Figure Legends for Supporting Information

Fig. S1. HR-ESI-MS/MS fragmentation analysis of compounds **1**–**4** isolated from all tissues of *Solanum viarum* fruit and purified by C_{18}-HPLC-DAD. Respectively, panels **A**, **B**, **C**, and **D** show the full mass spectral range *m*/*z* 150–850, and the partial ranges *m*/*z* 702–740, *m*/*z* 345–565, and *m*/*z* 177–338. In panel **D**, the abbreviations S, G, P, M, and W denote loss of sinapoyl, glucosyl, propanedioic acid, and methyl groups, and H_20, respectively.

Fig. S2. Proposed formation pathways for selected HR-ESI-MS ion fragments of compounds **1–4** isolated from fruit of *Solanum viarum* (see **Table 2** in Ma et al.). The structures shown in panel **A** are in accord with all but one of the ion fragments from compounds **1**–**4** that differ in their *m/z* values by ≤7.0 mDa (note that *m*/*z* values indicated in **A** are from mass spectra of compound **1**). A single exception was the ion fragment *m*/*z* 367.1028 from compound **4**, the formation of which is depicted in panel **B**.

Fig. S3. HR-ESI-MS fragmentation of compound **2** isolated from *S. viarum* fruit with the aperture 1volatage set to 80V. Panels **A** and **B**, respectively, show the full mass spectral range *m*/*z* 140–870, and the expanded partial range *m*/*z* 14–280. Presence of the ion fragments *m*/*z* 233.0668 (malonylquinic acid – COO – H) and 173.0452 (quinic acid – H_2O – H) > 191.0559 (quinic acid – H) are consistent with the inclusion of 4-*O*-malonylquinic acid in the structure, as deduced from the NMR analyses.

Fig. S4. ^{1}H-NMR spectra of compounds **1** and **2** isolated from fruit tissues of *S. viarum*. Panels **A** and **B** show the 300 and 500 MHz spectra of **1** plus the 300 MHz spectrum of **2** over the ranges 1.8–7.7 ppm and 3.10–3.95 ppm, respectively. Panels **C** and **D** show enlargements of the

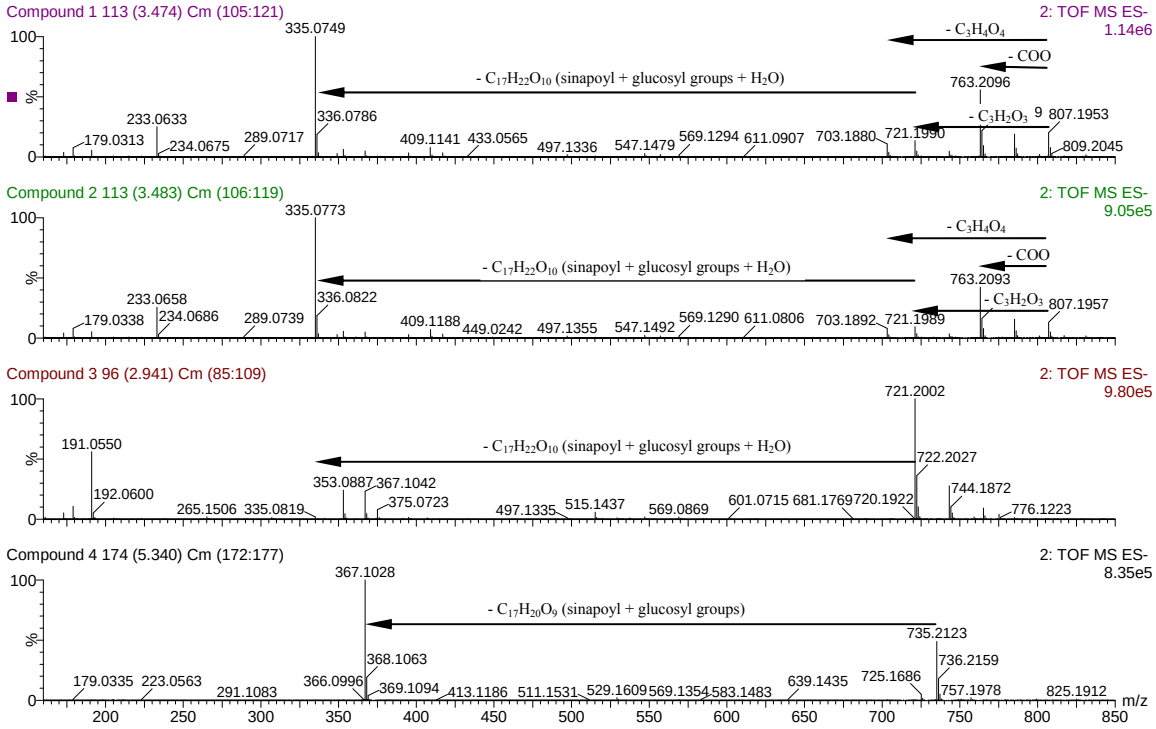
500 MHz spectra of **1** from panels **A** and **B**, respectively, including integration values along the X-axis for the individual and grouped peaks indicating the number of protons each represents.

Fig. S5. ^{13}C-NMR spectra of compound **1** isolated from fruit tissues of *S. viarum* over the full range from 33–181 ppm (**A**) and over the narrow range from 163.0–179.5 ppm (**B**), which includes the four carbonyl carbons representing the caffeoyl, sinapoyl, malonyl, and quinic acid moieties in the structure.

Fig. S6. Heteronuclear single quantum coherence (HSQC) spectrum of compound **1** isolated from fruit tissues of *S. viarum* over the ranges 1.8–7.7 ppm (^{1}H) and 33–150 ppm (^{13}C).

Fig. S7. Heteronuclear multiple band correlation (HMBC) spectra of compound **1** isolated from fruit tissues of *S. viarum* over the ranges: **A**, 1.6–7.8 ppm (^{1}H) and 33–185 ppm (^{13}C); **B**, 4.2–7.7 ppm (^{1}H) and 165.6–171.4 ppm (^{13}C); **C**, 6.70–7.12 ppm (^{1}H) and 144.5–152.0 ppm (^{13}C); **D**, 6.78–7.09 ppm (^{1}H) and 146.8–150.8 ppm (^{13}C); and **E**, 4.705–4.815 ppm (^{1}H) and 147.4–149.8 ppm (^{13}C).

