**SUPPORTING INFORMATION**

# Comparative chemical profiling and monacolins quantification in red yeast rice dietary supplements by $^{1}$H NMR and UHPLC-DAD-MS

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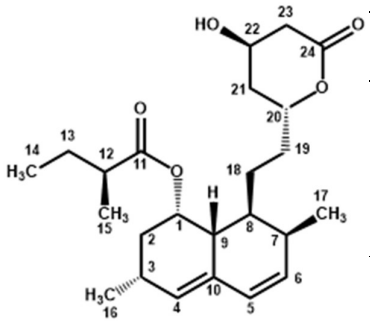
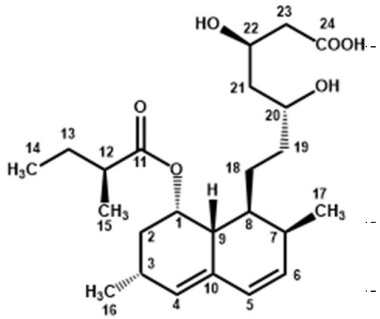
**Table S1.** $^{1}H$ and $^{13}C$ NMR data (solvent: $CD_3CN:D_2O$ 80:20) of monacolin K in lactone (MK) and hydroxyl acid (MKA) forms, compactin and dihydromonacolin K.

Monacolin K (MK)



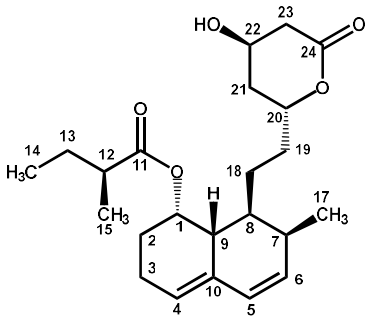

| Positions | | δ $^{1}H$ (ppm) | Multiplicity[1] (J (Hz)) | COSY $^{1}H$-$^{1}H$ correlations | | | δ $^{13}C$ (ppm) | HMBC $^{1}H$-$^{13}C$ correlations | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | $^{2}J_{HH}$ | $^{3}J_{HH}$ | $^{4}J_{HH}$ | | $^{2}J_{CH}$ | $^{3}J_{CH}$ |
| 5 | CH | 6.01 | d (9.6) | - | H6 | H7 | 131.0 | - | H4/H7 |
| 6 | CH | 5.84 | dd (6.1, 9.6) | - | H5/H7 | H17 | 136.4 | H7 | H17 |
| 4 | CH | 5.56 | app t (2.8) | - | H3 | H2/H9/H16 | 132.4 | - | H2/H9/H5/H16 |
| 1 | CH | 5.35 | q (3.2) | - | H2/H9 | - | 71.2 | H2 | - |
| 20 | CH | 4.59 | m | - | H19/H21 | - | 79.7 | H19/H21 | - |
| 22 | CH | 4.25 | app quint (3.9) | - | H21/H23 | - | 64.6 | H21/H23 | - |
| 23 | $CH_2$ | 2.69 | Ad (4.9, 17.6) | H23 | H22 | - | 40.8 | - | - |
| | | 2.51 | Bdd (1.7, 3.8, 17.6) | H23 | H22 | H21 | | | |
| 3 | CH | 2.45 | m | - | H2/H4/H16 | - | 30.1 | H2/H4/H16 | H1 |
| 7 | CH | 2.42 | m | - | H6/H8/H17 | H5 | 33.3 | H6 | H5/H18 |
| 9 | CH | 2.37 | m | - | H8/H1 | H4 | 39.7 | H1 | H2/H4/H5/H7/H18 |
| 12 | CH | 2.35 | m | - | H13/H15 | - | 44.3 | H13/H15 | H14 |
| 2 | $CH_2$ | 1.96 | m | - | H3/H1 | - | 35.3 | - | H4/H16 |
| 21 | $CH_2$ | 1.90 | m | H21 | H20/H22 | - | 37.9 | - | H19/H23 |
| | | 1.71 | m | H21 | H20/H22 | H23 | | - | |
| 8 | CH | 1.69 | m | - | H9/H7/H18 | - | 39.4 | H9/H7/H18 | H6 |
| 13 | $CH_2$ | 1.62 | app qd (7.4, 13.6) | H13 | H12/H14 | - | 29.5 | H12/H14 | H15 |
| | | 1.46 | m | H13 | H12/H14 | - | | | |
| 19 | $CH_2$ | 1.81 | m | H19 | H18/H20 | - | 35.0 | H18 | - |
| | | 1.37 | m | H19 | H18/H20 | - | | | |
| 18 | $CH_2$ | 1.46 | m | - | H8/H19 | - | 26.5 | H19 | - |
| | | 1.36 | m | - | H8/H19 | - | | | |
| 15 | $CH_3$ | 1.08 | d (6.9) | - | H12 | - | 18.5 | H12 | H13 |
| 16 | $CH_3$ | 1.06 | d (7.4) | - | H3 | - | 25.0 | - | H2 |
| 17 | $CH_3$ | 0.89 | d (6.9) | - | H7 | - | 15.9 | H7 | - |
| 14 | $CH_3$ | 0.88 | t (7.5) | - | H13 | - | 14.0 | H13 | H12 |
| 10 | Cq | - | - | - | - | - | 134.7 | H9/H5 | H6/H1 |
| 24 | Cq | - | - | - | - | - | 175.1 | H23 | - |
| 11 | Cq | - | - | - | - | - | 180.1 | H12 | H13/H15/H1 |

Monacolin K hydroxyl acid form (MKA)



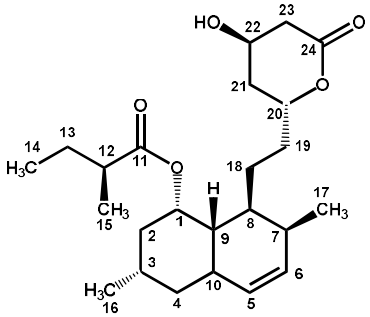

| Positions | | δ $^{1}$H (ppm) | Multiplicity$^{1}$ (J (Hz)) | COSY $^{1}$H-$^{1}$H correlations $^{2}J_{HH}$ | COSY $^{1}$H-$^{1}$H correlations $^{3}J_{HH}$ | COSY $^{1}$H-$^{1}$H correlations $^{4}J_{HH}$ | δ $^{13}$C (ppm) | HMBC $^{1}$H-$^{13}$C correlations $^{2}J_{CH}$ | HMBC $^{1}$H-$^{13}$C correlations $^{3}J_{CH}$ |
|---|---|---|---|---|---|---|---|---|---|
| 5 | CH | 5.99 | d (9.6) | - | H6 | H7 | 130.9 | - | H4/H7 |
| 6 | CH | 5.83 | dd (6.1, 9.6) | - | H5/H7 | H17 | 136.9 | H7 | H17 |
| 4 | CH | 5.53 | app t (2.8) | - | H3 | H2/H9/H16 | 132.2 | - | H2/H9/H5/H16 |
| 1 | CH | 5.33 | q (3.2) | - | H2/H9 | - | 71.6 | H2 | - |
| 20 | CH | 3.63 | app hept (4.1) | - | H19/H21 | - | 73.3 | H21 | H18 |
| 22 | CH | 4.05 | m | - | H21/H23 | - | 70.7 | H21/H23 | - |
| 23 | $CH_2$ | 2.33 | m | H23 | H22 | - | 46.6 | - | - |
| | | 2.16 | dd (8.7, 15.2) | H23 | H22 | - | | | |
| 3 | CH | 2.42 | m | - | H2/H4/H16 | - | 30.2 | H2/H4/H16 | H1 |
| 7 | CH | 2.39 | m | - | H6/H8/H17 | H5 | 33.4 | H6 | H5/H18 |
| 9 | CH | 2.35 | m | - | H8/H1 | H4 | 39.7 | H1 | H2/H4/H5/H7/H18 |
| 12 | CH | 2.33 | m | - | H13/H15 | - | 44.5 | H13/H15 | H14 |
| 2 | $CH_2$ | 1.93 | m | - | H3/H1 | - | 35.0 | - | H4/H16 |
| 21 | $CH_2$ | 1.57 | m | H21 | H20/H22 | - | 46.3 | - | H19/H23 |
| | | 1.51 | m | H21 | H20/H22 | - | | - | |
| 8 | CH | 1.63 | m | - | H9/H7/H18 | - | 39.7 | H9/H7/H18 | H6 |
| 13 | $CH_2$ | 1.59 | m | H13 | H12/H14 | - | 29.6 | H12/H14 | H15 |
| | | 1.45 | m | H13 | H12/H14 | - | | | |
| 19 | $CH_2$ | 1.53 | m | H19 | H18/H20 | - | 37.2 | H18 | - |
| | | 1.15 | m | H19 | H18/H20 | - | | | |
| 18 | $CH_2$ | 1.32 | m | - | H8/H19 | - | 27.3 | H19 | - |
| | | | | - | H8/H19 | - | | | |
| 15 | $CH_3$ | 1.08 | d (6.9) | - | H12 | - | 18.7 | H12 | H13 |
| 16 | $CH_3$ | 1.05 | d (7.4) | - | H3 | - | 25.1 | - | H2 |
| 17 | $CH_3$ | 0.87 | d (6.9) | - | H7 | - | 16.1 | H7 | - |
| 14 | $CH_3$ | 0.86 | t (7.4) | - | H13 | - | 14.1 | H13 | H12 |
| 10 | Cq | - | - | - | - | - | 135.0 | H9/H5 | H6/H1 |
| 24 | Cq | - | - | - | - | - | 181.5 | H23 | - |
| 11 | Cq | - | - | - | - | - | 180.9 | H12 | H13/H15/H1 |

Compactin (CP)
(mevastatin)



| Positions | | δ $^{1}$H (ppm) | Multiplicity[1] (J (Hz)) | COSY $^{1}$H-$^{1}$H correlations | | | δ $^{13}$C (ppm) | HMBC $^{1}$H-$^{13}$C correlations | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | $^{2}J_{HH}$ | $^{3}J_{HH}$ | $^{4}J_{HH}$ | | $^{2}J_{CH}$ | $^{3}J_{CH}$ |
| 5 | CH | 6.00 | d (9.7) | - | H6 | H7 | 130.8 | - | H4/H7 |
| 6 | CH | 5.79 | dd (6.0, 9.7) | - | H5/H7 | - | 135.9 | H7 | H17 |
| 4 | CH | 5.57 | m | - | H3 | H9 | 126.5 | - | H2/H5/H9 |
| 1 | CH | 5.30 | m | - | H2/H9 | - | 70.8 | - | H3 |
| 20 | CH | 4.60 | m | - | H19/H21 | - | 79.7 | H19 | H18/H22 |
| 22 | CH | 4.25 | app quint (3.9) | - | H21/H23 | - | 64.6 | H21/H23 | H20 |
| 23 | $CH_2$ | 2.69 | Ad (4.8, 17.6) | H23 | H22 | - | 40.7 | - | H21 |
| | | 2.51 | Bdd (1.7, 3.6, 17.6) | H23 | H22 | - | | | |
| 3 | $CH_2$ | 2.15 | m | - | H2/H4 | - | 23.4 | H2/H4 | H1 |
| 7 | CH | 2.42 | m | - | H6/H8/H17 | H5 | 33.5 | H6/H17 | H5/H18 |
| 9 | CH | 2.42 | m | - | H8/H1 | H4 | 39.8 | H1 | H2/H4/H5/H7/H18 |
| 12 | CH | 2.38 | m | - | H13/H15 | - | 44.5 | H13/H15 | H14 |
| 2 | $CH_2$ | 2.08 | m | - | H3/H1 | - | 28.6 | - | H4 |
| | | 1.72 | m | | H3/H1 | | | | |
| 21 | $CH_2$ | 1.90 | m | H21 | H20/H22 | - | 37.9 | - | H19/H23 |
| | | 1.72 | m | H21 | H20/H22 | - | | | |
| 8 | CH | 1.68 | m | - | H9/H7 | - | 39.6 | H7/H9/H18 | H6 |
| 13 | $CH_2$ | 1.62 | app qd (7.6, 13.6) | H13 | H12/H14 | - | 29.5 | H12/H14 | H15 |
| | | 1.46 | m | H13 | H12/H14 | - | | | |
| 19 | $CH_2$ | 1.81 | m | H19 | H18/H20 | - | 35.2 | H18 | - |
| | | 1.37 | m | H19 | H18/H20 | - | | | |
| 18 | $CH_2$ | 1.48 | m | - | H19 | - | 26.3 | H19 | - |
| | | 1.39 | m | - | H19 | - | | | |
| 15 | $CH_3$ | 1.11 | d (7.0) | - | H12 | - | 19.1 | H12 | H13 |
| 17 | $CH_3$ | 0.90 | d (7.0) | - | H7 | - | 15.9 | H7 | - |
| 14 | $CH_3$ | 0.89 | t (7.5) | - | H13 | - | 14.0 | H13 | H12 |
| 10 | Cq | - | - | - | - | - | 136.7 | H5/H9 | H1/H3/H6 |
| 24 | Cq | - | - | - | - | - | 174.2 | H23 | - |
| 11 | Cq | - | - | - | - | - | 179.2 | H12 | H1/H13/H15 |

Dihydromonacolin K
(DiMK)




| Positions | | δ $^{1}$H (ppm) | Multiplicity[1] (J (Hz)) | COSY $^{1}$H-$^{1}$H correlations | | | δ $^{13}$C (ppm) | HMBC $^{1}$H-$^{13}$C correlations | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | $^{2}J_{HH}$ | $^{3}J_{HH}$ | $^{4}J_{HH}$ | | $^{2}J_{CH}$ | $^{3}J_{CH}$ |
| 5 | CH | 5.42 | d (9.8) | - | H6 | H7 | 133.8 | H10 | H4/H7 |
| 6 | CH | 5.69 | ddd (2.7, 5.0, 9.8) | - | H5/H7 | - | 135.6 | H7 | H17 |
| 1 | CH | 5.15 | q (2.7) | - | H2/H9 | - | 73.1 | H2 | H3 |
| 20 | CH | 4.58 | m | - | H19/H21 | - | 79.7 | H19/H21 | - |
| 22 | CH | 4.25 | app quint (3.8) | - | H21/H23 | - | 64.6 | H21/H23 | - |
| 23 | $CH_2$ | 2.68 | Ad (4.9, 17.7) | H23 | H22 | - | 40.7 | - | - |
| | | 2.50 | Bdd (1.7, 3.7, 17.7) | H23 | H22 | H21 | | | |
| 3 | CH | 2.05 | m | - | H4/H16 | - | 29.5 | H2/H4/H16 | H1 |
| 7 | CH | 2.34 | m | - | H6/H8/H17 | H5 | 33.9 | H6 | H5/H18 |
| 9 | CH | 1.30 | m | - | H8/H1 | H4 | 44.3 | H1 | H2/H4/H5/H7/H18 |
| 10 | CH | 2.46 | m | - | H4/H5/H9 | - | 33.7 | H5 | H1/H3/H6 |
| 12 | CH | 2.39 | m | - | H13/H15 | - | 44.6 | H13/H15 | H14 |
| 2 | $CH_2$ | 1.80 | m | - | H3/H1 | - | 38.0 | - | H4/H16 |
| 4 | $CH_2$ | 1.61 | m | H4 | H10 | - | 41.1 | - | H16 |
| | | 1.35 | m | H4 | H10 | - | | | H16 |
| 21 | $CH_2$ | 1.88 | m | H21 | H20/H22 | - | 37.8 | - | H19/H23 |
| | | 1.72 | m | H21 | H20/H22 | H23 | | | |
| 8 | CH | 1.66 | m | - | H9/H7 | - | 40.2 | H9/H18 | H6 |
| 13 | $CH_2$ | 1.64 | m | H13 | H12/H14 | - | 29.3 | H12/H14 | H15 |
| | | 1.49 | app qd (7.4, 13.6) | H13 | H12/H14 | - | | | |
| 19 | $CH_2$ | 1.81 | m | H19 | H18/H20 | - | 35.3 | H18 | - |
| | | 1.37 | m | H19 | H18/H20 | - | | | |
| 18 | $CH_2$ | 1.35 | m | - | H8/H19 | - | 25.4 | H19 | - |
| | | 1.30 | m | - | H8/H19 | - | | | |
| 15 | $CH_3$ | 1.12 | d (7.0) | - | H12 | - | 18.8 | H12 | H13 |
| 16 | $CH_3$ | 1.11 | d (7.6) | - | H3 | - | 23.3 | - | H2/H4 |
| 17 | $CH_3$ | 0.86 | d (7.0) | - | H7 | - | 17.0 | H7 | - |
| 14 | $CH_3$ | 0.90 | t (7.5) | - | H13 | - | 14.0 | H13 | H12 |
| 24 | Cq | - | - | - | - | - | 175.2 | H23 | - |
| 11 | Cq | - | - | - | - | - | 179.9 | H12 | H13/H15/H1 |

[1] d: doublet, dd: doublet of doublet, ddd: doublet of doublet of doublet, t: triplet, q: quadruplet, qd: doublet of quadruplet, quint: quintuplet, hept: heptuplet, m: multiplet, A: part A of an AB system, B: part B of an AB system, app: apparent.

**Table S2.** [1]H NMR quantitative determination of monacolins in RYR dietary supplements.

| DS number | Amount of monacolins (mg per capsule or tablet)[1] ± CV (RSD) (n = 3) | | | | |
|---|---|---|---|---|---|
| | Signal at 5.84 ppm[2] H6 | Signal at 5.56 ppm[2] H4 | Signal at 5.33 ppm[2] H1 | Signal at 4.60 ppm[2] H20 | Signal at 4.25 ppm[2] H22 |
| 1 | 1.67 ± 0.11 (6.0%) | 1.70 ± 0.13 (7.6%) | 3.31 ± 0.22 (6.6%) | 1.40 ± 0.11 (7.9%) | 1.34 ± 0.07 (5.2%) |
| 2 | 9.14 ± 0.79 (8.7%) | 9.18 ± 0.73 (7.9%) | 9.26 ± 0.22 (2.4%) | | 7.10 ± 0.48 (6.8%) |
| 3 | 3.07 ± 0.36 (11.6%) | 3.07 ± 0.27 (8.8%) | 2.39 ± 0.07 (2.9%) | | |
| 4 | 1.02 ± 0.06 (5.9%) | 0.95 ± 0.07 (7.4%) | 1.64 ± 0.03 (1.8%) | | 0.71 ± 0.02 (2.8%) |
| 5 | 2.47 ± 0.14 (5.8%) | 2.53 ± 0.15 (5.8%) | 11.3 ± 1.1 (9.4%) | 2.15 ± 0.08 (3.8%) | |
| 6 | 2.92 ± 0.08 (2.7%) | 2.63 ± 0.20 (7.6%) | 3.27 ± 0.07 (2.1%) | | 2.19 ± 0.15 (6.9%) |
| 7 | 3.76 ± 0.29 (7.6%) | 3.73 ± 0.37 (10.0%) | | | |
| 8 | 8.68 ± 0.43 (4.9%) | 8.79 ± 0.29 (3.3%) | 8.65 ± 0.15 (1.7%) | 6.89 ± 0.46 (6.7%) | 7.73 ± 0.37 (4.8%) |
| 9 | 5.14 ± 0.44 (8.5%) | 5.21 ± 0.36 (6.9%) | 8.03 ± 0.20 (2.5%) | 4.55 ± 0.35 (7.6%) | 4.55 ± 0.40 (8.8%) |
| 10 | 2.10 ± 0.06 (3.0%) | 2.04 ± 0.27 (13.2%) | 8.67 ± 0.13 (1.5%) | | 1.22 ± 0.07 (5.8%) |
| 11 | | | | | |
| 12 | | | | | |
| 13 | 23.9 ± 1.8 (7.6%) | 23.9 ± 1.6 (6.9%) | 21.9 ± 0.5 (2.4%) | 23.9 ± 0.4 (1.7%) | 23.2 ± 1.9 (8.3%) |
| 14 | 3.45 ± 0.10 (2.8%) | 3.28 ± 0.26 (7.9%) | 10.8 ± 0.2 (1.5%) | | 2.26 ± 0.10 (4.2%) |
| 15 | 11.9 ± 0.2 (1.6%) | 12.3 ± 0.3 (2.6%) | | 9.85 ± 0.53 (5.4%) | |
| 16 | | 0.31 ± 0.03 (8.7%) | | | |
| 17 | 1.47 ± 0.04 (2.7%) | 1.51 ± 0.08 (5.0%) | 4.06 ± 0.07 (1.7%) | 1.28 ± 0.14 (11.0%) | |
| 18 | 8.84 ± 0.41 (5.0%) | 8.19 ± 0.30 (3.7%) | | 6.68 ± 0.39 (5.8%) | 7.04 ± 0.69 (9.8%) |

| | | | | | |
|---|---|---|---|---|---|
| 19 | 0.36 ± 0.02 (5.6%) | 0.44 ± 0.04 (6.9%) | | | |
| 20 | 1.75 ± 0.07 (4.0%) | 1.77 ± 0.08 (4.2%) | 3.51 ± 0.21 (6.0%) | 1.27 ± 0.08 (6.3%) | 1.49 ± 0.08 (5.4%) |
| 21 | 0.48 ± 0.06 (12.5%) | 0.47 ± 0.06 (12.8%) | | | |
| 22 | 3.09 ± 0.17 (5.4%) | 3.02 ± 0.26 (8.5%) | | | 2.26 ± 0.17 (7.6%) |
| 23 | 10.6 ± 0.2 (1.9%) | 10.7 ± 1.0 (9.2%) | 10.0 ± 0.9 (8.9%) | 10.0 ± 1.2 (11.8%) | 9.77 ± 0.71 (7.3%) |
| 24 | 11.5 ± 0.7 (5.9%) | 11.8 ± 0.8 (6.7%) | 9.38 ± 0.61 (6.5%) | | 5.97 ± 0.12 (2.0%) |
| 25 | 10.0 ± 0.3 (2.6%) | 9.72 ± 0.20 (2.1%) | | 5.97 ± 0.12 (2.0%) | 7.26 ± 0.63 (8.7%) |
| 26 | 4.51 ± 0.35 (7.4%) | 4.54 ± 0.19 (4.2%) | | | 3.88 ± 0.25 (6.5%) |
| 27 | 4.13 ± 0.21 (5.1%) | 3.84 ± 0.24 (6.3%) | | 2.97 ± 0.32 (10.8%) | 2.90 ± 0.26 (9.0%) |
| 28 | 1.64 ± 0.10 (6.1%) | 1.75 ± 0.15 (8.6%) | | 1.05 ± 0.09 (8.6%) | 1.31 ± 0.14 (10.7%) |
| 29 | | | | | |
| 30 | 2.99 ± 0.11 (3.7%) | 3.04 ± 0.12 (3.9%) | 2.61 ± 0.05 (1.9%) | | 2.43 ± 0.23 (9.5%) |
| 31 | 1.21 ± 0.10 (8.6%) | 1.28 ± 0.11 (8.6%) | 2.16 ± 0.09 (4.2%) | | |

[1] The amounts of monacolins (mg per dosage unit) were calculated from the measured areas using the equation presented in the paragraph 3.4.2.

[2] The resonances at 5.84, 5.56 ppm and 5.33 ppm are characteristic of all the monacolins bearing an hexahydronaphthalene ring but the 5.33 ppm signal does not characterize MJ and ML in lactone or in hydroxyl acid form; the resonances at 4.60 and 4.25 ppm are specific of all the monacolins in lactone form including dihydromonacolins.

**Table S3.** Comparison of monacolin amounts measured in RYR dietary supplements by [1]H NMR and UHPLC.

| NMR signal considered | Number of samples | Quantified monacolins (M)[1] | Linear regression equation y = a + bx [2] | | | p-value[3] |
|---|---|---|---|---|---|---|
| | | | b ± Sb | a ± Sa | $r^2$ | |
| 5.84 ppm | 27 | TotalM - DiMK | 0.986 ± 0.018 | 0.004 ± 0.130 | 0.992 | 0.9365 |
| 5.56 ppm | 28 | TotalM - DiMK | 0.984 ± 0.017 | 0.044 ± 0.117 | 0.993 | 0.6570 |
| Mean intensity of the two signals at 5.84 and 5.56 ppm | 28 | TotalM - DiMK | 0.985 ± 0.017 | 0.025 ± 0.117 | 0.993 | 0.6406 |
| 4.60 ppm or 4.25 ppm or mean intensity of the two signals | 22 | All M in lactone form (MJ, MN, MX, ML, CP, MK, DiMK) | 0.983 ± 0.015 | 0.013 ± 0.099 | 0.996 | 0.4953 |
| 5.33 ppm | 17 | MN, MX, MKA, CP, MK, DeML, DeMK | 0.952 ± 0.152 | -1.504 ± 1.321 | 0.723 | 0.0191 |
| Mean intensity of the two signals at 5.84 and 5.56 ppm | 28 | All M determined by [1]H NMR (TotalM - DiMK) vs TotalM determined by UHPLC | 1.001 ± 0.023 | 0.113 ± 0.166 | 0.986 | 0.2549 |

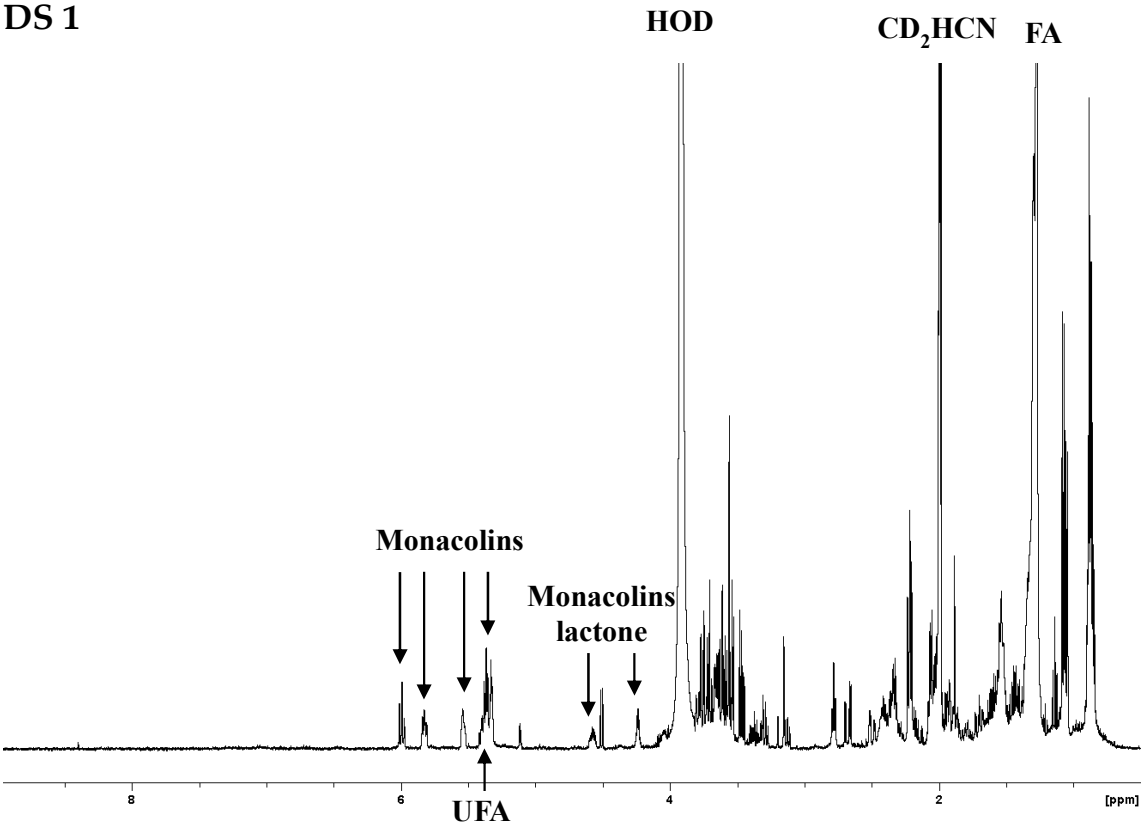
[1] The monacolin amount determined by [1]H NMR for each RYR dietary supplement (Table 3) was compared to that measured by UHPLC for the same group of monacolins (Table 5) except in the last line of the table.

