Supplementary material

3,3-Bis(4-(decyloxy)phenyl)benzofuranone (L-1)

Yield = 85.4%; melting point: 70–73 °C; Rf = 0.71 (acetate/hexane, 20:80). **^{1}H NMR (500 MHz, $CDCl_3$)**: δ (ppm) = 0.861 ($2CH_3$, t, J = 7 Hz); 1.252–1.415 ($14CH_2$, m); 1.712–1.769 ($2CH_2$, m); 3.909 ($2CH_2$, t, J = 6.75 Hz)); 6.765–6.825 (4H, H_{arom}, m); 7.191–7.248 (4H, H_{arom}, m); 7.491–7.532 (2H, H_{arom}, m); 7.658(1H, H_{arom}, t, J = 7.5 Hz); 7.901–7.916 (1H, H_{arom}, d, J = 7.5 Hz). **^{13}C NMR (125.76, $CDCl_3$)**: δ (ppm) = 14.208, 22.763, 26.107, 29.283, 29.397, 29.455, 29.633, 29.648, 31.975, 68.121 (C, alkyl chain), 91.854 (C_{spiro}), 114.288, 124.077, 125.672, 126.006, 128.596, 129.197, 132.109, 134.109, 152.790, 159.295 (C_{arom}), 170.0 (C═O). **IR-FT (ν, cm^{-1})**: 2,955 $(CH)_{arom}$, 2,916, 2,849 $(C–H)_{aliph}$, 1,756 $(C═O)_{ester}$, 1,610, 1,584, 1,509, 1,465 $(C═C)_{arom}$, 1,286 (C–O). **MS:** m/z $[C_{40}H_{54}O_4 + H]^+$ = 599.4.

3,3-Bis(4-(undecyloxy)phenyl)benzofuranone (L-2)

Yield = 82%; melting point: 64–68 °C; Rf = 0.86 (acetate/hexane, 20:80). **^{1}H NMR (500 MHz, $CDCl_3$)**: δ (ppm) = 0.851–0.879 (t, J = 7 Hz, $2CH_3$); 1.248–1.430 (m, 32H, $16CH_2$); 1.713–1.769 (m, 4H, $2CH_2$); 3.896–3.922 (t, J = 6.5 Hz, $2CH_2$); 6.796–6.826 (m, 4H, H_{arom}); 7.193–7.222 (m, 4H, H_{arom}); 7.492–7.532 (m, 2H, H_{arom}); 7.644–7.672 (t, J = 7 Hz, 1H, H_{arom}); 7.902–7.917 (d, J = 7.5 Hz, 1H, H_{arom}). **^{13}C NMR (125.76, $CDCl_3$)**: δ (ppm) = 14.222, 22.780, 26.111, 29.426–29.7, 31.994, 68.118 (C, alkyl chain), 91.857 (C_{spiro}), 114.284, 124.08, 125.668, 126.011, 128.596, 129.202, 132.919, 134.44, 152.787, 159.295 (C_{arom}), 170.064 (C═O). **IR-FT (ν, cm^{-1})**: 2,955 $(CH)_{arom}$, 2,916, 2,848 $(C–H)_{aliph}$, 1,755 $(C═O)_{ester}$, 1,609, 1,584, 1,509, 1,465 $(C═C)_{arom}$, 1,286 (C–O). **MS**: m/z $[C_{42}H_{58}O_4 + H]^+$ = 627.44.