A


Compound 1 113 (3.474) Cm (105:121)
2: TOF MS ES-
1.14e6
335.0749
- $C_3H_4O_4$
- COO
- $C_{17}H_{22}O_{10}$ (sinapoyl + glucosyl groups + H_2O)
763.2096
- $C_3H_2O_3$
807.1953
233.0633
336.0786
179.0313
234.0675
289.0717
409.1141
433.0565
497.1336
547.1479
569.1294
611.0907
703.1880
721.1990
809.2045
Compound 2 113 (3.483) Cm (106:119)
2: TOF MS ES-
9.05e5
335.0773
- $C_3H_4O_4$
- COO
- $C_{17}H_{22}O_{10}$ (sinapoyl + glucosyl groups + H_2O)
763.2093
- $C_3H_2O_3$
807.1957
233.0658
336.0822
179.0338
234.0686
289.0739
409.1188
449.0242
497.1355
547.1492
569.1290
611.0806
703.1892
721.1989
Compound 3 96 (2.941) Cm (85:109)
2: TOF MS ES-
9.80e5
721.2002
191.0550
- $C_{17}H_{22}O_{10}$ (sinapoyl + glucosyl groups + H_2O)
722.2027
353.0887
367.1042
192.0600
375.0723
744.1872
265.1506
335.0819
497.1335
515.1437
569.0869
601.0715
681.1769
720.1922
776.1223
Compound 4 174 (5.340) Cm (172:177)
2: TOF MS ES-
8.35e5
367.1028
- $C_{17}H_{20}O_9$ (sinapoyl + glucosyl groups)
735.2123
368.1063
736.2159
179.0335
223.0563
291.1083
366.0996
369.1094
413.1186
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529.1609
569.1354
583.1483
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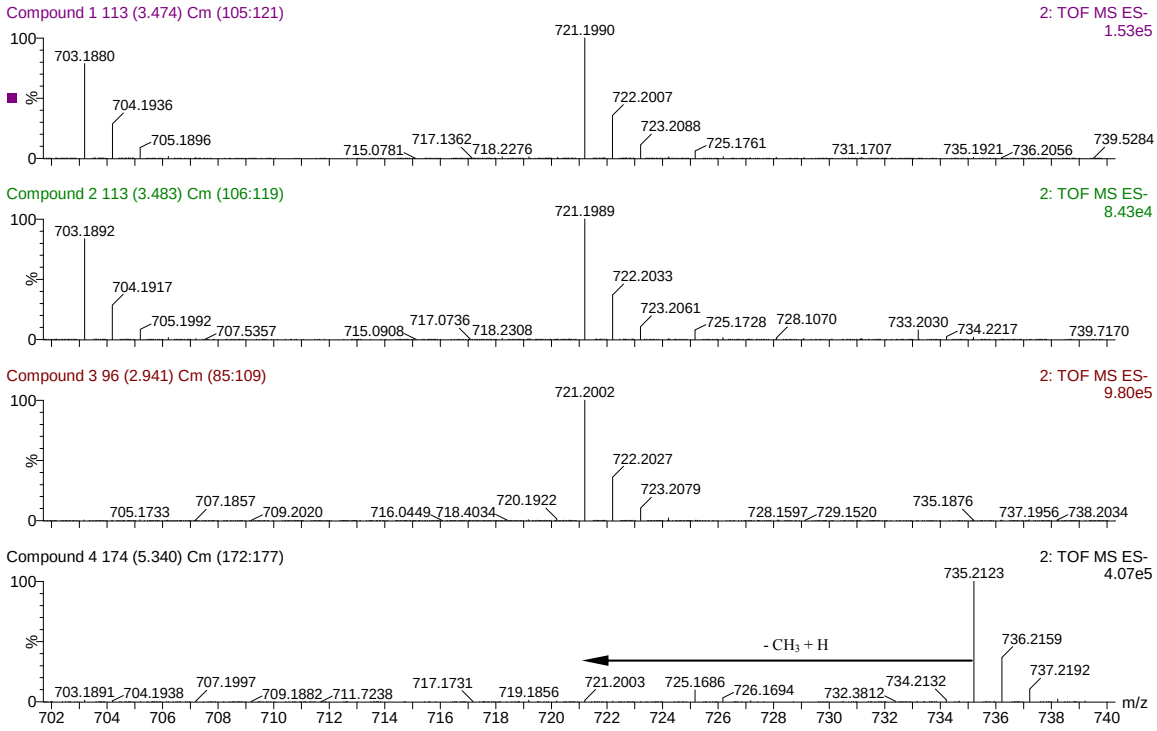
725.1686
757.1978
825.1912
m/z

B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705.1896
725.1761
715.0781
717.1362
718.2276
731.1707
735.1921
736.2056
739.5284
Compound 2 113 (3.483) Cm (106:119)
2: TOF MS ES-
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721.1989
703.1892
722.2033
704.1917
723.2061
705.1992
725.1728
728.1070
707.5357
715.0908
717.0736
718.2308
733.2030
734.2217
739.7170
Compound 3 96 (2.941) Cm (85:109)
2: TOF MS ES-
9.80e5
721.2002
722.2027
723.2079
705.1733
707.1857
709.2020
716.0449
718.4034
720.1922
728.1597
729.1520
735.1876
737.1956
738.2034
Compound 4 174 (5.340) Cm (172:177)
2: TOF MS ES-
4.07e5
735.2123
- CH_3 + H
736.2159
737.2192
703.1891
704.1938
707.1997
709.1882
711.7238
717.1731
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721.2003
725.1686
726.1694
732.3812
734.2132
m/z

