

**Appendix Information for:**

**NMR Studies of the Dynamics of High-Spin Nitrophorins:**

**Comparative Studies of NP4 and NP2 at Close to Physiological**

**pH**

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**Table A1. Assignments (in ppm) of the high-spin NP4  $^1\text{H}\{^{15}\text{N}\}$  HSQC experiment, pH 7.3.**

**Table A2. Assignments (in ppm) of the high-spin NP4 at pH 7.3 HNCA experiment.**

**Table A3. Assignments of high-spin NP4 at pH 7.3 from the HNCO and HN(CA)CO experiments.**

**Table A4. Assignments of high-spin NP4 at pH 7.3 from the HNCACB and CACB(CO)NH experiments.**

## Appendix A. Assignment Tables

Table A1. Assignments (in ppm) of the high-spin NP4  $^1\text{H}\{^{15}\text{N}\}$  HSQC experiment, pH 7.3.

| Assignment | N, ppm          | H, ppm       |
|------------|-----------------|--------------|
| A1         | <i>peak not</i> | <i>found</i> |
| C2         | <i>peak not</i> | <i>found</i> |
| T3         | <b>120.454</b>  | 9.891        |
| K4         | <b>124.021</b>  | 8.115        |
| N5         | <i>peak not</i> | <i>found</i> |
| A6         | <b>124.526</b>  | 7.785        |
| I7         | <b>124.81</b>   | 8.441        |
| A8         | <b>129.503</b>  | 8.477        |
| Q9         | <b>121.5</b>    | 8.53         |
| T10        | <b>127.063</b>  | 8.876        |
| G11        | <i>peak not</i> | <i>found</i> |
| F12        | <b>118.811</b>  | 7.014        |
| N13        | <b>128.097</b>  | 8.755        |
| K14        | <b>125.372</b>  | 7.986        |
| D15        | <b>120.18</b>   | 8.017        |
| K16        | <b>116.706</b>  | 7.066        |
| Y17        | <b>118.446</b>  | 7.012        |
| F18        | <b>118.382</b>  | 8.419        |
| N19        | <b>118.63</b>   | 7.856        |
| G20        | <b>110.377</b>  | 9.26         |
| D21        | <b>118.628</b>  | 7.644        |
| V22        | <b>119.129</b>  | 8.218        |
| W23        | <b>127.695</b>  | 9.625        |
| Y24        | <b>119.049</b>  | 8.999        |
| V25        | <b>120.66</b>   | 8.55         |
| T26        | <b>122.917</b>  | 10.072       |
| D27        | <b>120.548</b>  | 8.588        |
| Y28        | <b>119.276</b>  | 10.302       |
| L29        | <b>123.42</b>   | 9.225        |
| D30        | <b>127.386</b>  | 8.358        |

| Assignment | N, ppm          | H, ppm       |
|------------|-----------------|--------------|
| L31        | <b>123.631</b>  | 6.96         |
| E32        | <b>119.752</b>  | 7.212        |
| P33        | <i>peak not</i> | <i>found</i> |
| D34        | <b>120.8</b>    | 8.163        |
| D35        | <b>120.421</b>  | 8.357        |
| V36        | <b>119.19</b>   | 8.203        |
| P37        | <i>peak not</i> | <i>found</i> |
| K38        | <b>124.301</b>  | 9.9          |
| R39        | <b>127.483</b>  | 9.767        |
| Y40        | <i>peak not</i> | <i>found</i> |
| C41        | <i>peak not</i> | <i>found</i> |
| A42        | <i>peak not</i> | <i>found</i> |
| A43        | <i>peak not</i> | <i>found</i> |
| L44        | <b>116.178</b>  | 8.877        |
| A45        | <b>121.554</b>  | 8.994        |
| A46        | <b>125.805</b>  | 8.818        |
| G47        | <b>107.951</b>  | 9.213        |
| T48        | <b>113.214</b>  | 8.591        |
| A49        | <b>128.421</b>  | 8.984        |
| S50        | <i>peak not</i> | <i>found</i> |
| G51        | <b>106.739</b>  | 8.495        |
| K52        | <b>120.39</b>   | 7.879        |
| L53        | <b>123.356</b>  | 8.609        |
| K54        | <b>126.575</b>  | 8.955        |
| E55        | <b>118.759</b>  | 8.937        |
| A56        | <b>133.599</b>  | 9.858        |
| L57        | <b>121.601</b>  | 8.51         |
| Y58        | <i>peak not</i> | <i>found</i> |
| H59        | <i>peak not</i> | <i>found</i> |
| Y60        | <i>peak not</i> | <i>found</i> |
| D61        | <i>peak not</i> | <i>found</i> |
| P62        | <i>peak not</i> | <i>found</i> |
| K63        | <b>116.582</b>  | 7.983        |

| Assignment | N, ppm          | H, ppm       |
|------------|-----------------|--------------|
| T64        | <b>105.177</b>  | 6.603        |
| Q65        | <b>115.155</b>  | 8.009        |
| D66        | <b>119.676</b>  | 7.34         |
| T67        | <b>114.022</b>  | 7.189        |
| F68        | <b>114.64</b>   | 5.048        |
| Y69        | <b>117.756</b>  | 6.813        |
| D70        | <b>115.404</b>  | 7.422        |
| V71        | <b>118.112</b>  | 9.415        |
| S72        | <b>122.182</b>  | 9.185        |
| E73        | <b>124.232</b>  | 9.054        |
| L74        | <b>124.371</b>  | 8.607        |
| Q75        | <b>122.015</b>  | 9.437        |
| V76        | <b>126.157</b>  | 8.885        |
| E77        | <b>129.994</b>  | 8.689        |
| S78        | <b>111.536</b>  | 8.05         |
| L79        | <i>peak not</i> | <i>found</i> |
| G80        | <b>114.576</b>  | 8.374        |
| K81        | <b>121.828</b>  | 7.88         |
| Y82        | <b>121.063</b>  | 8.285        |
| T83        | <b>117.085</b>  | 9.079        |
| A84        | <b>132.388</b>  | 10.179       |
| N85        | <b>123.945</b>  | 8.425        |
| F86        | <b>120.033</b>  | 7.365        |
| K87        | <b>120.588</b>  | 9.284        |
| K88        | <b>127.293</b>  | 9.175        |
| V89        | <b>120.962</b>  | 8.418        |
| D90        | <b>118.614</b>  | 7.947        |
| K91        | <b>114.211</b>  | 7.789        |
| N92        | <b>114.29</b>   | 7.227        |
| G93        | <b>108.387</b>  | 7.933        |
| N94        | <b>120.295</b>  | 8.28         |
| V95        | <b>123.417</b>  | 8.763        |
| K96        | <b>128.108</b>  | 9.491        |

| Assignment | N, ppm          | H, ppm       |
|------------|-----------------|--------------|
| V97        | 119.618         | 7.995        |
| A98        | 128.223         | 8.595        |
| V99        | 122.189         | 8.546        |
| T100       | 126.137         | 9.975        |
| A101       | 131.269         | 8.9          |
| G102       | 110.228         | 9.142        |
| N103       | 121.028         | 8.198        |
| Y104       | 121.177         | 9.204        |
| Y105       | 116.235         | 10.222       |
| T106       | 113.605         | 8.476        |
| F107       | 119.697         | 9.471        |
| T108       | 117.611         | 9.34         |
| V109       | 127.898         | 9.343        |
| M110       | 129.521         | 8.78         |
| Y111       | 117.608         | 8.202        |
| A112       | 125.874         | 6.658        |
| D113       | 121.477         | 9.499        |
| D114       | 114.805         | 8.355        |
| S115       | 110.895         | 8.701        |
| S116       | 117.964         | 8.884        |
| A117       | 117.64          | 8.582        |
| L118       | 121.515         | 9.265        |
| I119       | 119.847         | 9.758        |
| H120       | 122.354         | 8.834        |
| T121       | 116.443         | 6.829        |
| C122       | 118.257         | 7.21         |
| L123       | 126.996         | 6.934        |
| H124       | <i>peak not</i> | <i>found</i> |
| K125       | 120.224         | 7.784        |
| G126       | 116.006         | 8.766        |
| N127       | <i>peak not</i> | <i>found</i> |
| K128       | 119.194         | 7.38         |
| D129       | 120.94          | 8.164        |

| Assignment | N, ppm          | H, ppm       |
|------------|-----------------|--------------|
| L130       | 123.138         | 6.906        |
| G131       | 103.714         | 5.159        |
| D132       | 116.476         | 6.516        |
| L133       | 120.795         | 5.511        |
| Y134       | 125.023         | 8.309        |
| A135       | 124.097         | 9.967        |
| V136       | 124.86          | 10.26        |
| L137       | 126.234         | 9.929        |
| N138       | 121.364         | 9.932        |
| R139       | 124.829         | 8.616        |
| N140       | 120.082         | 10.274       |
| K141       | 123.549         | 7.625        |
| D142       | 117.718         | 7.97         |
| A143       | 123.364         | 7.145        |
| A144       | 126.306         | 8.485        |
| A145       | 126.818         | 9.277        |
| G146       | 110.418         | 8.797        |
| D147       | 117.601         | 8.428        |
| K148       | <i>peak not</i> | <i>found</i> |
| V149       | 120.507         | 7.937        |
| K150       | 120.422         | 7.82         |
| S151       | 116.867         | 8.227        |
| A152       | 126.16          | 7.334        |
| V153       | 120.269         | 8.057        |
| S154       | 113.484         | 7.788        |
| A155       | 125.691         | 8.432        |
| A156       | 119.596         | 7.251        |
| T157       | 112.792         | 8.092        |
| L158       | 118.882         | 7.159        |
| E159       | 121.149         | 8.351        |
| F160       | 128.192         | 9.114        |
| S161       | 112.934         | 8.829        |
| K162       | 119.647         | 7.632        |

| Assignment | N, ppm  | H, ppm |
|------------|---------|--------|
| F163       | 120.19  | 7.986  |
| I164       | 124.464 | 9.573  |
| S165       | 119.407 | 8.748  |
| T166       | 118.197 | 9.387  |
| K167       | 125.338 | 8.932  |
| E168       | 116.891 | 8.629  |
| N169       | 117.484 | 7.767  |
| N170       | 115.158 | 8.51   |
| C171       | 114.733 | 8.473  |
| A172       | 123.198 | 5.222  |
| Y173       | 120.292 | 8.285  |
| D174       | 119.273 | 5.985  |
| N175       | 121.883 | 7.988  |
| D176       | 118.479 | 8.048  |
| S177       | 116.37  | 7.179  |
| L178       | 119.915 | 6.78   |
| K179       | 112.251 | 7.318  |
| S180       | 114.438 | 7.476  |
| L181       | 121.605 | 7.539  |
| L182       | 114.55  | 7.013  |
| T183       | 105.596 | 7.263  |
| K184       | 126.926 | 7.244  |

**Table A2. Assignments (in ppm) of the high-spin NP4 at pH 7.3 HNCA experiment.**

|              |        |         |        | Assignment   | C, ppm | N, ppm | H, ppm | Assignment   | C, ppm | N, ppm | H, ppm |
|--------------|--------|---------|--------|--------------|--------|--------|--------|--------------|--------|--------|--------|
| Assignment   | C, ppm | N, ppm  | H, ppm | Y17CA-N-H    | 62.32  | 118.46 | 7.013  | P33CA-D34N-H | 62.47  | 120.84 | 8.165  |
| A1CA-C2N-H   | peak   | not     | found  | Y17CA-F18N-H | 62.32  | 118.38 | 8.422  | D34CA-N-H    | 53.77  | 120.79 | 8.164  |
| C2CA-N-H     | peak   | not     | found  | F18CA-N-H    | 56.37  | 118.37 | 8.421  | D34CA-D35N-H | 53.74  | 120.3  | 8.359  |
| C2CA-T3N-H   | 53.66  | 120.41  | 9.894  | F18CA-N19N-H | 56.36  | 118.62 | 7.855  | D35CA-N-H    | 56.89  | 120.46 | 8.358  |
| T3CA-N-H     | 61.87  | 120.45  | 9.895  | N19CA-N-H    | 52.48  | 118.62 | 7.856  | D35CA-V36N-H | 56.87  | 119.17 | 8.203  |
| T3CA-K4N-H   | 61.82  | 124.02  | 8.113  | N19CA-G20N-H | 52.47  | 110.37 | 9.26   | V36CA-N-H    | 59.89  | 119.21 | 8.203  |
| K4CA-N-H     | 55.05  | 123.99  | 8.117  | G20CA-N-H    | 45.43  | 110.39 | 9.261  | V36CA-P37    | peak   | not    | found  |
| K4CA-N5N-H   | peak   | not     | found  | G20CA-D21N-H | 45.42  | 118.6  | 7.644  | P37CA        | peak   | not    | found  |
| N5CA-N-H     | peak   | not     | found  | D21CA-N-H    | 51.54  | 118.65 | 7.645  | P37CA-K38N-H | 63.89  | 124.25 | 9.901  |
| N5CA-A6N-H   | 52.37  | 124.53  | 7.787  | D21CA-V22N-H | 51.53  | 119.11 | 8.218  | K38CA-N-H    | 57.23  | 124.41 | 9.903  |
| A6CA-N-H     | 52.4   | 124.57  | 7.785  | V22CA-N-H    | 63.04  | 119.14 | 8.217  | K38CA-R39N-H | 57.14  | 127.57 | 9.788  |
| A6CA-I7N-H   | 52.34  | 124.73  | 8.443  | V22CA-W23N-H | 63.02  | 127.55 | 9.628  | R39CA-N-H    | 55.91  | 127.52 | 9.783  |
| I7CA-N-H     | 60.07  | 124.85  | 8.442  | W23CA-N-H    | 55.89  | 127.69 | 9.63   | R39CA-Y40N-H | peak   | not    | found  |
| I7CA-A8N-H   | 60.07  | 129.43  | 8.478  | W23CA-Y24N-H | 55.98  | 119.07 | 8.996  | Y40CA-N-H    | peak   | not    | found  |
| A8CA-N-H     | 51.32  | 129.47  | 8.479  | Y24CA-N-H    | 57.55  | 119.1  | 9.003  | Y40CA-C41N-H | peak   | not    | found  |
| A8CA-Q9N-H   | 51.36  | 121.44  | 8.533  | Y24CA-V25N-H | 57.5   | 120.59 | 8.551  | C41CA-N-H    | peak   | not    | found  |
| Q9CA-N-H     | 56.35  | 121.5   | 8.534  | V25CA-N-H    | 63.69  | 120.77 | 8.553  | D41CA-A42N-H | peak   | not    | found  |
| Q9CA-T10N-H  | 56.37  | 127.11  | 8.874  | V25CA-T26N-H | 63.7   | 122.91 | 10.067 | A42CA-N-H    | peak   | not    | found  |
| T10CA-N-H    | 64.33  | 127.11  | 8.874  | T26CA-N-H    | 64.01  | 122.93 | 10.069 | A42CA-A43N-H | peak   | not    | found  |
| T10CA-G11N-H | peak   | not     | found  | T26CA-D27N-H | 63.99  | 120.54 | 8.597  | A43CA-N-H    | peak   | not    | found  |
| G11CA-N-H    | peak   | not     | found  | D27CA-N-H    | 53.91  | 120.59 | 8.593  | A43CA-L44N-H | 49.75  | 116.15 | 8.876  |
| G11CA-F12N-H | 46.08  | 118.82  | 7.016  | D27CA-Y28N-H | 53.88  | 119.32 | 10.307 | L44CA-N-H    | 53.94  | 116.24 | 8.876  |
| F12CA-N-H    | 57.62  | 118.85  | 7.015  | Y28CA-N-H    | 58.19  | 119.3  | 10.306 | L44CA-A45N-H | 53.93  | 121.63 | 8.997  |
| F12CA-N13N-H | 57.54  | 128.03  | 8.754  | Y28CA-L29N-H | 58.19  | 123.41 | 9.225  | A45CA-N-H    | 51.96  | 121.55 | 8.996  |
| N13CA-N-H    | 51.3   | 128.07  | 8.755  | L29CA-N-H    | 53.52  | 123.43 | 9.229  | A45CA-A46N-H | 52.03  | 125.81 | 8.822  |
| N13CA-K14N-H | 51.28  | 125.34  | 7.988  | L29CA-D30N-H | 53.52  | 127.45 | 8.362  | A46CA-N-H    | 51.45  | 125.85 | 8.819  |
| K14CA-N-H    | 58.74  | 125.33  | 7.988  | D30CA-N-H    | 51.2   | 127.43 | 8.361  | A46CA-G47N-H | 51.44  | 107.93 | 9.216  |
| K14CA-D15N-H | 58.74  | 120.18  | 8.022  | D30CA-L31N-H | 51.2   | 123.68 | 6.963  | G47CA-N-H    | 45.73  | 107.94 | 9.216  |
| D15CA-N-H    | 57.27  | 120.17  | 8.02   | L31CA-N-H    | 55.3   | 123.63 | 6.96   | G47CA-T48N-H | 45.73  | 113.18 | 8.594  |
| D15CA-K16N-H | 57.28  | 116.71  | 7.067  | L31CA-E32N-H | 55.27  | 119.74 | 7.21   | T48CA-N-H    | 61.4   | 113.24 | 8.594  |
| K16CA-N-H    | 57.82  | 116.745 | 7.066  | E32CA-N-H    | 52.91  | 119.77 | 7.21   | T48CA-A49N-H | 61.37  | 128.45 | 8.986  |
| K16CA-Y17N-H | 57.87  | 118.46  | 7.013  | E32CA-P33    | peak   | not    | found  | A49CA-N-H    | 53.17  | 128.48 | 8.986  |
|              |        |         |        | P33CA        | peak   | not    | found  | A49CA-S50N-H | peak   | not    | found  |

| Assignment   | C,<br>ppm    | N, ppm     | H, ppm       | Assignment   | C,<br>ppm    | N, ppm     | H, ppm       | Assignment   | C,<br>ppm    | N, ppm | H, ppm |
|--------------|--------------|------------|--------------|--------------|--------------|------------|--------------|--------------|--------------|--------|--------|
| S50CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> | D66CA-T67N-H | <b>55.21</b> | 114.06     | 7.186        | T83CA-N-H    | <b>62.68</b> | 117.1  | 9.09   |
| S50CA-G51N-H | <b>59.06</b> | 106.76     | 8.496        | T67CA-N-H    | <b>58.49</b> | 114.05     | 7.186        | T83CA-A84N-H | <b>62.69</b> | 132.38 | 10.176 |
| G51CA-N-H    | <b>45.11</b> | 106.77     | 8.498        | T67CA-F68N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | A84CA-N-H    | <b>51.95</b> | 132.45 | 10.175 |
| G51CA-K52N-H | <b>45.12</b> | 120.37     | 7.879        | F68CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> | A84CA-N85N-H | <b>52.05</b> | 124.1  | 8.432  |
| K52CA-N-H    | <b>54.38</b> | 120.4      | 7.88         | F68CA-Y69N-H | <b>54.57</b> | 117.77     | 6.816        | N85CA-N-H    | <b>53.82</b> | 123.94 | 8.428  |
| K52CA-L53N-H | <b>54.43</b> | 123.49     | 8.61         | Y69CA-N-H    | <b>54.66</b> | 117.8      | 6.816        | N85CA-F86N-H | <b>53.93</b> | 119.96 | 7.368  |
| L53CA-N-H    | <b>55.34</b> | 123.4      | 8.611        | Y69CA-D70N-H | <b>54.7</b>  | 115.41     | 7.423        | F86CA-N-H    | <b>57.02</b> | 120.08 | 7.367  |
| L53CA-K54N-H | <b>55.28</b> | 126.61     | 8.952        | D70CA-N-H    | <b>52.07</b> | 115.42     | 7.423        | F86CA-K87N-H | <b>57.06</b> | 120.54 | 9.285  |
| K54CA-N-H    | <b>54.52</b> | 126.48     | 8.956        | D70CA-V71N-H | <b>52.07</b> | 118.06     | 9.412        | K87CA-N-H    | <b>54.68</b> | 120.75 | 9.282  |
| K54CA-E55N-H | <b>54.53</b> | 118.71     | 8.938        | V71CA-N-H    | <b>61.67</b> | 118.18     | 9.413        | K87CA-K88N-H | <b>54.75</b> | 127.34 | 9.179  |
| E55CA-N-H    | <b>56.41</b> | 118.8      | 8.94         | V71CA-S72N-H | <b>61.67</b> | 122.16     | 9.191        | K88CA-N-H    | <b>56.56</b> | 127.33 | 9.179  |
| E55CA-A56N-H | <b>56.4</b>  | 133.6      | 9.867        | S72CA-N-H    | <b>58.61</b> | 122.22     | 9.191        | K88CA-V89N-H | <b>56.67</b> | 120.87 | 8.415  |
| A56CA-N-H    | <b>49.92</b> | 133.62     | 9.865        | S72CA-E73N-H | <b>58.62</b> | 124.19     | 9.058        | V89CA-N-H    | <b>58.27</b> | 120.91 | 8.422  |
| A56CA-L57N-H | <b>49.96</b> | 121.52     | 8.51         | E73CA-N-H    | <b>56.25</b> | 124.26     | 9.058        | V89CA-D90N-H | <b>58.27</b> | 118.52 | 7.948  |
| L57CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> | E73CA-L74N-H | <b>56.3</b>  | 124.38     | 8.612        | D90CA-N-H    | <b>51.8</b>  | 118.64 | 7.949  |
| L57CA-Y58N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | L74CA-N-H    | <b>54.87</b> | 124.52     | 8.61         | D90CA-K91N-H | <b>51.8</b>  | 114.23 | 7.788  |
| Y58CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> | L74CA-Q75N-H | <b>54.88</b> | 122.07     | 9.44         | K91CA-N-H    | <b>57.94</b> | 114.28 | 7.789  |
| Y58CA-H59N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | Q75CA-N-H    | <b>54.07</b> | 122.04     | 9.435        | K91CA-N92N-H | <b>57.99</b> | 114.32 | 7.225  |
| H59CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> | Q75CA-V76N-H | <b>54.07</b> | 126.05     | 8.884        | N92CA-N-H    | <b>52.62</b> | 114.33 | 7.225  |
| H59CA-Y60N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | V76CA-N-H    | <b>62.84</b> | 126.17     | 8.884        | N92CA-G93N-H | <b>52.61</b> | 108.43 | 7.934  |
| Y60CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> | V76CA-E77N-H | <b>62.86</b> | 130.03     | 8.689        | G93CA-N-H    | <b>45.08</b> | 108.46 | 7.935  |
| Y60CA-D61N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | E77CA-N-H    | <b>57.58</b> | 130.07     | 8.689        | G93CA-N94N-H | <b>45.08</b> | 120.3  | 8.279  |
| D61CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> | E77CA-S78N-H | <b>57.63</b> | 111.55     | 8.053        | N94CA-N-H    | <b>53.61</b> | 120.31 | 8.28   |
| D61CA-P62N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | S78CA-N-H    | <b>57.05</b> | 111.56     | 8.051        | N94CA-V95N-H | <b>53.6</b>  | 123.43 | 8.762  |
| P62CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> | S78CA-L79N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | V95CA-N-H    | <b>65.04</b> | 123.41 | 8.763  |
| P62CA-K63N-H | <b>63.65</b> | 116.66     | 7.985        | L79CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> | V95CA-K96N-H | <b>65.04</b> | 128.04 | 9.489  |
| K63CA-N-H    | <b>58.73</b> | 116.58     | 7.985        | L79CA-G80N-H | <b>58.04</b> | 114.58     | 8.377        | K96CA-N-H    | <b>56.29</b> | 128.11 | 9.489  |
| K63CA-T64N-H | <b>58.72</b> | 105.17     | 6.601        | G80CA-N-H    | <b>46.28</b> | 114.59     | 8.377        | K96CA-V97N-H | <b>56.2</b>  | 119.62 | 7.99   |
| T64CA-N-H    | <b>61.3</b>  | 105.18     | 6.601        | G80CA-K81N-H | <b>46.27</b> | 121.87     | 7.881        | V97CA-N-H    | <b>62.91</b> | 119.64 | 7.997  |
| T64CA-Q65N-H | <b>61.31</b> | 115.16     | 8.01         | K81CA-N-H    | <b>56.1</b>  | 121.8      | 7.881        | V97CA-A98N-H | <b>62.92</b> | 128.18 | 8.597  |
| Q65CA-N-H    | <b>57.8</b>  | 115.19     | 8.01         | K81CA-Y82N-H | <b>56.15</b> | 121.12     | 8.286        | A98CA-N-H    | <b>52.39</b> | 128.23 | 8.597  |
| Q65CA-D66N-H | <b>57.8</b>  | 119.56     | 7.339        | Y82CA-N-H    | <b>56.96</b> | 121.13     | 8.287        | A98CA-V99N-H | <b>52.4</b>  | 122.17 | 8.548  |
| D66CA-N-H    | <b>55.19</b> | 119.62     | 7.343        | Y82CA-T83N-H | <b>56.93</b> | 117.1      | 9.085        | V99CA-N-H    | <b>64.88</b> | 122.18 | 8.547  |

| Assignment     | C, ppm | N, ppm | H, ppm | Assignment      | C, ppm | N, ppm | H, ppm | Assignment     | C, ppm | N, ppm | H, ppm |
|----------------|--------|--------|--------|-----------------|--------|--------|--------|----------------|--------|--------|--------|
| V99CA-T100N-H  | 64.91  | 126.19 | 9.973  | S116CA-N-H      | 58.55  | 117.99 | 8.884  | L133CA-N-H     | 52.75  | 120.8  | 5.507  |
| T100CA-N-H     | 61.81  | 126.15 | 9.974  | S116CA-A117N-H  | 58.55  | 117.59 | 8.584  | L133CA-Y134N-H | 52.77  | 124.89 | 8.314  |
| T100CA-A101N-H | 61.83  | 131.29 | 8.896  | A117CA-N-H      | 52.38  | 117.65 | 8.584  | Y134CA-N-H     | 56.69  | 125.06 | 8.312  |
| A101CA-N-H     | 54.19  | 131.35 | 8.903  | A117CA-L118N-H  | 52.39  | 121.51 | 9.266  | Y134CA-A135N-H | 56.68  | 124.11 | 9.969  |
| A101CA-G102N-H | 54.22  | 110.26 | 9.149  | L118CA-N-H      | 54.4   | 121.43 | 9.267  | A135CA-N-H     | 52.03  | 124.03 | 9.967  |
| G102CA-N-H     | 45.31  | 110.27 | 9.152  | L118CA-I119N-H  | 54.36  | 119.74 | 9.769  | A135CA-V136N-H | 52.03  | 124.83 | 10.263 |
| G102CA-N103N-H | 45.28  | 121.07 | 8.2    | I119CA-N-H      | 59.1   | 119.89 | 9.768  | V136CA-N-H     | 62.9   | 124.84 | 10.262 |
| N103CA-N-H     | 51.4   | 121.02 | 8.2    | I119CA-H120N-H  | 59.09  | 122.31 | 8.832  | V136CA-L137N-H | 62.91  | 126.2  | 9.93   |
| N103CA-Y104N-H | 51.39  | 121.05 | 9.211  | H120CA-N-H      | 56.07  | 122.33 | 8.83   | L137CA-N-H     | 52.2   | 126.24 | 9.931  |
| Y104CA-N-H     | 57.78  | 121.13 | 9.21   | H120CA-T121N-H  | 56.08  | 116.42 | 6.839  | L137CA-N138N-H | 52.2   | 121.32 | 9.936  |
| Y104CA-Y105N-H | 57.78  | 116.23 | 10.224 | T121CA-N-H      | 58.69  | 116.51 | 6.831  | N138CA-N-H     | 52.92  | 121.34 | 9.935  |
| Y105CA-N-H     | 56.23  | 116.25 | 10.221 | T121CA-C122N-H  | 58.67  | 118.3  | 7.205  | N138CA-R139N-H | 52.94  | 124.78 | 8.617  |
| Y105CA-T106N-H | 56.19  | 113.49 | 8.48   | C122CA-N-H      | 53.53  | 118.26 | 7.21   | R139CA-N-H     | 56.09  | 124.74 | 8.617  |
| T106CA-N-H     | 59.6   | 113.61 | 8.479  | C122CA-L123N-H  | 53.43  | 126.97 | 6.939  | R139CA-N140N-H | 55.93  | 120.06 | 10.28  |
| T106CA-F107N-H | 59.61  | 119.73 | 9.468  | L123CA-N-H      | 48.53  | 127.07 | 6.937  | N140CA-N-H     | 51.71  | 120.09 | 10.279 |
| F107CA-N-H     | 56.86  | 119.73 | 9.469  | L123CA-H124N-H  | peak   | not    | found  | N140CA-K141N-H | 51.7   | 123.51 | 7.626  |
| F107CA-T108N-H | 56.89  | 117.7  | 9.341  | H124CA-N-H      | peak   | not    | found  | K141CA-N-H     | 58.15  | 123.54 | 7.626  |
| T108CA-N-H     | 61     | 117.58 | 9.339  | H124CA-K125N-H  | 54.16  | 120.16 | 7.786  | K141CA-D142N-H | 58.14  | 117.72 | 7.969  |
| T108CA-V109N-H | peak   | not    | found  | K125CA-N-H      | 55.42  | 120.32 | 7.783  | D142CA-N-H     | 54.4   | 117.8  | 7.966  |
| V109CA-N-H     | 63.07  | 127.87 | 9.341  | K125CA-G126N-H  | 55.42  | 115.99 | 8.765  | D142CA-A143N-H | 54.36  | 123.44 | 7.142  |
| V109CA-M110N-H | 63.06  | 129.54 | 8.778  | G126CA-N-H      | 47.79  | 116.04 | 8.765  | A143CA-N-H     | 52.61  | 123.38 | 7.144  |
| M110CA-N-H     | 58.13  | 129.5  | 8.778  | N127CA-K128N-H  | 54.47  | 119.12 | 7.382  | A143CA-A144N-H | 52.63  | 126.24 | 8.489  |
| M110CA-Y111N-H | 58.1   | 117.61 | 8.205  | K128CA-N-H      | 55.13  | 119.26 | 7.379  | A144CA-N-H     | 51.29  | 126.31 | 8.488  |
| Y111CA-N-H     | 59.38  | 117.61 | 8.206  | K128CA-D129N-H  | 55.14  | 120.93 | 8.166  | A144CA-A145N-H | 51.29  | 126.7  | 9.278  |
| Y111CA-A112N-H | 59.39  | 125.92 | 6.658  | D129CA-N-H      | 52.71  | 120.94 | 8.163  | A145CA-N-H     | 53.28  | 126.81 | 9.278  |
| A112CA-N-H     | 52.93  | 125.93 | 6.658  | D129CA-L130N-H  | 52.68  | 123.06 | 6.911  | A145CA-G146N-H | 53.27  | 110.42 | 8.796  |
| A112CA-D113N-H | 52.95  | 121.49 | 9.5    | L130CA-N-H      | 53.44  | 123.14 | 6.91   | G146CA-N-H     | 43.68  | 110.42 | 8.796  |
| D113CA-N-H     | 53.17  | 121.49 | 9.498  | CL130CA-G131N-H | peak   | not    | found  | G146CA-D147N-H | 43.67  | 117.6  | 8.429  |
| D113CA-D114N-H | 53.17  | 114.79 | 8.357  | G131CA-N-H      | 42.62  | 103.71 | 5.152  | D147CA-N-H     | 57.86  | 117.68 | 8.429  |
| D114CA-N-H     | 58.1   | 114.74 | 8.361  | G131CA-D132N-H  | 42.62  | 116.48 | 6.514  | D147CA-K148N-H | peak   | not    | found  |
| D114CA-S115N-H | 58.09  | 110.95 | 8.701  | D132CA-N-H      | 53.2   | 116.49 | 6.515  | K148CA-N-H     | peak   | not    | found  |
| S115CA-N-H     | 59.43  | 110.93 | 8.701  | D132CB-N-H      | 42.83  | 116.51 | 6.515  | K148CA-V149N-H | 59.67  | 120.49 | 7.937  |
| S115CA-S116N-H | 59.42  | 117.98 | 8.885  | D132CA-L133N-H  | 53.19  | 120.81 | 5.501  | V149CA-N-H     | 65.54  | 120.57 | 7.938  |

| Assignment     | C, ppm | N, ppm  | H, ppm | Assignment     | C, ppm | N, ppm | H, ppm | Assignment     | C, ppm | N, ppm | H, ppm |
|----------------|--------|---------|--------|----------------|--------|--------|--------|----------------|--------|--------|--------|
| V149CA-K150N-H | 65.54  | 120.45  | 7.82   | T166CA-N-H     | 62.42  | 118.32 | 9.39   | L182CA-T183N-H | 56.9   | 105.62 | 7.262  |
| K150CA-N-H     | 61.23  | 120.45  | 7.819  | T166CA-K167N-H | 62.39  | 125.34 | 8.933  | T183CA-N-H     | 61.66  | 105.64 | 7.262  |
| K150CA-S151N-H | 61.27  | 116.88  | 8.23   | K167CA-N-H     | 59.69  | 125.32 | 8.933  | T183CA-K184N-H | 61.65  | 126.9  | 7.243  |
| S151CA-N-H     | 61.8   | 116.87  | 8.229  | K167CA-E168N-H | 59.61  | 116.93 | 8.639  | K184CA-N-H     | 56.98  | 126.94 | 7.243  |
| S151CA-A152N-H | 61.81  | 126.15  | 7.334  | E168CA-N-H     | 55.948 | 116.93 | 8.628  |                |        |        |        |
| A152CA-N-H     | 54.87  | 126.2   | 7.334  | E168CA-N169N-H | 56     | 117.49 | 7.769  |                |        |        |        |
| A152CA-V153N-H | 54.86  | 120.3   | 8.061  | N169CA-N-H     | 52.78  | 117.54 | 7.77   |                |        |        |        |
| V153CA-N-H     | 67.24  | 120.29  | 8.06   | N169CA-N170N-H | 52.8   | 115.17 | 8.513  |                |        |        |        |
| V153CA-S154N-H | 67.24  | 113.46  | 7.788  | N170CA-N-H     | 53.66  | 115.17 | 8.51   |                |        |        |        |
| S154CA-N-H     | 61.48  | 113.53  | 7.788  | N170CA-C171N-H | 53.69  | 114.76 | 8.478  |                |        |        |        |
| S154CA-A155N-H | 61.48  | 125.75  | 8.434  | C171CA-N-H     | 54.94  | 114.71 | 8.476  |                |        |        |        |
| A155CA-N-H     | 54.53  | 125.71  | 8.434  | C171CA-A172N-H | 54.95  | 123.28 | 5.217  |                |        |        |        |
| A155CA-A156N-H | 54.55  | 119.52  | 7.249  | A172CA-N-H     | 50.1   | 123.25 | 5.222  |                |        |        |        |
| A156CA-N-H     | 51.47  | 119.62  | 7.25   | A172CA-Y173N-H | 50.2   | 120.3  | 8.281  |                |        |        |        |
| A156CA-T157N-H | 51.47  | 112.81  | 8.094  | Y173CA-N-H     | 57.2   | 120.29 | 8.285  |                |        |        |        |
| T157CA-N-H     | 63.16  | 112.86  | 8.094  | Y173CA-D174N-H | 57.18  | 119.38 | 5.988  |                |        |        |        |
| T157CA-L158N-H | 63.17  | 118.88  | 7.158  | D174CA-N-H     | 50.94  | 119.24 | 5.986  |                |        |        |        |
| L158CA-N-H     | 52.59  | 118.91  | 7.158  | D174CA-N175N-H | 50.96  | 121.97 | 7.998  |                |        |        |        |
| L158CA-E159N-H | 52.57  | 121.08  | 8.354  | N175CA-N-H     | 55.59  | 121.91 | 7.996  |                |        |        |        |
| E159CA-N-H     | 54.44  | 121.24  | 8.353  | N175CA-D176N-H | 55.59  | 118.49 | 8.051  |                |        |        |        |
| E159CA-F160N-H | 54.44  | 128.05  | 9.12   | D176CA-N-H     | 57.35  | 118.52 | 8.05   |                |        |        |        |
| F160CA-N-H     | 61.02  | 128.16  | 9.118  | D176CA-S177N-H | 57.36  | 116.37 | 7.177  |                |        |        |        |
| F160CA-S161N-H | 61.01  | 112.93  | 8.831  | S177CA-N-H     | 61.25  | 116.41 | 7.176  |                |        |        |        |
| S161CA-N-H     | 60.74  | 112.97  | 8.828  | S177CA-L178N-H | 61.23  | 119.91 | 6.781  |                |        |        |        |
| S161CA-K162N-H | 60.69  | 119.62  | 7.634  | L178CA-N-H     | 57.98  | 119.92 | 6.782  |                |        |        |        |
| K162CA-N-H     | 56.19  | 119.66  | 7.633  | L178CA-K179N-H | 57.98  | 112.26 | 7.318  |                |        |        |        |
| K162CA-F163N-H | 56.19  | 120.21  | 7.989  | K179CA-N-H     | 59.8   | 112.3  | 7.318  |                |        |        |        |
| F163CA-N-H     | 58.512 | 120.19  | 7.986  | K179CA-S180N-H | 59.73  | 114.46 | 7.478  |                |        |        |        |
| F163CA-I164N-H | 58.46  | 124.44  | 9.575  | S180CA-N-H     | 60.87  | 114.46 | 7.477  |                |        |        |        |
| I164CA-N-H     | 59.64  | 124.54  | 9.575  | S180CA-L181N-H | 60.86  | 121.6  | 7.541  |                |        |        |        |
| I164CA-S165N-H | 59.642 | 119.359 | 8.747  | L181CA-N-H     | 56.73  | 121.65 | 7.541  |                |        |        |        |
| S165CA-N-H     | 57.09  | 119.49  | 8.747  | L181CA-L182N-H | 56.76  | 114.55 | 7.014  |                |        |        |        |
| S165CA-T166N-H | 57.09  | 118.19  | 9.389  | L182CA-N-H     | 56.9   | 114.55 | 7.014  |                |        |        |        |

**Table A3. Assignments of high-spin NP4 at pH 7.3 from the HNCO and HN(CA)CO experiments.**

|                 |               | HNCO       |              |  |               | HN(CA)-CO  |              |
|-----------------|---------------|------------|--------------|--|---------------|------------|--------------|
| Peak assignment | CO, ppm       | N, ppm     | H, ppm       |  | CO, ppm       | N, ppm     | H, ppm       |
|                 |               |            |              |  |               |            |              |
| A1C-C2N-H       | <i>peak</i>   | <i>not</i> | <i>found</i> |  | <i>peak</i>   | <i>not</i> | <i>found</i> |
| C2C-N-H         |               |            |              |  | <i>peak</i>   | <i>not</i> | <i>found</i> |
| C2C-T3N-H       | <b>174.65</b> | 120.46     | 9.896        |  | <b>174.65</b> | 120.46     | 9.896        |
| T3C-N-H         |               |            |              |  | <b>174.55</b> | 120.42     | 9.894        |
| T3C-K4N-H       | <b>174.55</b> | 124.02     | 8.116        |  | <b>174.55</b> | 124.02     | 8.116        |
| K4C-N-H         |               |            |              |  | <b>176.37</b> | 124.04     | 8.117        |
| K4C-N5N-H       | <i>peak</i>   | <i>not</i> | <i>found</i> |  | <i>Peak</i>   | <i>Not</i> | <i>found</i> |
| N5C-N-H         |               |            |              |  | <i>Peak</i>   | <i>Not</i> | <i>found</i> |
| N5C-A6N-H       | <b>174.23</b> | 124.53     | 7.785        |  | <b>174.22</b> | 124.5      | 7.785        |
| A6C-N-H         |               |            |              |  | <b>176.82</b> | 124.56     | 7.785        |
| A6C-I7N-H       | <b>176.83</b> | 124.83     | 8.443        |  | <b>176.81</b> | 124.83     | 8.442        |
| I7C-N-H         |               |            |              |  | <b>176.05</b> | 124.82     | 8.443        |
| I7C-A8N-H       | <b>176.09</b> | 129.55     | 8.48         |  | <b>176.07</b> | 129.45     | 8.478        |
| A8C-N-H         |               |            |              |  | <b>177.39</b> | 129.49     | 8.478        |
| A8C-Q9N-H       | <b>177.4</b>  | 121.51     | 8.534        |  | <b>177.4</b>  | 121.51     | 8.534        |
| Q9C-N-H         |               |            |              |  | <b>177.11</b> | 121.5      | 8.532        |
| Q9C-T10N-H      | <b>177.11</b> | 127.06     | 8.874        |  | <b>177.11</b> | 127.12     | 8.873        |
| T10C-N-H        |               |            |              |  | <b>176.04</b> | 127.06     | 8.873        |
| T10C-G11N-H     | <i>peak</i>   | <i>not</i> | <i>found</i> |  | <i>peak</i>   | <i>not</i> | <i>found</i> |
| G11C-N-H        |               |            |              |  | <i>peak</i>   | <i>not</i> | <i>found</i> |
| G11C-F12N-H     | <b>174.21</b> | 118.82     | 7.016        |  | <b>174.21</b> | 118.82     | 7.016        |
| F12C-N-H        |               |            |              |  | <b>174.12</b> | 118.83     | 7.017        |
| F12C-N13N-H     | <b>174.11</b> | 128.12     | 8.755        |  | <b>174.11</b> | 128.13     | 8.755        |
| N13C-N-H        |               |            |              |  | <b>174.99</b> | 128.08     | 8.754        |
| N13C-K14N-H     | <b>174.99</b> | 125.37     | 7.988        |  | <b>174.99</b> | 125.33     | 7.988        |
| K14C-N-H        |               |            |              |  | <b>176.81</b> | 125.35     | 7.989        |
| K14C-D15N-H     | <b>176.82</b> | 120.17     | 8.02         |  | <b>176.77</b> | 120.14     | 8.021        |
| D15C-N-H        |               |            |              |  | <b>177.93</b> | 120.18     | 8.02         |

|                 |               | HNCO   |        |  |               | HN(CA)-CO  |              |
|-----------------|---------------|--------|--------|--|---------------|------------|--------------|
| Peak assignment | CO, ppm       | N, ppm | H, ppm |  | CO, ppm       | N, ppm     | H, ppm       |
| D15C-K16N-H     | <b>177.95</b> | 116.7  | 7.066  |  | <b>177.95</b> | 116.73     | 7.068        |
| K16C-N-H        |               |        |        |  | <b>176.23</b> | 116.75     | 7.068        |
| K16C-Y17N-H     | <b>176.25</b> | 118.43 | 7.013  |  | <b>176.25</b> | 118.45     | 7.014        |
| Y17C-N-H        |               |        |        |  | <b>177.8</b>  | 118.45     | 7.015        |
| Y17C-F18N-H     | <b>177.9</b>  | 118.37 | 8.422  |  | <b>177.76</b> | 118.43     | 8.419        |
| F18C-N-H        |               |        |        |  | <b>176.80</b> | 118.38     | 8.422        |
| F18C-N19N-H     | <b>176.8</b>  | 118.62 | 7.857  |  | <b>176.80</b> | 118.62     | 7.857        |
| N19C-N-H        |               |        |        |  | <b>177.05</b> | 118.63     | 7.857        |
| N19C-G20N-H     | <b>177.07</b> | 110.35 | 9.262  |  | <b>177.06</b> | 110.37     | 9.259        |
| G20C-N-H        |               |        |        |  | <b>172.21</b> | 110.39     | 9.26         |
| G20C-D21N-H     | <b>172.21</b> | 118.62 | 7.646  |  | <b>172.21</b> | 118.66     | 7.647        |
| D21C-N-H        |               |        |        |  | <b>175.8</b>  | 118.6      | 7.646        |
| D21C-V22N-H     | <b>175.81</b> | 119.12 | 8.218  |  | <b>175.8</b>  | 119.1      | 8.219        |
| V22C-N-H        |               |        |        |  | <i>Peak</i>   | <i>not</i> | <i>found</i> |
| V22C-W23N-H     | <b>177.04</b> | 127.7  | 9.629  |  | <b>177.03</b> | 127.61     | 9.627        |
| W23C-N-H        |               |        |        |  | <b>174.66</b> | 127.7      | 9.627        |
| W23C-Y24N-H     | <b>174.66</b> | 119.05 | 9.003  |  | <b>174.63</b> | 118.99     | 8.992        |
| Y24C-N-H        |               |        |        |  | <b>177.19</b> | 119.08     | 9.003        |
| Y24C-V25N-H     | <b>177.2</b>  | 120.76 | 8.55   |  | <b>177.20</b> | 120.76     | 8.55         |
| V25C-N-H        |               |        |        |  | <b>178.08</b> | 120.66     | 8.552        |
| V25C-T26N-H     | <b>178.08</b> | 122.93 | 10.068 |  | <b>178.07</b> | 122.84     | 10.065       |
| T26C-N-H        |               |        |        |  | <b>175.30</b> | 122.86     | 10.065       |
| T26C-D27N-H     | <b>175.33</b> | 120.55 | 8.593  |  | <b>175.33</b> | 120.55     | 8.593        |
| D27C-N-H        |               |        |        |  | <b>175.52</b> | 120.58     | 8.593        |
| D27C-Y28N-H     | <b>175.52</b> | 119.29 | 10.307 |  | <b>175.52</b> | 119.29     | 10.307       |
| Y28C-N-H        |               |        |        |  | <b>172.03</b> | 119.31     | 10.304       |
| Y28C-L29N-H     | <b>172.03</b> | 123.45 | 9.228  |  | <b>172.01</b> | 123.45     | 9.226        |
| L29C-N-H        |               |        |        |  | <b>172.91</b> | 123.47     | 9.227        |
| L29C-D30N-H     | <b>172.92</b> | 127.4  | 8.361  |  | <b>172.92</b> | 127.37     | 8.358        |
| D30C-N-H        |               |        |        |  | <b>175.61</b> | 127.44     | 8.367        |
| D30C-L31N-H     | <b>175.61</b> | 123.66 | 6.963  |  | <b>175.61</b> | 123.66     | 6.966        |
|                 |               |        |        |  |               |            |              |

|                 |         | HNCO    |        |  |         | HN(CA)-CO |        |
|-----------------|---------|---------|--------|--|---------|-----------|--------|
| Peak assignment | CO, ppm | N, ppm  | H, ppm |  | CO, ppm | N, ppm    | H, ppm |
| L31C-N-H        |         |         |        |  | 176.73  | 123.58    | 6.963  |
| L31C-E32N-H     | 176.72  | 119.75  | 7.21   |  | 176.72  | 119.75    | 7.21   |
| E32C-N-H        |         |         |        |  | 171.79  | 119.79    | 7.212  |
| E32C-P33        | peak    | not     | found  |  | Peak    | not       | found  |
| P33C            |         |         |        |  | Peak    | not       | found  |
| P33C-D34N-H     | 176.96  | 120.78  | 8.165  |  | 176.97  | 120.80    | 8.162  |
| D34C-N-H        |         |         |        |  | 175.62  | 120.79    | 8.165  |
| D34C-D35N-H     | 175.66  | 120.43  | 8.359  |  | 175.65  | 120.39    | 8.357  |
| D35C-N-H        |         |         |        |  | 176.88  | 120.37    | 8.359  |
| D35C-V36N-H     | 176.89  | 119.17  | 8.204  |  | 176.89  | 119.17    | 8.204  |
| V36C-N-H        |         |         |        |  | 173.71  | 119.21    | 8.203  |
| V36C-P37        | peak    | not     | found  |  | Peak    | not       | found  |
| P37C            |         |         |        |  | Peak    | not       | found  |
| P37C-K38N-H     | 177.83  | 124.29  | 9.904  |  | 177.82  | 124.19    | 9.911  |
| K38C-N-H        |         |         |        |  | 178.81  | 124.44    | 9.9    |
| K38C-R39N-H     | 178.82  | 127.45  | 9.785  |  | 178.82  | 127.45    | 9.785  |
| R39C-N-H        |         |         |        |  | Peak    | not       | found  |
| R39C-Y40N-H     | peak    | not     | found  |  | Peak    | not       | found  |
| Y40C-N-H        |         |         |        |  | Peak    | not       | found  |
| Y40C-C41N-H     | peak    | not     | found  |  | Peak    | not       | found  |
| C41C-N-H        |         |         |        |  | Peak    | not       | found  |
| C41C-A42N-H     | peak    | not     | found  |  | Peak    | not       | found  |
| A42C-N-H        |         |         |        |  | Peak    | not       | found  |
| A42C-A43N-H     | peak    | not     | found  |  | Peak    | not       | found  |
| A43C-N-H        |         |         |        |  | Peak    | not       | found  |
| A43C-L44N-H     | 171.98  | 116.18  | 8.876  |  | 171.97  | 116.08    | 8.875  |
| L44C-N-H        |         |         |        |  | 174.2   | 116.22    | 8.874  |
| L44C-A45N-H     | 174.21  | 121.58  | 8.997  |  | 174.21  | 121.58    | 8.997  |
| A45C-N-H        |         |         |        |  | 174.16  | 121.55    | 8.996  |
| A45C-A46N-H     | 174.16  | 125.792 | 8.818  |  | 174.14  | 125.8     | 8.822  |
| A46C-N-H        |         |         |        |  | 177.35  | 125.85    | 8.818  |
| A46C-G47N-H     | 177.36  | 107.941 | 9.217  |  | 177.37  | 107.96    | 9.215  |

|                 |         | HNCO    |        |  |         | HN(CA)-CO |        |
|-----------------|---------|---------|--------|--|---------|-----------|--------|
| Peak assignment | CO, ppm | N, ppm  | H, ppm |  | CO, ppm | N, ppm    | H, ppm |
| G47C-N-H        |         |         |        |  | 172.23  | 107.94    | 9.215  |
| G47C-T48N-H     | 172.23  | 113.22  | 8.594  |  | 172.23  | 113.2     | 8.593  |
| T48C-N-H        |         |         |        |  | 175.29  | 113.23    | 8.593  |
| T48C-A49N-H     | 175.29  | 128.449 | 8.987  |  | 175.29  | 128.42    | 8.986  |
| A49C-N-H        |         |         |        |  | 177.63  | 128.45    | 8.986  |
| A49C-S50N-H     | peak    | not     | found  |  | Peak    | Not       | found  |
| S50C-N-H        |         |         |        |  | Peak    | Not       | found  |
| S50C-G51N-H     | 175.19  | 106.74  | 8.499  |  | Peak    | Not       | found  |
| G51C-N-H        |         |         |        |  | 173.6   | 106.76    | 8.492  |
| G51C-K52N-H     | 173.6   | 120.391 | 7.881  |  | 173.6   | 120.39    | 7.881  |
| K52C-N-H        |         |         |        |  | 174.63  | 120.42    | 7.881  |
| K52C-L53N-H     | 174.64  | 123.384 | 8.612  |  | 174.635 | 123.34    | 8.611  |
| L53C-N-H        |         |         |        |  | 176.1   | 123.41    | 8.61   |
| L53C-K54N-H     | 176.12  | 126.566 | 8.956  |  | 176.09  | 126.57    | 8.955  |
| K54C-N-H        |         |         |        |  | 174.15  | 126.53    | 8.956  |
| K54C-E55N-H     | 174.15  | 118.747 | 8.937  |  | 174.16  | 118.68    | 8.935  |
| E55C-N-H        |         |         |        |  | 174.59  | 118.79    | 8.937  |
| E55C-A56N-H     | 174.59  | 133.584 | 9.866  |  | 174.6   | 133.59    | 9.862  |
| A56C-N-H        |         |         |        |  | 173.42  | 133.61    | 9.862  |
| A56C-L57N-H     | 173.42  | 121.624 | 8.512  |  | 173.43  | 121.58    | 8.512  |
| L57C-N-H        |         |         |        |  | 171.45  | 121.73    | 8.504  |
| L57C-Y58N-H     | peak    | not     | found  |  | Peak    | Not       | found  |
| Y58C-N-H        |         |         |        |  | Peak    | Not       | found  |
| Y58C-H59N-H     | peak    | not     | found  |  | Peak    | not       | found  |
| H59C-N-H        |         |         |        |  | Peak    | not       | found  |
| H59C-Y60N-H     | peak    | not     | found  |  | Peak    | not       | found  |
| Y60C-N-H        |         |         |        |  | Peak    | not       | found  |
| Y60C-D61N-H     | peak    | not     | found  |  | Peak    | not       | found  |
| D61C-N-H        |         |         |        |  | Peak    | not       | found  |
| D61C-P62N-H     | peak    | not     | found  |  | Peak    | not       | found  |
| P62C-N-H        |         |         |        |  | Peak    | not       | found  |
| P62C-K63N-H     | 177.74  | 116.58  | 7.985  |  | 177.74  | 116.58    | 7.985  |

|                 |         | HNCO   |        |  |         | HN(CA)-CO |        |
|-----------------|---------|--------|--------|--|---------|-----------|--------|
| Peak assignment | CO, ppm | N, ppm | H, ppm |  | CO, ppm | N, ppm    | H, ppm |
| K63C-N-H        |         |        |        |  | 177.93  | 116.60    | 7.986  |
| K63C-T64N-H     | 177.96  | 105.17 | 6.602  |  | 177.95  | 105.18    | 6.605  |
| T64C-N-H        |         |        |        |  | 175.53  | 105.2     | 6.605  |
| T64C-Q65N-H     | 175.53  | 115.15 | 8.011  |  | 175.54  | 115.24    | 8.013  |
| Q65C-N-H        |         |        |        |  | 174.18  | 115.21    | 8.011  |
| Q65C-D66N-H     | 174.18  | 119.67 | 7.341  |  | 174.18  | 119.67    | 7.341  |
| D66C-N-H        |         |        |        |  | Peak    | Not       | found  |
| D66C-T67N-H     | 174.24  | 114.03 | 7.187  |  | 174.23  | 114.06    | 7.189  |
| T67C-N-H        |         |        |        |  | 172.9   | 114.03    | 7.192  |
| T67C-F68N-H     | peak    | Not    | found  |  | Peak    | Not       | found  |
| F68C-N-H        |         |        |        |  | Peak    | Not       | found  |
| F68C-Y69N-H     | 170.52  | 117.73 | 6.818  |  | 170.54  | 117.76    | 6.812  |
| Y69C-N-H        |         |        |        |  | 173.86  | 117.81    | 6.821  |
| Y69C-D70N-H     | 173.84  | 115.41 | 7.428  |  | 173.84  | 115.41    | 7.428  |
| D70C-N-H        |         |        |        |  | 173.67  | 115.41    | 7.424  |
| D70C-V71N-H     | 173.69  | 118.09 | 9.413  |  | 173.70  | 118.06    | 9.412  |
| V71C-N-H        |         |        |        |  | 175.04  | 118.2     | 9.411  |
| V71C-S72N-H     | 175.04  | 122.20 | 9.192  |  | 175.03  | 121.98    | 9.188  |
| S72C-N-H        |         |        |        |  | 174.22  | 122.08    | 9.189  |
| S72C-E73N-H     | 174.22  | 124.24 | 9.058  |  | 174.22  | 124.17    | 9.057  |
| E73C-N-H        |         |        |        |  | 177.06  | 124.28    | 9.057  |
| E73C-L74N-H     | 177.07  | 124.38 | 8.611  |  | 177.07  | 124.38    | 8.611  |
| L74C-N-H        |         |        |        |  | 176.89  | 124.38    | 8.61   |
| L74C-Q75N-H     | 176.87  | 122.03 | 9.434  |  | 176.86  | 122.02    | 9.433  |
| Q75C-N-H        |         |        |        |  | 175.56  | 122       | 9.433  |
| Q75C-V76N-H     | 175.56  | 126.14 | 8.884  |  | 175.60  | 126.02    | 8.88   |
| V76C-N-H        |         |        |        |  | 175.98  | 126.19    | 8.883  |
| V76C-E77N-H     | 175.98  | 130.04 | 8.69   |  | 175.99  | 130.05    | 8.691  |
| E77C-N-H        |         |        |        |  | 176.66  | 130.08    | 8.688  |
| E77C-S78N-H     | 176.66  | 111.53 | 8.051  |  | 176.66  | 111.65    | 8.053  |
| S78C-N-H        |         |        |        |  | 172.76  | 111.59    | 8.053  |
| S78C-L79N-H     | peak    | Not    | found  |  | Peak    | Not       | found  |