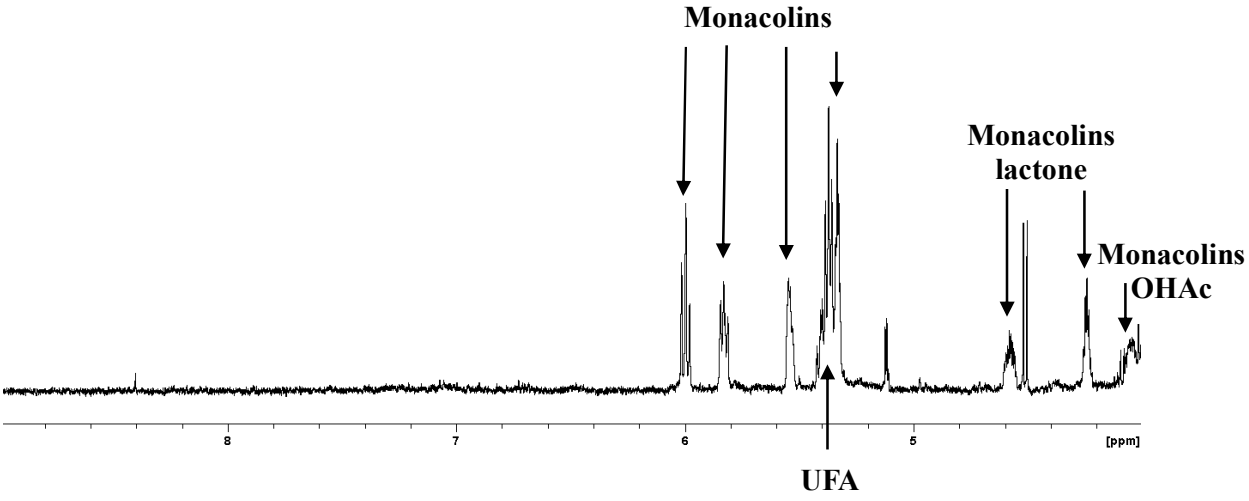
[2] The statistics for the straight lines were obtained with the LINEST function included in the Microsoft Excel software. b represents the slope of the linear regression and a the y-intercept. Sa and Sb correspond to the standard error values for the constants a and b, and $r^2$ is based on the Pearson's linear correlation coefficient.

[3] p-values were determined with the Wilcoxon signed-rank test.

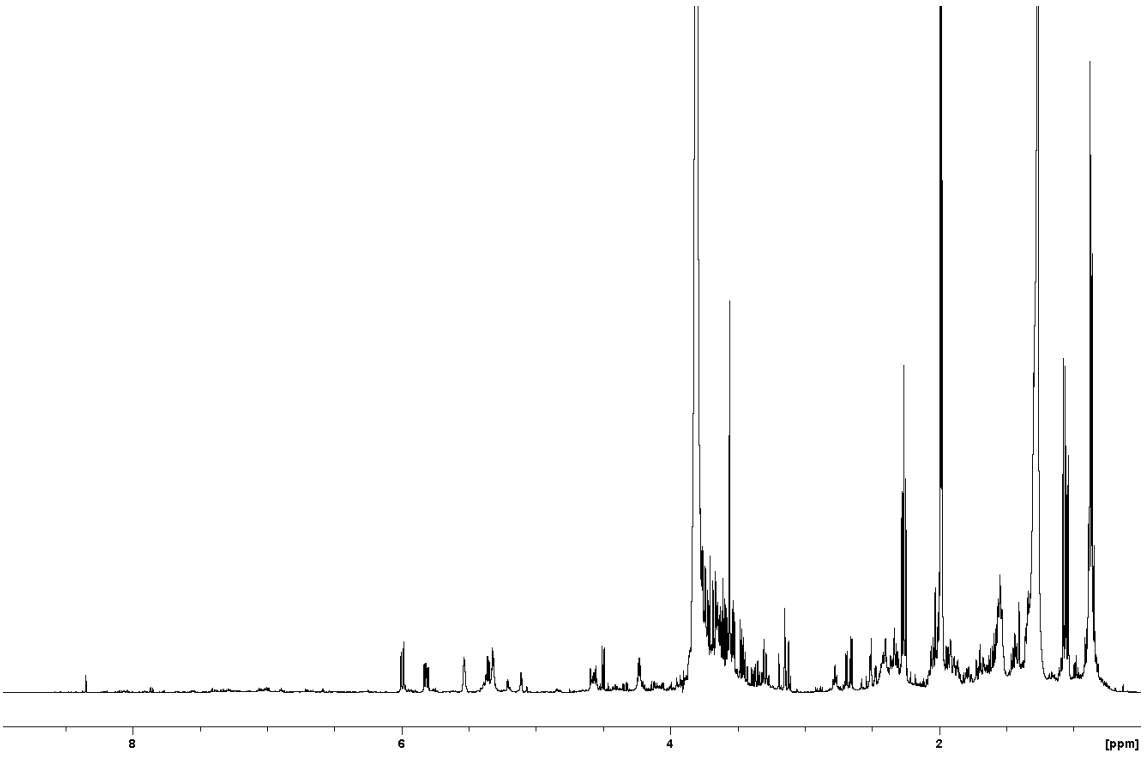
**Figure S1.** $^{1}H$ NMR spectra ($CD_3CN:D_2O$ (80:20)) of all the dietary supplements analyzed in the present study. Upper part: entire spectrum, lower part: enlarged downfield region (4-9 ppm). FA: fatty acids (saturated and unsaturated); UFA: non-conjugated unsaturated fatty acids; Monacolins OHAc: monacolins in hydroxyl acid form.

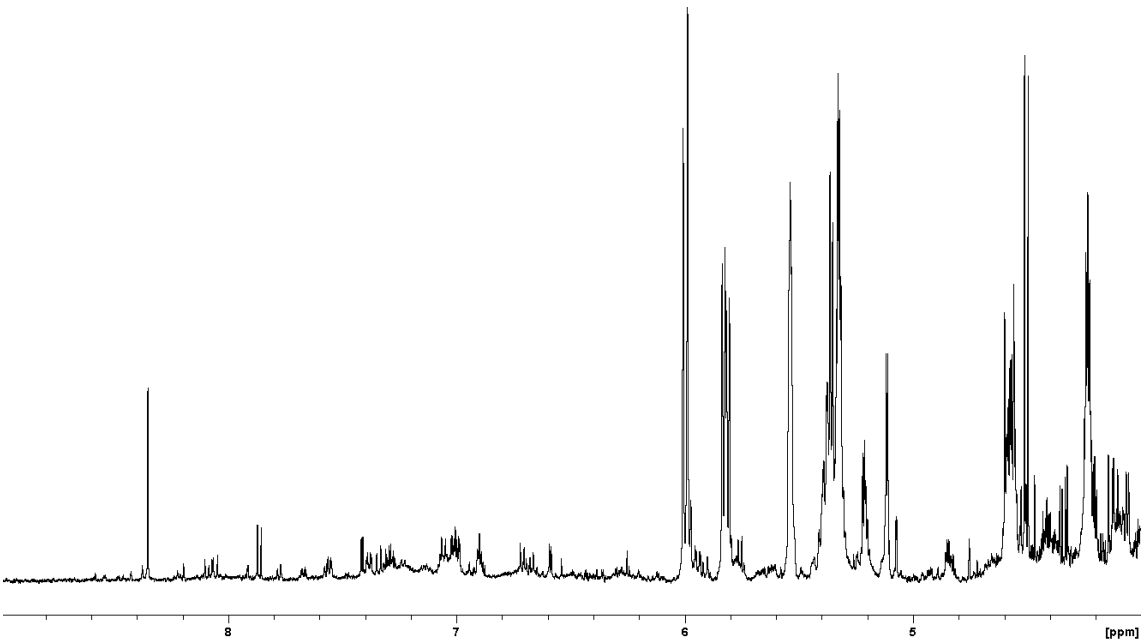
**DS 1**


HOD
CD2HCN
FA
Monacolins
Monacolins lactone
UFA
8
6
4
2
[ppm]


Monacolins
Monacolins lactone
Monacolins OHAc
UFA
8
7
6
5
[ppm]

**DS 2**



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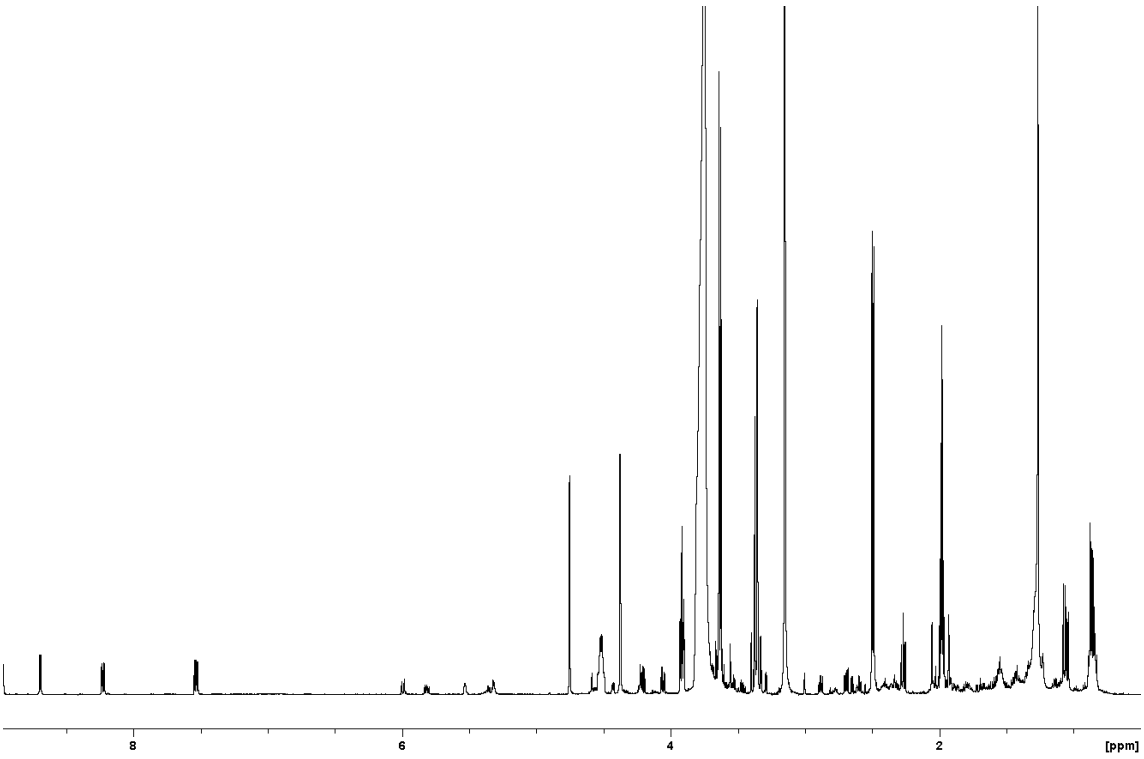


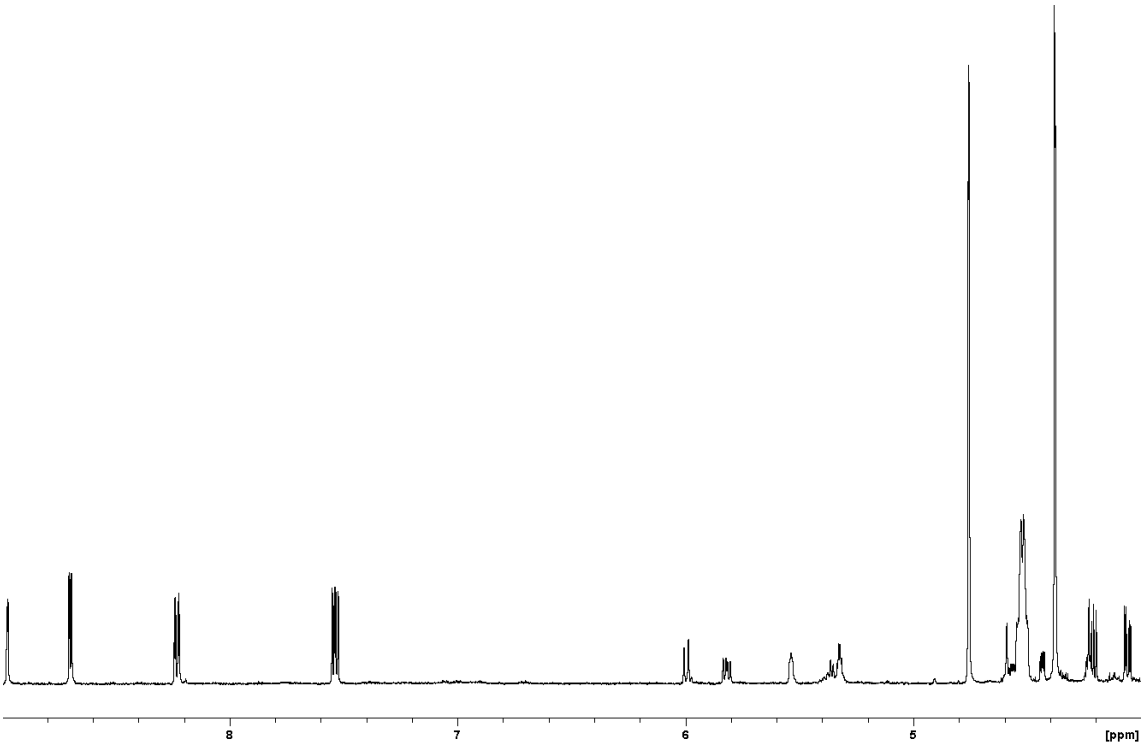

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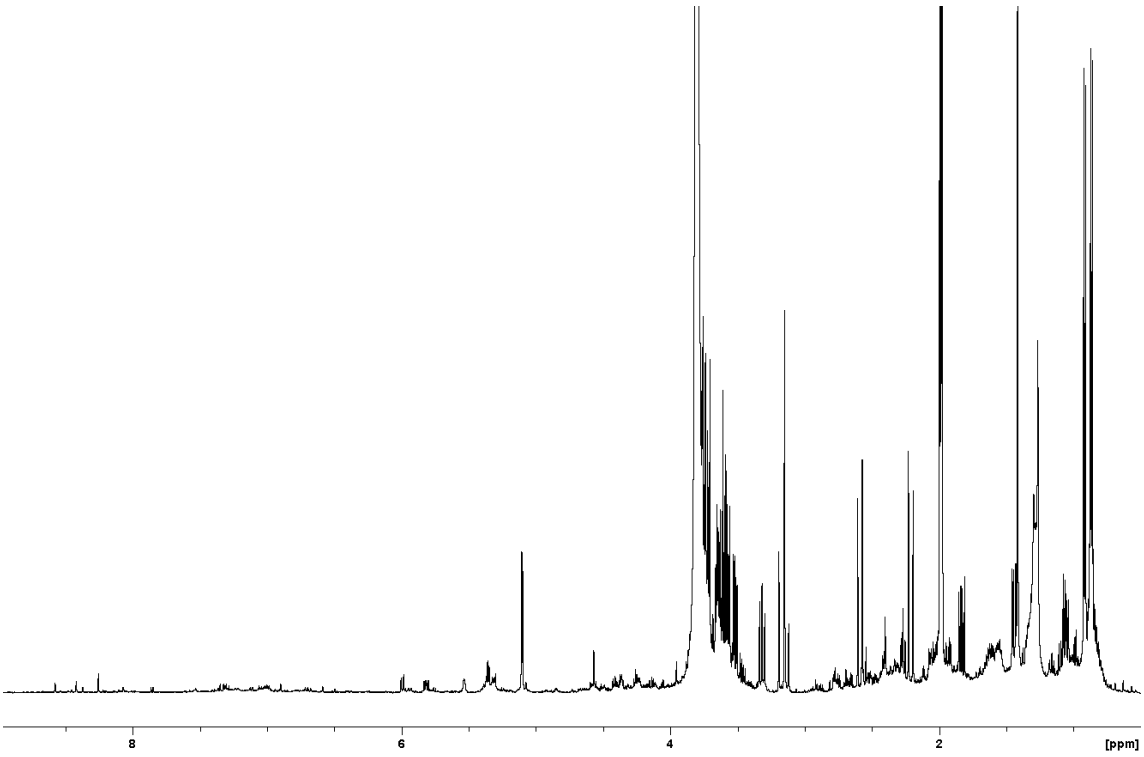


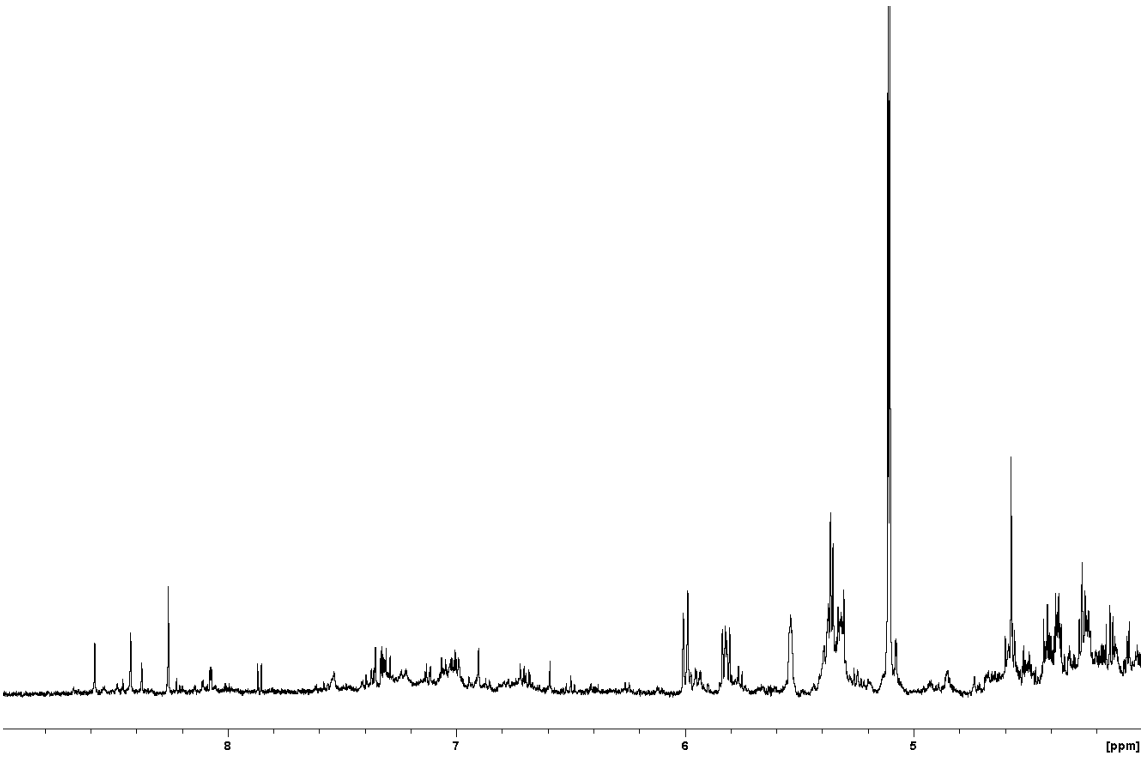

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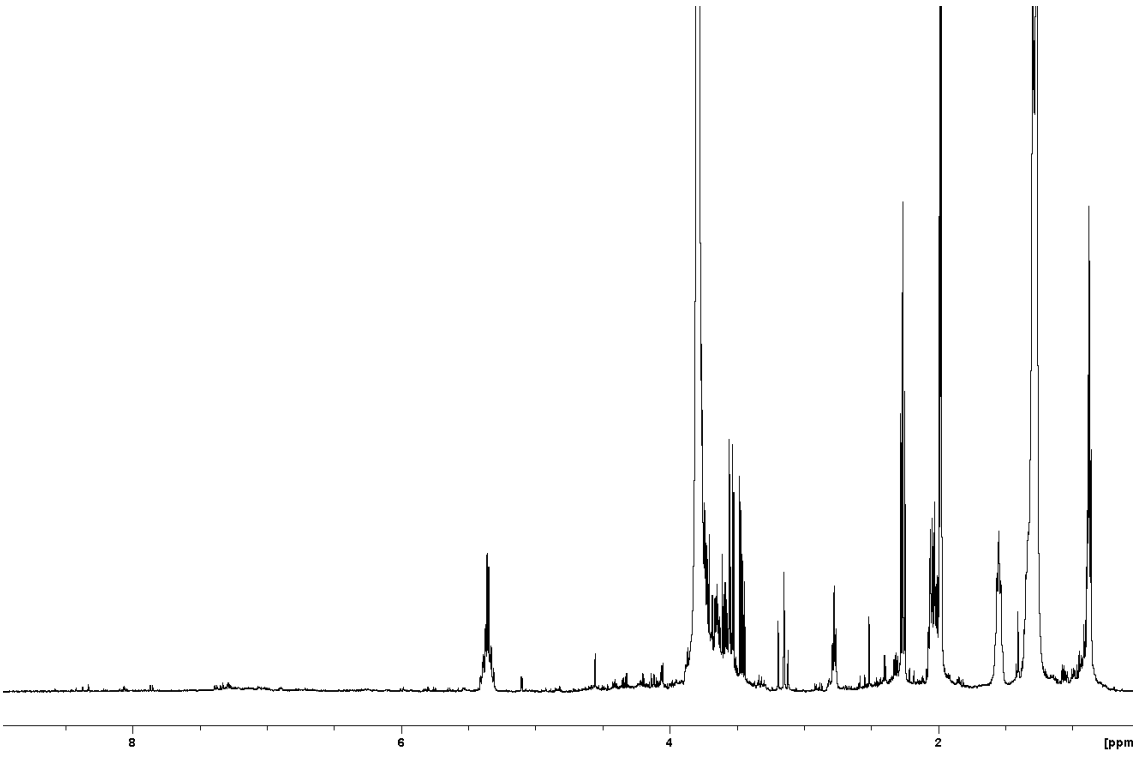


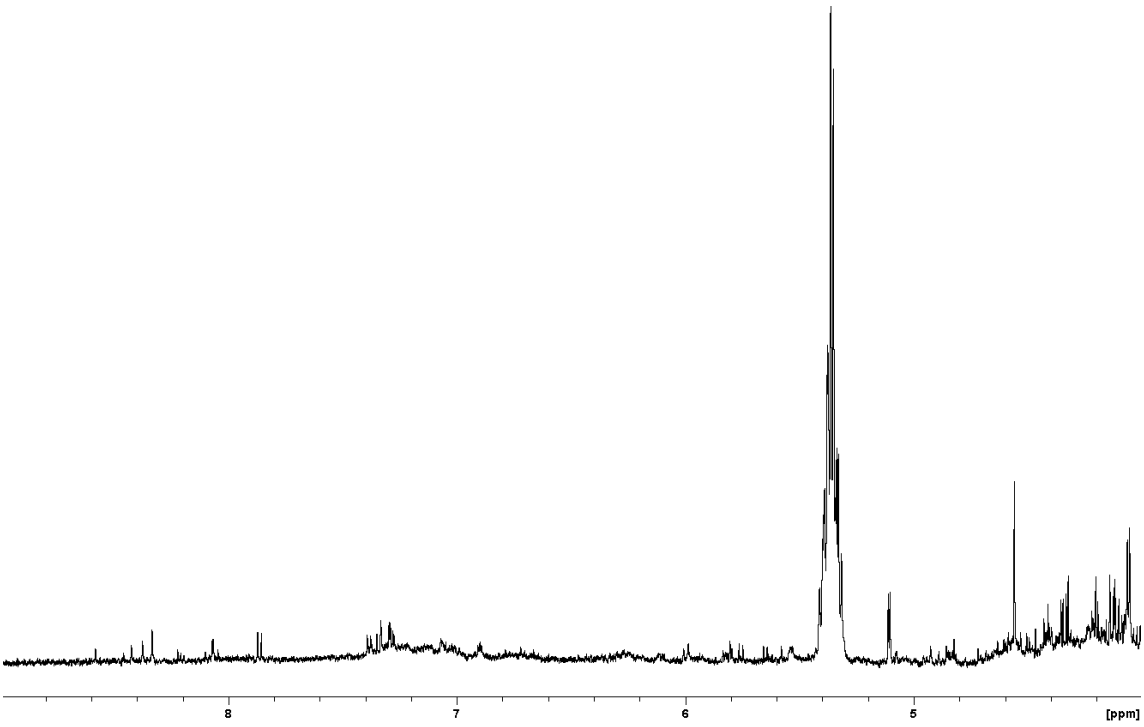

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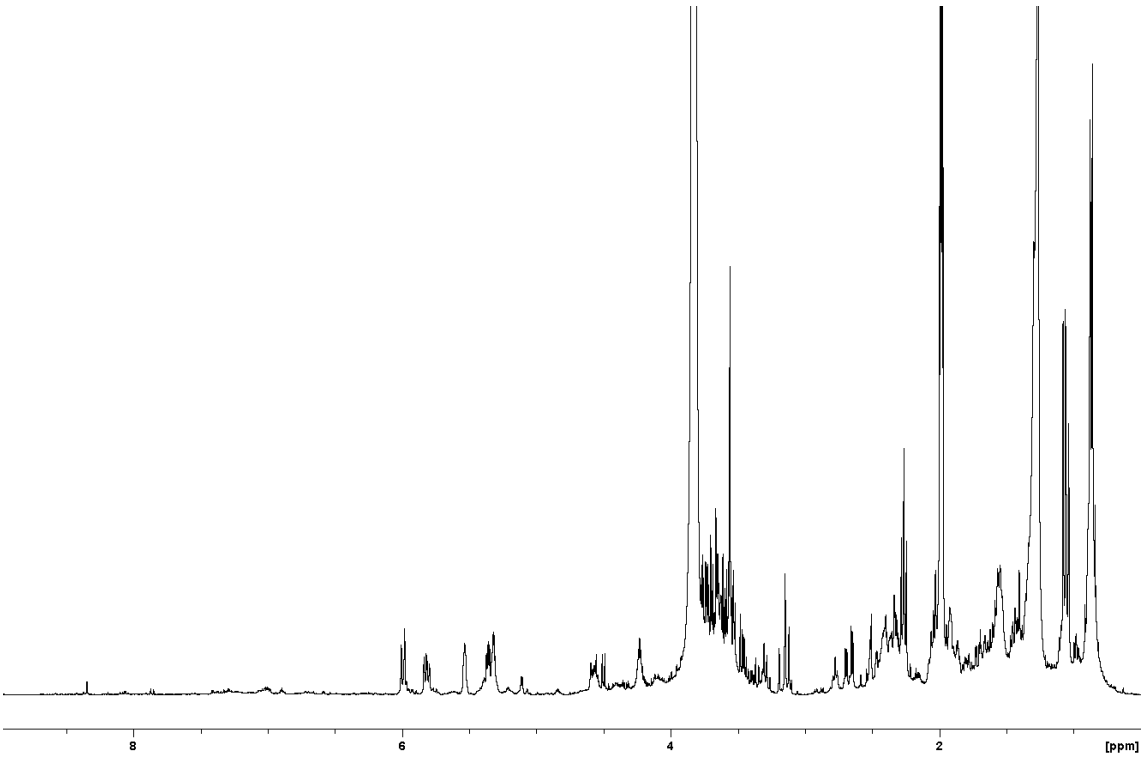