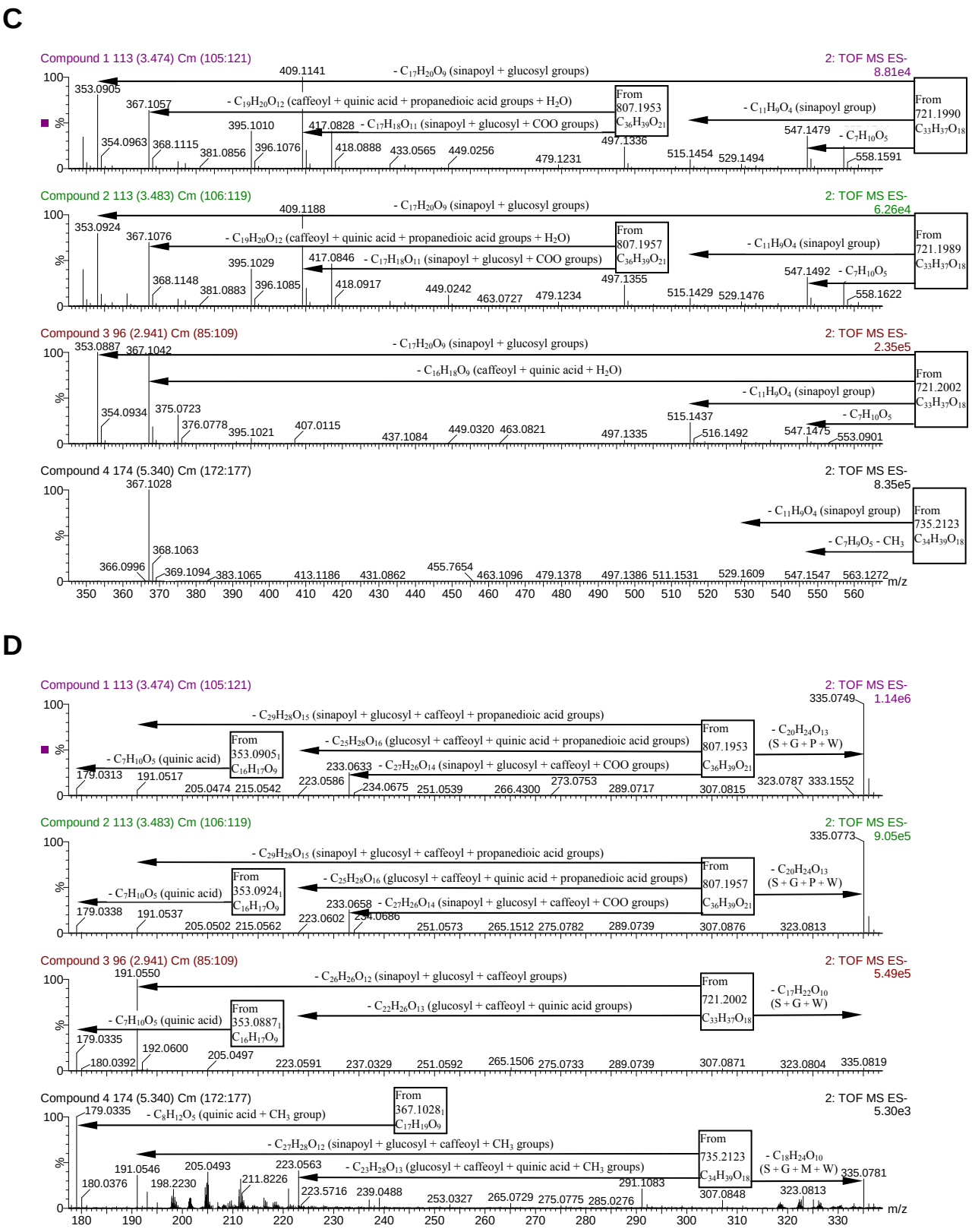


Fig. S1. (Supporting Information) Ma et al.

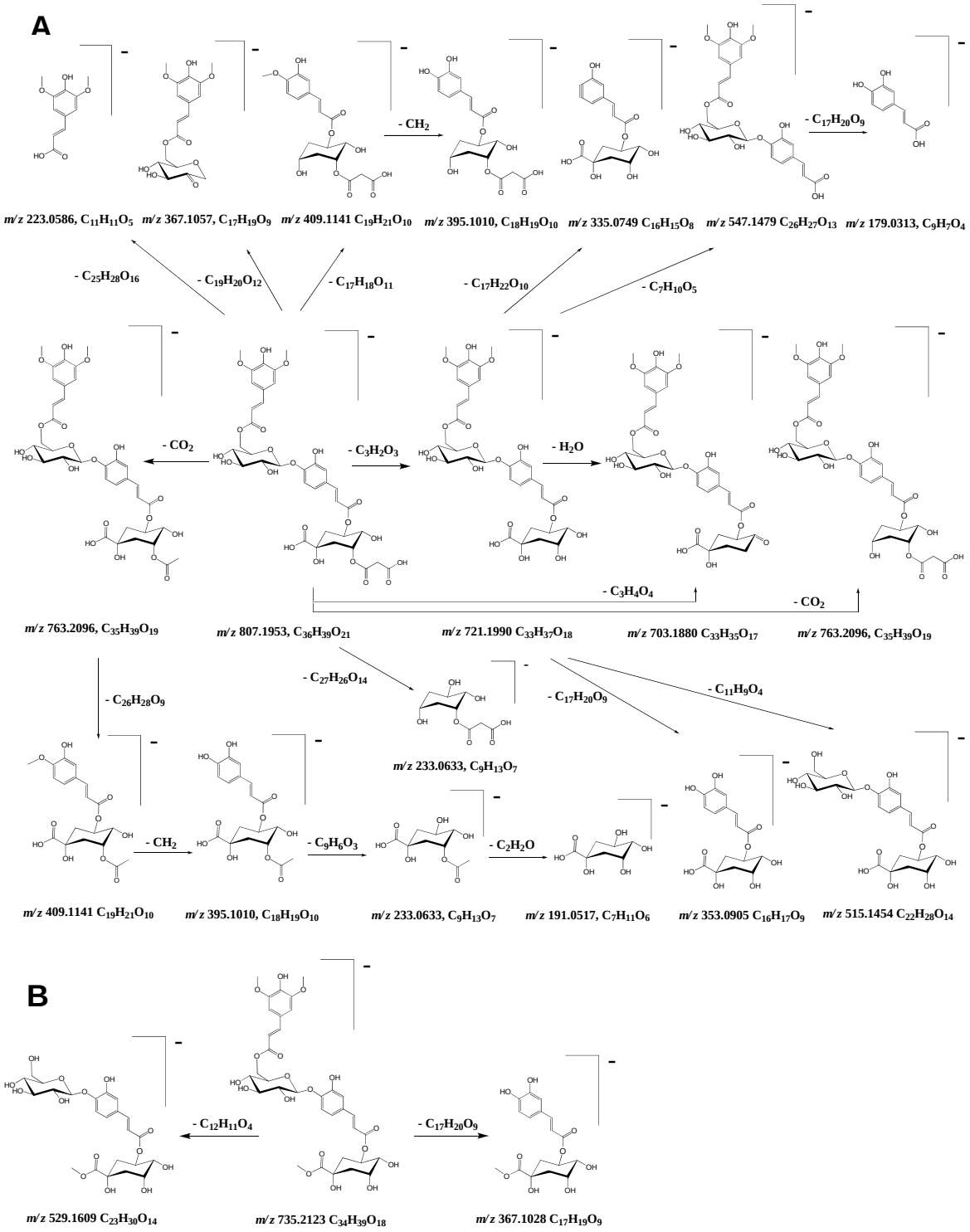
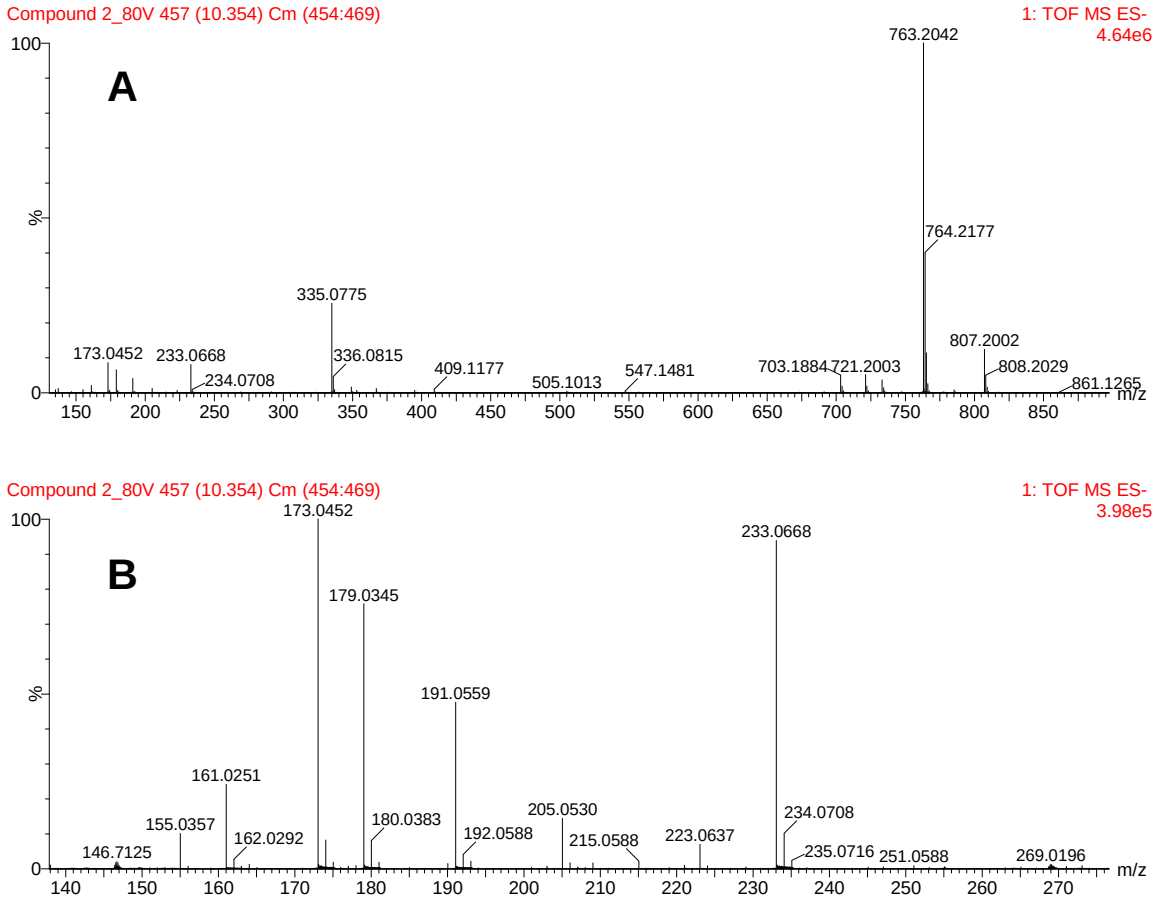


