

SUPPLEMENTARY MATERIAL

Naproxen based 1,3,4-oxadiazole derivatives as EGFR inhibitors: Design, Synthesis, Anticancer, and Computational Studies

S1. Characterization data of final compounds 8-16 and 19-26

4-((5-((S)-1-(2-methoxynaphthalen-6-yl)ethyl)-1,3,4-oxadiazol-2-ylthio)methyl)-1-(4-fluorophenyl)-1H-1,2,3-triazole (8)

M.p: 99-100; yield:70%; IR (ν , cm^{-1}): 3086, 2939, 1630, 1604, 1592, 1483, 1460, 1390, 1260, 1227, 1213, 1151, 1067, 1041, 1027, 864, 814, 780; ^1H NMR (850 MHz, CDCl_3): δ 1.83 (d, 3H, $-\text{CH}_3$), 3.93 (s, 3H, $\text{O}-\text{CH}_3$), 4.46 (brs, 1H, $-\text{CH}$), 4.60 (s, 2H, $\text{S}-\text{CH}_2$), 7.11 (d, $J = 7.6$ Hz, 1H, $1 \times \text{CH}$), 7.16 (dd, $J = 4.56, 8.50$ Hz, 1H, $1 \times \text{CH}$), 7.20 (t, $J = 8.50$ Hz, 2H, $2 \times \text{CH}$), 7.37 (d, $J = 8.50$ Hz, 1H, $1 \times \text{CH}$), 7.65-7.72 (m, 5H, $5 \times \text{CH}$), 8.26 (s, 1H, $1 \times \text{CH}$). ^{13}C NMR (213 MHz, CDCl_3): δ 19.24, 26.64, 37.50, 55.35, 105.61, 116.72, 116.83, 119.34, 122.77, 125.72, 125.94, 127.61, 129.31, 133.90, 134.75, 157.93, 161.87, 163.04. ESI MS: 462 $[\text{M}+\text{H}]^+$ $\text{C}_{24}\text{H}_{20}\text{N}_5\text{O}_2\text{S}$ (Calcd): C, 62.46; H, 4.37; N, 15.17; O, 6.93; S, 6.95. Obsd:C,62.44, H, 4.38; N,15.19; O, 6.96; S, 6.94

4-((5-((S)-1-(2-methoxynaphthalen-6-yl)ethyl)-1,3,4-oxadiazol-2-ylthio)methyl)-1-(2,4-difluorophenyl)-1H-1,2,3-triazole (9)

M.p: 119-120, yield: 72%; IR (ν , cm^{-1}): 3090, 2985, 1605, 1575, 1506, 1518, 1476, 1456, 1263, 1177, 1146, 1105, 1088, 1045, 958, 855, 823, 771; ^1H NMR (850 MHz, CDCl_3): δ 1.83 (d, $J = 7.60$ Hz, 3H, $-\text{CH}_3$), 3.93 (s, 3H, $-\text{O}-\text{CH}_3$), 4.47 (brs, 1H, $-\text{CH}$), 4.61 (brs, 2H, $-\text{S}-\text{CH}_2-$), 7.05-7.06 (m, 2H, $2 \times \text{CH}$), 7.11 (d, $J = 7.60$ Hz, 1H, $1 \times \text{CH}$), 7.17 (d, $J = 7.60$ Hz, 1H, $1 \times \text{CH}$), 7.37-7.38 (m, 1H, $1 \times \text{CH}$), 7.67-7.72 (m, 3H, $3 \times \text{CH}$), 7.85 (d, $J = 8.50$ Hz, 1H, $1 \times \text{CH}$), 8.34 (s, 1H, $1 \times \text{CH}$). ^{13}C NMR (213 MHz, CDCl_3): δ 19.27, 26.62, 37.49, 55.34, 105.34, 105.45, 105.60, 112.54, 112.64, 119.31, 125.73, 125.92, 127.59, 128.86, 129.31, 133.89, 134.79, 157.90, 161.98, 163.10. ESI MS: 480 $[\text{M}+\text{H}]^+$ $\text{C}_{24}\text{H}_{19}\text{N}_5\text{O}_2\text{S}$ (Calcd): C, 60.12; H, 3.99; N, 14.61; O, 6.67; S, 6.69. Obsd:C,60.09, H, 4.01; N,14.58; O, 6.65; S, 6.67

4-((5-((S)-1-(2-methoxynaphthalen-6-yl)ethyl)-1,3,4-oxadiazol-2-ylthio)methyl)-1-(2-chlorophenyl)-1H-1,2,3-triazole (10)

M.p: 90-92; yield:82 %; IR(ν , cm^{-1}): 3082, 2938, 1605, 1593, 1571, 1481, 1462, 1394, 1263, 1177, 1144, 1069, 1043, 1027, 895, 857, 784, 676; ^1H NMR (850 MHz, CDCl_3): δ 1.84 (d, $J = 7.61$ Hz, 3H, CH_3), 3.93 (s, 3H, $-\text{OCH}_3$), 4.47 (brs, 1H, $-\text{CH}$), 4.60 (s, 2H, $-\text{S}-\text{CH}_2-$), 7.11 (d, $J = 8.50$ Hz, 1H, $1 \times \text{CH}$), 7.16 (d, $J = 7.60$ Hz, 1H, $1 \times \text{CH}$), 7.32-7.78 (m, 8H, $8 \times \text{CH}$), 8.33 (s, 1H, $1 \times \text{CH}$). ^{13}C NMR (213 MHz, CDCl_3): δ 19.22, 26.61, 37.51, 55.35, 105.61, 118.78, 119.34, 121.01, 125.72, 125.94, 127.62, 128.86, 128.93, 129.30, 130.90, 133.90,

134.73, 135.71, 157.91, 161.48, 162.63. ESI MS: 478 [M+H]⁺, 480 [M+H+2]⁺ C₂₄H₂₀N₅O₂S(Calcd): C, 60.31; H, 4.22; N, 14.65; O, 6.69; S, 6.71. Obsd: C,60.28, H, 4.24; N,14.63; O, 6.73; S, 6.72

4-((5-((S)-1-(2-methoxynaphthalen-6-yl)ethyl)-1,3,4-oxadiazol-2-ylthio)methyl)-1-(3-chlorophenyl)-1H-1,2,3-triazole (11)

Semisolid; yield:73 %; IR(v, cm⁻¹): 3078, 2935, 1604, 1581, 1576, 1489, 1651, 1390, 1261, 1114, 1064, 857; ¹H NMR (850 MHz, CDCl₃): δ 1.83 (d, J = 8.50 Hz, 3H, -CH₃), 3.93 (s, 3H, -OCH₃), 4.45 (q, J = 8.50 Hz, 1H, C-H), 4.61 (s, 2H, -S-CH₂-), 7.11 (s, 1H, Ar-H), 7.15-7.16 (m, 1H, 1 × CH), 7.36 (d, J = 8.5Hz, 1H, 1 × CH), 7.42-7.44 (m, 1H, 1 × CH), 7.46 (t, J = 8.5 Hz, 1H, 1 × CH), 7.56-7.57 (m, 2H, 2 × CH), 7.67 (s, 1H, 1 × CH), 7.70-7.71 (m, 2H, 2 × CH), 8.10 (s, 1H, 1 × CH). ¹³C NMR (213 MHz, CDCl₃): δ 19.34, 26.17, 37.48, 55.34, 105.62, 119.32, 130.75, 133.34, 134.68, 134.87, 142.70, 157.75, 163.99. ESI MS: 478 [M+H]⁺, 480 [M+H+2]⁺ C₂₄H₂₀N₅O₂S(Calcd): C, 60.31; H, 4.22; N, 14.65; O, 6.69; S, 6.71. Obsd:C, 60.30; H, 4.23; N, 14.64; O, 6.67; S,6.73

4-((5-((S)-1-(2-methoxynaphthalen-6-yl)ethyl)-1,3,4-oxadiazol-2-ylthio)methyl)-1-(2,4-dichlorophenyl)-1H-1,2,3-triazole (12)

M.p: 102-103; yield:80%; IR (v, cm⁻¹): 3050, 2991, 2938, 1604, 1570, 1497, 1474, 1660, 1393, 1262, 1229, 1143, 1119, 1071, 1039, 1026, 894, 857, 822; ¹H NMR (850 MHz, CDCl₃): δ 1.84 (d, J = 8.50 Hz, 3H, -CH₃), 3.93 (s, 3H, -OCH₃), 4.47 (brs, s, 1H, C-H), 4.61 (s, 2H, -S-CH₂-), 7.11 (d, J = 7.60 Hz, 1H, 1 × CH), 7.15-7.17 (m, 1H, 1 × CH), 7.37 (d, J =8.5 Hz, 1H, 1 × CH), 7.41 (d, J = 7.6 Hz, 1H, 1 × CH), 7.50 (d, J = 8.5Hz, 1H, 1 × CH), 7.59 (s, 1H, 1 × CH), 7.67 (s, 1H, 1 × CH), 7.69-7.71 (m, 2H, 1 × CH), 8.26 (s, 1H, 1 × CH). ¹³C NMR (213 MHz, CDCl₃): δ 19.22, 26.63, 37.48, 55.35, 105.59, 119.33, 125.71, 125.92, 127.61, 128.26, 128.30, 128.85, 129.29, 130.62, 133.89, 136.35, 157.91, 160.34, 163.70. ESI MS: 512 [M+H]⁺, 514 [M+H+2]⁺ C₂₄H₁₉N₅O₂S(Calcd): C, 56.26; H, 3.74; N, 13.67; O, 6.24; S, 6.26. Obsd: C,56.29, H, 3.70; N,13.65; O, 6.28; S, 6.27

4-((5-((S)-1-(2-methoxynaphthalen-6-yl)ethyl)-1,3,4-oxadiazol-2-ylthio)methyl)-1-(3-bromophenyl)-1H-1,2,3-triazole (13)

M.p: 118-120; yield:86%; IR (v, cm⁻¹): 3086, 2939, 1604, 1504, 1483, 1461,1439, 1260, 1237, 1213, 1150, 1067, 1041, 1027, 923, 889, 865, 814, 780, 769, 674; ¹H NMR (850 MHz, CDCl₃): δ1.84 (d, J = 8.51 Hz, 3H, -CH₃), 3.93 (s, 3H, -OCH₃),4.48 (brs, 1H, CH), 4.61 (s, 2H, S-CH₂). 7.11-17 (m, 2H, 2 × CH), 7.37-7.39 (m, 2H, 2 × CH), 7.56-7.72 (m, 5H, 5 × CH), 7.93 (s, 1H, 1 × CH), 8.29 (s, 1H, 1 × CH). ¹³C

NMR (213 MHz, CDCl₃): δ 19.23, 26.57, 37.51, 55.35, 105.61, 119.34, 123.42, 123.82, 125.72, 125.96, 127.62, 129.30, 131.14, 131.92, 133.90, 134.67, 157.91, 160.35, 163.72. ESI MS: 522 [M+H]⁺, 524 [M+H+2]⁺ C₂₄H₂₀N₅O₂S(Calcd): C, 55.18; H, 3.86; N, 13.41; O, 6.13; S, 6.14. Obsd: C,55.15, H, 3.88; N,13.40; O, 6.17; S, 6.15

4-((5-((S)-1-(2-methoxynaphthalen-6-yl)ethyl)-1,3,4-oxadiazol-2-ylthio)methyl)-1-(4-bromophenyl)-1H-1,2,3-triazole (14)

M.p: 160-161; yield:81%; IR (ν , cm⁻¹): 3085, 2938, 1606, 1578, 1496, 1486, 1459, 1393, 1260, 1228, 1215, 1192, 1154, 1067, 1029, 987, 813; ¹H NMR (850 MHz, CDCl₃): δ 1.75 (brd s, 3H, -CH₃), 3.84 (s, 3H, -O-CH₃), 4.37 (brs, 1H, -CH), 4.51 (s, 2H, S-CH₂-), 7.02 (s, 1H, 1 \times CH), 7.08 (d, J = 8.5 Hz, 1H, 1 \times CH), 7.29 (d, J = 8.5 Hz, 1H, 1 \times CH), 7.48 (d, J = 8.5 Hz, 2H, 2 \times CH), 7.53 (d, J = 8.5Hz, 2H, 2 \times CH), 7.59 (s, 1H, 1 \times CH), 7.61-7.63 (m, 2H, 2 \times CH), 8.20 (s, 1H, 1 \times CH). ¹³C NMR (213 MHz, CDCl₃): δ 19.20, 26.93, 37.50, 55.36, 105.60, 119.36, 122.51, 125.72, 125.94, 127.62, 129.31, 132.98, 133.90, 134.68, 157.93, 159.46, 163.40. ESI MS: 522 [M+H]⁺, 524 [M+H+2]⁺ C₂₄H₂₀N₅O₂S(Calcd): C, 55.18; H, 3.86; N, 13.41; O, 6.13; S, 6.14. Obsd: C,55.15, H, 3.87; N,13.39; O, 6.15; S, 6.13.

2-(4-((5-((S)-1-(2-methoxynaphthalen-6-yl)ethyl)-1,3,4-oxadiazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)phenol (15)

M.p: 90-92; yield: 70%; IR (ν , cm⁻¹): 3150, 3045, 2937, 1605, 1506, 1480, 1457,1393, 1262, 1228, 1157, 1044, 1027, 895, 856, 822, 753; ¹H NMR (850 MHz, CDCl₃): δ 1.85 (brs, 3H, -CH₃), 3.93 (s, 3H, -OCH₃), 4.47 (brs, 1H, -CH), 4.62 (s, 2H, S-CH₂-), 7.00 (t, J = 8.50 Hz, 1H, 1 \times CH), 7.12 (s, 1H, 1 \times CH), 7.17 (d, J = 8.50 Hz, 1H, 1 \times CH), 7.19 (d, J = 8.50 Hz, 1H, 1 \times CH), 7.32 (t, J = 8.50 Hz, 1H, 1 \times CH), 7.37-7.38 (m, 2H, 2 \times CH), 7.68-7.72 (m, 3H, 3 \times CH), 8.46 (s, 1H, 1 \times CH), 9.70 (s, 1H, Ar-OH). ¹³C NMR (213 MHz, CDCl₃): δ 19.22, 25.84, 37.52, 55.35, 105.61, 119.35, 119.49, 120.41, 125.71, 125.96, 127.63, 128.30, 129.30, 129.85, 133.92, 134.68, 149.20, 157.93, 162.15, 164.50. ESI MS: 460 [M-H]⁺, C₂₄H₂₁N₅O₃S(Calcd): C, 62.73; H, 4.61; N, 15.24; O, 10.45; S, 6.98. Obsd:C,62.71, H, 4.63; N,15.22; O, 10.49; S, 6.99.

3-(4-((5-((S)-1-(2-methoxynaphthalen-6-yl)ethyl)-1,3,4-oxadiazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)benzoic acid (16)

M.p: 184-185; yield:89%; IR (ν , cm⁻¹): 3155, 3085, 2939, 1690, 1633, 1606, 1593, 1483, 1459, 1392, 1264, 1152, 1067, 813; ¹H NMR (850 MHz, CDCl₃): δ 1.84 (d, J = 7.6 Hz, 3H, CH-CH₃), 3.92 (s, -OCH₃, 3H), 4.47-4.49 (m, 1H, C-H), 4.64 (s, 2H, S-CH₂-), 7.10 (d, J = 7.6

Hz, 1H, 1 × CH), 7.15 (s, 1H, 1 × CH), 7.38 (s, 1H, 1 × CH), 7.64-7.72 (m, 4H, 4 × CH), 8.04 (d, $J = 8.50$ Hz, 1H, 1 × CH), 8.18 (d, $J = 8.50$ Hz, 1H, 1 × CH), 8.37 (s, 1H, 1 × CH), 8.44 (s, 1H, Ar-COOH). ^{13}C NMR (213 MHz, CDCl_3): δ 19.25, 26.64, 37.49, 55.34, 105.60, 119.32, 121.78, 125.43, 125.71, 127.63, 128.30, 129.31, 130.31, 131.29, 133.91, 134.67, 137.15, 157.90, 160.00, 163.31, 168.48. ESI MS: 486 $[\text{M}-\text{H}]^+$, $\text{C}_{25}\text{H}_{21}\text{N}_5\text{O}_4\text{S}$ (Calcd): C, 61.59; H, 4.34; N, 14.36; O, 13.13; S, 6.58. Obsd: C, 61.57; H, 4.35; N, 14.34; O, 13.15; S, 6.60.

2-(5-((S)-1-(2-methoxynaphthalen-6-yl)ethyl)-1,3,4-oxadiazol-2-ylthio)-N-(4-fluorophenyl) acetamide (19)

M.p: 220-221; yield:71%; IR (ν , cm^{-1}): 3195 (N-H), 3050, 2966, 1734, 1640, 1592, 1509, 1483, 1377, 1247, 1225, 1198, 1159, 1032, 939, 882; ^1H NMR (850 MHz, CDCl_3): δ 1.68 (d, $J = 8.50$ Hz, 3H, CH_3), 3.93-3.97 (m, 5H, -O- CH_3 , -S- CH_2 -), 4.06 (q, $J = 8.50$ Hz, 1H, -CH), 7.02 (d, $J = 8.5\text{Hz}$, 1H, 1 × CH), 7.10 (s, 1H, 1 × CH), 7.15 (d, $J = 8.5\text{Hz}$, 2H, 2 × CH), 7.19-7.21 (m, 2H, 2 × CH), 7.42 (d, $J = 8.50\text{Hz}$, 1H, 1 × CH), 7.58 (t, $J = 8.50$ Hz, 2H, 2 × CH), 7.72-7.77 (m, 2H, 2 × CH), 9.35(s, 1H, N-H). ^{13}C NMR (213 MHz, CDCl_3): δ 18.84, 33.05, 42.26, 55.34, 105.56, 105.68, 116.49, 116.60, 118.86, 119.40, 125.86, 126.61, 128.81, 129.66, 129.88, 129.93, 133.42, 135.20, 136.21, 157.52, 162.05, 163.21, 169.32, 175.49. ESI MS: 438 $[\text{M}+\text{H}]^+$, $\text{C}_{23}\text{H}_{20}\text{N}_3\text{O}_3\text{S}$ (Calcd): C, 63.14; H, 4.61; N, 9.60; O, 10.97; S, 7.33. Obsd: C, 63.15; H, 4.60; N, 9.59; O, 10.98; S, 7.34

2-(5-((S)-1-(2-methoxynaphthalen-6-yl)ethyl)-1,3,4-oxadiazol-2-ylthio)-N-(2,4-difluorophenyl)acetamide (20)

M.p: 102-103; yield:89%; IR (ν , cm^{-1}): 3150 (N-H), 3087, 2940, 1681, 1606, 1569, 1505, 1483, 1470, 1260, 1144, 1028, 850, 813; ^1H NMR (850 MHz, CDCl_3): δ 1.84 (d, $J = 8.50$ Hz, 3H, - CH_3), 3.94-4.06 (m, 3H, O- CH_3 , 2H, -S- CH_2 -), 4.49 (q, $J = 8.50$ Hz, 1H, -CH), 6.95-6.97 (m, 1H, 1 × CH), 7.13 (d, 7.60 Hz, 1H, 1 × CH), 7.17-7.19 (m, 1H, 1 × CH), 7.36-7.37 (m, 1H, 1 × CH), 7.52 (t, $J = 8.50$ Hz, 1H, 1 × CH), 7.67 (s, 1H, 1 × CH), 7.71-7.73 (m, 2H, 2 × CH), 8.26 (s, 1H, 1 × CH), 9.30 (s, 1H, N-H). ^{13}C NMR (213 MHz, CDCl_3): δ 19.25, 29.30, 37.52, 55.37, 105.82, 119.40, 122.77, 125.59, 125.91, 127.89, 128.94, 129.31, 133.94, 134.56, 157.98, 164.38, 165.89, 171.03. ESI MS: 456 $[\text{M}+\text{H}]^+$, $\text{C}_{23}\text{H}_{19}\text{N}_3\text{O}_3\text{S}$ (Calcd): C, 60.65; H, 4.20; N, 9.23; O, 10.54; S, 7.04. Obsd: C, 60.64; H, 4.21; N, 9.24; O, 10.55; S, 7.03

2-(5-((S)-1-(2-methoxynaphthalen-6-yl)ethyl)-1,3,4-oxadiazol-2-ylthio)-N-(3-chlorophenyl) acetamide (21)

M.p: 82-83; yield: 90%; IR (ν , cm^{-1}): 3148, 3050, 2934, 1634, 1593, 1480, 1263, 1158, 1029, 852; ^1H NMR (850 MHz, CDCl_3): δ 1.86 (d, $J = 8.50$ Hz, 3H, CH_3), 3.90-3.95 (m, 5H, $-\text{O}-\text{CH}_3$, $-\text{S}-\text{CH}_2-$), 4.49 (q, $J = 8.50$ Hz, 1H, $-\text{C}-\text{H}$), 7.10 (d, $J = 8.50$ Hz, 1H, $1 \times \text{CH}$), 7.13 (d, $J = 8.5$ Hz, 1H, $1 \times \text{CH}$), 7.18 (d, $J = 8.5$ Hz, 1H, $1 \times \text{CH}$), 7.24 (t, $J = 8.50$ Hz, $1 \times \text{CH}$), 7.33 (s, 1H, $1 \times \text{CH}$), 7.38 (d, $J = 8.5\text{Hz}$, 1H, $1 \times \text{CH}$), 7.69 (d, $J = 8.5\text{Hz}$, 2H, $2 \times \text{CH}$), 7.72-7.75 (m, 2H, $2 \times \text{CH}$), 9.47(s, 1H, N-H). ^{13}C NMR (213 MHz, CDCl_3): δ 19.21, 26.93, 37.55, 55.37, 105.64, 117.90, 119.44, 119.96, 124.65, 125.59, 126.00, 126.40, 127.78, 129.32, 129.96, 134.00, 134.67, 138.84, 158.00, 162.19, 165.64, 172.79. ESI MS: 454 $[\text{M}+\text{H}]^+$, 456 $[\text{M}+\text{H}+2]^+$ $\text{C}_{23}\text{H}_{20}\text{N}_3\text{O}_3\text{S}$ (Calcd): C, 60.86; H, 4.44; N, 9.26; O, 10.57; S, 7.06. Obsd: C, 60.85, H, 4.45; N, 9.25; O, 10.58; S, 7.05

2-(5-((S)-1-(2-methoxynaphthalen-6-yl)ethyl)-1,3,4-oxadiazol-2-ylthio)-N-(3-bromophenyl) acetamide (22)

M.p: 129-130; yield: 90%; IR (ν , cm^{-1}): 3111, 3040, 2933, 1671, 1595, 1539, 1471, 1456, 1263, 1214, 1028, 850; ^1H NMR (850 MHz, CDCl_3): δ 1.86 (d, $J = 8.50$ Hz, 3H, $-\text{CH}_3$), 3.92-3.94 (m, 5H, $-\text{O}-\text{CH}_3$, $-\text{S}-\text{CH}_2-$), 4.49 (q, $J = 8.50$ Hz, 1H, $-\text{CH}$), 7.13 (d, $J = 8.5\text{Hz}$, 1H, $1 \times \text{CH}$), 7.17-7.19 (m, 2H, $2 \times \text{CH}$), 7.25 (d, $J = 8.5\text{Hz}$, 1H, $1 \times \text{CH}$), 7.38 (d, $J = 8.5\text{Hz}$, 1H, $1 \times \text{CH}$), 7.43 (d, $J = 8.5\text{Hz}$, 1H, $1 \times \text{CH}$), 7.69 (s, 1H, $1 \times \text{CH}$), 7.72-7.75 (m, 2H, $2 \times \text{CH}$), 7.84 (s, 1H, $1 \times \text{CH}$), 9.45 (s, 1H, $-\text{N}-\text{H}$). ^{13}C NMR (213 MHz, CDCl_3): δ 19.22, 26.14, 37.56, 55.37, 105.64, 118.40, 119.45, 122.65, 122.77, 125.60, 126.00, 127.60, 127.76, 128.87, 129.32, 130.26, 134.01, 134.38, 138.97, 159.45, 161.71, 163.15, 175.43. ESI MS: 498 $[\text{M}+\text{H}]^+$, 500 $[\text{M}+\text{H}+2]^+$ $\text{C}_{23}\text{H}_{20}\text{N}_3\text{O}_3\text{S}$ (Calcd): C, 55.43; H, 4.04; N, 8.43; O, 9.63; S, 6.43. Obsd: C, 55.42, H, 4.06; N, 8.42; O, 9.62; S, 6.45

2-(5-((S)-1-(2-methoxynaphthalen-6-yl)ethyl)-1,3,4-oxadiazol-2-ylthio)-N-(4-bromophenyl) acetamide (23)

M.p: 148-149; yield: 71%; IR (ν , cm^{-1}): 3101, 3041, 2935, 1675, 1525, 1405, 1263, 1025, 855; ^1H NMR (850 MHz, CDCl_3): δ 1.86 (d, $J = 7.60$ Hz, 3H, $-\text{CH}_3$), 3.92-3.94 (m, 5H, $\text{O}-\text{CH}_3$, $\text{S}-\text{CH}_2-$), 4.48 (q, $J = 8.50$ Hz, 1H, $-\text{CH}$), 7.13 (d, $J = 8.50$, 1H, $1 \times \text{CH}$), 7.37 (d, $J = 8.5\text{Hz}$, 1H, $1 \times \text{CH}$), 7.42 (d, $J = 8.5\text{Hz}$, 2H, $2 \times \text{CH}$), 7.45 (d, $J = 8.5\text{Hz}$, 2H, $2 \times \text{CH}$), 7.59 (t, $J = 8.5\text{Hz}$, 1H, $1 \times \text{CH}$), 7.68 (s, 1H, $1 \times \text{CH}$), 7.71-7.75 (m, 2H, $1 \times \text{CH}$), 9.45 (s, 1H, N-H). ^{13}C NMR (213 MHz, CDCl_3): δ 19.22, 30.96, 37.54, 55.37, 105.64, 1117.18, 119.45, 121.43, 123.26, 125.58, 125.99, 126.89, 127.76, 128.86, 129.31, 129.62, 131.94, 132.72, 134.00, 134.36, 136.81, 158.01, 163.26, 165.51,

171.04. ESI MS: 498 [M+H]⁺, 500 [M+H+2]⁺ C₂₃H₂₀N₃O₃S(Calcd): C, 55.43; H, 4.04; N, 8.43; O, 9.63; S, 6.43. Obsd: C, 55.44, H, 4.03; N, 8.44; O, 9.64; S, 6.45

2-(5-((S)-1-(2-methoxynaphthalen-6-yl)ethyl)-1,3,4-oxadiazol-2-ylthio)-N-o-tolylacetamide (24)

M.p: 109-110; yield:75%; IR (ν, cm⁻¹): 3315, 2931, 1672, 1596, 1549, 1485, 1470, 1456, 1371, 1251, 1214, 1159, 1028, 850; ¹H NMR (850 MHz, CDCl₃): δ 1.85 (d, J = 7.60 Hz, 3H, -CH-CH₃), 2.27 (s, 3H, Ar-CH₃), 3.94 (s, 3H, O-CH₃), 4.0 (brs, 2H, -S-CH₂-), 4.49 (q, J = 8.5Hz, 1H, C-H), 7.08 (t, J = 8.5Hz, 1H, 1 × CH), 7.13 (s, 1H, 1 × CH), 7.17-7.22 (m, 3H, 3 × CH), 7.36 (d, J = 8.5Hz, 1H, 1 × CH), 7.68 (s, 1H, 1 × CH), 7.71-7.74 (m, 2H, 2 × CH), 7.90 (d, J = 8.5Hz, 1H, 1 × CH), 8.91 (s, 1H, -N-H). ¹³C NMR (213 MHz, CDCl₃): δ 18.04, 19.24, 26.93, 37.51, 55.36, 105.64, 119.41, 122.46, 125.24, 125.58, 125.93, 126.67, 127.73, 128.88, 129.05, 129.32, 130.55, 133.97, 135.71, 158.25, 160.55, 163.01, 176.59. ESI MS: 434 [M+H]⁺, C₂₄H₂₃N₃O₃S(Calcd): C, 66.49; H, 5.35; N, 9.69; O, 11.07; S, 7.40. Obsd: C, 66.50, H, 5.34, N, 9.68; O, 11.09; S, 7.41

2-(2-(5-((S)-1-(2-methoxynaphthalen-6-yl)ethyl)-1,3,4-oxadiazol-2-ylthio)acetamido)benzoic acid (25)

M.p: 130-131; yield:68%; IR (ν, cm⁻¹): 3150, 2976, 1690, 1684, 1605, 1576, 1483, 1470, 1393, 1262, 1228, 1214, 1152, 1028, 852, 767; ¹H NMR (850 MHz, CDCl₃): δ 1.72 (d, J = 8.50 Hz, 3H, CH₃), 3.92-3.94 (m, 5H, O-CH₃, S-CH₂-), 4.02-4.07 (m, 1H, -CH), 7.11-7.19 (m, 3H, 3 × CH), 7.42-7.54 (m, 3H, 3 × CH), 7.72-7.81 (m, 3H, 3 × CH), 7.84 (s, 1H, 1 × CH), 8.58 (s, 1H, NH), 10.71 (s, 1H, -COOH). ¹³C NMR (213 MHz, CDCl₃): δ 18.07, 33.93, 45.65, 55.38, 105.73, 119.52, 126.31, 127.00, 127.93, 129.03, 129.32, 133.99, 134.12, 135.64, 145.83, 158.04, 158.76, 160.18, 169.76, 174.15. ESI MS: 464 [M+H]⁺, C₂₄H₂₁N₃O₅S(Calcd): C, 62.19; H, 4.57; N, 9.07; O, 17.26; S, 6.92. Obsd: C, 62.20, H, 4.56, N, 9.08; O, 17.25; S, 6.93

2-(5-((S)-1-(2-methoxynaphthalen-6-yl)ethyl)-1,3,4-oxadiazol-2-ylthio)-1-morpholino ethanone (26)

M.p: 74-75; yield:70%; IR (ν, cm⁻¹): 3050, 2936, 1633, 1605, 1481, 1457, 1392, 1263, 1228, 1149, 1068, 1027, 850, 812; ¹H NMR (850 MHz, CDCl₃): δ 1.83 (d, J = 8.5 Hz, 3H, -CH₃), 3.59 (t, J = 8.5Hz, 2H, -N-CH₂-), 3.66 (t, J = 8.5Hz, 2H, N-CH₂-), 3.70 (t, J = 8.5Hz, 2H, O-CH₂-), 3.73 (t, J = 8.5Hz, 2H, O-CH₂-), 3.94 (brs, 5H, O-CH₃, S-CH₂-), 4.48 (q, J = 8.5Hz, 1H, -CH), 7.14-7.19 (m, 3H, 3 × CH), 7.36-

7.39 (m, 1H, 1 × CH), 7.68 (s, 1H, 1 × CH), 7.72-7.75 (m, 1H, 1 × CH). ¹³C NMR (213 MHz, CDCl₃): δ 19.35, 37.69, 42.63, 46.54, 55.36, 66.46, 105.64, 119.32, 119.45, 125.55, 125.74, 127.62, 127.76, 129.34, 133.91, 134.85, 157.91, 162.83, 164.38, 174.52. ESI MS: 414 [M+H]⁺, C₂₁H₂₃N₃O₄S(Calcd): C, 61.00; H, 5.61; N, 10.16; O, 15.48; S, 7.75. Obsd: C, 60.01, H, 5.60; N, 10.17; O, 15.50; S, 7.73

