

Supporting informations

**Cleaner enzymatic production of biodiesel with easy separation procedures
triggered by a biocompatible hydrophilic ionic liquid**

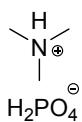
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|-------------------------------------------------------------------------|--------|
| 1HNMR, 13CNMR and FT-IR spectra data for the utilized ionic liquid..... | P2-9 |
| Spectrum for the utilized ionic liquids..... | P10-42 |
| Mass-spectrometry data of the biodiesel products..... | P43-48 |

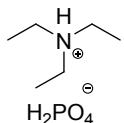
1. [TMA][H₂PO₄]



¹H NMR (400 MHz, D₂O) δ 2.66 (s, 9H) ppm; ¹³C NMR (100 MHz, D₂O) δ 44.5 ppm.

IR: ν 2924, 2364, 1642, 1534, 1483, 1228, 1042, 936, 482 cm⁻¹.

2. [TEA][H₂PO₄]

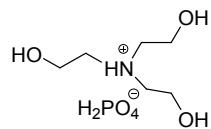


¹H NMR (400 MHz, D₂O) δ 2.42 (m, 6H), 0.51 (t, J = 6.3 Hz, 9H) ppm; ¹³C NMR

(100 MHz, D₂O) δ 45.9, 7.8 ppm.

IR: ν 3277, 2925, 2364, 1643, 1531, 1453, 1398, 1228, 1043, 945, 877, 837, 501 cm⁻¹.

3. [TEOA][H₂PO₄]

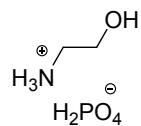


¹H NMR (400 MHz, D₂O) δ 3.91 (t, J = 4.0 Hz, 6H), 3.44 (t, J = 4.0 Hz, 6H) ppm;

¹³C NMR (100 MHz, D₂O) δ 55.2, 54.9 ppm.

IR: ν 3278, 2925, 1631, 1535, 1445, 1378, 1209, 1057, 932, 875, 689, 537, 496 cm⁻¹.

4. [EOA][H₂PO₄]

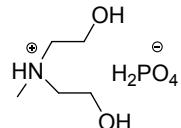


¹H NMR (400 MHz, D₂O) δ 3.78 - 3.75 (m, 2H), 3.10 - 3.07 (m, 2H) ppm; ¹³C NMR

(100 MHz, D₂O) δ 57.5, 41.2 ppm.

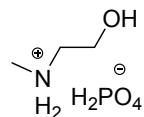
IR: ν 2749, 2168, 1636, 1501, 1456, 1344, 1205, 1135, 1112, 1075, 1014, 969, 933, 763, 550, 525, 491, 433 cm⁻¹.

5. [MDEOA][H₂PO₄]



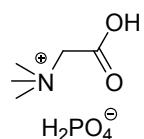
¹H NMR (400 MHz, D₂O) δ 3.94 (td, *J* = 5.3, 1.0 Hz, 4H), 3.37 (s, 4H), 2.96 (d, *J* = 1.1 Hz, 3H) ppm; ¹³C NMR (100 MHz, D₂O) δ 57.3, 55.1, 40.4 ppm.
 IR: ν 2767, 2334, 1643, 1466, 1062, 943, 480 cm⁻¹.

6. [MEOA][H₂PO₄]



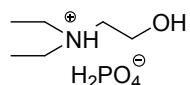
¹H NMR (400 MHz, D₂O) δ 3.73 (t, *J* = 4.0 Hz, 2H), 3.06 (t, *J* = 4.0 Hz, 2H), 2.64 (s, 3H) ppm; ¹³C NMR (100 MHz, D₂O) δ 56.3, 50.3, 32.5 ppm.
 IR: ν 2742, 2353, 1627, 1467, 1027, 930, 490 cm⁻¹.

7. [Betaine][H₂PO₄]



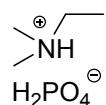
¹H NMR (400 MHz, D₂O) δ 4.03 (s, 2H), 3.25 (s, 9H) ppm; ¹³C NMR (100 MHz, D₂O) δ 168.1, 64.8, 53.5 ppm.
 IR: ν 2994, 2324, 1661, 1471, 1406, 1233, 956, 928, 894, 715, 436 cm⁻¹.

8. [DEEOA][H₂PO₄]



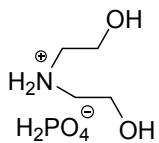
¹H NMR (400 MHz, D₂O) δ 3.88 - 3.85 (m, 2H), 3.28 - 3.20 (m, 6H), 1.27 (t, *J* = 4.0 Hz, 6H) ppm; ¹³C NMR (150 MHz, D₂O) δ 55.2, 53.1, 47.5, 7.9 ppm.
 IR: ν 2693, 2345, 1649, 1647, 1234, 1061, 946, 878, 499 cm⁻¹.

9. [DMEA][H₂PO₄]



¹H NMR (400 MHz, D₂O) δ 3.01 (q, *J* = 7.2 Hz, 2H), 2.69 (s, 6H), 1.14 (t, *J* = 7.2 Hz, 3H) ppm; ¹³C NMR (100 MHz, D₂O) δ 52.8, 41.9, 8.9 ppm.
 IR: ν 2695, 2343, 1644, 1470, 940, 479 cm⁻¹.

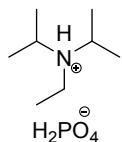
10. [DEOA][H₂PO₄]



^1H NMR (400 MHz, D₂O) δ 3.53 - 3.33 (m, 4H), 2.89 - 2.69 (m, 4H) ppm; ^{13}C NMR (100 MHz, D₂O) δ 56.2, 48.5 ppm.

IR: ν 2810, 2382, 1618, 1438, 1253, 926, 872, 826, 683, 502 cm⁻¹.

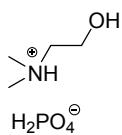
11. [DIPEA][H₂PO₄]



^1H NMR (400 MHz, D₂O) δ 3.73 (m, 2H), 3.22 (m, 2H), 1.35 (m, 15H) ppm; ^{13}C NMR (100 MHz, D₂O) δ 54.3, 42.5, 17.7, 16.2, 12.1 ppm.

IR: ν 2705, 2349, 1668, 1471, 1403, 1063, 945, 876, 503 cm⁻¹.

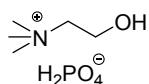
12. [DMEOA][H₂PO₄]



^1H NMR (400 MHz, D₂O) δ 3.67 - 3.65 (m, 2H), 3.06 - 3.03 (m, 2H), 2.68 (s, 6H) ppm; ^{13}C NMR (100 MHz, D₂O) δ 58.5, 55.1, 42.6 ppm.

IR: ν 2719, 2361, 1472, 1053, 933, 872, 494 cm⁻¹.

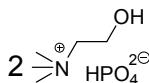
13. [Choline][H₂PO₄]



^1H NMR (400 MHz, D₂O) δ 4.02 - 3.96 (m, 2H), 3.47 - 3.41 (m, 2H), 3.13 (s, 9H) ppm; ^{13}C NMR (100 MHz, D₂O) δ 67.3, 55.5, 53.8 ppm.

IR: ν 3037, 2852, 2338, 1596, 1480, 1239, 1077, 936, 865, 507 cm⁻¹.

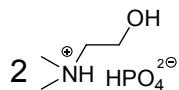
14. [Choline]₂[HPO₄]₂



^1H NMR (400 MHz, D₂O) δ 3.92 - 3.88 (m, 4H), 3.39 - 3.36 (m, 4H), 3.05 (s, 18H) ppm; ^{13}C NMR (100 MHz, D₂O) δ 67.3, 55.4, 53.8 ppm.

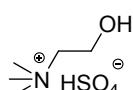
IR: ν 3030, 1655, 1479, 1373, 1033, 954, 843, 527 cm⁻¹.

15. [DMEA]₂[HPO₄]



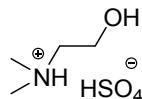
¹H NMR (400 MHz, D₂O) δ 3.79 - 3.77 (m, 4H), 3.18 - 3.16 (m, 4H), 2.80 (s, 12H) ppm; ¹³C NMR (100 MHz, D₂O) δ 56.4, 52.9, 40.4 ppm.
IR: ν 2713, 2345, 1655, 1471, 1053, 934, 872, 490 cm⁻¹.

16. [Choline][HSO₄]



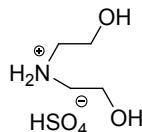
¹H NMR (400 MHz, D₂O) δ 4.00 - 3.96 (m, 2H), 3.45 - 3.43 (m, 2H), 3.12 (s, 9H) ppm; ¹³C NMR (100 MHz, D₂O) δ 67.3, 55.6, 53.8 ppm.
IR: ν 3371, 2893, 1480, 1161, 1083, 1030, 952, 849, 571, 435 cm⁻¹.

17. [DMEA][HSO₄]



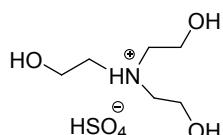
¹H NMR (400 MHz, D₂O) δ 3.71 - 3.68 (m, 2H), 3.10 - 3.07 (m, 2H), 2.72 (s, 6H) ppm; ¹³C NMR (100 MHz, D₂O) δ 58.5, 55.1, 42.6 ppm.
IR: ν 3387, 3059, 1653, 1472, 1151, 1030, 987, 852, 570, 436 cm⁻¹.

18. [DEOA][HSO₄]



¹H NMR (400 MHz, D₂O) δ 3.69 - 3.64 (m, 4H), 3.04 (s, 4H) ppm; ¹³C NMR (100 MHz, D₂O) δ 60.2, 49.8 ppm.
IR: ν 3407, 3051, 2842, 1600, 1448, 1171, 1006, 939, 855, 751, 572 cm⁻¹.

19. [TEOA][HSO₄]



¹H NMR (400 MHz, D₂O) δ 3.91 (t, *J* = 4.0 Hz, 6H), 3.44 (t, *J* = 4.0 Hz, 6H) ppm;

¹³C NMR (100 MHz, D₂O) δ 55.2, 54.9 ppm.

IR: ν 3387, 2899, 2162, 1707, 1162, 1091, 1025, 862, 755, 569 cm⁻¹.

20. [DMEA][HSO₄]

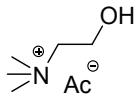


¹H NMR (400 MHz, D₂O) δ 2.98 (dt, *J* = 12.3, 4.9 Hz, 2H), 2.65 - 2.64 (m, 6H), 1.09

(td, *J* = 7.1, 2.4 Hz, 3H) ppm; ¹³C NMR (100 MHz, D₂O) δ 52.8, 41.9, 8.9 ppm.

IR: ν 3045, 2772, 1473, 1153, 1022, 926, 846, 870, 436 cm⁻¹.

21. [Choline][Ac]

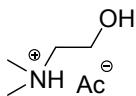


¹H NMR (600 MHz, D₂O) δ 4.07 - 4.07 (m, 2H), 3.53 - 3.52 (m, 2H), 3.21 (s, 9H),

1.93 (s, 3H) ppm; ¹³C NMR (100 MHz, D₂O) δ 181.0, 67.4, 55.5, 53.8, 23.3 ppm.

IR: ν 3144, 1568, 1481, 1384, 1330, 1139, 1089, 1008, 954, 915, 867, 640, 463 cm⁻¹.

22. [DMEOA][Ac]



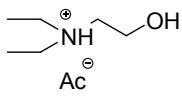
¹H NMR (400 MHz, D₂O) δ 3.88 - 3.85 (m, 2H), 3.27 - 3.25 (m, 2H), 2.89 (s, 6H),

1.97 (s, 3H) ppm; ¹³C NMR (100 MHz, D₂O) δ 178.9, 58.6, 55.0, 42.6, 21.8 ppm.

IR: ν 3268, 3028, 1572, 1474, 1397, 1258, 1080, 1013, 956, 919, 858, 799, 649, 613,

452 cm⁻¹.

23. [DEEOA][Ac]



¹H NMR (400 MHz, D₂O) δ 3.70 (m, 2H), 3.15 - 3.02 (m, 6H), 1.76 - 1.74 (m, 3H),

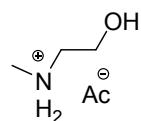
1.15 - 1.07 (m, 6H) ppm; ¹³C NMR (100 MHz, D₂O) δ 179.7, 55.1, 53.0, 47.3, 22.8,

7.9 ppm.

IR: ν 2979, 2479, 1709, 1570, 1396, 1256, 1131, 1082, 1012, 922, 877, 797, 647, 615,

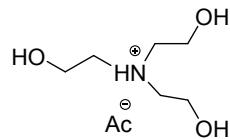
552, 450 cm⁻¹.

24. [MEOA][Ac]



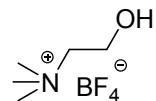
¹H NMR (400 MHz, D₂O) δ 3.57 - 3.54 (m, 2H), 2.90 - 2.88 (m, 2H), 2.47 (s, 3H), 1.65 (s, 3H) ppm; ¹³C NMR (100 MHz, D₂O) δ 180.8, 56.2, 50.2, 32.4, 23.1 ppm.
IR: ν 2731, 2441, 1556, 1392, 1334, 1149, 1082, 1039, 1012, 918, 648, 616, 533, 470 cm⁻¹.

25. [TEOA][Ac]



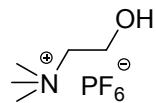
¹H NMR (400 MHz, D₂O) δ 3.83 - 3.80 (m, 6H), 3.21 - 3.19 (m, 6H), 1.85 (s, 3H) ppm; ¹³C NMR (100 MHz, D₂O) δ 181.2, 56.1, 55.3, 23.3 ppm.
IR: ν 3226, 2871, 1567, 1400, 1154, 1064, 1032, 913, 881, 648, 616 cm⁻¹.

26. [Choline][BF₄]



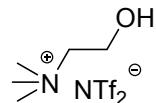
¹H NMR (400 MHz, D₂O) δ 4.19 - 4.15 (m, 2H), 3.63 - 3.60 (m, 2H), 3.30 (s, 9H) ppm; ¹³C NMR (100 MHz, D₂O) δ 67.5, 55.7, 53.9 ppm.
IR: ν 3545, 3048, 2170, 2040, 1993, 1962, 1588, 1478, 1345, 1287, 1029, 950, 869, 744, 521 cm⁻¹.

27. [Choline][PF₆]



¹H NMR (400 MHz, D₂O) δ 4.08 - 4.04 (m, 2H), 3.52 - 3.50 (m, 2H), 3.20 (s, 9H) ppm; ¹³C NMR (100 MHz, D₂O) δ 67.4, 55.6, 53.8 ppm.
IR: ν 2695, 2345, 2191, 2040, 2004, 1748, 1587, 1477, 1687, 954, 816, 669, 555 cm⁻¹.

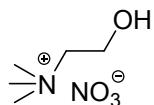
28. [Choline][NTf₂]



¹H NMR (400 MHz, DMSO) δ 4.44 (s, 1H), 2.97 (m, 2H), 2.53 - 2.45 (m, 2H), 2.22 (s, 9H) ppm; ¹³C NMR (100 MHz, DMSO) δ 124.7, 121.5, 118.3, 115.1, 67.6, 55.6, 53.6 ppm.

IR: ν 3536, 1478, 1346, 1180, 1132, 1052, 953, 865, 790, 763, 740, 654, 613, 570, 513 cm⁻¹.

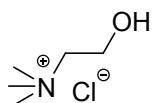
29. [Choline][NO₃]



¹H NMR (400 MHz, D₂O) δ 4.15 - 4.11 (m, 2H), 3.60 - 3.57 (m, 2H), 3.27 (s, 9H) ppm; ¹³C NMR (100 MHz, D₂O) δ 67.5, 55.7, 53.9 ppm.

IR: ν 3370, 3037, 1480, 1320, 1135, 1083, 1042, 1006, 925, 866, 830, 542, 454 cm⁻¹.

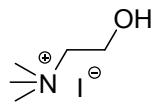
30. [Choline][Cl]



¹H NMR (400 MHz, D₂O) δ 4.12 - 4.08 (m, 2H), 3.58 - 3.56 (m, 2H), 3.25 (s, 9H) ppm; ¹³C NMR (100 MHz, D₂O) δ 67.4, 55.7, 54.0 ppm.

IR: ν 3219, 3005, 2843, 1580, 1482, 1460, 1349, 1275, 1141, 1084, 1057, 1012, 959, 893, 865, 635, 529, 466, 449 cm⁻¹.

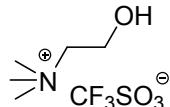
31. [Choline][I]



¹H NMR (400 MHz, D₂O) δ 4.14 - 4.10 (m, 2H), 3.60 - 3.57 (m, 2H), 3.26 (s, 9H) ppm; ¹³C NMR (100 MHz, D₂O) δ 67.5, 55.7, 54.1 ppm.

IR: ν 3330, 3025, 3005, 2347, 2043, 1963, 1588, 1478, 1409, 1355, 1130, 1079, 1054, 1010, 955, 945, 895, 860, 668, 528 cm⁻¹.

32. [Choline][CF₃SO₃]

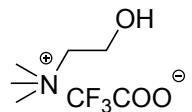


¹H NMR (400 MHz, D₂O) δ 4.13 - 4.10 (m, 2H), 3.58 - 3.55 (m, 2H), 3.26 (s, 9H) ppm;

¹³C NMR (100 MHz, D₂O) δ 124.5, 121.3, 118.2, 115.0, 67.5, 55.6, 53.9 ppm.

IR: ν 3457, 1479, 1247, 1224, 1152, 1086, 1026, 953, 868, 757, 635, 572, 516 cm^{-1} .

33. [Choline][CF₃COO]

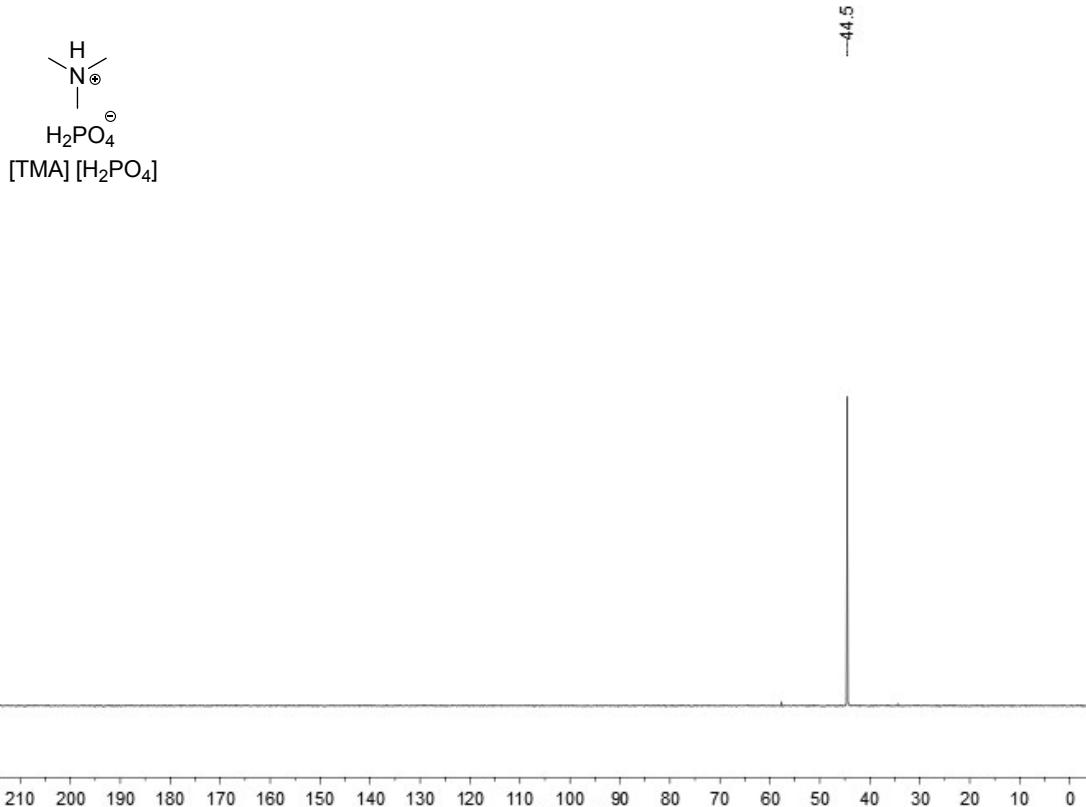
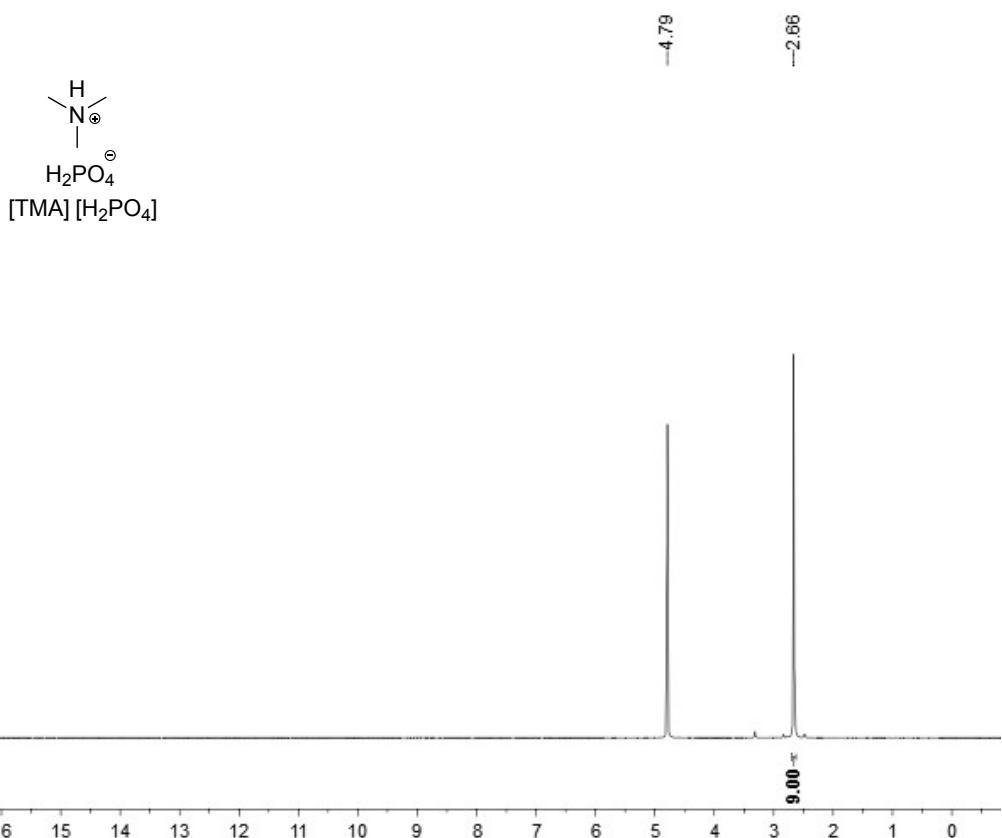


¹H NMR (400 MHz, D₂O) δ 4.08 - 4.04 (m, 2H), 3.53 - 3.50 (m, 2H), 3.21 (s, 9H) ppm;

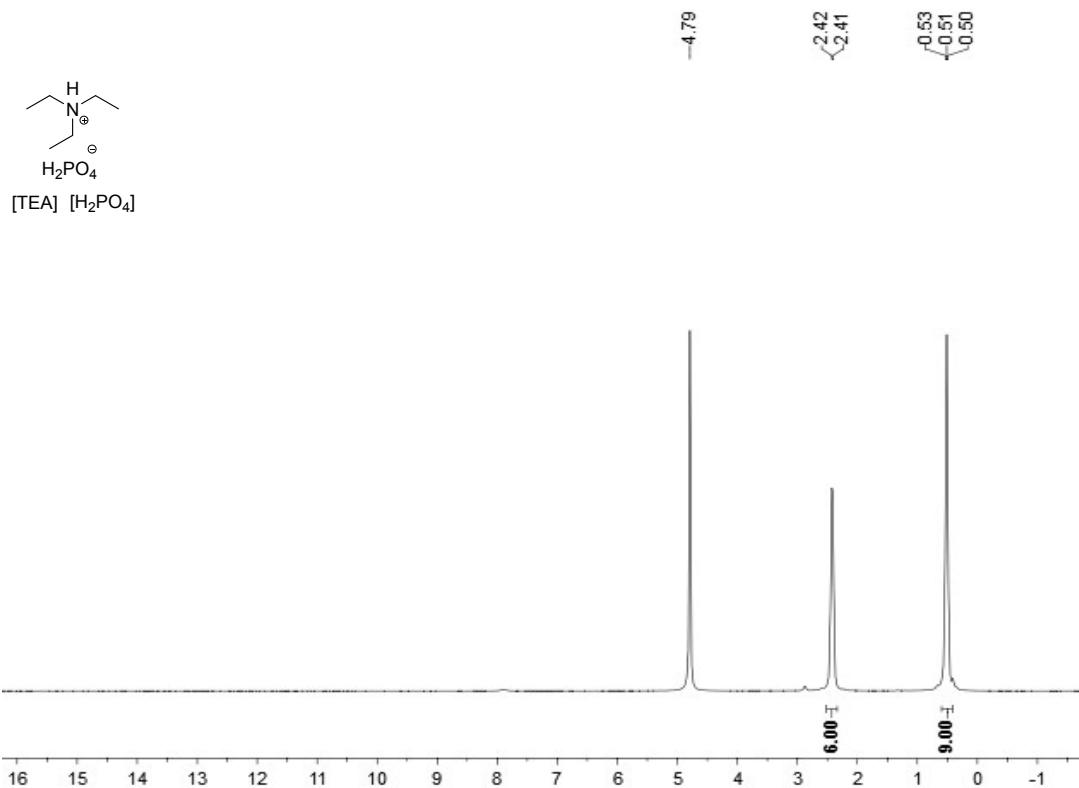
¹³C NMR (100 MHz, D₂O) δ 162.9, 162.6, 162.3, 161.9, 120.9, 118.0, 115.0, 112.1, 67.4, 55.6, 53.8 ppm.