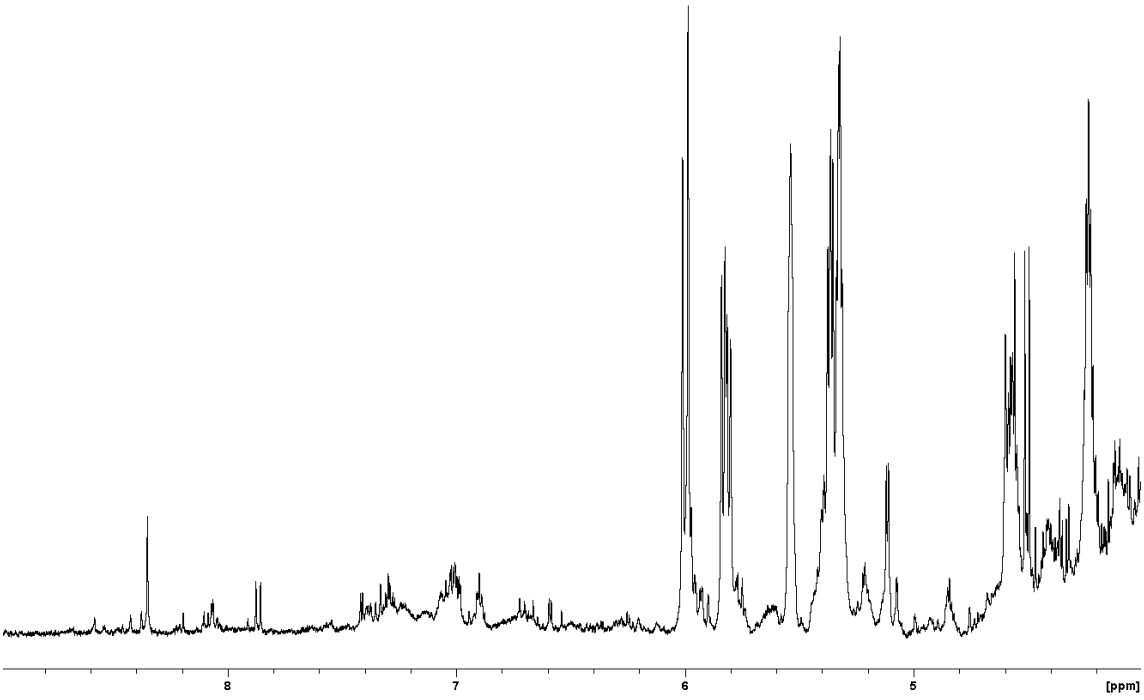

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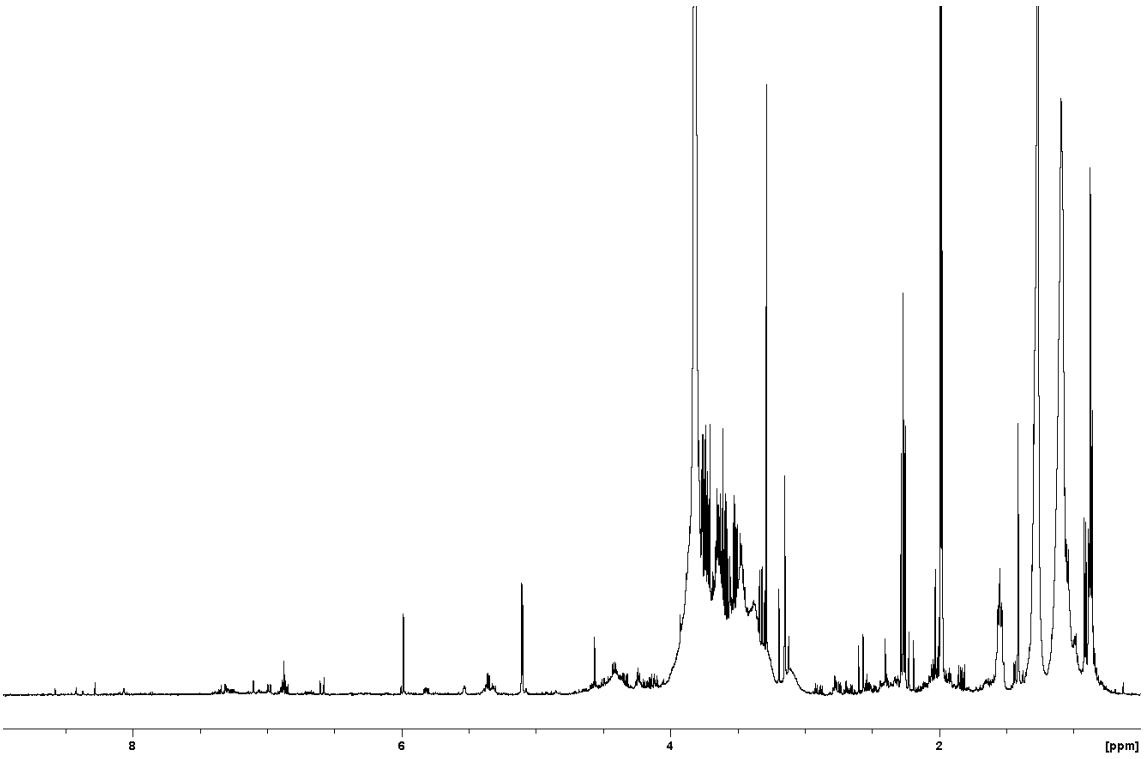


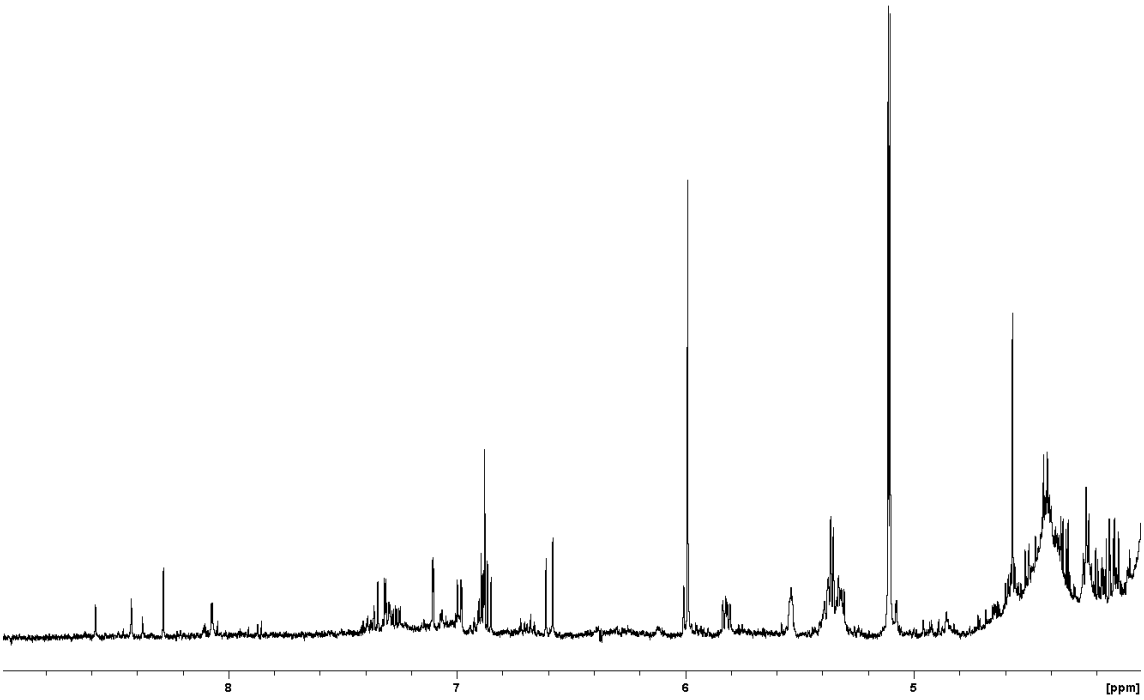

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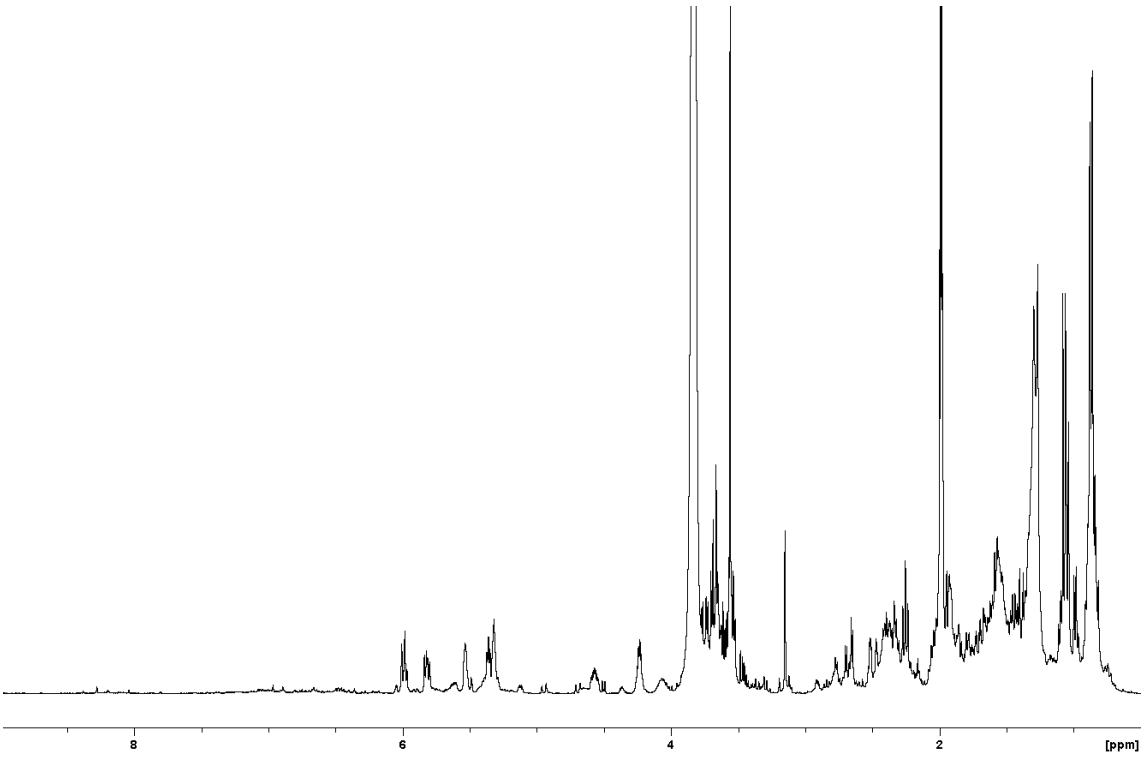


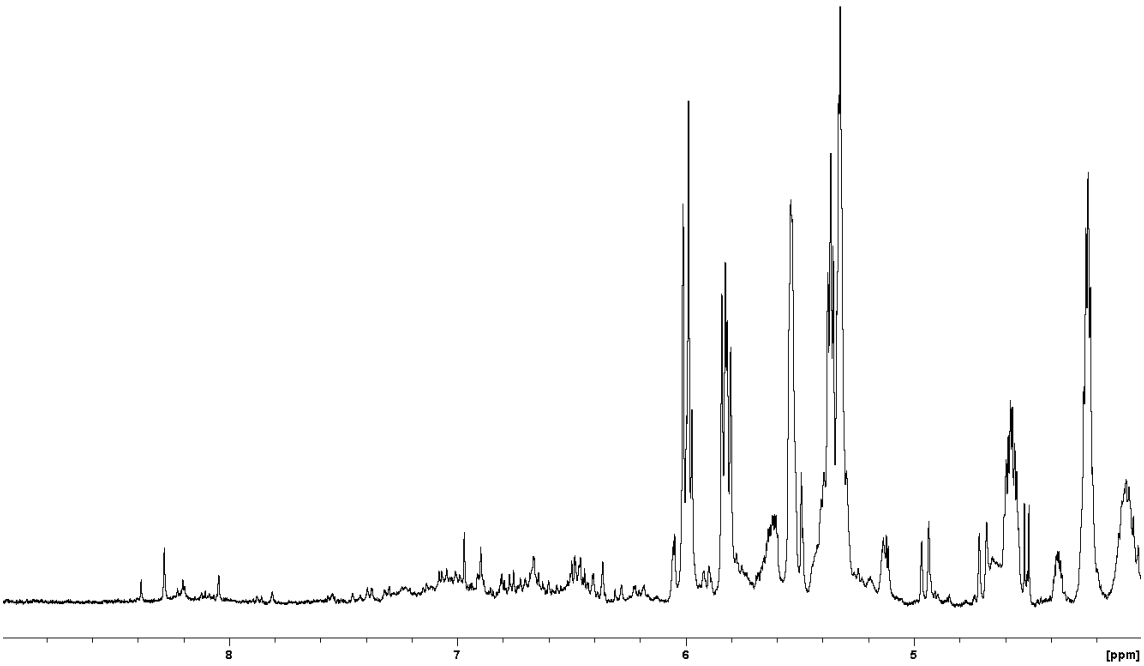

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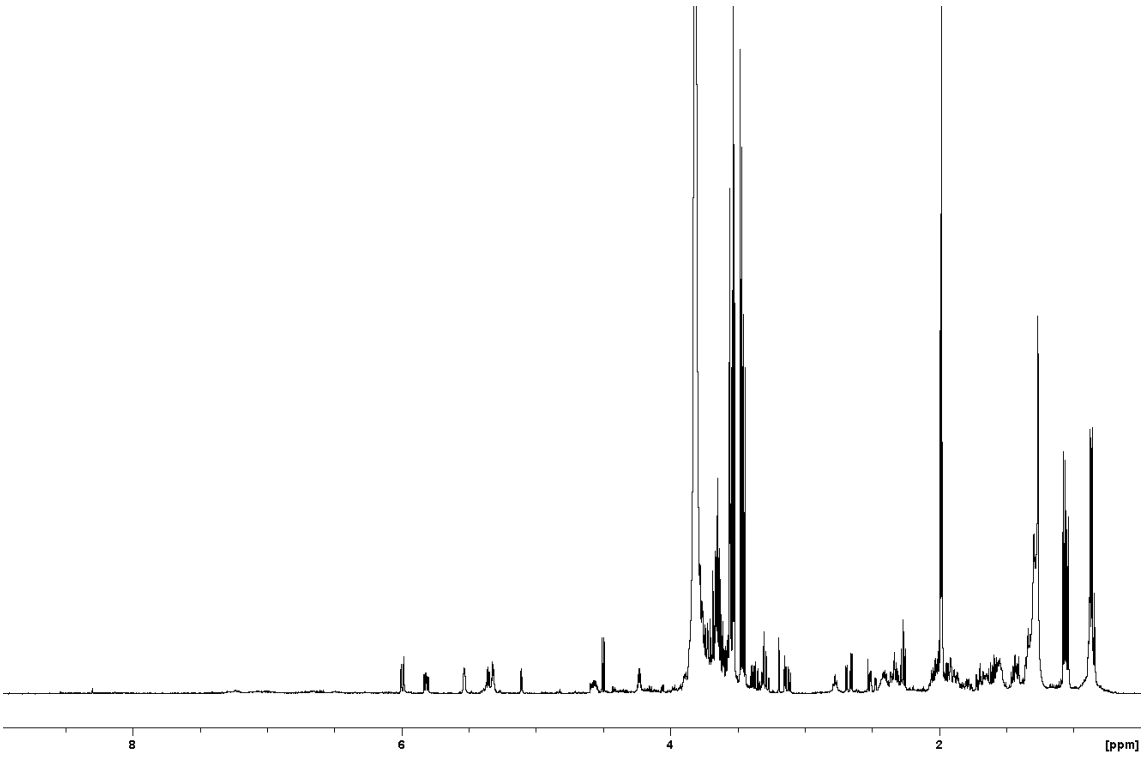


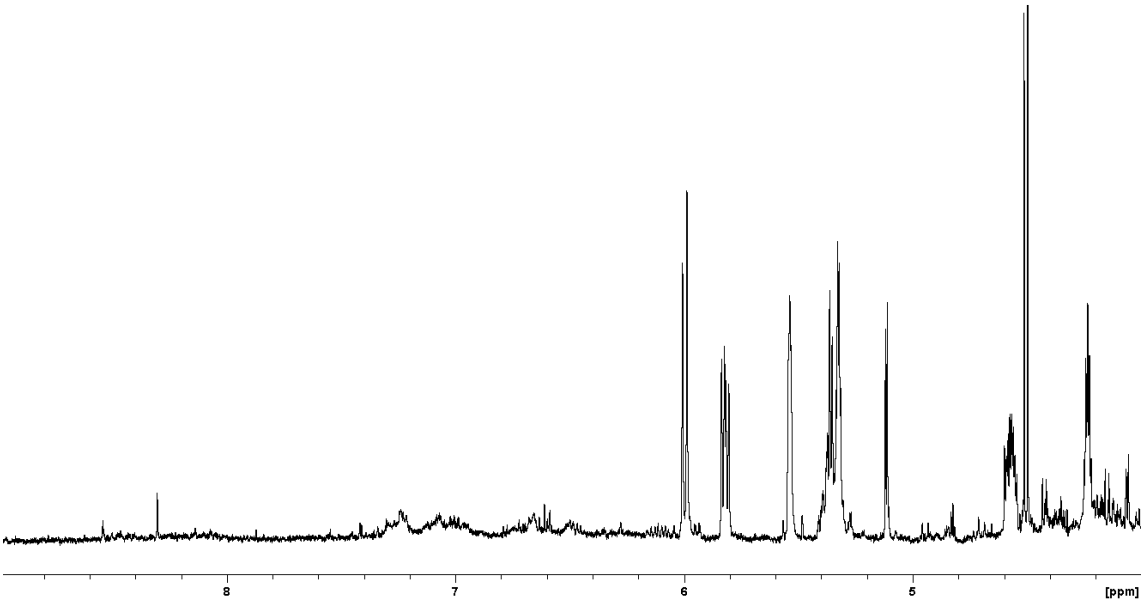

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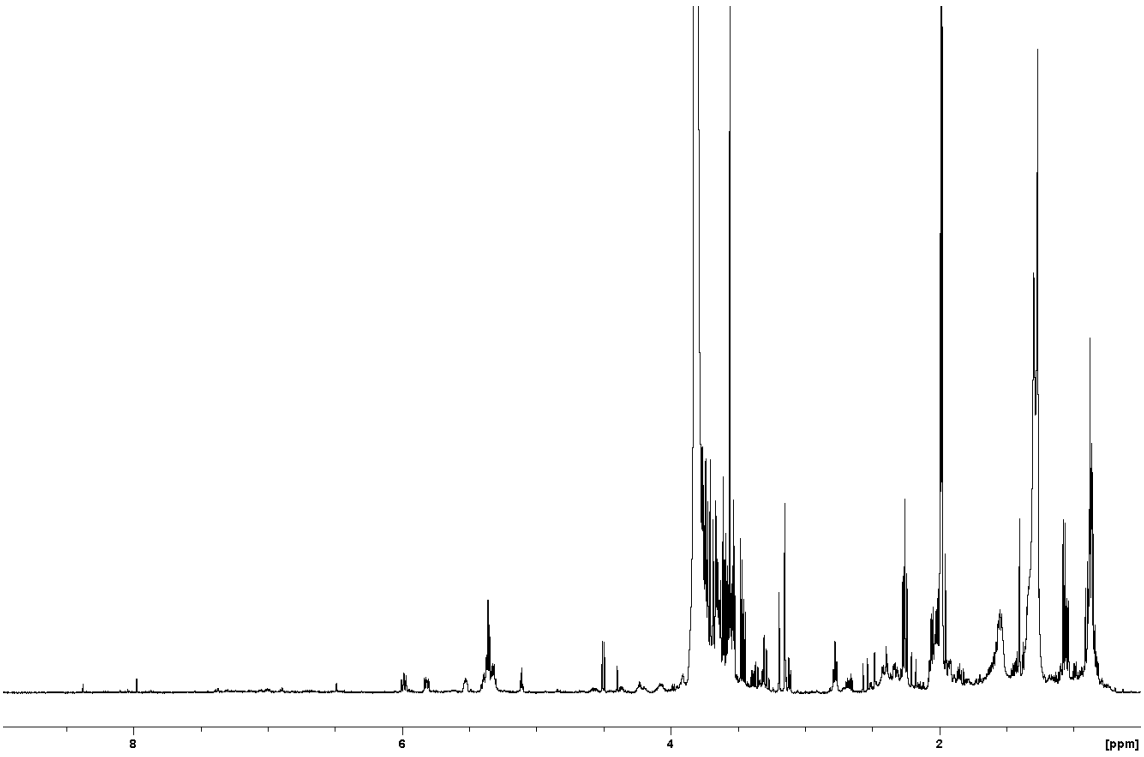
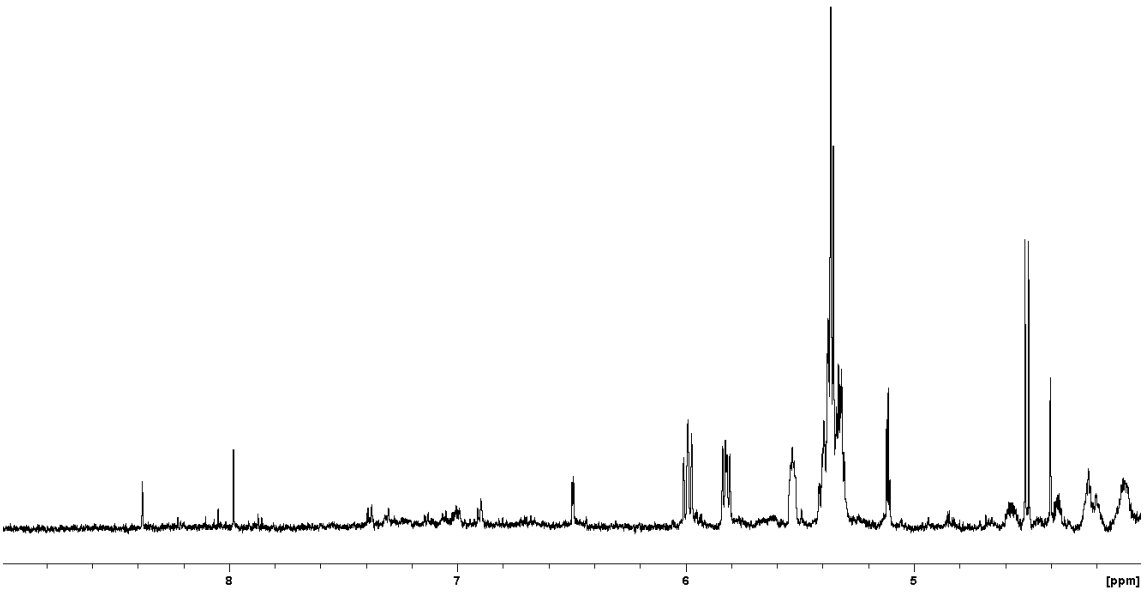
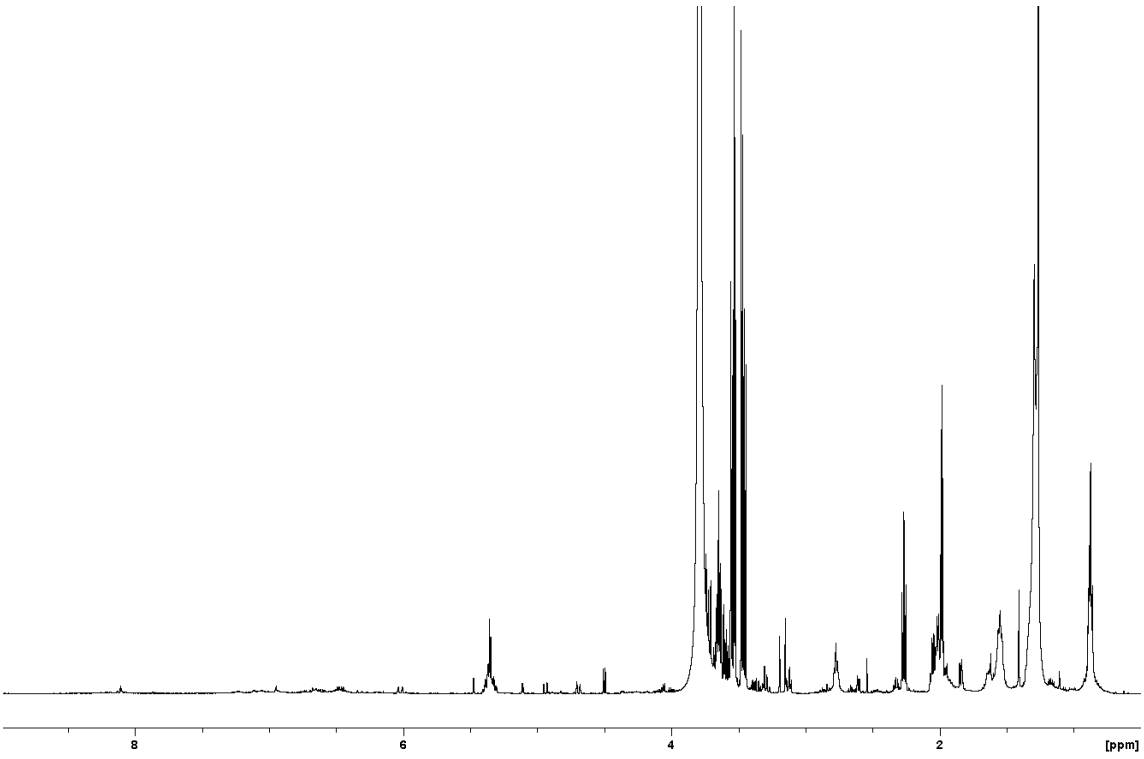
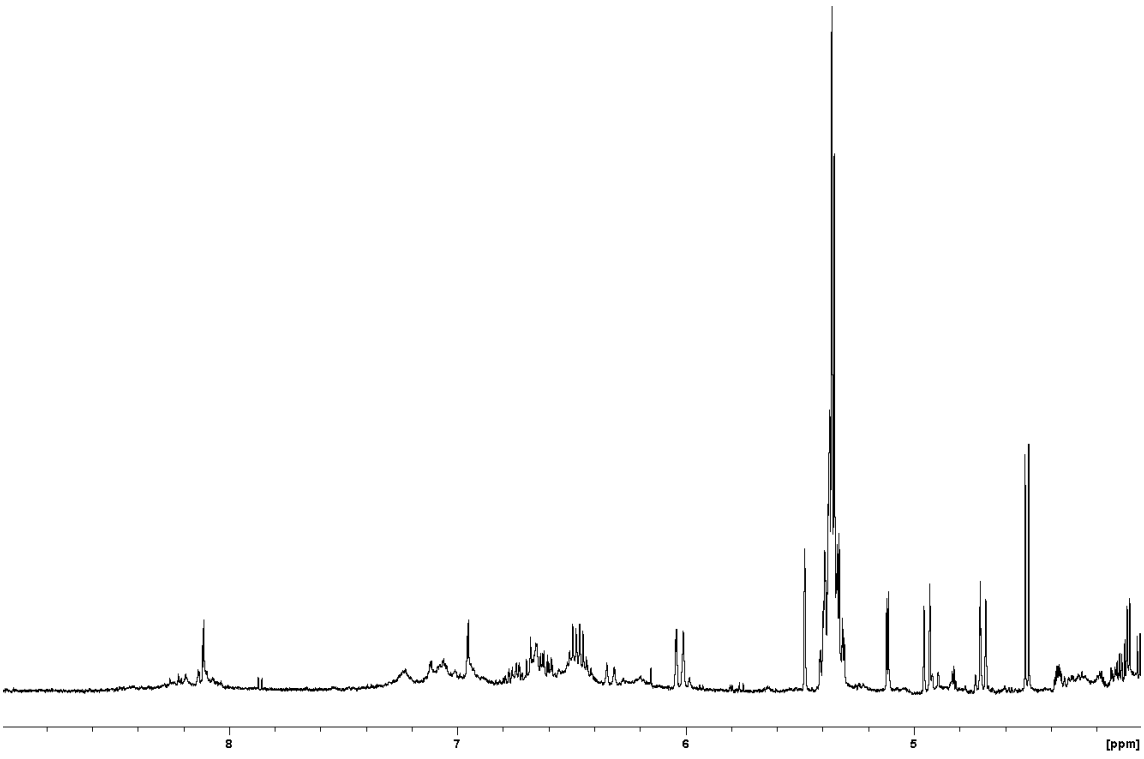