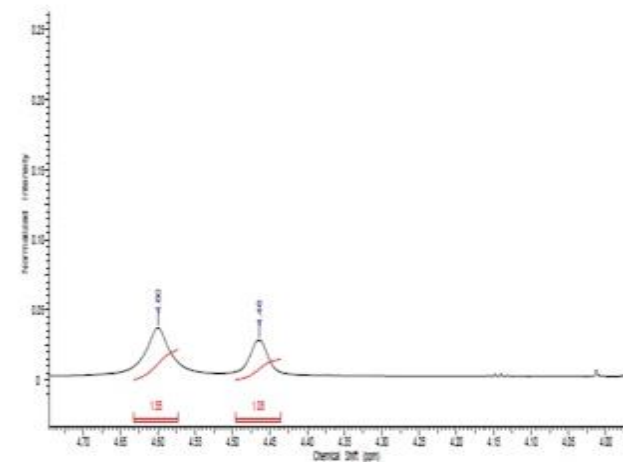
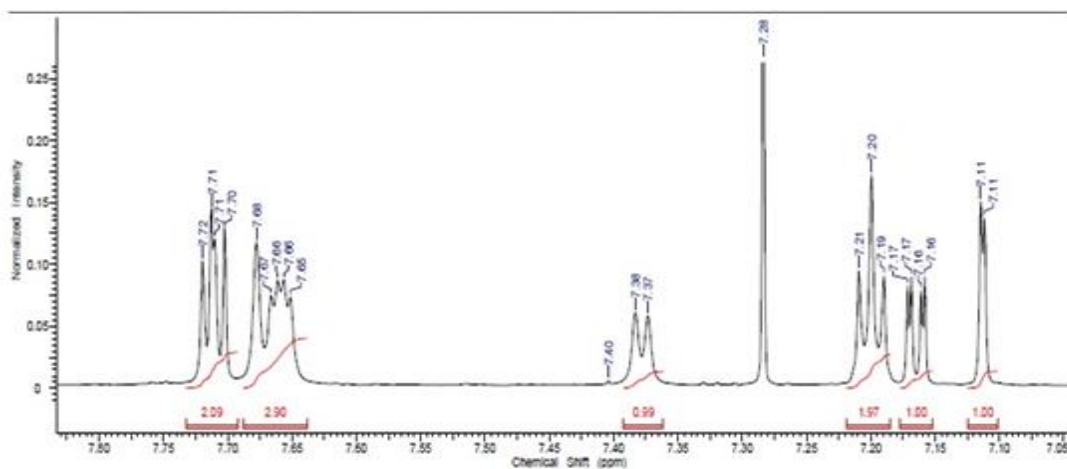
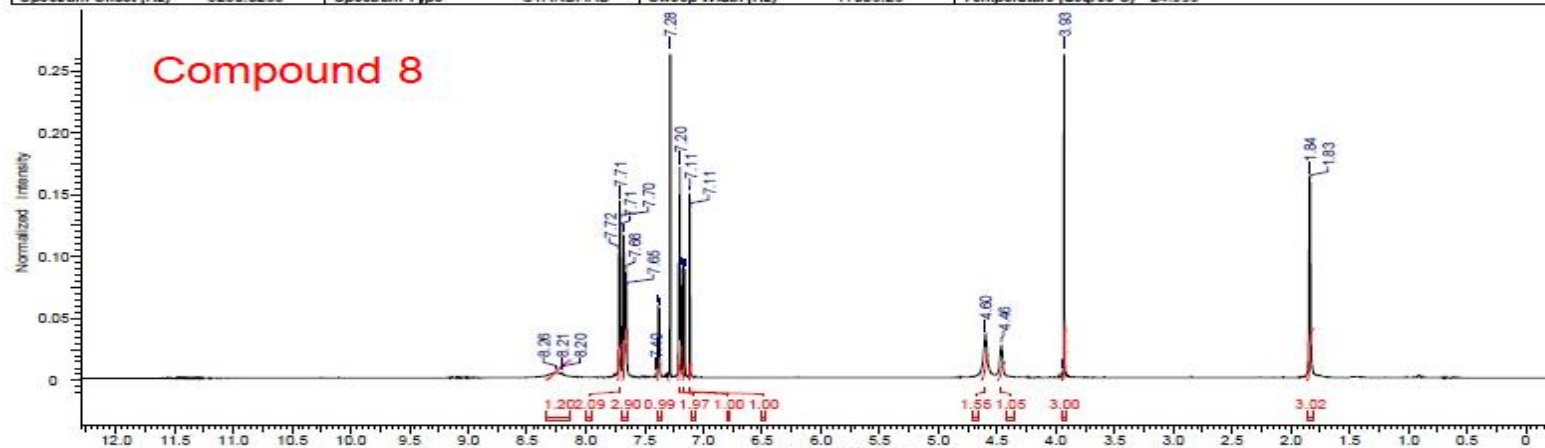
Table S1. The calculated GCRD derived from frontier molecular orbitals for **8-11** and **19-26**

| | E_{HOMO} | E_{LUMO} | E_{gap} | IP | EA | η | μ | S | χ | ω | ω^\pm |
|-----------|-------------------|-------------------|------------------|------|------|--------|-------|-------|--------|----------|--------------|
| 8 | -5.83 | -1.89 | -3.94 | 5.83 | 1.89 | 1.97 | -4.85 | 0.51 | 3.79 | -3.86 | 9.507 |
| 9 | -5.71 | -1.89 | -3.82 | 5.71 | 1.89 | 1.91 | -4.75 | 0.52 | 3.78 | -3.80 | 9.450 |
| 10 | -5.69 | -1.82 | -3.87 | 5.69 | 1.82 | 1.94 | -4.73 | 0.52 | 3.65 | -3.76 | 9.175 |
| 11 | -5.67 | -2.04 | -3.64 | 5.67 | 2.04 | 1.82 | -4.76 | 0.55 | 4.08 | -3.86 | 10.097 |
| 12 | -5.72 | -2.00 | -3.72 | 5.72 | 2.00 | 1.86 | -4.79 | 0.54 | 4.01 | -3.86 | 9.959 |
| 13 | -5.67 | -2.06 | -3.61 | 5.67 | 2.06 | 1.80 | -4.77 | 0.55 | 4.14 | -3.86 | 10.207 |
| 14 | -5.82 | -2.03 | -3.79 | 5.82 | 2.03 | 1.90 | -4.88 | 0.53 | 4.07 | -3.93 | 10.105 |
| 15 | -6.11 | -1.80 | -4.31 | 6.11 | 1.80 | 2.16 | -5.03 | 0.46 | 3.63 | -3.96 | 9.234 |
| 16 | -1.87 | -0.58 | -1.29 | 1.87 | 0.58 | 0.64 | -1.55 | 1.55 | 1.16 | -1.22 | 2.940 |
| 19 | -5.90 | -1.52 | -4.38 | 5.90 | 1.52 | 2.19 | -4.81 | 0.46 | 3.15 | -3.71 | 8.154 |
| 20 | -5.77 | -1.61 | -4.15 | 5.77 | 1.61 | 2.08 | -4.73 | 0.48 | 3.28 | -3.69 | 8.400 |
| 21 | -6.07 | -1.70 | -4.38 | 6.07 | 1.70 | 2.19 | -4.98 | 0.46 | 3.45 | -3.89 | 8.841 |
| 22 | -5.92 | -1.76 | -4.16 | 5.92 | 1.76 | 2.08 | -4.88 | 0.48 | 3.55 | -3.84 | 9.015 |
| 23 | -5.89 | -1.51 | -4.38 | 5.89 | 1.51 | 5.13 | -4.79 | -0.21 | 0.01 | 3.32 | 9.958 |
| 24 | -5.88 | -1.53 | -4.35 | 5.88 | 1.53 | 2.18 | -4.79 | 0.46 | 3.15 | -3.70 | 8.148 |
| 25 | -1.57 | -0.20 | -1.37 | 1.57 | 0.20 | 0.68 | -1.23 | 1.46 | 0.57 | -0.89 | 1.592 |
| 26 | -5.70 | -1.34 | -4.36 | 5.70 | 1.34 | 2.18 | -4.61 | 0.46 | 2.84 | -3.52 | 7.445 |

Figure S1-S17: ^1H NMR of compounds

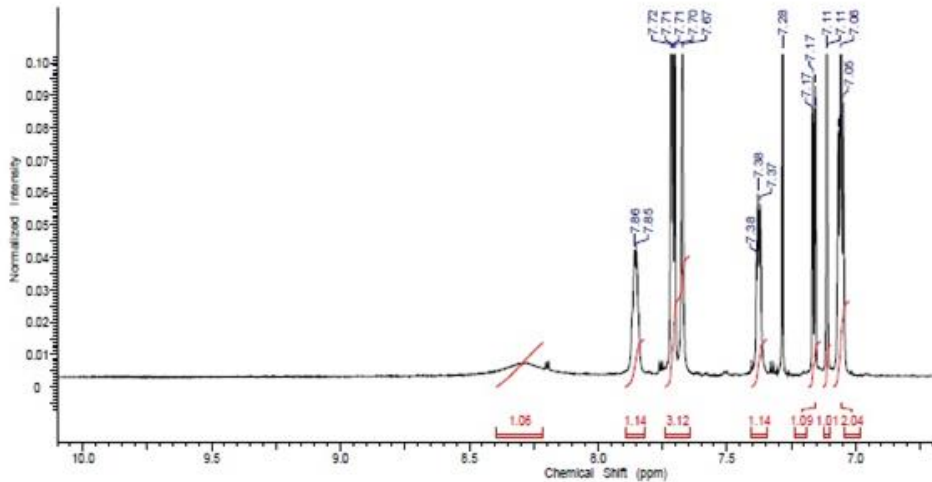
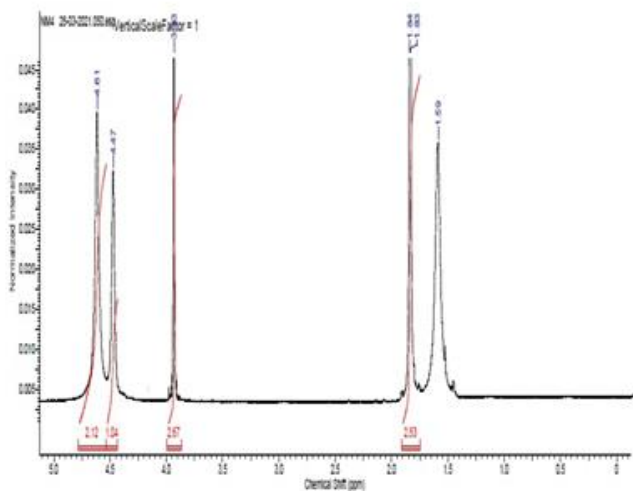
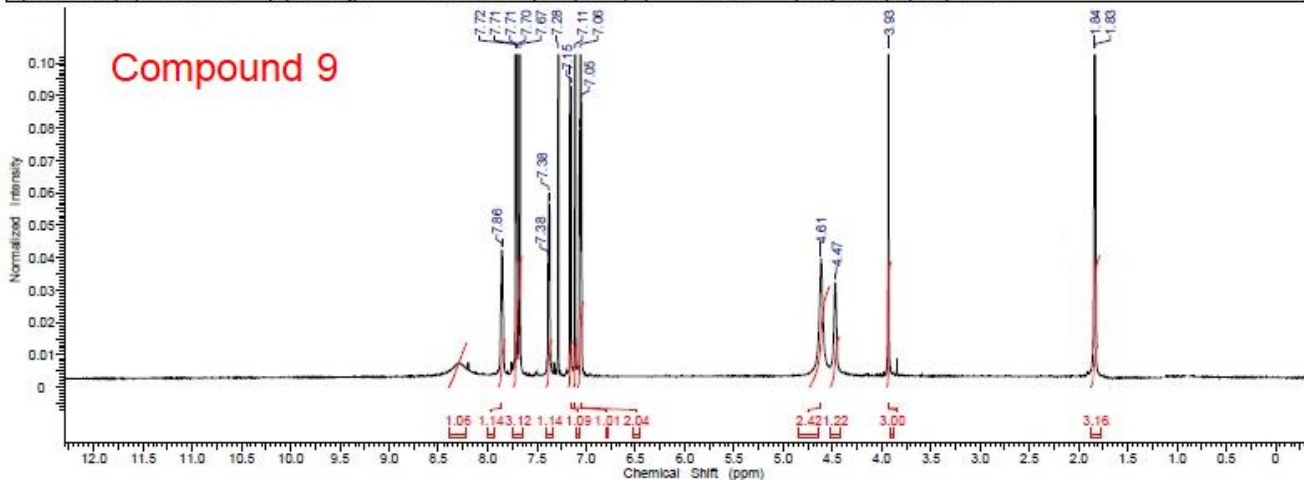
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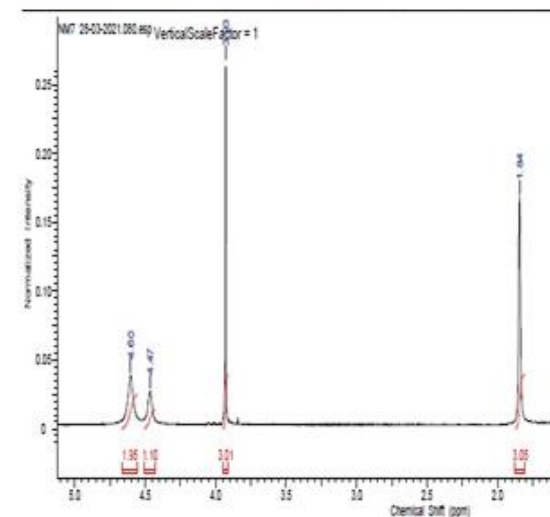
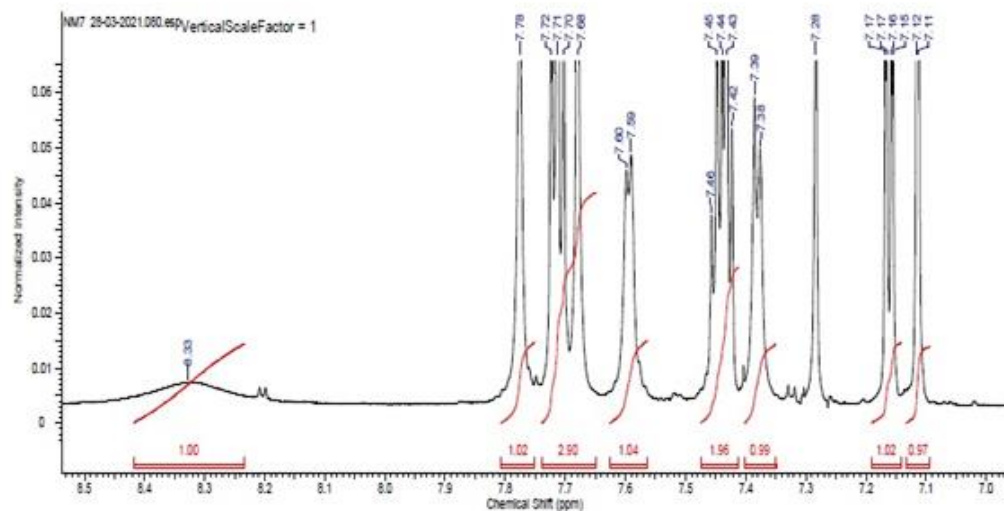
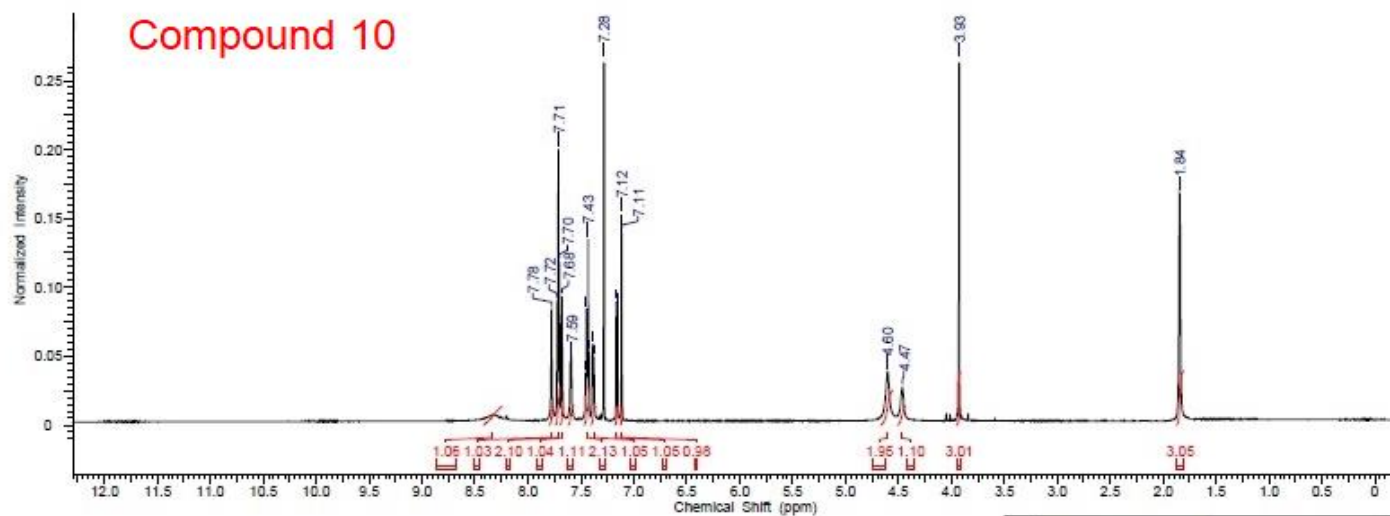
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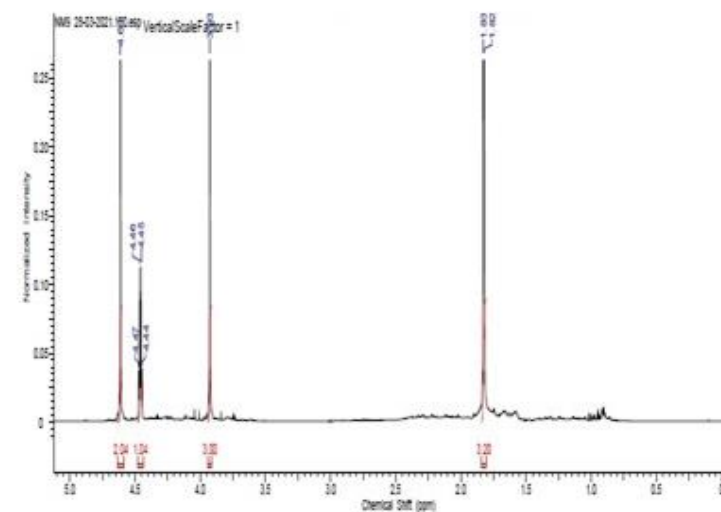
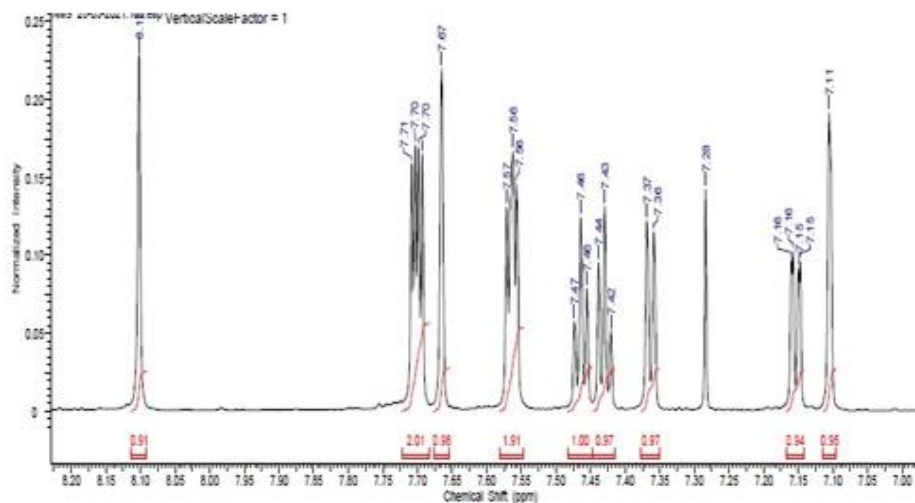
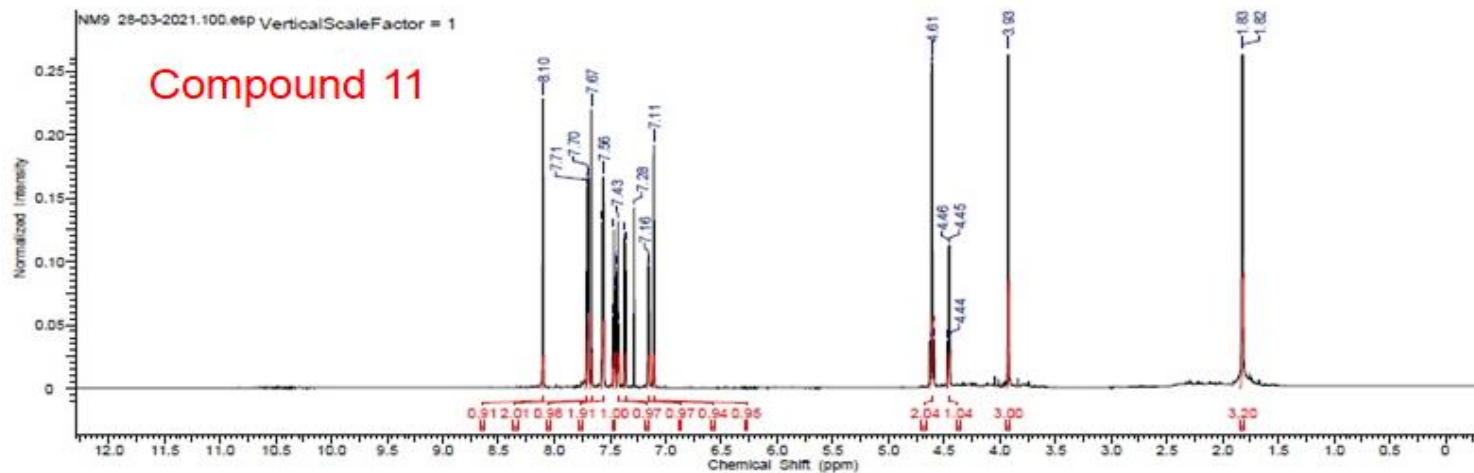
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Compound 10

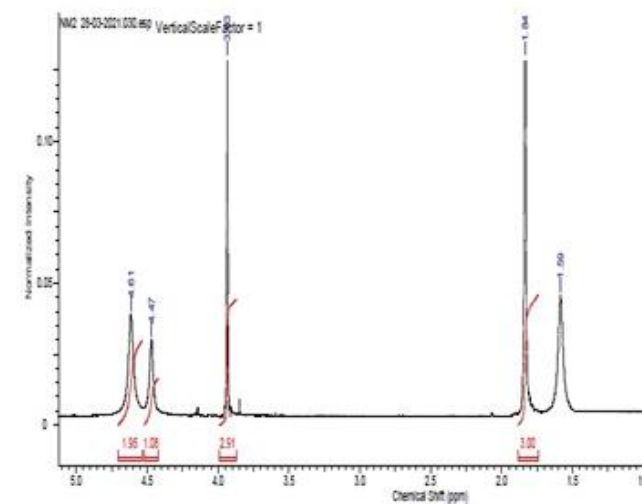
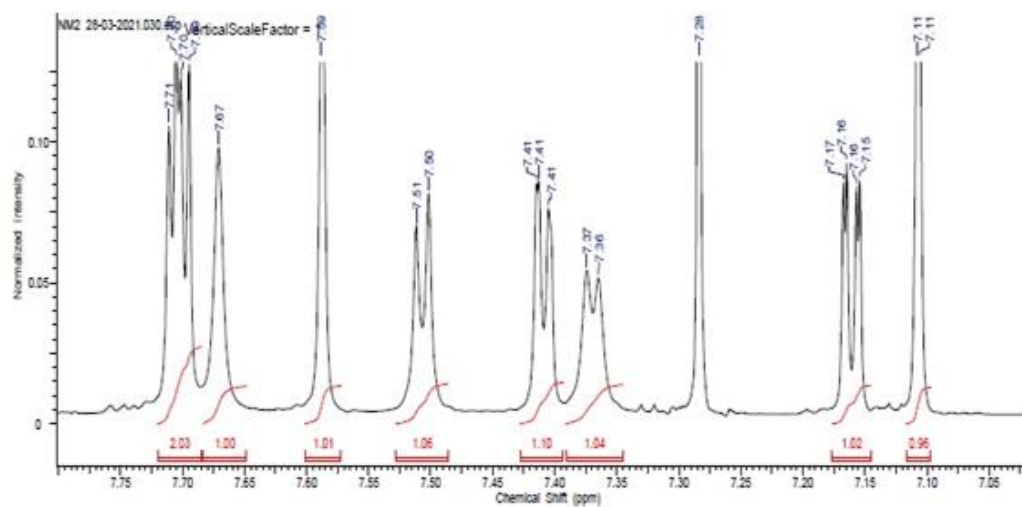
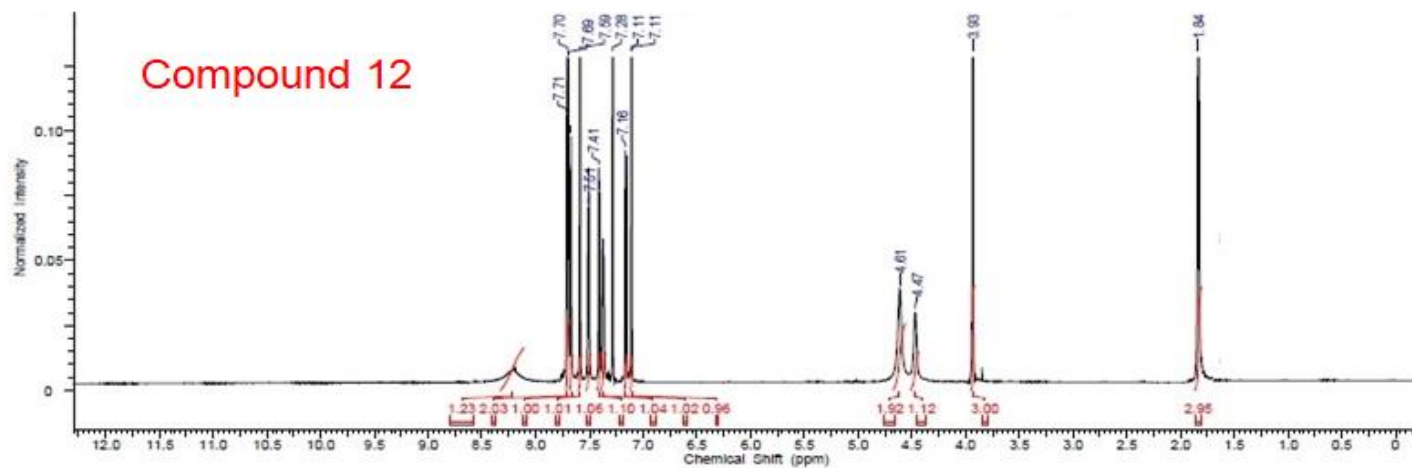


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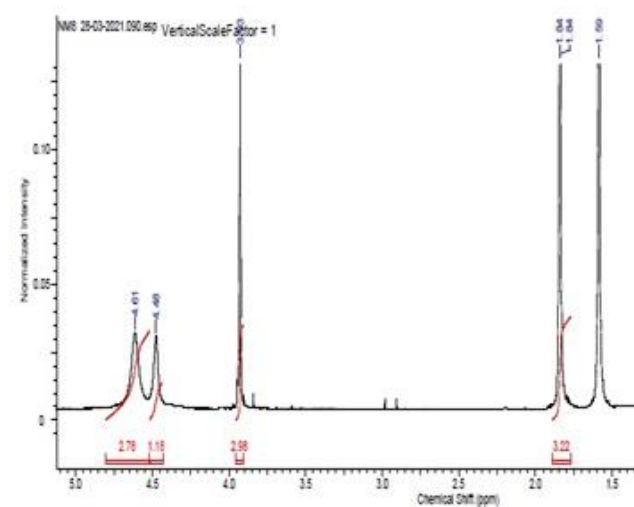
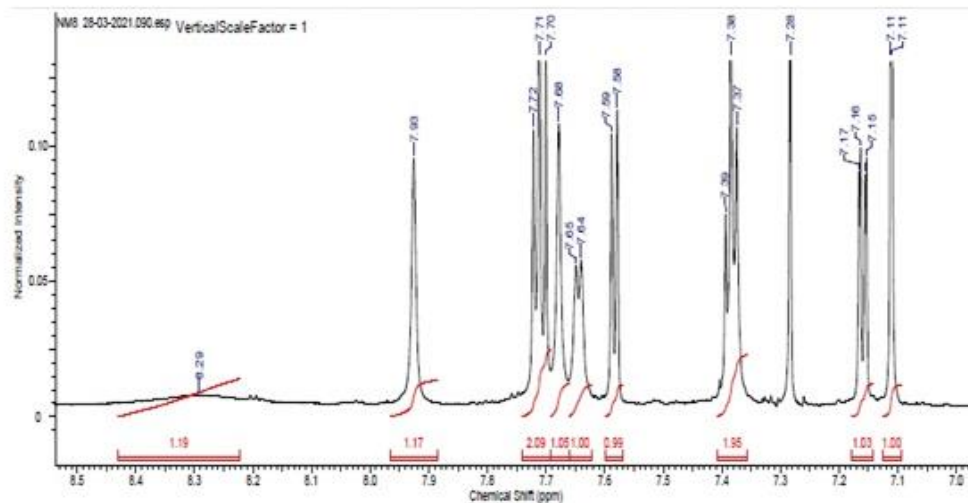
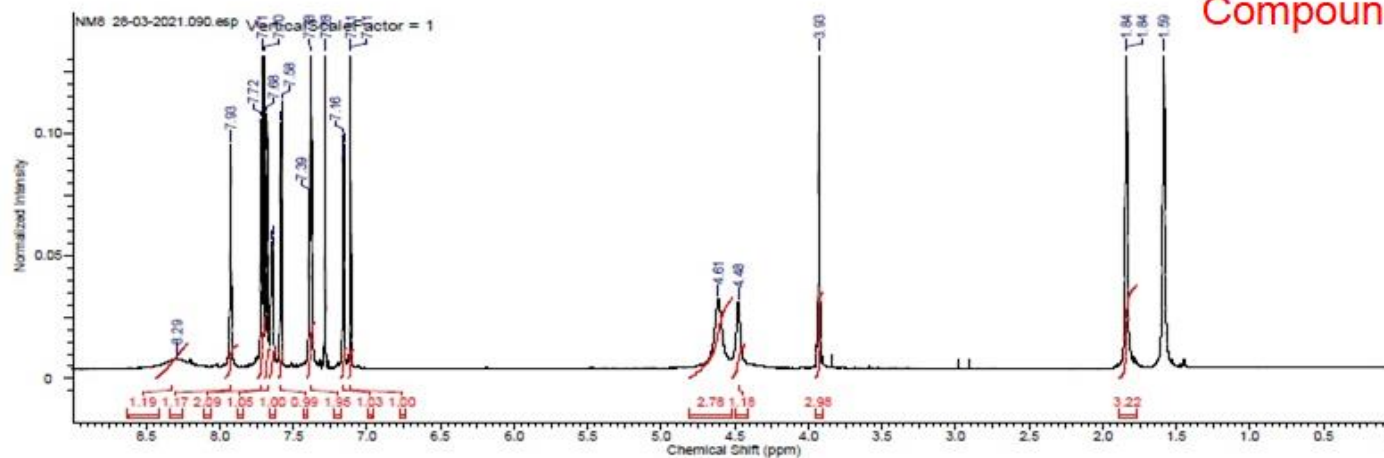