3,3-Bis(4-(decyloxy)phenyl)benzofuranone (L-3)

Yield = 84%; melting point: 51–55 °C; Rf = 0.89 (acetate/hexane, 20:80). **^{1}H NMR (500 MHz, $CDCl_3$)**: δ (ppm) = 0.850–0.878 (t, J = 7 Hz), 6H, $2CH_3$), 1.245–1.441 (m, 36H, $18CH_2$); 1.711–1.767 (m, 4H, $2CH_2$); 3.894–3.920 (t, J = 6.5 Hz, 4H, $2CH_2$); 6.793–6.817 (m, 4H, CH_{arom}); 7.189–7.247 (m, 4H, CH_{arom}); 7.489–7.532 (m, 2H, CH_{arom}); 7.642–7.672(t, J = 6.5 Hz), 1H, CH_{arom}); 7.9–7.915 (d, J = 7.5 Hz, 1 H, CH_{arom}). **^{13}C NMR (125.76, $CDCl_3$)**: δ (ppm) = 14.215, 22.778, 26.109, 29.285–29.714, 32.001, 68.123 (C, Alkyl chain), 91.852 (C_{spiro}), 114.286, 124.072, 125.672, 126.011, 128.594, 129.194, 132.919, 134.107, 152.790, 159.295 (C_{arom}), 170.054 (C═O). **IR-FT (ν, cm^{-1})**: 2,953 $(CH)_{arom}$, 2,916, 2,848 $(C–H)_{aliph}$, 1,754 $(C═O)_{ester}$, 1,610, 1,584, 1,510, 1,464 $(C═C)_{arom}$, 1,286 (C–O). **MS:** m/z $[C_{44}H_{62}O_4 + H]^+$ = 655.47.

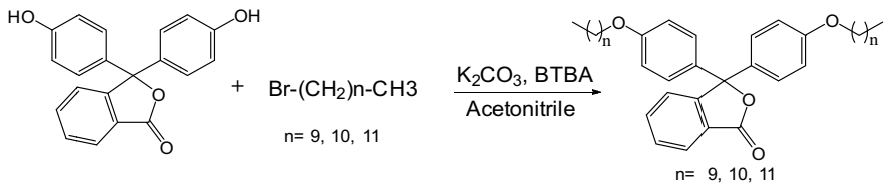
Gaussian calculations

Theoretical calculations provide important information about the chemical and biological properties of molecules. Many quantum chemical parameters are obtained from theoretical calculations. The calculated parameters are used to explain the chemical activities of the molecules. Many programs are used to calculate the molecules. These programs are Gaussian09 RevD.01 and GaussView 6.0 [1,2]. By using these programs, calculations were made using the HF [3–5] method with the 6-31++ g(d,p) basis set. As a result of these calculations, many quantum chemical parameters were found. Each parameter describes a different chemical property of the molecules, and the parameters are calculated as follows [34]:

$$\chi = -\left(\frac{\partial \mathrm{E}}{\partial \mathrm{N}}\right)_{\upsilon(r)} = \frac{1}{2}(I + A) \cong \frac{1}{2}(E_{\mathrm{HOMO}} + E_{\mathrm{LUMO}}),$$

$$\eta = -\left(\frac{\partial^2 \mathrm{E}}{\partial \mathrm{N}^2}\right)_{\upsilon(r)} = \frac{1}{2}(I - A) \cong -\frac{1}{2}(E_{\mathrm{HOMO}} - E_{\mathrm{LUMO}}),$$