|                 |         | HNCO   |        |  |         | HN(CA)-CO |        |
|-----------------|---------|--------|--------|--|---------|-----------|--------|
| Peak assignment | CO, ppm | N, ppm | H, ppm |  | CO, ppm | N, ppm    | H, ppm |
| L79C-N-H        |         |        |        |  | Peak    | not       | found  |
| L79C-G80N-H     | 178.31  | 114.57 | 8.377  |  | 178.29  | 114.58    | 8.377  |
| G80C-N-H        |         |        |        |  | 170.79  | 114.61    | 8.377  |
| G80C-K81N-H     | 170.79  | 121.85 | 7.882  |  | 170.8   | 121.84    | 7.881  |
| K81C-N-H        |         |        |        |  | 173.72  | 121.81    | 7.881  |
| K81C-Y82N-H     | 173.72  | 121.07 | 8.288  |  | 173.70  | 120.86    | 8.286  |
| Y82C-N-H        |         |        |        |  | 174.72  | 121.13    | 8.291  |
| Y82C-T83N-H     | 174.75  | 117.07 | 9.086  |  | 174.74  | 117.12    | 9.083  |
| T83C-N-H        |         |        |        |  | 173.05  | 117.09    | 9.084  |
| T83C-A84N-H     | 173.05  | 132.38 | 10.175 |  | 173.05  | 132.38    | 10.179 |
| A84C-N-H        |         |        |        |  | 175.87  | 132.44    | 10.172 |
| A84C-N85N-H     | 175.88  | 123.94 | 8.429  |  | 175.88  | 123.94    | 8.429  |
| N85C-N-H        |         |        |        |  | 173.88  | 123.95    | 8.426  |
| N85C-F86N-H     | 173.89  | 120.04 | 7.365  |  | 173.89  | 120.04    | 7.365  |
| F86C-N-H        |         |        |        |  | 175.86  | 120.09    | 7.371  |
| F86C-K87N-H     | 175.88  | 120.59 | 9.286  |  | 175.81  | 120.79    | 9.277  |
| K87C-N-H        |         |        |        |  | 174.82  | 120.59    | 9.281  |
| K87C-K88N-H     | 174.8   | 127.30 | 9.179  |  | 174.8   | 127.37    | 9.179  |
| K88C-N-H        |         |        |        |  | 177.21  | 127.32    | 9.178  |
| K88C-V89N-H     | 177.21  | 120.98 | 8.423  |  | 177.2   | 121.08    | 8.42   |
| V89C-N-H        |         |        |        |  | 175.4   | 120.92    | 8.423  |
| V89C-D90N-H     | 175.39  | 118.61 | 7.95   |  | 175.39  | 118.52    | 7.951  |
| D90C-N-H        |         |        |        |  | 176.82  | 118.66    | 7.95   |
| D90C-K91N-H     | 176.83  | 114.23 | 7.79   |  | 176.84  | 114.34    | 7.788  |
| K91C-N-H        |         |        |        |  | 174.70  | 114.3     | 7.79   |
| K91C-N92N-H     | 174.71  | 114.3  | 7.225  |  | 174.72  | 114.30    | 7.227  |
| N92C-N-H        |         |        |        |  | 175.51  | 114.33    | 7.227  |
| N92C-G93N-H     | 175.51  | 108.36 | 7.935  |  | 175.51  | 108.38    | 7.935  |
| G93C-N-H        |         |        |        |  | 173.52  | 108.47    | 7.934  |
| G93C-N94N-H     | 173.52  | 120.31 | 8.28   |  | 173.52  | 120.31    | 8.28   |
| N94C-N-H        |         |        |        |  | 175.61  | 120.31    | 8.28   |
| N94C-V95N-H     | 175.61  | 123.44 | 8.763  |  | 175.62  | 123.41    | 8.761  |

|                 |         | HNCO   |        |  |         | HN(CA)-CO |        |
|-----------------|---------|--------|--------|--|---------|-----------|--------|
| Peak assignment | CO, ppm | N, ppm | H, ppm |  | CO, ppm | N, ppm    | H, ppm |
| V95C-N-H        |         |        |        |  | 175.99  | 123.4     | 8.763  |
| V95C-K96N-H     | 176     | 128.13 | 9.49   |  | 175.99  | 128.05    | 9.489  |
| K96C-N-H        |         |        |        |  | 177.14  | 128.14    | 9.488  |
| K96C-V97N-H     | 177.14  | 119.61 | 7.997  |  | 177.14  | 119.6     | 7.997  |
| V97C-N-H        |         |        |        |  | 174.67  | 119.65    | 7.997  |
| V97C-A98N-H     | 174.68  | 128.24 | 8.597  |  | 174.67  | 128.18    | 8.597  |
| A98C-N-H        |         |        |        |  | 178.02  | 128.24    | 8.597  |
| A98C-V99N-H     | 178.03  | 122.21 | 8.548  |  | 178.01  | 122.10    | 8.546  |
| V99C-N-H        |         |        |        |  | 177.07  | 122.19    | 8.546  |
| V99C-T100N-H    | 177.06  | 126.11 | 9.975  |  | 177.07  | 126.08    | 9.974  |
| T100C-N-H       |         |        |        |  | 173.58  | 126.12    | 9.975  |
| T100C-A101N-H   | 173.58  | 131.29 | 8.904  |  | 173.58  | 131.29    | 8.904  |
| A101C-N-H       |         |        |        |  | 178.51  | 131.3     | 8.904  |
| A101C-G102N-H   | 178.51  | 110.19 | 9.151  |  | 178.51  | 110.21    | 9.142  |
| G102C-N-H       |         |        |        |  | 173.01  | 110.17    | 9.152  |
| G102C-N103N-H   | 173.02  | 121.06 | 8.201  |  | 173.02  | 121.09    | 8.202  |
| N103C-N-H       |         |        |        |  | 173.99  | 120.98    | 8.201  |
| N103C-Y104N-H   | 174     | 121.19 | 9.211  |  | 174     | 121.19    | 9.205  |
| Y104C-N-H       |         |        |        |  | 174.43  | 121.16    | 9.205  |
| Y104C-Y105N-H   | 174.45  | 116.24 | 10.222 |  | 174.45  | 116.24    | 10.222 |
| Y105C-N-H       |         |        |        |  | 174.29  | 116.19    | 10.219 |
| Y105C-T106N-H   | 174.24  | 113.62 | 8.48   |  | 174.28  | 113.61    | 8.483  |
| T106C-N-H       |         |        |        |  | 175.03  | 113.57    | 8.489  |
| T106C-F107N-H   | 175.01  | 119.69 | 9.469  |  | 175.01  | 119.69    | 9.469  |
| F107C-N-H       |         |        |        |  | 173.71  | 119.61    | 9.466  |
| F107C-T108N-H   | 173.73  | 117.61 | 9.34   |  | 173.75  | 117.59    | 9.336  |
| T108C-N-H       |         |        |        |  | 174.67  | 117.52    | 9.337  |
| T108C-V109N-H   | 174.7   | 127.91 | 9.343  |  | 174.7   | 127.91    | 9.343  |
| V109C-N-H       |         |        |        |  | 174.63  | 127.86    | 9.341  |
| V109C-M110N-H   | 174.61  | 129.58 | 8.779  |  | 174.61  | 129.49    | 8.779  |
| M110C-N-H       |         |        |        |  | 176.95  | 129.5     | 8.776  |
| M110C-Y111N-H   | 176.96  | 117.59 | 8.206  |  | 176.95  | 117.59    | 8.206  |

|                 |         | HNCO   |        |  |         | HN(CA)-CO |        |
|-----------------|---------|--------|--------|--|---------|-----------|--------|
| Peak assignment | CO, ppm | N, ppm | H, ppm |  | CO, ppm | N, ppm    | H, ppm |
| Y111C-N-H       |         |        |        |  | 172.24  | 117.6     | 8.207  |
| Y111C-A112N-H   | 172.25  | 125.86 | 6.659  |  | 172.24  | 125.93    | 6.659  |
| A112C-N-H       |         |        |        |  | 175.07  | 125.91    | 6.66   |
| A112C-D113N-H   | 175.07  | 121.5  | 9.498  |  | 175.07  | 121.5     | 9.496  |
| D113C-N-H       |         |        |        |  | 176.07  | 121.49    | 9.496  |
| D113C-D114N-H   | 176.09  | 114.82 | 8.357  |  | 176.09  | 114.83    | 8.357  |
| D114C-N-H       |         |        |        |  | 177.86  | 114.81    | 8.356  |
| D114C-S115N-H   | 177.87  | 110.88 | 8.702  |  | 177.85  | 110.89    | 8.701  |
| S115C-N-H       |         |        |        |  | 173     | 110.93    | 8.701  |
| S115C-S116N-H   | 173     | 117.95 | 8.884  |  | 173.01  | 117.92    | 8.884  |
| S116C-N-H       |         |        |        |  | 171.12  | 117.98    | 8.884  |
| S116C-A117N-H   | 171.12  | 117.62 | 8.584  |  | 171.12  | 117.55    | 8.583  |
| A117C-N-H       |         |        |        |  | 174.9   | 117.67    | 8.583  |
| A117C-L118N-H   | 174.9   | 121.54 | 9.266  |  | 174.9   | 121.54    | 9.266  |
| L118C-N-H       |         |        |        |  | 175.64  | 121.57    | 9.265  |
| L118C-I119N-H   | 175.63  | 119.83 | 9.769  |  | 175.61  | 119.85    | 9.758  |
| I119C-N-H       |         |        |        |  | 174.33  | 119.90    | 9.769  |
| I119C-H120N-H   | 174.33  | 122.38 | 8.832  |  | 174.33  | 122.38    | 8.832  |
| H120C-N-H       |         |        |        |  | 174.25  | 122.33    | 8.83   |
| H120C-T121N-H   | 174.23  | 116.42 | 6.837  |  | 174.23  | 116.42    | 6.837  |
| T121C-N-H       |         |        |        |  | 169.62  | 116.47    | 6.846  |
| T121C-C122N-H   | 169.65  | 118.22 | 7.212  |  | 169.64  | 118.2     | 7.211  |
| C122C-N-H       |         |        |        |  | 171.54  | 118.19    | 7.229  |
| C122C-L123N-H   | 171.58  | 126.99 | 6.939  |  | 171.59  | 126.97    | 6.94   |
| L123C-N-H       |         |        |        |  | 174.04  | 127.07    | 6.946  |
| L123C-H124H     | peak    | not    | found  |  | peak    | not       | found  |
| H124C-N-H       |         |        |        |  | peak    | not       | found  |
| H124C-K125N-H   | 173.67  | 120.23 | 7.785  |  | 173.67  | 120.24    | 7.788  |
| K125C-N-H       |         |        |        |  | 177.95  | 120.29    | 7.785  |
| K125C-G126N-H   | 177.97  | 116.01 | 8.766  |  | 177.96  | 116       | 8.765  |
| G126C-N-H       |         |        |        |  | 175.28  | 116.03    | 8.765  |
| G126C-N127N-H   | peak    | not    | found  |  | peak    | not       | found  |

|                 |         | HNCO   |        |  | HN(CA)-CO   |            |
|-----------------|---------|--------|--------|--|-------------|------------|
| Peak assignment | CO, ppm | N, ppm | H, ppm |  | CO, ppm     | N, ppm     |
| N127C-N-H       |         |        |        |  | <i>peak</i> | <i>not</i> |
| N127C-K128N-H   | 173.69  | 119.18 | 7.382  |  | 173.69      | 119.18     |
| K128C-N-H       |         |        |        |  | 173.7       | 119.23     |
| K128C-D129N-H   | 173.69  | 120.95 | 8.162  |  | 173.70      | 120.96     |
| D129C-N-H       |         |        |        |  | 175.42      | 120.94     |
| D129C-L130N-H   | 175.43  | 123.14 | 6.911  |  | 175.42      | 123.02     |
| L130C-N-H       |         |        |        |  | 174.70      | 123.20     |
| L130C-G131N-H   | 174.71  | 103.69 | 5.163  |  | <i>Peak</i> | <i>Not</i> |
| G131CN--H       |         |        |        |  | 169.76      | 103.71     |
| G131C-D132N-H   | 169.7   | 116.46 | 6.515  |  | 169.71      | 116.49     |
| D132C-N-H       |         |        |        |  | 172.42      | 116.52     |
| D132C-L133N-H   | 172.42  | 120.84 | 5.505  |  | 172.42      | 120.84     |
| L133C-N-H       |         |        |        |  | 175.04      | 120.8      |
| L133C-Y134N-H   | 175.08  | 125.02 | 8.309  |  | 175.08      | 125.02     |
| Y134C-N-H       |         |        |        |  | 175.39      | 125.11     |
| Y134C-A135N-H   | 175.41  | 124.12 | 9.966  |  | 175.41      | 124.12     |
| A135C-N-H       |         |        |        |  | 175.55      | 124.04     |
| A135C-V136N-H   | 175.59  | 124.87 | 10.264 |  | 175.59      | 124.87     |
| V136C-N-H       |         |        |        |  | 175.21      | 124.85     |
| V136C-L137N-H   | 175.22  | 126.22 | 9.931  |  | 175.22      | 126.2      |
| L137C-N-H       |         |        |        |  | 179.06      | 126.18     |
| L137C-N138N-H   | 179.07  | 121.39 | 9.935  |  | 179.06      | 121.22     |
| N138C-N-H       |         |        |        |  | 175.44      | 121.39     |
| N138C-R139N-H   | 175.45  | 124.83 | 8.619  |  | 175.51      | 124.88     |
| R139C-N-H       |         |        |        |  | 175.99      | 124.83     |
| R139C-N140N-H   | 176.02  | 120.08 | 10.279 |  | 176         | 120.05     |
| N140C-N-H       |         |        |        |  | 174.78      | 120.11     |
| N140C-K141N-H   | 174.81  | 123.57 | 7.627  |  | 174.82      | 123.59     |
| K141C-N-H       |         |        |        |  | 175.45      | 123.57     |
| K141C-D142N-H   | 175.44  | 117.64 | 7.965  |  | <i>peak</i> | <i>Not</i> |
| D142C-N-H       |         |        |        |  | <i>peak</i> | <i>Not</i> |
| D142C-A143N-H   | 175.21  | 123.39 | 7.144  |  | <i>Peak</i> | <i>Not</i> |

|                 |             | HNCO       |              |  | HN(CA)-CO   |            |
|-----------------|-------------|------------|--------------|--|-------------|------------|
| Peak assignment | CO, ppm     | N, ppm     | H, ppm       |  | CO, ppm     | N, ppm     |
| A143C-N-H       |             |            |              |  | 177.58      | 123.38     |
| A143C-A144N-H   | 177.59      | 126.29     | 8.488        |  | 177.59      | 126.29     |
| A144C-N-H       |             |            |              |  | 177.8       | 126.26     |
| A144C-A145N-H   | 177.82      | 126.81     | 9.278        |  | 177.80      | 126.73     |
| A145C-N-H       |             |            |              |  | 178.35      | 126.84     |
| A145C-G146N-H   | 178.35      | 110.4      | 8.796        |  | 178.34      | 110.42     |
| G146C-N-H       |             |            |              |  | 173.98      | 110.40     |
| G146C-D147N-H   | 173.97      | 117.57     | 8.431        |  | 173.97      | 117.57     |
| D147C-N-H       |             |            |              |  | 179.12      | 117.47     |
| D147C-K148N-H   | <i>peak</i> | <i>Not</i> | <i>found</i> |  | <i>Peak</i> | <i>Not</i> |
| K148C-N-H       |             |            |              |  | <i>Peak</i> | <i>Not</i> |
| K148C-V149N-H   | 179.94      | 120.52     | 7.939        |  | 179.92      | 120.50     |
| V149C-N-H       |             |            |              |  | 177.43      | 120.52     |
| V149C-K150N-H   | 177.44      | 120.43     | 7.82         |  | 177.45      | 120.41     |
| K150C-N-H       |             |            |              |  | 179.89      | 120.45     |
| K150C-S151N-H   | 179.9       | 116.86     | 8.228        |  | 179.89      | 116.90     |
| S151C-N-H       |             |            |              |  | <i>Peak</i> | <i>Not</i> |
| S151C-A152N-H   | 176.26      | 126.16     | 7.335        |  | <i>Peak</i> | <i>Not</i> |
| A152C-N-H       |             |            |              |  | 179.79      | 126.164    |
| A152C-V153N-H   | 179.8       | 120.28     | 8.06         |  | 179.8       | 120.27     |
| V153C-N-H       |             |            |              |  | 177.62      | 120.3      |
| V153C-S154N-H   | 177.63      | 113.49     | 7.788        |  | 177.64      | 113.39     |
| S154C-N-H       |             |            |              |  | <i>Peak</i> | <i>Not</i> |
| S154C-A155N-H   | 179.22      | 125.68     | 8.434        |  | <i>Peak</i> | <i>Not</i> |
| A155C-N-H       |             |            |              |  | 178.43      | 125.74     |
| A155C-A156N-H   | 178.44      | 119.58     | 7.25         |  | 178.43      | 119.57     |
| A156C-N-H       |             |            |              |  | 176.72      | 119.63     |
| A156C-T157N-H   | 176.73      | 112.79     | 8.094        |  | 176.73      | 112.82     |
| T157C-N-H       |             |            |              |  | 172.72      | 112.87     |
| T157C-L158N-H   | 172.73      | 118.87     | 7.158        |  | 172.69      | 118.79     |
| L158C-N-H       |             |            |              |  | 176.01      | 118.89     |
| L158C-E159N-H   | 176.02      | 121.18     | 8.354        |  | 176.02      | 121.09     |

|                 |         | HNCO   |        |  |         | HN(CA)-CO |        |
|-----------------|---------|--------|--------|--|---------|-----------|--------|
| Peak assignment | CO, ppm | N, ppm | H, ppm |  | CO, ppm | N, ppm    | H, ppm |
| E159C-N-H       |         |        |        |  | 176.64  | 121.24    | 8.354  |
| E159C-F160N-H   | 176.63  | 128.22 | 9.119  |  | 176.64  | 128.2     | 9.113  |
| F160C-N-H       |         |        |        |  | 177.83  | 128.16    | 9.114  |
| F160C-S161N-H   | 177.87  | 112.93 | 8.829  |  | 177.86  | 113.01    | 8.826  |
| S161C-N-H       |         |        |        |  | Peak    | Not       | found  |
| S161C-K162N-H   | 175.03  | 119.65 | 7.634  |  | Peak    | Not       | found  |
| K162C-N-H       |         |        |        |  | 176.57  | 119.67    | 7.635  |
| K162C-F163N-H   | 176.57  | 120.21 | 7.986  |  | 176.57  | 120.08    | 7.986  |
| F163C-N-H       |         |        |        |  | 175.85  | 120.16    | 7.987  |
| F163C-I164N-H   | 175.85  | 124.45 | 9.576  |  | 175.85  | 124.45    | 9.576  |
| I164C-N-H       |         |        |        |  | 176     | 124.5     | 9.573  |
| I164C-S165N-H   | 176.01  | 119.4  | 8.748  |  | 176     | 119.35    | 8.748  |
| S165C-N-H       |         |        |        |  | 178.95  | 119.47    | 8.747  |
| S165C-T166N-H   | 178.97  | 118.24 | 9.386  |  | 178.95  | 118.23    | 9.387  |
| T166C-N-H       |         |        |        |  | 176.86  | 118.22    | 9.386  |
| T166C-K167N-H   | 176.85  | 125.33 | 8.933  |  | 176.85  | 125.33    | 8.933  |
| K167C-N-H       |         |        |        |  | 177.44  | 125.41    | 8.932  |
| K167C-E168N-H   | 177.45  | 116.88 | 8.633  |  | 177.46  | 116.83    | 8.615  |
| E168C-N-H       |         |        |        |  | 176.21  | 116.85    | 8.629  |
| E168C-N169N-H   | 176.21  | 117.46 | 7.772  |  | 176.2   | 117.43    | 7.764  |
| N169C-N-H       |         |        |        |  | 174.3   | 117.57    | 7.777  |
| N169C-N170N-H   | 174.32  | 115.17 | 8.515  |  | 174.32  | 115.17    | 8.515  |
| N170C-N-H       |         |        |        |  | 174.77  | 115.15    | 8.507  |
| N170C-C171N-H   | 174.77  | 114.74 | 8.476  |  | 174.77  | 114.91    | 8.48   |
| C171C-N-H       |         |        |        |  | 173.03  | 114.75    | 8.476  |
| C171C-A172N-H   | 173.04  | 123.22 | 5.222  |  | 173.04  | 123.22    | 5.222  |
| A172C-N-H       |         |        |        |  | 175.26  | 123.17    | 5.227  |
| A172C-Y173N-H   | 175.26  | 120.3  | 8.284  |  | 175.26  | 120.3     | 8.284  |
| Y173C-N-H       |         |        |        |  | 172.81  | 120.22    | 8.287  |
| Y173C-D174N-H   | 172.76  | 119.27 | 5.986  |  | 172.76  | 119.26    | 5.987  |
| D174C-N-H       |         |        |        |  | 174.44  | 119.27    | 5.984  |
| D174C-N175N-H   | 174.45  | 121.89 | 7.995  |  | 174.45  | 121.89    | 7.995  |

|                 |         | HNCO    |        |  |         | HN(CA)-CO |        |
|-----------------|---------|---------|--------|--|---------|-----------|--------|
| Peak assignment | CO, ppm | N, ppm  | H, ppm |  | CO, ppm | N, ppm    | H, ppm |
| N175C-N-H       |         |         |        |  | 176.56  | 121.88    | 7.992  |
| N175C-D176N-H   | 176.59  | 118.472 | 8.051  |  | 176.59  | 118.47    | 8.051  |
| D176C-N-H       |         |         |        |  | 179.34  | 118.51    | 8.051  |
| D176C-S177N-H   | 179.34  | 116.362 | 7.177  |  | 179.34  | 116.35    | 7.179  |
| S177C-N-H       |         |         |        |  | 175.35  | 116.4     | 7.183  |
| S177C-L178N-H   | 175.35  | 119.917 | 6.783  |  | 175.35  | 119.92    | 6.783  |
| L178C-N-H       |         |         |        |  | 176.41  | 119.95    | 6.785  |
| L178C-K179N-H   | 176.43  | 112.242 | 7.318  |  | 176.42  | 112.22    | 7.319  |
| K179C-N-H       |         |         |        |  | 180.11  | 112.3     | 7.319  |
| K179C-S180N-H   | 180.12  | 114.447 | 7.478  |  | 180.11  | 114.46    | 7.48   |
| S180C-N-H       |         |         |        |  | Peak    | Not       | found  |
| S180C-L181N-H   | 176.62  | 121.622 | 7.542  |  | Peak    | Not       | found  |
| L181C-N-H       |         |         |        |  | 177.91  | 121.65    | 7.543  |
| L181C-L182N-H   | 177.93  | 114.552 | 7.014  |  | 177.93  | 114.55    | 7.014  |
| L182C-N-H       |         |         |        |  | 177.77  | 114.56    | 7.016  |
| L182C-T183N-H   | 177.78  | 105.598 | 7.262  |  | 177.77  | 105.6     | 7.264  |
| T183C-N-H       |         |         |        |  | 174.21  | 105.64    | 7.264  |
| T183C-K184N-H   | 174.22  | 126.916 | 7.243  |  | 174.21  | 126.89    | 7.245  |
| K184C-N-H       |         |         |        |  | 180.95  | 126.94    | 7.245  |

**Table A4. Assignments of high-spin NP4 at pH 7.3 from the HNCACB and CACB(CO)NH experiments.**

|            | HNCA-        | CB         |              | CACB-        | (CO)NH     |              |
|------------|--------------|------------|--------------|--------------|------------|--------------|
| Assignment | C, ppm       | N, ppm     | H, ppm       | C, ppm       | N, ppm     | H, ppm       |
| A1CA-C2N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | <i>peak</i>  | <i>not</i> | <i>found</i> |
| A1CB-C2N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | <i>peak</i>  | <i>not</i> | <i>found</i> |
| C2CA-N-H   | <i>peak</i>  | <i>not</i> | <i>found</i> |              |            |              |
| C2CA-T3N-H | <b>53.63</b> | 120.41     | 9.894        | <b>53.71</b> | 120.46     | 9.898        |
| C2CB-N-H   | <i>peak</i>  | <i>not</i> | <i>found</i> |              |            |              |
| C2CB-T3N-H | <b>42.93</b> | 120.44     | 9.895        | <b>43.01</b> | 120.46     | 9.898        |
| T3CA-N-H   | <b>61.85</b> | 120.43     | 9.897        |              |            |              |
| T3CA-K4N-H | <b>61.82</b> | 124.02     | 8.113        | <b>61.86</b> | 124        | 8.12         |
| T3CB-N-H   | <b>69.4</b>  | 120.41     | 9.896        |              |            |              |
| T3CB-K4N-H | <b>69.42</b> | 124.03     | 8.116        | <b>69.4</b>  | 124.04     | 8.116        |
| K4CA-N-H   | <b>55.02</b> | 124.06     | 8.113        |              |            |              |
| K4CA-N5N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | <i>peak</i>  | <i>not</i> | <i>found</i> |
| K4CB-N-H   | <b>32.29</b> | 124.02     | 8.116        |              |            |              |
| K4CB-N5N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | <i>peak</i>  | <i>not</i> | <i>found</i> |
| N5CA-N-H   | <i>peak</i>  | <i>not</i> | <i>found</i> |              |            |              |
| N5CA-A6N-H | <b>52.37</b> | 124.53     | 7.787        | <b>52.37</b> | 124.53     | 7.787        |
| N5CB-A6N-H | <b>39.02</b> | 124.57     | 7.783        | <b>38.89</b> | 124.53     | 7.787        |
| N5CB-A6N-H | <b>38.79</b> | 124.52     | 7.784        |              |            |              |
| A6CA-N-H   | <b>52.4</b>  | 124.54     | 7.785        |              |            |              |
| A6CA-I7N-H | <b>52.38</b> | 124.77     | 8.441        | <b>52.43</b> | 124.82     | 8.445        |
| A6CB-N-H   | <b>18.6</b>  | 124.55     | 7.785        |              |            |              |
| A6CB-I7N-H | <b>18.6</b>  | 124.76     | 8.443        | <b>18.64</b> | 124.84     | 8.445        |
| I7CA-N-H   | <b>60.09</b> | 124.75     | 8.444        |              |            |              |
| I7CA-A8N-H | <b>60.09</b> | 129.53     | 8.479        | <b>60.08</b> | 129.5      | 8.481        |
| I7CB-N-H   | <b>38.91</b> | 124.81     | 8.439        |              |            |              |
| I7CB-A8N-H | <b>38.89</b> | 129.53     | 8.478        | <b>38.85</b> | 129.49     | 8.481        |
| A8CA-N-H   | <b>51.33</b> | 129.55     | 8.478        |              |            |              |
| A8CA-Q9N-H | <b>51.31</b> | 121.52     | 8.534        | <b>51.33</b> | 121.52     | 8.536        |
| A8CB-N-H   | <b>20.66</b> | 129.54     | 8.479        |              |            |              |

|              | HNCA-        | CB         |              | CACB-        | (CO)NH     |              |
|--------------|--------------|------------|--------------|--------------|------------|--------------|
| Assignment   | C, ppm       | N, ppm     | H, ppm       | C, ppm       | N, ppm     | H, ppm       |
| A8CB-Q9N-H   | <b>20.64</b> | 121.5      | 8.534        | <b>20.71</b> | 121.43     | 8.535        |
| Q9CA-N-H     | <b>56.37</b> | 121.5      | 8.534        |              |            |              |
| Q9CA-T10N-H  | <b>56.35</b> | 127.10     | 8.874        | <b>56.39</b> | 127.07     | 8.876        |
| Q9CB-N-H     | <b>29.65</b> | 121.49     | 8.533        |              |            |              |
| Q9CB-N-H     | <b>29.37</b> | 121.53     | 8.533        |              |            |              |
| Q9CB-T10-N-H | <b>29.49</b> | 127.06     | 8.874        | <b>29.53</b> | 127.05     | 8.876        |
| T10CA-N-H    | <b>64.30</b> | 127.14     | 8.874        |              |            |              |
| T10CA-G11N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | <i>peak</i>  | <i>not</i> | <i>found</i> |
| T10CB-N-H    | <b>68.65</b> | 127.11     | 8.874        |              |            |              |
| T10CB-N-H    | <b>68.93</b> | 127.12     | 8.874        |              |            |              |
| T10CB-G11N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | <i>peak</i>  | <i>not</i> | <i>found</i> |
| G11CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> |              |            |              |
| G11CA-F12N-H | <b>46.08</b> | 118.83     | 7.015        | <b>46.12</b> | 118.83     | 7.017        |
| F12CA-N-H    | <b>57.62</b> | 118.85     | 7.015        |              |            |              |
| F12CA-N13N-H | <b>57.60</b> | 128.12     | 8.756        | <b>57.6</b>  | 128.1      | 8.757        |
| F12CB-N-H    | <b>39.94</b> | 118.85     | 7.015        |              |            |              |
| F12CB-N13N-H | <b>39.95</b> | 128.11     | 8.754        | <b>39.94</b> | 128.11     | 8.757        |
| N13CA-N-H    | <b>51.31</b> | 128.13     | 8.754        |              |            |              |
| N13CA-K14N-H | <b>51.27</b> | 125.41     | 7.987        | <b>51.29</b> | 125.39     | 7.99         |
| N13CB-N-H    | <b>37.36</b> | 128.16     | 8.755        |              |            |              |
| N13CB-K14N-H | <b>37.3</b>  | 125.34     | 7.988        | <b>37.32</b> | 125.38     | 7.99         |
| K14CA-N-H    | <b>58.74</b> | 125.41     | 7.987        |              |            |              |
| K14CA-D15N-H | <b>58.74</b> | 120.18     | 8.022        | <b>58.74</b> | 120.18     | 8.022        |
| K14CBN--H    | <b>32.17</b> | 125.38     | 7.988        |              |            |              |
| K14CB-D15N-H | <b>32.15</b> | 120.25     | 8.023        | <b>32.18</b> | 120.2      | 8.022        |
| D15CAN--H    | <b>57.3</b>  | 120.22     | 8.02         |              |            |              |
| D15CA-K16N-H | <b>57.28</b> | 116.71     | 7.067        | <b>57.28</b> | 116.71     | 7.067        |
| D15CB-N-H    | <b>40.42</b> | 120.18     | 8.02         |              |            |              |
| D15CB-K16N-H | <b>40.35</b> | 116.73     | 7.065        | <b>40.4</b>  | 116.72     | 7.068        |
| K16CA-N-H    | <b>57.85</b> | 116.74     | 7.066        |              |            |              |
| K16CA-Y17N-H | <b>57.87</b> | 118.46     | 7.013        | <b>57.87</b> | 118.46     | 7.013        |
| K16CB-N-H    | <b>33.42</b> | 116.74     | 7.066        |              |            |              |

|               | HNCA-  | CB     |        | CACB-  | (CO)NH  |        |
|---------------|--------|--------|--------|--------|---------|--------|
| Assignment    | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm  | H, ppm |
| K16CB-Y17N-H  | 33.43  | 118.47 | 7.013  | 33.45  | 118.45  | 7.013  |
| Y17CA-N-H     | 62.30  | 118.47 | 7.013  |        |         |        |
| Y17CA-F18N-H  | 62.30  | 118.41 | 8.421  | 62.31  | 118.39  | 8.424  |
| Y17CB-N-h     | 41.12  | 118.46 | 7.012  |        |         |        |
| Y17CB-F18N-H  | 41.11  | 118.33 | 8.422  | 41.12  | 118.41  | 8.424  |
| F18CA-N-H     | 56.38  | 118.42 | 8.421  |        |         |        |
| F18CA-N19N-H  | 56.41  | 118.71 | 7.856  | 56.41  | 118.64  | 7.858  |
| F18CB-N-H     | 36.74  | 118.42 | 8.421  |        |         |        |
| F18CB-N19N-H  | 36.74  | 118.65 | 7.857  | 36.75  | 118.64  | 7.858  |
| N19CA-N-H     | 52.48  | 118.65 | 7.855  |        |         |        |
| N19CA-G20-N-H | 52.49  | 110.38 | 9.265  | 52.50  | 110.38  | 9.263  |
| N19CB-N-H     | 38.49  | 118.64 | 7.856  |        |         |        |
| N19CB-G20-N-H | 38.47  | 110.39 | 9.261  | 38.49  | 110.38  | 9.264  |
| G20N-CA-H     | 45.41  | 110.42 | 9.262  |        |         |        |
| G20CA-D21N-H  | 45.4   | 118.55 | 7.645  | 45.43  | 118.63  | 7.648  |
| D21CA-N-H     | 51.56  | 118.68 | 7.645  |        |         |        |
| D21CA-V22N-H  | 51.53  | 119.09 | 8.217  | 51.57  | 119.14  | 8.219  |
| D21CB-N-H     | 42.51  | 118.65 | 7.645  |        |         |        |
| D21CB-V22N-H  | 42.57  | 119.12 | 8.217  | 42.58  | 119.15  | 8.219  |
| V22CA-N-H     | 63.06  | 119.17 | 8.217  |        |         |        |
| V22CA-W23N-H  | 63.06  | 127.69 | 9.632  | 63.06  | 127.69  | 9.632  |
| V22CB-N-H     | 33.01  | 119.15 | 8.222  |        |         |        |
| V22CB-W23N-H  | 33     | 127.59 | 9.63   | 33.005 | 127.683 | 9.631  |
| W23CA-N-H     | 55.93  | 127.69 | 9.629  |        |         |        |
| W23CA-Y24N-H  | 55.98  | 119.00 | 9.005  | 55.917 | 119.07  | 9.005  |
| W23CB-N-H     | 34.1   | 127.69 | 9.63   |        |         |        |
| W23CB-Y24N-H  | 34.05  | 119.06 | 9.009  | 34.122 | 119.071 | 9.006  |
| Y24CA-N-H     | 57.59  | 119.06 | 9.002  |        |         |        |
| Y24CA-V25N-H  | 57.59  | 120.55 | 8.547  | 57.625 | 120.726 | 8.551  |
| Y24CB-N-H     | 40.04  | 119.05 | 9.005  |        |         |        |
| Y24CB-V25N-H  | 40.03  | 120.61 | 8.552  | 40.047 | 120.682 | 8.555  |
| V25CA-N-H     | 63.66  | 120.77 | 8.55   |        |         |        |

|              | HNCA-  | CB     |        | CACB-  | (CO)NH  |        |
|--------------|--------|--------|--------|--------|---------|--------|
| Assignment   | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm  | H, ppm |
| V25CA-T26N-H | 63.7   | 122.91 | 10.067 | 63.7   | 122.91  | 10.067 |
| V25CB-N-H    | 32.63  | 120.74 | 8.559  |        |         |        |
| V25CB-T26N-H | 32.72  | 122.81 | 10.073 | 32.671 | 122.913 | 10.061 |
| T26CA-N-H    | 64.01  | 122.93 | 10.069 |        |         |        |
| T26CA-D27N-H | 63.99  | 120.54 | 8.597  | 63.99  | 120.54  | 8.597  |
| T26CB-N-H    | 69.01  | 122.94 | 10.072 |        |         |        |
| T26CB-N-H    | 69.24  | 122.88 | 10.072 |        |         |        |
| T26CB-D27N-H | 69.11  | 120.52 | 8.595  | 69.11  | 120.52  | 8.595  |
| D27CA-N-H    | 53.96  | 120.56 | 8.591  |        |         |        |
| D27CA-Y28N-H | 53.96  | 119.38 | 10.306 | 53.97  | 119.32  | 10.31  |
| D27CB-N-H    | 46.7   | 120.57 | 8.592  |        |         |        |
| D27CB-Y28N-H | 46.67  | 119.34 | 10.311 | 46.69  | 119.32  | 10.31  |
| Y28CA-N-H    | 58.2   | 119.33 | 10.308 |        |         |        |
| Y28CA-L29N-H | 58.2   | 123.41 | 9.235  | 58.21  | 123.45  | 9.232  |
| Y28CB-N-H    | 43.20  | 119.24 | 10.307 |        |         |        |
| Y28CB-L29N-H | 43.18  | 123.42 | 9.225  | 43.18  | 123.44  | 9.233  |
| L29CA-N-H    | 53.56  | 123.45 | 9.227  |        |         |        |
| L29CA-D30N-H | 53.55  | 127.36 | 8.366  | 53.56  | 127.41  | 8.363  |
| L29CB-N-H    | 43.42  | 123.45 | 9.222  |        |         |        |
| L29CB-D30N-H | 43.41  | 127.34 | 8.36   | 43.41  | 127.40  | 8.363  |
| D30CA-N-H    | 51.18  | 127.38 | 8.361  |        |         |        |
| D30CA-L31N-H | 51.17  | 123.62 | 6.96   | 51.21  | 123.69  | 6.964  |
| D30CB-N-H    | 40.86  | 127.38 | 8.363  |        |         |        |
| D30CB-L31N-H | 40.82  | 123.59 | 6.962  | 40.87  | 123.71  | 6.966  |
| L31CA-N-H    | 55.29  | 123.63 | 6.968  |        |         |        |
| L31CA-E32N-H | 55.28  | 119.66 | 7.206  | 55.34  | 119.78  | 7.21   |
| L31CB-N-H    | 40.89  | 123.63 | 6.962  |        |         |        |
| L31CB-E32N-H | 40.83  | 119.76 | 7.207  | 40.89  | 119.78  | 7.212  |
| E32CA-N-H    | 52.89  | 119.79 | 7.21   |        |         |        |
| E32CB-N-H    | 29.02  | 119.78 | 7.209  |        |         |        |
| E32CB-N-H    | 29.31  | 119.79 | 7.209  |        |         |        |
| P33CA-D34N-H | 62.47  | 120.80 | 8.166  | 62.48  | 120.77  | 8.167  |

|              | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|--------------|--------|--------|--------|--------|--------|--------|
| Assignment   | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| P33CB-D34N-H | 32.11  | 120.79 | 8.163  | 32.16  | 120.76 | 8.166  |
| D34CA-N-H    | 53.83  | 120.79 | 8.163  |        |        |        |
| D34CA-D35N-H | 53.81  | 120.41 | 8.358  | 53.85  | 120.45 | 8.36   |
| D34CB-N-H    | 42.26  | 120.74 | 8.163  |        |        |        |
| D34CB-D35N-H | 42.23  | 120.45 | 8.358  | 42.27  | 120.43 | 8.36   |
| D35CA-N-H    | 56.88  | 120.44 | 8.358  |        |        |        |
| D35CA-V36N-H | 56.87  | 119.18 | 8.203  | 56.88  | 119.18 | 8.205  |
| D35CB-N-H    | 40.75  | 120.5  | 8.358  |        |        |        |
| D35CB-V36N-H | 40.76  | 119.18 | 8.201  | 40.78  | 119.18 | 8.205  |
| V36CA-N-H    | 59.9   | 119.22 | 8.202  |        |        |        |
| V36CB-N-H    | 32.06  | 119.21 | 8.203  |        |        |        |
| V36CB-N-H    | 32.39  | 119.21 | 8.204  |        |        |        |
| P37CA-K38N-H | 63.85  | 124.29 | 9.905  | 63.89  | 124.29 | 9.908  |
| P37CB-K38N-H | 33.03  | 124.18 | 9.902  | 33.06  | 124.27 | 9.909  |
| K38N-CA-H    | 57.27  | 124.46 | 9.9    |        |        |        |
| K38CA-R39N-H | 57.21  | 127.48 | 9.78   | 57.21  | 127.48 | 9.78   |
| K38N-CB-H    | 35.29  | 124.46 | 9.905  |        |        |        |
| K38CB-R39N-H | 35.28  | 127.49 | 9.798  | 35.28  | 127.49 | 9.798  |
| R39CA-N-H    | 55.91  | 127.52 | 9.783  |        |        |        |
| R39CA-Y40N-H | peak   | not    | found  | peak   | not    | found  |
| R39CB-N-H    | 28.98  | 127.42 | 9.798  |        |        |        |
| R39CB-Y40N-H | peak   | not    | found  | peak   | not    | found  |
| Y40CA-C41N-H | peak   | not    | found  | peak   | not    | found  |
| Y40CB-C41N-H | peak   | not    | found  | peak   | not    | found  |
| C41CA-A42N-H | peak   | not    | found  | peak   | not    | found  |
| C41CB-A42N-H | peak   | not    | found  | peak   | not    | found  |
| A42CA-A43N-H | peak   | not    | found  | peak   | not    | found  |
| A42CB-A43N-H | peak   | not    | found  | peak   | not    | found  |
| A43CA-N-H    | peak   | not    | found  |        |        |        |
| A43CA-L44N-H | 49.78  | 116.14 | 8.875  | 49.77  | 116.18 | 8.881  |
| A43CB-L44N-H | 22.89  | 116.11 | 8.874  | 22.89  | 116.18 | 8.879  |
| L44CA-N-H    | 53.99  | 116.23 | 8.874  |        |        |        |

|              | HNCA-  | CB      |        | CACB-  | (CO)NH  |        |
|--------------|--------|---------|--------|--------|---------|--------|
| Assignment   | C, ppm | N, ppm  | H, ppm | C, ppm | N, ppm  | H, ppm |
| L44CA-A45N-H | 53.97  | 121.583 | 8.997  | 53.97  | 121.568 | 8.999  |
| L44CB-N-H    | 46.83  | 116.21  | 8.878  |        |         |        |
| L44CB-A45N-H | 46.84  | 121.65  | 8.997  | 46.79  | 121.57  | 8.999  |
| A45CA-N-H    | 52.00  | 121.51  | 8.997  |        |         |        |
| A45CA-A46N-H | 52.03  | 125.81  | 8.822  | 52.03  | 125.81  | 8.822  |
| A45CB-N-H    | 21.98  | 121.57  | 8.997  |        |         |        |
| A45CB-A46N-H | 21.99  | 125.84  | 8.819  | 22.01  | 125.81  | 8.82   |
| A46CA-N-H    | 51.45  | 125.85  | 8.819  |        |         |        |
| A46CA-G47N-H | 51.49  | 108.01  | 9.218  | 51.48  | 107.97  | 9.218  |
| A46CB-N-H    | 23.56  | 125.87  | 8.818  |        |         |        |
| A46CB-G47N-H | 23.55  | 107.97  | 9.216  | 23.57  | 107.97  | 9.218  |
| G47CA-N-H    | 45.72  | 107.96  | 9.217  |        |         |        |
| G47CA-T48N-H | 45.72  | 113.20  | 8.594  | 45.73  | 113.22  | 8.596  |
| T48CA-N-H    | 61.44  | 113.25  | 8.594  |        |         |        |
| T48CA-A49N-H | 61.45  | 128.48  | 8.987  | 61.42  | 128.43  | 8.989  |
| T48CB-N-H    | 69.83  | 113.27  | 8.594  |        |         |        |
| T48CB-N-H    | 69.63  | 113.26  | 8.594  |        |         |        |
| T48CB-A49N-H | 69.69  | 128.45  | 8.986  | 69.72  | 128.42  | 8.989  |
| A49CA-N-H    | 53.18  | 128.47  | 8.986  |        |         |        |
| A49CA-S50N-H | peak   | not     | found  | peak   | Not     | found  |
| A49CB-N-H    | 20.57  | 128.46  | 8.986  |        |         |        |
| A49CB-S50N-H | peak   | not     | found  | peak   | Not     | found  |
| S50CA-G51N-H | 59.05  | 106.84  | 8.497  | 59.12  | 106.74  | 8.502  |
| S50CB-G51N-H | 62.72  | 106.66  | 8.498  | 62.7   | 106.74  | 8.501  |
| G51CA-N-H    | 45.1   | 106.72  | 8.501  |        |         |        |
| G51CA-K52N-H | 45.07  | 120.38  | 7.88   | 45.12  | 120.39  | 7.882  |
| K52CA-N-H    | 54.4   | 120.41  | 7.88   |        |         |        |
| K52CA-L53N-H | 54.39  | 123.38  | 8.611  | 54.42  | 123.37  | 8.614  |
| K52CB-N-H    | 35.46  | 120.5   | 7.88   |        |         |        |
| K52CB-L53N-H | 35.45  | 123.36  | 8.612  | 35.45  | 123.37  | 8.614  |
| L53CA-N-H    | 55.38  | 123.36  | 8.611  |        |         |        |
| L53CA-K54N-H | 55.39  | 126.56  | 8.957  | 55.38  | 126.58  | 8.959  |

|              | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|--------------|--------|--------|--------|--------|--------|--------|
| Assignment   | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| L53CB-N-H    | 42.51  | 123.41 | 8.612  |        |        |        |
| L53CB-K54N-H | 42.50  | 126.53 | 8.958  | 42.532 | 126.60 | 8.959  |
| K54CA-N-H    | 54.55  | 126.56 | 8.957  |        |        |        |
| K54CA-E55N-H | 54.51  | 118.73 | 8.937  | 54.56  | 118.78 | 8.939  |
| K54CB-N-H    | 37.75  | 126.57 | 8.957  |        |        |        |
| K54CB-E55N-H | 37.77  | 118.72 | 8.936  | 37.76  | 118.76 | 8.939  |
| E55CA-N-H    | 56.41  | 118.80 | 8.937  |        |        |        |
| E55CA-A56N-H | 56.40  | 133.63 | 9.866  | 56.45  | 133.60 | 9.869  |
| E55CB-N-H    | 36.38  | 118.80 | 8.935  |        |        |        |
| E55CB-A56N-H | 36.45  | 133.64 | 9.865  | 36.39  | 133.62 | 9.868  |
| A56CA-N-H    | 49.98  | 133.62 | 9.863  |        |        |        |
| A56CA-L57N-H | 50.01  | 121.53 | 8.511  | 50.04  | 121.67 | 8.508  |
| A56CB-N-H    | 22.80  | 133.63 | 9.866  |        |        |        |
| A56CB-L57N-H | 22.76  | 121.61 | 8.511  | 22.81  | 121.65 | 8.511  |
| L57CB-N-H    | 46.77  | 121.51 | 8.511  |        |        |        |
| L57CA-Y58N-H | peak   | not    | found  | peak   | not    | found  |
| L57CB-Y58N-H | peak   | not    | found  | peak   | not    | found  |
| Y58CA-H59N-H | peak   | not    | found  | peak   | not    | found  |
| Y58CB-H59N-H | peak   | not    | found  | peak   | not    | found  |
| H59CA-Y60N-H | peak   | not    | found  | peak   | not    | found  |
| H59CB-Y60N-H | peak   | not    | found  | peak   | not    | found  |
| Y60CA-D61N-H | peak   | not    | found  | peak   | not    | found  |
| Y60CB-D61N-H | peak   | not    | found  | peak   | not    | found  |
| D61CA-P62N-H | peak   | not    | found  | peak   | not    | found  |
| D61CB-P62N-H | peak   | not    | found  | peak   | not    | found  |
| P62CA-K63N-H | 63.67  | 116.68 | 7.986  | 63.69  | 116.60 | 7.987  |
| P62CB-K63N-H | 32.95  | 116.58 | 7.987  | 32.95  | 116.60 | 7.987  |
| K63CA-N-H    | 58.72  | 116.59 | 7.985  |        |        |        |
| K63CA-T64N-H | 58.73  | 105.19 | 6.6    | 58.75  | 105.18 | 6.603  |
| K63CB-N-H    | 32.47  | 116.58 | 7.985  |        |        |        |
| K63CB-T64N-H | 32.46  | 105.21 | 6.602  | 32.48  | 105.18 | 6.603  |
| T64CA-N-H    | 61.36  | 105.21 | 6.601  |        |        |        |

|              | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|--------------|--------|--------|--------|--------|--------|--------|
| Assignment   | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| T64CA-Q65N-H | 61.36  | 115.13 | 8.011  | 61.31  | 115.16 | 8.012  |
| T64CB-N-H    | 71.03  | 105.19 | 6.601  |        |        |        |
| T64CB-Q65N-H | 71.05  | 115.15 | 8.009  | 71.08  | 115.16 | 8.013  |
| Q65CA-N-H    | 57.83  | 115.18 | 8.01   |        |        |        |
| Q65CA-D66N-H | 57.80  | 119.62 | 7.34   | 57.86  | 119.67 | 7.343  |
| Q65CB-N-H    | 25.40  | 115.19 | 8.01   |        |        |        |
| Q65CB-D66N-H | 25.39  | 119.66 | 7.341  | 25.45  | 119.68 | 7.342  |
| D66CA-N-H    | 55.20  | 119.64 | 7.342  |        |        |        |
| D66CA-T67N-H | 55.23  | 114.10 | 7.187  | 55.27  | 114.03 | 7.189  |
| D66CB-N-H    | 41.77  | 119.72 | 7.34   |        |        |        |
| D66CB-T67N-H | 41.78  | 114.12 | 7.184  | 41.75  | 114.03 | 7.188  |
| T67CA-N-H    | 58.48  | 114.06 | 7.186  |        |        |        |
| T67CA-F68N-H | peak   | not    | found  | 58.52  | 114.62 | 5.059  |
| T67CB-N-H    | 71.67  | 114.03 | 7.185  |        |        |        |
| T67CB-N-H    | 71.83  | 114.03 | 7.186  |        |        |        |
| T67CB-F68N-H | peak   | not    | found  | 71.74  | 114.64 | 5.05   |
| F68CA-Y69N-H | 54.57  | 117.77 | 6.816  | 54.57  | 117.77 | 6.816  |
| F68CB-Y69N-H | 39.35  | 117.87 | 6.813  | 39.4   | 117.78 | 6.82   |
| Y69CA-N-H    | 54.67  | 117.80 | 6.814  |        |        |        |
| Y69CA-D70N-H | 54.67  | 115.57 | 7.429  | 54.69  | 115.41 | 7.428  |
| Y69CB-N-H    | 41.06  | 117.85 | 6.807  |        |        |        |
| Y69CB-D70N-H | 41.04  | 115.29 | 7.417  | 41.07  | 115.45 | 7.415  |
| D70CA-N-H    | 52.07  | 115.42 | 7.423  |        |        |        |
| D70CA-V71N-H | 52.10  | 118.01 | 9.413  | 52.14  | 118.11 | 9.415  |
| D70CB-N-H    | 43.89  | 115.51 | 7.427  |        |        |        |
| D70CB-V71N-H | 43.98  | 118.07 | 9.412  | 43.99  | 118.09 | 9.415  |
| V71CA-N-H    | 61.69  | 118.18 | 9.412  |        |        |        |
| V71CA-S72N-H | 61.68  | 122.18 | 9.192  | 61.68  | 122.19 | 9.195  |
| V71CB-N-H    | 35.83  | 118.20 | 9.411  |        |        |        |
| V71CB-S72N-H | 35.92  | 122.09 | 9.196  | 35.91  | 122.19 | 9.194  |
| S72CA-N-H    | 58.62  | 122.20 | 9.192  |        |        |        |
| S72CA-E73N-H | 58.61  | 124.21 | 9.057  | 58.61  | 124.24 | 9.06   |

|              | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|--------------|--------|--------|--------|--------|--------|--------|
| Assignment   | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| S72CB-N-H    | 67.62  | 122.16 | 9.191  |        |        |        |
| S72CB-E73N-H | 67.61  | 124.23 | 9.058  | 67.62  | 124.25 | 9.06   |
| E73CA-N-H    | 56.25  | 124.27 | 9.06   |        |        |        |
| E73CA-L74N-H | 56.30  | 124.38 | 8.612  | 56.30  | 124.38 | 8.612  |
| E73CB-N-H    | 29.81  | 124.31 | 9.058  |        |        |        |
| E73CB-N-H    | 30.09  | 124.31 | 9.058  |        |        |        |
| E73CB-L74N-H | 29.94  | 124.41 | 8.612  | 29.984 | 124.38 | 8.613  |
| L74CA-N-H    | 54.87  | 124.39 | 8.61   |        |        |        |
| L74CA-Q75N-H | 54.87  | 122.04 | 9.434  | 54.91  | 122.02 | 9.436  |
| L74CB-N-H    | 43.11  | 124.40 | 8.61   |        |        |        |
| L74CB-Q75N-H | 43.14  | 122.04 | 9.431  | 43.13  | 122.03 | 9.437  |
| Q75CA-N-H    | 54.11  | 122.01 | 9.434  |        |        |        |
| Q75CA-V76N-H | 54.10  | 126.08 | 8.882  | 54.12  | 126.16 | 8.886  |
| Q75CB-N-H    | 30.49  | 122.02 | 9.435  |        |        |        |
| Q75CB-N-H    | 30.72  | 122.01 | 9.433  |        |        |        |
| Q75CB-V76N-H | 30.65  | 126.06 | 8.883  | 30.63  | 126.17 | 8.886  |
| V76CA-N-H    | 62.89  | 126.11 | 8.883  |        |        |        |
| V76CA-E77N-H | 62.89  | 129.98 | 8.689  | 62.88  | 130.01 | 8.692  |
| V76CB-N-H    | 32.35  | 126.07 | 8.886  |        |        |        |
| V76CB-N-H    | 32.61  | 126.12 | 8.882  |        |        |        |
| V76CB-E77N-H | 32.44  | 130.   | 8.686  | 32.47  | 130.   | 8.692  |
| E77CA-N-H    | 57.62  | 129.96 | 8.688  |        |        |        |
| E77CA-S78N-H | 57.63  | 111.55 | 8.053  | 57.63  | 111.55 | 8.053  |
| E77CB-N-H    | 29.74  | 129.99 | 8.691  |        |        |        |
| E77CB-S78N-H | 29.75  | 111.65 | 8.052  | 29.87  | 111.55 | 8.053  |
| S78CA-N-H    | 57.07  | 111.60 | 8.051  |        |        |        |
| S78CA-L79N-H | peak   | not    | found  | peak   | not    | found  |
| S78CB-N-H    | 62.94  | 111.60 | 8.052  |        |        |        |
| S78CB-L79N-H | peak   | not    | found  | peak   | not    | found  |
| L79CA-N-H    |        |        |        |        |        |        |
| L79CA-G80N-H | 58.04  | 114.58 | 8.377  | 58.042 | 114.58 | 8.377  |
| L79CB-N-H    |        |        |        |        |        |        |
| L79CB-G80N-H | 40.99  | 114.58 | 8.377  | 40.99  | 114.58 | 8.377  |

|              | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|--------------|--------|--------|--------|--------|--------|--------|
| Assignment   | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
|              |        |        |        |        |        |        |
| G80CA-N-H    | 46.29  | 114.61 | 8.376  |        |        |        |
| G80CA-K81N-H | 46.28  | 121.83 | 7.881  | 46.31  | 121.84 | 7.883  |
| K81CA-N-H    | 56.15  | 121.83 | 7.881  |        |        |        |
| K81CA-Y82H   | 56.16  | 120.95 | 8.286  | 56.14  | 121.08 | 8.29   |
| K81CB-N-H    | 35.44  | 121.83 | 7.88   |        |        |        |
| K81CB-Y82N-H | 35.44  | 120.93 | 8.285  | 35.45  | 121.05 | 8.29   |
| Y82CA-N-H    | 56.93  | 121.12 | 8.286  |        |        |        |
| Y82CA-T83N-H | 56.93  | 117.10 | 9.087  | 56.95  | 117.09 | 9.087  |
| Y82CB-N-H    | 44.08  | 121.14 | 8.286  |        |        |        |
| Y82CB-T83N-H | 44.03  | 117.13 | 9.086  | 44.06  | 117.09 | 9.088  |
| T83CA-N-H    | 62.69  | 117.08 | 9.085  |        |        |        |
| T83CA-A84N-H | 62.68  | 132.39 | 10.179 | 62.66  | 132.38 | 10.179 |
| T83CB-N-H    | 70.93  | 117.11 | 9.085  |        |        |        |
| T83CB-N-H    | 70.63  | 117.10 | 9.085  |        |        |        |
| T83CB-A84N-H | 70.79  | 132.39 | 10.176 | 70.79  | 132.39 | 10.179 |
| A84CA-N-H    | 51.99  | 132.47 | 10.176 |        |        |        |
| A84CA-N85N-H | 52.06  | 124.01 | 8.43   | 52.02  | 123.95 | 8.43   |
| A84CB-N-H    | 21.51  | 132.45 | 10.175 |        |        |        |
| A84CB-N85N-H | 21.53  | 123.91 | 8.428  | 21.51  | 123.94 | 8.43   |
| N85CA-N-H    | 53.81  | 123.95 | 8.428  |        |        |        |
| N85CA-F86N-H | 53.89  | 119.99 | 7.368  | 53.82  | 120.11 | 7.369  |
| N85CB-N-H    | 39.02  | 123.94 | 8.432  |        |        |        |
| N85CB-F86N-H | 39.10  | 120.06 | 7.364  | 39.05  | 120.09 | 7.368  |
| F86CA-N-H    | 57.05  | 120.08 | 7.366  |        |        |        |
| F86CA-K87N-H | 57.06  | 120.57 | 9.283  | 57.07  | 120.60 | 9.288  |
| F86CB-N-H    | 42.79  | 120.11 | 7.366  |        |        |        |
| F86CB-K87N-H | 42.84  | 120.43 | 9.288  | 42.78  | 120.59 | 9.288  |
| K87CA-N-H    | 54.74  | 120.68 | 9.287  |        |        |        |
| K87CA-K88N-H | 54.76  | 127.32 | 9.179  | 54.77  | 127.31 | 9.182  |
| K87CB-N-H    | 35.51  | 120.64 | 9.287  |        |        |        |
| K87CB-K88N-H | 35.55  | 127.26 | 9.18   | 35.57  | 127.30 | 9.182  |

