Supporting Information

Redox Property of Enamines

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1. Cyclic Voltammograms of enamines

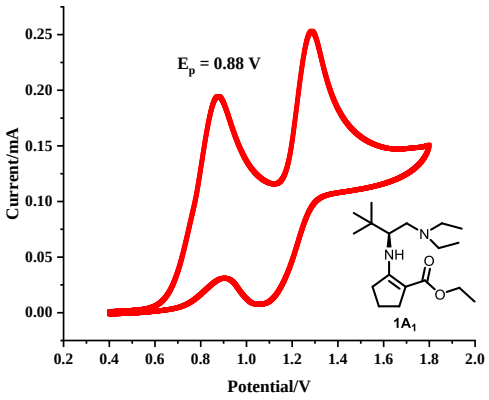


Figure S1. Cyclic voltammogram of 1A$_1$.

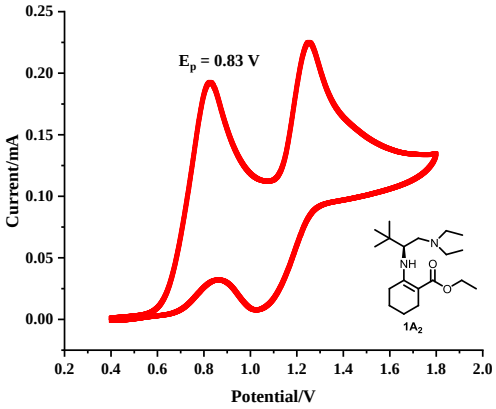


Figure S2. Cyclic voltammogram of 1A$_2$.

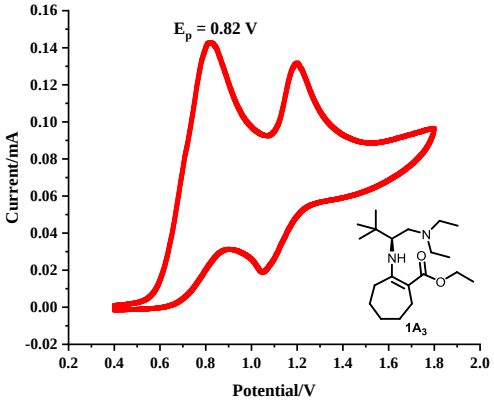


Figure S3. Cyclic voltammogram of 1A$_3$.

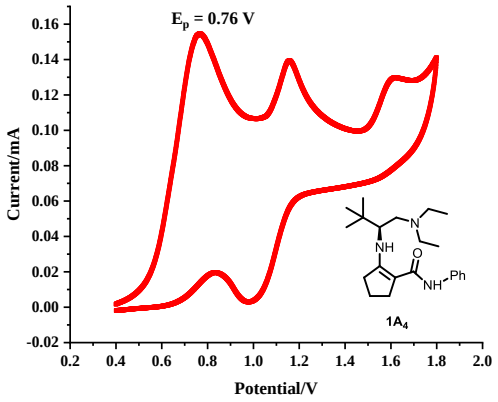


Figure S4. Cyclic voltammogram of $1A_4$.

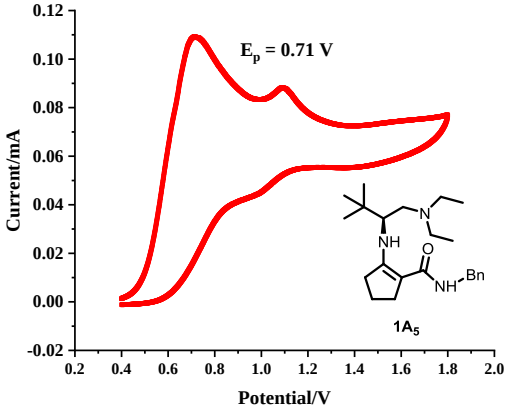


Figure S5. Cyclic voltammogram of $1A_5$.

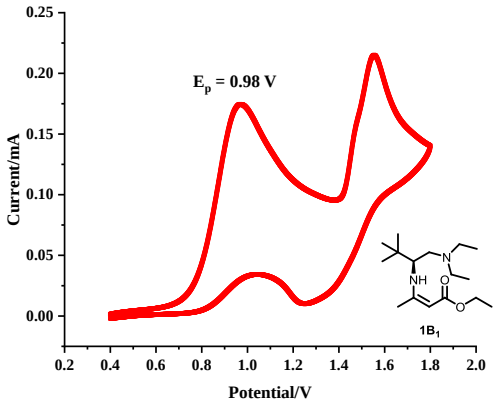


Figure S6. Cyclic voltammogram of $1B_1$.

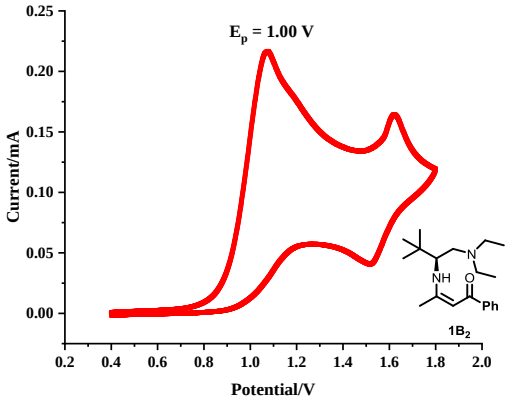


Figure S7. Cyclic voltammogram of 1B$_2$.

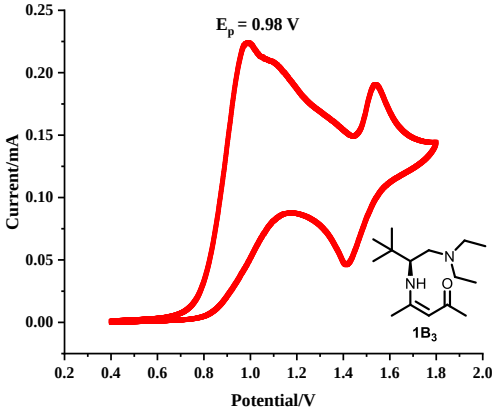


Figure S8. Cyclic voltammogram of 1B$_3$.

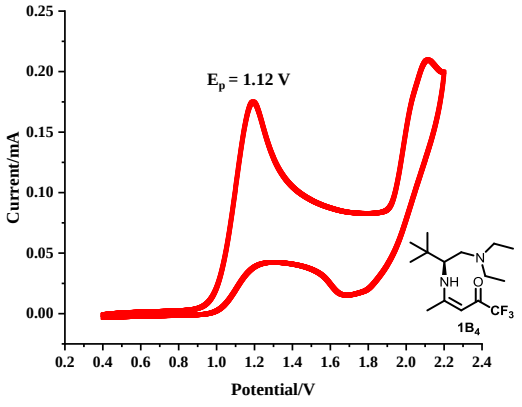


Figure S9. Cyclic voltammogram of 1B$_4$.

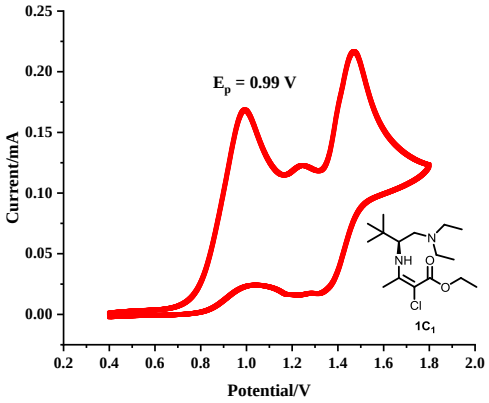


Figure S10. Cyclic voltammogram of 1C$_1$.

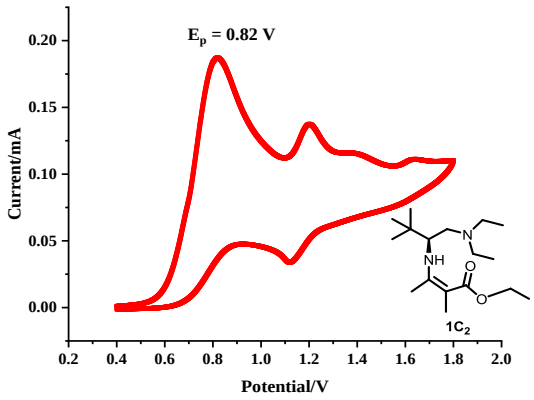


Figure S11. Cyclic voltammogram of 1C$_2$.

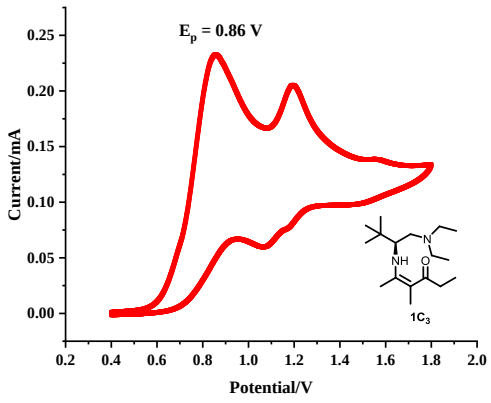


Figure S12. Cyclic voltammogram of 1C$_3$.

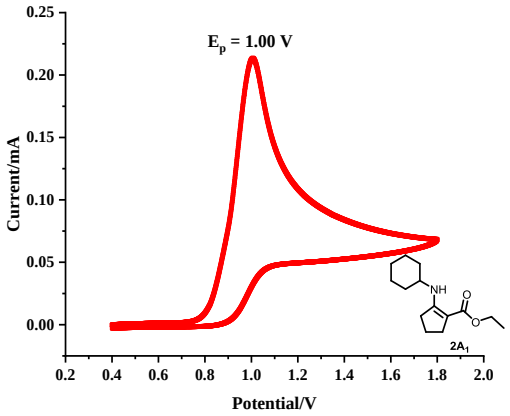


Figure S13. Cyclic voltammogram of $2A_1$.

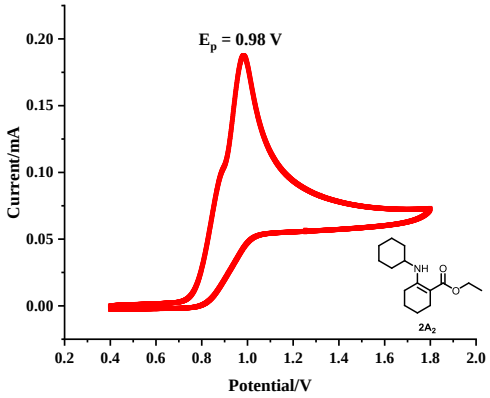


Figure S14. Cyclic voltammogram of $2A_2$.

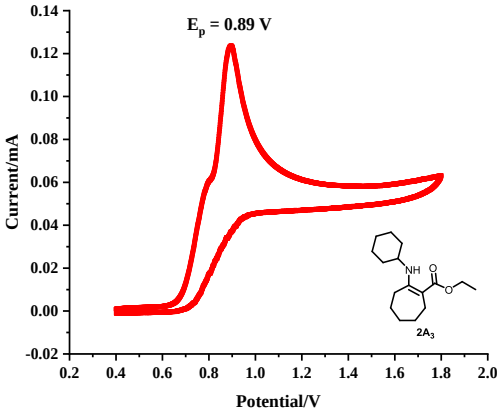


Figure S15. Cyclic voltammogram of $2A_3$.

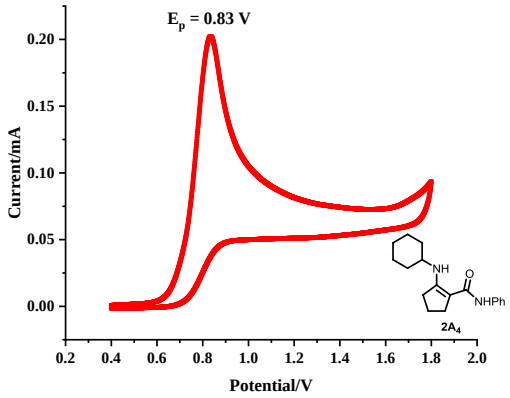


Figure S16. Cyclic voltammogram of $2A_4$.

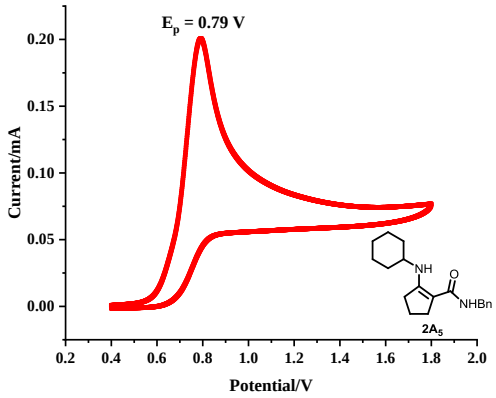
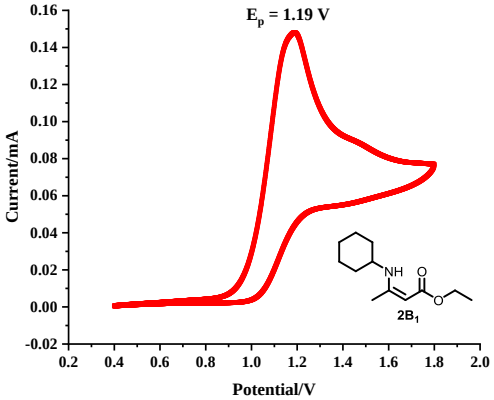


Figure S17. Cyclic voltammogram of $2A_5$.



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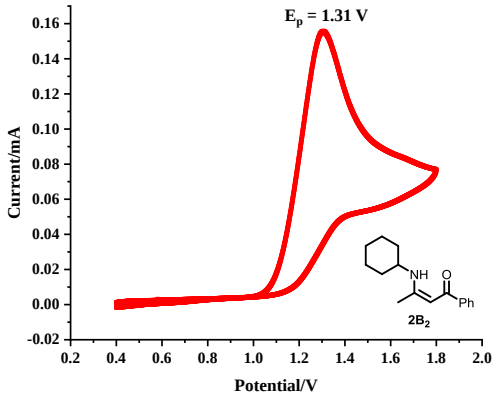


Figure S19. Cyclic voltammogram of $2B_2$.

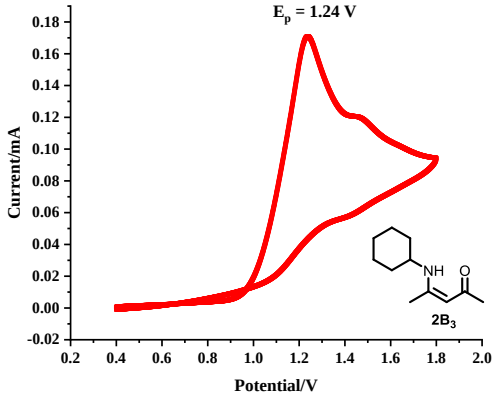


Figure S20. Cyclic voltammogram of $2B_3$.

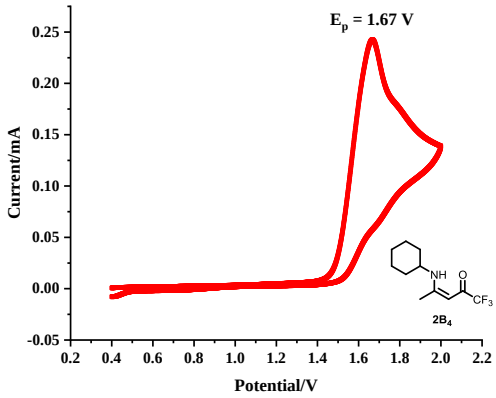


Figure S21. Cyclic voltammogram of $2B_4$.

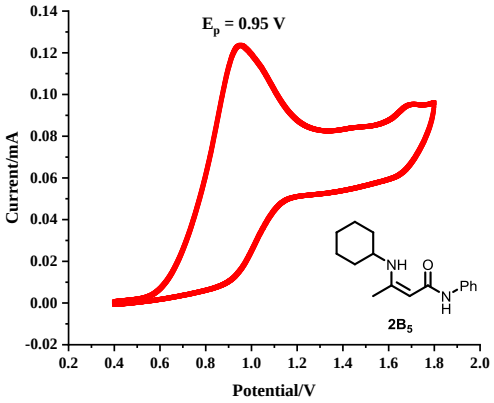


Figure S22. Cyclic voltammogram of 2B$_5$.

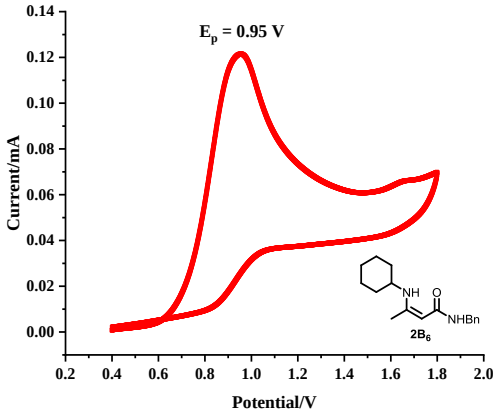


Figure S23. Cyclic voltammogram of 2B$_6$.

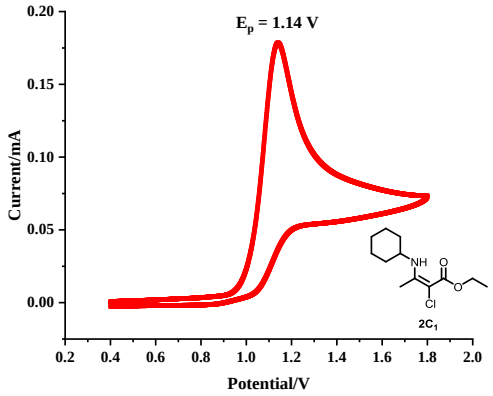


Figure S24. Cyclic voltammogram of 2C$_1$.

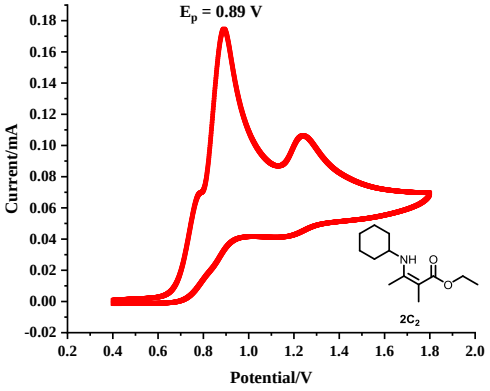


Figure S25. Cyclic voltammogram of $2C_2$.

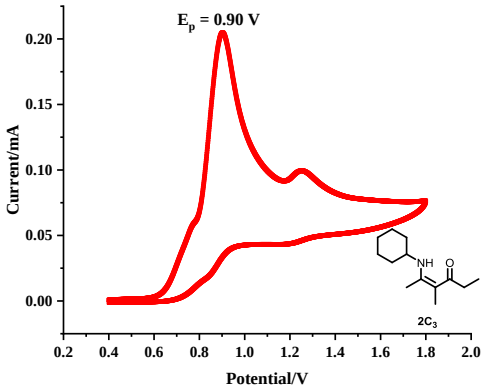


Figure S26. Cyclic voltammogram of $2C_3$.

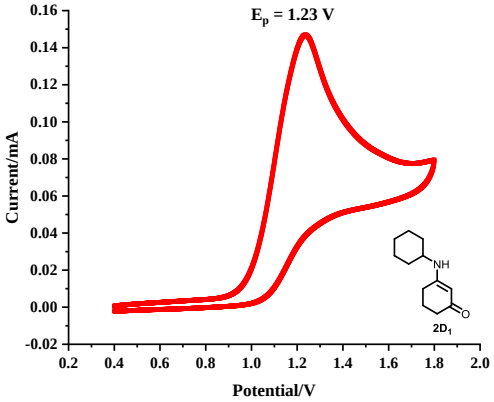


Figure S27. Cyclic voltammogram of $2D_1$.

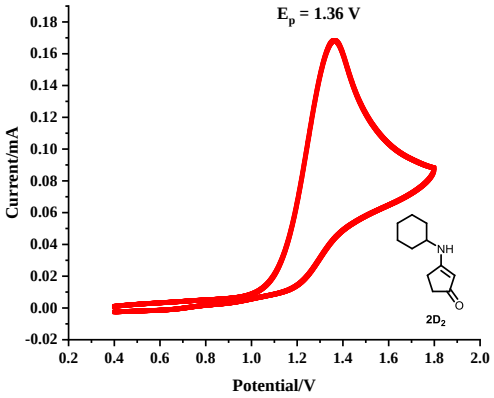


Figure S28. Cyclic voltammogram of $2D_2$.

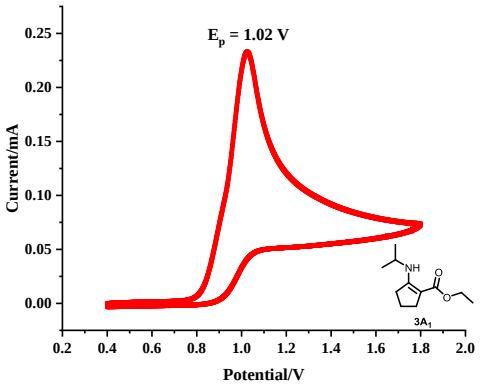


Figure S29. Cyclic voltammogram of $3A_1$.

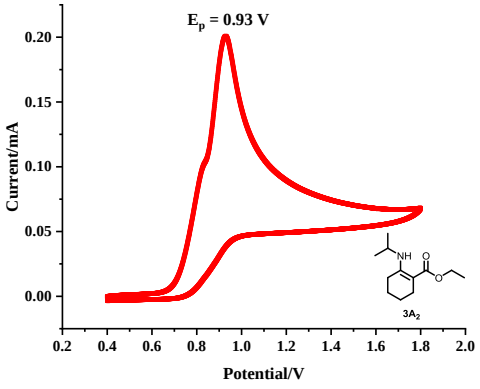


Figure S30. Cyclic voltammogram of $3A_2$.

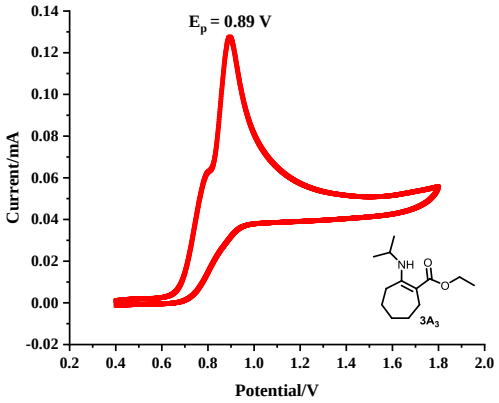


Figure S31. Cyclic voltammogram of 3A$_3$.

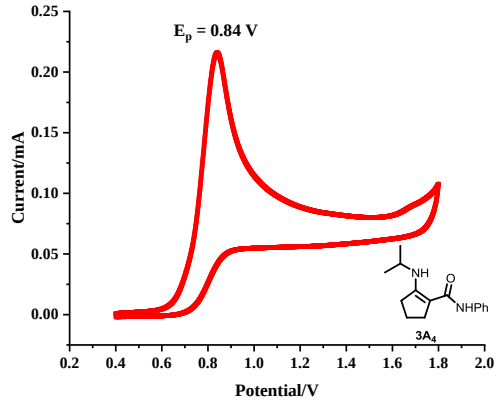


Figure S32. Cyclic voltammogram of 3A$_4$.

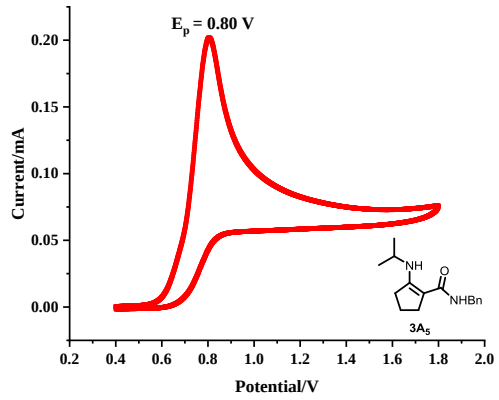


Figure S33. Cyclic voltammogram of 3A$_5$.

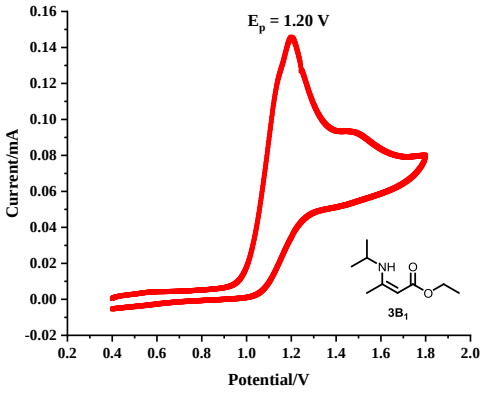


Figure S34. Cyclic voltammogram of $3B_1$.

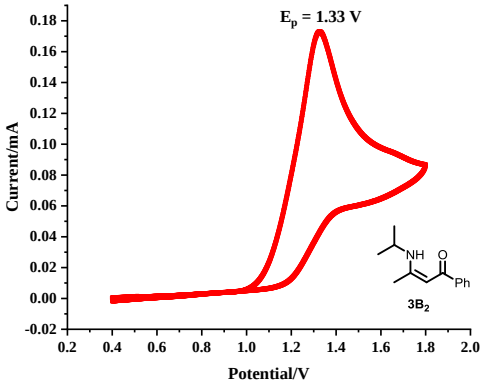


Figure S35. Cyclic voltammogram of $3B_2$.

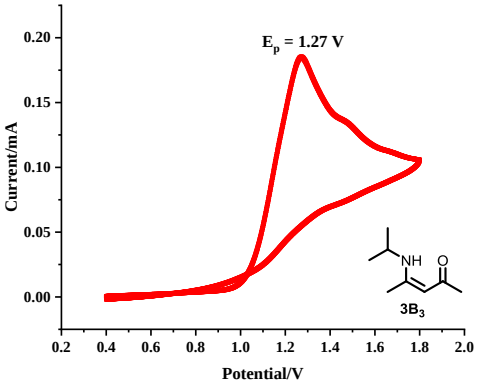


Figure S36. Cyclic voltammogram of $3B_3$.

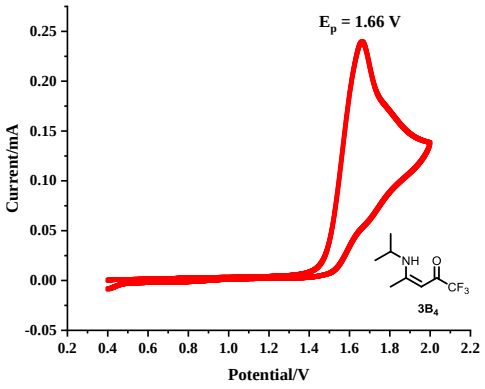


Figure S37. Cyclic voltammogram of $3B_4$.

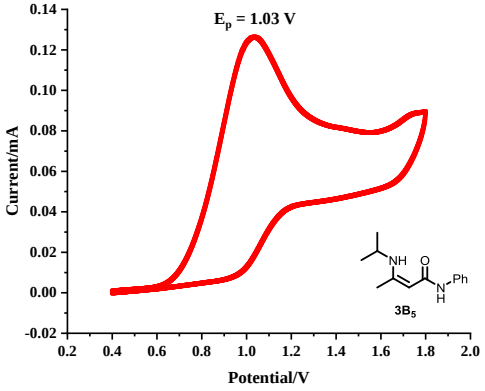


Figure S38. Cyclic voltammogram of $3B_5$.

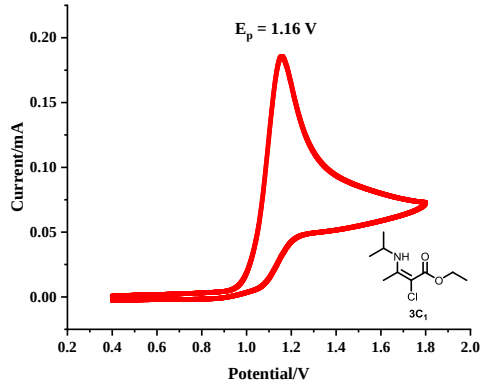


Figure S39. Cyclic voltammogram of $3C_1$.

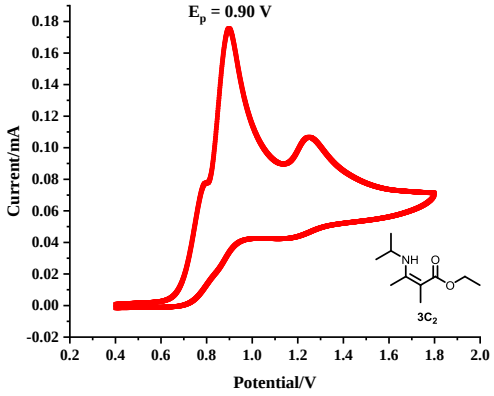


Figure S40. Cyclic voltammogram of 3C$_2$.

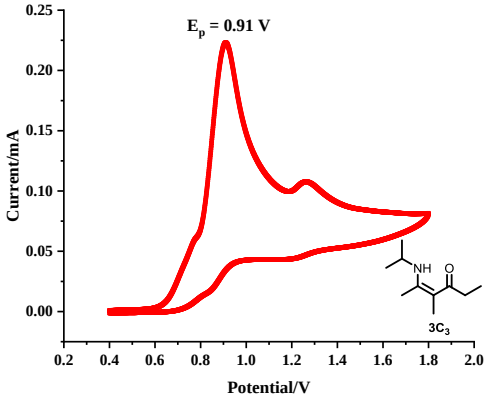


Figure S41. Cyclic voltammogram of 3C$_3$.

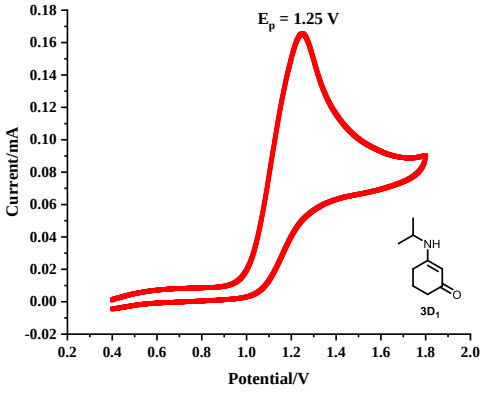


Figure S42. Cyclic voltammogram of 3D$_1$.

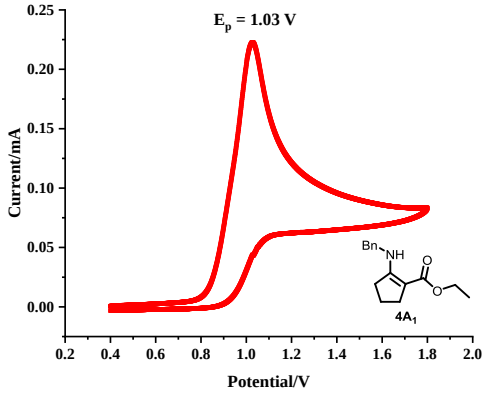


Figure S43. Cyclic voltammogram of $4A_1$.

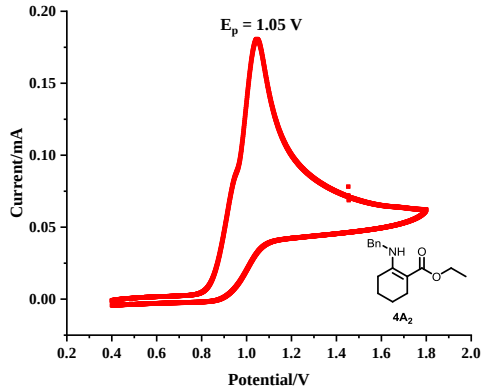


Figure S44. Cyclic voltammogram of $4A_2$.

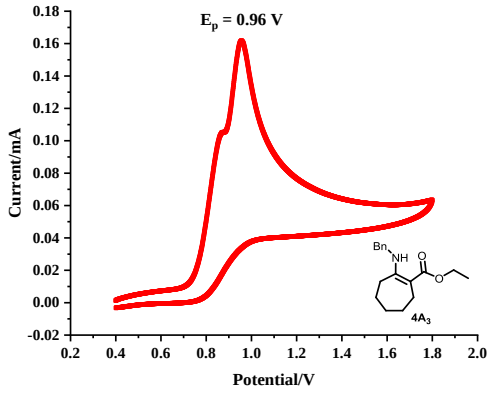


Figure S45. Cyclic voltammogram of $4A_3$.

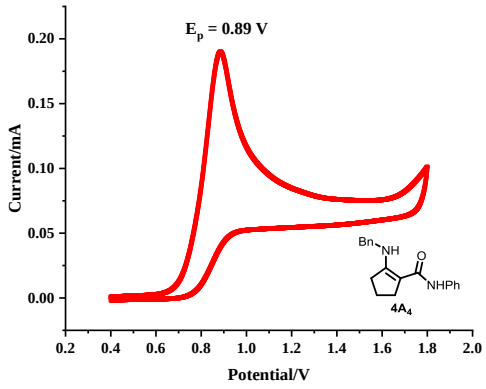


Figure S46. Cyclic voltammogram of 4A$_4$.

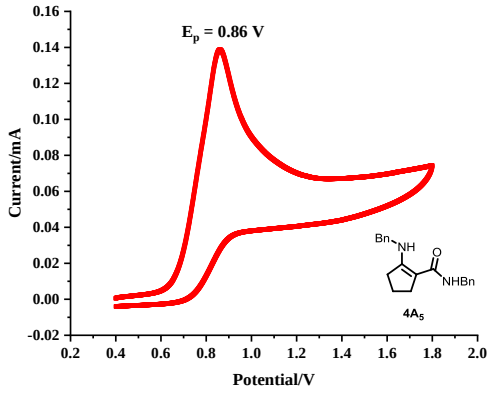


Figure S47. Cyclic voltammogram of 4A$_5$.

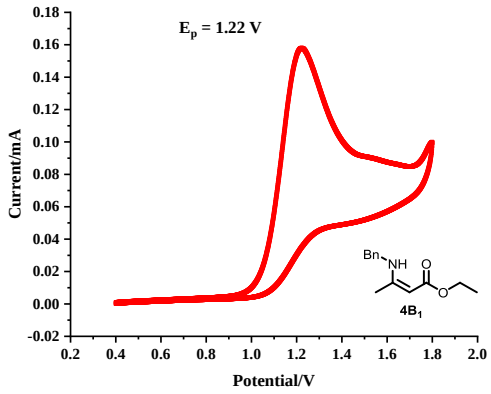


Figure S48. Cyclic voltammogram of 4B$_1$.

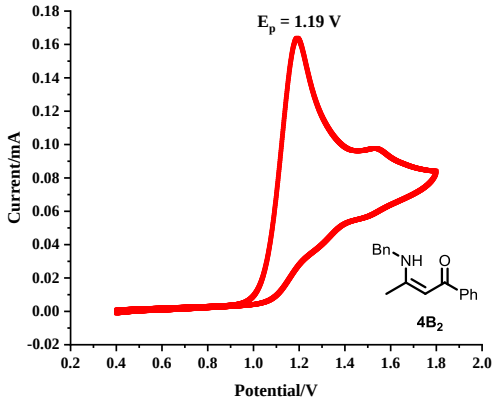


Figure S49. Cyclic voltammogram of 4B$_2$.

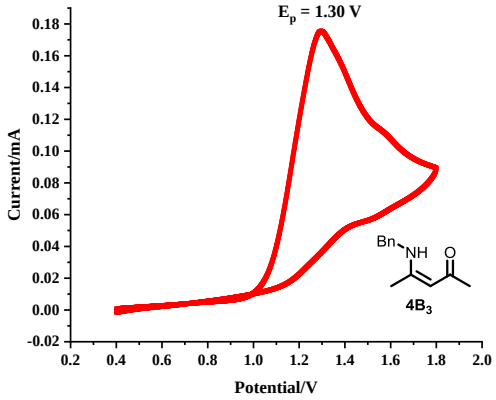


Figure S50. Cyclic voltammogram of 4B$_3$.

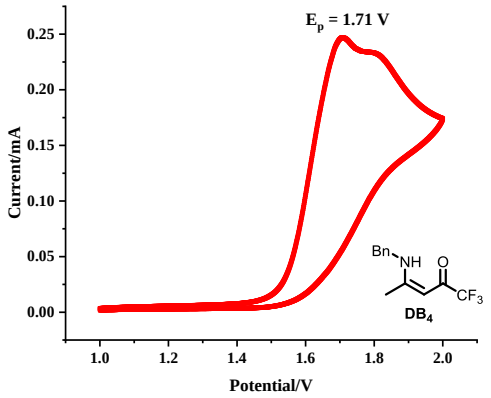


Figure S51. Cyclic voltammogram of 4B$_4$.

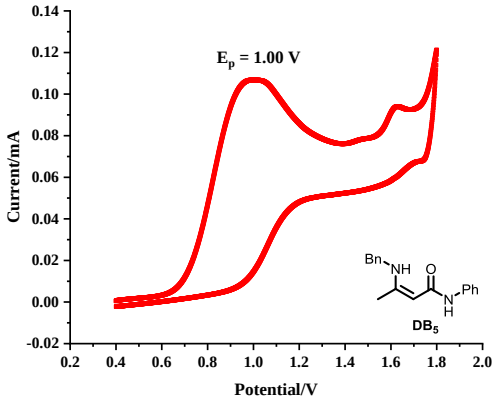


Figure S52. Cyclic voltammogram of 4B$_5$.

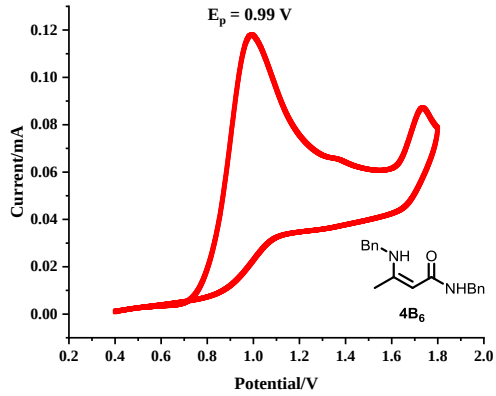


Figure S53. Cyclic voltammogram of 4B$_6$.

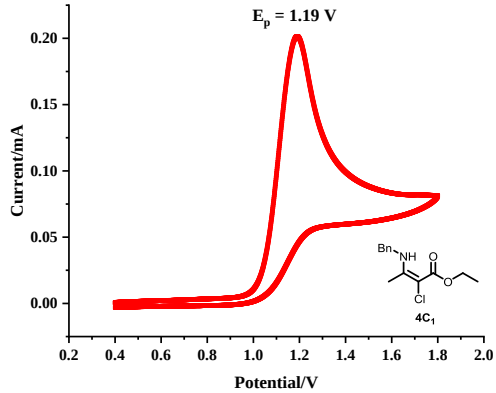


Figure S54. Cyclic voltammogram of 4C$_1$.

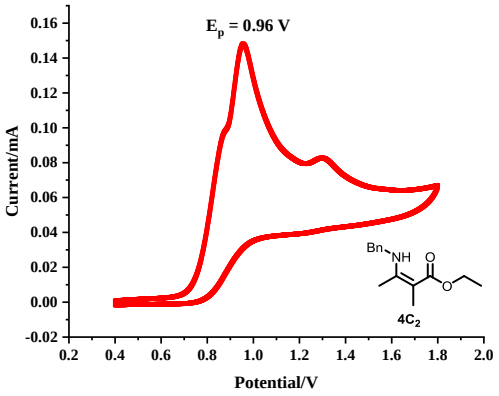


Figure S55. Cyclic voltammogram of 4C$_2$.

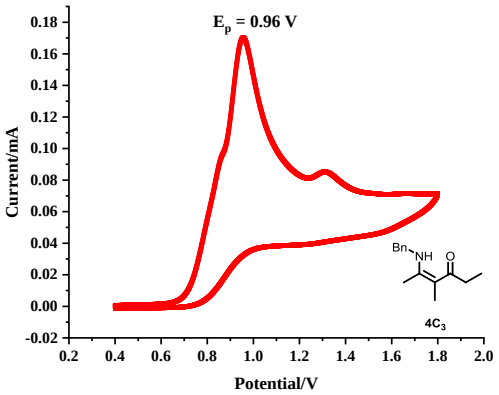


Figure S56. Cyclic voltammogram of 4C$_3$.

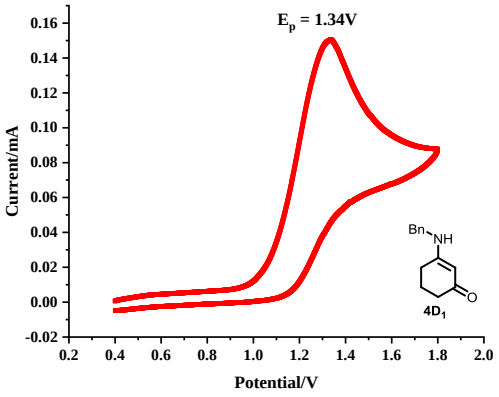


Figure S57. Cyclic voltammogram of 4D$_1$.

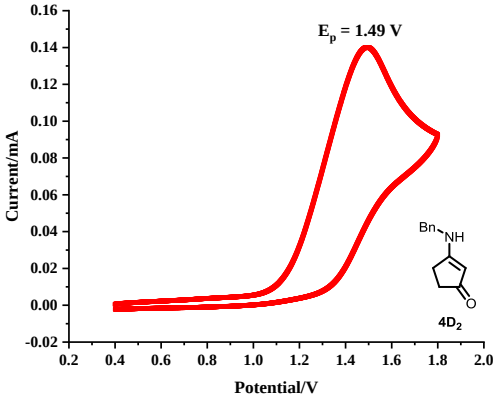


Figure S58. Cyclic voltammogram of 4D$_2$.

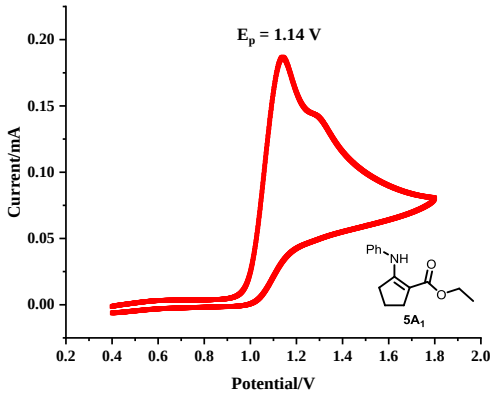


Figure S59. Cyclic voltammogram of 5A$_1$.

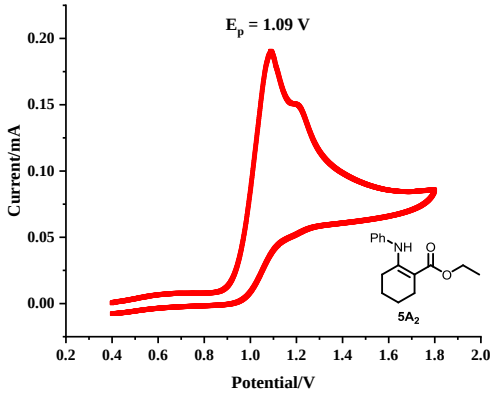


Figure S60. Cyclic voltammogram of 5A$_2$.

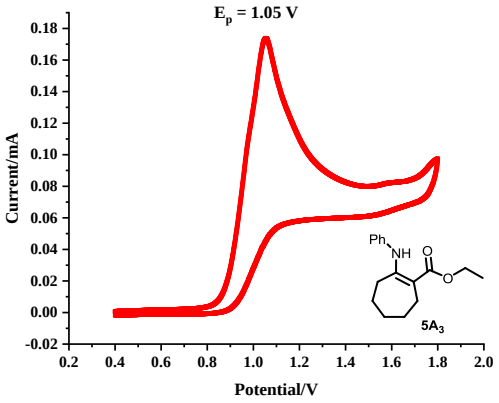


Figure S61. Cyclic voltammogram of $5A_3$.

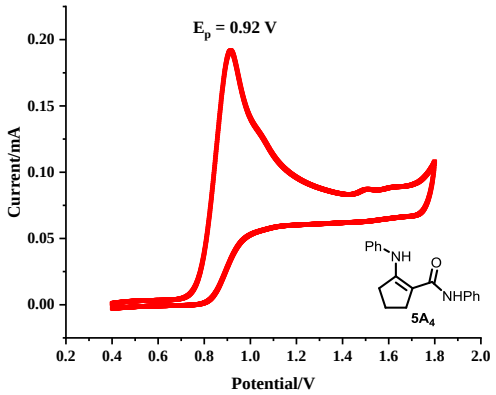


Figure S62. Cyclic voltammogram of $5A_4$.

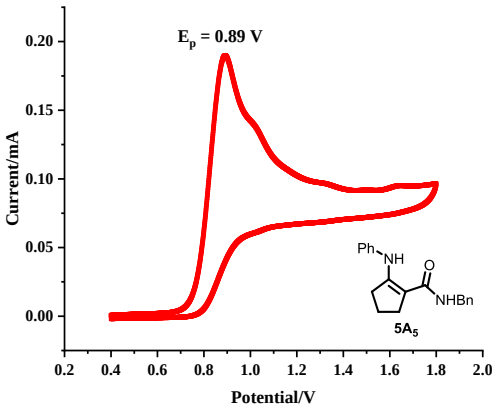


Figure S63. Cyclic voltammogram of $5A_5$.

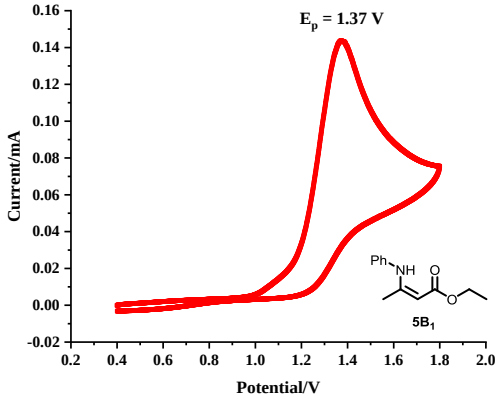


Figure S64. Cyclic voltammogram of 5B$_1$.

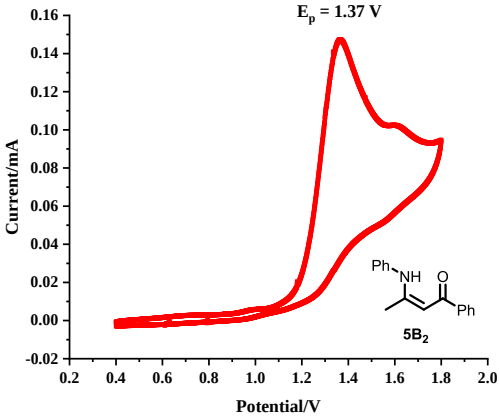


Figure S65. Cyclic voltammogram of 5B$_2$.

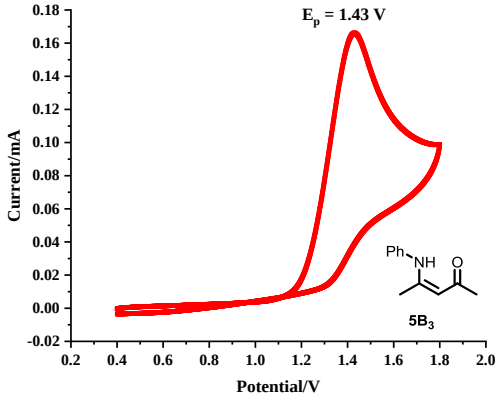


Figure S66. Cyclic voltammogram of 5B$_3$.

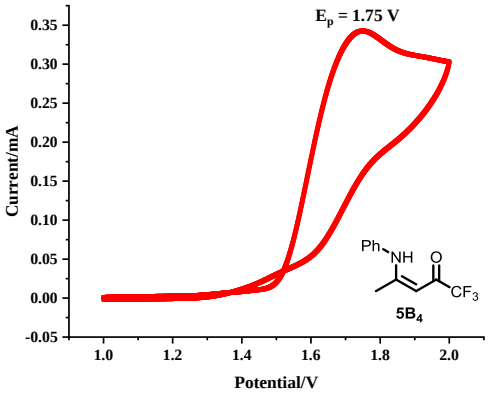


Figure S67. Cyclic voltammogram of 5B$_4$.

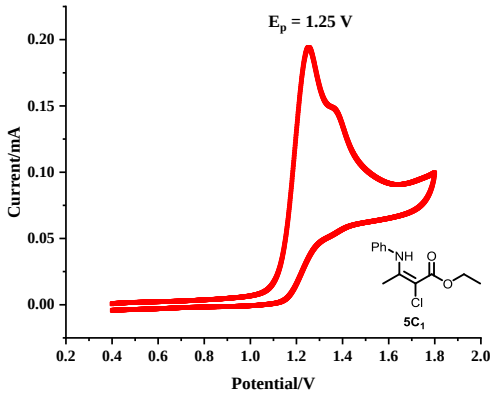


Figure S68. Cyclic voltammogram of 5C$_1$.

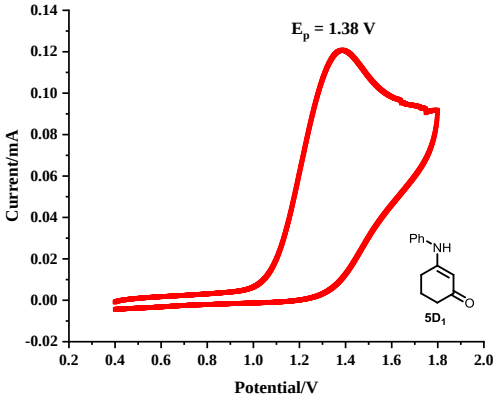


Figure S69. Cyclic voltammogram of 5D$_1$.

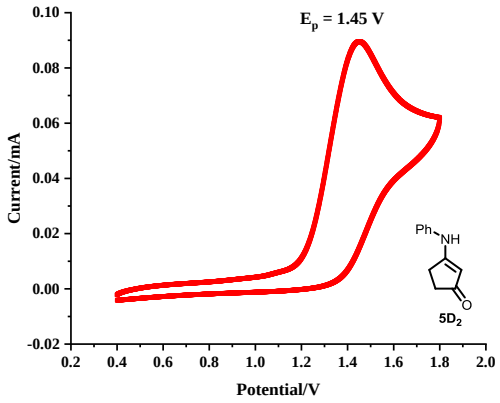


Figure S70. Cyclic voltammogram of 5D$_2$.

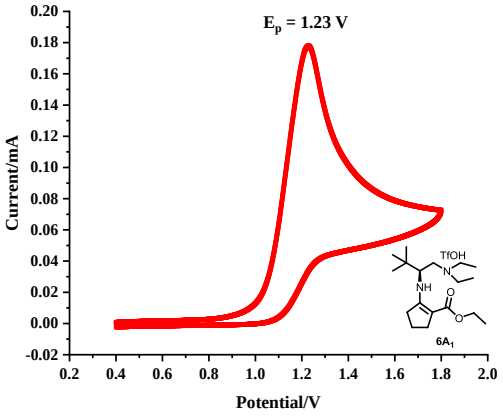


Figure S71. Cyclic voltammogram of 6A$_1$.

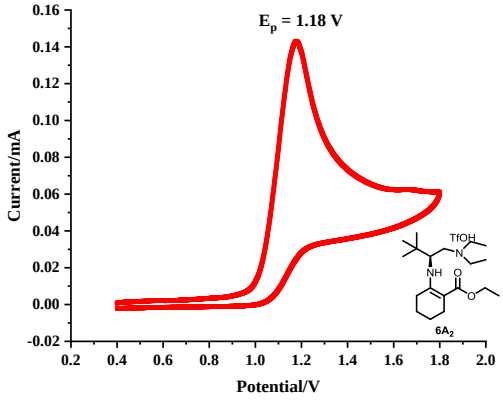


Figure S72. Cyclic voltammogram of 6A$_2$.

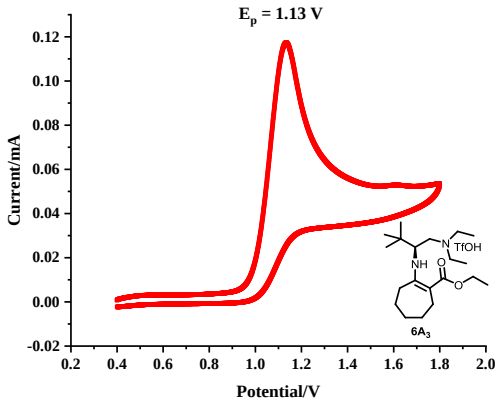


Figure S73. Cyclic voltammogram of 6A$_3$.

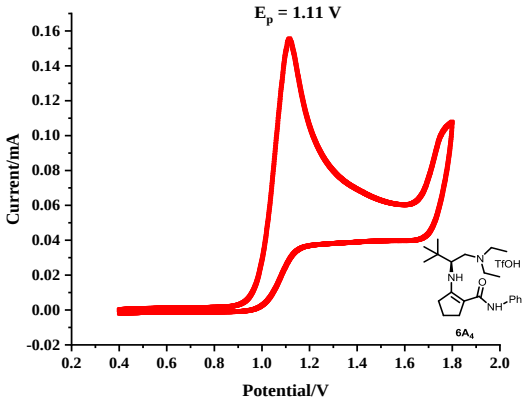


Figure S74. Cyclic voltammogram of 6A$_4$.

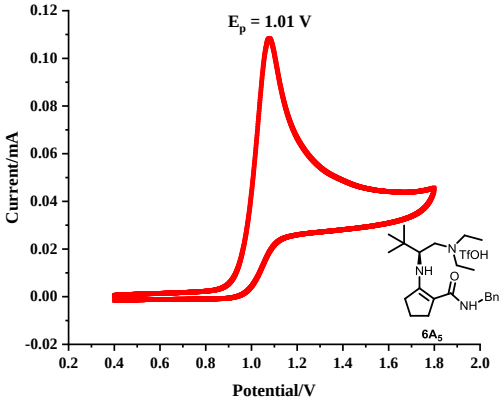


Figure S75. Cyclic voltammogram of 6A$_5$.

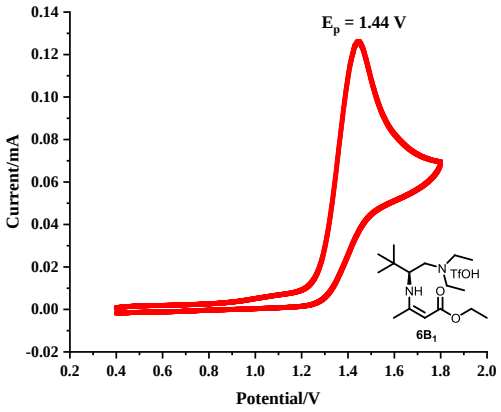


Figure S76. Cyclic voltammogram of 6B$_1$.

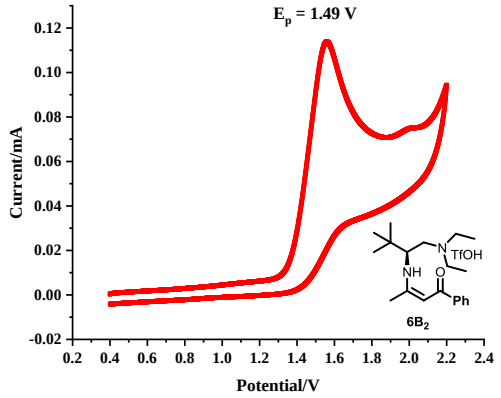


Figure S77. Cyclic voltammogram of 6B$_2$.

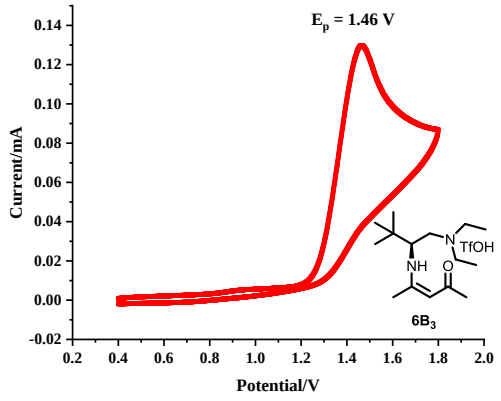


Figure S78. Cyclic voltammogram of 6B$_3$.