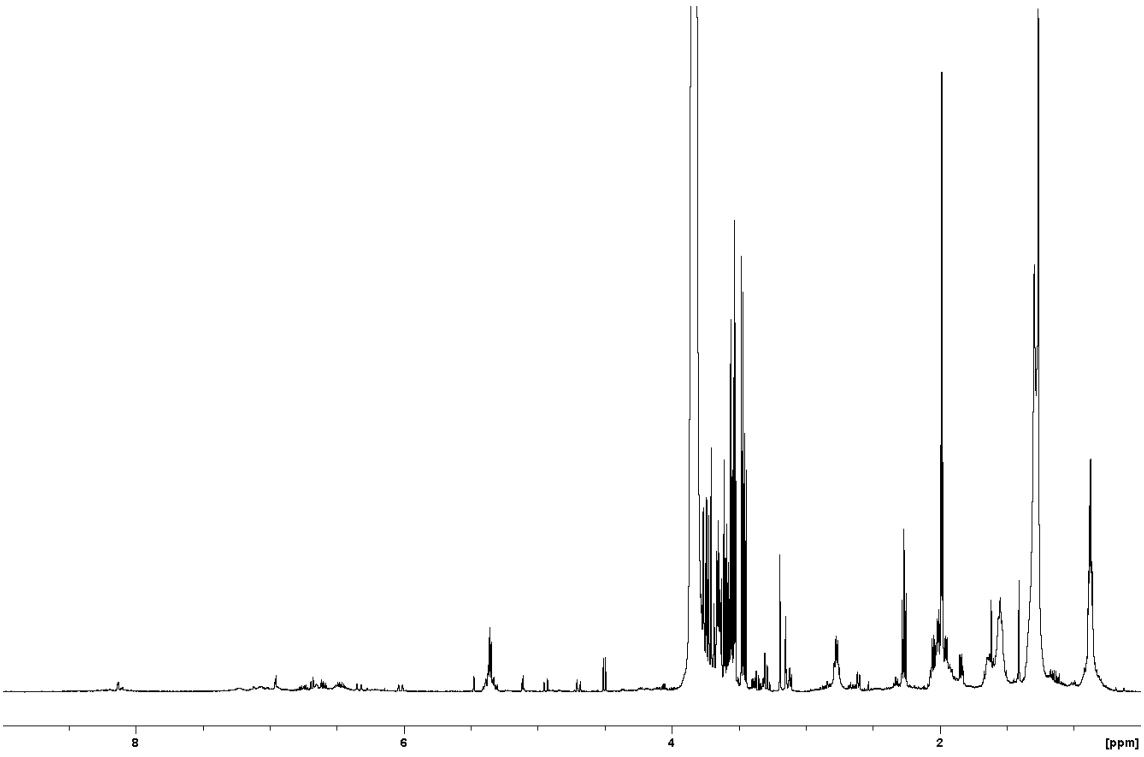



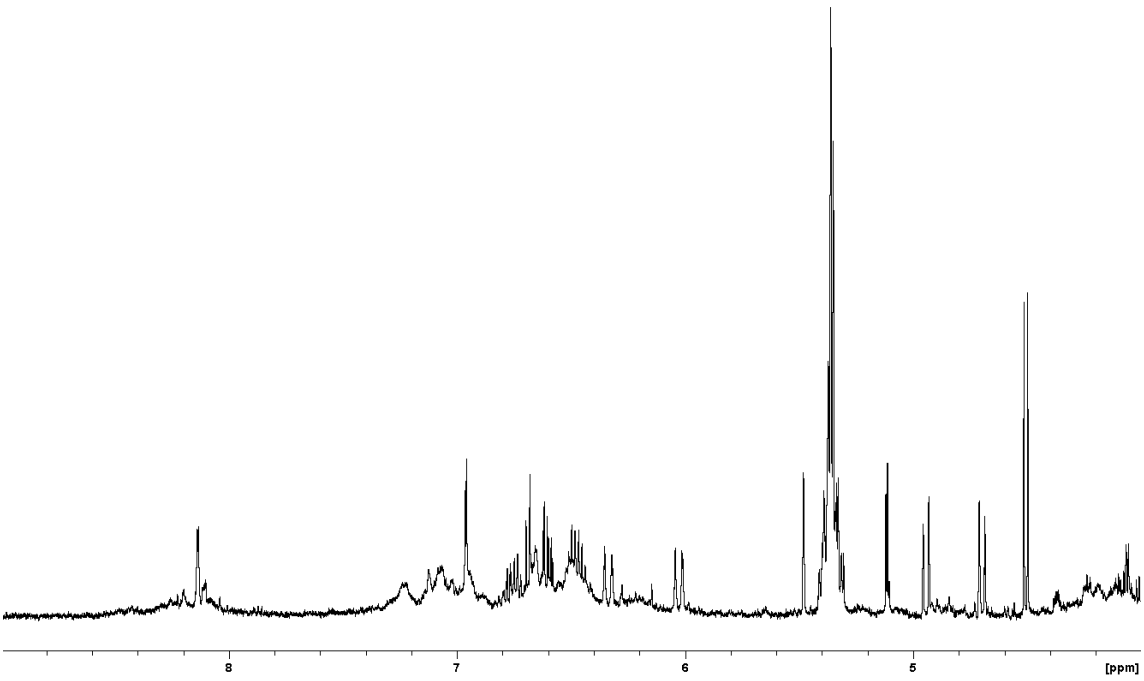
## DS 11 No monacolins detected



## DS 12 No monacolins detected



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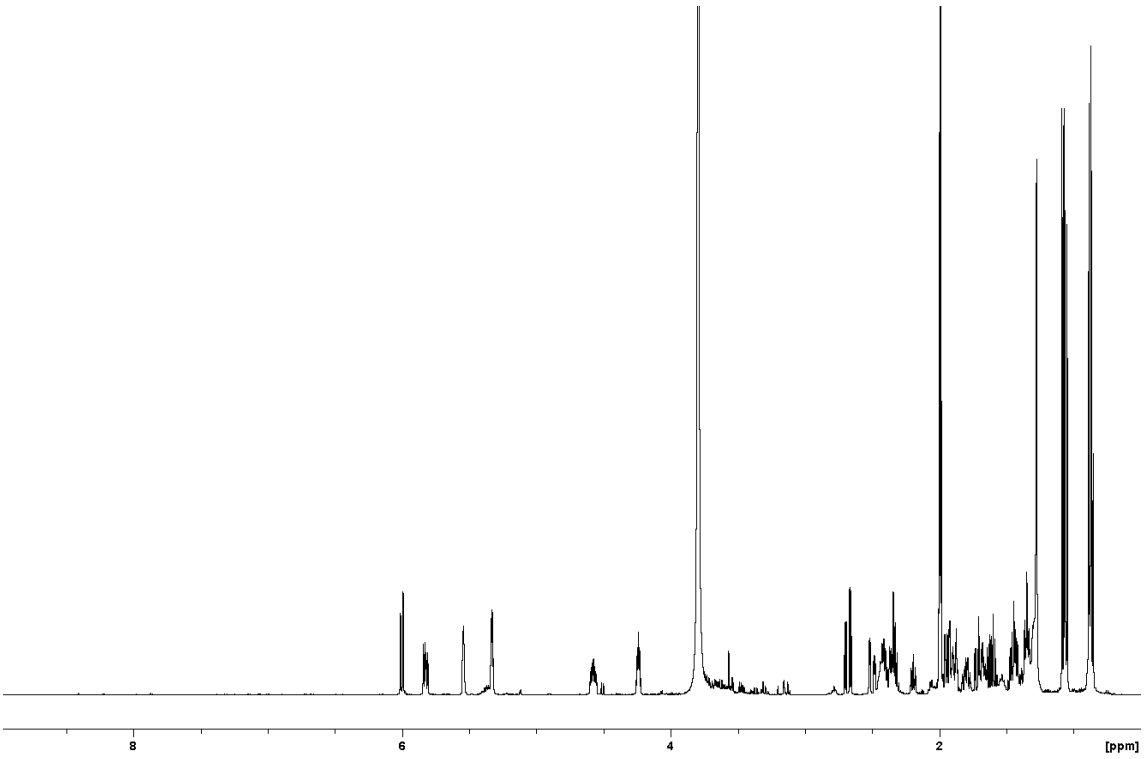


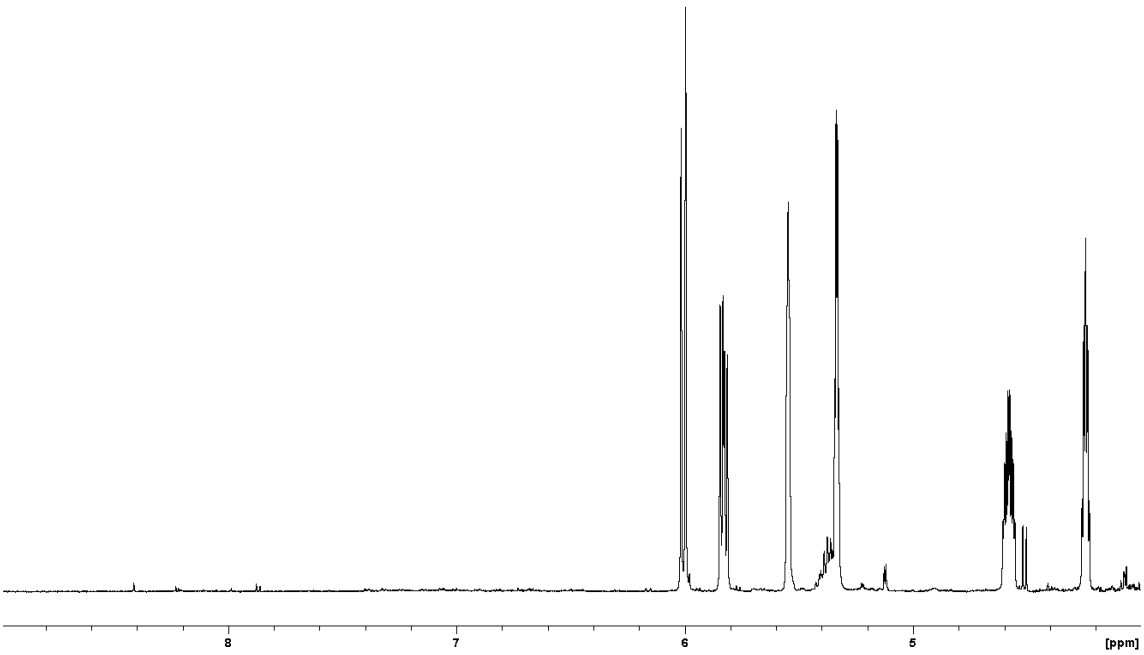

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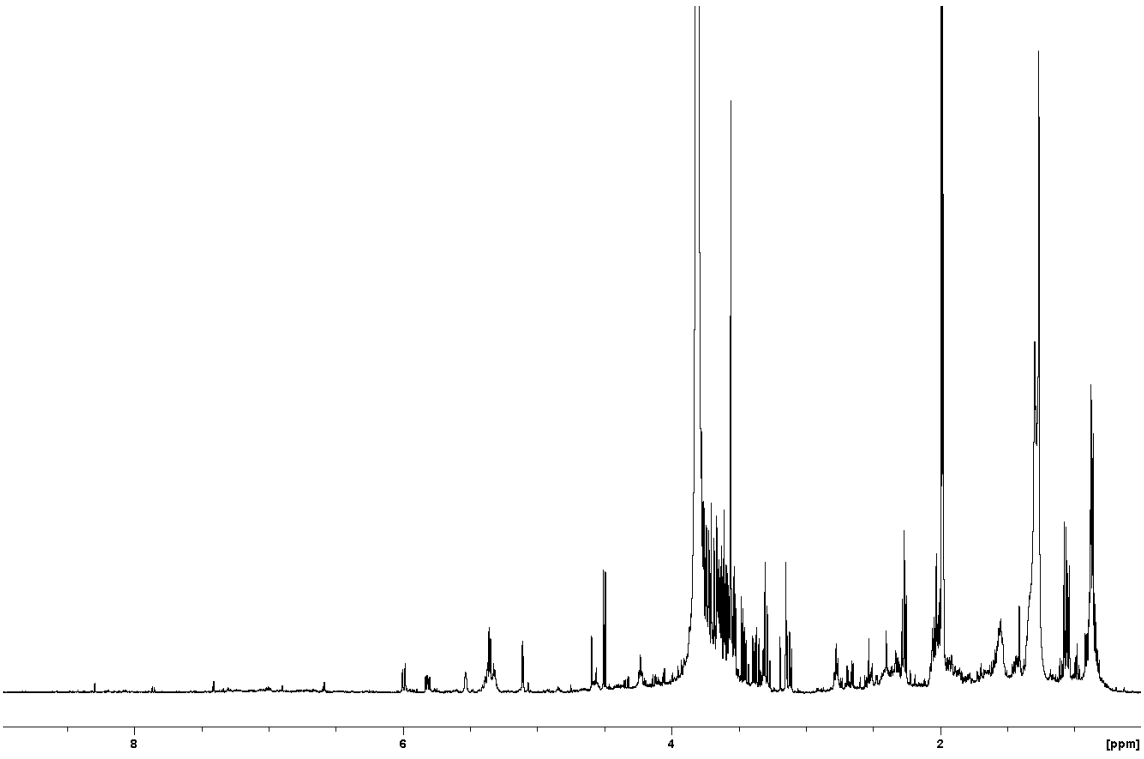


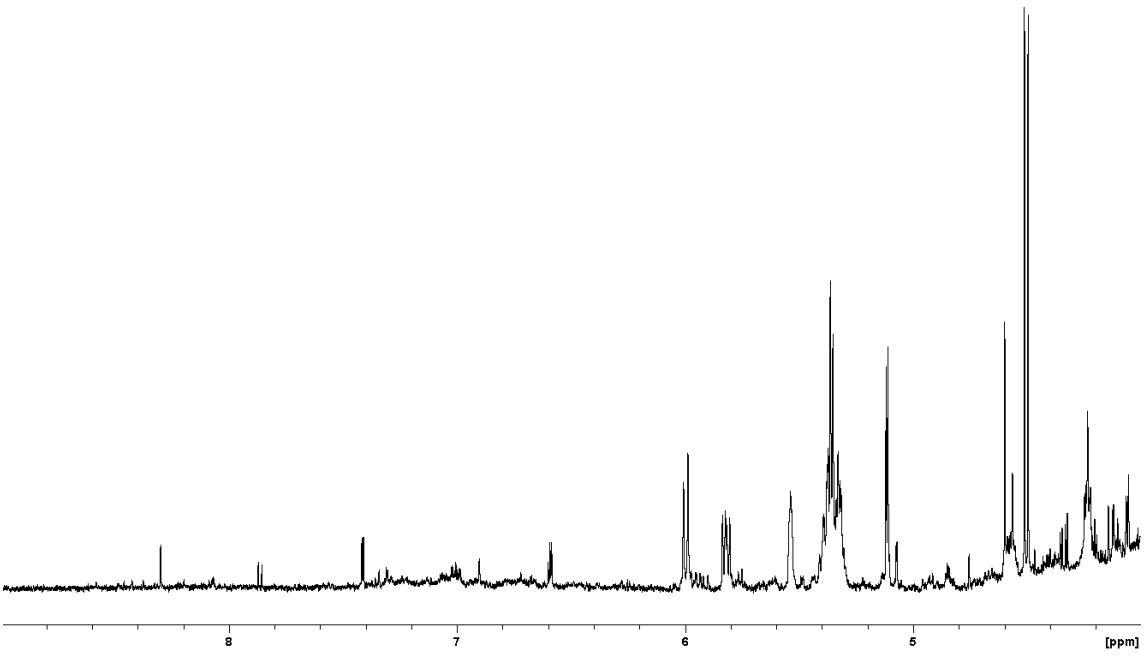

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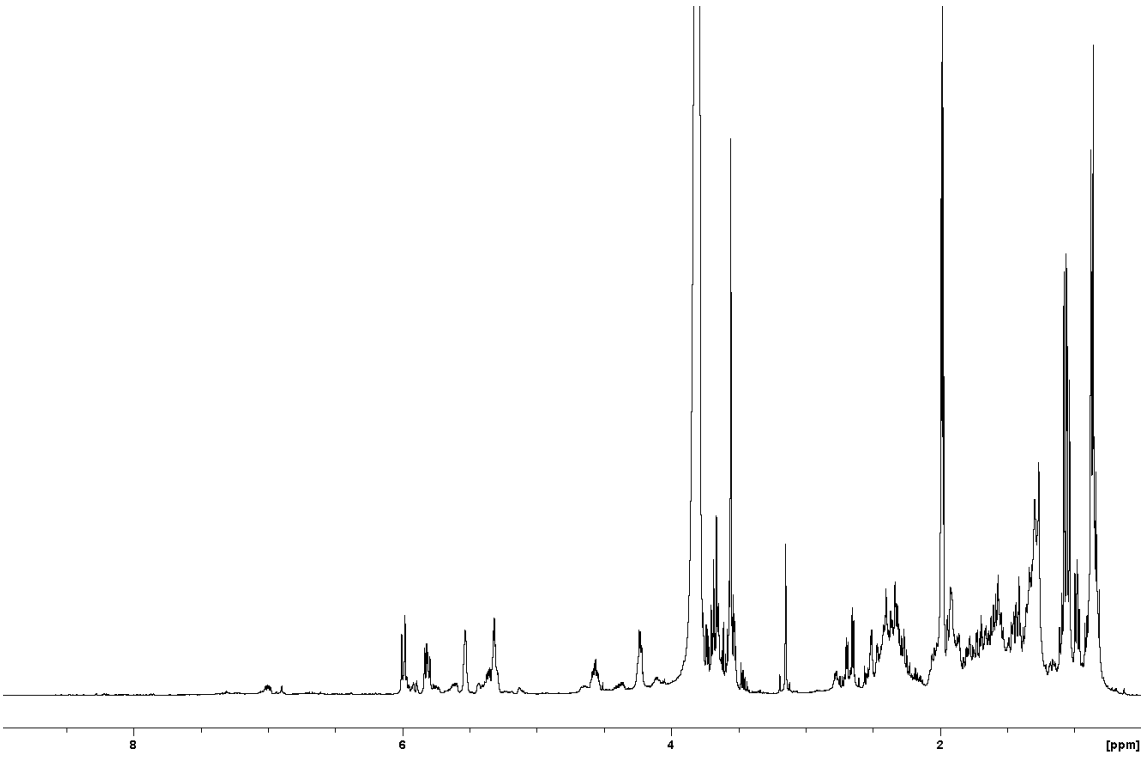
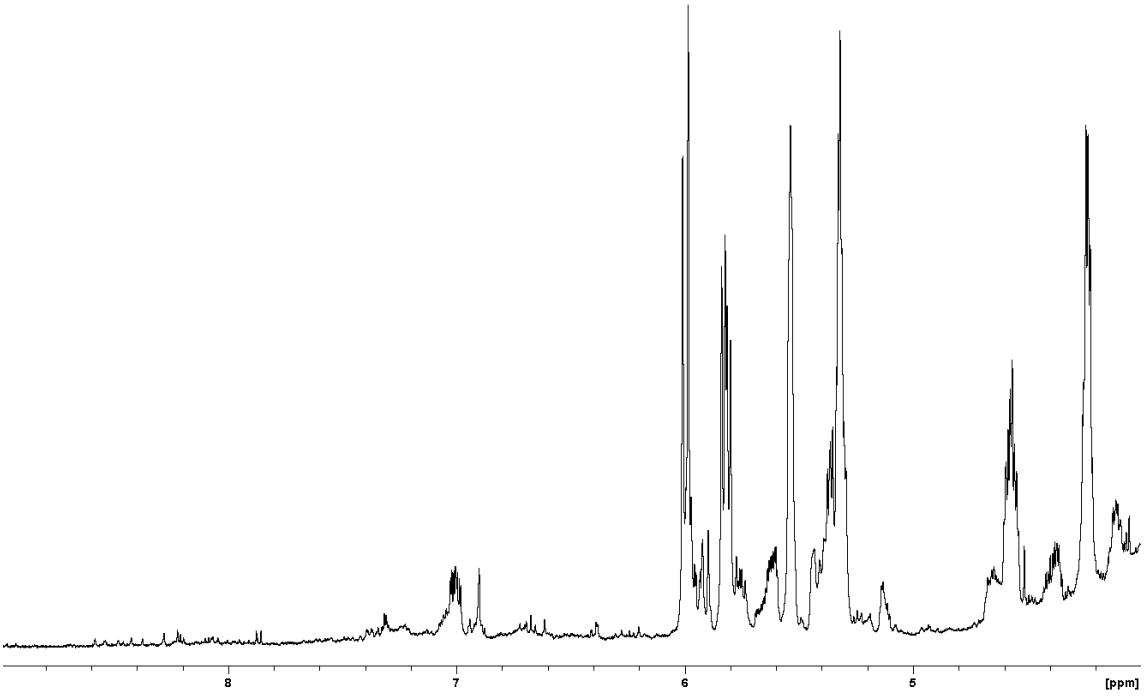
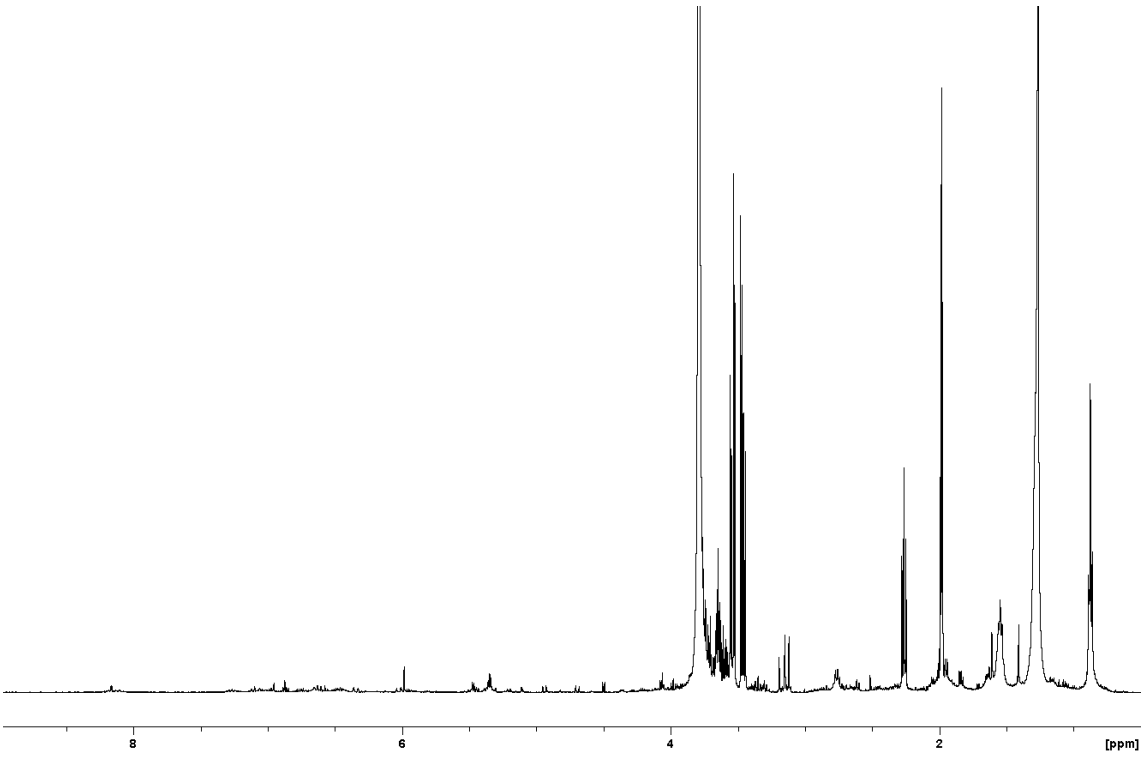
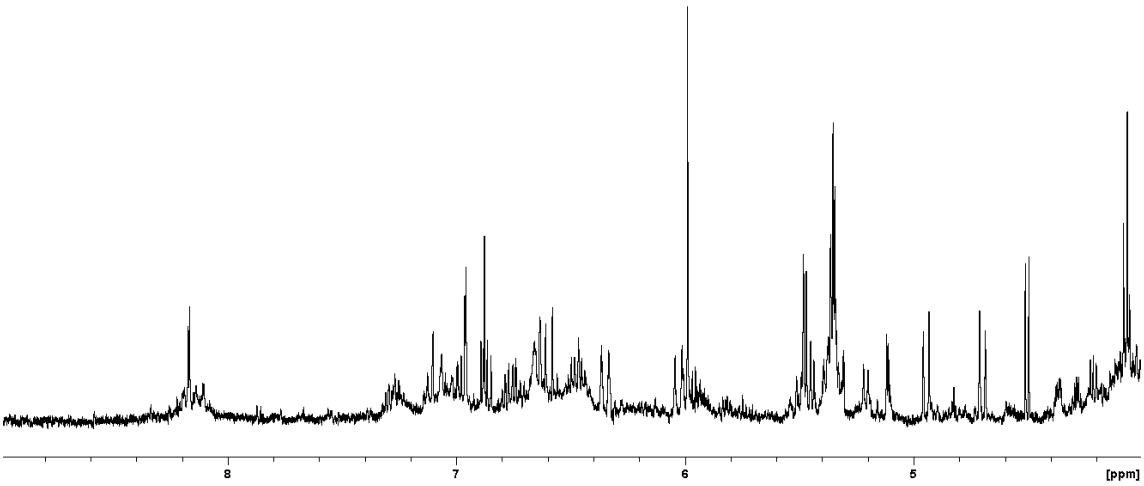