$$\sigma = 1/\eta \ \omega = \chi^2/2\eta \ \varepsilon = 1/\omega.$$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O
+
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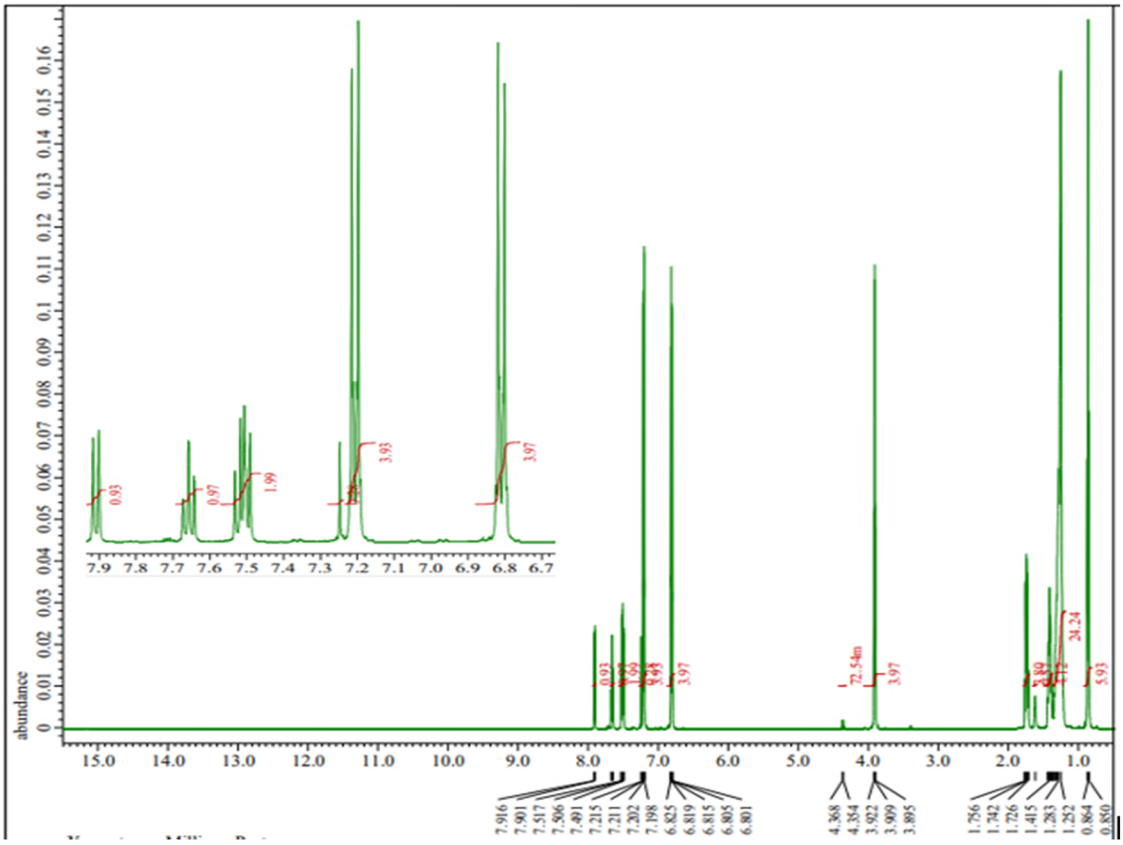
K2CO3, BTBA
Acetonitrile
O
n
O
n
O
O
n= 9, 10, 11