IR: ν 3288, 1674, 1480, 1414, 1197, 1170, 1117, 1088, 1006, 953, 867, 826, 800, 718, 595, 518 cm^{-1} .

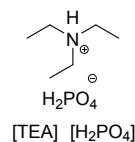
1.



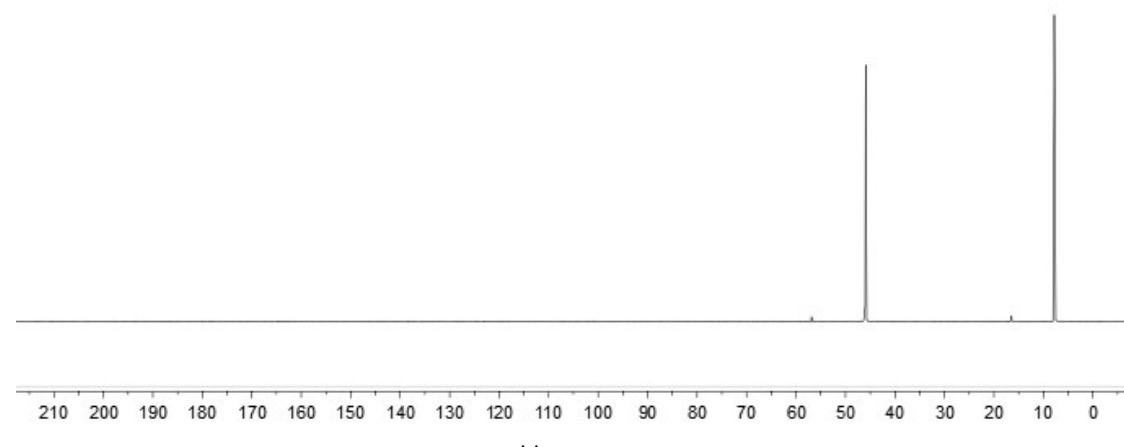
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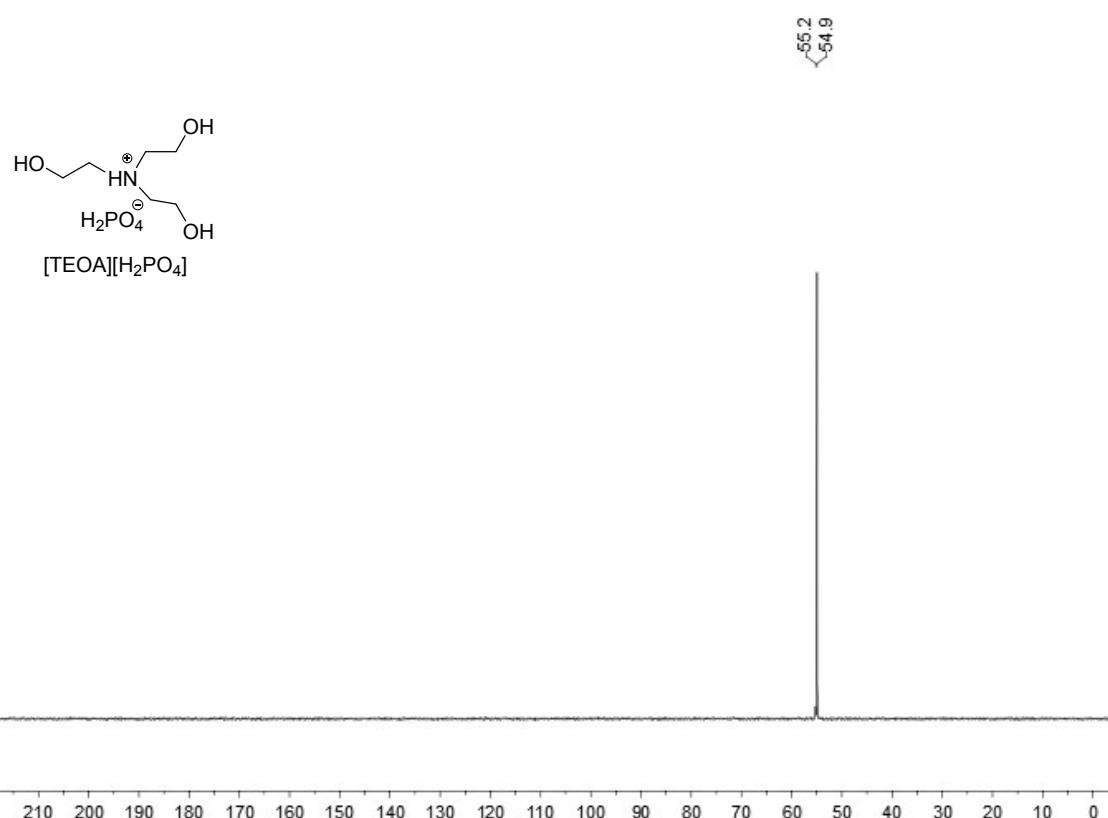
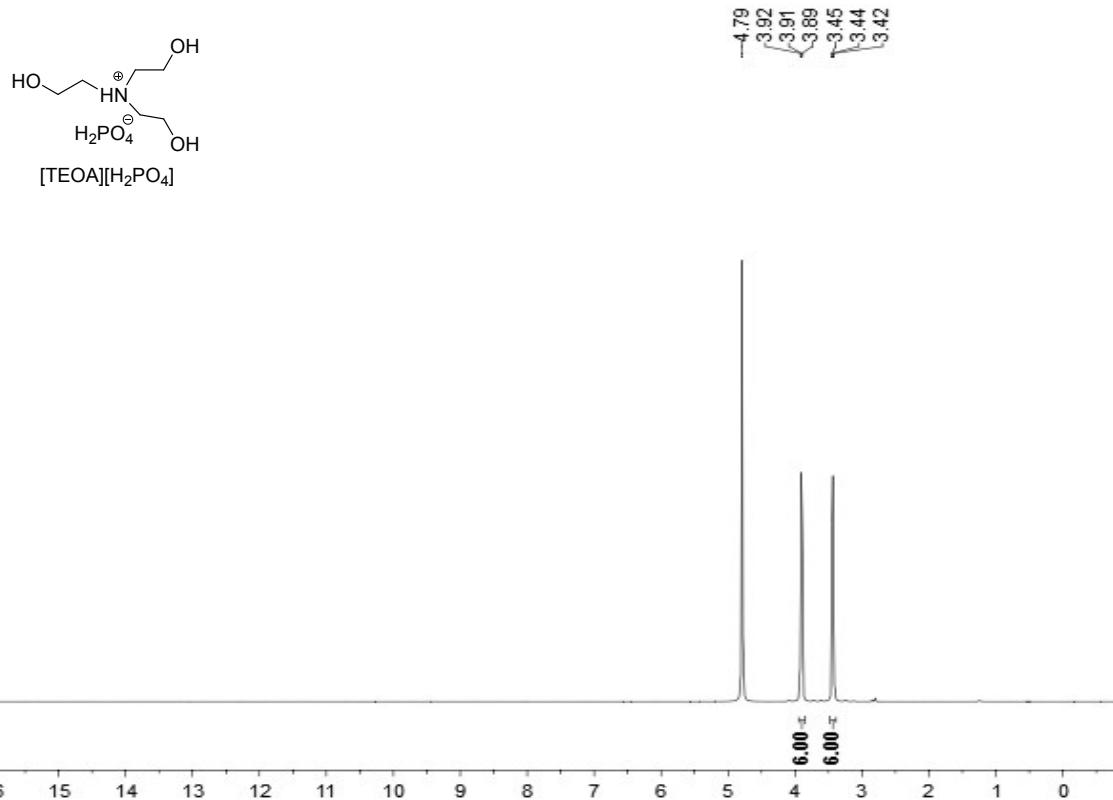
-45.9 -7.8



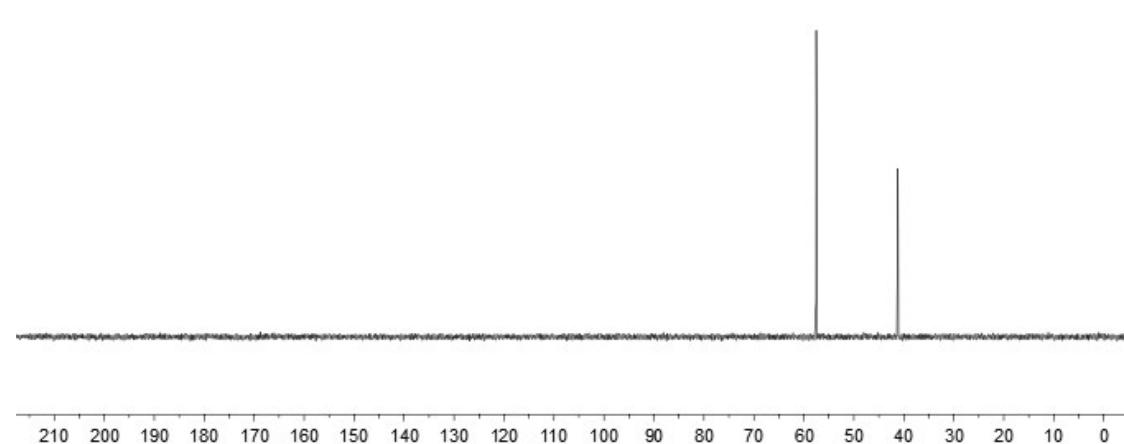
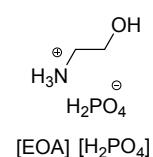
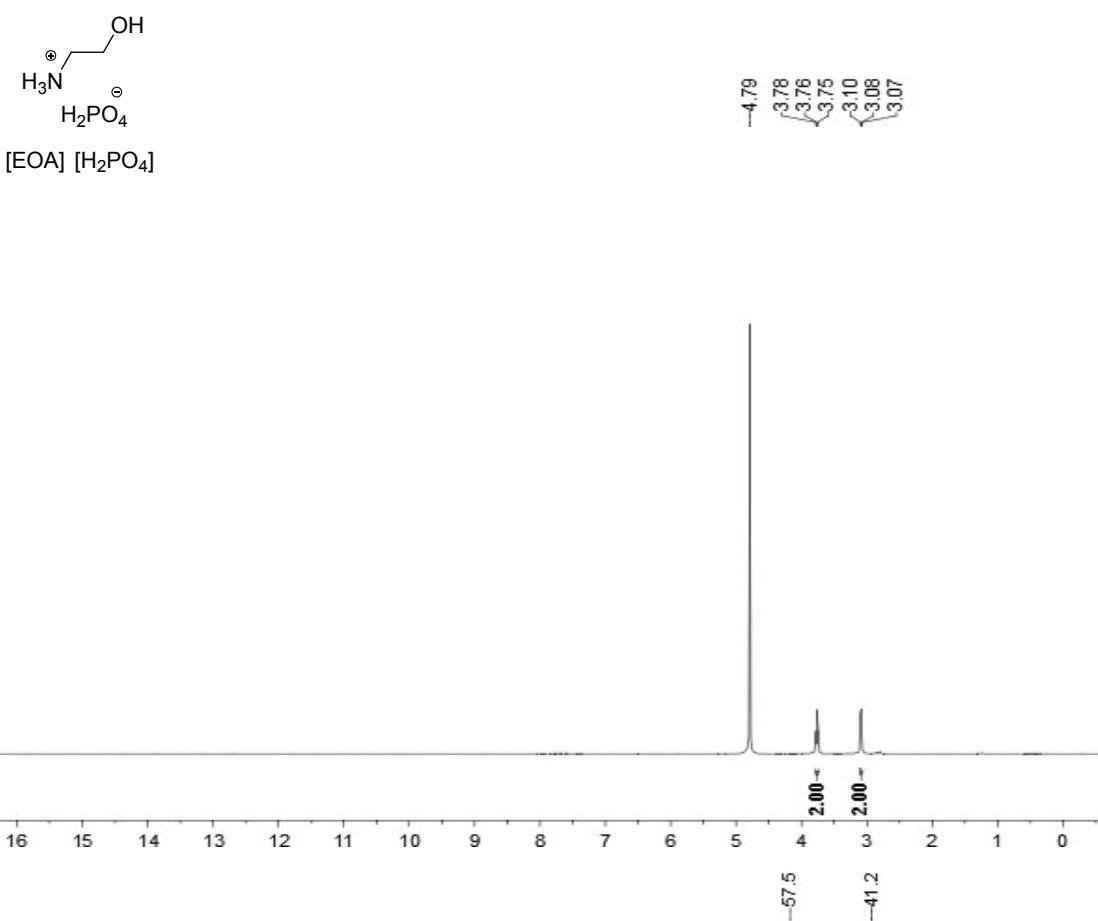
[TEA] [H₂PO₄]



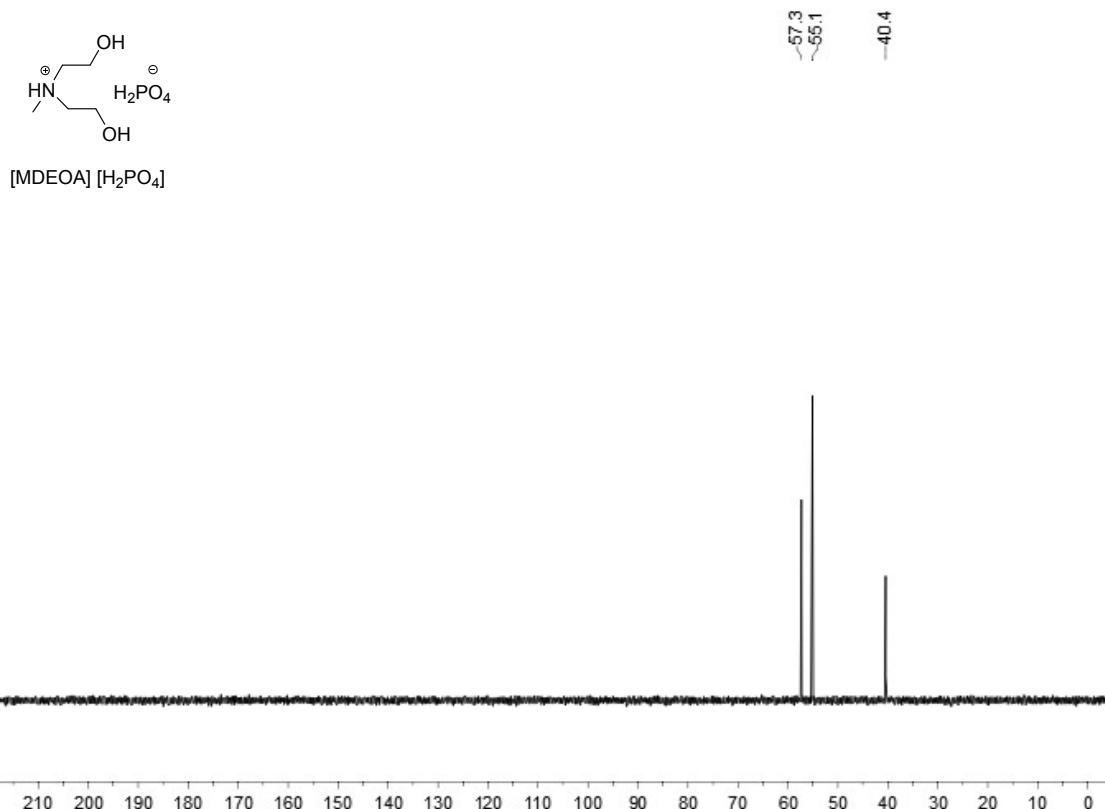
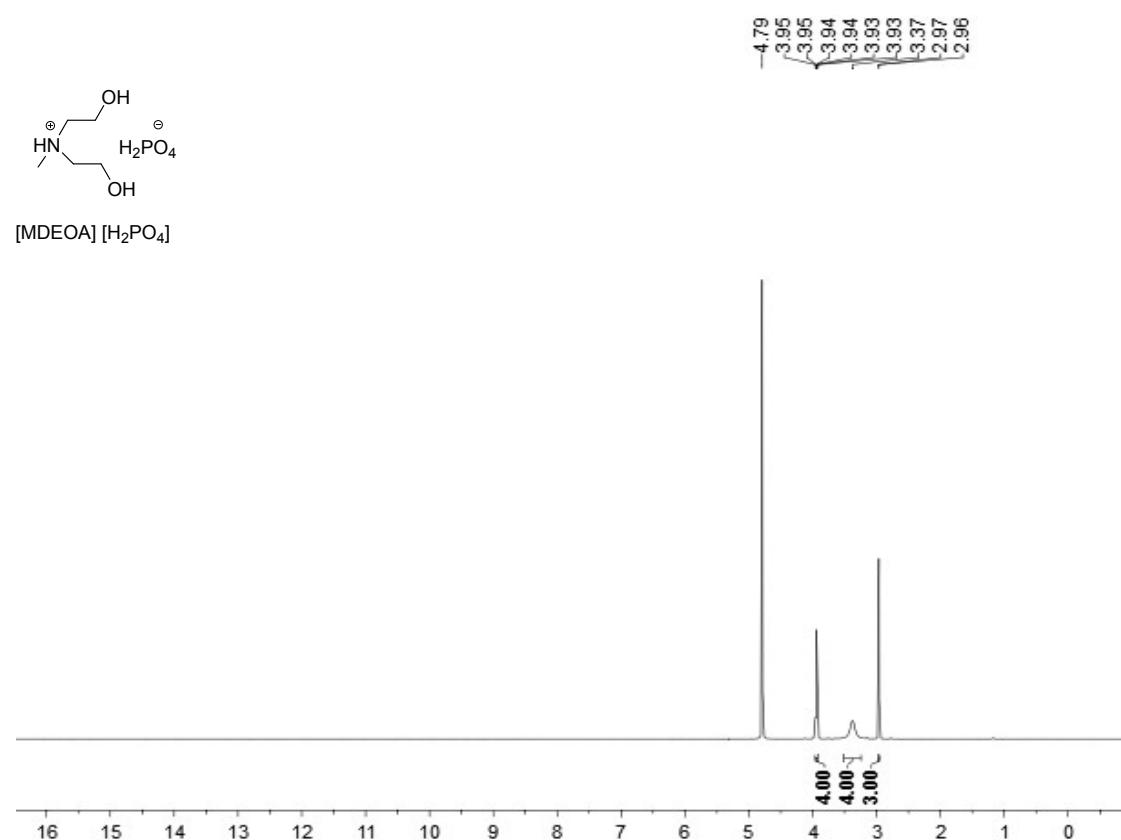
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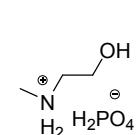
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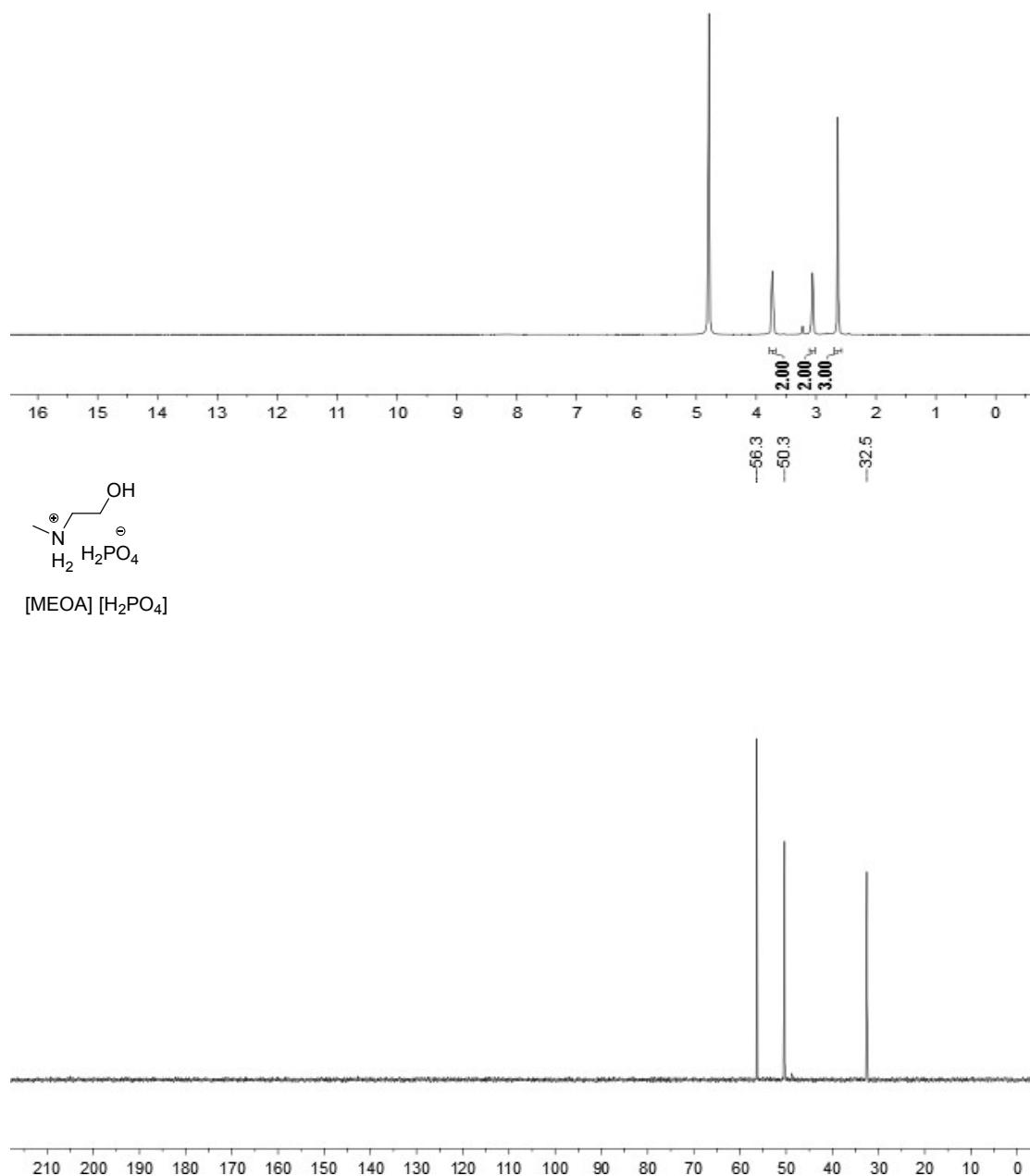
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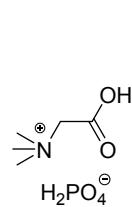
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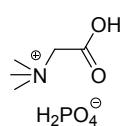
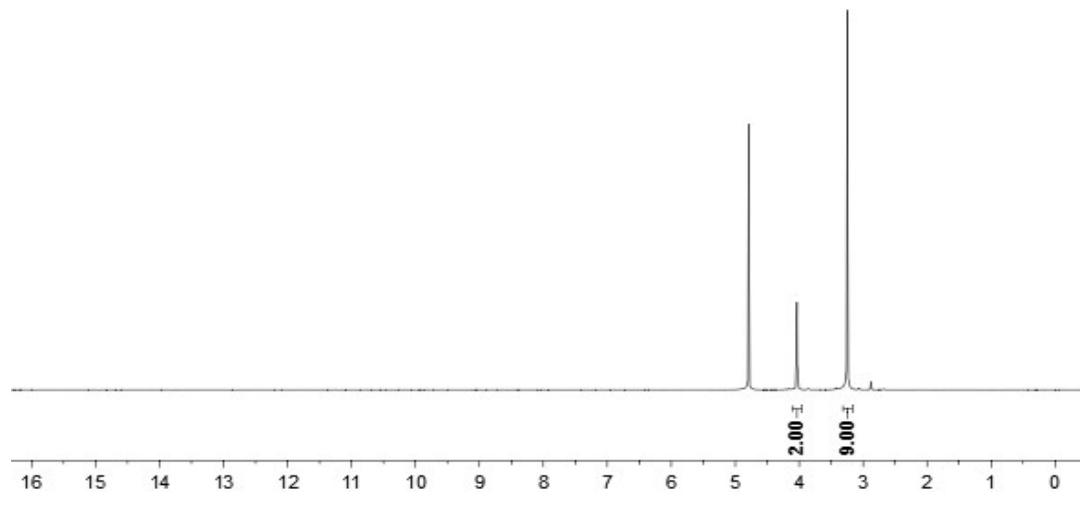
[MEOA] [H₂PO₄]