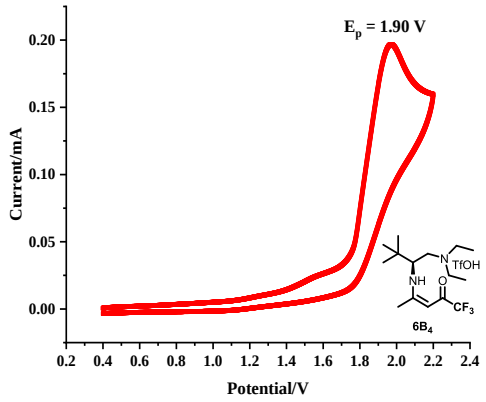


Figure S79. Cyclic voltammogram of $6B_4$.

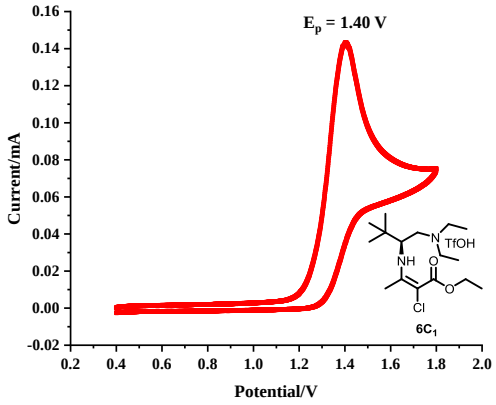


Figure S80. Cyclic voltammogram of $6C_1$.

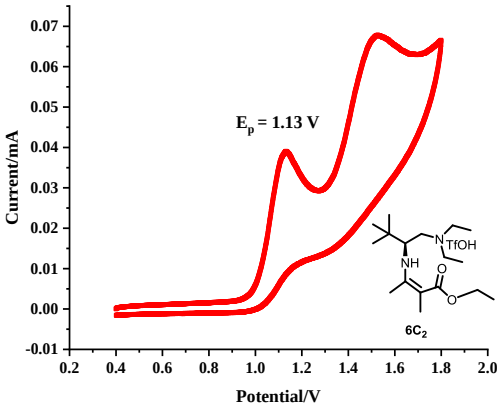


Figure S81. Cyclic voltammogram of $6C_2$.

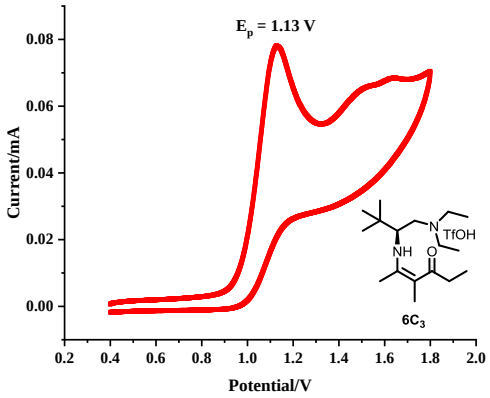
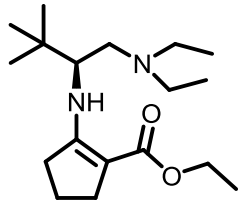
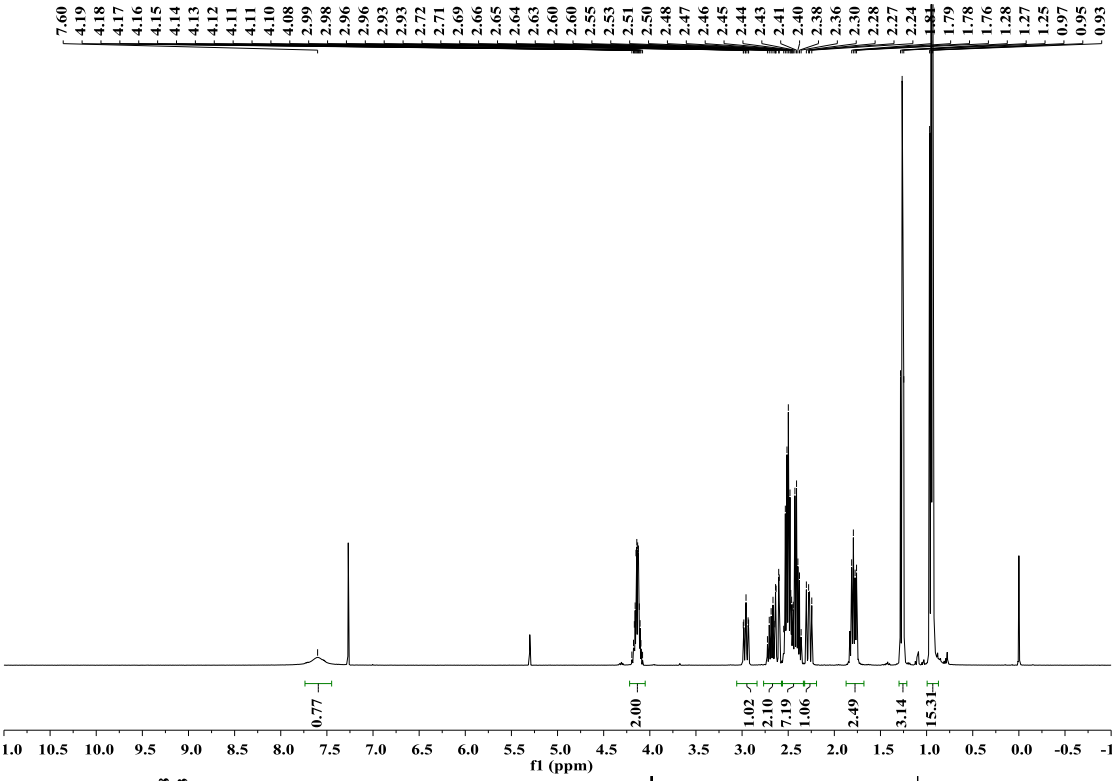


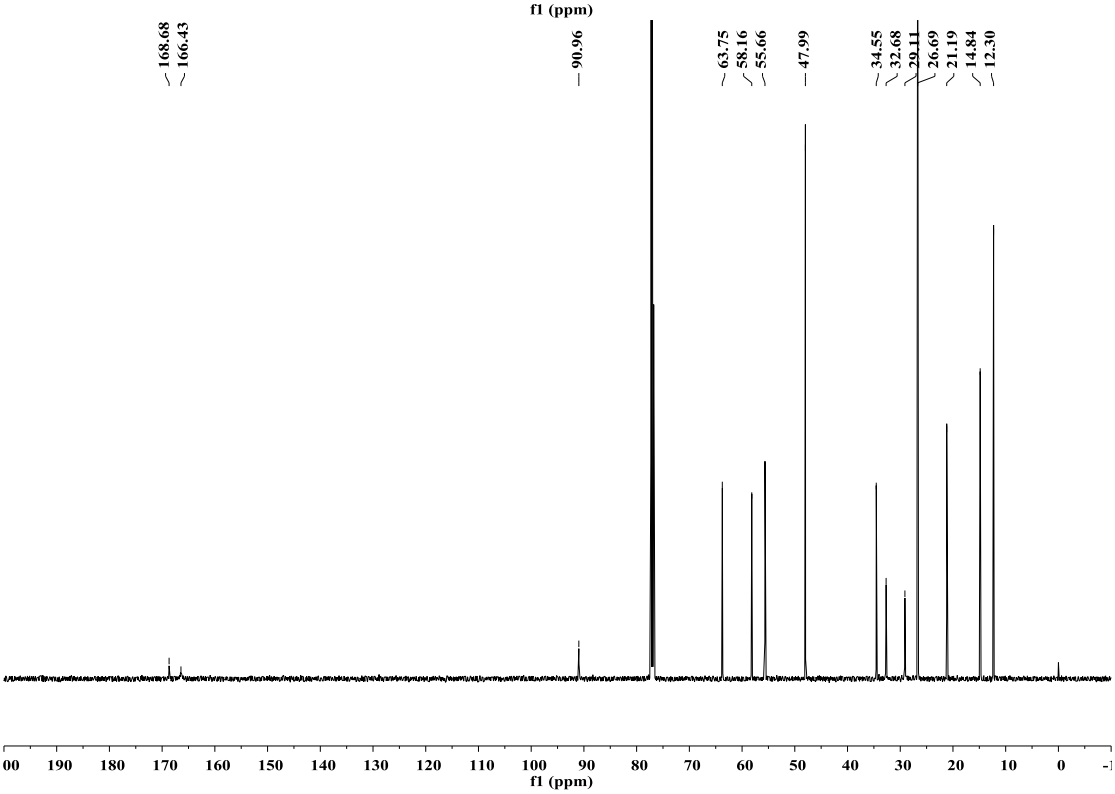
Figure S82. Cyclic voltammogram of $6C_3$.

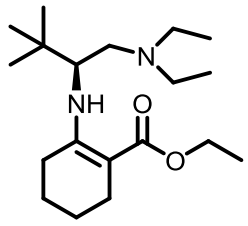
2. NMR spectra of enamines



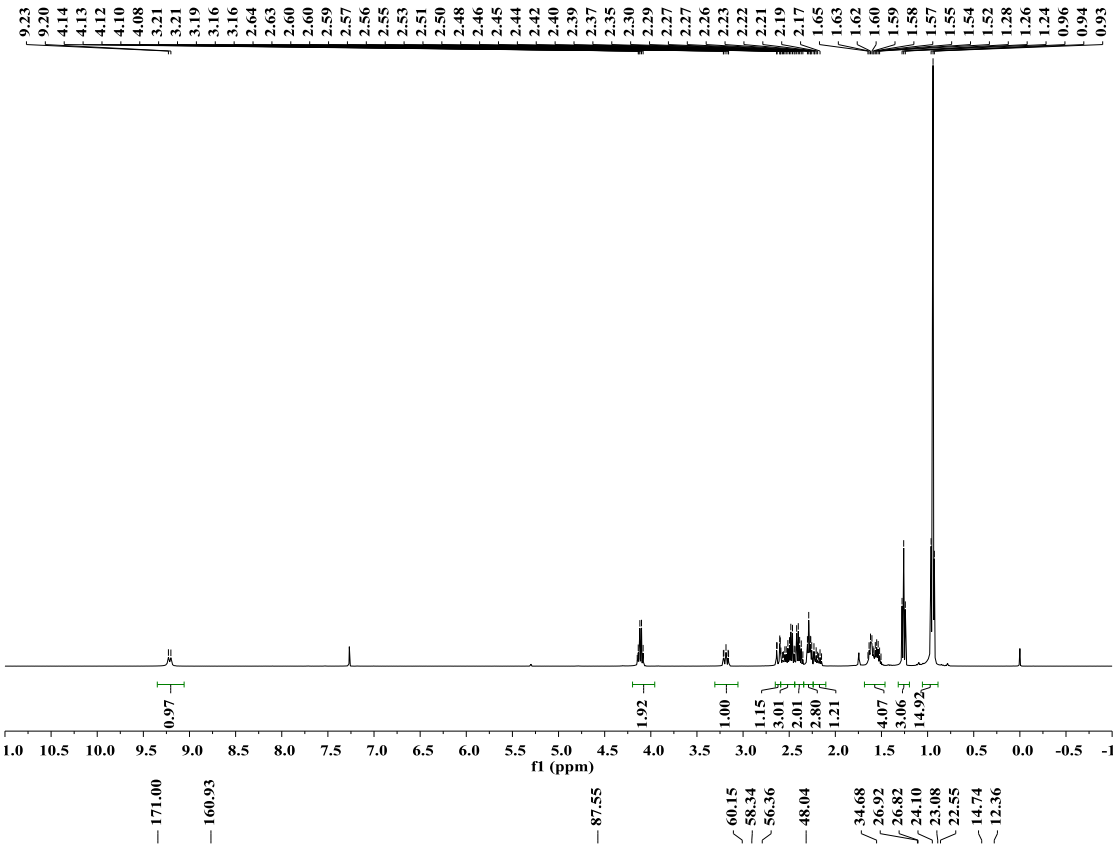
1A$_1$

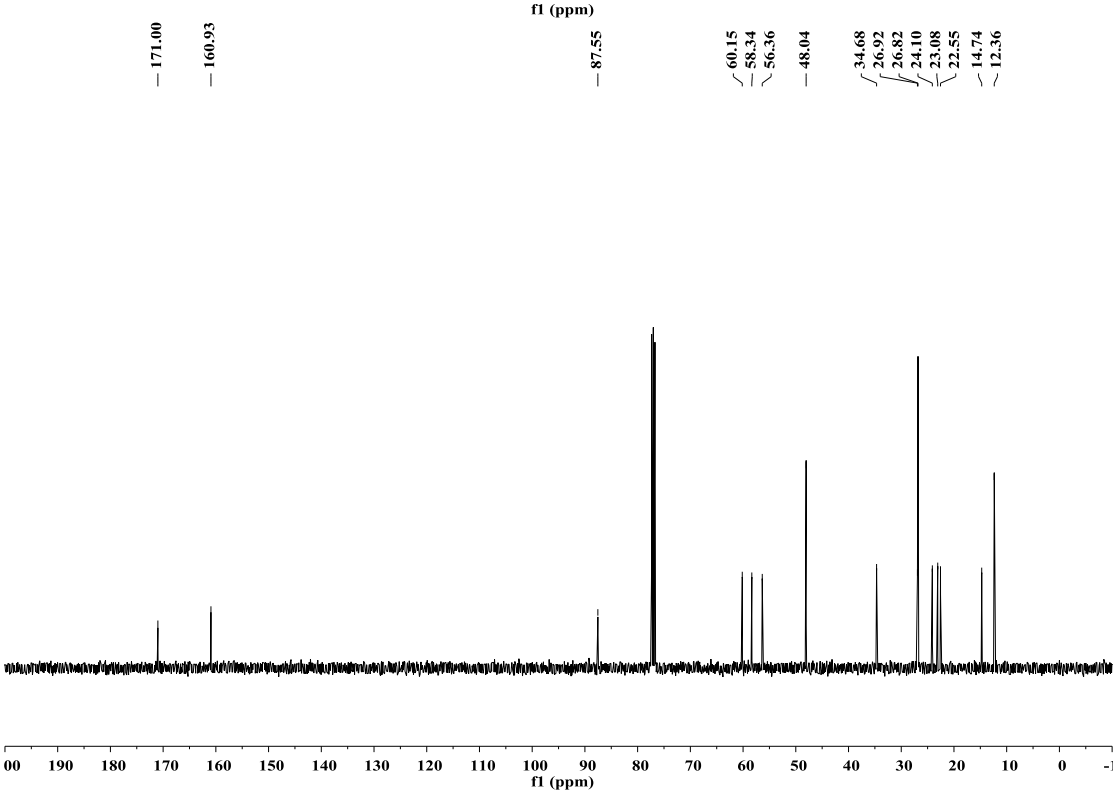


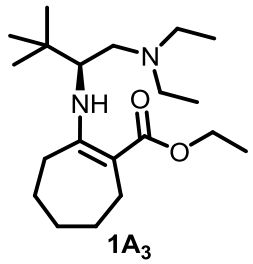



NH
O
N
O

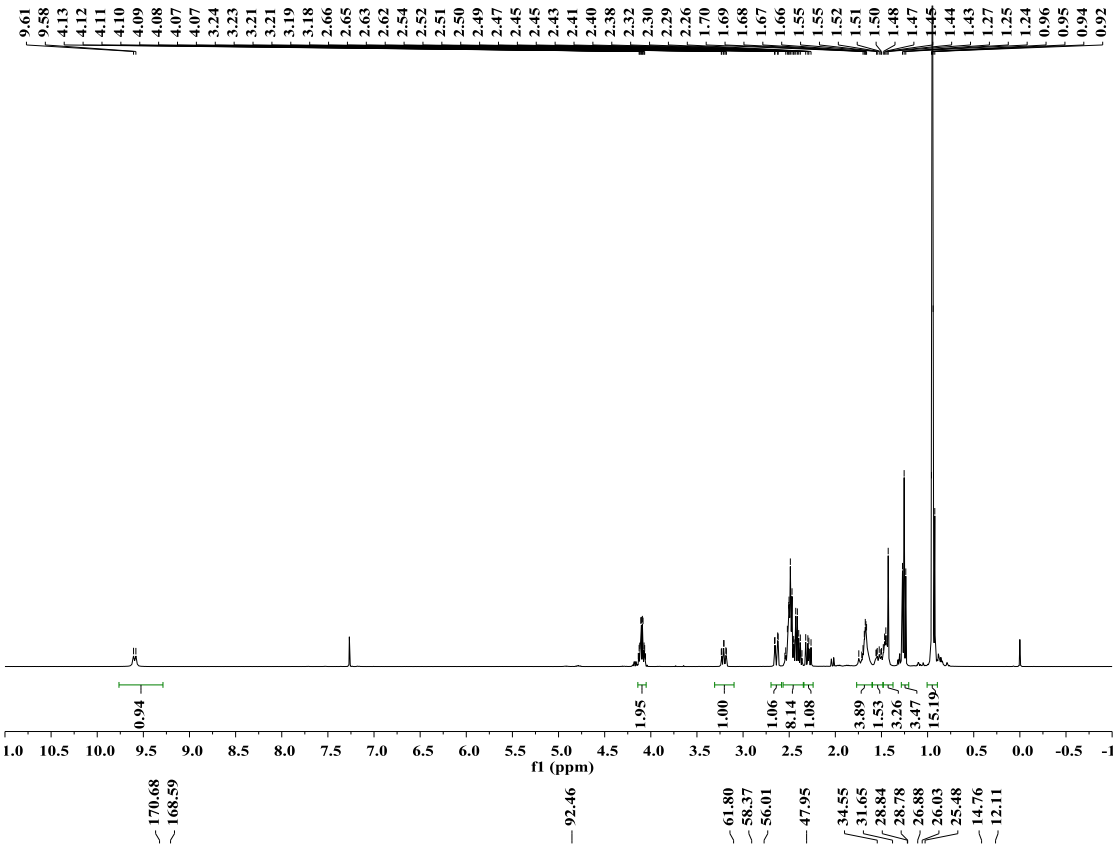
1A$_2$


9.23 9.20 4.14 4.13 4.12 4.10 4.08 3.21 3.21 3.19 3.16 3.16 2.64 2.63 2.60 2.60 2.59 2.57 2.56 2.55 2.53 2.51 2.50 2.48 2.46 2.45 2.44 2.42 2.40 2.39 2.37 2.35 2.30 2.29 2.27 2.27 2.26 2.23 2.22 2.21 2.19 2.17 1.65 1.63 1.62 1.60 1.59 1.58 1.57 1.55 1.54 1.52 1.28 1.26 1.24 0.96 0.94 0.93
0.97 1.92 1.00 1.15 3.01 2.01 2.80 1.21 4.07 3.06 14.92
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

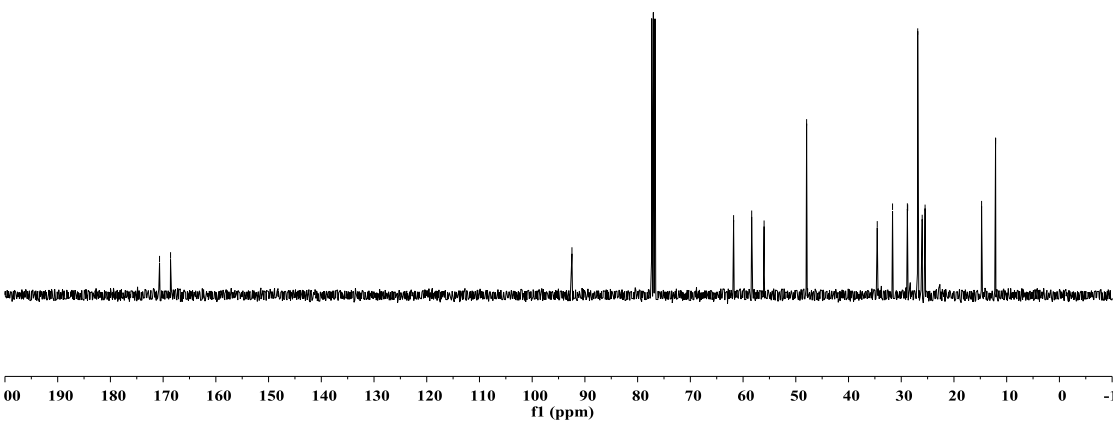

171.00 160.93 87.55 60.15 58.34 56.36 48.04 34.68 26.92 26.82 24.10 23.08 22.55 14.74 12.36
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

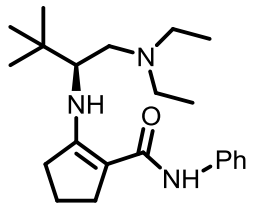

NH
O
N
O

1A$_3$

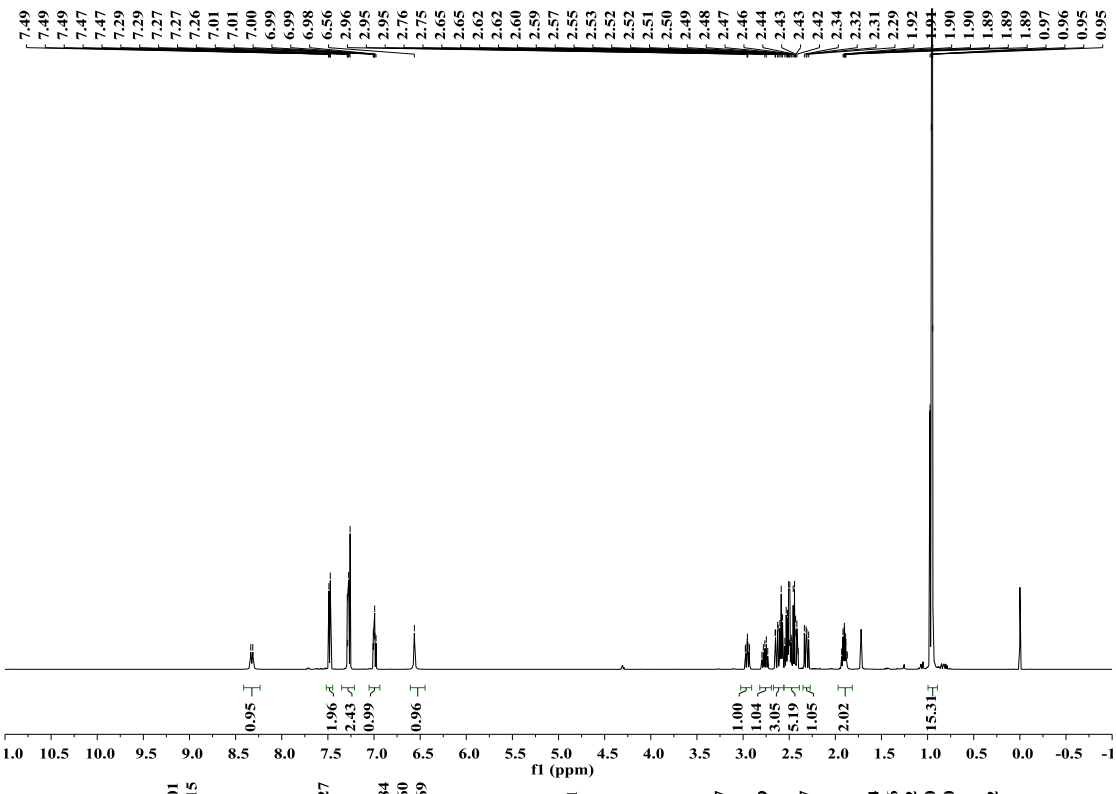

9.61 9.58 4.13 4.12 4.11 4.10 4.09 4.08 4.07 4.07 3.24 3.23 3.21 3.21 3.19 3.18 2.66 2.65 2.63 2.62 2.54 2.52 2.51 2.50 2.49 2.47 2.45 2.45 2.43 2.41 2.40 2.38 2.32 2.30 2.29 2.26 1.70 1.69 1.68 1.67 1.66 1.55 1.55 1.52 1.51 1.50 1.48 1.47 1.45 1.44 1.43 1.27 1.25 1.24 0.96 0.95 0.94 0.92
0.94 1.95 1.00 1.06 8.14 1.08 3.89 1.53 3.26 3.47 15.19
f1 (ppm)

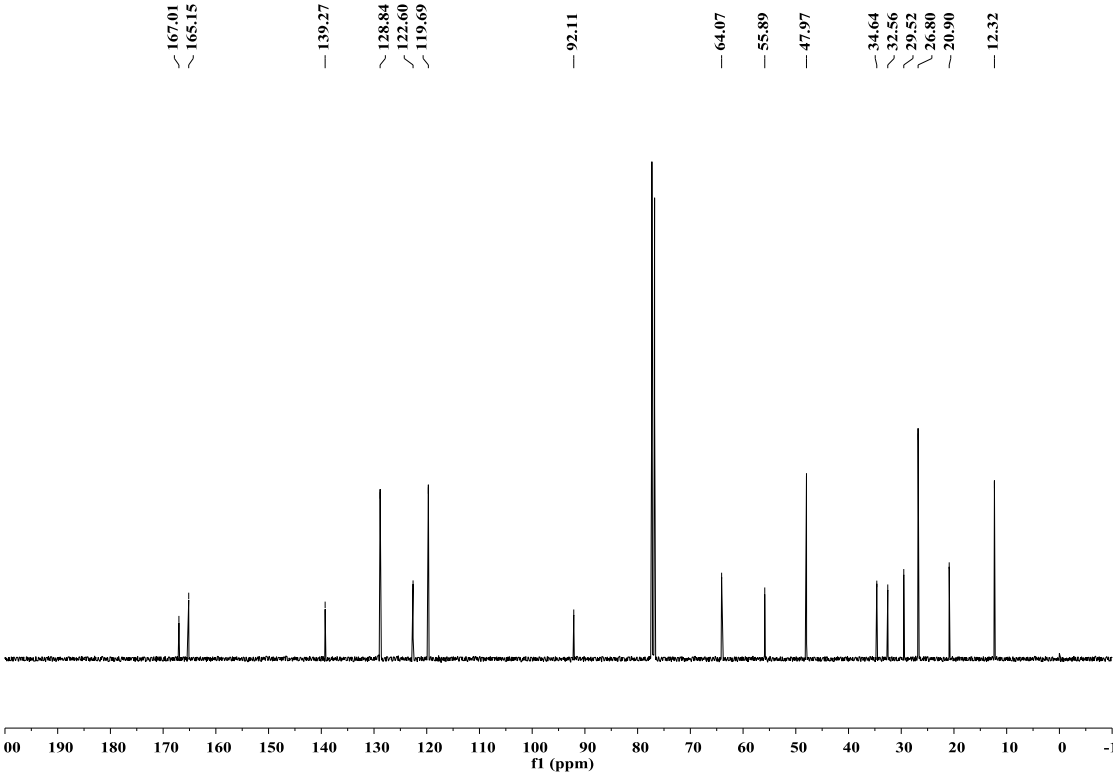
170.68 168.59 92.46 61.80 58.37 56.01 47.95 34.55 31.65 28.84 28.78 26.88 26.03 25.48 14.76 12.11

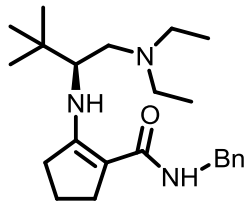

f1 (ppm)


N
NH
O
NH
Ph

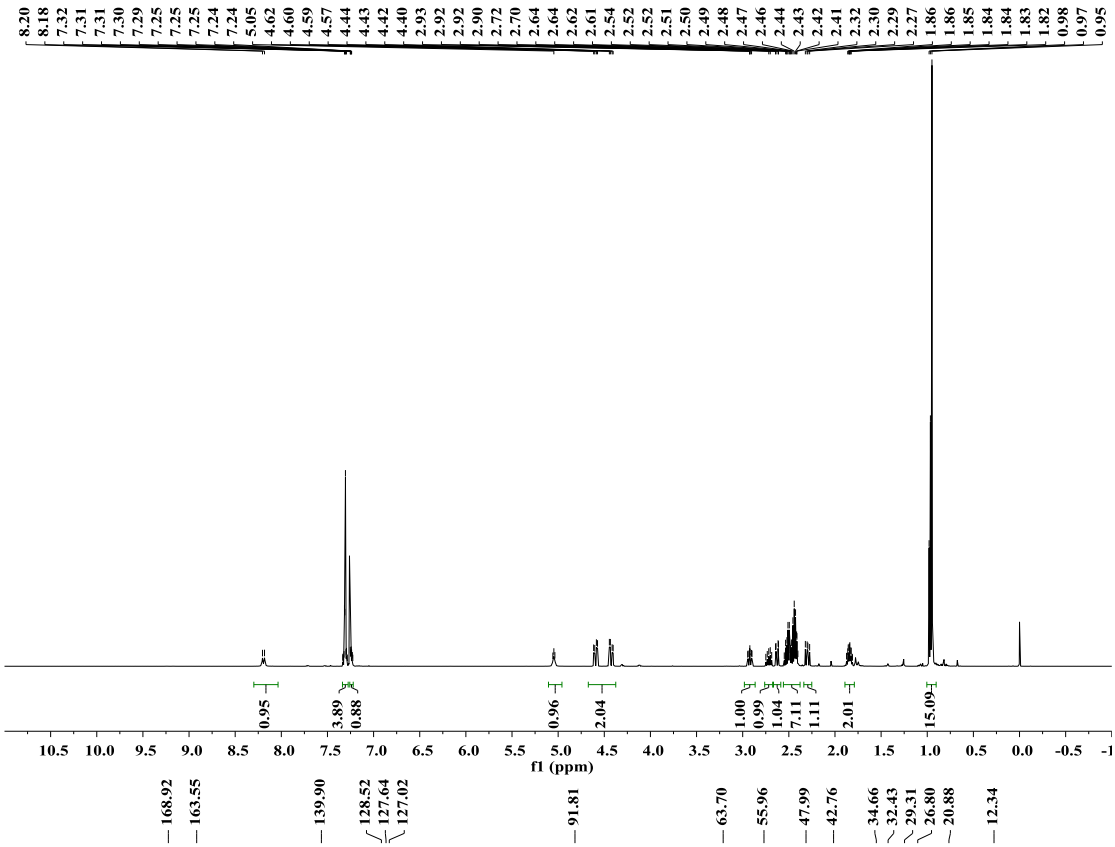
1A$_4$

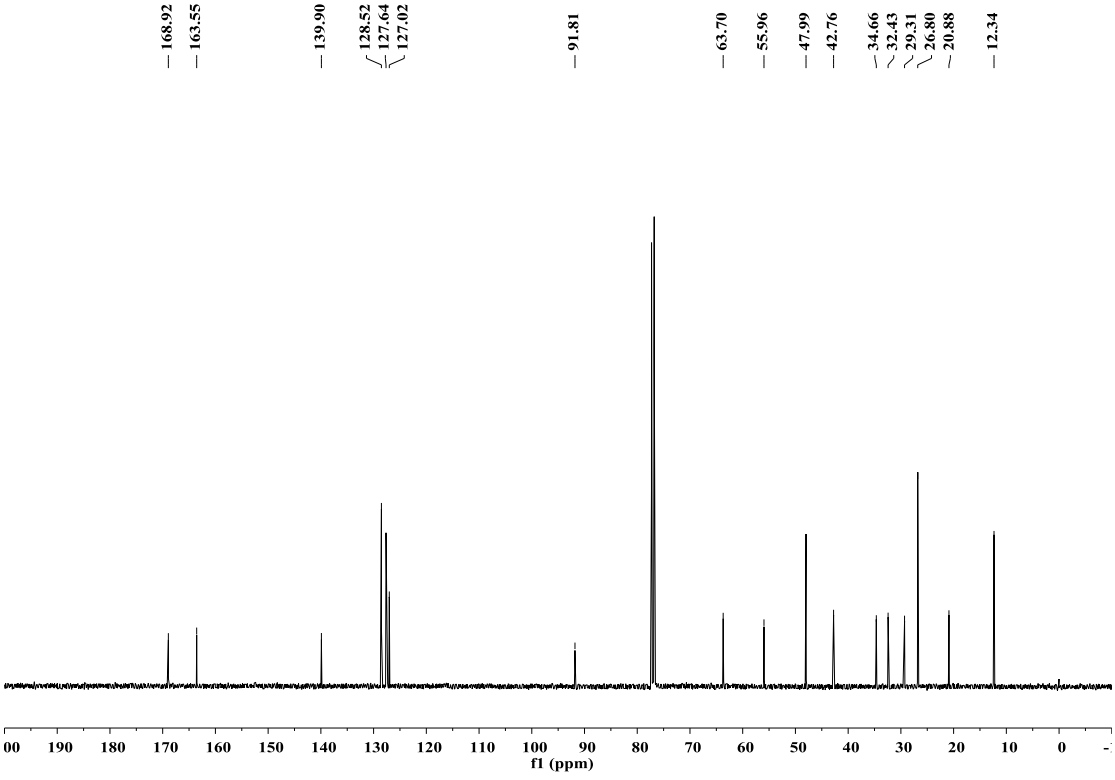

7.49 7.49 7.49 7.47 7.47 7.29 7.29 7.27 7.27 7.26 7.01 7.01 7.00 6.99 6.99 6.98 6.56 2.96 2.95 2.95 2.76 2.75 2.65 2.65 2.62 2.62 2.60 2.59 2.57 2.55 2.53 2.52 2.52 2.51 2.50 2.49 2.48 2.47 2.46 2.44 2.43 2.43 2.42 2.34 2.32 2.31 2.29 1.92 1.91 1.90 1.90 1.89 1.89 1.89 0.97 0.96 0.95 0.95
0.95 1.96 2.43 0.99 0.96 1.00 1.04 3.05 5.19 1.05 2.02 15.31
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

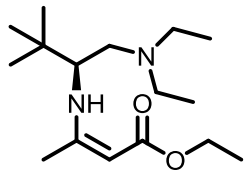

167.01 165.15 139.27 128.84 122.60 119.69 92.11 64.07 55.89 47.97 34.64 32.56 29.52 26.80 20.90 12.32
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)


N
NH
O
NH
Bn

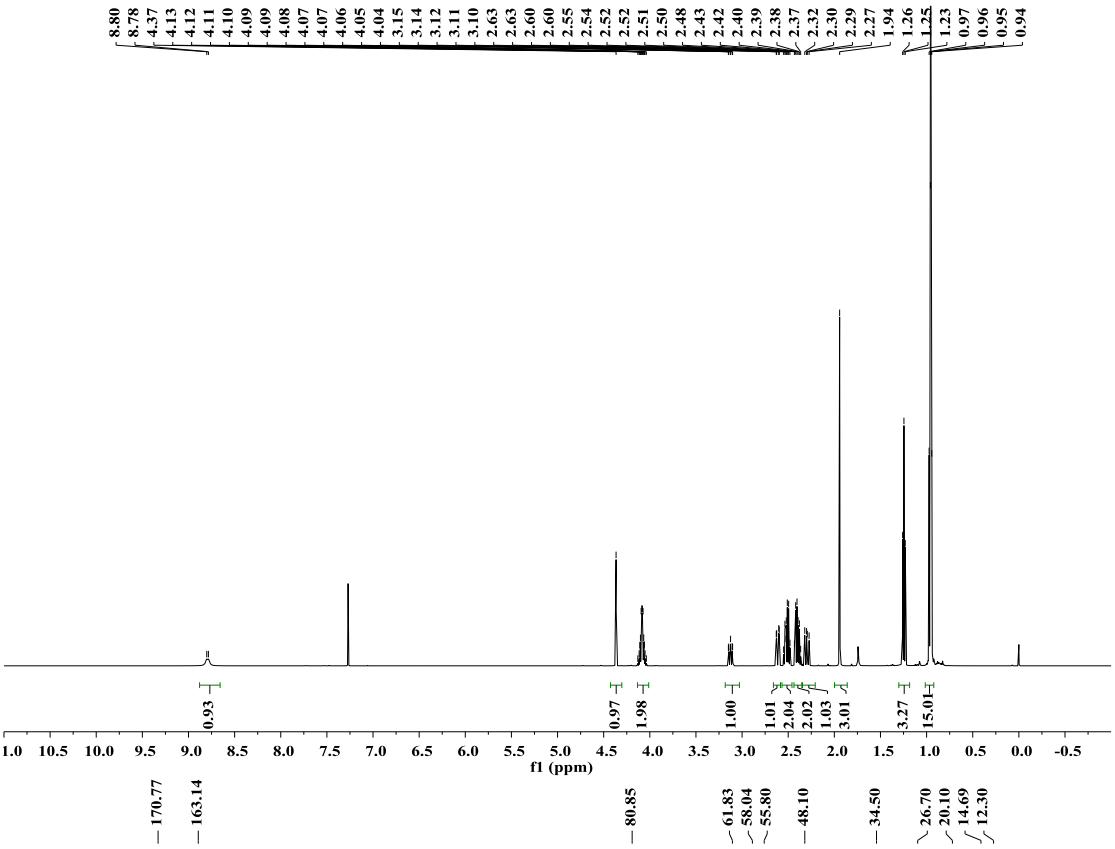
1A$_5$

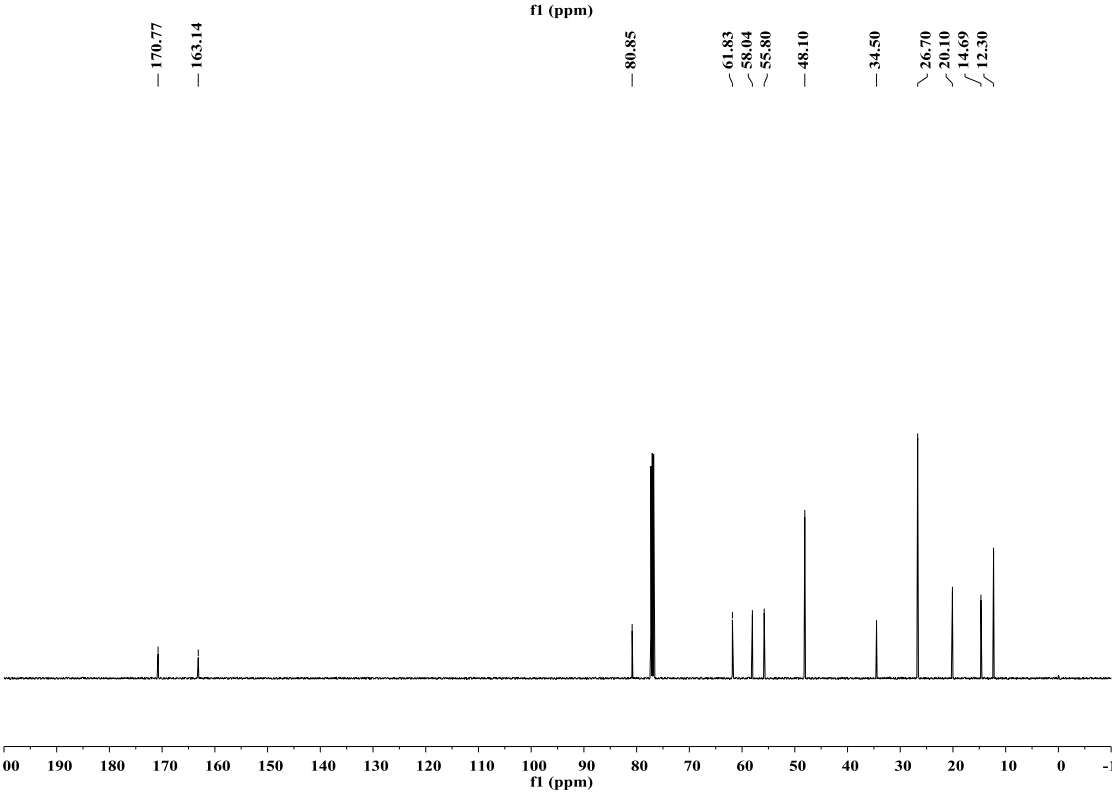

8.20 8.18 7.32 7.31 7.31 7.30 7.29 7.25 7.25 7.25 7.24 7.24 5.05 4.62 4.60 4.59 4.57 4.44 4.43 4.42 4.40 2.93 2.92 2.92 2.90 2.72 2.70 2.64 2.64 2.62 2.61 2.54 2.52 2.52 2.51 2.50 2.49 2.48 2.47 2.46 2.44 2.43 2.42 2.41 2.32 2.30 2.29 2.27 1.86 1.86 1.85 1.84 1.84 1.83 1.82 0.98 0.97 0.95
0.95 3.89 0.88 0.96 2.04 1.00 0.99 1.04 7.11 1.11 2.01 15.09
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

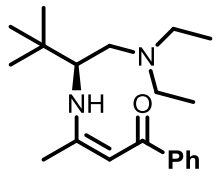

168.92 163.55 139.90 128.52 127.64 127.02 91.81 63.70 55.96 47.99 42.76 34.66 32.43 29.31 26.80 20.88 12.34
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


N
NH
O
O

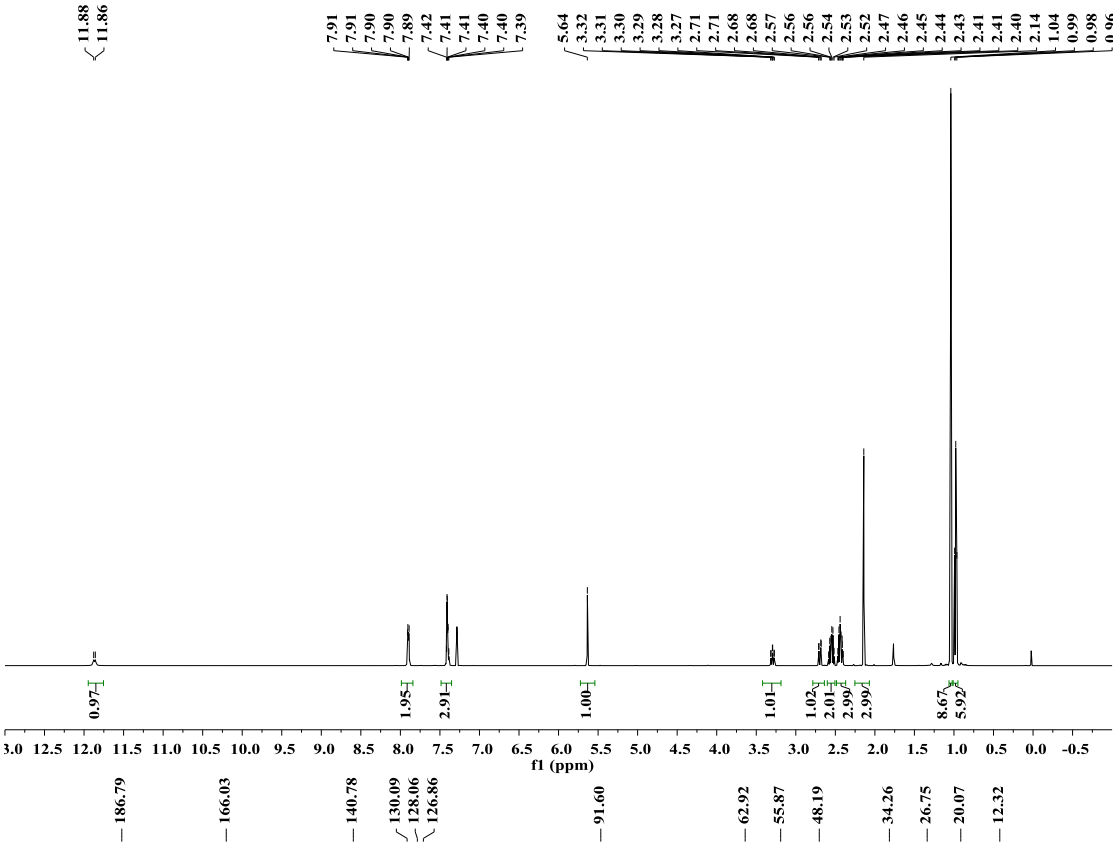
1B$_1$

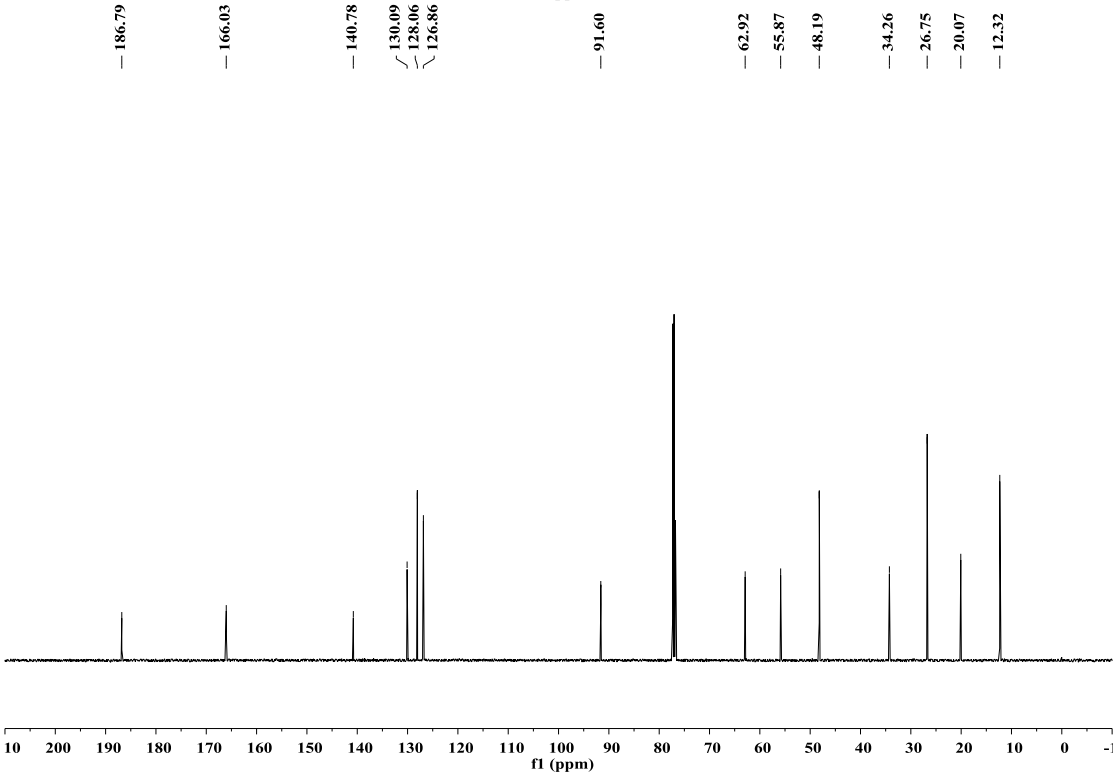

8.80
8.78
4.37
4.13
4.12
4.11
4.10
4.09
4.09
4.08
4.07
4.07
4.06
4.05
4.04
3.15
3.14
3.12
3.11
3.10
2.63
2.63
2.60
2.60
2.55
2.54
2.52
2.52
2.51
2.50
2.48
2.43
2.42
2.40
2.39
2.38
2.37
2.32
2.30
2.29
2.27
1.94
1.26
1.25
1.23
0.97
0.96
0.95
0.94
0.93
0.97
1.98
1.00
1.01
2.04
2.02
1.03
3.01
3.27
15.01
f1 (ppm)

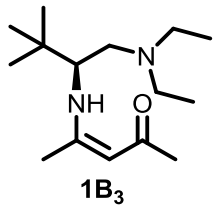

170.77
163.14
80.85
61.83
58.04
55.80
48.10
34.50
26.70
20.10
14.69
12.30
f1 (ppm)


N
NH
O
Ph

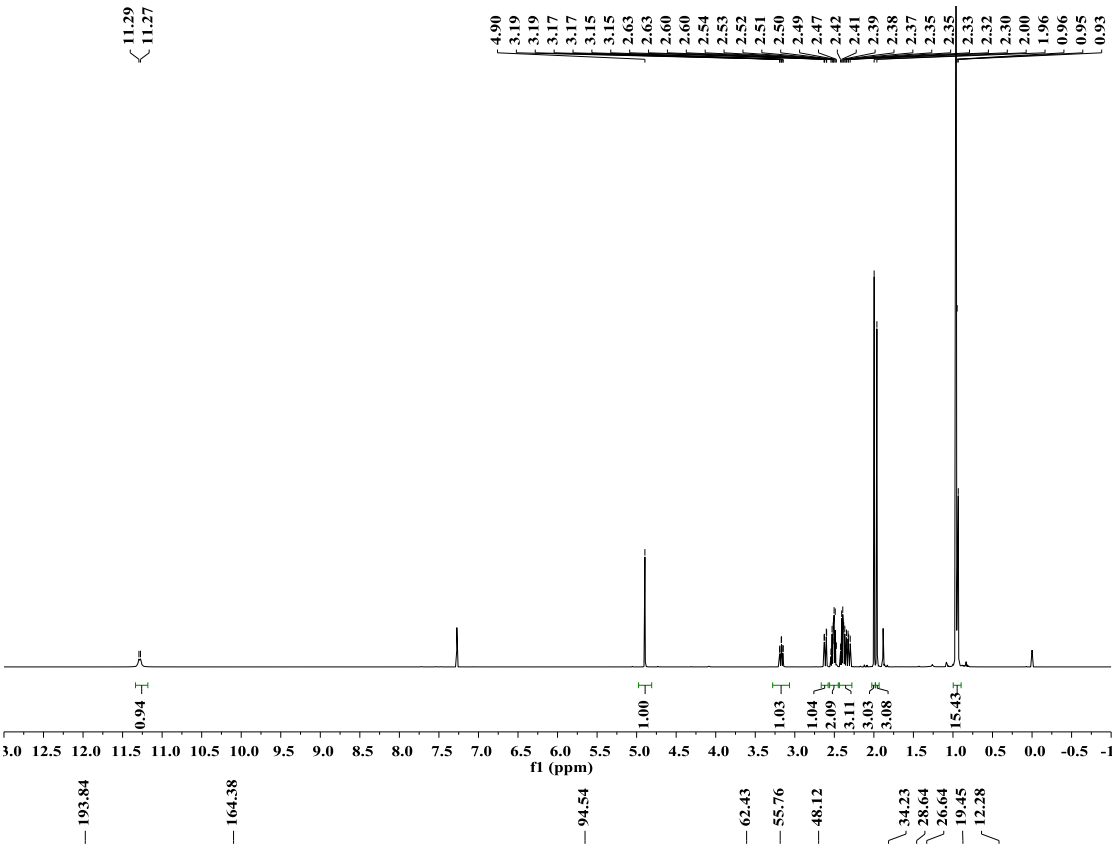
1B$_2$

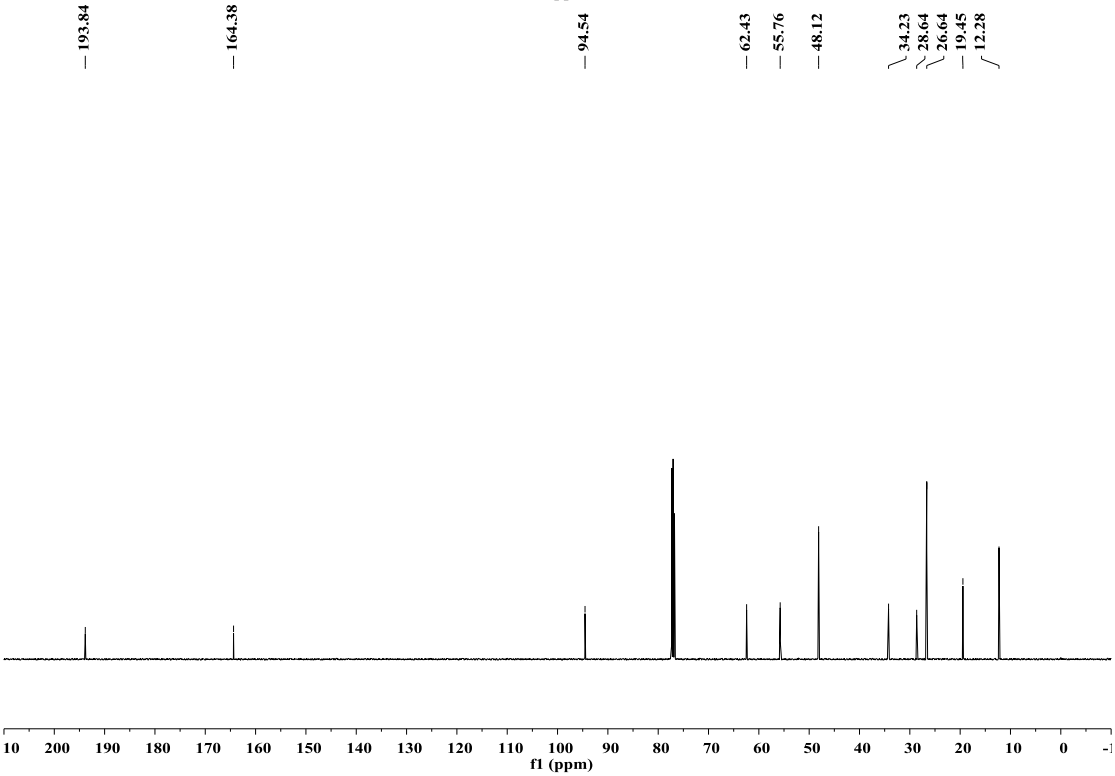

11.88
11.86
7.91
7.91
7.90
7.90
7.89
7.42
7.41
7.41
7.40
7.40
7.39
5.64
3.32
3.31
3.30
3.29
3.28
3.27
2.71
2.71
2.68
2.68
2.57
2.56
2.56
2.54
2.53
2.52
2.47
2.46
2.45
2.44
2.43
2.41
2.41
2.40
2.14
1.04
0.99
0.98
0.97
1.95
2.91
1.00
1.01
1.02
2.01
2.99
2.99
8.67
5.92
f1 (ppm)

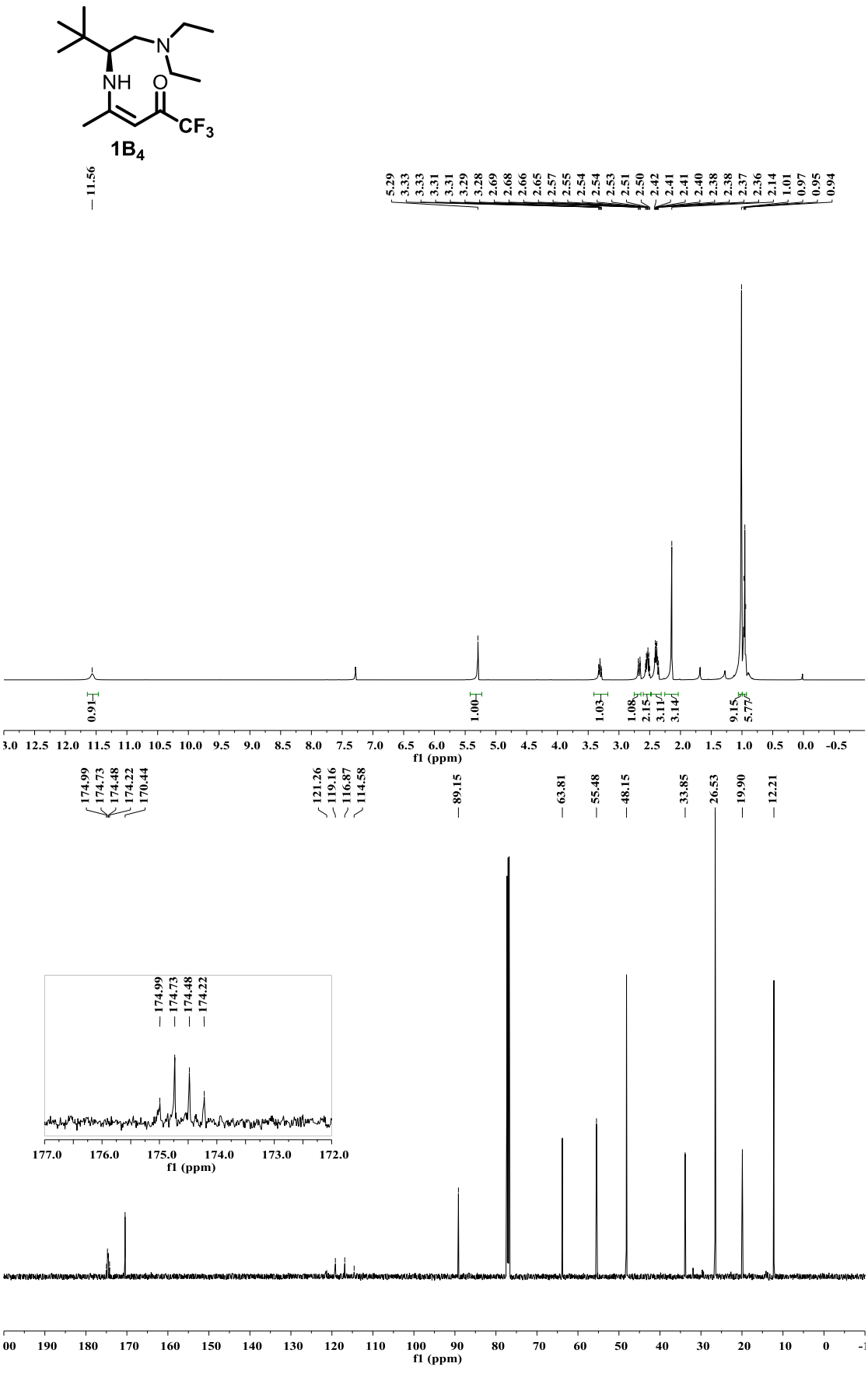

186.79
166.03
140.78
130.09
128.06
126.86
91.60
62.92
55.87
48.19
34.26
26.75
20.07
12.32
f1 (ppm)