L-1

L-1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7.211
7.202
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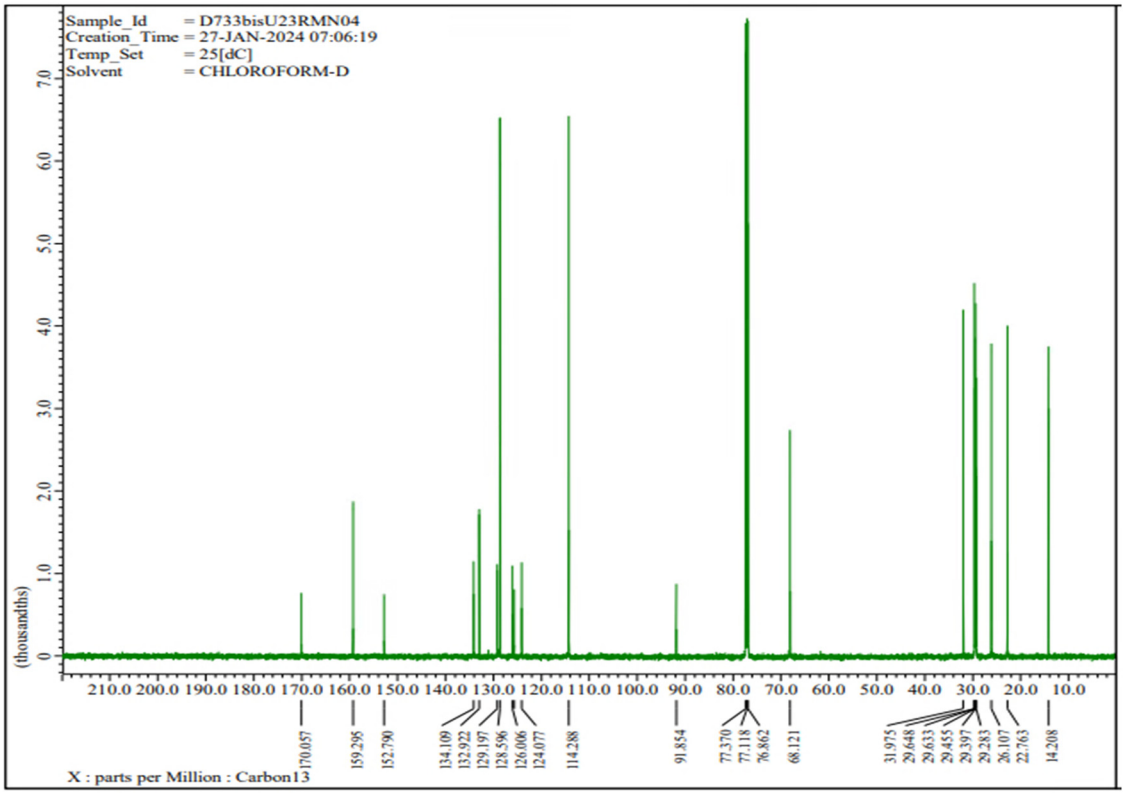