|              | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|--------------|--------|--------|--------|--------|--------|--------|
| Assignment   | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| K88CA-N-H    | 56.55  | 127.26 | 9.181  |        |        |        |
| K88CA-V89N-H | 56.6   | 120.96 | 8.42   | 56.59  | 121.04 | 8.424  |
| K88CB-N-H    | 34.42  | 127.26 | 9.18   |        |        |        |
| K88CB-V89N-H | 34.44  | 121.01 | 8.421  | 34.45  | 121.00 | 8.425  |
| V89CA-N-H    | 58.27  | 120.90 | 8.422  |        |        |        |
| V89CA-D90N-H | 58.26  | 118.48 | 7.949  | 58.30  | 118.62 | 7.952  |
| V89CB-N-H    | 36.95  | 120.91 | 8.422  |        |        |        |
| V89CB-D90N-H | 36.94  | 118.56 | 7.95   | 36.90  | 118.63 | 7.952  |
| D90CA-N-H    | 51.84  | 118.64 | 7.949  |        |        |        |
| D90CA-K91N-H | 51.86  | 114.27 | 7.79   | 51.86  | 114.23 | 7.791  |
| D90CB-N-H    | 41.50  | 118.64 | 7.949  |        |        |        |
| D90CB-K91N-H | 41.45  | 114.34 | 7.788  | 41.52  | 114.22 | 7.791  |
| K91CA-N-H    | 57.97  | 114.29 | 7.789  |        |        |        |
| K91CA-N92N-H | 57.95  | 114.32 | 7.223  | 58.00  | 114.30 | 7.227  |
| K91CB-N-H    | 30.72  | 114.27 | 7.788  |        |        |        |
| K91CB-N92N-H | 30.69  | 114.34 | 7.224  | 30.75  | 114.31 | 7.227  |
| N92CA-N-H    | 52.62  | 114.34 | 7.225  |        |        |        |
| N92CA-G93N-H | 52.62  | 108.38 | 7.936  | 52.66  | 108.40 | 7.937  |
| N92CB-N-H    | 39.94  | 114.35 | 7.225  |        |        |        |
| N92CB-G93N-H | 39.92  | 108.44 | 7.933  | 39.94  | 108.39 | 7.937  |
| G93CA-N-H    | 45.07  | 108.42 | 7.934  |        |        |        |
| G93CA-N94N-H | 45.05  | 120.25 | 8.279  | 45.08  | 120.34 | 8.282  |
| N94CA-N-H    | 53.64  | 120.35 | 8.279  |        |        |        |
| N94CA-V95N-H | 53.65  | 123.44 | 8.762  | 53.63  | 123.43 | 8.764  |
| N94CB-N-H    | 37.99  | 120.34 | 8.28   |        |        |        |
| N94CB-V95N-H | 37.96  | 123.39 | 8.762  | 37.99  | 123.42 | 8.764  |
| V95CA-N-H    | 65.06  | 123.39 | 8.762  |        |        |        |
| V95CA-K96N-H | 65.06  | 128.09 | 9.49   | 65.06  | 128.12 | 9.492  |
| V95CB-N-H    | 31.98  | 123.40 | 8.762  |        |        |        |
| V95CB-K96N-H | 32.09  | 128.14 | 9.488  | 32.10  | 128.12 | 9.492  |
| K96CA-N-H    | 56.30  | 128.16 | 9.49   |        |        |        |
| K96CA-V97N-H | 56.25  | 119.62 | 7.99   | 56.29  | 119.62 | 7.991  |

|                | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|----------------|--------|--------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| K96CB-N-H      | 32.95  | 128.15 | 9.487  |        |        |        |
| K96CB-V97N-H   | 32.95  | 119.62 | 7.994  | 32.95  | 119.62 | 7.994  |
| V97CA-N-H      | 62.95  | 119.63 | 7.997  |        |        |        |
| V97CA-A98N-H   | 62.96  | 128.24 | 8.597  | 62.94  | 128.22 | 8.599  |
| V97CB-N-H      | 34.83  | 119.67 | 7.997  |        |        |        |
| V97CB-A98N-H   | 34.83  | 128.26 | 8.597  | 34.90  | 128.23 | 8.599  |
| A98CA-N-H      | 52.41  | 128.28 | 8.597  |        |        |        |
| A98CA-V99N-H   | 52.40  | 122.19 | 8.548  | 52.45  | 122.17 | 8.549  |
| A98CB-N-H      | 19.99  | 128.32 | 8.598  |        |        |        |
| A98CB-V99N-H   | 19.98  | 122.13 | 8.547  | 19.99  | 122.25 | 8.549  |
| V99CA-N-H      | 64.92  | 122.19 | 8.547  |        |        |        |
| V99CA-T100N-H  | 64.93  | 126.07 | 9.973  | 64.91  | 126.11 | 9.979  |
| V99CB-N-H      | 31.77  | 122.16 | 8.546  |        |        |        |
| V99CB-T100N-H  | 31.73  | 126.04 | 9.977  | 31.79  | 126.11 | 9.978  |
| T100CA-N-H     | 61.80  | 126.10 | 9.975  |        |        |        |
| T100CA-A101N-H | 61.83  | 131.29 | 8.896  | 61.80  | 131.27 | 8.902  |
| T100CB-N-H     | 72.64  | 126.07 | 9.974  |        |        |        |
| T100CB-A101N-H | 72.67  | 131.26 | 8.903  | 72.67  | 131.26 | 8.903  |
| A101CA-N-H     | 54.20  | 131.32 | 8.902  |        |        |        |
| A101CA-G102N-H | 54.21  | 110.28 | 9.152  | 54.25  | 110.23 | 9.153  |
| A101CB-N-H     | 18.04  | 131.23 | 8.898  |        |        |        |
| A101CB-G102N-H | 18.08  | 110.26 | 9.16   | 18.06  | 110.24 | 9.151  |
| G102N-CA-H     | 45.29  | 110.36 | 9.15   |        |        |        |
| G102CA-N103N-H | 45.24  | 121.11 | 8.202  | 45.28  | 121.06 | 8.203  |
| N103CA-N-H     | 51.42  | 121.04 | 8.2    |        |        |        |
| N103CA-Y104N-H | 51.42  | 121.16 | 9.214  | 51.41  | 121.19 | 9.213  |
| N103CB-N-H     | 37.89  | 121.01 | 8.2    |        |        |        |
| N103CB-Y104N-H | 37.85  | 121.16 | 9.214  | 37.91  | 121.18 | 9.213  |
| Y104CA-N-H     | 57.83  | 121.22 | 9.21   |        |        |        |
| Y104CA-Y105N-H | 57.84  | 116.21 | 10.223 | 57.83  | 116.26 | 10.224 |
| Y104CB-N-H     | 39.75  | 121.21 | 9.209  |        |        |        |
| Y104CB-Y105N-H | 39.77  | 116.24 | 10.218 | 39.77  | 116.25 | 10.227 |

|                | HNCA-  | CB      |        | CACB-  | (CO)NH |        |
|----------------|--------|---------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm  | H, ppm | C, ppm | N, ppm | H, ppm |
| Y105CA-N-H     | 56.24  | 116.19  | 10.223 |        |        |        |
| Y105CA-T106N-H | 56.28  | 113.57  | 8.475  | 56.25  | 113.60 | 8.484  |
| Y105CB-N-H     | 43.57  | 116.18  | 10.217 |        |        |        |
| Y105CB-T106N-H | 43.55  | 113.67  | 8.485  | 43.56  | 113.67 | 8.48   |
| T106CA-N-H     | 59.62  | 113.61  | 8.474  |        |        |        |
| T106CA-F107N-H | 59.63  | 119.77  | 9.471  | 59.63  | 119.69 | 9.471  |
| T106CB-N-H     | 70.98  | 113.60  | 8.484  |        |        |        |
| T106CB-N-H     | 71.15  | 113.62  | 8.477  |        |        |        |
| T106CB-F107N-H | 71.10  | 119.73  | 9.468  | 71.09  | 119.70 | 9.471  |
| F107CA-N-H     | 56.82  | 119.63  | 9.468  |        |        |        |
| F107CA-T108N-H | 56.85  | 117.73  | 9.34   | 56.89  | 117.61 | 9.341  |
| F107CB-N-H     | 44.11  | 119.70  | 9.47   |        |        |        |
| F107CB-T108N-H | 44.11  | 117.68  | 9.335  | 44.17  | 117.61 | 9.342  |
| T108CA-N-H     | 61.06  | 117.56  | 9.339  |        |        |        |
| T108CA-V109N-H | 61.03  | 127.86  | 9.343  | 61.04  | 127.9  | 9.345  |
| T108CB-N-H     | 72.29  | 117.59  | 9.34   |        |        |        |
| T108CB-N-H     | 71.92  | 117.60  | 9.339  |        |        |        |
| T108CB-V109N-H | 72.07  | 127.85  | 9.341  | 72.12  | 127.90 | 9.344  |
| V109CA-N-H     | 63.10  | 127.92  | 9.344  |        |        |        |
| V109CA-M110N-H | 63.12  | 129.62  | 8.783  | 63.09  | 129.56 | 8.781  |
| V109CB-N-H     | 29.615 | 127.9   | 9.343  |        |        |        |
| V109CB-N-H     | 30.007 | 127.947 | 9.342  |        |        |        |
| V109CB-M110N-H | 29.813 | 129.65  | 8.778  | 29.80  | 129.51 | 8.783  |
| M110CA-N-H     | 58.138 | 129.563 | 8.78   |        |        |        |
| M110CA-Y111N-H | 58.144 | 117.67  | 8.204  | 58.15  | 117.60 | 8.209  |
| M110CB-N-H     | 35.149 | 129.561 | 8.778  |        |        |        |
| M110CB-Y111N-H | 35.198 | 117.621 | 8.205  | 35.20  | 117.67 | 8.207  |
| Y111CA-N-H     | 59.4   | 117.598 | 8.207  |        |        |        |
| Y111CA-A112N-H | 59.42  | 125.898 | 6.658  | 59.43  | 125.88 | 6.66   |
| Y111CB-N-H     | 42.371 | 117.649 | 8.205  |        |        |        |
| Y111CB-A112N-H | 42.418 | 125.941 | 6.656  | 42.40  | 125.88 | 6.66   |
| A112CA-N-H     | 52.938 | 125.889 | 6.658  |        |        |        |

|                | HNCA-  | CB      |        | CACB-  | (CO)NH |        |
|----------------|--------|---------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm  | H, ppm | C, ppm | N, ppm | H, ppm |
| A112CA-D113N-H | 52.95  | 121.49  | 9.5    | 52.95  | 121.49 | 9.5    |
| A112CB-N-H     | 22.32  | 125.9   | 6.658  |        |        |        |
| A112CB-D113N-H | 22.31  | 121.48  | 9.498  | 22.35  | 121.49 | 9.501  |
| D113CA-N-H     | 53.17  | 121.48  | 9.499  |        |        |        |
| D113CA-D114N-H | 53.17  | 114.79  | 8.356  | 53.17  | 114.83 | 8.358  |
| D113CB-N-H     | 40.80  | 121.50  | 9.498  |        |        |        |
| D113CB-D114N-H | 40.88  | 114.79  | 8.361  | 40.88  | 114.79 | 8.361  |
| D114N-CA-H     | 58.12  | 114.76  | 8.36   |        |        |        |
| D114CA-S115N-H | 58.13  | 110.88  | 8.699  | Peak   | Not    | found  |
| D114N-CB-H     | 40.95  | 114.78  | 8.358  |        |        |        |
| D114CB-S115N-H | 40.96  | 110.89  | 8.702  | Peak   | Not    | found  |
| S115CA-N-H     | 59.48  | 110.89  | 8.702  |        |        |        |
| S115CA-S116N-H | 59.45  | 118.01  | 8.884  | 40.96  | 110.91 | 8.704  |
| S115CB-N-H     | 66.70  | 110.89  | 8.702  |        |        |        |
| S115CB-S116N-H | 66.68  | 118.03  | 8.883  | 66.69  | 117.97 | 8.887  |
| S116CA-N-H     | 58.55  | 117.99  | 8.884  |        |        |        |
| S116CA-A117N-H | 58.55  | 117.61  | 8.585  | 58.55  | 117.64 | 8.586  |
| S116CB-N-H     | 69.33  | 117.99  | 8.884  |        |        |        |
| S116CB-A117N-H | 69.35  | 117.59  | 8.583  | 69.34  | 117.64 | 8.586  |
| A117CA-N-H     | 52.40  | 117.66  | 8.584  |        |        |        |
| A117CA-L118N-H | 52.406 | 121.539 | 9.267  | 52.43  | 121.52 | 9.268  |
| A117CB-N-H     | 22.863 | 117.668 | 8.584  |        |        |        |
| A117CB-L118N-H | 22.851 | 121.514 | 9.266  | 22.90  | 121.52 | 9.269  |
| L118CA-N-H     | 54.385 | 121.504 | 9.266  |        |        |        |
| L118CA-N-H     | 54.385 | 121.504 | 9.266  |        |        |        |
| L118CA-I119N-H | 54.361 | 119.793 | 9.767  | 54.40  | 119.85 | 9.772  |
| L118CB-N-H     | 46.675 | 121.563 | 9.266  |        |        |        |
| L118CB-I119N-H | 46.712 | 119.736 | 9.769  | 46.77  | 119.85 | 9.772  |
| I119CA-N-H     | 59.122 | 119.934 | 9.769  |        |        |        |
| I119CA-H120N-H | 59.086 | 122.314 | 8.831  | 59.12  | 122.36 | 8.836  |
| I119CB-N-H     | 42.83  | 119.916 | 9.77   |        |        |        |
| I119CB-H120N-H | 42.828 | 122.246 | 8.829  | 42.76  | 122.37 | 8.834  |

|                | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|----------------|--------|--------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| H120CA-N-H     | 56.09  | 122.39 | 8.831  |        |        |        |
| H120CA-T121N-H | 56.08  | 116.42 | 6.839  | 56.17  | 116.46 | 6.832  |
| H120CB-N-H     | 34.97  | 122.32 | 8.832  |        |        |        |
| H120CB-T121N-H | 34.95  | 116.43 | 6.833  | 34.95  | 116.43 | 6.833  |
| T121CA-N-H     | 58.71  | 116.51 | 6.828  |        |        |        |
| T121CA-C122N-H | 58.71  | 118.31 | 7.212  | 58.68  | 118.21 | 7.206  |
| T121CB-N-H     | 71.60  | 116.44 | 6.829  |        |        |        |
| T121CB-C122N-H | 71.62  | 118.33 | 7.207  | 71.66  | 118.27 | 7.242  |
| C122CA-N-H     | 53.48  | 118.23 | 7.216  |        |        |        |
| C122CA-L123N-H | 53.49  | 127.01 | 6.935  | 53.45  | 127.00 | 6.939  |
| C122CB-N-H     | 42.74  | 118.22 | 7.216  |        |        |        |
| C122CB-L123N-H | 42.74  | 126.95 | 6.931  | 42.69  | 127.01 | 6.938  |
| L123CA-N-H     | 48.54  | 127.07 | 6.941  |        |        |        |
| L123CA-H124N-H | peak   | Not    | found  | Peak   | Not    | found  |
| L123CB-N-H     | 41.89  | 127.11 | 6.941  |        |        |        |
| L123CB-H124N-H | peak   | Not    | found  | Peak   | Not    | found  |
| H124CA-K125N-H | 54.16  | 120.22 | 7.786  | 54.11  | 120.21 | 7.786  |
| H124CB-K125N-H | 29.94  | 120.19 | 7.781  | 30.02  | 120.24 | 7.785  |
| K125CA-N-H     | 55.45  | 120.26 | 7.782  |        |        |        |
| K125CA-G126N-H | 55.45  | 115.99 | 8.767  | 55.43  | 116.04 | 8.767  |
| K125CB-N-H     | 36.19  | 120.30 | 7.781  |        |        |        |
| K125CB-G126N-H | 36.22  | 115.99 | 8.764  | 36.17  | 116.03 | 8.768  |
| G126CA-N-H     | 47.80  | 116.05 | 8.765  |        |        |        |
| G126CA-N127N-H | Peak   | Not    | found  | Peak   | Not    | found  |
| N127CA-K128N-H | 54.35  | 119.20 | 7.382  | 54.41  | 119.17 | 7.385  |
| N127CB-K128N-H | 38.34  | 119.23 | 7.38   | 38.35  | 119.19 | 7.383  |
| K128CA-N-H     | 55.11  | 119.26 | 7.379  |        |        |        |
| K128CA-D129N-H | 55.10  | 120.96 | 8.162  | 55.12  | 120.94 | 8.164  |
| K128CB-N-H     | 34.50  | 119.24 | 7.381  |        |        |        |
| K128CB-D129N-H | 34.59  | 120.97 | 8.163  | 34.56  | 120.95 | 8.164  |
| D129CA-N-H     | 52.71  | 120.92 | 8.163  |        |        |        |
| D129CA-L130N-H | 52.69  | 122.99 | 6.909  | 52.74  | 123.12 | 6.912  |

|                | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|----------------|--------|--------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| D129CB-N-H     | 40.17  | 120.91 | 8.162  |        |        |        |
| D129CB-L130N-H | 40.20  | 123.07 | 6.907  | 40.16  | 123.11 | 6.912  |
| L130CA-N-H     | 53.47  | 123.17 | 6.913  |        |        |        |
| L130CA-G131N-H |        |        |        | 53.4   | 103.72 | 5.161  |
| L130CB-N-H     | 38.3   | 123.14 | 6.912  |        |        |        |
| L130CB-G131N-H |        |        |        | 38.29  | 103.77 | 5.162  |
| G131CA-N-H     | 42.64  | 103.71 | 5.16   |        |        |        |
| G131CA-D132N-H | 42.61  | 116.41 | 6.51   | 42.64  | 116.47 | 6.517  |
| D132CA-N-H     | 53.22  | 116.51 | 6.513  |        |        |        |
| D132CA-L133N-H | 53.19  | 120.81 | 5.501  | 53.19  | 120.81 | 5.501  |
| D132CB-N-H     | 42.91  | 116.51 | 6.515  |        |        |        |
| D132CB-L133N-H | Peak   | Not    | found  | 42.75  | 120.83 | 5.505  |
| L133CA-N-H     | 52.75  | 120.8  | 5.507  |        |        |        |
| L133CA-Y134N-H | 52.74  | 125.04 | 8.311  | 52.74  | 125.04 | 8.311  |
| L133CB-Y134N-H | Peak   | Not    | found  | Peak   | Not    | found  |
| Y134CA-N-H     | 56.67  | 125.05 | 8.305  |        |        |        |
| Y134CA-A135N-H | 56.66  | 124.00 | 9.973  | 56.68  | 124.11 | 9.969  |
| Y134CB-N-H     | 40.88  | 125.08 | 8.308  |        |        |        |
| Y134CB-A135N-H | 40.85  | 124.04 | 9.963  | 40.91  | 124.10 | 9.969  |
| A135CA-N-H     | 52.11  | 124.01 | 9.964  |        |        |        |
| A135CA-V136N-H | 52.08  | 124.82 | 10.262 | 52.08  | 124.88 | 10.266 |
| A135CB-N-H     | 23.93  | 124.19 | 9.966  |        |        |        |
| A135CB-V136N-H | 23.92  | 124.84 | 10.266 | 23.93  | 124.88 | 10.267 |
| V136CA-N-H     | 62.87  | 124.75 | 10.262 |        |        |        |
| V136CA-L137N-H | 62.91  | 126.22 | 9.932  | 62.91  | 126.23 | 9.936  |
| V136CB-N-H     | 33.16  | 124.91 | 10.259 |        |        |        |
| V136CB-N-H     | 33.00  | 124.86 | 10.265 |        |        |        |
| V136CB-L137N-H | 33.03  | 126.25 | 9.931  | 33.11  | 126.24 | 9.931  |
| V136CB-L137N-H | 33.19  | 126.17 | 9.931  |        |        |        |
| L137CA-N-H     | 52.21  | 126.24 | 9.932  |        |        |        |
| L137CA-N138N-H | 52.24  | 121.43 | 9.935  | 52.26  | 121.38 | 9.938  |
| L137CB-N-H     | 45.94  | 126.20 | 9.931  |        |        |        |

|                | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|----------------|--------|--------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| L137CB-N138N-H | 45.97  | 121.45 | 9.935  | 45.98  | 121.39 | 9.937  |
| N138CA-N-H     | 52.9   | 121.34 | 9.936  |        |        |        |
| N138CA-R139N-H | 52.92  | 124.79 | 8.619  | 52.96  | 124.87 | 8.621  |
| N138CB-N-H     | 44.39  | 121.34 | 9.936  |        |        |        |
| N138CB-R139N-H | 44.39  | 124.75 | 8.619  | 44.42  | 124.84 | 8.621  |
| R139CA-N-H     | 56.06  | 124.74 | 8.617  |        |        |        |
| R139CA-N140N-H | 55.97  | 120.13 | 10.277 | 56.00  | 120.08 | 10.281 |
| R139CB-N-H     | 31.15  | 124.77 | 8.619  |        |        |        |
| R139CB-N140N-H | 31.17  | 120.06 | 10.282 | 31.15  | 120.08 | 10.282 |
| N140CA-N-H     | 51.74  | 120.12 | 10.278 |        |        |        |
| N140CA-K141N-H | 51.75  | 123.53 | 7.627  | 51.75  | 123.53 | 7.627  |
| N140CB-N-H     | 40.58  | 120.10 | 10.278 |        |        |        |
| N140CB-K141N-H | 40.61  | 123.52 | 7.626  | 40.55  | 123.58 | 7.619  |
| K141CA-N-H     | 58.14  | 123.52 | 7.627  |        |        |        |
| K141CA-D142N-H | 58.14  | 117.72 | 7.969  | Peak   | Not    | found  |
| K141CB-N-H     | 30.62  | 123.52 | 7.626  |        |        |        |
| K141CB-D142N-H | 30.62  | 117.72 | 7.969  | 30.59  | 117.72 | 7.964  |
| D142CA-N-H     | 54.40  | 117.72 | 7.966  |        |        |        |
| D142CB-A143N-H | 20.49  | 123.37 | 7.144  | peak   | Not    | found  |
| A143CA-N-H     | 52.62  | 123.38 | 7.143  |        |        |        |
| A143CA-A144N-H | 52.61  | 126.19 | 8.487  | 52.65  | 126.31 | 8.49   |
| A143CB-N-H     | 20.49  | 123.37 | 7.144  |        |        |        |
| A143CB-A144N-H | 20.47  | 126.25 | 8.487  | 20.53  | 126.31 | 8.49   |
| A144CA-N-H     | 51.29  | 126.29 | 8.488  |        |        |        |
| A144CA-A145N-H | 51.28  | 126.82 | 9.277  | 51.29  | 126.83 | 9.28   |
| A144CB-N-H     | 19.53  | 126.25 | 8.486  |        |        |        |
| A144CB-A145N-H | 19.52  | 126.83 | 9.28   | 19.52  | 126.83 | 9.28   |
| A145CA-N-H     | 53.26  | 126.86 | 9.277  |        |        |        |
| A145CA-G146N-H | 53.28  | 110.48 | 8.795  | 53.29  | 110.43 | 8.798  |
| A145CB-N-H     | 19.17  | 126.85 | 9.277  |        |        |        |
| A145CB-G146N-H | 19.15  | 110.51 | 8.797  | 19.19  | 110.43 | 8.798  |
| G146CA-N-H     | 43.66  | 110.47 | 8.796  |        |        |        |

|                | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|----------------|--------|--------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| G146CA-D147N-H | 43.63  | 117.59 | 8.433  | 43.66  | 117.59 | 8.433  |
| D147CA-N-H     | 57.87  | 117.60 | 8.43   | Peak   | Not    | found  |
| D147CB-N-H     | 40.91  | 117.60 | 8.432  |        |        |        |
| D147CB-K148N-H | peak   | Not    | found  | Peak   | Not    | found  |
| K148CA-V149N-H | 59.7   | 120.53 | 7.937  | 59.73  | 120.52 | 7.94   |
| K148CB-V149N-H | 31.55  | 120.53 | 7.94   | 31.55  | 120.53 | 7.94   |
| V149CA-N-H     | 65.53  | 120.54 | 7.938  |        |        |        |
| V149CA-K150N-H | 65.55  | 120.43 | 7.82   | 65.55  | 120.44 | 7.821  |
| V149CB-N-H     | 31.23  | 120.53 | 7.94   |        |        |        |
| V149CB-K150N-H | 31.23  | 120.44 | 7.821  | 31.23  | 120.44 | 7.821  |
| K150CA-N-H     | 61.27  | 120.46 | 7.819  |        |        |        |
| K150CA-S151N-H | 61.35  | 116.95 | 8.228  | 61.27  | 116.88 | 8.23   |
| K150CB-N-H     | 31.34  | 120.46 | 7.819  |        |        |        |
| K150CB-S151N-H | 31.34  | 116.87 | 8.229  | 31.35  | 116.86 | 8.231  |
| S151CA-N-H     | 61.8   | 116.87 | 8.229  |        |        |        |
| S151CA-A152N-H | 61.80  | 126.16 | 7.331  | 61.81  | 126.15 | 7.334  |
| S151CB-N-H     | 62.73  | 116.87 | 8.229  |        |        |        |
| S151CB-N-H     | 62.15  | 117.02 | 8.227  |        |        |        |
| S151CB-A152N-H | 62.16  | 126.04 | 7.33   | 62.48  | 126.16 | 7.337  |
| S151CB-A152N-H | 62.76  | 126.19 | 7.336  |        |        |        |
| A152CA-N-H     | 54.85  | 126.15 | 7.334  |        |        |        |
| A152CA-V153N-H | 54.85  | 120.27 | 8.06   | 54.91  | 120.30 | 8.062  |
| A152CB-N-H     | 17.77  | 126.13 | 7.334  |        |        |        |
| A152CB-V153N-H | 17.76  | 120.28 | 8.06   | 17.76  | 120.29 | 8.062  |
| V153CA-N-H     | 67.24  | 120.31 | 8.06   |        |        |        |
| V153CA-S154N-H | 67.26  | 113.45 | 7.788  | 67.26  | 113.48 | 7.79   |
| V153CB-N-H     | 31.85  | 120.34 | 8.06   |        |        |        |
| V153CB-S154N-H | 31.88  | 113.45 | 7.788  | 31.86  | 113.49 | 7.79   |
| S154CA-N-H     | 61.5   | 113.52 | 7.787  |        |        |        |
| S154CA-A155N-H | 61.47  | 125.76 | 8.433  | 61.53  | 125.68 | 8.436  |
| S154CB-N-H     | 62.65  | 113.52 | 7.788  |        |        |        |
| S154CB-A155N-H | 62.62  | 125.75 | 8.434  | 62.67  | 125.70 | 8.436  |

|                | HNCA-  | CB     |        | CACB-  | (CO)NH  |        |
|----------------|--------|--------|--------|--------|---------|--------|
| Assignment     | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm  | H, ppm |
| A155CA-N-H     | 54.53  | 125.70 | 8.434  |        |         |        |
| A155CA-A156N-H | 54.52  | 119.58 | 7.249  | 54.57  | 119.60  | 7.252  |
| A155CB-N-H     | 17.78  | 125.74 | 8.434  |        |         |        |
| A155CB-A156N-H | 17.77  | 119.60 | 7.251  | 17.77  | 119.60  | 7.251  |
| A156CA-N-H     | 51.48  | 119.61 | 7.249  |        |         |        |
| A156CA-T157N-H | 51.47  | 112.83 | 8.094  | 51.52  | 112.8   | 8.096  |
| A156CB-N-H     | 18.09  | 119.63 | 7.25   |        |         |        |
| A156CB-T157N-H | 18.08  | 112.82 | 8.094  | 18.10  | 112.81  | 8.096  |
| T157CA-N-H     | 63.27  | 112.88 | 8.093  |        |         |        |
| T157CA-L158N-H | 63.20  | 118.85 | 7.157  | 63.20  | 118.89  | 7.16   |
| T157CB-N-H     | 67.88  | 112.85 | 8.094  |        |         |        |
| T157CB-N-H     | 67.62  | 112.86 | 8.094  |        |         |        |
| T157CB-L158N-H | 67.64  | 118.92 | 7.157  | 67.75  | 118.90  | 7.16   |
| L158CA-N-H     | 52.59  | 118.91 | 7.158  |        |         |        |
| L158CA-E159N-H | 52.59  | 121.15 | 8.353  | 52.66  | 121.20  | 8.357  |
| L158CB-N-H     | 44.59  | 118.90 | 7.158  |        |         |        |
| L158CB-E159N-H | 44.60  | 121.11 | 8.354  | 44.61  | 121.25  | 8.354  |
| E159CA-N-H     | 54.45  | 121.14 | 8.354  |        |         |        |
| E159CA-F160N-H | 54.46  | 128.15 | 9.12   | 54.50  | 128.19  | 9.121  |
| E159CB-N-H     | 30.21  | 121.15 | 8.353  |        |         |        |
| E159CB-N-H     | 30.49  | 121.17 | 8.354  |        |         |        |
| E159CB-F160N-H | 30.34  | 128.24 | 9.121  | 30.37  | 128.191 | 9.122  |
| F160CA-N-H     | 61.03  | 128.24 | 9.121  |        |         |        |
| F160CA-S161N-H | 61.01  | 112.93 | 8.831  | 61.01  | 112.931 | 8.831  |
| F160CB-N-H     | 38.46  | 128.27 | 9.11   |        |         |        |
| F160CB-S161N-H | 38.43  | 113.02 | 8.83   | 38.42  | 112.94  | 8.83   |
| S161CA-N-H     | 60.71  | 113.05 | 8.825  |        |         |        |
| S161CA-K162N-H | 60.67  | 119.60 | 7.634  | 60.73  | 119.607 | 7.635  |
| S161CB-N-H     | 62.46  | 113.01 | 8.828  |        |         |        |
| S161CB-K162N-H | 62.52  | 119.65 | 7.636  | 62.50  | 119.657 | 7.635  |
| K162CA-N-H     | 56.22  | 119.67 | 7.633  |        |         |        |
| K162CA-F163N-H | 56.25  | 120.21 | 7.987  | 56.27  | 120.208 | 7.991  |

|                | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|----------------|--------|--------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| K162CB-N-H     | 33.11  | 119.69 | 7.634  |        |        |        |
| K162CB-F163N-H | 33.04  | 120.00 | 7.986  | 33.10  | 120.10 | 7.989  |
| F163CA-N-H     | 58.49  | 120.23 | 7.986  |        |        |        |
| F163CA-I164N-H | 58.48  | 124.39 | 9.575  | 58.51  | 124.45 | 9.577  |
| I164CA-N-H     | 59.65  | 124.55 | 9.575  |        |        |        |
| F163CB-I164N-H | peak   | Not    | found  | 38.62  | 124.45 | 9.578  |
| I164CA-S165N-H | 59.67  | 119.40 | 8.747  | 59.66  | 119.41 | 8.749  |
| I164CB-N-H     | 38.9   | 124.49 | 9.575  |        |        |        |
| I164CB-S165N-H | 38.94  | 119.30 | 8.746  | 38.87  | 119.41 | 8.75   |
| S165CA-N-H     | 57.12  | 119.45 | 8.747  |        |        |        |
| S165CA-T166N-H | 57.05  | 118.05 | 9.383  | 57.09  | 118.19 | 9.389  |
| S165CB-N-H     | 64.85  | 119.46 | 8.749  |        |        |        |
| S165CB-T166N-H | 64.83  | 118.16 | 9.38   | 64.87  | 118.26 | 9.39   |
| T166CA-N-H     | 62.29  | 118.3  | 9.387  |        |        |        |
| T166CA-K167N-H | 62.30  | 125.24 | 8.931  | 62.35  | 125.34 | 8.936  |
| T166CB-N-H     | 70.36  | 118.2  | 9.386  |        |        |        |
| T166CB-K167N-H | 70.41  | 125.26 | 8.929  | 70.38  | 125.34 | 8.935  |
| K167CA-N-H     | 59.72  | 125.40 | 8.932  |        |        |        |
| K167CA-E168N-H | 59.78  | 116.87 | 8.641  | 59.75  | 116.95 | 8.627  |
| K167CB-N-H     | 32.38  | 125.47 | 8.932  |        |        |        |
| K167CB-N-H     | 32.56  | 125.47 | 8.931  |        |        |        |
| K167CB-E168N-H | Peak   | Not    | found  | 32.45  | 116.89 | 8.63   |
| E168CA-N-H     | 56.02  | 116.84 | 8.629  |        |        |        |
| E168CA-N169N-H | 56.00  | 117.46 | 7.776  | 56.04  | 117.48 | 7.773  |
| E168CB-N-H     | 28.65  | 116.91 | 8.622  |        |        |        |
| E168CB-N169N-H | 28.63  | 117.46 | 7.771  | 28.59  | 117.46 | 7.774  |
| N169CA-N-H     | 52.81  | 117.54 | 7.771  |        |        |        |
| N169CA-N170N-H | 52.77  | 115.04 | 8.511  | 52.81  | 115.20 | 8.516  |
| N169CB-N-H     | 41.18  | 117.48 | 7.767  |        |        |        |
| N169CB-N170N-H | 41.09  | 115.16 | 8.512  | 41.18  | 115.16 | 8.517  |
| N170CA-N-H     | 53.70  | 115.13 | 8.508  |        |        |        |
| N170CA-C171N-H | 53.70  | 114.84 | 8.476  | 53.69  | 114.76 | 8.478  |

|                | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|----------------|--------|--------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| N170CB-N-H     | 36.69  | 115.16 | 8.512  |        |        |        |
| N170CB-C171N-H | 36.70  | 114.85 | 8.479  | 36.85  | 114.75 | 8.478  |
| C171CA-N-H     | 54.92  | 114.75 | 8.476  |        |        |        |
| C171CA-A172N-H | 54.95  | 123.22 | 5.226  | 54.98  | 123.20 | 5.224  |
| C171CB-N-H     | 41.96  | 114.78 | 8.476  |        |        |        |
| C171CB-A172N-H | 41.97  | 123.31 | 5.221  | 41.94  | 123.20 | 5.223  |
| A172CA-N-H     | 50.18  | 123.20 | 5.216  |        |        |        |
| A172CA-Y173N-H | Peak   | Not    | found  | 50.2   | 120.30 | 8.281  |
| A172CB-N-H     | 20.26  | 123.29 | 5.22   |        |        |        |
| A172CB-Y173N-H | 20.21  | 120.32 | 8.288  | 20.28  | 120.32 | 8.284  |
| Y173CA-H       | 57.20  | 120.29 | 8.289  |        |        |        |
| Y173CA-D174N-H | 57.21  | 119.29 | 5.988  | 57.20  | 119.28 | 5.988  |
| Y173CB-D174N-H | 40.58  | 119.31 | 5.988  | 40.65  | 119.27 | 5.986  |
| D174CA-N-H     | 50.91  | 119.32 | 5.98   |        |        |        |
| D174CA-N175N-H | 50.96  | 121.97 | 7.998  | 50.96  | 121.97 | 7.998  |
| D174CB-N-H     | 38.74  | 119.26 | 5.986  |        |        |        |
| D174CB-N175N-H | Peak   | Not    | found  | 38.77  | 121.87 | 7.999  |
| N175CA-N-H     | 55.59  | 121.91 | 7.996  |        |        |        |
| N175CA-D176N-H | 55.62  | 118.47 | 8.048  | 55.61  | 118.48 | 8.052  |
| N175CB-N-H     | 37.60  | 121.87 | 7.99   |        |        |        |
| N175CB-D176N-H | 37.65  | 118.45 | 8.051  | 37.67  | 118.49 | 8.052  |
| D176CA-N-H     | 57.40  | 118.50 | 8.051  |        |        |        |
| D176CA-S177N-H | 57.38  | 116.38 | 7.178  | 57.39  | 116.39 | 7.178  |
| D176CB-N-H     | 39.91  | 118.54 | 8.052  |        |        |        |
| D176CB-S177N-H | 39.94  | 116.37 | 7.176  | 39.91  | 116.37 | 7.179  |
| S177CA-N-H     | 61.25  | 116.41 | 7.176  |        |        |        |
| S177CA-L178N-H | 61.25  | 119.92 | 6.783  | 61.20  | 119.92 | 6.784  |
| S177CB-L178N-H | Peak   | Not    | found  | Peak   | Not    | found  |
| L178CA-N-H     | 57.99  | 119.97 | 6.781  |        |        |        |
| L178CA-K179N-H | 57.99  | 112.26 | 7.317  | 58.04  | 112.25 | 7.32   |
| L178CB-N-H     | 42.28  | 119.95 | 6.781  |        |        |        |
| L178CB-K179N-H | 42.34  | 112.21 | 7.317  | 42.31  | 112.26 | 7.32   |

|                | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|----------------|--------|--------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| K179CA-N-H     | 59.81  | 112.30 | 7.316  |        |        |        |
| K179CA-S180N-H | 59.83  | 114.47 | 7.477  | 59.83  | 114.45 | 7.479  |
| K179CB-N-H     | 31.89  | 112.27 | 7.318  |        |        |        |
| K179CB-S180N-H | 31.88  | 114.45 | 7.478  | 31.92  | 114.44 | 7.479  |
| S180CA-N-H     | 60.86  | 114.49 | 7.477  |        |        |        |
| S180CA-L181N-H | 60.86  | 121.55 | 7.541  | 60.89  | 121.59 | 7.544  |
| S180CB-N-H     | 62.67  | 114.48 | 7.477  |        |        |        |
| S180CB-L181N-H | 62.66  | 121.60 | 7.541  | 62.67  | 121.60 | 7.543  |
| L181CA-N-H     | 56.71  | 121.65 | 7.54   |        |        |        |
| L181CA-L182N-H | 56.76  | 114.55 | 7.016  | 56.76  | 114.55 | 7.016  |
| L181CB-N-H     | 41.87  | 121.63 | 7.541  |        |        |        |
| L181CB-L182N-H | 41.86  | 114.55 | 7.016  | 41.86  | 114.55 | 7.016  |
| L182CA-N-H     | 56.90  | 114.61 | 7.014  |        |        |        |
| L182CA-T183N-H | 56.88  | 105.57 | 7.261  | 56.92  | 105.60 | 7.264  |
| L182CB-N-H     | 42.28  | 114.58 | 7.013  |        |        |        |
| L182CB-T183N-H | 42.31  | 105.51 | 7.262  | 42.28  | 105.60 | 7.264  |
| T183CA-N-H     | 61.69  | 105.58 | 7.261  |        |        |        |
| T183CA-K184N-H | 61.69  | 126.95 | 7.243  | 61.67  | 126.93 | 7.245  |
| T183CB-N-H     | 69.43  | 105.6  | 7.262  |        |        |        |
| T183CB-K184N-H | 69.43  | 126.95 | 7.242  | 69.47  | 126.93 | 7.245  |
| K184CA-N-H     | 56.98  | 126.97 | 7.243  |        |        |        |
| K184CB-N-H     | 33.46  | 126.97 | 7.243  |        |        |        |

## Appendix A. Assignment Tables

Table A1. Assignments (in ppm) of the high-spin NP4  $^1\text{H}\{^{15}\text{N}\}$  HSQC experiment, pH 7.3.

| Assignment | N, ppm          | H, ppm       |
|------------|-----------------|--------------|
| A1         | <i>peak not</i> | <i>found</i> |
| C2         | <i>peak not</i> | <i>found</i> |
| T3         | <b>120.454</b>  | 9.891        |
| K4         | <b>124.021</b>  | 8.115        |
| N5         | <i>peak not</i> | <i>found</i> |
| A6         | <b>124.526</b>  | 7.785        |
| I7         | <b>124.81</b>   | 8.441        |
| A8         | <b>129.503</b>  | 8.477        |
| Q9         | <b>121.5</b>    | 8.53         |
| T10        | <b>127.063</b>  | 8.876        |
| G11        | <i>peak not</i> | <i>found</i> |
| F12        | <b>118.811</b>  | 7.014        |
| N13        | <b>128.097</b>  | 8.755        |
| K14        | <b>125.372</b>  | 7.986        |
| D15        | <b>120.18</b>   | 8.017        |
| K16        | <b>116.706</b>  | 7.066        |
| Y17        | <b>118.446</b>  | 7.012        |
| F18        | <b>118.382</b>  | 8.419        |
| N19        | <b>118.63</b>   | 7.856        |
| G20        | <b>110.377</b>  | 9.26         |
| D21        | <b>118.628</b>  | 7.644        |
| V22        | <b>119.129</b>  | 8.218        |
| W23        | <b>127.695</b>  | 9.625        |
| Y24        | <b>119.049</b>  | 8.999        |
| V25        | <b>120.66</b>   | 8.55         |
| T26        | <b>122.917</b>  | 10.072       |
| D27        | <b>120.548</b>  | 8.588        |
| Y28        | <b>119.276</b>  | 10.302       |
| L29        | <b>123.42</b>   | 9.225        |
| D30        | <b>127.386</b>  | 8.358        |

| Assignment | N, ppm          | H, ppm       |
|------------|-----------------|--------------|
| L31        | <b>123.631</b>  | 6.96         |
| E32        | <b>119.752</b>  | 7.212        |
| P33        | <i>peak not</i> | <i>found</i> |
| D34        | <b>120.8</b>    | 8.163        |
| D35        | <b>120.421</b>  | 8.357        |
| V36        | <b>119.19</b>   | 8.203        |
| P37        | <i>peak not</i> | <i>found</i> |
| K38        | <b>124.301</b>  | 9.9          |
| R39        | <b>127.483</b>  | 9.767        |
| Y40        | <i>peak not</i> | <i>found</i> |
| C41        | <i>peak not</i> | <i>found</i> |
| A42        | <i>peak not</i> | <i>found</i> |
| A43        | <i>peak not</i> | <i>found</i> |
| L44        | <b>116.178</b>  | 8.877        |
| A45        | <b>121.554</b>  | 8.994        |
| A46        | <b>125.805</b>  | 8.818        |
| G47        | <b>107.951</b>  | 9.213        |
| T48        | <b>113.214</b>  | 8.591        |
| A49        | <b>128.421</b>  | 8.984        |
| S50        | <i>peak not</i> | <i>found</i> |
| G51        | <b>106.739</b>  | 8.495        |
| K52        | <b>120.39</b>   | 7.879        |
| L53        | <b>123.356</b>  | 8.609        |
| K54        | <b>126.575</b>  | 8.955        |
| E55        | <b>118.759</b>  | 8.937        |
| A56        | <b>133.599</b>  | 9.858        |
| L57        | <b>121.601</b>  | 8.51         |
| Y58        | <i>peak not</i> | <i>found</i> |
| H59        | <i>peak not</i> | <i>found</i> |
| Y60        | <i>peak not</i> | <i>found</i> |
| D61        | <i>peak not</i> | <i>found</i> |
| P62        | <i>peak not</i> | <i>found</i> |
| K63        | <b>116.582</b>  | 7.983        |

| Assignment | N, ppm          | H, ppm       |
|------------|-----------------|--------------|
| T64        | <b>105.177</b>  | 6.603        |
| Q65        | <b>115.155</b>  | 8.009        |
| D66        | <b>119.676</b>  | 7.34         |
| T67        | <b>114.022</b>  | 7.189        |
| F68        | <b>114.64</b>   | 5.048        |
| Y69        | <b>117.756</b>  | 6.813        |
| D70        | <b>115.404</b>  | 7.422        |
| V71        | <b>118.112</b>  | 9.415        |
| S72        | <b>122.182</b>  | 9.185        |
| E73        | <b>124.232</b>  | 9.054        |
| L74        | <b>124.371</b>  | 8.607        |
| Q75        | <b>122.015</b>  | 9.437        |
| V76        | <b>126.157</b>  | 8.885        |
| E77        | <b>129.994</b>  | 8.689        |
| S78        | <b>111.536</b>  | 8.05         |
| L79        | <i>peak not</i> | <i>found</i> |
| G80        | <b>114.576</b>  | 8.374        |
| K81        | <b>121.828</b>  | 7.88         |
| Y82        | <b>121.063</b>  | 8.285        |
| T83        | <b>117.085</b>  | 9.079        |
| A84        | <b>132.388</b>  | 10.179       |
| N85        | <b>123.945</b>  | 8.425        |
| F86        | <b>120.033</b>  | 7.365        |
| K87        | <b>120.588</b>  | 9.284        |
| K88        | <b>127.293</b>  | 9.175        |
| V89        | <b>120.962</b>  | 8.418        |
| D90        | <b>118.614</b>  | 7.947        |
| K91        | <b>114.211</b>  | 7.789        |
| N92        | <b>114.29</b>   | 7.227        |
| G93        | <b>108.387</b>  | 7.933        |
| N94        | <b>120.295</b>  | 8.28         |
| V95        | <b>123.417</b>  | 8.763        |
| K96        | <b>128.108</b>  | 9.491        |

| Assignment | N, ppm          | H, ppm       |
|------------|-----------------|--------------|
| V97        | 119.618         | 7.995        |
| A98        | 128.223         | 8.595        |
| V99        | 122.189         | 8.546        |
| T100       | 126.137         | 9.975        |
| A101       | 131.269         | 8.9          |
| G102       | 110.228         | 9.142        |
| N103       | 121.028         | 8.198        |
| Y104       | 121.177         | 9.204        |
| Y105       | 116.235         | 10.222       |
| T106       | 113.605         | 8.476        |
| F107       | 119.697         | 9.471        |
| T108       | 117.611         | 9.34         |
| V109       | 127.898         | 9.343        |
| M110       | 129.521         | 8.78         |
| Y111       | 117.608         | 8.202        |
| A112       | 125.874         | 6.658        |
| D113       | 121.477         | 9.499        |
| D114       | 114.805         | 8.355        |
| S115       | 110.895         | 8.701        |
| S116       | 117.964         | 8.884        |
| A117       | 117.64          | 8.582        |
| L118       | 121.515         | 9.265        |
| I119       | 119.847         | 9.758        |
| H120       | 122.354         | 8.834        |
| T121       | 116.443         | 6.829        |
| C122       | 118.257         | 7.21         |
| L123       | 126.996         | 6.934        |
| H124       | <i>peak not</i> | <i>found</i> |
| K125       | 120.224         | 7.784        |
| G126       | 116.006         | 8.766        |
| N127       | <i>peak not</i> | <i>found</i> |
| K128       | 119.194         | 7.38         |
| D129       | 120.94          | 8.164        |

| Assignment | N, ppm          | H, ppm       |
|------------|-----------------|--------------|
| L130       | 123.138         | 6.906        |
| G131       | 103.714         | 5.159        |
| D132       | 116.476         | 6.516        |
| L133       | 120.795         | 5.511        |
| Y134       | 125.023         | 8.309        |
| A135       | 124.097         | 9.967        |
| V136       | 124.86          | 10.26        |
| L137       | 126.234         | 9.929        |
| N138       | 121.364         | 9.932        |
| R139       | 124.829         | 8.616        |
| N140       | 120.082         | 10.274       |
| K141       | 123.549         | 7.625        |
| D142       | 117.718         | 7.97         |
| A143       | 123.364         | 7.145        |
| A144       | 126.306         | 8.485        |
| A145       | 126.818         | 9.277        |
| G146       | 110.418         | 8.797        |
| D147       | 117.601         | 8.428        |
| K148       | <i>peak not</i> | <i>found</i> |
| V149       | 120.507         | 7.937        |
| K150       | 120.422         | 7.82         |
| S151       | 116.867         | 8.227        |
| A152       | 126.16          | 7.334        |
| V153       | 120.269         | 8.057        |
| S154       | 113.484         | 7.788        |
| A155       | 125.691         | 8.432        |
| A156       | 119.596         | 7.251        |
| T157       | 112.792         | 8.092        |
| L158       | 118.882         | 7.159        |
| E159       | 121.149         | 8.351        |
| F160       | 128.192         | 9.114        |
| S161       | 112.934         | 8.829        |
| K162       | 119.647         | 7.632        |

| Assignment | N, ppm  | H, ppm |
|------------|---------|--------|
| F163       | 120.19  | 7.986  |
| I164       | 124.464 | 9.573  |
| S165       | 119.407 | 8.748  |
| T166       | 118.197 | 9.387  |
| K167       | 125.338 | 8.932  |
| E168       | 116.891 | 8.629  |
| N169       | 117.484 | 7.767  |
| N170       | 115.158 | 8.51   |
| C171       | 114.733 | 8.473  |
| A172       | 123.198 | 5.222  |
| Y173       | 120.292 | 8.285  |
| D174       | 119.273 | 5.985  |
| N175       | 121.883 | 7.988  |
| D176       | 118.479 | 8.048  |
| S177       | 116.37  | 7.179  |
| L178       | 119.915 | 6.78   |
| K179       | 112.251 | 7.318  |
| S180       | 114.438 | 7.476  |
| L181       | 121.605 | 7.539  |
| L182       | 114.55  | 7.013  |
| T183       | 105.596 | 7.263  |
| K184       | 126.926 | 7.244  |

**Table A2. Assignments (in ppm) of the high-spin NP4 at pH 7.3 HNCA experiment.**

|              |        |         |        | Assignment   | C, ppm | N, ppm | H, ppm | Assignment   | C, ppm | N, ppm | H, ppm |
|--------------|--------|---------|--------|--------------|--------|--------|--------|--------------|--------|--------|--------|
| Assignment   | C, ppm | N, ppm  | H, ppm | Y17CA-N-H    | 62.32  | 118.46 | 7.013  | P33CA-D34N-H | 62.47  | 120.84 | 8.165  |
| A1CA-C2N-H   | peak   | not     | found  | Y17CA-F18N-H | 62.32  | 118.38 | 8.422  | D34CA-N-H    | 53.77  | 120.79 | 8.164  |
| C2CA-N-H     | peak   | not     | found  | F18CA-N-H    | 56.37  | 118.37 | 8.421  | D34CA-D35N-H | 53.74  | 120.3  | 8.359  |
| C2CA-T3N-H   | 53.66  | 120.41  | 9.894  | F18CA-N19N-H | 56.36  | 118.62 | 7.855  | D35CA-N-H    | 56.89  | 120.46 | 8.358  |
| T3CA-N-H     | 61.87  | 120.45  | 9.895  | N19CA-N-H    | 52.48  | 118.62 | 7.856  | D35CA-V36N-H | 56.87  | 119.17 | 8.203  |
| T3CA-K4N-H   | 61.82  | 124.02  | 8.113  | N19CA-G20N-H | 52.47  | 110.37 | 9.26   | V36CA-N-H    | 59.89  | 119.21 | 8.203  |
| K4CA-N-H     | 55.05  | 123.99  | 8.117  | G20CA-N-H    | 45.43  | 110.39 | 9.261  | V36CA-P37    | peak   | not    | found  |
| K4CA-N5N-H   | peak   | not     | found  | G20CA-D21N-H | 45.42  | 118.6  | 7.644  | P37CA        | peak   | not    | found  |
| N5CA-N-H     | peak   | not     | found  | D21CA-N-H    | 51.54  | 118.65 | 7.645  | P37CA-K38N-H | 63.89  | 124.25 | 9.901  |
| N5CA-A6N-H   | 52.37  | 124.53  | 7.787  | D21CA-V22N-H | 51.53  | 119.11 | 8.218  | K38CA-N-H    | 57.23  | 124.41 | 9.903  |
| A6CA-N-H     | 52.4   | 124.57  | 7.785  | V22CA-N-H    | 63.04  | 119.14 | 8.217  | K38CA-R39N-H | 57.14  | 127.57 | 9.788  |
| A6CA-I7N-H   | 52.34  | 124.73  | 8.443  | V22CA-W23N-H | 63.02  | 127.55 | 9.628  | R39CA-N-H    | 55.91  | 127.52 | 9.783  |
| I7CA-N-H     | 60.07  | 124.85  | 8.442  | W23CA-N-H    | 55.89  | 127.69 | 9.63   | R39CA-Y40N-H | peak   | not    | found  |
| I7CA-A8N-H   | 60.07  | 129.43  | 8.478  | W23CA-Y24N-H | 55.98  | 119.07 | 8.996  | Y40CA-N-H    | peak   | not    | found  |
| A8CA-N-H     | 51.32  | 129.47  | 8.479  | Y24CA-N-H    | 57.55  | 119.1  | 9.003  | Y40CA-C41N-H | peak   | not    | found  |
| A8CA-Q9N-H   | 51.36  | 121.44  | 8.533  | Y24CA-V25N-H | 57.5   | 120.59 | 8.551  | C41CA-N-H    | peak   | not    | found  |
| Q9CA-N-H     | 56.35  | 121.5   | 8.534  | V25CA-N-H    | 63.69  | 120.77 | 8.553  | D41CA-A42N-H | peak   | not    | found  |
| Q9CA-T10N-H  | 56.37  | 127.11  | 8.874  | V25CA-T26N-H | 63.7   | 122.91 | 10.067 | A42CA-N-H    | peak   | not    | found  |
| T10CA-N-H    | 64.33  | 127.11  | 8.874  | T26CA-N-H    | 64.01  | 122.93 | 10.069 | A42CA-A43N-H | peak   | not    | found  |
| T10CA-G11N-H | peak   | not     | found  | T26CA-D27N-H | 63.99  | 120.54 | 8.597  | A43CA-N-H    | peak   | not    | found  |
| G11CA-N-H    | peak   | not     | found  | D27CA-N-H    | 53.91  | 120.59 | 8.593  | A43CA-L44N-H | 49.75  | 116.15 | 8.876  |
| G11CA-F12N-H | 46.08  | 118.82  | 7.016  | D27CA-Y28N-H | 53.88  | 119.32 | 10.307 | L44CA-N-H    | 53.94  | 116.24 | 8.876  |
| F12CA-N-H    | 57.62  | 118.85  | 7.015  | Y28CA-N-H    | 58.19  | 119.3  | 10.306 | L44CA-A45N-H | 53.93  | 121.63 | 8.997  |
| F12CA-N13N-H | 57.54  | 128.03  | 8.754  | Y28CA-L29N-H | 58.19  | 123.41 | 9.225  | A45CA-N-H    | 51.96  | 121.55 | 8.996  |
| N13CA-N-H    | 51.3   | 128.07  | 8.755  | L29CA-N-H    | 53.52  | 123.43 | 9.229  | A45CA-A46N-H | 52.03  | 125.81 | 8.822  |
| N13CA-K14N-H | 51.28  | 125.34  | 7.988  | L29CA-D30N-H | 53.52  | 127.45 | 8.362  | A46CA-N-H    | 51.45  | 125.85 | 8.819  |
| K14CA-N-H    | 58.74  | 125.33  | 7.988  | D30CA-N-H    | 51.2   | 127.43 | 8.361  | A46CA-G47N-H | 51.44  | 107.93 | 9.216  |
| K14CA-D15N-H | 58.74  | 120.18  | 8.022  | D30CA-L31N-H | 51.2   | 123.68 | 6.963  | G47CA-N-H    | 45.73  | 107.94 | 9.216  |
| D15CA-N-H    | 57.27  | 120.17  | 8.02   | L31CA-N-H    | 55.3   | 123.63 | 6.96   | G47CA-T48N-H | 45.73  | 113.18 | 8.594  |
| D15CA-K16N-H | 57.28  | 116.71  | 7.067  | L31CA-E32N-H | 55.27  | 119.74 | 7.21   | T48CA-N-H    | 61.4   | 113.24 | 8.594  |
| K16CA-N-H    | 57.82  | 116.745 | 7.066  | E32CA-N-H    | 52.91  | 119.77 | 7.21   | T48CA-A49N-H | 61.37  | 128.45 | 8.986  |
| K16CA-Y17N-H | 57.87  | 118.46  | 7.013  | E32CA-P33    | peak   | not    | found  | A49CA-N-H    | 53.17  | 128.48 | 8.986  |
|              |        |         |        | P33CA        | peak   | not    | found  | A49CA-S50N-H | peak   | not    | found  |