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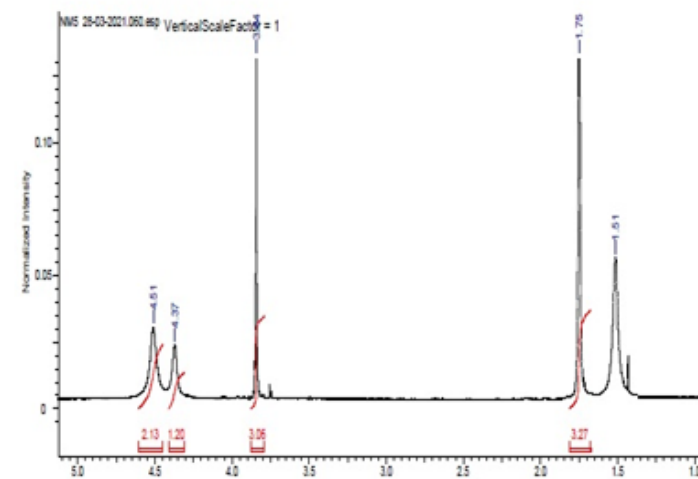
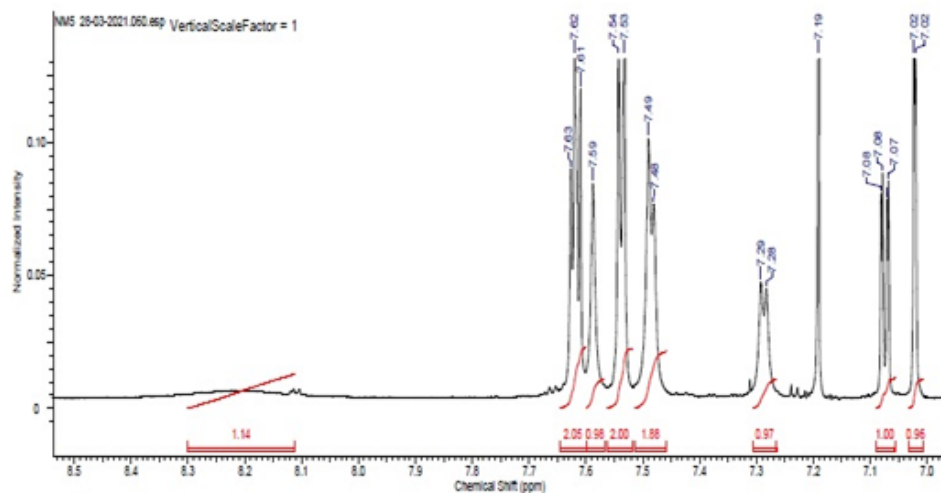
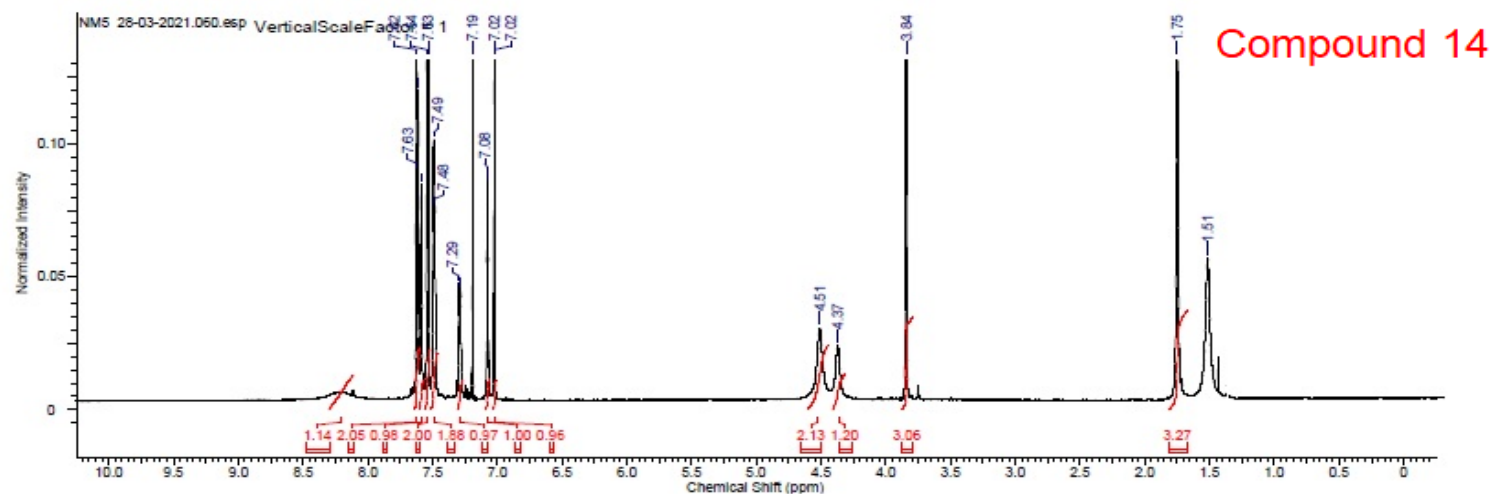
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Compound 13



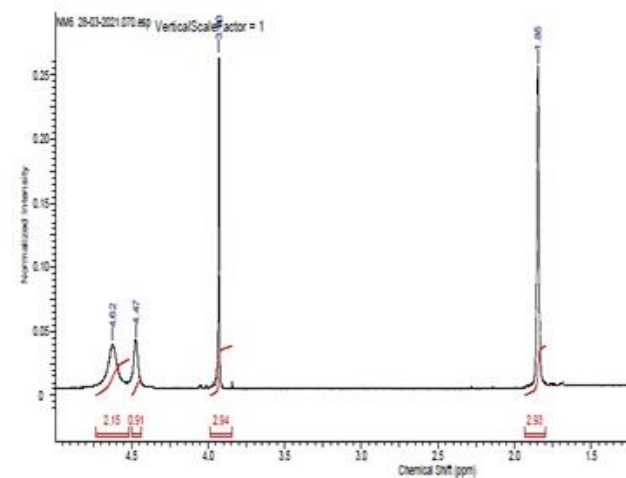
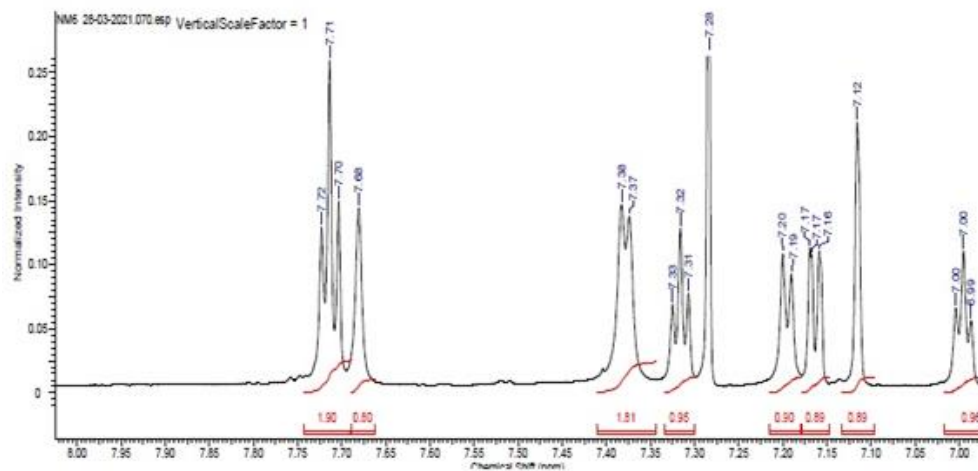
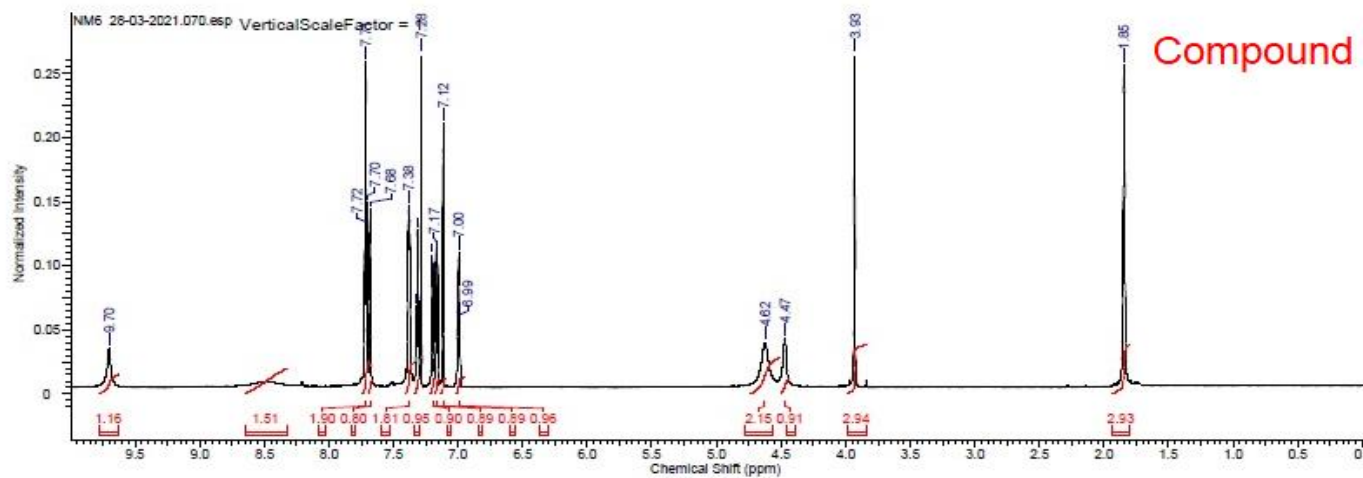
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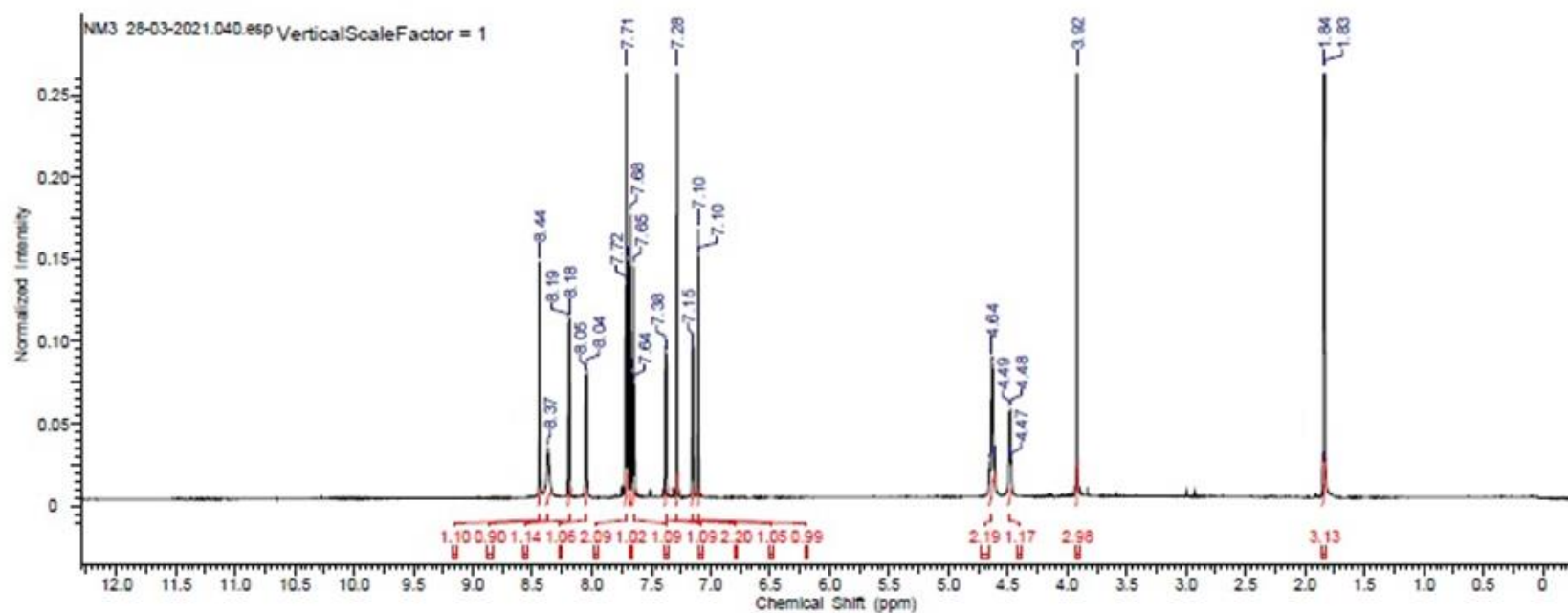
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Compound 16

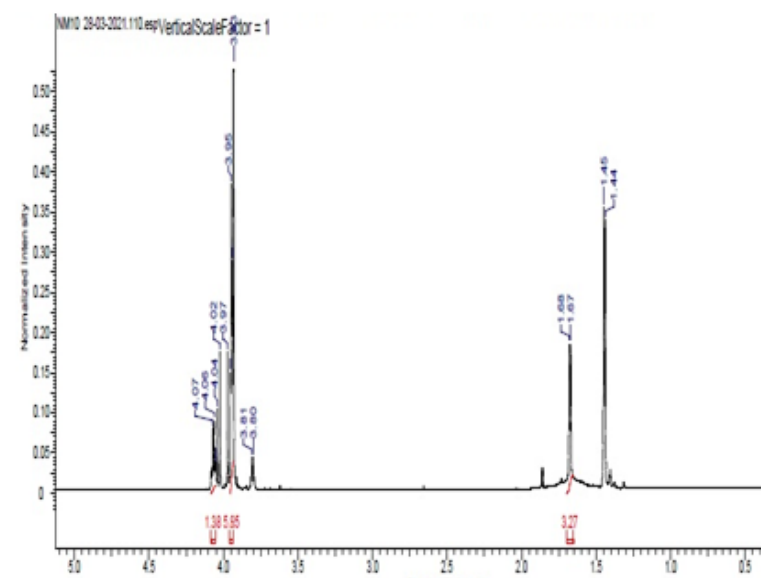
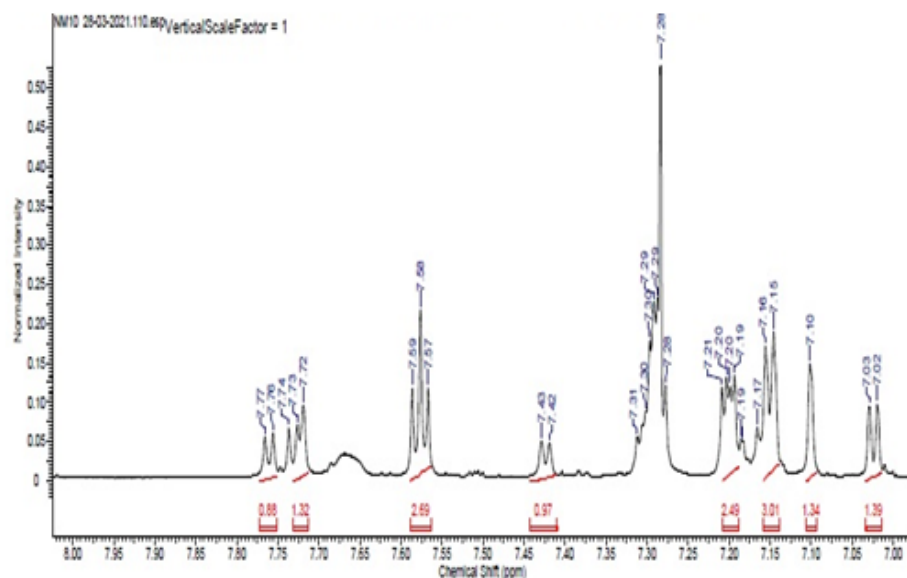
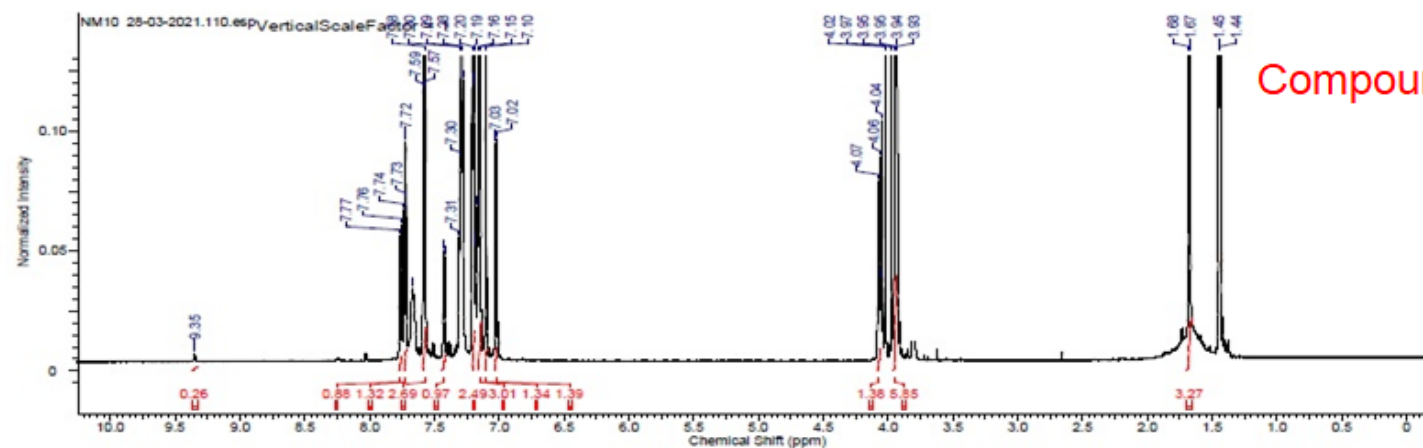
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| Receiver Gain | 12.46 | SW (cycles) | 17006.80 | Pulse Sequence | zg30 |
| Spectrum Offset (Hz) | 5250.0283 | Spectrum Type | STANDARD | Solvent | CHLOROFORM-d |
| | | | | Temperature (degree C) | 25.000 |

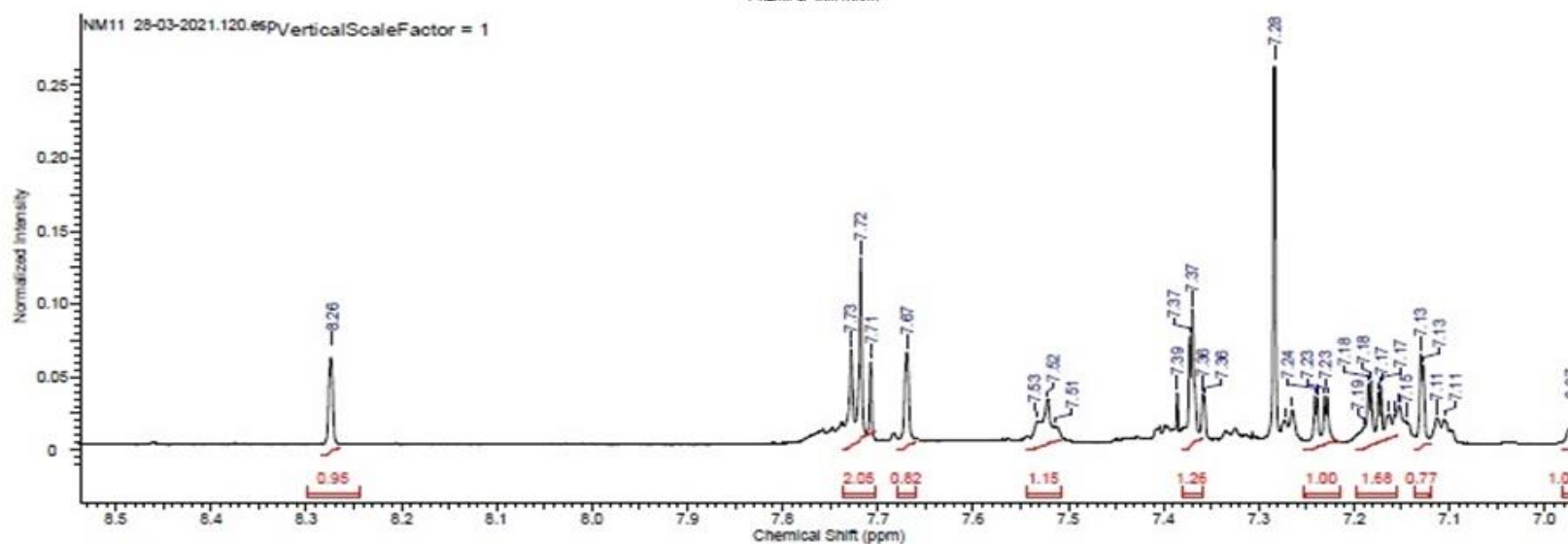
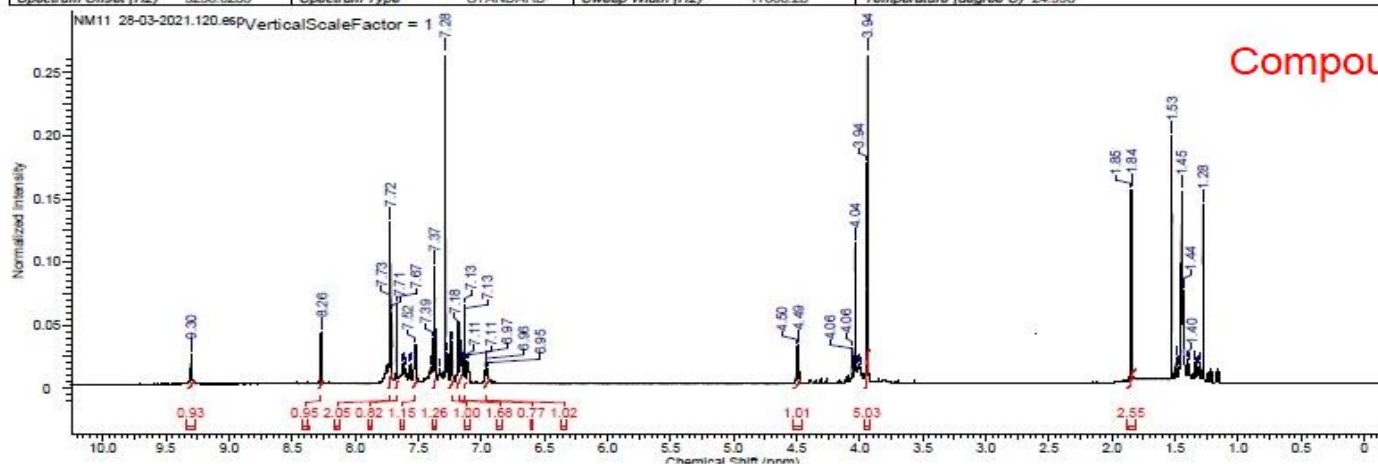


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| Date Stamp | 28 Mar 2021 21:22:56 | | File Name | C:\Users\hp\Desktop\Naproxen NMR\NM10_28-03-2021\110.fid | |
| Frequency (MHz) | 850.15 | Nucleus | ¹ H | Number of Transients | 32 |
| Original Points Count | 32768 | Owner | nmr | Points Count | 32768 |
| Receiver Gain | 11.37 | SW(cyclical) (Hz) | 17006.80 | Solvent | CHLOROFORM-d |
| Spectrum Offset (Hz) | 5250.0283 | Spectrum Type | STANDARD | Sweep Width (Hz) | 17006.28 |
| | | | | Temperature (degree C) | 25.000 |

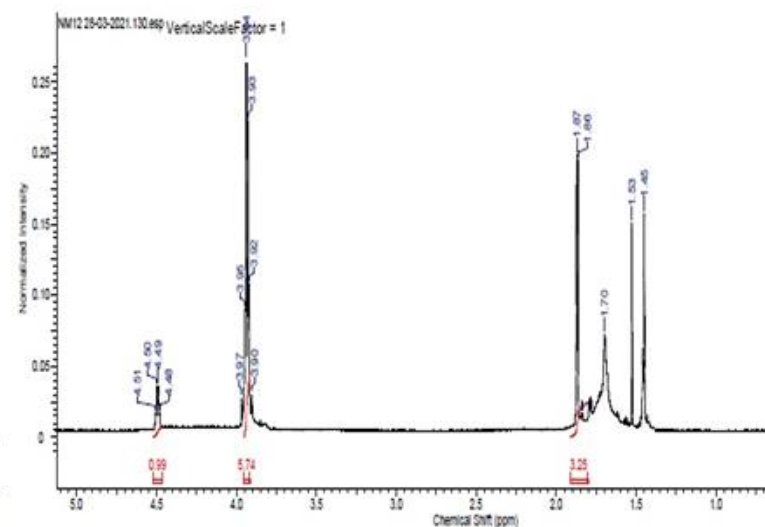
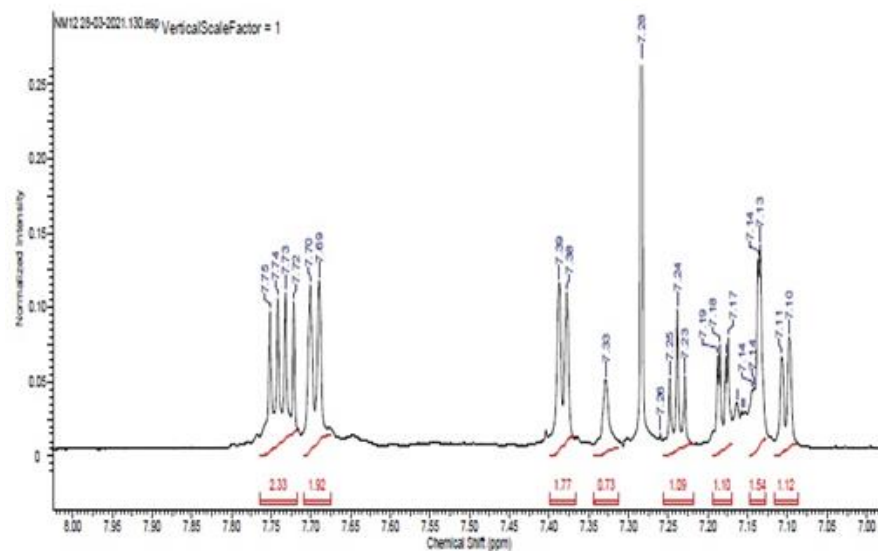
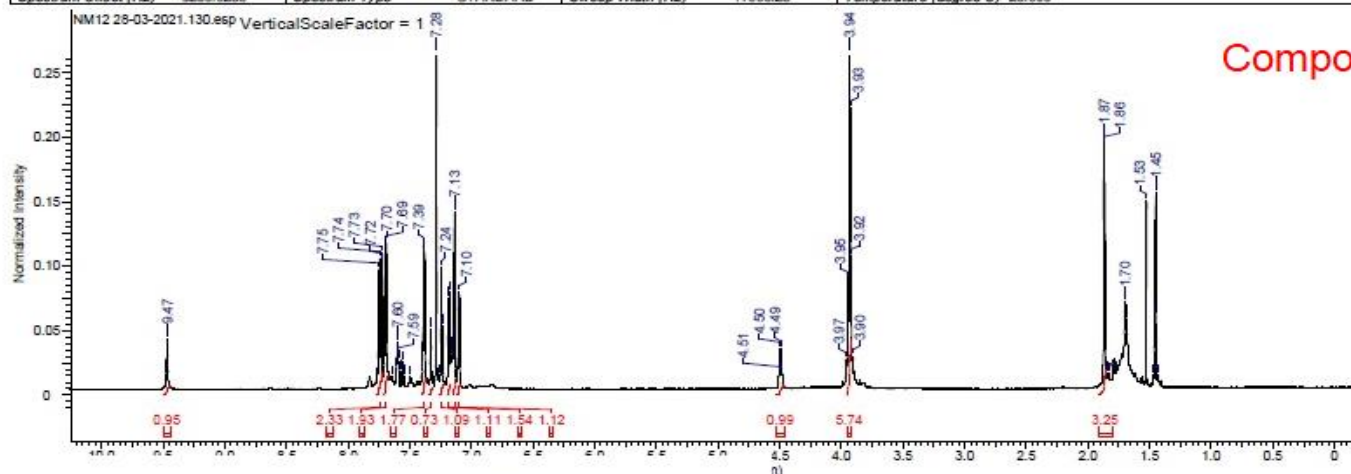


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| Acquisition Time (sec) | 1.9268 | Comment | Dr. Abdusattar Sample 27-03 CDCL3 | | | Date | 28 Mar 2021 22:16:16 |
| Date Stamp | 28 Mar 2021 22:16:16 | | File Name | C:\Users\shp\Desktop\Naproxen NMR\NM11 | | | 28-03-2021\120fid |
| Frequency (MHz) | 850.15 | Nucleus | ¹ H | Number of Transients | 32 | Origin | spect |
| Original Points Count | 32768 | Owner | nmr | Points Count | 32768 | Pulse Sequence | zg30 |
| Receiver Gain | 11.37 | SW(cyclical) (Hz) | 17006.80 | Solvent | CHLOROFORM-d | | |
| Spectrum Offset (Hz) | 5250.0283 | Spectrum Type | STANDARD | Sweep Width (Hz) | 17006.28 | Temperature (degree C) | 24.998 |

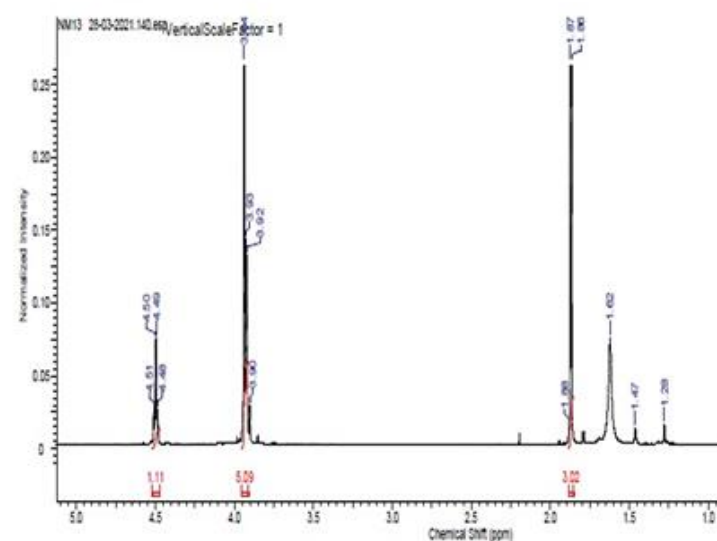
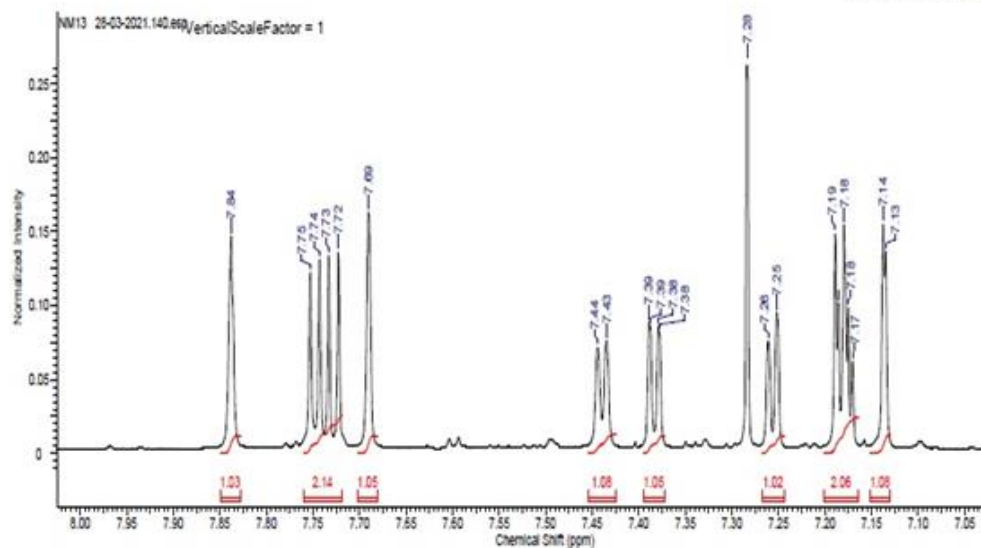
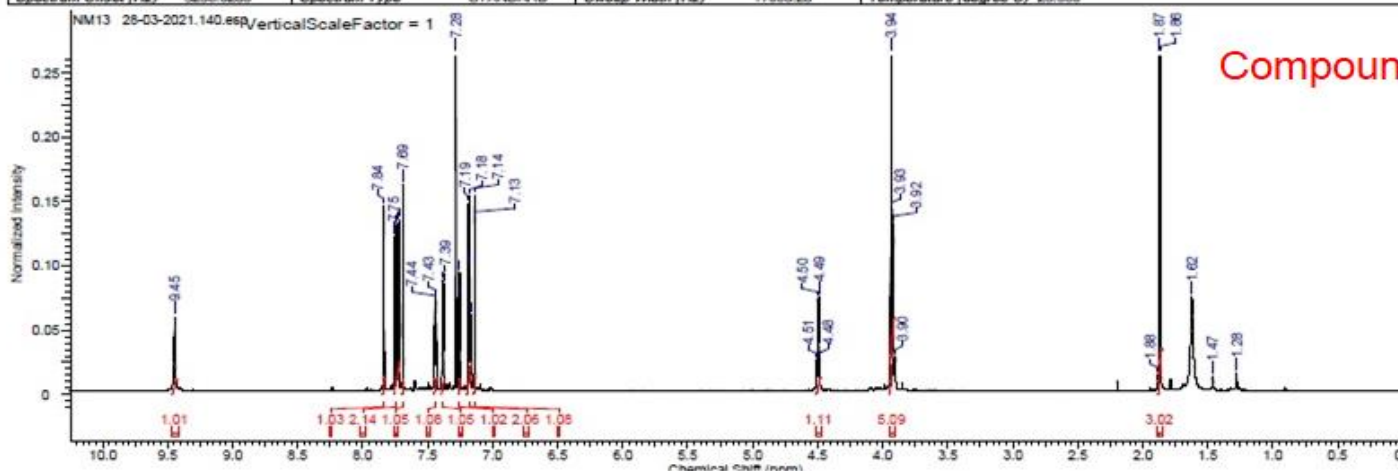


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| | | | | | | | |
|------------------------|----------------------|-------------------|-----------------------|----------------------|--------------|------------------------|---|
| Acquisition Time (sec) | 1.9268 | Comment | Dr. Abdussattar Sampe | 28-03 | CDCL3 | Date | 28 Mar 2021 23:09:36 |
| Date Stamp | 28 Mar 2021 23:09:36 | | | | | File Name | C:\Users\shp\Desktop\Naproxen NMR\NM12 28-03-2021\130\fid |
| Frequency (MHz) | 850.15 | Nucleus | 1H | Number of Transients | 32 | Origin | spect |
| Original Points Count | 32768 | Owner | nmr | Points Count | 32768 | Pulse Sequence | zg30 |
| Receiver Gain | 12.46 | SW(cyclical) (Hz) | 17006.80 | Solvent | CHLOROFORM-d | | |
| Spectrum Offset (Hz) | 5250.0283 | Spectrum Type | STANDARD | Sweep Width (Hz) | 17006.28 | Temperature (degree C) | 25.000 |