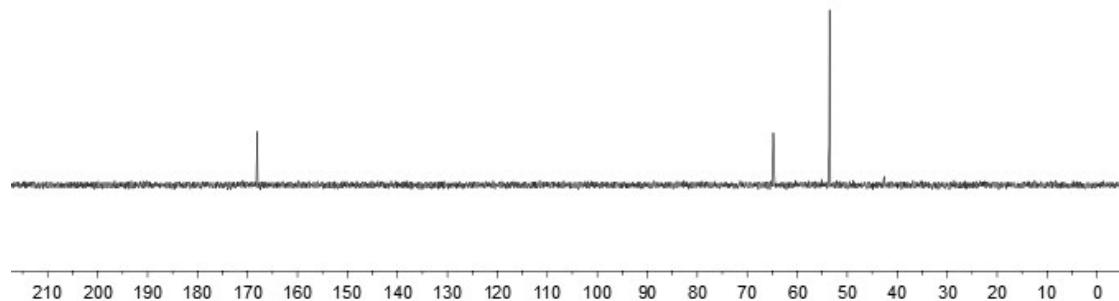
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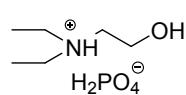
[Betaine][H₂PO₄]



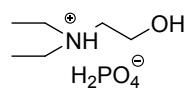
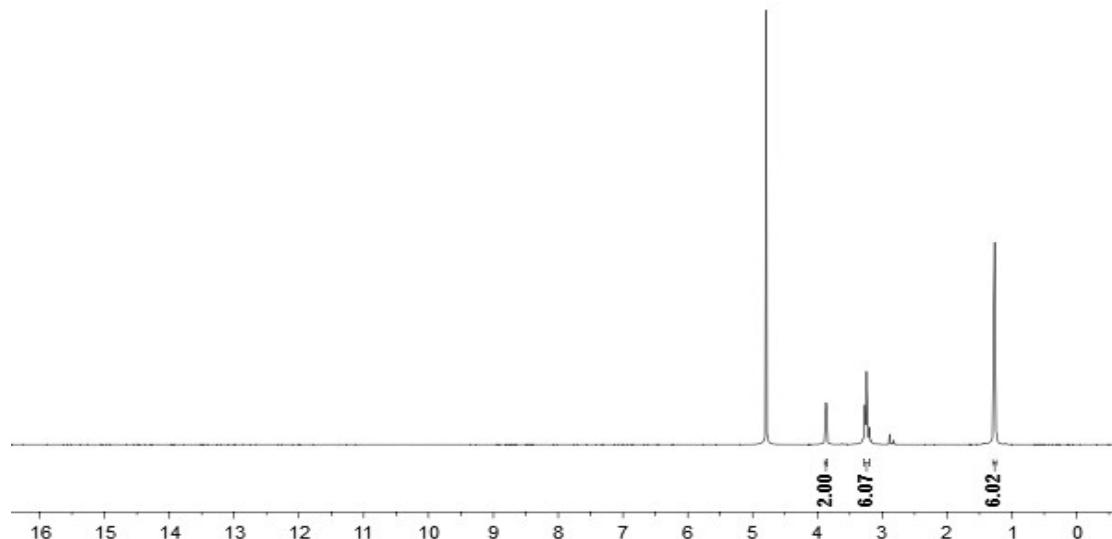
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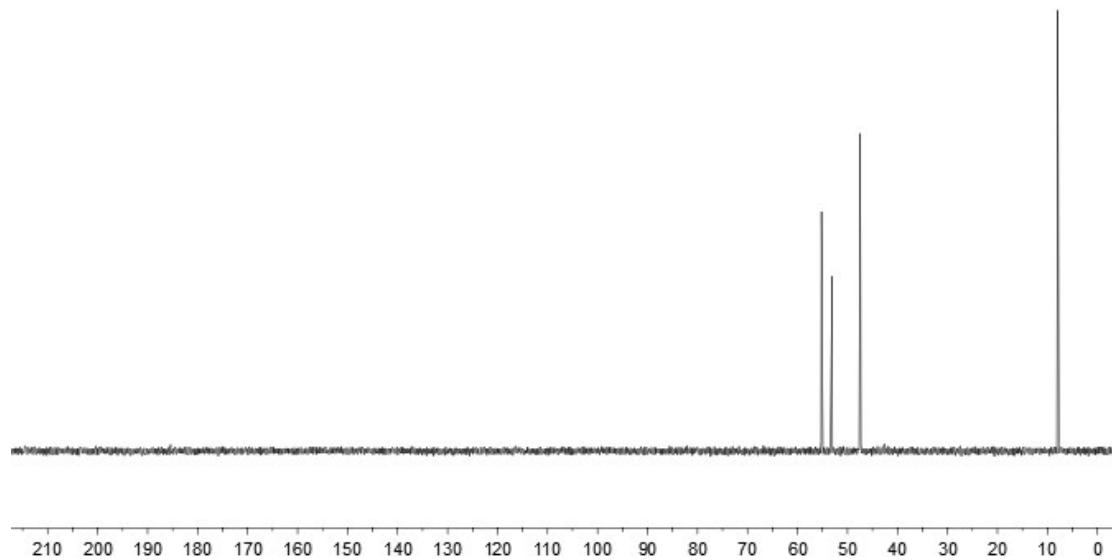
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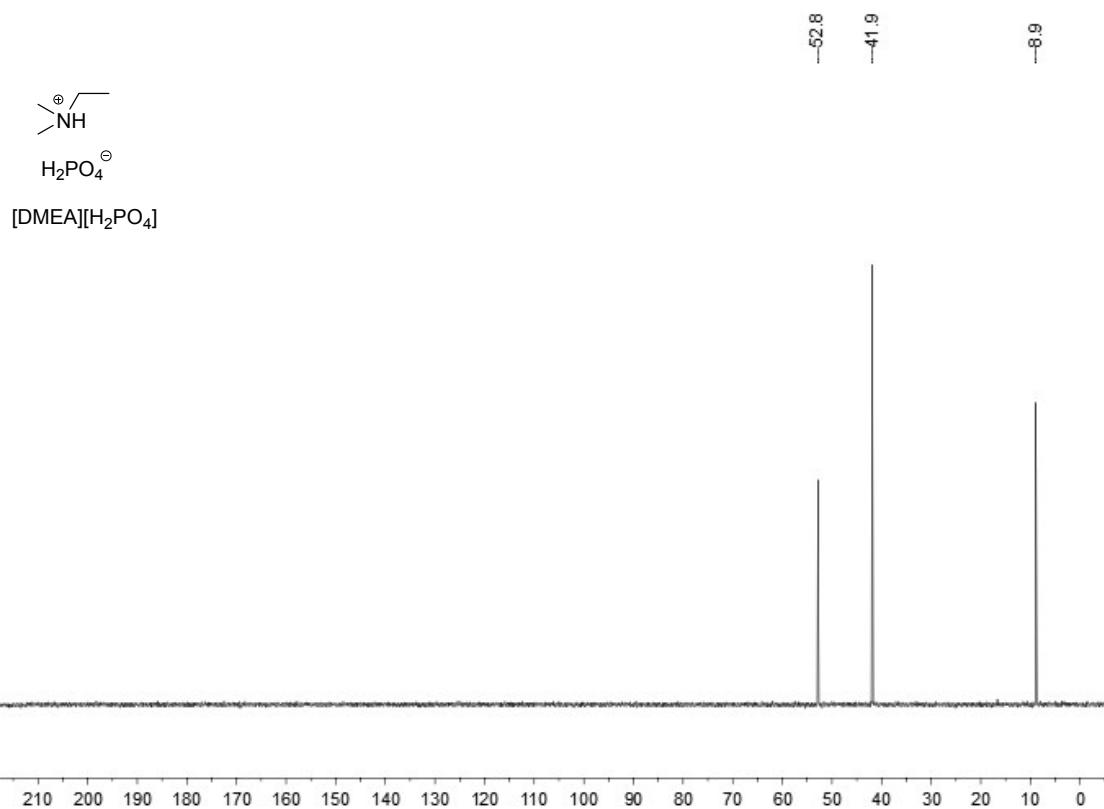
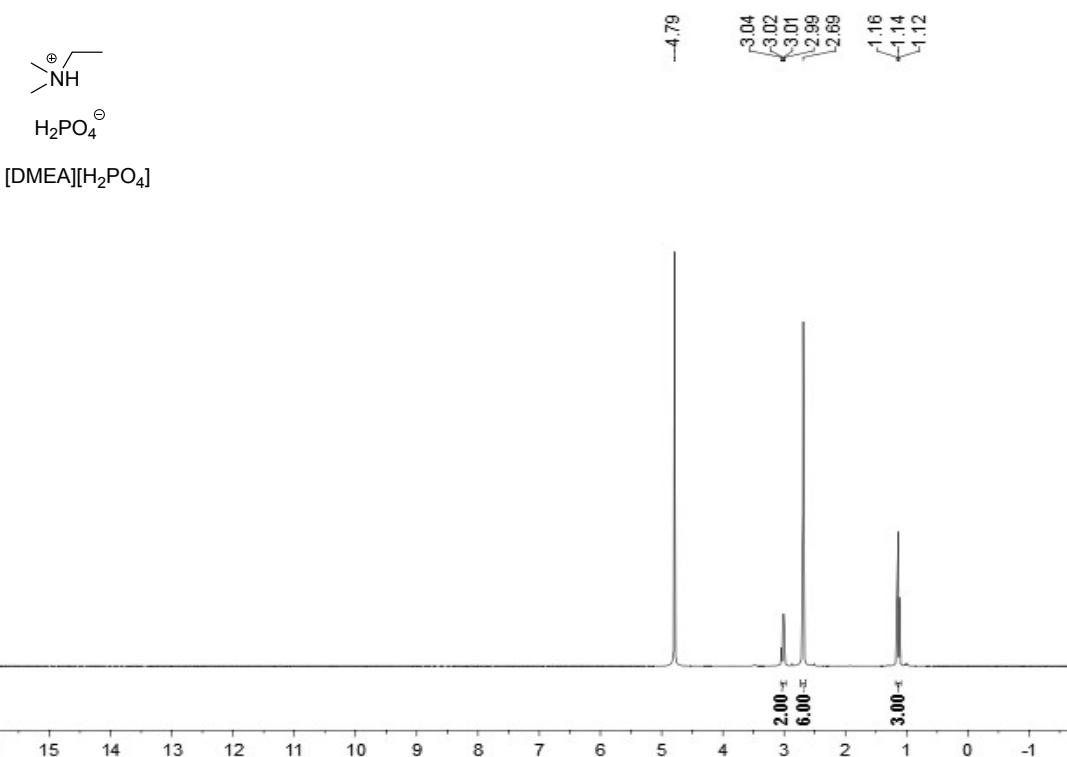
[DEEOA][H₂PO₄]



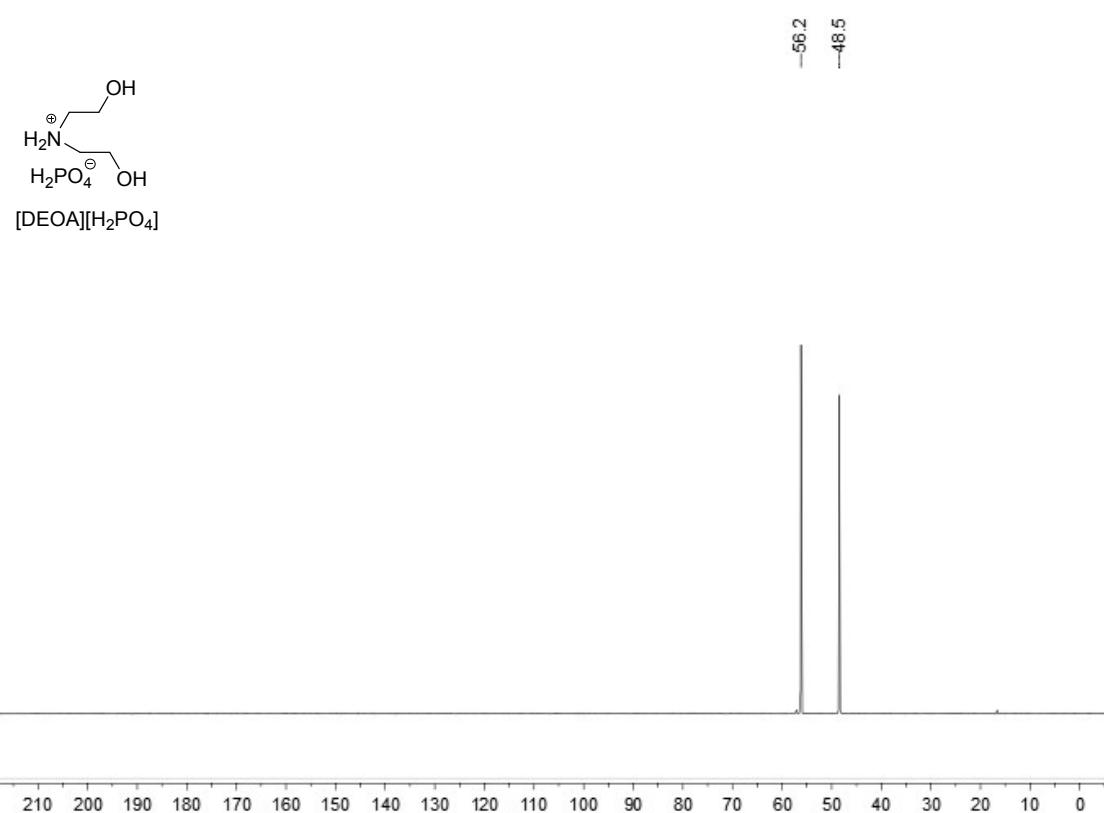
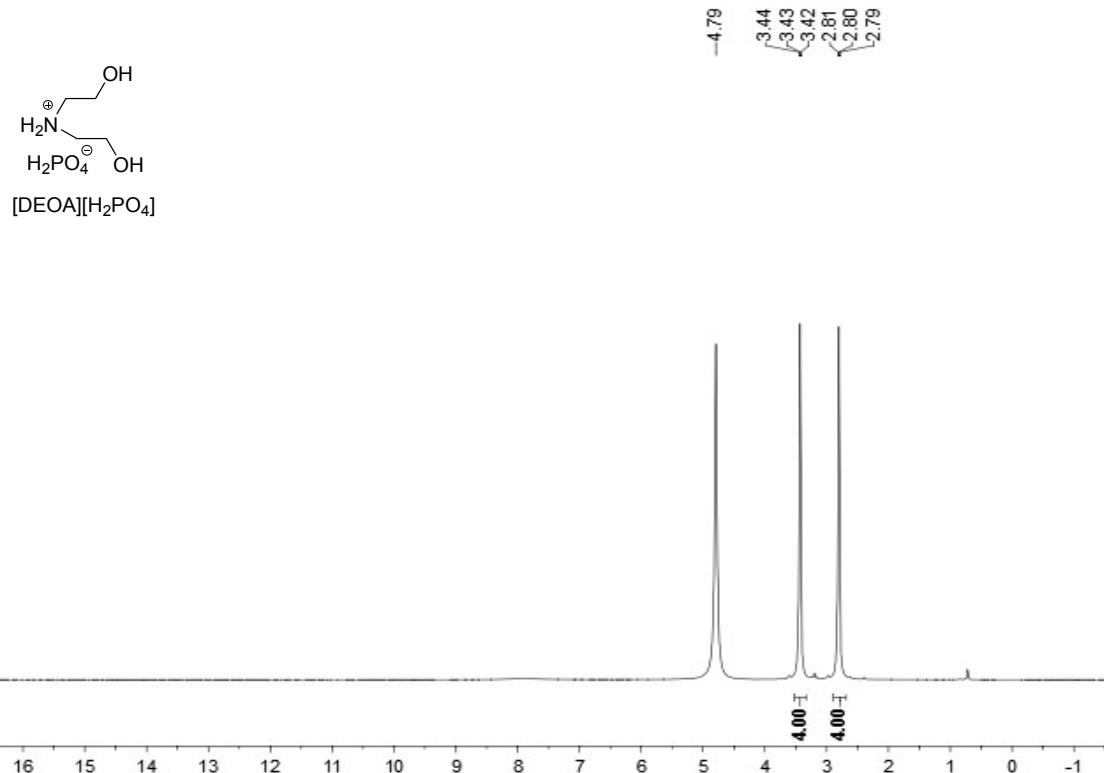
[DEEOA][H₂PO₄]