## DS 16 Monacolins hardly detected



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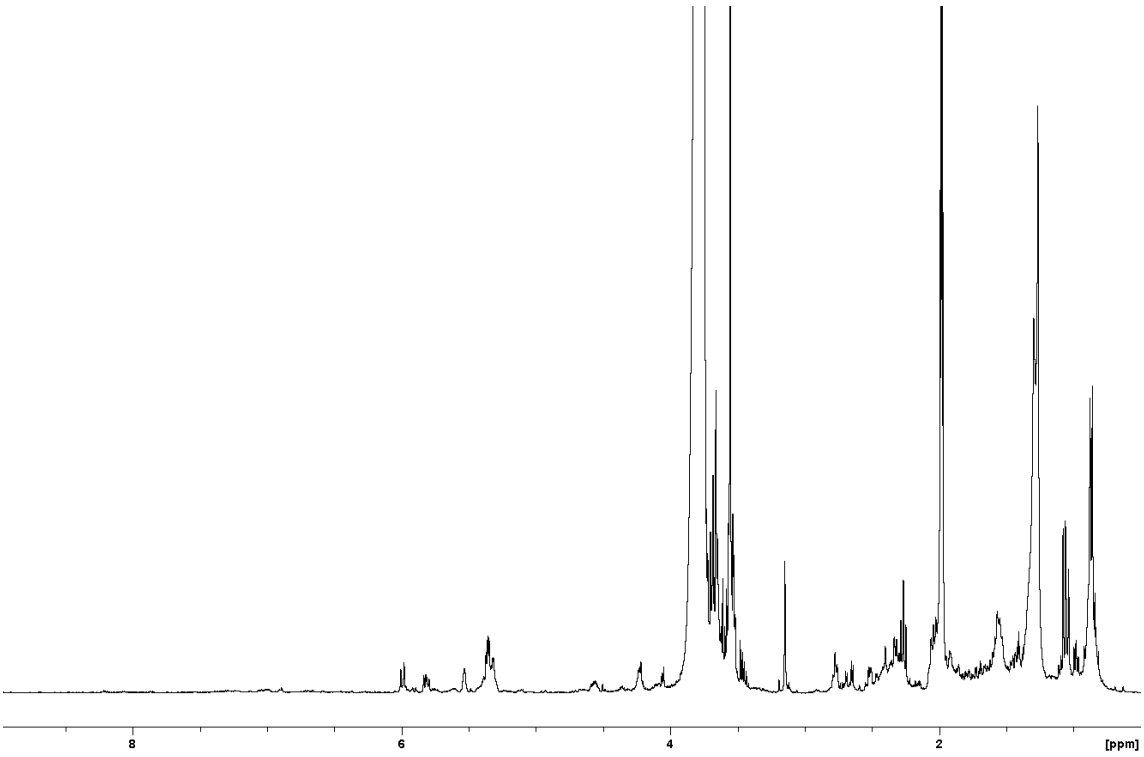


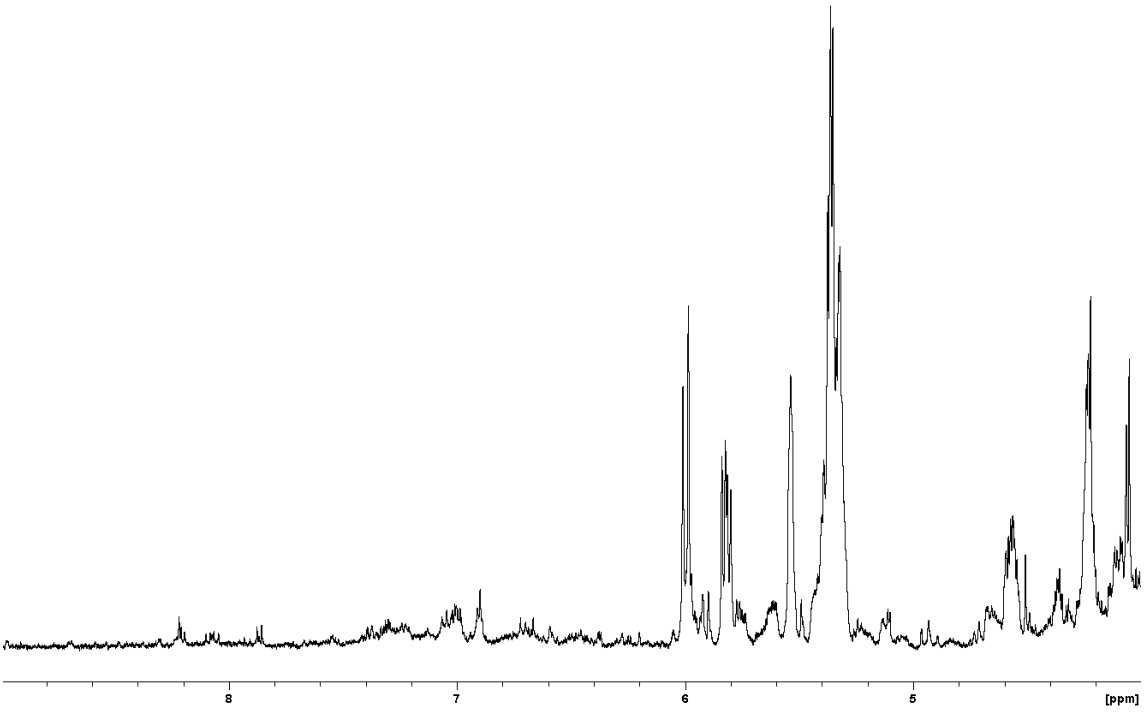

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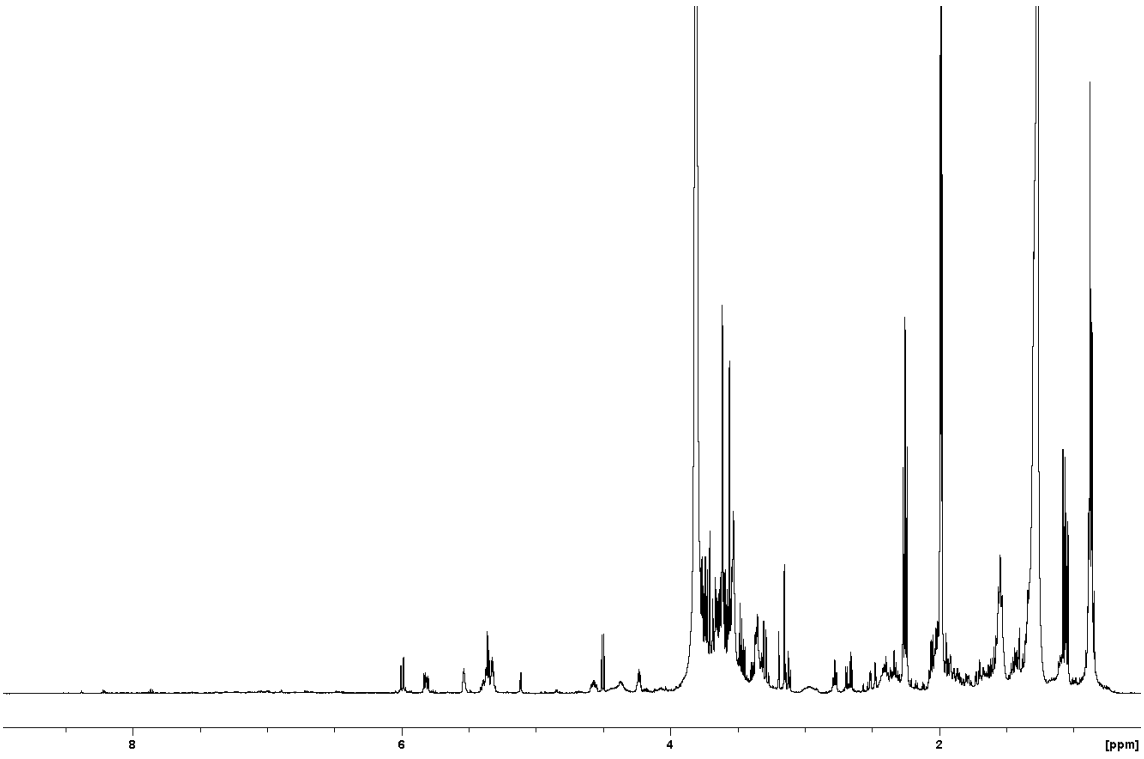


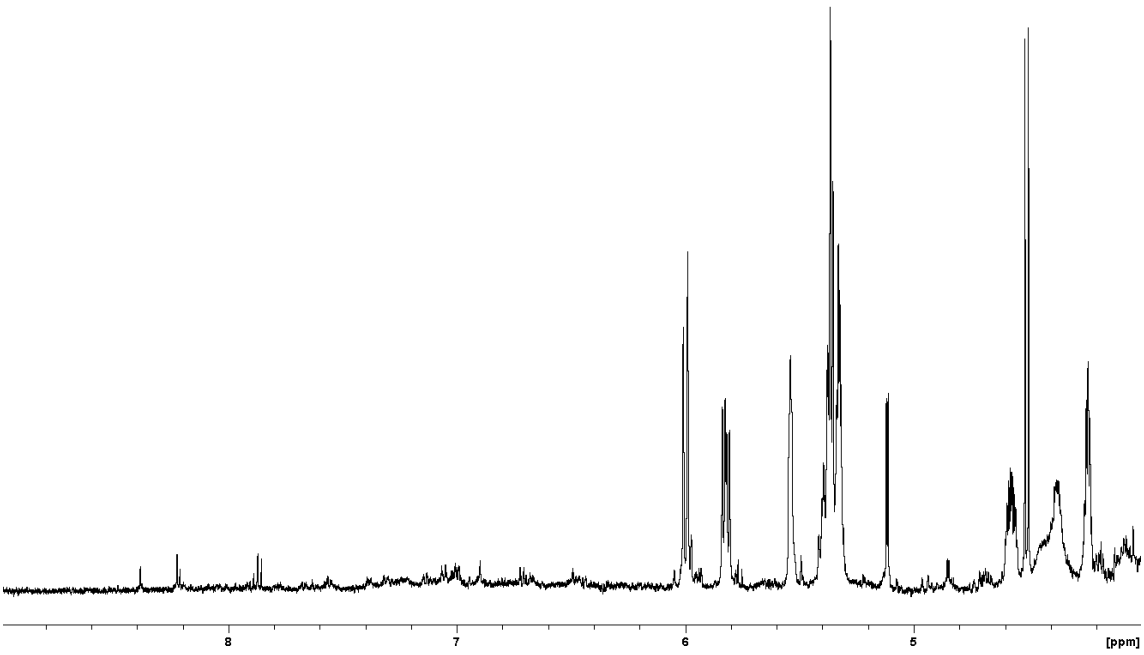

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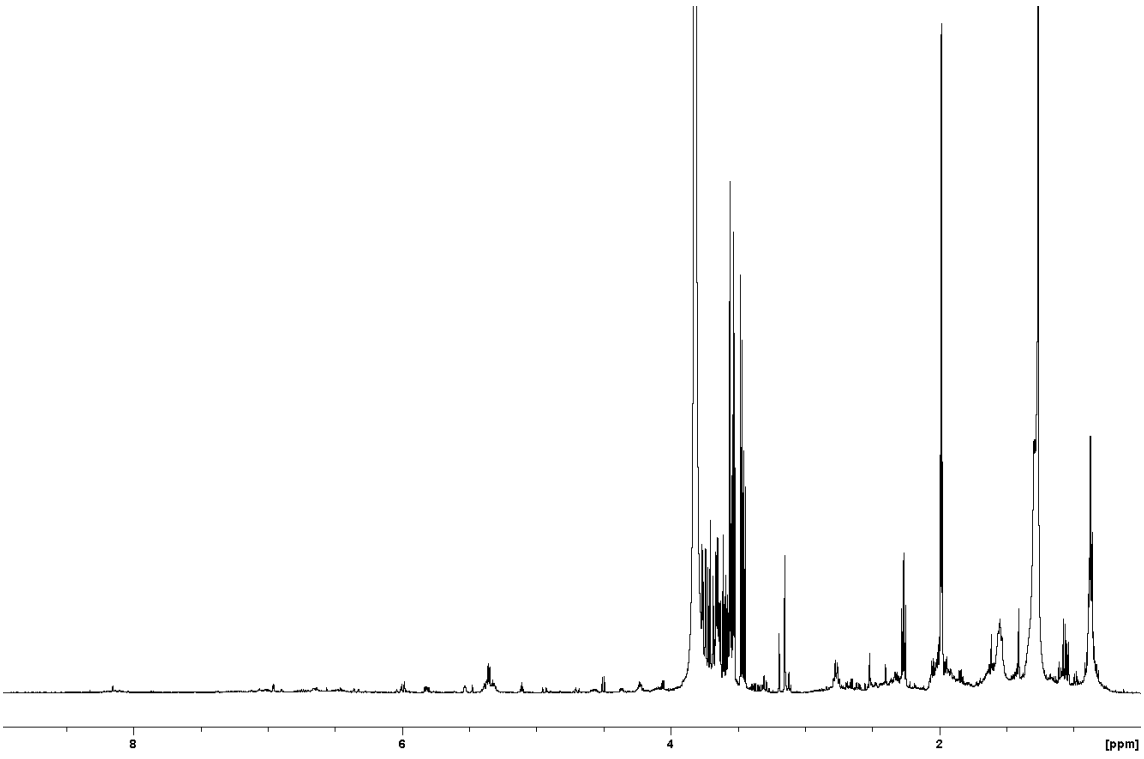


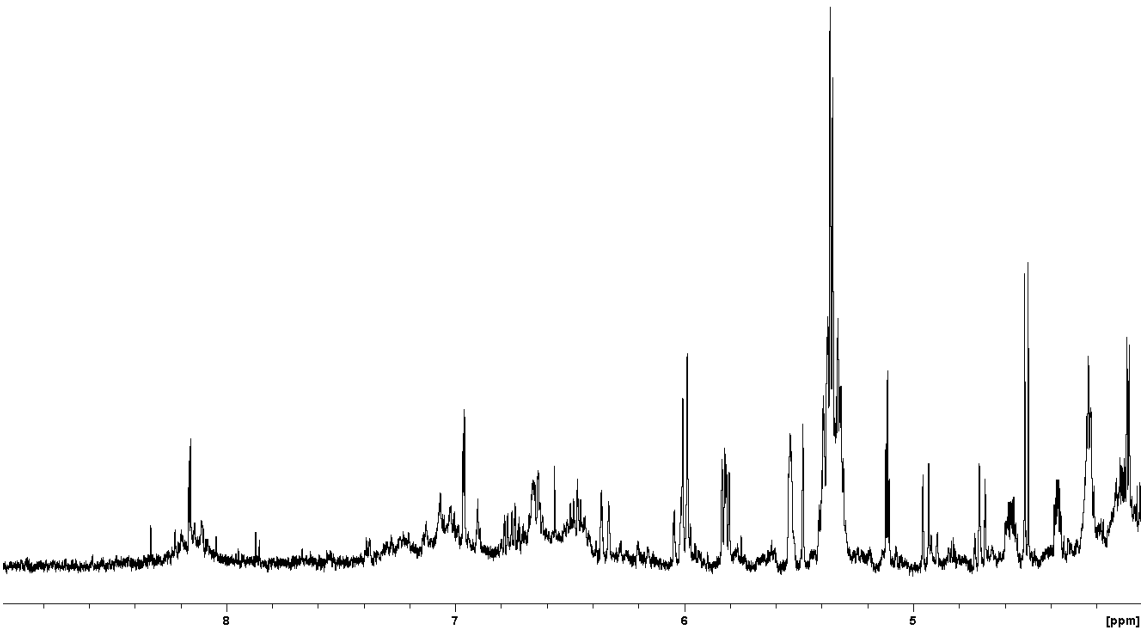

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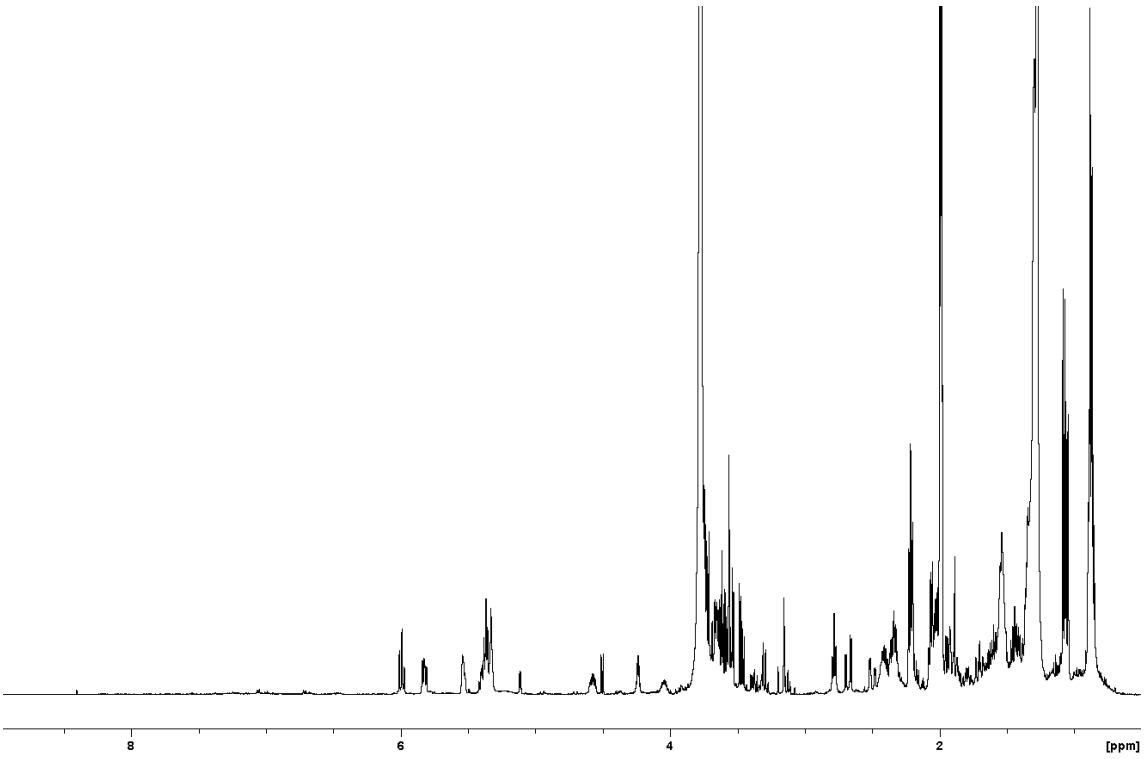


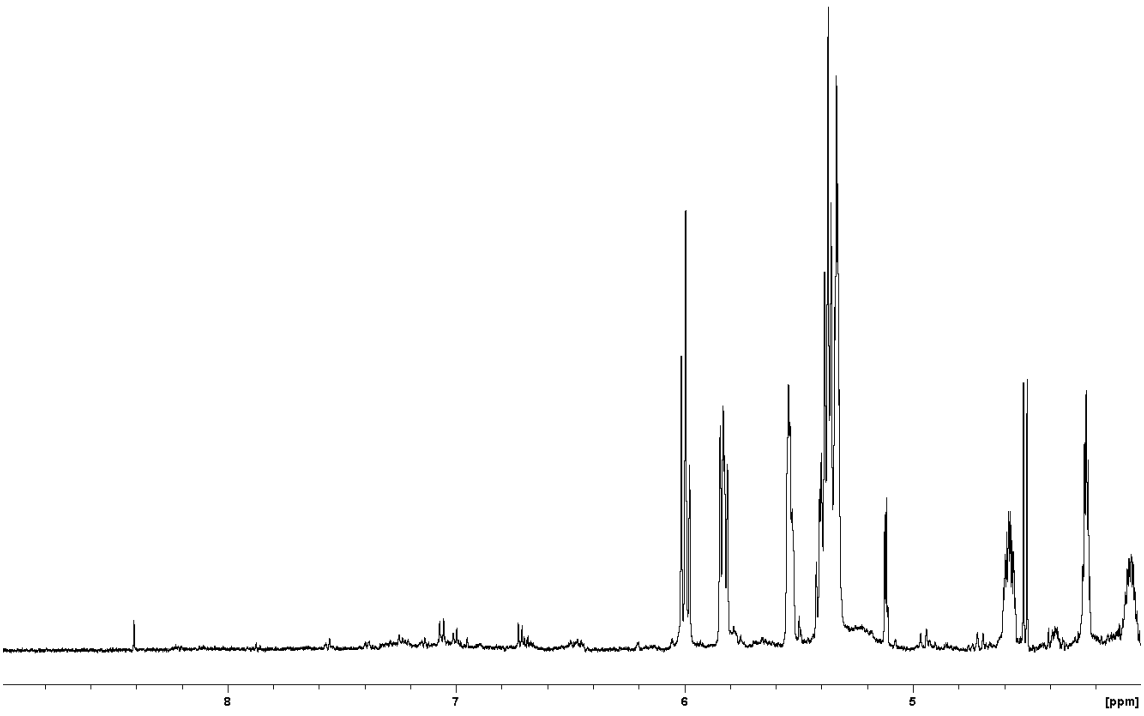

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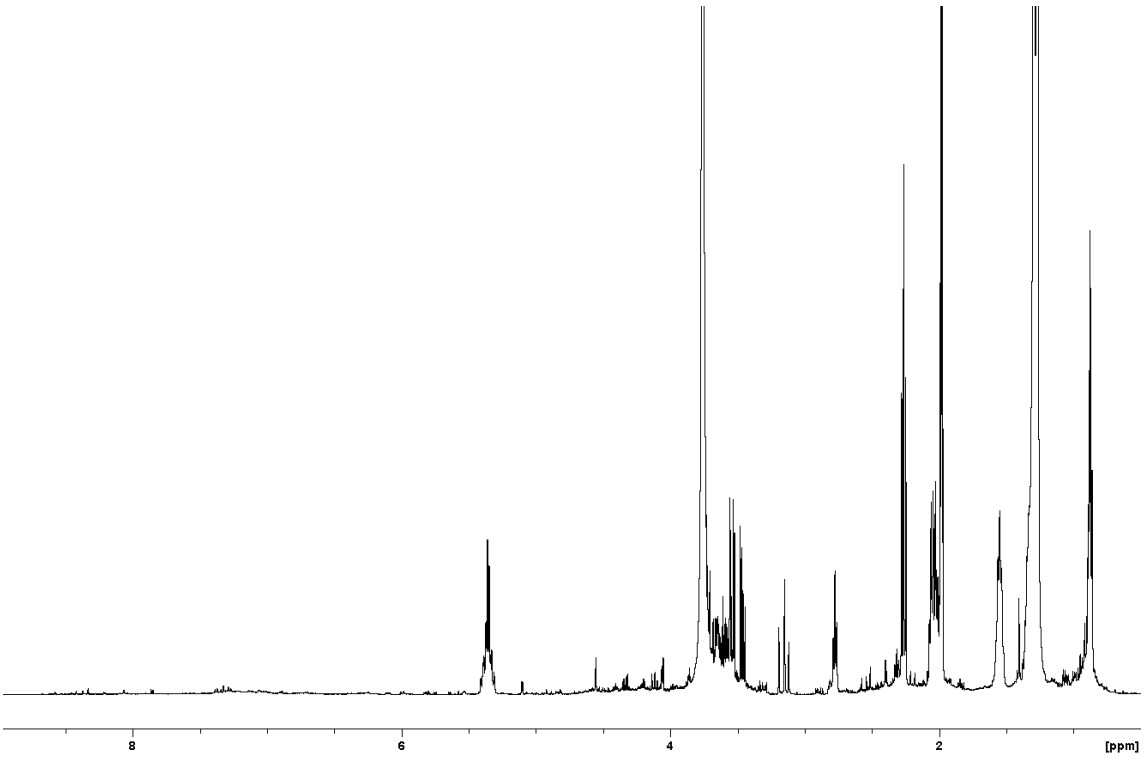


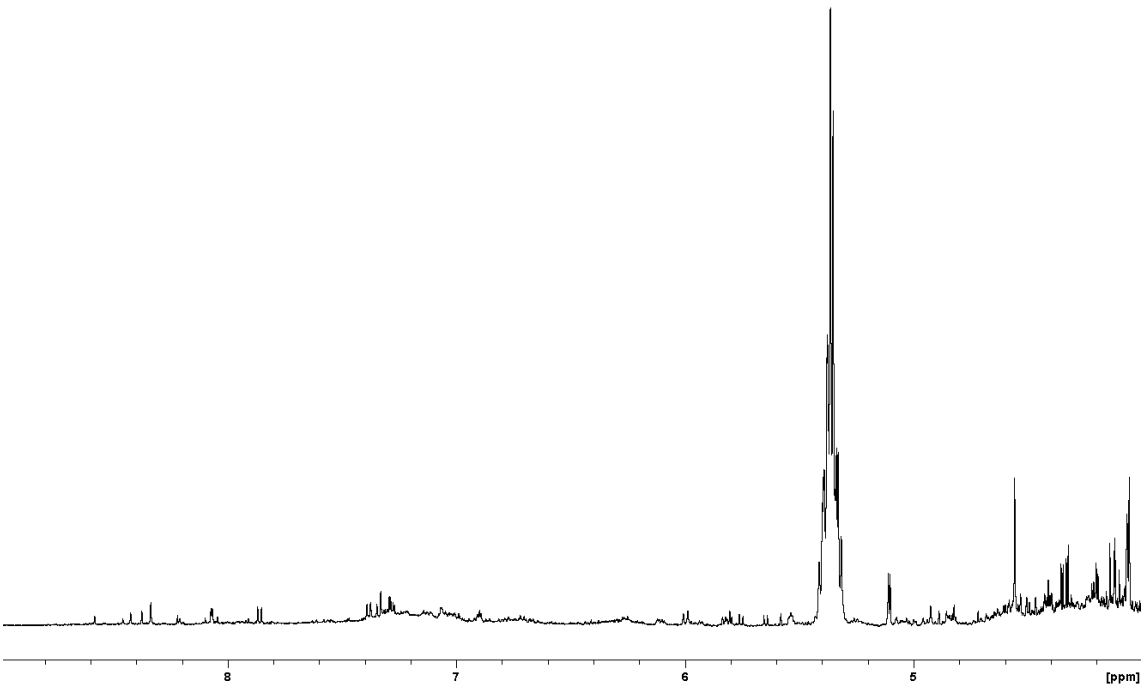

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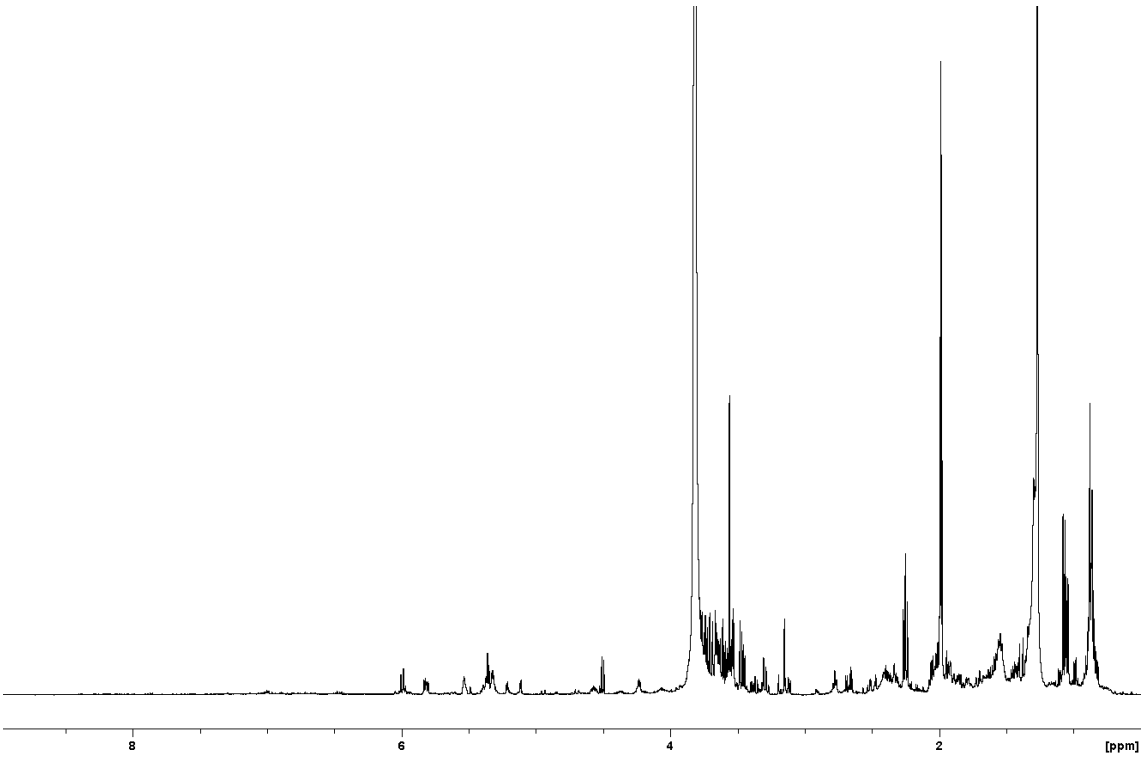