| Assignment   | C,<br>ppm    | N, ppm     | H, ppm       | Assignment   | C,<br>ppm    | N, ppm     | H, ppm       | Assignment   | C,<br>ppm    | N, ppm | H, ppm |
|--------------|--------------|------------|--------------|--------------|--------------|------------|--------------|--------------|--------------|--------|--------|
| S50CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> | D66CA-T67N-H | <b>55.21</b> | 114.06     | 7.186        | T83CA-N-H    | <b>62.68</b> | 117.1  | 9.09   |
| S50CA-G51N-H | <b>59.06</b> | 106.76     | 8.496        | T67CA-N-H    | <b>58.49</b> | 114.05     | 7.186        | T83CA-A84N-H | <b>62.69</b> | 132.38 | 10.176 |
| G51CA-N-H    | <b>45.11</b> | 106.77     | 8.498        | T67CA-F68N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | A84CA-N-H    | <b>51.95</b> | 132.45 | 10.175 |
| G51CA-K52N-H | <b>45.12</b> | 120.37     | 7.879        | F68CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> | A84CA-N85N-H | <b>52.05</b> | 124.1  | 8.432  |
| K52CA-N-H    | <b>54.38</b> | 120.4      | 7.88         | F68CA-Y69N-H | <b>54.57</b> | 117.77     | 6.816        | N85CA-N-H    | <b>53.82</b> | 123.94 | 8.428  |
| K52CA-L53N-H | <b>54.43</b> | 123.49     | 8.61         | Y69CA-N-H    | <b>54.66</b> | 117.8      | 6.816        | N85CA-F86N-H | <b>53.93</b> | 119.96 | 7.368  |
| L53CA-N-H    | <b>55.34</b> | 123.4      | 8.611        | Y69CA-D70N-H | <b>54.7</b>  | 115.41     | 7.423        | F86CA-N-H    | <b>57.02</b> | 120.08 | 7.367  |
| L53CA-K54N-H | <b>55.28</b> | 126.61     | 8.952        | D70CA-N-H    | <b>52.07</b> | 115.42     | 7.423        | F86CA-K87N-H | <b>57.06</b> | 120.54 | 9.285  |
| K54CA-N-H    | <b>54.52</b> | 126.48     | 8.956        | D70CA-V71N-H | <b>52.07</b> | 118.06     | 9.412        | K87CA-N-H    | <b>54.68</b> | 120.75 | 9.282  |
| K54CA-E55N-H | <b>54.53</b> | 118.71     | 8.938        | V71CA-N-H    | <b>61.67</b> | 118.18     | 9.413        | K87CA-K88N-H | <b>54.75</b> | 127.34 | 9.179  |
| E55CA-N-H    | <b>56.41</b> | 118.8      | 8.94         | V71CA-S72N-H | <b>61.67</b> | 122.16     | 9.191        | K88CA-N-H    | <b>56.56</b> | 127.33 | 9.179  |
| E55CA-A56N-H | <b>56.4</b>  | 133.6      | 9.867        | S72CA-N-H    | <b>58.61</b> | 122.22     | 9.191        | K88CA-V89N-H | <b>56.67</b> | 120.87 | 8.415  |
| A56CA-N-H    | <b>49.92</b> | 133.62     | 9.865        | S72CA-E73N-H | <b>58.62</b> | 124.19     | 9.058        | V89CA-N-H    | <b>58.27</b> | 120.91 | 8.422  |
| A56CA-L57N-H | <b>49.96</b> | 121.52     | 8.51         | E73CA-N-H    | <b>56.25</b> | 124.26     | 9.058        | V89CA-D90N-H | <b>58.27</b> | 118.52 | 7.948  |
| L57CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> | E73CA-L74N-H | <b>56.3</b>  | 124.38     | 8.612        | D90CA-N-H    | <b>51.8</b>  | 118.64 | 7.949  |
| L57CA-Y58N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | L74CA-N-H    | <b>54.87</b> | 124.52     | 8.61         | D90CA-K91N-H | <b>51.8</b>  | 114.23 | 7.788  |
| Y58CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> | L74CA-Q75N-H | <b>54.88</b> | 122.07     | 9.44         | K91CA-N-H    | <b>57.94</b> | 114.28 | 7.789  |
| Y58CA-H59N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | Q75CA-N-H    | <b>54.07</b> | 122.04     | 9.435        | K91CA-N92N-H | <b>57.99</b> | 114.32 | 7.225  |
| H59CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> | Q75CA-V76N-H | <b>54.07</b> | 126.05     | 8.884        | N92CA-N-H    | <b>52.62</b> | 114.33 | 7.225  |
| H59CA-Y60N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | V76CA-N-H    | <b>62.84</b> | 126.17     | 8.884        | N92CA-G93N-H | <b>52.61</b> | 108.43 | 7.934  |
| Y60CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> | V76CA-E77N-H | <b>62.86</b> | 130.03     | 8.689        | G93CA-N-H    | <b>45.08</b> | 108.46 | 7.935  |
| Y60CA-D61N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | E77CA-N-H    | <b>57.58</b> | 130.07     | 8.689        | G93CA-N94N-H | <b>45.08</b> | 120.3  | 8.279  |
| D61CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> | E77CA-S78N-H | <b>57.63</b> | 111.55     | 8.053        | N94CA-N-H    | <b>53.61</b> | 120.31 | 8.28   |
| D61CA-P62N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | S78CA-N-H    | <b>57.05</b> | 111.56     | 8.051        | N94CA-V95N-H | <b>53.6</b>  | 123.43 | 8.762  |
| P62CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> | S78CA-L79N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | V95CA-N-H    | <b>65.04</b> | 123.41 | 8.763  |
| P62CA-K63N-H | <b>63.65</b> | 116.66     | 7.985        | L79CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> | V95CA-K96N-H | <b>65.04</b> | 128.04 | 9.489  |
| K63CA-N-H    | <b>58.73</b> | 116.58     | 7.985        | L79CA-G80N-H | <b>58.04</b> | 114.58     | 8.377        | K96CA-N-H    | <b>56.29</b> | 128.11 | 9.489  |
| K63CA-T64N-H | <b>58.72</b> | 105.17     | 6.601        | G80CA-N-H    | <b>46.28</b> | 114.59     | 8.377        | K96CA-V97N-H | <b>56.2</b>  | 119.62 | 7.99   |
| T64CA-N-H    | <b>61.3</b>  | 105.18     | 6.601        | G80CA-K81N-H | <b>46.27</b> | 121.87     | 7.881        | V97CA-N-H    | <b>62.91</b> | 119.64 | 7.997  |
| T64CA-Q65N-H | <b>61.31</b> | 115.16     | 8.01         | K81CA-N-H    | <b>56.1</b>  | 121.8      | 7.881        | V97CA-A98N-H | <b>62.92</b> | 128.18 | 8.597  |
| Q65CA-N-H    | <b>57.8</b>  | 115.19     | 8.01         | K81CA-Y82N-H | <b>56.15</b> | 121.12     | 8.286        | A98CA-N-H    | <b>52.39</b> | 128.23 | 8.597  |
| Q65CA-D66N-H | <b>57.8</b>  | 119.56     | 7.339        | Y82CA-N-H    | <b>56.96</b> | 121.13     | 8.287        | A98CA-V99N-H | <b>52.4</b>  | 122.17 | 8.548  |
| D66CA-N-H    | <b>55.19</b> | 119.62     | 7.343        | Y82CA-T83N-H | <b>56.93</b> | 117.1      | 9.085        | V99CA-N-H    | <b>64.88</b> | 122.18 | 8.547  |

| Assignment     | C, ppm | N, ppm | H, ppm | Assignment      | C, ppm | N, ppm | H, ppm | Assignment     | C, ppm | N, ppm | H, ppm |
|----------------|--------|--------|--------|-----------------|--------|--------|--------|----------------|--------|--------|--------|
| V99CA-T100N-H  | 64.91  | 126.19 | 9.973  | S116CA-N-H      | 58.55  | 117.99 | 8.884  | L133CA-N-H     | 52.75  | 120.8  | 5.507  |
| T100CA-N-H     | 61.81  | 126.15 | 9.974  | S116CA-A117N-H  | 58.55  | 117.59 | 8.584  | L133CA-Y134N-H | 52.77  | 124.89 | 8.314  |
| T100CA-A101N-H | 61.83  | 131.29 | 8.896  | A117CA-N-H      | 52.38  | 117.65 | 8.584  | Y134CA-N-H     | 56.69  | 125.06 | 8.312  |
| A101CA-N-H     | 54.19  | 131.35 | 8.903  | A117CA-L118N-H  | 52.39  | 121.51 | 9.266  | Y134CA-A135N-H | 56.68  | 124.11 | 9.969  |
| A101CA-G102N-H | 54.22  | 110.26 | 9.149  | L118CA-N-H      | 54.4   | 121.43 | 9.267  | A135CA-N-H     | 52.03  | 124.03 | 9.967  |
| G102CA-N-H     | 45.31  | 110.27 | 9.152  | L118CA-I119N-H  | 54.36  | 119.74 | 9.769  | A135CA-V136N-H | 52.03  | 124.83 | 10.263 |
| G102CA-N103N-H | 45.28  | 121.07 | 8.2    | I119CA-N-H      | 59.1   | 119.89 | 9.768  | V136CA-N-H     | 62.9   | 124.84 | 10.262 |
| N103CA-N-H     | 51.4   | 121.02 | 8.2    | I119CA-H120N-H  | 59.09  | 122.31 | 8.832  | V136CA-L137N-H | 62.91  | 126.2  | 9.93   |
| N103CA-Y104N-H | 51.39  | 121.05 | 9.211  | H120CA-N-H      | 56.07  | 122.33 | 8.83   | L137CA-N-H     | 52.2   | 126.24 | 9.931  |
| Y104CA-N-H     | 57.78  | 121.13 | 9.21   | H120CA-T121N-H  | 56.08  | 116.42 | 6.839  | L137CA-N138N-H | 52.2   | 121.32 | 9.936  |
| Y104CA-Y105N-H | 57.78  | 116.23 | 10.224 | T121CA-N-H      | 58.69  | 116.51 | 6.831  | N138CA-N-H     | 52.92  | 121.34 | 9.935  |
| Y105CA-N-H     | 56.23  | 116.25 | 10.221 | T121CA-C122N-H  | 58.67  | 118.3  | 7.205  | N138CA-R139N-H | 52.94  | 124.78 | 8.617  |
| Y105CA-T106N-H | 56.19  | 113.49 | 8.48   | C122CA-N-H      | 53.53  | 118.26 | 7.21   | R139CA-N-H     | 56.09  | 124.74 | 8.617  |
| T106CA-N-H     | 59.6   | 113.61 | 8.479  | C122CA-L123N-H  | 53.43  | 126.97 | 6.939  | R139CA-N140N-H | 55.93  | 120.06 | 10.28  |
| T106CA-F107N-H | 59.61  | 119.73 | 9.468  | L123CA-N-H      | 48.53  | 127.07 | 6.937  | N140CA-N-H     | 51.71  | 120.09 | 10.279 |
| F107CA-N-H     | 56.86  | 119.73 | 9.469  | L123CA-H124N-H  | peak   | not    | found  | N140CA-K141N-H | 51.7   | 123.51 | 7.626  |
| F107CA-T108N-H | 56.89  | 117.7  | 9.341  | H124CA-N-H      | peak   | not    | found  | K141CA-N-H     | 58.15  | 123.54 | 7.626  |
| T108CA-N-H     | 61     | 117.58 | 9.339  | H124CA-K125N-H  | 54.16  | 120.16 | 7.786  | K141CA-D142N-H | 58.14  | 117.72 | 7.969  |
| T108CA-V109N-H | peak   | not    | found  | K125CA-N-H      | 55.42  | 120.32 | 7.783  | D142CA-N-H     | 54.4   | 117.8  | 7.966  |
| V109CA-N-H     | 63.07  | 127.87 | 9.341  | K125CA-G126N-H  | 55.42  | 115.99 | 8.765  | D142CA-A143N-H | 54.36  | 123.44 | 7.142  |
| V109CA-M110N-H | 63.06  | 129.54 | 8.778  | G126CA-N-H      | 47.79  | 116.04 | 8.765  | A143CA-N-H     | 52.61  | 123.38 | 7.144  |
| M110CA-N-H     | 58.13  | 129.5  | 8.778  | N127CA-K128N-H  | 54.47  | 119.12 | 7.382  | A143CA-A144N-H | 52.63  | 126.24 | 8.489  |
| M110CA-Y111N-H | 58.1   | 117.61 | 8.205  | K128CA-N-H      | 55.13  | 119.26 | 7.379  | A144CA-N-H     | 51.29  | 126.31 | 8.488  |
| Y111CA-N-H     | 59.38  | 117.61 | 8.206  | K128CA-D129N-H  | 55.14  | 120.93 | 8.166  | A144CA-A145N-H | 51.29  | 126.7  | 9.278  |
| Y111CA-A112N-H | 59.39  | 125.92 | 6.658  | D129CA-N-H      | 52.71  | 120.94 | 8.163  | A145CA-N-H     | 53.28  | 126.81 | 9.278  |
| A112CA-N-H     | 52.93  | 125.93 | 6.658  | D129CA-L130N-H  | 52.68  | 123.06 | 6.911  | A145CA-G146N-H | 53.27  | 110.42 | 8.796  |
| A112CA-D113N-H | 52.95  | 121.49 | 9.5    | L130CA-N-H      | 53.44  | 123.14 | 6.91   | G146CA-N-H     | 43.68  | 110.42 | 8.796  |
| D113CA-N-H     | 53.17  | 121.49 | 9.498  | CL130CA-G131N-H | peak   | not    | found  | G146CA-D147N-H | 43.67  | 117.6  | 8.429  |
| D113CA-D114N-H | 53.17  | 114.79 | 8.357  | G131CA-N-H      | 42.62  | 103.71 | 5.152  | D147CA-N-H     | 57.86  | 117.68 | 8.429  |
| D114CA-N-H     | 58.1   | 114.74 | 8.361  | G131CA-D132N-H  | 42.62  | 116.48 | 6.514  | D147CA-K148N-H | peak   | not    | found  |
| D114CA-S115N-H | 58.09  | 110.95 | 8.701  | D132CA-N-H      | 53.2   | 116.49 | 6.515  | K148CA-N-H     | peak   | not    | found  |
| S115CA-N-H     | 59.43  | 110.93 | 8.701  | D132CB-N-H      | 42.83  | 116.51 | 6.515  | K148CA-V149N-H | 59.67  | 120.49 | 7.937  |
| S115CA-S116N-H | 59.42  | 117.98 | 8.885  | D132CA-L133N-H  | 53.19  | 120.81 | 5.501  | V149CA-N-H     | 65.54  | 120.57 | 7.938  |

| Assignment     | C, ppm | N, ppm  | H, ppm | Assignment     | C, ppm | N, ppm | H, ppm | Assignment     | C, ppm | N, ppm | H, ppm |
|----------------|--------|---------|--------|----------------|--------|--------|--------|----------------|--------|--------|--------|
| V149CA-K150N-H | 65.54  | 120.45  | 7.82   | T166CA-N-H     | 62.42  | 118.32 | 9.39   | L182CA-T183N-H | 56.9   | 105.62 | 7.262  |
| K150CA-N-H     | 61.23  | 120.45  | 7.819  | T166CA-K167N-H | 62.39  | 125.34 | 8.933  | T183CA-N-H     | 61.66  | 105.64 | 7.262  |
| K150CA-S151N-H | 61.27  | 116.88  | 8.23   | K167CA-N-H     | 59.69  | 125.32 | 8.933  | T183CA-K184N-H | 61.65  | 126.9  | 7.243  |
| S151CA-N-H     | 61.8   | 116.87  | 8.229  | K167CA-E168N-H | 59.61  | 116.93 | 8.639  | K184CA-N-H     | 56.98  | 126.94 | 7.243  |
| S151CA-A152N-H | 61.81  | 126.15  | 7.334  | E168CA-N-H     | 55.948 | 116.93 | 8.628  |                |        |        |        |
| A152CA-N-H     | 54.87  | 126.2   | 7.334  | E168CA-N169N-H | 56     | 117.49 | 7.769  |                |        |        |        |
| A152CA-V153N-H | 54.86  | 120.3   | 8.061  | N169CA-N-H     | 52.78  | 117.54 | 7.77   |                |        |        |        |
| V153CA-N-H     | 67.24  | 120.29  | 8.06   | N169CA-N170N-H | 52.8   | 115.17 | 8.513  |                |        |        |        |
| V153CA-S154N-H | 67.24  | 113.46  | 7.788  | N170CA-N-H     | 53.66  | 115.17 | 8.51   |                |        |        |        |
| S154CA-N-H     | 61.48  | 113.53  | 7.788  | N170CA-C171N-H | 53.69  | 114.76 | 8.478  |                |        |        |        |
| S154CA-A155N-H | 61.48  | 125.75  | 8.434  | C171CA-N-H     | 54.94  | 114.71 | 8.476  |                |        |        |        |
| A155CA-N-H     | 54.53  | 125.71  | 8.434  | C171CA-A172N-H | 54.95  | 123.28 | 5.217  |                |        |        |        |
| A155CA-A156N-H | 54.55  | 119.52  | 7.249  | A172CA-N-H     | 50.1   | 123.25 | 5.222  |                |        |        |        |
| A156CA-N-H     | 51.47  | 119.62  | 7.25   | A172CA-Y173N-H | 50.2   | 120.3  | 8.281  |                |        |        |        |
| A156CA-T157N-H | 51.47  | 112.81  | 8.094  | Y173CA-N-H     | 57.2   | 120.29 | 8.285  |                |        |        |        |
| T157CA-N-H     | 63.16  | 112.86  | 8.094  | Y173CA-D174N-H | 57.18  | 119.38 | 5.988  |                |        |        |        |
| T157CA-L158N-H | 63.17  | 118.88  | 7.158  | D174CA-N-H     | 50.94  | 119.24 | 5.986  |                |        |        |        |
| L158CA-N-H     | 52.59  | 118.91  | 7.158  | D174CA-N175N-H | 50.96  | 121.97 | 7.998  |                |        |        |        |
| L158CA-E159N-H | 52.57  | 121.08  | 8.354  | N175CA-N-H     | 55.59  | 121.91 | 7.996  |                |        |        |        |
| E159CA-N-H     | 54.44  | 121.24  | 8.353  | N175CA-D176N-H | 55.59  | 118.49 | 8.051  |                |        |        |        |
| E159CA-F160N-H | 54.44  | 128.05  | 9.12   | D176CA-N-H     | 57.35  | 118.52 | 8.05   |                |        |        |        |
| F160CA-N-H     | 61.02  | 128.16  | 9.118  | D176CA-S177N-H | 57.36  | 116.37 | 7.177  |                |        |        |        |
| F160CA-S161N-H | 61.01  | 112.93  | 8.831  | S177CA-N-H     | 61.25  | 116.41 | 7.176  |                |        |        |        |
| S161CA-N-H     | 60.74  | 112.97  | 8.828  | S177CA-L178N-H | 61.23  | 119.91 | 6.781  |                |        |        |        |
| S161CA-K162N-H | 60.69  | 119.62  | 7.634  | L178CA-N-H     | 57.98  | 119.92 | 6.782  |                |        |        |        |
| K162CA-N-H     | 56.19  | 119.66  | 7.633  | L178CA-K179N-H | 57.98  | 112.26 | 7.318  |                |        |        |        |
| K162CA-F163N-H | 56.19  | 120.21  | 7.989  | K179CA-N-H     | 59.8   | 112.3  | 7.318  |                |        |        |        |
| F163CA-N-H     | 58.512 | 120.19  | 7.986  | K179CA-S180N-H | 59.73  | 114.46 | 7.478  |                |        |        |        |
| F163CA-I164N-H | 58.46  | 124.44  | 9.575  | S180CA-N-H     | 60.87  | 114.46 | 7.477  |                |        |        |        |
| I164CA-N-H     | 59.64  | 124.54  | 9.575  | S180CA-L181N-H | 60.86  | 121.6  | 7.541  |                |        |        |        |
| I164CA-S165N-H | 59.642 | 119.359 | 8.747  | L181CA-N-H     | 56.73  | 121.65 | 7.541  |                |        |        |        |
| S165CA-N-H     | 57.09  | 119.49  | 8.747  | L181CA-L182N-H | 56.76  | 114.55 | 7.014  |                |        |        |        |
| S165CA-T166N-H | 57.09  | 118.19  | 9.389  | L182CA-N-H     | 56.9   | 114.55 | 7.014  |                |        |        |        |

**Table A3. Assignments of high-spin NP4 at pH 7.3 from the HNCO and HN(CA)CO experiments.**

|                 |               | HNCO       |              |  |               | HN(CA)-CO  |              |
|-----------------|---------------|------------|--------------|--|---------------|------------|--------------|
| Peak assignment | CO, ppm       | N, ppm     | H, ppm       |  | CO, ppm       | N, ppm     | H, ppm       |
|                 |               |            |              |  |               |            |              |
| A1C-C2N-H       | <i>peak</i>   | <i>not</i> | <i>found</i> |  | <i>peak</i>   | <i>not</i> | <i>found</i> |
| C2C-N-H         |               |            |              |  | <i>peak</i>   | <i>not</i> | <i>found</i> |
| C2C-T3N-H       | <b>174.65</b> | 120.46     | 9.896        |  | <b>174.65</b> | 120.46     | 9.896        |
| T3C-N-H         |               |            |              |  | <b>174.55</b> | 120.42     | 9.894        |
| T3C-K4N-H       | <b>174.55</b> | 124.02     | 8.116        |  | <b>174.55</b> | 124.02     | 8.116        |
| K4C-N-H         |               |            |              |  | <b>176.37</b> | 124.04     | 8.117        |
| K4C-N5N-H       | <i>peak</i>   | <i>not</i> | <i>found</i> |  | <i>Peak</i>   | <i>Not</i> | <i>found</i> |
| N5-C-N-H        |               |            |              |  | <i>Peak</i>   | <i>Not</i> | <i>found</i> |
| N5C-A6N-H       | <b>174.23</b> | 124.53     | 7.785        |  | <b>174.22</b> | 124.5      | 7.785        |
| A6C-N-H         |               |            |              |  | <b>176.82</b> | 124.56     | 7.785        |
| A6C-I7N-H       | <b>176.83</b> | 124.83     | 8.443        |  | <b>176.81</b> | 124.83     | 8.442        |
| I7C-N-H         |               |            |              |  | <b>176.05</b> | 124.82     | 8.443        |
| I7C-A8N-H       | <b>176.09</b> | 129.55     | 8.48         |  | <b>176.07</b> | 129.45     | 8.478        |
| A8C-N-H         |               |            |              |  | <b>177.39</b> | 129.49     | 8.478        |
| A8C-Q9N-H       | <b>177.4</b>  | 121.51     | 8.534        |  | <b>177.4</b>  | 121.51     | 8.534        |
| Q9C-N-H         |               |            |              |  | <b>177.11</b> | 121.5      | 8.532        |
| Q9C-T10N-H      | <b>177.11</b> | 127.06     | 8.874        |  | <b>177.11</b> | 127.12     | 8.873        |
| T10C-N-H        |               |            |              |  | <b>176.04</b> | 127.06     | 8.873        |
| T10C-G11N-H     | <i>peak</i>   | <i>not</i> | <i>found</i> |  | <i>peak</i>   | <i>not</i> | <i>found</i> |
| G11C-N-H        |               |            |              |  | <i>peak</i>   | <i>not</i> | <i>found</i> |
| G11C-F12N-H     | <b>174.21</b> | 118.82     | 7.016        |  | <b>174.21</b> | 118.82     | 7.016        |
| F12C-N-H        |               |            |              |  | <b>174.12</b> | 118.83     | 7.017        |
| F12C-N13N-H     | <b>174.11</b> | 128.12     | 8.755        |  | <b>174.11</b> | 128.13     | 8.755        |
| N13C-N-H        |               |            |              |  | <b>174.99</b> | 128.08     | 8.754        |
| N13C-K14N-H     | <b>174.99</b> | 125.37     | 7.988        |  | <b>174.99</b> | 125.33     | 7.988        |
| K14C-N-H        |               |            |              |  | <b>176.81</b> | 125.35     | 7.989        |
| K14C-D15N-H     | <b>176.82</b> | 120.17     | 8.02         |  | <b>176.77</b> | 120.14     | 8.021        |
| D15C-N-H        |               |            |              |  | <b>177.93</b> | 120.18     | 8.02         |

|                 |               | HNCO   |        |  |               | HN(CA)-CO  |              |
|-----------------|---------------|--------|--------|--|---------------|------------|--------------|
| Peak assignment | CO, ppm       | N, ppm | H, ppm |  | CO, ppm       | N, ppm     | H, ppm       |
| D15C-K16N-H     | <b>177.95</b> | 116.7  | 7.066  |  | <b>177.95</b> | 116.73     | 7.068        |
| K16C-N-H        |               |        |        |  | <b>176.23</b> | 116.75     | 7.068        |
| K16C-Y17N-H     | <b>176.25</b> | 118.43 | 7.013  |  | <b>176.25</b> | 118.45     | 7.014        |
| Y17C-N-H        |               |        |        |  | <b>177.8</b>  | 118.45     | 7.015        |
| Y17C-F18N-H     | <b>177.9</b>  | 118.37 | 8.422  |  | <b>177.76</b> | 118.43     | 8.419        |
| F18C-N-H        |               |        |        |  | <b>176.80</b> | 118.38     | 8.422        |
| F18C-N19N-H     | <b>176.8</b>  | 118.62 | 7.857  |  | <b>176.80</b> | 118.62     | 7.857        |
| N19C-N-H        |               |        |        |  | <b>177.05</b> | 118.63     | 7.857        |
| N19C-G20N-H     | <b>177.07</b> | 110.35 | 9.262  |  | <b>177.06</b> | 110.37     | 9.259        |
| G20C-N-H        |               |        |        |  | <b>172.21</b> | 110.39     | 9.26         |
| G20C-D21N-H     | <b>172.21</b> | 118.62 | 7.646  |  | <b>172.21</b> | 118.66     | 7.647        |
| D21C-N-H        |               |        |        |  | <b>175.8</b>  | 118.6      | 7.646        |
| D21C-V22N-H     | <b>175.81</b> | 119.12 | 8.218  |  | <b>175.8</b>  | 119.1      | 8.219        |
| V22C-N-H        |               |        |        |  | <i>Peak</i>   | <i>not</i> | <i>found</i> |
| V22C-W23N-H     | <b>177.04</b> | 127.7  | 9.629  |  | <b>177.03</b> | 127.61     | 9.627        |
| W23C-N-H        |               |        |        |  | <b>174.66</b> | 127.7      | 9.627        |
| W23C-Y24N-H     | <b>174.66</b> | 119.05 | 9.003  |  | <b>174.63</b> | 118.99     | 8.992        |
| Y24C-N-H        |               |        |        |  | <b>177.19</b> | 119.08     | 9.003        |
| Y24C-V25N-H     | <b>177.2</b>  | 120.76 | 8.55   |  | <b>177.20</b> | 120.76     | 8.55         |
| V25C-N-H        |               |        |        |  | <b>178.08</b> | 120.66     | 8.552        |
| V25C-T26N-H     | <b>178.08</b> | 122.93 | 10.068 |  | <b>178.07</b> | 122.84     | 10.065       |
| T26C-N-H        |               |        |        |  | <b>175.30</b> | 122.86     | 10.065       |
| T26C-D27N-H     | <b>175.33</b> | 120.55 | 8.593  |  | <b>175.33</b> | 120.55     | 8.593        |
| D27C-N-H        |               |        |        |  | <b>175.52</b> | 120.58     | 8.593        |
| D27C-Y28N-H     | <b>175.52</b> | 119.29 | 10.307 |  | <b>175.52</b> | 119.29     | 10.307       |
| Y28C-N-H        |               |        |        |  | <b>172.03</b> | 119.31     | 10.304       |
| Y28C-L29N-H     | <b>172.03</b> | 123.45 | 9.228  |  | <b>172.01</b> | 123.45     | 9.226        |
| L29C-N-H        |               |        |        |  | <b>172.91</b> | 123.47     | 9.227        |
| L29C-D30N-H     | <b>172.92</b> | 127.4  | 8.361  |  | <b>172.92</b> | 127.37     | 8.358        |
| D30C-N-H        |               |        |        |  | <b>175.61</b> | 127.44     | 8.367        |
| D30C-L31N-H     | <b>175.61</b> | 123.66 | 6.963  |  | <b>175.61</b> | 123.66     | 6.966        |
|                 |               |        |        |  |               |            |              |

|                 |         | HNCO    |        |  |         | HN(CA)-CO |        |
|-----------------|---------|---------|--------|--|---------|-----------|--------|
| Peak assignment | CO, ppm | N, ppm  | H, ppm |  | CO, ppm | N, ppm    | H, ppm |
| L31C-N-H        |         |         |        |  | 176.73  | 123.58    | 6.963  |
| L31C-E32N-H     | 176.72  | 119.75  | 7.21   |  | 176.72  | 119.75    | 7.21   |
| E32C-N-H        |         |         |        |  | 171.79  | 119.79    | 7.212  |
| E32C-P33        | peak    | not     | found  |  | Peak    | not       | found  |
| P33C            |         |         |        |  | Peak    | not       | found  |
| P33C-D34N-H     | 176.96  | 120.78  | 8.165  |  | 176.97  | 120.80    | 8.162  |
| D34C-N-H        |         |         |        |  | 175.62  | 120.79    | 8.165  |
| D34C-D35N-H     | 175.66  | 120.43  | 8.359  |  | 175.65  | 120.39    | 8.357  |
| D35C-N-H        |         |         |        |  | 176.88  | 120.37    | 8.359  |
| D35C-V36N-H     | 176.89  | 119.17  | 8.204  |  | 176.89  | 119.17    | 8.204  |
| V36C-N-H        |         |         |        |  | 173.71  | 119.21    | 8.203  |
| V36C-P37        | peak    | not     | found  |  | Peak    | not       | found  |
| P37C            |         |         |        |  | Peak    | not       | found  |
| P37C-K38N-H     | 177.83  | 124.29  | 9.904  |  | 177.82  | 124.19    | 9.911  |
| K38C-N-H        |         |         |        |  | 178.81  | 124.44    | 9.9    |
| K38C-R39N-H     | 178.82  | 127.45  | 9.785  |  | 178.82  | 127.45    | 9.785  |
| R39C-N-H        |         |         |        |  | Peak    | not       | found  |
| R39C-Y40N-H     | peak    | not     | found  |  | Peak    | not       | found  |
| Y40C-N-H        |         |         |        |  | Peak    | not       | found  |
| Y40C-C41N-H     | peak    | not     | found  |  | Peak    | not       | found  |
| C41C-N-H        |         |         |        |  | Peak    | not       | found  |
| C41C-A42N-H     | peak    | not     | found  |  | Peak    | not       | found  |
| A42C-N-H        |         |         |        |  | Peak    | not       | found  |
| A42C-A43N-H     | peak    | not     | found  |  | Peak    | not       | found  |
| A43C-N-H        |         |         |        |  | Peak    | not       | found  |
| A43C-L44N-H     | 171.98  | 116.18  | 8.876  |  | 171.97  | 116.08    | 8.875  |
| L44C-N-H        |         |         |        |  | 174.2   | 116.22    | 8.874  |
| L44C-A45N-H     | 174.21  | 121.58  | 8.997  |  | 174.21  | 121.58    | 8.997  |
| A45C-N-H        |         |         |        |  | 174.16  | 121.55    | 8.996  |
| A45C-A46N-H     | 174.16  | 125.792 | 8.818  |  | 174.14  | 125.8     | 8.822  |
| A46C-N-H        |         |         |        |  | 177.35  | 125.85    | 8.818  |
| A46C-G47N-H     | 177.36  | 107.941 | 9.217  |  | 177.37  | 107.96    | 9.215  |

|                 |         | HNCO    |        |  |         | HN(CA)-CO |        |
|-----------------|---------|---------|--------|--|---------|-----------|--------|
| Peak assignment | CO, ppm | N, ppm  | H, ppm |  | CO, ppm | N, ppm    | H, ppm |
| G47C-N-H        |         |         |        |  | 172.23  | 107.94    | 9.215  |
| G47C-T48N-H     | 172.23  | 113.22  | 8.594  |  | 172.23  | 113.2     | 8.593  |
| T48C-N-H        |         |         |        |  | 175.29  | 113.23    | 8.593  |
| T48C-A49N-H     | 175.29  | 128.449 | 8.987  |  | 175.29  | 128.42    | 8.986  |
| A49C-N-H        |         |         |        |  | 177.63  | 128.45    | 8.986  |
| A49C-S50N-H     | peak    | not     | found  |  | Peak    | Not       | found  |
| S50C-N-H        |         |         |        |  | Peak    | Not       | found  |
| S50C-G51N-H     | 175.19  | 106.74  | 8.499  |  | Peak    | Not       | found  |
| G51C-N-H        |         |         |        |  | 173.6   | 106.76    | 8.492  |
| G51C-K52N-H     | 173.6   | 120.391 | 7.881  |  | 173.6   | 120.39    | 7.881  |
| K52C-N-H        |         |         |        |  | 174.63  | 120.42    | 7.881  |
| K52C-L53N-H     | 174.64  | 123.384 | 8.612  |  | 174.635 | 123.34    | 8.611  |
| L53C-N-H        |         |         |        |  | 176.1   | 123.41    | 8.61   |
| L53C-K54N-H     | 176.12  | 126.566 | 8.956  |  | 176.09  | 126.57    | 8.955  |
| K54C-N-H        |         |         |        |  | 174.15  | 126.53    | 8.956  |
| K54C-E55N-H     | 174.15  | 118.747 | 8.937  |  | 174.16  | 118.68    | 8.935  |
| E55C-N-H        |         |         |        |  | 174.59  | 118.79    | 8.937  |
| E55C-A56N-H     | 174.59  | 133.584 | 9.866  |  | 174.6   | 133.59    | 9.862  |
| A56C-N-H        |         |         |        |  | 173.42  | 133.61    | 9.862  |
| A56C-L57N-H     | 173.42  | 121.624 | 8.512  |  | 173.43  | 121.58    | 8.512  |
| L57C-N-H        |         |         |        |  | 171.45  | 121.73    | 8.504  |
| L57C-Y58N-H     | peak    | not     | found  |  | Peak    | Not       | found  |
| Y58C-N-H        |         |         |        |  | Peak    | Not       | found  |
| Y58C-H59N-H     | peak    | not     | found  |  | Peak    | not       | found  |
| H59C-N-H        |         |         |        |  | Peak    | not       | found  |
| H59C-Y60N-H     | peak    | not     | found  |  | Peak    | not       | found  |
| Y60C-N-H        |         |         |        |  | Peak    | not       | found  |
| Y60C-D61N-H     | peak    | not     | found  |  | Peak    | not       | found  |
| D61C-N-H        |         |         |        |  | Peak    | not       | found  |
| D61C-P62N-H     | peak    | not     | found  |  | Peak    | not       | found  |
| P62C-N-H        |         |         |        |  | Peak    | not       | found  |
| P62C-K63N-H     | 177.74  | 116.58  | 7.985  |  | 177.74  | 116.58    | 7.985  |

|                 |         | HNCO   |        |  |         | HN(CA)-CO |        |
|-----------------|---------|--------|--------|--|---------|-----------|--------|
| Peak assignment | CO, ppm | N, ppm | H, ppm |  | CO, ppm | N, ppm    | H, ppm |
| K63C-N-H        |         |        |        |  | 177.93  | 116.60    | 7.986  |
| K63C-T64N-H     | 177.96  | 105.17 | 6.602  |  | 177.95  | 105.18    | 6.605  |
| T64C-N-H        |         |        |        |  | 175.53  | 105.2     | 6.605  |
| T64C-Q65N-H     | 175.53  | 115.15 | 8.011  |  | 175.54  | 115.24    | 8.013  |
| Q65C-N-H        |         |        |        |  | 174.18  | 115.21    | 8.011  |
| Q65C-D66N-H     | 174.18  | 119.67 | 7.341  |  | 174.18  | 119.67    | 7.341  |
| D66C-N-H        |         |        |        |  | Peak    | Not       | found  |
| D66C-T67N-H     | 174.24  | 114.03 | 7.187  |  | 174.23  | 114.06    | 7.189  |
| T67C-N-H        |         |        |        |  | 172.9   | 114.03    | 7.192  |
| T67C-F68N-H     | peak    | Not    | found  |  | Peak    | Not       | found  |
| F68C-N-H        |         |        |        |  | Peak    | Not       | found  |
| F68C-Y69N-H     | 170.52  | 117.73 | 6.818  |  | 170.54  | 117.76    | 6.812  |
| Y69C-N-H        |         |        |        |  | 173.86  | 117.81    | 6.821  |
| Y69C-D70N-H     | 173.84  | 115.41 | 7.428  |  | 173.84  | 115.41    | 7.428  |
| D70C-N-H        |         |        |        |  | 173.67  | 115.41    | 7.424  |
| D70C-V71N-H     | 173.69  | 118.09 | 9.413  |  | 173.70  | 118.06    | 9.412  |
| V71C-N-H        |         |        |        |  | 175.04  | 118.2     | 9.411  |
| V71C-S72N-H     | 175.04  | 122.20 | 9.192  |  | 175.03  | 121.98    | 9.188  |
| S72C-N-H        |         |        |        |  | 174.22  | 122.08    | 9.189  |
| S72C-E73N-H     | 174.22  | 124.24 | 9.058  |  | 174.22  | 124.17    | 9.057  |
| E73C-N-H        |         |        |        |  | 177.06  | 124.28    | 9.057  |
| E73C-L74N-H     | 177.07  | 124.38 | 8.611  |  | 177.07  | 124.38    | 8.611  |
| L74C-N-H        |         |        |        |  | 176.89  | 124.38    | 8.61   |
| L74C-Q75N-H     | 176.87  | 122.03 | 9.434  |  | 176.86  | 122.02    | 9.433  |
| Q75C-N-H        |         |        |        |  | 175.56  | 122       | 9.433  |
| Q75C-V76N-H     | 175.56  | 126.14 | 8.884  |  | 175.60  | 126.02    | 8.88   |
| V76C-N-H        |         |        |        |  | 175.98  | 126.19    | 8.883  |
| V76C-E77N-H     | 175.98  | 130.04 | 8.69   |  | 175.99  | 130.05    | 8.691  |
| E77C-N-H        |         |        |        |  | 176.66  | 130.08    | 8.688  |
| E77C-S78N-H     | 176.66  | 111.53 | 8.051  |  | 176.66  | 111.65    | 8.053  |
| S78C-N-H        |         |        |        |  | 172.76  | 111.59    | 8.053  |
| S78C-L79N-H     | peak    | Not    | found  |  | Peak    | Not       | found  |

|                 |         | HNCO   |        |  |         | HN(CA)-CO |        |
|-----------------|---------|--------|--------|--|---------|-----------|--------|
| Peak assignment | CO, ppm | N, ppm | H, ppm |  | CO, ppm | N, ppm    | H, ppm |
| L79C-N-H        |         |        |        |  | Peak    | not       | found  |
| L79C-G80N-H     | 178.31  | 114.57 | 8.377  |  | 178.29  | 114.58    | 8.377  |
| G80C-N-H        |         |        |        |  | 170.79  | 114.61    | 8.377  |
| G80C-K81N-H     | 170.79  | 121.85 | 7.882  |  | 170.8   | 121.84    | 7.881  |
| K81C-N-H        |         |        |        |  | 173.72  | 121.81    | 7.881  |
| K81C-Y82N-H     | 173.72  | 121.07 | 8.288  |  | 173.70  | 120.86    | 8.286  |
| Y82C-N-H        |         |        |        |  | 174.72  | 121.13    | 8.291  |
| Y82C-T83N-H     | 174.75  | 117.07 | 9.086  |  | 174.74  | 117.12    | 9.083  |
| T83C-N-H        |         |        |        |  | 173.05  | 117.09    | 9.084  |
| T83C-A84N-H     | 173.05  | 132.38 | 10.175 |  | 173.05  | 132.38    | 10.179 |
| A84C-N-H        |         |        |        |  | 175.87  | 132.44    | 10.172 |
| A84C-N85N-H     | 175.88  | 123.94 | 8.429  |  | 175.88  | 123.94    | 8.429  |
| N85C-N-H        |         |        |        |  | 173.88  | 123.95    | 8.426  |
| N85C-F86N-H     | 173.89  | 120.04 | 7.365  |  | 173.89  | 120.04    | 7.365  |
| F86C-N-H        |         |        |        |  | 175.86  | 120.09    | 7.371  |
| F86C-K87N-H     | 175.88  | 120.59 | 9.286  |  | 175.81  | 120.79    | 9.277  |
| K87C-N-H        |         |        |        |  | 174.82  | 120.59    | 9.281  |
| K87C-K88N-H     | 174.8   | 127.30 | 9.179  |  | 174.8   | 127.37    | 9.179  |
| K88C-N-H        |         |        |        |  | 177.21  | 127.32    | 9.178  |
| K88C-V89N-H     | 177.21  | 120.98 | 8.423  |  | 177.2   | 121.08    | 8.42   |
| V89C-N-H        |         |        |        |  | 175.4   | 120.92    | 8.423  |
| V89C-D90N-H     | 175.39  | 118.61 | 7.95   |  | 175.39  | 118.52    | 7.951  |
| D90C-N-H        |         |        |        |  | 176.82  | 118.66    | 7.95   |
| D90C-K91N-H     | 176.83  | 114.23 | 7.79   |  | 176.84  | 114.34    | 7.788  |
| K91C-N-H        |         |        |        |  | 174.70  | 114.3     | 7.79   |
| K91C-N92N-H     | 174.71  | 114.3  | 7.225  |  | 174.72  | 114.30    | 7.227  |
| N92C-N-H        |         |        |        |  | 175.51  | 114.33    | 7.227  |
| N92C-G93N-H     | 175.51  | 108.36 | 7.935  |  | 175.51  | 108.38    | 7.935  |
| G93C-N-H        |         |        |        |  | 173.52  | 108.47    | 7.934  |
| G93C-N94N-H     | 173.52  | 120.31 | 8.28   |  | 173.52  | 120.31    | 8.28   |
| N94C-N-H        |         |        |        |  | 175.61  | 120.31    | 8.28   |
| N94C-V95N-H     | 175.61  | 123.44 | 8.763  |  | 175.62  | 123.41    | 8.761  |

|                 |         | HNCO   |        |  |         | HN(CA)-CO |        |
|-----------------|---------|--------|--------|--|---------|-----------|--------|
| Peak assignment | CO, ppm | N, ppm | H, ppm |  | CO, ppm | N, ppm    | H, ppm |
| V95C-N-H        |         |        |        |  | 175.99  | 123.4     | 8.763  |
| V95C-K96N-H     | 176     | 128.13 | 9.49   |  | 175.99  | 128.05    | 9.489  |
| K96C-N-H        |         |        |        |  | 177.14  | 128.14    | 9.488  |
| K96C-V97N-H     | 177.14  | 119.61 | 7.997  |  | 177.14  | 119.6     | 7.997  |
| V97C-N-H        |         |        |        |  | 174.67  | 119.65    | 7.997  |
| V97C-A98N-H     | 174.68  | 128.24 | 8.597  |  | 174.67  | 128.18    | 8.597  |
| A98C-N-H        |         |        |        |  | 178.02  | 128.24    | 8.597  |
| A98C-V99N-H     | 178.03  | 122.21 | 8.548  |  | 178.01  | 122.10    | 8.546  |
| V99C-N-H        |         |        |        |  | 177.07  | 122.19    | 8.546  |
| V99C-T100N-H    | 177.06  | 126.11 | 9.975  |  | 177.07  | 126.08    | 9.974  |
| T100C-N-H       |         |        |        |  | 173.58  | 126.12    | 9.975  |
| T100C-A101N-H   | 173.58  | 131.29 | 8.904  |  | 173.58  | 131.29    | 8.904  |
| A101C-N-H       |         |        |        |  | 178.51  | 131.3     | 8.904  |
| A101C-G102N-H   | 178.51  | 110.19 | 9.151  |  | 178.51  | 110.21    | 9.142  |
| G102C-N-H       |         |        |        |  | 173.01  | 110.17    | 9.152  |
| G102C-N103N-H   | 173.02  | 121.06 | 8.201  |  | 173.02  | 121.09    | 8.202  |
| N103C-N-H       |         |        |        |  | 173.99  | 120.98    | 8.201  |
| N103C-Y104N-H   | 174     | 121.19 | 9.211  |  | 174     | 121.19    | 9.205  |
| Y104C-N-H       |         |        |        |  | 174.43  | 121.16    | 9.205  |
| Y104C-Y105N-H   | 174.45  | 116.24 | 10.222 |  | 174.45  | 116.24    | 10.222 |
| Y105C-N-H       |         |        |        |  | 174.29  | 116.19    | 10.219 |
| Y105C-T106N-H   | 174.24  | 113.62 | 8.48   |  | 174.28  | 113.61    | 8.483  |
| T106C-N-H       |         |        |        |  | 175.03  | 113.57    | 8.489  |
| T106C-F107N-H   | 175.01  | 119.69 | 9.469  |  | 175.01  | 119.69    | 9.469  |
| F107C-N-H       |         |        |        |  | 173.71  | 119.61    | 9.466  |
| F107C-T108N-H   | 173.73  | 117.61 | 9.34   |  | 173.75  | 117.59    | 9.336  |
| T108C-N-H       |         |        |        |  | 174.67  | 117.52    | 9.337  |
| T108C-V109N-H   | 174.7   | 127.91 | 9.343  |  | 174.7   | 127.91    | 9.343  |
| V109C-N-H       |         |        |        |  | 174.63  | 127.86    | 9.341  |
| V109C-M110N-H   | 174.61  | 129.58 | 8.779  |  | 174.61  | 129.49    | 8.779  |
| M110C-N-H       |         |        |        |  | 176.95  | 129.5     | 8.776  |
| M110C-Y111N-H   | 176.96  | 117.59 | 8.206  |  | 176.95  | 117.59    | 8.206  |

|                 |         | HNCO   |        |  |         | HN(CA)-CO |        |
|-----------------|---------|--------|--------|--|---------|-----------|--------|
| Peak assignment | CO, ppm | N, ppm | H, ppm |  | CO, ppm | N, ppm    | H, ppm |
| Y111C-N-H       |         |        |        |  | 172.24  | 117.6     | 8.207  |
| Y111C-A112N-H   | 172.25  | 125.86 | 6.659  |  | 172.24  | 125.93    | 6.659  |
| A112C-N-H       |         |        |        |  | 175.07  | 125.91    | 6.66   |
| A112C-D113N-H   | 175.07  | 121.5  | 9.498  |  | 175.07  | 121.5     | 9.496  |
| D113C-N-H       |         |        |        |  | 176.07  | 121.49    | 9.496  |
| D113C-D114N-H   | 176.09  | 114.82 | 8.357  |  | 176.09  | 114.83    | 8.357  |
| D114C-N-H       |         |        |        |  | 177.86  | 114.81    | 8.356  |
| D114C-S115N-H   | 177.87  | 110.88 | 8.702  |  | 177.85  | 110.89    | 8.701  |
| S115C-N-H       |         |        |        |  | 173     | 110.93    | 8.701  |
| S115C-S116N-H   | 173     | 117.95 | 8.884  |  | 173.01  | 117.92    | 8.884  |
| S116C-N-H       |         |        |        |  | 171.12  | 117.98    | 8.884  |
| S116C-A117N-H   | 171.12  | 117.62 | 8.584  |  | 171.12  | 117.55    | 8.583  |
| A117C-N-H       |         |        |        |  | 174.9   | 117.67    | 8.583  |
| A117C-L118N-H   | 174.9   | 121.54 | 9.266  |  | 174.9   | 121.54    | 9.266  |
| L118C-N-H       |         |        |        |  | 175.64  | 121.57    | 9.265  |
| L118C-I119N-H   | 175.63  | 119.83 | 9.769  |  | 175.61  | 119.85    | 9.758  |
| I119C-N-H       |         |        |        |  | 174.33  | 119.90    | 9.769  |
| I119C-H120N-H   | 174.33  | 122.38 | 8.832  |  | 174.33  | 122.38    | 8.832  |
| H120C-N-H       |         |        |        |  | 174.25  | 122.33    | 8.83   |
| H120C-T121N-H   | 174.23  | 116.42 | 6.837  |  | 174.23  | 116.42    | 6.837  |
| T121C-N-H       |         |        |        |  | 169.62  | 116.47    | 6.846  |
| T121C-C122N-H   | 169.65  | 118.22 | 7.212  |  | 169.64  | 118.2     | 7.211  |
| C122C-N-H       |         |        |        |  | 171.54  | 118.19    | 7.229  |
| C122C-L123N-H   | 171.58  | 126.99 | 6.939  |  | 171.59  | 126.97    | 6.94   |
| L123C-N-H       |         |        |        |  | 174.04  | 127.07    | 6.946  |
| L123C-H124H     | peak    | not    | found  |  | peak    | not       | found  |
| H124C-N-H       |         |        |        |  | peak    | not       | found  |
| H124C-K125N-H   | 173.67  | 120.23 | 7.785  |  | 173.67  | 120.24    | 7.788  |
| K125C-N-H       |         |        |        |  | 177.95  | 120.29    | 7.785  |
| K125C-G126N-H   | 177.97  | 116.01 | 8.766  |  | 177.96  | 116       | 8.765  |
| G126C-N-H       |         |        |        |  | 175.28  | 116.03    | 8.765  |
| G126C-N127N-H   | peak    | not    | found  |  | peak    | not       | found  |

|                 |         | HNCO   |        |  | HN(CA)-CO   |            |
|-----------------|---------|--------|--------|--|-------------|------------|
| Peak assignment | CO, ppm | N, ppm | H, ppm |  | CO, ppm     | N, ppm     |
| N127C-N-H       |         |        |        |  | <i>peak</i> | <i>not</i> |
| N127C-K128N-H   | 173.69  | 119.18 | 7.382  |  | 173.69      | 119.18     |
| K128C-N-H       |         |        |        |  | 173.7       | 119.23     |
| K128C-D129N-H   | 173.69  | 120.95 | 8.162  |  | 173.70      | 120.96     |
| D129C-N-H       |         |        |        |  | 175.42      | 120.94     |
| D129C-L130N-H   | 175.43  | 123.14 | 6.911  |  | 175.42      | 123.02     |
| L130C-N-H       |         |        |        |  | 174.70      | 123.20     |
| L130C-G131N-H   | 174.71  | 103.69 | 5.163  |  | <i>Peak</i> | <i>Not</i> |
| G131CN--H       |         |        |        |  | 169.76      | 103.71     |
| G131C-D132N-H   | 169.7   | 116.46 | 6.515  |  | 169.71      | 116.49     |
| D132C-N-H       |         |        |        |  | 172.42      | 116.52     |
| D132C-L133N-H   | 172.42  | 120.84 | 5.505  |  | 172.42      | 120.84     |
| L133C-N-H       |         |        |        |  | 175.04      | 120.8      |
| L133C-Y134N-H   | 175.08  | 125.02 | 8.309  |  | 175.08      | 125.02     |
| Y134C-N-H       |         |        |        |  | 175.39      | 125.11     |
| Y134C-A135N-H   | 175.41  | 124.12 | 9.966  |  | 175.41      | 124.12     |
| A135C-N-H       |         |        |        |  | 175.55      | 124.04     |
| A135C-V136N-H   | 175.59  | 124.87 | 10.264 |  | 175.59      | 124.87     |
| V136C-N-H       |         |        |        |  | 175.21      | 124.85     |
| V136C-L137N-H   | 175.22  | 126.22 | 9.931  |  | 175.22      | 126.2      |
| L137C-N-H       |         |        |        |  | 179.06      | 126.18     |
| L137C-N138N-H   | 179.07  | 121.39 | 9.935  |  | 179.06      | 121.22     |
| N138C-N-H       |         |        |        |  | 175.44      | 121.39     |
| N138C-R139N-H   | 175.45  | 124.83 | 8.619  |  | 175.51      | 124.88     |
| R139C-N-H       |         |        |        |  | 175.99      | 124.83     |
| R139C-N140N-H   | 176.02  | 120.08 | 10.279 |  | 176         | 120.05     |
| N140C-N-H       |         |        |        |  | 174.78      | 120.11     |
| N140C-K141N-H   | 174.81  | 123.57 | 7.627  |  | 174.82      | 123.59     |
| K141C-N-H       |         |        |        |  | 175.45      | 123.57     |
| K141C-D142N-H   | 175.44  | 117.64 | 7.965  |  | <i>peak</i> | <i>Not</i> |
| D142C-N-H       |         |        |        |  | <i>peak</i> | <i>Not</i> |
| D142C-A143N-H   | 175.21  | 123.39 | 7.144  |  | <i>Peak</i> | <i>Not</i> |

|                 |             | HNCO       |              |  | HN(CA)-CO   |            |
|-----------------|-------------|------------|--------------|--|-------------|------------|
| Peak assignment | CO, ppm     | N, ppm     | H, ppm       |  | CO, ppm     | N, ppm     |
| A143C-N-H       |             |            |              |  | 177.58      | 123.38     |
| A143C-A144N-H   | 177.59      | 126.29     | 8.488        |  | 177.59      | 126.29     |
| A144C-N-H       |             |            |              |  | 177.8       | 126.26     |
| A144C-A145N-H   | 177.82      | 126.81     | 9.278        |  | 177.80      | 126.73     |
| A145C-N-H       |             |            |              |  | 178.35      | 126.84     |
| A145C-G146N-H   | 178.35      | 110.4      | 8.796        |  | 178.34      | 110.42     |
| G146C-N-H       |             |            |              |  | 173.98      | 110.40     |
| G146C-D147N-H   | 173.97      | 117.57     | 8.431        |  | 173.97      | 117.57     |
| D147C-N-H       |             |            |              |  | 179.12      | 117.47     |
| D147C-K148N-H   | <i>peak</i> | <i>Not</i> | <i>found</i> |  | <i>Peak</i> | <i>Not</i> |
| K148C-N-H       |             |            |              |  | <i>Peak</i> | <i>Not</i> |
| K148C-V149N-H   | 179.94      | 120.52     | 7.939        |  | 179.92      | 120.50     |
| V149C-N-H       |             |            |              |  | 177.43      | 120.52     |
| V149C-K150N-H   | 177.44      | 120.43     | 7.82         |  | 177.45      | 120.41     |
| K150C-N-H       |             |            |              |  | 179.89      | 120.45     |
| K150C-S151N-H   | 179.9       | 116.86     | 8.228        |  | 179.89      | 116.90     |
| S151C-N-H       |             |            |              |  | <i>Peak</i> | <i>Not</i> |
| S151C-A152N-H   | 176.26      | 126.16     | 7.335        |  | <i>Peak</i> | <i>Not</i> |
| A152C-N-H       |             |            |              |  | 179.79      | 126.164    |
| A152C-V153N-H   | 179.8       | 120.28     | 8.06         |  | 179.8       | 120.27     |
| V153C-N-H       |             |            |              |  | 177.62      | 120.3      |
| V153C-S154N-H   | 177.63      | 113.49     | 7.788        |  | 177.64      | 113.39     |
| S154C-N-H       |             |            |              |  | <i>Peak</i> | <i>Not</i> |
| S154C-A155N-H   | 179.22      | 125.68     | 8.434        |  | <i>Peak</i> | <i>Not</i> |
| A155C-N-H       |             |            |              |  | 178.43      | 125.74     |
| A155C-A156N-H   | 178.44      | 119.58     | 7.25         |  | 178.43      | 119.57     |
| A156C-N-H       |             |            |              |  | 176.72      | 119.63     |
| A156C-T157N-H   | 176.73      | 112.79     | 8.094        |  | 176.73      | 112.82     |
| T157C-N-H       |             |            |              |  | 172.72      | 112.87     |
| T157C-L158N-H   | 172.73      | 118.87     | 7.158        |  | 172.69      | 118.79     |
| L158C-N-H       |             |            |              |  | 176.01      | 118.89     |
| L158C-E159N-H   | 176.02      | 121.18     | 8.354        |  | 176.02      | 121.09     |

|                 |         | HNCO   |        |  |         | HN(CA)-CO |        |
|-----------------|---------|--------|--------|--|---------|-----------|--------|
| Peak assignment | CO, ppm | N, ppm | H, ppm |  | CO, ppm | N, ppm    | H, ppm |
| E159C-N-H       |         |        |        |  | 176.64  | 121.24    | 8.354  |
| E159C-F160N-H   | 176.63  | 128.22 | 9.119  |  | 176.64  | 128.2     | 9.113  |
| F160C-N-H       |         |        |        |  | 177.83  | 128.16    | 9.114  |
| F160C-S161N-H   | 177.87  | 112.93 | 8.829  |  | 177.86  | 113.01    | 8.826  |
| S161C-N-H       |         |        |        |  | Peak    | Not       | found  |
| S161C-K162N-H   | 175.03  | 119.65 | 7.634  |  | Peak    | Not       | found  |
| K162C-N-H       |         |        |        |  | 176.57  | 119.67    | 7.635  |
| K162C-F163N-H   | 176.57  | 120.21 | 7.986  |  | 176.57  | 120.08    | 7.986  |
| F163C-N-H       |         |        |        |  | 175.85  | 120.16    | 7.987  |
| F163C-I164N-H   | 175.85  | 124.45 | 9.576  |  | 175.85  | 124.45    | 9.576  |
| I164C-N-H       |         |        |        |  | 176     | 124.5     | 9.573  |
| I164C-S165N-H   | 176.01  | 119.4  | 8.748  |  | 176     | 119.35    | 8.748  |
| S165C-N-H       |         |        |        |  | 178.95  | 119.47    | 8.747  |
| S165C-T166N-H   | 178.97  | 118.24 | 9.386  |  | 178.95  | 118.23    | 9.387  |
| T166C-N-H       |         |        |        |  | 176.86  | 118.22    | 9.386  |
| T166C-K167N-H   | 176.85  | 125.33 | 8.933  |  | 176.85  | 125.33    | 8.933  |
| K167C-N-H       |         |        |        |  | 177.44  | 125.41    | 8.932  |
| K167C-E168N-H   | 177.45  | 116.88 | 8.633  |  | 177.46  | 116.83    | 8.615  |
| E168C-N-H       |         |        |        |  | 176.21  | 116.85    | 8.629  |
| E168C-N169N-H   | 176.21  | 117.46 | 7.772  |  | 176.2   | 117.43    | 7.764  |
| N169C-N-H       |         |        |        |  | 174.3   | 117.57    | 7.777  |
| N169C-N170N-H   | 174.32  | 115.17 | 8.515  |  | 174.32  | 115.17    | 8.515  |
| N170C-N-H       |         |        |        |  | 174.77  | 115.15    | 8.507  |
| N170C-C171N-H   | 174.77  | 114.74 | 8.476  |  | 174.77  | 114.91    | 8.48   |
| C171C-N-H       |         |        |        |  | 173.03  | 114.75    | 8.476  |
| C171C-A172N-H   | 173.04  | 123.22 | 5.222  |  | 173.04  | 123.22    | 5.222  |
| A172C-N-H       |         |        |        |  | 175.26  | 123.17    | 5.227  |
| A172C-Y173N-H   | 175.26  | 120.3  | 8.284  |  | 175.26  | 120.3     | 8.284  |
| Y173C-N-H       |         |        |        |  | 172.81  | 120.22    | 8.287  |
| Y173C-D174N-H   | 172.76  | 119.27 | 5.986  |  | 172.76  | 119.26    | 5.987  |
| D174C-N-H       |         |        |        |  | 174.44  | 119.27    | 5.984  |
| D174C-N175N-H   | 174.45  | 121.89 | 7.995  |  | 174.45  | 121.89    | 7.995  |

|                 |         | HNCO    |        |  |         | HN(CA)-CO |        |
|-----------------|---------|---------|--------|--|---------|-----------|--------|
| Peak assignment | CO, ppm | N, ppm  | H, ppm |  | CO, ppm | N, ppm    | H, ppm |
| N175C-N-H       |         |         |        |  | 176.56  | 121.88    | 7.992  |
| N175C-D176N-H   | 176.59  | 118.472 | 8.051  |  | 176.59  | 118.47    | 8.051  |
| D176C-N-H       |         |         |        |  | 179.34  | 118.51    | 8.051  |
| D176C-S177N-H   | 179.34  | 116.362 | 7.177  |  | 179.34  | 116.35    | 7.179  |
| S177C-N-H       |         |         |        |  | 175.35  | 116.4     | 7.183  |
| S177C-L178N-H   | 175.35  | 119.917 | 6.783  |  | 175.35  | 119.92    | 6.783  |
| L178C-N-H       |         |         |        |  | 176.41  | 119.95    | 6.785  |
| L178C-K179N-H   | 176.43  | 112.242 | 7.318  |  | 176.42  | 112.22    | 7.319  |
| K179C-N-H       |         |         |        |  | 180.11  | 112.3     | 7.319  |
| K179C-S180N-H   | 180.12  | 114.447 | 7.478  |  | 180.11  | 114.46    | 7.48   |
| S180C-N-H       |         |         |        |  | Peak    | Not       | found  |
| S180C-L181N-H   | 176.62  | 121.622 | 7.542  |  | Peak    | Not       | found  |
| L181C-N-H       |         |         |        |  | 177.91  | 121.65    | 7.543  |
| L181C-L182N-H   | 177.93  | 114.552 | 7.014  |  | 177.93  | 114.55    | 7.014  |
| L182C-N-H       |         |         |        |  | 177.77  | 114.56    | 7.016  |
| L182C-T183N-H   | 177.78  | 105.598 | 7.262  |  | 177.77  | 105.6     | 7.264  |
| T183C-N-H       |         |         |        |  | 174.21  | 105.64    | 7.264  |
| T183C-K184N-H   | 174.22  | 126.916 | 7.243  |  | 174.21  | 126.89    | 7.245  |
| K184C-N-H       |         |         |        |  | 180.95  | 126.94    | 7.245  |