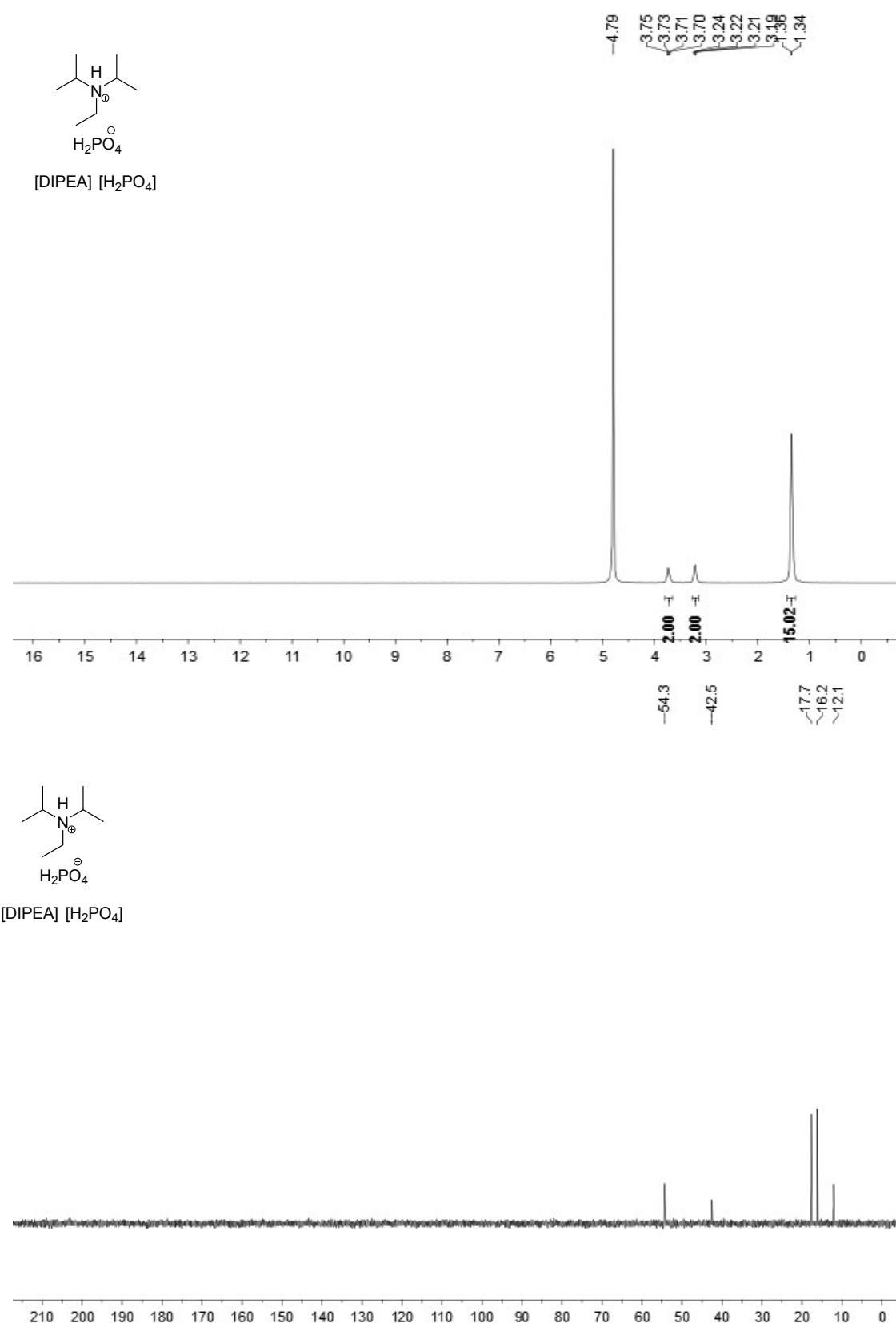
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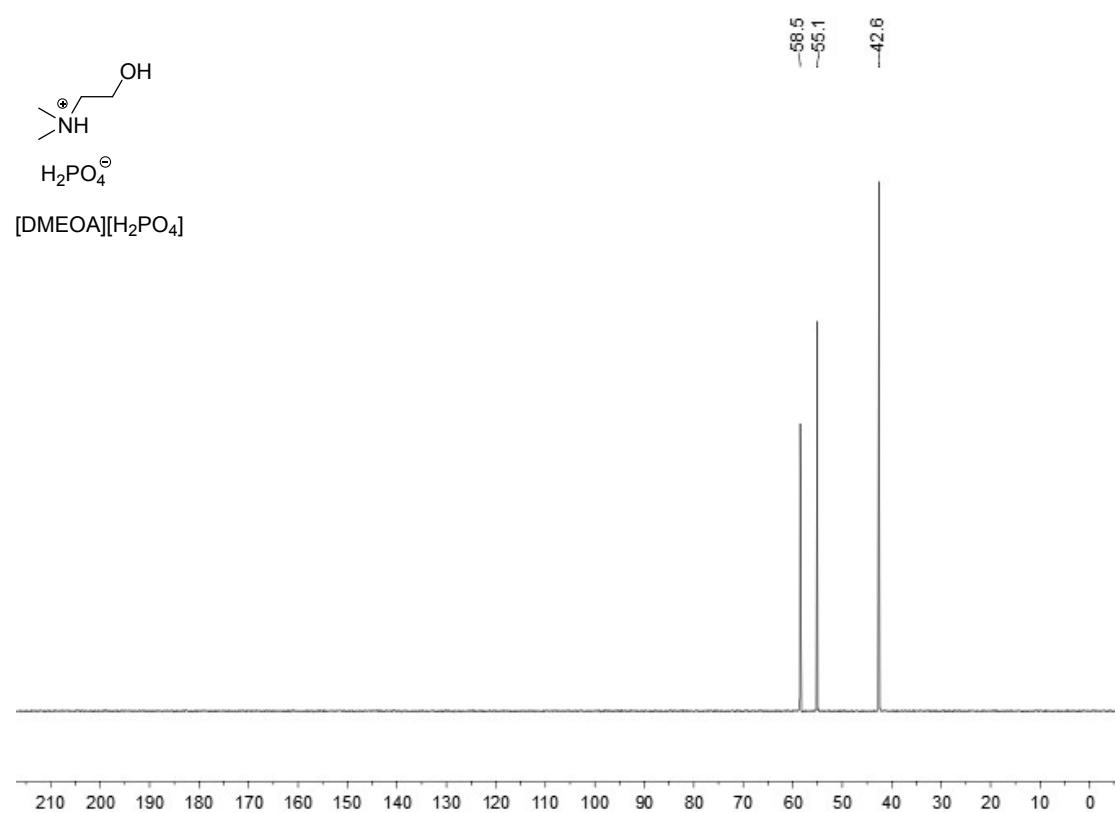
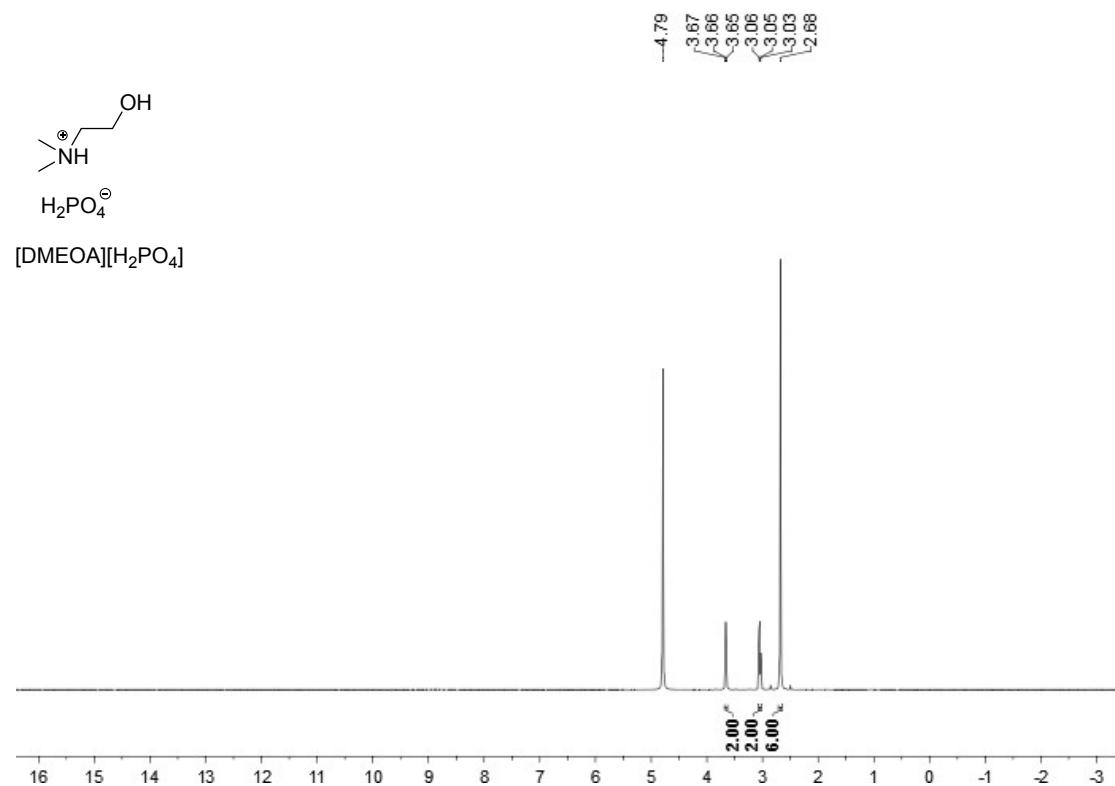
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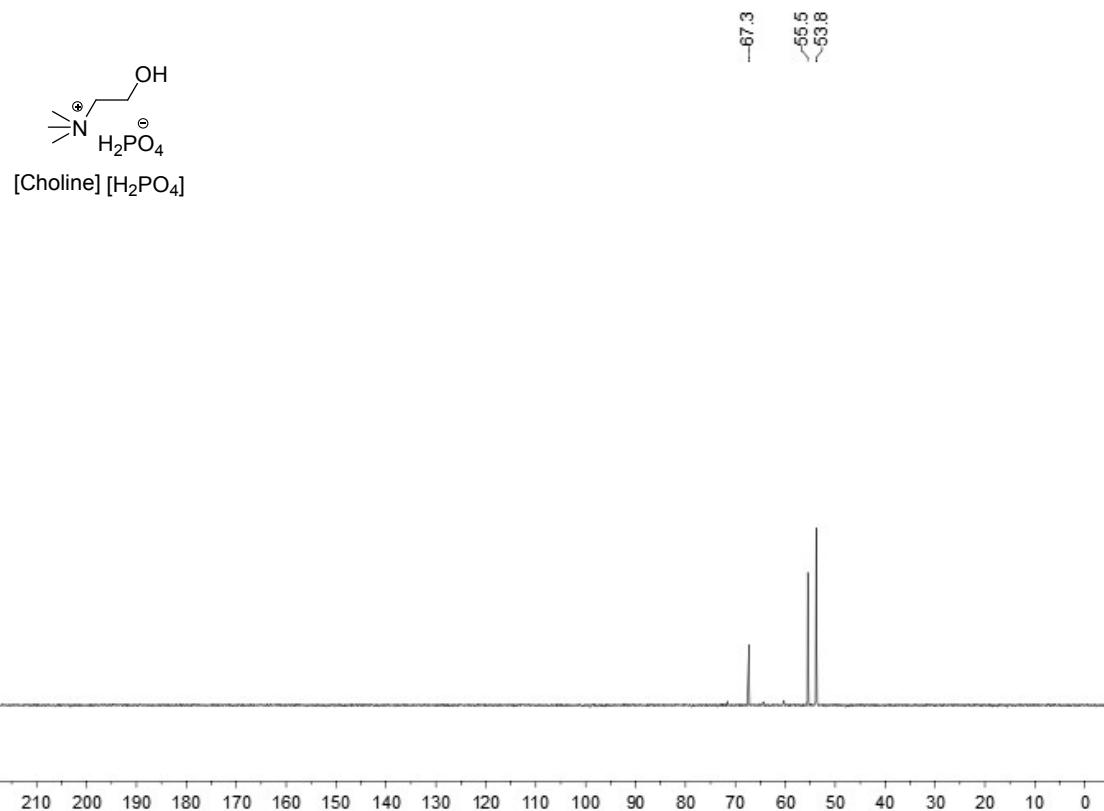
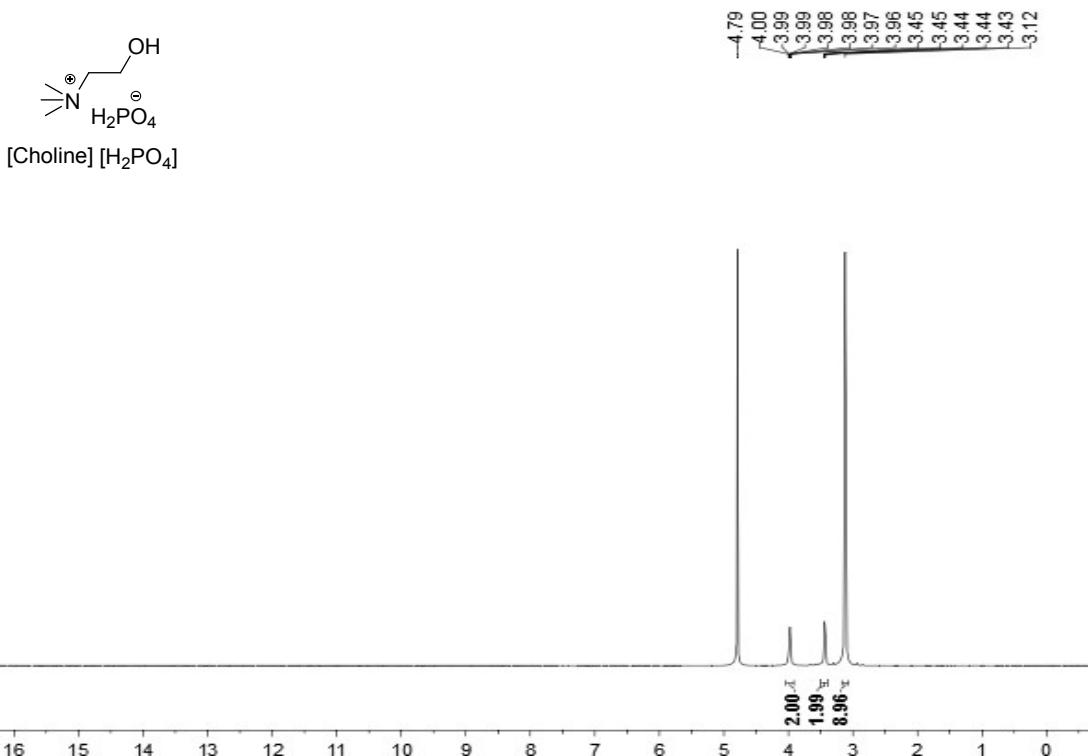
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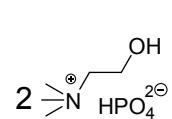
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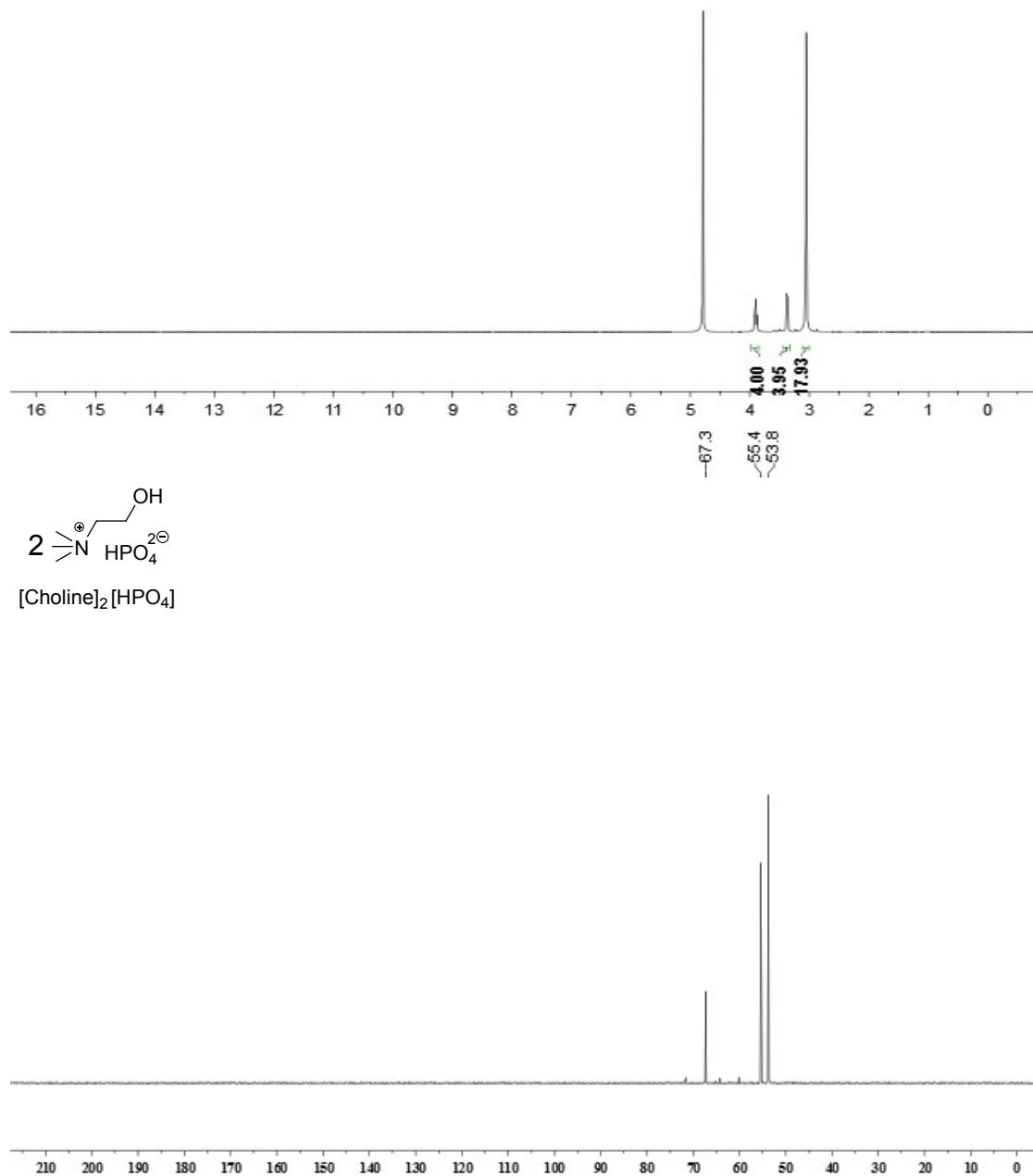
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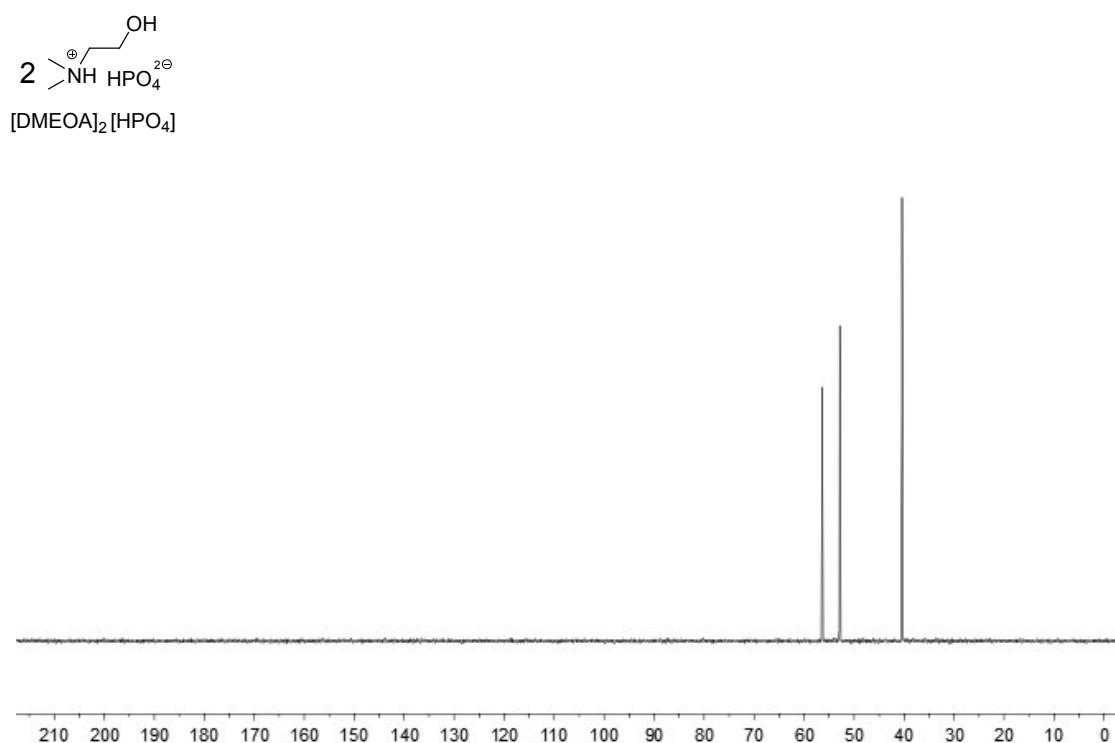
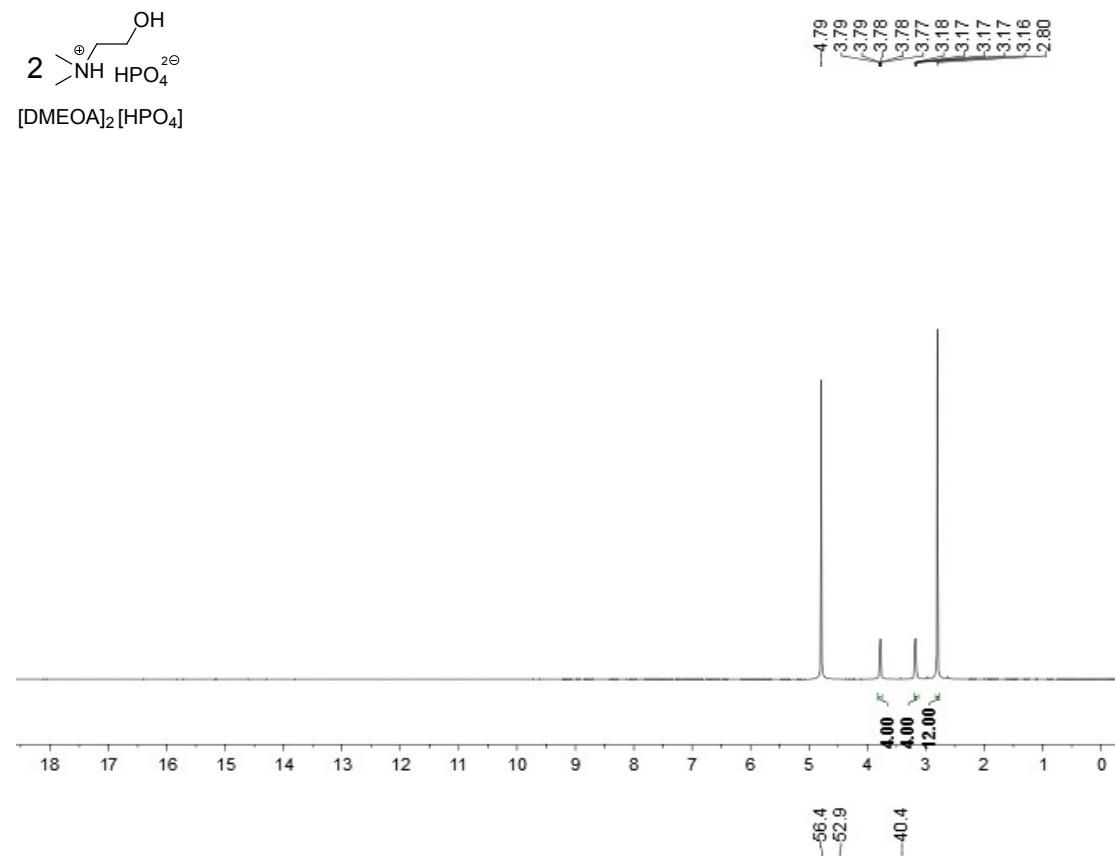
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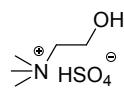
[Choline]₂[HPO₄]



15.

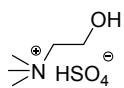
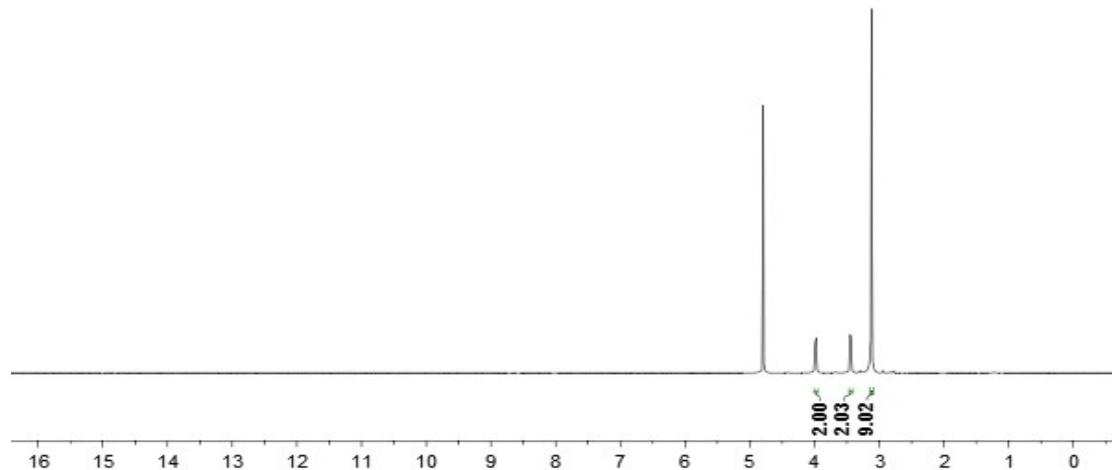


16.