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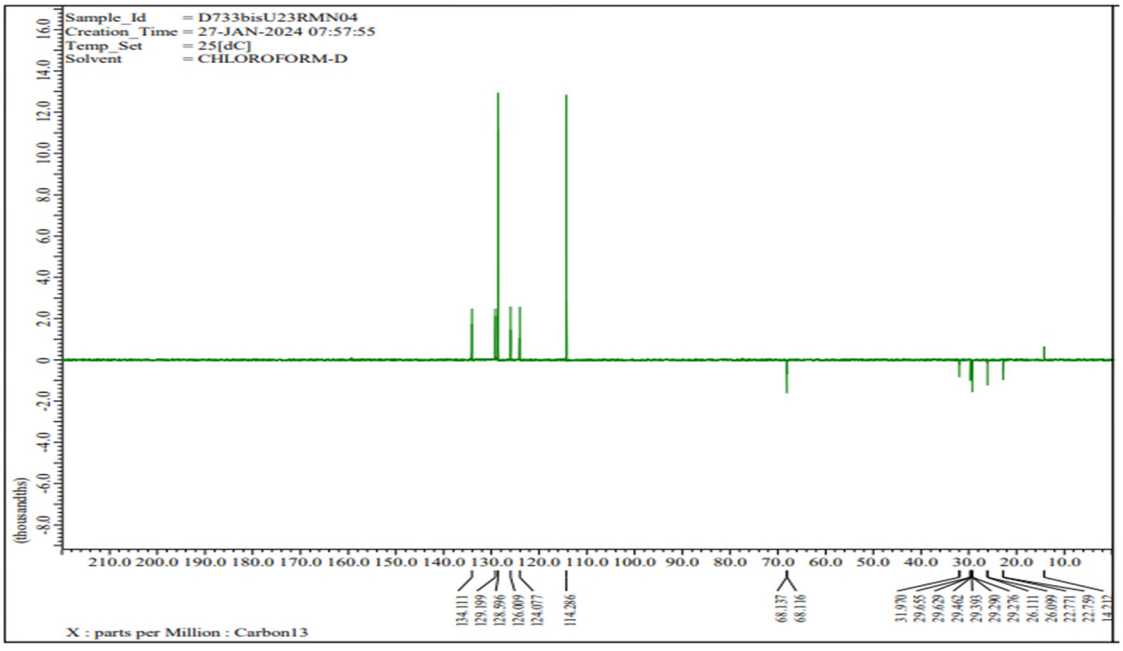
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