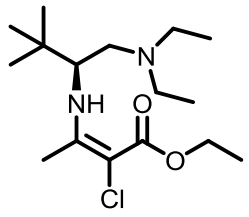

NH
O
N

1B$_3$

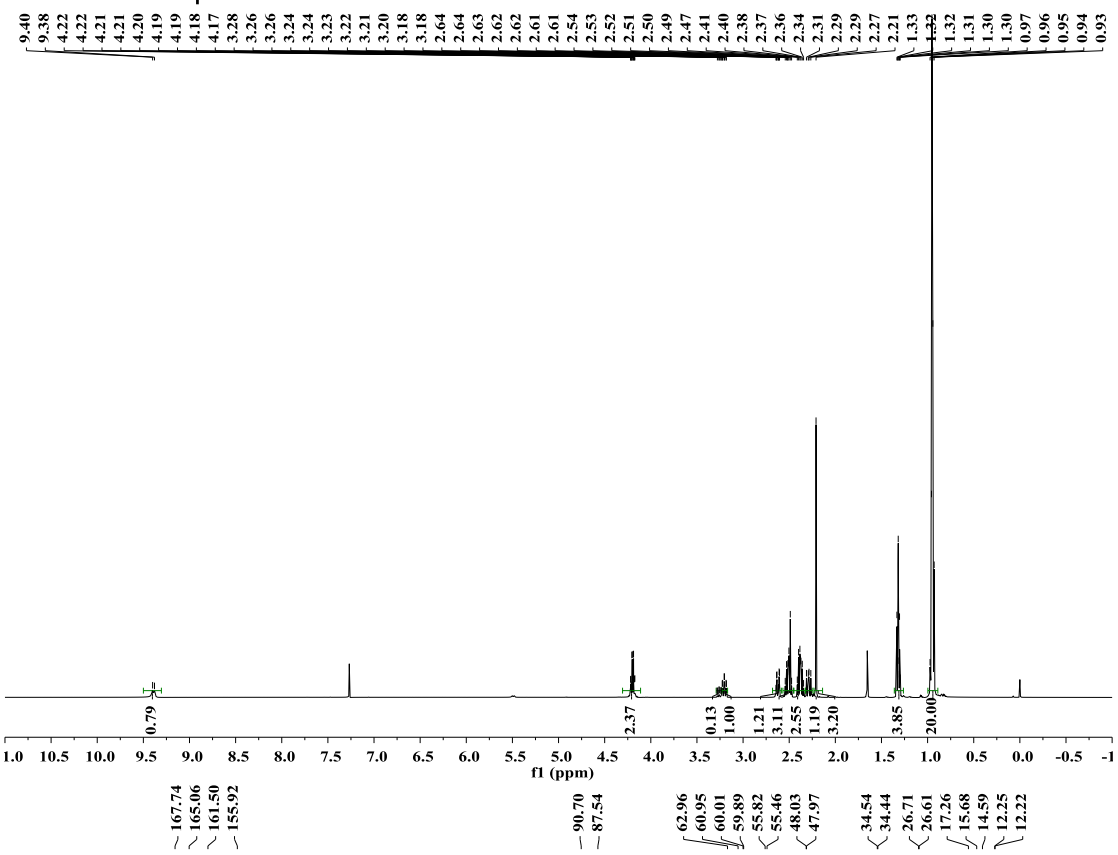

11.29
11.27
4.90
3.19
3.19
3.17
3.17
3.15
3.15
2.63
2.63
2.60
2.60
2.54
2.53
2.52
2.51
2.50
2.49
2.47
2.42
2.41
2.39
2.38
2.37
2.35
2.35
2.33
2.32
2.30
2.00
1.96
0.96
0.95
0.93
0.94
1.00
1.03
1.04
2.09
3.11
3.03
3.08
15.43
f1 (ppm)

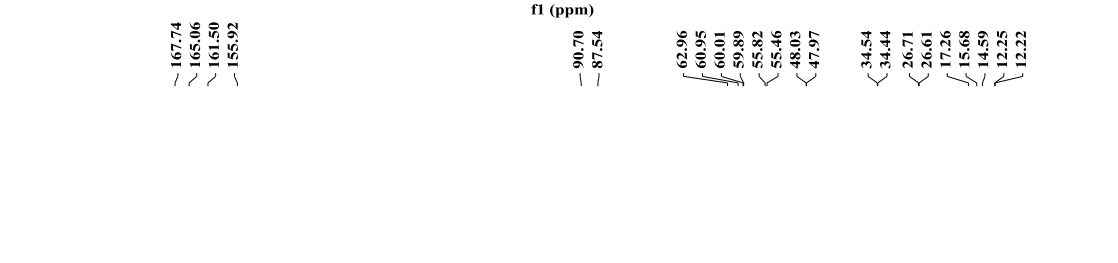

193.84
164.38
94.54
62.43
55.76
48.12
34.23
28.64
26.64
19.45
12.28
f1 (ppm)

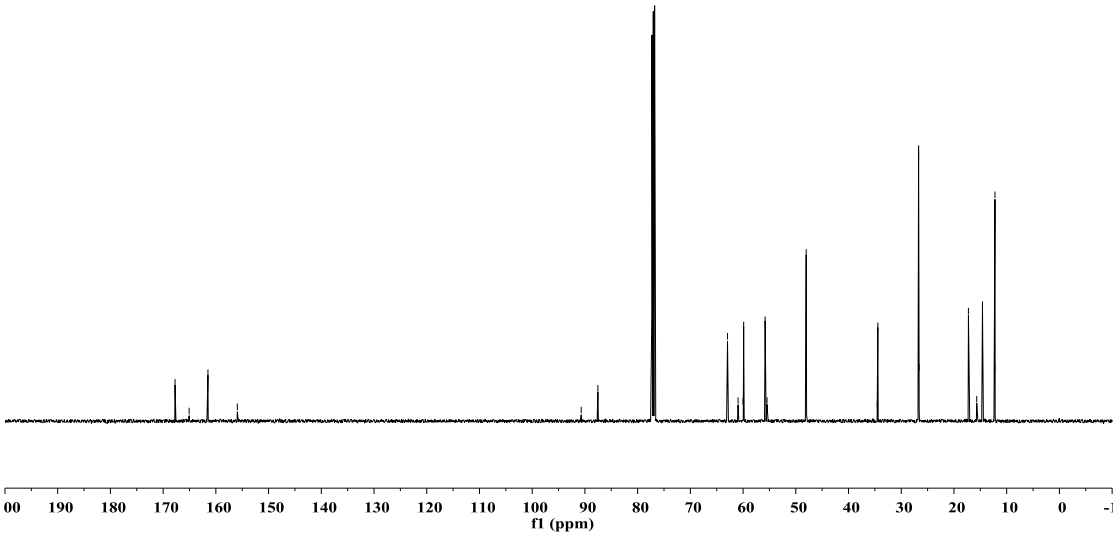

NH
O
N
CF3
1B4
11.56
5.29
3.33
3.33
3.31
3.31
3.29
3.28
2.69
2.68
2.66
2.65
2.57
2.55
2.54
2.54
2.53
2.51
2.50
2.42
2.41
2.41
2.40
2.38
2.38
2.37
2.36
2.14
1.01
0.97
0.95
0.94
0.91
1.00
1.03
1.08
2.15
3.11
3.14
9.15
5.77
f1 (ppm)
174.99
174.73
174.48
174.22
170.44
121.26
119.16
116.87
114.58
89.15
63.81
55.48
48.15
33.85
26.53
19.90
12.21
177.0
176.0
175.0
174.0
173.0
172.0
f1 (ppm)

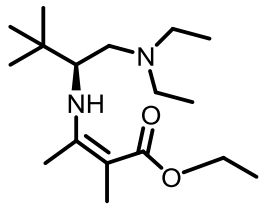

N
NH
O
O
Cl

1C$_1$

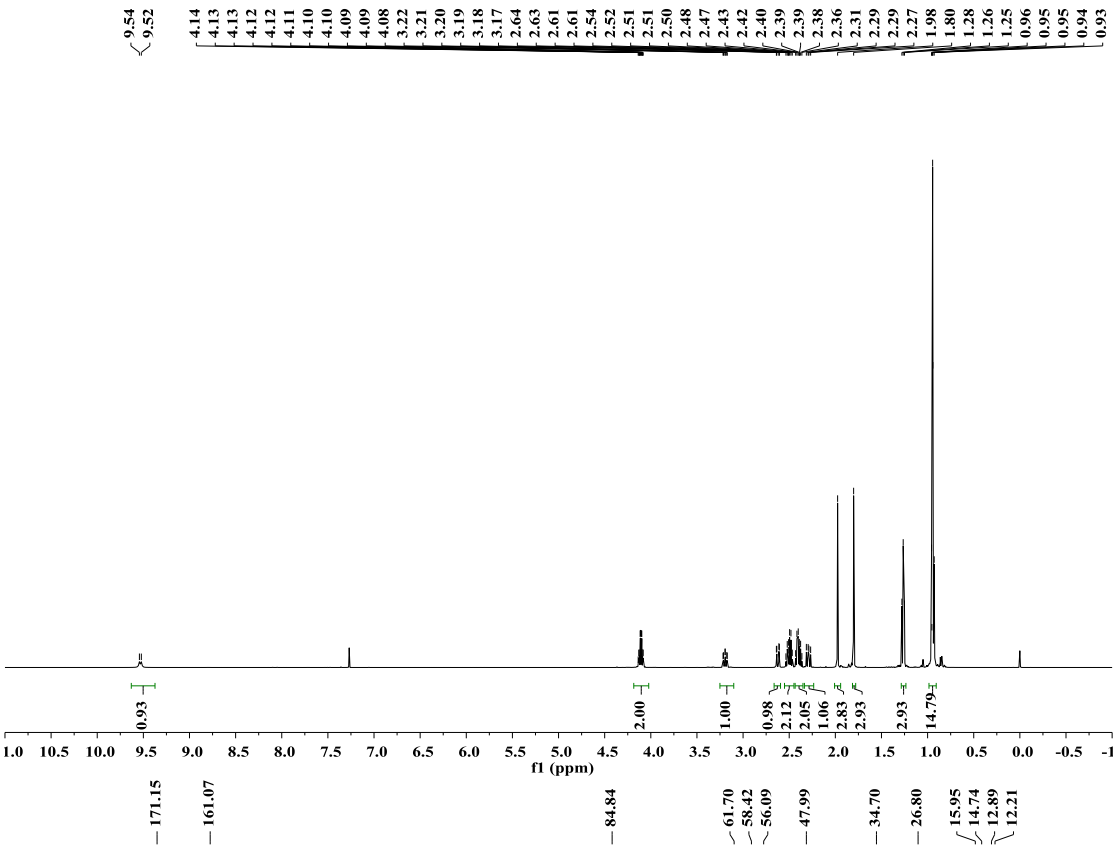

9.40 9.38 4.22 4.22 4.21 4.21 4.20 4.19 4.19 4.18 4.17 3.28 3.26 3.26 3.24 3.24 3.23 3.22 3.21 3.20 3.18 3.18 2.64 2.64 2.63 2.62 2.62 2.61 2.61 2.54 2.53 2.52 2.51 2.50 2.49 2.47 2.41 2.40 2.38 2.37 2.36 2.34 2.31 2.29 2.29 2.27 2.21 1.33 1.32 1.32 1.31 1.30 1.30 0.97 0.96 0.95 0.94 0.93
0.79 2.37 0.13 1.00 1.21 3.11 2.55 1.19 3.20 3.85 20.00
f1 (ppm)

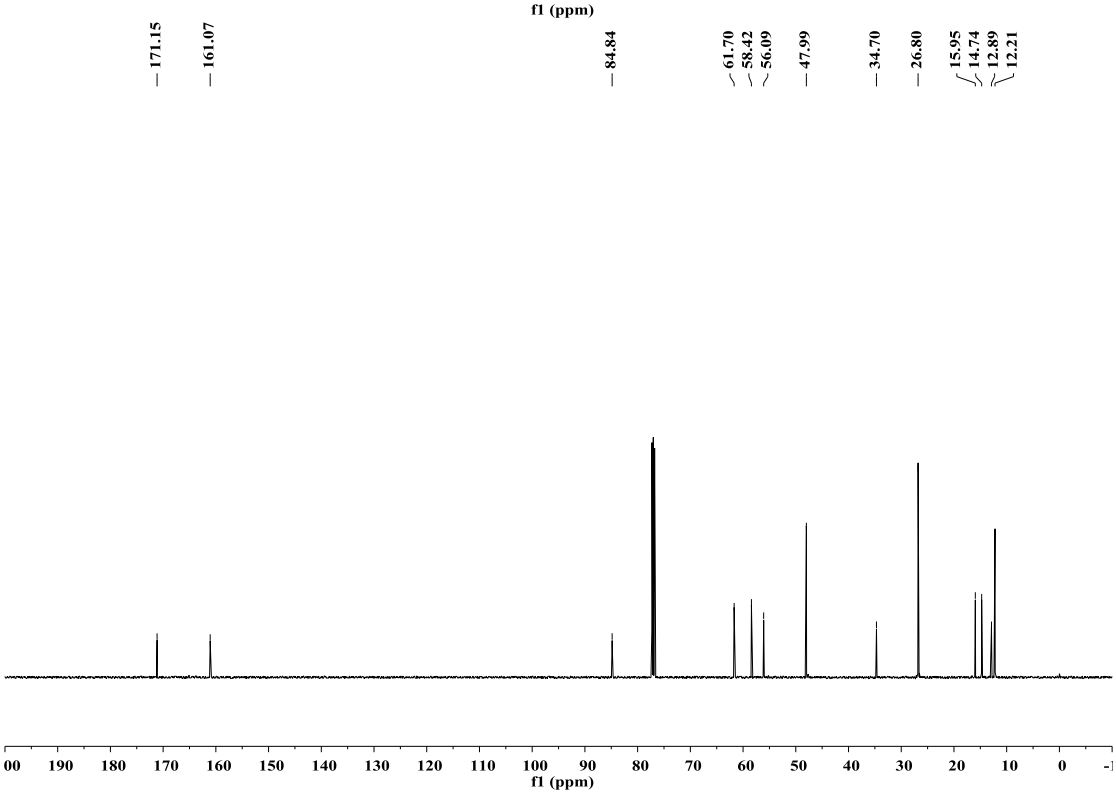

167.74 165.06 161.50 155.92 90.70 87.54 62.96 60.95 60.01 59.89 55.82 55.46 48.03 47.97 34.54 34.44 26.71 26.61 17.26 15.68 14.59 12.25 12.22

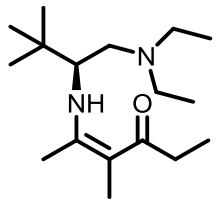

f1 (ppm)


N
NH
O
O

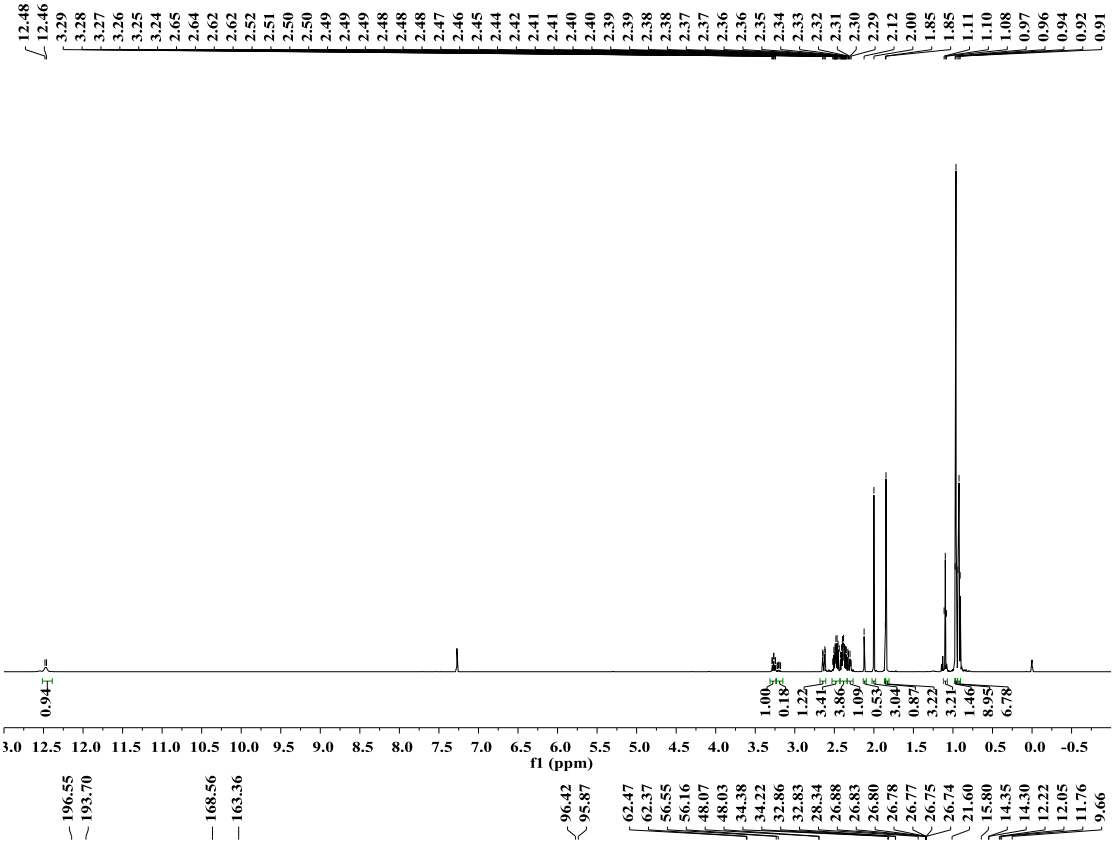
1C$_2$

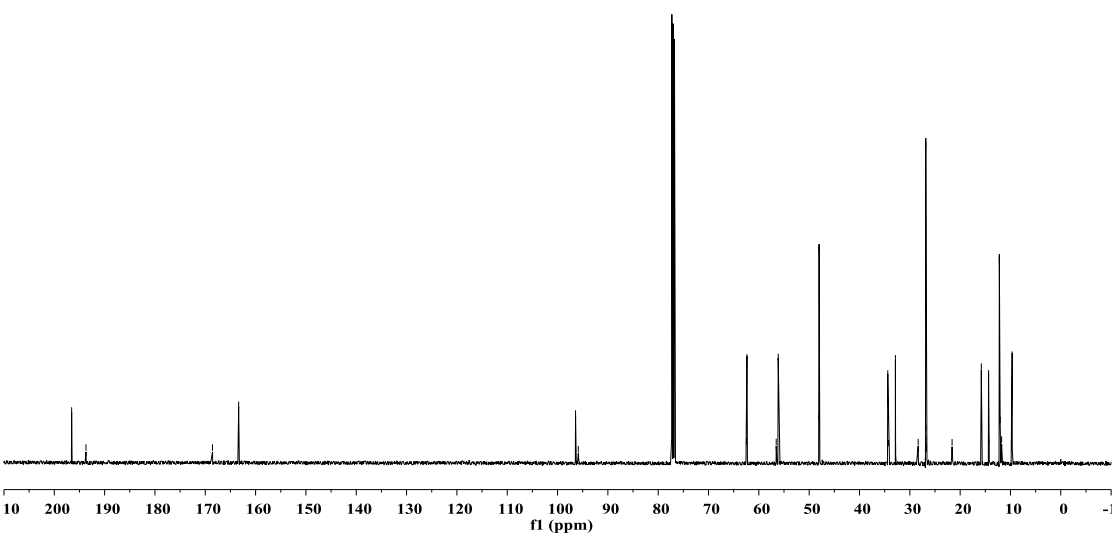

9.54
9.52
4.14
4.13
4.13
4.12
4.12
4.11
4.10
4.10
4.09
4.09
4.08
3.22
3.21
3.20
3.19
3.18
3.17
2.64
2.63
2.61
2.61
2.54
2.52
2.51
2.51
2.50
2.48
2.47
2.43
2.42
2.40
2.39
2.39
2.38
2.36
2.31
2.29
2.29
2.27
1.98
1.80
1.28
1.26
1.25
0.96
0.95
0.95
0.94
0.93
0.93
2.00
1.00
0.98
2.12
2.05
1.06
2.83
2.93
2.93
14.79
f1 (ppm)

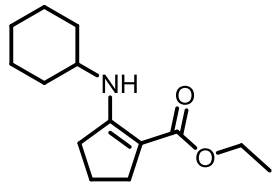

171.15
161.07
84.84
61.70
58.42
56.09
47.99
34.70
26.80
15.95
14.74
12.89
12.21
f1 (ppm)



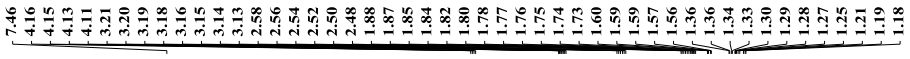
1C$_3$






NH
O
O

2A$_1$


7.46
4.16
4.15
4.13
4.11
3.21
3.20
3.19
3.18
3.16
3.15
3.14
3.13
2.58
2.56
2.54
2.52
2.50
2.48
1.88
1.87
1.85
1.84
1.82
1.80
1.78
1.77
1.76
1.75
1.74
1.73
1.60
1.59
1.59
1.57
1.56
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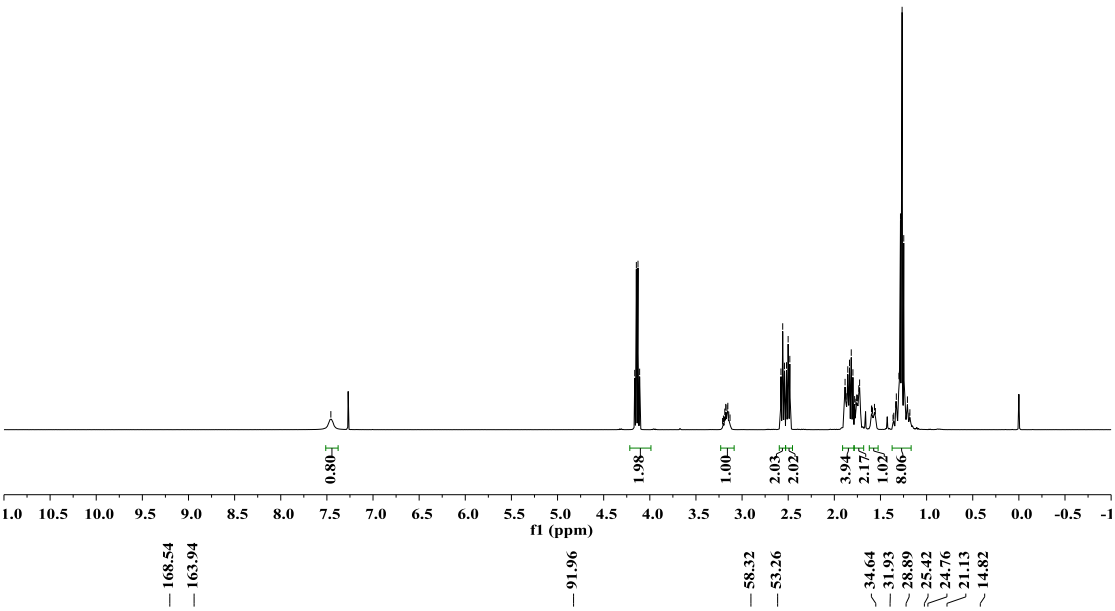
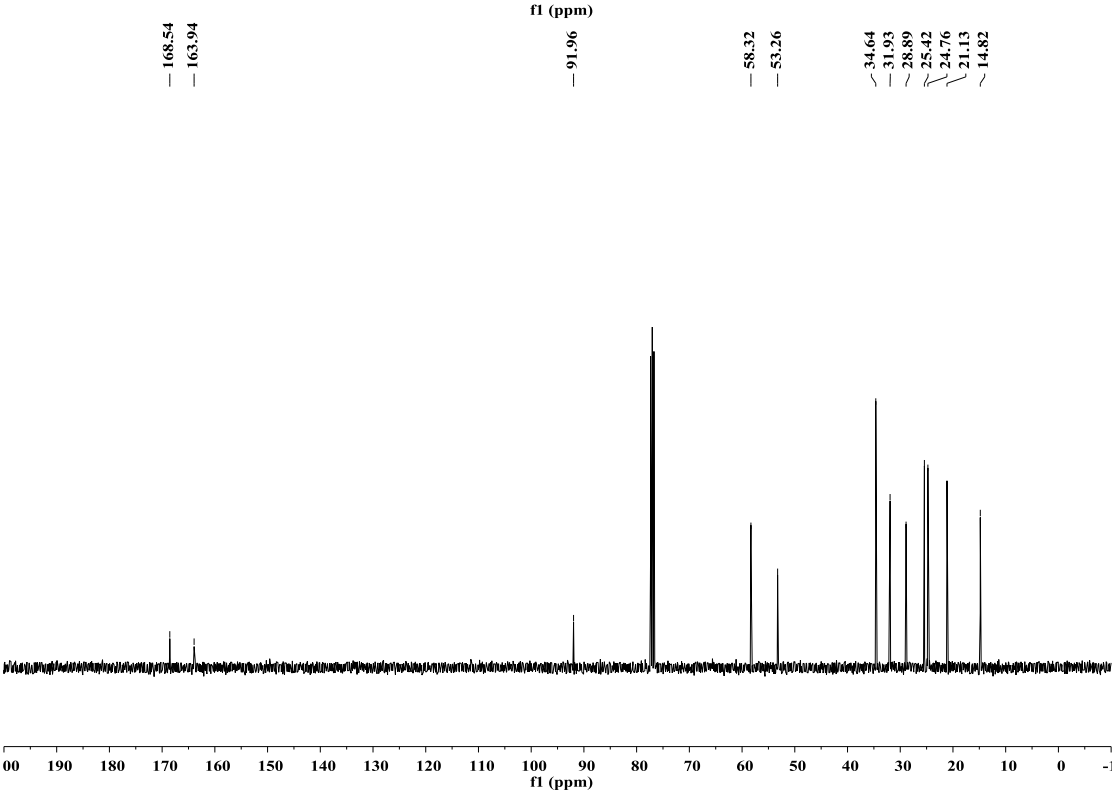
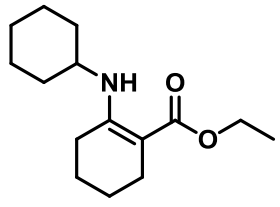
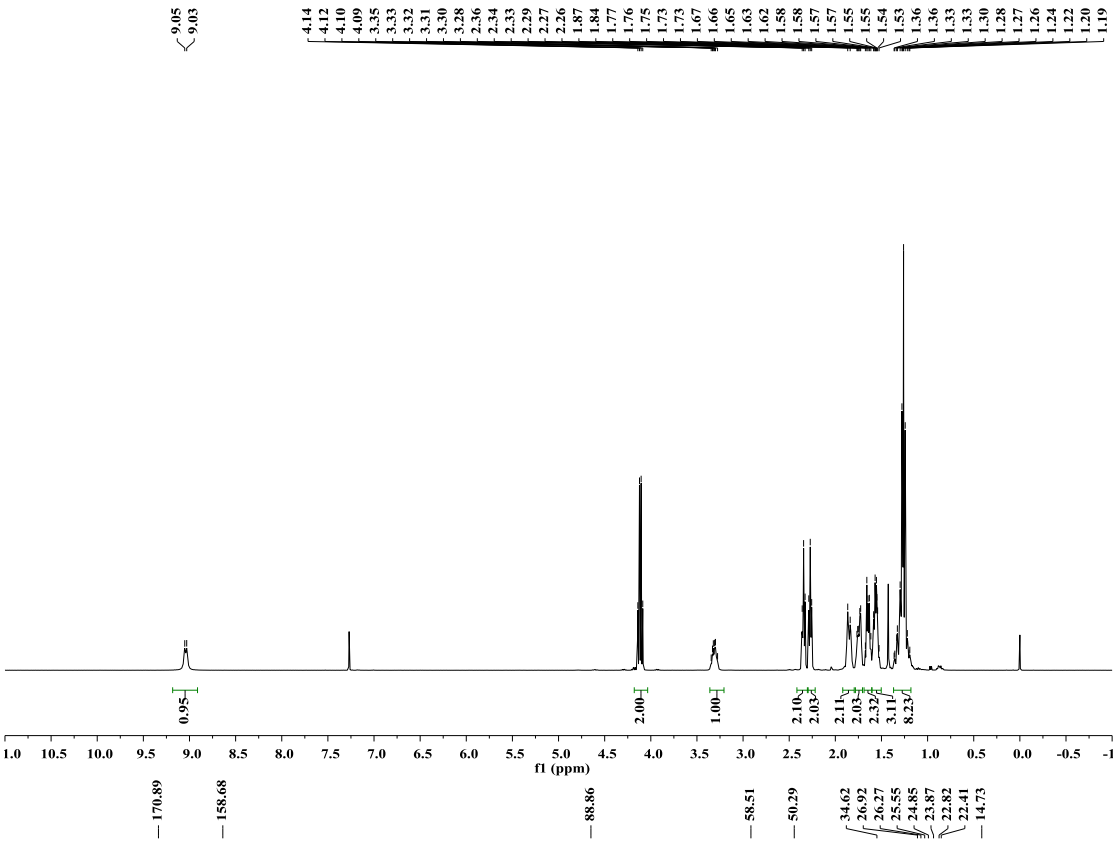
1.28
1.27
1.25
1.21
1.19
1.18

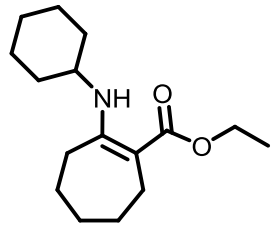

0.80
1.98
1.00
2.03
2.02
3.94
2.17
1.02
8.06
f1 (ppm)


168.54
163.94
91.96
58.32
53.26
34.64
31.93
28.89
25.42
24.76
21.13
14.82
f1 (ppm)

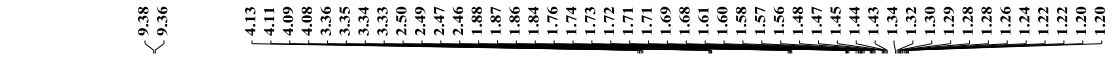

NH
O
O

$2A_2$


9.05
9.03
4.14
4.12
4.10
4.09
3.35
3.33
3.32
3.31
3.30
3.28
2.36
2.34
2.33
2.29
2.27
2.26
1.87
1.84
1.77
1.76
1.75
1.73
1.73
1.67
1.66
1.65
1.63
1.62
1.58
1.58
1.57
1.57
1.55
1.55
1.54
1.53
1.36
1.36
1.33
1.33
1.30
1.28
1.27
1.26
1.24
1.22
1.20
1.19
0.95
2.00
1.00
2.10
2.03
2.11
2.03
2.32
3.11
8.23
f1 (ppm)
170.89
158.68
88.86
58.51
50.29
34.62
26.92
26.27
25.55
24.85
23.87
22.82
22.41
14.73
f1 (ppm)


NH
O
O

2A$_3$


9.38
9.36
4.13
4.11
4.09
4.08
3.36
3.35
3.34
3.33
2.50
2.49
2.47
2.46
1.88
1.87
1.86
1.84
1.76
1.74
1.73
1.72
1.71
1.71
1.69
1.68
1.61
1.60
1.58
1.57
1.56
1.48
1.47
1.45
1.44
1.43
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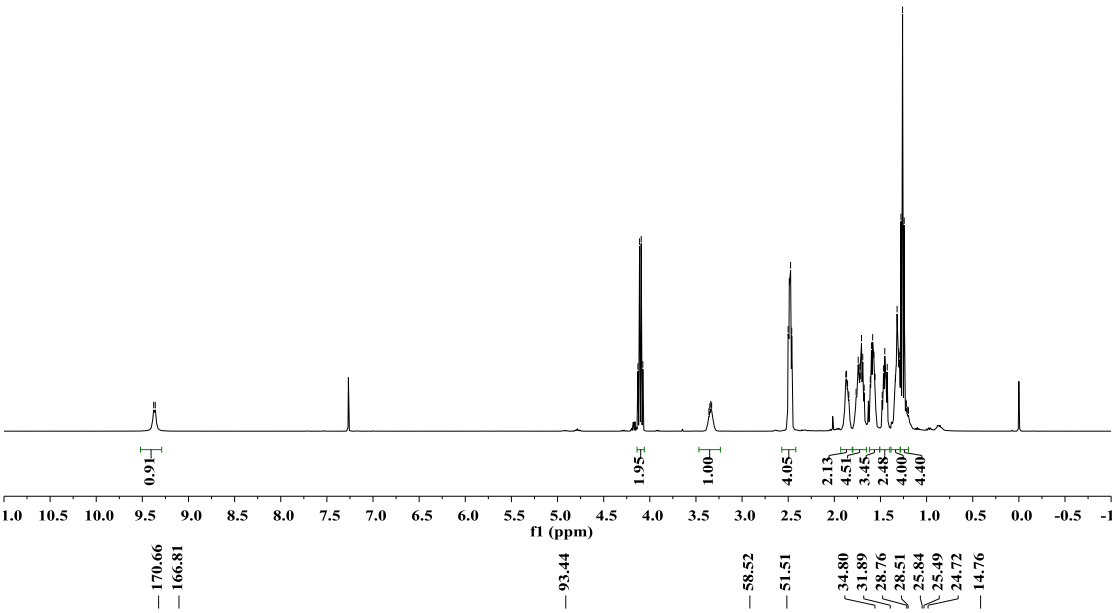
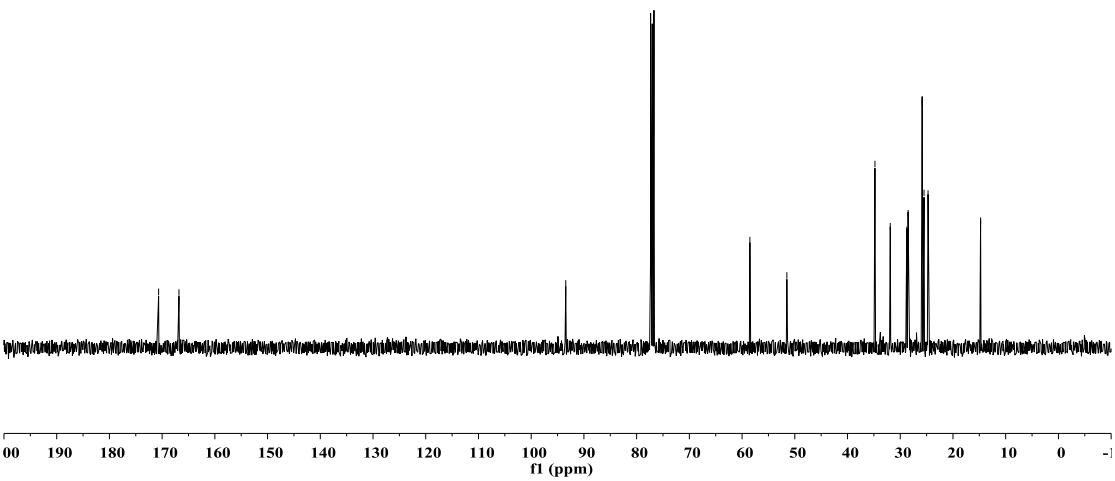
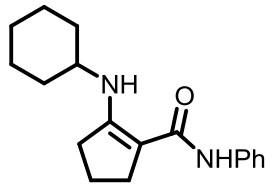
1.26
1.24
1.22
1.22
1.20
1.20

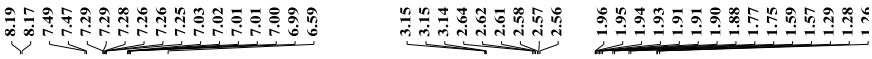

0.91
1.95
1.00
4.05
2.13
4.51
3.45
2.48
4.00
4.40
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

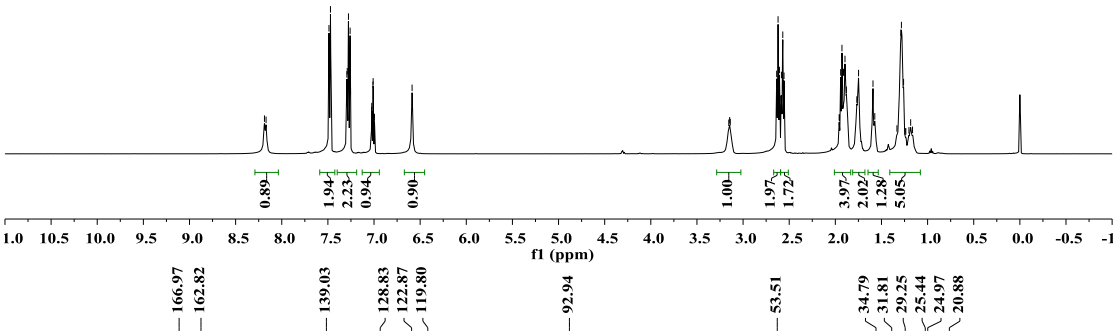
170.66
166.81
93.44
58.52
51.51
34.80
31.89
28.76
28.51
25.84
25.49
24.72
14.76


00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

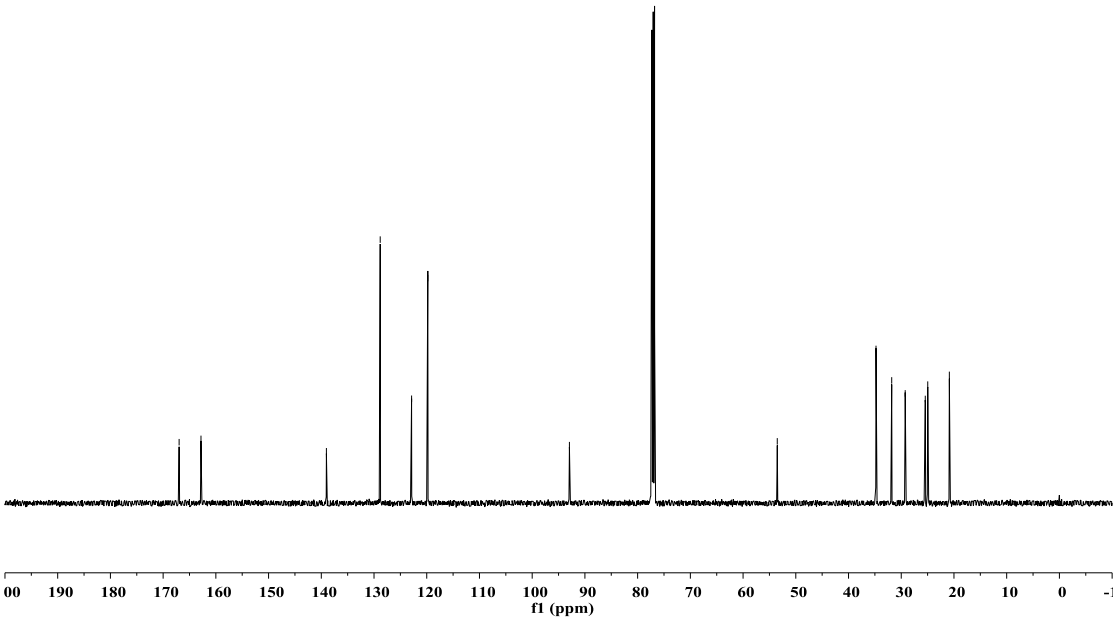

NH
O
NHPh

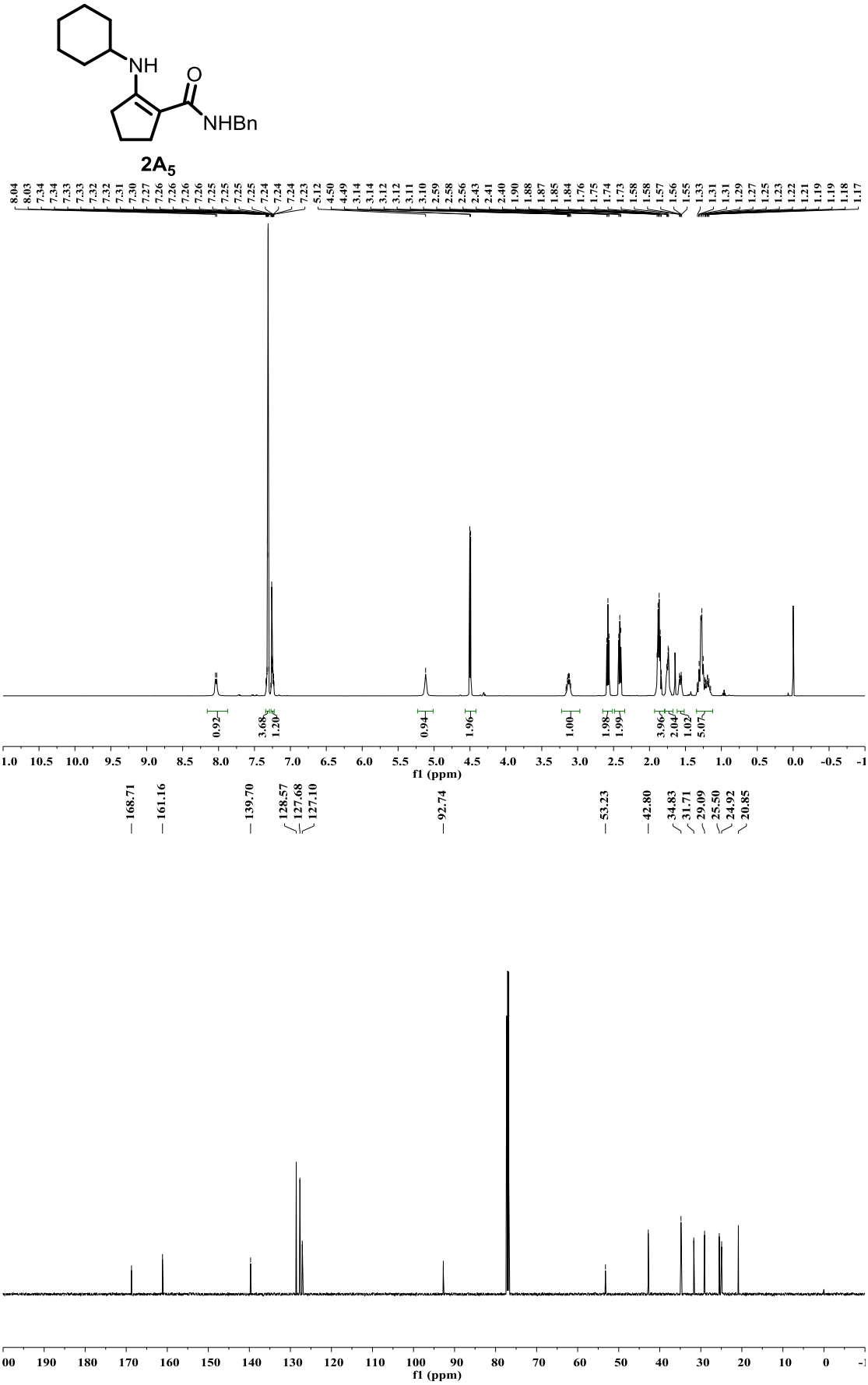
2A$_4$

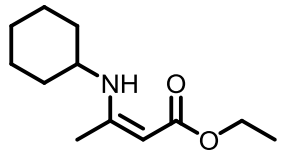

8.19
8.17
7.49
7.47
7.29
7.29
7.28
7.26
7.26
7.25
7.03
7.02
7.01
7.01
7.00
6.99
6.59
3.15
3.15
3.14
2.64
2.62
2.61
2.58
2.57
2.56
1.96
1.95
1.94
1.93
1.91
1.91
1.90
1.88
1.77
1.75
1.59
1.57
1.29
1.28


0.89
1.94
2.23
0.94
0.90
1.00
1.97
1.72
3.97
2.02
1.28
5.05
f1 (ppm)

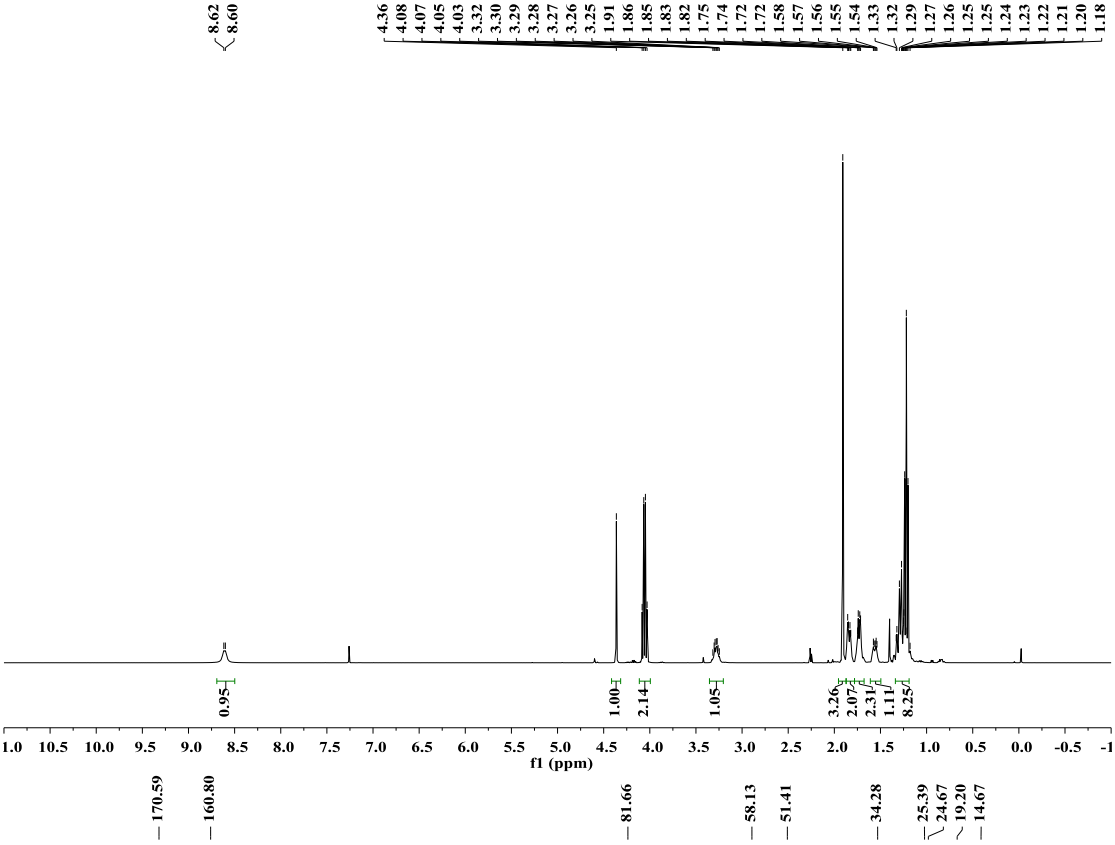
166.97
162.82
139.03
128.83
122.87
119.80
92.94
53.51
34.79
31.81
29.25
25.44
24.97
20.88

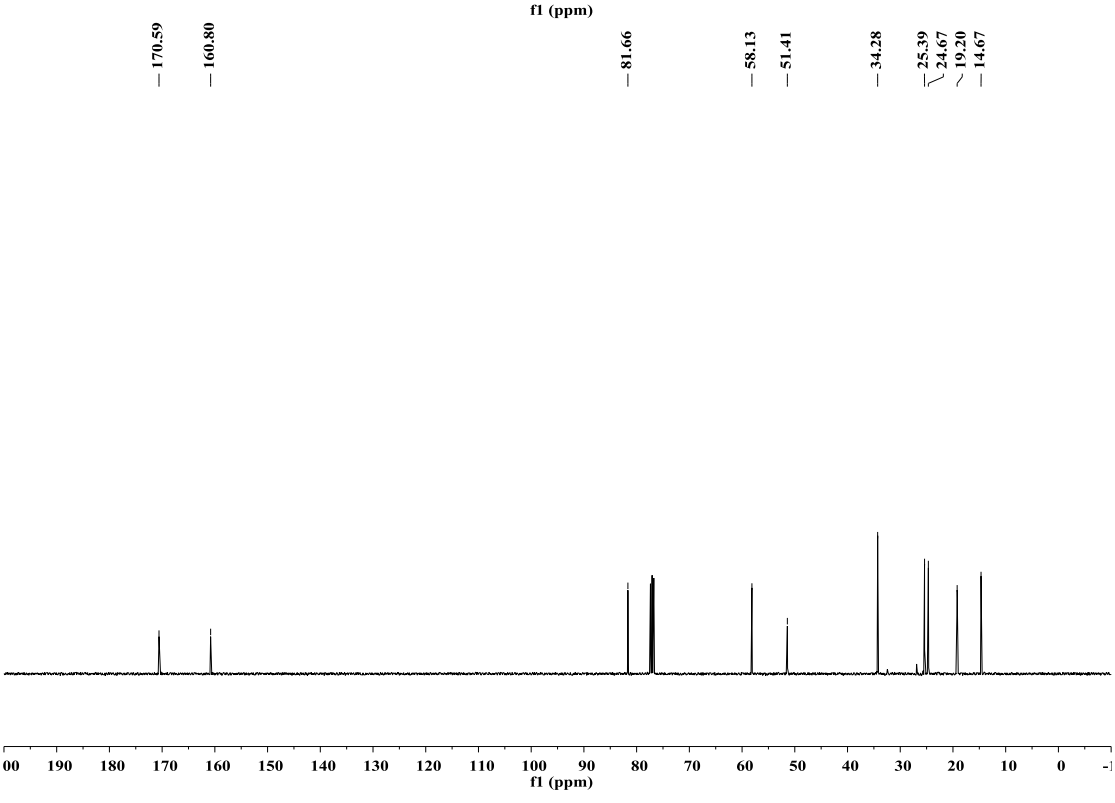

f1 (ppm)

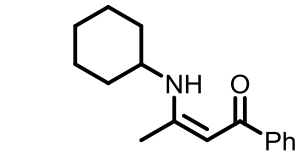

NH
O
NHBn
2A5
f1 (ppm)


NH
O
O

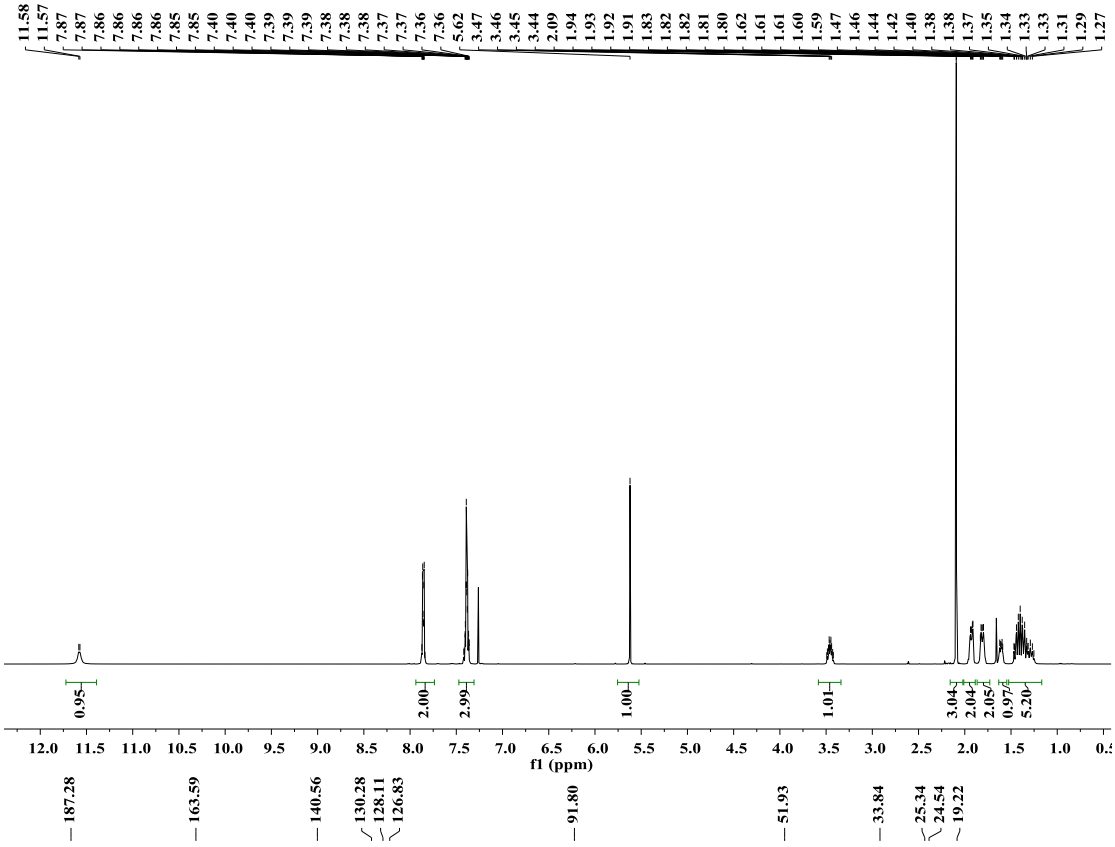
2B$_1$

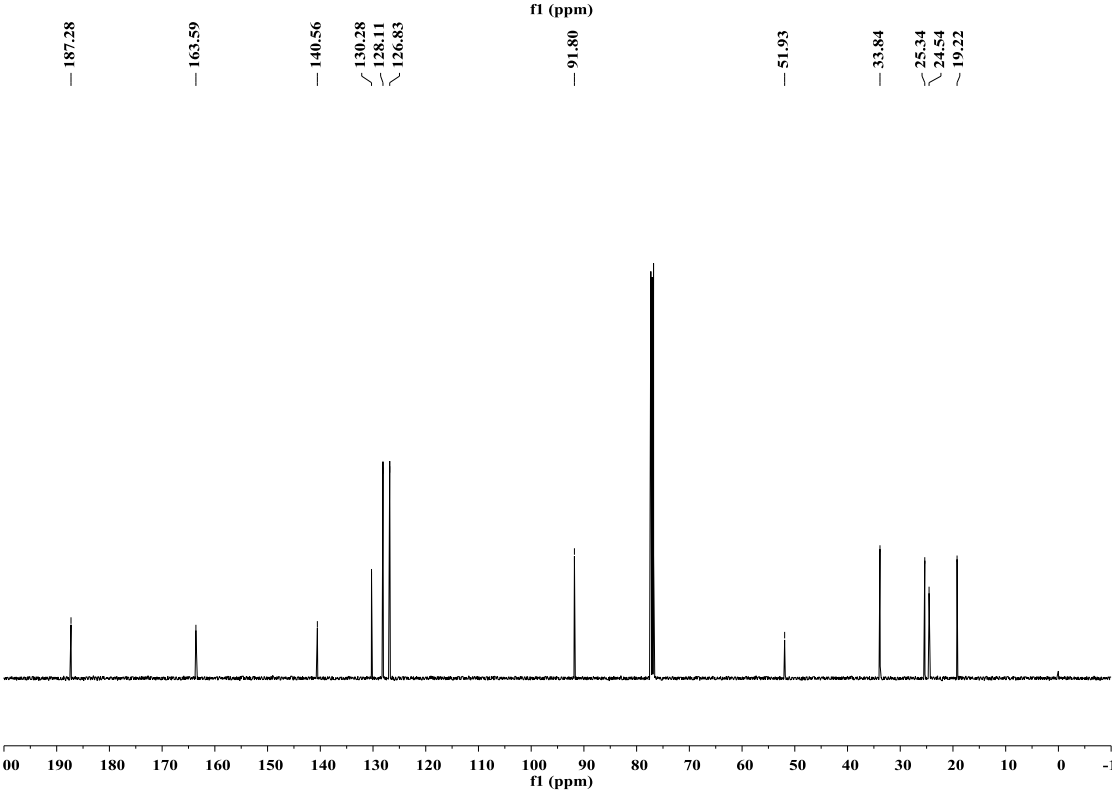

8.62
8.60
4.36
4.08
4.07
4.05
4.03
3.32
3.30
3.29
3.28
3.27
3.26
3.25
1.91
1.86
1.85
1.83
1.82
1.75
1.74
1.72
1.72
1.58
1.57
1.56
1.55
1.54
1.33
1.32
1.29
1.27
1.26
1.25
1.25
1.24
1.23
1.22
1.21
1.20
1.18
0.95
1.00
2.14
1.05
3.26
2.07
2.31
1.11
8.25
f1 (ppm)