Fig. S2. (Supporting Information) Ma et al.



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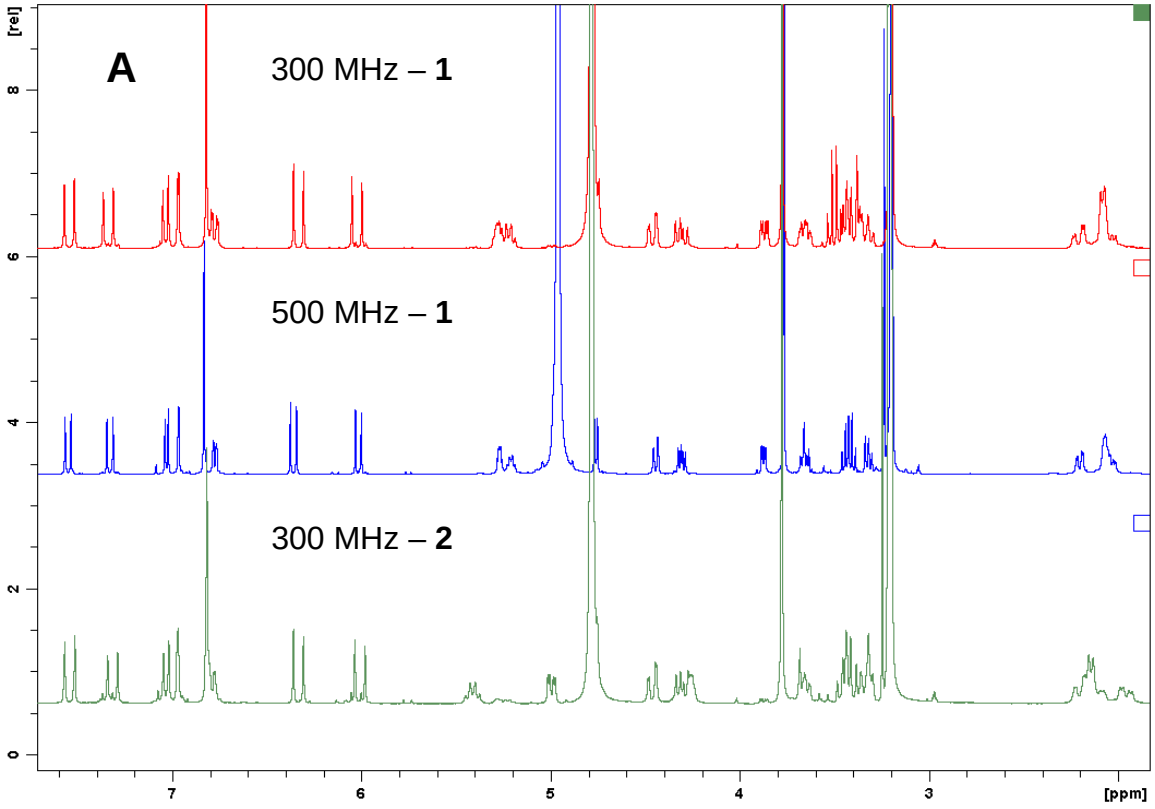
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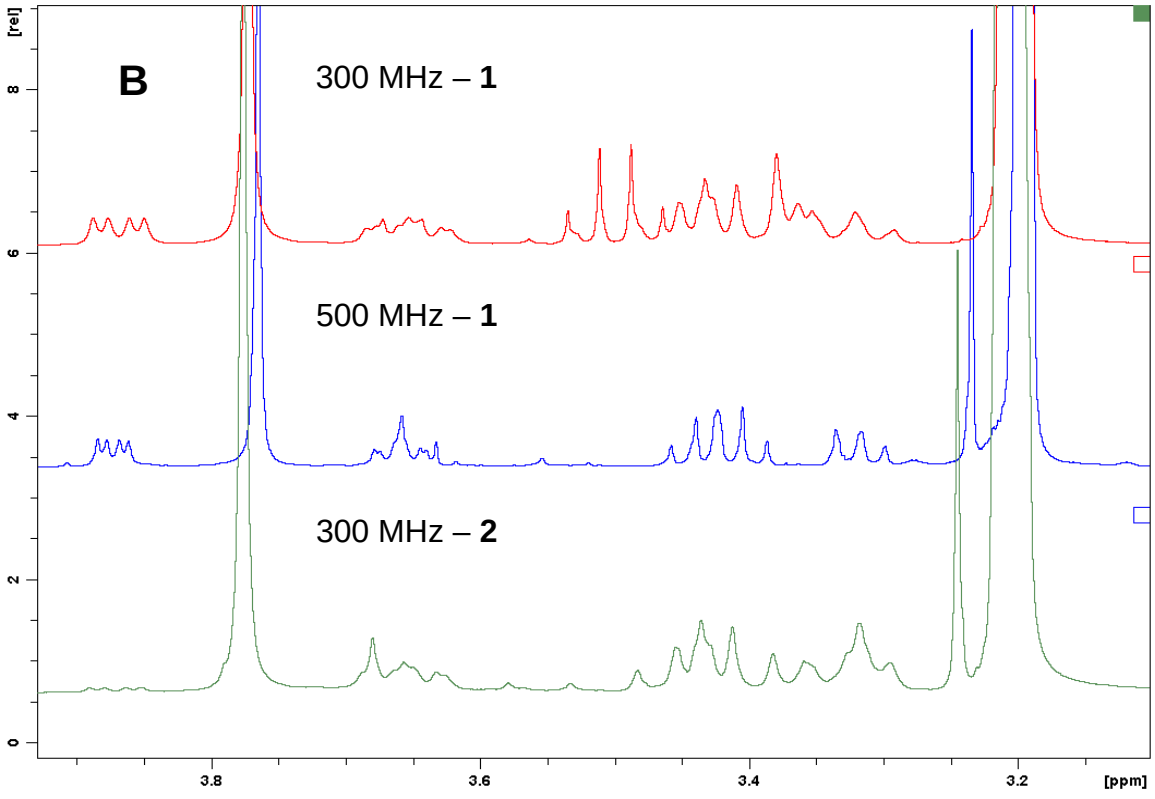
500 MHz – 1
300 MHz – 2
[rel]
0
2
4
6
8
7
6
5
4
3
[ppm]