**Table A4. Assignments of high-spin NP4 at pH 7.3 from the HNCACB and CACB(CO)NH experiments.**

|            | HNCA-        | CB         |              | CACB-        | (CO)NH     |              |
|------------|--------------|------------|--------------|--------------|------------|--------------|
| Assignment | C, ppm       | N, ppm     | H, ppm       | C, ppm       | N, ppm     | H, ppm       |
| A1CA-C2N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | <i>peak</i>  | <i>not</i> | <i>found</i> |
| A1CB-C2N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | <i>peak</i>  | <i>not</i> | <i>found</i> |
| C2CA-N-H   | <i>peak</i>  | <i>not</i> | <i>found</i> |              |            |              |
| C2CA-T3N-H | <b>53.63</b> | 120.41     | 9.894        | <b>53.71</b> | 120.46     | 9.898        |
| C2CB-N-H   | <i>peak</i>  | <i>not</i> | <i>found</i> |              |            |              |
| C2CB-T3N-H | <b>42.93</b> | 120.44     | 9.895        | <b>43.01</b> | 120.46     | 9.898        |
| T3CA-N-H   | <b>61.85</b> | 120.43     | 9.897        |              |            |              |
| T3CA-K4N-H | <b>61.82</b> | 124.02     | 8.113        | <b>61.86</b> | 124        | 8.12         |
| T3CB-N-H   | <b>69.4</b>  | 120.41     | 9.896        |              |            |              |
| T3CB-K4N-H | <b>69.42</b> | 124.03     | 8.116        | <b>69.4</b>  | 124.04     | 8.116        |
| K4CA-N-H   | <b>55.02</b> | 124.06     | 8.113        |              |            |              |
| K4CA-N5N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | <i>peak</i>  | <i>not</i> | <i>found</i> |
| K4CB-N-H   | <b>32.29</b> | 124.02     | 8.116        |              |            |              |
| K4CB-N5N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | <i>peak</i>  | <i>not</i> | <i>found</i> |
| N5CA-N-H   | <i>peak</i>  | <i>not</i> | <i>found</i> |              |            |              |
| N5CA-A6N-H | <b>52.37</b> | 124.53     | 7.787        | <b>52.37</b> | 124.53     | 7.787        |
| N5CB-A6N-H | <b>39.02</b> | 124.57     | 7.783        | <b>38.89</b> | 124.53     | 7.787        |
| N5CB-A6N-H | <b>38.79</b> | 124.52     | 7.784        |              |            |              |
| A6CA-N-H   | <b>52.4</b>  | 124.54     | 7.785        |              |            |              |
| A6CA-I7N-H | <b>52.38</b> | 124.77     | 8.441        | <b>52.43</b> | 124.82     | 8.445        |
| A6CB-N-H   | <b>18.6</b>  | 124.55     | 7.785        |              |            |              |
| A6CB-I7N-H | <b>18.6</b>  | 124.76     | 8.443        | <b>18.64</b> | 124.84     | 8.445        |
| I7CA-N-H   | <b>60.09</b> | 124.75     | 8.444        |              |            |              |
| I7CA-A8N-H | <b>60.09</b> | 129.53     | 8.479        | <b>60.08</b> | 129.5      | 8.481        |
| I7CB-N-H   | <b>38.91</b> | 124.81     | 8.439        |              |            |              |
| I7CB-A8N-H | <b>38.89</b> | 129.53     | 8.478        | <b>38.85</b> | 129.49     | 8.481        |
| A8CA-N-H   | <b>51.33</b> | 129.55     | 8.478        |              |            |              |
| A8CA-Q9N-H | <b>51.31</b> | 121.52     | 8.534        | <b>51.33</b> | 121.52     | 8.536        |
| A8CB-N-H   | <b>20.66</b> | 129.54     | 8.479        |              |            |              |

|              | HNCA-        | CB         |              | CACB-        | (CO)NH     |              |
|--------------|--------------|------------|--------------|--------------|------------|--------------|
| Assignment   | C, ppm       | N, ppm     | H, ppm       | C, ppm       | N, ppm     | H, ppm       |
| A8CB-Q9N-H   | <b>20.64</b> | 121.5      | 8.534        | <b>20.71</b> | 121.43     | 8.535        |
| Q9CA-N-H     | <b>56.37</b> | 121.5      | 8.534        |              |            |              |
| Q9CA-T10N-H  | <b>56.35</b> | 127.10     | 8.874        | <b>56.39</b> | 127.07     | 8.876        |
| Q9CB-N-H     | <b>29.65</b> | 121.49     | 8.533        |              |            |              |
| Q9CB-N-H     | <b>29.37</b> | 121.53     | 8.533        |              |            |              |
| Q9CB-T10-N-H | <b>29.49</b> | 127.06     | 8.874        | <b>29.53</b> | 127.05     | 8.876        |
| T10CA-N-H    | <b>64.30</b> | 127.14     | 8.874        |              |            |              |
| T10CA-G11N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | <i>peak</i>  | <i>not</i> | <i>found</i> |
| T10CB-N-H    | <b>68.65</b> | 127.11     | 8.874        |              |            |              |
| T10CB-N-H    | <b>68.93</b> | 127.12     | 8.874        |              |            |              |
| T10CB-G11N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | <i>peak</i>  | <i>not</i> | <i>found</i> |
| G11CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> |              |            |              |
| G11CA-F12N-H | <b>46.08</b> | 118.83     | 7.015        | <b>46.12</b> | 118.83     | 7.017        |
| F12CA-N-H    | <b>57.62</b> | 118.85     | 7.015        |              |            |              |
| F12CA-N13N-H | <b>57.60</b> | 128.12     | 8.756        | <b>57.6</b>  | 128.1      | 8.757        |
| F12CB-N-H    | <b>39.94</b> | 118.85     | 7.015        |              |            |              |
| F12CB-N13N-H | <b>39.95</b> | 128.11     | 8.754        | <b>39.94</b> | 128.11     | 8.757        |
| N13CA-N-H    | <b>51.31</b> | 128.13     | 8.754        |              |            |              |
| N13CA-K14N-H | <b>51.27</b> | 125.41     | 7.987        | <b>51.29</b> | 125.39     | 7.99         |
| N13CB-N-H    | <b>37.36</b> | 128.16     | 8.755        |              |            |              |
| N13CB-K14N-H | <b>37.3</b>  | 125.34     | 7.988        | <b>37.32</b> | 125.38     | 7.99         |
| K14CA-N-H    | <b>58.74</b> | 125.41     | 7.987        |              |            |              |
| K14CA-D15N-H | <b>58.74</b> | 120.18     | 8.022        | <b>58.74</b> | 120.18     | 8.022        |
| K14CBN--H    | <b>32.17</b> | 125.38     | 7.988        |              |            |              |
| K14CB-D15N-H | <b>32.15</b> | 120.25     | 8.023        | <b>32.18</b> | 120.2      | 8.022        |
| D15CAN--H    | <b>57.3</b>  | 120.22     | 8.02         |              |            |              |
| D15CA-K16N-H | <b>57.28</b> | 116.71     | 7.067        | <b>57.28</b> | 116.71     | 7.067        |
| D15CB-N-H    | <b>40.42</b> | 120.18     | 8.02         |              |            |              |
| D15CB-K16N-H | <b>40.35</b> | 116.73     | 7.065        | <b>40.4</b>  | 116.72     | 7.068        |
| K16CA-N-H    | <b>57.85</b> | 116.74     | 7.066        |              |            |              |
| K16CA-Y17N-H | <b>57.87</b> | 118.46     | 7.013        | <b>57.87</b> | 118.46     | 7.013        |
| K16CB-N-H    | <b>33.42</b> | 116.74     | 7.066        |              |            |              |

|               | HNCA-  | CB     |        | CACB-  | (CO)NH  |        |
|---------------|--------|--------|--------|--------|---------|--------|
| Assignment    | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm  | H, ppm |
| K16CB-Y17N-H  | 33.43  | 118.47 | 7.013  | 33.45  | 118.45  | 7.013  |
| Y17CA-N-H     | 62.30  | 118.47 | 7.013  |        |         |        |
| Y17CA-F18N-H  | 62.30  | 118.41 | 8.421  | 62.31  | 118.39  | 8.424  |
| Y17CB-N-h     | 41.12  | 118.46 | 7.012  |        |         |        |
| Y17CB-F18N-H  | 41.11  | 118.33 | 8.422  | 41.12  | 118.41  | 8.424  |
| F18CA-N-H     | 56.38  | 118.42 | 8.421  |        |         |        |
| F18CA-N19N-H  | 56.41  | 118.71 | 7.856  | 56.41  | 118.64  | 7.858  |
| F18CB-N-H     | 36.74  | 118.42 | 8.421  |        |         |        |
| F18CB-N19N-H  | 36.74  | 118.65 | 7.857  | 36.75  | 118.64  | 7.858  |
| N19CA-N-H     | 52.48  | 118.65 | 7.855  |        |         |        |
| N19CA-G20-N-H | 52.49  | 110.38 | 9.265  | 52.50  | 110.38  | 9.263  |
| N19CB-N-H     | 38.49  | 118.64 | 7.856  |        |         |        |
| N19CB-G20-N-H | 38.47  | 110.39 | 9.261  | 38.49  | 110.38  | 9.264  |
| G20N-CA-H     | 45.41  | 110.42 | 9.262  |        |         |        |
| G20CA-D21N-H  | 45.4   | 118.55 | 7.645  | 45.43  | 118.63  | 7.648  |
| D21CA-N-H     | 51.56  | 118.68 | 7.645  |        |         |        |
| D21CA-V22N-H  | 51.53  | 119.09 | 8.217  | 51.57  | 119.14  | 8.219  |
| D21CB-N-H     | 42.51  | 118.65 | 7.645  |        |         |        |
| D21CB-V22N-H  | 42.57  | 119.12 | 8.217  | 42.58  | 119.15  | 8.219  |
| V22CA-N-H     | 63.06  | 119.17 | 8.217  |        |         |        |
| V22CA-W23N-H  | 63.06  | 127.69 | 9.632  | 63.06  | 127.69  | 9.632  |
| V22CB-N-H     | 33.01  | 119.15 | 8.222  |        |         |        |
| V22CB-W23N-H  | 33     | 127.59 | 9.63   | 33.005 | 127.683 | 9.631  |
| W23CA-N-H     | 55.93  | 127.69 | 9.629  |        |         |        |
| W23CA-Y24N-H  | 55.98  | 119.00 | 9.005  | 55.917 | 119.07  | 9.005  |
| W23CB-N-H     | 34.1   | 127.69 | 9.63   |        |         |        |
| W23CB-Y24N-H  | 34.05  | 119.06 | 9.009  | 34.122 | 119.071 | 9.006  |
| Y24CA-N-H     | 57.59  | 119.06 | 9.002  |        |         |        |
| Y24CA-V25N-H  | 57.59  | 120.55 | 8.547  | 57.625 | 120.726 | 8.551  |
| Y24CB-N-H     | 40.04  | 119.05 | 9.005  |        |         |        |
| Y24CB-V25N-H  | 40.03  | 120.61 | 8.552  | 40.047 | 120.682 | 8.555  |
| V25CA-N-H     | 63.66  | 120.77 | 8.55   |        |         |        |

|              | HNCA-  | CB     |        | CACB-  | (CO)NH  |        |
|--------------|--------|--------|--------|--------|---------|--------|
| Assignment   | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm  | H, ppm |
| V25CA-T26N-H | 63.7   | 122.91 | 10.067 | 63.7   | 122.91  | 10.067 |
| V25CB-N-H    | 32.63  | 120.74 | 8.559  |        |         |        |
| V25CB-T26N-H | 32.72  | 122.81 | 10.073 | 32.671 | 122.913 | 10.061 |
| T26CA-N-H    | 64.01  | 122.93 | 10.069 |        |         |        |
| T26CA-D27N-H | 63.99  | 120.54 | 8.597  | 63.99  | 120.54  | 8.597  |
| T26CB-N-H    | 69.01  | 122.94 | 10.072 |        |         |        |
| T26CB-N-H    | 69.24  | 122.88 | 10.072 |        |         |        |
| T26CB-D27N-H | 69.11  | 120.52 | 8.595  | 69.11  | 120.52  | 8.595  |
| D27CA-N-H    | 53.96  | 120.56 | 8.591  |        |         |        |
| D27CA-Y28N-H | 53.96  | 119.38 | 10.306 | 53.97  | 119.32  | 10.31  |
| D27CB-N-H    | 46.7   | 120.57 | 8.592  |        |         |        |
| D27CB-Y28N-H | 46.67  | 119.34 | 10.311 | 46.69  | 119.32  | 10.31  |
| Y28CA-N-H    | 58.2   | 119.33 | 10.308 |        |         |        |
| Y28CA-L29N-H | 58.2   | 123.41 | 9.235  | 58.21  | 123.45  | 9.232  |
| Y28CB-N-H    | 43.20  | 119.24 | 10.307 |        |         |        |
| Y28CB-L29N-H | 43.18  | 123.42 | 9.225  | 43.18  | 123.44  | 9.233  |
| L29CA-N-H    | 53.56  | 123.45 | 9.227  |        |         |        |
| L29CA-D30N-H | 53.55  | 127.36 | 8.366  | 53.56  | 127.41  | 8.363  |
| L29CB-N-H    | 43.42  | 123.45 | 9.222  |        |         |        |
| L29CB-D30N-H | 43.41  | 127.34 | 8.36   | 43.41  | 127.40  | 8.363  |
| D30CA-N-H    | 51.18  | 127.38 | 8.361  |        |         |        |
| D30CA-L31N-H | 51.17  | 123.62 | 6.96   | 51.21  | 123.69  | 6.964  |
| D30CB-N-H    | 40.86  | 127.38 | 8.363  |        |         |        |
| D30CB-L31N-H | 40.82  | 123.59 | 6.962  | 40.87  | 123.71  | 6.966  |
| L31CA-N-H    | 55.29  | 123.63 | 6.968  |        |         |        |
| L31CA-E32N-H | 55.28  | 119.66 | 7.206  | 55.34  | 119.78  | 7.21   |
| L31CB-N-H    | 40.89  | 123.63 | 6.962  |        |         |        |
| L31CB-E32N-H | 40.83  | 119.76 | 7.207  | 40.89  | 119.78  | 7.212  |
| E32CA-N-H    | 52.89  | 119.79 | 7.21   |        |         |        |
| E32CB-N-H    | 29.02  | 119.78 | 7.209  |        |         |        |
| E32CB-N-H    | 29.31  | 119.79 | 7.209  |        |         |        |
| P33CA-D34N-H | 62.47  | 120.80 | 8.166  | 62.48  | 120.77  | 8.167  |

|              | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|--------------|--------|--------|--------|--------|--------|--------|
| Assignment   | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| P33CB-D34N-H | 32.11  | 120.79 | 8.163  | 32.16  | 120.76 | 8.166  |
| D34CA-N-H    | 53.83  | 120.79 | 8.163  |        |        |        |
| D34CA-D35N-H | 53.81  | 120.41 | 8.358  | 53.85  | 120.45 | 8.36   |
| D34CB-N-H    | 42.26  | 120.74 | 8.163  |        |        |        |
| D34CB-D35N-H | 42.23  | 120.45 | 8.358  | 42.27  | 120.43 | 8.36   |
| D35CA-N-H    | 56.88  | 120.44 | 8.358  |        |        |        |
| D35CA-V36N-H | 56.87  | 119.18 | 8.203  | 56.88  | 119.18 | 8.205  |
| D35CB-N-H    | 40.75  | 120.5  | 8.358  |        |        |        |
| D35CB-V36N-H | 40.76  | 119.18 | 8.201  | 40.78  | 119.18 | 8.205  |
| V36CA-N-H    | 59.9   | 119.22 | 8.202  |        |        |        |
| V36CB-N-H    | 32.06  | 119.21 | 8.203  |        |        |        |
| V36CB-N-H    | 32.39  | 119.21 | 8.204  |        |        |        |
| P37CA-K38N-H | 63.85  | 124.29 | 9.905  | 63.89  | 124.29 | 9.908  |
| P37CB-K38N-H | 33.03  | 124.18 | 9.902  | 33.06  | 124.27 | 9.909  |
| K38N-CA-H    | 57.27  | 124.46 | 9.9    |        |        |        |
| K38CA-R39N-H | 57.21  | 127.48 | 9.78   | 57.21  | 127.48 | 9.78   |
| K38N-CB-H    | 35.29  | 124.46 | 9.905  |        |        |        |
| K38CB-R39N-H | 35.28  | 127.49 | 9.798  | 35.28  | 127.49 | 9.798  |
| R39CA-N-H    | 55.91  | 127.52 | 9.783  |        |        |        |
| R39CA-Y40N-H | peak   | not    | found  | peak   | not    | found  |
| R39CB-N-H    | 28.98  | 127.42 | 9.798  |        |        |        |
| R39CB-Y40N-H | peak   | not    | found  | peak   | not    | found  |
| Y40CA-C41N-H | peak   | not    | found  | peak   | not    | found  |
| Y40CB-C41N-H | peak   | not    | found  | peak   | not    | found  |
| C41CA-A42N-H | peak   | not    | found  | peak   | not    | found  |
| C41CB-A42N-H | peak   | not    | found  | peak   | not    | found  |
| A42CA-A43N-H | peak   | not    | found  | peak   | not    | found  |
| A42CB-A43N-H | peak   | not    | found  | peak   | not    | found  |
| A43CA-N-H    | peak   | not    | found  |        |        |        |
| A43CA-L44N-H | 49.78  | 116.14 | 8.875  | 49.77  | 116.18 | 8.881  |
| A43CB-L44N-H | 22.89  | 116.11 | 8.874  | 22.89  | 116.18 | 8.879  |
| L44CA-N-H    | 53.99  | 116.23 | 8.874  |        |        |        |

|              | HNCA-  | CB      |        | CACB-  | (CO)NH  |        |
|--------------|--------|---------|--------|--------|---------|--------|
| Assignment   | C, ppm | N, ppm  | H, ppm | C, ppm | N, ppm  | H, ppm |
| L44CA-A45N-H | 53.97  | 121.583 | 8.997  | 53.97  | 121.568 | 8.999  |
| L44CB-N-H    | 46.83  | 116.21  | 8.878  |        |         |        |
| L44CB-A45N-H | 46.84  | 121.65  | 8.997  | 46.79  | 121.57  | 8.999  |
| A45CA-N-H    | 52.00  | 121.51  | 8.997  |        |         |        |
| A45CA-A46N-H | 52.03  | 125.81  | 8.822  | 52.03  | 125.81  | 8.822  |
| A45CB-N-H    | 21.98  | 121.57  | 8.997  |        |         |        |
| A45CB-A46N-H | 21.99  | 125.84  | 8.819  | 22.01  | 125.81  | 8.82   |
| A46CA-N-H    | 51.45  | 125.85  | 8.819  |        |         |        |
| A46CA-G47N-H | 51.49  | 108.01  | 9.218  | 51.48  | 107.97  | 9.218  |
| A46CB-N-H    | 23.56  | 125.87  | 8.818  |        |         |        |
| A46CB-G47N-H | 23.55  | 107.97  | 9.216  | 23.57  | 107.97  | 9.218  |
| G47CA-N-H    | 45.72  | 107.96  | 9.217  |        |         |        |
| G47CA-T48N-H | 45.72  | 113.20  | 8.594  | 45.73  | 113.22  | 8.596  |
| T48CA-N-H    | 61.44  | 113.25  | 8.594  |        |         |        |
| T48CA-A49N-H | 61.45  | 128.48  | 8.987  | 61.42  | 128.43  | 8.989  |
| T48CB-N-H    | 69.83  | 113.27  | 8.594  |        |         |        |
| T48CB-N-H    | 69.63  | 113.26  | 8.594  |        |         |        |
| T48CB-A49N-H | 69.69  | 128.45  | 8.986  | 69.72  | 128.42  | 8.989  |
| A49CA-N-H    | 53.18  | 128.47  | 8.986  |        |         |        |
| A49CA-S50N-H | peak   | not     | found  | peak   | Not     | found  |
| A49CB-N-H    | 20.57  | 128.46  | 8.986  |        |         |        |
| A49CB-S50N-H | peak   | not     | found  | peak   | Not     | found  |
| S50CA-G51N-H | 59.05  | 106.84  | 8.497  | 59.12  | 106.74  | 8.502  |
| S50CB-G51N-H | 62.72  | 106.66  | 8.498  | 62.7   | 106.74  | 8.501  |
| G51CA-N-H    | 45.1   | 106.72  | 8.501  |        |         |        |
| G51CA-K52N-H | 45.07  | 120.38  | 7.88   | 45.12  | 120.39  | 7.882  |
| K52CA-N-H    | 54.4   | 120.41  | 7.88   |        |         |        |
| K52CA-L53N-H | 54.39  | 123.38  | 8.611  | 54.42  | 123.37  | 8.614  |
| K52CB-N-H    | 35.46  | 120.5   | 7.88   |        |         |        |
| K52CB-L53N-H | 35.45  | 123.36  | 8.612  | 35.45  | 123.37  | 8.614  |
| L53CA-N-H    | 55.38  | 123.36  | 8.611  |        |         |        |
| L53CA-K54N-H | 55.39  | 126.56  | 8.957  | 55.38  | 126.58  | 8.959  |

|              | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|--------------|--------|--------|--------|--------|--------|--------|
| Assignment   | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| L53CB-N-H    | 42.51  | 123.41 | 8.612  |        |        |        |
| L53CB-K54N-H | 42.50  | 126.53 | 8.958  | 42.532 | 126.60 | 8.959  |
| K54CA-N-H    | 54.55  | 126.56 | 8.957  |        |        |        |
| K54CA-E55N-H | 54.51  | 118.73 | 8.937  | 54.56  | 118.78 | 8.939  |
| K54CB-N-H    | 37.75  | 126.57 | 8.957  |        |        |        |
| K54CB-E55N-H | 37.77  | 118.72 | 8.936  | 37.76  | 118.76 | 8.939  |
| E55CA-N-H    | 56.41  | 118.80 | 8.937  |        |        |        |
| E55CA-A56N-H | 56.40  | 133.63 | 9.866  | 56.45  | 133.60 | 9.869  |
| E55CB-N-H    | 36.38  | 118.80 | 8.935  |        |        |        |
| E55CB-A56N-H | 36.45  | 133.64 | 9.865  | 36.39  | 133.62 | 9.868  |
| A56CA-N-H    | 49.98  | 133.62 | 9.863  |        |        |        |
| A56CA-L57N-H | 50.01  | 121.53 | 8.511  | 50.04  | 121.67 | 8.508  |
| A56CB-N-H    | 22.80  | 133.63 | 9.866  |        |        |        |
| A56CB-L57N-H | 22.76  | 121.61 | 8.511  | 22.81  | 121.65 | 8.511  |
| L57CB-N-H    | 46.77  | 121.51 | 8.511  |        |        |        |
| L57CA-Y58N-H | peak   | not    | found  | peak   | not    | found  |
| L57CB-Y58N-H | peak   | not    | found  | peak   | not    | found  |
| Y58CA-H59N-H | peak   | not    | found  | peak   | not    | found  |
| Y58CB-H59N-H | peak   | not    | found  | peak   | not    | found  |
| H59CA-Y60N-H | peak   | not    | found  | peak   | not    | found  |
| H59CB-Y60N-H | peak   | not    | found  | peak   | not    | found  |
| Y60CA-D61N-H | peak   | not    | found  | peak   | not    | found  |
| Y60CB-D61N-H | peak   | not    | found  | peak   | not    | found  |
| D61CA-P62N-H | peak   | not    | found  | peak   | not    | found  |
| D61CB-P62N-H | peak   | not    | found  | peak   | not    | found  |
| P62CA-K63N-H | 63.67  | 116.68 | 7.986  | 63.69  | 116.60 | 7.987  |
| P62CB-K63N-H | 32.95  | 116.58 | 7.987  | 32.95  | 116.60 | 7.987  |
| K63CA-N-H    | 58.72  | 116.59 | 7.985  |        |        |        |
| K63CA-T64N-H | 58.73  | 105.19 | 6.6    | 58.75  | 105.18 | 6.603  |
| K63CB-N-H    | 32.47  | 116.58 | 7.985  |        |        |        |
| K63CB-T64N-H | 32.46  | 105.21 | 6.602  | 32.48  | 105.18 | 6.603  |
| T64CA-N-H    | 61.36  | 105.21 | 6.601  |        |        |        |

|              | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|--------------|--------|--------|--------|--------|--------|--------|
| Assignment   | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| T64CA-Q65N-H | 61.36  | 115.13 | 8.011  | 61.31  | 115.16 | 8.012  |
| T64CB-N-H    | 71.03  | 105.19 | 6.601  |        |        |        |
| T64CB-Q65N-H | 71.05  | 115.15 | 8.009  | 71.08  | 115.16 | 8.013  |
| Q65CA-N-H    | 57.83  | 115.18 | 8.01   |        |        |        |
| Q65CA-D66N-H | 57.80  | 119.62 | 7.34   | 57.86  | 119.67 | 7.343  |
| Q65CB-N-H    | 25.40  | 115.19 | 8.01   |        |        |        |
| Q65CB-D66N-H | 25.39  | 119.66 | 7.341  | 25.45  | 119.68 | 7.342  |
| D66CA-N-H    | 55.20  | 119.64 | 7.342  |        |        |        |
| D66CA-T67N-H | 55.23  | 114.10 | 7.187  | 55.27  | 114.03 | 7.189  |
| D66CB-N-H    | 41.77  | 119.72 | 7.34   |        |        |        |
| D66CB-T67N-H | 41.78  | 114.12 | 7.184  | 41.75  | 114.03 | 7.188  |
| T67CA-N-H    | 58.48  | 114.06 | 7.186  |        |        |        |
| T67CA-F68N-H | peak   | not    | found  | 58.52  | 114.62 | 5.059  |
| T67CB-N-H    | 71.67  | 114.03 | 7.185  |        |        |        |
| T67CB-N-H    | 71.83  | 114.03 | 7.186  |        |        |        |
| T67CB-F68N-H | peak   | not    | found  | 71.74  | 114.64 | 5.05   |
| F68CA-Y69N-H | 54.57  | 117.77 | 6.816  | 54.57  | 117.77 | 6.816  |
| F68CB-Y69N-H | 39.35  | 117.87 | 6.813  | 39.4   | 117.78 | 6.82   |
| Y69CA-N-H    | 54.67  | 117.80 | 6.814  |        |        |        |
| Y69CA-D70N-H | 54.67  | 115.57 | 7.429  | 54.69  | 115.41 | 7.428  |
| Y69CB-N-H    | 41.06  | 117.85 | 6.807  |        |        |        |
| Y69CB-D70N-H | 41.04  | 115.29 | 7.417  | 41.07  | 115.45 | 7.415  |
| D70CA-N-H    | 52.07  | 115.42 | 7.423  |        |        |        |
| D70CA-V71N-H | 52.10  | 118.01 | 9.413  | 52.14  | 118.11 | 9.415  |
| D70CB-N-H    | 43.89  | 115.51 | 7.427  |        |        |        |
| D70CB-V71N-H | 43.98  | 118.07 | 9.412  | 43.99  | 118.09 | 9.415  |
| V71CA-N-H    | 61.69  | 118.18 | 9.412  |        |        |        |
| V71CA-S72N-H | 61.68  | 122.18 | 9.192  | 61.68  | 122.19 | 9.195  |
| V71CB-N-H    | 35.83  | 118.20 | 9.411  |        |        |        |
| V71CB-S72N-H | 35.92  | 122.09 | 9.196  | 35.91  | 122.19 | 9.194  |
| S72CA-N-H    | 58.62  | 122.20 | 9.192  |        |        |        |
| S72CA-E73N-H | 58.61  | 124.21 | 9.057  | 58.61  | 124.24 | 9.06   |

|              | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|--------------|--------|--------|--------|--------|--------|--------|
| Assignment   | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| S72CB-N-H    | 67.62  | 122.16 | 9.191  |        |        |        |
| S72CB-E73N-H | 67.61  | 124.23 | 9.058  | 67.62  | 124.25 | 9.06   |
| E73CA-N-H    | 56.25  | 124.27 | 9.06   |        |        |        |
| E73CA-L74N-H | 56.30  | 124.38 | 8.612  | 56.30  | 124.38 | 8.612  |
| E73CB-N-H    | 29.81  | 124.31 | 9.058  |        |        |        |
| E73CB-N-H    | 30.09  | 124.31 | 9.058  |        |        |        |
| E73CB-L74N-H | 29.94  | 124.41 | 8.612  | 29.984 | 124.38 | 8.613  |
| L74CA-N-H    | 54.87  | 124.39 | 8.61   |        |        |        |
| L74CA-Q75N-H | 54.87  | 122.04 | 9.434  | 54.91  | 122.02 | 9.436  |
| L74CB-N-H    | 43.11  | 124.40 | 8.61   |        |        |        |
| L74CB-Q75N-H | 43.14  | 122.04 | 9.431  | 43.13  | 122.03 | 9.437  |
| Q75CA-N-H    | 54.11  | 122.01 | 9.434  |        |        |        |
| Q75CA-V76N-H | 54.10  | 126.08 | 8.882  | 54.12  | 126.16 | 8.886  |
| Q75CB-N-H    | 30.49  | 122.02 | 9.435  |        |        |        |
| Q75CB-N-H    | 30.72  | 122.01 | 9.433  |        |        |        |
| Q75CB-V76N-H | 30.65  | 126.06 | 8.883  | 30.63  | 126.17 | 8.886  |
| V76CA-N-H    | 62.89  | 126.11 | 8.883  |        |        |        |
| V76CA-E77N-H | 62.89  | 129.98 | 8.689  | 62.88  | 130.01 | 8.692  |
| V76CB-N-H    | 32.35  | 126.07 | 8.886  |        |        |        |
| V76CB-N-H    | 32.61  | 126.12 | 8.882  |        |        |        |
| V76CB-E77N-H | 32.44  | 130.   | 8.686  | 32.47  | 130.   | 8.692  |
| E77CA-N-H    | 57.62  | 129.96 | 8.688  |        |        |        |
| E77CA-S78N-H | 57.63  | 111.55 | 8.053  | 57.63  | 111.55 | 8.053  |
| E77CB-N-H    | 29.74  | 129.99 | 8.691  |        |        |        |
| E77CB-S78N-H | 29.75  | 111.65 | 8.052  | 29.87  | 111.55 | 8.053  |
| S78CA-N-H    | 57.07  | 111.60 | 8.051  |        |        |        |
| S78CA-L79N-H | peak   | not    | found  | peak   | not    | found  |
| S78CB-N-H    | 62.94  | 111.60 | 8.052  |        |        |        |
| S78CB-L79N-H | peak   | not    | found  | peak   | not    | found  |
| L79CA-N-H    |        |        |        |        |        |        |
| L79CA-G80N-H | 58.04  | 114.58 | 8.377  | 58.042 | 114.58 | 8.377  |
| L79CB-N-H    |        |        |        |        |        |        |
| L79CB-G80N-H | 40.99  | 114.58 | 8.377  | 40.99  | 114.58 | 8.377  |

|              | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|--------------|--------|--------|--------|--------|--------|--------|
| Assignment   | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
|              |        |        |        |        |        |        |
| G80CA-N-H    | 46.29  | 114.61 | 8.376  |        |        |        |
| G80CA-K81N-H | 46.28  | 121.83 | 7.881  | 46.31  | 121.84 | 7.883  |
| K81CA-N-H    | 56.15  | 121.83 | 7.881  |        |        |        |
| K81CA-Y82H   | 56.16  | 120.95 | 8.286  | 56.14  | 121.08 | 8.29   |
| K81CB-N-H    | 35.44  | 121.83 | 7.88   |        |        |        |
| K81CB-Y82N-H | 35.44  | 120.93 | 8.285  | 35.45  | 121.05 | 8.29   |
| Y82CA-N-H    | 56.93  | 121.12 | 8.286  |        |        |        |
| Y82CA-T83N-H | 56.93  | 117.10 | 9.087  | 56.95  | 117.09 | 9.087  |
| Y82CB-N-H    | 44.08  | 121.14 | 8.286  |        |        |        |
| Y82CB-T83N-H | 44.03  | 117.13 | 9.086  | 44.06  | 117.09 | 9.088  |
| T83CA-N-H    | 62.69  | 117.08 | 9.085  |        |        |        |
| T83CA-A84N-H | 62.68  | 132.39 | 10.179 | 62.66  | 132.38 | 10.179 |
| T83CB-N-H    | 70.93  | 117.11 | 9.085  |        |        |        |
| T83CB-N-H    | 70.63  | 117.10 | 9.085  |        |        |        |
| T83CB-A84N-H | 70.79  | 132.39 | 10.176 | 70.79  | 132.39 | 10.179 |
| A84CA-N-H    | 51.99  | 132.47 | 10.176 |        |        |        |
| A84CA-N85N-H | 52.06  | 124.01 | 8.43   | 52.02  | 123.95 | 8.43   |
| A84CB-N-H    | 21.51  | 132.45 | 10.175 |        |        |        |
| A84CB-N85N-H | 21.53  | 123.91 | 8.428  | 21.51  | 123.94 | 8.43   |
| N85CA-N-H    | 53.81  | 123.95 | 8.428  |        |        |        |
| N85CA-F86N-H | 53.89  | 119.99 | 7.368  | 53.82  | 120.11 | 7.369  |
| N85CB-N-H    | 39.02  | 123.94 | 8.432  |        |        |        |
| N85CB-F86N-H | 39.10  | 120.06 | 7.364  | 39.05  | 120.09 | 7.368  |
| F86CA-N-H    | 57.05  | 120.08 | 7.366  |        |        |        |
| F86CA-K87N-H | 57.06  | 120.57 | 9.283  | 57.07  | 120.60 | 9.288  |
| F86CB-N-H    | 42.79  | 120.11 | 7.366  |        |        |        |
| F86CB-K87N-H | 42.84  | 120.43 | 9.288  | 42.78  | 120.59 | 9.288  |
| K87CA-N-H    | 54.74  | 120.68 | 9.287  |        |        |        |
| K87CA-K88N-H | 54.76  | 127.32 | 9.179  | 54.77  | 127.31 | 9.182  |
| K87CB-N-H    | 35.51  | 120.64 | 9.287  |        |        |        |
| K87CB-K88N-H | 35.55  | 127.26 | 9.18   | 35.57  | 127.30 | 9.182  |

|              | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|--------------|--------|--------|--------|--------|--------|--------|
| Assignment   | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| K88CA-N-H    | 56.55  | 127.26 | 9.181  |        |        |        |
| K88CA-V89N-H | 56.6   | 120.96 | 8.42   | 56.59  | 121.04 | 8.424  |
| K88CB-N-H    | 34.42  | 127.26 | 9.18   |        |        |        |
| K88CB-V89N-H | 34.44  | 121.01 | 8.421  | 34.45  | 121.00 | 8.425  |
| V89CA-N-H    | 58.27  | 120.90 | 8.422  |        |        |        |
| V89CA-D90N-H | 58.26  | 118.48 | 7.949  | 58.30  | 118.62 | 7.952  |
| V89CB-N-H    | 36.95  | 120.91 | 8.422  |        |        |        |
| V89CB-D90N-H | 36.94  | 118.56 | 7.95   | 36.90  | 118.63 | 7.952  |
| D90CA-N-H    | 51.84  | 118.64 | 7.949  |        |        |        |
| D90CA-K91N-H | 51.86  | 114.27 | 7.79   | 51.86  | 114.23 | 7.791  |
| D90CB-N-H    | 41.50  | 118.64 | 7.949  |        |        |        |
| D90CB-K91N-H | 41.45  | 114.34 | 7.788  | 41.52  | 114.22 | 7.791  |
| K91CA-N-H    | 57.97  | 114.29 | 7.789  |        |        |        |
| K91CA-N92N-H | 57.95  | 114.32 | 7.223  | 58.00  | 114.30 | 7.227  |
| K91CB-N-H    | 30.72  | 114.27 | 7.788  |        |        |        |
| K91CB-N92N-H | 30.69  | 114.34 | 7.224  | 30.75  | 114.31 | 7.227  |
| N92CA-N-H    | 52.62  | 114.34 | 7.225  |        |        |        |
| N92CA-G93N-H | 52.62  | 108.38 | 7.936  | 52.66  | 108.40 | 7.937  |
| N92CB-N-H    | 39.94  | 114.35 | 7.225  |        |        |        |
| N92CB-G93N-H | 39.92  | 108.44 | 7.933  | 39.94  | 108.39 | 7.937  |
| G93CA-N-H    | 45.07  | 108.42 | 7.934  |        |        |        |
| G93CA-N94N-H | 45.05  | 120.25 | 8.279  | 45.08  | 120.34 | 8.282  |
| N94CA-N-H    | 53.64  | 120.35 | 8.279  |        |        |        |
| N94CA-V95N-H | 53.65  | 123.44 | 8.762  | 53.63  | 123.43 | 8.764  |
| N94CB-N-H    | 37.99  | 120.34 | 8.28   |        |        |        |
| N94CB-V95N-H | 37.96  | 123.39 | 8.762  | 37.99  | 123.42 | 8.764  |
| V95CA-N-H    | 65.06  | 123.39 | 8.762  |        |        |        |
| V95CA-K96N-H | 65.06  | 128.09 | 9.49   | 65.06  | 128.12 | 9.492  |
| V95CB-N-H    | 31.98  | 123.40 | 8.762  |        |        |        |
| V95CB-K96N-H | 32.09  | 128.14 | 9.488  | 32.10  | 128.12 | 9.492  |
| K96CA-N-H    | 56.30  | 128.16 | 9.49   |        |        |        |
| K96CA-V97N-H | 56.25  | 119.62 | 7.99   | 56.29  | 119.62 | 7.991  |

|                | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|----------------|--------|--------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| K96CB-N-H      | 32.95  | 128.15 | 9.487  |        |        |        |
| K96CB-V97N-H   | 32.95  | 119.62 | 7.994  | 32.95  | 119.62 | 7.994  |
| V97CA-N-H      | 62.95  | 119.63 | 7.997  |        |        |        |
| V97CA-A98N-H   | 62.96  | 128.24 | 8.597  | 62.94  | 128.22 | 8.599  |
| V97CB-N-H      | 34.83  | 119.67 | 7.997  |        |        |        |
| V97CB-A98N-H   | 34.83  | 128.26 | 8.597  | 34.90  | 128.23 | 8.599  |
| A98CA-N-H      | 52.41  | 128.28 | 8.597  |        |        |        |
| A98CA-V99N-H   | 52.40  | 122.19 | 8.548  | 52.45  | 122.17 | 8.549  |
| A98CB-N-H      | 19.99  | 128.32 | 8.598  |        |        |        |
| A98CB-V99N-H   | 19.98  | 122.13 | 8.547  | 19.99  | 122.25 | 8.549  |
| V99CA-N-H      | 64.92  | 122.19 | 8.547  |        |        |        |
| V99CA-T100N-H  | 64.93  | 126.07 | 9.973  | 64.91  | 126.11 | 9.979  |
| V99CB-N-H      | 31.77  | 122.16 | 8.546  |        |        |        |
| V99CB-T100N-H  | 31.73  | 126.04 | 9.977  | 31.79  | 126.11 | 9.978  |
| T100CA-N-H     | 61.80  | 126.10 | 9.975  |        |        |        |
| T100CA-A101N-H | 61.83  | 131.29 | 8.896  | 61.80  | 131.27 | 8.902  |
| T100CB-N-H     | 72.64  | 126.07 | 9.974  |        |        |        |
| T100CB-A101N-H | 72.67  | 131.26 | 8.903  | 72.67  | 131.26 | 8.903  |
| A101CA-N-H     | 54.20  | 131.32 | 8.902  |        |        |        |
| A101CA-G102N-H | 54.21  | 110.28 | 9.152  | 54.25  | 110.23 | 9.153  |
| A101CB-N-H     | 18.04  | 131.23 | 8.898  |        |        |        |
| A101CB-G102N-H | 18.08  | 110.26 | 9.16   | 18.06  | 110.24 | 9.151  |
| G102N-CA-H     | 45.29  | 110.36 | 9.15   |        |        |        |
| G102CA-N103N-H | 45.24  | 121.11 | 8.202  | 45.28  | 121.06 | 8.203  |
| N103CA-N-H     | 51.42  | 121.04 | 8.2    |        |        |        |
| N103CA-Y104N-H | 51.42  | 121.16 | 9.214  | 51.41  | 121.19 | 9.213  |
| N103CB-N-H     | 37.89  | 121.01 | 8.2    |        |        |        |
| N103CB-Y104N-H | 37.85  | 121.16 | 9.214  | 37.91  | 121.18 | 9.213  |
| Y104CA-N-H     | 57.83  | 121.22 | 9.21   |        |        |        |
| Y104CA-Y105N-H | 57.84  | 116.21 | 10.223 | 57.83  | 116.26 | 10.224 |
| Y104CB-N-H     | 39.75  | 121.21 | 9.209  |        |        |        |
| Y104CB-Y105N-H | 39.77  | 116.24 | 10.218 | 39.77  | 116.25 | 10.227 |

|                | HNCA-  | CB      |        | CACB-  | (CO)NH |        |
|----------------|--------|---------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm  | H, ppm | C, ppm | N, ppm | H, ppm |
| Y105CA-N-H     | 56.24  | 116.19  | 10.223 |        |        |        |
| Y105CA-T106N-H | 56.28  | 113.57  | 8.475  | 56.25  | 113.60 | 8.484  |
| Y105CB-N-H     | 43.57  | 116.18  | 10.217 |        |        |        |
| Y105CB-T106N-H | 43.55  | 113.67  | 8.485  | 43.56  | 113.67 | 8.48   |
| T106CA-N-H     | 59.62  | 113.61  | 8.474  |        |        |        |
| T106CA-F107N-H | 59.63  | 119.77  | 9.471  | 59.63  | 119.69 | 9.471  |
| T106CB-N-H     | 70.98  | 113.60  | 8.484  |        |        |        |
| T106CB-N-H     | 71.15  | 113.62  | 8.477  |        |        |        |
| T106CB-F107N-H | 71.10  | 119.73  | 9.468  | 71.09  | 119.70 | 9.471  |
| F107CA-N-H     | 56.82  | 119.63  | 9.468  |        |        |        |
| F107CA-T108N-H | 56.85  | 117.73  | 9.34   | 56.89  | 117.61 | 9.341  |
| F107CB-N-H     | 44.11  | 119.70  | 9.47   |        |        |        |
| F107CB-T108N-H | 44.11  | 117.68  | 9.335  | 44.17  | 117.61 | 9.342  |
| T108CA-N-H     | 61.06  | 117.56  | 9.339  |        |        |        |
| T108CA-V109N-H | 61.03  | 127.86  | 9.343  | 61.04  | 127.9  | 9.345  |
| T108CB-N-H     | 72.29  | 117.59  | 9.34   |        |        |        |
| T108CB-N-H     | 71.92  | 117.60  | 9.339  |        |        |        |
| T108CB-V109N-H | 72.07  | 127.85  | 9.341  | 72.12  | 127.90 | 9.344  |
| V109CA-N-H     | 63.10  | 127.92  | 9.344  |        |        |        |
| V109CA-M110N-H | 63.12  | 129.62  | 8.783  | 63.09  | 129.56 | 8.781  |
| V109CB-N-H     | 29.615 | 127.9   | 9.343  |        |        |        |
| V109CB-N-H     | 30.007 | 127.947 | 9.342  |        |        |        |
| V109CB-M110N-H | 29.813 | 129.65  | 8.778  | 29.80  | 129.51 | 8.783  |
| M110CA-N-H     | 58.138 | 129.563 | 8.78   |        |        |        |
| M110CA-Y111N-H | 58.144 | 117.67  | 8.204  | 58.15  | 117.60 | 8.209  |
| M110CB-N-H     | 35.149 | 129.561 | 8.778  |        |        |        |
| M110CB-Y111N-H | 35.198 | 117.621 | 8.205  | 35.20  | 117.67 | 8.207  |
| Y111CA-N-H     | 59.4   | 117.598 | 8.207  |        |        |        |
| Y111CA-A112N-H | 59.42  | 125.898 | 6.658  | 59.43  | 125.88 | 6.66   |
| Y111CB-N-H     | 42.371 | 117.649 | 8.205  |        |        |        |
| Y111CB-A112N-H | 42.418 | 125.941 | 6.656  | 42.40  | 125.88 | 6.66   |
| A112CA-N-H     | 52.938 | 125.889 | 6.658  |        |        |        |

|                | HNCA-  | CB      |        | CACB-  | (CO)NH |        |
|----------------|--------|---------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm  | H, ppm | C, ppm | N, ppm | H, ppm |
| A112CA-D113N-H | 52.95  | 121.49  | 9.5    | 52.95  | 121.49 | 9.5    |
| A112CB-N-H     | 22.32  | 125.9   | 6.658  |        |        |        |
| A112CB-D113N-H | 22.31  | 121.48  | 9.498  | 22.35  | 121.49 | 9.501  |
| D113CA-N-H     | 53.17  | 121.48  | 9.499  |        |        |        |
| D113CA-D114N-H | 53.17  | 114.79  | 8.356  | 53.17  | 114.83 | 8.358  |
| D113CB-N-H     | 40.80  | 121.50  | 9.498  |        |        |        |
| D113CB-D114N-H | 40.88  | 114.79  | 8.361  | 40.88  | 114.79 | 8.361  |
| D114N-CA-H     | 58.12  | 114.76  | 8.36   |        |        |        |
| D114CA-S115N-H | 58.13  | 110.88  | 8.699  | Peak   | Not    | found  |
| D114N-CB-H     | 40.95  | 114.78  | 8.358  |        |        |        |
| D114CB-S115N-H | 40.96  | 110.89  | 8.702  | Peak   | Not    | found  |
| S115CA-N-H     | 59.48  | 110.89  | 8.702  |        |        |        |
| S115CA-S116N-H | 59.45  | 118.01  | 8.884  | 40.96  | 110.91 | 8.704  |
| S115CB-N-H     | 66.70  | 110.89  | 8.702  |        |        |        |
| S115CB-S116N-H | 66.68  | 118.03  | 8.883  | 66.69  | 117.97 | 8.887  |
| S116CA-N-H     | 58.55  | 117.99  | 8.884  |        |        |        |
| S116CA-A117N-H | 58.55  | 117.61  | 8.585  | 58.55  | 117.64 | 8.586  |
| S116CB-N-H     | 69.33  | 117.99  | 8.884  |        |        |        |
| S116CB-A117N-H | 69.35  | 117.59  | 8.583  | 69.34  | 117.64 | 8.586  |
| A117CA-N-H     | 52.40  | 117.66  | 8.584  |        |        |        |
| A117CA-L118N-H | 52.406 | 121.539 | 9.267  | 52.43  | 121.52 | 9.268  |
| A117CB-N-H     | 22.863 | 117.668 | 8.584  |        |        |        |
| A117CB-L118N-H | 22.851 | 121.514 | 9.266  | 22.90  | 121.52 | 9.269  |
| L118CA-N-H     | 54.385 | 121.504 | 9.266  |        |        |        |
| L118CA-N-H     | 54.385 | 121.504 | 9.266  |        |        |        |
| L118CA-I119N-H | 54.361 | 119.793 | 9.767  | 54.40  | 119.85 | 9.772  |
| L118CB-N-H     | 46.675 | 121.563 | 9.266  |        |        |        |
| L118CB-I119N-H | 46.712 | 119.736 | 9.769  | 46.77  | 119.85 | 9.772  |
| I119CA-N-H     | 59.122 | 119.934 | 9.769  |        |        |        |
| I119CA-H120N-H | 59.086 | 122.314 | 8.831  | 59.12  | 122.36 | 8.836  |
| I119CB-N-H     | 42.83  | 119.916 | 9.77   |        |        |        |
| I119CB-H120N-H | 42.828 | 122.246 | 8.829  | 42.76  | 122.37 | 8.834  |

|                | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|----------------|--------|--------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| H120CA-N-H     | 56.09  | 122.39 | 8.831  |        |        |        |
| H120CA-T121N-H | 56.08  | 116.42 | 6.839  | 56.17  | 116.46 | 6.832  |
| H120CB-N-H     | 34.97  | 122.32 | 8.832  |        |        |        |
| H120CB-T121N-H | 34.95  | 116.43 | 6.833  | 34.95  | 116.43 | 6.833  |
| T121CA-N-H     | 58.71  | 116.51 | 6.828  |        |        |        |
| T121CA-C122N-H | 58.71  | 118.31 | 7.212  | 58.68  | 118.21 | 7.206  |
| T121CB-N-H     | 71.60  | 116.44 | 6.829  |        |        |        |
| T121CB-C122N-H | 71.62  | 118.33 | 7.207  | 71.66  | 118.27 | 7.242  |
| C122CA-N-H     | 53.48  | 118.23 | 7.216  |        |        |        |
| C122CA-L123N-H | 53.49  | 127.01 | 6.935  | 53.45  | 127.00 | 6.939  |
| C122CB-N-H     | 42.74  | 118.22 | 7.216  |        |        |        |
| C122CB-L123N-H | 42.74  | 126.95 | 6.931  | 42.69  | 127.01 | 6.938  |
| L123CA-N-H     | 48.54  | 127.07 | 6.941  |        |        |        |
| L123CA-H124N-H | peak   | Not    | found  | Peak   | Not    | found  |
| L123CB-N-H     | 41.89  | 127.11 | 6.941  |        |        |        |
| L123CB-H124N-H | peak   | Not    | found  | Peak   | Not    | found  |
| H124CA-K125N-H | 54.16  | 120.22 | 7.786  | 54.11  | 120.21 | 7.786  |
| H124CB-K125N-H | 29.94  | 120.19 | 7.781  | 30.02  | 120.24 | 7.785  |
| K125CA-N-H     | 55.45  | 120.26 | 7.782  |        |        |        |
| K125CA-G126N-H | 55.45  | 115.99 | 8.767  | 55.43  | 116.04 | 8.767  |
| K125CB-N-H     | 36.19  | 120.30 | 7.781  |        |        |        |
| K125CB-G126N-H | 36.22  | 115.99 | 8.764  | 36.17  | 116.03 | 8.768  |
| G126CA-N-H     | 47.80  | 116.05 | 8.765  |        |        |        |
| G126CA-N127N-H | Peak   | Not    | found  | Peak   | Not    | found  |
| N127CA-K128N-H | 54.35  | 119.20 | 7.382  | 54.41  | 119.17 | 7.385  |
| N127CB-K128N-H | 38.34  | 119.23 | 7.38   | 38.35  | 119.19 | 7.383  |
| K128CA-N-H     | 55.11  | 119.26 | 7.379  |        |        |        |
| K128CA-D129N-H | 55.10  | 120.96 | 8.162  | 55.12  | 120.94 | 8.164  |
| K128CB-N-H     | 34.50  | 119.24 | 7.381  |        |        |        |
| K128CB-D129N-H | 34.59  | 120.97 | 8.163  | 34.56  | 120.95 | 8.164  |
| D129CA-N-H     | 52.71  | 120.92 | 8.163  |        |        |        |
| D129CA-L130N-H | 52.69  | 122.99 | 6.909  | 52.74  | 123.12 | 6.912  |

|                | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|----------------|--------|--------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| D129CB-N-H     | 40.17  | 120.91 | 8.162  |        |        |        |
| D129CB-L130N-H | 40.20  | 123.07 | 6.907  | 40.16  | 123.11 | 6.912  |
| L130CA-N-H     | 53.47  | 123.17 | 6.913  |        |        |        |
| L130CA-G131N-H |        |        |        | 53.4   | 103.72 | 5.161  |
| L130CB-N-H     | 38.3   | 123.14 | 6.912  |        |        |        |
| L130CB-G131N-H |        |        |        | 38.29  | 103.77 | 5.162  |
| G131CA-N-H     | 42.64  | 103.71 | 5.16   |        |        |        |
| G131CA-D132N-H | 42.61  | 116.41 | 6.51   | 42.64  | 116.47 | 6.517  |
| D132CA-N-H     | 53.22  | 116.51 | 6.513  |        |        |        |
| D132CA-L133N-H | 53.19  | 120.81 | 5.501  | 53.19  | 120.81 | 5.501  |
| D132CB-N-H     | 42.91  | 116.51 | 6.515  |        |        |        |
| D132CB-L133N-H | Peak   | Not    | found  | 42.75  | 120.83 | 5.505  |
| L133CA-N-H     | 52.75  | 120.8  | 5.507  |        |        |        |
| L133CA-Y134N-H | 52.74  | 125.04 | 8.311  | 52.74  | 125.04 | 8.311  |
| L133CB-Y134N-H | Peak   | Not    | found  | Peak   | Not    | found  |
| Y134CA-N-H     | 56.67  | 125.05 | 8.305  |        |        |        |
| Y134CA-A135N-H | 56.66  | 124.00 | 9.973  | 56.68  | 124.11 | 9.969  |
| Y134CB-N-H     | 40.88  | 125.08 | 8.308  |        |        |        |
| Y134CB-A135N-H | 40.85  | 124.04 | 9.963  | 40.91  | 124.10 | 9.969  |
| A135CA-N-H     | 52.11  | 124.01 | 9.964  |        |        |        |
| A135CA-V136N-H | 52.08  | 124.82 | 10.262 | 52.08  | 124.88 | 10.266 |
| A135CB-N-H     | 23.93  | 124.19 | 9.966  |        |        |        |
| A135CB-V136N-H | 23.92  | 124.84 | 10.266 | 23.93  | 124.88 | 10.267 |
| V136CA-N-H     | 62.87  | 124.75 | 10.262 |        |        |        |
| V136CA-L137N-H | 62.91  | 126.22 | 9.932  | 62.91  | 126.23 | 9.936  |
| V136CB-N-H     | 33.16  | 124.91 | 10.259 |        |        |        |
| V136CB-N-H     | 33.00  | 124.86 | 10.265 |        |        |        |
| V136CB-L137N-H | 33.03  | 126.25 | 9.931  | 33.11  | 126.24 | 9.931  |
| V136CB-L137N-H | 33.19  | 126.17 | 9.931  |        |        |        |
| L137CA-N-H     | 52.21  | 126.24 | 9.932  |        |        |        |
| L137CA-N138N-H | 52.24  | 121.43 | 9.935  | 52.26  | 121.38 | 9.938  |
| L137CB-N-H     | 45.94  | 126.20 | 9.931  |        |        |        |