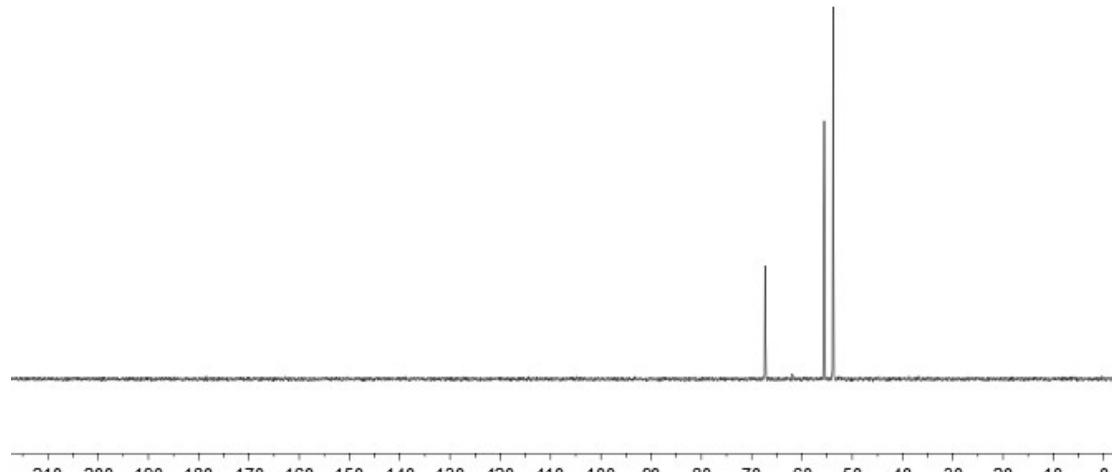
[Choline] [HSO₄]

-4.79
-4.00
-3.99
-3.99
-3.98
-3.98
-3.97
-3.97
-3.96
-3.45
-3.44
-3.44
-3.43
-3.43
-3.12

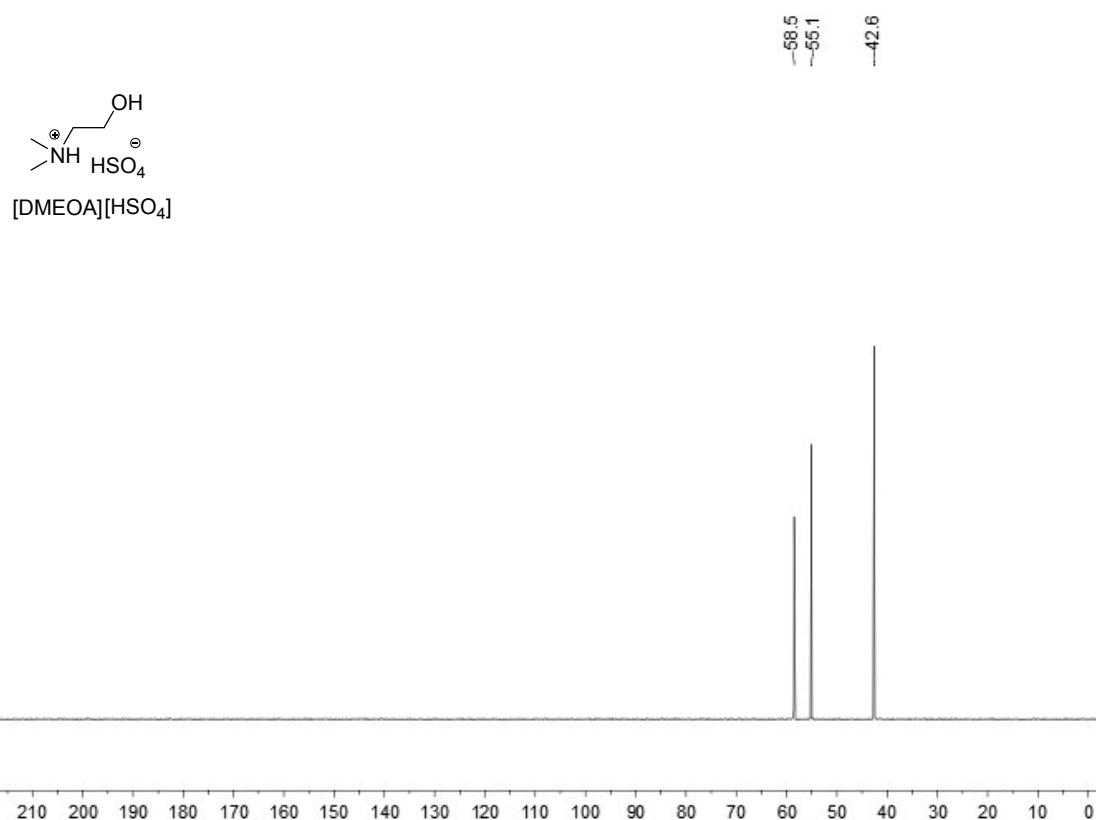
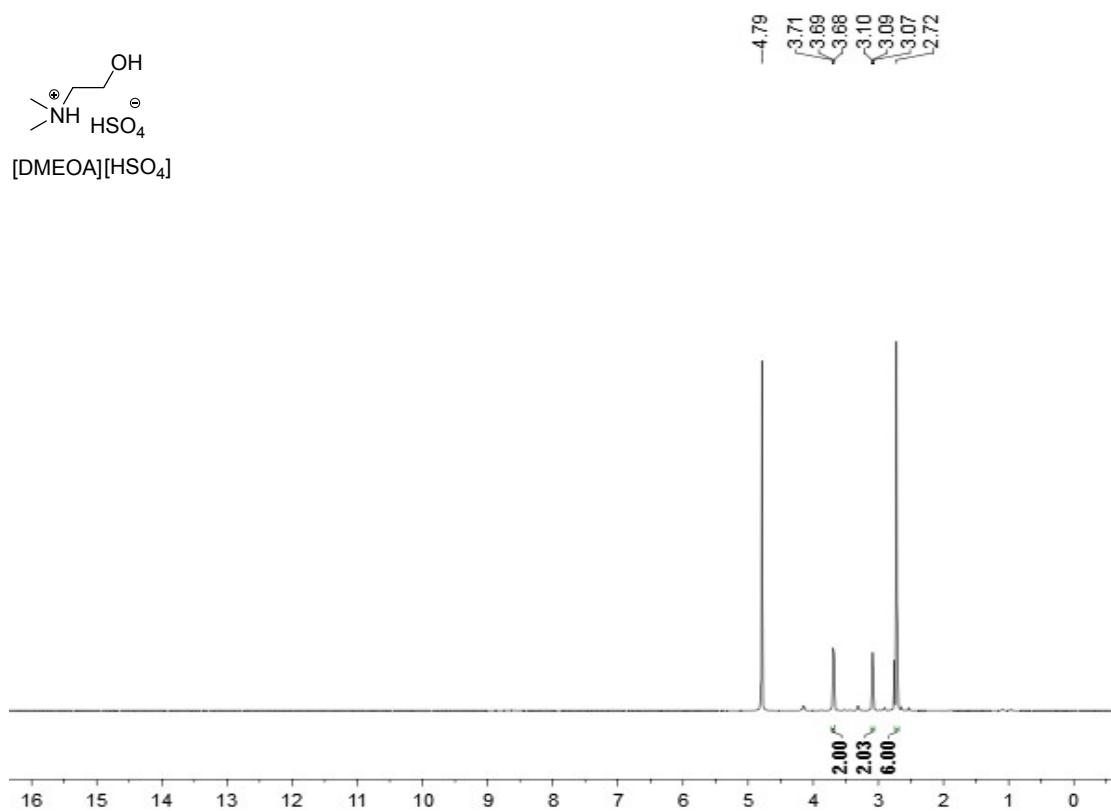


[Choline] [HSO₄]

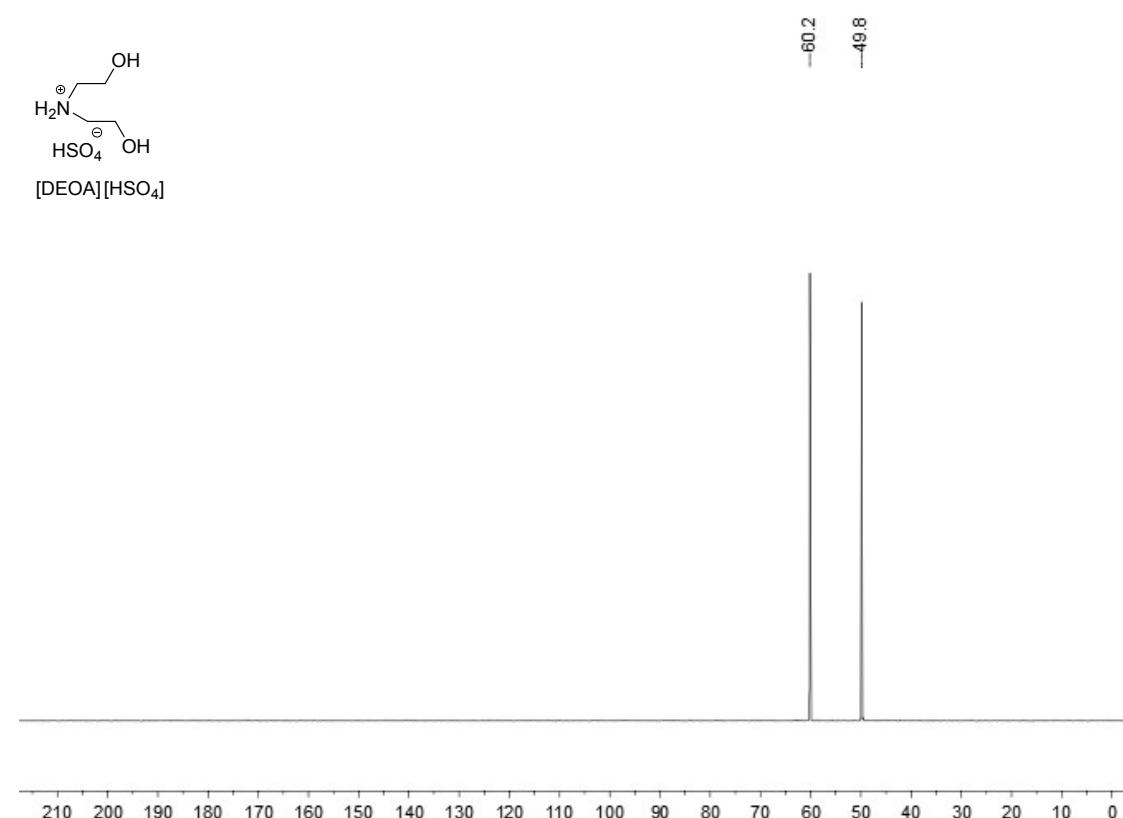
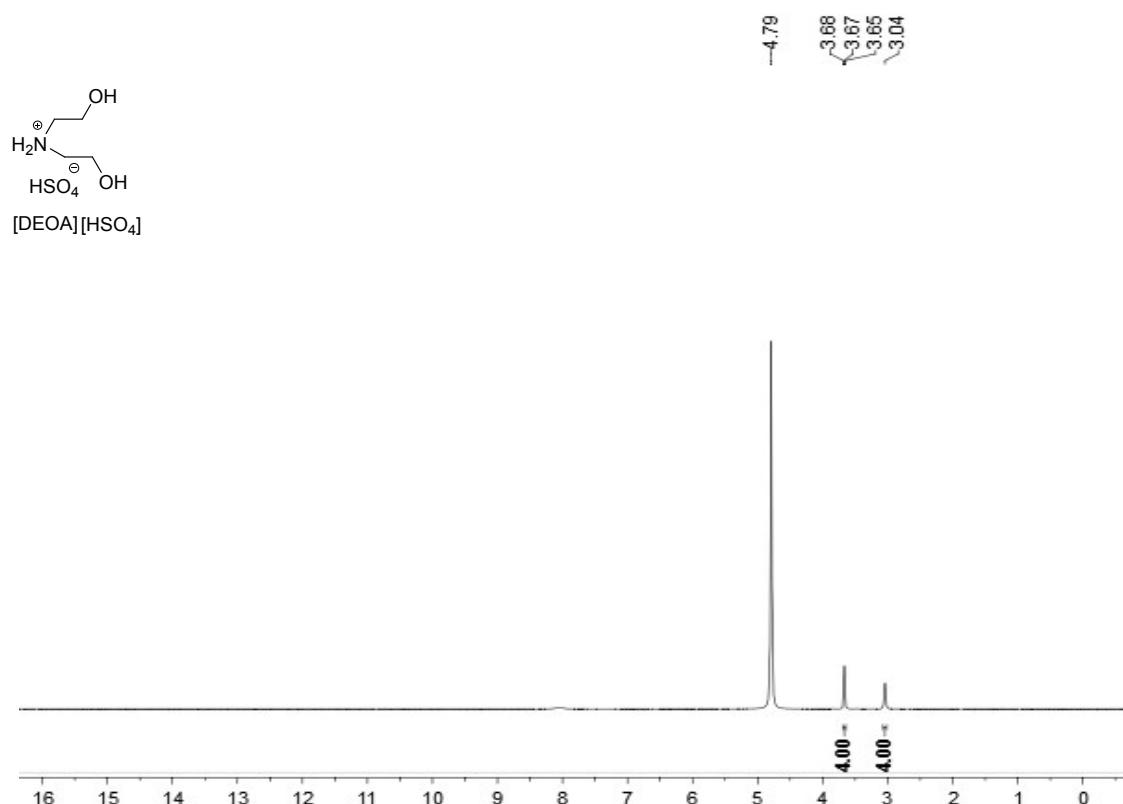
-67.3
-55.6
-53.8



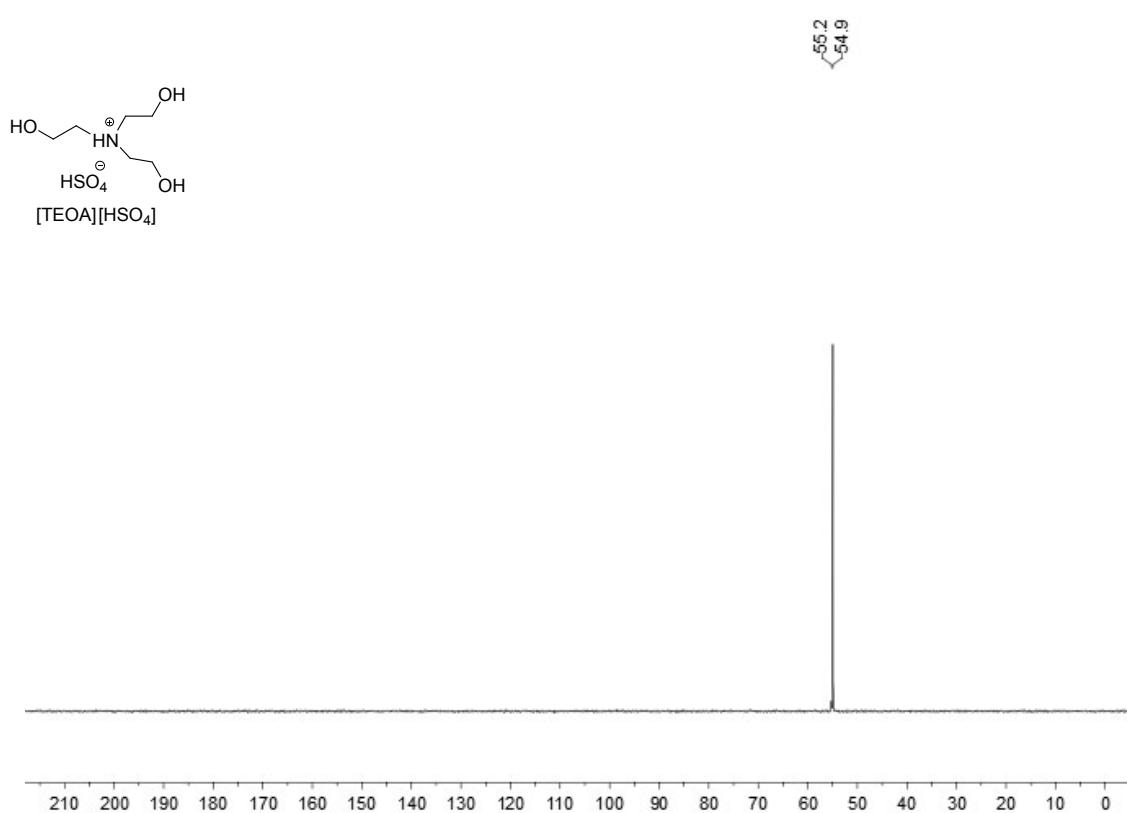
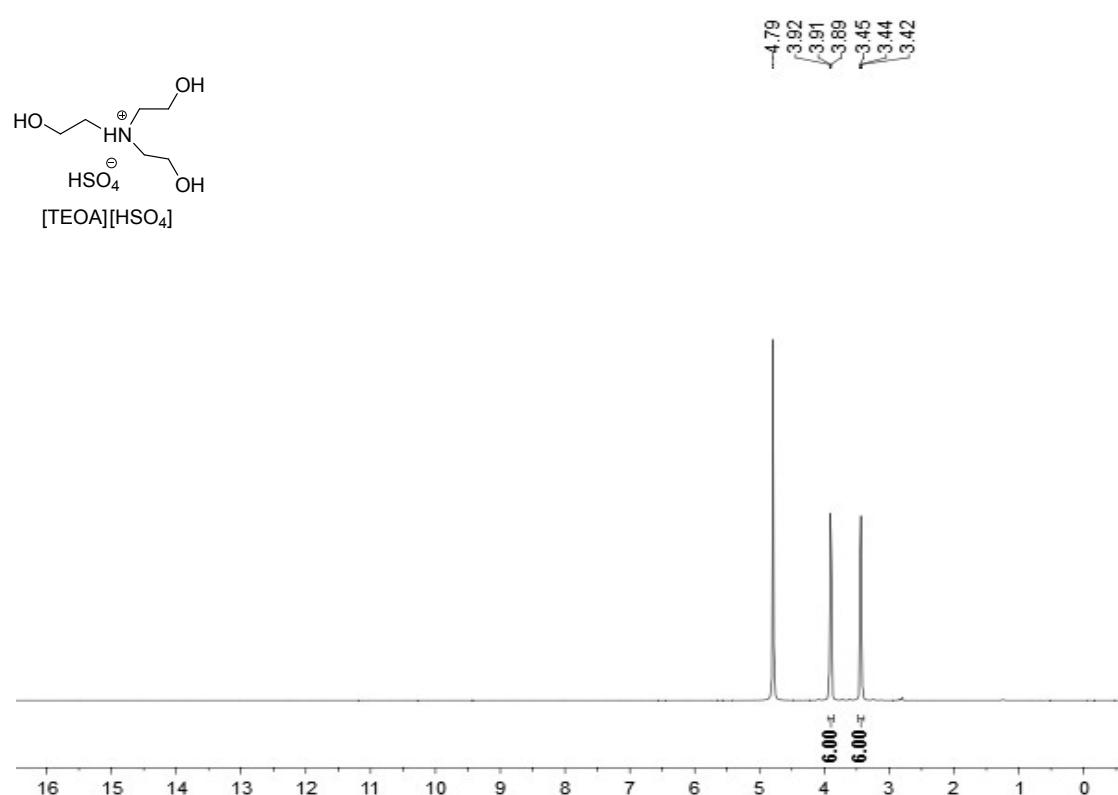
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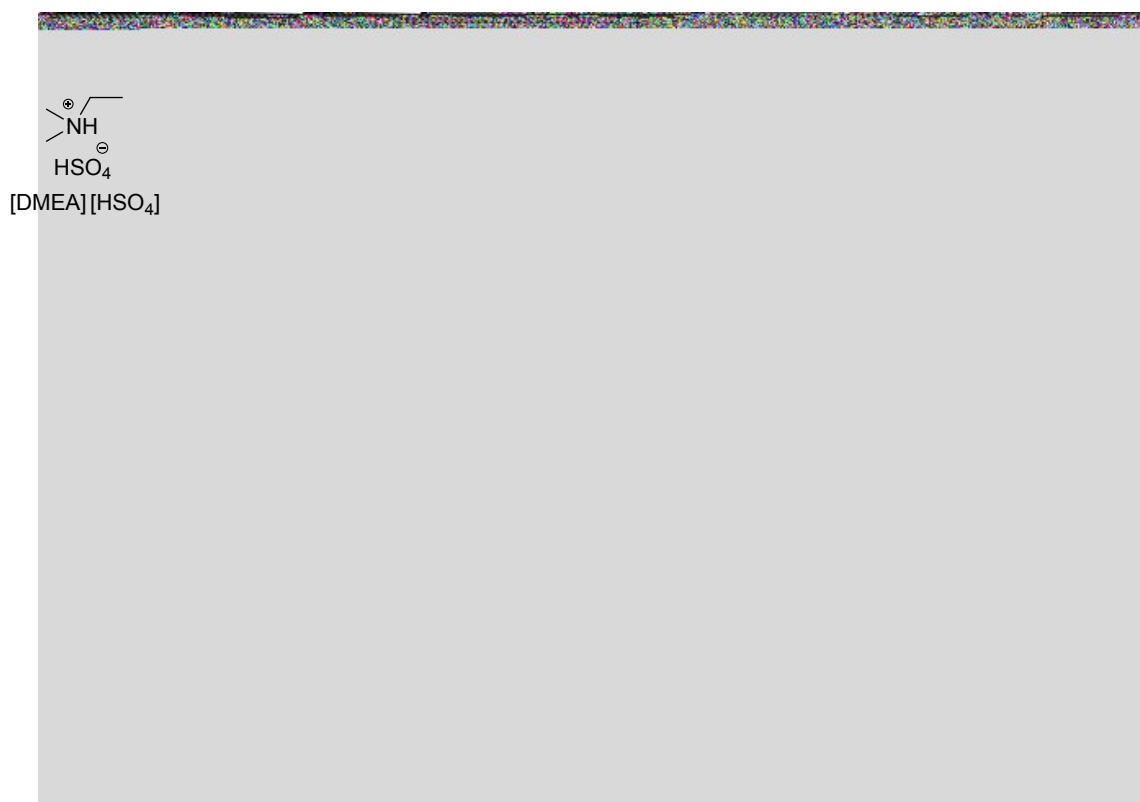
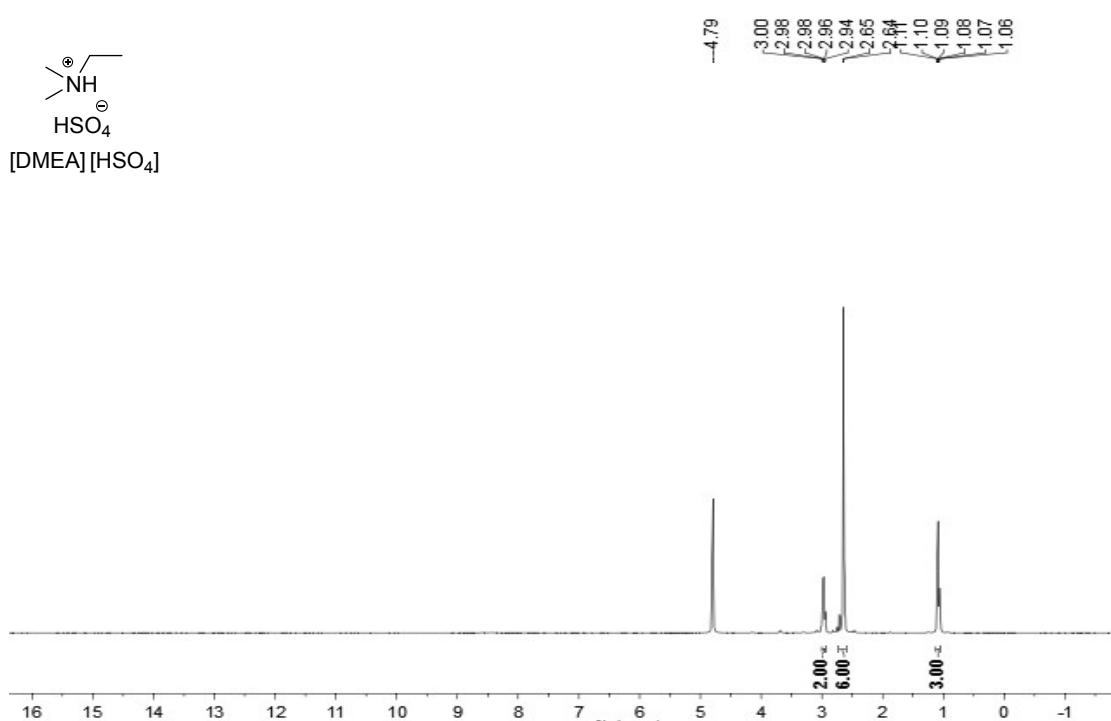
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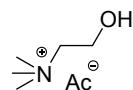
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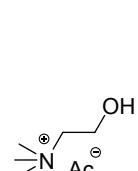
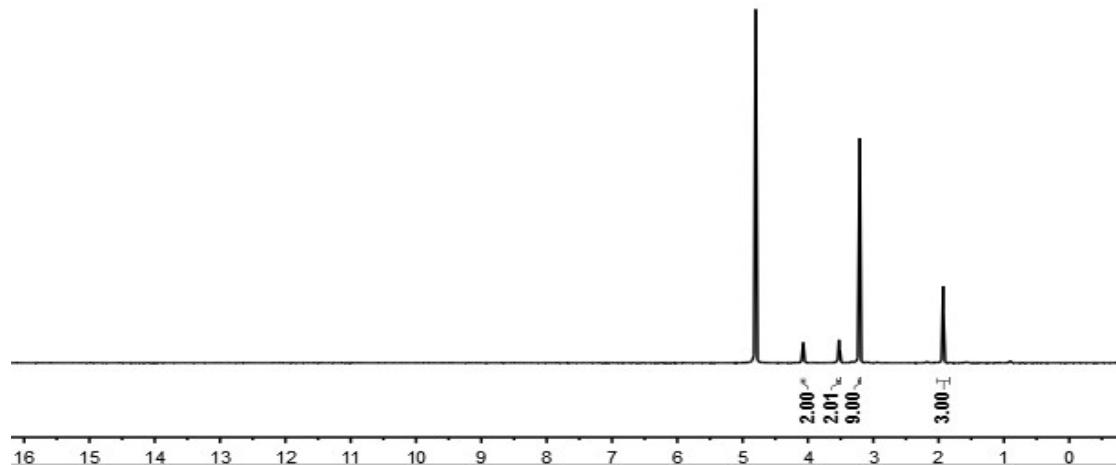
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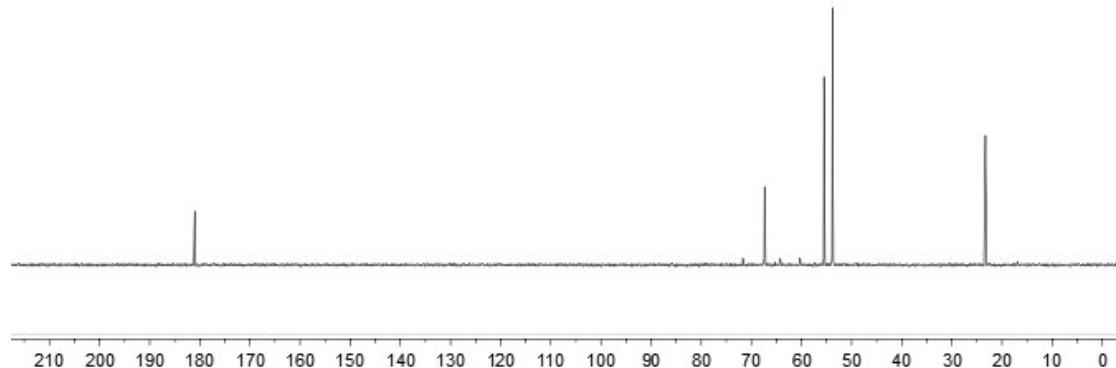
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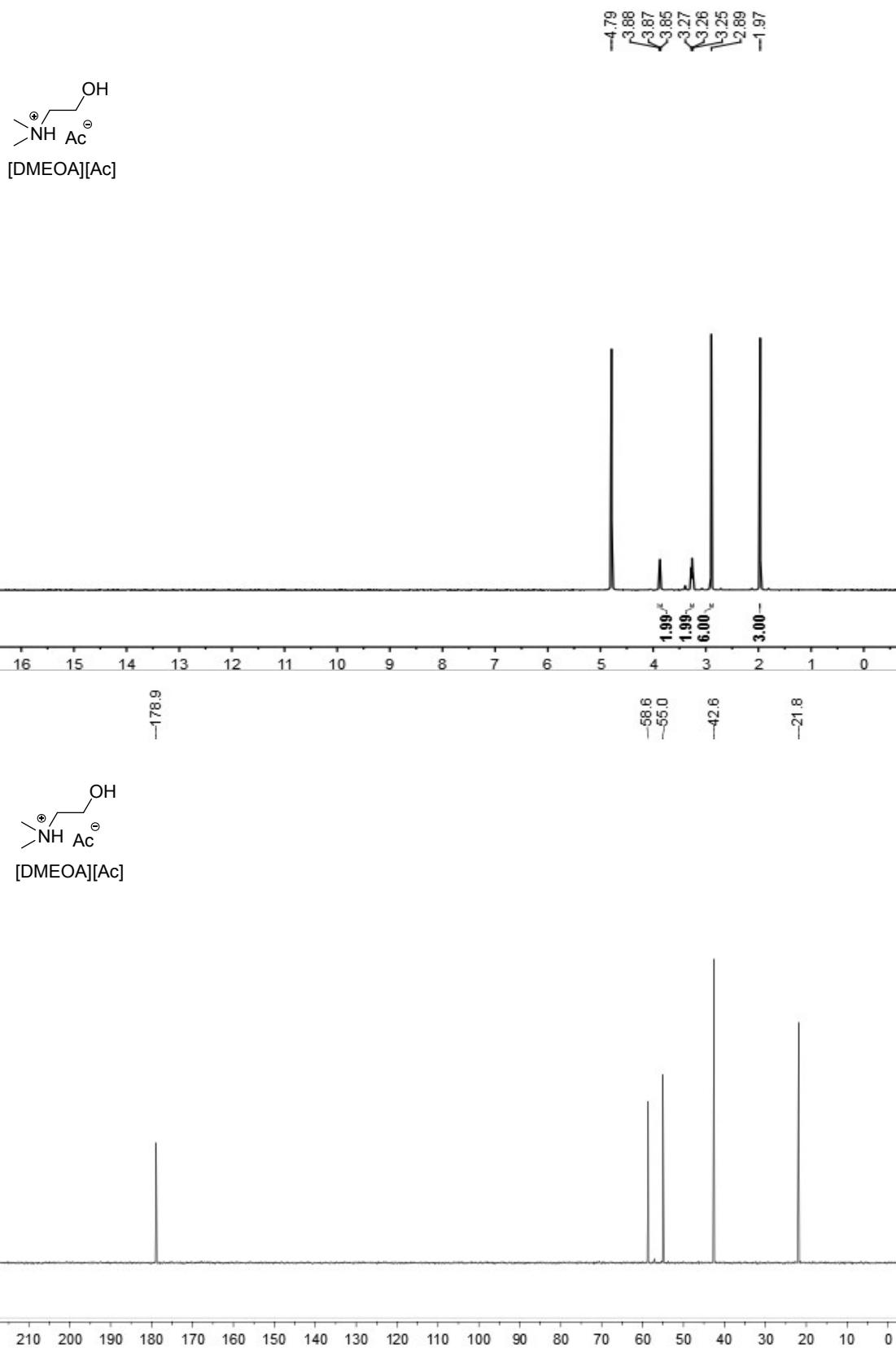
[Choline] [Ac]