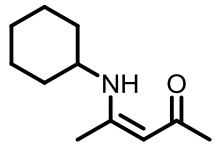

170.59
160.80
81.66
58.13
51.41
34.28
25.39
24.67
19.20
14.67
f1 (ppm)


NH
O
Ph

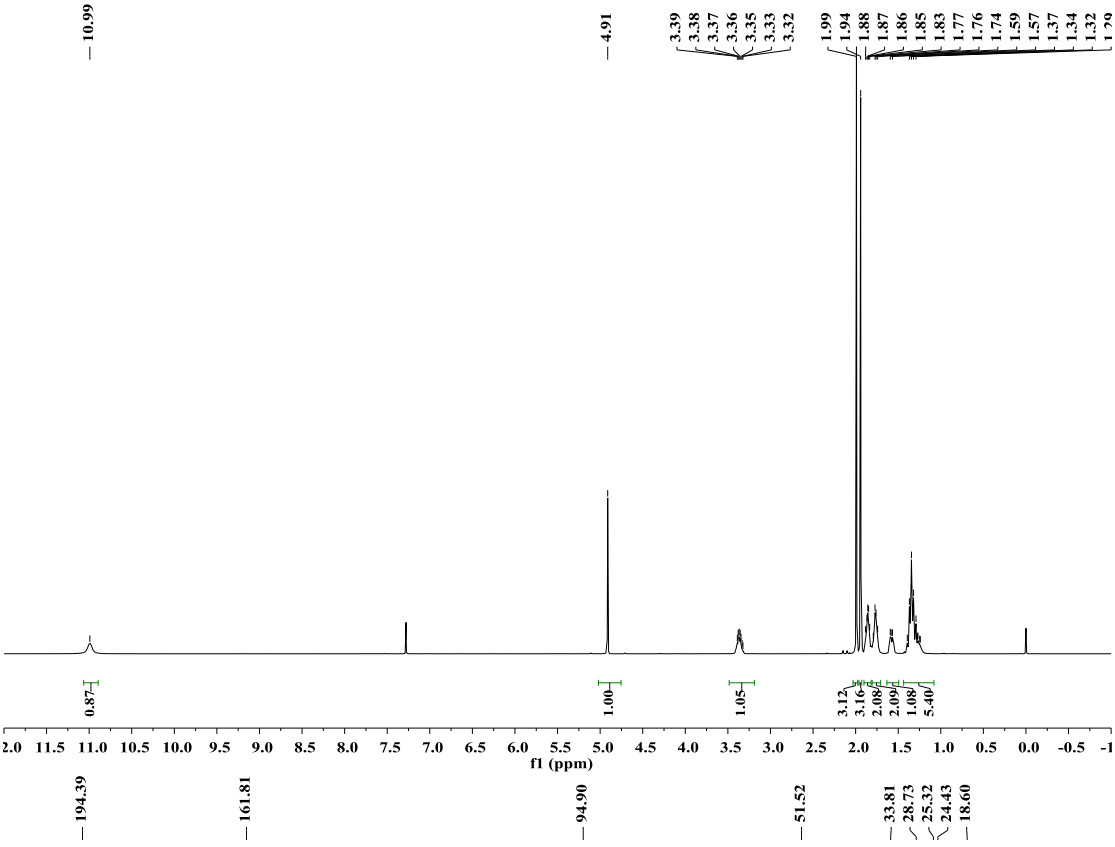
2B$_2$

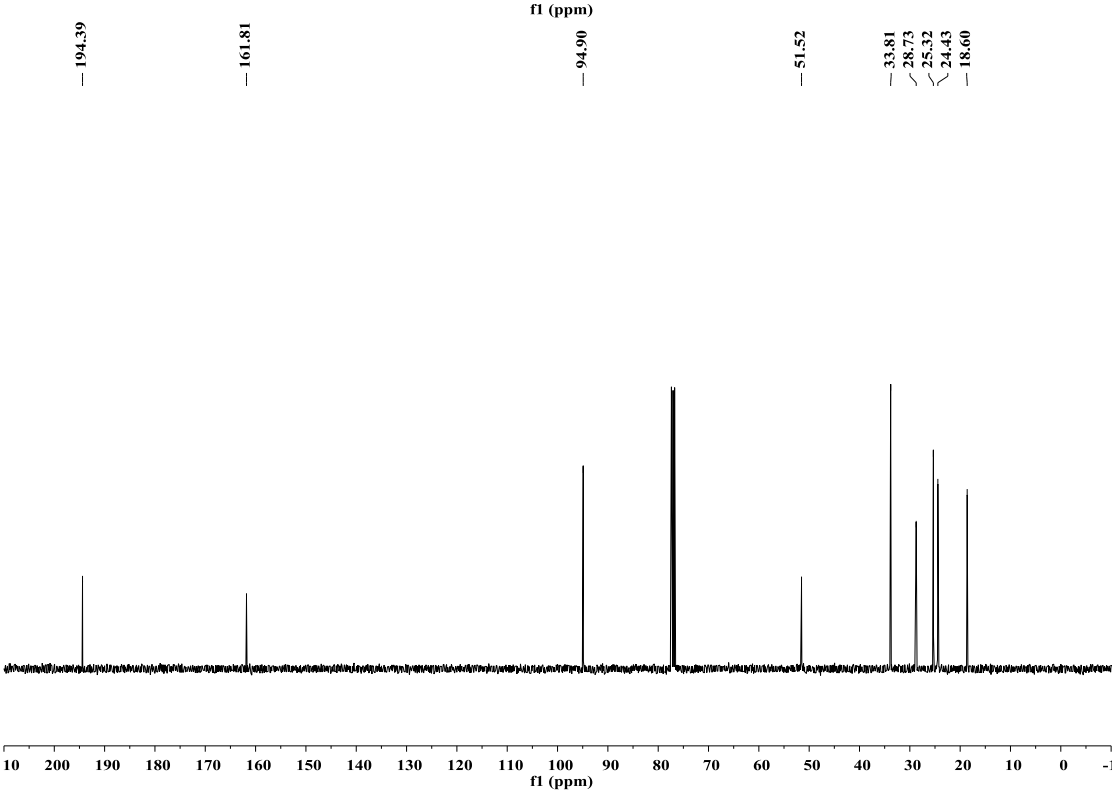

11.58
11.57
7.87
7.87
7.86
7.86
7.86
7.86
7.85
7.85
7.40
7.40
7.40
7.39
7.39
7.39
7.38
7.38
7.38
7.37
7.37
7.36
7.36
5.62
3.47
3.46
3.45
3.44
2.09
1.94
1.93
1.92
1.91
1.83
1.82
1.82
1.81
1.80
1.62
1.61
1.61
1.60
1.59
1.47
1.46
1.44
1.42
1.40
1.38
1.38
1.37
1.35
1.34
1.33
1.33
1.31
1.29
1.27
0.95
2.00
2.99
1.00
1.01
3.04
2.04
2.05
0.97
5.20
f1 (ppm)

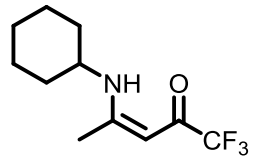

187.28
163.59
140.56
130.28
128.11
126.83
91.80
51.93
33.84
25.34
24.54
19.22
f1 (ppm)


NH
O

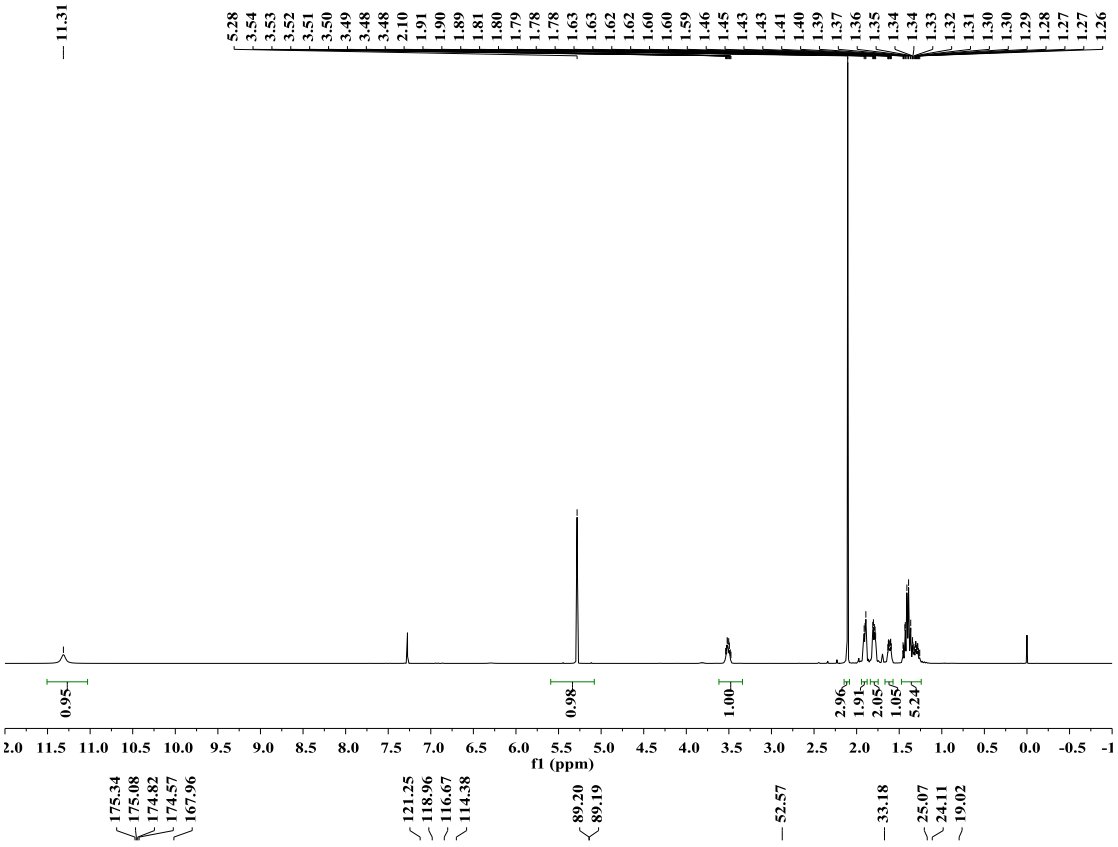
2B$_3$

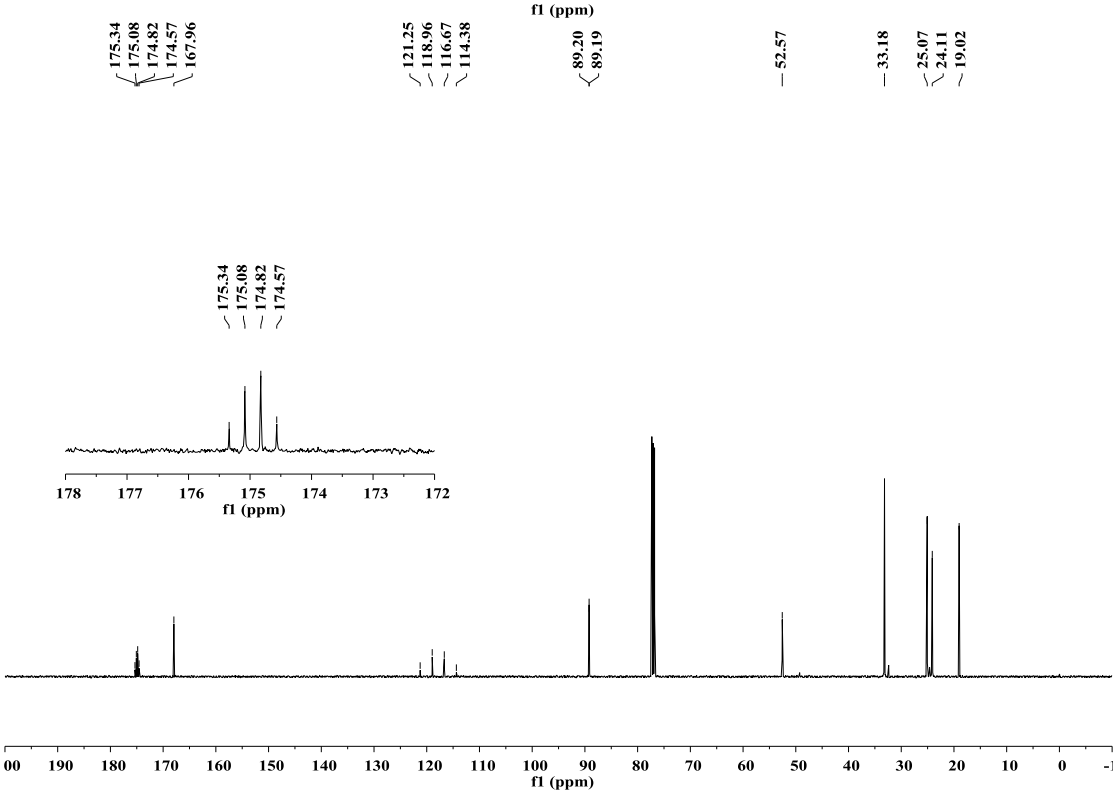

10.99
4.91
3.39
3.38
3.37
3.36
3.35
3.33
3.32
1.99
1.94
1.88
1.87
1.86
1.85
1.83
1.77
1.76
1.74
1.59
1.57
1.37
1.34
1.32
0.87
1.00
1.05
3.12
3.16
2.08
2.09
1.08
5.40
f1 (ppm)

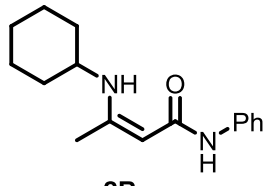

194.39
161.81
94.90
51.52
33.81
28.73
25.32
24.43
18.60
f1 (ppm)


NH
O
CF3

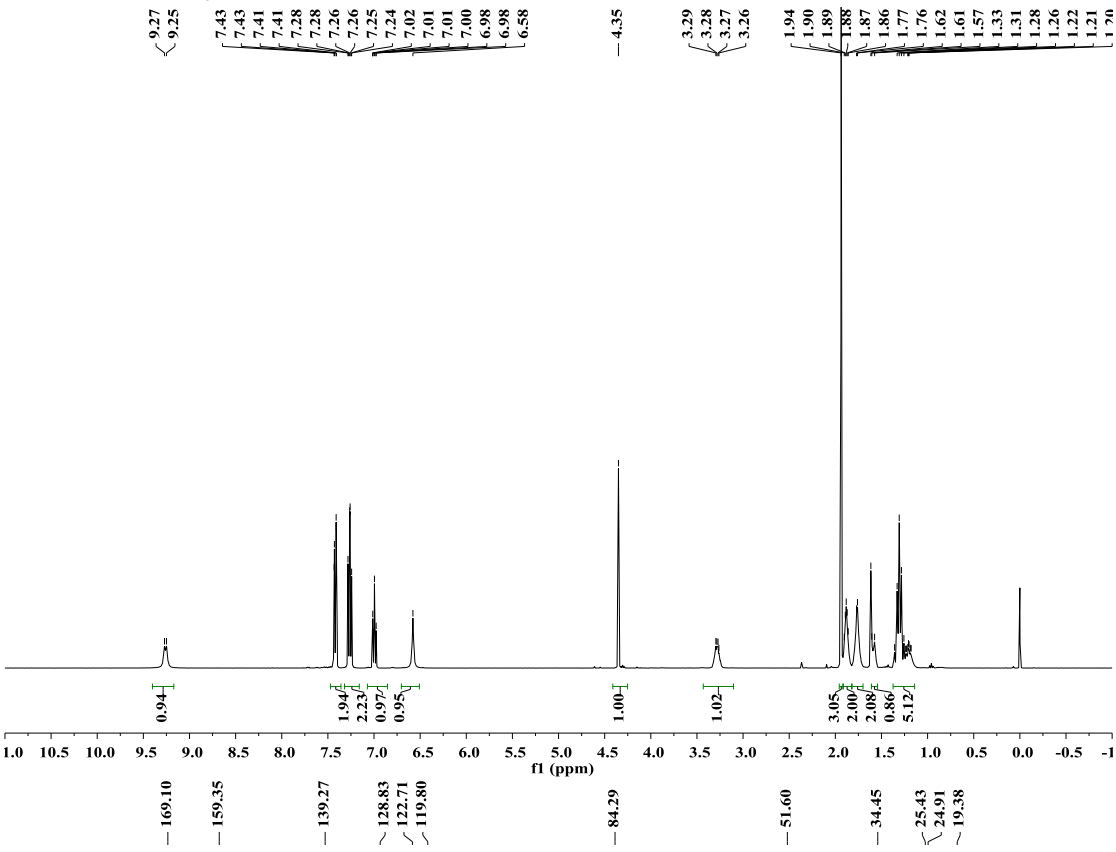
2B$_4$

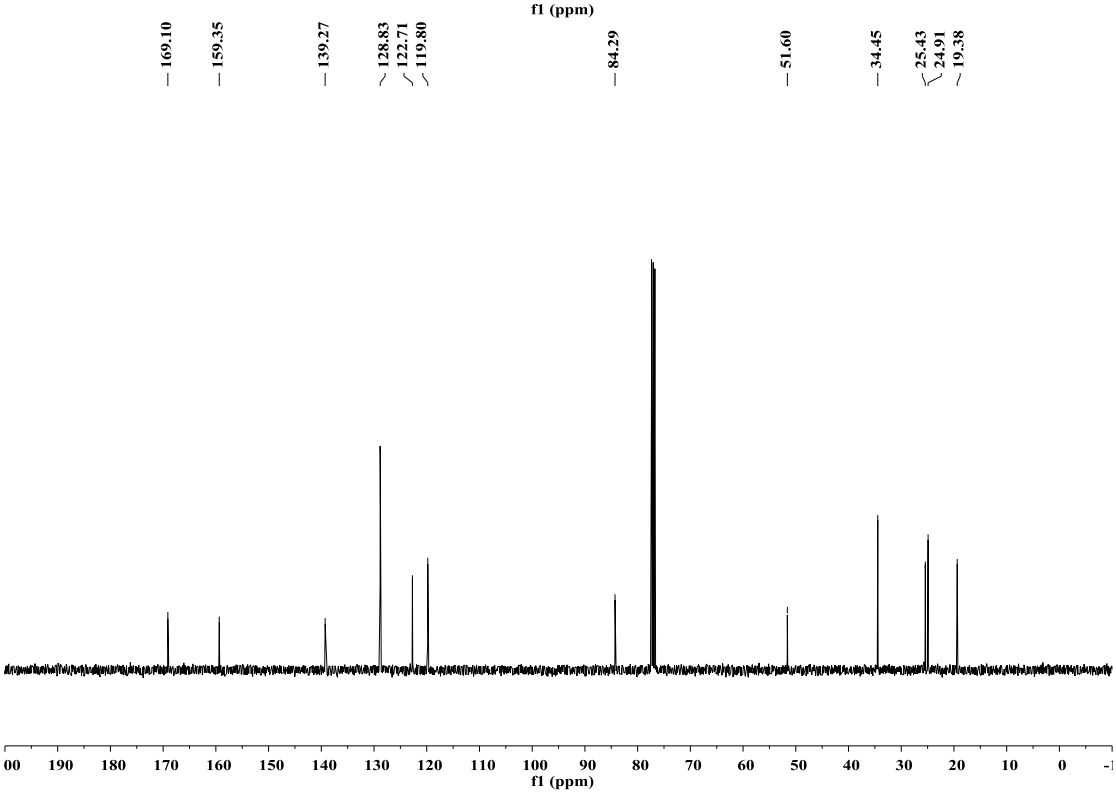

11.31
5.28
3.54
3.53
3.52
3.51
3.50
3.49
3.48
3.48
2.10
1.91
1.90
1.89
1.81
1.80
1.79
1.78
1.78
1.63
1.63
1.62
1.62
1.60
1.60
1.59
1.46
1.45
1.43
1.43
1.41
1.40
1.39
1.37
1.36
1.35
1.34
1.34
1.33
1.32
1.31
1.30
1.30
1.29
1.28
1.27
1.27
1.26
0.95
0.98
1.00
2.96
1.91
2.05
1.05
5.24
f1 (ppm)

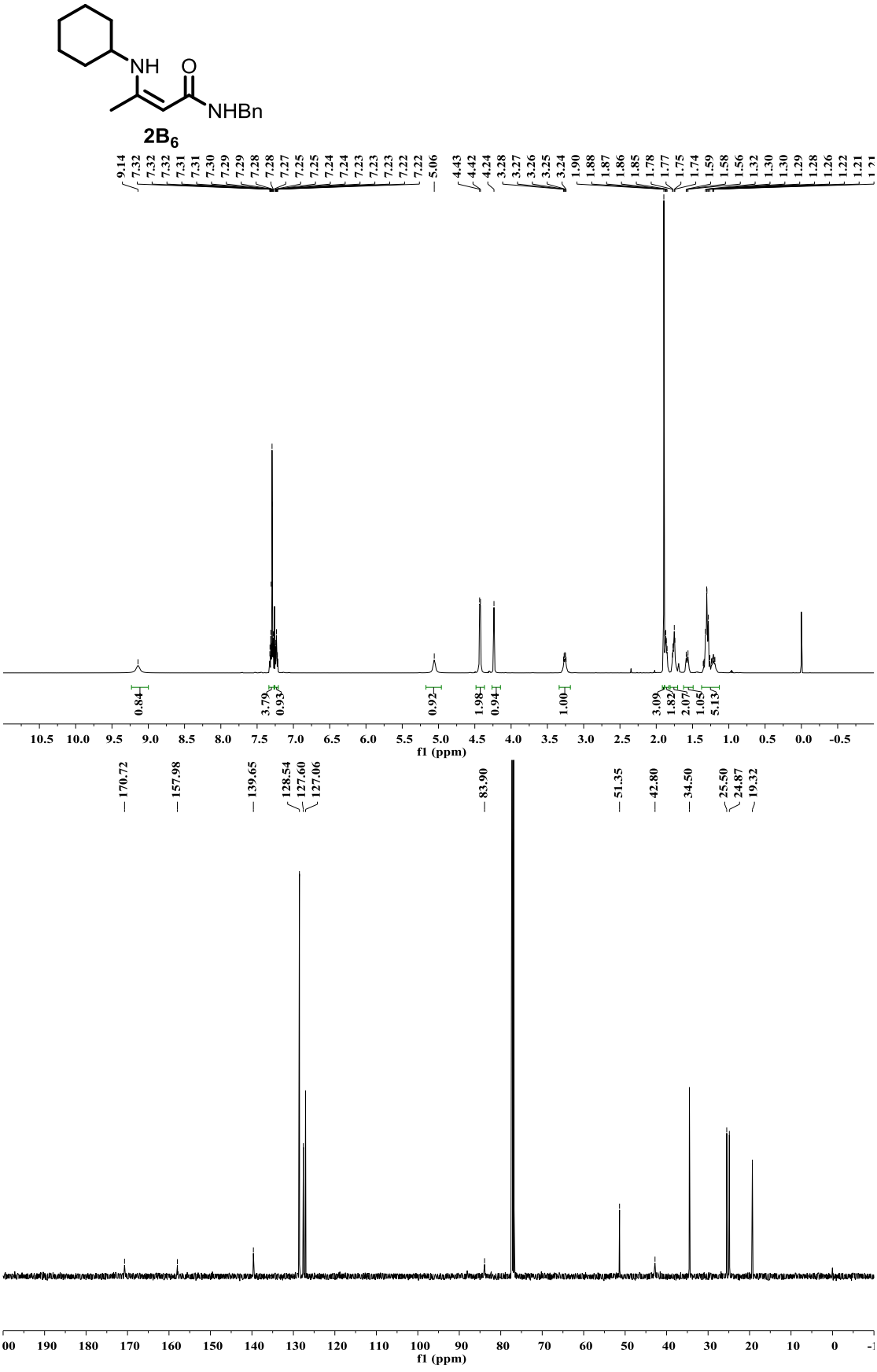

175.34
175.08
174.82
174.57
167.96
121.25
118.96
116.67
114.38
89.20
89.19
52.57
33.18
25.07
24.11
19.02
175.34
175.08
174.82
174.57
f1 (ppm)
f1 (ppm)

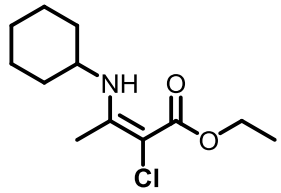

NH
O
N
Ph
H

2B$_5$

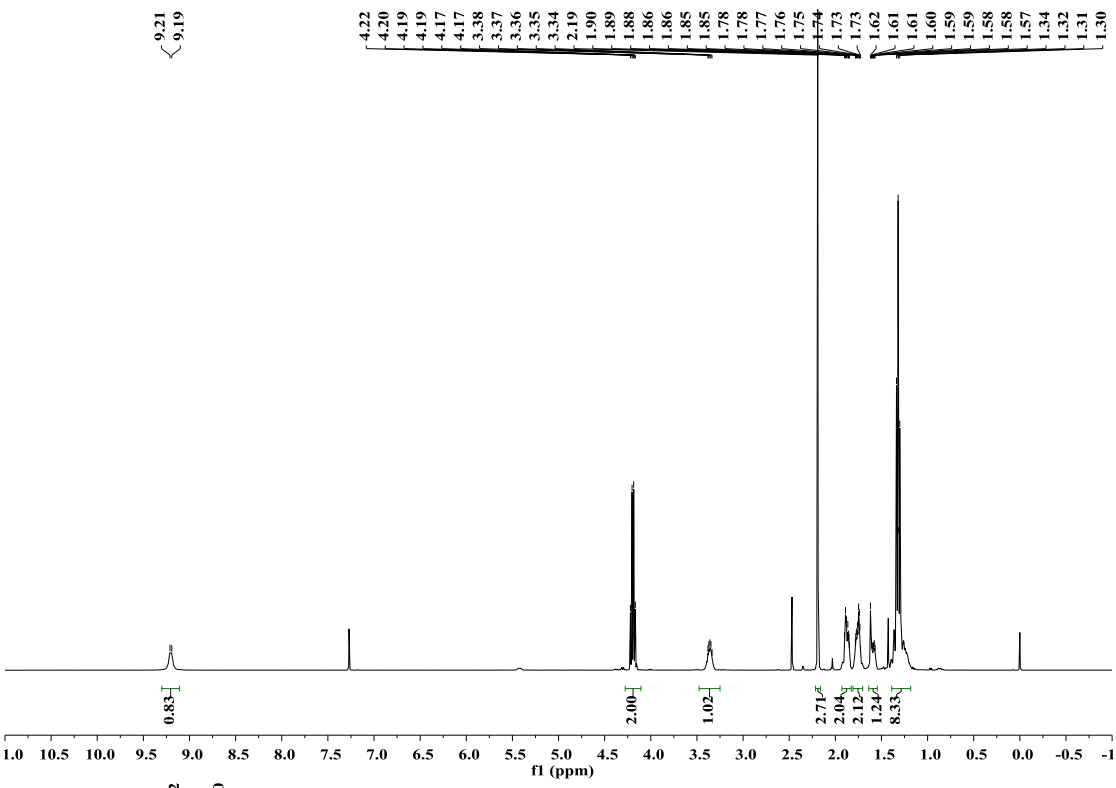

9.27
9.25
7.43
7.43
7.41
7.41
7.28
7.28
7.26
7.26
7.25
7.24
7.02
7.01
7.01
7.00
6.98
6.98
6.58
4.35
3.29
3.28
3.27
3.26
1.94
1.90
1.89
1.88
1.87
1.86
1.77
1.76
1.62
1.61
1.57
1.33
1.31
1.28
1.26
1.22
1.21
0.94
1.94
2.23
0.97
0.95
1.00
1.02
3.05
2.00
2.08
0.86
5.12
f1 (ppm)

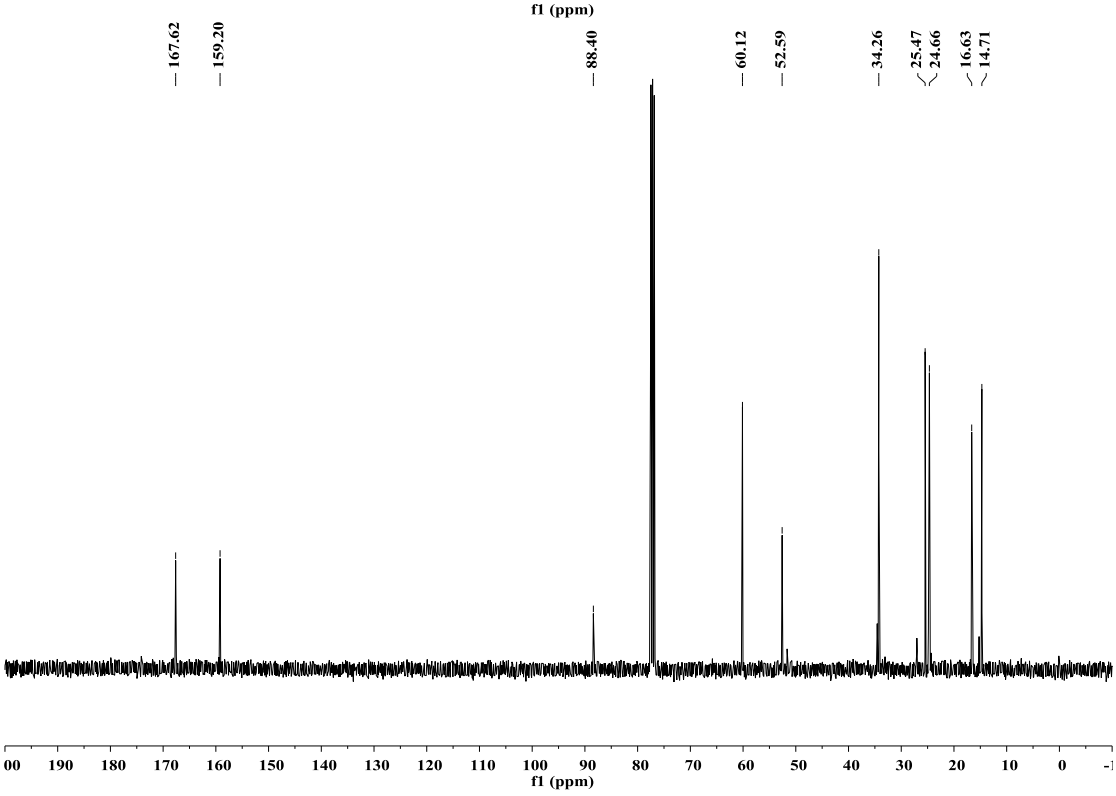

169.10
159.35
139.27
128.83
122.71
119.80
84.29
51.60
34.45
25.43
24.91
19.38
f1 (ppm)

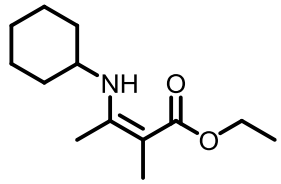

NH
O
NHBn
2B6
9.14
7.32
7.32
7.32
7.31
7.31
7.30
7.29
7.29
7.28
7.28
7.27
7.25
7.25
7.24
7.24
7.23
7.23
7.23
7.22
7.22
5.06
4.43
4.42
4.24
3.28
3.27
3.26
3.25
3.24
1.90
1.88
1.87
1.86
1.85
1.78
1.77
1.75
1.74
1.59
1.58
1.56
1.32
1.30
1.30
1.29
1.28
1.26
1.22
1.21
0.84
3.79
0.93
0.92
1.98
0.94
1.00
3.09
1.82
2.07
1.05
5.13
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
170.72
157.98
139.65
128.54
127.60
127.06
83.90
51.35
42.80
34.50
25.50
24.87
19.32
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


NH
O
O
Cl

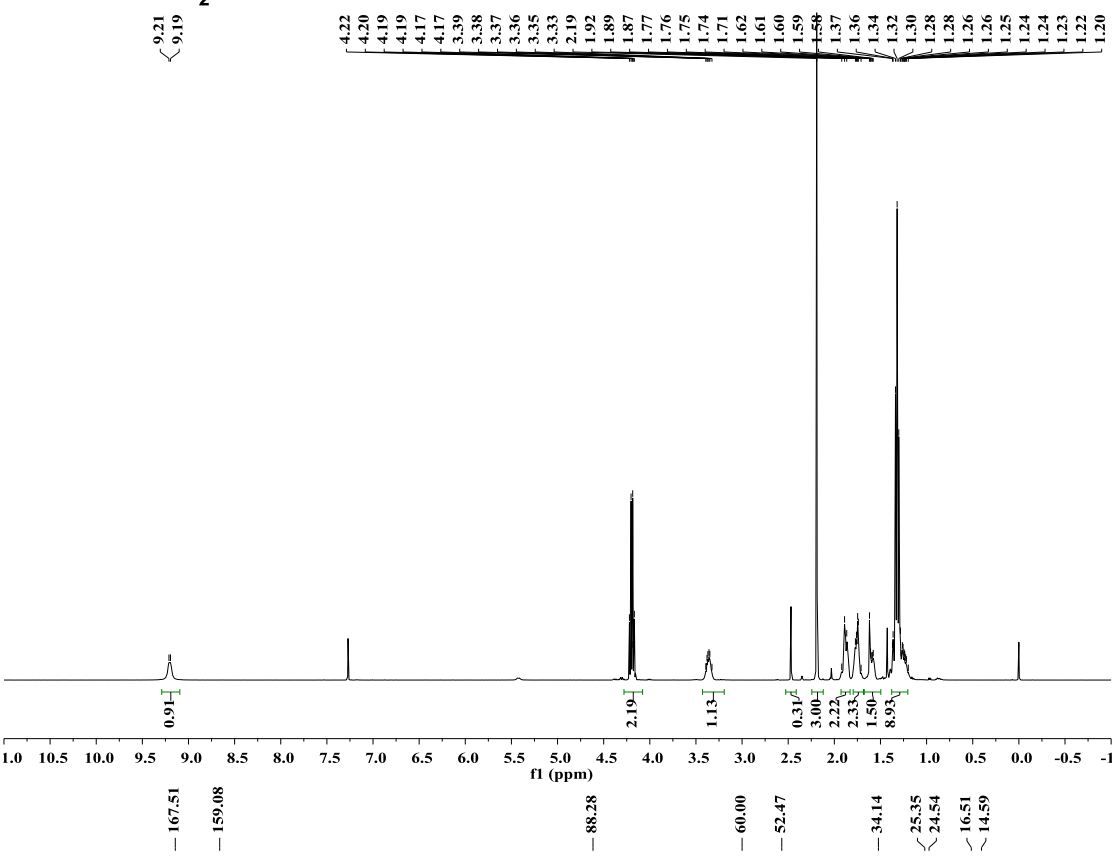
2C$_1$

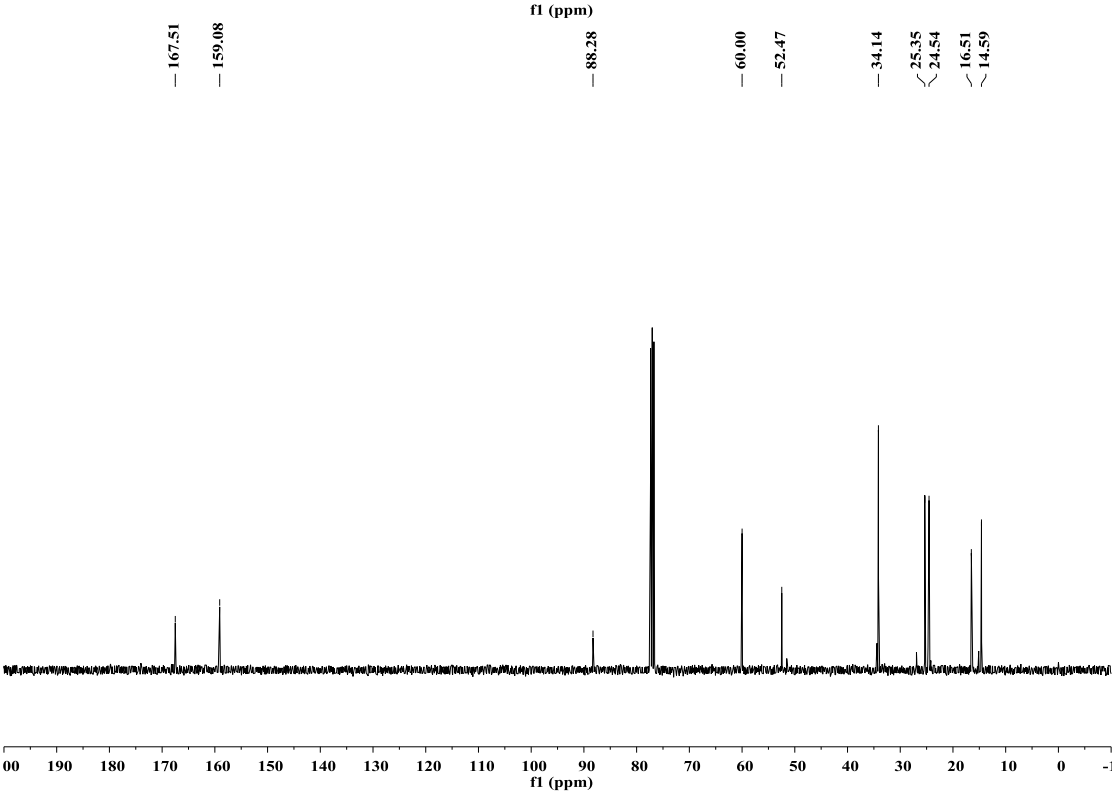

9.21
9.19
4.22
4.20
4.19
4.19
4.17
4.17
3.38
3.37
3.36
3.35
3.34
2.19
1.90
1.89
1.88
1.86
1.86
1.85
1.85
1.78
1.78
1.77
1.76
1.75
1.74
1.73
1.73
1.62
1.61
1.61
1.60
1.59
1.59
1.58
1.58
1.57
1.34
1.32
1.31
1.30
0.83
2.00
1.02
2.71
2.04
2.12
1.24
8.33
f1 (ppm)

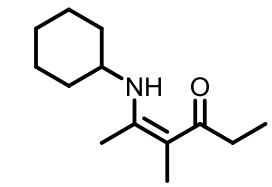

167.62
159.20
88.40
60.12
52.59
34.26
25.47
24.66
16.63
14.71
f1 (ppm)


NH
O
O

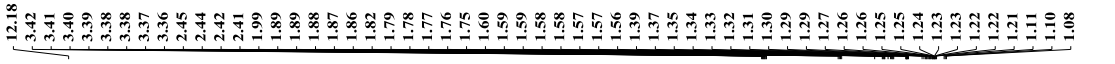
2C$_2$


9.21
9.19
4.22
4.20
4.19
4.19
4.17
4.17
3.39
3.38
3.37
3.36
3.35
3.33
2.19
1.92
1.89
1.87
1.77
1.76
1.75
1.74
1.71
1.62
1.61
1.60
1.59
1.58
1.37
1.36
1.34
1.32
1.30
1.28
1.28
1.26
1.26
1.25
1.24
1.24
1.23
1.22
1.20
0.91
2.19
1.13
0.31
3.00
2.22
2.33
1.50
8.93
f1 (ppm)


167.51
159.08
88.28
60.00
52.47
34.14
25.35
24.54
16.51
14.59
f1 (ppm)


NH
O

2C$_3$


12.18
3.42
3.41
3.40
3.39
3.38
3.38
3.37
3.36
2.45
2.44
2.42
2.41
1.99
1.89
1.89
1.88
1.87
1.86
1.82
1.79
1.78
1.77
1.76
1.75
1.60
1.59
1.59
1.58
1.58
1.57
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1.56
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1.33
1.32
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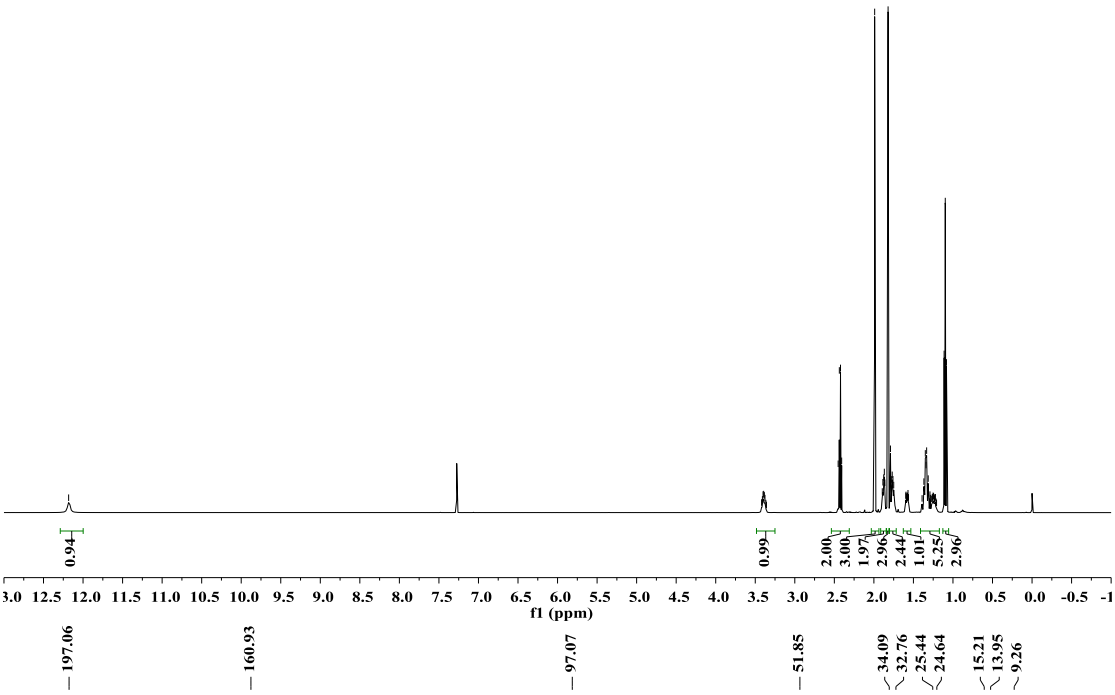
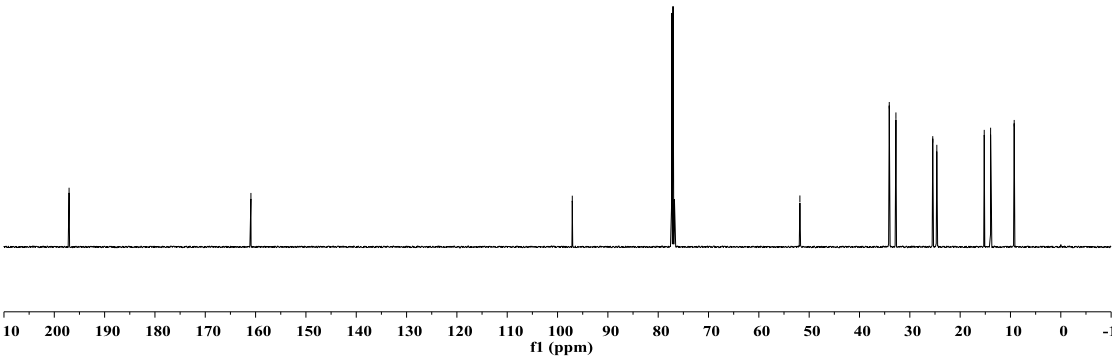
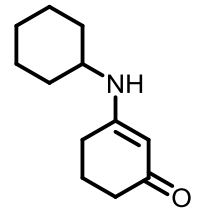
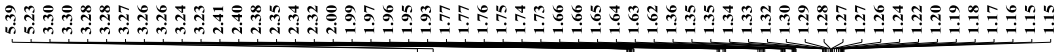
1.22
1.22
1.21
1.11
1.10
1.08

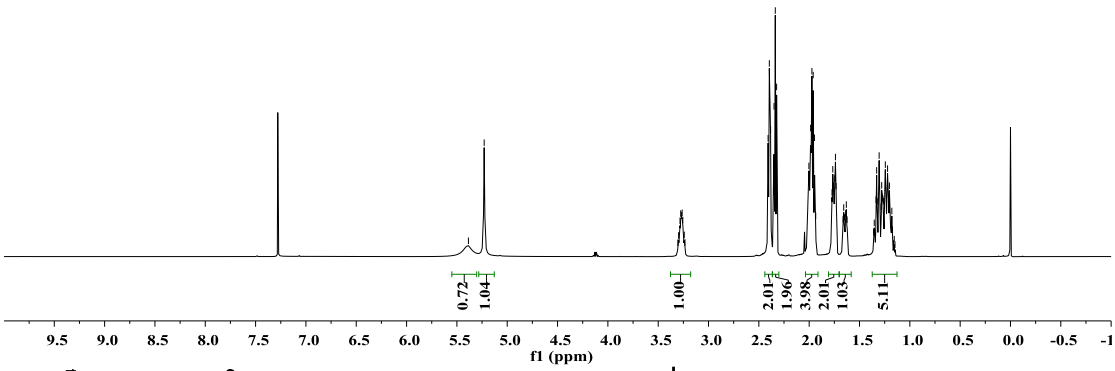

0.94
0.99
2.00
3.00
1.97
2.96
2.44
1.01
5.25
2.96
f1 (ppm)
197.06
160.93
97.07
51.85
34.09
32.76
25.44
24.64
15.21
13.95
9.26

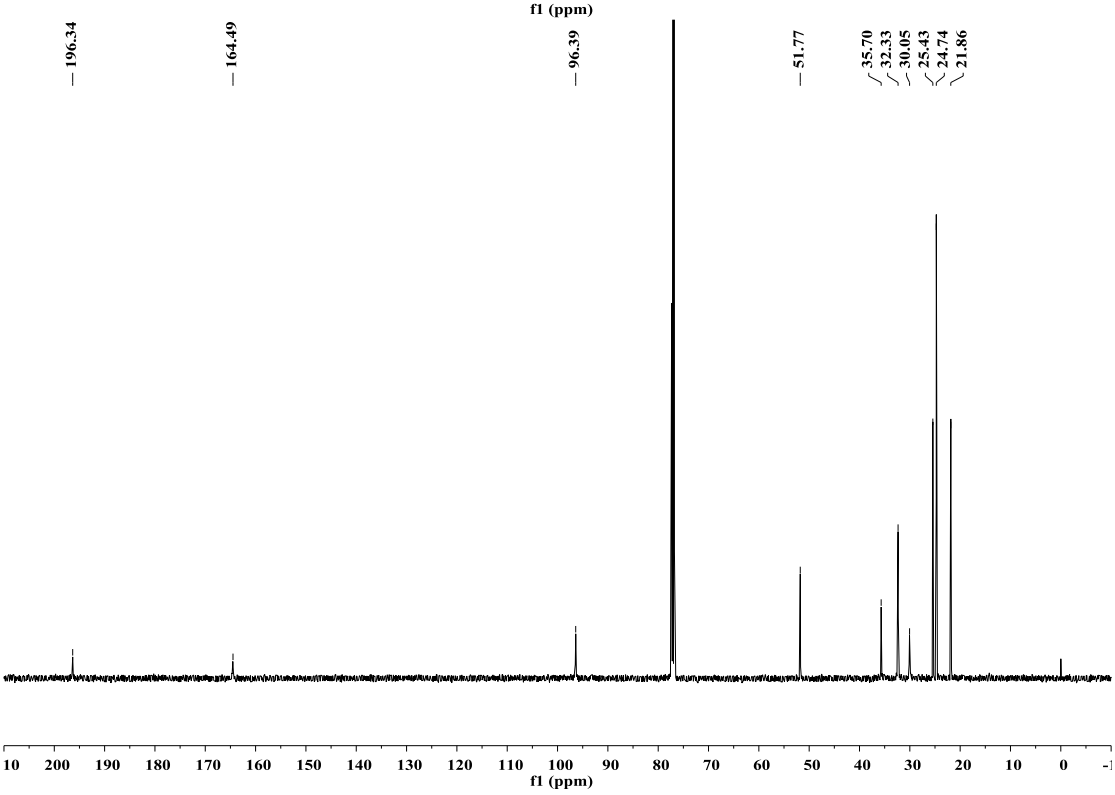

f1 (ppm)

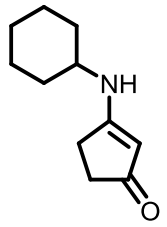

NH
O

2D$_1$

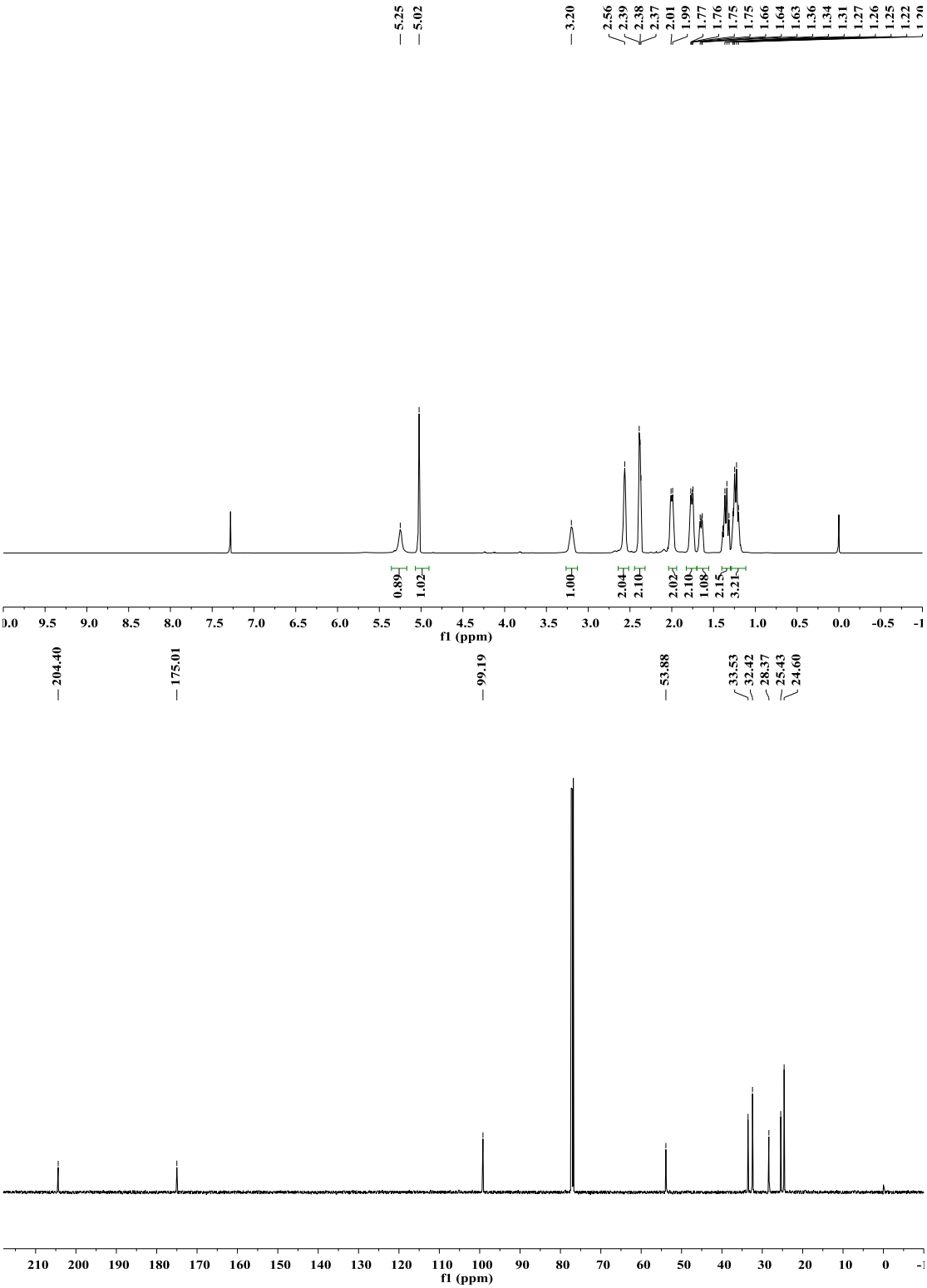

5.39 5.23 3.30 3.30 3.28 3.28 3.27 3.26 3.26 3.24 3.23 2.41 2.40 2.38 2.35 2.34 2.32 2.00 1.99 1.97 1.96 1.95 1.93 1.77 1.77 1.76 1.75 1.74 1.73 1.66 1.66 1.65 1.64 1.63 1.62 1.36 1.35 1.35 1.34 1.33 1.32 1.30 1.29 1.28 1.27 1.27 1.26 1.24 1.22 1.20 1.19 1.18 1.17 1.16 1.15 1.15

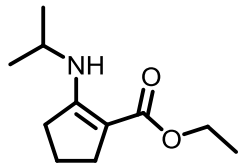

0.72
1.04
1.00
2.01
1.96
3.98
2.01
1.03
5.11
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


196.34
164.49
96.39
51.77
35.70
32.33
30.05
25.43
24.74
21.86
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