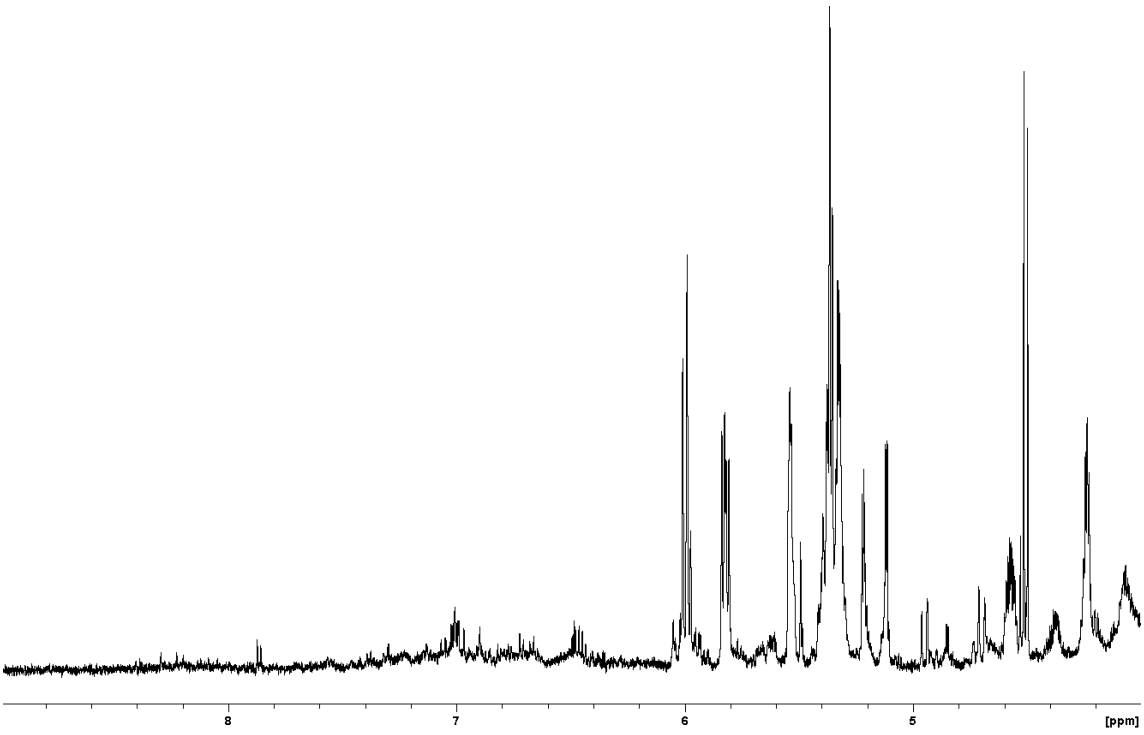

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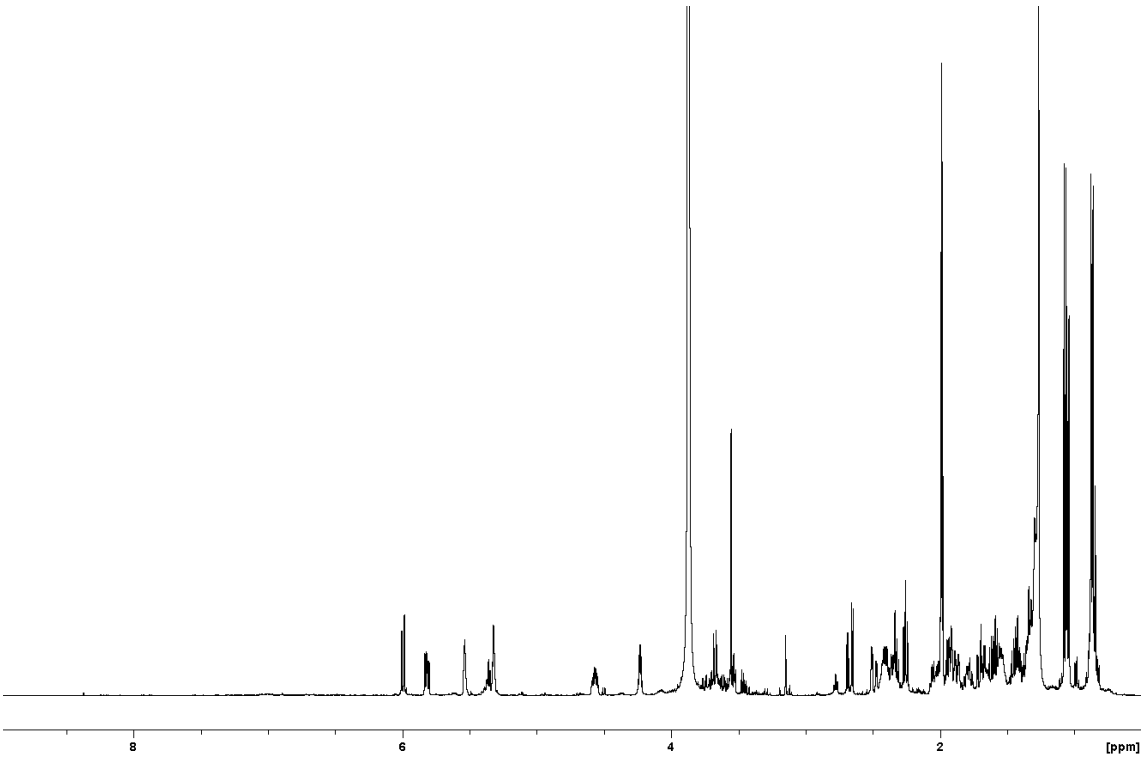


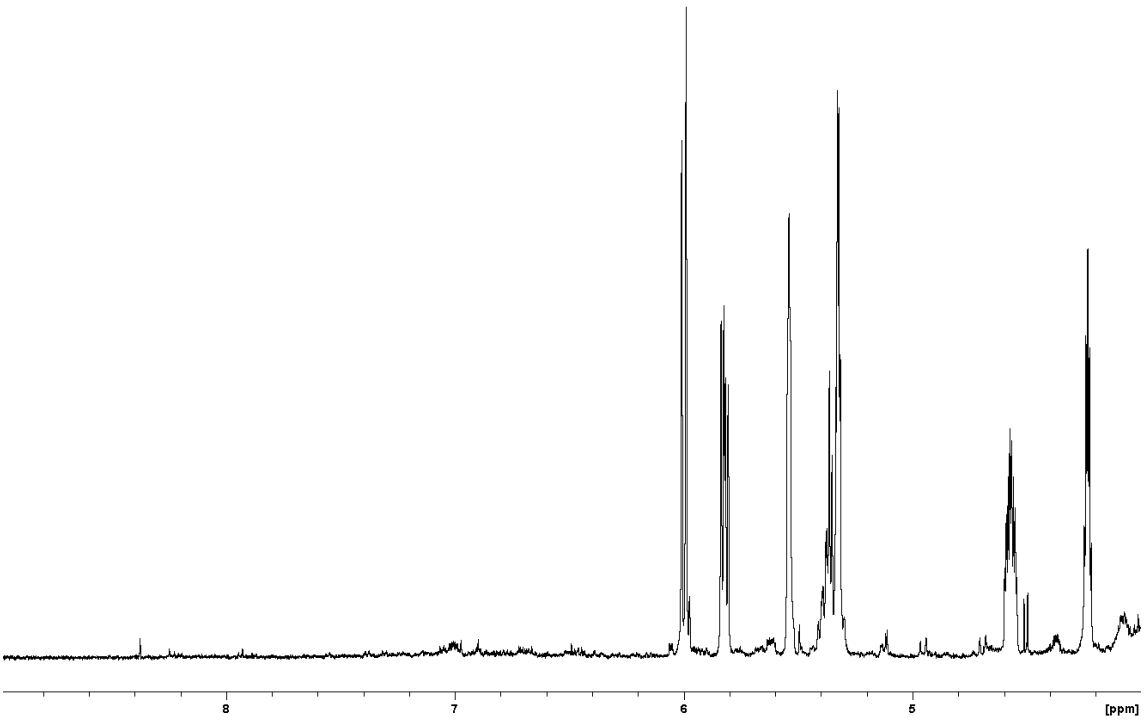

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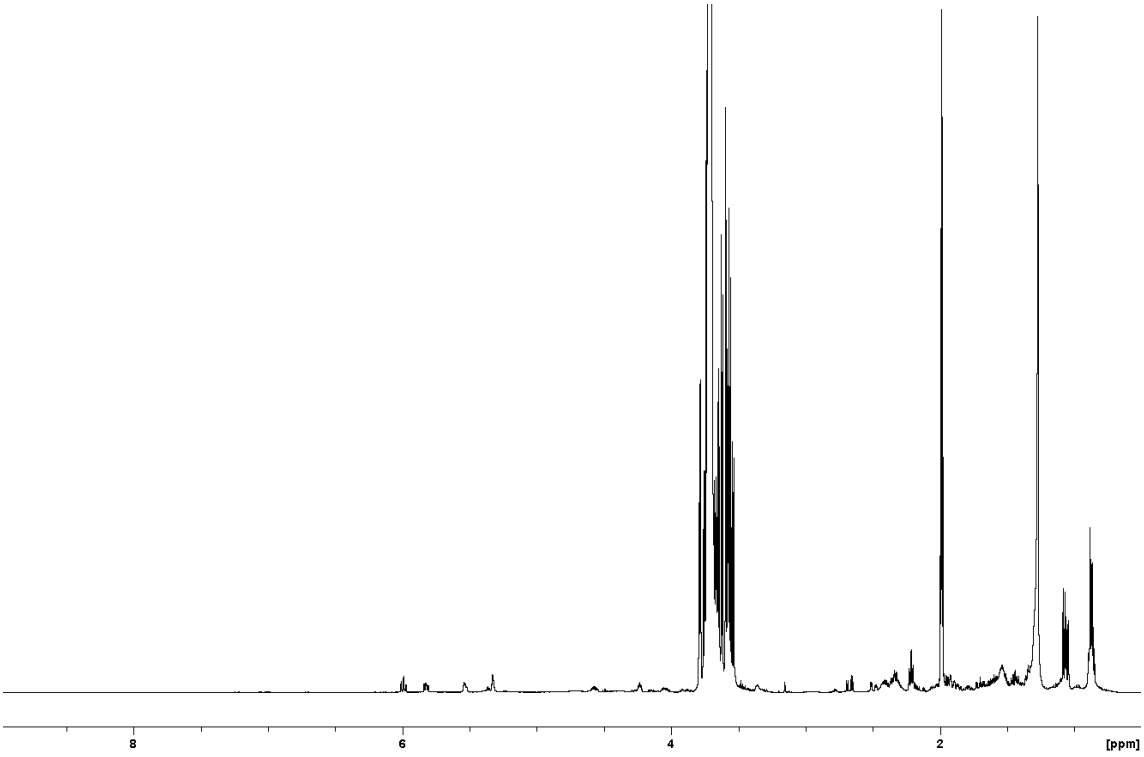


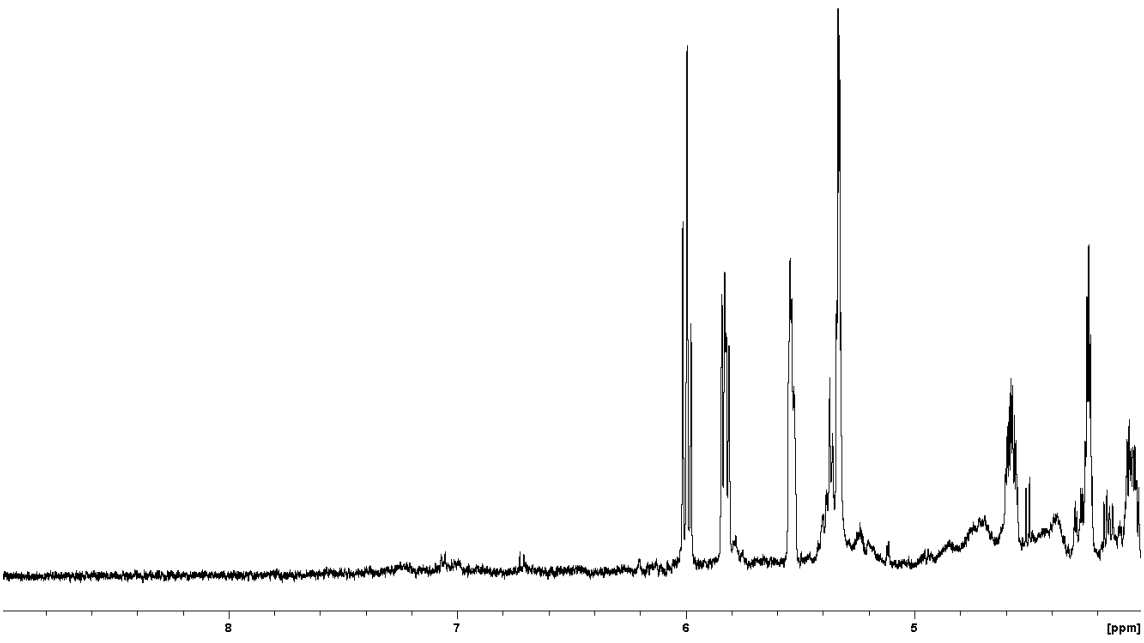

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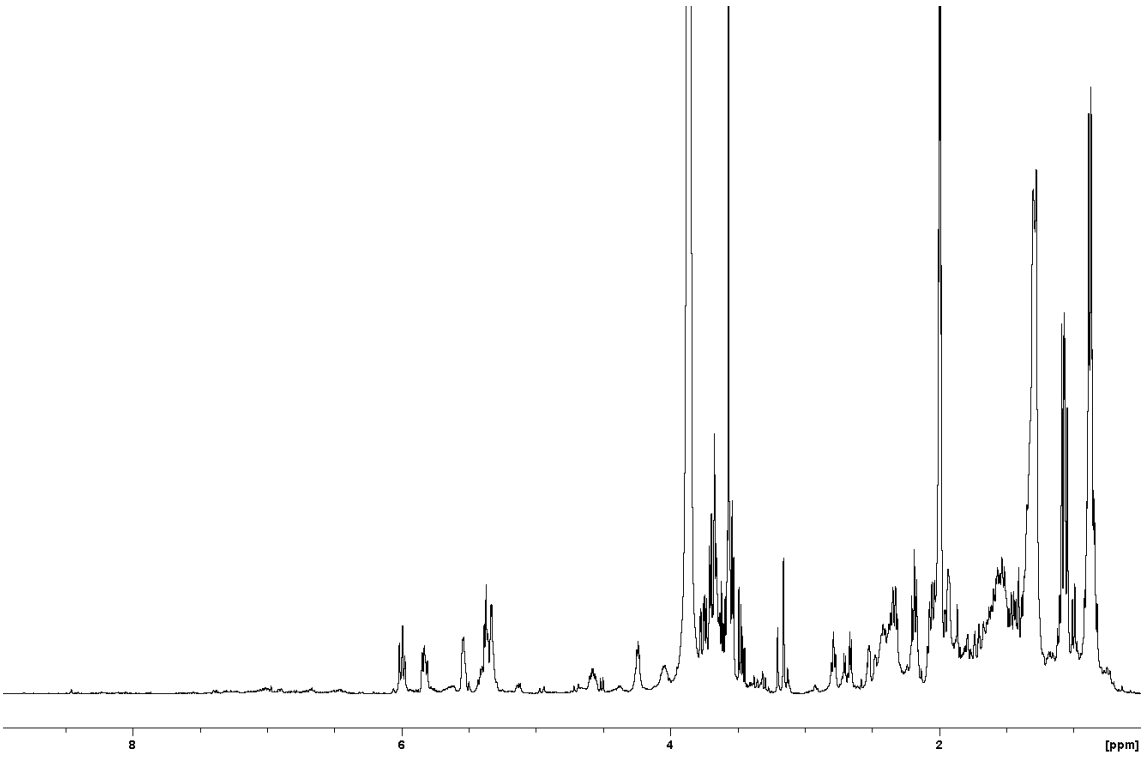


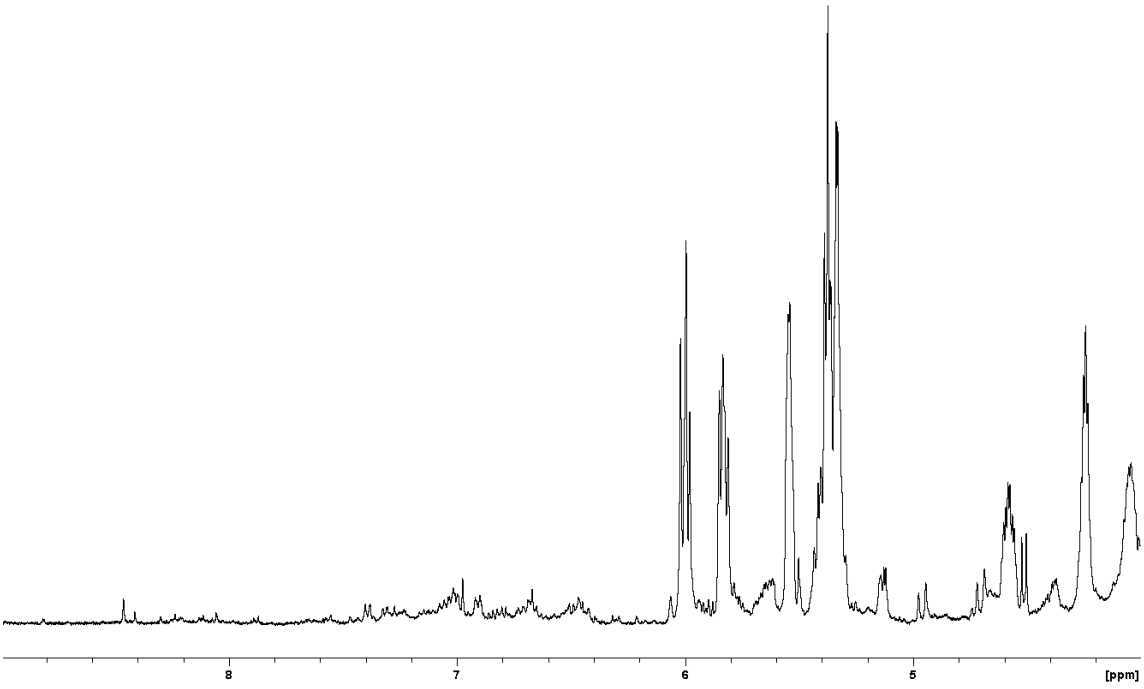

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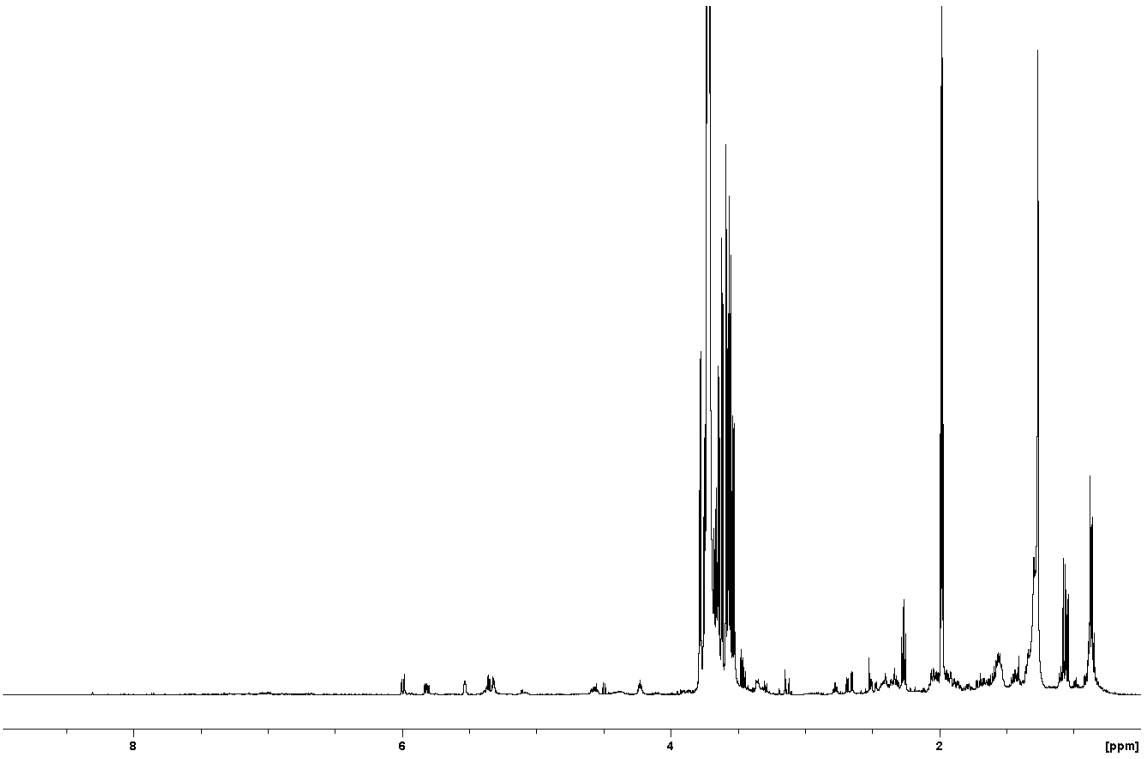


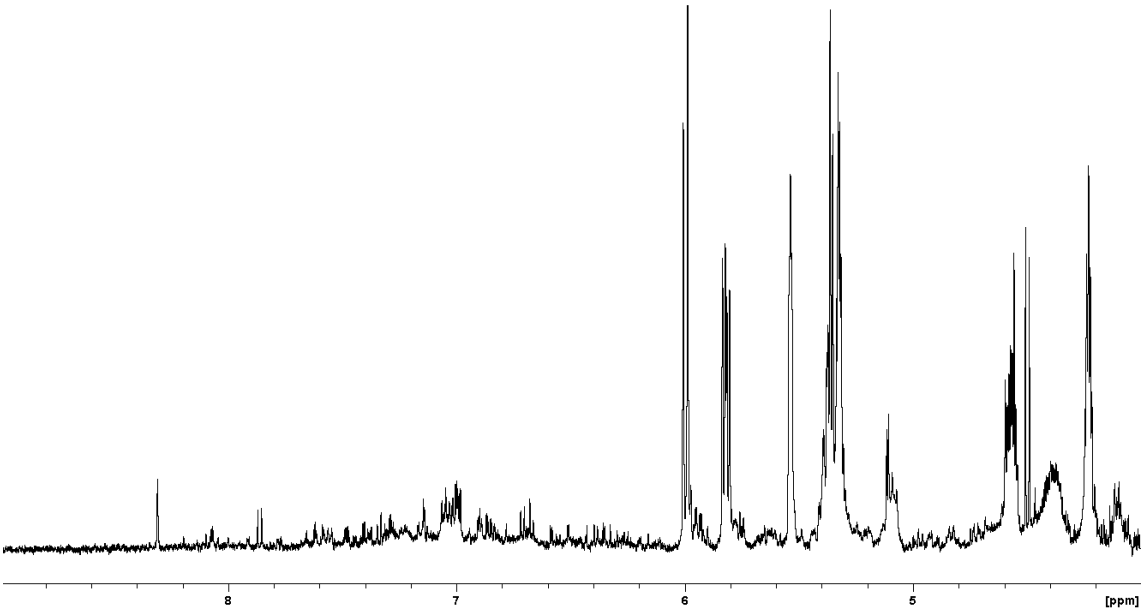

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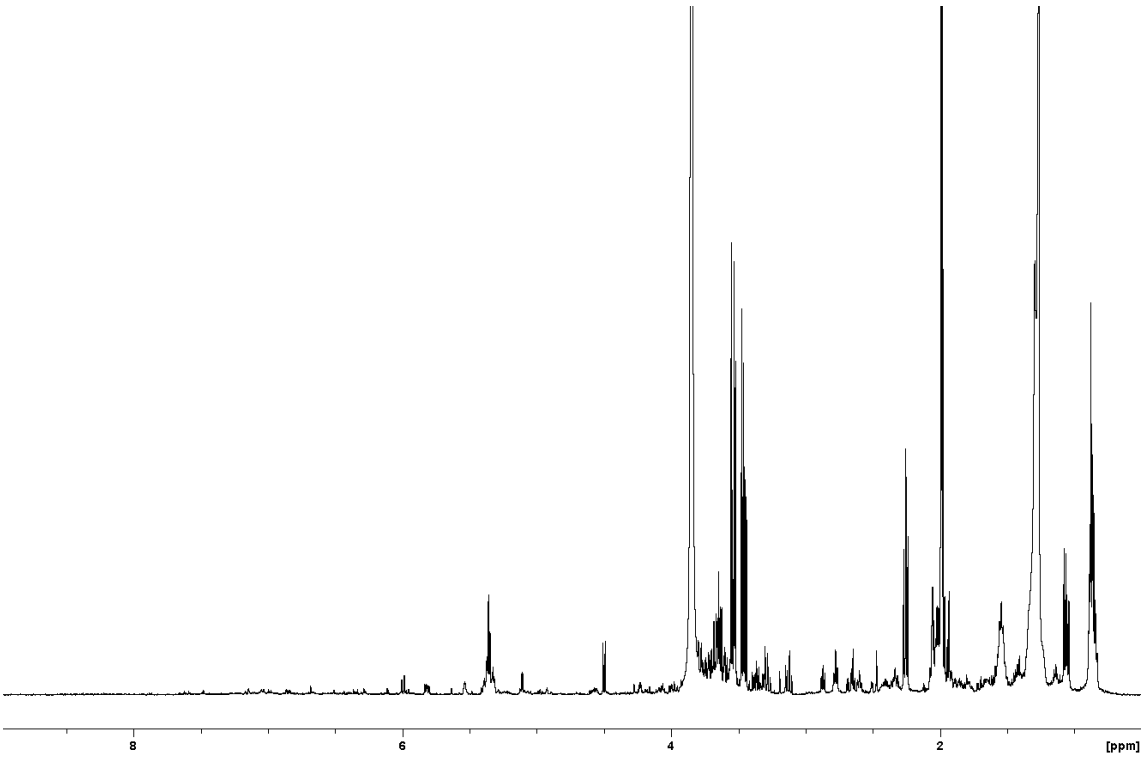