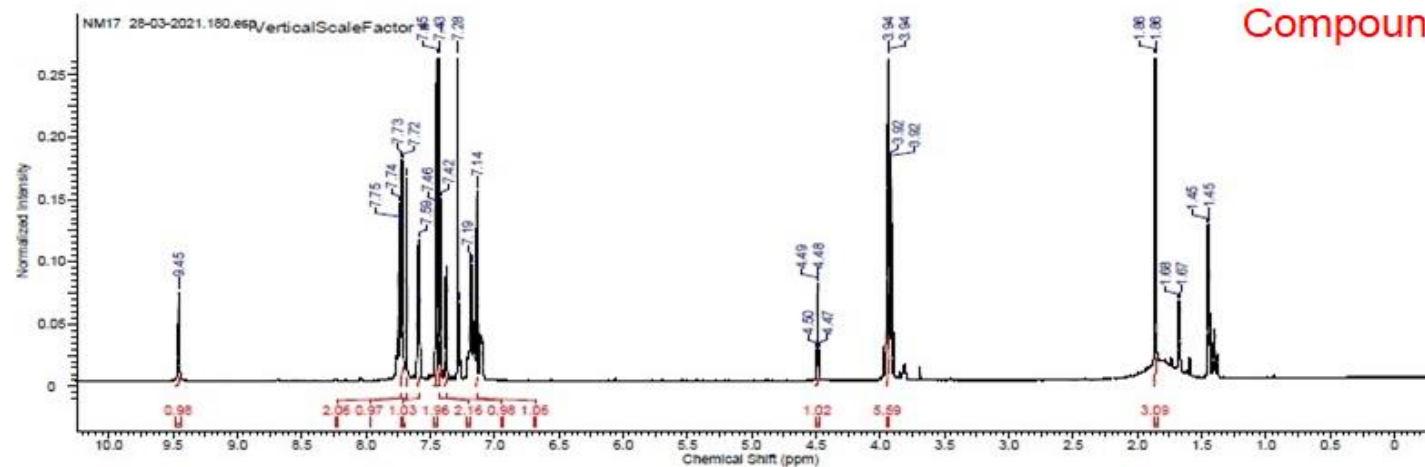


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|------------------------|----------------------|-------------------|-----------------------------------|---|--------------|------------------------|----------------------|
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| Date Stamp | 29 Mar 2021 00:00:48 | | File Name | C:\Users\vip\Desktop\Naproxen NMR\NM13_28-03-2021\140.fid | | | |
| Frequency (MHz) | 850.15 | Nucleus | ¹ H | Number of Transients | 32 | Origin | spect |
| Original Points Count | 32768 | Owner | nmr | Points Count | 32768 | Pulse Sequence | zg30 |
| Receiver Gain | 12.46 | SW(cyclical) (Hz) | 17006.80 | Solvent | CHLOROFORM-d | | |
| Spectrum Offset (Hz) | 5250.0283 | Spectrum Type | STANDARD | Sweep Width (Hz) | 17006.28 | Temperature (degree C) | 25.000 |

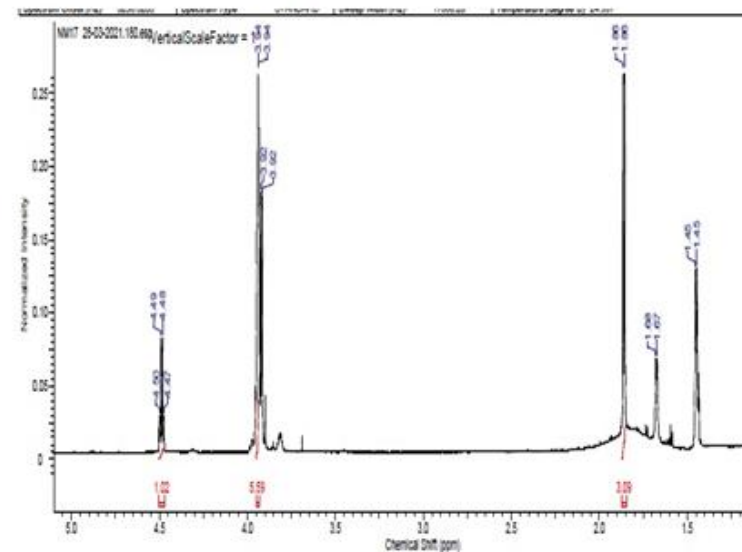
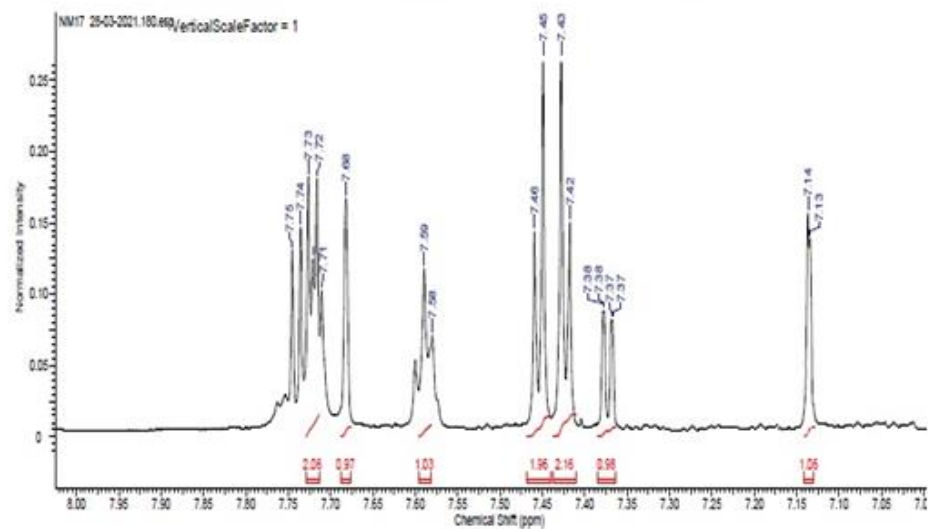


4/30/2021 4:08:32 PM

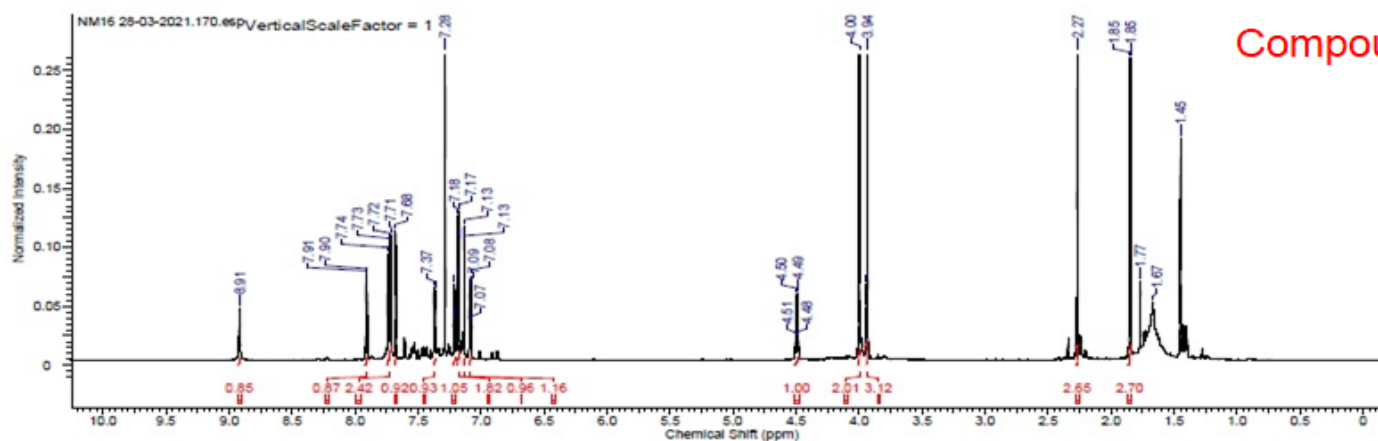
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| Acquisition Time (sec) | 1.9268 | Comment | Dr. Abdusattar Sample 33-03 CDCL3 | Date | 29 Mar 2021 03:34:08 |
| Date Stamp | 29 Mar 2021 03:34:08 | File Name | C:\Users\hdp\Desktop\Naproxen NMR\ NM17_ 29-03-2021\180.fid | Origin | spect |
| Frequency (MHz) | 850.15 | Nucleus | 1H | Number of Transients | 32 |
| Original Points Count | 32768 | Owner | nmr | Points Count | 32768 |
| Receiver Gain | 12.46 | SW(cyclical) (Hz) | 17006.80 | Solvent | CHLOROFORM-d |
| Spectrum Offset (Hz) | 5250.0283 | Spectrum Type | STANDARD | Sweep Width (Hz) | 17006.28 |
| | | | | Temperature (degree C) | 24.997 |



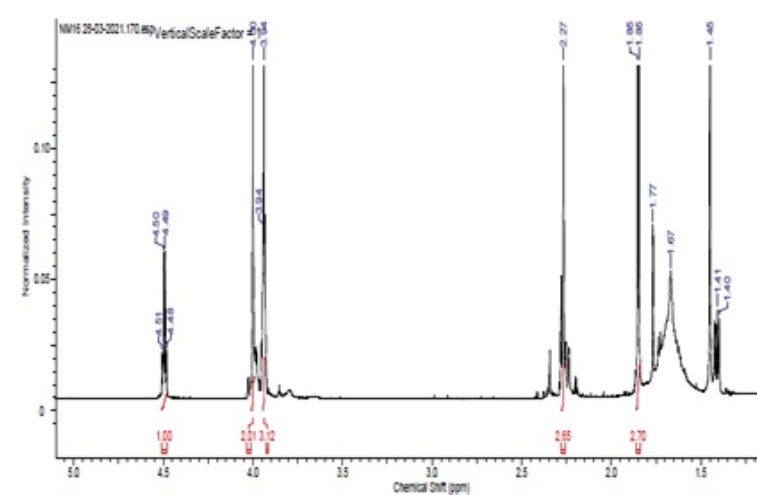
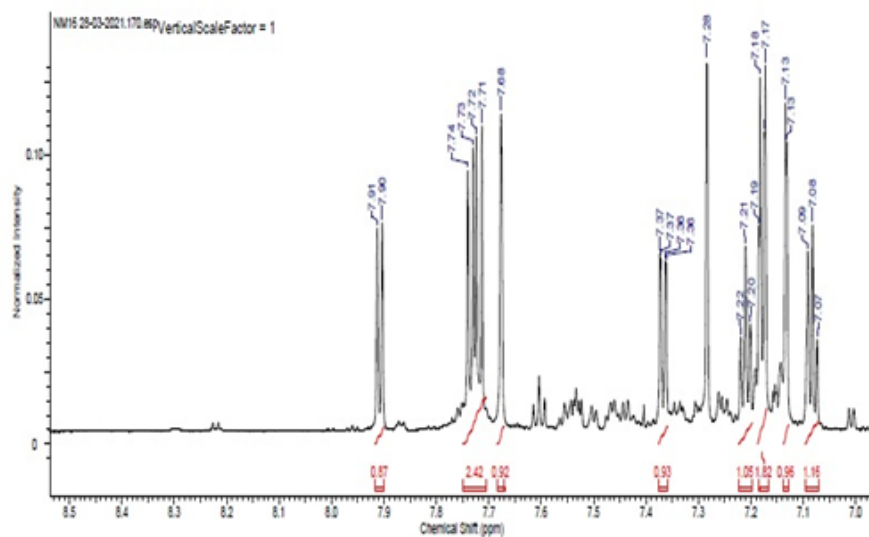
Compound 23



| | | | | | |
|------------------------|----------------------|-------------------|--|------------------------|----------------------|
| Acquisition Time (sec) | 1.9268 | Comment | Dr. Abdussattar Sample 32-03 CDCL3 | Date | 29 Mar 2021 02:40:48 |
| Date Stamp | 29 Mar 2021 02:40:48 | File Name | C:\Users\hp\Desktop\Naproxen NMR\ NM16 28-03-2021\1706fd | Origin | spect |
| Frequency (MHz) | 850.15 | Nucleus | 1H | Number of Transients | 32 |
| Original Points Count | 32768 | Owner | nmr | Points Count | 32768 |
| Receiver Gain | 12.46 | SW(cyclical) (Hz) | 17006.80 | Pulse Sequence | zg30 |
| Spectrum Offset (Hz) | 6250.0283 | Spectrum Type | STANDARD | Solvent | CHLOROFORM-d |
| | | Sweep Width (Hz) | 17006.28 | Temperature (degree C) | 24.999 |

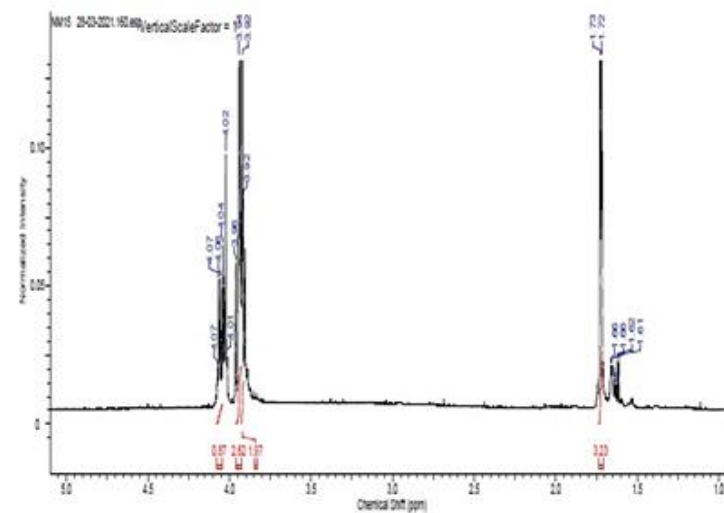
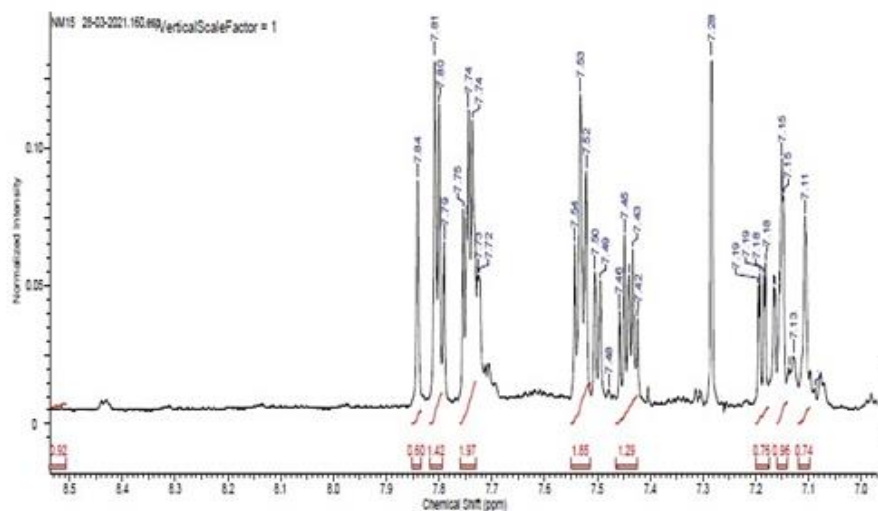
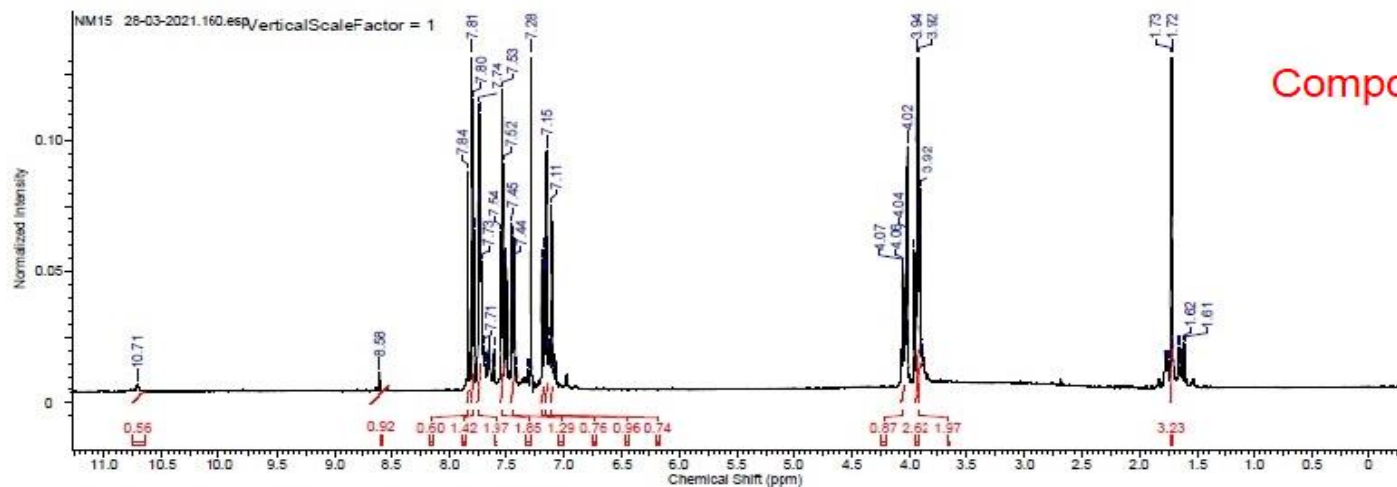


Compound 24



4/30/2021 3:32:40 PM

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|------------------------|----------------------|-------------------|-----------------------------------|---|----------------------|
| Acquisition Time (sec) | 1.9268 | Comment | Dr. Abdusattar Sample 31-03 CDCL3 | Date | 29 Mar 2021 01:47:28 |
| Date Samp | 29 Mar 2021 01:47:28 | | File Name | C:\Users\hpl\Desktop\Naproxen NMR\NM15_28-03-2021\160.fid | |
| Frequency (MHz) | 850.15 | Nucleus | 1H | Number of Transients | 32 |
| Original Points Count | 32758 | Owner | nmr | Points Count | 32768 |
| Receiver Gain | 12.46 | SW(cyclical) (Hz) | 17006.80 | Solvent | CHLOROFORM-d |
| Spectrum Offset (Hz) | 5250.0283 | Spectrum Type | STANDARD | Sweep Width (Hz) | 17006.26 |
| | | | | Temperature (degree C) | 24.958 |



| | | | | | |
|------------------------|----------------------|-------------------|---|------------------------|----------------------|
| Acquisition Time (sec) | 1.9258 | Comment | Dr. Abdusattar Sample 30-03_CDCL3 | Date | 29 Mar 2021 00:56:16 |
| Date Stamp | 29 Mar 2021 00:56:16 | File Name | C:\Users\hp\Desktop\Naproxen NMR\NM14_28-03-2021\150v6d | Origin | spect |
| Frequency (MHz) | 850.15 | Nucleus | ¹ H | Number of Transients | 32 |
| Original Points Count | 32768 | Owner | nmr | Points Count | 32768 |
| Receiver Gain | 11.37 | SW(cyclical) (Hz) | 17006.80 | Pulse Sequence | zg30 |
| Spectrum Offset (Hz) | 5250.0283 | Spectrum Type | STANDARD | Solvent | CHLOROFORM-d |
| | | Sweep Width (Hz) | 17006.28 | Temperature (degree C) | 25.000 |

Compound 26

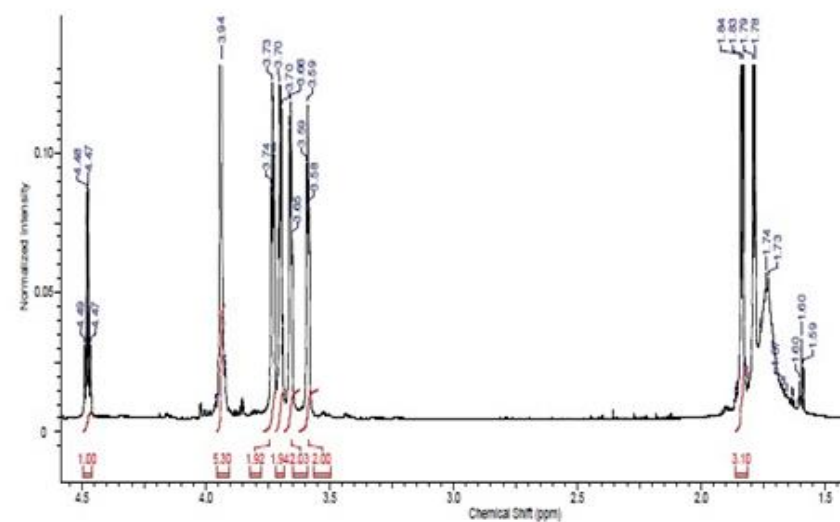
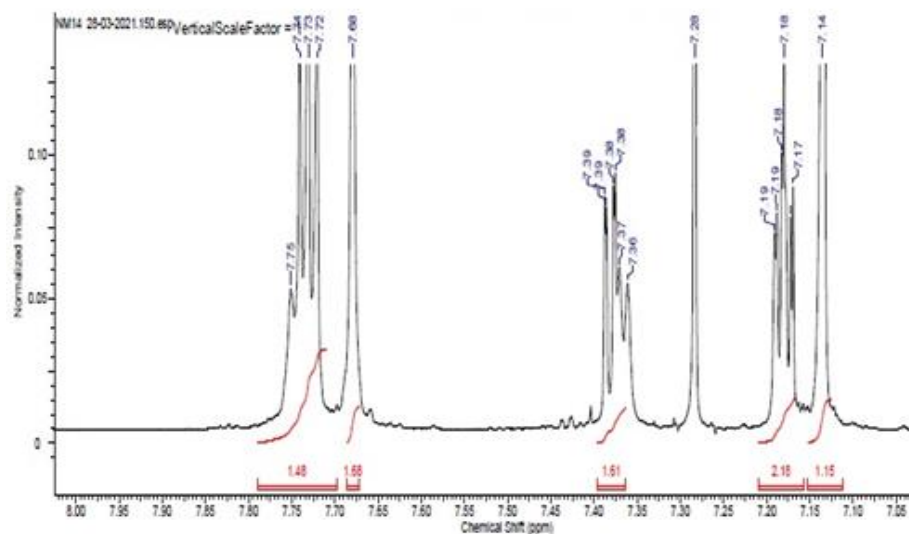
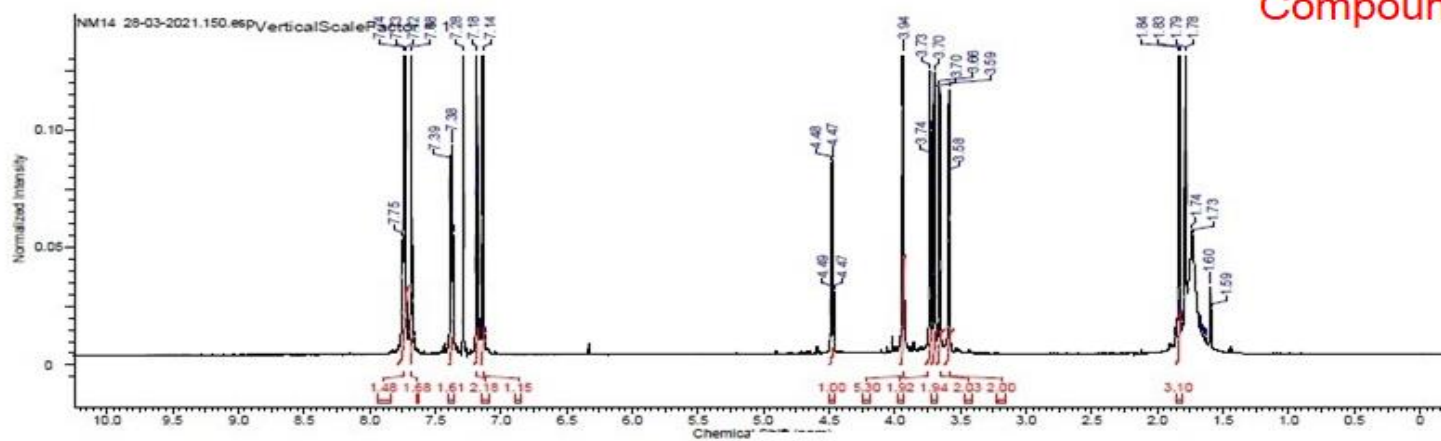
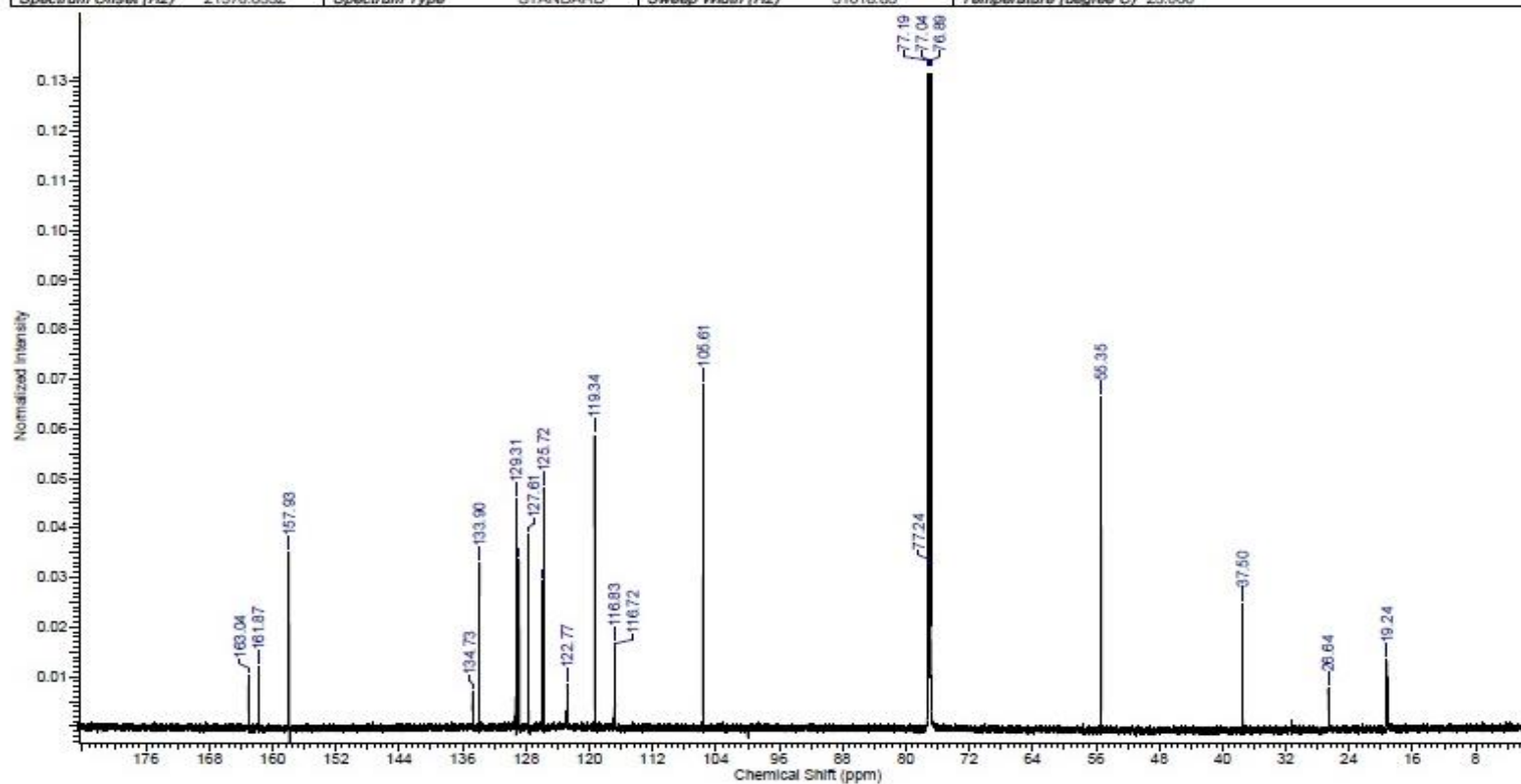


Figure S18-S34: ^{13}C NMR of compounds

Compound 8

4/28/2021 11:14:55 PM

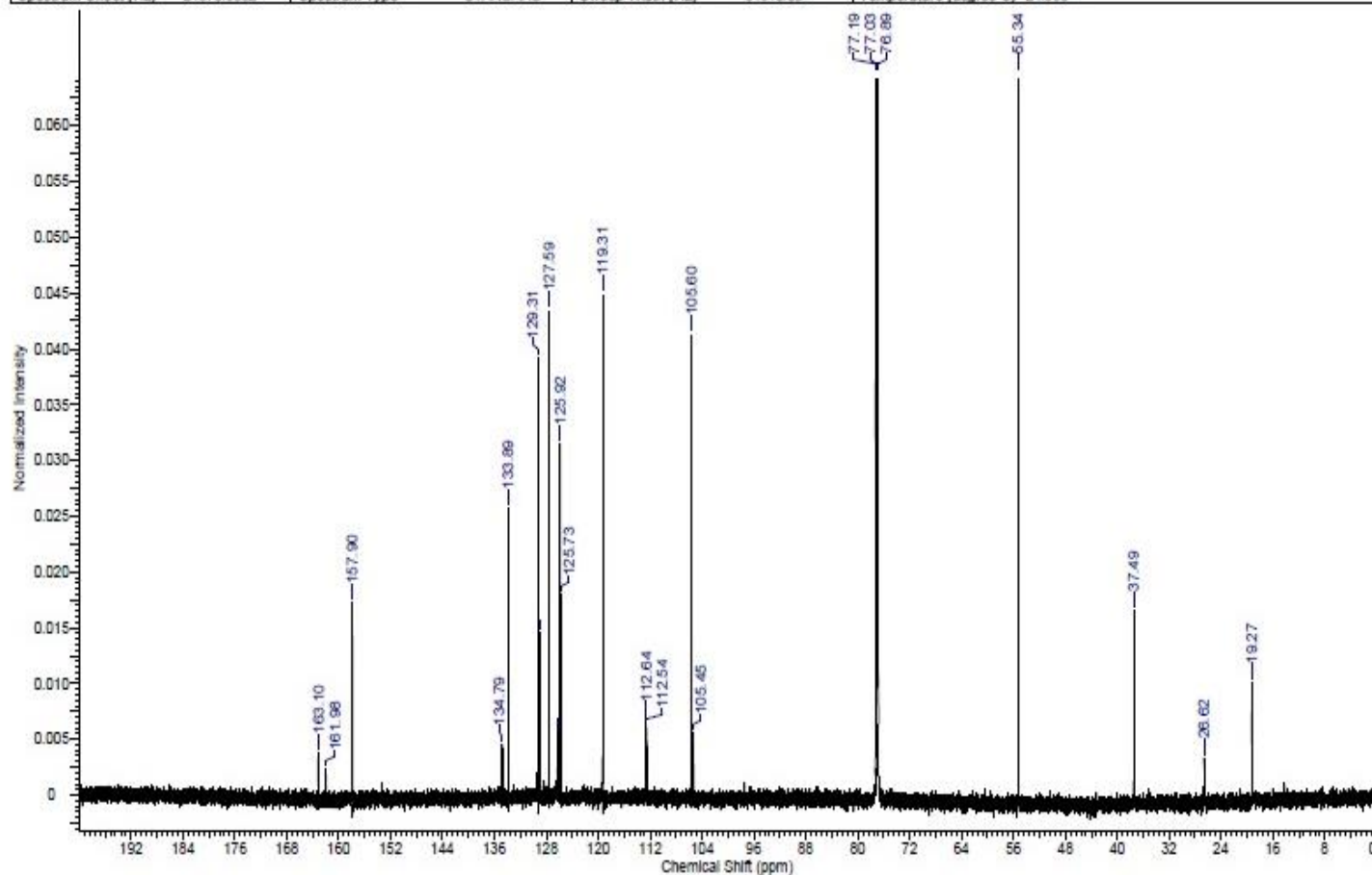
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|------------------------|----------------------|-------------------|----------------------------------|------------------------|---|
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| Date Stamp | 28 Mar 2021 14:12:00 | | | File Name | C:\Users\hp\Desktop\Naproxen NMR\NM1 28-03-2021\21f5d |
| Frequency (MHz) | 213.77 | Nucleus | ^{13}C | Number of Transients | 1024 |
| Original Points Count | 32768 | Owner | nmr | Points Count | 32768 |
| Receiver Gain | 186.93 | SW(cyclical) (Hz) | 51020.41 | Solvent | CHLOROFORM-d |
| Spectrum Offset (Hz) | 21376.0332 | Spectrum Type | STANDARD | Sweep Width (Hz) | 51018.85 |
| | | | | Temperature (degree C) | 25.000 |