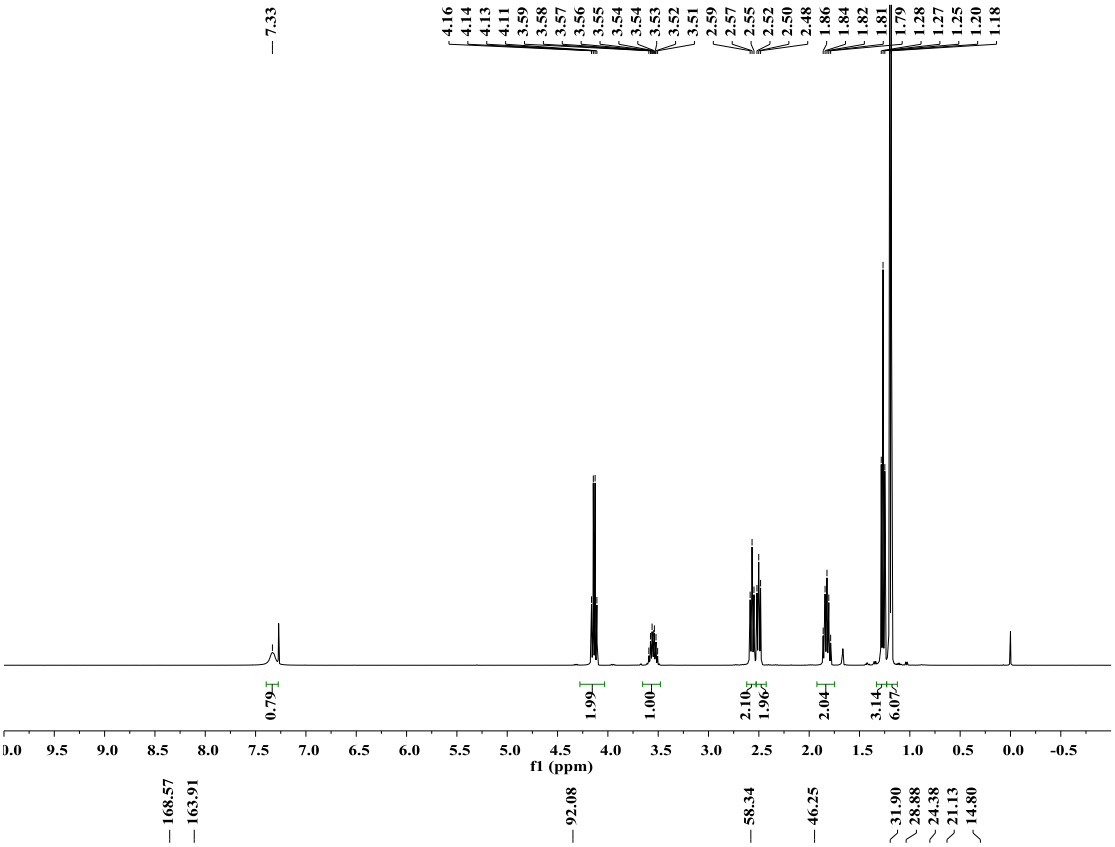

NH
O

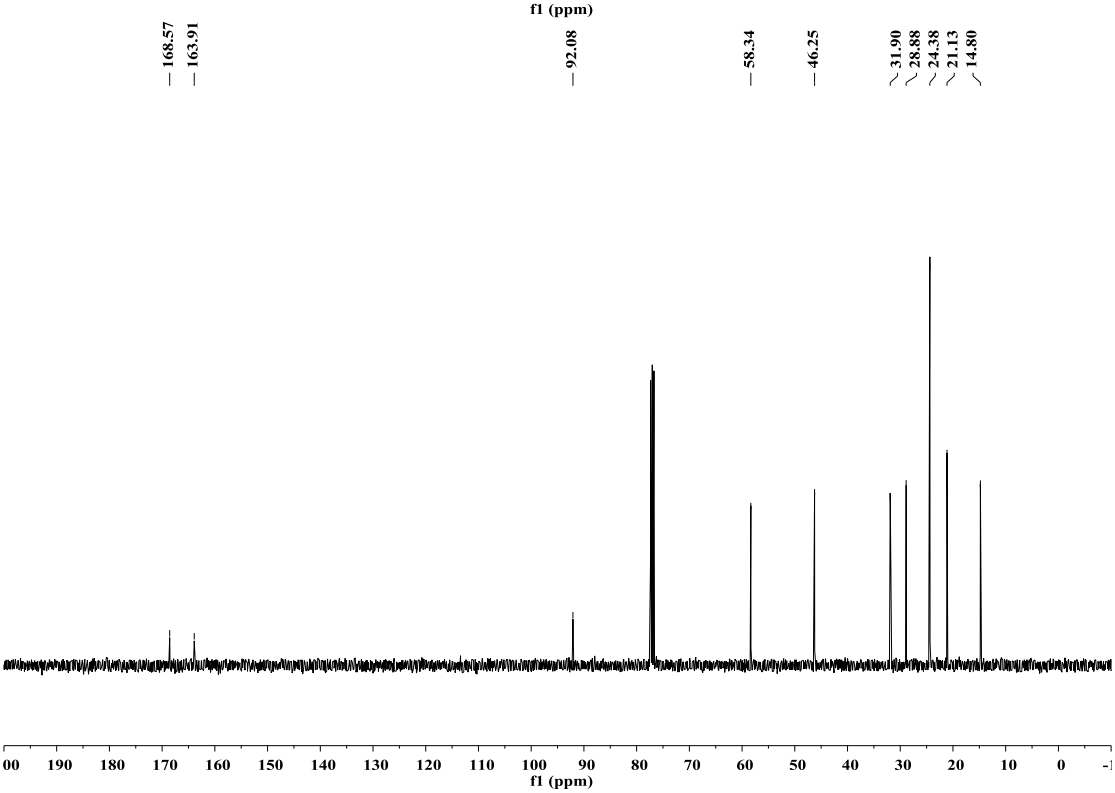
2D$_2$

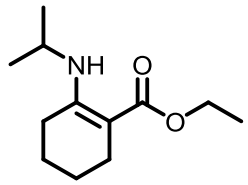

5.25
5.02
3.20
2.56
2.39
2.38
2.37
2.01
1.99
1.77
1.76
1.75
1.75
1.66
1.64
1.63
1.36
1.34
1.31
1.27
1.26
1.25
1.22
0.89
1.02
1.00
2.04
2.10
2.02
2.10
1.08
2.15
3.21
f1 (ppm)
204.40
175.01
99.19
53.88
33.53
32.42
28.37
25.43
24.60
f1 (ppm)


NH
O
O

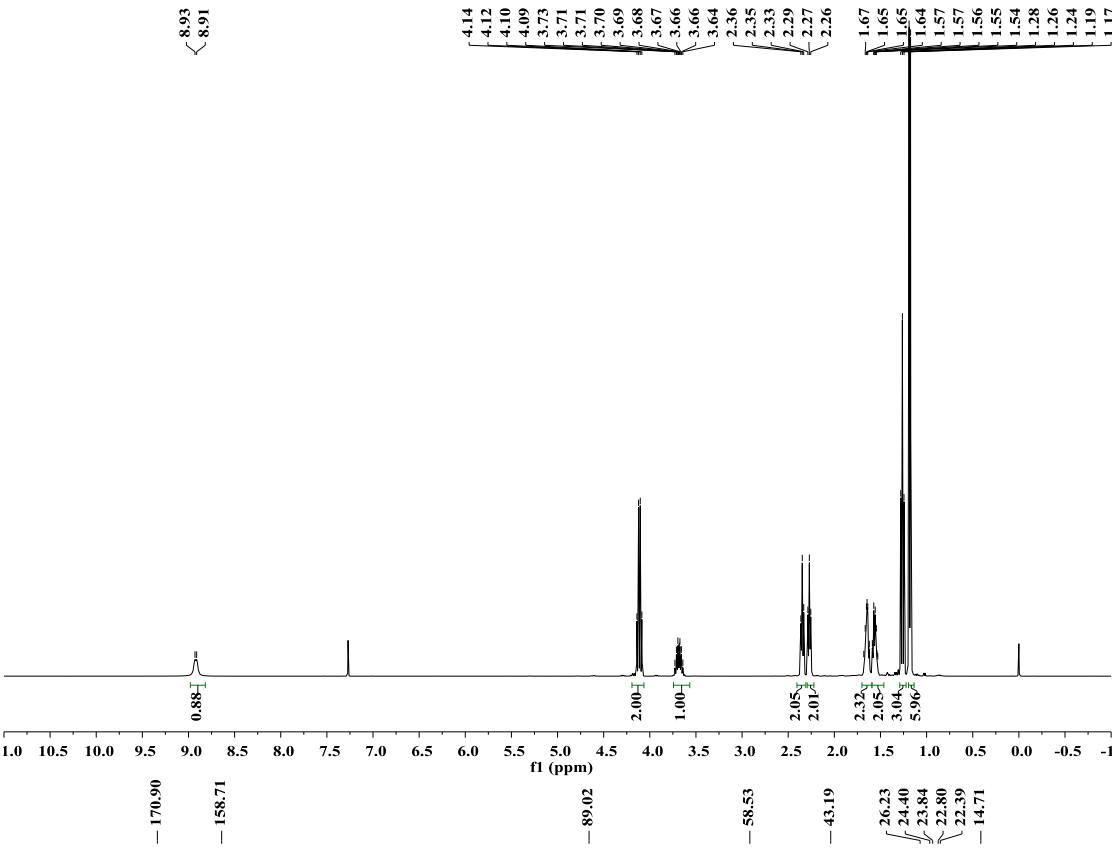
3A$_1$

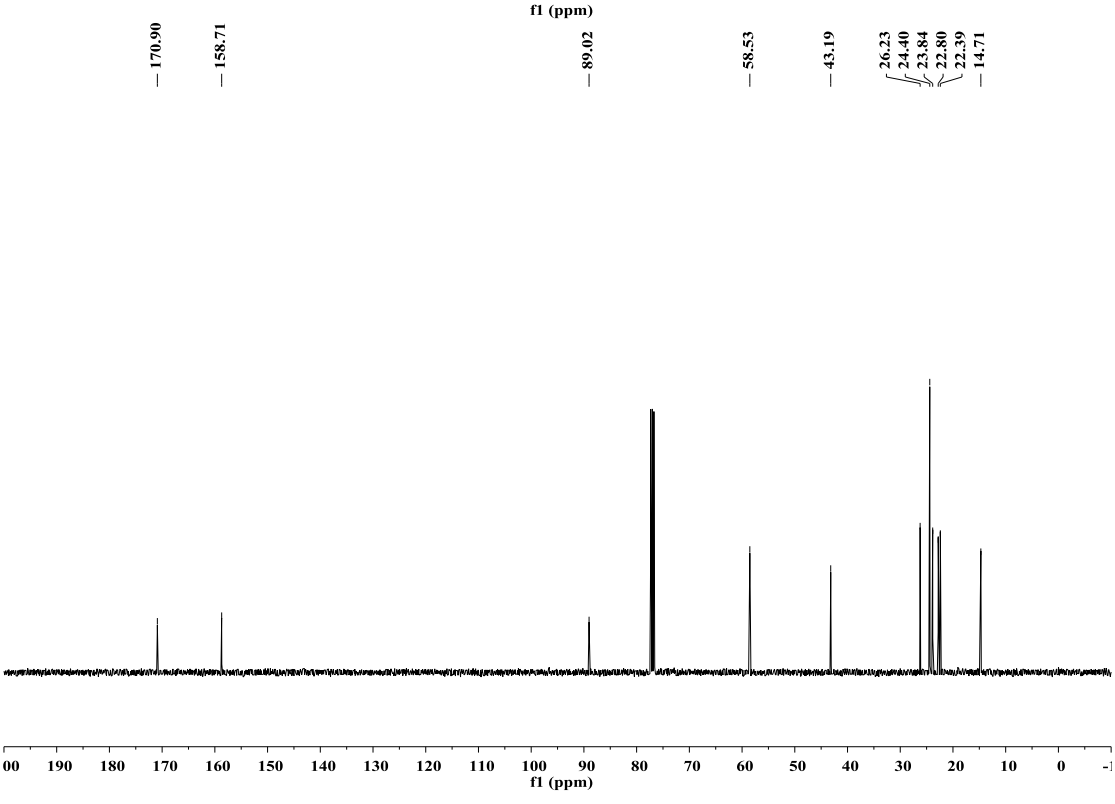

7.33
4.16
4.14
4.13
4.11
3.59
3.58
3.57
3.56
3.55
3.54
3.54
3.53
3.52
3.51
2.59
2.57
2.55
2.52
2.50
2.48
1.86
1.84
1.82
1.81
1.79
1.28
1.27
1.25
1.20
1.18
0.79
1.99
1.00
2.10
1.96
2.04
3.14
6.07
f1 (ppm)

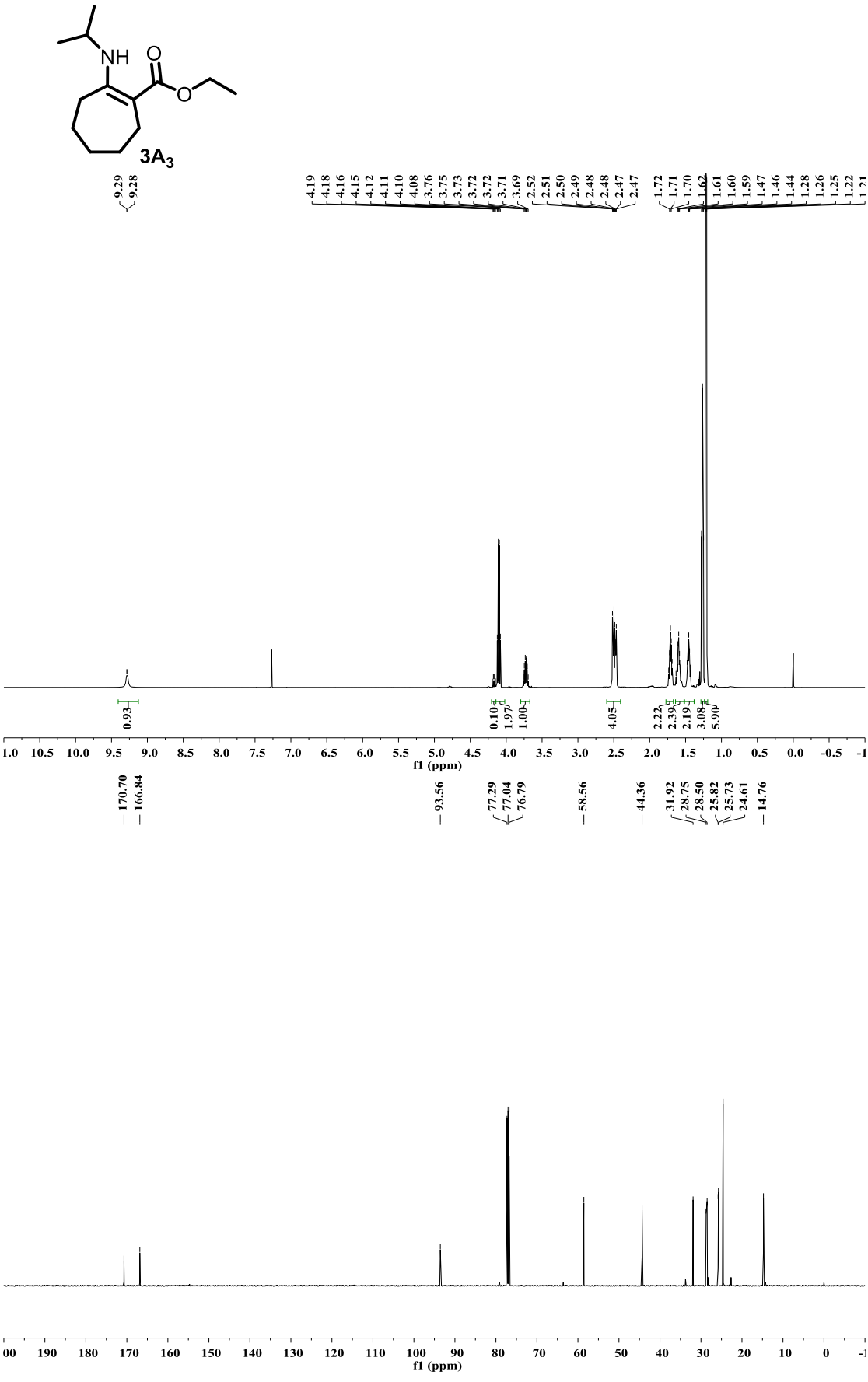

168.57
163.91
92.08
58.34
46.25
31.90
28.88
24.38
21.13
14.80
f1 (ppm)

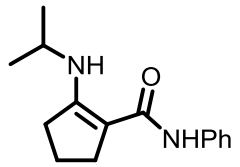

NH
O
O

3A$_2$

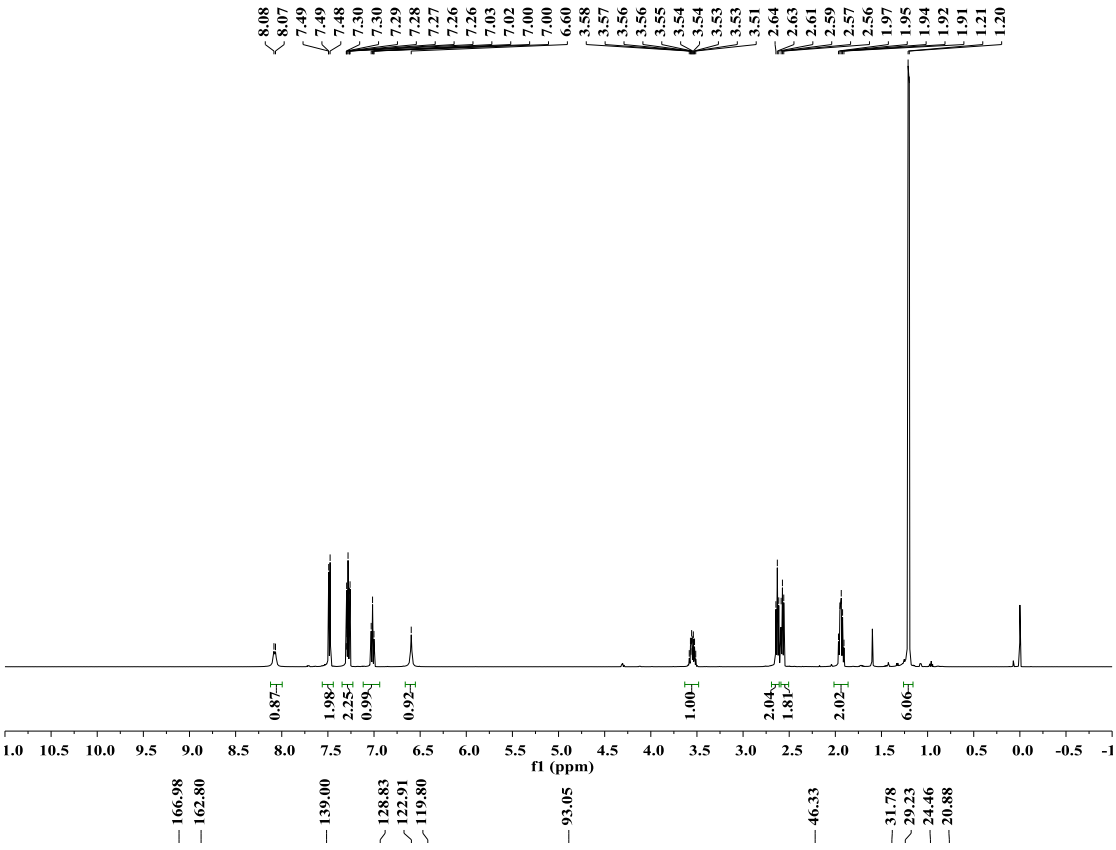

8.93
8.91
4.14
4.12
4.10
4.09
3.73
3.71
3.71
3.70
3.69
3.68
3.67
3.66
3.66
3.64
2.36
2.35
2.33
2.29
2.27
2.26
1.67
1.65
1.65
1.64
1.57
1.57
1.56
1.55
1.54
1.28
1.26
1.24
1.19
0.88
2.00
1.00
2.05
2.01
2.32
2.05
3.04
5.96
f1 (ppm)

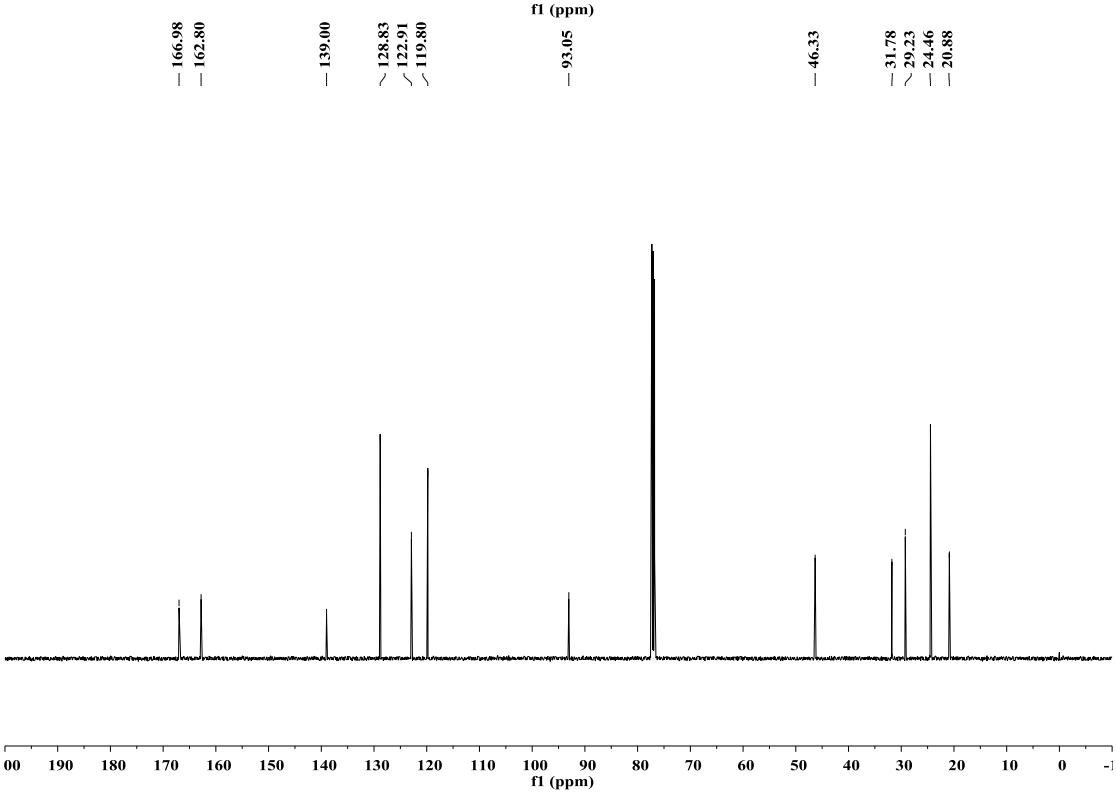

170.90
158.71
89.02
58.53
43.19
26.23
24.40
23.84
22.80
22.39
14.71
f1 (ppm)

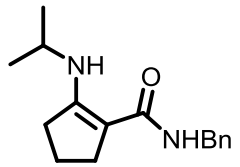

NH
O
O
3A3
f1 (ppm)
f1 (ppm)


NH
O
NHPh

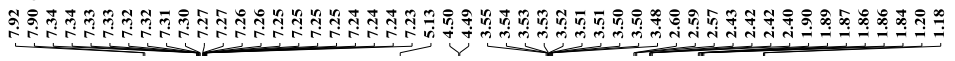
3A$_4$

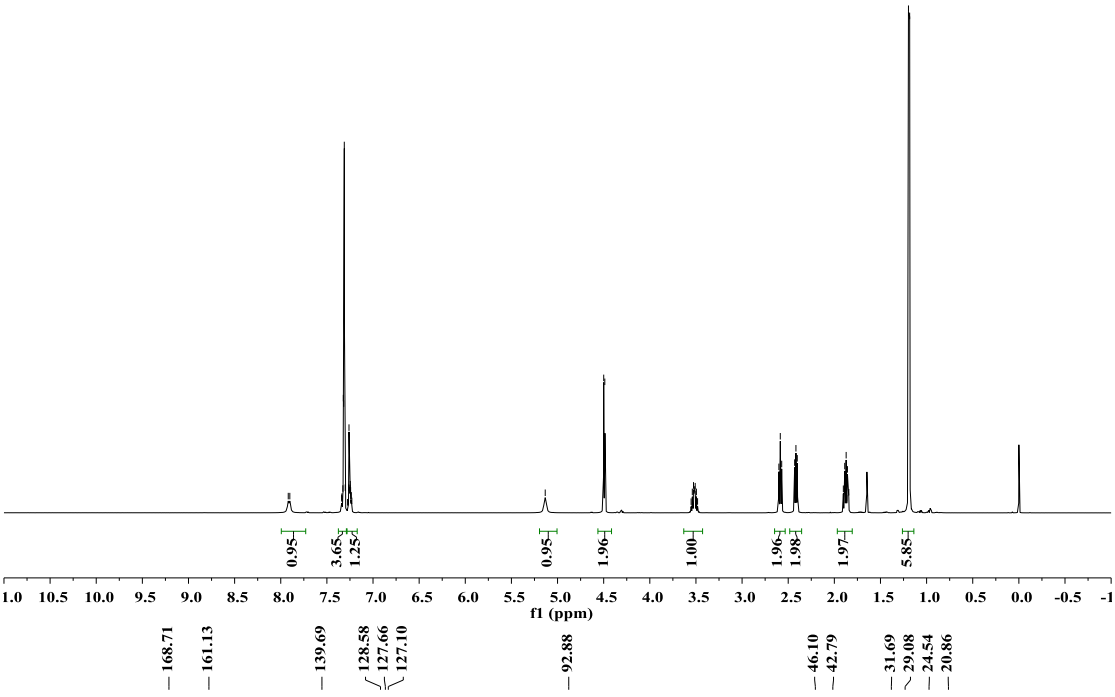

8.08
8.07
7.49
7.49
7.48
7.30
7.30
7.29
7.28
7.27
7.26
7.26
7.03
7.02
7.00
7.00
7.00
6.60
3.58
3.57
3.56
3.56
3.55
3.54
3.54
3.53
3.53
3.51
2.64
2.63
2.61
2.59
2.57
2.56
1.97
1.95
1.94
1.92
1.91
1.21
1.20
0.87
1.98
2.25
0.99
0.92
1.00
2.04
1.81
2.02
6.06
f1 (ppm)


166.98
162.80
139.00
128.83
122.91
119.80
93.05
46.33
31.78
29.23
24.46
20.88
f1 (ppm)

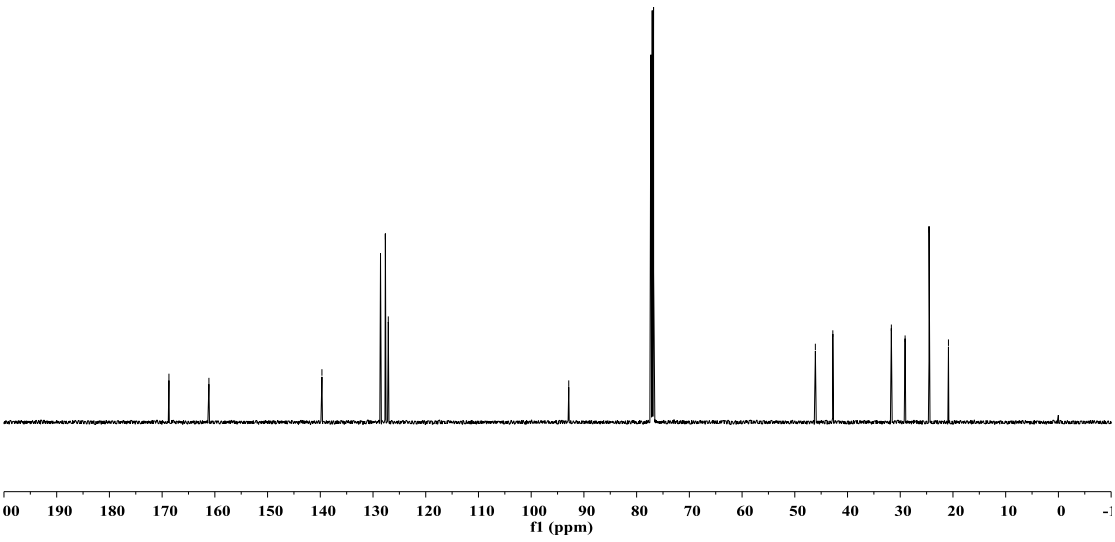

NH
O
NHBn

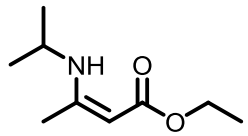
3A$_5$


7.92
7.90
7.34
7.34
7.33
7.33
7.32
7.32
7.31
7.30
7.27
7.27
7.26
7.26
7.25
7.25
7.25
7.25
7.24
7.24
7.24
7.23
5.13
4.50
4.49
3.55
3.54
3.53
3.53
3.52
3.51
3.51
3.50
3.50
3.48
2.60
2.59
2.57
2.43
2.42
2.42
2.40
1.90
1.89
1.87
1.86
1.86
1.84
1.20
1.18

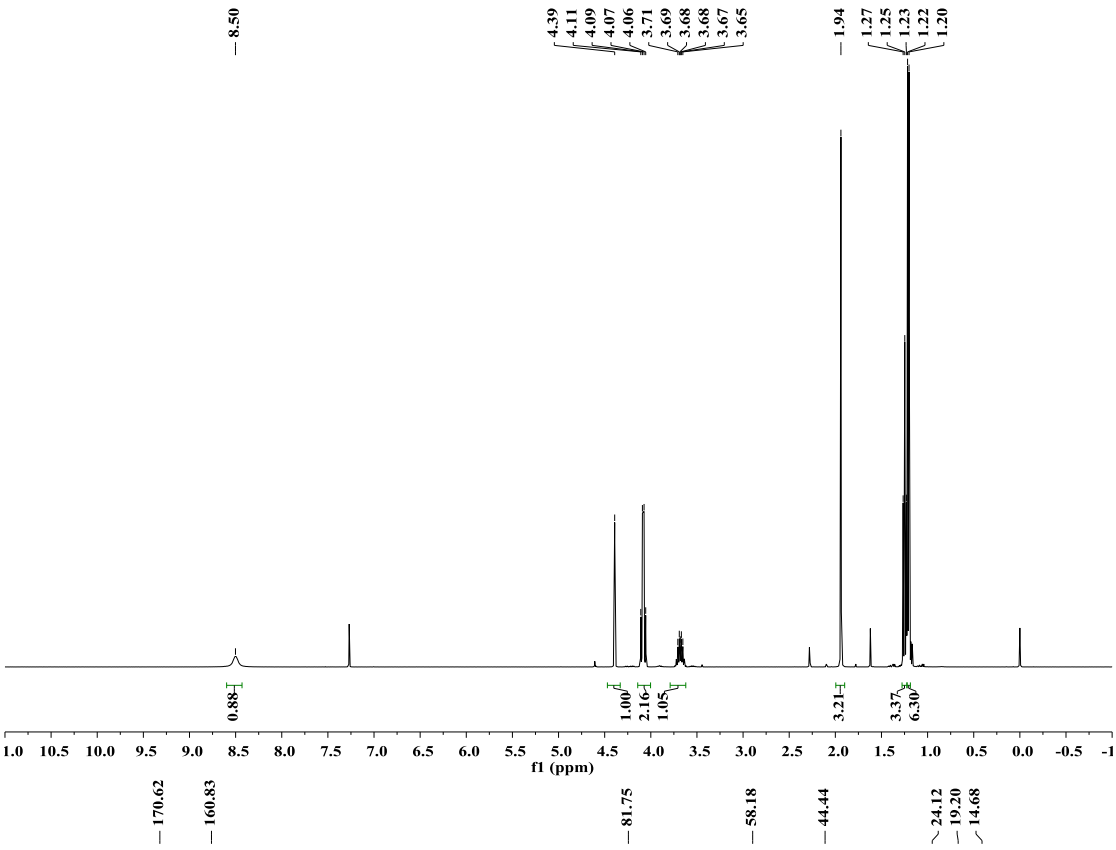

0.95
3.65
1.25
0.95
1.96
1.00
1.96
1.98
1.97
5.85
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

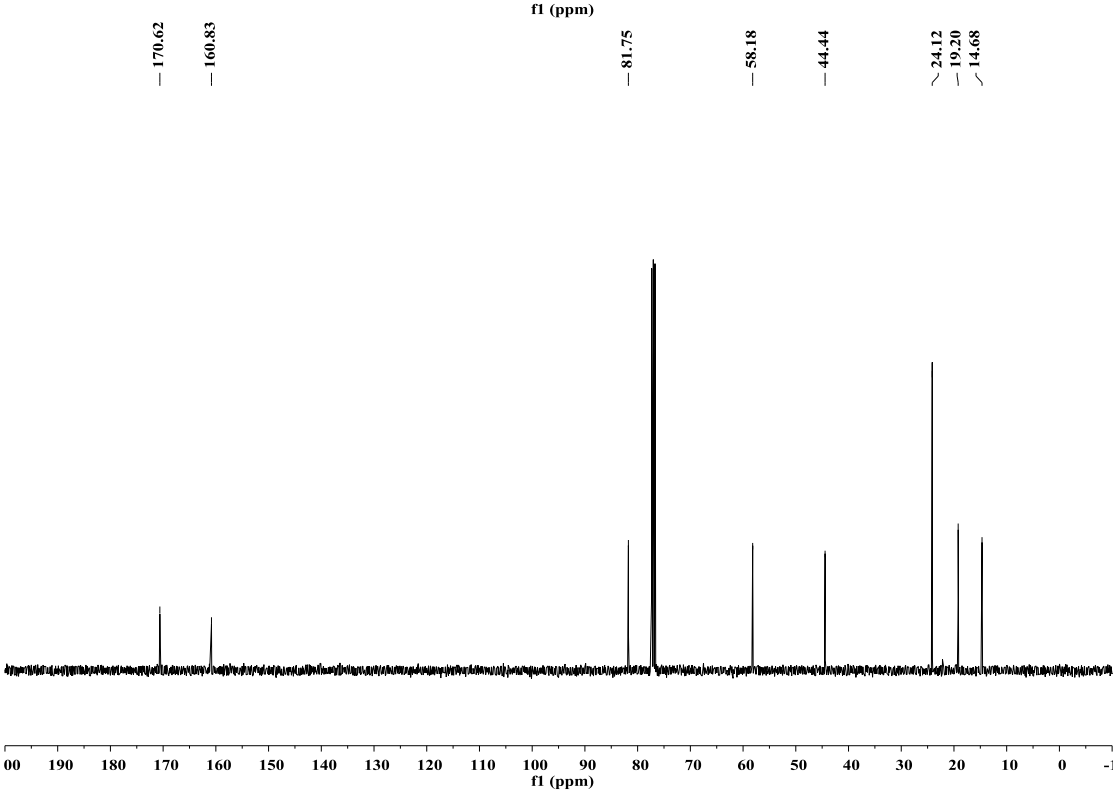
168.71
161.13
139.69
128.58
127.66
127.10
92.88
46.10
42.79
31.69
29.08
24.54
20.86

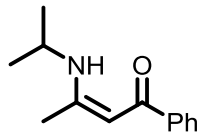

00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)


NH
O
O

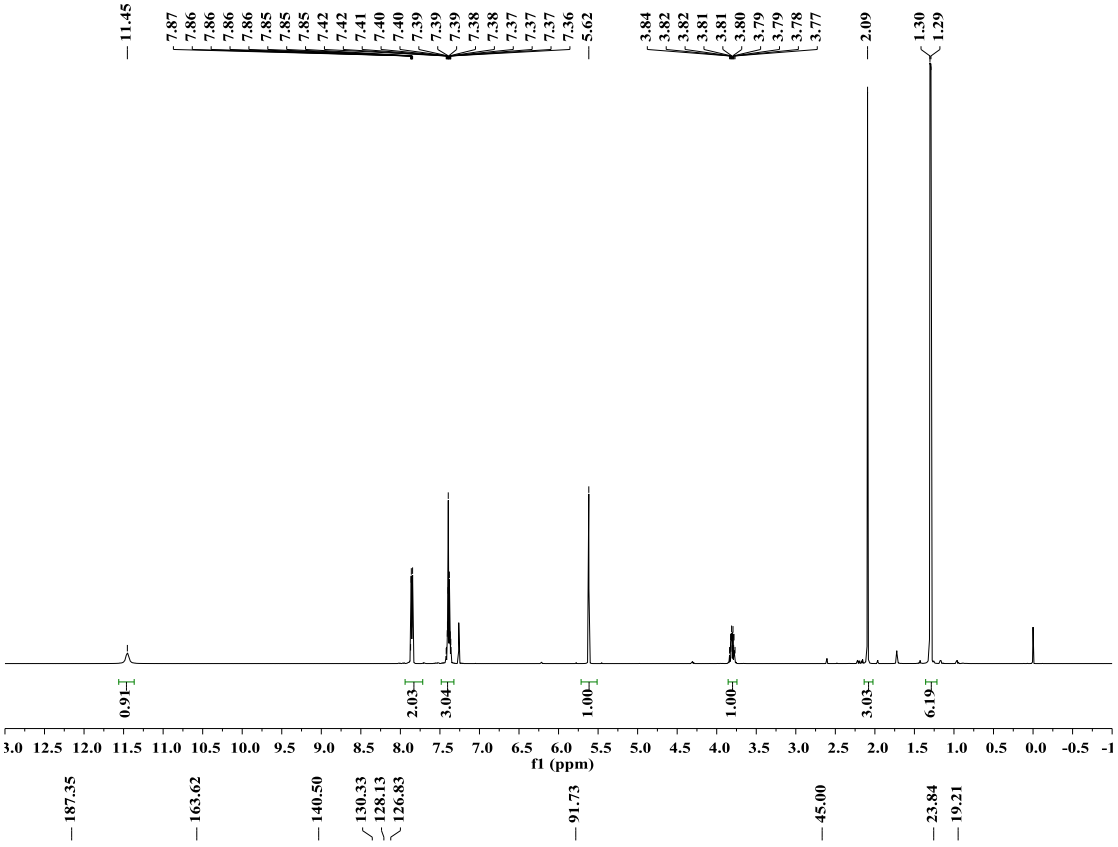
3B$_1$

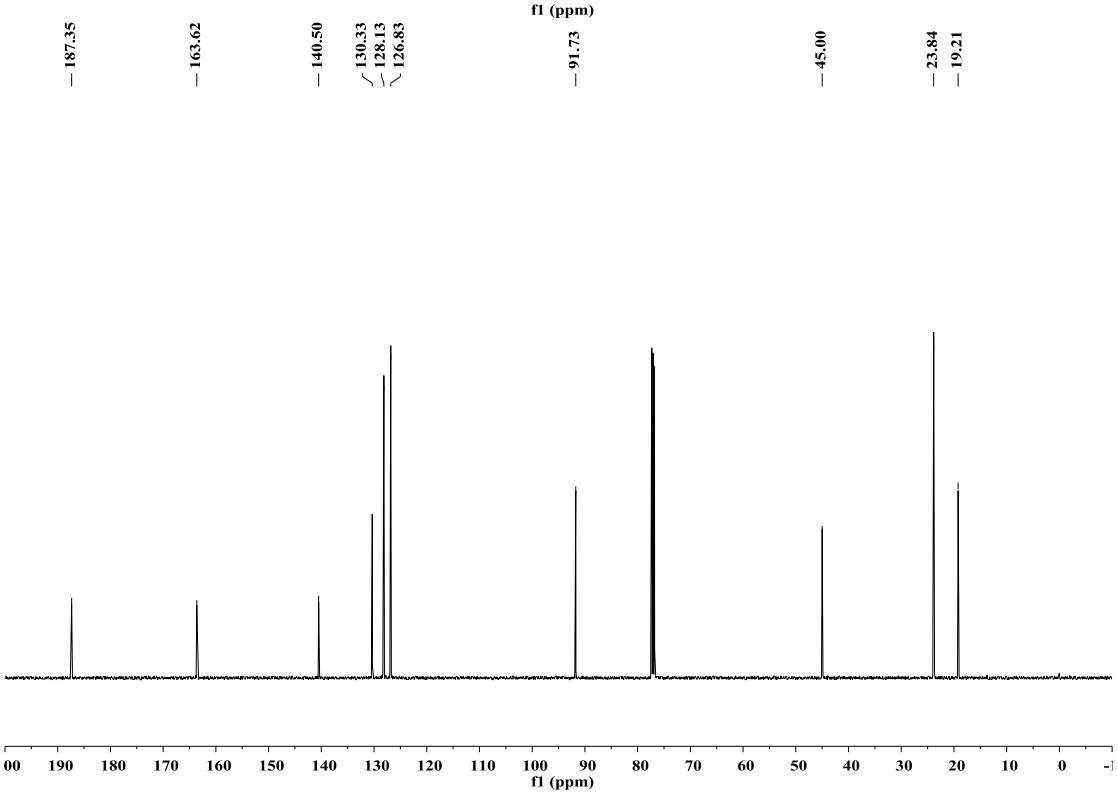

8.50
4.39
4.11
4.09
4.07
4.06
3.71
3.69
3.68
3.68
3.67
3.65
1.94
1.27
1.25
1.23
1.22
1.20
0.88
1.00
2.16
1.05
3.21
3.37
6.30
f1 (ppm)

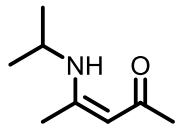

170.62
160.83
81.75
58.18
44.44
24.12
19.20
14.68
f1 (ppm)


NH
O
Ph

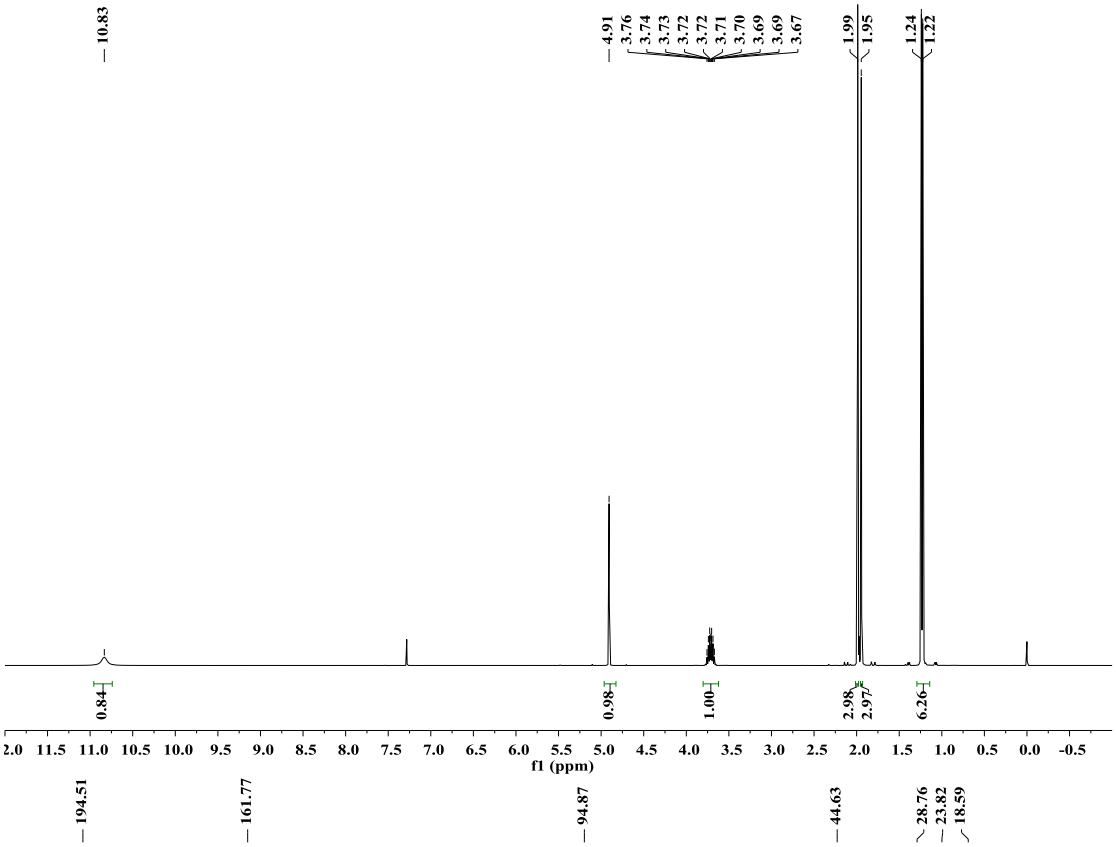
3B$_2$

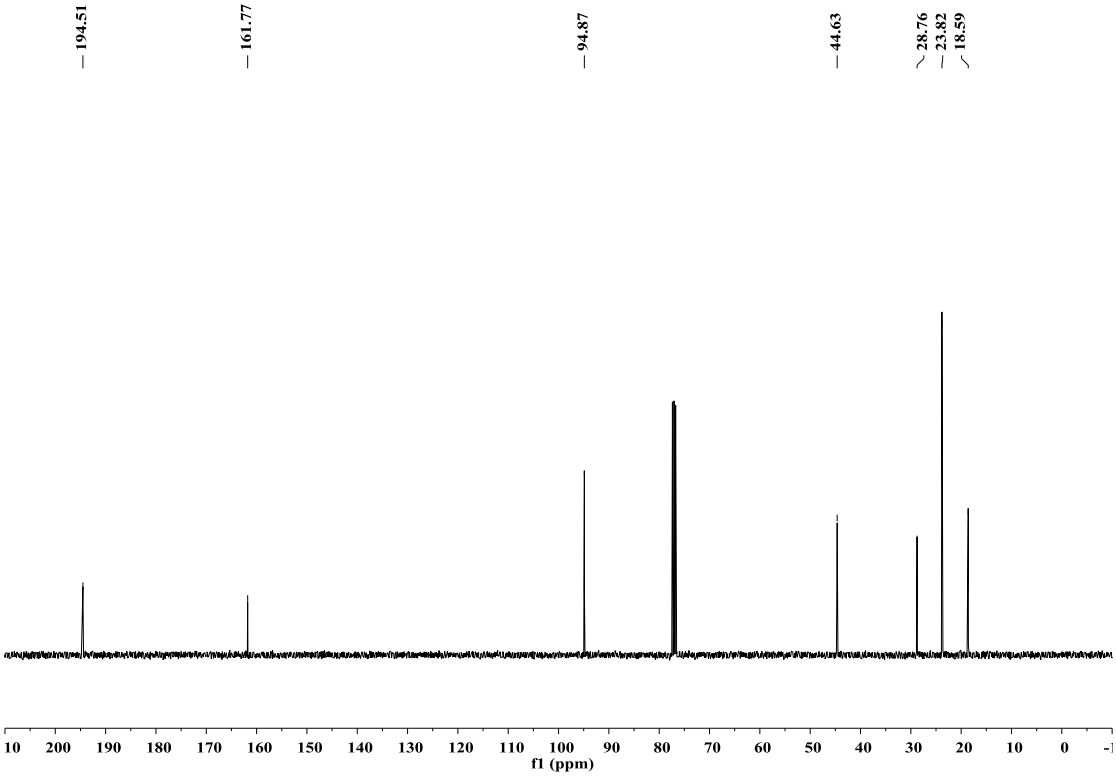

11.45
7.87 7.86 7.86 7.86 7.86 7.85 7.85 7.85 7.42 7.42 7.41 7.40 7.40 7.39 7.39 7.39 7.38 7.38 7.37 7.37 7.37 7.36
5.62
3.84 3.82 3.82 3.81 3.81 3.80 3.79 3.79 3.78 3.77
2.09
1.30 1.29
0.91 2.03 3.04 1.00 1.00 3.03 6.19
f1 (ppm)

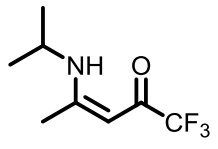

187.35
163.62
140.50
130.33
128.13
126.83
91.73
45.00
23.84
19.21
f1 (ppm)


NH
O

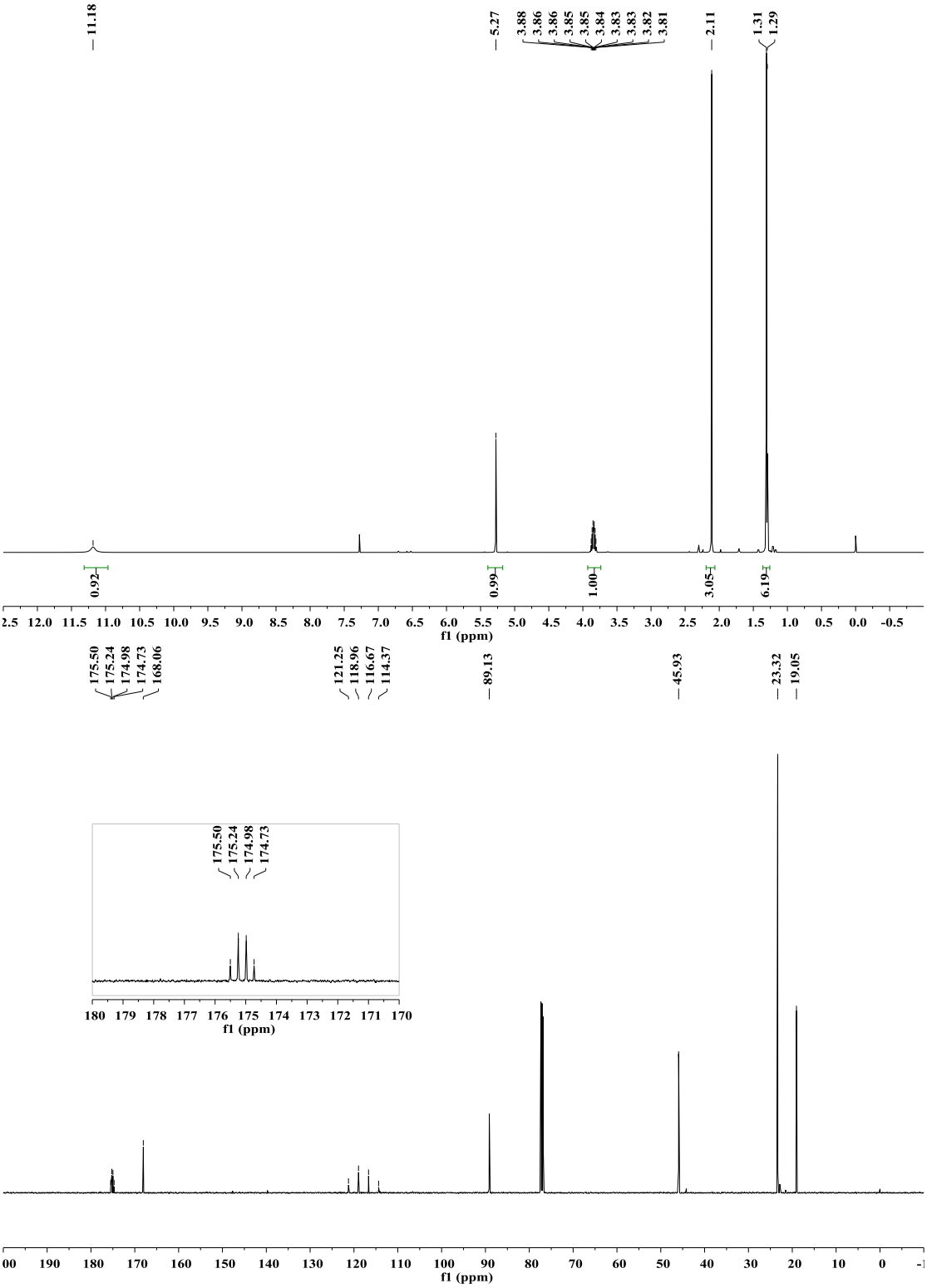
3B$_3$

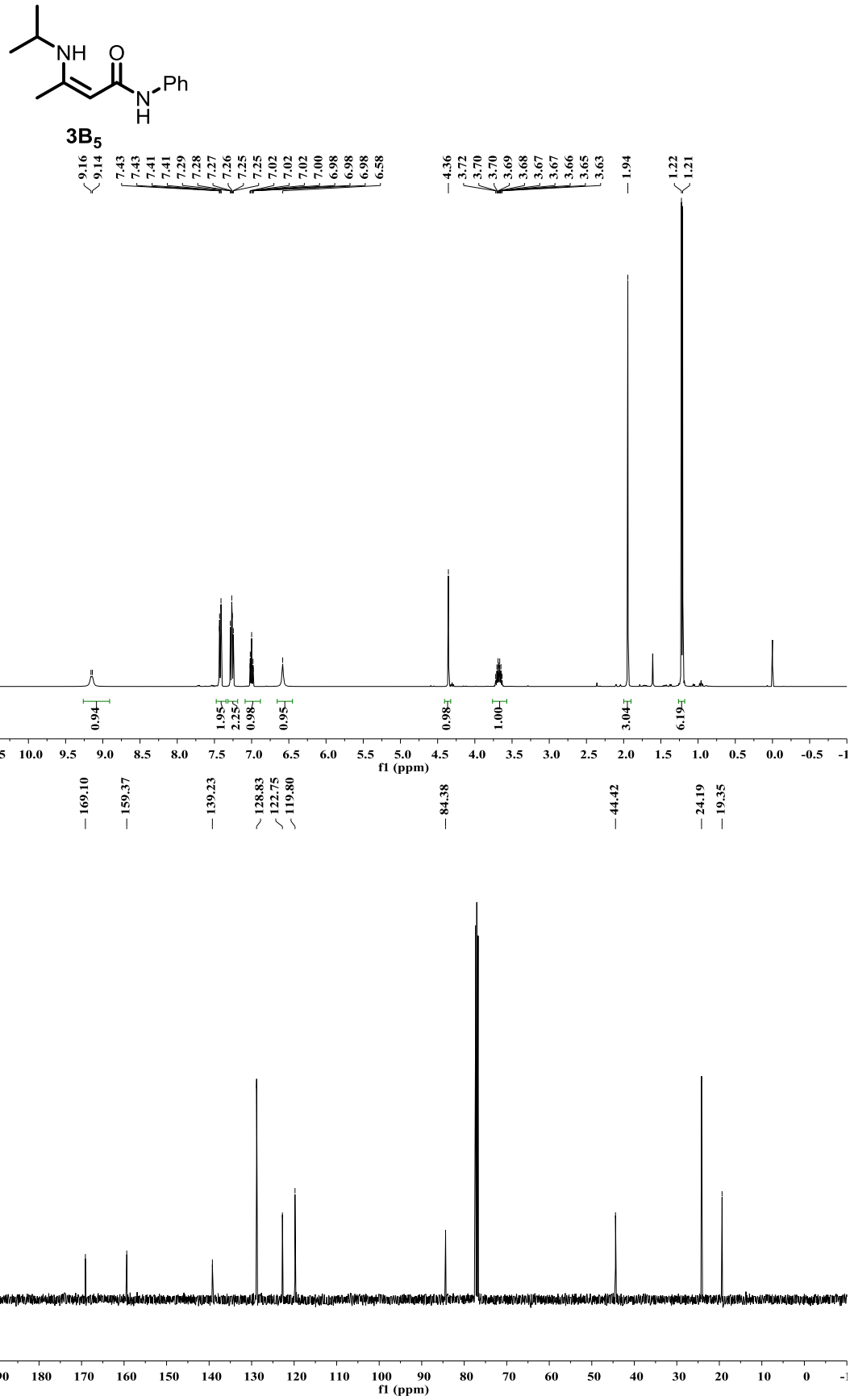

10.83
4.91
3.76
3.74
3.73
3.72
3.72
3.71
3.70
3.69
3.69
3.67
1.99
1.95
1.24
1.22
0.84
0.98
1.00
2.98
2.97
6.26
f1 (ppm)

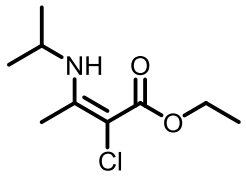

194.51
161.77
94.87
44.63
28.76
23.82
18.59
f1 (ppm)


NH
O
CF3

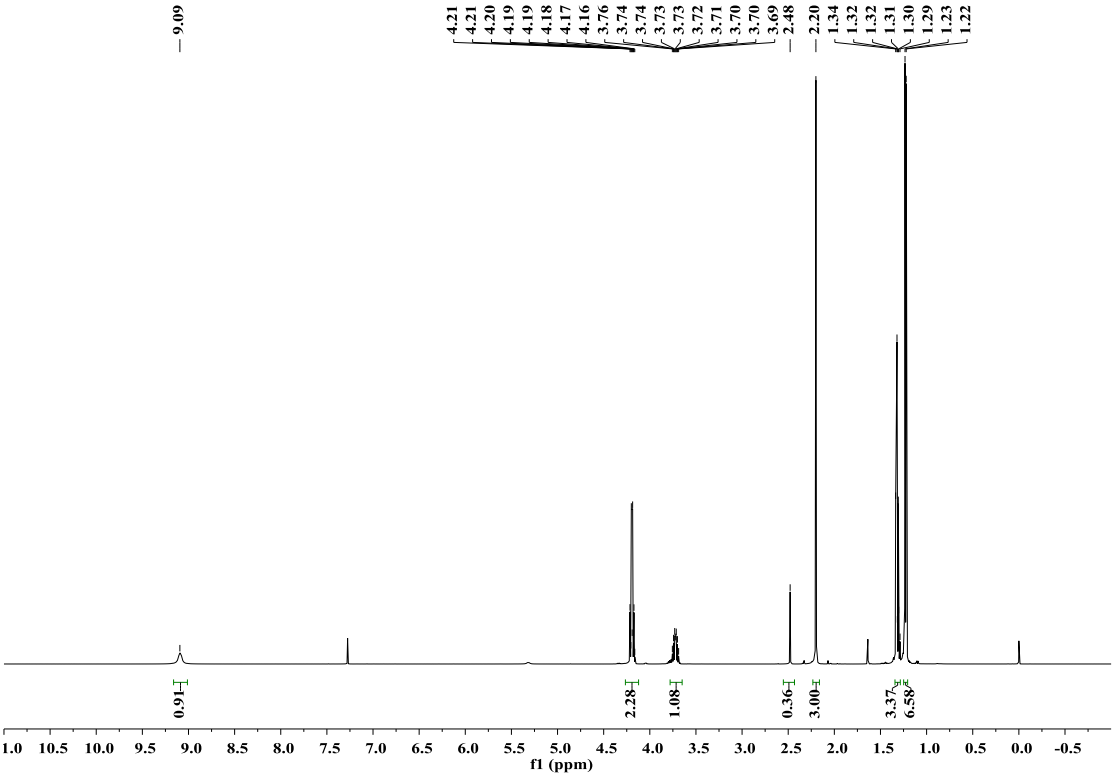
3B$_4$

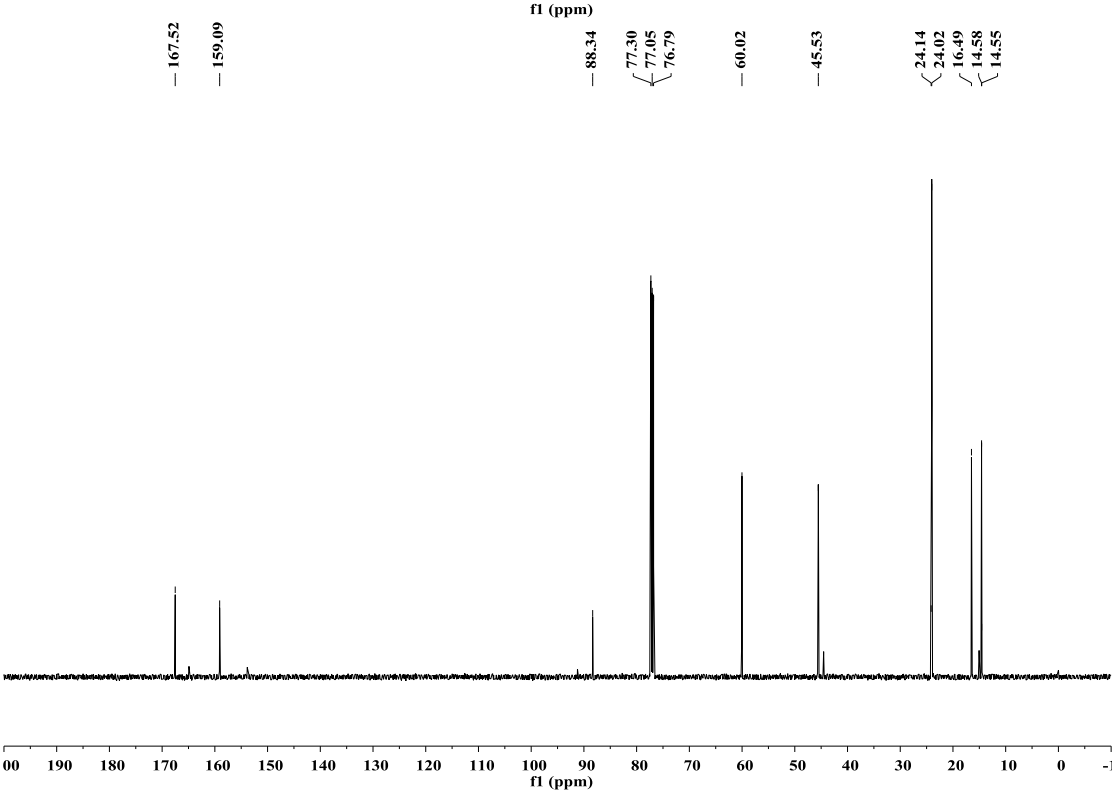

11.18
5.27
3.88
3.86
3.86
3.85
3.85
3.84
3.83
3.83
3.82
3.81
2.11
1.31
1.29
0.92
0.99
1.00
3.05
6.19
f1 (ppm)
175.50
175.24
174.98
174.73
168.06
121.25
118.96
116.67
114.37
89.13
45.93
23.32
19.05
180 179 178 177 176 175 174 173 172 171 170
f1 (ppm)
f1 (ppm)