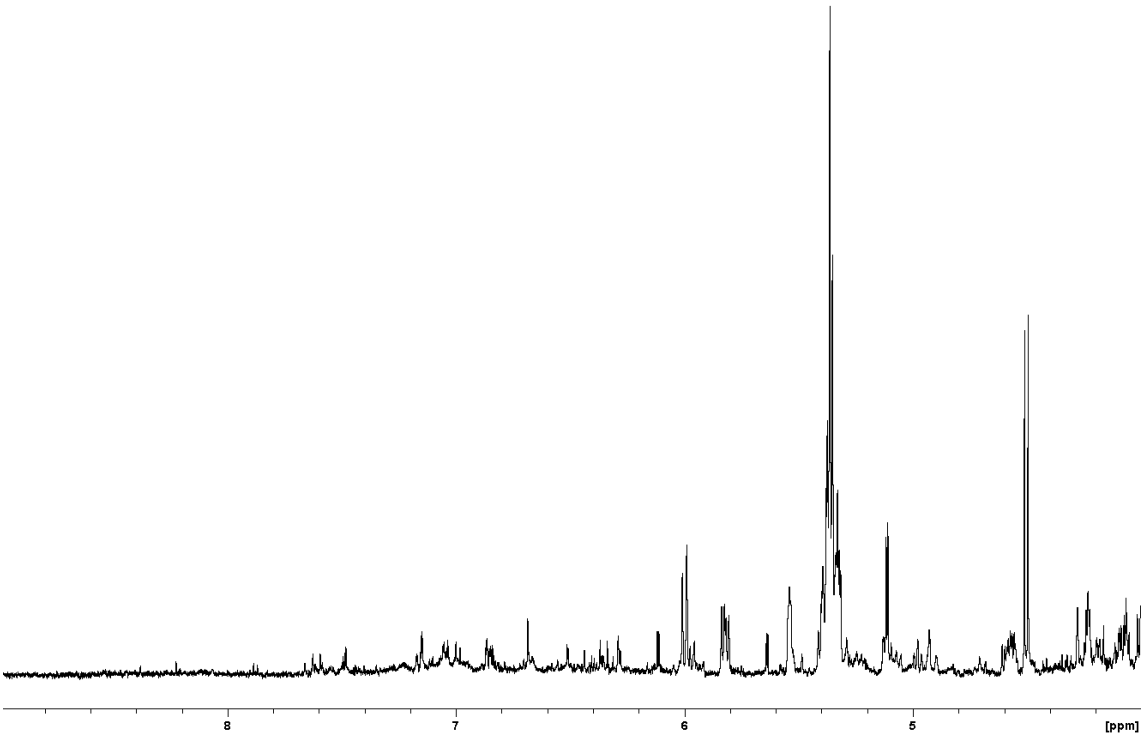

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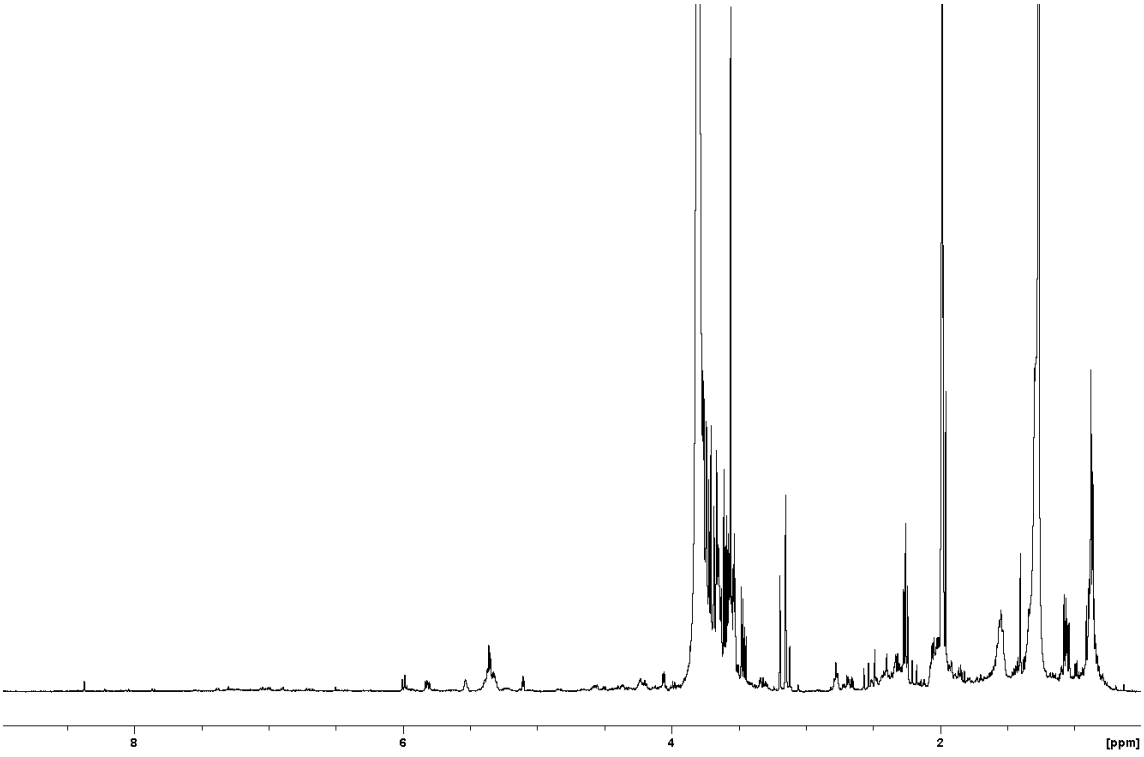
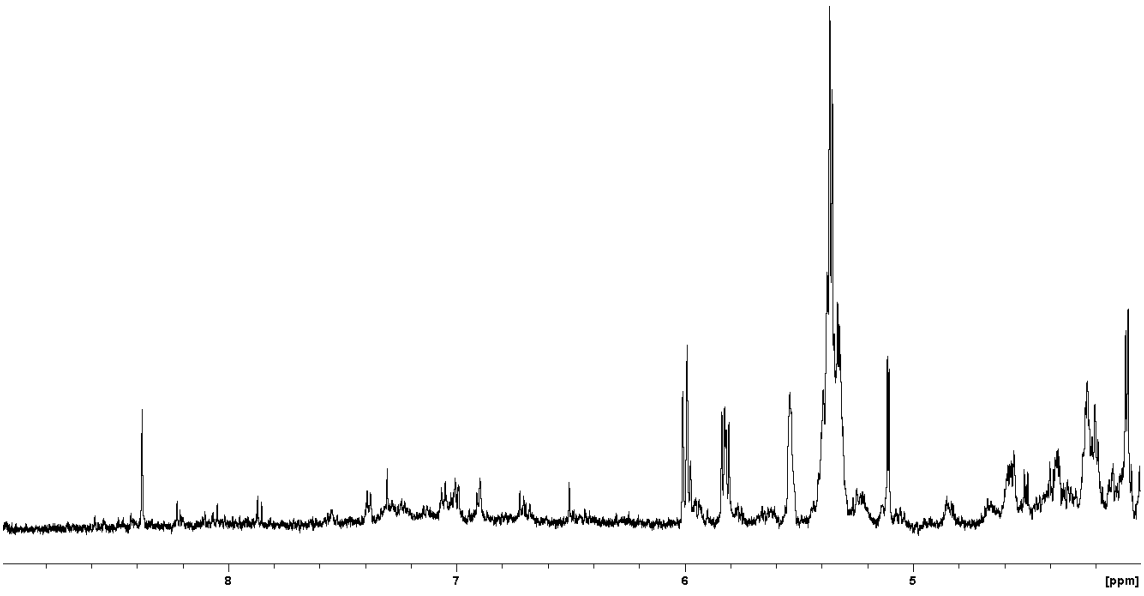
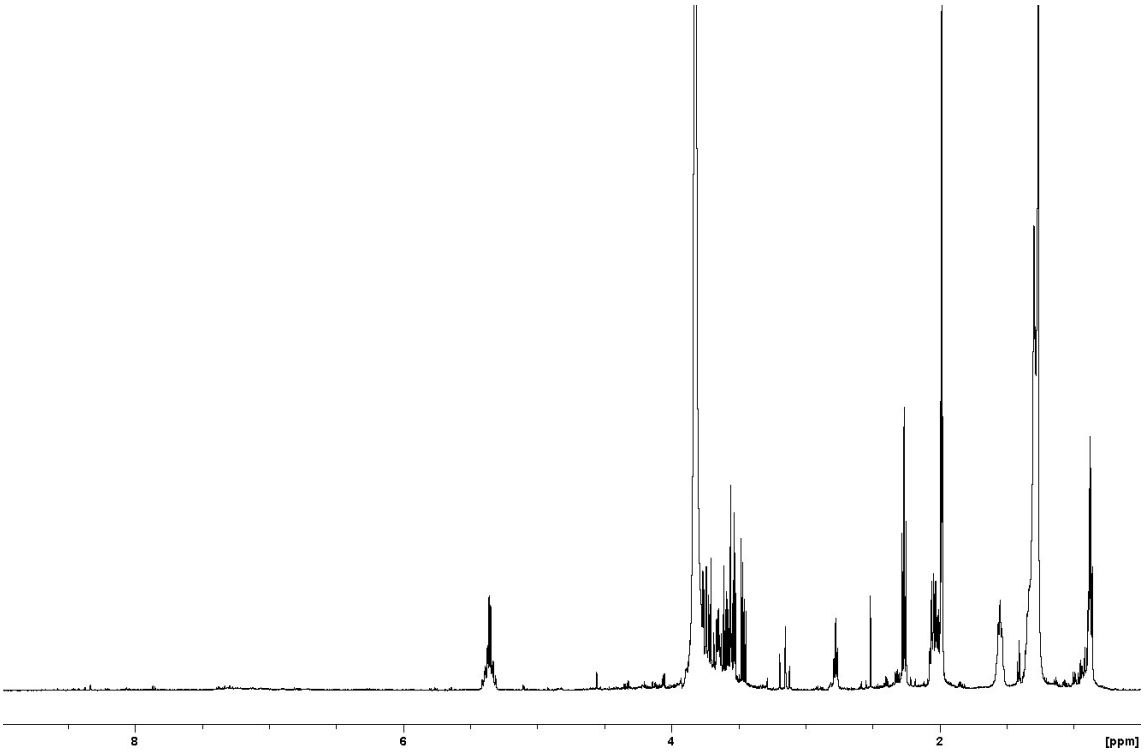
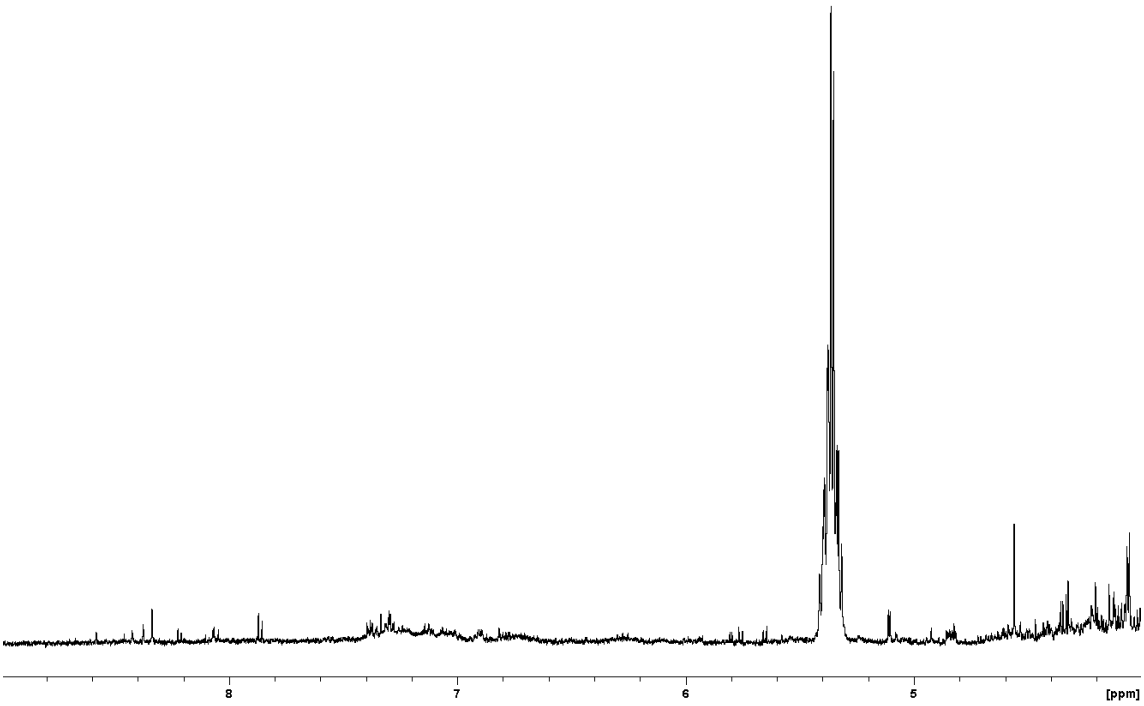


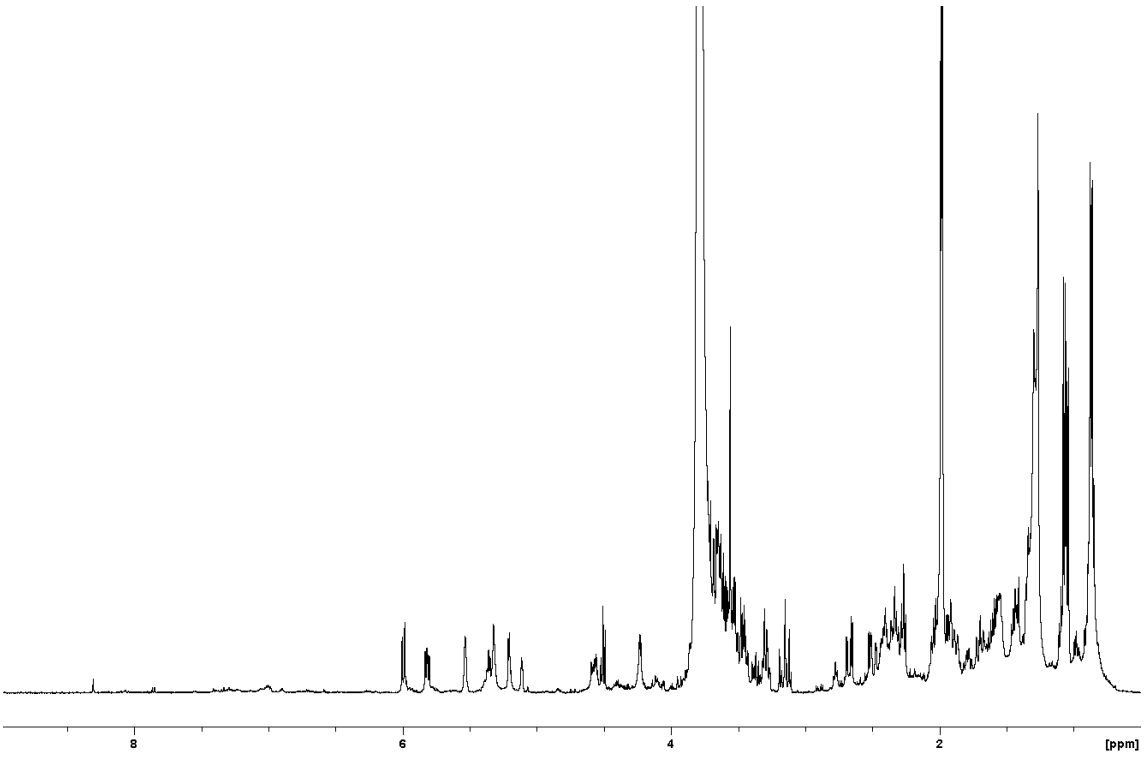



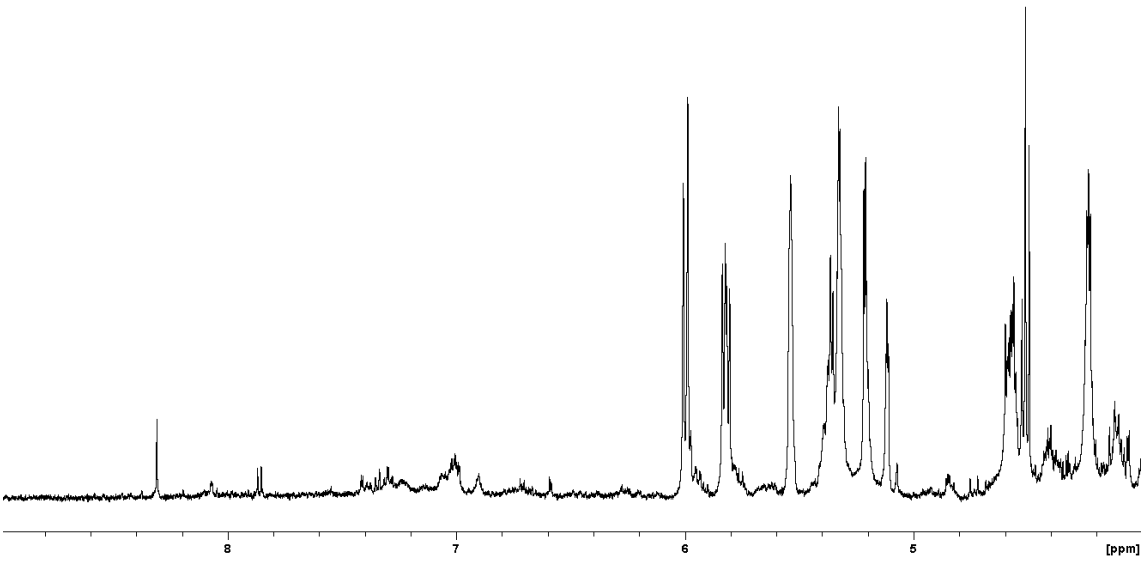
**DS 29 No monacolins detected**



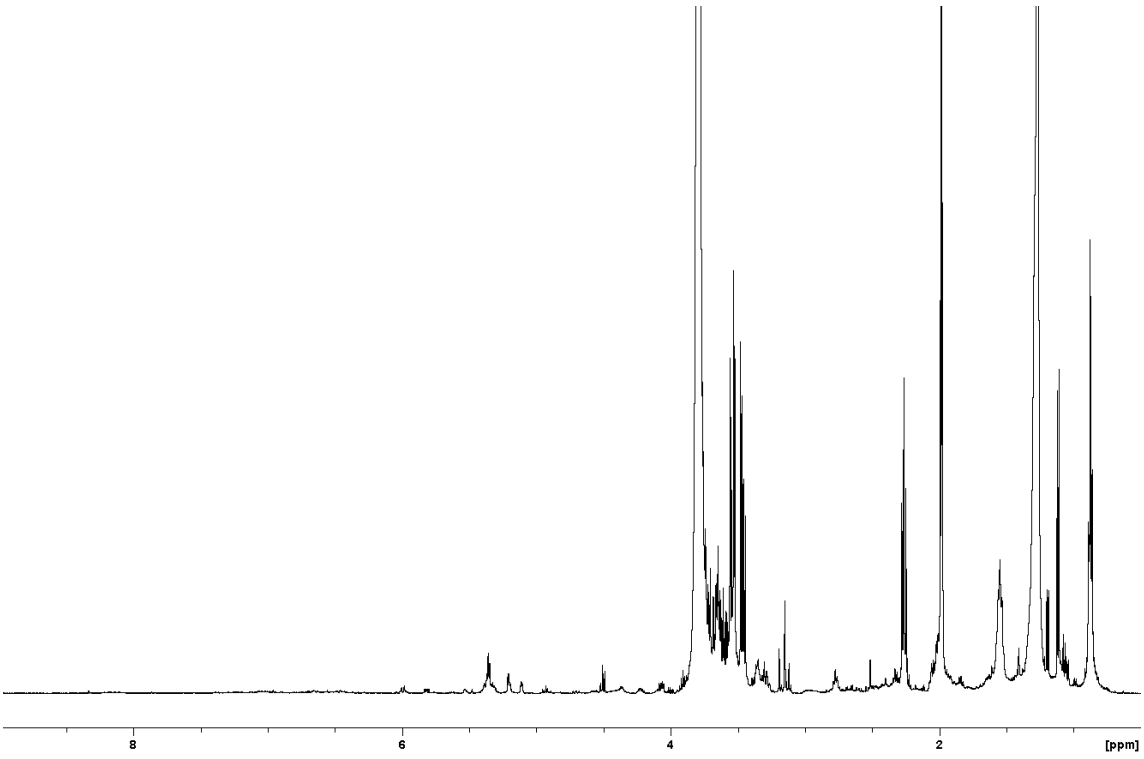



**DS 30**



**DS 31**



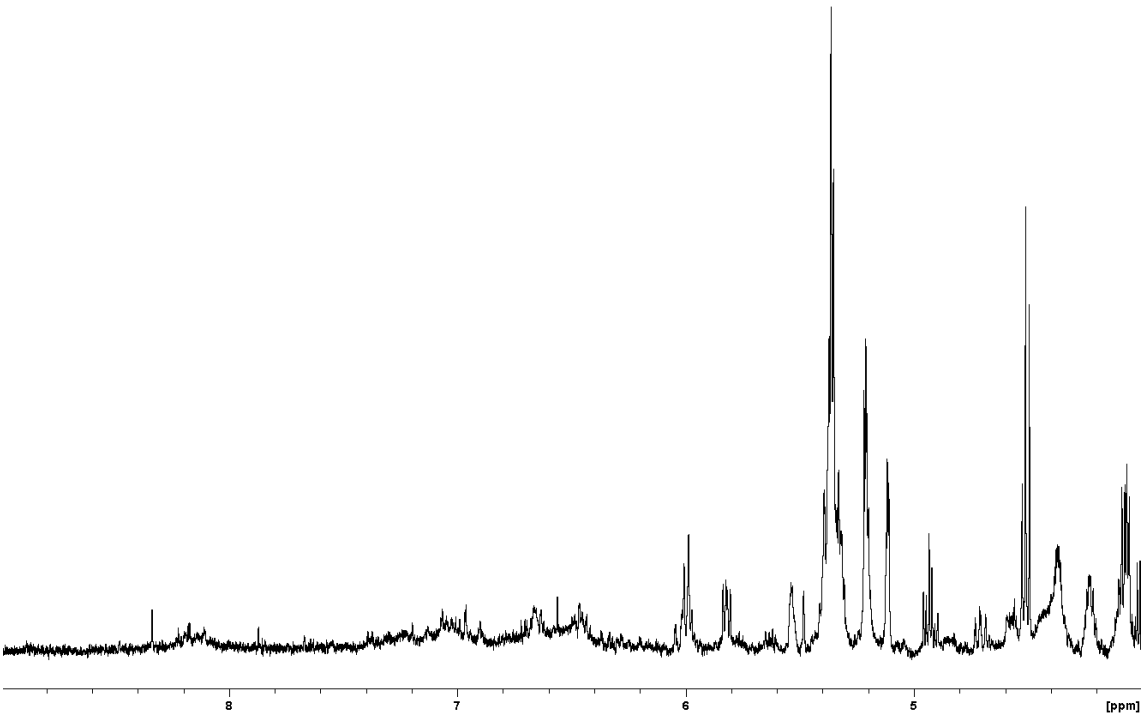
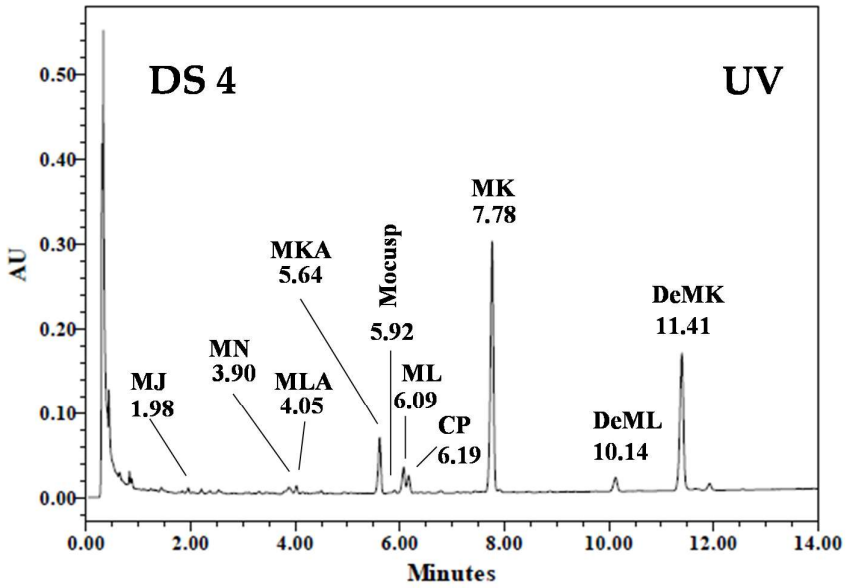
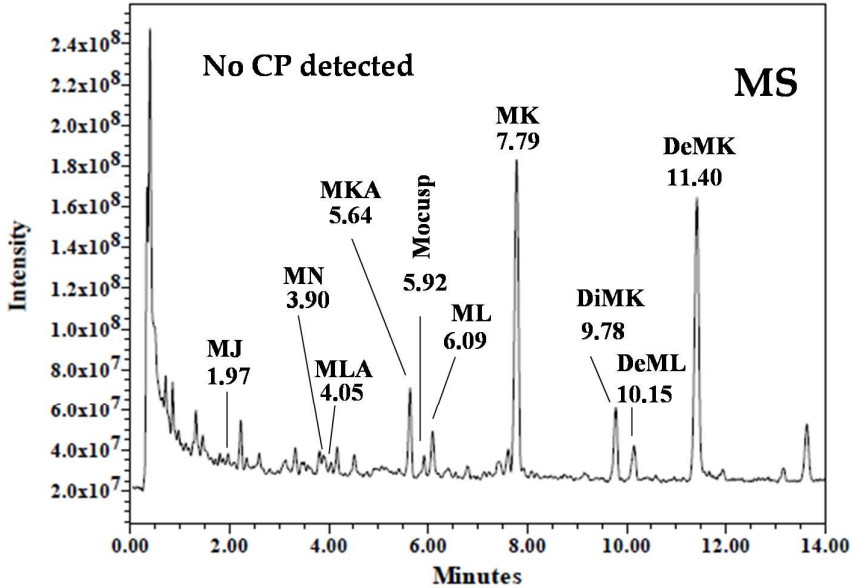
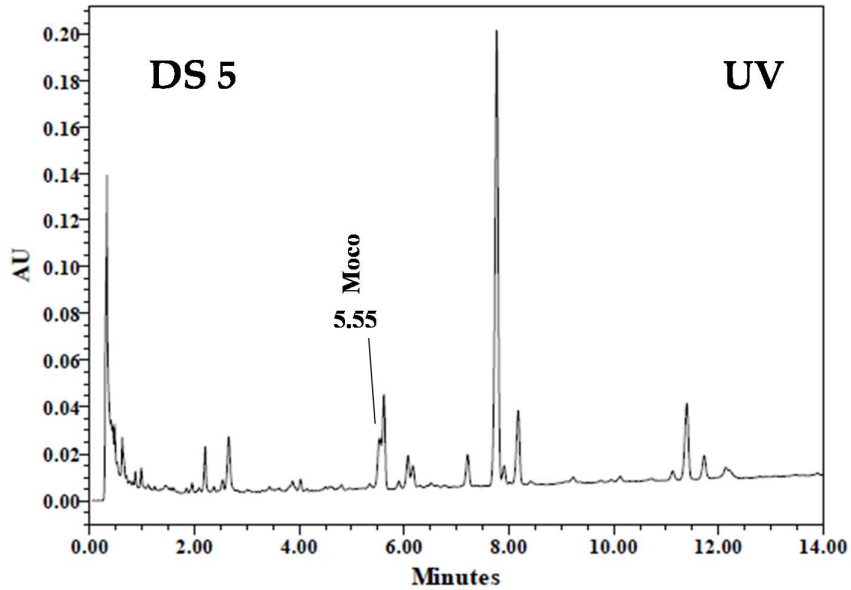
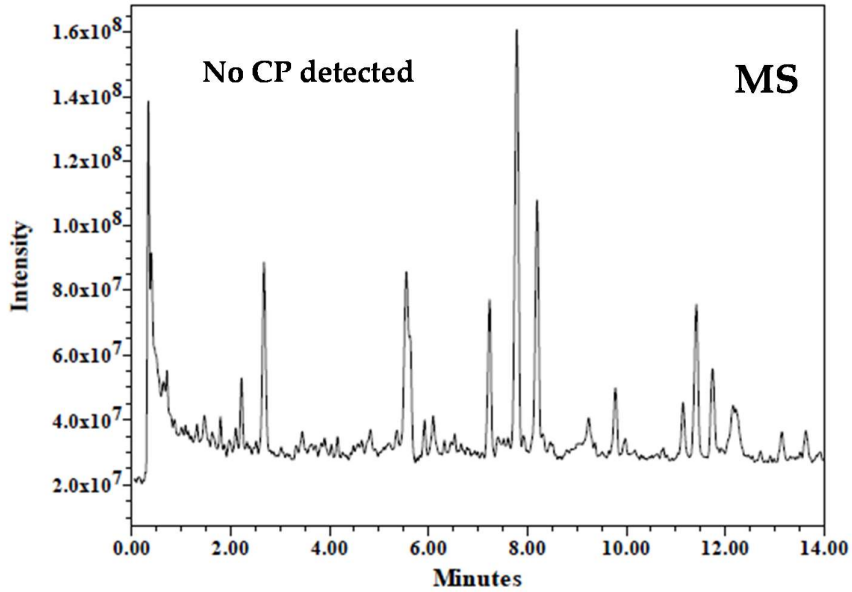