B
300 MHz – 1
500 MHz – 1
300 MHz – 2
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2
4
6
8
3.8
3.6
3.4
3.2
[ppm]

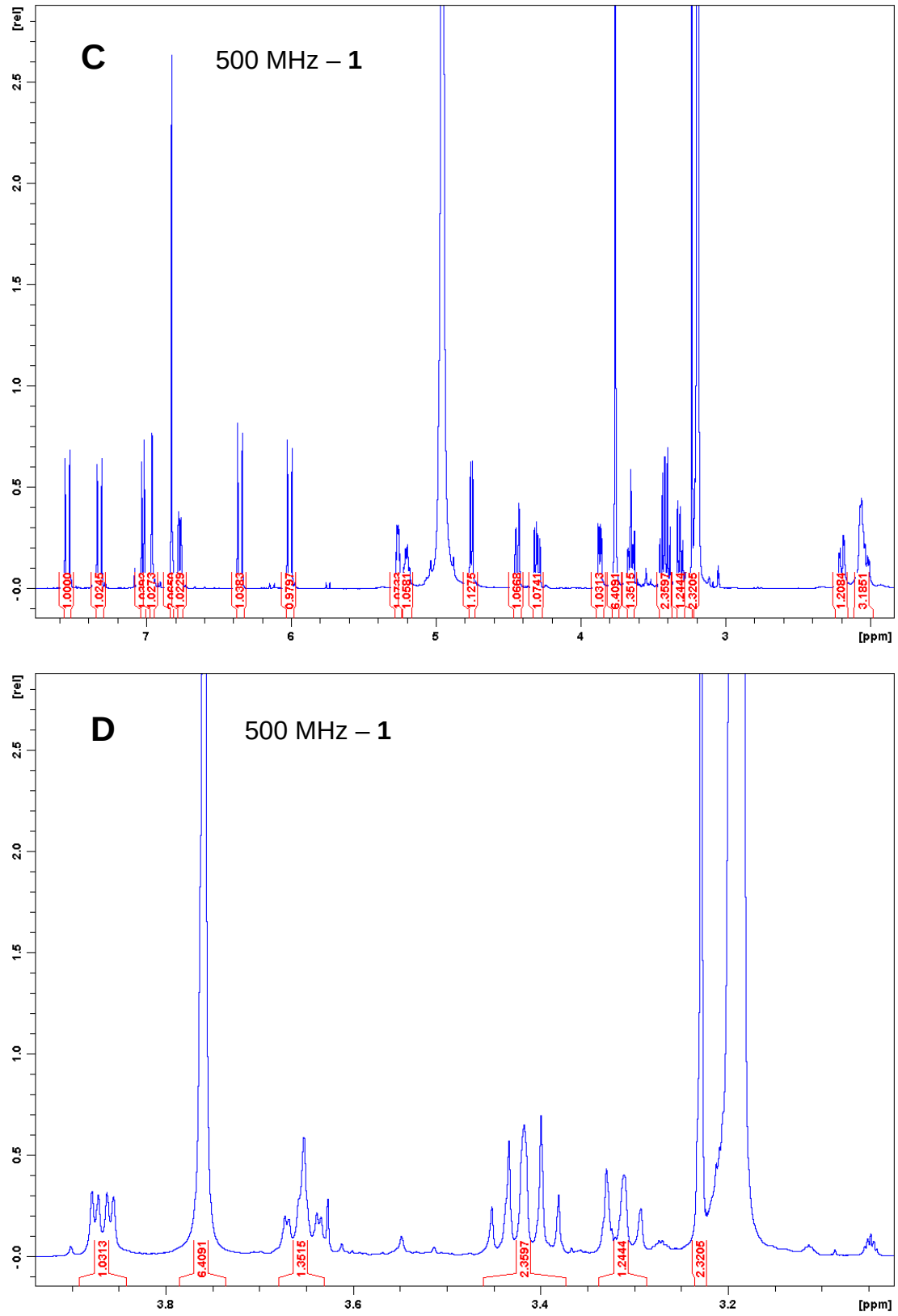


Fig. S4. (Supporting Information) Ma et al.