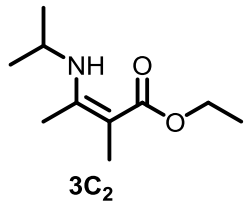

NH
O
N
H
Ph
3B5
9.16
9.14
7.43
7.43
7.41
7.41
7.29
7.28
7.27
7.26
7.25
7.25
7.02
7.02
7.02
7.00
6.98
6.98
6.98
6.58
4.36
3.72
3.70
3.70
3.69
3.68
3.67
3.67
3.66
3.65
3.63
1.94
1.22
1.21
0.94
1.95
2.25
0.98
0.95
0.98
1.00
3.04
6.19
f1 (ppm)
169.10
159.37
139.23
128.83
122.75
119.80
84.38
44.42
24.19
19.35
f1 (ppm)


NH
O
O
Cl

3C$_1$

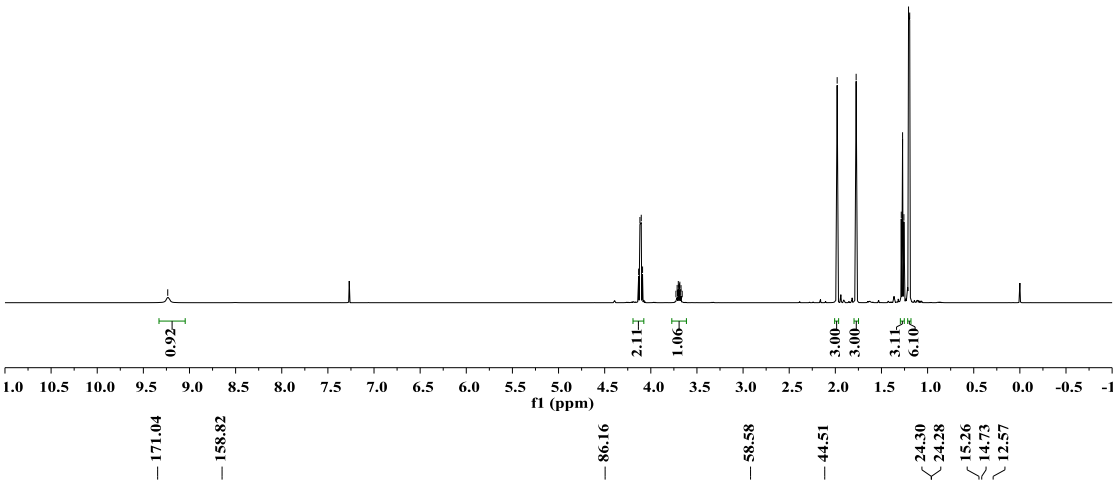

9.09
4.21
4.21
4.20
4.19
4.19
4.18
4.17
4.16
3.76
3.74
3.74
3.73
3.73
3.72
3.71
3.70
3.70
3.69
2.48
2.20
1.34
1.32
1.32
1.31
1.30
1.29
1.23
1.22
0.91
2.28
1.08
0.36
3.00
3.37
6.58
f1 (ppm)

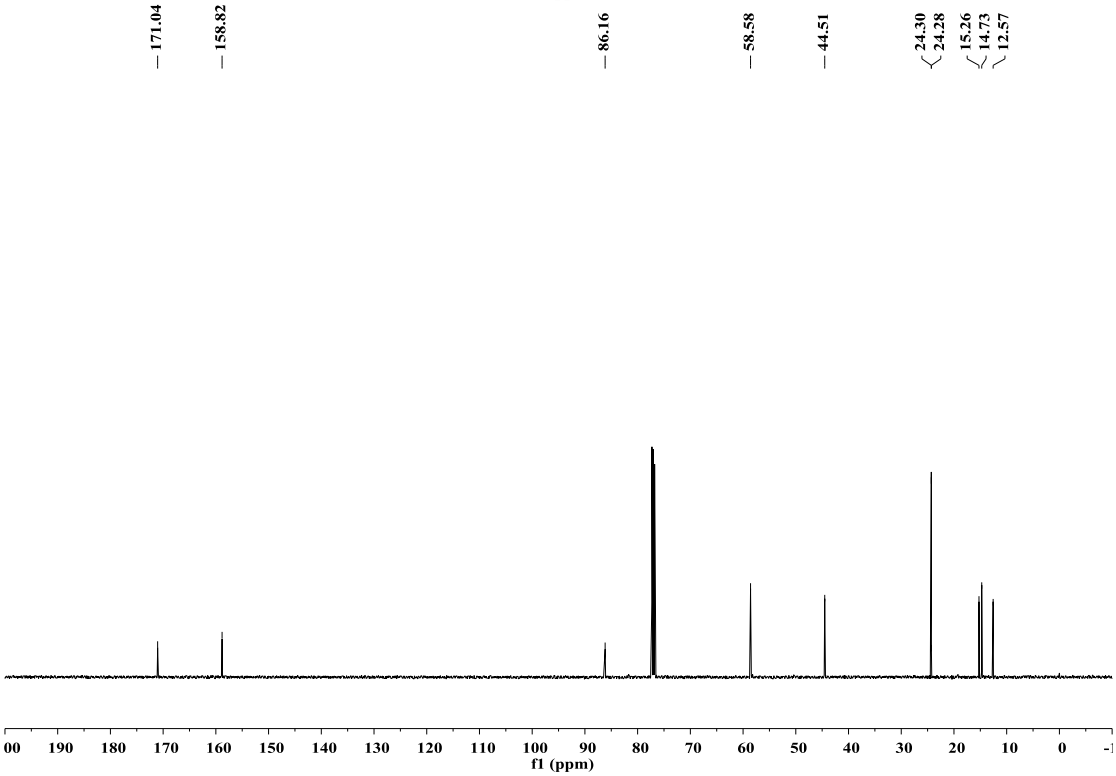

167.52
159.09
88.34
77.30
77.05
76.79
60.02
45.53
24.14
24.02
16.49
14.58
14.55
f1 (ppm)

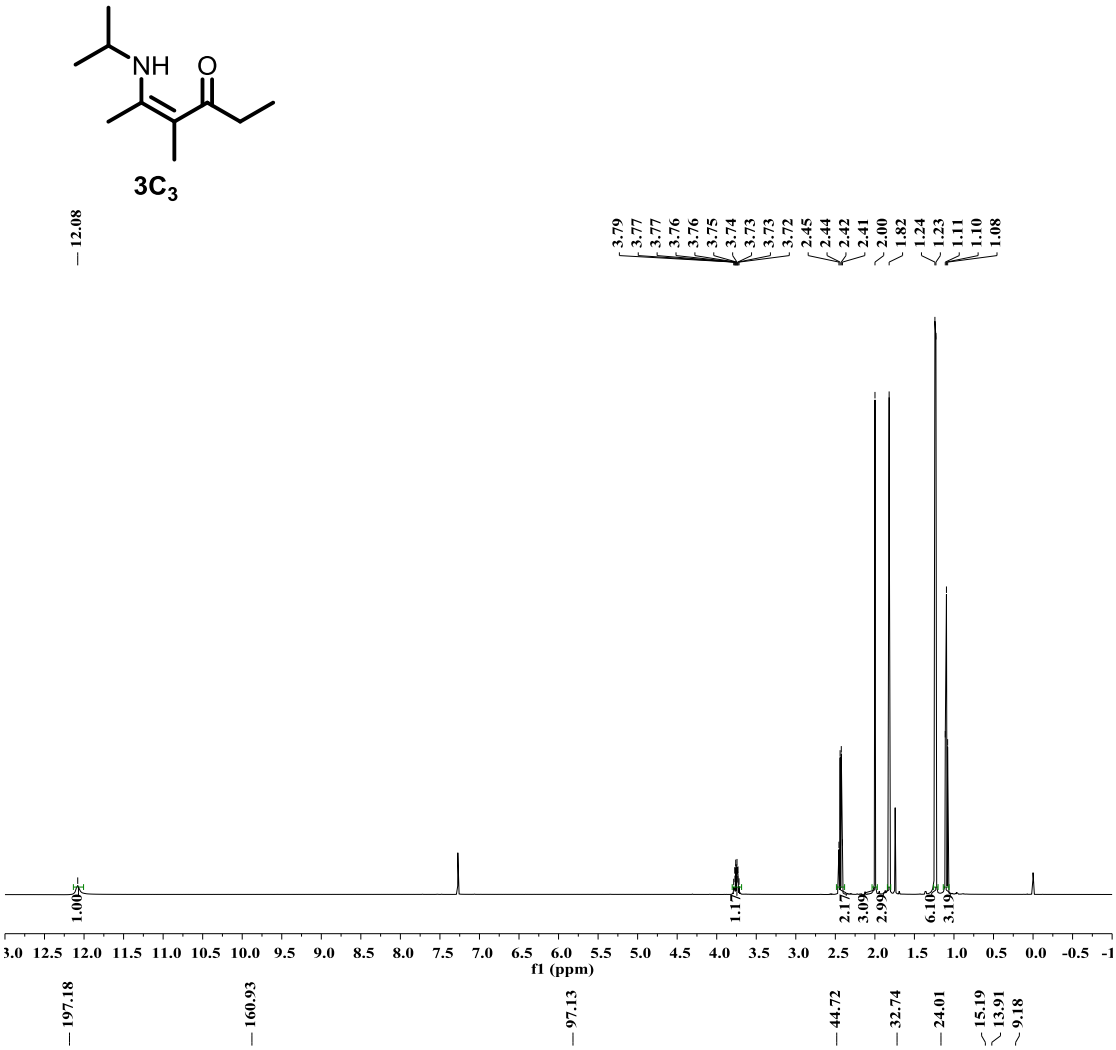

NH
O
O

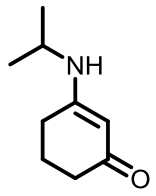
3C$_2$


9.24
4.13
4.12
4.10
4.09
3.73
3.71
3.71
3.70
3.70
3.69
3.69
3.68
3.67
3.66
1.98
1.77
1.29
1.27
1.26
1.21
1.19

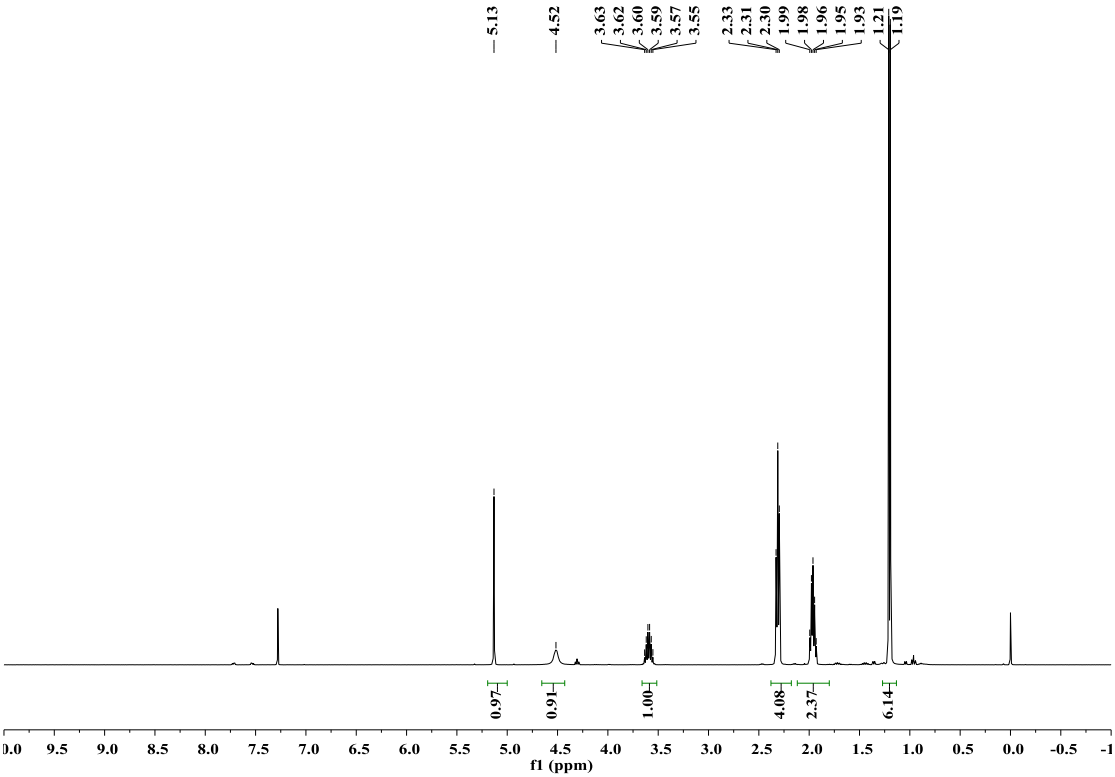

0.92
2.11
1.06
3.00
3.00
3.11
6.10
f1 (ppm)

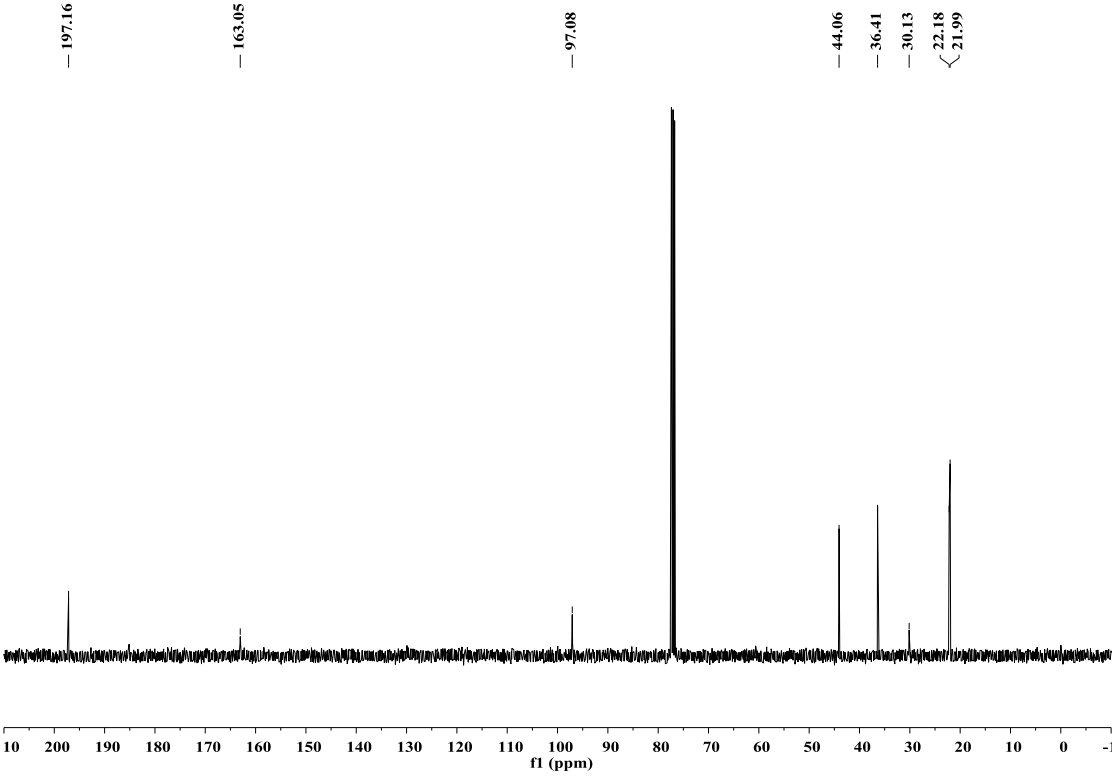

171.04
158.82
86.16
58.58
44.51
24.30
24.28
15.26
14.73
12.57
f1 (ppm)

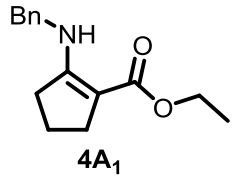

NH
O
3C3
12.08
3.79
3.77
3.77
3.76
3.76
3.75
3.74
3.73
3.73
3.72
2.45
2.44
2.42
2.41
2.00
1.82
1.24
1.23
1.11
1.10
1.08
1.00
1.17
2.17
3.09
2.99
6.10
3.19
f1 (ppm)
197.18
160.93
97.13
44.72
32.74
24.01
15.19
13.91
9.18
f1 (ppm)


NH
O

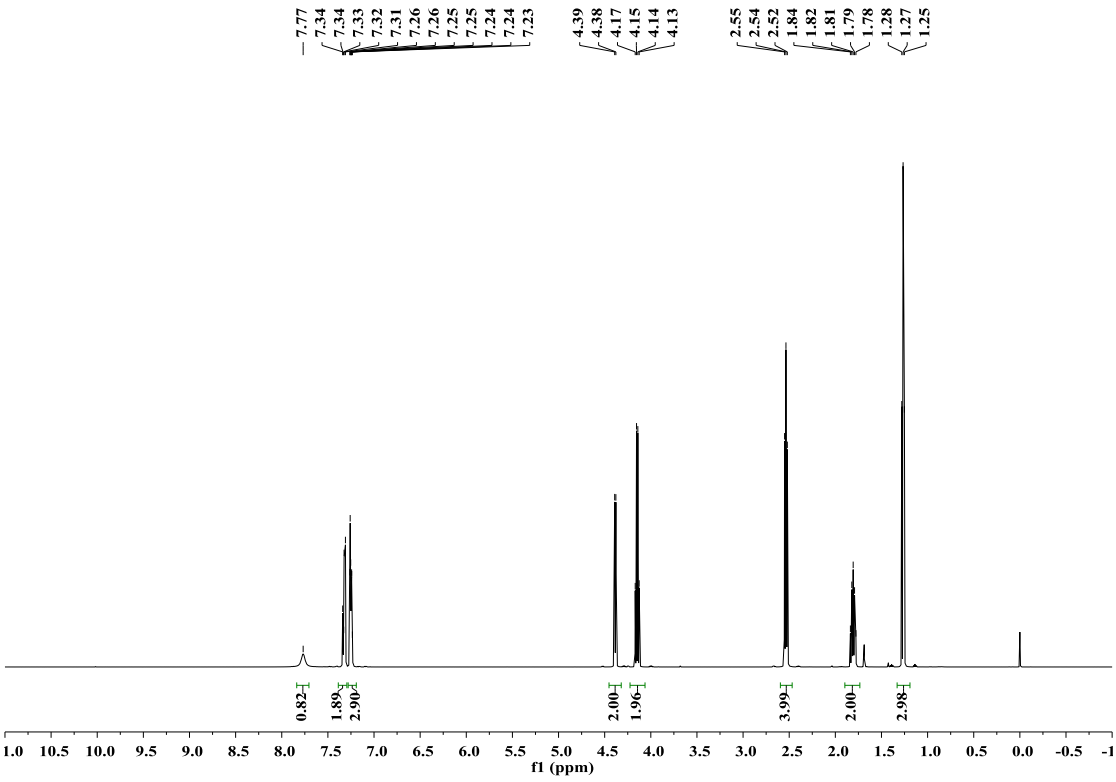
3D$_1$

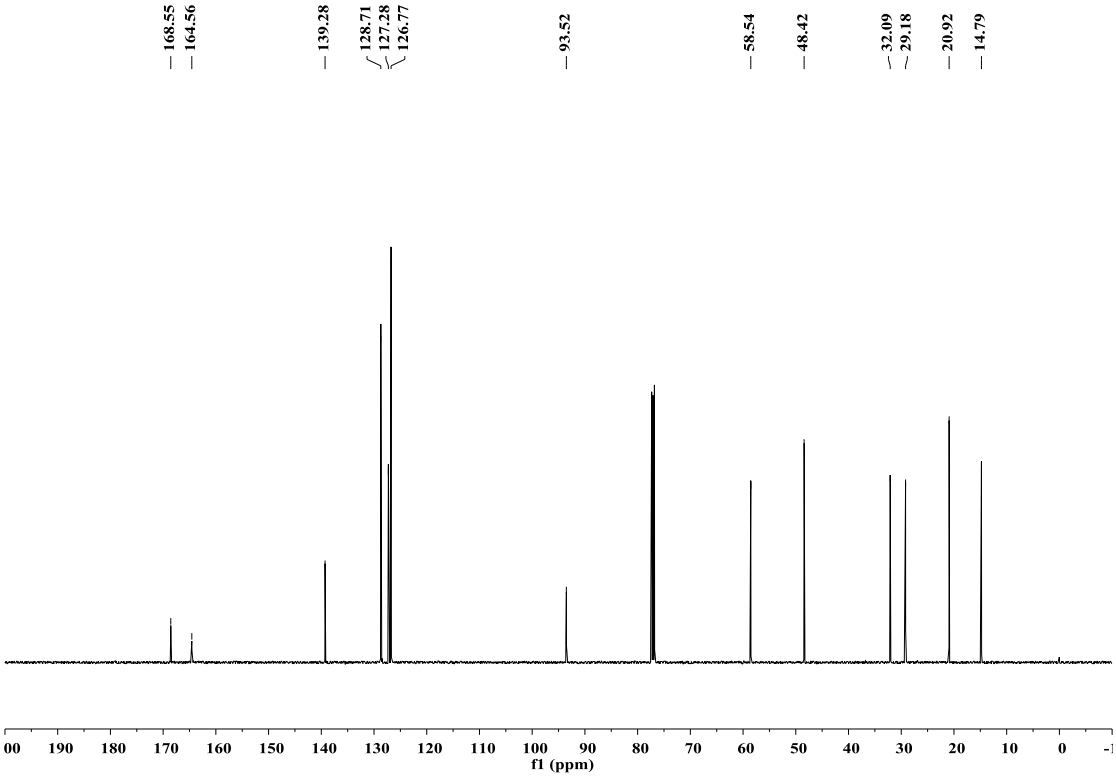

5.13
4.52
3.63
3.62
3.60
3.59
3.57
3.55
2.33
2.31
2.30
1.99
1.98
1.96
1.95
1.93
1.21
1.19
0.97
0.91
1.00
4.08
2.37
6.14
f1 (ppm)

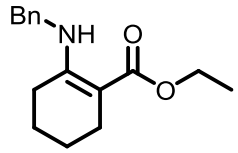

197.16
163.05
97.08
44.06
36.41
30.13
22.18
21.99
f1 (ppm)


Bn
NH
O
O

4A$_1$

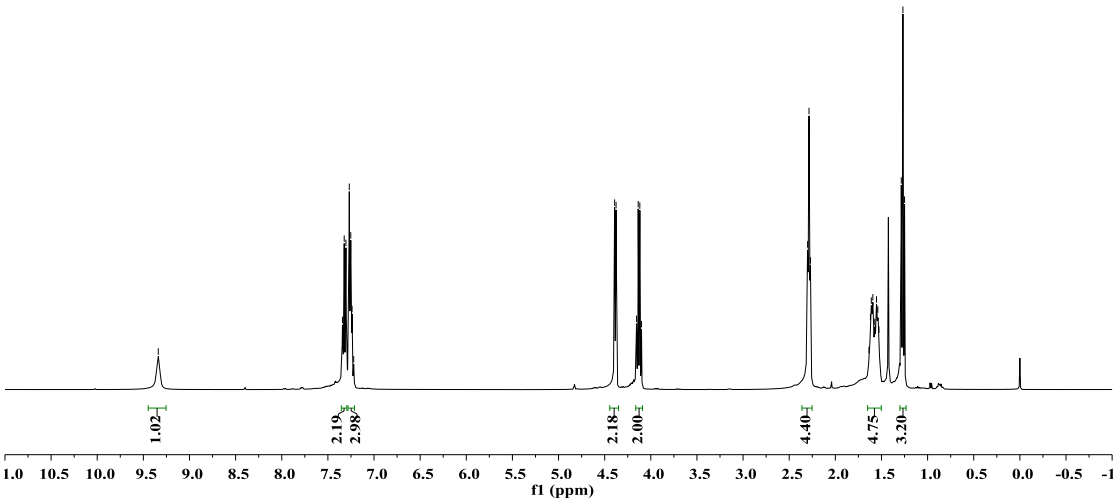

7.77
7.34
7.34
7.33
7.32
7.31
7.26
7.26
7.25
7.25
7.24
7.24
7.23
4.39
4.38
4.17
4.15
4.14
4.13
2.55
2.54
2.52
1.84
1.82
1.81
1.79
1.78
1.28
1.27
1.25
0.82
1.89
2.90
2.00
1.96
3.99
2.00
2.98
f1 (ppm)

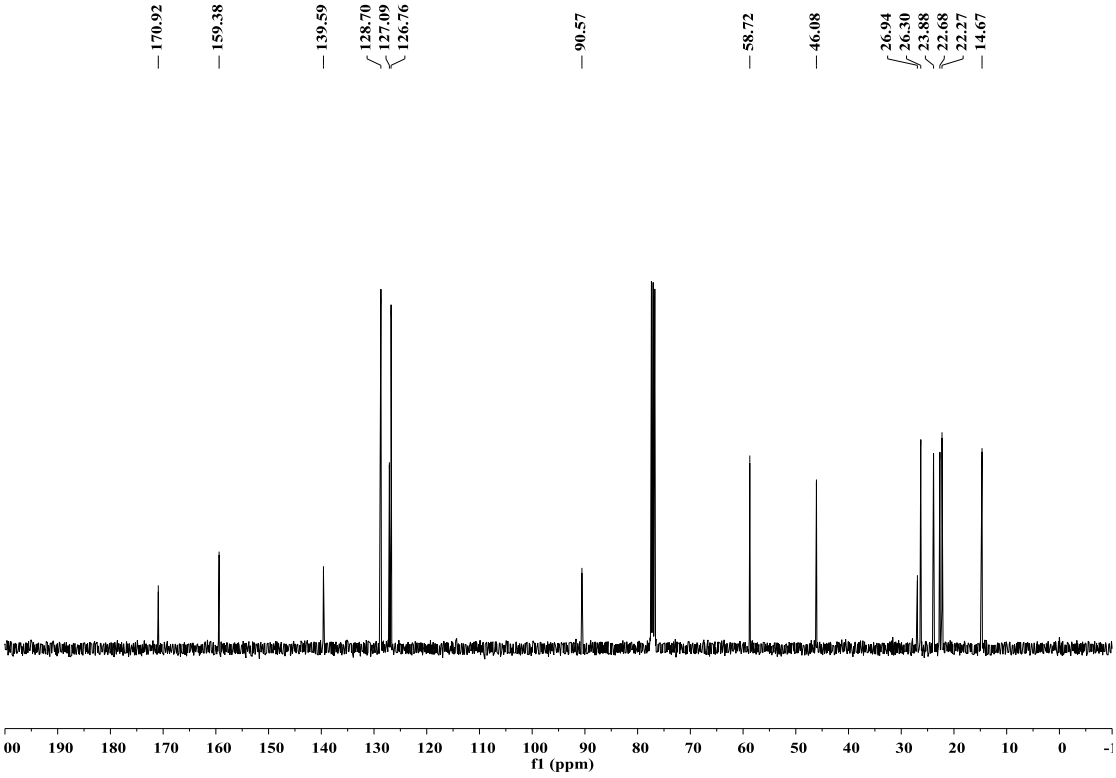

168.55
164.56
139.28
128.71
127.28
126.77
93.52
58.54
48.42
32.09
29.18
20.92
14.79
f1 (ppm)

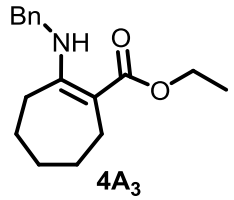

Bn
NH
O
O

4A$_2$

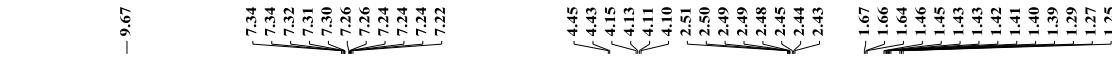

9.34
7.34
7.32
7.30
7.27
7.25
7.24
7.22
4.39
4.38
4.15
4.14
4.12
4.10
2.30
2.29
2.27
1.64
1.62
1.61
1.59
1.57
1.56
1.55
1.54
1.53
1.29
1.27
1.25

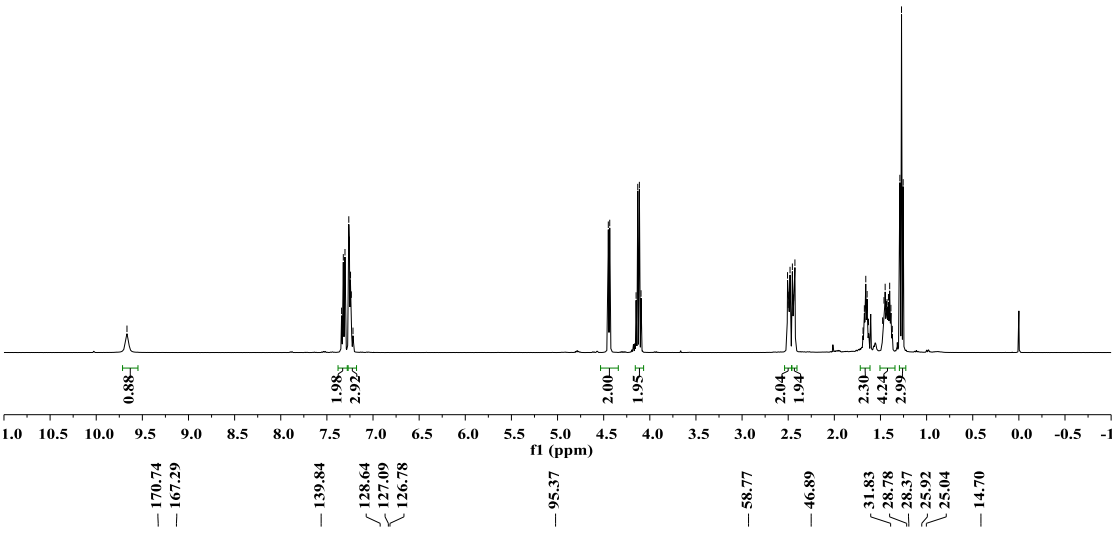

1.02
2.19
2.98
2.18
2.00
4.40
4.75
3.20
f1 (ppm)


170.92
159.38
139.59
128.70
127.09
126.76
90.57
58.72
46.08
26.94
26.30
23.88
22.68
22.27
14.67
f1 (ppm)

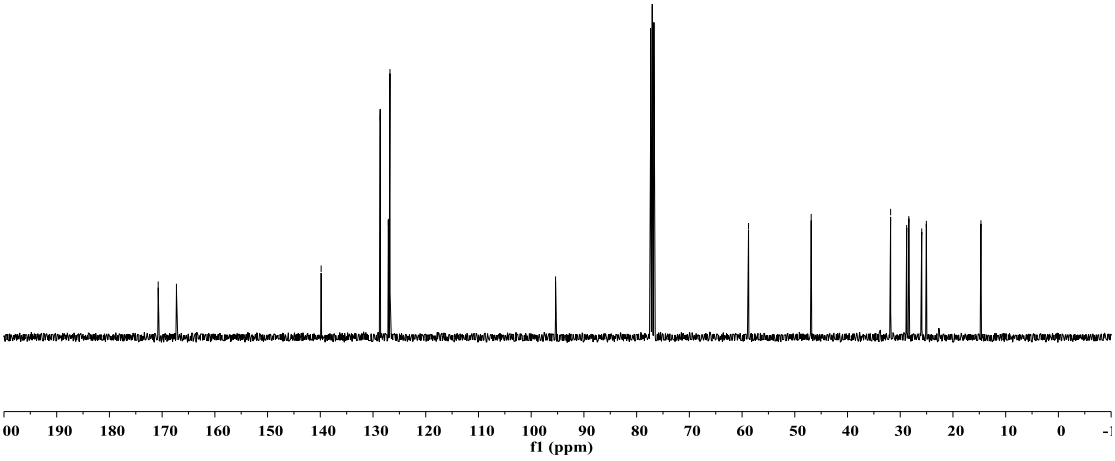

Bn
NH
O
O

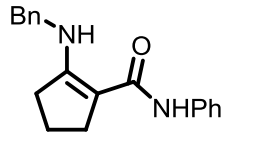
4A$_3$


9.67
7.34
7.34
7.32
7.31
7.30
7.26
7.26
7.24
7.24
7.24
7.22
4.45
4.43
4.15
4.13
4.11
4.10
2.51
2.50
2.49
2.49
2.48
2.45
2.44
2.43
1.67
1.66
1.64
1.46
1.45
1.43
1.43
1.42
1.41
1.40
1.39
1.29
1.27


0.88
1.98
2.92
2.00
1.95
2.04
1.94
2.30
4.24
2.99
f1 (ppm)

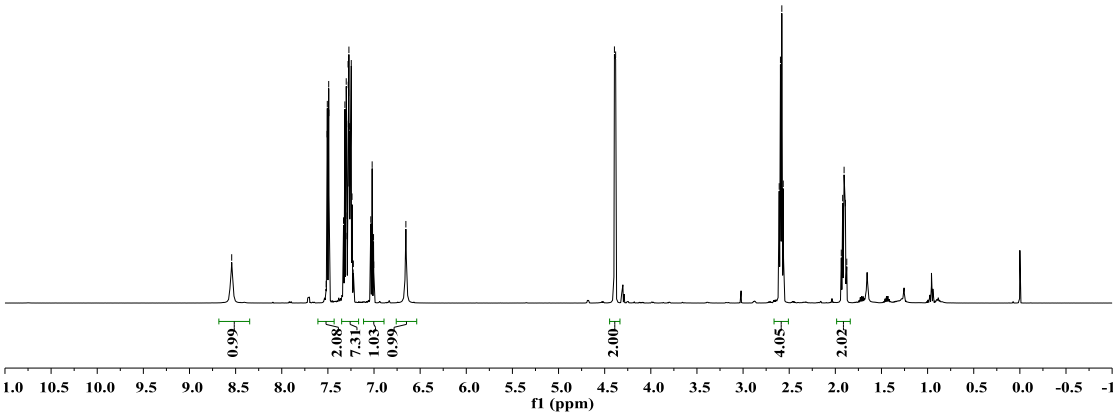
170.74
167.29
139.84
128.64
127.09
126.78
95.37
58.77
46.89
31.83
28.78
28.37
25.92
25.04
14.70


f1 (ppm)

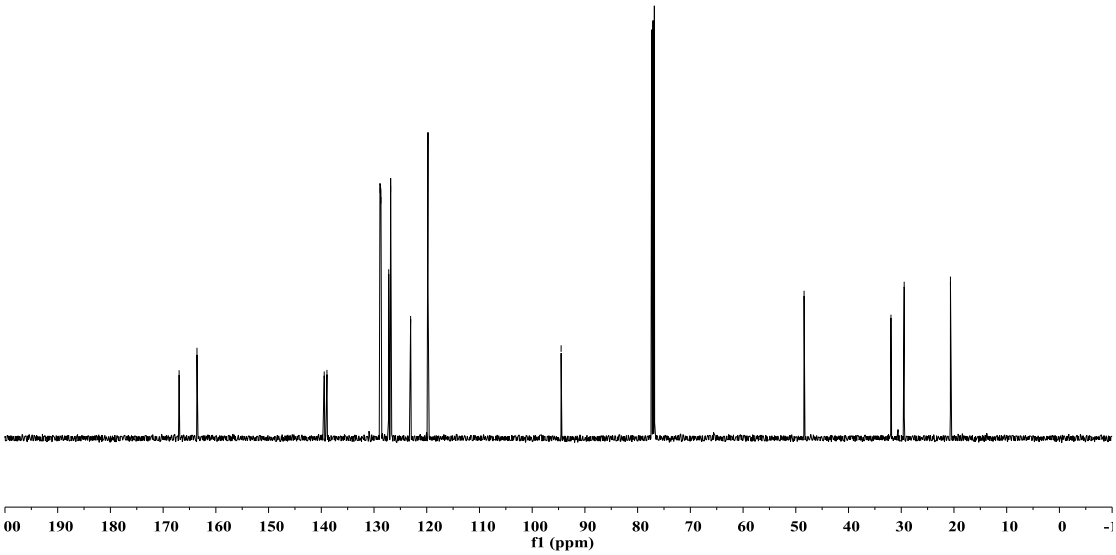


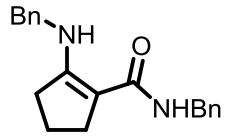
4A$_4$

8.54 7.52 7.51 7.51 7.49 7.49 7.33 7.33 7.32 7.30 7.30 7.30 7.29 7.28 7.28 7.27 7.27 7.26 7.26 7.26 7.25 7.24 7.23 7.22 7.04 7.03 7.03 7.02 7.01 7.01 7.00 6.65 4.39 4.38 2.61 2.59 2.58 2.56 1.94 1.92 1.91 1.89 1.88

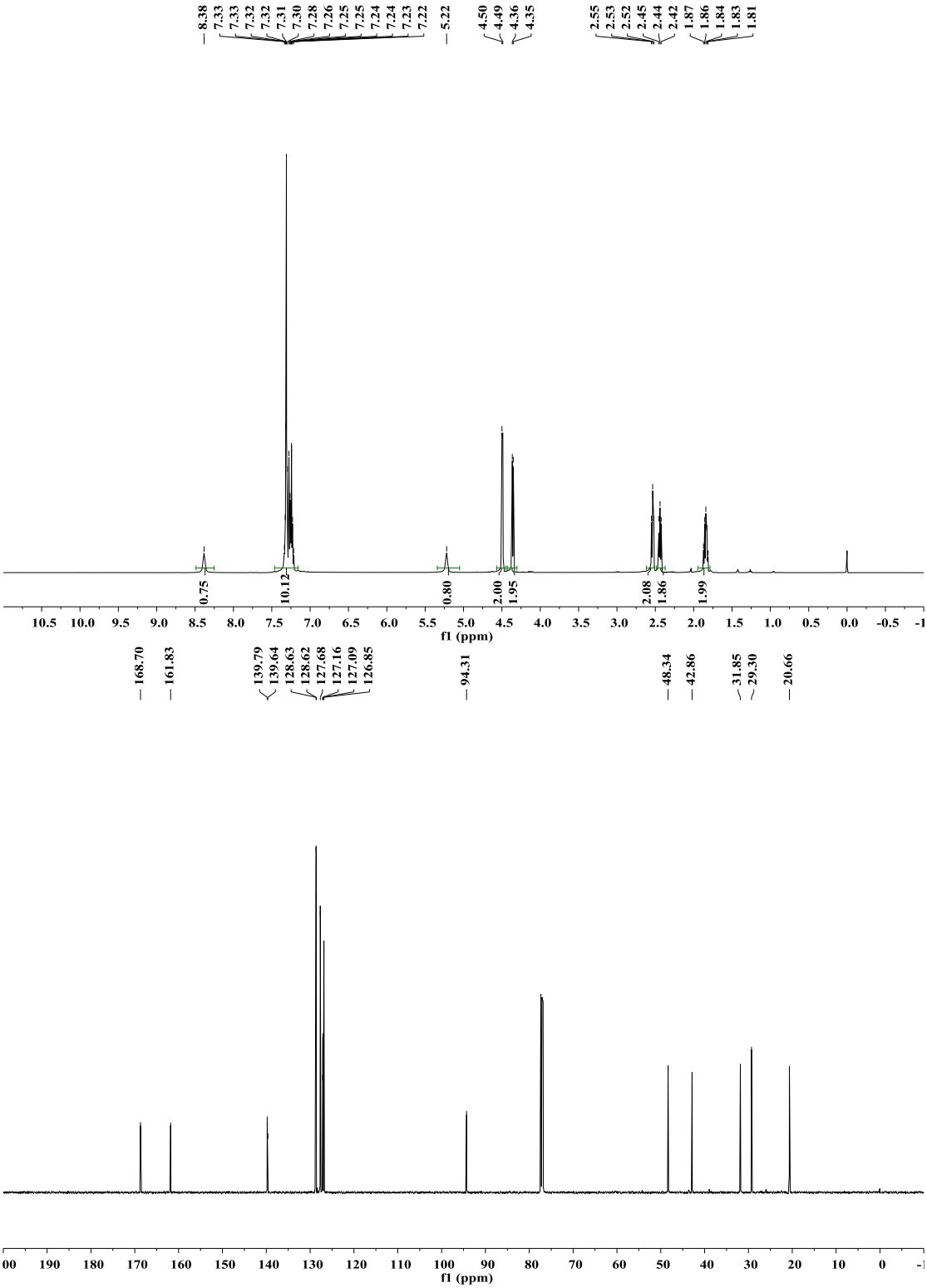


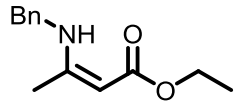
166.97 163.58 139.44 138.92 128.87 128.69 127.21 126.85 123.06 119.76 94.51 48.43 31.95 29.44 20.67



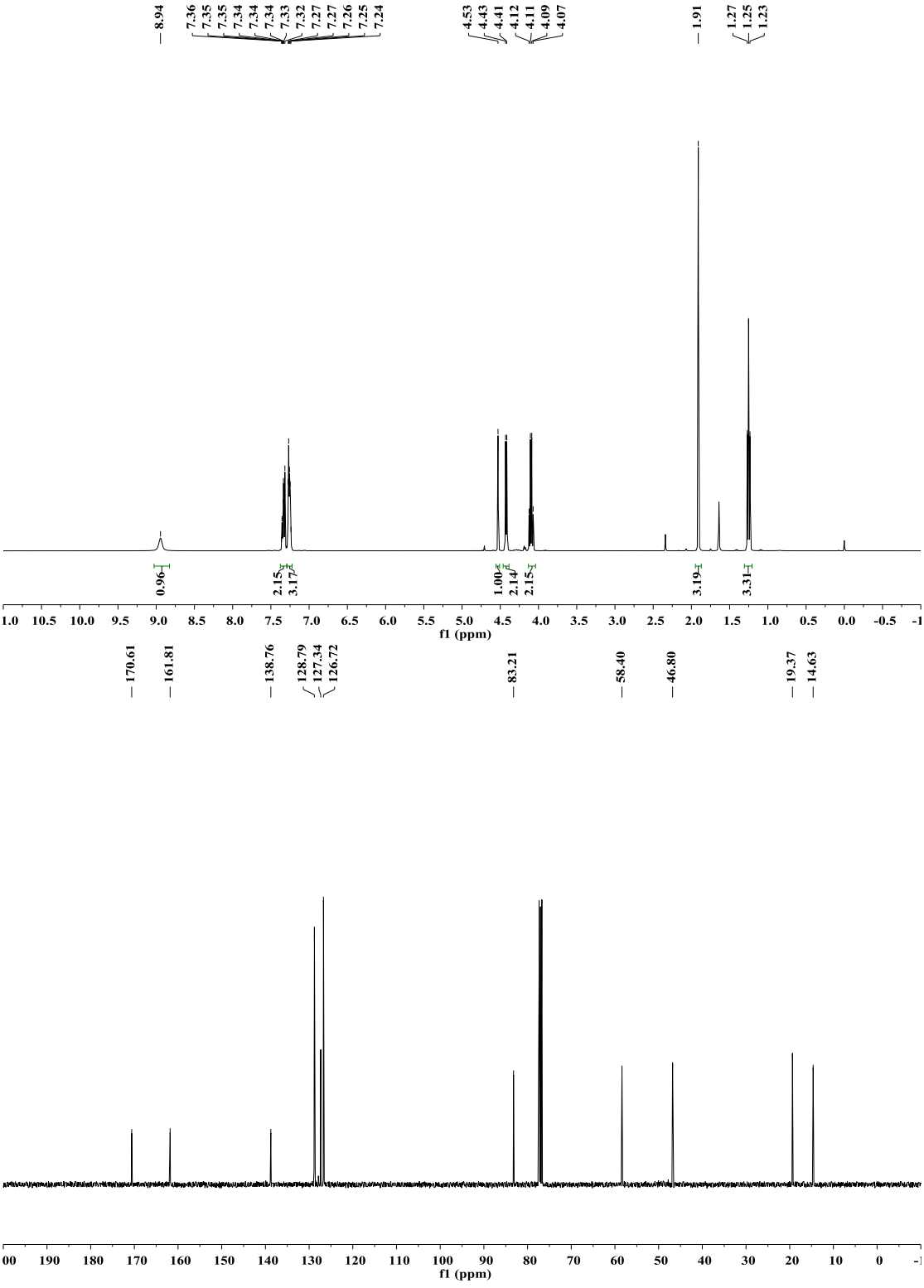

Bn
NH
O
NHBn

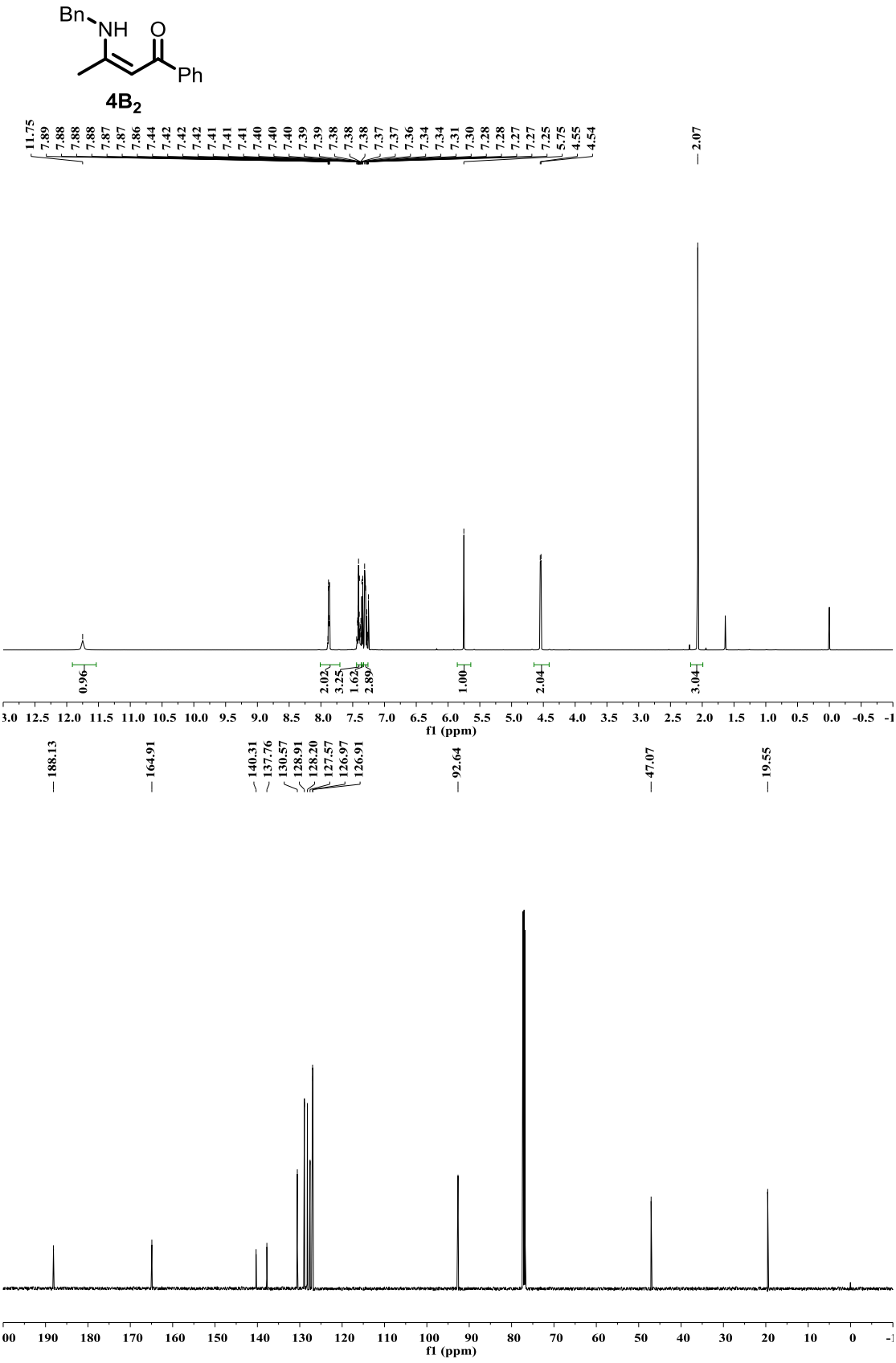
4A$_5$

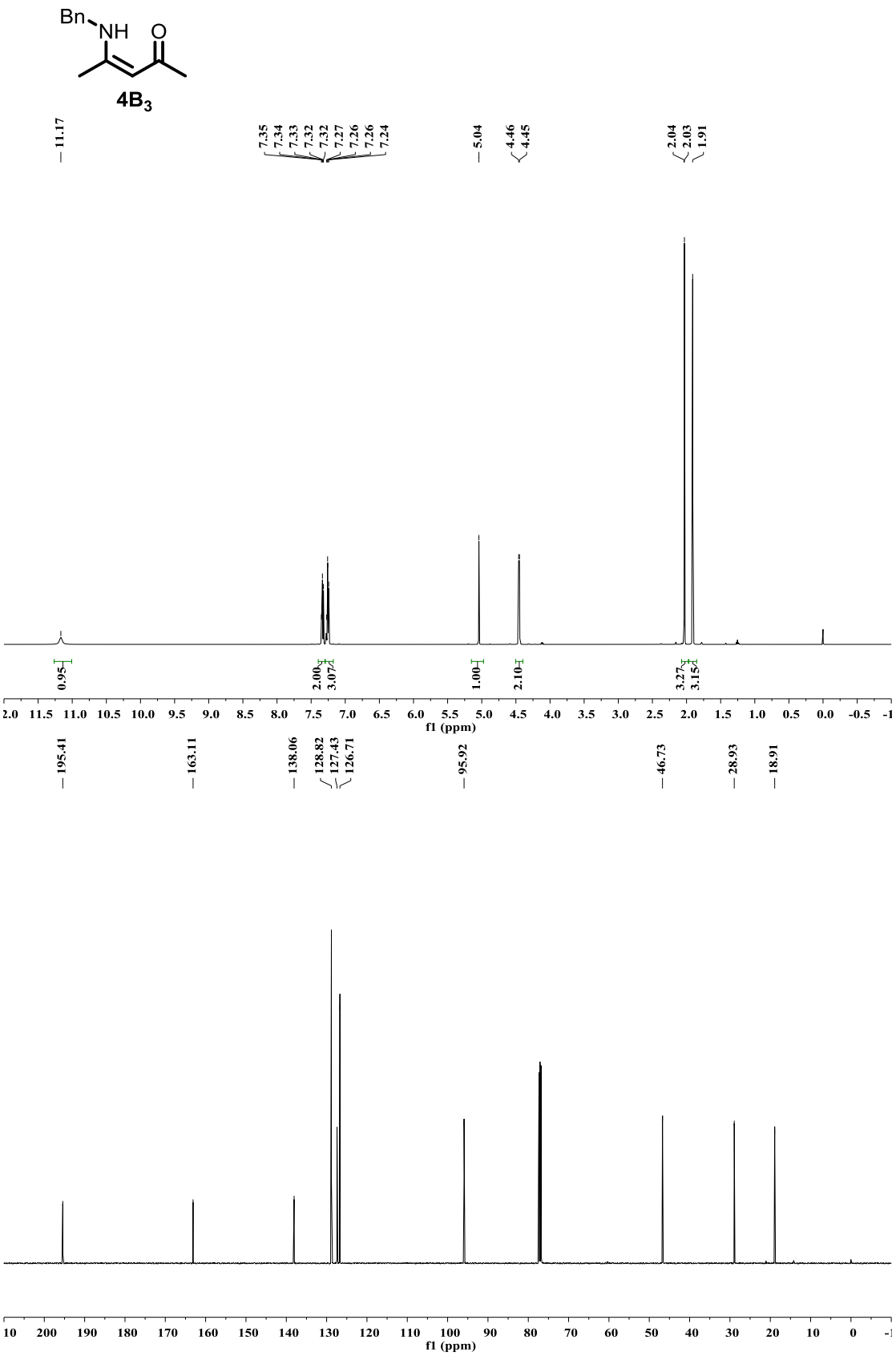

8.38
7.33
7.33
7.32
7.32
7.31
7.30
7.28
7.26
7.25
7.25
7.24
7.24
7.23
7.22
5.22
4.50
4.49
4.36
4.35
2.55
2.53
2.52
2.45
2.44
2.42
1.87
1.86
1.84
1.83
1.81
0.75
10.12
0.80
2.00
1.95
2.08
1.86
1.99
f1 (ppm)
168.70
161.83
139.79
139.64
128.63
128.62
127.68
127.16
127.09
126.85
94.31
48.34
42.86
31.85
29.30
20.66
f1 (ppm)