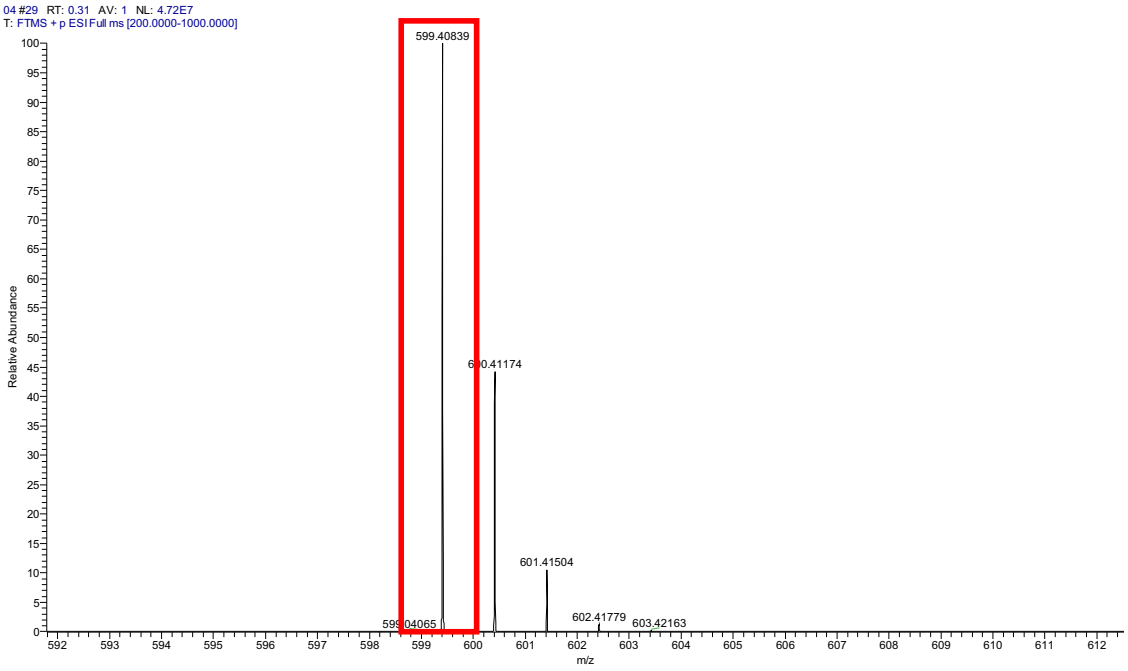
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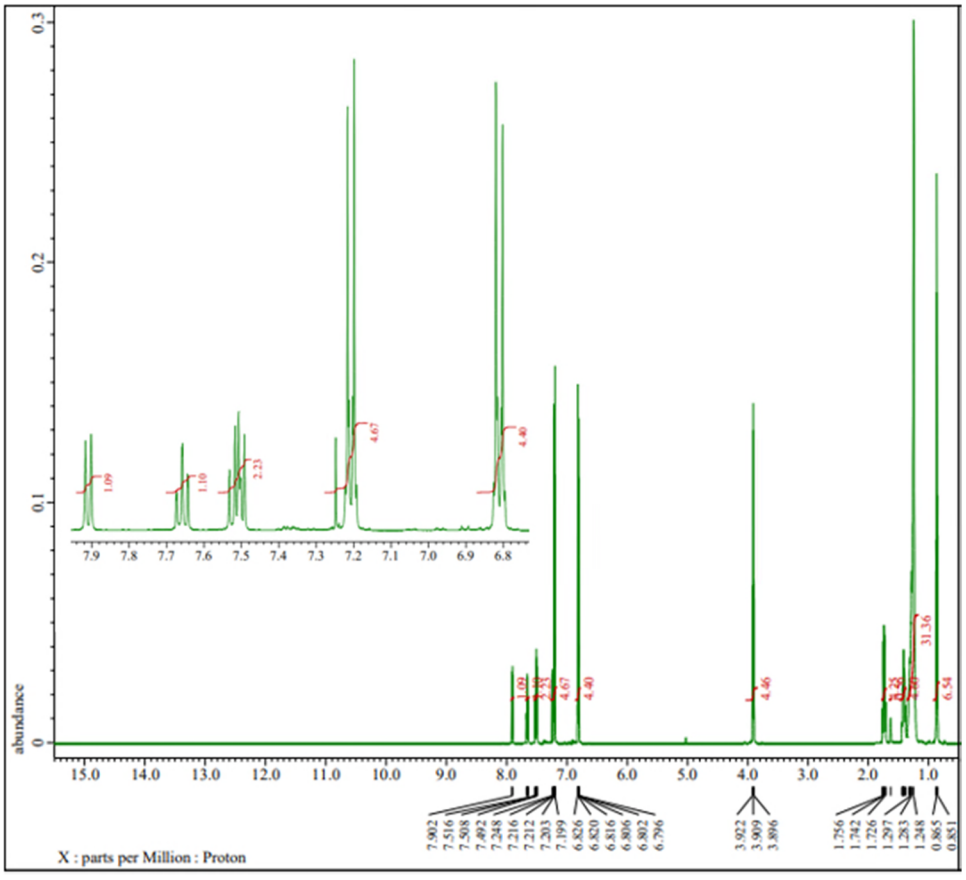
Relative Abundance
m/z