Compound 9

4/28/2021 10:44:41 PM

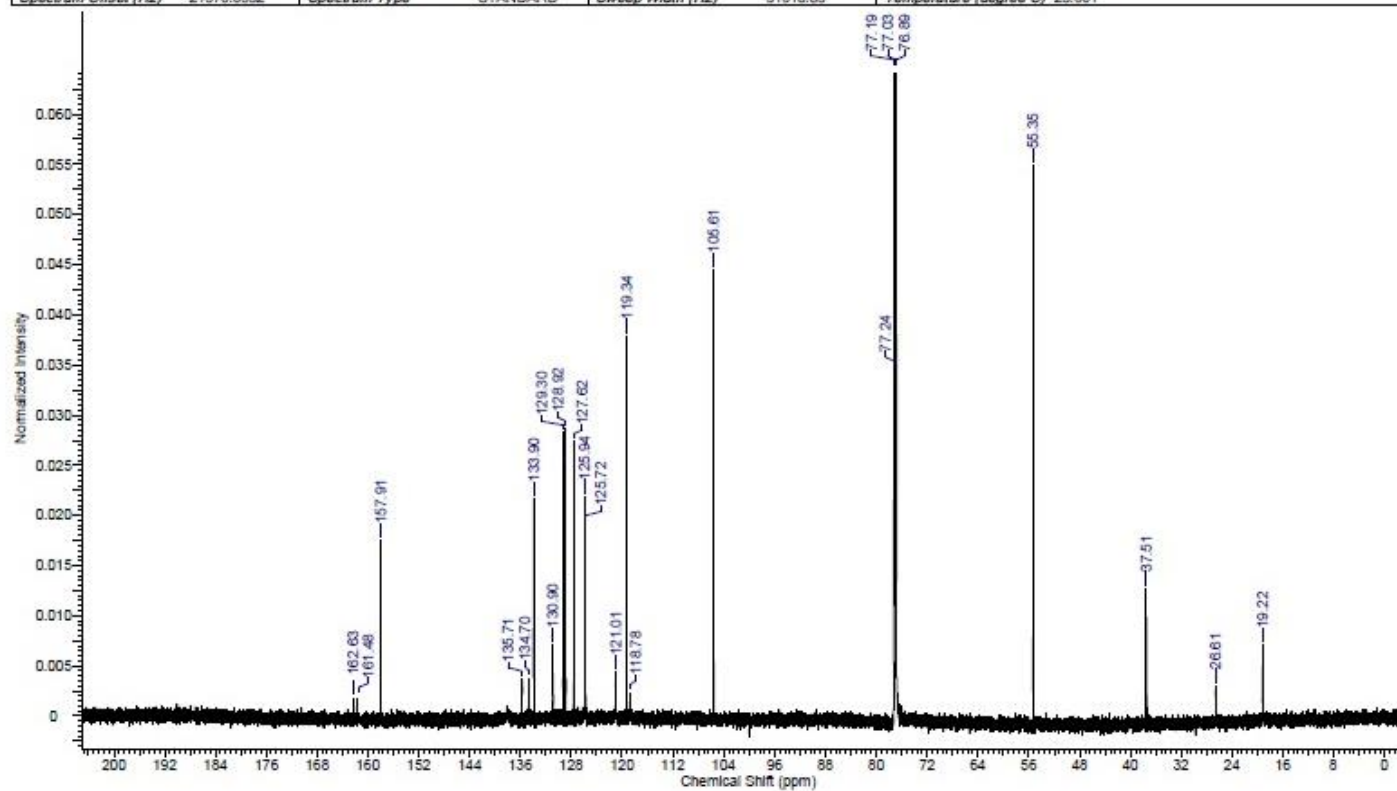
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| Acquisition Time (sec) | 0.6423 | Comment | Dr. Abdusattir Sampe 20-03 CDCL3 | Date | 28 Mar 2021 16:52:00 |
| Date Stamp | 28 Mar 2021 16:52:00 | | File Name | C:\Users\hpl\Desktop\Naproxen NMR\NM4 | 28-03-2021\51\6d |
| Frequency (MHz) | 213.77 | Nucleus | ¹³ C | Number of Transients | 1024 |
| Original Points Count | 32768 | Owner | nmr | Points Count | 32768 |
| Receiver Gain | 186.93 | SW(cyclical) (Hz) | 51020.41 | Solvent | CHLOROFORM-d |
| Spectrum Offset (Hz) | 21376.0332 | Spectrum Type | STANDARD | Sweep Width (Hz) | 51018.85 |
| | | | | Temperature (degree C) | 24.999 |



Compound 10

4/28/2021 10:39:20 PM

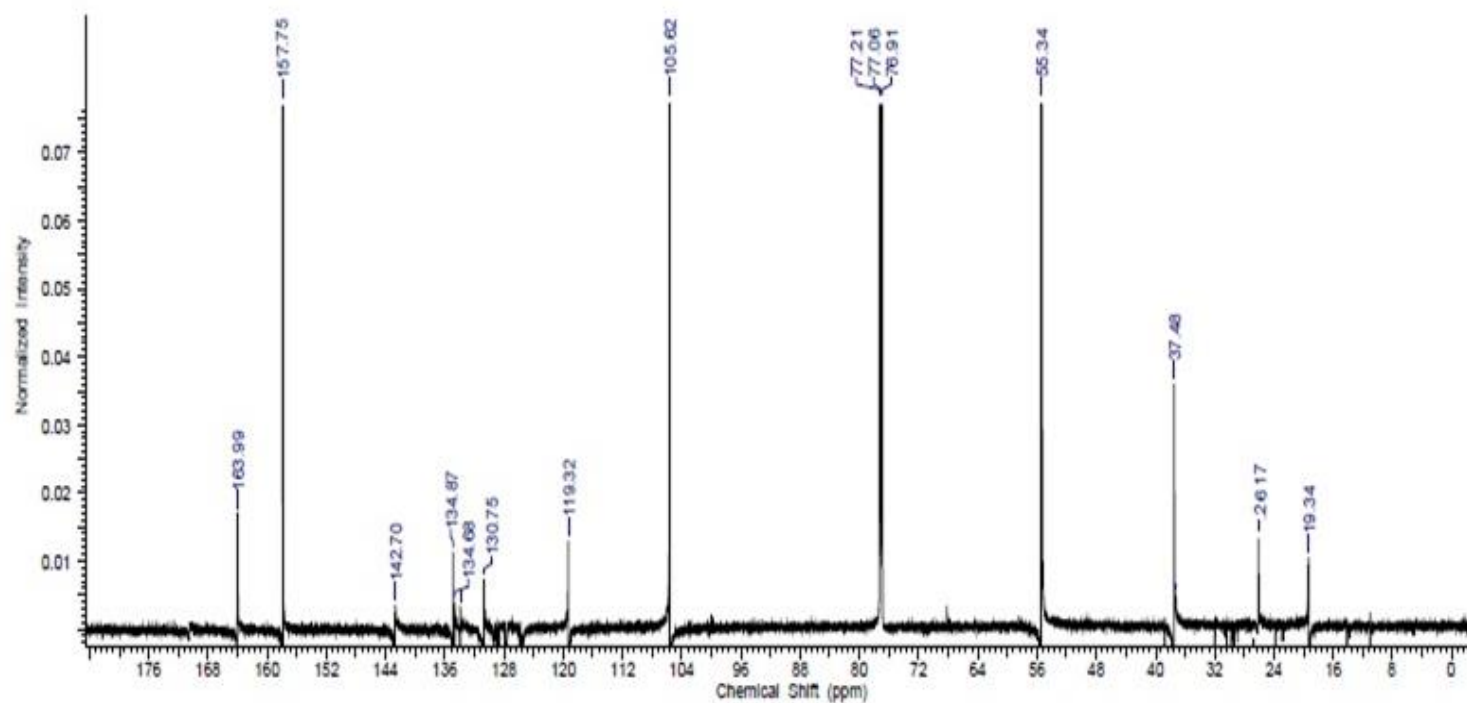
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|------------------------|----------------------|-------------------|----------------------------------|------------------------|---|
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| Date Stamp | 28 Mar 2021 19:32:00 | | | File Name | C:\Users\shp\Desktop\Naproxen NMR\NM7 28-03-2021\81.fid |
| Frequency (MHz) | 213.77 | Nucleus | ¹³ C | Number of Transients | 1024 |
| Original Points Count | 32768 | Owner | nmr | Points Count | 32768 |
| Receiver Gain | 186.93 | SW(cyclical) (Hz) | 51020.41 | Solvent | CHLOROFORM-d |
| Spectrum Offset (Hz) | 21376.0332 | Spectrum Type | STANDARD | Sweep Width (Hz) | 51018.85 |
| | | | | Temperature (degree C) | 25.001 |



Compound 11

3/30/2021 2:05:53 AM

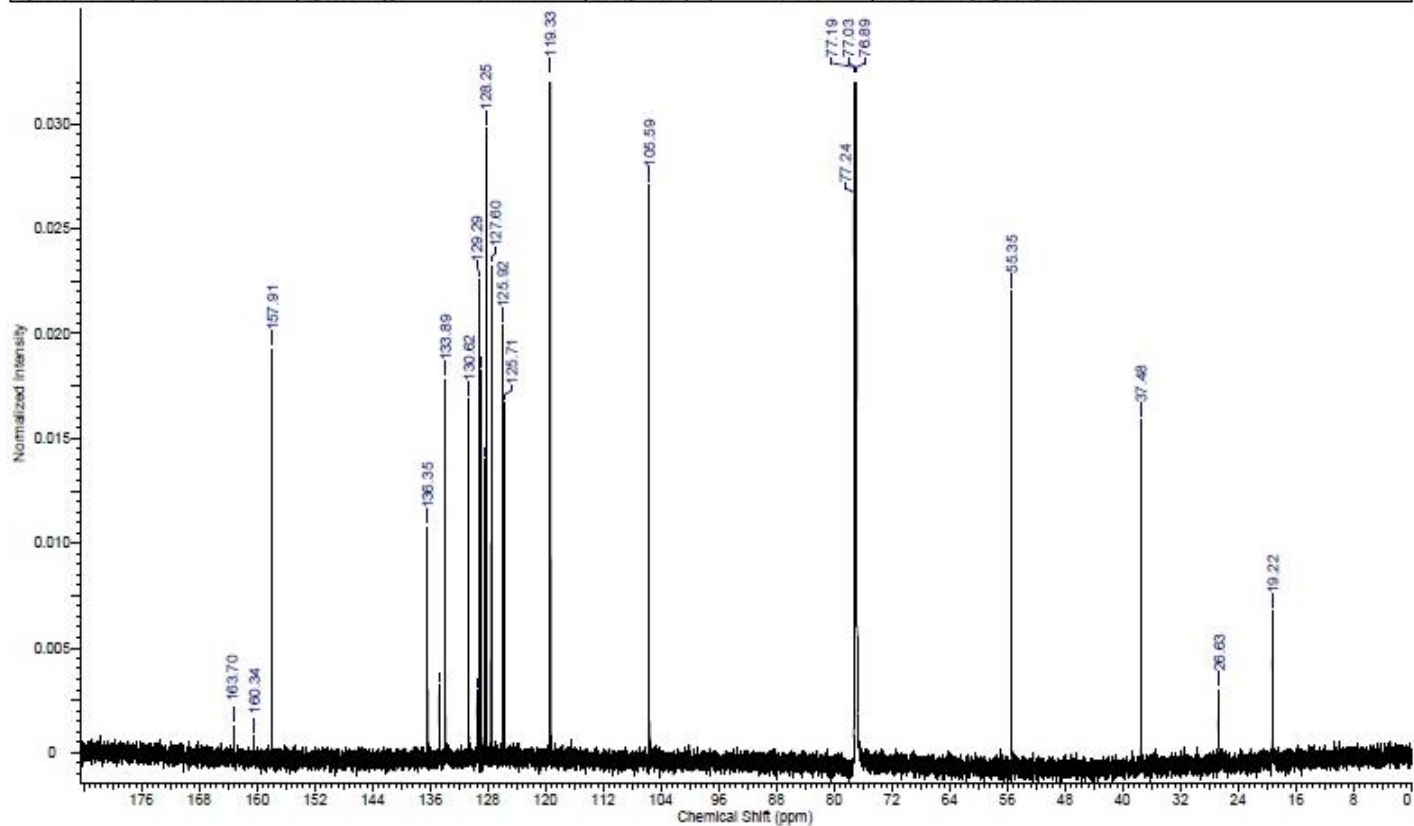
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| Date Stamp | 28 Mar 2021 21:18:40 | File Name | C:\Users\hpl\Desktop\Naproxen NMR\NM9_28-03-2021\1102.fid | | |
| Frequency (MHz) | 213.77 | Nucleus | ¹³ C | Number of Transients | 1024 |
| Original Points Count | 32768 | Owner | nmr | Points Count | 32768 |
| Receiver Gain | 186.93 | SW (cycles) | 51020.41 | Pulse Sequence | zgpg30 |
| Spectrum Offset (Hz) | 21376.0332 | Solvent | CHLOROFORM-d | | |
| | | Spectrum Type | STANDARD | Sweep Width (Hz) | 51018.85 |
| | | | | Temperature (degree C) | 24.999 |



Compound 12

4/28/2021 10:49:36 PM

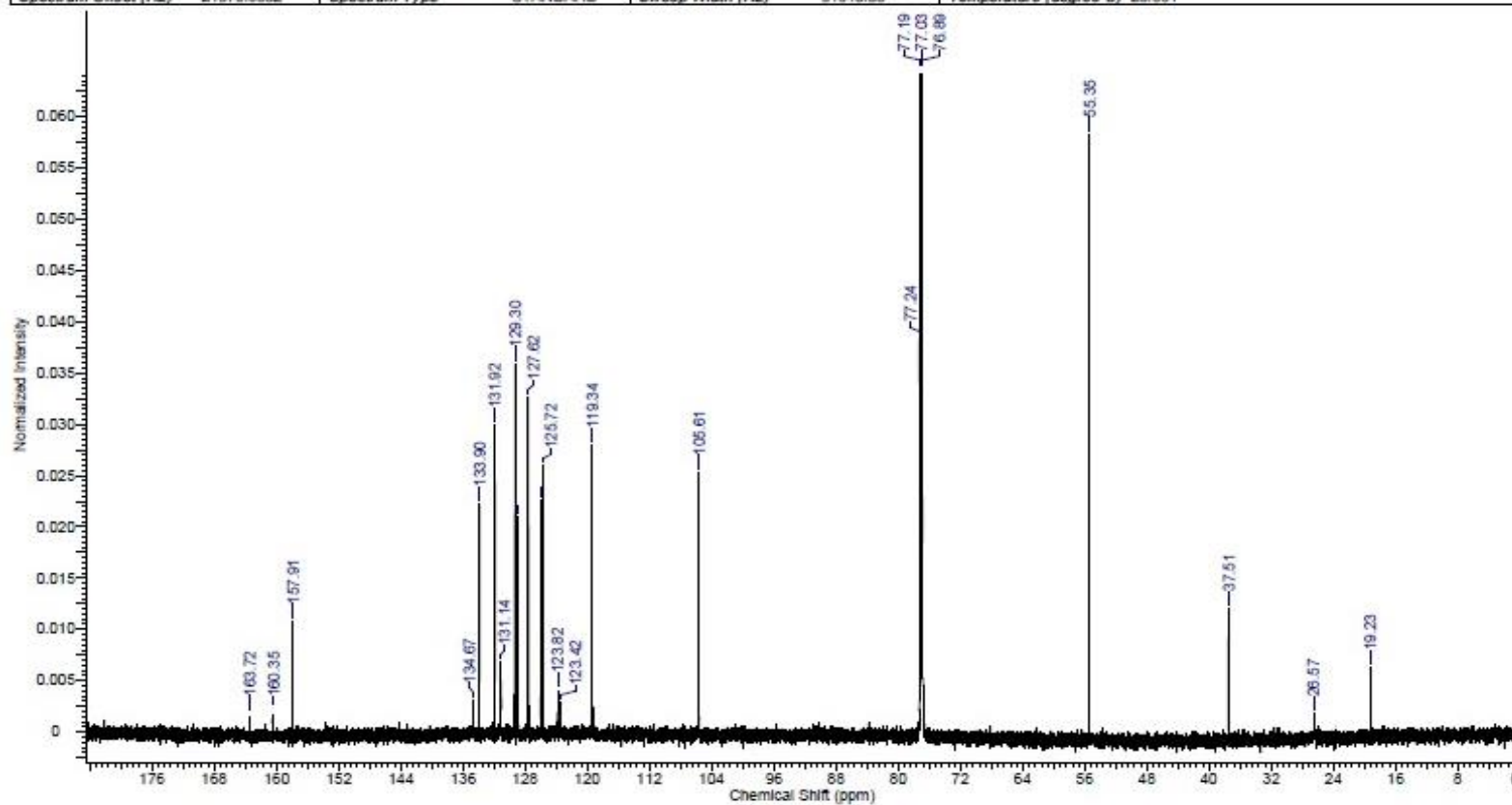
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| Date Stamp | 28 Mar 2021 15:07:28 | File Name | C:\Users\hp\Desktop\Naproxen NMR\NM2 28-03-2021\31fid | | |
| Frequency (MHz) | 213.77 | Nucleus | ¹³ C | Number of Transients | 1024 |
| Original Points Count | 32768 | Owner | nmr | Points Count | 32768 |
| Receiver Gain | 186.93 | SW(cyclical) (Hz) | 51020.41 | Solvent | CHLOROFORM-d |
| Spectrum Offset (Hz) | 21376.0332 | Spectrum Type | STANDARD | Sweep Width (Hz) | 51018.85 |
| | | | | Temperature (degree C) | 25.000 |



Compound 13

4/28/2021 10:53:28 PM

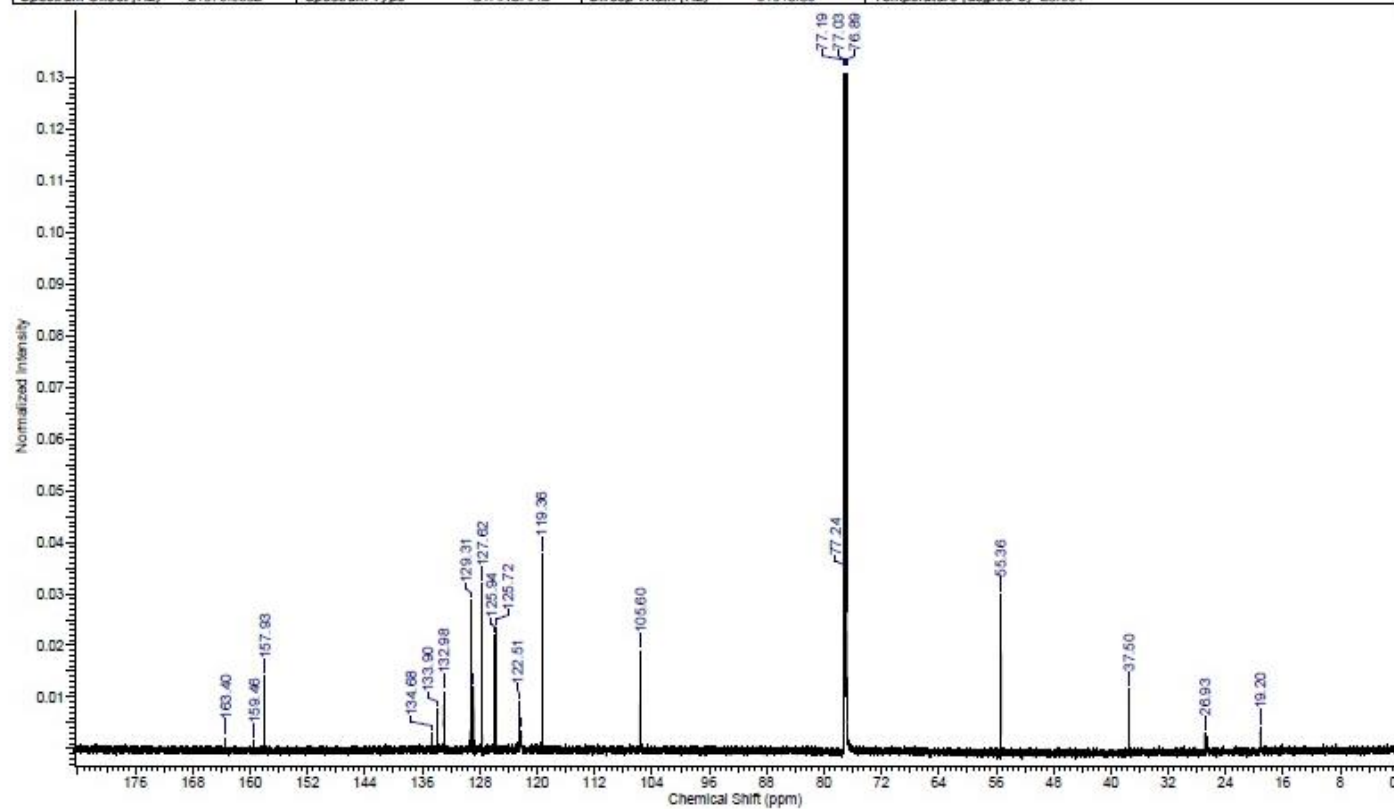
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| Date Stamp | 28 Mar 2021 20:25:20 | File Name | C:\Users\hnp\Desktop\Naproxen NMR\NM8 | 28-03-2021\92fid | |
| Frequency (MHz) | 213.77 | Nucleus | ¹³ C | Number of Transients | 1024 |
| Original Points Count | 32768 | Owner | nmr | Points Count | 32768 |
| Receiver Gain | 186.93 | SW(cyclical) (Hz) | 51020.41 | Pulse Sequence | zgpg30 |
| Spectrum Offset (Hz) | 21376.0332 | Solvent | CHLOROFORM-d | Temperature (degree C) | 25.001 |
| Spectrum Type | STANDARD | Sweep Width (Hz) | 51018.85 | | |



Compound 14

4/28/2021 11:01:03 PM

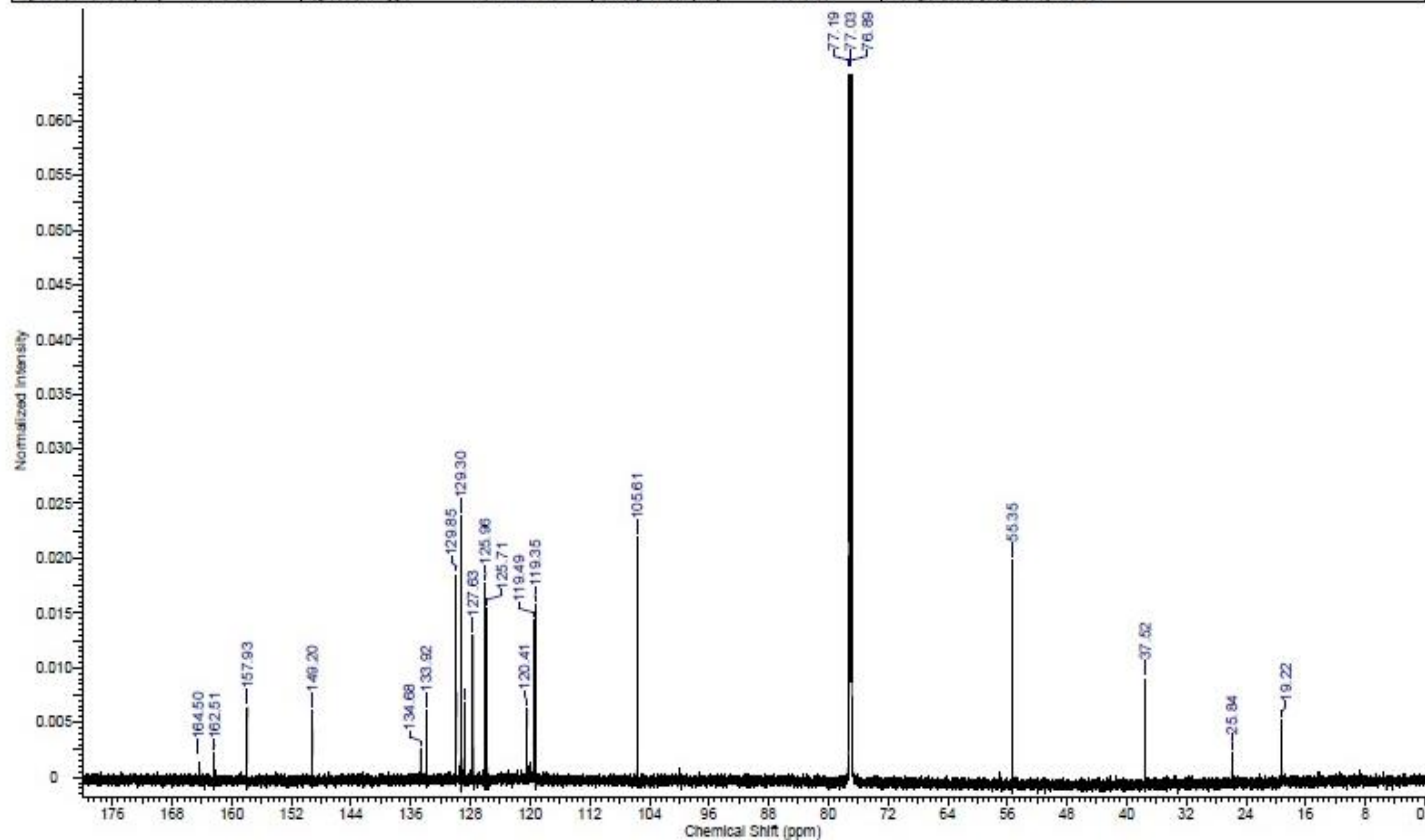
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| Date Stamp | 28 Mar 2021 17:45:20 | | File Name | C:\Users\hp\Desktop\Naproxen NMR\NM5 28-03-2021\61.fid | | | |
| Frequency (MHz) | 213.77 | Nucleus | ¹³ C | Number of Transients | 1024 | Origin | spect |
| Original Points Count | 32768 | Owner | nmr | Points Count | 32768 | Pulse Sequence | zgpg30 |
| Receiver Gain | 186.93 | SW(cyclical) (Hz) | 51020.41 | Solvent | CHLOROFORM-d | | |
| Spectrum Offset (Hz) | 21376.0332 | Spectrum Type | STANDARD | Sweep Width (Hz) | 51018.85 | Temperature (degree C) | 25.001 |



Compound 15

4/28/2021 11:05:23 PM

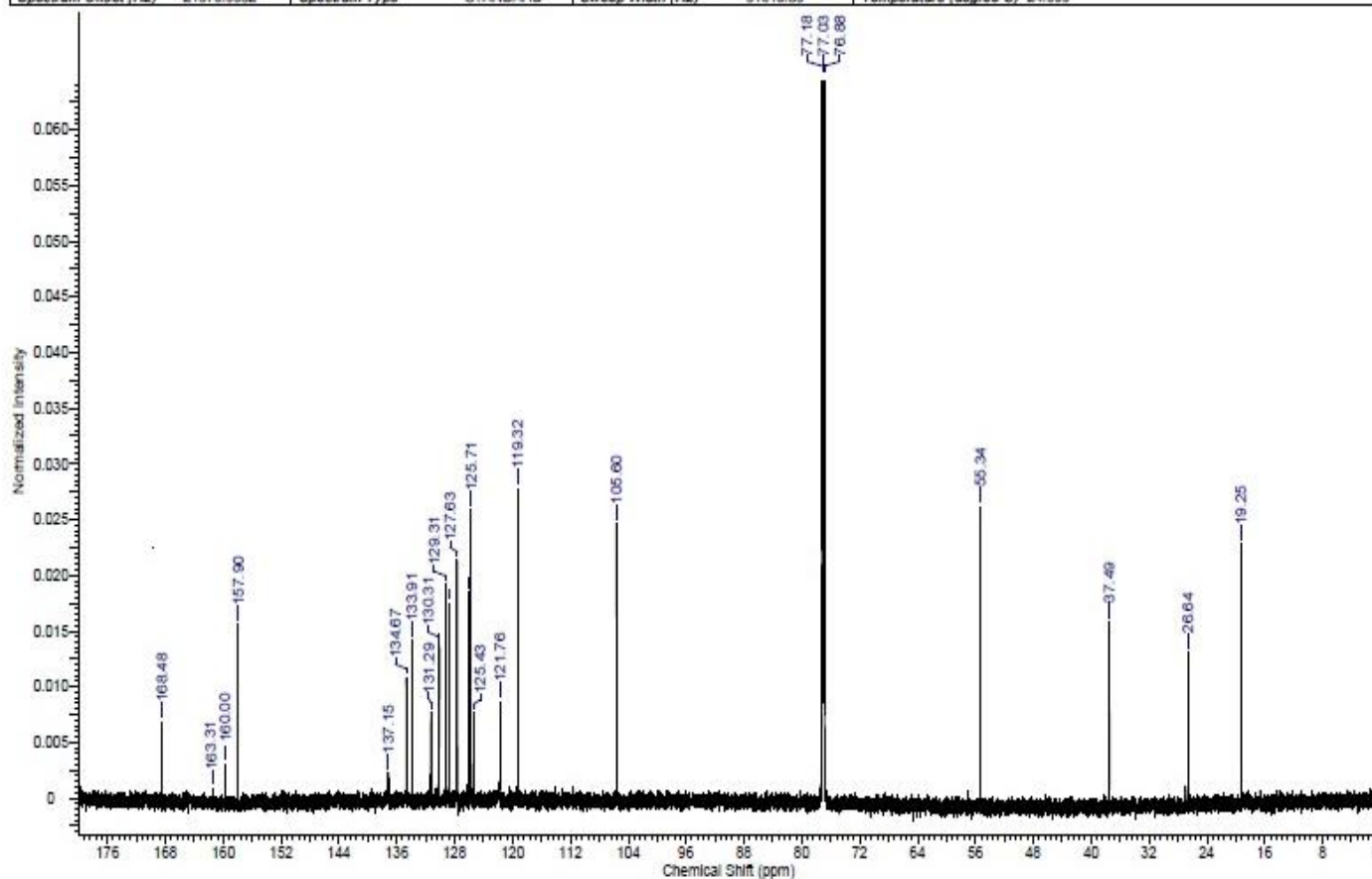
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| Date Stamp | 28 Mar 2021 18:15:12 | File Name | C:\Users\hpl\Desktop\Naproxen NMR\NM6 | 28-03-2021\71.fid | |
| Frequency (MHz) | 213.77 | Nucleus | 13C | Number of Transients | 1024 |
| Original Points Count | 32768 | Owner | nmr | Points Count | 32768 |
| Receiver Gain | 186.93 | SW(cyclical) (Hz) | 51020.41 | Solvent | CHLOROFORM-d |
| Spectrum Offset (Hz) | 21376.0332 | Spectrum Type | STANDARD | Sweep Width (Hz) | 51018.85 |
| | | | | Temperature (degree C) | 25.001 |