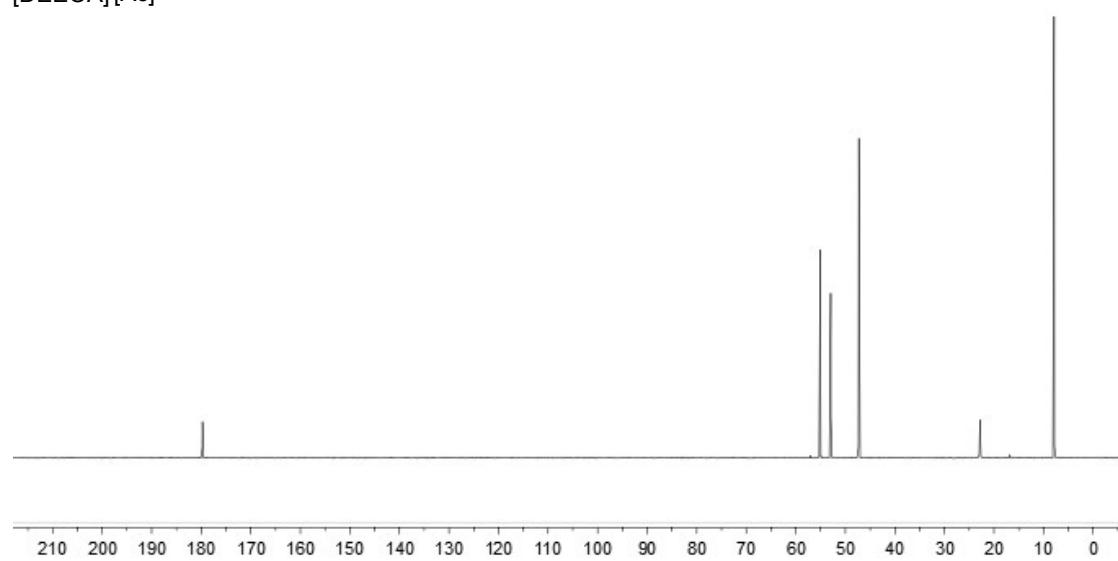
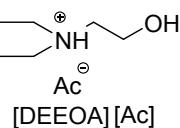
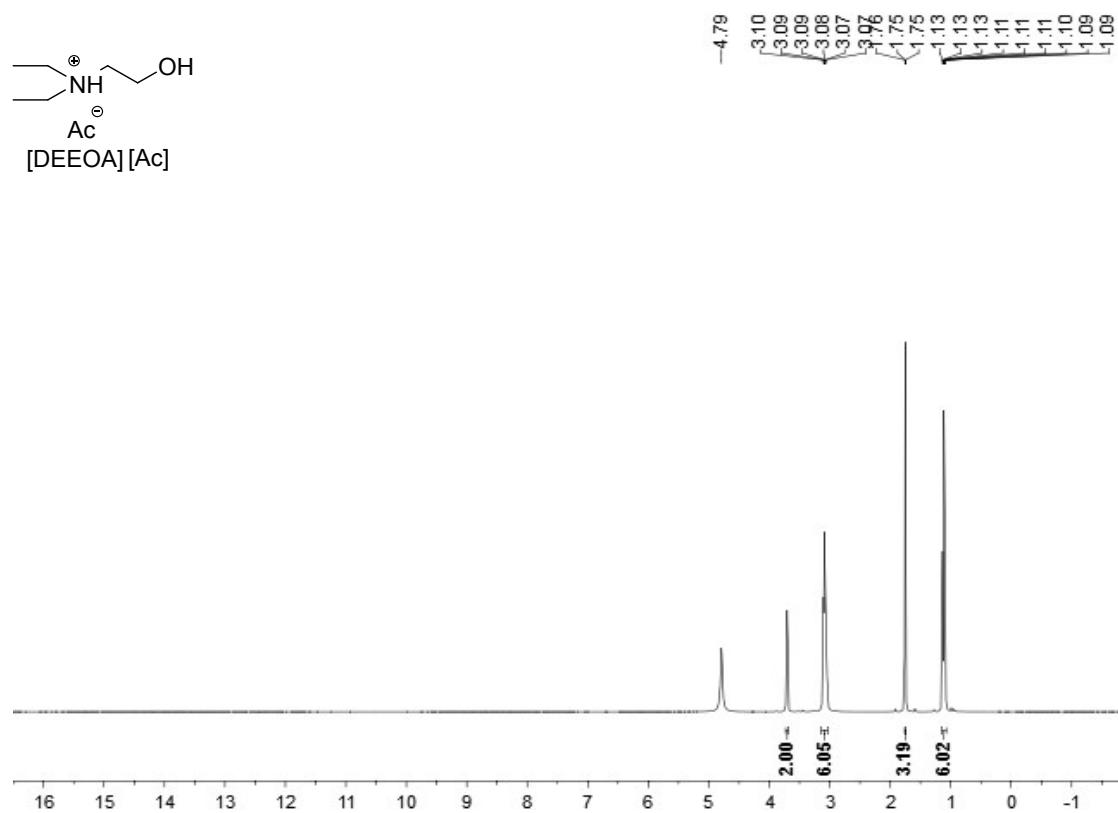
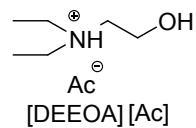
[Choline] [Ac]



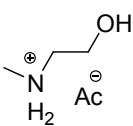
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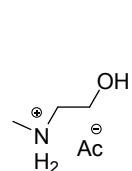
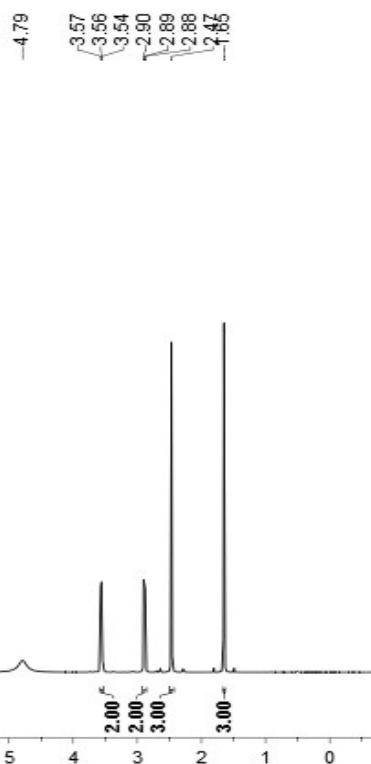
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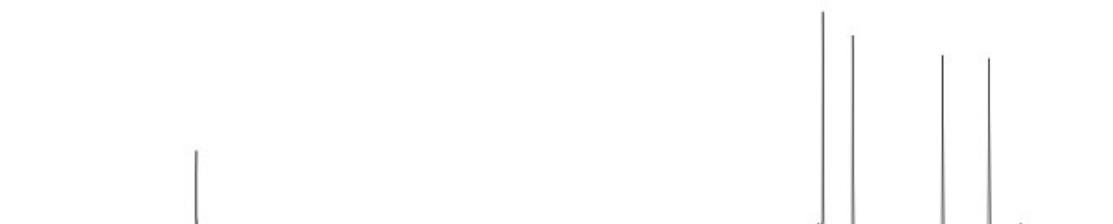
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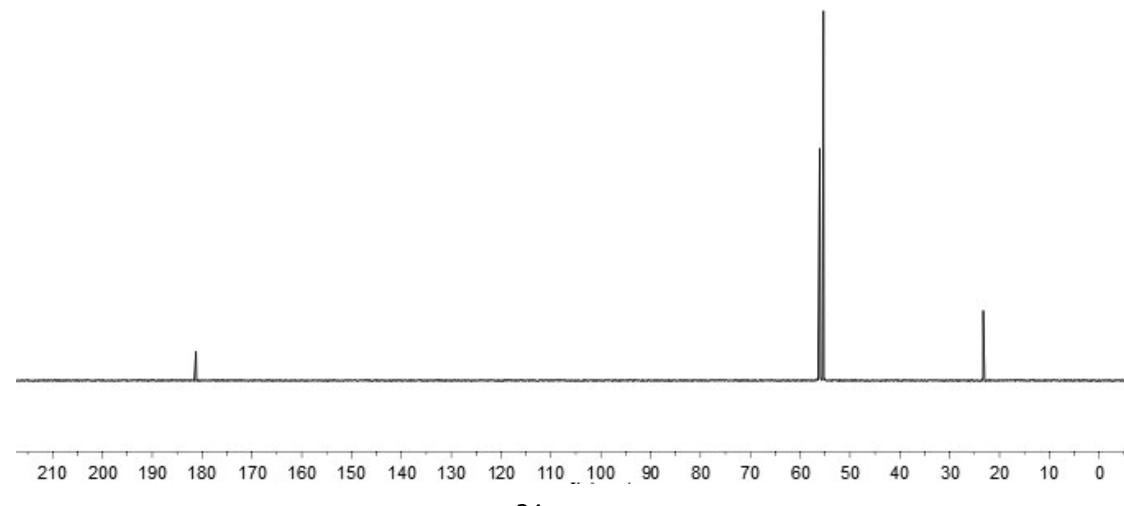
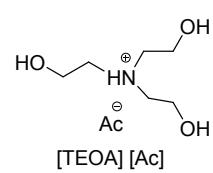
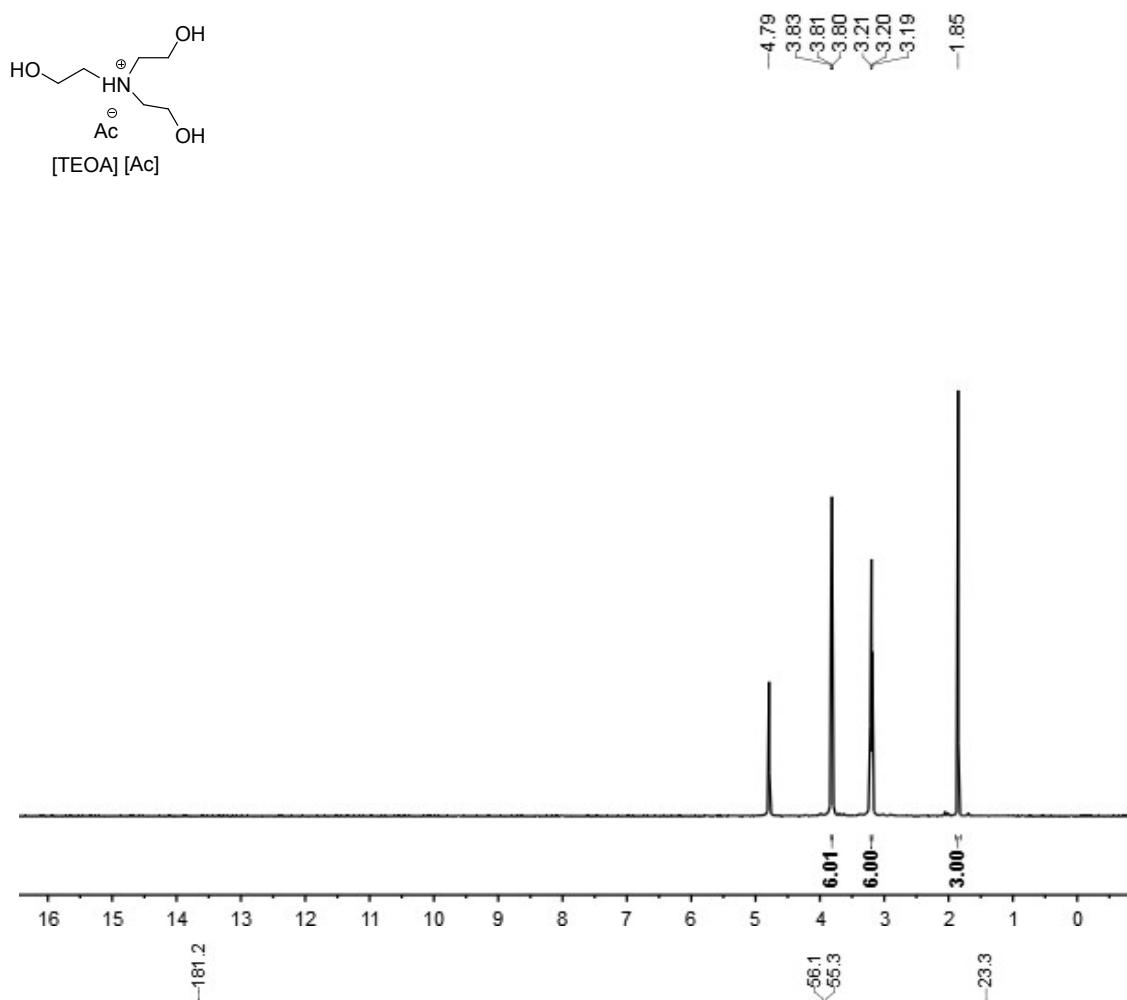
[MEOA][Ac]



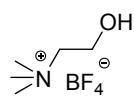
[MEOA][Ac]



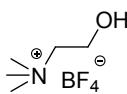
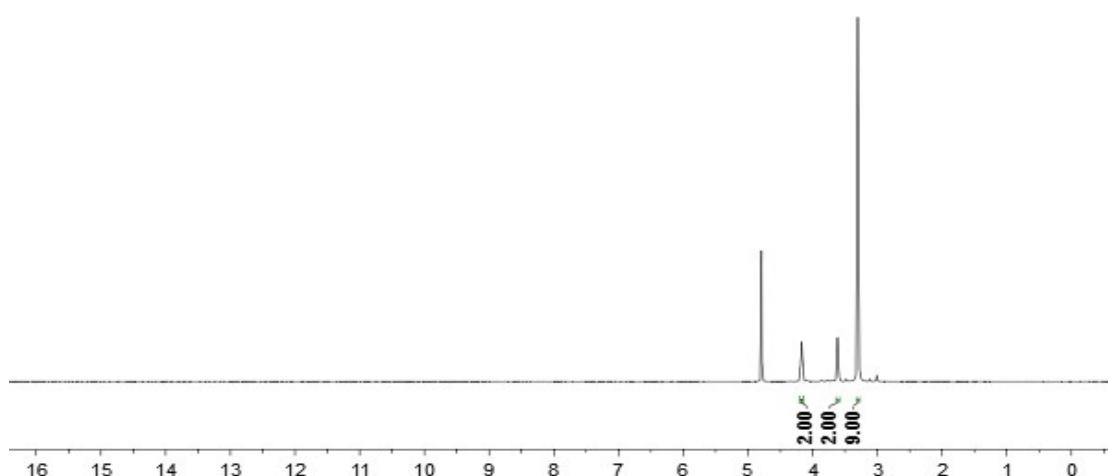
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26.