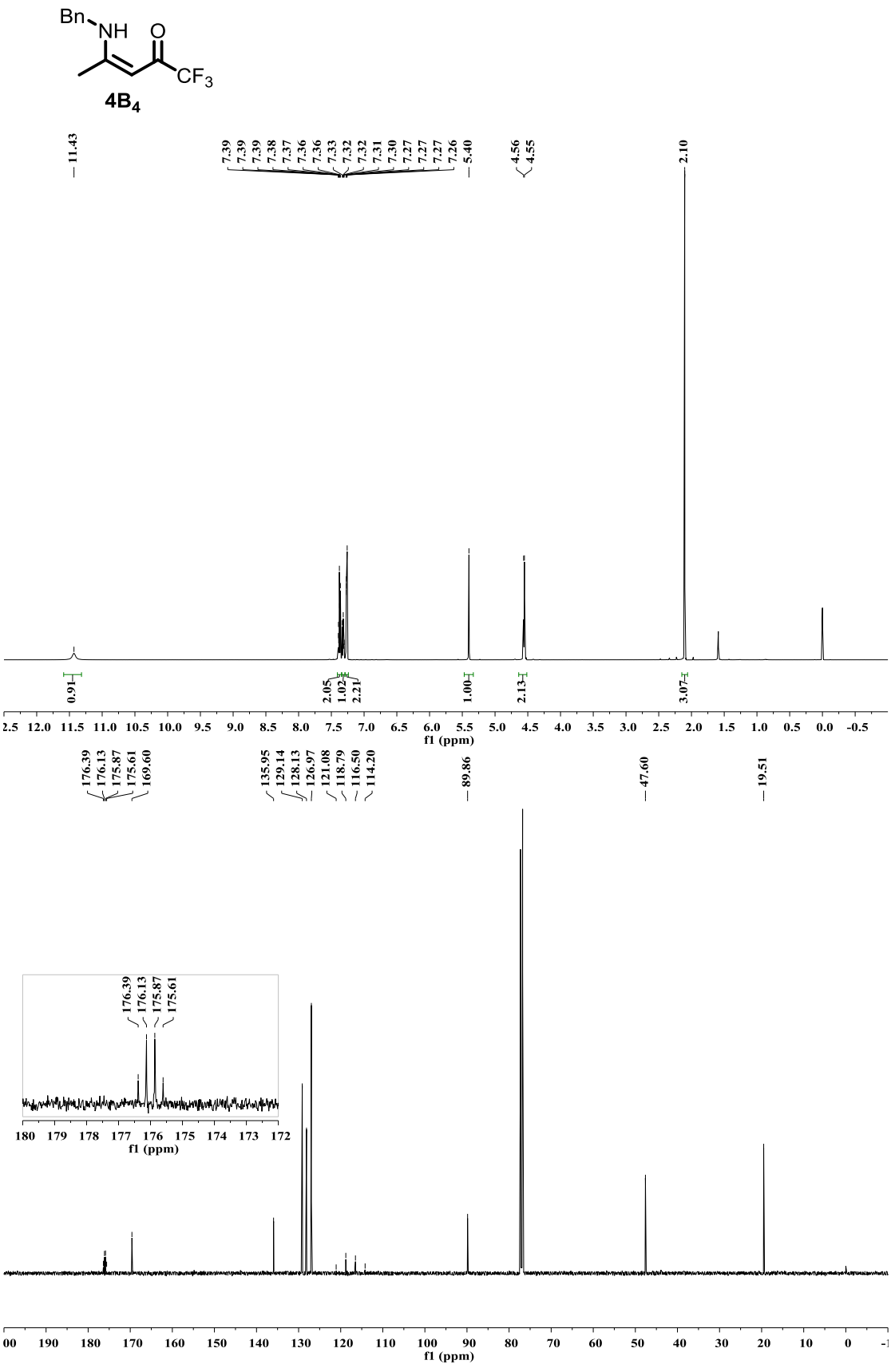

Bn
NH
O
O

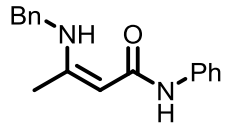
4B$_1$


8.94
7.36
7.35
7.35
7.34
7.34
7.34
7.33
7.32
7.27
7.27
7.26
7.25
7.24
4.53
4.43
4.41
4.12
4.11
4.09
4.07
1.91
1.27
1.25
1.23
0.96
2.15
3.17
1.00
2.14
2.15
3.19
3.31
f1 (ppm)
170.61
161.81
138.76
128.79
127.34
126.72
83.21
58.40
46.80
19.37
14.63
f1 (ppm)

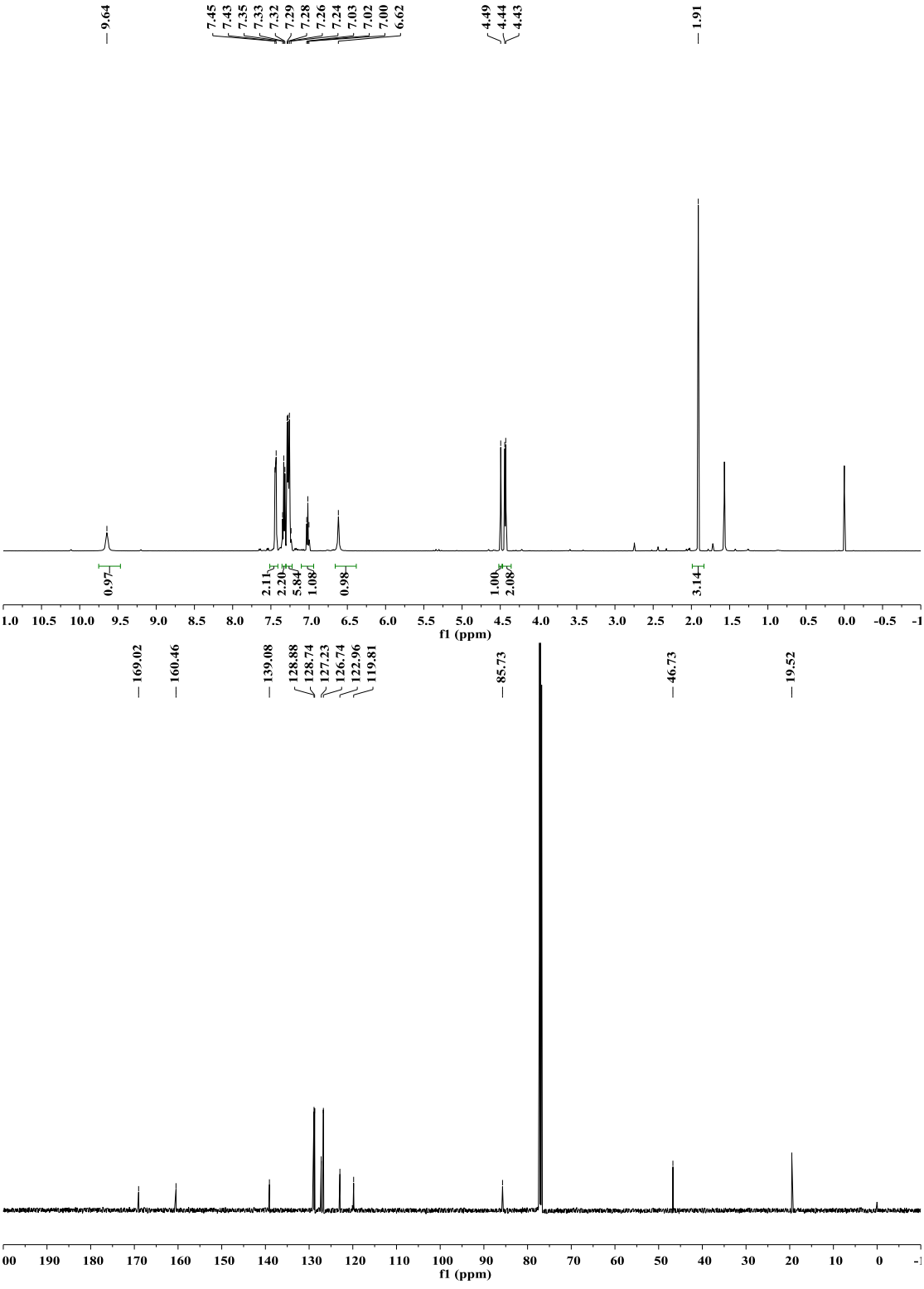

Bn
NH
O
Ph
4B2
11.75
7.89
7.88
7.88
7.88
7.87
7.87
7.86
7.44
7.42
7.42
7.42
7.41
7.41
7.41
7.40
7.40
7.40
7.40
7.39
7.39
7.38
7.38
7.38
7.37
7.37
7.36
7.34
7.34
7.31
7.30
7.28
7.28
7.27
7.27
7.25
5.75
4.55
4.54
2.07
0.96
2.02
3.25
1.62
2.89
1.00
2.04
3.04
f1 (ppm)
188.13
164.91
140.31
137.76
130.57
128.91
128.20
127.57
126.97
126.91
92.64
47.07
19.55
f1 (ppm)

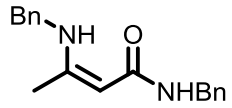

Bn
NH
O
4B3
11.17
7.35
7.34
7.33
7.32
7.32
7.27
7.26
7.26
7.24
5.04
4.46
4.45
2.04
2.03
1.91
0.95
2.00
3.07
1.00
2.10
3.27
3.15
f1 (ppm)
195.41
163.11
138.06
128.82
127.43
126.71
95.92
46.73
28.93
18.91
f1 (ppm)


Bn
NH
O
CF3
4B4
11.43
7.39
7.39
7.39
7.38
7.37
7.36
7.36
7.33
7.32
7.32
7.31
7.30
7.27
7.27
7.27
7.26
5.40
4.56
4.55
2.10
0.91
2.05
1.02
2.21
1.00
2.13
3.07
f1 (ppm)
176.39
176.13
175.87
175.61
169.60
135.95
129.14
128.13
126.97
121.08
118.79
116.50
114.20
89.86
47.60
19.51
f1 (ppm)

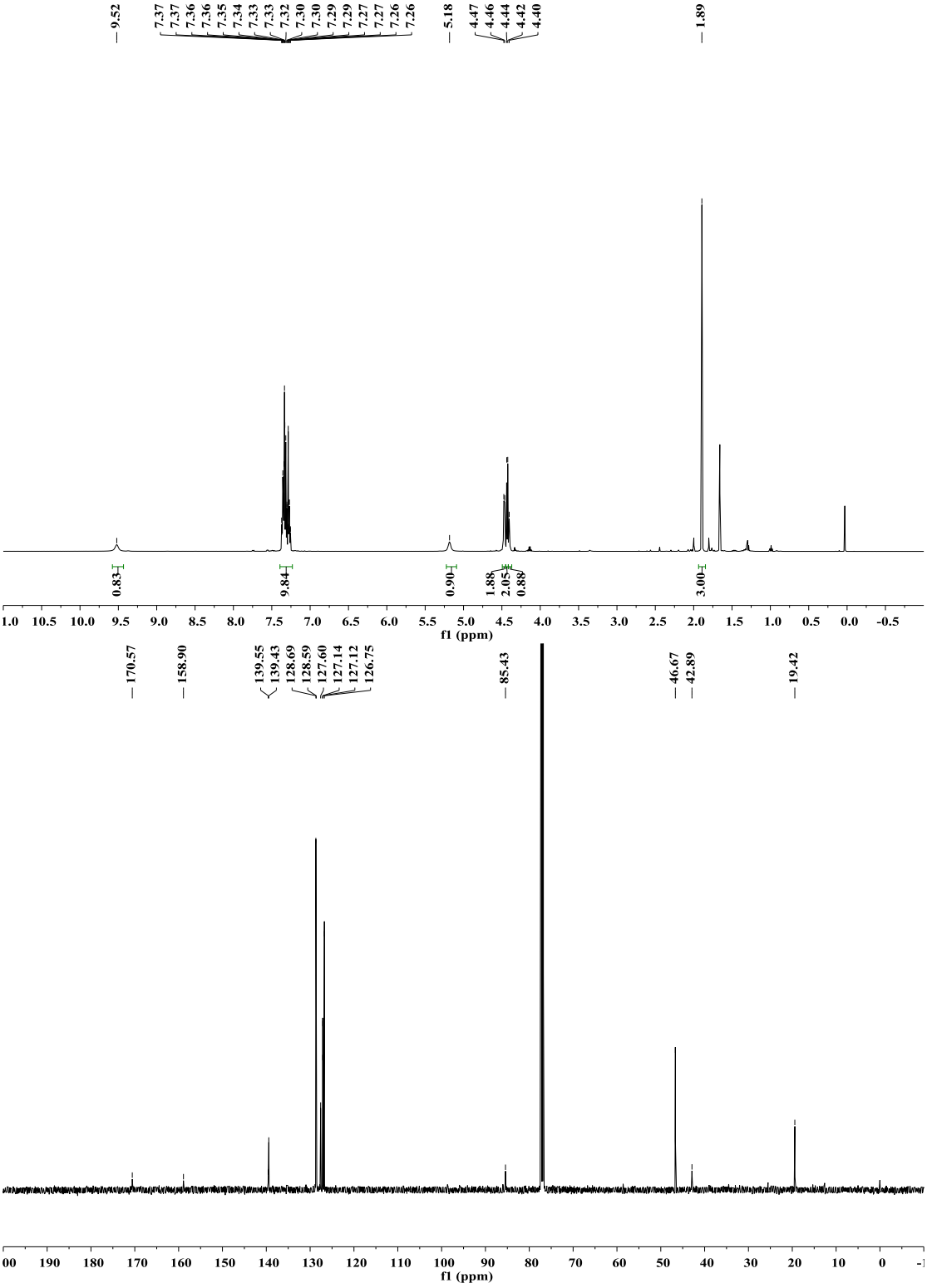

Bn
NH
O
N
Ph
H

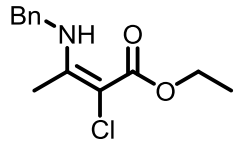
4B$_5$


9.64
7.45
7.43
7.35
7.33
7.32
7.29
7.28
7.26
7.24
7.03
7.02
7.00
6.62
4.49
4.44
4.43
1.91
0.97
2.11
2.20
5.84
1.08
0.98
1.00
2.08
3.14
f1 (ppm)
169.02
160.46
139.08
128.88
128.74
127.23
126.74
122.96
119.81
85.73
46.73
19.52
f1 (ppm)

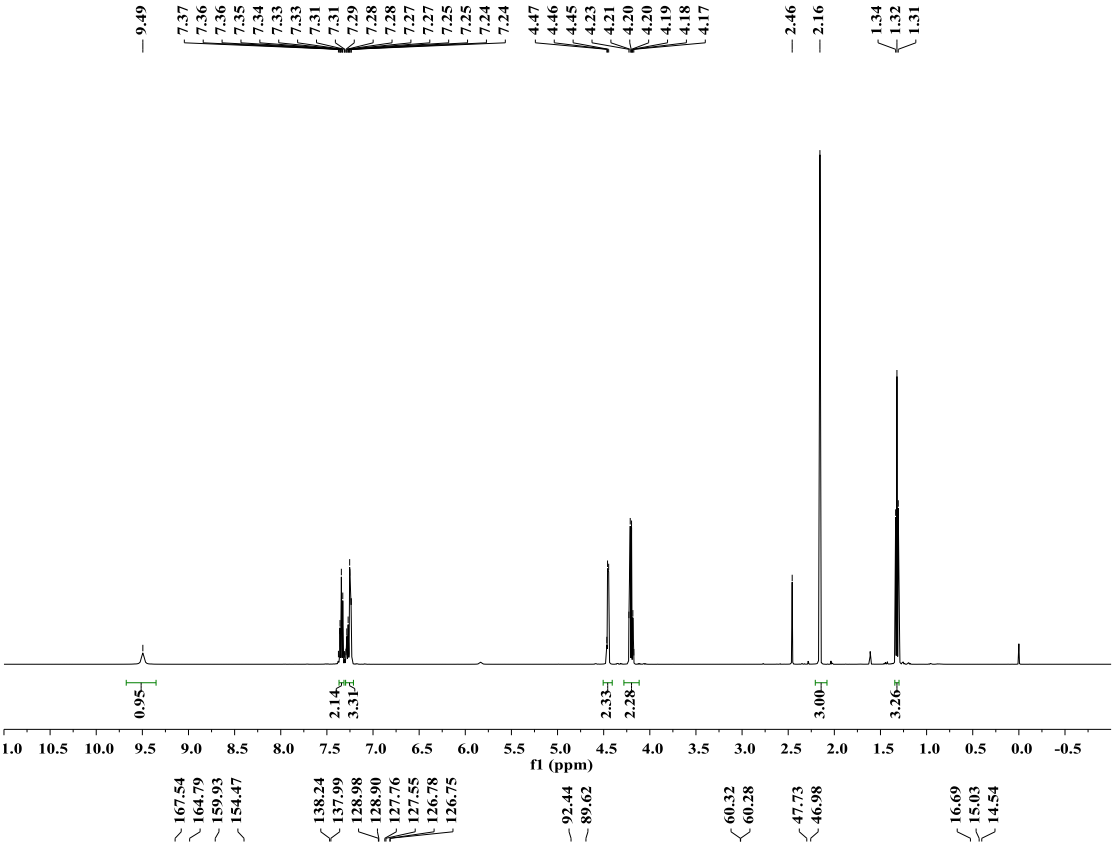

Bn
NH
O
NHBn

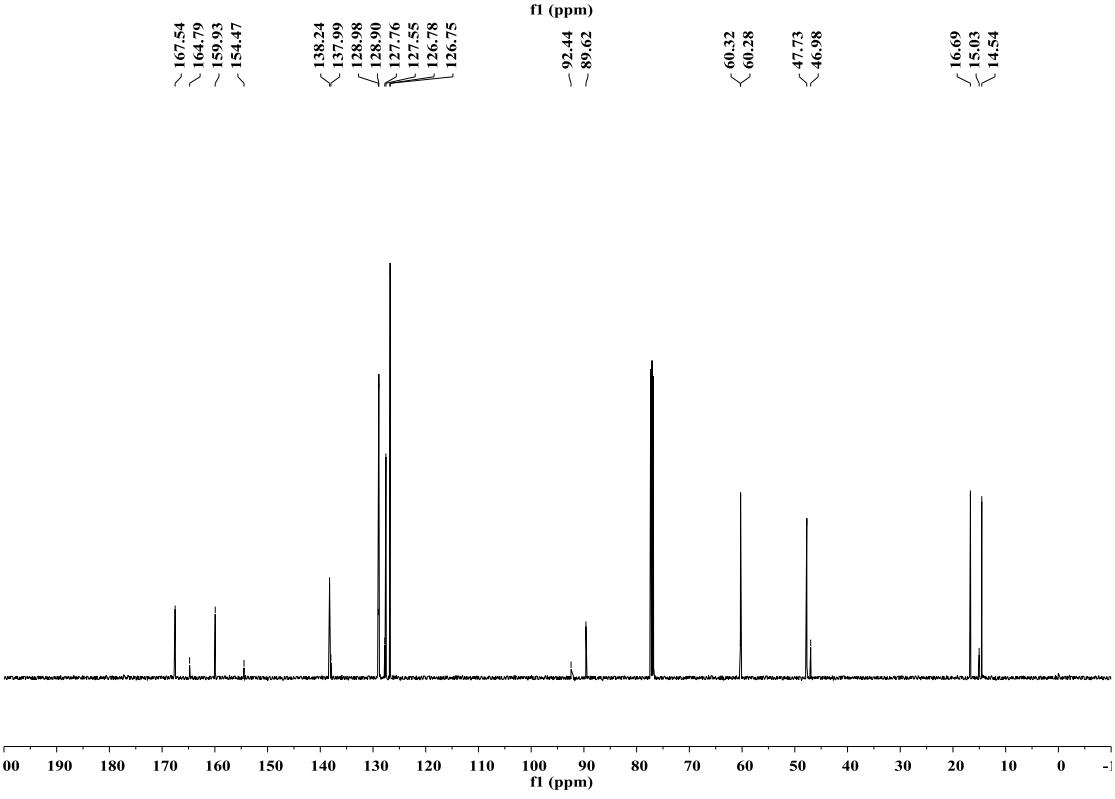
4B$_6$

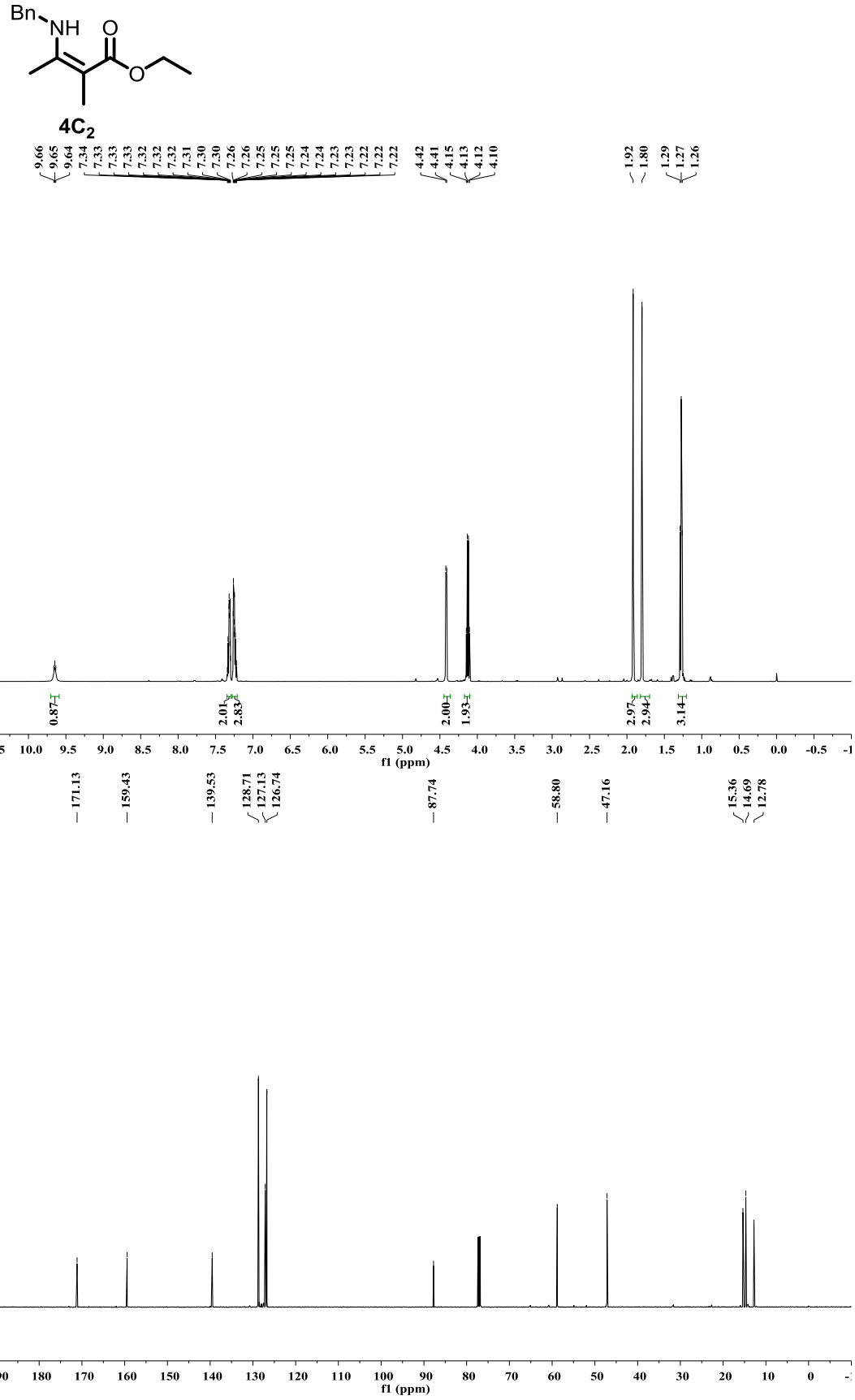

9.52
7.37
7.37
7.36
7.36
7.35
7.34
7.33
7.33
7.32
7.30
7.30
7.29
7.29
7.27
7.27
7.26
7.26
5.18
4.47
4.46
4.44
4.42
4.40
1.89
0.83
9.84
0.90
1.88
2.05
0.88
3.00
f1 (ppm)
170.57
158.90
139.55
139.43
128.69
128.59
127.60
127.14
127.12
126.75
85.43
46.67
42.89
19.42
f1 (ppm)

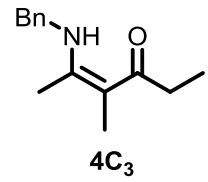

Bn
NH
O
O
Cl

4C$_1$

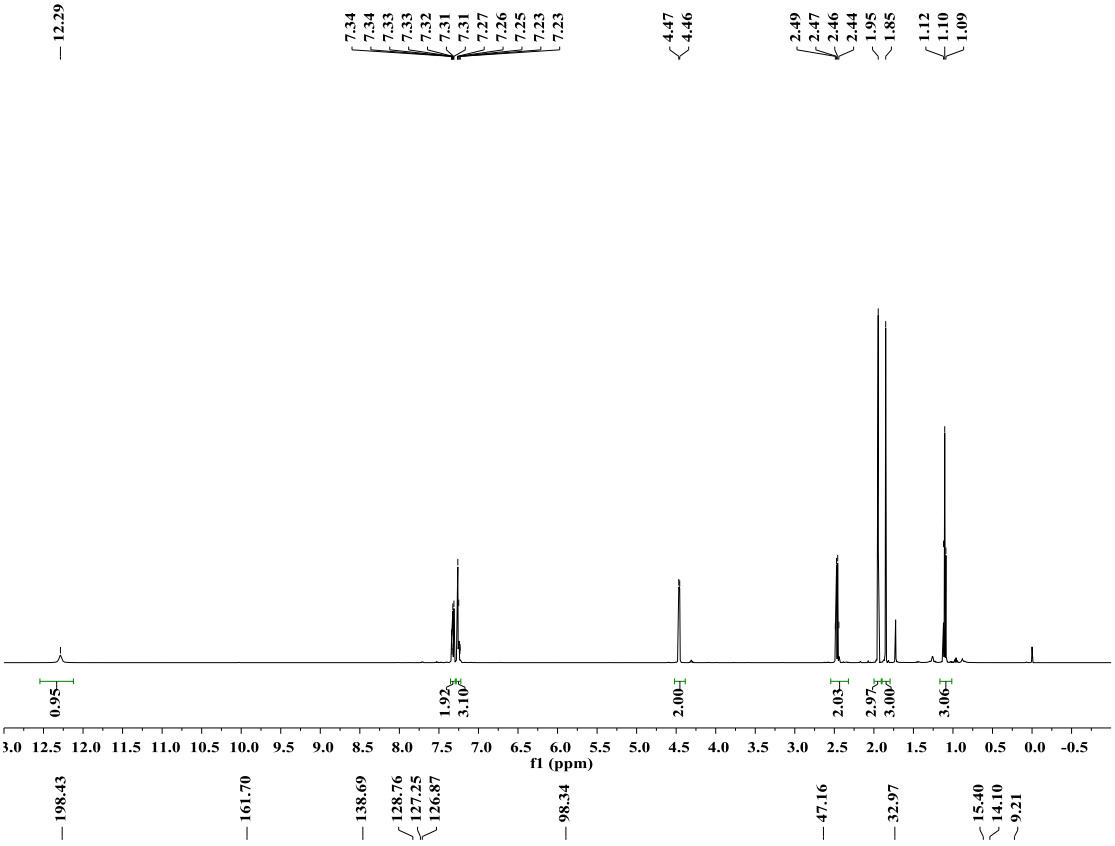

9.49
7.37
7.36
7.36
7.35
7.34
7.33
7.33
7.31
7.31
7.29
7.28
7.28
7.27
7.27
7.25
7.25
7.24
7.24
4.47
4.46
4.45
4.23
4.21
4.20
4.20
4.19
4.18
4.17
2.46
2.16
1.34
1.32
1.31
0.95
2.14
3.31
2.33
2.28
3.00
3.26
f1 (ppm)

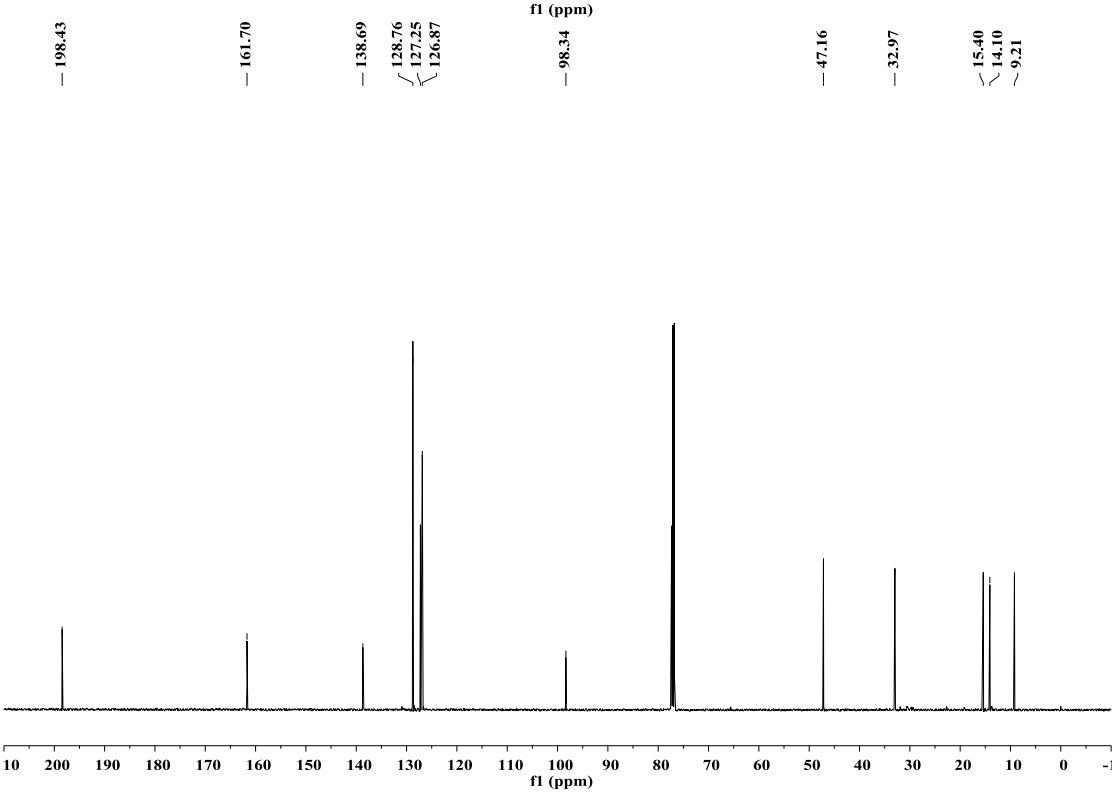

167.54
164.79
159.93
154.47
138.24
137.99
128.98
128.90
127.76
127.55
126.78
126.75
92.44
89.62
60.32
60.28
47.73
46.98
16.69
15.03
14.54
f1 (ppm)

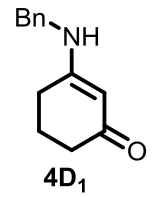

Bn
NH
O
O
4C2
9.66
9.65
9.64
7.34
7.33
7.33
7.33
7.32
7.32
7.32
7.31
7.30
7.30
7.26
7.26
7.25
7.25
7.25
7.24
7.24
7.23
7.23
7.22
7.22
7.22
4.42
4.41
4.15
4.13
4.12
4.10
1.92
1.80
1.29
1.27
1.26
0.87
2.01
2.83
2.00
1.93
2.97
2.94
3.14
f1 (ppm)
171.13
159.43
139.53
128.71
127.13
126.74
87.74
58.80
47.16
15.36
14.69
12.78
f1 (ppm)


Bn
NH
O

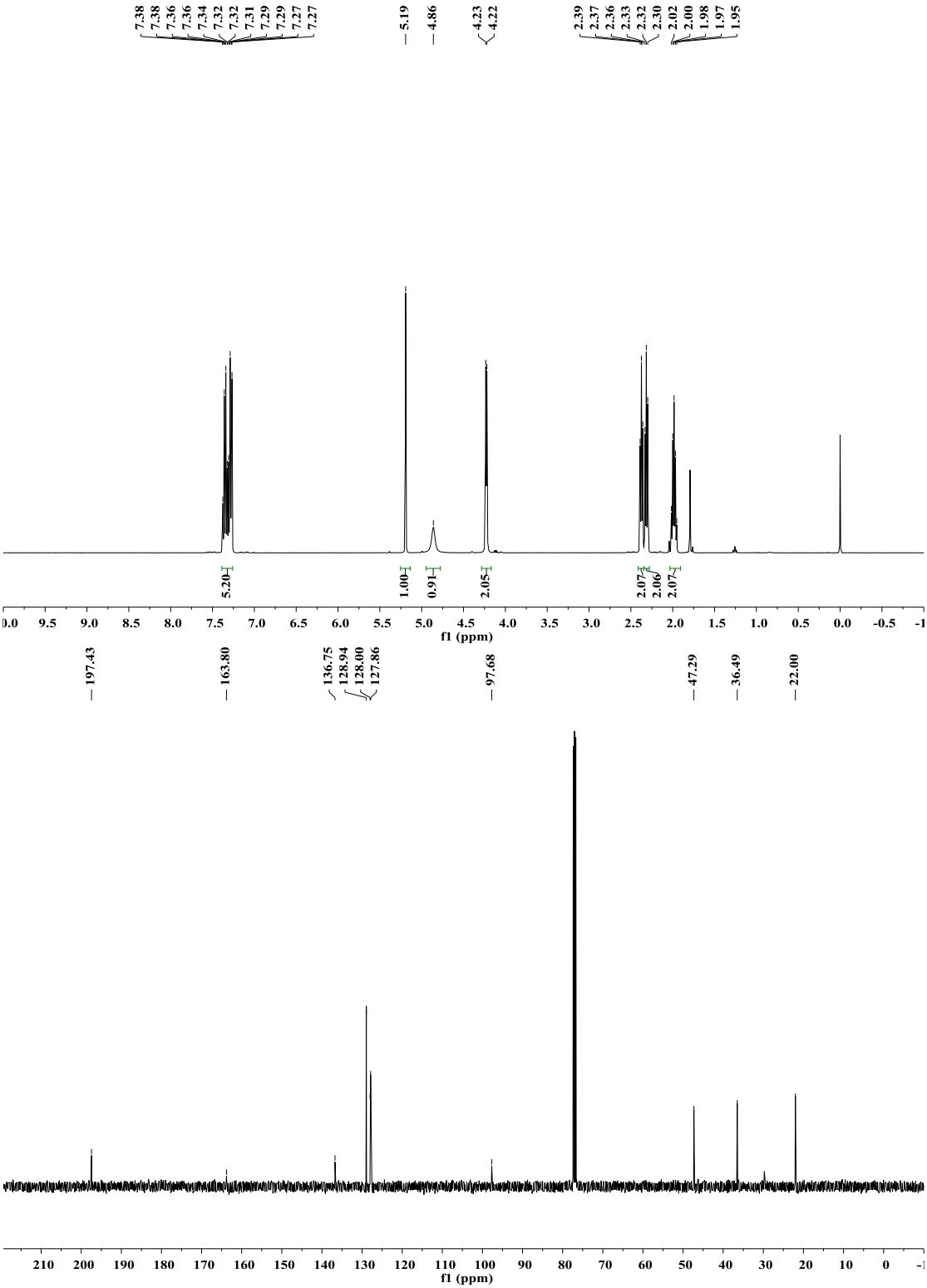
4C$_3$

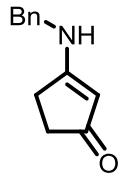

12.29
7.34
7.34
7.33
7.33
7.32
7.31
7.31
7.27
7.26
7.25
7.23
7.23
4.47
4.46
2.49
2.47
2.46
2.44
1.95
1.85
1.12
1.10
1.09
0.95
1.92
3.10
2.00
2.03
2.97
3.00
3.06
f1 (ppm)


198.43
161.70
138.69
128.76
127.25
126.87
98.34
47.16
32.97
15.40
14.10
9.21
f1 (ppm)

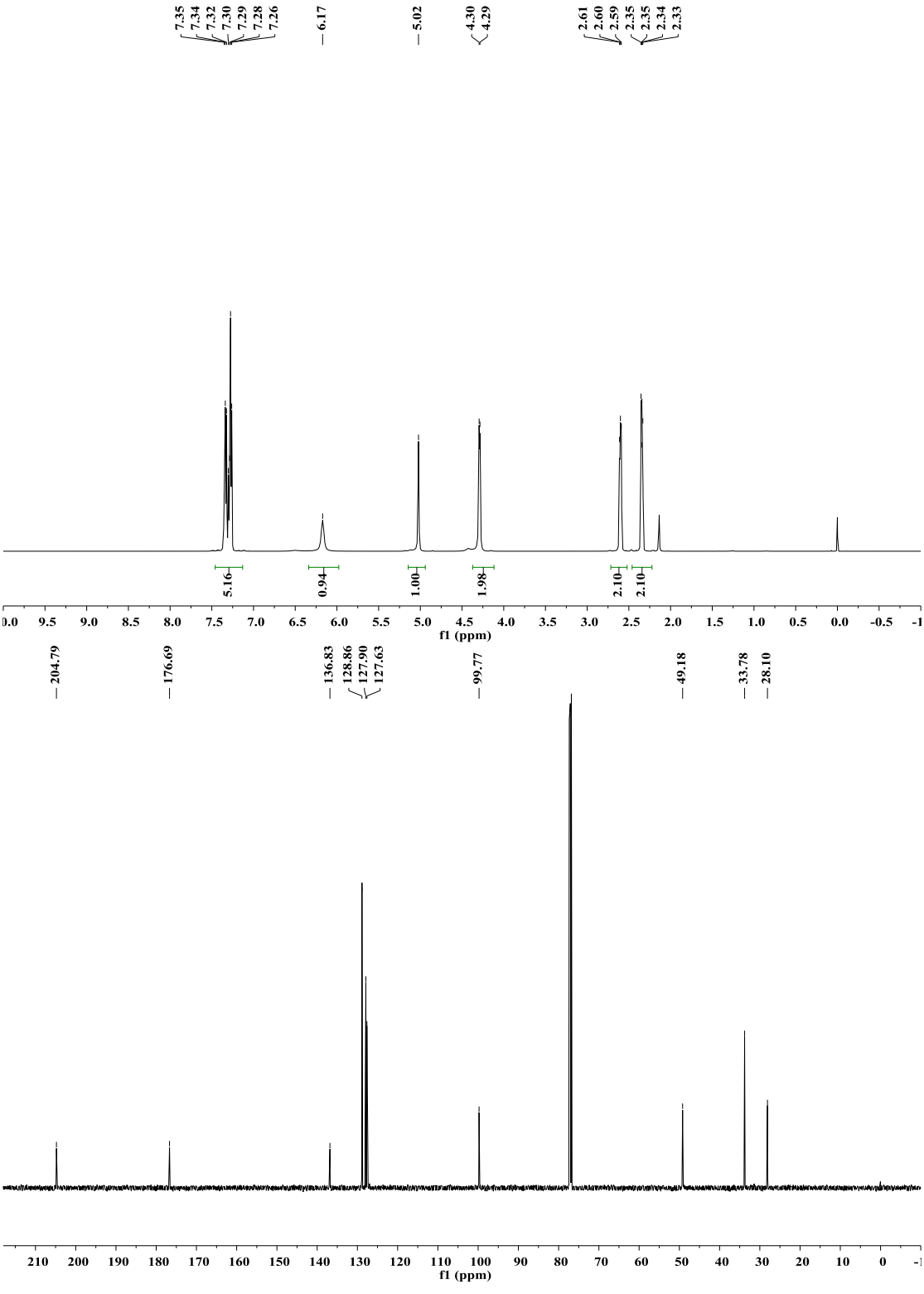

Bn
NH
O

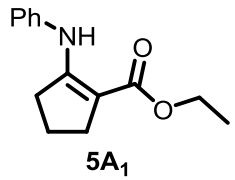
4D$_1$


7.38
7.38
7.36
7.36
7.34
7.32
7.32
7.31
7.29
7.29
7.27
7.27
5.19
4.86
4.23
4.22
2.39
2.37
2.36
2.33
2.32
2.30
2.02
2.00
1.98
1.97
1.95
5.20
1.00
0.91
2.05
2.07
2.06
2.07
f1 (ppm)
197.43
163.80
136.75
128.94
128.00
127.86
97.68
47.29
36.49
22.00
f1 (ppm)

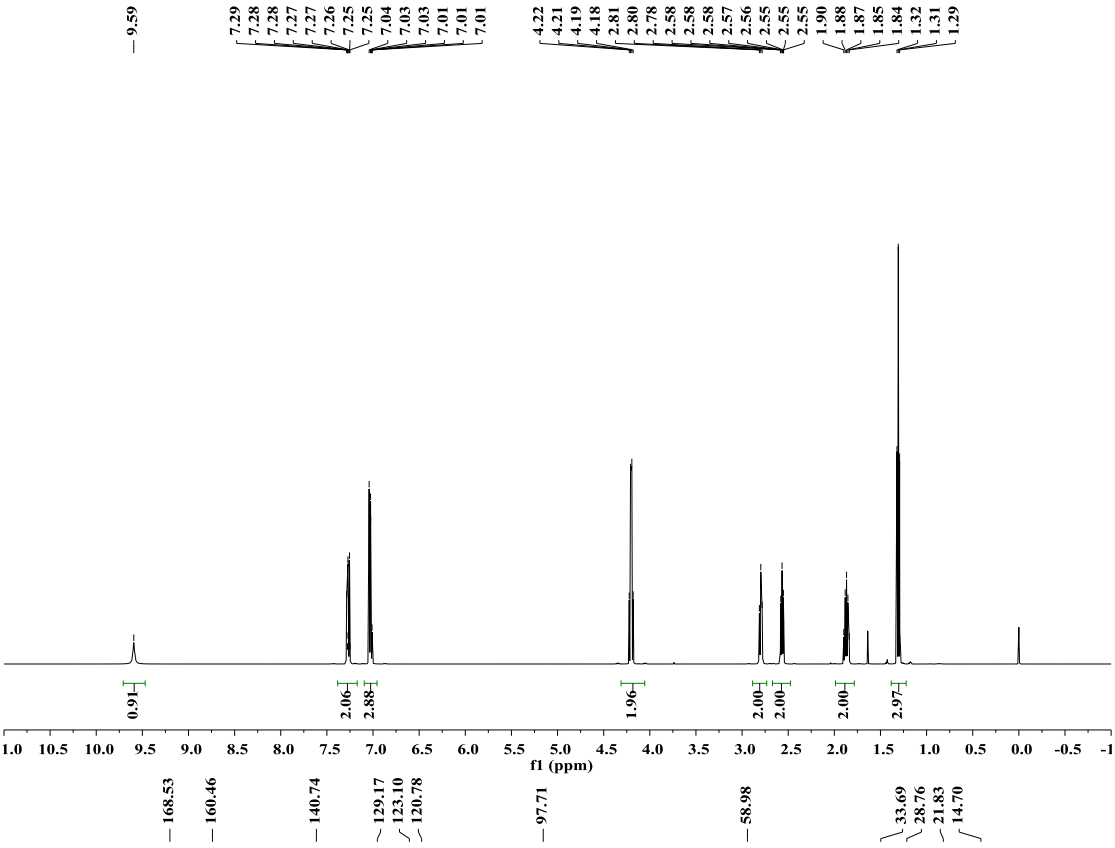

Bn
NH
O

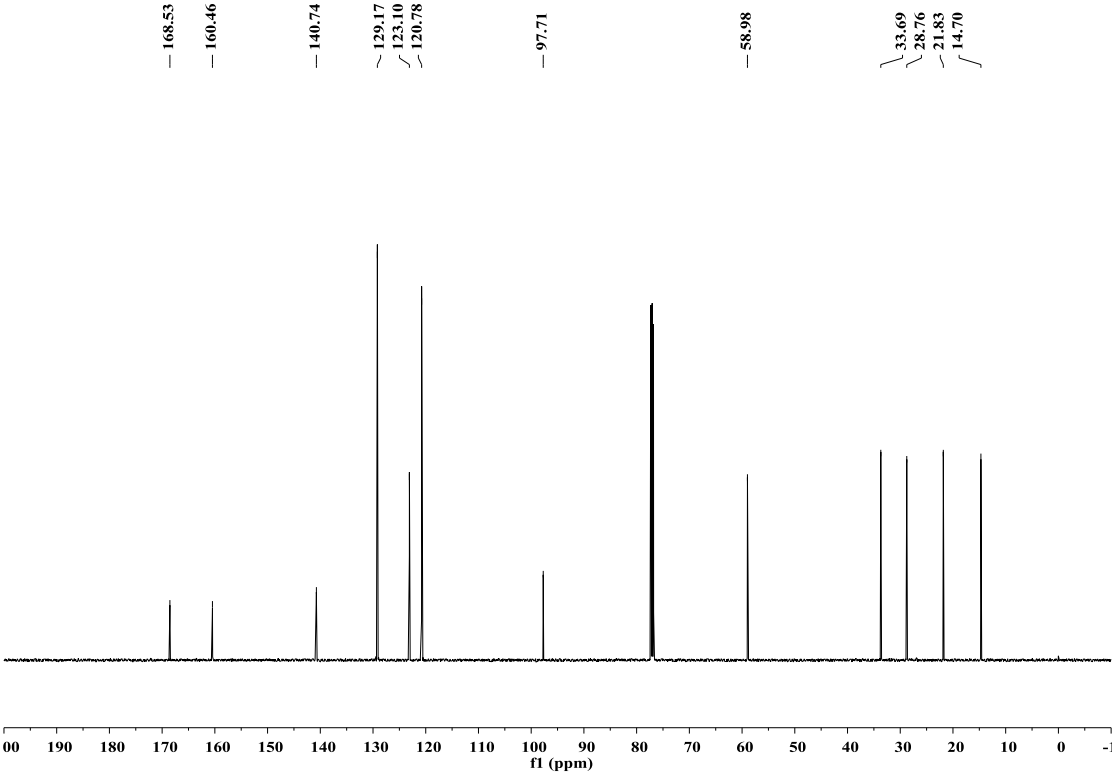
4D$_2$

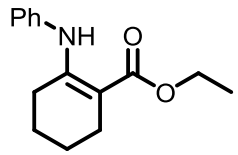

7.35
7.34
7.32
7.30
7.29
7.28
7.26
6.17
5.02
4.30
4.29
2.61
2.60
2.59
2.35
2.35
2.34
2.33
5.16
0.94
1.00
1.98
2.10
2.10
f1 (ppm)
204.79
176.69
136.83
128.86
127.90
127.63
99.77
49.18
33.78
28.10
f1 (ppm)


Ph
NH
O
O

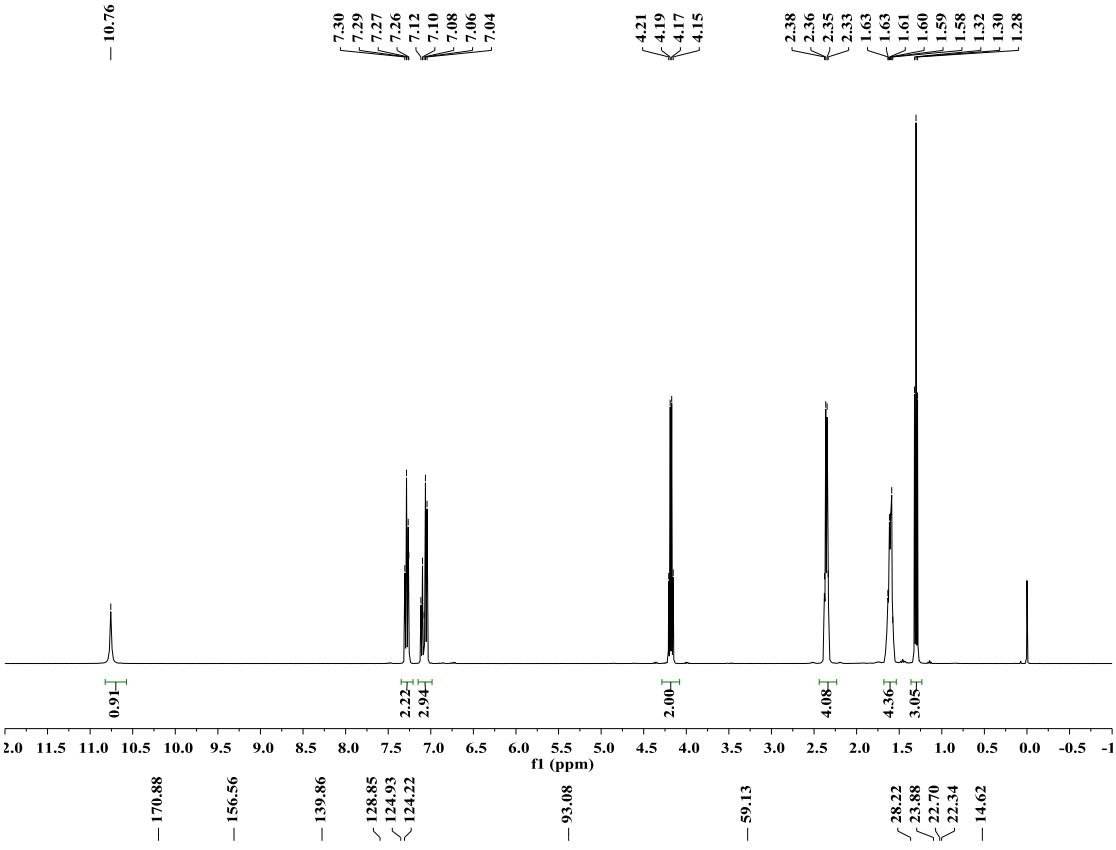
5A$_1$

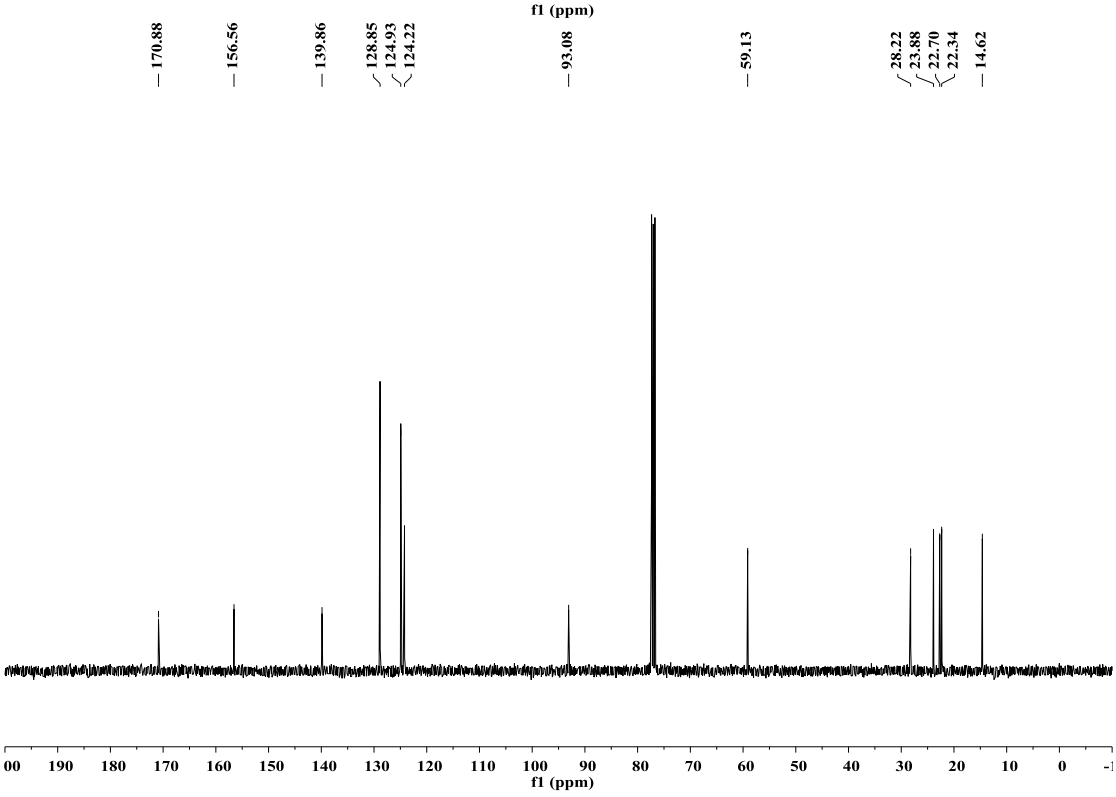

9.59
7.29 7.28 7.28 7.27 7.27 7.26 7.25 7.25 7.04 7.03 7.03 7.01 7.01 7.01
4.22 4.21 4.19 4.18 2.81 2.80 2.78 2.58 2.58 2.58 2.57 2.56 2.55 2.55 2.55
1.90 1.88 1.87 1.85 1.84 1.32 1.31 1.29
0.91 2.06 2.88 1.96 2.00 2.00 2.00 2.97
f1 (ppm)

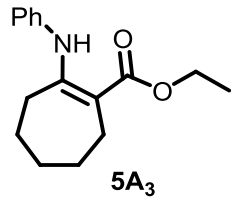

168.53
160.46
140.74
129.17
123.10
120.78
97.71
58.98
33.69
28.76
21.83
14.70
f1 (ppm)


Ph
NH
O
O

5A$_2$

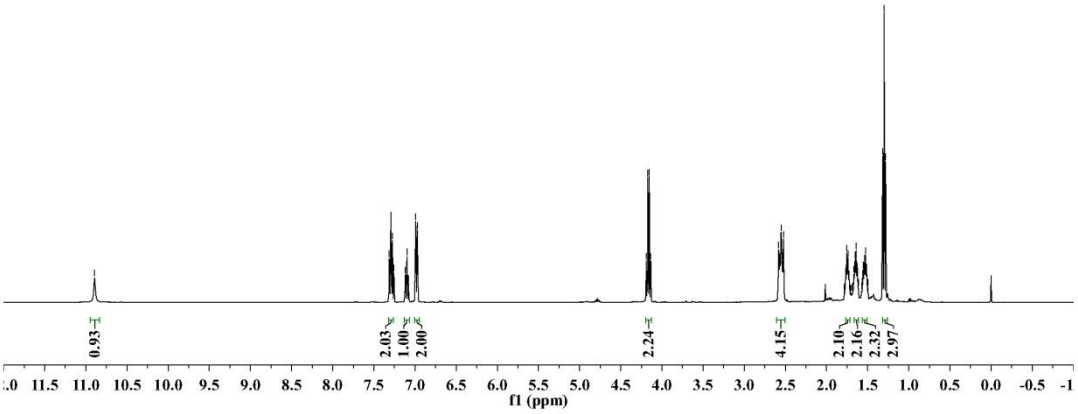

10.76
7.30
7.29
7.27
7.26
7.12
7.10
7.08
7.06
7.04
4.21
4.19
4.17
4.15
2.38
2.36
2.35
2.33
1.63
1.63
1.61
1.60
1.59
1.58
1.32
1.30
1.28
0.91
2.22
2.94
2.00
4.08
4.36
3.05
f1 (ppm)

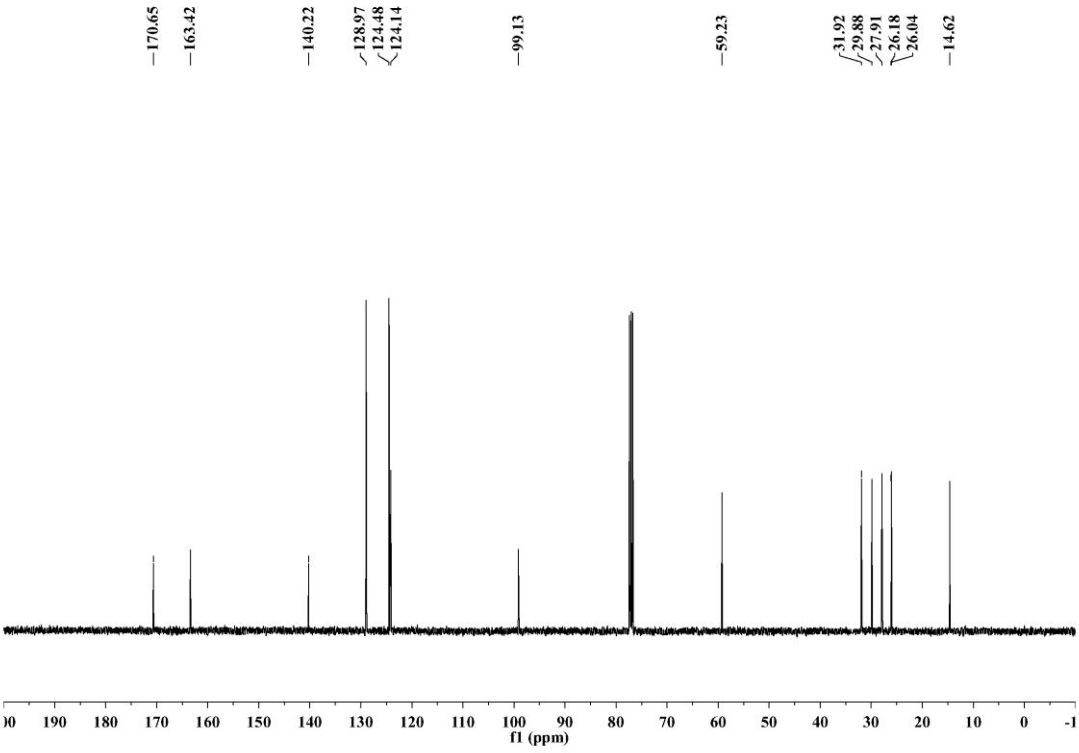

170.88
156.56
139.86
128.85
124.93
124.22
93.08
59.13
28.22
23.88
22.70
22.34
14.62
f1 (ppm)