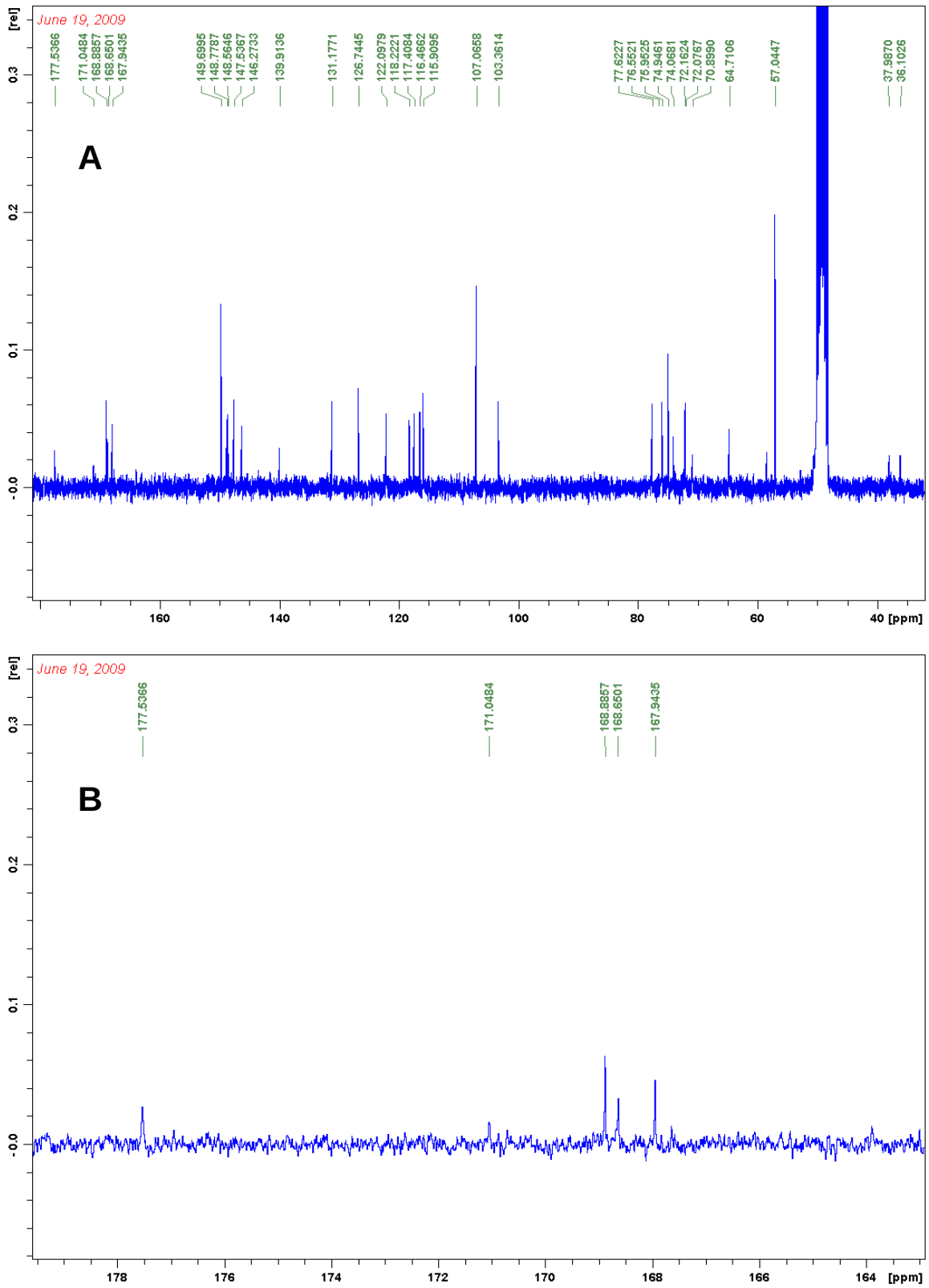


Fig. S5. (Supporting Information) Ma et al.

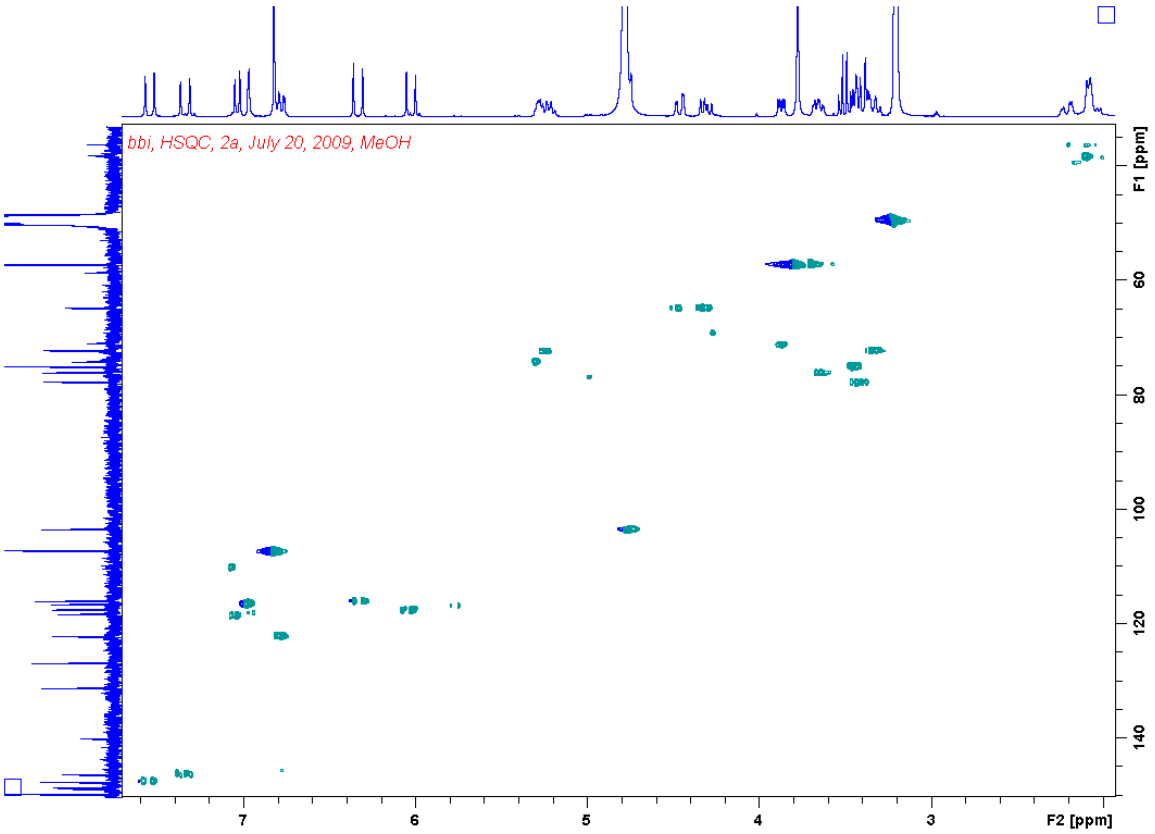
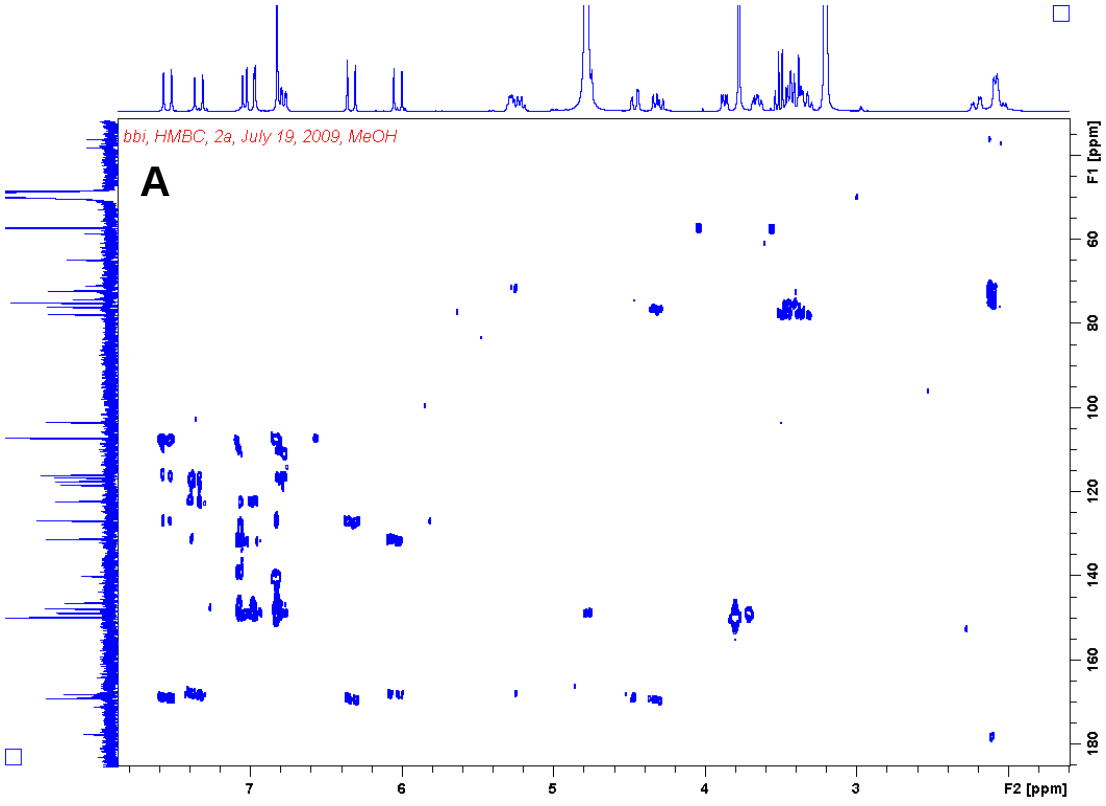