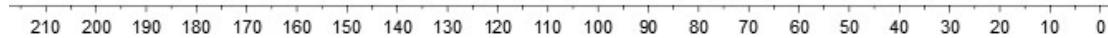


[Choline][BF₄]

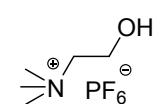


[Choline][BF₄]

-67.5
~55.7
~53.9

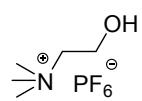
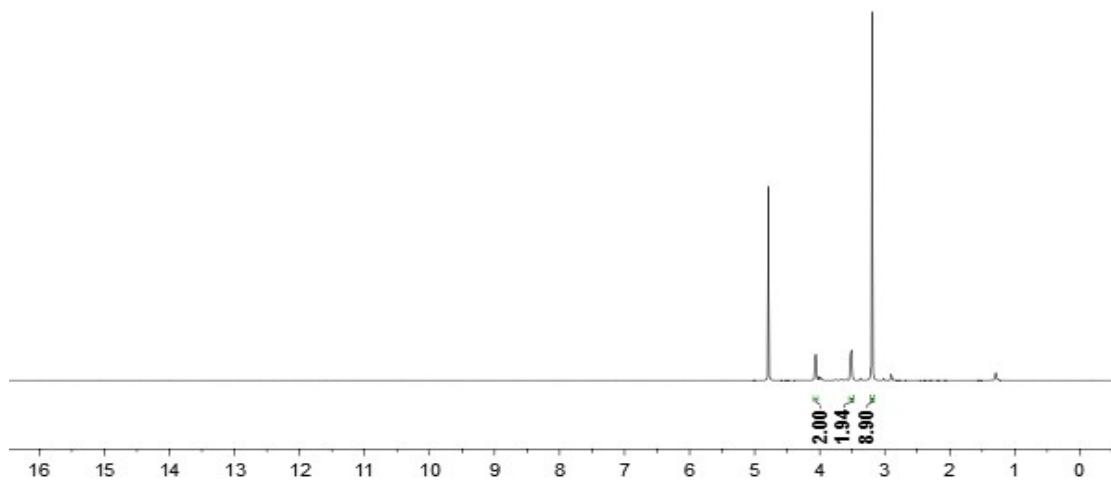


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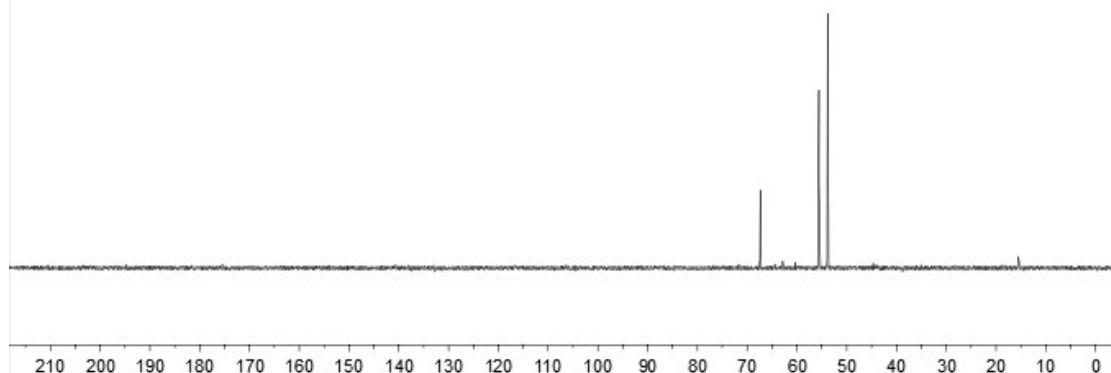
[Choline][PF₆]

4.79
4.08
4.07
4.06
4.05
4.04
3.52
3.51
3.50
3.20

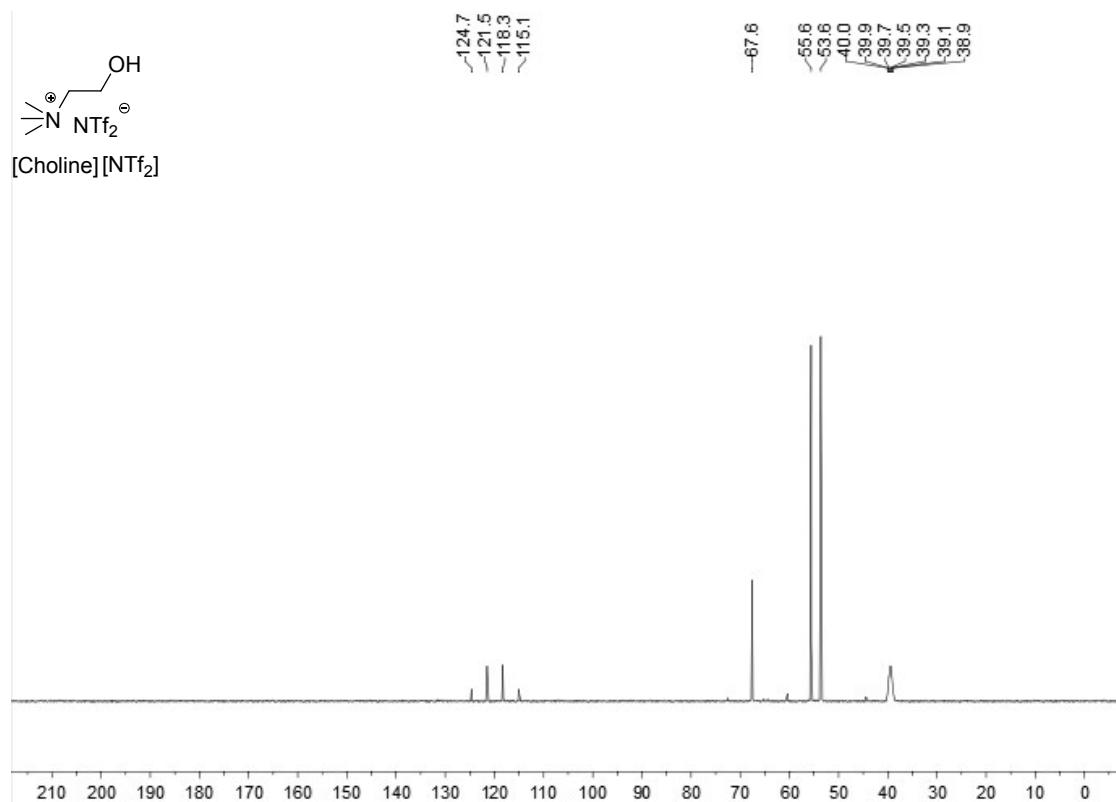
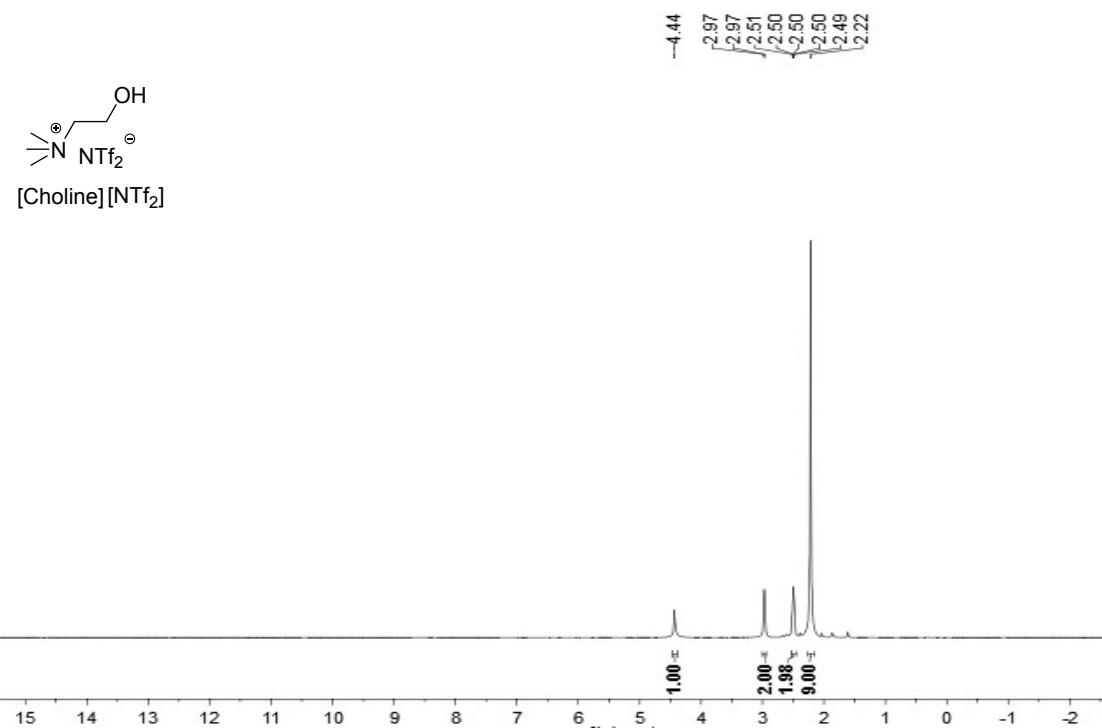


[Choline][PF₆]

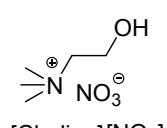
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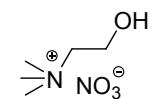
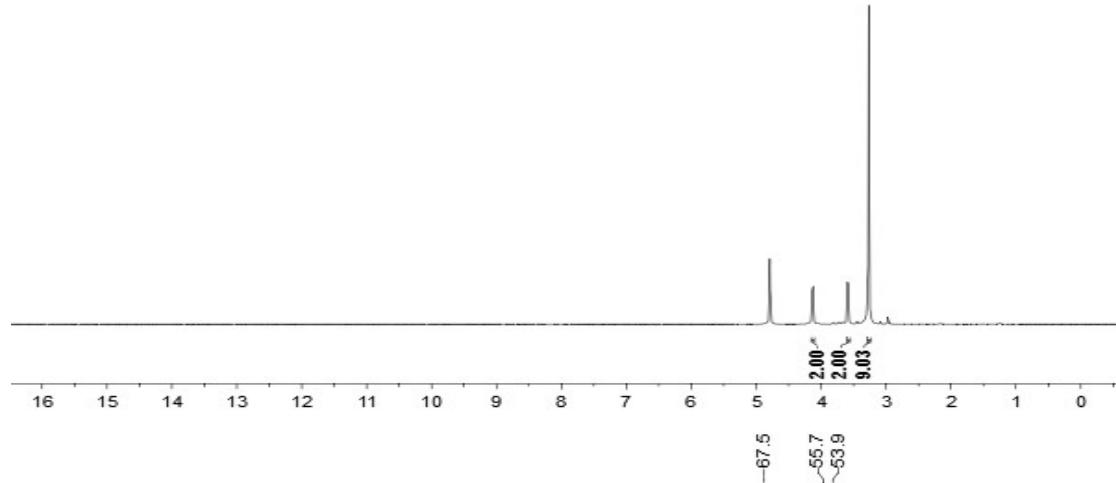
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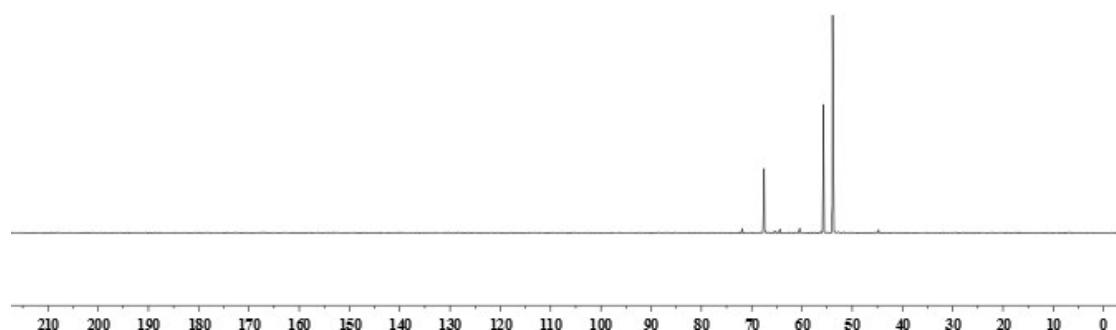
29.



[Choline][NO₃]

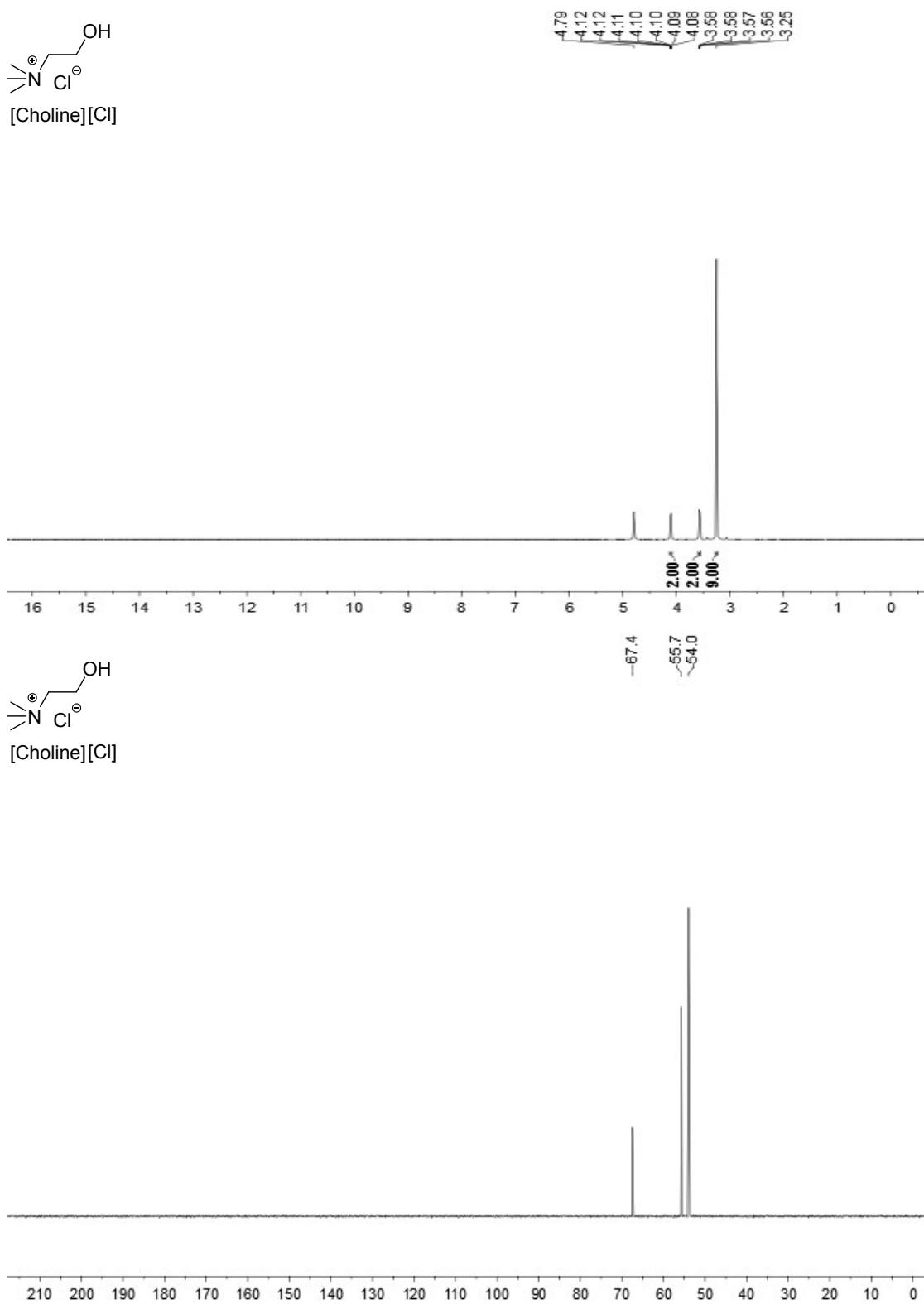
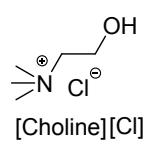


[Choline][NO₃]

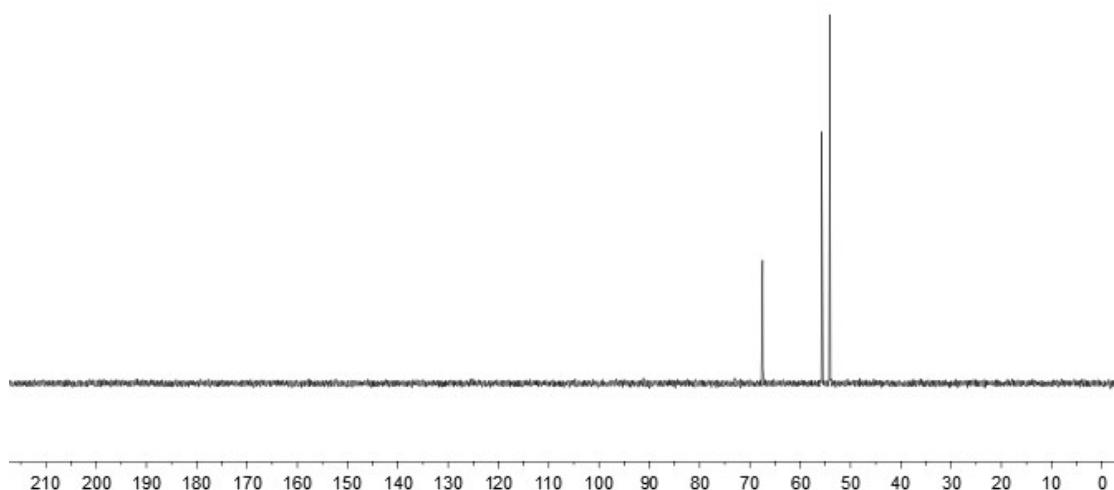
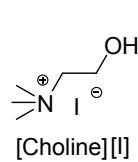
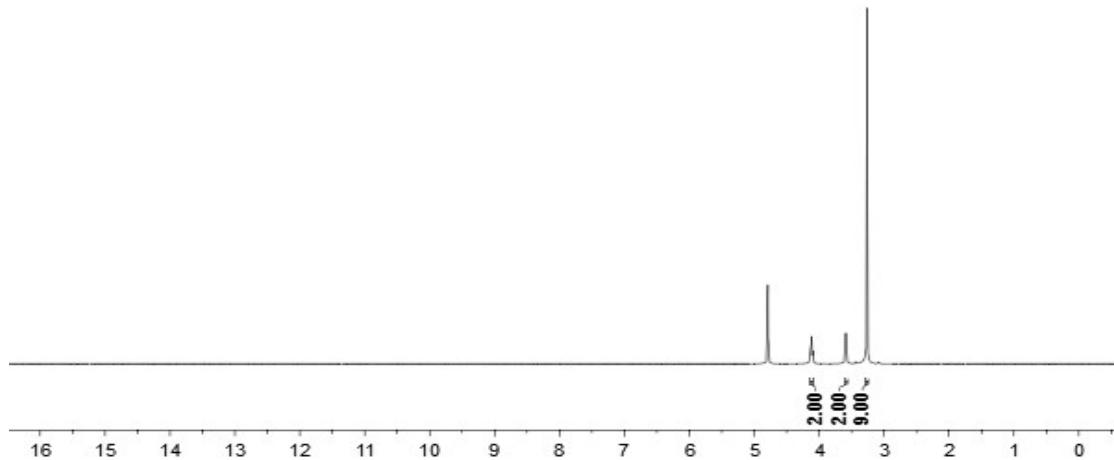
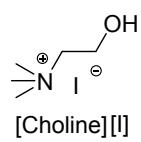


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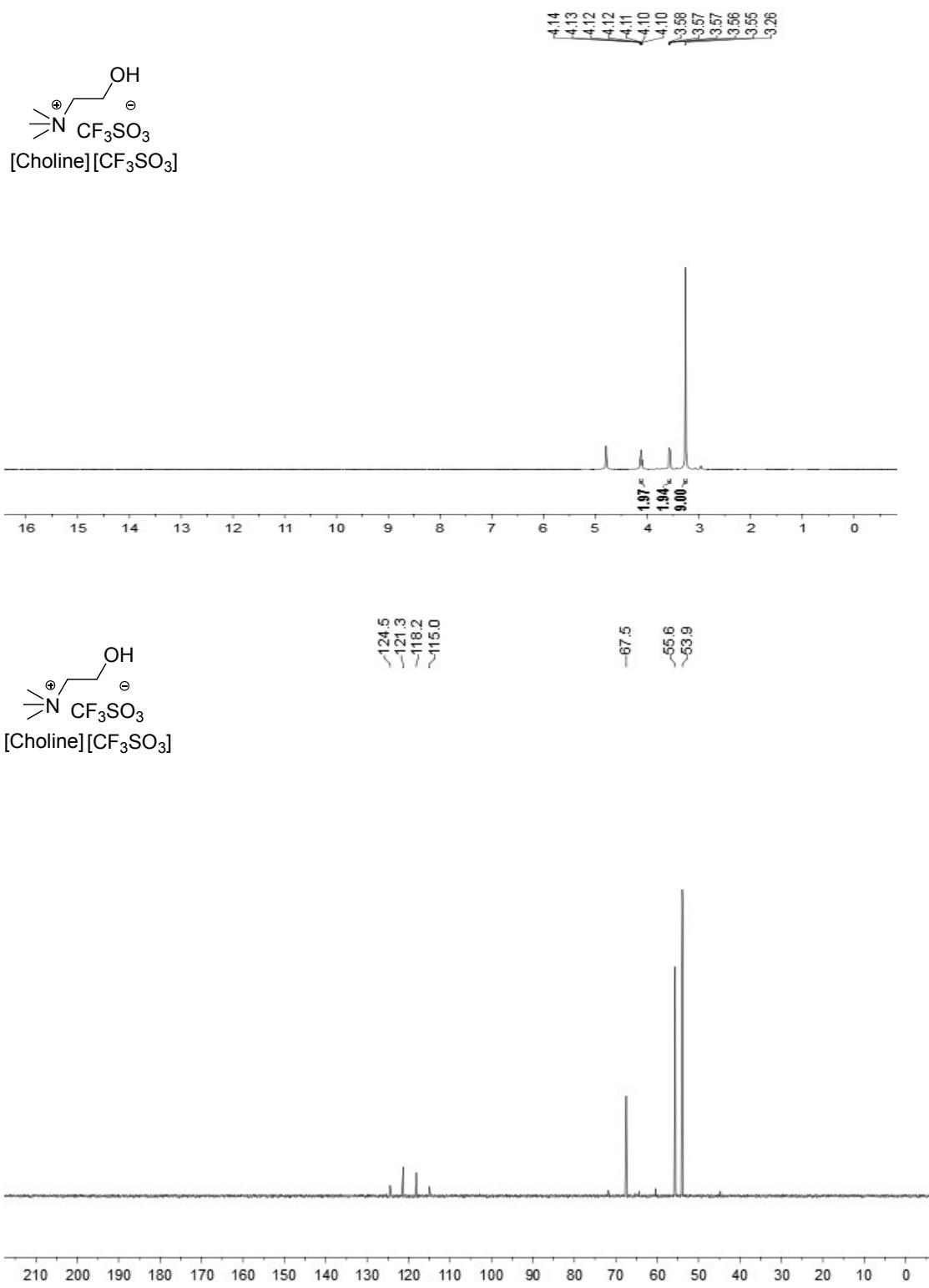
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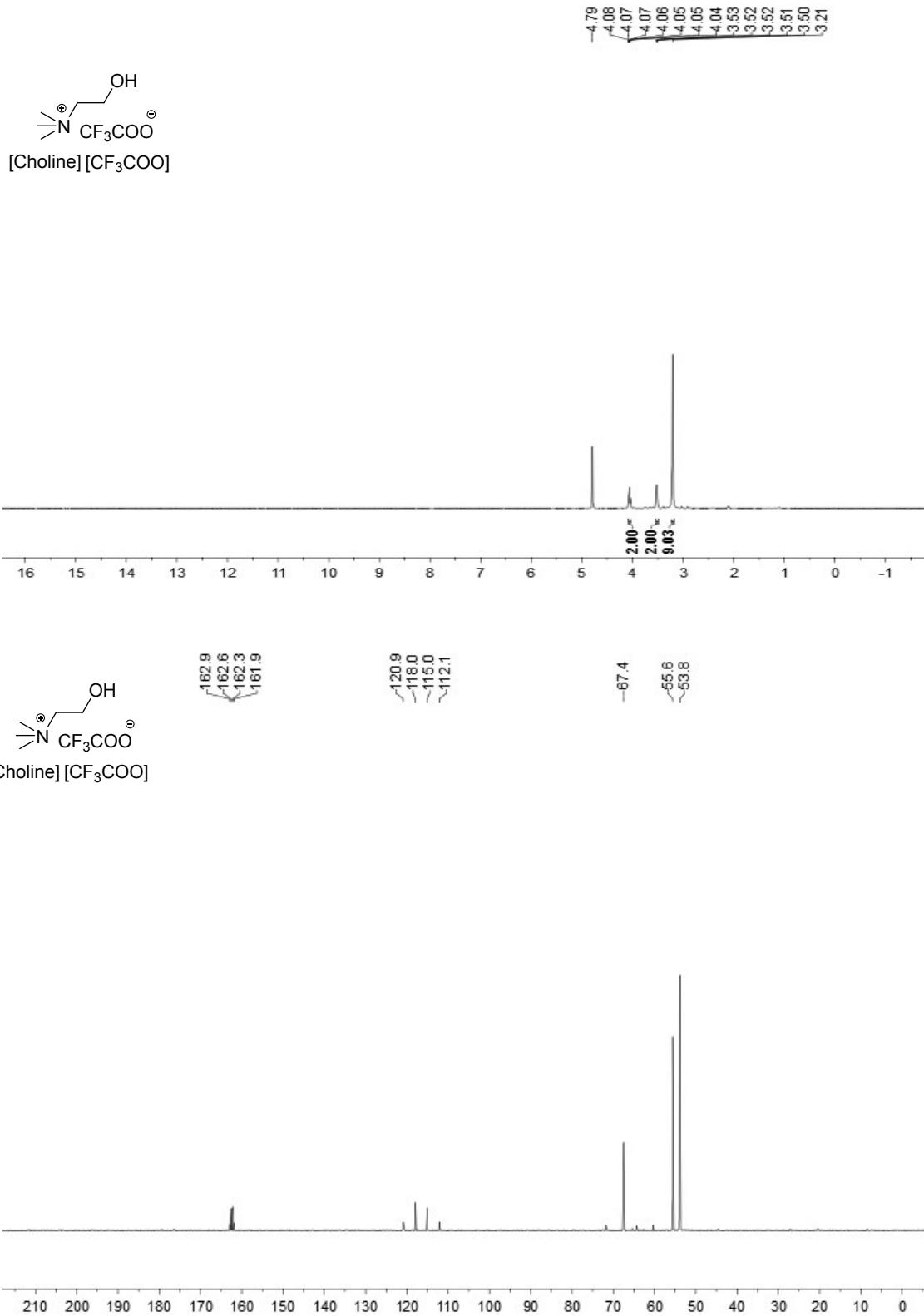


31.