Compound 16

4/28/2021 11:11:25 PM

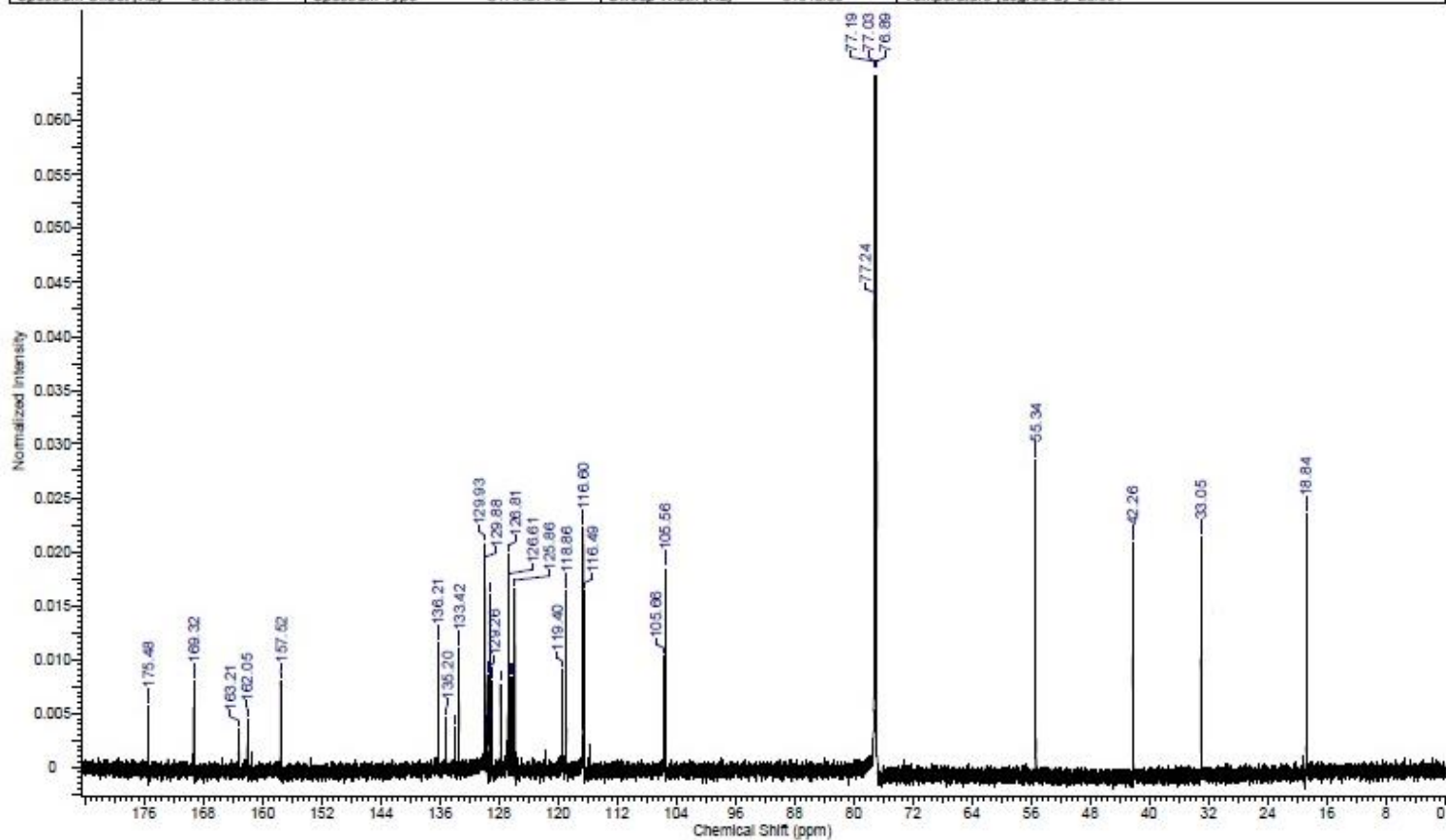
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| Frequency (MHz) | 213.77 | Nucleus | ¹³ C | Number of Transients | 1024 |
| Original Points Count | 32768 | Owner | nmr | Points Count | 32768 |
| Receiver Gain | 186.93 | SW(cyclical) (Hz) | 51020.41 | Solvent | CHLOROFORM-d |
| Spectrum Offset (Hz) | 21376.0332 | Spectrum Type | STANDARD | Sweep Width (Hz) | 51018.85 |
| | | | | Temperature (degree C) | 24.999 |



Compound 19

4/28/2021 11:25:19 PM

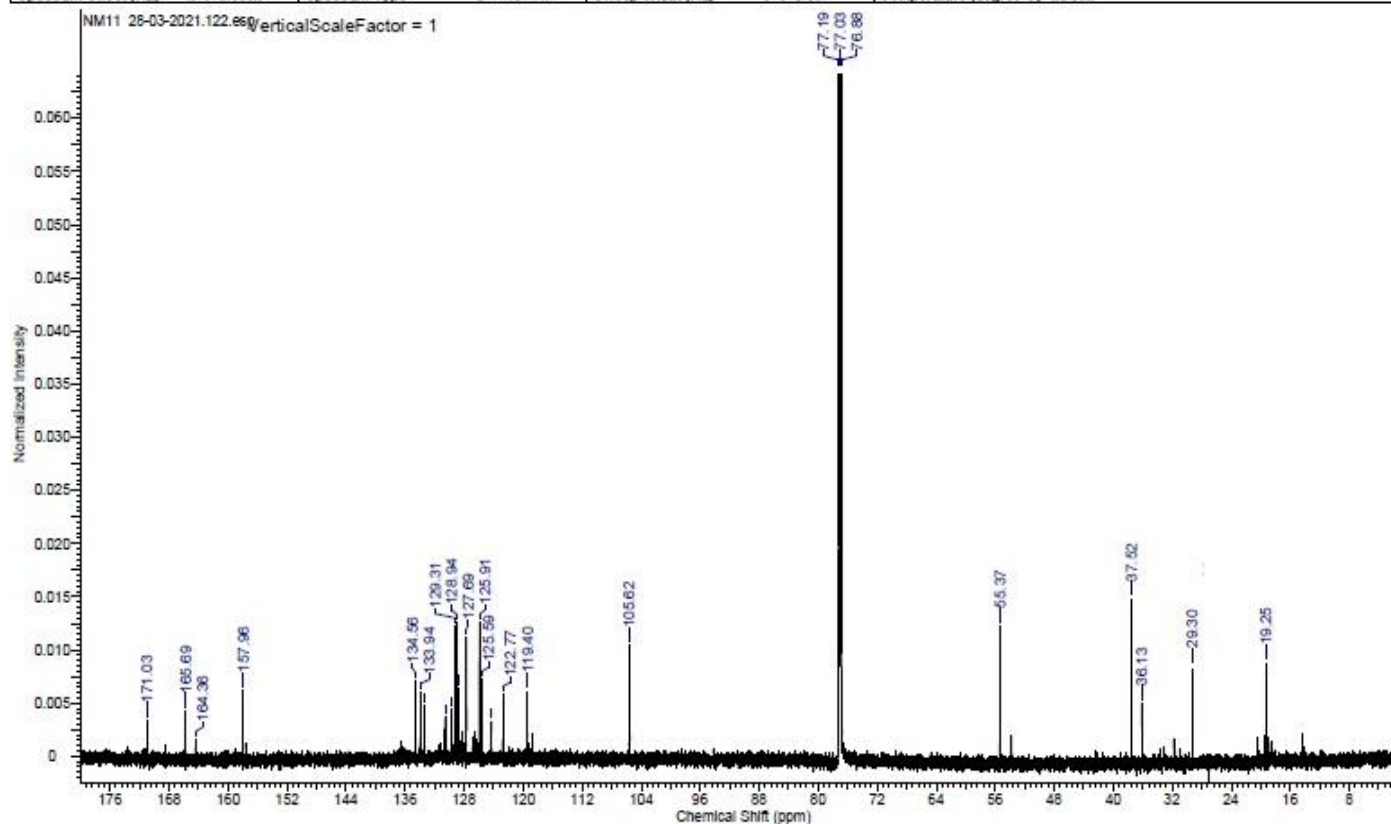
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|------------------------|----------------------|-------------------|---|------------------------|----------------------|
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| Date Stamp | 28 Mar 2021 22:12:00 | File Name | C:\Users\hpi\Desktop\Naproxen NMR\NM10 26-03-2021\112.fid | | |
| Frequency (MHz) | 213.77 | Nucleus | 13C | Number of Transients | 1024 |
| Original Points Count | 32768 | Owner | nmr | Points Count | 32768 |
| Receiver Gain | 186.93 | SW(cyclical) (Hz) | 51020.41 | Solvent | CHLOROFORM-d |
| Spectrum Offset (Hz) | 21376.0332 | Spectrum Type | STANDARD | Sweep Width (Hz) | 51018.85 |
| | | | | Temperature (degree C) | 25.001 |



Compound 20

4/28/2021 11:30:24 PM

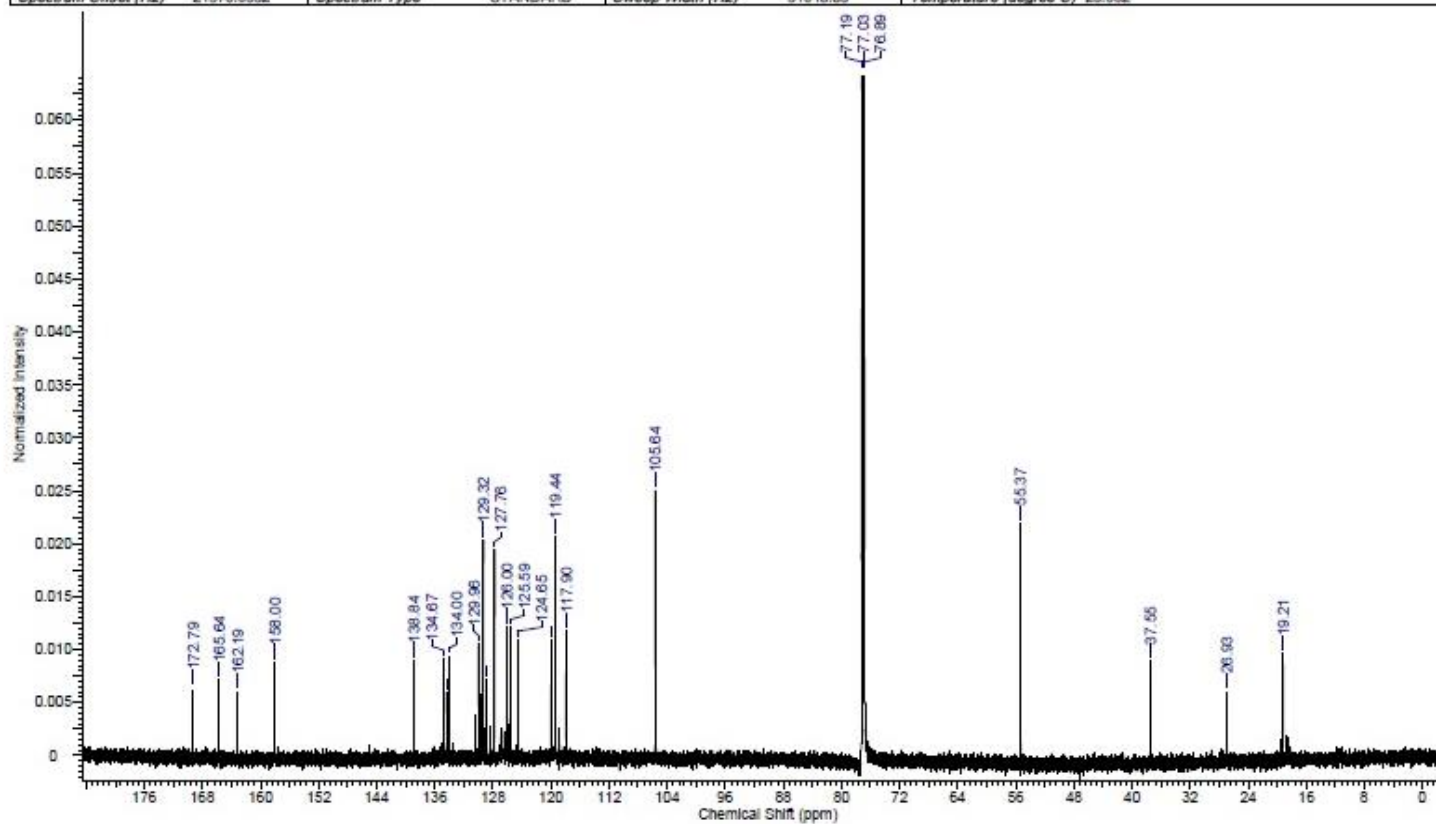
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|------------------------|----------------------|-------------------|-----------------------------------|--|----------------------|
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| Date Stamp | 28 Mar 2021 23:03:12 | | File Name | C:\Users\hp\Desktop\Naproxen NMR\NM11 28-03-2021\122\fid | |
| Frequency (MHz) | 213.77 | Nucleus | ¹³ C | Number of Transients | 1024 |
| Original Points Count | 32768 | Owner | nmr | Points Count | 32768 |
| Receiver Gain | 186.93 | SW(cyclical) (Hz) | 51020.41 | Solvent | CHLOROFORM-d |
| Spectrum Offset (Hz) | 21376.0332 | Spectrum Type | STANDARD | Sweep Width (Hz) | 51018.85 |
| | | | | Temperature (degree C) | 25.002 |



Compound 21

4/28/2021 11:34:12 PM

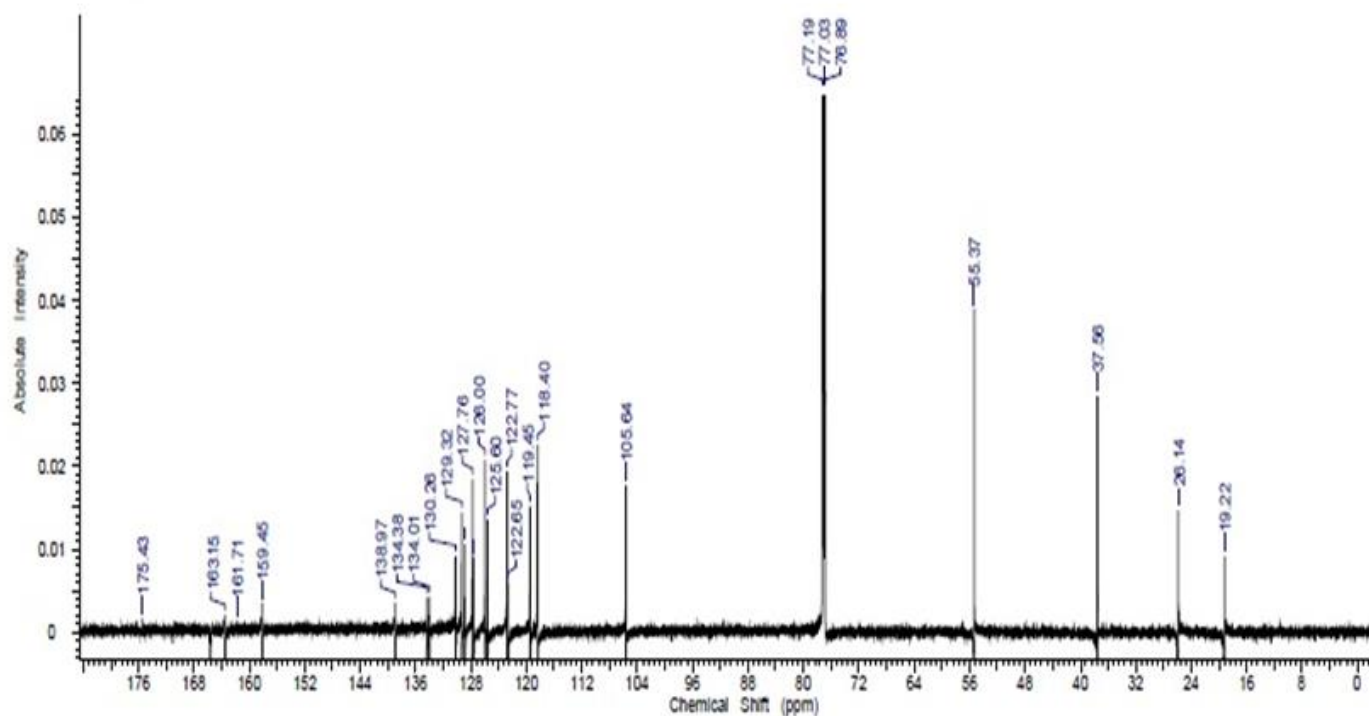
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|------------------------|----------------------|--------------------|------------------------------------|--|----------------------|
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| Frequency (MHz) | 213.77 | Nucleus | ¹³ C | Number of Transients | 1024 |
| Original Points Count | 32768 | Owner | nmr | Points Count | 32768 |
| Receiver Gain | 186.93 | SW (cyclical) (Hz) | 51020.41 | Solvent | CHLOROFORM-d |
| Spectrum Offset (Hz) | 21376.0332 | Spectrum Type | STANDARD | Sweep Width (Hz) | 51018.85 |
| | | | | Temperature (degree C) | 25.002 |



Compound 22

3/31/2021 12:42:44 AM

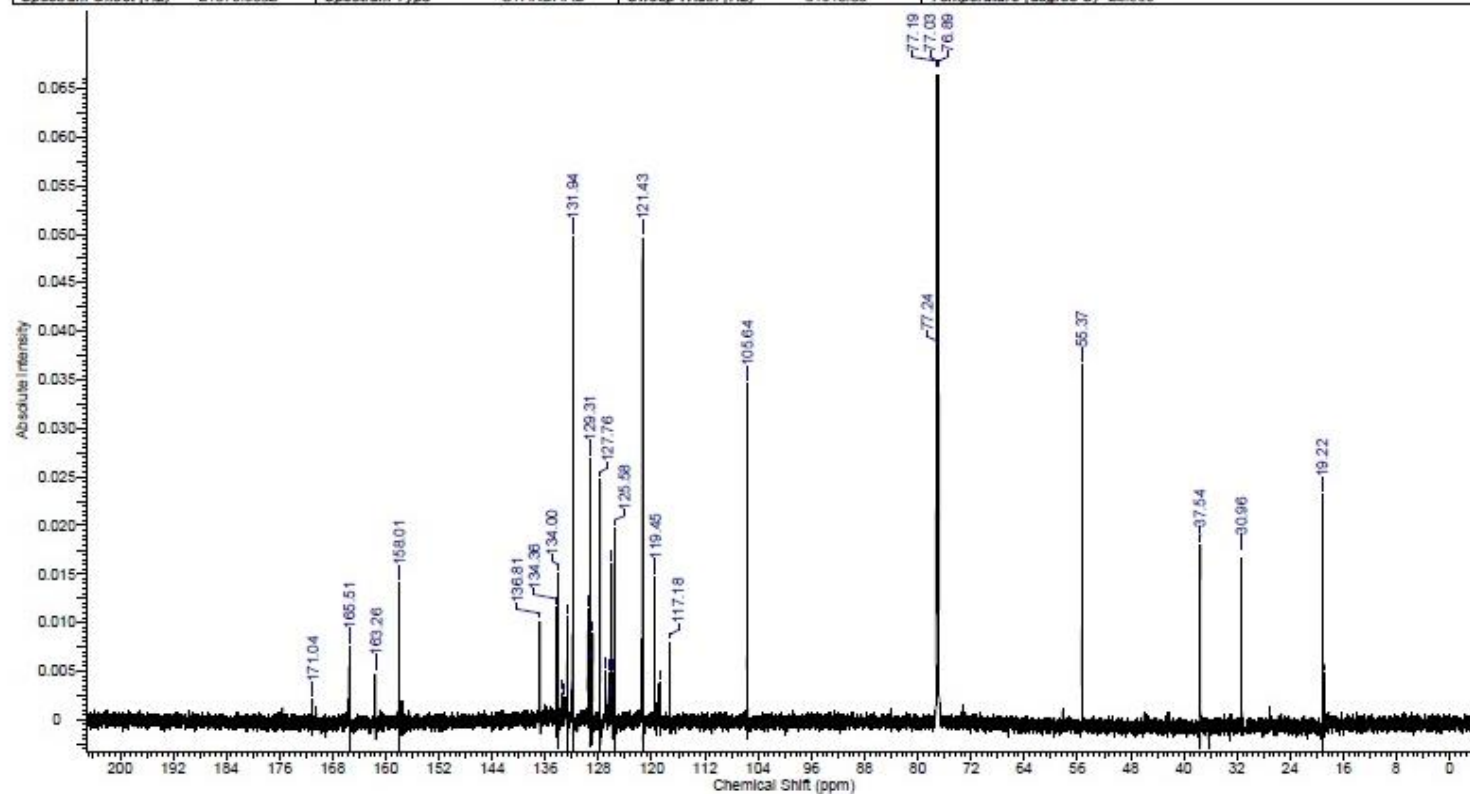
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|------------------------|----------------------|-------------------|-----------------------------------|--|----------------------|
| Acquisition Time (sec) | 0.6423 | Comment | Dr. Abdusattar Sample 29-03 CDCL3 | Date | 29 Mar 2021 00:49:52 |
| Date Stamp | 29 Mar 2021 00:49:52 | | File Name | C:\Users\hpi\Desktop\Naproxen NMR\NM13 28-03-2021\1141.fid | |
| Frequency (MHz) | 213.77 | Nucleus | ¹³ C | Number of Transients | 1024 |
| Original Points Count | 32768 | Owner | nmr | Points Count | 32768 |
| Receiver Gain | 186.93 | SW(cyclical) (Hz) | 51020.41 | Solvent | CHLOROFORM-d |
| Spectrum Offset (Hz) | 21376.0332 | Spectrum Type | STANDARD | Sweep Width (Hz) | 51018.85 |
| | | | | Temperature (degree C) | 25.000 |



Compound 23

4/16/2021 6:03:48 PM

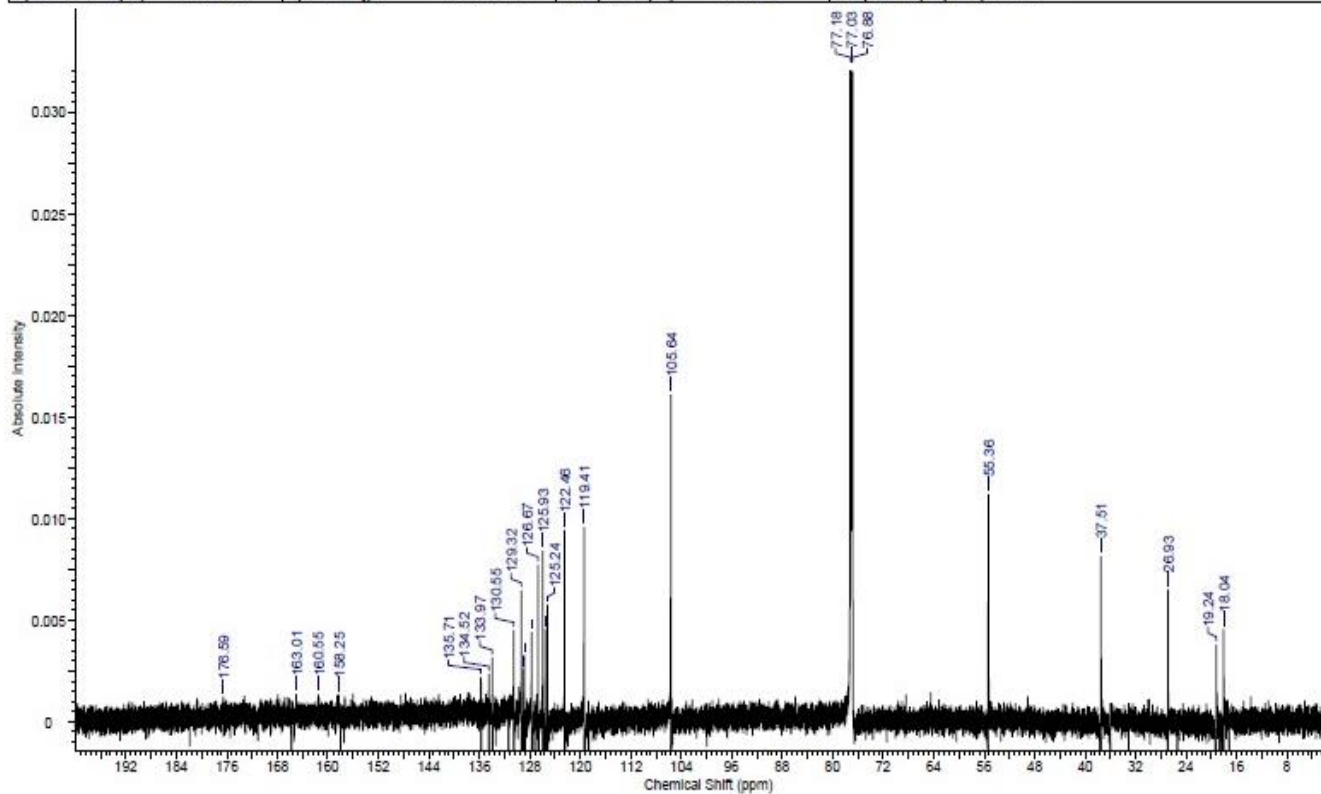
| | | | | | |
|--------------------------|----------------------|-------------------|---|------------------------|----------------------|
| RMS of Noise 507469.5313 | | | | | |
| Acquisition Time (sec) | 0.6423 | Comment | Dr. Abdussattar Sampe 33-03 CDCL3 | Date | 29 Mar 2021 04:21:04 |
| Date Stamp | 29 Mar 2021 04:21:04 | File Name | C:\Users\thp\Desktop\Naproxen NMR\ NM17 28-03-2021\181fid | | |
| Frequency (MHz) | 213.77 | Nucleus | ¹³ C | Number of Transients | 1024 |
| Original Points Count | 32768 | Owner | nmr | Points Count | 32768 |
| Receiver Gain | 186.93 | SW(cyclical) (Hz) | 51020.41 | Solvent | CHLOROFORM-d |
| Spectrum Offset (Hz) | 21376.0332 | Spectrum Type | STANDARD | Sweep Width (Hz) | 51018.85 |
| | | | | Temperature (degree C) | 25.000 |



Compound 24

4/17/2021 2:16:28 AM

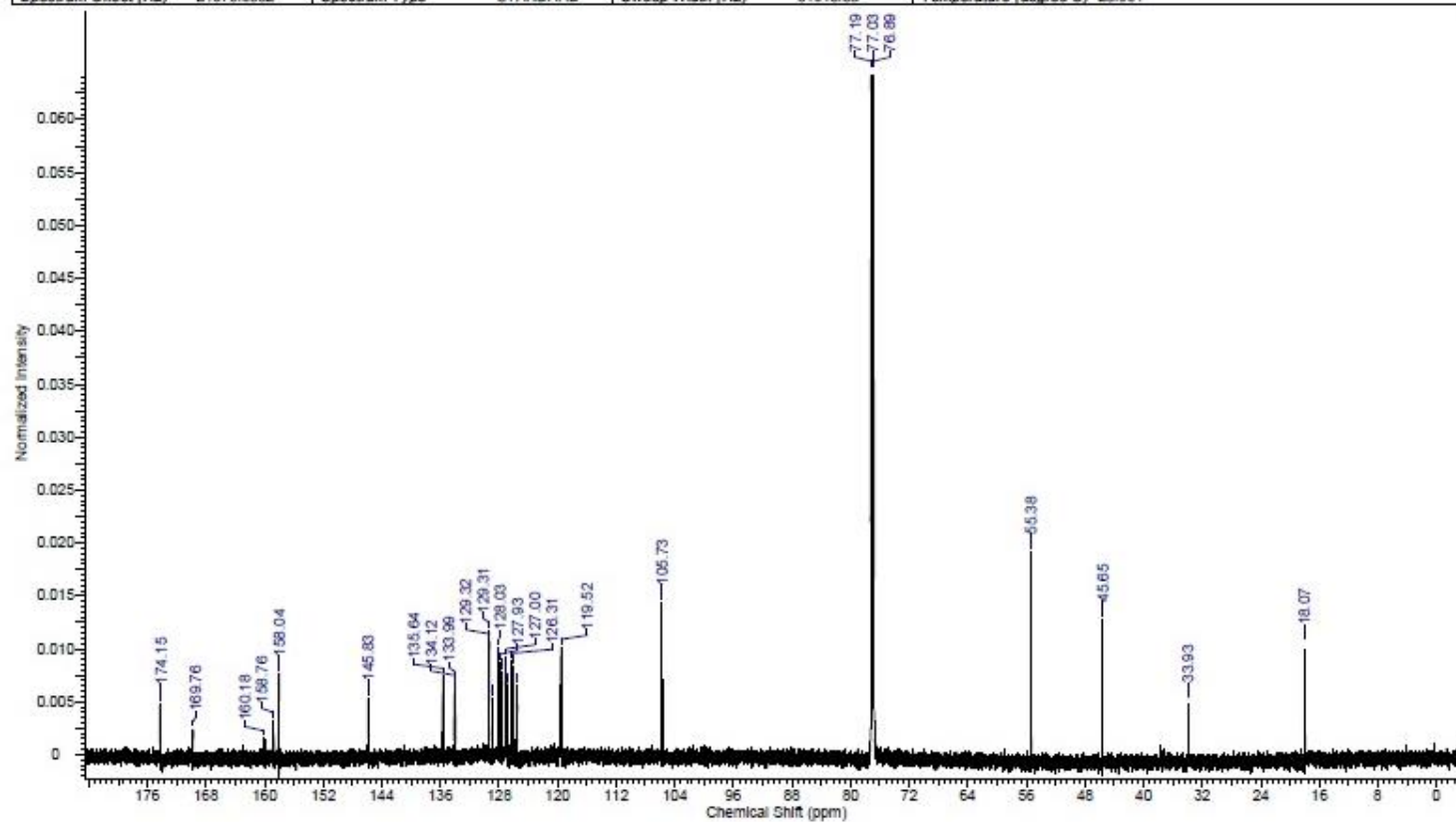
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|------------------------|----------------------|------------------|----------------------------------|---|----------------------|
| Acquisition Time (sec) | 0.6423 | Comment | Dr. Abdusattar Sampe 32-03 CDCL3 | Date | 29 Mar 2021 03:27:44 |
| Date Stamp | 29 Mar 2021 03:27:44 | | File Name | C:\Users\hp\Desktop\Naproxen NMR\ NM16 28-03-2021\171.fid | |
| Frequency (MHz) | 213.77 | Nucleus | ¹³ C | Number of Transients | 1024 |
| Original Points Count | 32768 | Owner | nmr | Points Count | 32768 |
| Receiver Gain | 186.93 | SW (cycles) (Hz) | 51020.41 | Solvent | CHLOROFORM-d |
| Spectrum Offset (Hz) | 21376.0332 | Spectrum Type | STANDARD | Sweep Width (Hz) | 51018.85 |
| | | | | Temperature (degree C) | 25.000 |



Compound 25

4/28/2021 11:42:53 PM

| | | | | | |
|------------------------|----------------------|-------------------|--|------------------------|----------------------|
| Acquisition Time (sec) | 0.6423 | Comment | Dr. Abdusattar Sampe 31-03 CDCL3 | Date | 29 Mar 2021 02:36:32 |
| Date Stamp | 29 Mar 2021 02:36:32 | File Name | C:\Users\hpl\Desktop\Naproxen NMR\NM15 | 28-03-2021\161\fid | |
| Frequency (MHz) | 213.77 | Nucleus | 13C | Number of Transients | 1024 |
| Original Points Count | 32768 | Owner | nmr | Points Count | 32768 |
| Receiver Gain | 186.93 | SW(cyclical) (Hz) | 51020.41 | Solvent | CHLOROFORM-d |
| Spectrum Offset (Hz) | 21376.0332 | Spectrum Type | STANDARD | Sweep Width (Hz) | 51018.85 |
| | | | | Temperature (degree C) | 25.001 |



Compound 26

4/17/2021 1:29:47 AM

| | | | | | |
|------------------------|----------------------|--------------------|---|------------------------|----------------------|
| Acquisition Time (sec) | 0.6423 | Comment | Dr. Abdusattar Sampe 30-03 CDCL3 | Date | 29 Mar 2021 01:43:12 |
| Date Stamp | 29 Mar 2021 01:43:12 | File Name | C:\Users\hp\Desktop\Naproxen NMR\NM14 26-03-2021\1511.fid | | |
| Frequency (MHz) | 213.77 | Nucleus | ¹³ C | Number of Transients | 1024 |
| Original Points Count | 32768 | Owner | nmr | Points Count | 32768 |
| Receiver Gain | 186.93 | SW (cyclical) (Hz) | 51020.41 | Pulse Sequence | zgpg30 |
| Spectrum Offset (Hz) | 21376.0332 | Solvent | CHLOROFORM-d | Temperature (degree C) | 25.001 |
| | | Spectrum Type | STANDARD | Sweep Width (Hz) | 51018.85 |