Fig. S6. (Supporting Information) Ma et al.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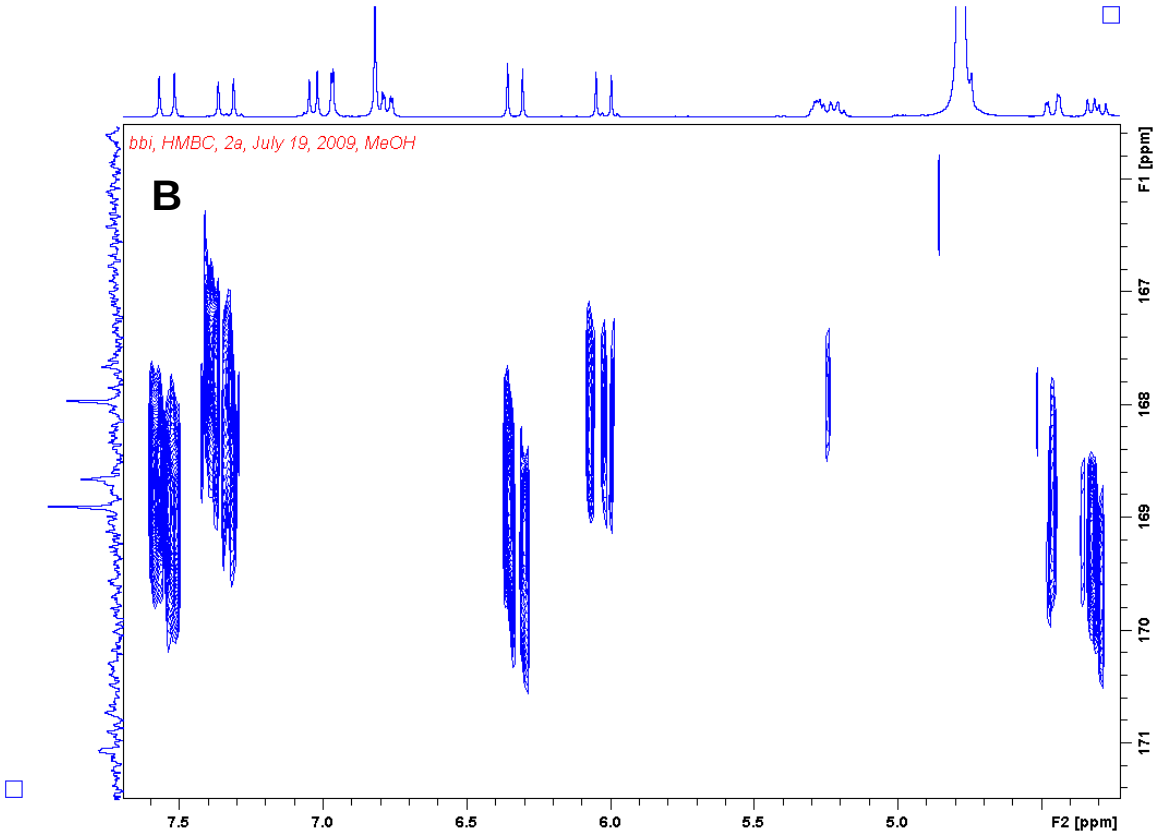
80
100
120
140
160
180
7
6
5
4
3
F2 [ppm]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B
F1 [ppm]
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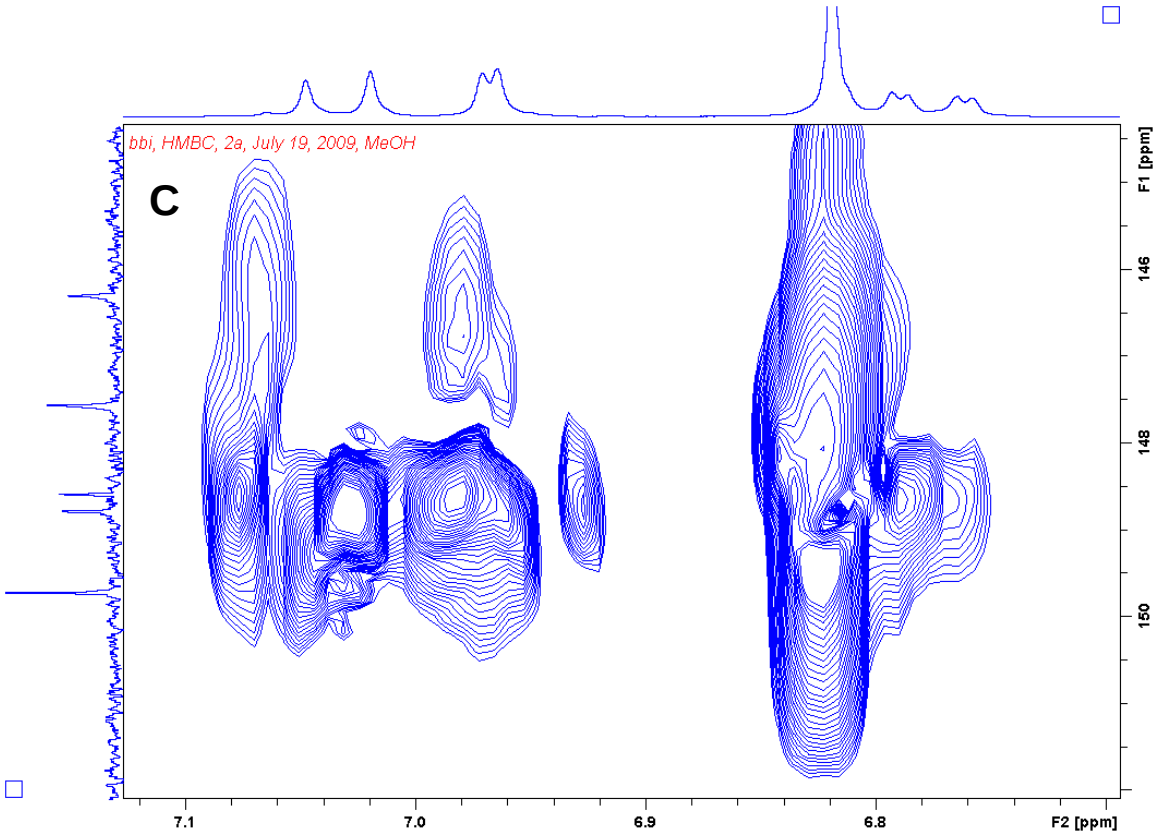
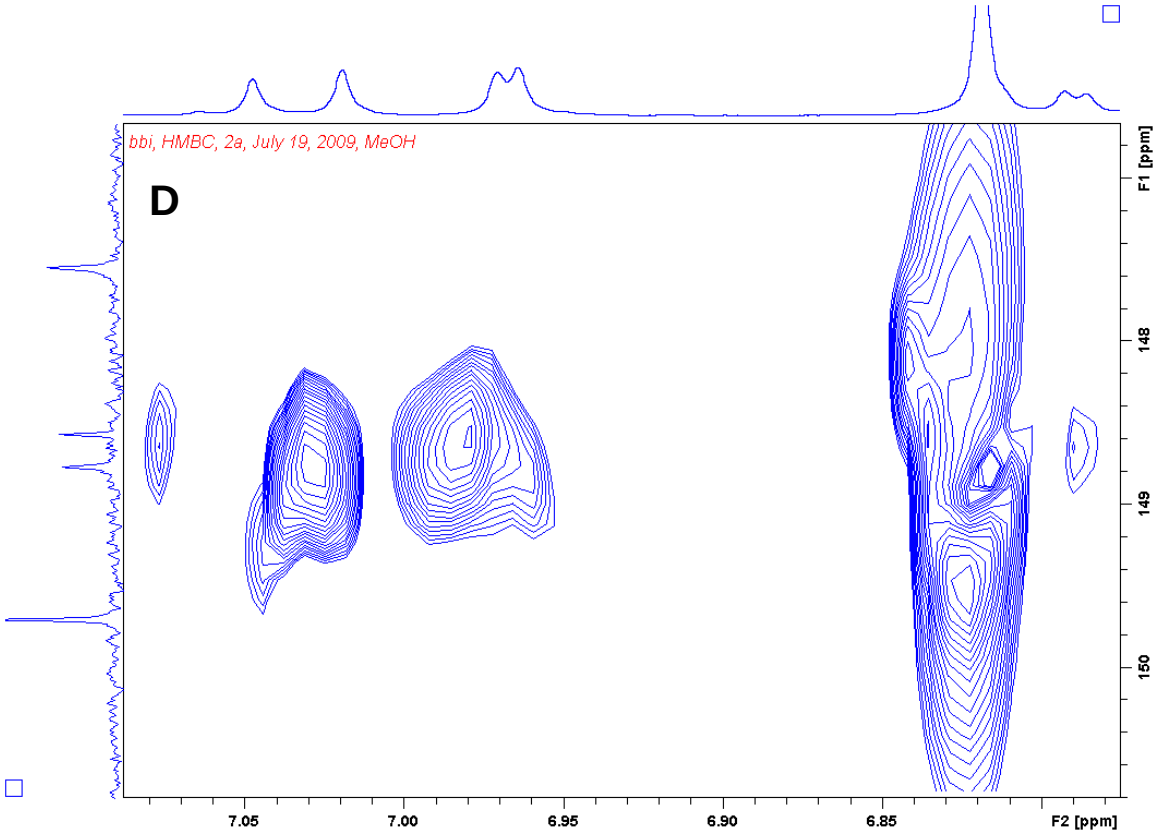
168
169
170
171
7.5
7.0
6.5
6.0
5.5
5.0
F2 [ppm]