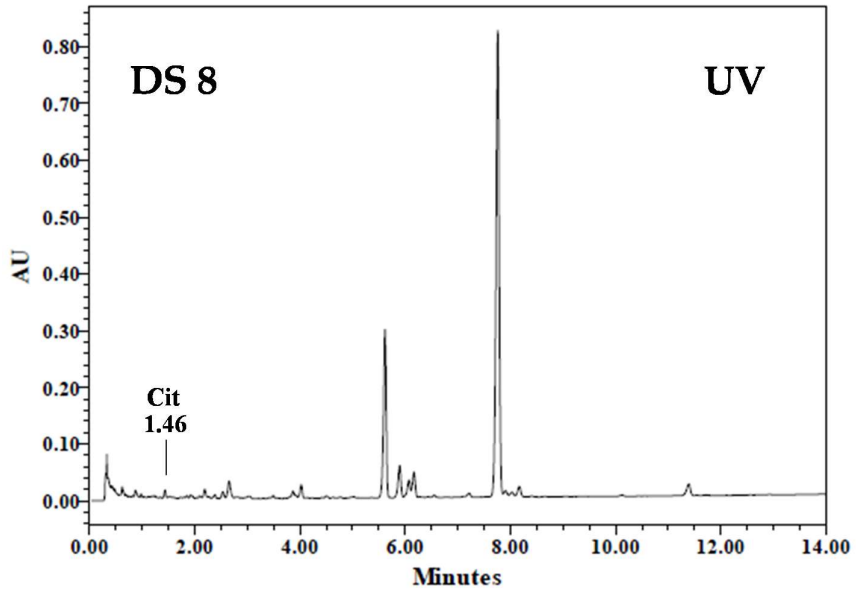
**Figure S2.** UHPLC chromatograms with UV detection at 238 nm (left) and full scan MS profile in positive ESI mode (right) of 9 RYR dietary supplements. MJ, MN, ML, MK: monacolins J, N, L, K; MLA, MKA: monacolins L, K in hydroxyl acid forms; CP: compactin; DiMK: dihydromonacolin K; DeML, DeMK: dehydromonacolins L,K; Cit: citrinin; Mo: monascin; Moco: monascorubramine; Mocusp: monascuspiloin.

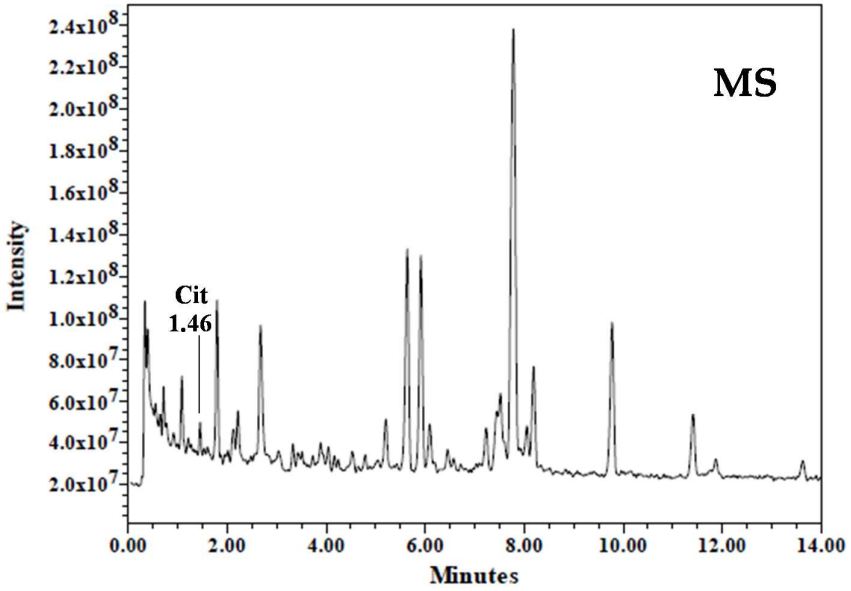

DS 4
UV
AU
MJ
1.98
MN
3.90
MLA
4.05
MKA
5.64
Mocusp
5.92
ML
6.09
CP
6.19
MK
7.78
DeML
10.14
DeMK
11.41
Minutes

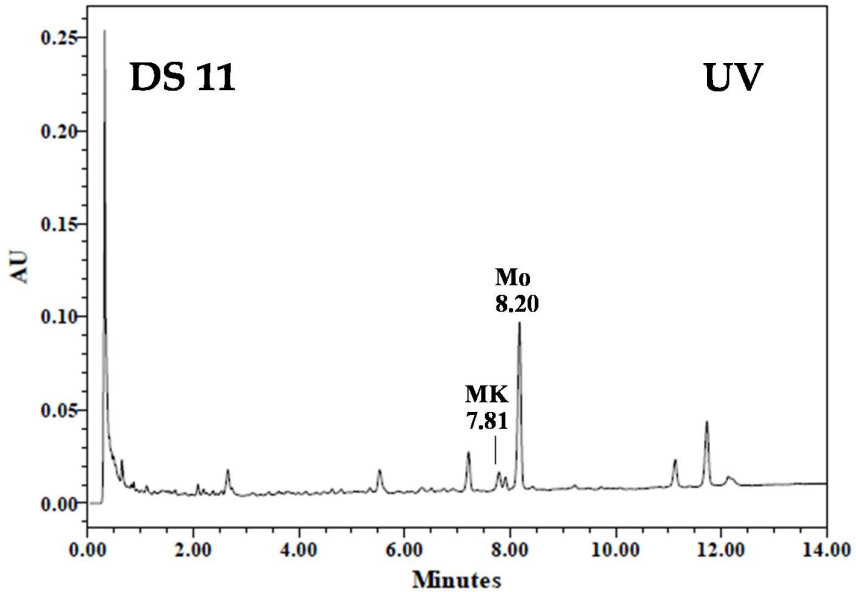

No CP detected
MS
Intensity
MJ
1.97
MN
3.90
MLA
4.05
MKA
5.64
Mocusp
5.92
ML
6.09
MK
7.79
DiMK
9.78
DeML
10.15
DeMK
11.40
Minutes

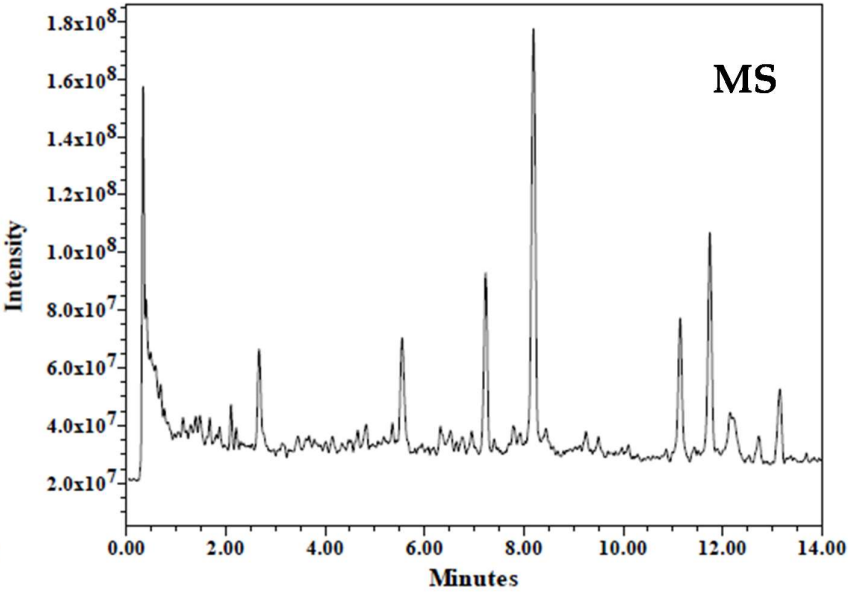

DS 5
UV
AU
Moco
5.55
Minutes

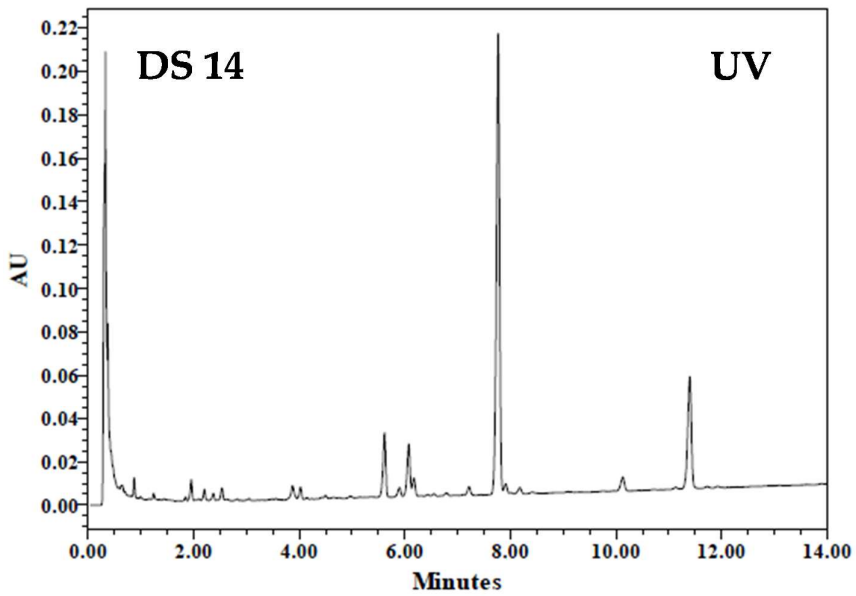

No CP detected
MS
Intensity
Minutes

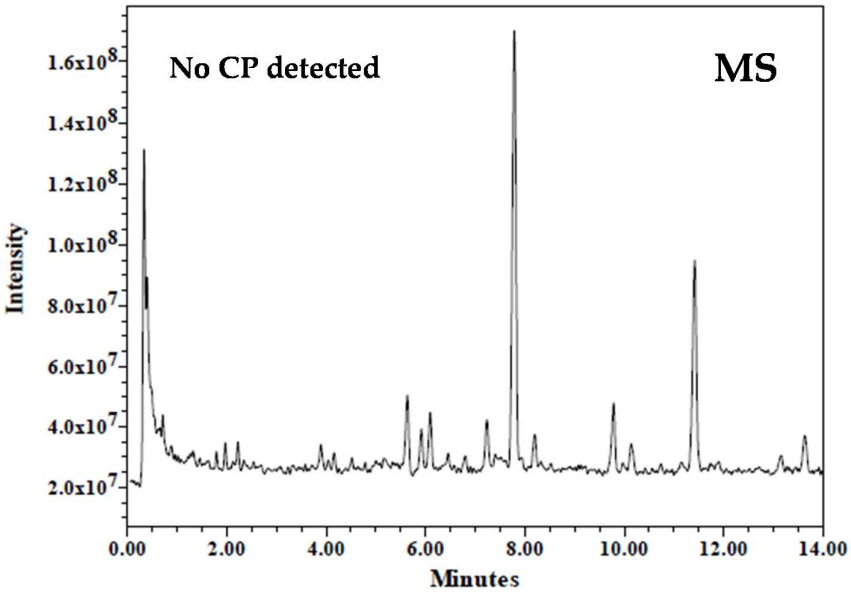

DS 8
UV
AU
Cit
1.46
Minutes

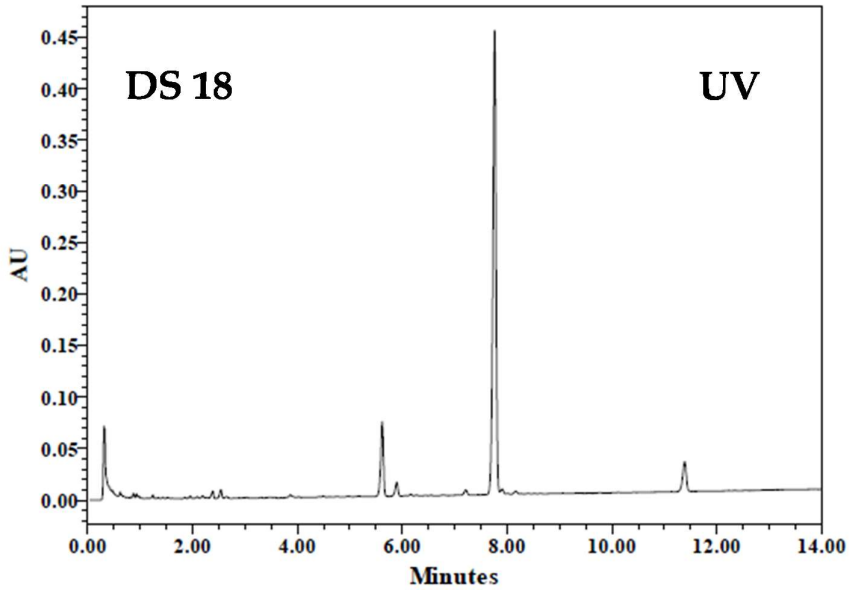

MS
Intensity
Cit
1.46
Minutes

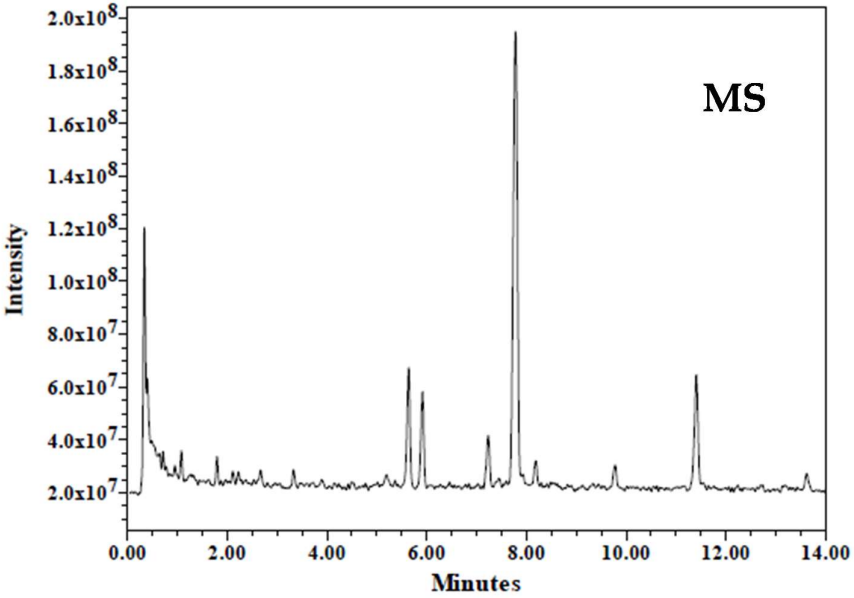

DS 11
UV
AU
Mo
8.20
MK
7.81
Minutes

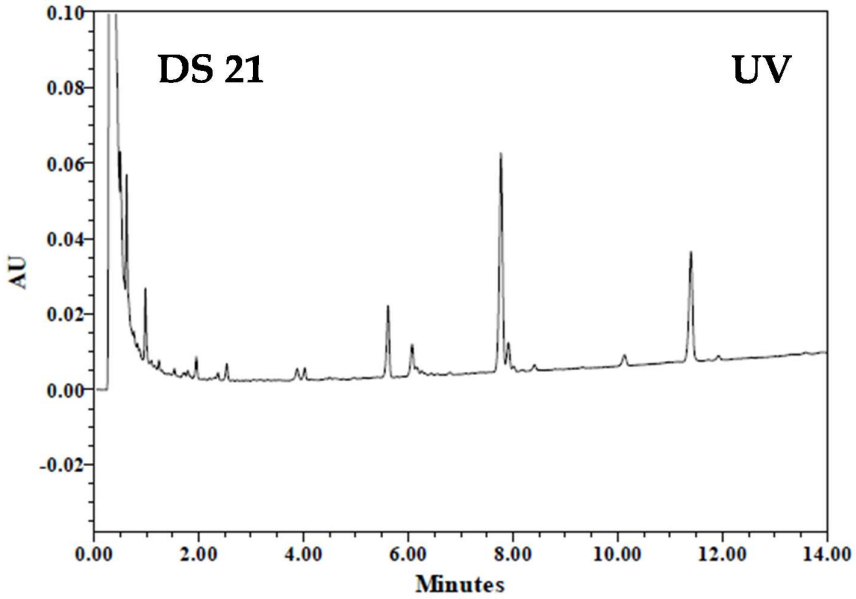

MS
Intensity
Minutes

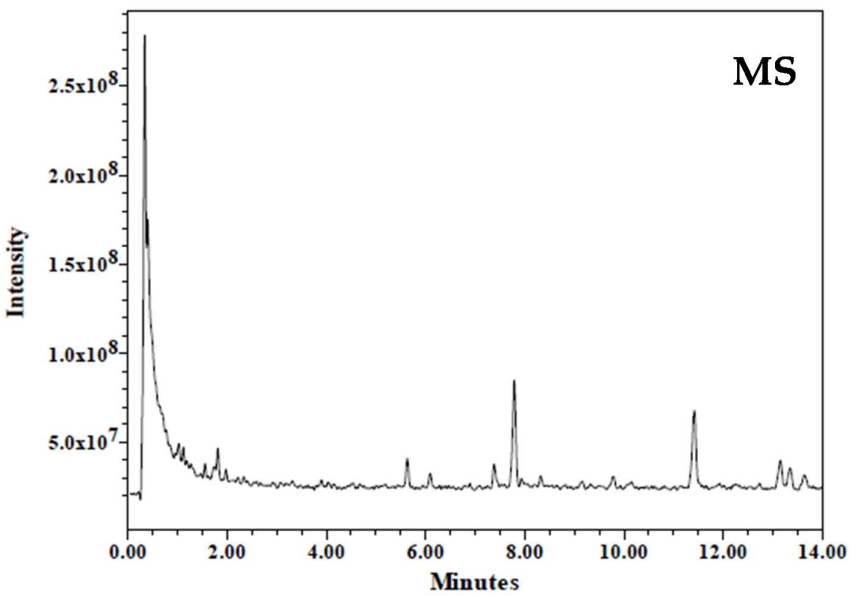

DS 14
UV
AU
Minutes

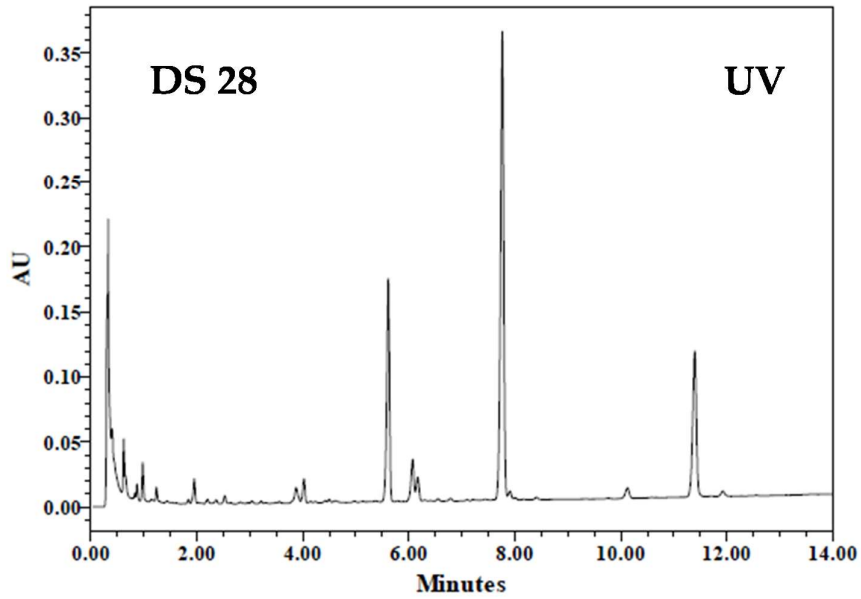

No CP detected
MS
Intensity
Minutes

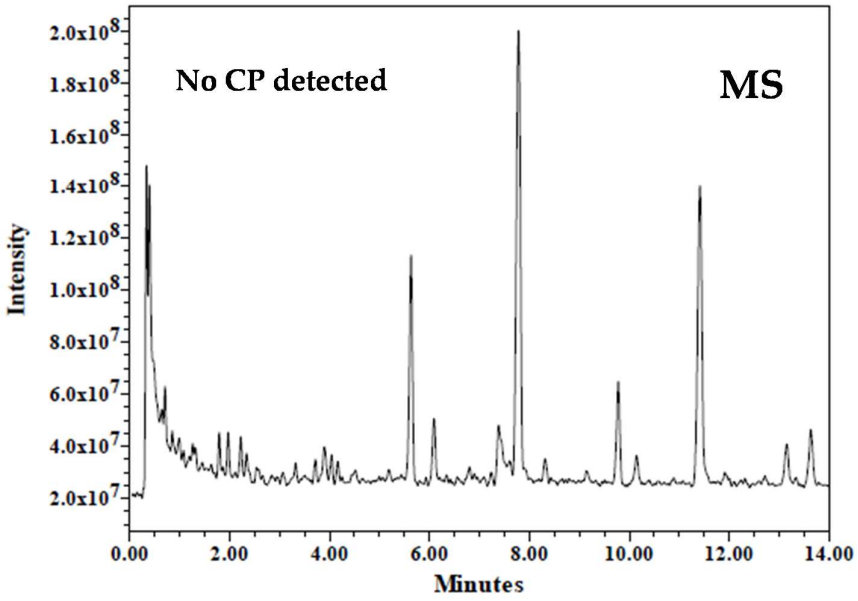

DS 18
UV
AU
Minutes

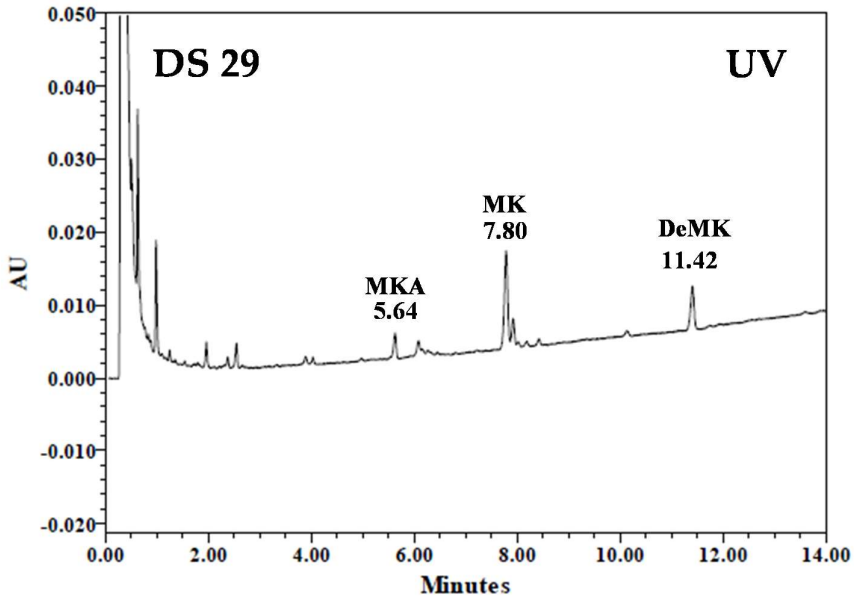

MS
Intensity
Minutes

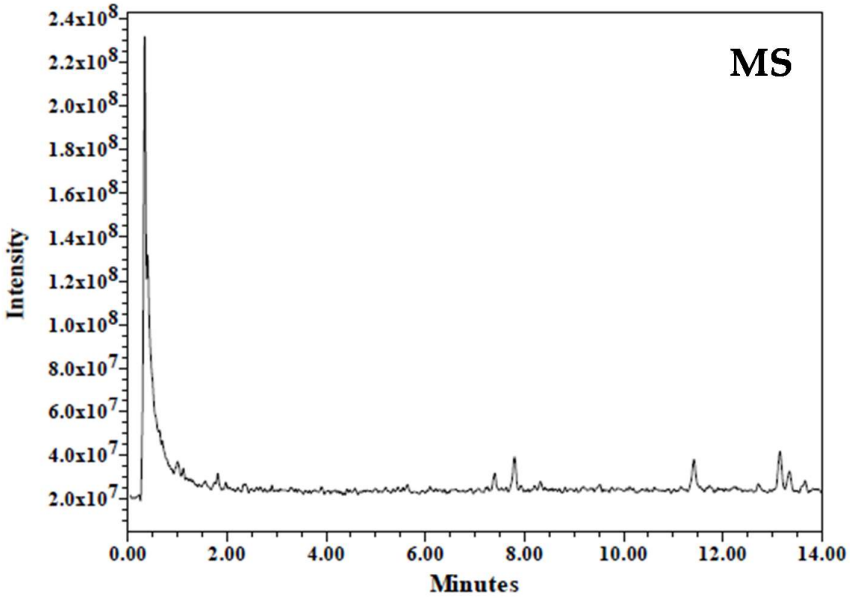

DS 21
UV
AU
Minutes


MS
Intensity
Minutes


DS 28
UV
AU
Minutes


No CP detected
MS
Intensity
Minutes


DS 29
UV
AU
MKA
5.64
MK
7.80
DeMK
11.42
Minutes


MS
Intensity
Minutes