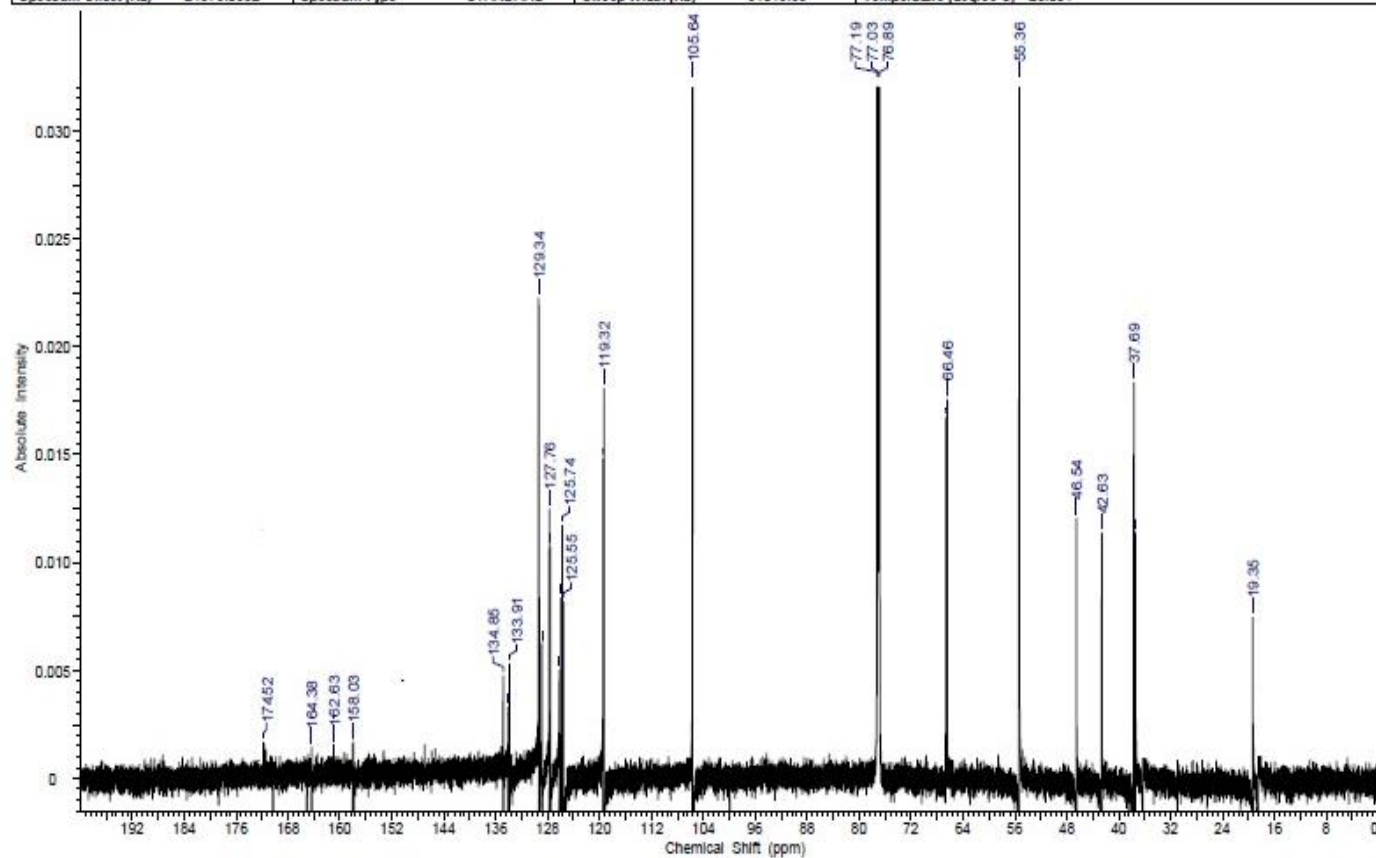
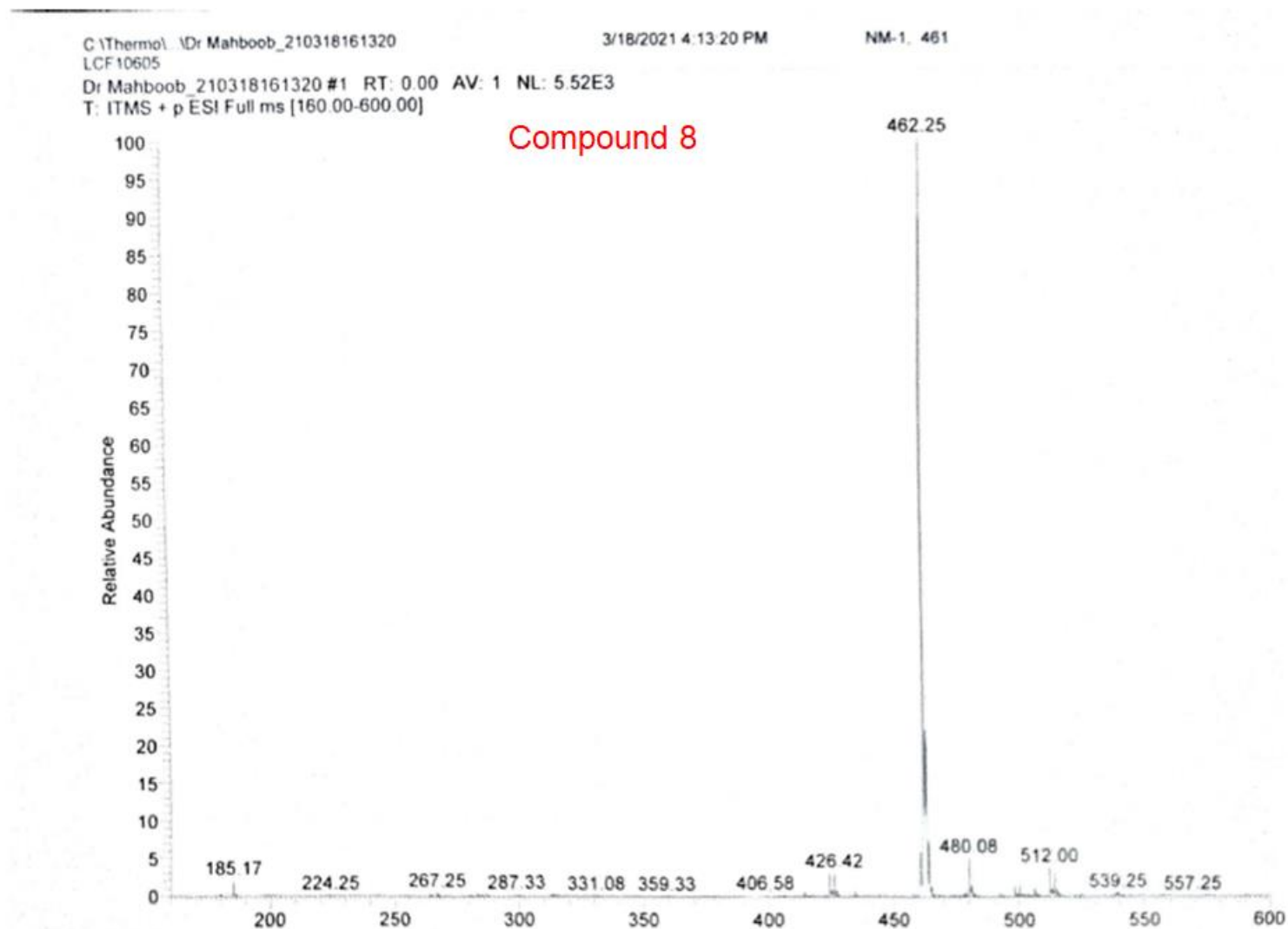
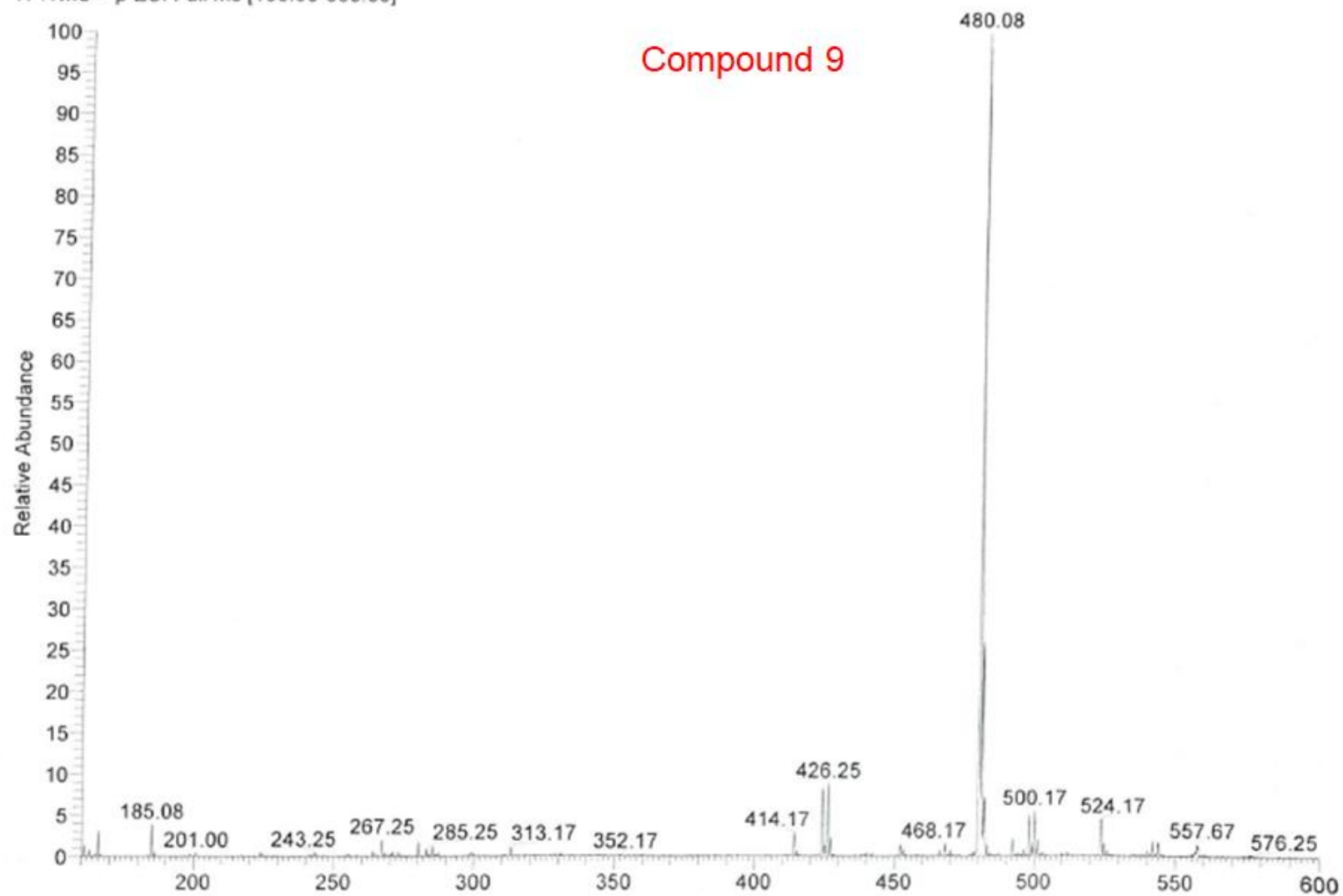


Figure S35-S50:- Mass spectra of compounds





C:\Thermo\...\\Dr Mahboob_210318162611

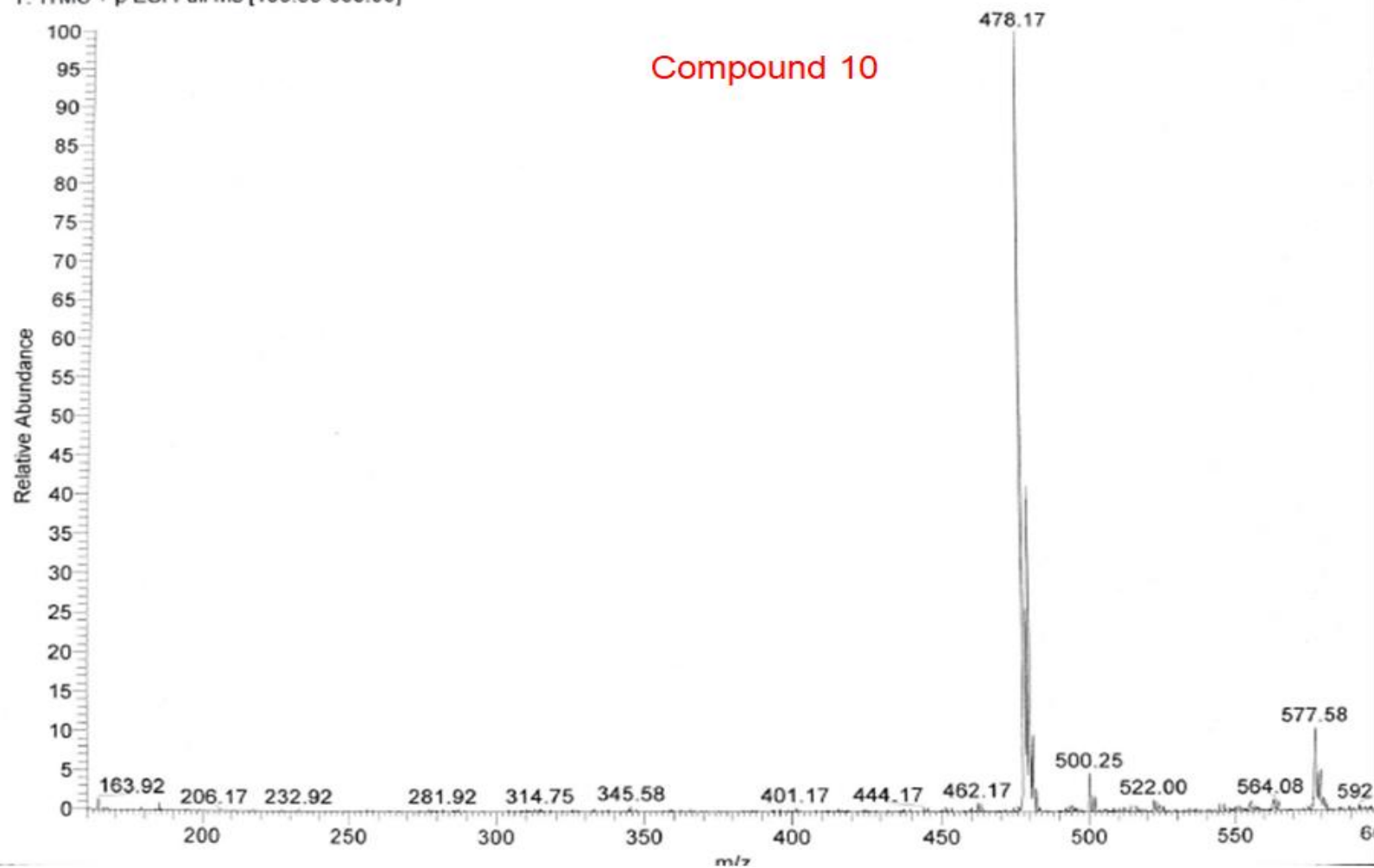
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NM-7, 478

LCF10605

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T: ITMS + p ESI Full ms [160.00-600.00]

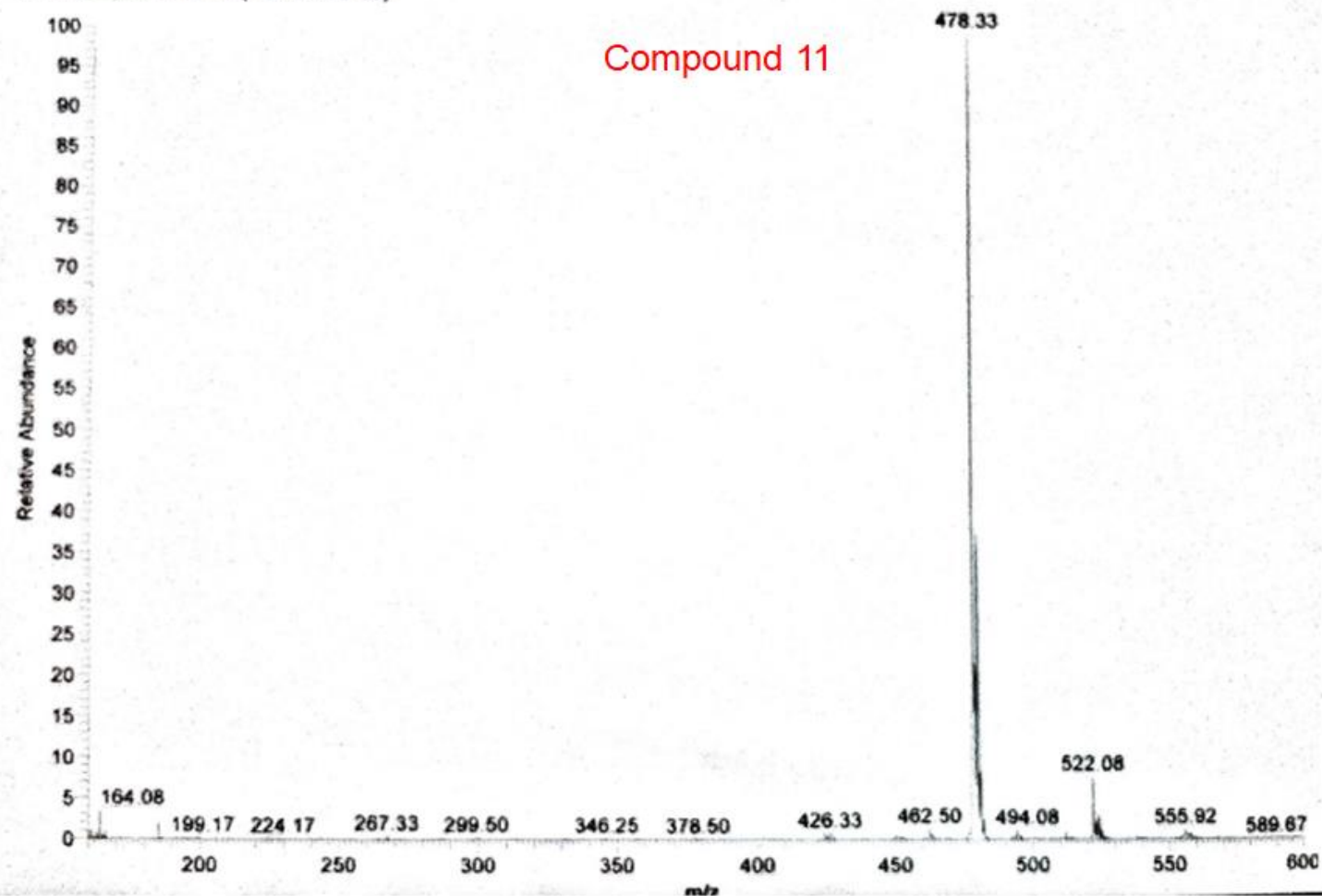


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LCF10805

3/18/2021 4:37:51 PM

NM-9. 478

Dr Mahboob_210318163751 #1 RT: 0.00 AV: 1 NL: 6.11E3
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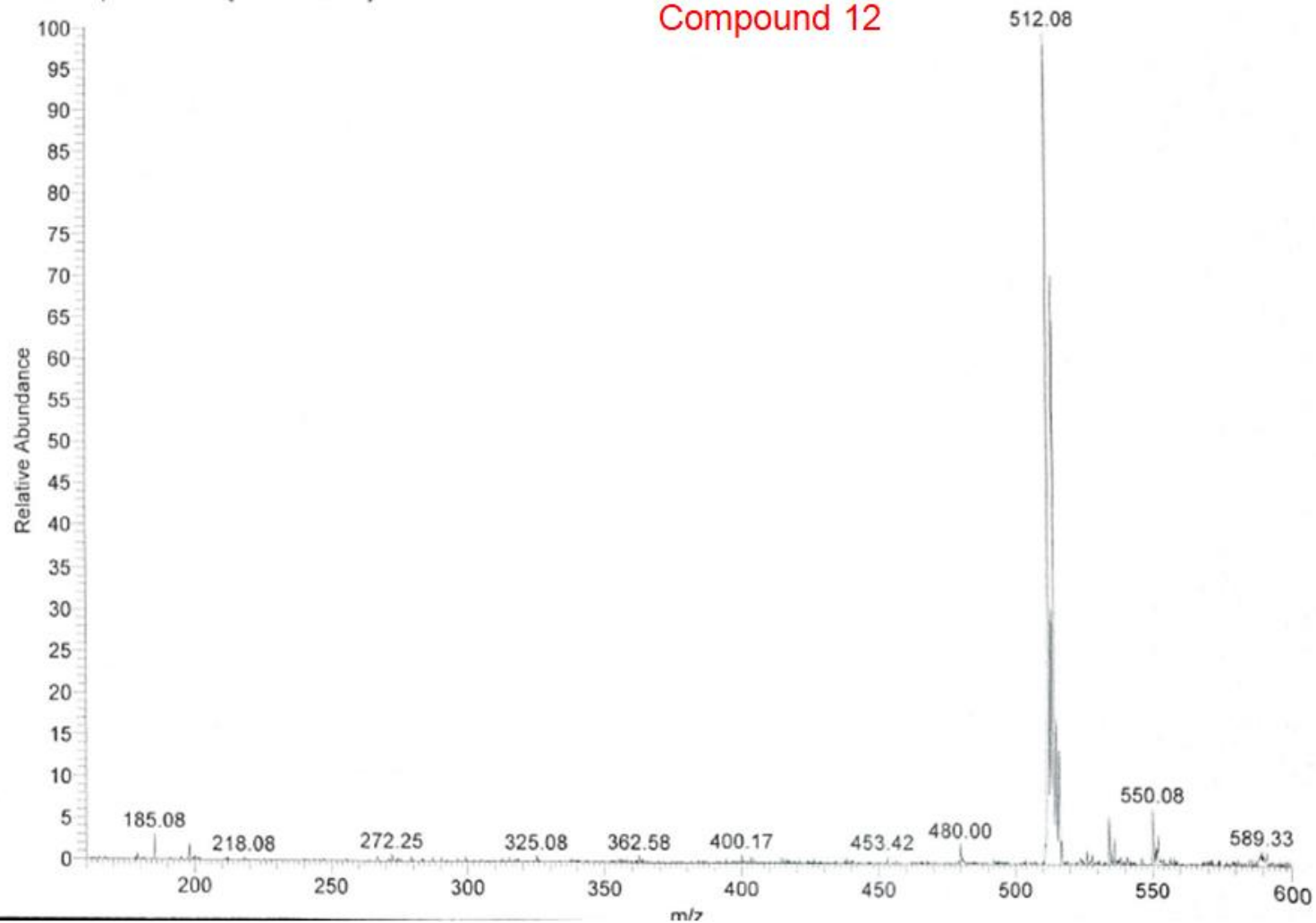
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3/18/2021 4:01:51 PM

NM-2, 512

Dr Mahboob_210318160150 #1 RT: 0.00 AV: 1 NL: 6.13E2
T: ITMS + p ESI Full ms [160.00-600.00]

Compound 12



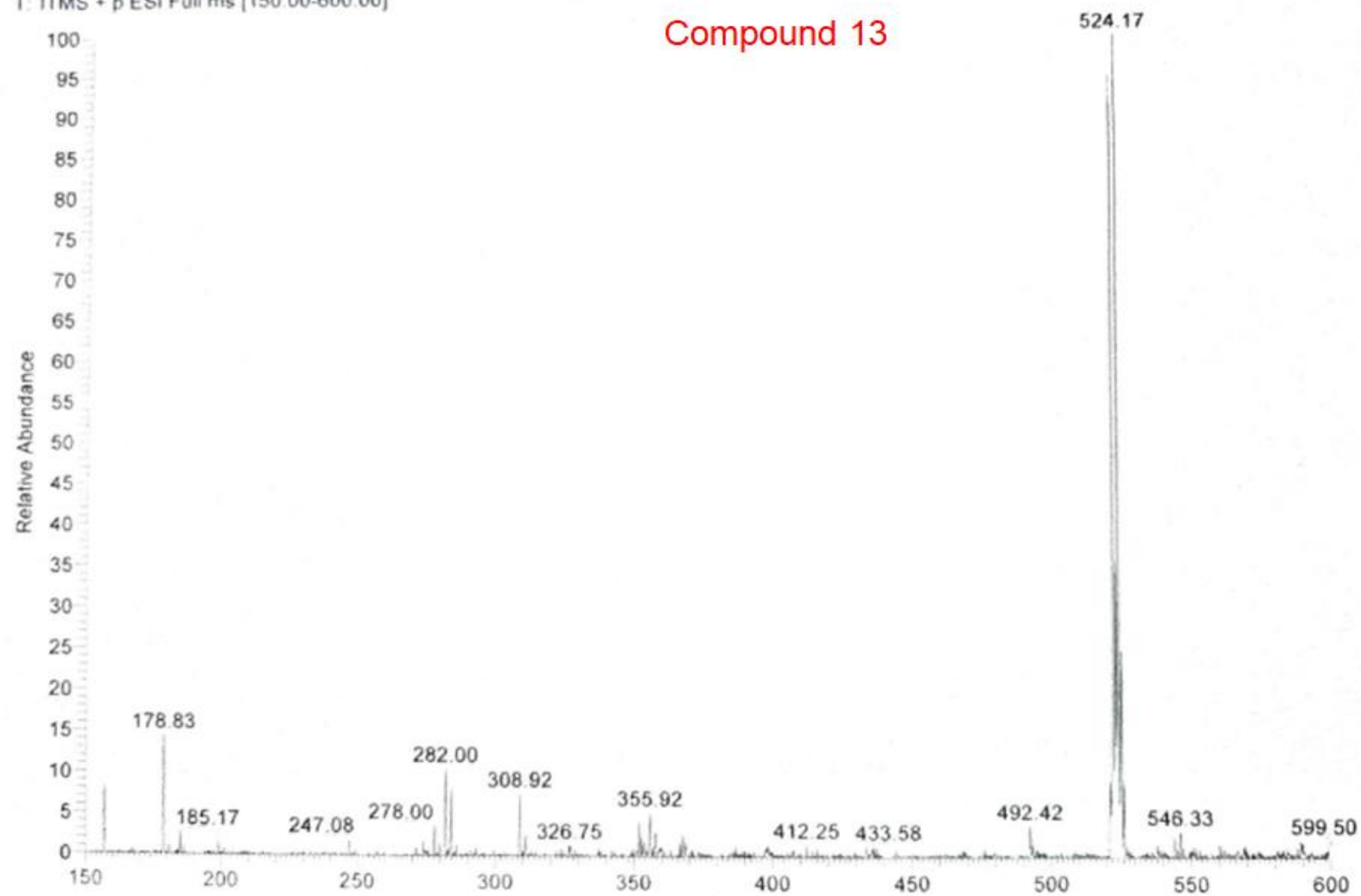
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3/18/2021 3:30:56 PM

NM-8, 522

Dr Mahboob_210318153056 #1 RT: 0.00 AV: 1 NL: 6.73E2
T: ITMS + p ESI Full ms [150.00-600.00]

Compound 13



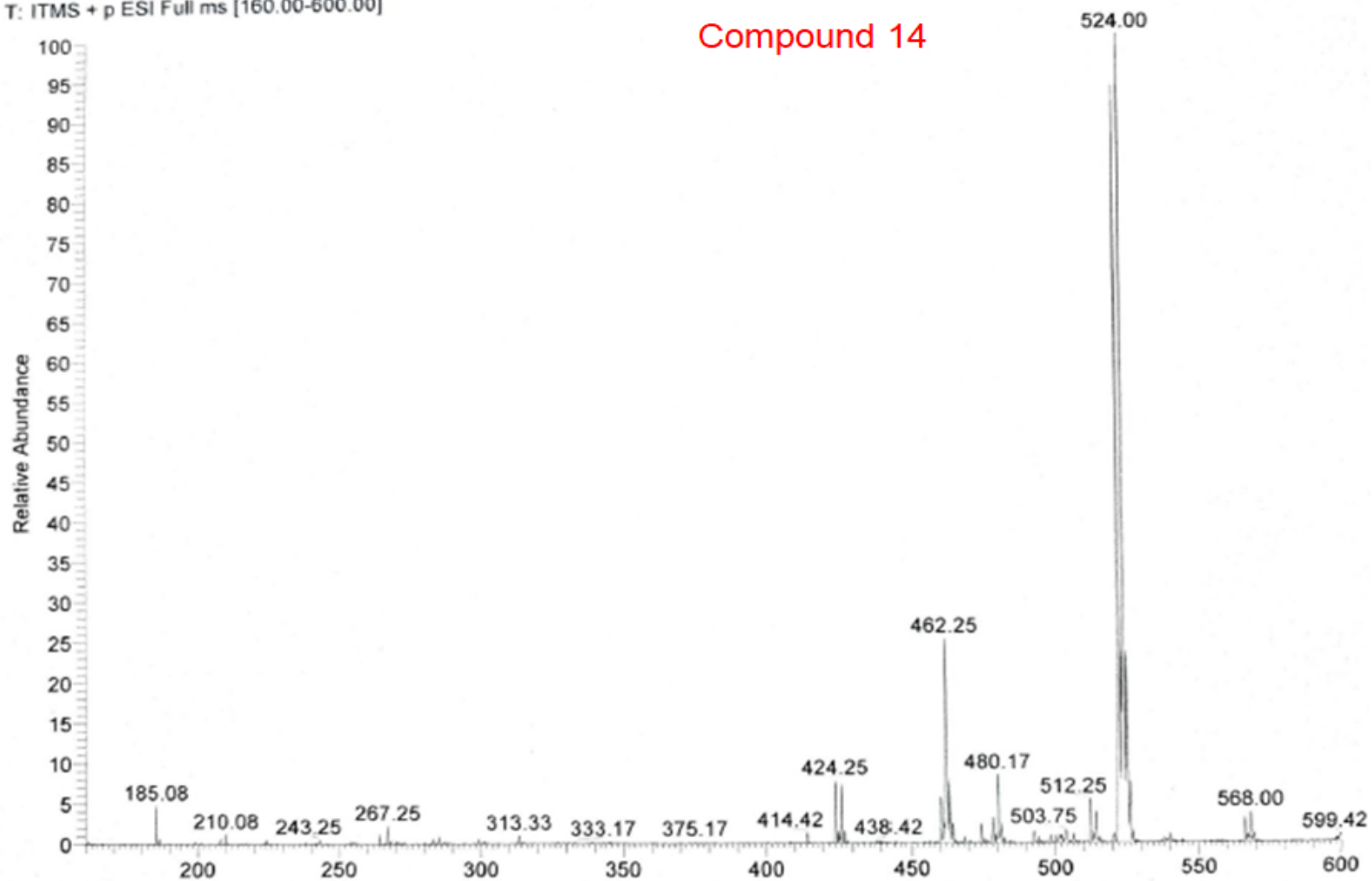
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3/18/2021 4:20:30 PM

NM-5, 522

Dr Mahboob_210318162030 #1 RT: 0.00 AV: 1 NL: 1.97E3
T: ITMS + p ESI Full ms [160.00-600.00]