L-2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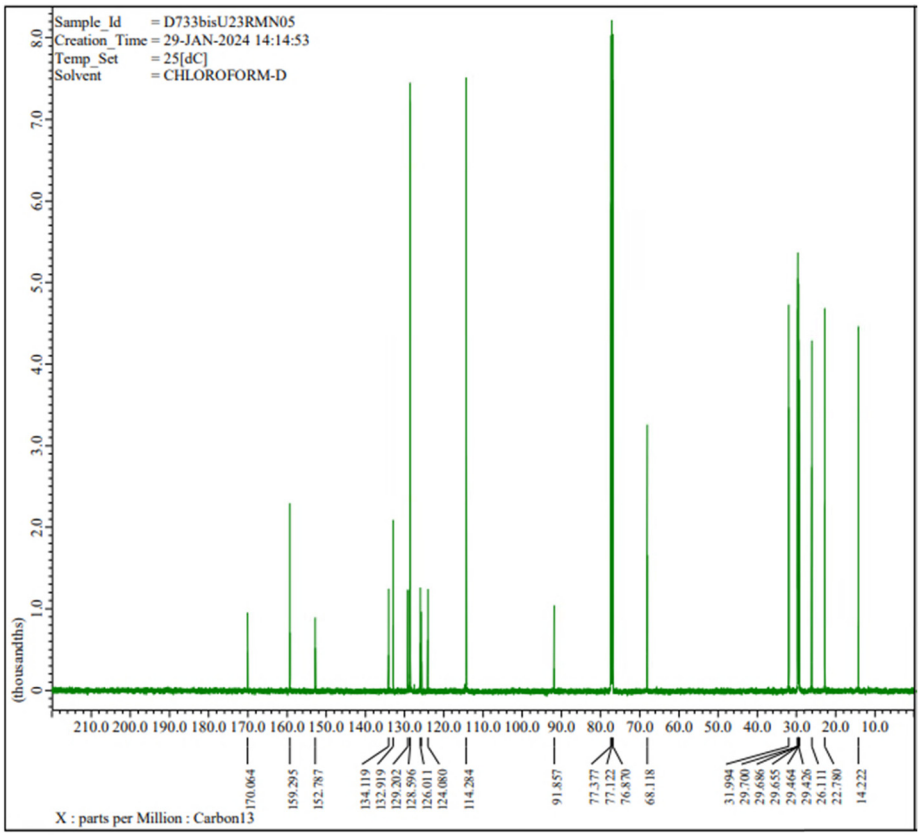
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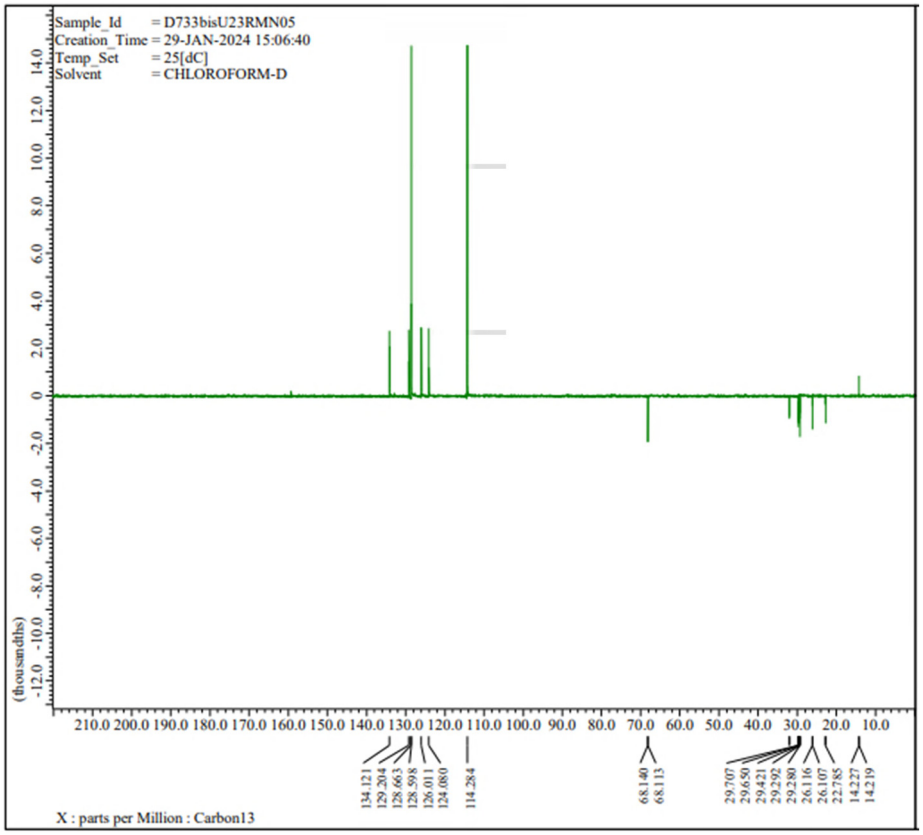
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