|                | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|----------------|--------|--------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| L137CB-N138N-H | 45.97  | 121.45 | 9.935  | 45.98  | 121.39 | 9.937  |
| N138CA-N-H     | 52.9   | 121.34 | 9.936  |        |        |        |
| N138CA-R139N-H | 52.92  | 124.79 | 8.619  | 52.96  | 124.87 | 8.621  |
| N138CB-N-H     | 44.39  | 121.34 | 9.936  |        |        |        |
| N138CB-R139N-H | 44.39  | 124.75 | 8.619  | 44.42  | 124.84 | 8.621  |
| R139CA-N-H     | 56.06  | 124.74 | 8.617  |        |        |        |
| R139CA-N140N-H | 55.97  | 120.13 | 10.277 | 56.00  | 120.08 | 10.281 |
| R139CB-N-H     | 31.15  | 124.77 | 8.619  |        |        |        |
| R139CB-N140N-H | 31.17  | 120.06 | 10.282 | 31.15  | 120.08 | 10.282 |
| N140CA-N-H     | 51.74  | 120.12 | 10.278 |        |        |        |
| N140CA-K141N-H | 51.75  | 123.53 | 7.627  | 51.75  | 123.53 | 7.627  |
| N140CB-N-H     | 40.58  | 120.10 | 10.278 |        |        |        |
| N140CB-K141N-H | 40.61  | 123.52 | 7.626  | 40.55  | 123.58 | 7.619  |
| K141CA-N-H     | 58.14  | 123.52 | 7.627  |        |        |        |
| K141CA-D142N-H | 58.14  | 117.72 | 7.969  | Peak   | Not    | found  |
| K141CB-N-H     | 30.62  | 123.52 | 7.626  |        |        |        |
| K141CB-D142N-H | 30.62  | 117.72 | 7.969  | 30.59  | 117.72 | 7.964  |
| D142CA-N-H     | 54.40  | 117.72 | 7.966  |        |        |        |
| D142CB-A143N-H | 20.49  | 123.37 | 7.144  | peak   | Not    | found  |
| A143CA-N-H     | 52.62  | 123.38 | 7.143  |        |        |        |
| A143CA-A144N-H | 52.61  | 126.19 | 8.487  | 52.65  | 126.31 | 8.49   |
| A143CB-N-H     | 20.49  | 123.37 | 7.144  |        |        |        |
| A143CB-A144N-H | 20.47  | 126.25 | 8.487  | 20.53  | 126.31 | 8.49   |
| A144CA-N-H     | 51.29  | 126.29 | 8.488  |        |        |        |
| A144CA-A145N-H | 51.28  | 126.82 | 9.277  | 51.29  | 126.83 | 9.28   |
| A144CB-N-H     | 19.53  | 126.25 | 8.486  |        |        |        |
| A144CB-A145N-H | 19.52  | 126.83 | 9.28   | 19.52  | 126.83 | 9.28   |
| A145CA-N-H     | 53.26  | 126.86 | 9.277  |        |        |        |
| A145CA-G146N-H | 53.28  | 110.48 | 8.795  | 53.29  | 110.43 | 8.798  |
| A145CB-N-H     | 19.17  | 126.85 | 9.277  |        |        |        |
| A145CB-G146N-H | 19.15  | 110.51 | 8.797  | 19.19  | 110.43 | 8.798  |
| G146CA-N-H     | 43.66  | 110.47 | 8.796  |        |        |        |

|                | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|----------------|--------|--------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| G146CA-D147N-H | 43.63  | 117.59 | 8.433  | 43.66  | 117.59 | 8.433  |
| D147CA-N-H     | 57.87  | 117.60 | 8.43   | Peak   | Not    | found  |
| D147CB-N-H     | 40.91  | 117.60 | 8.432  |        |        |        |
| D147CB-K148N-H | peak   | Not    | found  | Peak   | Not    | found  |
| K148CA-V149N-H | 59.7   | 120.53 | 7.937  | 59.73  | 120.52 | 7.94   |
| K148CB-V149N-H | 31.55  | 120.53 | 7.94   | 31.55  | 120.53 | 7.94   |
| V149CA-N-H     | 65.53  | 120.54 | 7.938  |        |        |        |
| V149CA-K150N-H | 65.55  | 120.43 | 7.82   | 65.55  | 120.44 | 7.821  |
| V149CB-N-H     | 31.23  | 120.53 | 7.94   |        |        |        |
| V149CB-K150N-H | 31.23  | 120.44 | 7.821  | 31.23  | 120.44 | 7.821  |
| K150CA-N-H     | 61.27  | 120.46 | 7.819  |        |        |        |
| K150CA-S151N-H | 61.35  | 116.95 | 8.228  | 61.27  | 116.88 | 8.23   |
| K150CB-N-H     | 31.34  | 120.46 | 7.819  |        |        |        |
| K150CB-S151N-H | 31.34  | 116.87 | 8.229  | 31.35  | 116.86 | 8.231  |
| S151CA-N-H     | 61.8   | 116.87 | 8.229  |        |        |        |
| S151CA-A152N-H | 61.80  | 126.16 | 7.331  | 61.81  | 126.15 | 7.334  |
| S151CB-N-H     | 62.73  | 116.87 | 8.229  |        |        |        |
| S151CB-N-H     | 62.15  | 117.02 | 8.227  |        |        |        |
| S151CB-A152N-H | 62.16  | 126.04 | 7.33   | 62.48  | 126.16 | 7.337  |
| S151CB-A152N-H | 62.76  | 126.19 | 7.336  |        |        |        |
| A152CA-N-H     | 54.85  | 126.15 | 7.334  |        |        |        |
| A152CA-V153N-H | 54.85  | 120.27 | 8.06   | 54.91  | 120.30 | 8.062  |
| A152CB-N-H     | 17.77  | 126.13 | 7.334  |        |        |        |
| A152CB-V153N-H | 17.76  | 120.28 | 8.06   | 17.76  | 120.29 | 8.062  |
| V153CA-N-H     | 67.24  | 120.31 | 8.06   |        |        |        |
| V153CA-S154N-H | 67.26  | 113.45 | 7.788  | 67.26  | 113.48 | 7.79   |
| V153CB-N-H     | 31.85  | 120.34 | 8.06   |        |        |        |
| V153CB-S154N-H | 31.88  | 113.45 | 7.788  | 31.86  | 113.49 | 7.79   |
| S154CA-N-H     | 61.5   | 113.52 | 7.787  |        |        |        |
| S154CA-A155N-H | 61.47  | 125.76 | 8.433  | 61.53  | 125.68 | 8.436  |
| S154CB-N-H     | 62.65  | 113.52 | 7.788  |        |        |        |
| S154CB-A155N-H | 62.62  | 125.75 | 8.434  | 62.67  | 125.70 | 8.436  |

|                | HNCA-  | CB     |        | CACB-  | (CO)NH  |        |
|----------------|--------|--------|--------|--------|---------|--------|
| Assignment     | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm  | H, ppm |
| A155CA-N-H     | 54.53  | 125.70 | 8.434  |        |         |        |
| A155CA-A156N-H | 54.52  | 119.58 | 7.249  | 54.57  | 119.60  | 7.252  |
| A155CB-N-H     | 17.78  | 125.74 | 8.434  |        |         |        |
| A155CB-A156N-H | 17.77  | 119.60 | 7.251  | 17.77  | 119.60  | 7.251  |
| A156CA-N-H     | 51.48  | 119.61 | 7.249  |        |         |        |
| A156CA-T157N-H | 51.47  | 112.83 | 8.094  | 51.52  | 112.8   | 8.096  |
| A156CB-N-H     | 18.09  | 119.63 | 7.25   |        |         |        |
| A156CB-T157N-H | 18.08  | 112.82 | 8.094  | 18.10  | 112.81  | 8.096  |
| T157CA-N-H     | 63.27  | 112.88 | 8.093  |        |         |        |
| T157CA-L158N-H | 63.20  | 118.85 | 7.157  | 63.20  | 118.89  | 7.16   |
| T157CB-N-H     | 67.88  | 112.85 | 8.094  |        |         |        |
| T157CB-N-H     | 67.62  | 112.86 | 8.094  |        |         |        |
| T157CB-L158N-H | 67.64  | 118.92 | 7.157  | 67.75  | 118.90  | 7.16   |
| L158CA-N-H     | 52.59  | 118.91 | 7.158  |        |         |        |
| L158CA-E159N-H | 52.59  | 121.15 | 8.353  | 52.66  | 121.20  | 8.357  |
| L158CB-N-H     | 44.59  | 118.90 | 7.158  |        |         |        |
| L158CB-E159N-H | 44.60  | 121.11 | 8.354  | 44.61  | 121.25  | 8.354  |
| E159CA-N-H     | 54.45  | 121.14 | 8.354  |        |         |        |
| E159CA-F160N-H | 54.46  | 128.15 | 9.12   | 54.50  | 128.19  | 9.121  |
| E159CB-N-H     | 30.21  | 121.15 | 8.353  |        |         |        |
| E159CB-N-H     | 30.49  | 121.17 | 8.354  |        |         |        |
| E159CB-F160N-H | 30.34  | 128.24 | 9.121  | 30.37  | 128.191 | 9.122  |
| F160CA-N-H     | 61.03  | 128.24 | 9.121  |        |         |        |
| F160CA-S161N-H | 61.01  | 112.93 | 8.831  | 61.01  | 112.931 | 8.831  |
| F160CB-N-H     | 38.46  | 128.27 | 9.11   |        |         |        |
| F160CB-S161N-H | 38.43  | 113.02 | 8.83   | 38.42  | 112.94  | 8.83   |
| S161CA-N-H     | 60.71  | 113.05 | 8.825  |        |         |        |
| S161CA-K162N-H | 60.67  | 119.60 | 7.634  | 60.73  | 119.607 | 7.635  |
| S161CB-N-H     | 62.46  | 113.01 | 8.828  |        |         |        |
| S161CB-K162N-H | 62.52  | 119.65 | 7.636  | 62.50  | 119.657 | 7.635  |
| K162CA-N-H     | 56.22  | 119.67 | 7.633  |        |         |        |
| K162CA-F163N-H | 56.25  | 120.21 | 7.987  | 56.27  | 120.208 | 7.991  |

|                | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|----------------|--------|--------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| K162CB-N-H     | 33.11  | 119.69 | 7.634  |        |        |        |
| K162CB-F163N-H | 33.04  | 120.00 | 7.986  | 33.10  | 120.10 | 7.989  |
| F163CA-N-H     | 58.49  | 120.23 | 7.986  |        |        |        |
| F163CA-I164N-H | 58.48  | 124.39 | 9.575  | 58.51  | 124.45 | 9.577  |
| I164CA-N-H     | 59.65  | 124.55 | 9.575  |        |        |        |
| F163CB-I164N-H | peak   | Not    | found  | 38.62  | 124.45 | 9.578  |
| I164CA-S165N-H | 59.67  | 119.40 | 8.747  | 59.66  | 119.41 | 8.749  |
| I164CB-N-H     | 38.9   | 124.49 | 9.575  |        |        |        |
| I164CB-S165N-H | 38.94  | 119.30 | 8.746  | 38.87  | 119.41 | 8.75   |
| S165CA-N-H     | 57.12  | 119.45 | 8.747  |        |        |        |
| S165CA-T166N-H | 57.05  | 118.05 | 9.383  | 57.09  | 118.19 | 9.389  |
| S165CB-N-H     | 64.85  | 119.46 | 8.749  |        |        |        |
| S165CB-T166N-H | 64.83  | 118.16 | 9.38   | 64.87  | 118.26 | 9.39   |
| T166CA-N-H     | 62.29  | 118.3  | 9.387  |        |        |        |
| T166CA-K167N-H | 62.30  | 125.24 | 8.931  | 62.35  | 125.34 | 8.936  |
| T166CB-N-H     | 70.36  | 118.2  | 9.386  |        |        |        |
| T166CB-K167N-H | 70.41  | 125.26 | 8.929  | 70.38  | 125.34 | 8.935  |
| K167CA-N-H     | 59.72  | 125.40 | 8.932  |        |        |        |
| K167CA-E168N-H | 59.78  | 116.87 | 8.641  | 59.75  | 116.95 | 8.627  |
| K167CB-N-H     | 32.38  | 125.47 | 8.932  |        |        |        |
| K167CB-N-H     | 32.56  | 125.47 | 8.931  |        |        |        |
| K167CB-E168N-H | Peak   | Not    | found  | 32.45  | 116.89 | 8.63   |
| E168CA-N-H     | 56.02  | 116.84 | 8.629  |        |        |        |
| E168CA-N169N-H | 56.00  | 117.46 | 7.776  | 56.04  | 117.48 | 7.773  |
| E168CB-N-H     | 28.65  | 116.91 | 8.622  |        |        |        |
| E168CB-N169N-H | 28.63  | 117.46 | 7.771  | 28.59  | 117.46 | 7.774  |
| N169CA-N-H     | 52.81  | 117.54 | 7.771  |        |        |        |
| N169CA-N170N-H | 52.77  | 115.04 | 8.511  | 52.81  | 115.20 | 8.516  |
| N169CB-N-H     | 41.18  | 117.48 | 7.767  |        |        |        |
| N169CB-N170N-H | 41.09  | 115.16 | 8.512  | 41.18  | 115.16 | 8.517  |
| N170CA-N-H     | 53.70  | 115.13 | 8.508  |        |        |        |
| N170CA-C171N-H | 53.70  | 114.84 | 8.476  | 53.69  | 114.76 | 8.478  |

|                | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|----------------|--------|--------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| N170CB-N-H     | 36.69  | 115.16 | 8.512  |        |        |        |
| N170CB-C171N-H | 36.70  | 114.85 | 8.479  | 36.85  | 114.75 | 8.478  |
| C171CA-N-H     | 54.92  | 114.75 | 8.476  |        |        |        |
| C171CA-A172N-H | 54.95  | 123.22 | 5.226  | 54.98  | 123.20 | 5.224  |
| C171CB-N-H     | 41.96  | 114.78 | 8.476  |        |        |        |
| C171CB-A172N-H | 41.97  | 123.31 | 5.221  | 41.94  | 123.20 | 5.223  |
| A172CA-N-H     | 50.18  | 123.20 | 5.216  |        |        |        |
| A172CA-Y173N-H | Peak   | Not    | found  | 50.2   | 120.30 | 8.281  |
| A172CB-N-H     | 20.26  | 123.29 | 5.22   |        |        |        |
| A172CB-Y173N-H | 20.21  | 120.32 | 8.288  | 20.28  | 120.32 | 8.284  |
| Y173CA-H       | 57.20  | 120.29 | 8.289  |        |        |        |
| Y173CA-D174N-H | 57.21  | 119.29 | 5.988  | 57.20  | 119.28 | 5.988  |
| Y173CB-D174N-H | 40.58  | 119.31 | 5.988  | 40.65  | 119.27 | 5.986  |
| D174CA-N-H     | 50.91  | 119.32 | 5.98   |        |        |        |
| D174CA-N175N-H | 50.96  | 121.97 | 7.998  | 50.96  | 121.97 | 7.998  |
| D174CB-N-H     | 38.74  | 119.26 | 5.986  |        |        |        |
| D174CB-N175N-H | Peak   | Not    | found  | 38.77  | 121.87 | 7.999  |
| N175CA-N-H     | 55.59  | 121.91 | 7.996  |        |        |        |
| N175CA-D176N-H | 55.62  | 118.47 | 8.048  | 55.61  | 118.48 | 8.052  |
| N175CB-N-H     | 37.60  | 121.87 | 7.99   |        |        |        |
| N175CB-D176N-H | 37.65  | 118.45 | 8.051  | 37.67  | 118.49 | 8.052  |
| D176CA-N-H     | 57.40  | 118.50 | 8.051  |        |        |        |
| D176CA-S177N-H | 57.38  | 116.38 | 7.178  | 57.39  | 116.39 | 7.178  |
| D176CB-N-H     | 39.91  | 118.54 | 8.052  |        |        |        |
| D176CB-S177N-H | 39.94  | 116.37 | 7.176  | 39.91  | 116.37 | 7.179  |
| S177CA-N-H     | 61.25  | 116.41 | 7.176  |        |        |        |
| S177CA-L178N-H | 61.25  | 119.92 | 6.783  | 61.20  | 119.92 | 6.784  |
| S177CB-L178N-H | Peak   | Not    | found  | Peak   | Not    | found  |
| L178CA-N-H     | 57.99  | 119.97 | 6.781  |        |        |        |
| L178CA-K179N-H | 57.99  | 112.26 | 7.317  | 58.04  | 112.25 | 7.32   |
| L178CB-N-H     | 42.28  | 119.95 | 6.781  |        |        |        |
| L178CB-K179N-H | 42.34  | 112.21 | 7.317  | 42.31  | 112.26 | 7.32   |

|                | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|----------------|--------|--------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| K179CA-N-H     | 59.81  | 112.30 | 7.316  |        |        |        |
| K179CA-S180N-H | 59.83  | 114.47 | 7.477  | 59.83  | 114.45 | 7.479  |
| K179CB-N-H     | 31.89  | 112.27 | 7.318  |        |        |        |
| K179CB-S180N-H | 31.88  | 114.45 | 7.478  | 31.92  | 114.44 | 7.479  |
| S180CA-N-H     | 60.86  | 114.49 | 7.477  |        |        |        |
| S180CA-L181N-H | 60.86  | 121.55 | 7.541  | 60.89  | 121.59 | 7.544  |
| S180CB-N-H     | 62.67  | 114.48 | 7.477  |        |        |        |
| S180CB-L181N-H | 62.66  | 121.60 | 7.541  | 62.67  | 121.60 | 7.543  |
| L181CA-N-H     | 56.71  | 121.65 | 7.54   |        |        |        |
| L181CA-L182N-H | 56.76  | 114.55 | 7.016  | 56.76  | 114.55 | 7.016  |
| L181CB-N-H     | 41.87  | 121.63 | 7.541  |        |        |        |
| L181CB-L182N-H | 41.86  | 114.55 | 7.016  | 41.86  | 114.55 | 7.016  |
| L182CA-N-H     | 56.90  | 114.61 | 7.014  |        |        |        |
| L182CA-T183N-H | 56.88  | 105.57 | 7.261  | 56.92  | 105.60 | 7.264  |
| L182CB-N-H     | 42.28  | 114.58 | 7.013  |        |        |        |
| L182CB-T183N-H | 42.31  | 105.51 | 7.262  | 42.28  | 105.60 | 7.264  |
| T183CA-N-H     | 61.69  | 105.58 | 7.261  |        |        |        |
| T183CA-K184N-H | 61.69  | 126.95 | 7.243  | 61.67  | 126.93 | 7.245  |
| T183CB-N-H     | 69.43  | 105.6  | 7.262  |        |        |        |
| T183CB-K184N-H | 69.43  | 126.95 | 7.242  | 69.47  | 126.93 | 7.245  |
| K184CA-N-H     | 56.98  | 126.97 | 7.243  |        |        |        |
| K184CB-N-H     | 33.46  | 126.97 | 7.243  |        |        |        |

## Appendix A. Assignment Tables

Table A1. Assignments (in ppm) of the high-spin NP4  $^1\text{H}\{^{15}\text{N}\}$  HSQC experiment, pH 7.3.

| Assignment | N, ppm          | H, ppm       |
|------------|-----------------|--------------|
| A1         | <i>peak not</i> | <i>found</i> |
| C2         | <i>peak not</i> | <i>found</i> |
| T3         | <b>120.454</b>  | 9.891        |
| K4         | <b>124.021</b>  | 8.115        |
| N5         | <i>peak not</i> | <i>found</i> |
| A6         | <b>124.526</b>  | 7.785        |
| I7         | <b>124.81</b>   | 8.441        |
| A8         | <b>129.503</b>  | 8.477        |
| Q9         | <b>121.5</b>    | 8.53         |
| T10        | <b>127.063</b>  | 8.876        |
| G11        | <i>peak not</i> | <i>found</i> |
| F12        | <b>118.811</b>  | 7.014        |
| N13        | <b>128.097</b>  | 8.755        |
| K14        | <b>125.372</b>  | 7.986        |
| D15        | <b>120.18</b>   | 8.017        |
| K16        | <b>116.706</b>  | 7.066        |
| Y17        | <b>118.446</b>  | 7.012        |
| F18        | <b>118.382</b>  | 8.419        |
| N19        | <b>118.63</b>   | 7.856        |
| G20        | <b>110.377</b>  | 9.26         |
| D21        | <b>118.628</b>  | 7.644        |
| V22        | <b>119.129</b>  | 8.218        |
| W23        | <b>127.695</b>  | 9.625        |
| Y24        | <b>119.049</b>  | 8.999        |
| V25        | <b>120.66</b>   | 8.55         |
| T26        | <b>122.917</b>  | 10.072       |
| D27        | <b>120.548</b>  | 8.588        |
| Y28        | <b>119.276</b>  | 10.302       |
| L29        | <b>123.42</b>   | 9.225        |
| D30        | <b>127.386</b>  | 8.358        |

| Assignment | N, ppm          | H, ppm       |
|------------|-----------------|--------------|
| L31        | <b>123.631</b>  | 6.96         |
| E32        | <b>119.752</b>  | 7.212        |
| P33        | <i>peak not</i> | <i>found</i> |
| D34        | <b>120.8</b>    | 8.163        |
| D35        | <b>120.421</b>  | 8.357        |
| V36        | <b>119.19</b>   | 8.203        |
| P37        | <i>peak not</i> | <i>found</i> |
| K38        | <b>124.301</b>  | 9.9          |
| R39        | <b>127.483</b>  | 9.767        |
| Y40        | <i>peak not</i> | <i>found</i> |
| C41        | <i>peak not</i> | <i>found</i> |
| A42        | <i>peak not</i> | <i>found</i> |
| A43        | <i>peak not</i> | <i>found</i> |
| L44        | <b>116.178</b>  | 8.877        |
| A45        | <b>121.554</b>  | 8.994        |
| A46        | <b>125.805</b>  | 8.818        |
| G47        | <b>107.951</b>  | 9.213        |
| T48        | <b>113.214</b>  | 8.591        |
| A49        | <b>128.421</b>  | 8.984        |
| S50        | <i>peak not</i> | <i>found</i> |
| G51        | <b>106.739</b>  | 8.495        |
| K52        | <b>120.39</b>   | 7.879        |
| L53        | <b>123.356</b>  | 8.609        |
| K54        | <b>126.575</b>  | 8.955        |
| E55        | <b>118.759</b>  | 8.937        |
| A56        | <b>133.599</b>  | 9.858        |
| L57        | <b>121.601</b>  | 8.51         |
| Y58        | <i>peak not</i> | <i>found</i> |
| H59        | <i>peak not</i> | <i>found</i> |
| Y60        | <i>peak not</i> | <i>found</i> |
| D61        | <i>peak not</i> | <i>found</i> |
| P62        | <i>peak not</i> | <i>found</i> |
| K63        | <b>116.582</b>  | 7.983        |

| Assignment | N, ppm          | H, ppm       |
|------------|-----------------|--------------|
| T64        | <b>105.177</b>  | 6.603        |
| Q65        | <b>115.155</b>  | 8.009        |
| D66        | <b>119.676</b>  | 7.34         |
| T67        | <b>114.022</b>  | 7.189        |
| F68        | <b>114.64</b>   | 5.048        |
| Y69        | <b>117.756</b>  | 6.813        |
| D70        | <b>115.404</b>  | 7.422        |
| V71        | <b>118.112</b>  | 9.415        |
| S72        | <b>122.182</b>  | 9.185        |
| E73        | <b>124.232</b>  | 9.054        |
| L74        | <b>124.371</b>  | 8.607        |
| Q75        | <b>122.015</b>  | 9.437        |
| V76        | <b>126.157</b>  | 8.885        |
| E77        | <b>129.994</b>  | 8.689        |
| S78        | <b>111.536</b>  | 8.05         |
| L79        | <i>peak not</i> | <i>found</i> |
| G80        | <b>114.576</b>  | 8.374        |
| K81        | <b>121.828</b>  | 7.88         |
| Y82        | <b>121.063</b>  | 8.285        |
| T83        | <b>117.085</b>  | 9.079        |
| A84        | <b>132.388</b>  | 10.179       |
| N85        | <b>123.945</b>  | 8.425        |
| F86        | <b>120.033</b>  | 7.365        |
| K87        | <b>120.588</b>  | 9.284        |
| K88        | <b>127.293</b>  | 9.175        |
| V89        | <b>120.962</b>  | 8.418        |
| D90        | <b>118.614</b>  | 7.947        |
| K91        | <b>114.211</b>  | 7.789        |
| N92        | <b>114.29</b>   | 7.227        |
| G93        | <b>108.387</b>  | 7.933        |
| N94        | <b>120.295</b>  | 8.28         |
| V95        | <b>123.417</b>  | 8.763        |
| K96        | <b>128.108</b>  | 9.491        |

| Assignment | N, ppm          | H, ppm       |
|------------|-----------------|--------------|
| V97        | 119.618         | 7.995        |
| A98        | 128.223         | 8.595        |
| V99        | 122.189         | 8.546        |
| T100       | 126.137         | 9.975        |
| A101       | 131.269         | 8.9          |
| G102       | 110.228         | 9.142        |
| N103       | 121.028         | 8.198        |
| Y104       | 121.177         | 9.204        |
| Y105       | 116.235         | 10.222       |
| T106       | 113.605         | 8.476        |
| F107       | 119.697         | 9.471        |
| T108       | 117.611         | 9.34         |
| V109       | 127.898         | 9.343        |
| M110       | 129.521         | 8.78         |
| Y111       | 117.608         | 8.202        |
| A112       | 125.874         | 6.658        |
| D113       | 121.477         | 9.499        |
| D114       | 114.805         | 8.355        |
| S115       | 110.895         | 8.701        |
| S116       | 117.964         | 8.884        |
| A117       | 117.64          | 8.582        |
| L118       | 121.515         | 9.265        |
| I119       | 119.847         | 9.758        |
| H120       | 122.354         | 8.834        |
| T121       | 116.443         | 6.829        |
| C122       | 118.257         | 7.21         |
| L123       | 126.996         | 6.934        |
| H124       | <i>peak not</i> | <i>found</i> |
| K125       | 120.224         | 7.784        |
| G126       | 116.006         | 8.766        |
| N127       | <i>peak not</i> | <i>found</i> |
| K128       | 119.194         | 7.38         |
| D129       | 120.94          | 8.164        |

| Assignment | N, ppm          | H, ppm       |
|------------|-----------------|--------------|
| L130       | 123.138         | 6.906        |
| G131       | 103.714         | 5.159        |
| D132       | 116.476         | 6.516        |
| L133       | 120.795         | 5.511        |
| Y134       | 125.023         | 8.309        |
| A135       | 124.097         | 9.967        |
| V136       | 124.86          | 10.26        |
| L137       | 126.234         | 9.929        |
| N138       | 121.364         | 9.932        |
| R139       | 124.829         | 8.616        |
| N140       | 120.082         | 10.274       |
| K141       | 123.549         | 7.625        |
| D142       | 117.718         | 7.97         |
| A143       | 123.364         | 7.145        |
| A144       | 126.306         | 8.485        |
| A145       | 126.818         | 9.277        |
| G146       | 110.418         | 8.797        |
| D147       | 117.601         | 8.428        |
| K148       | <i>peak not</i> | <i>found</i> |
| V149       | 120.507         | 7.937        |
| K150       | 120.422         | 7.82         |
| S151       | 116.867         | 8.227        |
| A152       | 126.16          | 7.334        |
| V153       | 120.269         | 8.057        |
| S154       | 113.484         | 7.788        |
| A155       | 125.691         | 8.432        |
| A156       | 119.596         | 7.251        |
| T157       | 112.792         | 8.092        |
| L158       | 118.882         | 7.159        |
| E159       | 121.149         | 8.351        |
| F160       | 128.192         | 9.114        |
| S161       | 112.934         | 8.829        |
| K162       | 119.647         | 7.632        |

| Assignment | N, ppm  | H, ppm |
|------------|---------|--------|
| F163       | 120.19  | 7.986  |
| I164       | 124.464 | 9.573  |
| S165       | 119.407 | 8.748  |
| T166       | 118.197 | 9.387  |
| K167       | 125.338 | 8.932  |
| E168       | 116.891 | 8.629  |
| N169       | 117.484 | 7.767  |
| N170       | 115.158 | 8.51   |
| C171       | 114.733 | 8.473  |
| A172       | 123.198 | 5.222  |
| Y173       | 120.292 | 8.285  |
| D174       | 119.273 | 5.985  |
| N175       | 121.883 | 7.988  |
| D176       | 118.479 | 8.048  |
| S177       | 116.37  | 7.179  |
| L178       | 119.915 | 6.78   |
| K179       | 112.251 | 7.318  |
| S180       | 114.438 | 7.476  |
| L181       | 121.605 | 7.539  |
| L182       | 114.55  | 7.013  |
| T183       | 105.596 | 7.263  |
| K184       | 126.926 | 7.244  |

**Table A2. Assignments (in ppm) of the high-spin NP4 at pH 7.3 HNCA experiment.**

|              |        |         |        | Assignment   | C, ppm | N, ppm | H, ppm | Assignment   | C, ppm | N, ppm | H, ppm |
|--------------|--------|---------|--------|--------------|--------|--------|--------|--------------|--------|--------|--------|
| Assignment   | C, ppm | N, ppm  | H, ppm | Y17CA-N-H    | 62.32  | 118.46 | 7.013  | P33CA-D34N-H | 62.47  | 120.84 | 8.165  |
| A1CA-C2N-H   | peak   | not     | found  | Y17CA-F18N-H | 62.32  | 118.38 | 8.422  | D34CA-N-H    | 53.77  | 120.79 | 8.164  |
| C2CA-N-H     | peak   | not     | found  | F18CA-N-H    | 56.37  | 118.37 | 8.421  | D34CA-D35N-H | 53.74  | 120.3  | 8.359  |
| C2CA-T3N-H   | 53.66  | 120.41  | 9.894  | F18CA-N19N-H | 56.36  | 118.62 | 7.855  | D35CA-N-H    | 56.89  | 120.46 | 8.358  |
| T3CA-N-H     | 61.87  | 120.45  | 9.895  | N19CA-N-H    | 52.48  | 118.62 | 7.856  | D35CA-V36N-H | 56.87  | 119.17 | 8.203  |
| T3CA-K4N-H   | 61.82  | 124.02  | 8.113  | N19CA-G20N-H | 52.47  | 110.37 | 9.26   | V36CA-N-H    | 59.89  | 119.21 | 8.203  |
| K4CA-N-H     | 55.05  | 123.99  | 8.117  | G20CA-N-H    | 45.43  | 110.39 | 9.261  | V36CA-P37    | peak   | not    | found  |
| K4CA-N5N-H   | peak   | not     | found  | G20CA-D21N-H | 45.42  | 118.6  | 7.644  | P37CA        | peak   | not    | found  |
| N5CA-N-H     | peak   | not     | found  | D21CA-N-H    | 51.54  | 118.65 | 7.645  | P37CA-K38N-H | 63.89  | 124.25 | 9.901  |
| N5CA-A6N-H   | 52.37  | 124.53  | 7.787  | D21CA-V22N-H | 51.53  | 119.11 | 8.218  | K38CA-N-H    | 57.23  | 124.41 | 9.903  |
| A6CA-N-H     | 52.4   | 124.57  | 7.785  | V22CA-N-H    | 63.04  | 119.14 | 8.217  | K38CA-R39N-H | 57.14  | 127.57 | 9.788  |
| A6CA-I7N-H   | 52.34  | 124.73  | 8.443  | V22CA-W23N-H | 63.02  | 127.55 | 9.628  | R39CA-N-H    | 55.91  | 127.52 | 9.783  |
| I7CA-N-H     | 60.07  | 124.85  | 8.442  | W23CA-N-H    | 55.89  | 127.69 | 9.63   | R39CA-Y40N-H | peak   | not    | found  |
| I7CA-A8N-H   | 60.07  | 129.43  | 8.478  | W23CA-Y24N-H | 55.98  | 119.07 | 8.996  | Y40CA-N-H    | peak   | not    | found  |
| A8CA-N-H     | 51.32  | 129.47  | 8.479  | Y24CA-N-H    | 57.55  | 119.1  | 9.003  | Y40CA-C41N-H | peak   | not    | found  |
| A8CA-Q9N-H   | 51.36  | 121.44  | 8.533  | Y24CA-V25N-H | 57.5   | 120.59 | 8.551  | C41CA-N-H    | peak   | not    | found  |
| Q9CA-N-H     | 56.35  | 121.5   | 8.534  | V25CA-N-H    | 63.69  | 120.77 | 8.553  | D41CA-A42N-H | peak   | not    | found  |
| Q9CA-T10N-H  | 56.37  | 127.11  | 8.874  | V25CA-T26N-H | 63.7   | 122.91 | 10.067 | A42CA-N-H    | peak   | not    | found  |
| T10CA-N-H    | 64.33  | 127.11  | 8.874  | T26CA-N-H    | 64.01  | 122.93 | 10.069 | A42CA-A43N-H | peak   | not    | found  |
| T10CA-G11N-H | peak   | not     | found  | T26CA-D27N-H | 63.99  | 120.54 | 8.597  | A43CA-N-H    | peak   | not    | found  |
| G11CA-N-H    | peak   | not     | found  | D27CA-N-H    | 53.91  | 120.59 | 8.593  | A43CA-L44N-H | 49.75  | 116.15 | 8.876  |
| G11CA-F12N-H | 46.08  | 118.82  | 7.016  | D27CA-Y28N-H | 53.88  | 119.32 | 10.307 | L44CA-N-H    | 53.94  | 116.24 | 8.876  |
| F12CA-N-H    | 57.62  | 118.85  | 7.015  | Y28CA-N-H    | 58.19  | 119.3  | 10.306 | L44CA-A45N-H | 53.93  | 121.63 | 8.997  |
| F12CA-N13N-H | 57.54  | 128.03  | 8.754  | Y28CA-L29N-H | 58.19  | 123.41 | 9.225  | A45CA-N-H    | 51.96  | 121.55 | 8.996  |
| N13CA-N-H    | 51.3   | 128.07  | 8.755  | L29CA-N-H    | 53.52  | 123.43 | 9.229  | A45CA-A46N-H | 52.03  | 125.81 | 8.822  |
| N13CA-K14N-H | 51.28  | 125.34  | 7.988  | L29CA-D30N-H | 53.52  | 127.45 | 8.362  | A46CA-N-H    | 51.45  | 125.85 | 8.819  |
| K14CA-N-H    | 58.74  | 125.33  | 7.988  | D30CA-N-H    | 51.2   | 127.43 | 8.361  | A46CA-G47N-H | 51.44  | 107.93 | 9.216  |
| K14CA-D15N-H | 58.74  | 120.18  | 8.022  | D30CA-L31N-H | 51.2   | 123.68 | 6.963  | G47CA-N-H    | 45.73  | 107.94 | 9.216  |
| D15CA-N-H    | 57.27  | 120.17  | 8.02   | L31CA-N-H    | 55.3   | 123.63 | 6.96   | G47CA-T48N-H | 45.73  | 113.18 | 8.594  |
| D15CA-K16N-H | 57.28  | 116.71  | 7.067  | L31CA-E32N-H | 55.27  | 119.74 | 7.21   | T48CA-N-H    | 61.4   | 113.24 | 8.594  |
| K16CA-N-H    | 57.82  | 116.745 | 7.066  | E32CA-N-H    | 52.91  | 119.77 | 7.21   | T48CA-A49N-H | 61.37  | 128.45 | 8.986  |
| K16CA-Y17N-H | 57.87  | 118.46  | 7.013  | E32CA-P33    | peak   | not    | found  | A49CA-N-H    | 53.17  | 128.48 | 8.986  |
|              |        |         |        | P33CA        | peak   | not    | found  | A49CA-S50N-H | peak   | not    | found  |

| Assignment   | C,<br>ppm    | N, ppm     | H, ppm       | Assignment   | C,<br>ppm    | N, ppm     | H, ppm       | Assignment   | C,<br>ppm    | N, ppm | H, ppm |
|--------------|--------------|------------|--------------|--------------|--------------|------------|--------------|--------------|--------------|--------|--------|
| S50CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> | D66CA-T67N-H | <b>55.21</b> | 114.06     | 7.186        | T83CA-N-H    | <b>62.68</b> | 117.1  | 9.09   |
| S50CA-G51N-H | <b>59.06</b> | 106.76     | 8.496        | T67CA-N-H    | <b>58.49</b> | 114.05     | 7.186        | T83CA-A84N-H | <b>62.69</b> | 132.38 | 10.176 |
| G51CA-N-H    | <b>45.11</b> | 106.77     | 8.498        | T67CA-F68N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | A84CA-N-H    | <b>51.95</b> | 132.45 | 10.175 |
| G51CA-K52N-H | <b>45.12</b> | 120.37     | 7.879        | F68CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> | A84CA-N85N-H | <b>52.05</b> | 124.1  | 8.432  |
| K52CA-N-H    | <b>54.38</b> | 120.4      | 7.88         | F68CA-Y69N-H | <b>54.57</b> | 117.77     | 6.816        | N85CA-N-H    | <b>53.82</b> | 123.94 | 8.428  |
| K52CA-L53N-H | <b>54.43</b> | 123.49     | 8.61         | Y69CA-N-H    | <b>54.66</b> | 117.8      | 6.816        | N85CA-F86N-H | <b>53.93</b> | 119.96 | 7.368  |
| L53CA-N-H    | <b>55.34</b> | 123.4      | 8.611        | Y69CA-D70N-H | <b>54.7</b>  | 115.41     | 7.423        | F86CA-N-H    | <b>57.02</b> | 120.08 | 7.367  |
| L53CA-K54N-H | <b>55.28</b> | 126.61     | 8.952        | D70CA-N-H    | <b>52.07</b> | 115.42     | 7.423        | F86CA-K87N-H | <b>57.06</b> | 120.54 | 9.285  |
| K54CA-N-H    | <b>54.52</b> | 126.48     | 8.956        | D70CA-V71N-H | <b>52.07</b> | 118.06     | 9.412        | K87CA-N-H    | <b>54.68</b> | 120.75 | 9.282  |
| K54CA-E55N-H | <b>54.53</b> | 118.71     | 8.938        | V71CA-N-H    | <b>61.67</b> | 118.18     | 9.413        | K87CA-K88N-H | <b>54.75</b> | 127.34 | 9.179  |
| E55CA-N-H    | <b>56.41</b> | 118.8      | 8.94         | V71CA-S72N-H | <b>61.67</b> | 122.16     | 9.191        | K88CA-N-H    | <b>56.56</b> | 127.33 | 9.179  |
| E55CA-A56N-H | <b>56.4</b>  | 133.6      | 9.867        | S72CA-N-H    | <b>58.61</b> | 122.22     | 9.191        | K88CA-V89N-H | <b>56.67</b> | 120.87 | 8.415  |
| A56CA-N-H    | <b>49.92</b> | 133.62     | 9.865        | S72CA-E73N-H | <b>58.62</b> | 124.19     | 9.058        | V89CA-N-H    | <b>58.27</b> | 120.91 | 8.422  |
| A56CA-L57N-H | <b>49.96</b> | 121.52     | 8.51         | E73CA-N-H    | <b>56.25</b> | 124.26     | 9.058        | V89CA-D90N-H | <b>58.27</b> | 118.52 | 7.948  |
| L57CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> | E73CA-L74N-H | <b>56.3</b>  | 124.38     | 8.612        | D90CA-N-H    | <b>51.8</b>  | 118.64 | 7.949  |
| L57CA-Y58N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | L74CA-N-H    | <b>54.87</b> | 124.52     | 8.61         | D90CA-K91N-H | <b>51.8</b>  | 114.23 | 7.788  |
| Y58CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> | L74CA-Q75N-H | <b>54.88</b> | 122.07     | 9.44         | K91CA-N-H    | <b>57.94</b> | 114.28 | 7.789  |
| Y58CA-H59N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | Q75CA-N-H    | <b>54.07</b> | 122.04     | 9.435        | K91CA-N92N-H | <b>57.99</b> | 114.32 | 7.225  |
| H59CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> | Q75CA-V76N-H | <b>54.07</b> | 126.05     | 8.884        | N92CA-N-H    | <b>52.62</b> | 114.33 | 7.225  |
| H59CA-Y60N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | V76CA-N-H    | <b>62.84</b> | 126.17     | 8.884        | N92CA-G93N-H | <b>52.61</b> | 108.43 | 7.934  |
| Y60CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> | V76CA-E77N-H | <b>62.86</b> | 130.03     | 8.689        | G93CA-N-H    | <b>45.08</b> | 108.46 | 7.935  |
| Y60CA-D61N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | E77CA-N-H    | <b>57.58</b> | 130.07     | 8.689        | G93CA-N94N-H | <b>45.08</b> | 120.3  | 8.279  |
| D61CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> | E77CA-S78N-H | <b>57.63</b> | 111.55     | 8.053        | N94CA-N-H    | <b>53.61</b> | 120.31 | 8.28   |
| D61CA-P62N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | S78CA-N-H    | <b>57.05</b> | 111.56     | 8.051        | N94CA-V95N-H | <b>53.6</b>  | 123.43 | 8.762  |
| P62CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> | S78CA-L79N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | V95CA-N-H    | <b>65.04</b> | 123.41 | 8.763  |
| P62CA-K63N-H | <b>63.65</b> | 116.66     | 7.985        | L79CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> | V95CA-K96N-H | <b>65.04</b> | 128.04 | 9.489  |
| K63CA-N-H    | <b>58.73</b> | 116.58     | 7.985        | L79CA-G80N-H | <b>58.04</b> | 114.58     | 8.377        | K96CA-N-H    | <b>56.29</b> | 128.11 | 9.489  |
| K63CA-T64N-H | <b>58.72</b> | 105.17     | 6.601        | G80CA-N-H    | <b>46.28</b> | 114.59     | 8.377        | K96CA-V97N-H | <b>56.2</b>  | 119.62 | 7.99   |
| T64CA-N-H    | <b>61.3</b>  | 105.18     | 6.601        | G80CA-K81N-H | <b>46.27</b> | 121.87     | 7.881        | V97CA-N-H    | <b>62.91</b> | 119.64 | 7.997  |
| T64CA-Q65N-H | <b>61.31</b> | 115.16     | 8.01         | K81CA-N-H    | <b>56.1</b>  | 121.8      | 7.881        | V97CA-A98N-H | <b>62.92</b> | 128.18 | 8.597  |
| Q65CA-N-H    | <b>57.8</b>  | 115.19     | 8.01         | K81CA-Y82N-H | <b>56.15</b> | 121.12     | 8.286        | A98CA-N-H    | <b>52.39</b> | 128.23 | 8.597  |
| Q65CA-D66N-H | <b>57.8</b>  | 119.56     | 7.339        | Y82CA-N-H    | <b>56.96</b> | 121.13     | 8.287        | A98CA-V99N-H | <b>52.4</b>  | 122.17 | 8.548  |
| D66CA-N-H    | <b>55.19</b> | 119.62     | 7.343        | Y82CA-T83N-H | <b>56.93</b> | 117.1      | 9.085        | V99CA-N-H    | <b>64.88</b> | 122.18 | 8.547  |

| Assignment     | C, ppm | N, ppm | H, ppm | Assignment      | C, ppm | N, ppm | H, ppm | Assignment     | C, ppm | N, ppm | H, ppm |
|----------------|--------|--------|--------|-----------------|--------|--------|--------|----------------|--------|--------|--------|
| V99CA-T100N-H  | 64.91  | 126.19 | 9.973  | S116CA-N-H      | 58.55  | 117.99 | 8.884  | L133CA-N-H     | 52.75  | 120.8  | 5.507  |
| T100CA-N-H     | 61.81  | 126.15 | 9.974  | S116CA-A117N-H  | 58.55  | 117.59 | 8.584  | L133CA-Y134N-H | 52.77  | 124.89 | 8.314  |
| T100CA-A101N-H | 61.83  | 131.29 | 8.896  | A117CA-N-H      | 52.38  | 117.65 | 8.584  | Y134CA-N-H     | 56.69  | 125.06 | 8.312  |
| A101CA-N-H     | 54.19  | 131.35 | 8.903  | A117CA-L118N-H  | 52.39  | 121.51 | 9.266  | Y134CA-A135N-H | 56.68  | 124.11 | 9.969  |
| A101CA-G102N-H | 54.22  | 110.26 | 9.149  | L118CA-N-H      | 54.4   | 121.43 | 9.267  | A135CA-N-H     | 52.03  | 124.03 | 9.967  |
| G102CA-N-H     | 45.31  | 110.27 | 9.152  | L118CA-I119N-H  | 54.36  | 119.74 | 9.769  | A135CA-V136N-H | 52.03  | 124.83 | 10.263 |
| G102CA-N103N-H | 45.28  | 121.07 | 8.2    | I119CA-N-H      | 59.1   | 119.89 | 9.768  | V136CA-N-H     | 62.9   | 124.84 | 10.262 |
| N103CA-N-H     | 51.4   | 121.02 | 8.2    | I119CA-H120N-H  | 59.09  | 122.31 | 8.832  | V136CA-L137N-H | 62.91  | 126.2  | 9.93   |
| N103CA-Y104N-H | 51.39  | 121.05 | 9.211  | H120CA-N-H      | 56.07  | 122.33 | 8.83   | L137CA-N-H     | 52.2   | 126.24 | 9.931  |
| Y104CA-N-H     | 57.78  | 121.13 | 9.21   | H120CA-T121N-H  | 56.08  | 116.42 | 6.839  | L137CA-N138N-H | 52.2   | 121.32 | 9.936  |
| Y104CA-Y105N-H | 57.78  | 116.23 | 10.224 | T121CA-N-H      | 58.69  | 116.51 | 6.831  | N138CA-N-H     | 52.92  | 121.34 | 9.935  |
| Y105CA-N-H     | 56.23  | 116.25 | 10.221 | T121CA-C122N-H  | 58.67  | 118.3  | 7.205  | N138CA-R139N-H | 52.94  | 124.78 | 8.617  |
| Y105CA-T106N-H | 56.19  | 113.49 | 8.48   | C122CA-N-H      | 53.53  | 118.26 | 7.21   | R139CA-N-H     | 56.09  | 124.74 | 8.617  |
| T106CA-N-H     | 59.6   | 113.61 | 8.479  | C122CA-L123N-H  | 53.43  | 126.97 | 6.939  | R139CA-N140N-H | 55.93  | 120.06 | 10.28  |
| T106CA-F107N-H | 59.61  | 119.73 | 9.468  | L123CA-N-H      | 48.53  | 127.07 | 6.937  | N140CA-N-H     | 51.71  | 120.09 | 10.279 |
| F107CA-N-H     | 56.86  | 119.73 | 9.469  | L123CA-H124N-H  | peak   | not    | found  | N140CA-K141N-H | 51.7   | 123.51 | 7.626  |
| F107CA-T108N-H | 56.89  | 117.7  | 9.341  | H124CA-N-H      | peak   | not    | found  | K141CA-N-H     | 58.15  | 123.54 | 7.626  |
| T108CA-N-H     | 61     | 117.58 | 9.339  | H124CA-K125N-H  | 54.16  | 120.16 | 7.786  | K141CA-D142N-H | 58.14  | 117.72 | 7.969  |
| T108CA-V109N-H | peak   | not    | found  | K125CA-N-H      | 55.42  | 120.32 | 7.783  | D142CA-N-H     | 54.4   | 117.8  | 7.966  |
| V109CA-N-H     | 63.07  | 127.87 | 9.341  | K125CA-G126N-H  | 55.42  | 115.99 | 8.765  | D142CA-A143N-H | 54.36  | 123.44 | 7.142  |
| V109CA-M110N-H | 63.06  | 129.54 | 8.778  | G126CA-N-H      | 47.79  | 116.04 | 8.765  | A143CA-N-H     | 52.61  | 123.38 | 7.144  |
| M110CA-N-H     | 58.13  | 129.5  | 8.778  | N127CA-K128N-H  | 54.47  | 119.12 | 7.382  | A143CA-A144N-H | 52.63  | 126.24 | 8.489  |
| M110CA-Y111N-H | 58.1   | 117.61 | 8.205  | K128CA-N-H      | 55.13  | 119.26 | 7.379  | A144CA-N-H     | 51.29  | 126.31 | 8.488  |
| Y111CA-N-H     | 59.38  | 117.61 | 8.206  | K128CA-D129N-H  | 55.14  | 120.93 | 8.166  | A144CA-A145N-H | 51.29  | 126.7  | 9.278  |
| Y111CA-A112N-H | 59.39  | 125.92 | 6.658  | D129CA-N-H      | 52.71  | 120.94 | 8.163  | A145CA-N-H     | 53.28  | 126.81 | 9.278  |
| A112CA-N-H     | 52.93  | 125.93 | 6.658  | D129CA-L130N-H  | 52.68  | 123.06 | 6.911  | A145CA-G146N-H | 53.27  | 110.42 | 8.796  |
| A112CA-D113N-H | 52.95  | 121.49 | 9.5    | L130CA-N-H      | 53.44  | 123.14 | 6.91   | G146CA-N-H     | 43.68  | 110.42 | 8.796  |
| D113CA-N-H     | 53.17  | 121.49 | 9.498  | CL130CA-G131N-H | peak   | not    | found  | G146CA-D147N-H | 43.67  | 117.6  | 8.429  |
| D113CA-D114N-H | 53.17  | 114.79 | 8.357  | G131CA-N-H      | 42.62  | 103.71 | 5.152  | D147CA-N-H     | 57.86  | 117.68 | 8.429  |
| D114CA-N-H     | 58.1   | 114.74 | 8.361  | G131CA-D132N-H  | 42.62  | 116.48 | 6.514  | D147CA-K148N-H | peak   | not    | found  |
| D114CA-S115N-H | 58.09  | 110.95 | 8.701  | D132CA-N-H      | 53.2   | 116.49 | 6.515  | K148CA-N-H     | peak   | not    | found  |
| S115CA-N-H     | 59.43  | 110.93 | 8.701  | D132CB-N-H      | 42.83  | 116.51 | 6.515  | K148CA-V149N-H | 59.67  | 120.49 | 7.937  |
| S115CA-S116N-H | 59.42  | 117.98 | 8.885  | D132CA-L133N-H  | 53.19  | 120.81 | 5.501  | V149CA-N-H     | 65.54  | 120.57 | 7.938  |

| Assignment     | C, ppm | N, ppm  | H, ppm | Assignment     | C, ppm | N, ppm | H, ppm | Assignment     | C, ppm | N, ppm | H, ppm |
|----------------|--------|---------|--------|----------------|--------|--------|--------|----------------|--------|--------|--------|
| V149CA-K150N-H | 65.54  | 120.45  | 7.82   | T166CA-N-H     | 62.42  | 118.32 | 9.39   | L182CA-T183N-H | 56.9   | 105.62 | 7.262  |
| K150CA-N-H     | 61.23  | 120.45  | 7.819  | T166CA-K167N-H | 62.39  | 125.34 | 8.933  | T183CA-N-H     | 61.66  | 105.64 | 7.262  |
| K150CA-S151N-H | 61.27  | 116.88  | 8.23   | K167CA-N-H     | 59.69  | 125.32 | 8.933  | T183CA-K184N-H | 61.65  | 126.9  | 7.243  |
| S151CA-N-H     | 61.8   | 116.87  | 8.229  | K167CA-E168N-H | 59.61  | 116.93 | 8.639  | K184CA-N-H     | 56.98  | 126.94 | 7.243  |
| S151CA-A152N-H | 61.81  | 126.15  | 7.334  | E168CA-N-H     | 55.948 | 116.93 | 8.628  |                |        |        |        |
| A152CA-N-H     | 54.87  | 126.2   | 7.334  | E168CA-N169N-H | 56     | 117.49 | 7.769  |                |        |        |        |
| A152CA-V153N-H | 54.86  | 120.3   | 8.061  | N169CA-N-H     | 52.78  | 117.54 | 7.77   |                |        |        |        |
| V153CA-N-H     | 67.24  | 120.29  | 8.06   | N169CA-N170N-H | 52.8   | 115.17 | 8.513  |                |        |        |        |
| V153CA-S154N-H | 67.24  | 113.46  | 7.788  | N170CA-N-H     | 53.66  | 115.17 | 8.51   |                |        |        |        |
| S154CA-N-H     | 61.48  | 113.53  | 7.788  | N170CA-C171N-H | 53.69  | 114.76 | 8.478  |                |        |        |        |
| S154CA-A155N-H | 61.48  | 125.75  | 8.434  | C171CA-N-H     | 54.94  | 114.71 | 8.476  |                |        |        |        |
| A155CA-N-H     | 54.53  | 125.71  | 8.434  | C171CA-A172N-H | 54.95  | 123.28 | 5.217  |                |        |        |        |
| A155CA-A156N-H | 54.55  | 119.52  | 7.249  | A172CA-N-H     | 50.1   | 123.25 | 5.222  |                |        |        |        |
| A156CA-N-H     | 51.47  | 119.62  | 7.25   | A172CA-Y173N-H | 50.2   | 120.3  | 8.281  |                |        |        |        |
| A156CA-T157N-H | 51.47  | 112.81  | 8.094  | Y173CA-N-H     | 57.2   | 120.29 | 8.285  |                |        |        |        |
| T157CA-N-H     | 63.16  | 112.86  | 8.094  | Y173CA-D174N-H | 57.18  | 119.38 | 5.988  |                |        |        |        |
| T157CA-L158N-H | 63.17  | 118.88  | 7.158  | D174CA-N-H     | 50.94  | 119.24 | 5.986  |                |        |        |        |
| L158CA-N-H     | 52.59  | 118.91  | 7.158  | D174CA-N175N-H | 50.96  | 121.97 | 7.998  |                |        |        |        |
| L158CA-E159N-H | 52.57  | 121.08  | 8.354  | N175CA-N-H     | 55.59  | 121.91 | 7.996  |                |        |        |        |
| E159CA-N-H     | 54.44  | 121.24  | 8.353  | N175CA-D176N-H | 55.59  | 118.49 | 8.051  |                |        |        |        |
| E159CA-F160N-H | 54.44  | 128.05  | 9.12   | D176CA-N-H     | 57.35  | 118.52 | 8.05   |                |        |        |        |
| F160CA-N-H     | 61.02  | 128.16  | 9.118  | D176CA-S177N-H | 57.36  | 116.37 | 7.177  |                |        |        |        |
| F160CA-S161N-H | 61.01  | 112.93  | 8.831  | S177CA-N-H     | 61.25  | 116.41 | 7.176  |                |        |        |        |
| S161CA-N-H     | 60.74  | 112.97  | 8.828  | S177CA-L178N-H | 61.23  | 119.91 | 6.781  |                |        |        |        |
| S161CA-K162N-H | 60.69  | 119.62  | 7.634  | L178CA-N-H     | 57.98  | 119.92 | 6.782  |                |        |        |        |
| K162CA-N-H     | 56.19  | 119.66  | 7.633  | L178CA-K179N-H | 57.98  | 112.26 | 7.318  |                |        |        |        |
| K162CA-F163N-H | 56.19  | 120.21  | 7.989  | K179CA-N-H     | 59.8   | 112.3  | 7.318  |                |        |        |        |
| F163CA-N-H     | 58.512 | 120.19  | 7.986  | K179CA-S180N-H | 59.73  | 114.46 | 7.478  |                |        |        |        |
| F163CA-I164N-H | 58.46  | 124.44  | 9.575  | S180CA-N-H     | 60.87  | 114.46 | 7.477  |                |        |        |        |
| I164CA-N-H     | 59.64  | 124.54  | 9.575  | S180CA-L181N-H | 60.86  | 121.6  | 7.541  |                |        |        |        |
| I164CA-S165N-H | 59.642 | 119.359 | 8.747  | L181CA-N-H     | 56.73  | 121.65 | 7.541  |                |        |        |        |
| S165CA-N-H     | 57.09  | 119.49  | 8.747  | L181CA-L182N-H | 56.76  | 114.55 | 7.014  |                |        |        |        |
| S165CA-T166N-H | 57.09  | 118.19  | 9.389  | L182CA-N-H     | 56.9   | 114.55 | 7.014  |                |        |        |        |