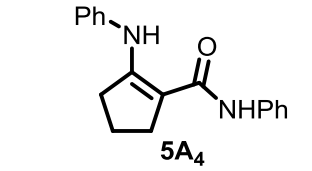

Ph
NH
O
O

5A$_3$

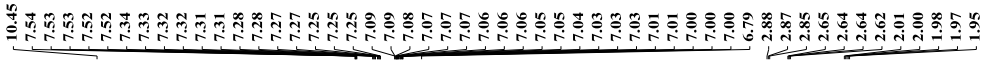

10.89
7.31
7.31
7.29
7.29
7.28
7.27
7.26
7.12
7.12
7.11
7.10
7.10
7.09
7.08
7.08
6.99
6.99
6.98
6.97
6.97
4.19
4.17
4.15
4.14
2.58
2.57
2.57
2.56
2.55
2.55
2.53
2.52
1.77
1.77
1.76
1.75
1.74
1.73
1.72
1.67
1.65
1.64
1.63
1.62
1.61
1.57
1.56
1.55
1.55
1.54
1.54
1.52
1.51
1.50
1.32
1.30
1.28


0.93
2.03
1.00
2.00
2.24
4.15
2.10
2.16
2.32
2.97
f1 (ppm)


170.65
163.42
140.22
128.97
124.48
124.14
99.13
59.23
31.92
29.88
27.91
26.18
26.04
14.62
f1 (ppm)


Ph
NH
O
NHPh

5A$_4$


10.45
7.54
7.53
7.53
7.52
7.52
7.34
7.33
7.32
7.32
7.31
7.31
7.28
7.28
7.27
7.27
7.25
7.25
7.25
7.09
7.09
7.08
7.07
7.07
7.07
7.06
7.06
7.06
7.05
7.05
7.04
7.03
7.03
7.03
7.01
7.01
7.00
7.00
7.00
6.79
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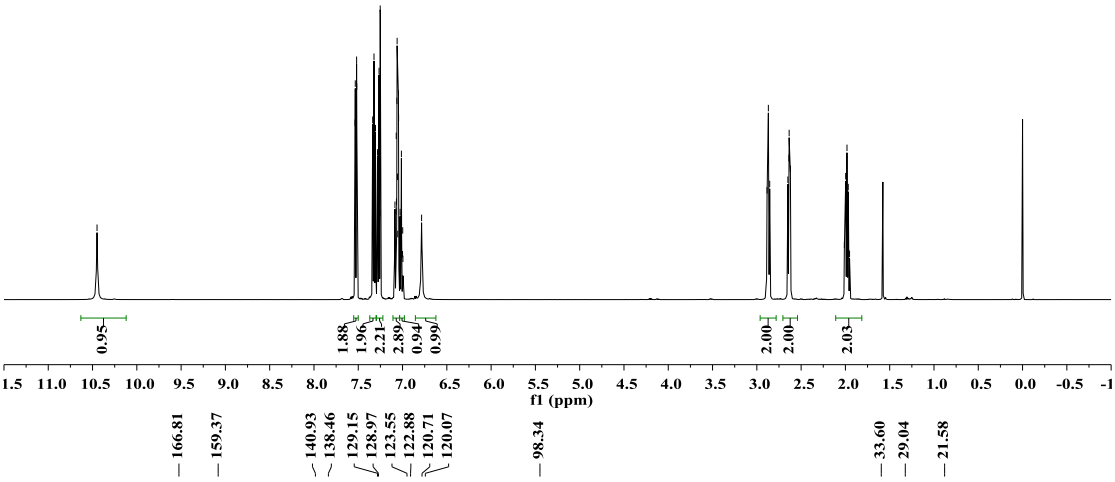
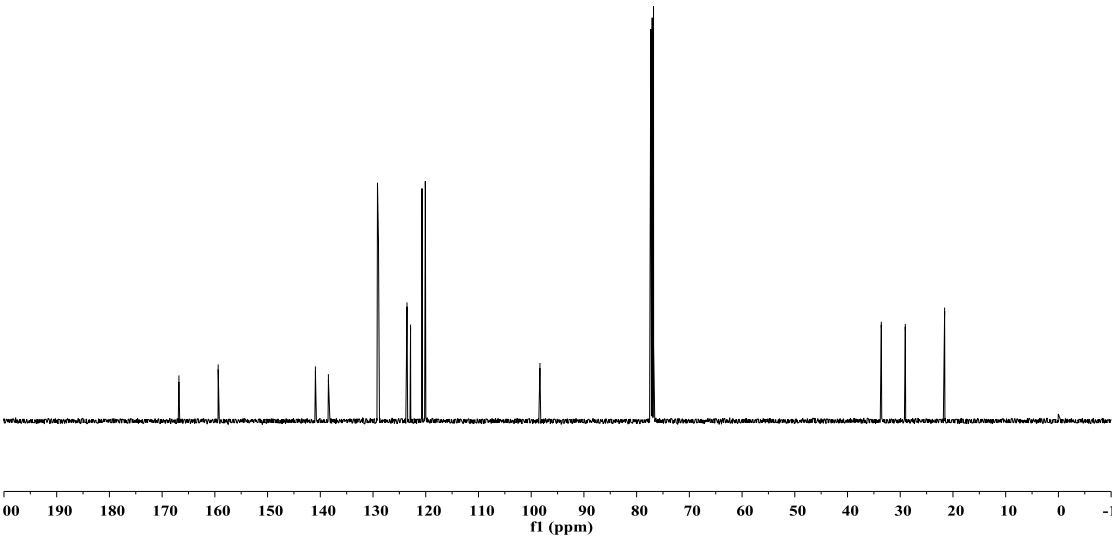
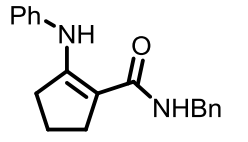
2.62
2.01
2.00
1.98
1.97
1.95

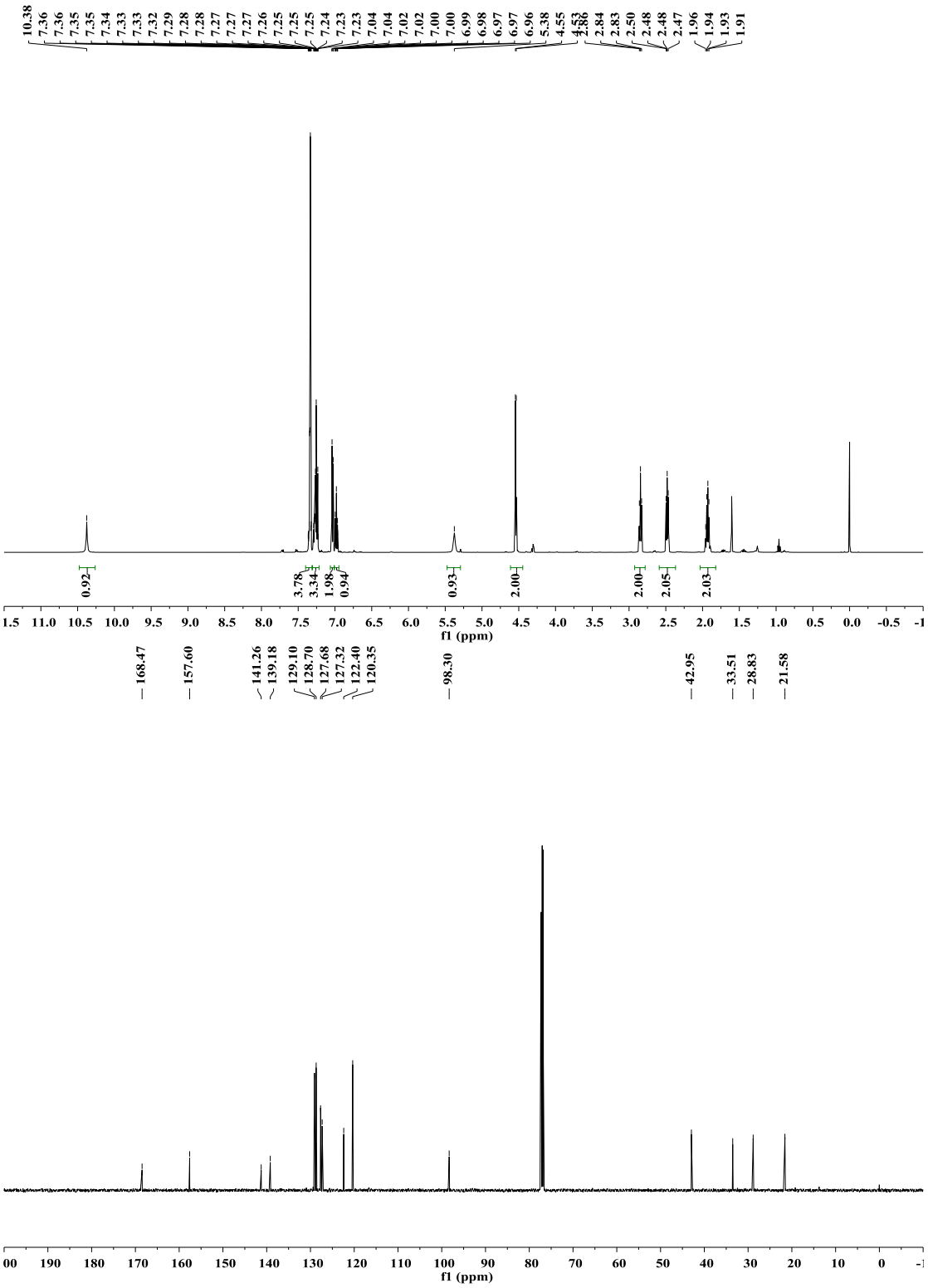

0.95
1.88
1.96
2.21
2.89
0.94
0.99
2.00
2.00
2.03
f1 (ppm)

166.81
159.37
140.93
138.46
129.15
128.97
123.55
122.88
120.71
120.07
98.34
33.60
29.04
21.58


f1 (ppm)


Ph
NH
O
NHBn

5A$_5$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7.36
7.36
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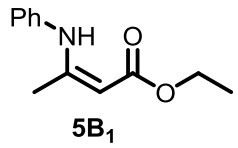
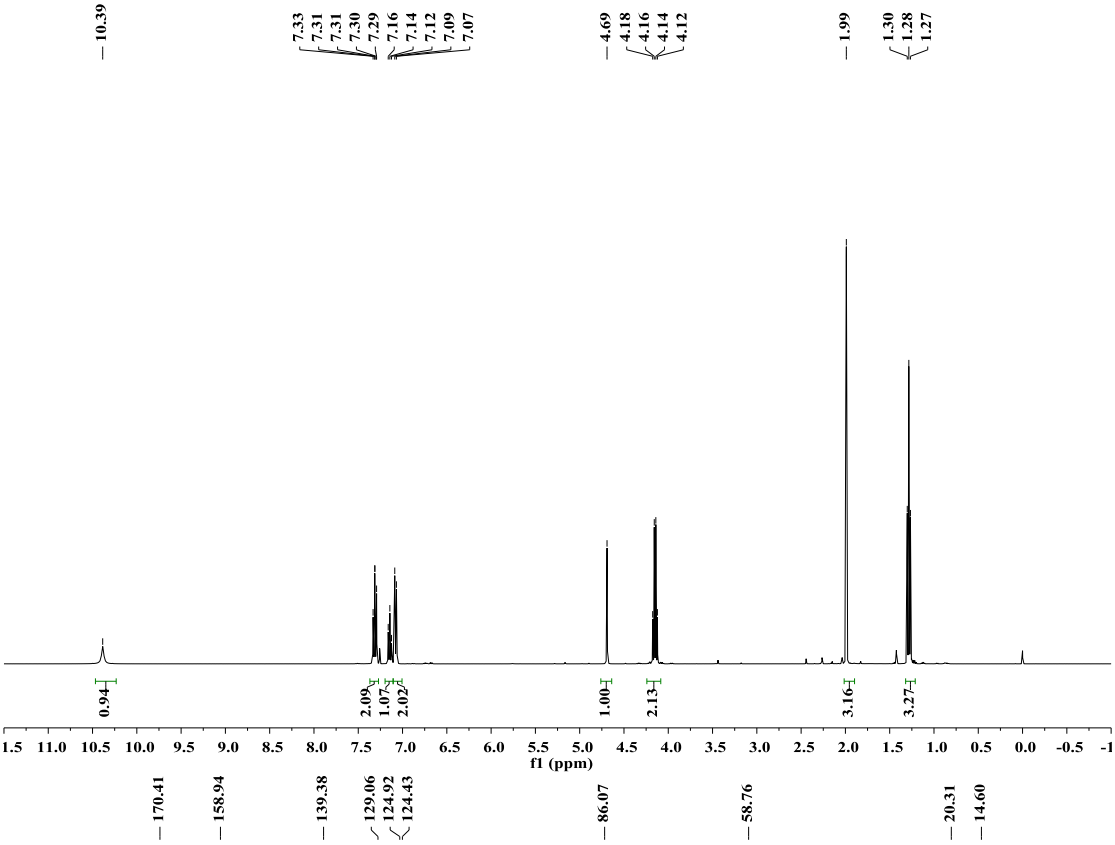
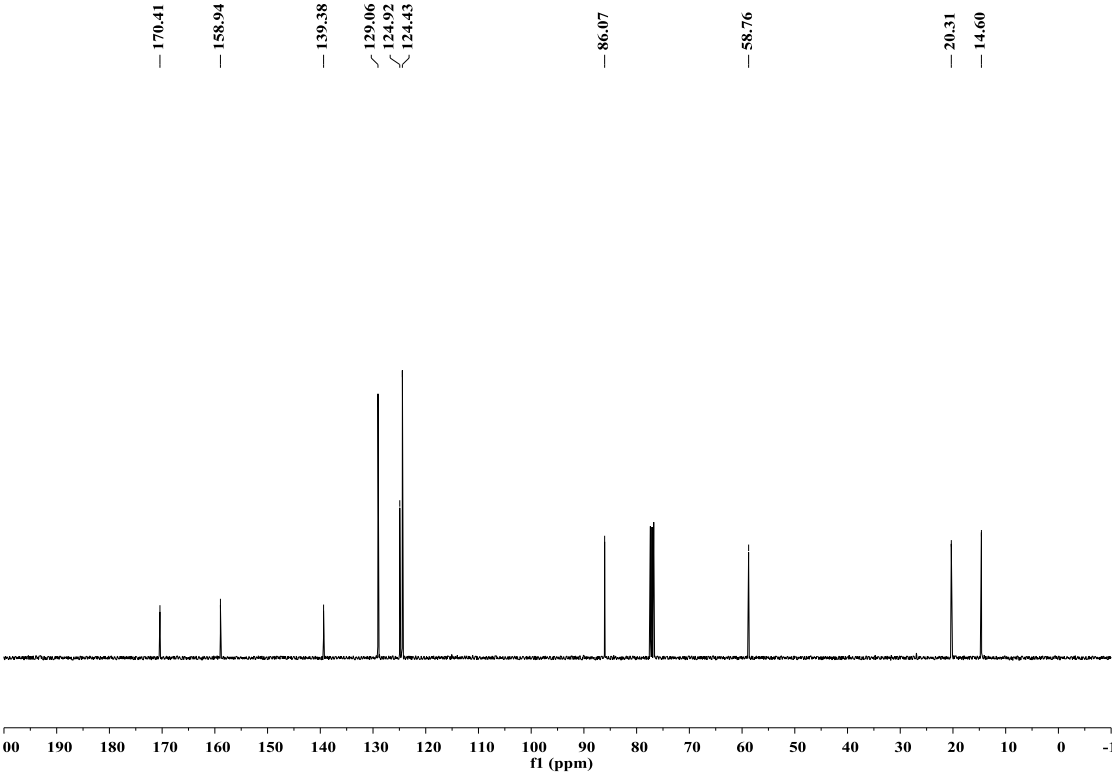
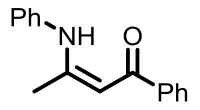
7.35
7.34
7.33
7.33
7.32
7.29
7.28
7.28
7.27
7.27
7.27
7.26
7.25
7.25
7.25
7.24
7.23
7.23
7.04
7.04
7.02
7.02
7.00
7.00
6.99
6.98
6.97
6.97
6.96
5.38
4.55
2.86
2.84
2.83
2.50
2.48
2.48
2.47
1.96
1.94
1.93
1.91
0.92
3.78
3.34
1.98
0.94
0.93
2.00
2.00
2.05
2.03
f1 (ppm)
168.47
157.60
141.26
139.18
129.10
128.70
127.68
127.32
122.40
120.35
98.30
42.95
33.51
28.83
21.58
f1 (ppm)


Ph
NH
O
O

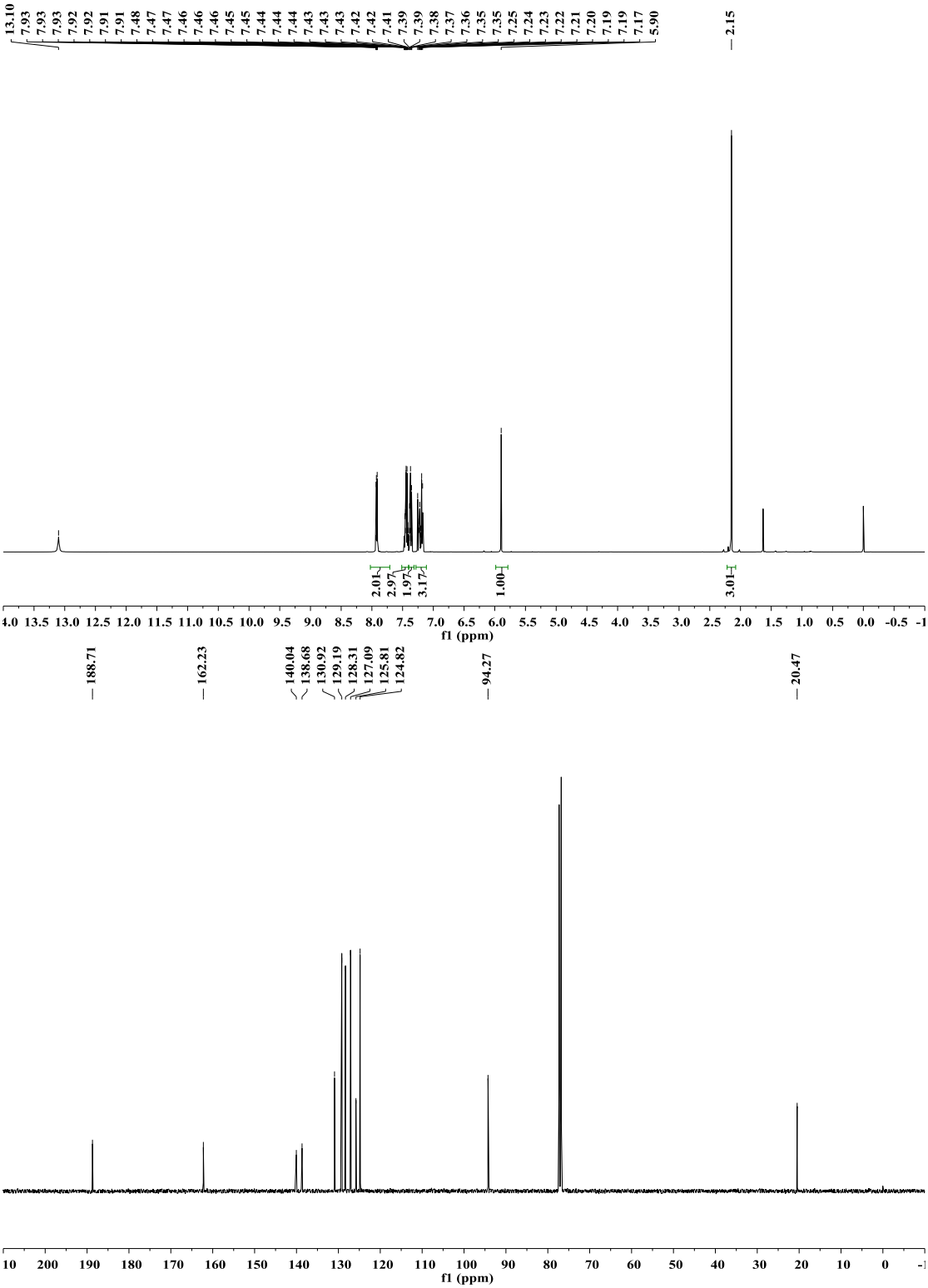
5B$_1$

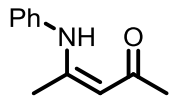

10.39
7.33
7.31
7.31
7.30
7.29
7.16
7.14
7.12
7.09
7.07
4.69
4.18
4.16
4.14
4.12
1.99
1.30
1.28
1.27
0.94
2.09
1.07
2.02
1.00
2.13
3.16
3.27
f1 (ppm)


170.41
158.94
139.38
129.06
124.92
124.43
86.07
58.76
20.31
14.60
f1 (ppm)

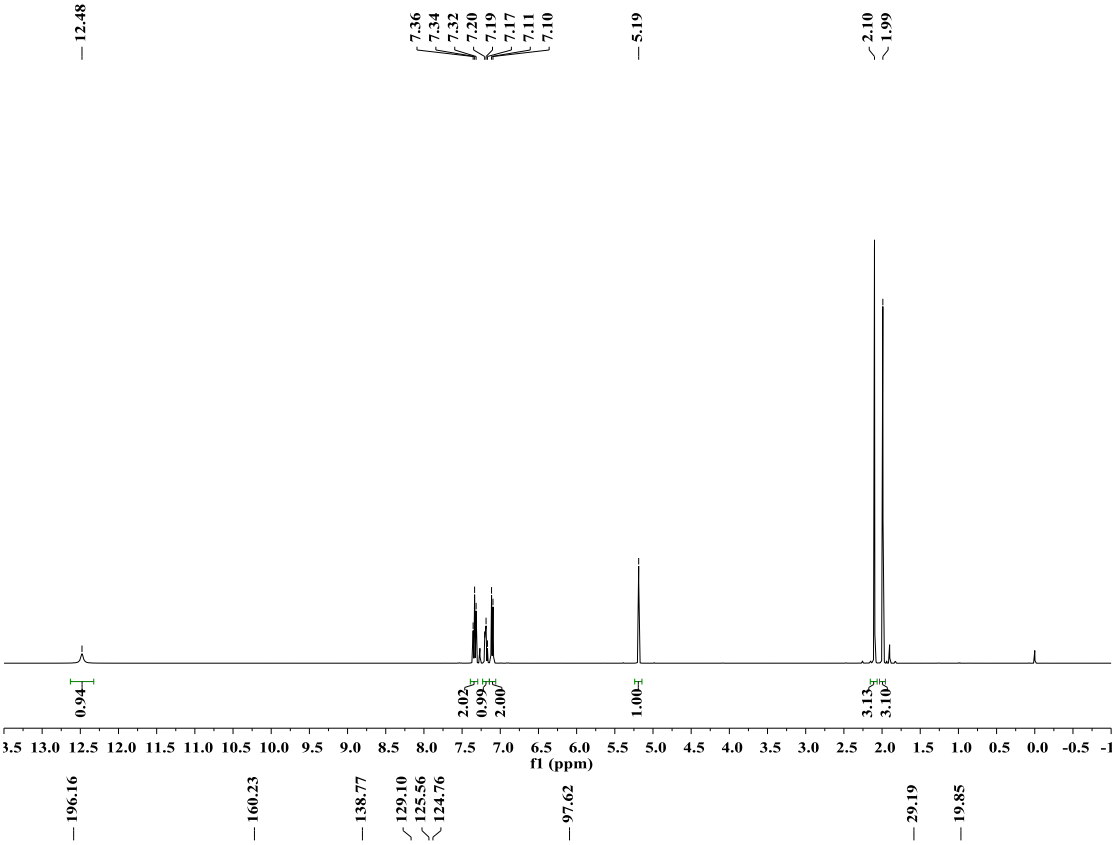

Ph
NH
O
Ph

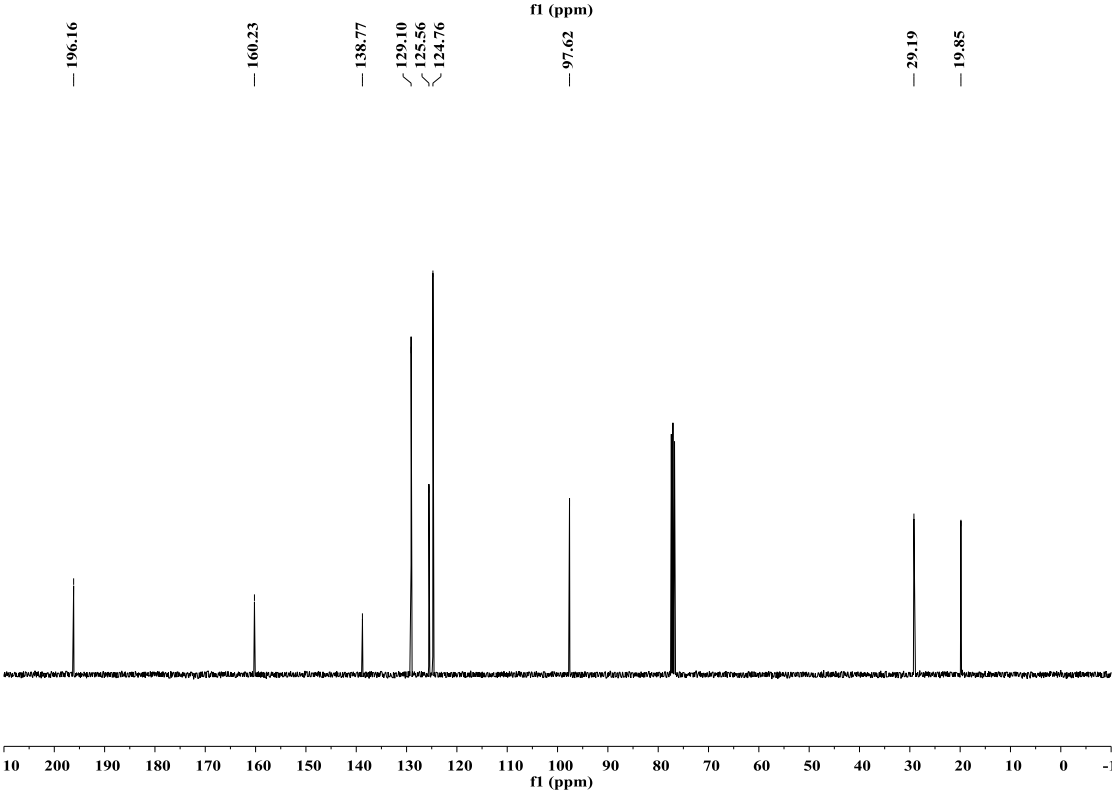
5B$_2$

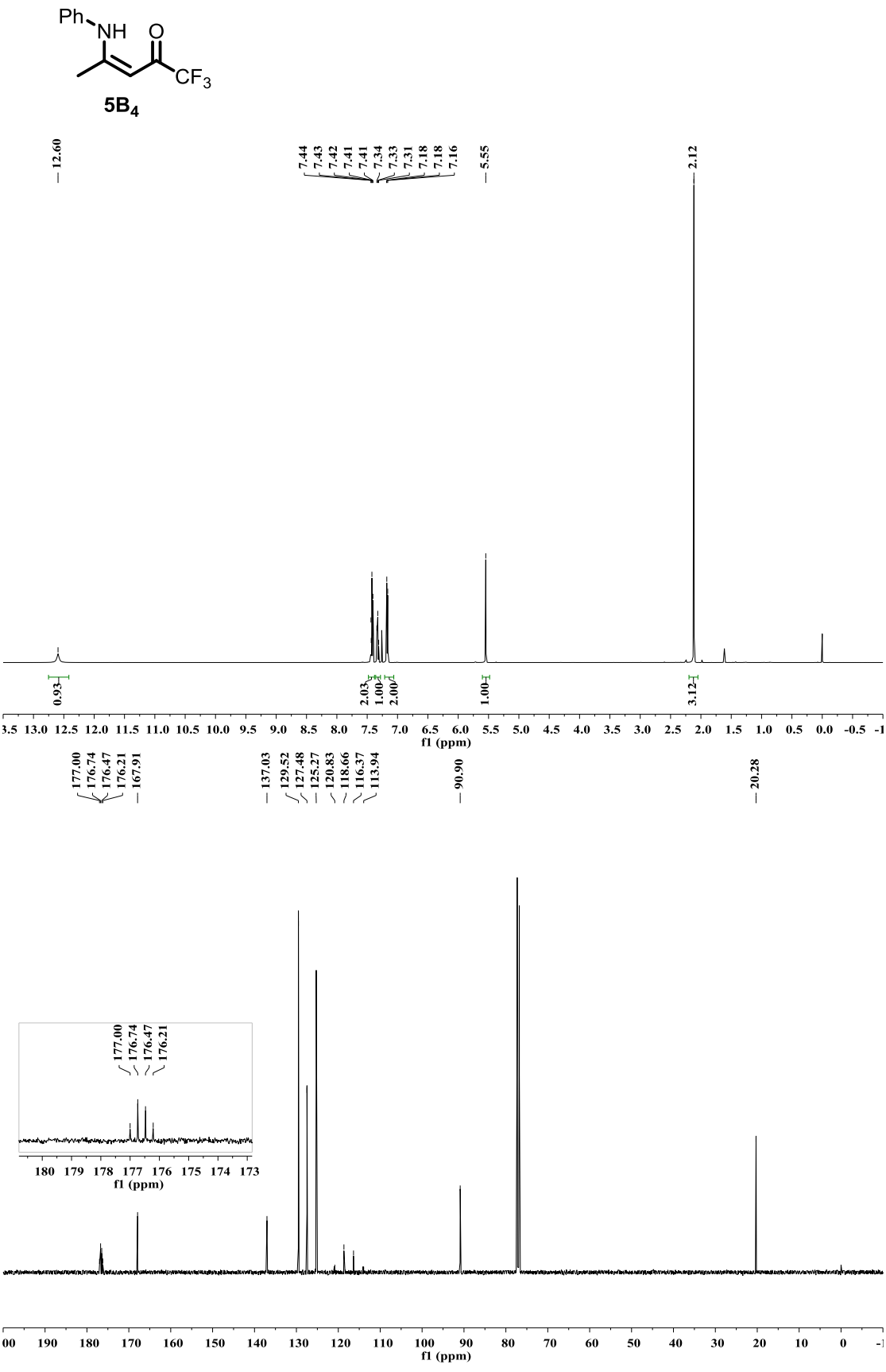

13.10
7.93
7.93
7.93
7.92
7.92
7.91
7.91
7.48
7.47
7.47
7.46
7.46
7.46
7.45
7.45
7.44
7.44
7.44
7.43
7.43
7.43
7.42
7.42
7.41
7.39
7.39
7.38
7.37
7.36
7.35
7.35
7.25
7.24
7.23
7.22
7.21
7.20
7.19
7.19
7.17
5.90
2.15
2.01
2.97
1.97
3.17
1.00
3.01
f1 (ppm)
188.71
162.23
140.04
138.68
130.92
129.19
128.31
127.09
125.81
124.82
94.27
20.47
f1 (ppm)


Ph
NH
O

5B$_3$


12.48
7.36
7.34
7.32
7.20
7.19
7.17
7.11
7.10
5.19
2.10
1.99
0.94
2.02
0.99
2.00
1.00
3.13
3.10
f1 (ppm)


196.16
160.23
138.77
129.10
125.56
124.76
97.62
29.19
19.85
f1 (ppm)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7.31
7.18
7.18
7.16
5.55
2.12
0.93
2.03
1.00
2.00
1.00
3.12
f1 (ppm)
177.00
176.74
176.47
176.21
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137.03
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113.94
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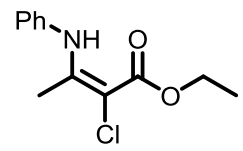
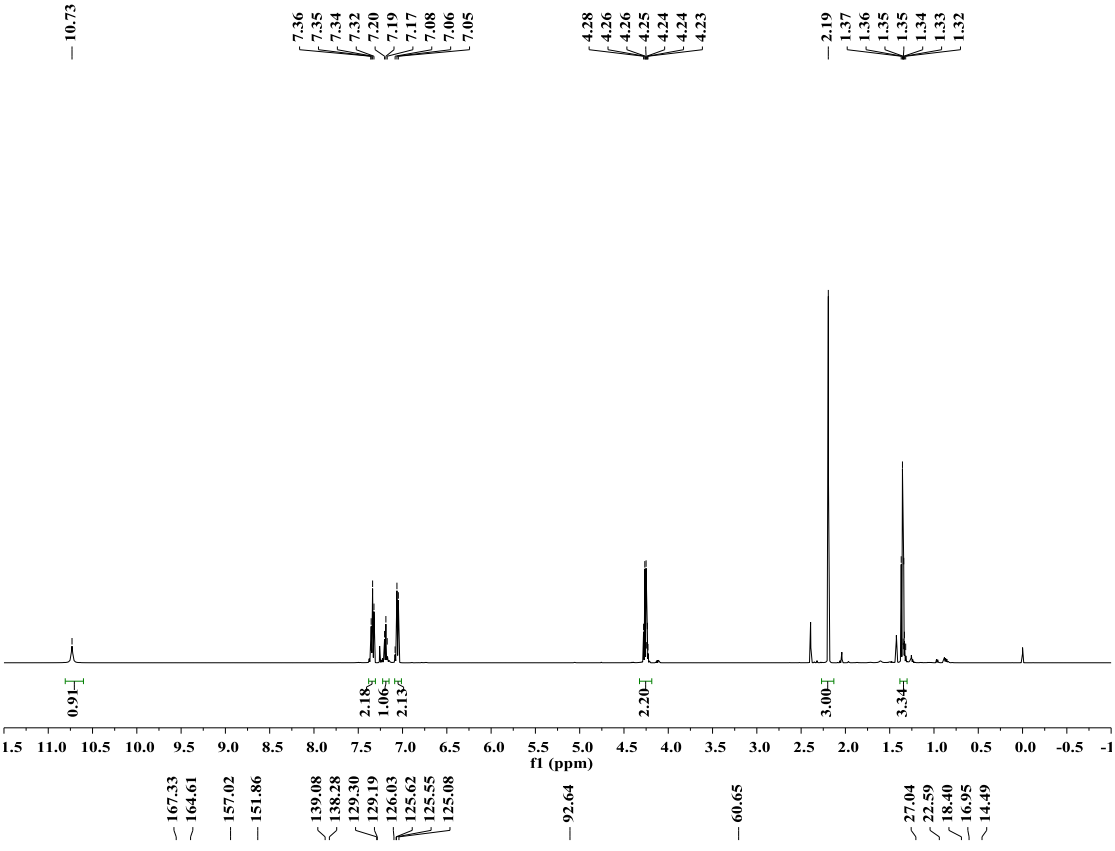
20.28
f1 (ppm)


Ph
NH
O
O
Cl

5C$_1$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4.26
4.25
4.24
4.24
4.23
2.19
1.37
1.36
1.35
1.35
1.34
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1.06
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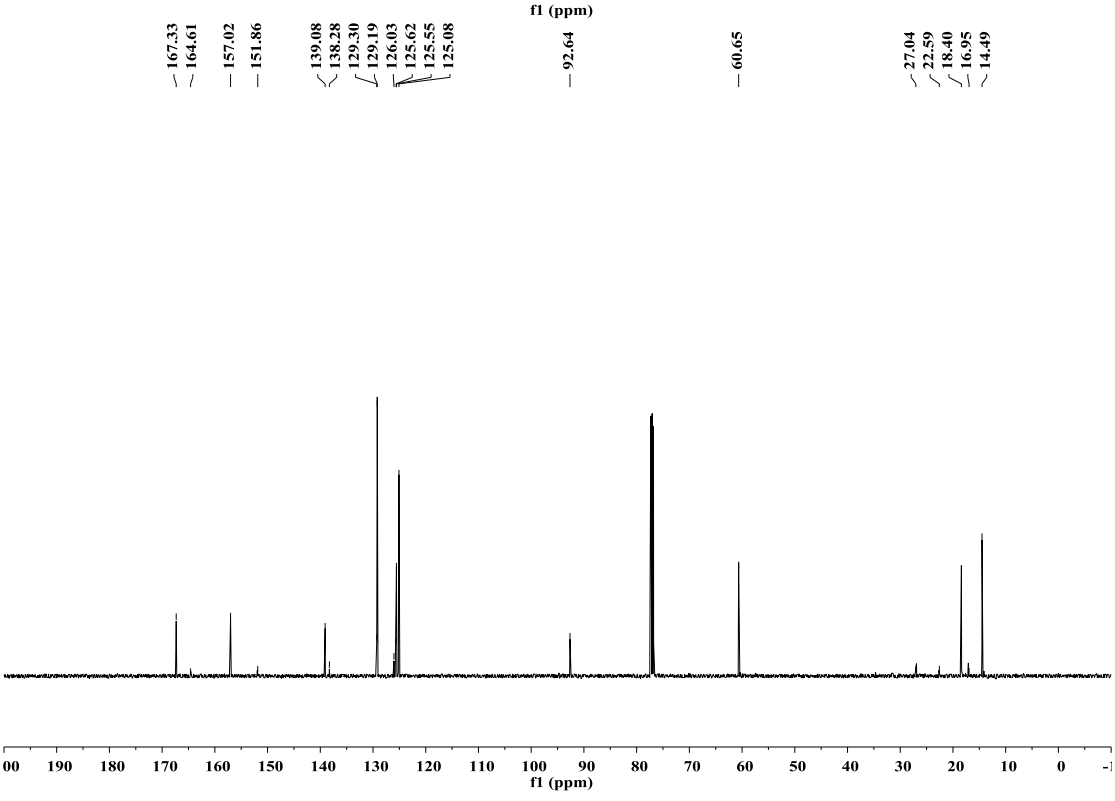
2.20
3.00
3.34
f1 (ppm)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18.40
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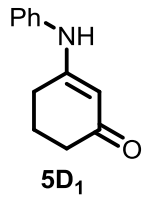
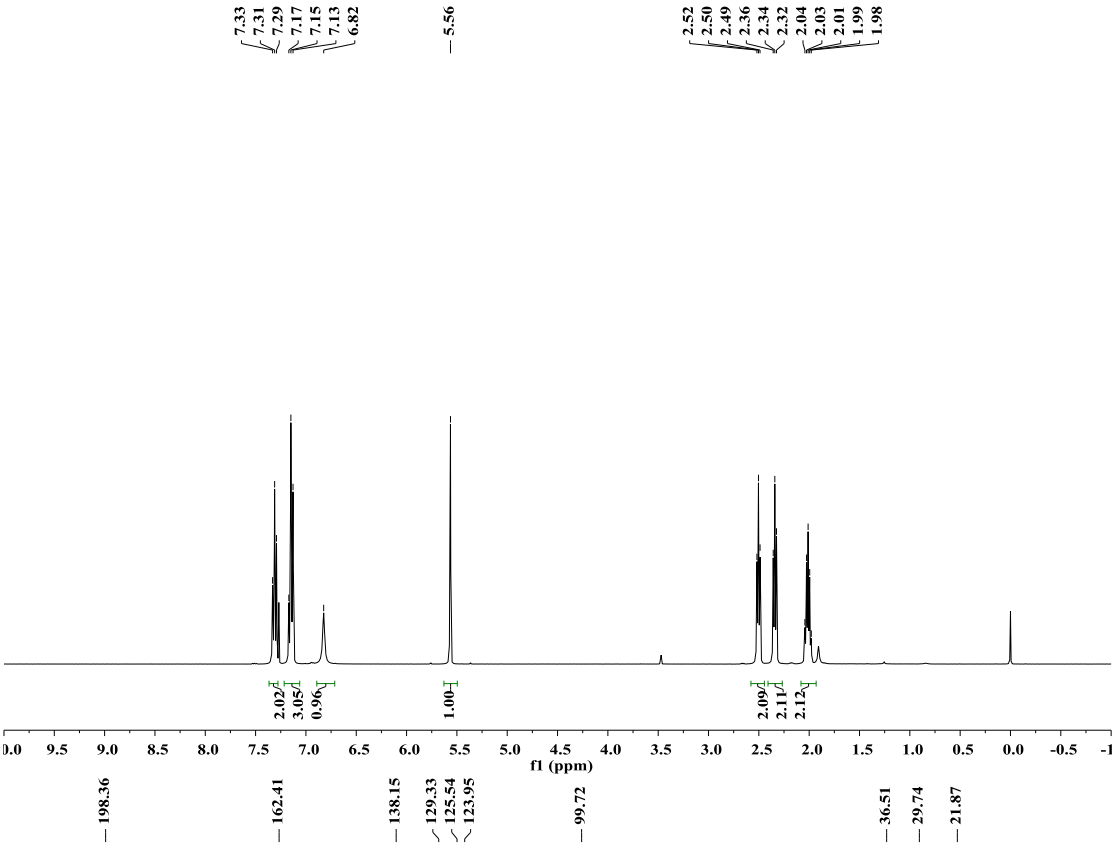
14.49
f1 (ppm)


Ph
NH
O

5D$_1$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7.17
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2.34
2.32
2.04
2.03
2.01
1.99
1.98
2.02
3.05
0.96
1.00
2.09
2.11
2.12
f1 (ppm)
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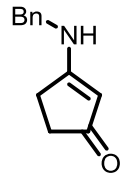
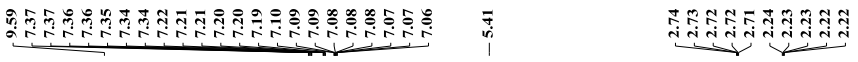

Bn
NH
O

4D$_2$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7.20
7.19
7.10
7.09
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7.08
7.08
7.08
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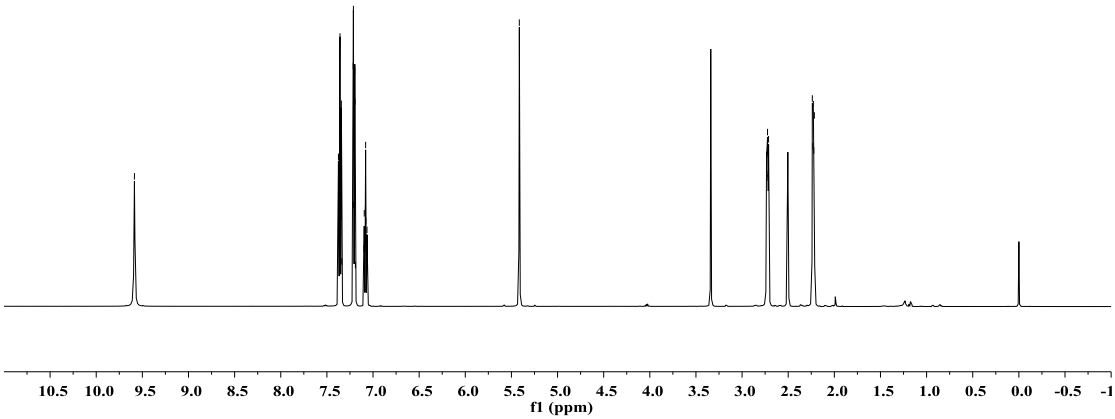
2.22
2.22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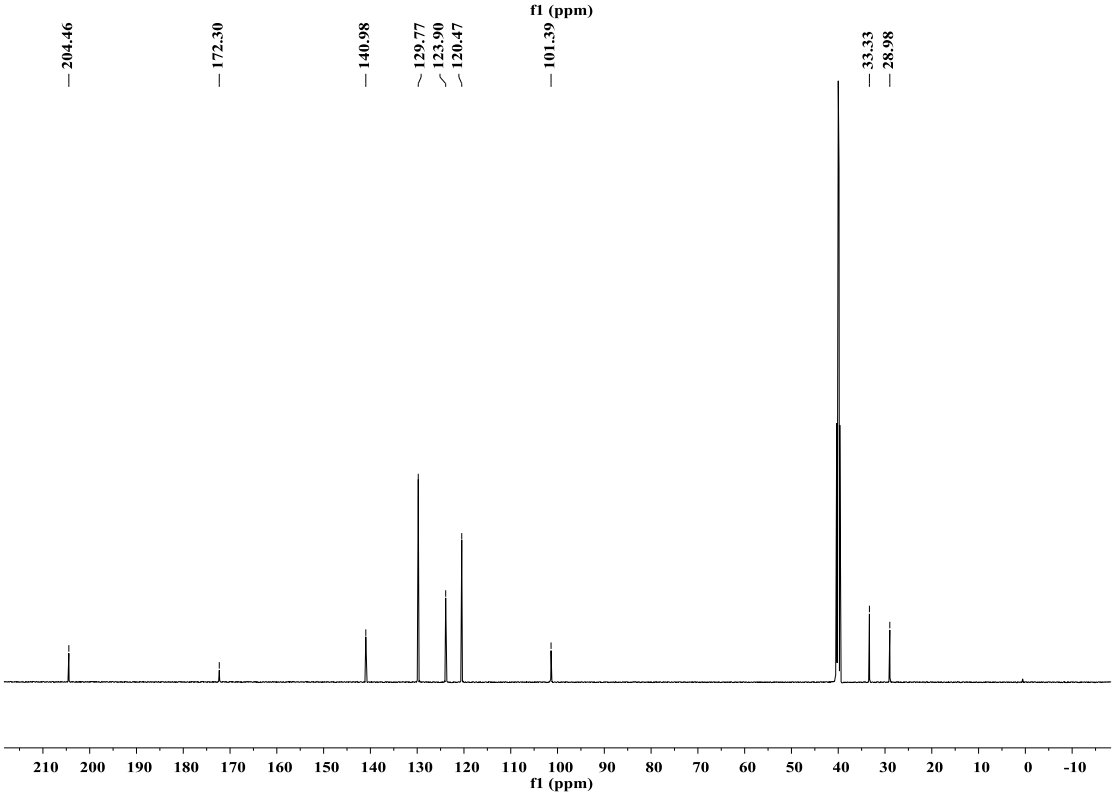
f1 (ppm)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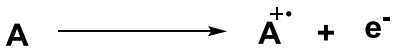
172.30
140.98
129.77
123.90
120.47
101.39
33.33
28.98
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3. Calculation details and additional data

Since Truhlar et al.'s M06-2X hybrid functional was shown to provide accurate predictions of main group thermochemistry,[1] geometry optimizations and frequency computations were performed using Gaussian 09 at the M06-2X/6-311G(d,p) level of theory, in conjunction with the IEF-PCM model to account for the solvation effects of acetonitrile.[1-3] Free energies include unscaled zero-point vibrational energies. Where indicated, low frequencies (<100 cm^{-1}) were corrected in the vibrational component of the entropy using a free rotor approximation according to the method of Grimme et al., since entropy associated with these loose vibrational modes was the most prone to computational error.[4] The quasi-harmonic oscillator corrections were obtained using the GoodVibes.[5] NBO analysis was conducted at the same level of geometry optimization using NBO package build-in Gaussian 09. [6]

The oxidation potentials of enamines were calculated using the free energies of enamine and enamine radical cation according the equation below.

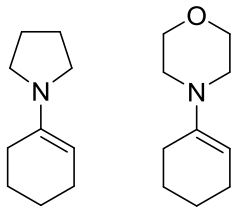


$$E = (G(A^{+\cdot}) + G(e^-) - G(A))/F - E^{o/SCE} \quad \text{(Eq. S1)}$$

The value of -0.86 kcal/mol for the gas phase energy of the electron based on the Fermi-Dirac statistical formalism is employed.[7] $E^{o/SCE}$ is the standard potential of the saturated calomel electrode (SCE) in acetonitrile (value = 4.429 V).[8]

We benchmarked several conventional density functions to calculated the oxidation potential of enamine **9H** (Table S1). The experimental oxidation peak potential of **9H** is 0.361 V (*vs.* SCE).[9] This approach also gave an accurate prediction oxidation potential of enamine **22H**.[9] M06-2X hybrid functional gave the best results and it has been shown to provide accurate predictions of redox potentials in DFT methods.[10]

Table S1. Tested several density functions for prediction of oxidation potentials (V *vs.* SCE).



	9H	22H
Experimental E_p	0.361 V	0.574 V

function	Basis set	Solvating model	E_{ox}(9H)
B3LYP	6-311g(d,p)	pcm	0.172
PBE	6-311g(d,p)	pcm	0.108
PBE0	6-311g(d,p)	pcm	0.141
M06-2X	**6-311g(d,p)**	**pcm**	**0.326** **0.567**[a]
M06L	6-311g(d,p)	pcm	0.107
ωB97XD	6-311g(d,p)	pcm	0.178
B97D	6-311g(d,p)	pcm	0.026

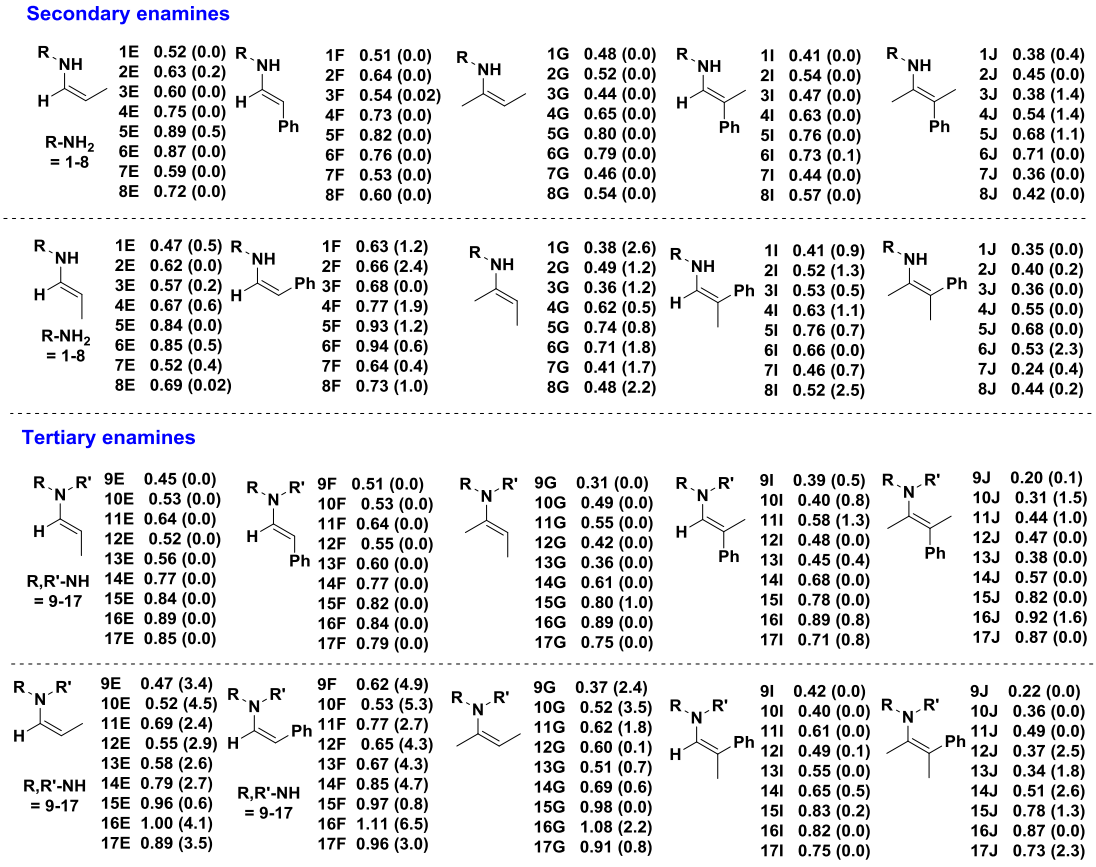
[a] Calculated oxidation potentials of enamine **22H**.

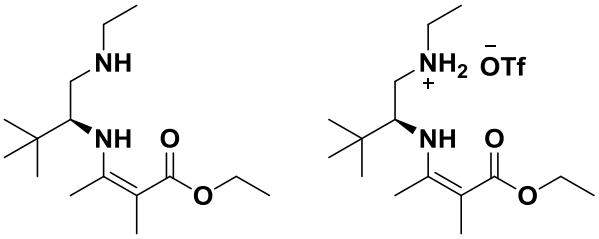
Table S2. Comparison of experimental and calculated oxidation potentials (V *vs.* SCE) of enamines deriving from β-ketocarbonyls

Enamines	Experimental oxidation peak potentials	Calculated oxidation potentials
$1A_1$	0.85	0.91
$1A_5$	0.68	0.83
$1C_2$	0.79	0.93
$2B_3$	1.21	1.23
$3A_1$	0.99	0.99
$3A_3$	0.86	0.92
$3A_4$	0.81	0.91
$3B_1$	1.17	1.28
$3B_2$	1.30	1.32
$3B_3$	1.24	1.27

$3C_1$	1.13	1.25
$3C_2$	0.87	0.92
$3C_3$	0.88	0.91
$3D_1$	1.22	1.28
4C2	0.96	1.04
$5A_1$	1.11	1.14
$5A_2$	1.06	1.14
$5B_4$	1.72	1.80
$5D_2$	1.42	1.51
$6C_2$	1.10	1.05

Table S3. Calculated oxidation potentials (V *vs.* SCE) of enamines in different conformations and relative free energies (in parentheses).

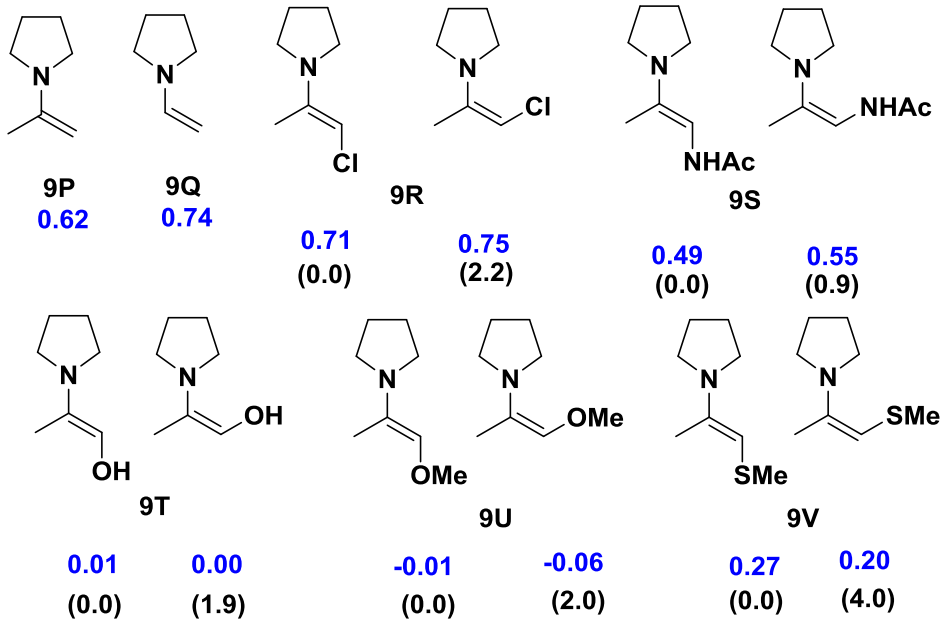




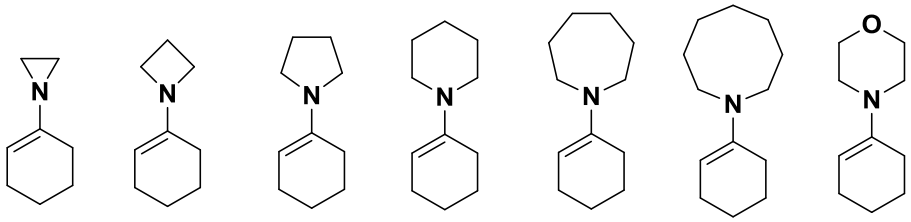
0.95 1.23

1'C_2 6'C_2

Scheme S1. Calculated oxidation potentials (V *vs.* SCE) of enamines deriving from 1', 6' and C_2. The numbers in parentheses are the relative free energies.



Scheme S2. Calculated oxidation potentials (V *vs.* SCE) of enamines deriving from acetaldehyde and α-substituted acetones. The numbers in parentheses are the relative free energies.



E_{ox}(V *vs.* SCE)	0.91	0.38	0.32	0.49	0.39	0.43	0.57

Scheme S3. Calculated oxidation potentials (V *vs.* SCE) of enamines deriving from cyclohexanone and various cyclic amines.

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