bbi, HMBC, 2a, July 19, 2009, MeOH
C
F1 [ppm]
146
148
150
7.1
7.0
6.9
6.8
F2 [ppm]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D
F1 [ppm]
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149
150
7.05
7.00
6.95
6.90
6.85
F2 [ppm]

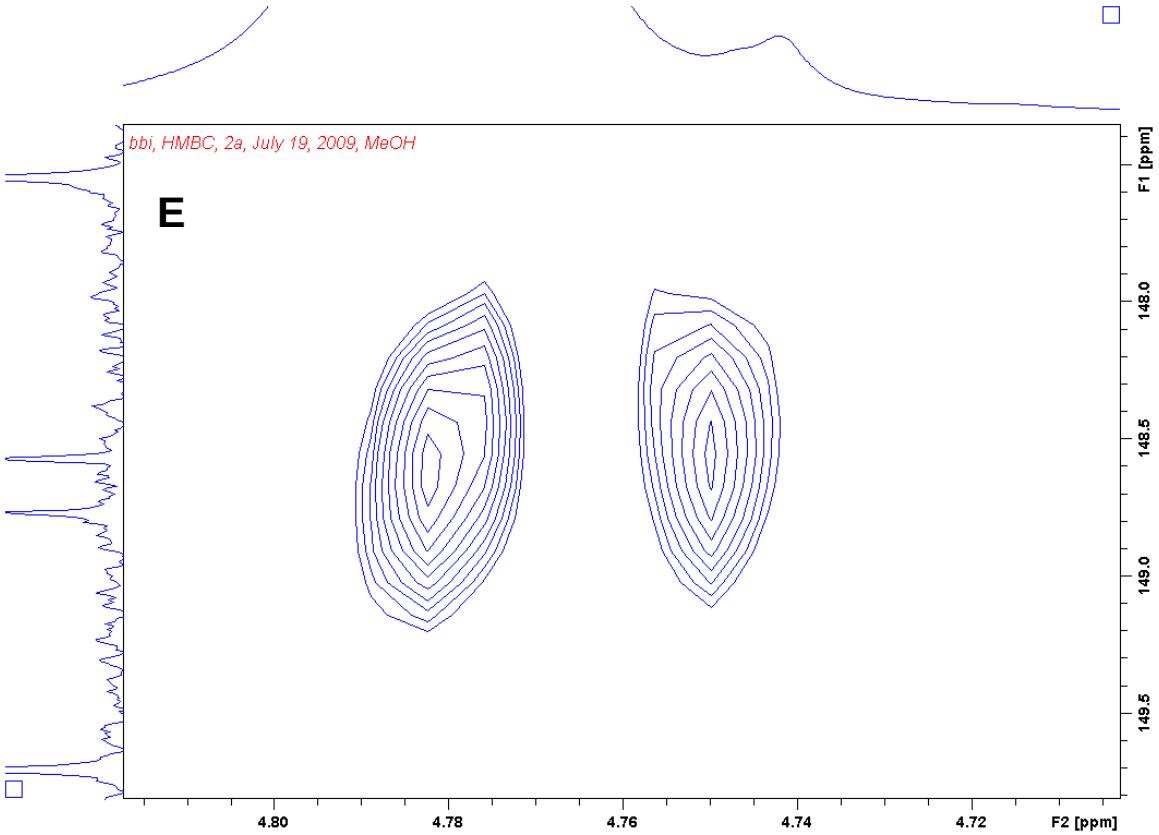

Fig. S7. (Supporting Information) Ma et al.