**Table A3. Assignments of high-spin NP4 at pH 7.3 from the HNCO and HN(CA)CO experiments.**

|                 |               | HNCO       |              |  |               | HN(CA)-CO  |              |
|-----------------|---------------|------------|--------------|--|---------------|------------|--------------|
| Peak assignment | CO, ppm       | N, ppm     | H, ppm       |  | CO, ppm       | N, ppm     | H, ppm       |
|                 |               |            |              |  |               |            |              |
| A1C-C2N-H       | <i>peak</i>   | <i>not</i> | <i>found</i> |  | <i>peak</i>   | <i>not</i> | <i>found</i> |
| C2C-N-H         |               |            |              |  | <i>peak</i>   | <i>not</i> | <i>found</i> |
| C2C-T3N-H       | <b>174.65</b> | 120.46     | 9.896        |  | <b>174.65</b> | 120.46     | 9.896        |
| T3C-N-H         |               |            |              |  | <b>174.55</b> | 120.42     | 9.894        |
| T3C-K4N-H       | <b>174.55</b> | 124.02     | 8.116        |  | <b>174.55</b> | 124.02     | 8.116        |
| K4C-N-H         |               |            |              |  | <b>176.37</b> | 124.04     | 8.117        |
| K4C-N5N-H       | <i>peak</i>   | <i>not</i> | <i>found</i> |  | <i>Peak</i>   | <i>Not</i> | <i>found</i> |
| N5-C-N-H        |               |            |              |  | <i>Peak</i>   | <i>Not</i> | <i>found</i> |
| N5C-A6N-H       | <b>174.23</b> | 124.53     | 7.785        |  | <b>174.22</b> | 124.5      | 7.785        |
| A6C-N-H         |               |            |              |  | <b>176.82</b> | 124.56     | 7.785        |
| A6C-I7N-H       | <b>176.83</b> | 124.83     | 8.443        |  | <b>176.81</b> | 124.83     | 8.442        |
| I7C-N-H         |               |            |              |  | <b>176.05</b> | 124.82     | 8.443        |
| I7C-A8N-H       | <b>176.09</b> | 129.55     | 8.48         |  | <b>176.07</b> | 129.45     | 8.478        |
| A8C-N-H         |               |            |              |  | <b>177.39</b> | 129.49     | 8.478        |
| A8C-Q9N-H       | <b>177.4</b>  | 121.51     | 8.534        |  | <b>177.4</b>  | 121.51     | 8.534        |
| Q9C-N-H         |               |            |              |  | <b>177.11</b> | 121.5      | 8.532        |
| Q9C-T10N-H      | <b>177.11</b> | 127.06     | 8.874        |  | <b>177.11</b> | 127.12     | 8.873        |
| T10C-N-H        |               |            |              |  | <b>176.04</b> | 127.06     | 8.873        |
| T10C-G11N-H     | <i>peak</i>   | <i>not</i> | <i>found</i> |  | <i>peak</i>   | <i>not</i> | <i>found</i> |
| G11C-N-H        |               |            |              |  | <i>peak</i>   | <i>not</i> | <i>found</i> |
| G11C-F12N-H     | <b>174.21</b> | 118.82     | 7.016        |  | <b>174.21</b> | 118.82     | 7.016        |
| F12C-N-H        |               |            |              |  | <b>174.12</b> | 118.83     | 7.017        |
| F12C-N13N-H     | <b>174.11</b> | 128.12     | 8.755        |  | <b>174.11</b> | 128.13     | 8.755        |
| N13C-N-H        |               |            |              |  | <b>174.99</b> | 128.08     | 8.754        |
| N13C-K14N-H     | <b>174.99</b> | 125.37     | 7.988        |  | <b>174.99</b> | 125.33     | 7.988        |
| K14C-N-H        |               |            |              |  | <b>176.81</b> | 125.35     | 7.989        |
| K14C-D15N-H     | <b>176.82</b> | 120.17     | 8.02         |  | <b>176.77</b> | 120.14     | 8.021        |
| D15C-N-H        |               |            |              |  | <b>177.93</b> | 120.18     | 8.02         |

|                 |               | HNCO   |        |  |               | HN(CA)-CO  |              |
|-----------------|---------------|--------|--------|--|---------------|------------|--------------|
| Peak assignment | CO, ppm       | N, ppm | H, ppm |  | CO, ppm       | N, ppm     | H, ppm       |
| D15C-K16N-H     | <b>177.95</b> | 116.7  | 7.066  |  | <b>177.95</b> | 116.73     | 7.068        |
| K16C-N-H        |               |        |        |  | <b>176.23</b> | 116.75     | 7.068        |
| K16C-Y17N-H     | <b>176.25</b> | 118.43 | 7.013  |  | <b>176.25</b> | 118.45     | 7.014        |
| Y17C-N-H        |               |        |        |  | <b>177.8</b>  | 118.45     | 7.015        |
| Y17C-F18N-H     | <b>177.9</b>  | 118.37 | 8.422  |  | <b>177.76</b> | 118.43     | 8.419        |
| F18C-N-H        |               |        |        |  | <b>176.80</b> | 118.38     | 8.422        |
| F18C-N19N-H     | <b>176.8</b>  | 118.62 | 7.857  |  | <b>176.80</b> | 118.62     | 7.857        |
| N19C-N-H        |               |        |        |  | <b>177.05</b> | 118.63     | 7.857        |
| N19C-G20N-H     | <b>177.07</b> | 110.35 | 9.262  |  | <b>177.06</b> | 110.37     | 9.259        |
| G20C-N-H        |               |        |        |  | <b>172.21</b> | 110.39     | 9.26         |
| G20C-D21N-H     | <b>172.21</b> | 118.62 | 7.646  |  | <b>172.21</b> | 118.66     | 7.647        |
| D21C-N-H        |               |        |        |  | <b>175.8</b>  | 118.6      | 7.646        |
| D21C-V22N-H     | <b>175.81</b> | 119.12 | 8.218  |  | <b>175.8</b>  | 119.1      | 8.219        |
| V22C-N-H        |               |        |        |  | <i>Peak</i>   | <i>not</i> | <i>found</i> |
| V22C-W23N-H     | <b>177.04</b> | 127.7  | 9.629  |  | <b>177.03</b> | 127.61     | 9.627        |
| W23C-N-H        |               |        |        |  | <b>174.66</b> | 127.7      | 9.627        |
| W23C-Y24N-H     | <b>174.66</b> | 119.05 | 9.003  |  | <b>174.63</b> | 118.99     | 8.992        |
| Y24C-N-H        |               |        |        |  | <b>177.19</b> | 119.08     | 9.003        |
| Y24C-V25N-H     | <b>177.2</b>  | 120.76 | 8.55   |  | <b>177.20</b> | 120.76     | 8.55         |
| V25C-N-H        |               |        |        |  | <b>178.08</b> | 120.66     | 8.552        |
| V25C-T26N-H     | <b>178.08</b> | 122.93 | 10.068 |  | <b>178.07</b> | 122.84     | 10.065       |
| T26C-N-H        |               |        |        |  | <b>175.30</b> | 122.86     | 10.065       |
| T26C-D27N-H     | <b>175.33</b> | 120.55 | 8.593  |  | <b>175.33</b> | 120.55     | 8.593        |
| D27C-N-H        |               |        |        |  | <b>175.52</b> | 120.58     | 8.593        |
| D27C-Y28N-H     | <b>175.52</b> | 119.29 | 10.307 |  | <b>175.52</b> | 119.29     | 10.307       |
| Y28C-N-H        |               |        |        |  | <b>172.03</b> | 119.31     | 10.304       |
| Y28C-L29N-H     | <b>172.03</b> | 123.45 | 9.228  |  | <b>172.01</b> | 123.45     | 9.226        |
| L29C-N-H        |               |        |        |  | <b>172.91</b> | 123.47     | 9.227        |
| L29C-D30N-H     | <b>172.92</b> | 127.4  | 8.361  |  | <b>172.92</b> | 127.37     | 8.358        |
| D30C-N-H        |               |        |        |  | <b>175.61</b> | 127.44     | 8.367        |
| D30C-L31N-H     | <b>175.61</b> | 123.66 | 6.963  |  | <b>175.61</b> | 123.66     | 6.966        |
|                 |               |        |        |  |               |            |              |

|                 |         | HNCO    |        |  |         | HN(CA)-CO |        |
|-----------------|---------|---------|--------|--|---------|-----------|--------|
| Peak assignment | CO, ppm | N, ppm  | H, ppm |  | CO, ppm | N, ppm    | H, ppm |
| L31C-N-H        |         |         |        |  | 176.73  | 123.58    | 6.963  |
| L31C-E32N-H     | 176.72  | 119.75  | 7.21   |  | 176.72  | 119.75    | 7.21   |
| E32C-N-H        |         |         |        |  | 171.79  | 119.79    | 7.212  |
| E32C-P33        | peak    | not     | found  |  | Peak    | not       | found  |
| P33C            |         |         |        |  | Peak    | not       | found  |
| P33C-D34N-H     | 176.96  | 120.78  | 8.165  |  | 176.97  | 120.80    | 8.162  |
| D34C-N-H        |         |         |        |  | 175.62  | 120.79    | 8.165  |
| D34C-D35N-H     | 175.66  | 120.43  | 8.359  |  | 175.65  | 120.39    | 8.357  |
| D35C-N-H        |         |         |        |  | 176.88  | 120.37    | 8.359  |
| D35C-V36N-H     | 176.89  | 119.17  | 8.204  |  | 176.89  | 119.17    | 8.204  |
| V36C-N-H        |         |         |        |  | 173.71  | 119.21    | 8.203  |
| V36C-P37        | peak    | not     | found  |  | Peak    | not       | found  |
| P37C            |         |         |        |  | Peak    | not       | found  |
| P37C-K38N-H     | 177.83  | 124.29  | 9.904  |  | 177.82  | 124.19    | 9.911  |
| K38C-N-H        |         |         |        |  | 178.81  | 124.44    | 9.9    |
| K38C-R39N-H     | 178.82  | 127.45  | 9.785  |  | 178.82  | 127.45    | 9.785  |
| R39C-N-H        |         |         |        |  | Peak    | not       | found  |
| R39C-Y40N-H     | peak    | not     | found  |  | Peak    | not       | found  |
| Y40C-N-H        |         |         |        |  | Peak    | not       | found  |
| Y40C-C41N-H     | peak    | not     | found  |  | Peak    | not       | found  |
| C41C-N-H        |         |         |        |  | Peak    | not       | found  |
| C41C-A42N-H     | peak    | not     | found  |  | Peak    | not       | found  |
| A42C-N-H        |         |         |        |  | Peak    | not       | found  |
| A42C-A43N-H     | peak    | not     | found  |  | Peak    | not       | found  |
| A43C-N-H        |         |         |        |  | Peak    | not       | found  |
| A43C-L44N-H     | 171.98  | 116.18  | 8.876  |  | 171.97  | 116.08    | 8.875  |
| L44C-N-H        |         |         |        |  | 174.2   | 116.22    | 8.874  |
| L44C-A45N-H     | 174.21  | 121.58  | 8.997  |  | 174.21  | 121.58    | 8.997  |
| A45C-N-H        |         |         |        |  | 174.16  | 121.55    | 8.996  |
| A45C-A46N-H     | 174.16  | 125.792 | 8.818  |  | 174.14  | 125.8     | 8.822  |
| A46C-N-H        |         |         |        |  | 177.35  | 125.85    | 8.818  |
| A46C-G47N-H     | 177.36  | 107.941 | 9.217  |  | 177.37  | 107.96    | 9.215  |

|                 |         | HNCO    |        |  |         | HN(CA)-CO |        |
|-----------------|---------|---------|--------|--|---------|-----------|--------|
| Peak assignment | CO, ppm | N, ppm  | H, ppm |  | CO, ppm | N, ppm    | H, ppm |
| G47C-N-H        |         |         |        |  | 172.23  | 107.94    | 9.215  |
| G47C-T48N-H     | 172.23  | 113.22  | 8.594  |  | 172.23  | 113.2     | 8.593  |
| T48C-N-H        |         |         |        |  | 175.29  | 113.23    | 8.593  |
| T48C-A49N-H     | 175.29  | 128.449 | 8.987  |  | 175.29  | 128.42    | 8.986  |
| A49C-N-H        |         |         |        |  | 177.63  | 128.45    | 8.986  |
| A49C-S50N-H     | peak    | not     | found  |  | Peak    | Not       | found  |
| S50C-N-H        |         |         |        |  | Peak    | Not       | found  |
| S50C-G51N-H     | 175.19  | 106.74  | 8.499  |  | Peak    | Not       | found  |
| G51C-N-H        |         |         |        |  | 173.6   | 106.76    | 8.492  |
| G51C-K52N-H     | 173.6   | 120.391 | 7.881  |  | 173.6   | 120.39    | 7.881  |
| K52C-N-H        |         |         |        |  | 174.63  | 120.42    | 7.881  |
| K52C-L53N-H     | 174.64  | 123.384 | 8.612  |  | 174.635 | 123.34    | 8.611  |
| L53C-N-H        |         |         |        |  | 176.1   | 123.41    | 8.61   |
| L53C-K54N-H     | 176.12  | 126.566 | 8.956  |  | 176.09  | 126.57    | 8.955  |
| K54C-N-H        |         |         |        |  | 174.15  | 126.53    | 8.956  |
| K54C-E55N-H     | 174.15  | 118.747 | 8.937  |  | 174.16  | 118.68    | 8.935  |
| E55C-N-H        |         |         |        |  | 174.59  | 118.79    | 8.937  |
| E55C-A56N-H     | 174.59  | 133.584 | 9.866  |  | 174.6   | 133.59    | 9.862  |
| A56C-N-H        |         |         |        |  | 173.42  | 133.61    | 9.862  |
| A56C-L57N-H     | 173.42  | 121.624 | 8.512  |  | 173.43  | 121.58    | 8.512  |
| L57C-N-H        |         |         |        |  | 171.45  | 121.73    | 8.504  |
| L57C-Y58N-H     | peak    | not     | found  |  | Peak    | Not       | found  |
| Y58C-N-H        |         |         |        |  | Peak    | Not       | found  |
| Y58C-H59N-H     | peak    | not     | found  |  | Peak    | not       | found  |
| H59C-N-H        |         |         |        |  | Peak    | not       | found  |
| H59C-Y60N-H     | peak    | not     | found  |  | Peak    | not       | found  |
| Y60C-N-H        |         |         |        |  | Peak    | not       | found  |
| Y60C-D61N-H     | peak    | not     | found  |  | Peak    | not       | found  |
| D61C-N-H        |         |         |        |  | Peak    | not       | found  |
| D61C-P62N-H     | peak    | not     | found  |  | Peak    | not       | found  |
| P62C-N-H        |         |         |        |  | Peak    | not       | found  |
| P62C-K63N-H     | 177.74  | 116.58  | 7.985  |  | 177.74  | 116.58    | 7.985  |

|                 |         | HNCO   |        |  |         | HN(CA)-CO |        |
|-----------------|---------|--------|--------|--|---------|-----------|--------|
| Peak assignment | CO, ppm | N, ppm | H, ppm |  | CO, ppm | N, ppm    | H, ppm |
| K63C-N-H        |         |        |        |  | 177.93  | 116.60    | 7.986  |
| K63C-T64N-H     | 177.96  | 105.17 | 6.602  |  | 177.95  | 105.18    | 6.605  |
| T64C-N-H        |         |        |        |  | 175.53  | 105.2     | 6.605  |
| T64C-Q65N-H     | 175.53  | 115.15 | 8.011  |  | 175.54  | 115.24    | 8.013  |
| Q65C-N-H        |         |        |        |  | 174.18  | 115.21    | 8.011  |
| Q65C-D66N-H     | 174.18  | 119.67 | 7.341  |  | 174.18  | 119.67    | 7.341  |
| D66C-N-H        |         |        |        |  | Peak    | Not       | found  |
| D66C-T67N-H     | 174.24  | 114.03 | 7.187  |  | 174.23  | 114.06    | 7.189  |
| T67C-N-H        |         |        |        |  | 172.9   | 114.03    | 7.192  |
| T67C-F68N-H     | peak    | Not    | found  |  | Peak    | Not       | found  |
| F68C-N-H        |         |        |        |  | Peak    | Not       | found  |
| F68C-Y69N-H     | 170.52  | 117.73 | 6.818  |  | 170.54  | 117.76    | 6.812  |
| Y69C-N-H        |         |        |        |  | 173.86  | 117.81    | 6.821  |
| Y69C-D70N-H     | 173.84  | 115.41 | 7.428  |  | 173.84  | 115.41    | 7.428  |
| D70C-N-H        |         |        |        |  | 173.67  | 115.41    | 7.424  |
| D70C-V71N-H     | 173.69  | 118.09 | 9.413  |  | 173.70  | 118.06    | 9.412  |
| V71C-N-H        |         |        |        |  | 175.04  | 118.2     | 9.411  |
| V71C-S72N-H     | 175.04  | 122.20 | 9.192  |  | 175.03  | 121.98    | 9.188  |
| S72C-N-H        |         |        |        |  | 174.22  | 122.08    | 9.189  |
| S72C-E73N-H     | 174.22  | 124.24 | 9.058  |  | 174.22  | 124.17    | 9.057  |
| E73C-N-H        |         |        |        |  | 177.06  | 124.28    | 9.057  |
| E73C-L74N-H     | 177.07  | 124.38 | 8.611  |  | 177.07  | 124.38    | 8.611  |
| L74C-N-H        |         |        |        |  | 176.89  | 124.38    | 8.61   |
| L74C-Q75N-H     | 176.87  | 122.03 | 9.434  |  | 176.86  | 122.02    | 9.433  |
| Q75C-N-H        |         |        |        |  | 175.56  | 122       | 9.433  |
| Q75C-V76N-H     | 175.56  | 126.14 | 8.884  |  | 175.60  | 126.02    | 8.88   |
| V76C-N-H        |         |        |        |  | 175.98  | 126.19    | 8.883  |
| V76C-E77N-H     | 175.98  | 130.04 | 8.69   |  | 175.99  | 130.05    | 8.691  |
| E77C-N-H        |         |        |        |  | 176.66  | 130.08    | 8.688  |
| E77C-S78N-H     | 176.66  | 111.53 | 8.051  |  | 176.66  | 111.65    | 8.053  |
| S78C-N-H        |         |        |        |  | 172.76  | 111.59    | 8.053  |
| S78C-L79N-H     | peak    | Not    | found  |  | Peak    | Not       | found  |

|                 |         | HNCO   |        |  |         | HN(CA)-CO |        |
|-----------------|---------|--------|--------|--|---------|-----------|--------|
| Peak assignment | CO, ppm | N, ppm | H, ppm |  | CO, ppm | N, ppm    | H, ppm |
| L79C-N-H        |         |        |        |  | Peak    | not       | found  |
| L79C-G80N-H     | 178.31  | 114.57 | 8.377  |  | 178.29  | 114.58    | 8.377  |
| G80C-N-H        |         |        |        |  | 170.79  | 114.61    | 8.377  |
| G80C-K81N-H     | 170.79  | 121.85 | 7.882  |  | 170.8   | 121.84    | 7.881  |
| K81C-N-H        |         |        |        |  | 173.72  | 121.81    | 7.881  |
| K81C-Y82N-H     | 173.72  | 121.07 | 8.288  |  | 173.70  | 120.86    | 8.286  |
| Y82C-N-H        |         |        |        |  | 174.72  | 121.13    | 8.291  |
| Y82C-T83N-H     | 174.75  | 117.07 | 9.086  |  | 174.74  | 117.12    | 9.083  |
| T83C-N-H        |         |        |        |  | 173.05  | 117.09    | 9.084  |
| T83C-A84N-H     | 173.05  | 132.38 | 10.175 |  | 173.05  | 132.38    | 10.179 |
| A84C-N-H        |         |        |        |  | 175.87  | 132.44    | 10.172 |
| A84C-N85N-H     | 175.88  | 123.94 | 8.429  |  | 175.88  | 123.94    | 8.429  |
| N85C-N-H        |         |        |        |  | 173.88  | 123.95    | 8.426  |
| N85C-F86N-H     | 173.89  | 120.04 | 7.365  |  | 173.89  | 120.04    | 7.365  |
| F86C-N-H        |         |        |        |  | 175.86  | 120.09    | 7.371  |
| F86C-K87N-H     | 175.88  | 120.59 | 9.286  |  | 175.81  | 120.79    | 9.277  |
| K87C-N-H        |         |        |        |  | 174.82  | 120.59    | 9.281  |
| K87C-K88N-H     | 174.8   | 127.30 | 9.179  |  | 174.8   | 127.37    | 9.179  |
| K88C-N-H        |         |        |        |  | 177.21  | 127.32    | 9.178  |
| K88C-V89N-H     | 177.21  | 120.98 | 8.423  |  | 177.2   | 121.08    | 8.42   |
| V89C-N-H        |         |        |        |  | 175.4   | 120.92    | 8.423  |
| V89C-D90N-H     | 175.39  | 118.61 | 7.95   |  | 175.39  | 118.52    | 7.951  |
| D90C-N-H        |         |        |        |  | 176.82  | 118.66    | 7.95   |
| D90C-K91N-H     | 176.83  | 114.23 | 7.79   |  | 176.84  | 114.34    | 7.788  |
| K91C-N-H        |         |        |        |  | 174.70  | 114.3     | 7.79   |
| K91C-N92N-H     | 174.71  | 114.3  | 7.225  |  | 174.72  | 114.30    | 7.227  |
| N92C-N-H        |         |        |        |  | 175.51  | 114.33    | 7.227  |
| N92C-G93N-H     | 175.51  | 108.36 | 7.935  |  | 175.51  | 108.38    | 7.935  |
| G93C-N-H        |         |        |        |  | 173.52  | 108.47    | 7.934  |
| G93C-N94N-H     | 173.52  | 120.31 | 8.28   |  | 173.52  | 120.31    | 8.28   |
| N94C-N-H        |         |        |        |  | 175.61  | 120.31    | 8.28   |
| N94C-V95N-H     | 175.61  | 123.44 | 8.763  |  | 175.62  | 123.41    | 8.761  |

|                 |         | HNCO   |        |  |         | HN(CA)-CO |        |
|-----------------|---------|--------|--------|--|---------|-----------|--------|
| Peak assignment | CO, ppm | N, ppm | H, ppm |  | CO, ppm | N, ppm    | H, ppm |
| V95C-N-H        |         |        |        |  | 175.99  | 123.4     | 8.763  |
| V95C-K96N-H     | 176     | 128.13 | 9.49   |  | 175.99  | 128.05    | 9.489  |
| K96C-N-H        |         |        |        |  | 177.14  | 128.14    | 9.488  |
| K96C-V97N-H     | 177.14  | 119.61 | 7.997  |  | 177.14  | 119.6     | 7.997  |
| V97C-N-H        |         |        |        |  | 174.67  | 119.65    | 7.997  |
| V97C-A98N-H     | 174.68  | 128.24 | 8.597  |  | 174.67  | 128.18    | 8.597  |
| A98C-N-H        |         |        |        |  | 178.02  | 128.24    | 8.597  |
| A98C-V99N-H     | 178.03  | 122.21 | 8.548  |  | 178.01  | 122.10    | 8.546  |
| V99C-N-H        |         |        |        |  | 177.07  | 122.19    | 8.546  |
| V99C-T100N-H    | 177.06  | 126.11 | 9.975  |  | 177.07  | 126.08    | 9.974  |
| T100C-N-H       |         |        |        |  | 173.58  | 126.12    | 9.975  |
| T100C-A101N-H   | 173.58  | 131.29 | 8.904  |  | 173.58  | 131.29    | 8.904  |
| A101C-N-H       |         |        |        |  | 178.51  | 131.3     | 8.904  |
| A101C-G102N-H   | 178.51  | 110.19 | 9.151  |  | 178.51  | 110.21    | 9.142  |
| G102C-N-H       |         |        |        |  | 173.01  | 110.17    | 9.152  |
| G102C-N103N-H   | 173.02  | 121.06 | 8.201  |  | 173.02  | 121.09    | 8.202  |
| N103C-N-H       |         |        |        |  | 173.99  | 120.98    | 8.201  |
| N103C-Y104N-H   | 174     | 121.19 | 9.211  |  | 174     | 121.19    | 9.205  |
| Y104C-N-H       |         |        |        |  | 174.43  | 121.16    | 9.205  |
| Y104C-Y105N-H   | 174.45  | 116.24 | 10.222 |  | 174.45  | 116.24    | 10.222 |
| Y105C-N-H       |         |        |        |  | 174.29  | 116.19    | 10.219 |
| Y105C-T106N-H   | 174.24  | 113.62 | 8.48   |  | 174.28  | 113.61    | 8.483  |
| T106C-N-H       |         |        |        |  | 175.03  | 113.57    | 8.489  |
| T106C-F107N-H   | 175.01  | 119.69 | 9.469  |  | 175.01  | 119.69    | 9.469  |
| F107C-N-H       |         |        |        |  | 173.71  | 119.61    | 9.466  |
| F107C-T108N-H   | 173.73  | 117.61 | 9.34   |  | 173.75  | 117.59    | 9.336  |
| T108C-N-H       |         |        |        |  | 174.67  | 117.52    | 9.337  |
| T108C-V109N-H   | 174.7   | 127.91 | 9.343  |  | 174.7   | 127.91    | 9.343  |
| V109C-N-H       |         |        |        |  | 174.63  | 127.86    | 9.341  |
| V109C-M110N-H   | 174.61  | 129.58 | 8.779  |  | 174.61  | 129.49    | 8.779  |
| M110C-N-H       |         |        |        |  | 176.95  | 129.5     | 8.776  |
| M110C-Y111N-H   | 176.96  | 117.59 | 8.206  |  | 176.95  | 117.59    | 8.206  |

|                 |         | HNCO   |        |  |         | HN(CA)-CO |        |
|-----------------|---------|--------|--------|--|---------|-----------|--------|
| Peak assignment | CO, ppm | N, ppm | H, ppm |  | CO, ppm | N, ppm    | H, ppm |
| Y111C-N-H       |         |        |        |  | 172.24  | 117.6     | 8.207  |
| Y111C-A112N-H   | 172.25  | 125.86 | 6.659  |  | 172.24  | 125.93    | 6.659  |
| A112C-N-H       |         |        |        |  | 175.07  | 125.91    | 6.66   |
| A112C-D113N-H   | 175.07  | 121.5  | 9.498  |  | 175.07  | 121.5     | 9.496  |
| D113C-N-H       |         |        |        |  | 176.07  | 121.49    | 9.496  |
| D113C-D114N-H   | 176.09  | 114.82 | 8.357  |  | 176.09  | 114.83    | 8.357  |
| D114C-N-H       |         |        |        |  | 177.86  | 114.81    | 8.356  |
| D114C-S115N-H   | 177.87  | 110.88 | 8.702  |  | 177.85  | 110.89    | 8.701  |
| S115C-N-H       |         |        |        |  | 173     | 110.93    | 8.701  |
| S115C-S116N-H   | 173     | 117.95 | 8.884  |  | 173.01  | 117.92    | 8.884  |
| S116C-N-H       |         |        |        |  | 171.12  | 117.98    | 8.884  |
| S116C-A117N-H   | 171.12  | 117.62 | 8.584  |  | 171.12  | 117.55    | 8.583  |
| A117C-N-H       |         |        |        |  | 174.9   | 117.67    | 8.583  |
| A117C-L118N-H   | 174.9   | 121.54 | 9.266  |  | 174.9   | 121.54    | 9.266  |
| L118C-N-H       |         |        |        |  | 175.64  | 121.57    | 9.265  |
| L118C-I119N-H   | 175.63  | 119.83 | 9.769  |  | 175.61  | 119.85    | 9.758  |
| I119C-N-H       |         |        |        |  | 174.33  | 119.90    | 9.769  |
| I119C-H120N-H   | 174.33  | 122.38 | 8.832  |  | 174.33  | 122.38    | 8.832  |
| H120C-N-H       |         |        |        |  | 174.25  | 122.33    | 8.83   |
| H120C-T121N-H   | 174.23  | 116.42 | 6.837  |  | 174.23  | 116.42    | 6.837  |
| T121C-N-H       |         |        |        |  | 169.62  | 116.47    | 6.846  |
| T121C-C122N-H   | 169.65  | 118.22 | 7.212  |  | 169.64  | 118.2     | 7.211  |
| C122C-N-H       |         |        |        |  | 171.54  | 118.19    | 7.229  |
| C122C-L123N-H   | 171.58  | 126.99 | 6.939  |  | 171.59  | 126.97    | 6.94   |
| L123C-N-H       |         |        |        |  | 174.04  | 127.07    | 6.946  |
| L123C-H124H     | peak    | not    | found  |  | peak    | not       | found  |
| H124C-N-H       |         |        |        |  | peak    | not       | found  |
| H124C-K125N-H   | 173.67  | 120.23 | 7.785  |  | 173.67  | 120.24    | 7.788  |
| K125C-N-H       |         |        |        |  | 177.95  | 120.29    | 7.785  |
| K125C-G126N-H   | 177.97  | 116.01 | 8.766  |  | 177.96  | 116       | 8.765  |
| G126C-N-H       |         |        |        |  | 175.28  | 116.03    | 8.765  |
| G126C-N127N-H   | peak    | not    | found  |  | peak    | not       | found  |

|                 |         | HNCO   |        |  | HN(CA)-CO   |            |
|-----------------|---------|--------|--------|--|-------------|------------|
| Peak assignment | CO, ppm | N, ppm | H, ppm |  | CO, ppm     | N, ppm     |
| N127C-N-H       |         |        |        |  | <i>peak</i> | <i>not</i> |
| N127C-K128N-H   | 173.69  | 119.18 | 7.382  |  | 173.69      | 119.18     |
| K128C-N-H       |         |        |        |  | 173.7       | 119.23     |
| K128C-D129N-H   | 173.69  | 120.95 | 8.162  |  | 173.70      | 120.96     |
| D129C-N-H       |         |        |        |  | 175.42      | 120.94     |
| D129C-L130N-H   | 175.43  | 123.14 | 6.911  |  | 175.42      | 123.02     |
| L130C-N-H       |         |        |        |  | 174.70      | 123.20     |
| L130C-G131N-H   | 174.71  | 103.69 | 5.163  |  | <i>Peak</i> | <i>Not</i> |
| G131CN--H       |         |        |        |  | 169.76      | 103.71     |
| G131C-D132N-H   | 169.7   | 116.46 | 6.515  |  | 169.71      | 116.49     |
| D132C-N-H       |         |        |        |  | 172.42      | 116.52     |
| D132C-L133N-H   | 172.42  | 120.84 | 5.505  |  | 172.42      | 120.84     |
| L133C-N-H       |         |        |        |  | 175.04      | 120.8      |
| L133C-Y134N-H   | 175.08  | 125.02 | 8.309  |  | 175.08      | 125.02     |
| Y134C-N-H       |         |        |        |  | 175.39      | 125.11     |
| Y134C-A135N-H   | 175.41  | 124.12 | 9.966  |  | 175.41      | 124.12     |
| A135C-N-H       |         |        |        |  | 175.55      | 124.04     |
| A135C-V136N-H   | 175.59  | 124.87 | 10.264 |  | 175.59      | 124.87     |
| V136C-N-H       |         |        |        |  | 175.21      | 124.85     |
| V136C-L137N-H   | 175.22  | 126.22 | 9.931  |  | 175.22      | 126.2      |
| L137C-N-H       |         |        |        |  | 179.06      | 126.18     |
| L137C-N138N-H   | 179.07  | 121.39 | 9.935  |  | 179.06      | 121.22     |
| N138C-N-H       |         |        |        |  | 175.44      | 121.39     |
| N138C-R139N-H   | 175.45  | 124.83 | 8.619  |  | 175.51      | 124.88     |
| R139C-N-H       |         |        |        |  | 175.99      | 124.83     |
| R139C-N140N-H   | 176.02  | 120.08 | 10.279 |  | 176         | 120.05     |
| N140C-N-H       |         |        |        |  | 174.78      | 120.11     |
| N140C-K141N-H   | 174.81  | 123.57 | 7.627  |  | 174.82      | 123.59     |
| K141C-N-H       |         |        |        |  | 175.45      | 123.57     |
| K141C-D142N-H   | 175.44  | 117.64 | 7.965  |  | <i>peak</i> | <i>Not</i> |
| D142C-N-H       |         |        |        |  | <i>peak</i> | <i>Not</i> |
| D142C-A143N-H   | 175.21  | 123.39 | 7.144  |  | <i>Peak</i> | <i>Not</i> |

|                 |             | HNCO       |              |  | HN(CA)-CO   |            |
|-----------------|-------------|------------|--------------|--|-------------|------------|
| Peak assignment | CO, ppm     | N, ppm     | H, ppm       |  | CO, ppm     | N, ppm     |
| A143C-N-H       |             |            |              |  | 177.58      | 123.38     |
| A143C-A144N-H   | 177.59      | 126.29     | 8.488        |  | 177.59      | 126.29     |
| A144C-N-H       |             |            |              |  | 177.8       | 126.26     |
| A144C-A145N-H   | 177.82      | 126.81     | 9.278        |  | 177.80      | 126.73     |
| A145C-N-H       |             |            |              |  | 178.35      | 126.84     |
| A145C-G146N-H   | 178.35      | 110.4      | 8.796        |  | 178.34      | 110.42     |
| G146C-N-H       |             |            |              |  | 173.98      | 110.40     |
| G146C-D147N-H   | 173.97      | 117.57     | 8.431        |  | 173.97      | 117.57     |
| D147C-N-H       |             |            |              |  | 179.12      | 117.47     |
| D147C-K148N-H   | <i>peak</i> | <i>Not</i> | <i>found</i> |  | <i>Peak</i> | <i>Not</i> |
| K148C-N-H       |             |            |              |  | <i>Peak</i> | <i>Not</i> |
| K148C-V149N-H   | 179.94      | 120.52     | 7.939        |  | 179.92      | 120.50     |
| V149C-N-H       |             |            |              |  | 177.43      | 120.52     |
| V149C-K150N-H   | 177.44      | 120.43     | 7.82         |  | 177.45      | 120.41     |
| K150C-N-H       |             |            |              |  | 179.89      | 120.45     |
| K150C-S151N-H   | 179.9       | 116.86     | 8.228        |  | 179.89      | 116.90     |
| S151C-N-H       |             |            |              |  | <i>Peak</i> | <i>Not</i> |
| S151C-A152N-H   | 176.26      | 126.16     | 7.335        |  | <i>Peak</i> | <i>Not</i> |
| A152C-N-H       |             |            |              |  | 179.79      | 126.164    |
| A152C-V153N-H   | 179.8       | 120.28     | 8.06         |  | 179.8       | 120.27     |
| V153C-N-H       |             |            |              |  | 177.62      | 120.3      |
| V153C-S154N-H   | 177.63      | 113.49     | 7.788        |  | 177.64      | 113.39     |
| S154C-N-H       |             |            |              |  | <i>Peak</i> | <i>Not</i> |
| S154C-A155N-H   | 179.22      | 125.68     | 8.434        |  | <i>Peak</i> | <i>Not</i> |
| A155C-N-H       |             |            |              |  | 178.43      | 125.74     |
| A155C-A156N-H   | 178.44      | 119.58     | 7.25         |  | 178.43      | 119.57     |
| A156C-N-H       |             |            |              |  | 176.72      | 119.63     |
| A156C-T157N-H   | 176.73      | 112.79     | 8.094        |  | 176.73      | 112.82     |
| T157C-N-H       |             |            |              |  | 172.72      | 112.87     |
| T157C-L158N-H   | 172.73      | 118.87     | 7.158        |  | 172.69      | 118.79     |
| L158C-N-H       |             |            |              |  | 176.01      | 118.89     |
| L158C-E159N-H   | 176.02      | 121.18     | 8.354        |  | 176.02      | 121.09     |

|                 |         | HNCO   |        |  |         | HN(CA)-CO |        |
|-----------------|---------|--------|--------|--|---------|-----------|--------|
| Peak assignment | CO, ppm | N, ppm | H, ppm |  | CO, ppm | N, ppm    | H, ppm |
| E159C-N-H       |         |        |        |  | 176.64  | 121.24    | 8.354  |
| E159C-F160N-H   | 176.63  | 128.22 | 9.119  |  | 176.64  | 128.2     | 9.113  |
| F160C-N-H       |         |        |        |  | 177.83  | 128.16    | 9.114  |
| F160C-S161N-H   | 177.87  | 112.93 | 8.829  |  | 177.86  | 113.01    | 8.826  |
| S161C-N-H       |         |        |        |  | Peak    | Not       | found  |
| S161C-K162N-H   | 175.03  | 119.65 | 7.634  |  | Peak    | Not       | found  |
| K162C-N-H       |         |        |        |  | 176.57  | 119.67    | 7.635  |
| K162C-F163N-H   | 176.57  | 120.21 | 7.986  |  | 176.57  | 120.08    | 7.986  |
| F163C-N-H       |         |        |        |  | 175.85  | 120.16    | 7.987  |
| F163C-I164N-H   | 175.85  | 124.45 | 9.576  |  | 175.85  | 124.45    | 9.576  |
| I164C-N-H       |         |        |        |  | 176     | 124.5     | 9.573  |
| I164C-S165N-H   | 176.01  | 119.4  | 8.748  |  | 176     | 119.35    | 8.748  |
| S165C-N-H       |         |        |        |  | 178.95  | 119.47    | 8.747  |
| S165C-T166N-H   | 178.97  | 118.24 | 9.386  |  | 178.95  | 118.23    | 9.387  |
| T166C-N-H       |         |        |        |  | 176.86  | 118.22    | 9.386  |
| T166C-K167N-H   | 176.85  | 125.33 | 8.933  |  | 176.85  | 125.33    | 8.933  |
| K167C-N-H       |         |        |        |  | 177.44  | 125.41    | 8.932  |
| K167C-E168N-H   | 177.45  | 116.88 | 8.633  |  | 177.46  | 116.83    | 8.615  |
| E168C-N-H       |         |        |        |  | 176.21  | 116.85    | 8.629  |
| E168C-N169N-H   | 176.21  | 117.46 | 7.772  |  | 176.2   | 117.43    | 7.764  |
| N169C-N-H       |         |        |        |  | 174.3   | 117.57    | 7.777  |
| N169C-N170N-H   | 174.32  | 115.17 | 8.515  |  | 174.32  | 115.17    | 8.515  |
| N170C-N-H       |         |        |        |  | 174.77  | 115.15    | 8.507  |
| N170C-C171N-H   | 174.77  | 114.74 | 8.476  |  | 174.77  | 114.91    | 8.48   |
| C171C-N-H       |         |        |        |  | 173.03  | 114.75    | 8.476  |
| C171C-A172N-H   | 173.04  | 123.22 | 5.222  |  | 173.04  | 123.22    | 5.222  |
| A172C-N-H       |         |        |        |  | 175.26  | 123.17    | 5.227  |
| A172C-Y173N-H   | 175.26  | 120.3  | 8.284  |  | 175.26  | 120.3     | 8.284  |
| Y173C-N-H       |         |        |        |  | 172.81  | 120.22    | 8.287  |
| Y173C-D174N-H   | 172.76  | 119.27 | 5.986  |  | 172.76  | 119.26    | 5.987  |
| D174C-N-H       |         |        |        |  | 174.44  | 119.27    | 5.984  |
| D174C-N175N-H   | 174.45  | 121.89 | 7.995  |  | 174.45  | 121.89    | 7.995  |

|                 |         | HNCO    |        |  |         | HN(CA)-CO |        |
|-----------------|---------|---------|--------|--|---------|-----------|--------|
| Peak assignment | CO, ppm | N, ppm  | H, ppm |  | CO, ppm | N, ppm    | H, ppm |
| N175C-N-H       |         |         |        |  | 176.56  | 121.88    | 7.992  |
| N175C-D176N-H   | 176.59  | 118.472 | 8.051  |  | 176.59  | 118.47    | 8.051  |
| D176C-N-H       |         |         |        |  | 179.34  | 118.51    | 8.051  |
| D176C-S177N-H   | 179.34  | 116.362 | 7.177  |  | 179.34  | 116.35    | 7.179  |
| S177C-N-H       |         |         |        |  | 175.35  | 116.4     | 7.183  |
| S177C-L178N-H   | 175.35  | 119.917 | 6.783  |  | 175.35  | 119.92    | 6.783  |
| L178C-N-H       |         |         |        |  | 176.41  | 119.95    | 6.785  |
| L178C-K179N-H   | 176.43  | 112.242 | 7.318  |  | 176.42  | 112.22    | 7.319  |
| K179C-N-H       |         |         |        |  | 180.11  | 112.3     | 7.319  |
| K179C-S180N-H   | 180.12  | 114.447 | 7.478  |  | 180.11  | 114.46    | 7.48   |
| S180C-N-H       |         |         |        |  | Peak    | Not       | found  |
| S180C-L181N-H   | 176.62  | 121.622 | 7.542  |  | Peak    | Not       | found  |
| L181C-N-H       |         |         |        |  | 177.91  | 121.65    | 7.543  |
| L181C-L182N-H   | 177.93  | 114.552 | 7.014  |  | 177.93  | 114.55    | 7.014  |
| L182C-N-H       |         |         |        |  | 177.77  | 114.56    | 7.016  |
| L182C-T183N-H   | 177.78  | 105.598 | 7.262  |  | 177.77  | 105.6     | 7.264  |
| T183C-N-H       |         |         |        |  | 174.21  | 105.64    | 7.264  |
| T183C-K184N-H   | 174.22  | 126.916 | 7.243  |  | 174.21  | 126.89    | 7.245  |
| K184C-N-H       |         |         |        |  | 180.95  | 126.94    | 7.245  |

**Table A4. Assignments of high-spin NP4 at pH 7.3 from the HNCACB and CACB(CO)NH experiments.**

|            | HNCA-        | CB         |              | CACB-        | (CO)NH     |              |
|------------|--------------|------------|--------------|--------------|------------|--------------|
| Assignment | C, ppm       | N, ppm     | H, ppm       | C, ppm       | N, ppm     | H, ppm       |
| A1CA-C2N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | <i>peak</i>  | <i>not</i> | <i>found</i> |
| A1CB-C2N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | <i>peak</i>  | <i>not</i> | <i>found</i> |
| C2CA-N-H   | <i>peak</i>  | <i>not</i> | <i>found</i> |              |            |              |
| C2CA-T3N-H | <b>53.63</b> | 120.41     | 9.894        | <b>53.71</b> | 120.46     | 9.898        |
| C2CB-N-H   | <i>peak</i>  | <i>not</i> | <i>found</i> |              |            |              |
| C2CB-T3N-H | <b>42.93</b> | 120.44     | 9.895        | <b>43.01</b> | 120.46     | 9.898        |
| T3CA-N-H   | <b>61.85</b> | 120.43     | 9.897        |              |            |              |
| T3CA-K4N-H | <b>61.82</b> | 124.02     | 8.113        | <b>61.86</b> | 124        | 8.12         |
| T3CB-N-H   | <b>69.4</b>  | 120.41     | 9.896        |              |            |              |
| T3CB-K4N-H | <b>69.42</b> | 124.03     | 8.116        | <b>69.4</b>  | 124.04     | 8.116        |
| K4CA-N-H   | <b>55.02</b> | 124.06     | 8.113        |              |            |              |
| K4CA-N5N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | <i>peak</i>  | <i>not</i> | <i>found</i> |
| K4CB-N-H   | <b>32.29</b> | 124.02     | 8.116        |              |            |              |
| K4CB-N5N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | <i>peak</i>  | <i>not</i> | <i>found</i> |
| N5CA-N-H   | <i>peak</i>  | <i>not</i> | <i>found</i> |              |            |              |
| N5CA-A6N-H | <b>52.37</b> | 124.53     | 7.787        | <b>52.37</b> | 124.53     | 7.787        |
| N5CB-A6N-H | <b>39.02</b> | 124.57     | 7.783        | <b>38.89</b> | 124.53     | 7.787        |
| N5CB-A6N-H | <b>38.79</b> | 124.52     | 7.784        |              |            |              |
| A6CA-N-H   | <b>52.4</b>  | 124.54     | 7.785        |              |            |              |
| A6CA-I7N-H | <b>52.38</b> | 124.77     | 8.441        | <b>52.43</b> | 124.82     | 8.445        |
| A6CB-N-H   | <b>18.6</b>  | 124.55     | 7.785        |              |            |              |
| A6CB-I7N-H | <b>18.6</b>  | 124.76     | 8.443        | <b>18.64</b> | 124.84     | 8.445        |
| I7CA-N-H   | <b>60.09</b> | 124.75     | 8.444        |              |            |              |
| I7CA-A8N-H | <b>60.09</b> | 129.53     | 8.479        | <b>60.08</b> | 129.5      | 8.481        |
| I7CB-N-H   | <b>38.91</b> | 124.81     | 8.439        |              |            |              |
| I7CB-A8N-H | <b>38.89</b> | 129.53     | 8.478        | <b>38.85</b> | 129.49     | 8.481        |
| A8CA-N-H   | <b>51.33</b> | 129.55     | 8.478        |              |            |              |
| A8CA-Q9N-H | <b>51.31</b> | 121.52     | 8.534        | <b>51.33</b> | 121.52     | 8.536        |
| A8CB-N-H   | <b>20.66</b> | 129.54     | 8.479        |              |            |              |

|              | HNCA-        | CB         |              | CACB-        | (CO)NH     |              |
|--------------|--------------|------------|--------------|--------------|------------|--------------|
| Assignment   | C, ppm       | N, ppm     | H, ppm       | C, ppm       | N, ppm     | H, ppm       |
| A8CB-Q9N-H   | <b>20.64</b> | 121.5      | 8.534        | <b>20.71</b> | 121.43     | 8.535        |
| Q9CA-N-H     | <b>56.37</b> | 121.5      | 8.534        |              |            |              |
| Q9CA-T10N-H  | <b>56.35</b> | 127.10     | 8.874        | <b>56.39</b> | 127.07     | 8.876        |
| Q9CB-N-H     | <b>29.65</b> | 121.49     | 8.533        |              |            |              |
| Q9CB-N-H     | <b>29.37</b> | 121.53     | 8.533        |              |            |              |
| Q9CB-T10-N-H | <b>29.49</b> | 127.06     | 8.874        | <b>29.53</b> | 127.05     | 8.876        |
| T10CA-N-H    | <b>64.30</b> | 127.14     | 8.874        |              |            |              |
| T10CA-G11N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | <i>peak</i>  | <i>not</i> | <i>found</i> |
| T10CB-N-H    | <b>68.65</b> | 127.11     | 8.874        |              |            |              |
| T10CB-N-H    | <b>68.93</b> | 127.12     | 8.874        |              |            |              |
| T10CB-G11N-H | <i>peak</i>  | <i>not</i> | <i>found</i> | <i>peak</i>  | <i>not</i> | <i>found</i> |
| G11CA-N-H    | <i>peak</i>  | <i>not</i> | <i>found</i> |              |            |              |
| G11CA-F12N-H | <b>46.08</b> | 118.83     | 7.015        | <b>46.12</b> | 118.83     | 7.017        |
| F12CA-N-H    | <b>57.62</b> | 118.85     | 7.015        |              |            |              |
| F12CA-N13N-H | <b>57.60</b> | 128.12     | 8.756        | <b>57.6</b>  | 128.1      | 8.757        |
| F12CB-N-H    | <b>39.94</b> | 118.85     | 7.015        |              |            |              |
| F12CB-N13N-H | <b>39.95</b> | 128.11     | 8.754        | <b>39.94</b> | 128.11     | 8.757        |
| N13CA-N-H    | <b>51.31</b> | 128.13     | 8.754        |              |            |              |
| N13CA-K14N-H | <b>51.27</b> | 125.41     | 7.987        | <b>51.29</b> | 125.39     | 7.99         |
| N13CB-N-H    | <b>37.36</b> | 128.16     | 8.755        |              |            |              |
| N13CB-K14N-H | <b>37.3</b>  | 125.34     | 7.988        | <b>37.32</b> | 125.38     | 7.99         |
| K14CA-N-H    | <b>58.74</b> | 125.41     | 7.987        |              |            |              |
| K14CA-D15N-H | <b>58.74</b> | 120.18     | 8.022        | <b>58.74</b> | 120.18     | 8.022        |
| K14CBN--H    | <b>32.17</b> | 125.38     | 7.988        |              |            |              |
| K14CB-D15N-H | <b>32.15</b> | 120.25     | 8.023        | <b>32.18</b> | 120.2      | 8.022        |
| D15CAN--H    | <b>57.3</b>  | 120.22     | 8.02         |              |            |              |
| D15CA-K16N-H | <b>57.28</b> | 116.71     | 7.067        | <b>57.28</b> | 116.71     | 7.067        |
| D15CB-N-H    | <b>40.42</b> | 120.18     | 8.02         |              |            |              |
| D15CB-K16N-H | <b>40.35</b> | 116.73     | 7.065        | <b>40.4</b>  | 116.72     | 7.068        |
| K16CA-N-H    | <b>57.85</b> | 116.74     | 7.066        |              |            |              |
| K16CA-Y17N-H | <b>57.87</b> | 118.46     | 7.013        | <b>57.87</b> | 118.46     | 7.013        |
| K16CB-N-H    | <b>33.42</b> | 116.74     | 7.066        |              |            |              |

|               | HNCA-  | CB     |        | CACB-  | (CO)NH  |        |
|---------------|--------|--------|--------|--------|---------|--------|
| Assignment    | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm  | H, ppm |
| K16CB-Y17N-H  | 33.43  | 118.47 | 7.013  | 33.45  | 118.45  | 7.013  |
| Y17CA-N-H     | 62.30  | 118.47 | 7.013  |        |         |        |
| Y17CA-F18N-H  | 62.30  | 118.41 | 8.421  | 62.31  | 118.39  | 8.424  |
| Y17CB-N-h     | 41.12  | 118.46 | 7.012  |        |         |        |
| Y17CB-F18N-H  | 41.11  | 118.33 | 8.422  | 41.12  | 118.41  | 8.424  |
| F18CA-N-H     | 56.38  | 118.42 | 8.421  |        |         |        |
| F18CA-N19N-H  | 56.41  | 118.71 | 7.856  | 56.41  | 118.64  | 7.858  |
| F18CB-N-H     | 36.74  | 118.42 | 8.421  |        |         |        |
| F18CB-N19N-H  | 36.74  | 118.65 | 7.857  | 36.75  | 118.64  | 7.858  |
| N19CA-N-H     | 52.48  | 118.65 | 7.855  |        |         |        |
| N19CA-G20-N-H | 52.49  | 110.38 | 9.265  | 52.50  | 110.38  | 9.263  |
| N19CB-N-H     | 38.49  | 118.64 | 7.856  |        |         |        |
| N19CB-G20-N-H | 38.47  | 110.39 | 9.261  | 38.49  | 110.38  | 9.264  |
| G20N-CA-H     | 45.41  | 110.42 | 9.262  |        |         |        |
| G20CA-D21N-H  | 45.4   | 118.55 | 7.645  | 45.43  | 118.63  | 7.648  |
| D21CA-N-H     | 51.56  | 118.68 | 7.645  |        |         |        |
| D21CA-V22N-H  | 51.53  | 119.09 | 8.217  | 51.57  | 119.14  | 8.219  |
| D21CB-N-H     | 42.51  | 118.65 | 7.645  |        |         |        |
| D21CB-V22N-H  | 42.57  | 119.12 | 8.217  | 42.58  | 119.15  | 8.219  |
| V22CA-N-H     | 63.06  | 119.17 | 8.217  |        |         |        |
| V22CA-W23N-H  | 63.06  | 127.69 | 9.632  | 63.06  | 127.69  | 9.632  |
| V22CB-N-H     | 33.01  | 119.15 | 8.222  |        |         |        |
| V22CB-W23N-H  | 33     | 127.59 | 9.63   | 33.005 | 127.683 | 9.631  |
| W23CA-N-H     | 55.93  | 127.69 | 9.629  |        |         |        |
| W23CA-Y24N-H  | 55.98  | 119.00 | 9.005  | 55.917 | 119.07  | 9.005  |
| W23CB-N-H     | 34.1   | 127.69 | 9.63   |        |         |        |
| W23CB-Y24N-H  | 34.05  | 119.06 | 9.009  | 34.122 | 119.071 | 9.006  |
| Y24CA-N-H     | 57.59  | 119.06 | 9.002  |        |         |        |
| Y24CA-V25N-H  | 57.59  | 120.55 | 8.547  | 57.625 | 120.726 | 8.551  |
| Y24CB-N-H     | 40.04  | 119.05 | 9.005  |        |         |        |
| Y24CB-V25N-H  | 40.03  | 120.61 | 8.552  | 40.047 | 120.682 | 8.555  |
| V25CA-N-H     | 63.66  | 120.77 | 8.55   |        |         |        |

|              | HNCA-  | CB     |        | CACB-  | (CO)NH  |        |
|--------------|--------|--------|--------|--------|---------|--------|
| Assignment   | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm  | H, ppm |
| V25CA-T26N-H | 63.7   | 122.91 | 10.067 | 63.7   | 122.91  | 10.067 |
| V25CB-N-H    | 32.63  | 120.74 | 8.559  |        |         |        |
| V25CB-T26N-H | 32.72  | 122.81 | 10.073 | 32.671 | 122.913 | 10.061 |
| T26CA-N-H    | 64.01  | 122.93 | 10.069 |        |         |        |
| T26CA-D27N-H | 63.99  | 120.54 | 8.597  | 63.99  | 120.54  | 8.597  |
| T26CB-N-H    | 69.01  | 122.94 | 10.072 |        |         |        |
| T26CB-N-H    | 69.24  | 122.88 | 10.072 |        |         |        |
| T26CB-D27N-H | 69.11  | 120.52 | 8.595  | 69.11  | 120.52  | 8.595  |
| D27CA-N-H    | 53.96  | 120.56 | 8.591  |        |         |        |
| D27CA-Y28N-H | 53.96  | 119.38 | 10.306 | 53.97  | 119.32  | 10.31  |
| D27CB-N-H    | 46.7   | 120.57 | 8.592  |        |         |        |
| D27CB-Y28N-H | 46.67  | 119.34 | 10.311 | 46.69  | 119.32  | 10.31  |
| Y28CA-N-H    | 58.2   | 119.33 | 10.308 |        |         |        |
| Y28CA-L29N-H | 58.2   | 123.41 | 9.235  | 58.21  | 123.45  | 9.232  |
| Y28CB-N-H    | 43.20  | 119.24 | 10.307 |        |         |        |
| Y28CB-L29N-H | 43.18  | 123.42 | 9.225  | 43.18  | 123.44  | 9.233  |
| L29CA-N-H    | 53.56  | 123.45 | 9.227  |        |         |        |
| L29CA-D30N-H | 53.55  | 127.36 | 8.366  | 53.56  | 127.41  | 8.363  |
| L29CB-N-H    | 43.42  | 123.45 | 9.222  |        |         |        |
| L29CB-D30N-H | 43.41  | 127.34 | 8.36   | 43.41  | 127.40  | 8.363  |
| D30CA-N-H    | 51.18  | 127.38 | 8.361  |        |         |        |
| D30CA-L31N-H | 51.17  | 123.62 | 6.96   | 51.21  | 123.69  | 6.964  |
| D30CB-N-H    | 40.86  | 127.38 | 8.363  |        |         |        |
| D30CB-L31N-H | 40.82  | 123.59 | 6.962  | 40.87  | 123.71  | 6.966  |
| L31CA-N-H    | 55.29  | 123.63 | 6.968  |        |         |        |
| L31CA-E32N-H | 55.28  | 119.66 | 7.206  | 55.34  | 119.78  | 7.21   |
| L31CB-N-H    | 40.89  | 123.63 | 6.962  |        |         |        |
| L31CB-E32N-H | 40.83  | 119.76 | 7.207  | 40.89  | 119.78  | 7.212  |
| E32CA-N-H    | 52.89  | 119.79 | 7.21   |        |         |        |
| E32CB-N-H    | 29.02  | 119.78 | 7.209  |        |         |        |
| E32CB-N-H    | 29.31  | 119.79 | 7.209  |        |         |        |
| P33CA-D34N-H | 62.47  | 120.80 | 8.166  | 62.48  | 120.77  | 8.167  |

|              | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|--------------|--------|--------|--------|--------|--------|--------|
| Assignment   | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| P33CB-D34N-H | 32.11  | 120.79 | 8.163  | 32.16  | 120.76 | 8.166  |
| D34CA-N-H    | 53.83  | 120.79 | 8.163  |        |        |        |
| D34CA-D35N-H | 53.81  | 120.41 | 8.358  | 53.85  | 120.45 | 8.36   |
| D34CB-N-H    | 42.26  | 120.74 | 8.163  |        |        |        |
| D34CB-D35N-H | 42.23  | 120.45 | 8.358  | 42.27  | 120.43 | 8.36   |
| D35CA-N-H    | 56.88  | 120.44 | 8.358  |        |        |        |
| D35CA-V36N-H | 56.87  | 119.18 | 8.203  | 56.88  | 119.18 | 8.205  |
| D35CB-N-H    | 40.75  | 120.5  | 8.358  |        |        |        |
| D35CB-V36N-H | 40.76  | 119.18 | 8.201  | 40.78  | 119.18 | 8.205  |
| V36CA-N-H    | 59.9   | 119.22 | 8.202  |        |        |        |
| V36CB-N-H    | 32.06  | 119.21 | 8.203  |        |        |        |
| V36CB-N-H    | 32.39  | 119.21 | 8.204  |        |        |        |
| P37CA-K38N-H | 63.85  | 124.29 | 9.905  | 63.89  | 124.29 | 9.908  |
| P37CB-K38N-H | 33.03  | 124.18 | 9.902  | 33.06  | 124.27 | 9.909  |
| K38N-CA-H    | 57.27  | 124.46 | 9.9    |        |        |        |
| K38CA-R39N-H | 57.21  | 127.48 | 9.78   | 57.21  | 127.48 | 9.78   |
| K38N-CB-H    | 35.29  | 124.46 | 9.905  |        |        |        |
| K38CB-R39N-H | 35.28  | 127.49 | 9.798  | 35.28  | 127.49 | 9.798  |
| R39CA-N-H    | 55.91  | 127.52 | 9.783  |        |        |        |
| R39CA-Y40N-H | peak   | not    | found  | peak   | not    | found  |
| R39CB-N-H    | 28.98  | 127.42 | 9.798  |        |        |        |
| R39CB-Y40N-H | peak   | not    | found  | peak   | not    | found  |
| Y40CA-C41N-H | peak   | not    | found  | peak   | not    | found  |
| Y40CB-C41N-H | peak   | not    | found  | peak   | not    | found  |
| C41CA-A42N-H | peak   | not    | found  | peak   | not    | found  |
| C41CB-A42N-H | peak   | not    | found  | peak   | not    | found  |
| A42CA-A43N-H | peak   | not    | found  | peak   | not    | found  |
| A42CB-A43N-H | peak   | not    | found  | peak   | not    | found  |
| A43CA-N-H    | peak   | not    | found  |        |        |        |
| A43CA-L44N-H | 49.78  | 116.14 | 8.875  | 49.77  | 116.18 | 8.881  |
| A43CB-L44N-H | 22.89  | 116.11 | 8.874  | 22.89  | 116.18 | 8.879  |
| L44CA-N-H    | 53.99  | 116.23 | 8.874  |        |        |        |