Compound 14

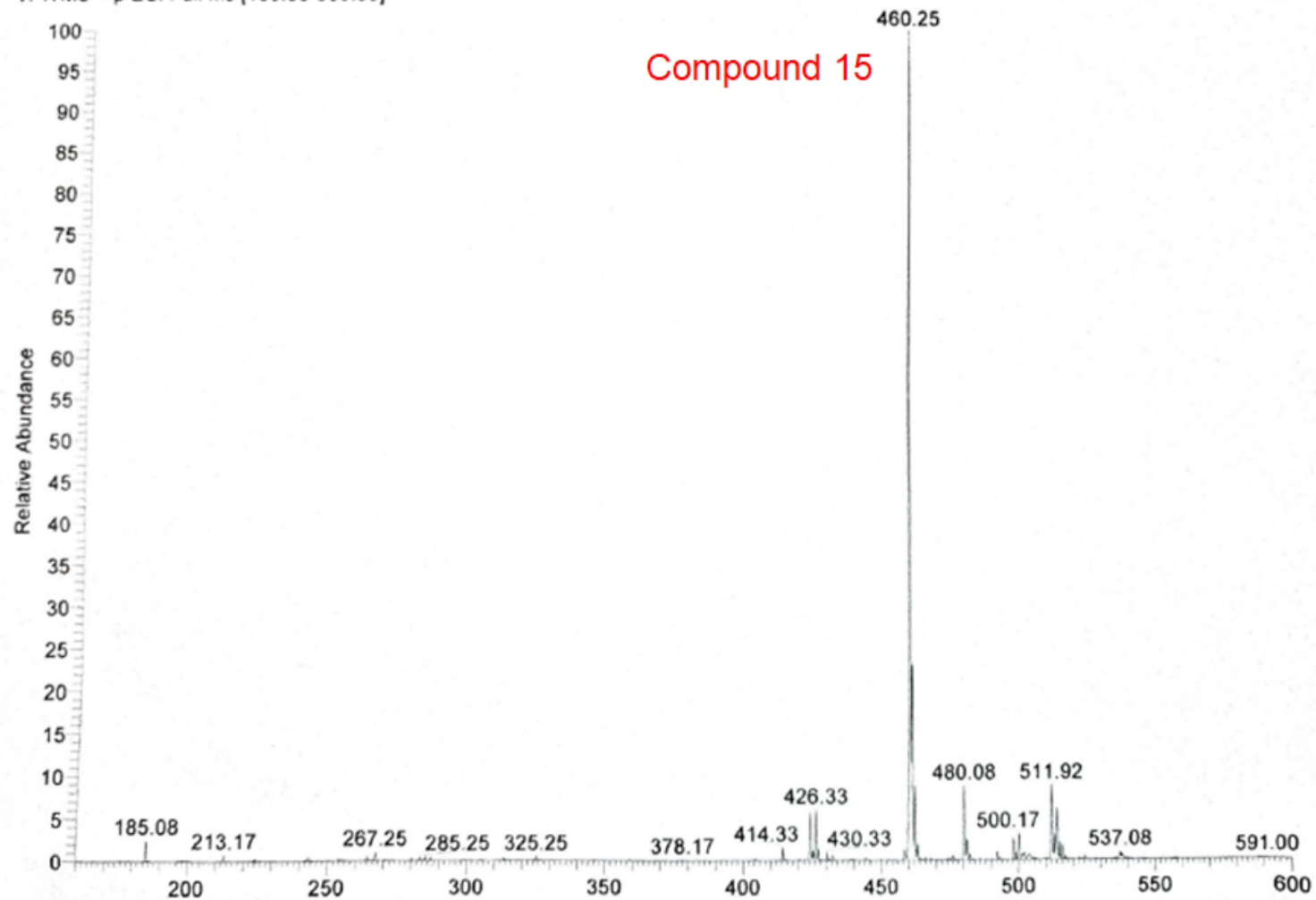


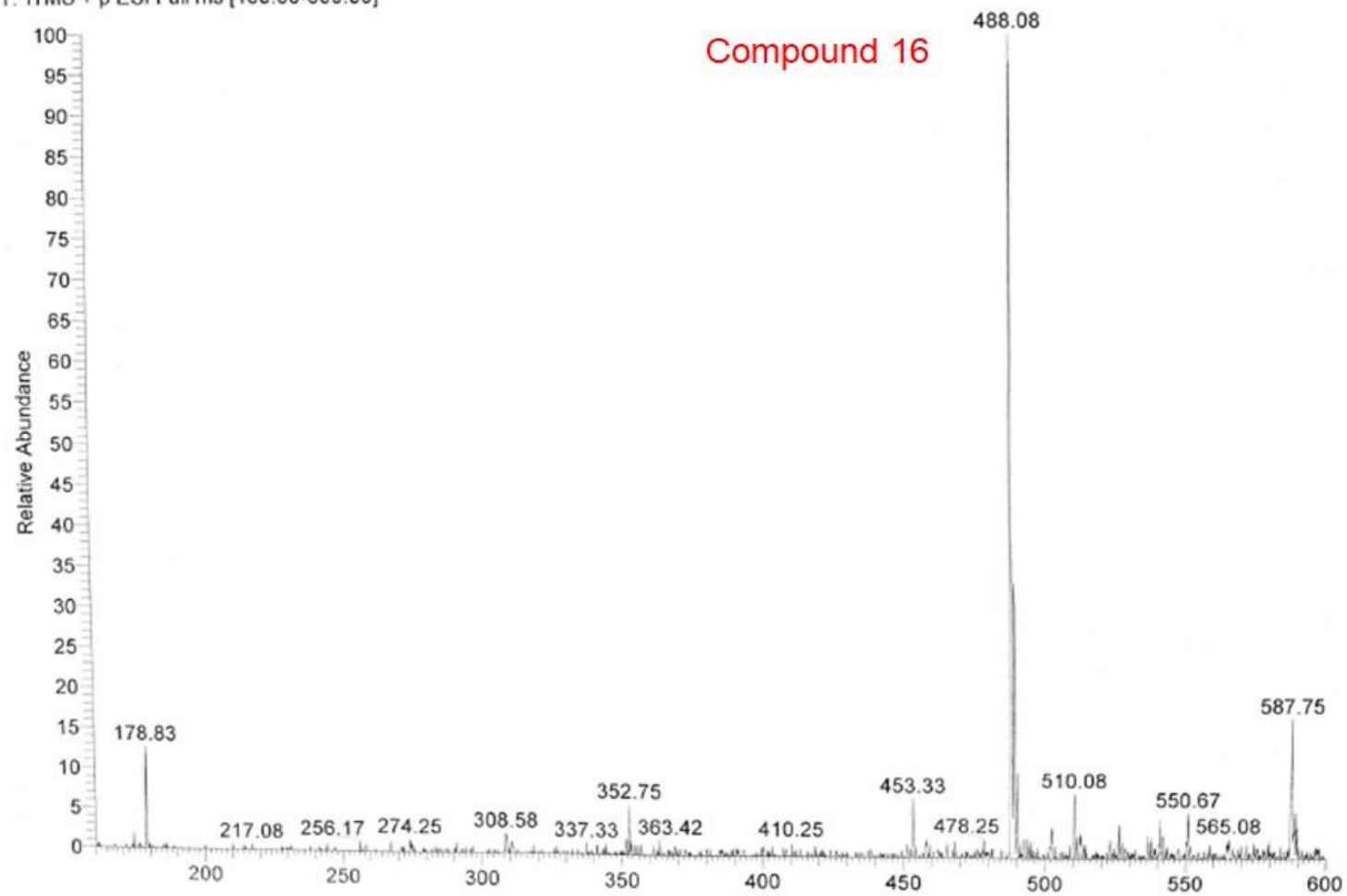
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LCF10605

3/18/2021 4:07:34 PM

NM-6, 459

Dr Mahboob_210318160733 #1 RT: 0.00 AV: 1 NL: 3.70E3
T: ITMS + p ESI Full ms [160.00-600.00]



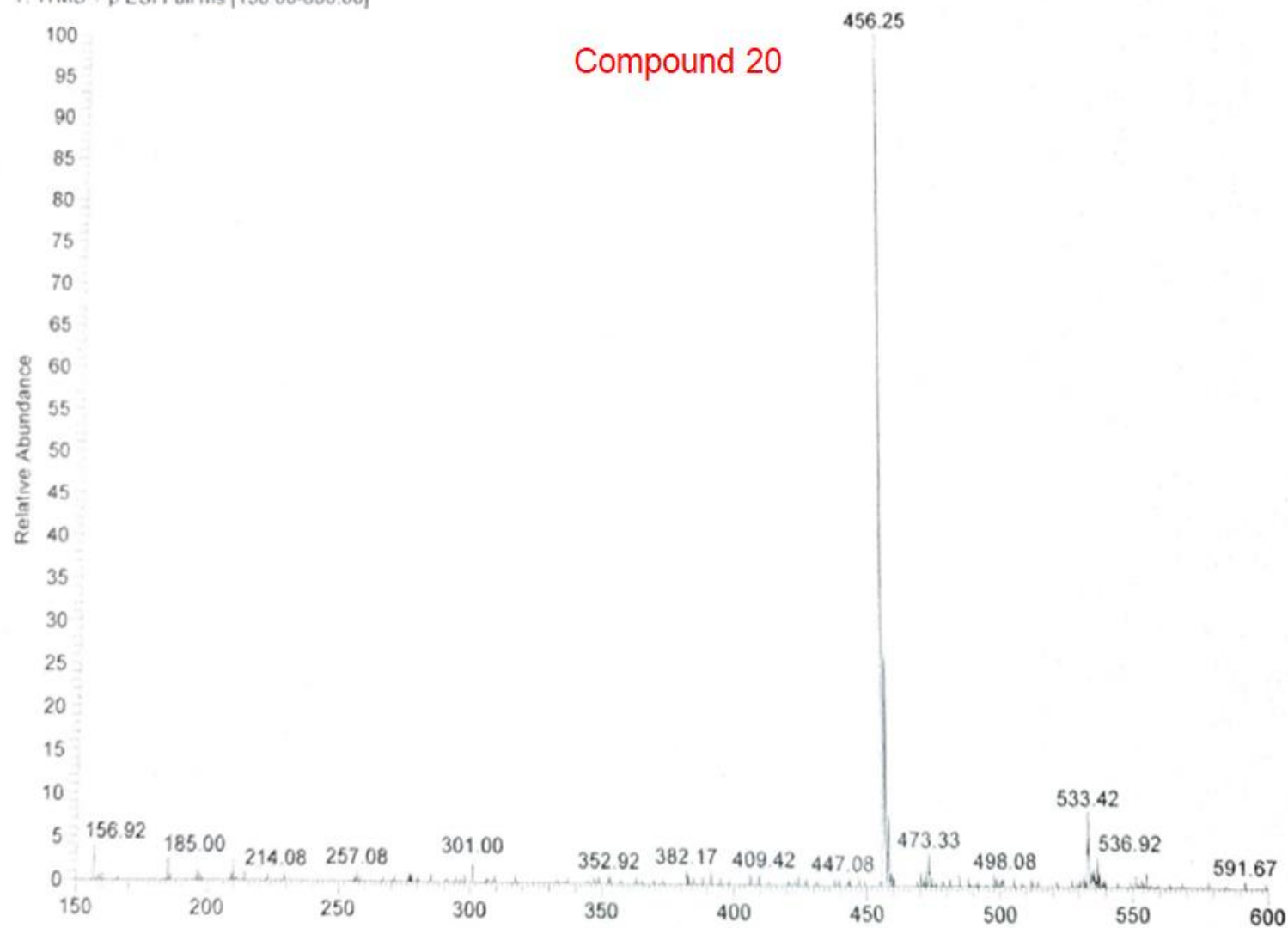


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LCF10605

5/1/2021 3:10:26 PM

NM-11 2,4-F acetamide 455

Dr Mahboob_210501151026 #1 RT: 0.00 AV: 1 NL: 1.80E2
T: ITMS + p ESI Full ms [150.00-600.00]



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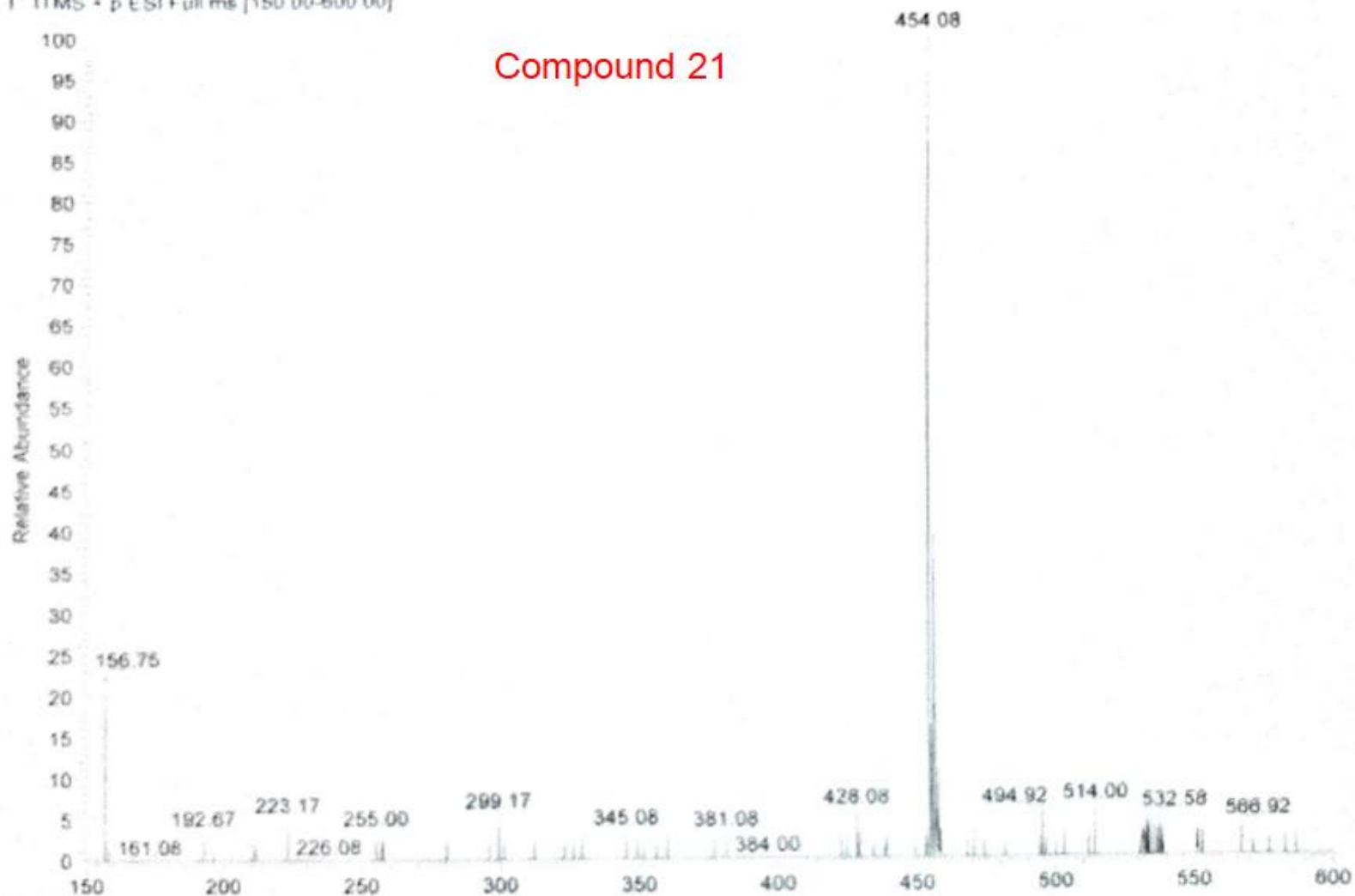
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NM-12 3-Cl acetamide 453

LCF10605

Dr Mahboob_210501151545 #1 RT: 0.00 AV: 1 NL: 4.46E1

1 ITMS + p ESI Full ms [150.00-600.00]

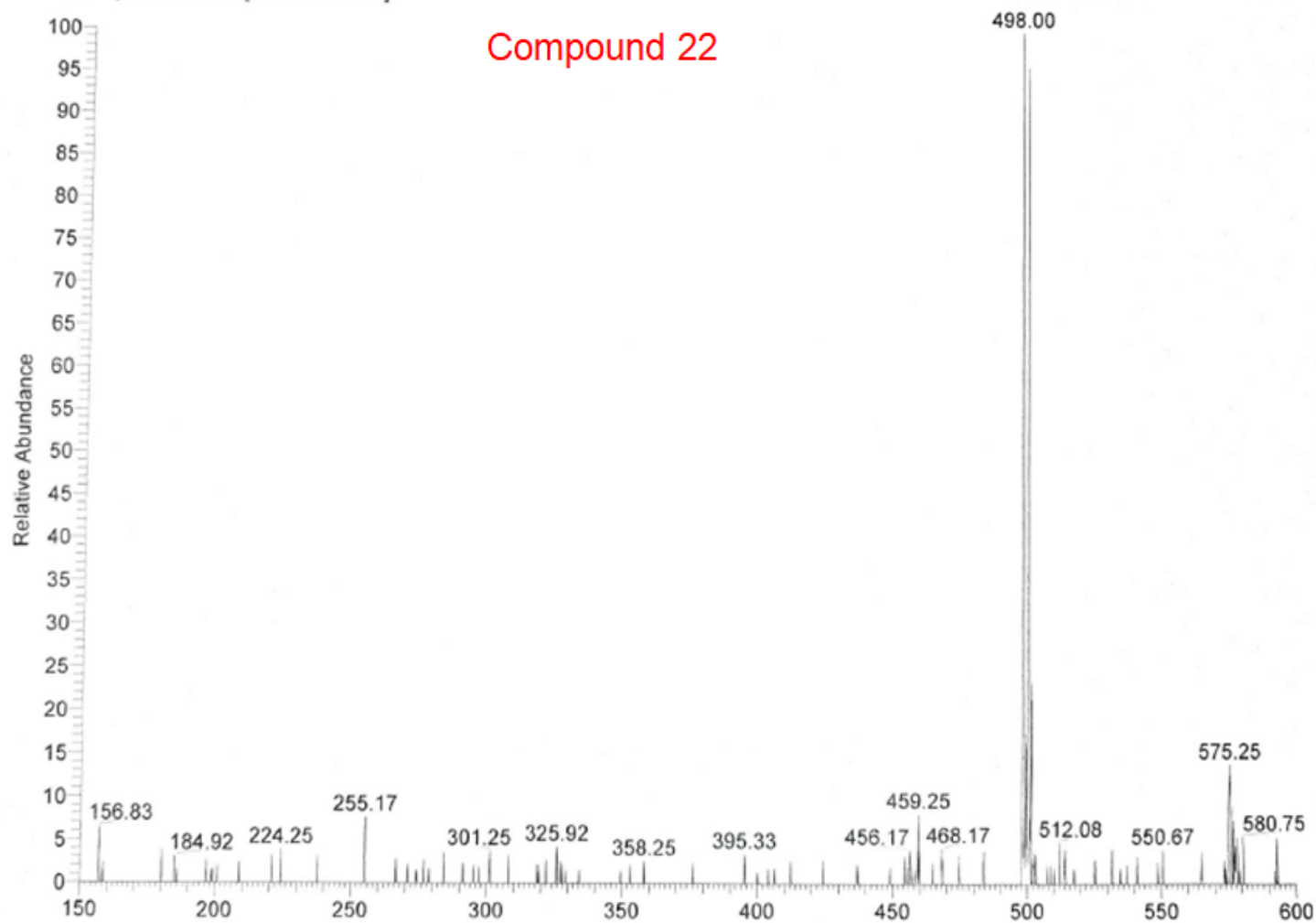


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LCF10605

5/1/2021 3:22:04 PM

NM-13 3-Bracetamide 497

Dr Mahboob_210501152204 #1 RT: 0.00 AV: 1 NL: 5.41E1
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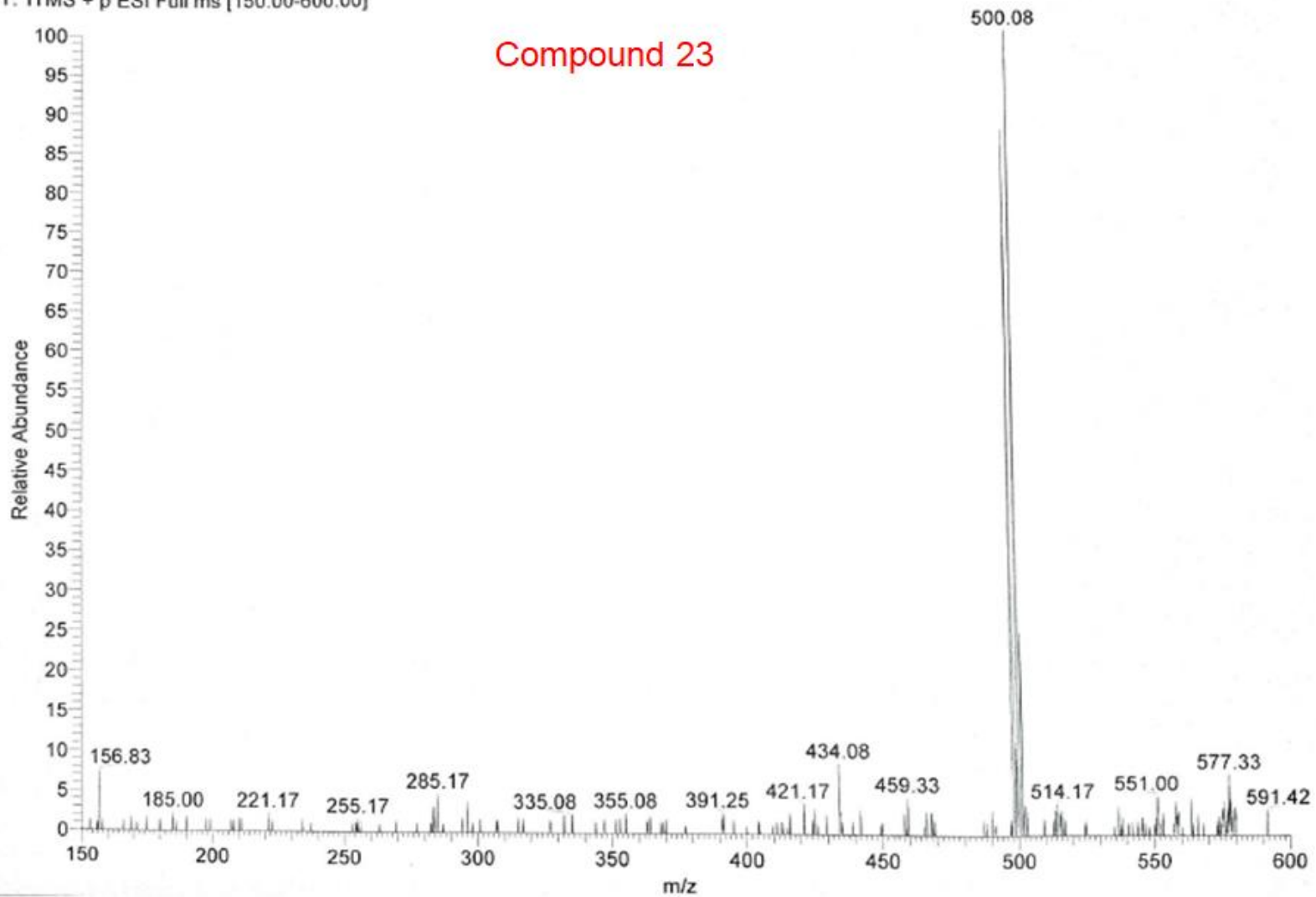


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LCF10605

5/1/2021 3:33:09 PM

NM-17 4-Br acetamide 497

Dr Mahboob_210501153309 #1 RT: 0.00 AV: 1 NL: 7.48E1
T: ITMS + p ESI Full ms [150.00-600.00]



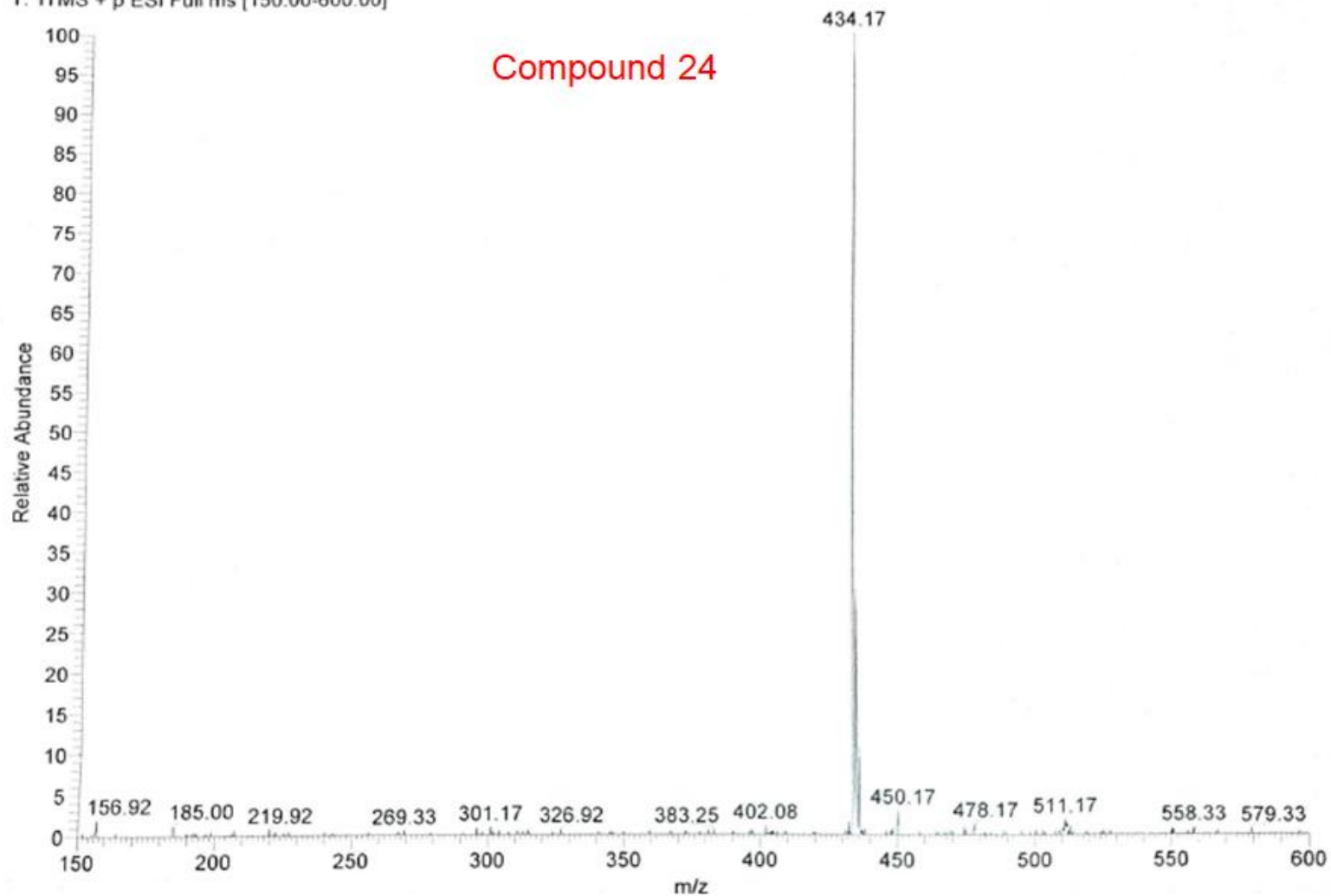
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5/1/2021 3:28:38 PM

NM-16 2-Me acetamide 433

Dr Mahboob_210501152838 #1 RT: 0.00 AV: 1 NL: 2.80E2

T: ITMS + p ESI Full ms [150.00-600.00]



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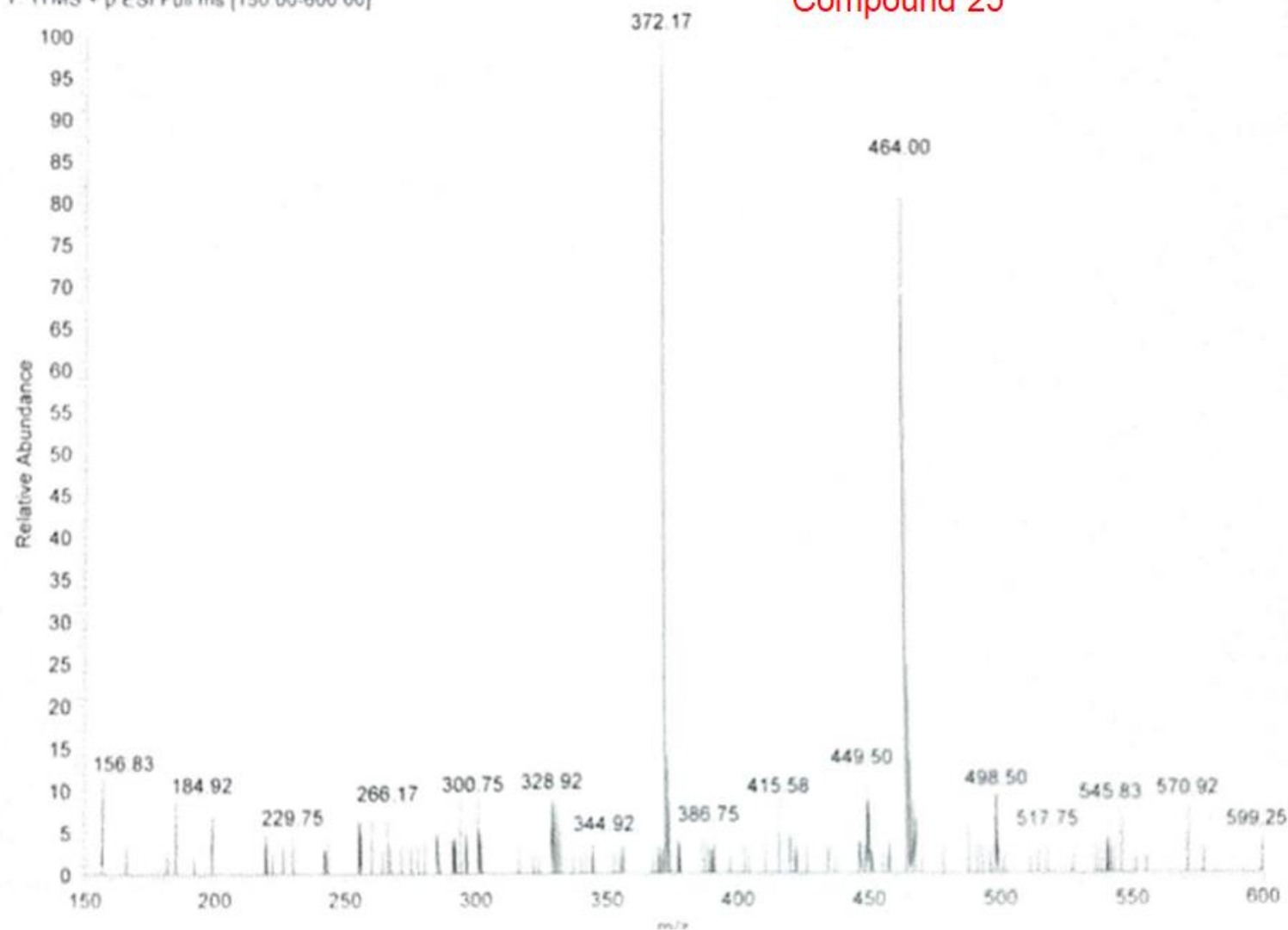
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NM-15: 2-COOH acetamide 463

Dr Mahboob_210501153859 #1 RT: 0.00 AV: 1 NL: 3.27E1

T: ITMS + p ESI Full ms [150.00-600.00]

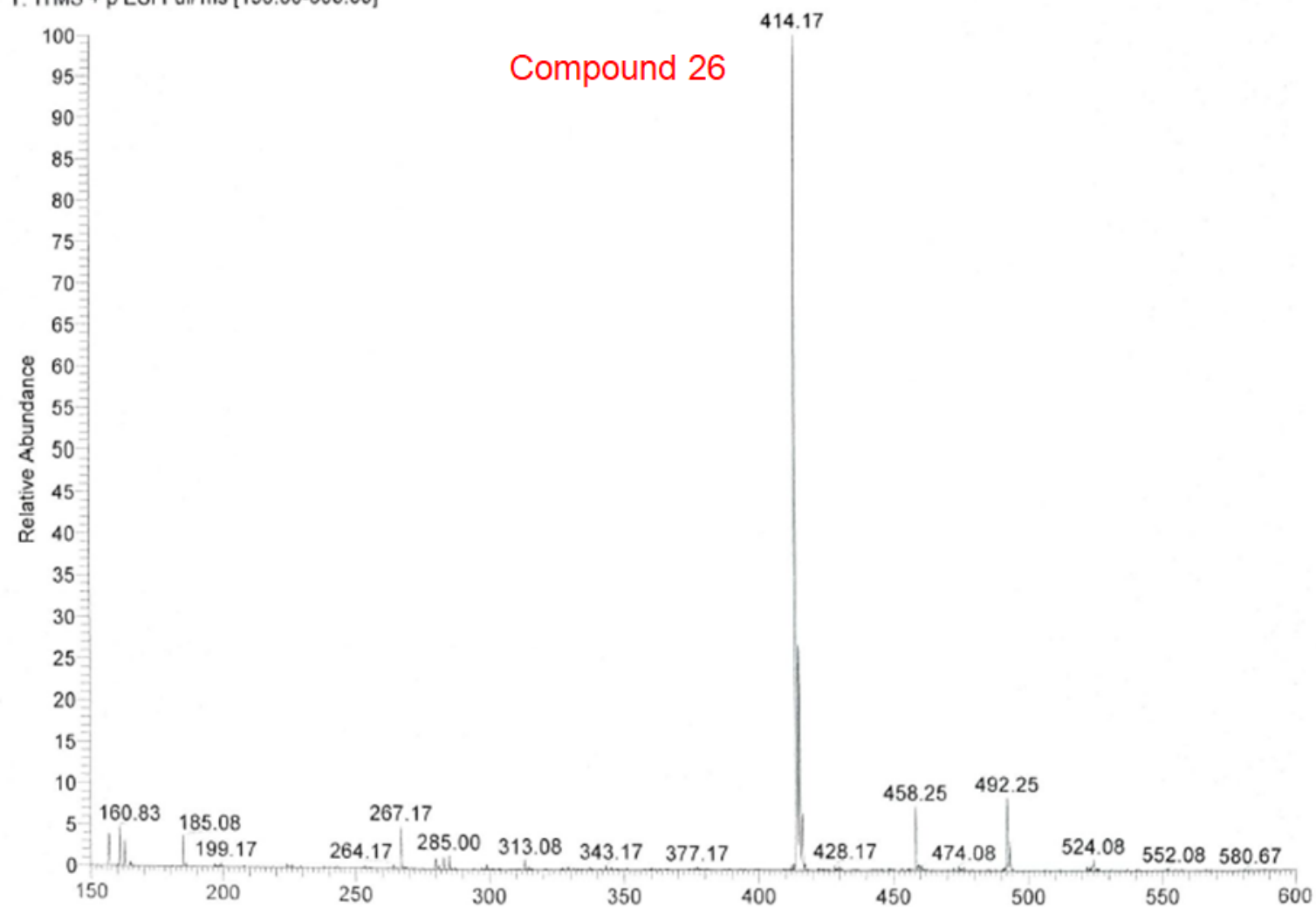
Compound 25



LCF10605

Dr Mahboob_210318153646 #1 RT: 0.00 AV: 1 NL: 8.96E2

T: ITMS + p ESI Full ms [150.00-600.00]



ALIE is represented as sum $E_{orbitals}$ weighted by the orbital densities (supplementary material) according equation:

$$(I(r) = \sum_i \frac{p_i(\vec{r}) |\epsilon_i|}{p(\vec{r})}). \text{ Where } I(r) = \sum_i \frac{p_i(\vec{r}) |\epsilon_i|}{p(\vec{r})} \text{ where } p_i(\vec{r}) \text{ :is electronic cloud for the orbital (i) at the exact point } (\vec{r}), |\epsilon_i| :$$

is energy orbital and $p(\vec{r})$: reflecting the summation electronic density function.