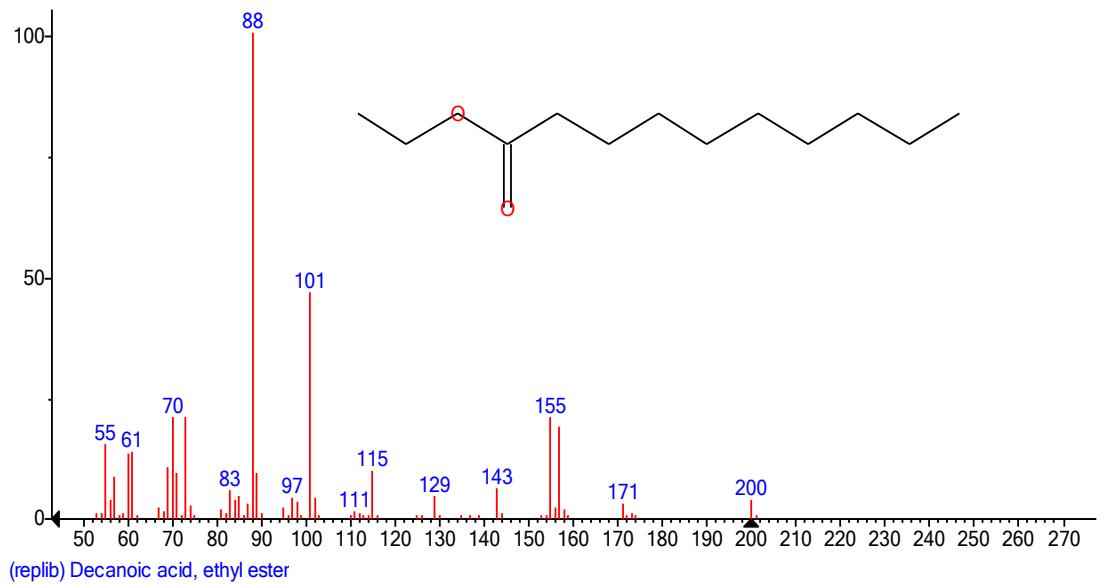


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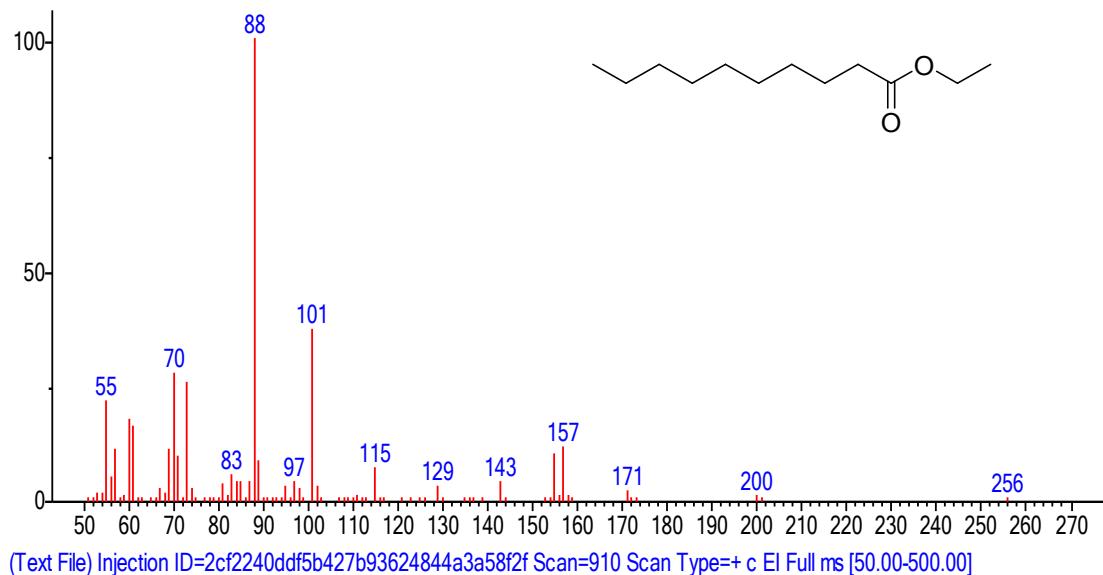




Component 1
The standard mass spectrum

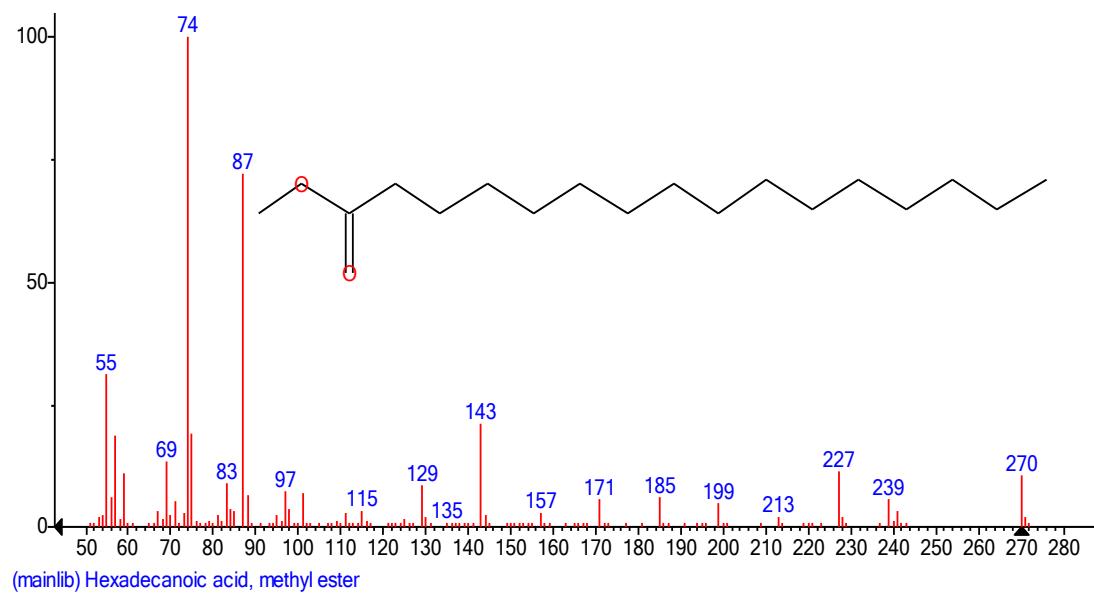


Mass Spectrum of the detected sample

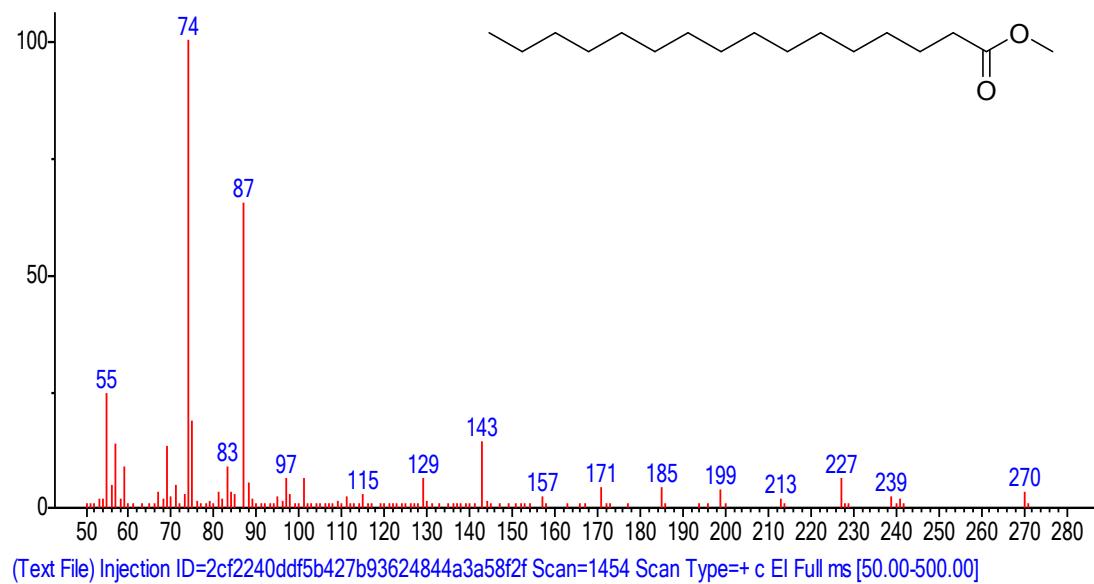


Component 2

The standard mass spectrum

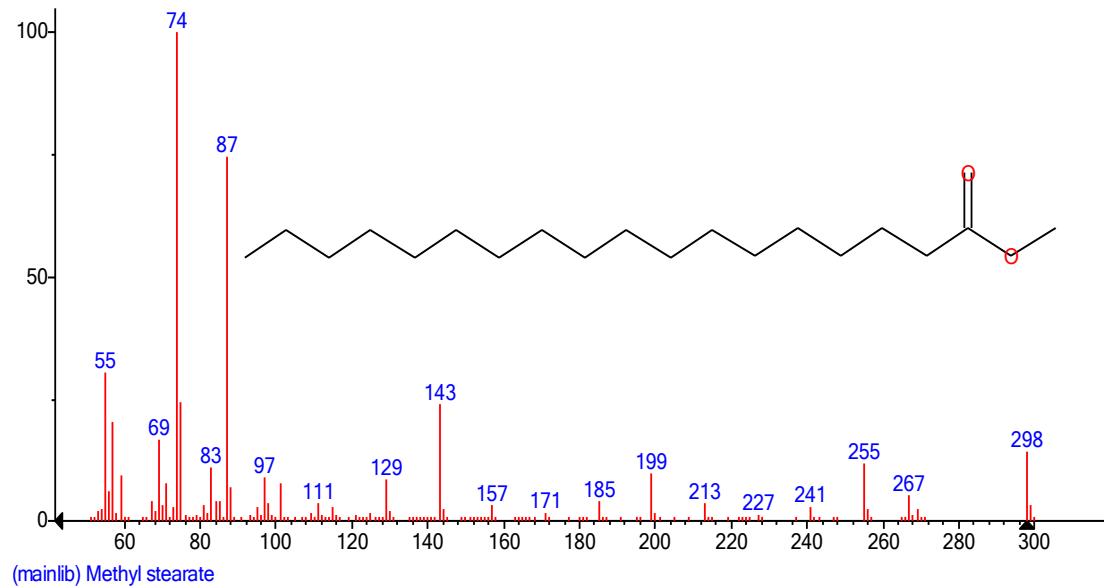


Mass Spectrum of the detected sample

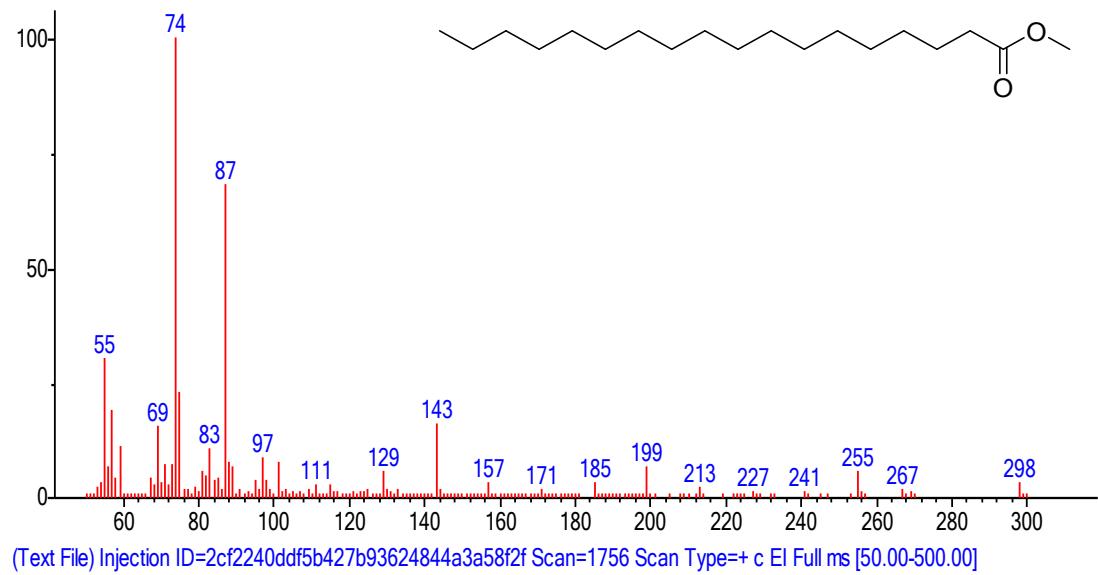


Component 3

The standard mass spectrum

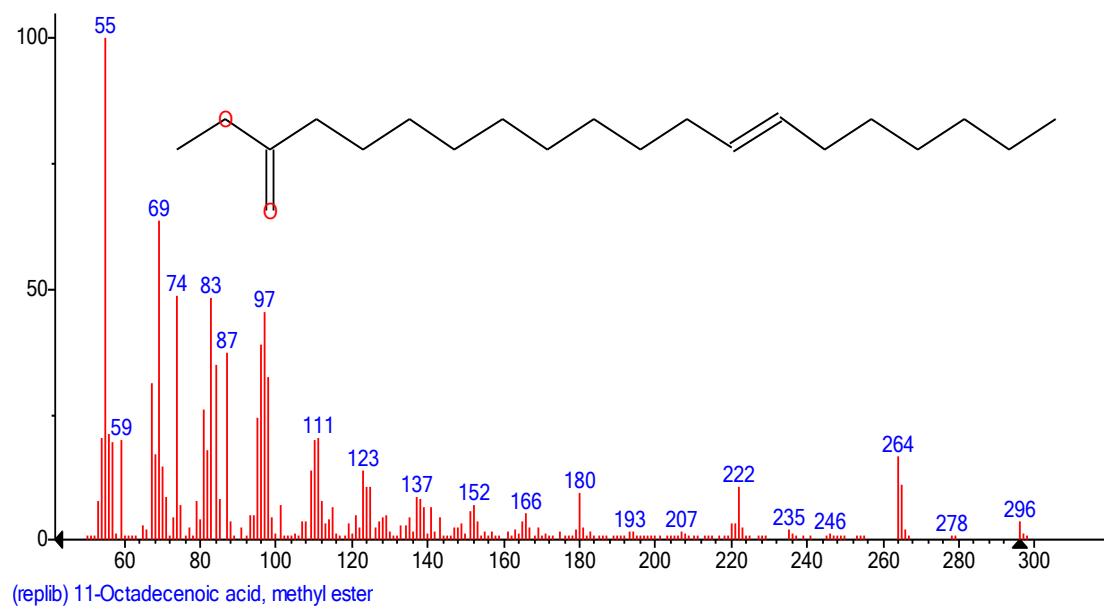


Mass Spectrum of the detected sample

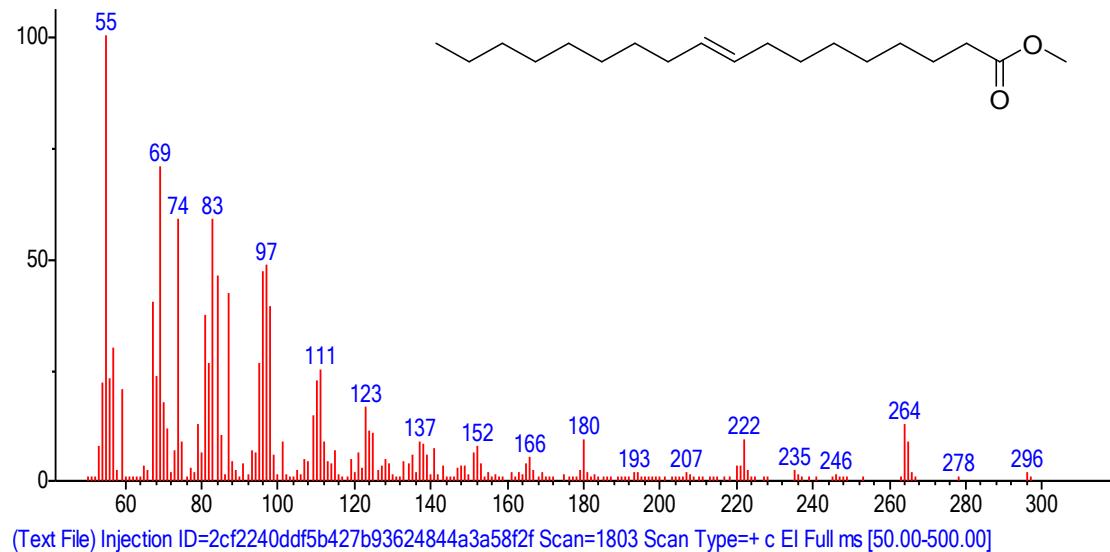


Component 4

The standard mass spectrum

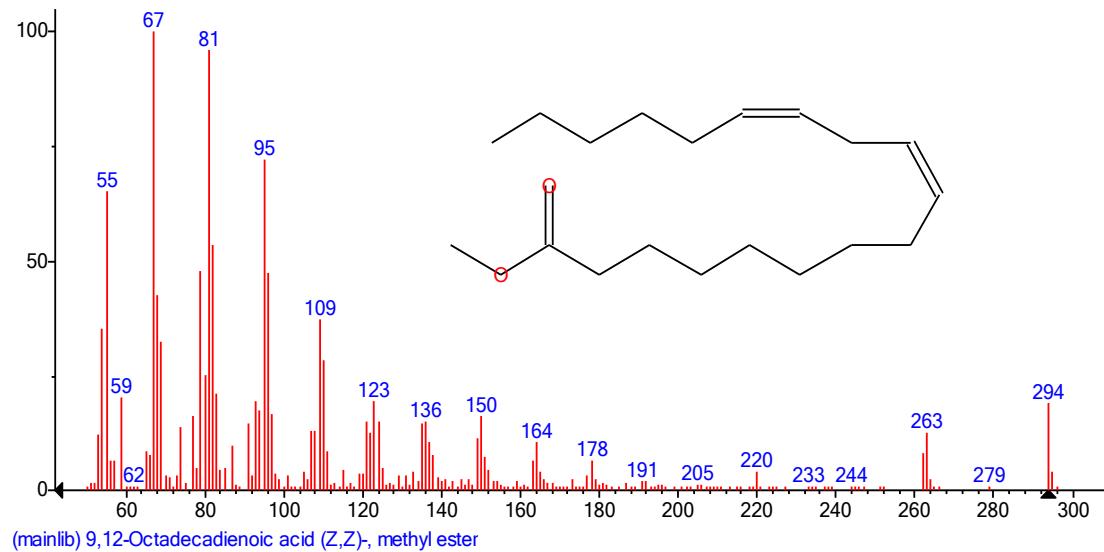


Mass Spectrum of the detected sample

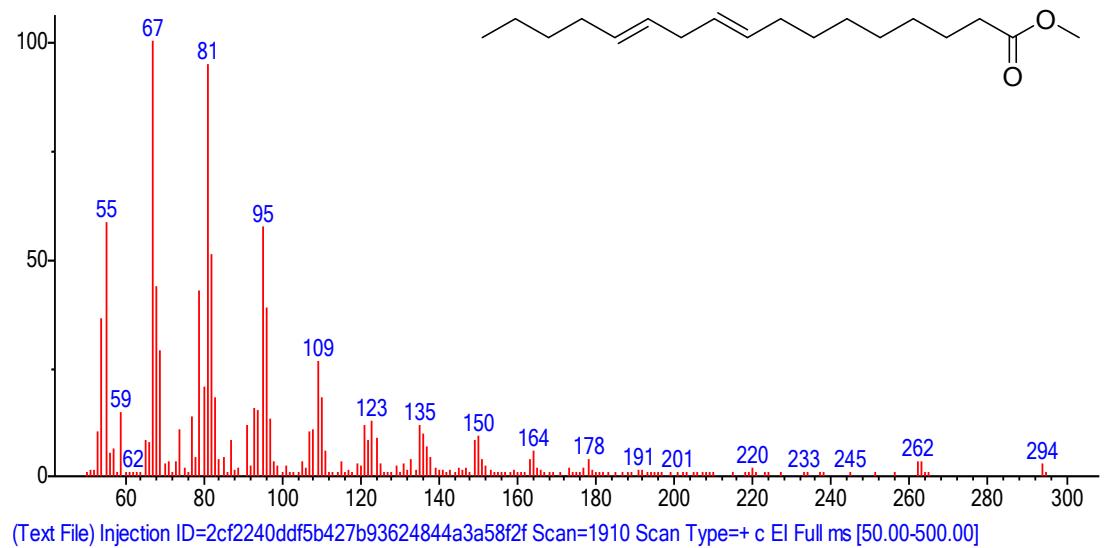


Component 5

The standard mass spectrum

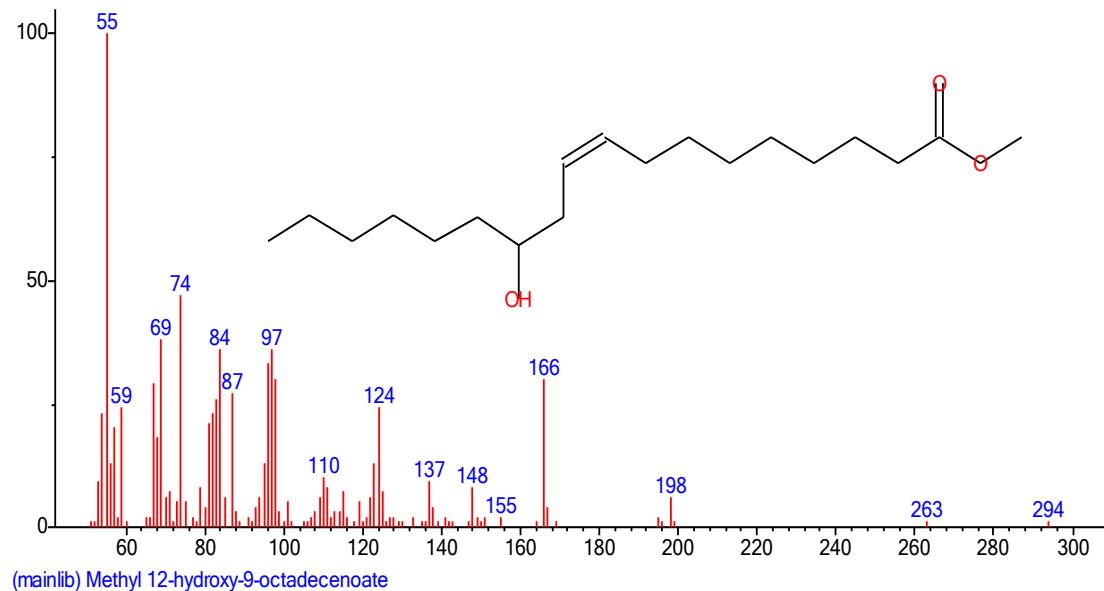


Mass Spectrum of the detected sample



Component 6

The standard mass spectrum



Mass Spectrum of the detected sample