|              | HNCA-  | CB      |        | CACB-  | (CO)NH  |        |
|--------------|--------|---------|--------|--------|---------|--------|
| Assignment   | C, ppm | N, ppm  | H, ppm | C, ppm | N, ppm  | H, ppm |
| L44CA-A45N-H | 53.97  | 121.583 | 8.997  | 53.97  | 121.568 | 8.999  |
| L44CB-N-H    | 46.83  | 116.21  | 8.878  |        |         |        |
| L44CB-A45N-H | 46.84  | 121.65  | 8.997  | 46.79  | 121.57  | 8.999  |
| A45CA-N-H    | 52.00  | 121.51  | 8.997  |        |         |        |
| A45CA-A46N-H | 52.03  | 125.81  | 8.822  | 52.03  | 125.81  | 8.822  |
| A45CB-N-H    | 21.98  | 121.57  | 8.997  |        |         |        |
| A45CB-A46N-H | 21.99  | 125.84  | 8.819  | 22.01  | 125.81  | 8.82   |
| A46CA-N-H    | 51.45  | 125.85  | 8.819  |        |         |        |
| A46CA-G47N-H | 51.49  | 108.01  | 9.218  | 51.48  | 107.97  | 9.218  |
| A46CB-N-H    | 23.56  | 125.87  | 8.818  |        |         |        |
| A46CB-G47N-H | 23.55  | 107.97  | 9.216  | 23.57  | 107.97  | 9.218  |
| G47CA-N-H    | 45.72  | 107.96  | 9.217  |        |         |        |
| G47CA-T48N-H | 45.72  | 113.20  | 8.594  | 45.73  | 113.22  | 8.596  |
| T48CA-N-H    | 61.44  | 113.25  | 8.594  |        |         |        |
| T48CA-A49N-H | 61.45  | 128.48  | 8.987  | 61.42  | 128.43  | 8.989  |
| T48CB-N-H    | 69.83  | 113.27  | 8.594  |        |         |        |
| T48CB-N-H    | 69.63  | 113.26  | 8.594  |        |         |        |
| T48CB-A49N-H | 69.69  | 128.45  | 8.986  | 69.72  | 128.42  | 8.989  |
| A49CA-N-H    | 53.18  | 128.47  | 8.986  |        |         |        |
| A49CA-S50N-H | peak   | not     | found  | peak   | Not     | found  |
| A49CB-N-H    | 20.57  | 128.46  | 8.986  |        |         |        |
| A49CB-S50N-H | peak   | not     | found  | peak   | Not     | found  |
| S50CA-G51N-H | 59.05  | 106.84  | 8.497  | 59.12  | 106.74  | 8.502  |
| S50CB-G51N-H | 62.72  | 106.66  | 8.498  | 62.7   | 106.74  | 8.501  |
| G51CA-N-H    | 45.1   | 106.72  | 8.501  |        |         |        |
| G51CA-K52N-H | 45.07  | 120.38  | 7.88   | 45.12  | 120.39  | 7.882  |
| K52CA-N-H    | 54.4   | 120.41  | 7.88   |        |         |        |
| K52CA-L53N-H | 54.39  | 123.38  | 8.611  | 54.42  | 123.37  | 8.614  |
| K52CB-N-H    | 35.46  | 120.5   | 7.88   |        |         |        |
| K52CB-L53N-H | 35.45  | 123.36  | 8.612  | 35.45  | 123.37  | 8.614  |
| L53CA-N-H    | 55.38  | 123.36  | 8.611  |        |         |        |
| L53CA-K54N-H | 55.39  | 126.56  | 8.957  | 55.38  | 126.58  | 8.959  |

|              | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|--------------|--------|--------|--------|--------|--------|--------|
| Assignment   | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| L53CB-N-H    | 42.51  | 123.41 | 8.612  |        |        |        |
| L53CB-K54N-H | 42.50  | 126.53 | 8.958  | 42.532 | 126.60 | 8.959  |
| K54CA-N-H    | 54.55  | 126.56 | 8.957  |        |        |        |
| K54CA-E55N-H | 54.51  | 118.73 | 8.937  | 54.56  | 118.78 | 8.939  |
| K54CB-N-H    | 37.75  | 126.57 | 8.957  |        |        |        |
| K54CB-E55N-H | 37.77  | 118.72 | 8.936  | 37.76  | 118.76 | 8.939  |
| E55CA-N-H    | 56.41  | 118.80 | 8.937  |        |        |        |
| E55CA-A56N-H | 56.40  | 133.63 | 9.866  | 56.45  | 133.60 | 9.869  |
| E55CB-N-H    | 36.38  | 118.80 | 8.935  |        |        |        |
| E55CB-A56N-H | 36.45  | 133.64 | 9.865  | 36.39  | 133.62 | 9.868  |
| A56CA-N-H    | 49.98  | 133.62 | 9.863  |        |        |        |
| A56CA-L57N-H | 50.01  | 121.53 | 8.511  | 50.04  | 121.67 | 8.508  |
| A56CB-N-H    | 22.80  | 133.63 | 9.866  |        |        |        |
| A56CB-L57N-H | 22.76  | 121.61 | 8.511  | 22.81  | 121.65 | 8.511  |
| L57CB-N-H    | 46.77  | 121.51 | 8.511  |        |        |        |
| L57CA-Y58N-H | peak   | not    | found  | peak   | not    | found  |
| L57CB-Y58N-H | peak   | not    | found  | peak   | not    | found  |
| Y58CA-H59N-H | peak   | not    | found  | peak   | not    | found  |
| Y58CB-H59N-H | peak   | not    | found  | peak   | not    | found  |
| H59CA-Y60N-H | peak   | not    | found  | peak   | not    | found  |
| H59CB-Y60N-H | peak   | not    | found  | peak   | not    | found  |
| Y60CA-D61N-H | peak   | not    | found  | peak   | not    | found  |
| Y60CB-D61N-H | peak   | not    | found  | peak   | not    | found  |
| D61CA-P62N-H | peak   | not    | found  | peak   | not    | found  |
| D61CB-P62N-H | peak   | not    | found  | peak   | not    | found  |
| P62CA-K63N-H | 63.67  | 116.68 | 7.986  | 63.69  | 116.60 | 7.987  |
| P62CB-K63N-H | 32.95  | 116.58 | 7.987  | 32.95  | 116.60 | 7.987  |
| K63CA-N-H    | 58.72  | 116.59 | 7.985  |        |        |        |
| K63CA-T64N-H | 58.73  | 105.19 | 6.6    | 58.75  | 105.18 | 6.603  |
| K63CB-N-H    | 32.47  | 116.58 | 7.985  |        |        |        |
| K63CB-T64N-H | 32.46  | 105.21 | 6.602  | 32.48  | 105.18 | 6.603  |
| T64CA-N-H    | 61.36  | 105.21 | 6.601  |        |        |        |

|              | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|--------------|--------|--------|--------|--------|--------|--------|
| Assignment   | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| T64CA-Q65N-H | 61.36  | 115.13 | 8.011  | 61.31  | 115.16 | 8.012  |
| T64CB-N-H    | 71.03  | 105.19 | 6.601  |        |        |        |
| T64CB-Q65N-H | 71.05  | 115.15 | 8.009  | 71.08  | 115.16 | 8.013  |
| Q65CA-N-H    | 57.83  | 115.18 | 8.01   |        |        |        |
| Q65CA-D66N-H | 57.80  | 119.62 | 7.34   | 57.86  | 119.67 | 7.343  |
| Q65CB-N-H    | 25.40  | 115.19 | 8.01   |        |        |        |
| Q65CB-D66N-H | 25.39  | 119.66 | 7.341  | 25.45  | 119.68 | 7.342  |
| D66CA-N-H    | 55.20  | 119.64 | 7.342  |        |        |        |
| D66CA-T67N-H | 55.23  | 114.10 | 7.187  | 55.27  | 114.03 | 7.189  |
| D66CB-N-H    | 41.77  | 119.72 | 7.34   |        |        |        |
| D66CB-T67N-H | 41.78  | 114.12 | 7.184  | 41.75  | 114.03 | 7.188  |
| T67CA-N-H    | 58.48  | 114.06 | 7.186  |        |        |        |
| T67CA-F68N-H | peak   | not    | found  | 58.52  | 114.62 | 5.059  |
| T67CB-N-H    | 71.67  | 114.03 | 7.185  |        |        |        |
| T67CB-N-H    | 71.83  | 114.03 | 7.186  |        |        |        |
| T67CB-F68N-H | peak   | not    | found  | 71.74  | 114.64 | 5.05   |
| F68CA-Y69N-H | 54.57  | 117.77 | 6.816  | 54.57  | 117.77 | 6.816  |
| F68CB-Y69N-H | 39.35  | 117.87 | 6.813  | 39.4   | 117.78 | 6.82   |
| Y69CA-N-H    | 54.67  | 117.80 | 6.814  |        |        |        |
| Y69CA-D70N-H | 54.67  | 115.57 | 7.429  | 54.69  | 115.41 | 7.428  |
| Y69CB-N-H    | 41.06  | 117.85 | 6.807  |        |        |        |
| Y69CB-D70N-H | 41.04  | 115.29 | 7.417  | 41.07  | 115.45 | 7.415  |
| D70CA-N-H    | 52.07  | 115.42 | 7.423  |        |        |        |
| D70CA-V71N-H | 52.10  | 118.01 | 9.413  | 52.14  | 118.11 | 9.415  |
| D70CB-N-H    | 43.89  | 115.51 | 7.427  |        |        |        |
| D70CB-V71N-H | 43.98  | 118.07 | 9.412  | 43.99  | 118.09 | 9.415  |
| V71CA-N-H    | 61.69  | 118.18 | 9.412  |        |        |        |
| V71CA-S72N-H | 61.68  | 122.18 | 9.192  | 61.68  | 122.19 | 9.195  |
| V71CB-N-H    | 35.83  | 118.20 | 9.411  |        |        |        |
| V71CB-S72N-H | 35.92  | 122.09 | 9.196  | 35.91  | 122.19 | 9.194  |
| S72CA-N-H    | 58.62  | 122.20 | 9.192  |        |        |        |
| S72CA-E73N-H | 58.61  | 124.21 | 9.057  | 58.61  | 124.24 | 9.06   |

|              | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|--------------|--------|--------|--------|--------|--------|--------|
| Assignment   | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| S72CB-N-H    | 67.62  | 122.16 | 9.191  |        |        |        |
| S72CB-E73N-H | 67.61  | 124.23 | 9.058  | 67.62  | 124.25 | 9.06   |
| E73CA-N-H    | 56.25  | 124.27 | 9.06   |        |        |        |
| E73CA-L74N-H | 56.30  | 124.38 | 8.612  | 56.30  | 124.38 | 8.612  |
| E73CB-N-H    | 29.81  | 124.31 | 9.058  |        |        |        |
| E73CB-N-H    | 30.09  | 124.31 | 9.058  |        |        |        |
| E73CB-L74N-H | 29.94  | 124.41 | 8.612  | 29.984 | 124.38 | 8.613  |
| L74CA-N-H    | 54.87  | 124.39 | 8.61   |        |        |        |
| L74CA-Q75N-H | 54.87  | 122.04 | 9.434  | 54.91  | 122.02 | 9.436  |
| L74CB-N-H    | 43.11  | 124.40 | 8.61   |        |        |        |
| L74CB-Q75N-H | 43.14  | 122.04 | 9.431  | 43.13  | 122.03 | 9.437  |
| Q75CA-N-H    | 54.11  | 122.01 | 9.434  |        |        |        |
| Q75CA-V76N-H | 54.10  | 126.08 | 8.882  | 54.12  | 126.16 | 8.886  |
| Q75CB-N-H    | 30.49  | 122.02 | 9.435  |        |        |        |
| Q75CB-N-H    | 30.72  | 122.01 | 9.433  |        |        |        |
| Q75CB-V76N-H | 30.65  | 126.06 | 8.883  | 30.63  | 126.17 | 8.886  |
| V76CA-N-H    | 62.89  | 126.11 | 8.883  |        |        |        |
| V76CA-E77N-H | 62.89  | 129.98 | 8.689  | 62.88  | 130.01 | 8.692  |
| V76CB-N-H    | 32.35  | 126.07 | 8.886  |        |        |        |
| V76CB-N-H    | 32.61  | 126.12 | 8.882  |        |        |        |
| V76CB-E77N-H | 32.44  | 130.   | 8.686  | 32.47  | 130.   | 8.692  |
| E77CA-N-H    | 57.62  | 129.96 | 8.688  |        |        |        |
| E77CA-S78N-H | 57.63  | 111.55 | 8.053  | 57.63  | 111.55 | 8.053  |
| E77CB-N-H    | 29.74  | 129.99 | 8.691  |        |        |        |
| E77CB-S78N-H | 29.75  | 111.65 | 8.052  | 29.87  | 111.55 | 8.053  |
| S78CA-N-H    | 57.07  | 111.60 | 8.051  |        |        |        |
| S78CA-L79N-H | peak   | not    | found  | peak   | not    | found  |
| S78CB-N-H    | 62.94  | 111.60 | 8.052  |        |        |        |
| S78CB-L79N-H | peak   | not    | found  | peak   | not    | found  |
| L79CA-N-H    |        |        |        |        |        |        |
| L79CA-G80N-H | 58.04  | 114.58 | 8.377  | 58.042 | 114.58 | 8.377  |
| L79CB-N-H    |        |        |        |        |        |        |
| L79CB-G80N-H | 40.99  | 114.58 | 8.377  | 40.99  | 114.58 | 8.377  |

|              | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|--------------|--------|--------|--------|--------|--------|--------|
| Assignment   | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
|              |        |        |        |        |        |        |
| G80CA-N-H    | 46.29  | 114.61 | 8.376  |        |        |        |
| G80CA-K81N-H | 46.28  | 121.83 | 7.881  | 46.31  | 121.84 | 7.883  |
| K81CA-N-H    | 56.15  | 121.83 | 7.881  |        |        |        |
| K81CA-Y82H   | 56.16  | 120.95 | 8.286  | 56.14  | 121.08 | 8.29   |
| K81CB-N-H    | 35.44  | 121.83 | 7.88   |        |        |        |
| K81CB-Y82N-H | 35.44  | 120.93 | 8.285  | 35.45  | 121.05 | 8.29   |
| Y82CA-N-H    | 56.93  | 121.12 | 8.286  |        |        |        |
| Y82CA-T83N-H | 56.93  | 117.10 | 9.087  | 56.95  | 117.09 | 9.087  |
| Y82CB-N-H    | 44.08  | 121.14 | 8.286  |        |        |        |
| Y82CB-T83N-H | 44.03  | 117.13 | 9.086  | 44.06  | 117.09 | 9.088  |
| T83CA-N-H    | 62.69  | 117.08 | 9.085  |        |        |        |
| T83CA-A84N-H | 62.68  | 132.39 | 10.179 | 62.66  | 132.38 | 10.179 |
| T83CB-N-H    | 70.93  | 117.11 | 9.085  |        |        |        |
| T83CB-N-H    | 70.63  | 117.10 | 9.085  |        |        |        |
| T83CB-A84N-H | 70.79  | 132.39 | 10.176 | 70.79  | 132.39 | 10.179 |
| A84CA-N-H    | 51.99  | 132.47 | 10.176 |        |        |        |
| A84CA-N85N-H | 52.06  | 124.01 | 8.43   | 52.02  | 123.95 | 8.43   |
| A84CB-N-H    | 21.51  | 132.45 | 10.175 |        |        |        |
| A84CB-N85N-H | 21.53  | 123.91 | 8.428  | 21.51  | 123.94 | 8.43   |
| N85CA-N-H    | 53.81  | 123.95 | 8.428  |        |        |        |
| N85CA-F86N-H | 53.89  | 119.99 | 7.368  | 53.82  | 120.11 | 7.369  |
| N85CB-N-H    | 39.02  | 123.94 | 8.432  |        |        |        |
| N85CB-F86N-H | 39.10  | 120.06 | 7.364  | 39.05  | 120.09 | 7.368  |
| F86CA-N-H    | 57.05  | 120.08 | 7.366  |        |        |        |
| F86CA-K87N-H | 57.06  | 120.57 | 9.283  | 57.07  | 120.60 | 9.288  |
| F86CB-N-H    | 42.79  | 120.11 | 7.366  |        |        |        |
| F86CB-K87N-H | 42.84  | 120.43 | 9.288  | 42.78  | 120.59 | 9.288  |
| K87CA-N-H    | 54.74  | 120.68 | 9.287  |        |        |        |
| K87CA-K88N-H | 54.76  | 127.32 | 9.179  | 54.77  | 127.31 | 9.182  |
| K87CB-N-H    | 35.51  | 120.64 | 9.287  |        |        |        |
| K87CB-K88N-H | 35.55  | 127.26 | 9.18   | 35.57  | 127.30 | 9.182  |

|              | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|--------------|--------|--------|--------|--------|--------|--------|
| Assignment   | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| K88CA-N-H    | 56.55  | 127.26 | 9.181  |        |        |        |
| K88CA-V89N-H | 56.6   | 120.96 | 8.42   | 56.59  | 121.04 | 8.424  |
| K88CB-N-H    | 34.42  | 127.26 | 9.18   |        |        |        |
| K88CB-V89N-H | 34.44  | 121.01 | 8.421  | 34.45  | 121.00 | 8.425  |
| V89CA-N-H    | 58.27  | 120.90 | 8.422  |        |        |        |
| V89CA-D90N-H | 58.26  | 118.48 | 7.949  | 58.30  | 118.62 | 7.952  |
| V89CB-N-H    | 36.95  | 120.91 | 8.422  |        |        |        |
| V89CB-D90N-H | 36.94  | 118.56 | 7.95   | 36.90  | 118.63 | 7.952  |
| D90CA-N-H    | 51.84  | 118.64 | 7.949  |        |        |        |
| D90CA-K91N-H | 51.86  | 114.27 | 7.79   | 51.86  | 114.23 | 7.791  |
| D90CB-N-H    | 41.50  | 118.64 | 7.949  |        |        |        |
| D90CB-K91N-H | 41.45  | 114.34 | 7.788  | 41.52  | 114.22 | 7.791  |
| K91CA-N-H    | 57.97  | 114.29 | 7.789  |        |        |        |
| K91CA-N92N-H | 57.95  | 114.32 | 7.223  | 58.00  | 114.30 | 7.227  |
| K91CB-N-H    | 30.72  | 114.27 | 7.788  |        |        |        |
| K91CB-N92N-H | 30.69  | 114.34 | 7.224  | 30.75  | 114.31 | 7.227  |
| N92CA-N-H    | 52.62  | 114.34 | 7.225  |        |        |        |
| N92CA-G93N-H | 52.62  | 108.38 | 7.936  | 52.66  | 108.40 | 7.937  |
| N92CB-N-H    | 39.94  | 114.35 | 7.225  |        |        |        |
| N92CB-G93N-H | 39.92  | 108.44 | 7.933  | 39.94  | 108.39 | 7.937  |
| G93CA-N-H    | 45.07  | 108.42 | 7.934  |        |        |        |
| G93CA-N94N-H | 45.05  | 120.25 | 8.279  | 45.08  | 120.34 | 8.282  |
| N94CA-N-H    | 53.64  | 120.35 | 8.279  |        |        |        |
| N94CA-V95N-H | 53.65  | 123.44 | 8.762  | 53.63  | 123.43 | 8.764  |
| N94CB-N-H    | 37.99  | 120.34 | 8.28   |        |        |        |
| N94CB-V95N-H | 37.96  | 123.39 | 8.762  | 37.99  | 123.42 | 8.764  |
| V95CA-N-H    | 65.06  | 123.39 | 8.762  |        |        |        |
| V95CA-K96N-H | 65.06  | 128.09 | 9.49   | 65.06  | 128.12 | 9.492  |
| V95CB-N-H    | 31.98  | 123.40 | 8.762  |        |        |        |
| V95CB-K96N-H | 32.09  | 128.14 | 9.488  | 32.10  | 128.12 | 9.492  |
| K96CA-N-H    | 56.30  | 128.16 | 9.49   |        |        |        |
| K96CA-V97N-H | 56.25  | 119.62 | 7.99   | 56.29  | 119.62 | 7.991  |

|                | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|----------------|--------|--------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| K96CB-N-H      | 32.95  | 128.15 | 9.487  |        |        |        |
| K96CB-V97N-H   | 32.95  | 119.62 | 7.994  | 32.95  | 119.62 | 7.994  |
| V97CA-N-H      | 62.95  | 119.63 | 7.997  |        |        |        |
| V97CA-A98N-H   | 62.96  | 128.24 | 8.597  | 62.94  | 128.22 | 8.599  |
| V97CB-N-H      | 34.83  | 119.67 | 7.997  |        |        |        |
| V97CB-A98N-H   | 34.83  | 128.26 | 8.597  | 34.90  | 128.23 | 8.599  |
| A98CA-N-H      | 52.41  | 128.28 | 8.597  |        |        |        |
| A98CA-V99N-H   | 52.40  | 122.19 | 8.548  | 52.45  | 122.17 | 8.549  |
| A98CB-N-H      | 19.99  | 128.32 | 8.598  |        |        |        |
| A98CB-V99N-H   | 19.98  | 122.13 | 8.547  | 19.99  | 122.25 | 8.549  |
| V99CA-N-H      | 64.92  | 122.19 | 8.547  |        |        |        |
| V99CA-T100N-H  | 64.93  | 126.07 | 9.973  | 64.91  | 126.11 | 9.979  |
| V99CB-N-H      | 31.77  | 122.16 | 8.546  |        |        |        |
| V99CB-T100N-H  | 31.73  | 126.04 | 9.977  | 31.79  | 126.11 | 9.978  |
| T100CA-N-H     | 61.80  | 126.10 | 9.975  |        |        |        |
| T100CA-A101N-H | 61.83  | 131.29 | 8.896  | 61.80  | 131.27 | 8.902  |
| T100CB-N-H     | 72.64  | 126.07 | 9.974  |        |        |        |
| T100CB-A101N-H | 72.67  | 131.26 | 8.903  | 72.67  | 131.26 | 8.903  |
| A101CA-N-H     | 54.20  | 131.32 | 8.902  |        |        |        |
| A101CA-G102N-H | 54.21  | 110.28 | 9.152  | 54.25  | 110.23 | 9.153  |
| A101CB-N-H     | 18.04  | 131.23 | 8.898  |        |        |        |
| A101CB-G102N-H | 18.08  | 110.26 | 9.16   | 18.06  | 110.24 | 9.151  |
| G102N-CA-H     | 45.29  | 110.36 | 9.15   |        |        |        |
| G102CA-N103N-H | 45.24  | 121.11 | 8.202  | 45.28  | 121.06 | 8.203  |
| N103CA-N-H     | 51.42  | 121.04 | 8.2    |        |        |        |
| N103CA-Y104N-H | 51.42  | 121.16 | 9.214  | 51.41  | 121.19 | 9.213  |
| N103CB-N-H     | 37.89  | 121.01 | 8.2    |        |        |        |
| N103CB-Y104N-H | 37.85  | 121.16 | 9.214  | 37.91  | 121.18 | 9.213  |
| Y104CA-N-H     | 57.83  | 121.22 | 9.21   |        |        |        |
| Y104CA-Y105N-H | 57.84  | 116.21 | 10.223 | 57.83  | 116.26 | 10.224 |
| Y104CB-N-H     | 39.75  | 121.21 | 9.209  |        |        |        |
| Y104CB-Y105N-H | 39.77  | 116.24 | 10.218 | 39.77  | 116.25 | 10.227 |

|                | HNCA-  | CB      |        | CACB-  | (CO)NH |        |
|----------------|--------|---------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm  | H, ppm | C, ppm | N, ppm | H, ppm |
| Y105CA-N-H     | 56.24  | 116.19  | 10.223 |        |        |        |
| Y105CA-T106N-H | 56.28  | 113.57  | 8.475  | 56.25  | 113.60 | 8.484  |
| Y105CB-N-H     | 43.57  | 116.18  | 10.217 |        |        |        |
| Y105CB-T106N-H | 43.55  | 113.67  | 8.485  | 43.56  | 113.67 | 8.48   |
| T106CA-N-H     | 59.62  | 113.61  | 8.474  |        |        |        |
| T106CA-F107N-H | 59.63  | 119.77  | 9.471  | 59.63  | 119.69 | 9.471  |
| T106CB-N-H     | 70.98  | 113.60  | 8.484  |        |        |        |
| T106CB-N-H     | 71.15  | 113.62  | 8.477  |        |        |        |
| T106CB-F107N-H | 71.10  | 119.73  | 9.468  | 71.09  | 119.70 | 9.471  |
| F107CA-N-H     | 56.82  | 119.63  | 9.468  |        |        |        |
| F107CA-T108N-H | 56.85  | 117.73  | 9.34   | 56.89  | 117.61 | 9.341  |
| F107CB-N-H     | 44.11  | 119.70  | 9.47   |        |        |        |
| F107CB-T108N-H | 44.11  | 117.68  | 9.335  | 44.17  | 117.61 | 9.342  |
| T108CA-N-H     | 61.06  | 117.56  | 9.339  |        |        |        |
| T108CA-V109N-H | 61.03  | 127.86  | 9.343  | 61.04  | 127.9  | 9.345  |
| T108CB-N-H     | 72.29  | 117.59  | 9.34   |        |        |        |
| T108CB-N-H     | 71.92  | 117.60  | 9.339  |        |        |        |
| T108CB-V109N-H | 72.07  | 127.85  | 9.341  | 72.12  | 127.90 | 9.344  |
| V109CA-N-H     | 63.10  | 127.92  | 9.344  |        |        |        |
| V109CA-M110N-H | 63.12  | 129.62  | 8.783  | 63.09  | 129.56 | 8.781  |
| V109CB-N-H     | 29.615 | 127.9   | 9.343  |        |        |        |
| V109CB-N-H     | 30.007 | 127.947 | 9.342  |        |        |        |
| V109CB-M110N-H | 29.813 | 129.65  | 8.778  | 29.80  | 129.51 | 8.783  |
| M110CA-N-H     | 58.138 | 129.563 | 8.78   |        |        |        |
| M110CA-Y111N-H | 58.144 | 117.67  | 8.204  | 58.15  | 117.60 | 8.209  |
| M110CB-N-H     | 35.149 | 129.561 | 8.778  |        |        |        |
| M110CB-Y111N-H | 35.198 | 117.621 | 8.205  | 35.20  | 117.67 | 8.207  |
| Y111CA-N-H     | 59.4   | 117.598 | 8.207  |        |        |        |
| Y111CA-A112N-H | 59.42  | 125.898 | 6.658  | 59.43  | 125.88 | 6.66   |
| Y111CB-N-H     | 42.371 | 117.649 | 8.205  |        |        |        |
| Y111CB-A112N-H | 42.418 | 125.941 | 6.656  | 42.40  | 125.88 | 6.66   |
| A112CA-N-H     | 52.938 | 125.889 | 6.658  |        |        |        |

|                | HNCA-  | CB      |        | CACB-  | (CO)NH |        |
|----------------|--------|---------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm  | H, ppm | C, ppm | N, ppm | H, ppm |
| A112CA-D113N-H | 52.95  | 121.49  | 9.5    | 52.95  | 121.49 | 9.5    |
| A112CB-N-H     | 22.32  | 125.9   | 6.658  |        |        |        |
| A112CB-D113N-H | 22.31  | 121.48  | 9.498  | 22.35  | 121.49 | 9.501  |
| D113CA-N-H     | 53.17  | 121.48  | 9.499  |        |        |        |
| D113CA-D114N-H | 53.17  | 114.79  | 8.356  | 53.17  | 114.83 | 8.358  |
| D113CB-N-H     | 40.80  | 121.50  | 9.498  |        |        |        |
| D113CB-D114N-H | 40.88  | 114.79  | 8.361  | 40.88  | 114.79 | 8.361  |
| D114N-CA-H     | 58.12  | 114.76  | 8.36   |        |        |        |
| D114CA-S115N-H | 58.13  | 110.88  | 8.699  | Peak   | Not    | found  |
| D114N-CB-H     | 40.95  | 114.78  | 8.358  |        |        |        |
| D114CB-S115N-H | 40.96  | 110.89  | 8.702  | Peak   | Not    | found  |
| S115CA-N-H     | 59.48  | 110.89  | 8.702  |        |        |        |
| S115CA-S116N-H | 59.45  | 118.01  | 8.884  | 40.96  | 110.91 | 8.704  |
| S115CB-N-H     | 66.70  | 110.89  | 8.702  |        |        |        |
| S115CB-S116N-H | 66.68  | 118.03  | 8.883  | 66.69  | 117.97 | 8.887  |
| S116CA-N-H     | 58.55  | 117.99  | 8.884  |        |        |        |
| S116CA-A117N-H | 58.55  | 117.61  | 8.585  | 58.55  | 117.64 | 8.586  |
| S116CB-N-H     | 69.33  | 117.99  | 8.884  |        |        |        |
| S116CB-A117N-H | 69.35  | 117.59  | 8.583  | 69.34  | 117.64 | 8.586  |
| A117CA-N-H     | 52.40  | 117.66  | 8.584  |        |        |        |
| A117CA-L118N-H | 52.406 | 121.539 | 9.267  | 52.43  | 121.52 | 9.268  |
| A117CB-N-H     | 22.863 | 117.668 | 8.584  |        |        |        |
| A117CB-L118N-H | 22.851 | 121.514 | 9.266  | 22.90  | 121.52 | 9.269  |
| L118CA-N-H     | 54.385 | 121.504 | 9.266  |        |        |        |
| L118CA-N-H     | 54.385 | 121.504 | 9.266  |        |        |        |
| L118CA-I119N-H | 54.361 | 119.793 | 9.767  | 54.40  | 119.85 | 9.772  |
| L118CB-N-H     | 46.675 | 121.563 | 9.266  |        |        |        |
| L118CB-I119N-H | 46.712 | 119.736 | 9.769  | 46.77  | 119.85 | 9.772  |
| I119CA-N-H     | 59.122 | 119.934 | 9.769  |        |        |        |
| I119CA-H120N-H | 59.086 | 122.314 | 8.831  | 59.12  | 122.36 | 8.836  |
| I119CB-N-H     | 42.83  | 119.916 | 9.77   |        |        |        |
| I119CB-H120N-H | 42.828 | 122.246 | 8.829  | 42.76  | 122.37 | 8.834  |

|                | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|----------------|--------|--------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| H120CA-N-H     | 56.09  | 122.39 | 8.831  |        |        |        |
| H120CA-T121N-H | 56.08  | 116.42 | 6.839  | 56.17  | 116.46 | 6.832  |
| H120CB-N-H     | 34.97  | 122.32 | 8.832  |        |        |        |
| H120CB-T121N-H | 34.95  | 116.43 | 6.833  | 34.95  | 116.43 | 6.833  |
| T121CA-N-H     | 58.71  | 116.51 | 6.828  |        |        |        |
| T121CA-C122N-H | 58.71  | 118.31 | 7.212  | 58.68  | 118.21 | 7.206  |
| T121CB-N-H     | 71.60  | 116.44 | 6.829  |        |        |        |
| T121CB-C122N-H | 71.62  | 118.33 | 7.207  | 71.66  | 118.27 | 7.242  |
| C122CA-N-H     | 53.48  | 118.23 | 7.216  |        |        |        |
| C122CA-L123N-H | 53.49  | 127.01 | 6.935  | 53.45  | 127.00 | 6.939  |
| C122CB-N-H     | 42.74  | 118.22 | 7.216  |        |        |        |
| C122CB-L123N-H | 42.74  | 126.95 | 6.931  | 42.69  | 127.01 | 6.938  |
| L123CA-N-H     | 48.54  | 127.07 | 6.941  |        |        |        |
| L123CA-H124N-H | peak   | Not    | found  | Peak   | Not    | found  |
| L123CB-N-H     | 41.89  | 127.11 | 6.941  |        |        |        |
| L123CB-H124N-H | peak   | Not    | found  | Peak   | Not    | found  |
| H124CA-K125N-H | 54.16  | 120.22 | 7.786  | 54.11  | 120.21 | 7.786  |
| H124CB-K125N-H | 29.94  | 120.19 | 7.781  | 30.02  | 120.24 | 7.785  |
| K125CA-N-H     | 55.45  | 120.26 | 7.782  |        |        |        |
| K125CA-G126N-H | 55.45  | 115.99 | 8.767  | 55.43  | 116.04 | 8.767  |
| K125CB-N-H     | 36.19  | 120.30 | 7.781  |        |        |        |
| K125CB-G126N-H | 36.22  | 115.99 | 8.764  | 36.17  | 116.03 | 8.768  |
| G126CA-N-H     | 47.80  | 116.05 | 8.765  |        |        |        |
| G126CA-N127N-H | Peak   | Not    | found  | Peak   | Not    | found  |
| N127CA-K128N-H | 54.35  | 119.20 | 7.382  | 54.41  | 119.17 | 7.385  |
| N127CB-K128N-H | 38.34  | 119.23 | 7.38   | 38.35  | 119.19 | 7.383  |
| K128CA-N-H     | 55.11  | 119.26 | 7.379  |        |        |        |
| K128CA-D129N-H | 55.10  | 120.96 | 8.162  | 55.12  | 120.94 | 8.164  |
| K128CB-N-H     | 34.50  | 119.24 | 7.381  |        |        |        |
| K128CB-D129N-H | 34.59  | 120.97 | 8.163  | 34.56  | 120.95 | 8.164  |
| D129CA-N-H     | 52.71  | 120.92 | 8.163  |        |        |        |
| D129CA-L130N-H | 52.69  | 122.99 | 6.909  | 52.74  | 123.12 | 6.912  |

|                | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|----------------|--------|--------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| D129CB-N-H     | 40.17  | 120.91 | 8.162  |        |        |        |
| D129CB-L130N-H | 40.20  | 123.07 | 6.907  | 40.16  | 123.11 | 6.912  |
| L130CA-N-H     | 53.47  | 123.17 | 6.913  |        |        |        |
| L130CA-G131N-H |        |        |        | 53.4   | 103.72 | 5.161  |
| L130CB-N-H     | 38.3   | 123.14 | 6.912  |        |        |        |
| L130CB-G131N-H |        |        |        | 38.29  | 103.77 | 5.162  |
| G131CA-N-H     | 42.64  | 103.71 | 5.16   |        |        |        |
| G131CA-D132N-H | 42.61  | 116.41 | 6.51   | 42.64  | 116.47 | 6.517  |
| D132CA-N-H     | 53.22  | 116.51 | 6.513  |        |        |        |
| D132CA-L133N-H | 53.19  | 120.81 | 5.501  | 53.19  | 120.81 | 5.501  |
| D132CB-N-H     | 42.91  | 116.51 | 6.515  |        |        |        |
| D132CB-L133N-H | Peak   | Not    | found  | 42.75  | 120.83 | 5.505  |
| L133CA-N-H     | 52.75  | 120.8  | 5.507  |        |        |        |
| L133CA-Y134N-H | 52.74  | 125.04 | 8.311  | 52.74  | 125.04 | 8.311  |
| L133CB-Y134N-H | Peak   | Not    | found  | Peak   | Not    | found  |
| Y134CA-N-H     | 56.67  | 125.05 | 8.305  |        |        |        |
| Y134CA-A135N-H | 56.66  | 124.00 | 9.973  | 56.68  | 124.11 | 9.969  |
| Y134CB-N-H     | 40.88  | 125.08 | 8.308  |        |        |        |
| Y134CB-A135N-H | 40.85  | 124.04 | 9.963  | 40.91  | 124.10 | 9.969  |
| A135CA-N-H     | 52.11  | 124.01 | 9.964  |        |        |        |
| A135CA-V136N-H | 52.08  | 124.82 | 10.262 | 52.08  | 124.88 | 10.266 |
| A135CB-N-H     | 23.93  | 124.19 | 9.966  |        |        |        |
| A135CB-V136N-H | 23.92  | 124.84 | 10.266 | 23.93  | 124.88 | 10.267 |
| V136CA-N-H     | 62.87  | 124.75 | 10.262 |        |        |        |
| V136CA-L137N-H | 62.91  | 126.22 | 9.932  | 62.91  | 126.23 | 9.936  |
| V136CB-N-H     | 33.16  | 124.91 | 10.259 |        |        |        |
| V136CB-N-H     | 33.00  | 124.86 | 10.265 |        |        |        |
| V136CB-L137N-H | 33.03  | 126.25 | 9.931  | 33.11  | 126.24 | 9.931  |
| V136CB-L137N-H | 33.19  | 126.17 | 9.931  |        |        |        |
| L137CA-N-H     | 52.21  | 126.24 | 9.932  |        |        |        |
| L137CA-N138N-H | 52.24  | 121.43 | 9.935  | 52.26  | 121.38 | 9.938  |
| L137CB-N-H     | 45.94  | 126.20 | 9.931  |        |        |        |

|                | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|----------------|--------|--------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| L137CB-N138N-H | 45.97  | 121.45 | 9.935  | 45.98  | 121.39 | 9.937  |
| N138CA-N-H     | 52.9   | 121.34 | 9.936  |        |        |        |
| N138CA-R139N-H | 52.92  | 124.79 | 8.619  | 52.96  | 124.87 | 8.621  |
| N138CB-N-H     | 44.39  | 121.34 | 9.936  |        |        |        |
| N138CB-R139N-H | 44.39  | 124.75 | 8.619  | 44.42  | 124.84 | 8.621  |
| R139CA-N-H     | 56.06  | 124.74 | 8.617  |        |        |        |
| R139CA-N140N-H | 55.97  | 120.13 | 10.277 | 56.00  | 120.08 | 10.281 |
| R139CB-N-H     | 31.15  | 124.77 | 8.619  |        |        |        |
| R139CB-N140N-H | 31.17  | 120.06 | 10.282 | 31.15  | 120.08 | 10.282 |
| N140CA-N-H     | 51.74  | 120.12 | 10.278 |        |        |        |
| N140CA-K141N-H | 51.75  | 123.53 | 7.627  | 51.75  | 123.53 | 7.627  |
| N140CB-N-H     | 40.58  | 120.10 | 10.278 |        |        |        |
| N140CB-K141N-H | 40.61  | 123.52 | 7.626  | 40.55  | 123.58 | 7.619  |
| K141CA-N-H     | 58.14  | 123.52 | 7.627  |        |        |        |
| K141CA-D142N-H | 58.14  | 117.72 | 7.969  | Peak   | Not    | found  |
| K141CB-N-H     | 30.62  | 123.52 | 7.626  |        |        |        |
| K141CB-D142N-H | 30.62  | 117.72 | 7.969  | 30.59  | 117.72 | 7.964  |
| D142CA-N-H     | 54.40  | 117.72 | 7.966  |        |        |        |
| D142CB-A143N-H | 20.49  | 123.37 | 7.144  | peak   | Not    | found  |
| A143CA-N-H     | 52.62  | 123.38 | 7.143  |        |        |        |
| A143CA-A144N-H | 52.61  | 126.19 | 8.487  | 52.65  | 126.31 | 8.49   |
| A143CB-N-H     | 20.49  | 123.37 | 7.144  |        |        |        |
| A143CB-A144N-H | 20.47  | 126.25 | 8.487  | 20.53  | 126.31 | 8.49   |
| A144CA-N-H     | 51.29  | 126.29 | 8.488  |        |        |        |
| A144CA-A145N-H | 51.28  | 126.82 | 9.277  | 51.29  | 126.83 | 9.28   |
| A144CB-N-H     | 19.53  | 126.25 | 8.486  |        |        |        |
| A144CB-A145N-H | 19.52  | 126.83 | 9.28   | 19.52  | 126.83 | 9.28   |
| A145CA-N-H     | 53.26  | 126.86 | 9.277  |        |        |        |
| A145CA-G146N-H | 53.28  | 110.48 | 8.795  | 53.29  | 110.43 | 8.798  |
| A145CB-N-H     | 19.17  | 126.85 | 9.277  |        |        |        |
| A145CB-G146N-H | 19.15  | 110.51 | 8.797  | 19.19  | 110.43 | 8.798  |
| G146CA-N-H     | 43.66  | 110.47 | 8.796  |        |        |        |

|                | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|----------------|--------|--------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| G146CA-D147N-H | 43.63  | 117.59 | 8.433  | 43.66  | 117.59 | 8.433  |
| D147CA-N-H     | 57.87  | 117.60 | 8.43   | Peak   | Not    | found  |
| D147CB-N-H     | 40.91  | 117.60 | 8.432  |        |        |        |
| D147CB-K148N-H | peak   | Not    | found  | Peak   | Not    | found  |
| K148CA-V149N-H | 59.7   | 120.53 | 7.937  | 59.73  | 120.52 | 7.94   |
| K148CB-V149N-H | 31.55  | 120.53 | 7.94   | 31.55  | 120.53 | 7.94   |
| V149CA-N-H     | 65.53  | 120.54 | 7.938  |        |        |        |
| V149CA-K150N-H | 65.55  | 120.43 | 7.82   | 65.55  | 120.44 | 7.821  |
| V149CB-N-H     | 31.23  | 120.53 | 7.94   |        |        |        |
| V149CB-K150N-H | 31.23  | 120.44 | 7.821  | 31.23  | 120.44 | 7.821  |
| K150CA-N-H     | 61.27  | 120.46 | 7.819  |        |        |        |
| K150CA-S151N-H | 61.35  | 116.95 | 8.228  | 61.27  | 116.88 | 8.23   |
| K150CB-N-H     | 31.34  | 120.46 | 7.819  |        |        |        |
| K150CB-S151N-H | 31.34  | 116.87 | 8.229  | 31.35  | 116.86 | 8.231  |
| S151CA-N-H     | 61.8   | 116.87 | 8.229  |        |        |        |
| S151CA-A152N-H | 61.80  | 126.16 | 7.331  | 61.81  | 126.15 | 7.334  |
| S151CB-N-H     | 62.73  | 116.87 | 8.229  |        |        |        |
| S151CB-N-H     | 62.15  | 117.02 | 8.227  |        |        |        |
| S151CB-A152N-H | 62.16  | 126.04 | 7.33   | 62.48  | 126.16 | 7.337  |
| S151CB-A152N-H | 62.76  | 126.19 | 7.336  |        |        |        |
| A152CA-N-H     | 54.85  | 126.15 | 7.334  |        |        |        |
| A152CA-V153N-H | 54.85  | 120.27 | 8.06   | 54.91  | 120.30 | 8.062  |
| A152CB-N-H     | 17.77  | 126.13 | 7.334  |        |        |        |
| A152CB-V153N-H | 17.76  | 120.28 | 8.06   | 17.76  | 120.29 | 8.062  |
| V153CA-N-H     | 67.24  | 120.31 | 8.06   |        |        |        |
| V153CA-S154N-H | 67.26  | 113.45 | 7.788  | 67.26  | 113.48 | 7.79   |
| V153CB-N-H     | 31.85  | 120.34 | 8.06   |        |        |        |
| V153CB-S154N-H | 31.88  | 113.45 | 7.788  | 31.86  | 113.49 | 7.79   |
| S154CA-N-H     | 61.5   | 113.52 | 7.787  |        |        |        |
| S154CA-A155N-H | 61.47  | 125.76 | 8.433  | 61.53  | 125.68 | 8.436  |
| S154CB-N-H     | 62.65  | 113.52 | 7.788  |        |        |        |
| S154CB-A155N-H | 62.62  | 125.75 | 8.434  | 62.67  | 125.70 | 8.436  |

|                | HNCA-  | CB     |        | CACB-  | (CO)NH  |        |
|----------------|--------|--------|--------|--------|---------|--------|
| Assignment     | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm  | H, ppm |
| A155CA-N-H     | 54.53  | 125.70 | 8.434  |        |         |        |
| A155CA-A156N-H | 54.52  | 119.58 | 7.249  | 54.57  | 119.60  | 7.252  |
| A155CB-N-H     | 17.78  | 125.74 | 8.434  |        |         |        |
| A155CB-A156N-H | 17.77  | 119.60 | 7.251  | 17.77  | 119.60  | 7.251  |
| A156CA-N-H     | 51.48  | 119.61 | 7.249  |        |         |        |
| A156CA-T157N-H | 51.47  | 112.83 | 8.094  | 51.52  | 112.8   | 8.096  |
| A156CB-N-H     | 18.09  | 119.63 | 7.25   |        |         |        |
| A156CB-T157N-H | 18.08  | 112.82 | 8.094  | 18.10  | 112.81  | 8.096  |
| T157CA-N-H     | 63.27  | 112.88 | 8.093  |        |         |        |
| T157CA-L158N-H | 63.20  | 118.85 | 7.157  | 63.20  | 118.89  | 7.16   |
| T157CB-N-H     | 67.88  | 112.85 | 8.094  |        |         |        |
| T157CB-N-H     | 67.62  | 112.86 | 8.094  |        |         |        |
| T157CB-L158N-H | 67.64  | 118.92 | 7.157  | 67.75  | 118.90  | 7.16   |
| L158CA-N-H     | 52.59  | 118.91 | 7.158  |        |         |        |
| L158CA-E159N-H | 52.59  | 121.15 | 8.353  | 52.66  | 121.20  | 8.357  |
| L158CB-N-H     | 44.59  | 118.90 | 7.158  |        |         |        |
| L158CB-E159N-H | 44.60  | 121.11 | 8.354  | 44.61  | 121.25  | 8.354  |
| E159CA-N-H     | 54.45  | 121.14 | 8.354  |        |         |        |
| E159CA-F160N-H | 54.46  | 128.15 | 9.12   | 54.50  | 128.19  | 9.121  |
| E159CB-N-H     | 30.21  | 121.15 | 8.353  |        |         |        |
| E159CB-N-H     | 30.49  | 121.17 | 8.354  |        |         |        |
| E159CB-F160N-H | 30.34  | 128.24 | 9.121  | 30.37  | 128.191 | 9.122  |
| F160CA-N-H     | 61.03  | 128.24 | 9.121  |        |         |        |
| F160CA-S161N-H | 61.01  | 112.93 | 8.831  | 61.01  | 112.931 | 8.831  |
| F160CB-N-H     | 38.46  | 128.27 | 9.11   |        |         |        |
| F160CB-S161N-H | 38.43  | 113.02 | 8.83   | 38.42  | 112.94  | 8.83   |
| S161CA-N-H     | 60.71  | 113.05 | 8.825  |        |         |        |
| S161CA-K162N-H | 60.67  | 119.60 | 7.634  | 60.73  | 119.607 | 7.635  |
| S161CB-N-H     | 62.46  | 113.01 | 8.828  |        |         |        |
| S161CB-K162N-H | 62.52  | 119.65 | 7.636  | 62.50  | 119.657 | 7.635  |
| K162CA-N-H     | 56.22  | 119.67 | 7.633  |        |         |        |
| K162CA-F163N-H | 56.25  | 120.21 | 7.987  | 56.27  | 120.208 | 7.991  |

|                | HNCA-       | CB         |              | CACB-  | (CO)NH |        |
|----------------|-------------|------------|--------------|--------|--------|--------|
| Assignment     | C, ppm      | N, ppm     | H, ppm       | C, ppm | N, ppm | H, ppm |
| K162CB-N-H     | 33.11       | 119.69     | 7.634        |        |        |        |
| K162CB-F163N-H | 33.04       | 120.00     | 7.986        | 33.10  | 120.10 | 7.989  |
| F163CA-N-H     | 58.49       | 120.23     | 7.986        |        |        |        |
| F163CA-I164N-H | 58.48       | 124.39     | 9.575        | 58.51  | 124.45 | 9.577  |
| I164CA-N-H     | 59.65       | 124.55     | 9.575        |        |        |        |
| F163CB-I164N-H | <i>peak</i> | <i>Not</i> | <i>found</i> | 38.62  | 124.45 | 9.578  |
| I164CA-S165N-H | 59.67       | 119.40     | 8.747        | 59.66  | 119.41 | 8.749  |
| I164CB-N-H     | 38.9        | 124.49     | 9.575        |        |        |        |
| I164CB-S165N-H | 38.94       | 119.30     | 8.746        | 38.87  | 119.41 | 8.75   |
| S165CA-N-H     | 57.12       | 119.45     | 8.747        |        |        |        |
| S165CA-T166N-H | 57.05       | 118.05     | 9.383        | 57.09  | 118.19 | 9.389  |
| S165CB-N-H     | 64.85       | 119.46     | 8.749        |        |        |        |
| S165CB-T166N-H | 64.83       | 118.16     | 9.38         | 64.87  | 118.26 | 9.39   |
| T166CA-N-H     | 62.29       | 118.3      | 9.387        |        |        |        |
| T166CA-K167N-H | 62.30       | 125.24     | 8.931        | 62.35  | 125.34 | 8.936  |
| T166CB-N-H     | 70.36       | 118.2      | 9.386        |        |        |        |
| T166CB-K167N-H | 70.41       | 125.26     | 8.929        | 70.38  | 125.34 | 8.935  |
| K167CA-N-H     | 59.72       | 125.40     | 8.932        |        |        |        |
| K167CA-E168N-H | 59.78       | 116.87     | 8.641        | 59.75  | 116.95 | 8.627  |
| K167CB-N-H     | 32.38       | 125.47     | 8.932        |        |        |        |
| K167CB-N-H     | 32.56       | 125.47     | 8.931        |        |        |        |
| K167CB-E168N-H | <i>Peak</i> | <i>Not</i> | <i>found</i> | 32.45  | 116.89 | 8.63   |
| E168CA-N-H     | 56.02       | 116.84     | 8.629        |        |        |        |
| E168CA-N169N-H | 56.00       | 117.46     | 7.776        | 56.04  | 117.48 | 7.773  |
| E168CB-N-H     | 28.65       | 116.91     | 8.622        |        |        |        |
| E168CB-N169N-H | 28.63       | 117.46     | 7.771        | 28.59  | 117.46 | 7.774  |
| N169CA-N-H     | 52.81       | 117.54     | 7.771        |        |        |        |
| N169CA-N170N-H | 52.77       | 115.04     | 8.511        | 52.81  | 115.20 | 8.516  |
| N169CB-N-H     | 41.18       | 117.48     | 7.767        |        |        |        |
| N169CB-N170N-H | 41.09       | 115.16     | 8.512        | 41.18  | 115.16 | 8.517  |
| N170CA-N-H     | 53.70       | 115.13     | 8.508        |        |        |        |
| N170CA-C171N-H | 53.70       | 114.84     | 8.476        | 53.69  | 114.76 | 8.478  |

|                | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|----------------|--------|--------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| N170CB-N-H     | 36.69  | 115.16 | 8.512  |        |        |        |
| N170CB-C171N-H | 36.70  | 114.85 | 8.479  | 36.85  | 114.75 | 8.478  |
| C171CA-N-H     | 54.92  | 114.75 | 8.476  |        |        |        |
| C171CA-A172N-H | 54.95  | 123.22 | 5.226  | 54.98  | 123.20 | 5.224  |
| C171CB-N-H     | 41.96  | 114.78 | 8.476  |        |        |        |
| C171CB-A172N-H | 41.97  | 123.31 | 5.221  | 41.94  | 123.20 | 5.223  |
| A172CA-N-H     | 50.18  | 123.20 | 5.216  |        |        |        |
| A172CA-Y173N-H | Peak   | Not    | found  | 50.2   | 120.30 | 8.281  |
| A172CB-N-H     | 20.26  | 123.29 | 5.22   |        |        |        |
| A172CB-Y173N-H | 20.21  | 120.32 | 8.288  | 20.28  | 120.32 | 8.284  |
| Y173CA-H       | 57.20  | 120.29 | 8.289  |        |        |        |
| Y173CA-D174N-H | 57.21  | 119.29 | 5.988  | 57.20  | 119.28 | 5.988  |
| Y173CB-D174N-H | 40.58  | 119.31 | 5.988  | 40.65  | 119.27 | 5.986  |
| D174CA-N-H     | 50.91  | 119.32 | 5.98   |        |        |        |
| D174CA-N175N-H | 50.96  | 121.97 | 7.998  | 50.96  | 121.97 | 7.998  |
| D174CB-N-H     | 38.74  | 119.26 | 5.986  |        |        |        |
| D174CB-N175N-H | Peak   | Not    | found  | 38.77  | 121.87 | 7.999  |
| N175CA-N-H     | 55.59  | 121.91 | 7.996  |        |        |        |
| N175CA-D176N-H | 55.62  | 118.47 | 8.048  | 55.61  | 118.48 | 8.052  |
| N175CB-N-H     | 37.60  | 121.87 | 7.99   |        |        |        |
| N175CB-D176N-H | 37.65  | 118.45 | 8.051  | 37.67  | 118.49 | 8.052  |
| D176CA-N-H     | 57.40  | 118.50 | 8.051  |        |        |        |
| D176CA-S177N-H | 57.38  | 116.38 | 7.178  | 57.39  | 116.39 | 7.178  |
| D176CB-N-H     | 39.91  | 118.54 | 8.052  |        |        |        |
| D176CB-S177N-H | 39.94  | 116.37 | 7.176  | 39.91  | 116.37 | 7.179  |
| S177CA-N-H     | 61.25  | 116.41 | 7.176  |        |        |        |
| S177CA-L178N-H | 61.25  | 119.92 | 6.783  | 61.20  | 119.92 | 6.784  |
| S177CB-L178N-H | Peak   | Not    | found  | Peak   | Not    | found  |
| L178CA-N-H     | 57.99  | 119.97 | 6.781  |        |        |        |
| L178CA-K179N-H | 57.99  | 112.26 | 7.317  | 58.04  | 112.25 | 7.32   |
| L178CB-N-H     | 42.28  | 119.95 | 6.781  |        |        |        |
| L178CB-K179N-H | 42.34  | 112.21 | 7.317  | 42.31  | 112.26 | 7.32   |

|                | HNCA-  | CB     |        | CACB-  | (CO)NH |        |
|----------------|--------|--------|--------|--------|--------|--------|
| Assignment     | C, ppm | N, ppm | H, ppm | C, ppm | N, ppm | H, ppm |
| K179CA-N-H     | 59.81  | 112.30 | 7.316  |        |        |        |
| K179CA-S180N-H | 59.83  | 114.47 | 7.477  | 59.83  | 114.45 | 7.479  |
| K179CB-N-H     | 31.89  | 112.27 | 7.318  |        |        |        |
| K179CB-S180N-H | 31.88  | 114.45 | 7.478  | 31.92  | 114.44 | 7.479  |
| S180CA-N-H     | 60.86  | 114.49 | 7.477  |        |        |        |
| S180CA-L181N-H | 60.86  | 121.55 | 7.541  | 60.89  | 121.59 | 7.544  |
| S180CB-N-H     | 62.67  | 114.48 | 7.477  |        |        |        |
| S180CB-L181N-H | 62.66  | 121.60 | 7.541  | 62.67  | 121.60 | 7.543  |
| L181CA-N-H     | 56.71  | 121.65 | 7.54   |        |        |        |
| L181CA-L182N-H | 56.76  | 114.55 | 7.016  | 56.76  | 114.55 | 7.016  |
| L181CB-N-H     | 41.87  | 121.63 | 7.541  |        |        |        |
| L181CB-L182N-H | 41.86  | 114.55 | 7.016  | 41.86  | 114.55 | 7.016  |
| L182CA-N-H     | 56.90  | 114.61 | 7.014  |        |        |        |
| L182CA-T183N-H | 56.88  | 105.57 | 7.261  | 56.92  | 105.60 | 7.264  |
| L182CB-N-H     | 42.28  | 114.58 | 7.013  |        |        |        |
| L182CB-T183N-H | 42.31  | 105.51 | 7.262  | 42.28  | 105.60 | 7.264  |
| T183CA-N-H     | 61.69  | 105.58 | 7.261  |        |        |        |
| T183CA-K184N-H | 61.69  | 126.95 | 7.243  | 61.67  | 126.93 | 7.245  |
| T183CB-N-H     | 69.43  | 105.6  | 7.262  |        |        |        |
| T183CB-K184N-H | 69.43  | 126.95 | 7.242  | 69.47  | 126.93 | 7.245  |
| K184CA-N-H     | 56.98  | 126.97 | 7.243  |        |        |        |
| K184CB-N-H     | 33.46  | 126.97 | 7.243  |        |        |        |