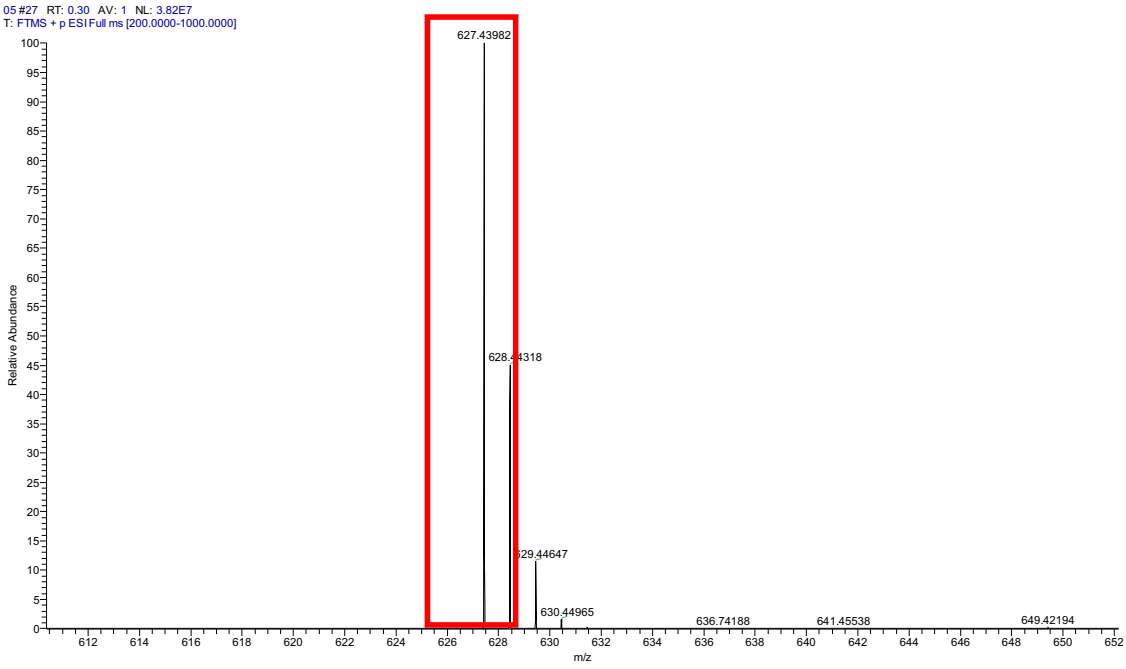
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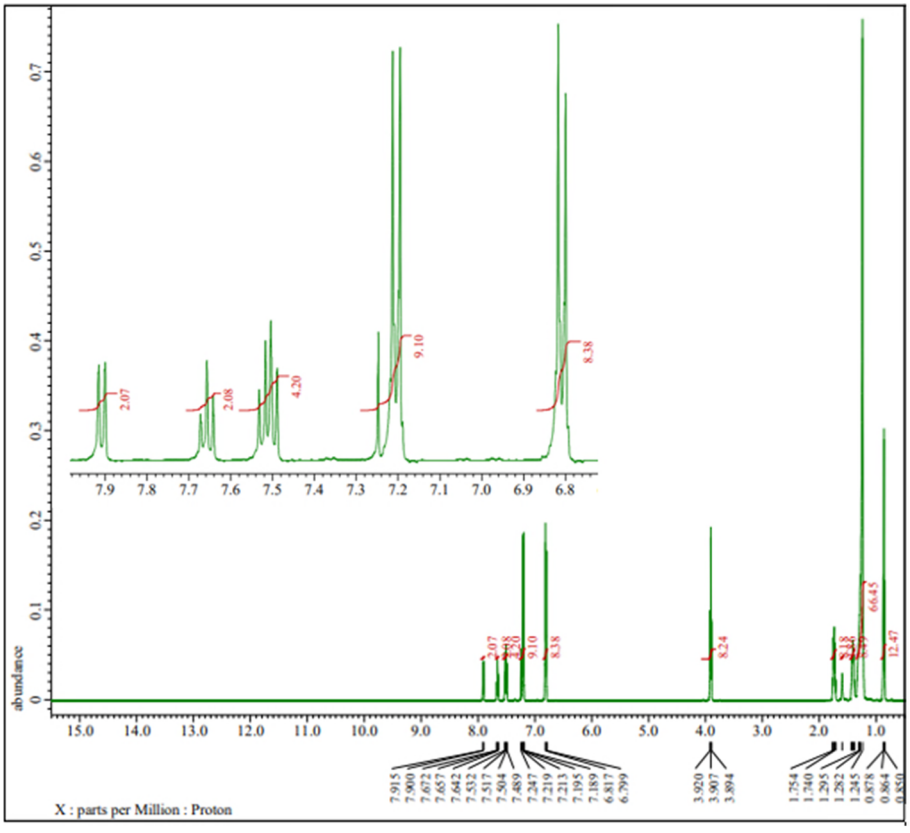
Relative Abundance
m/z

L-3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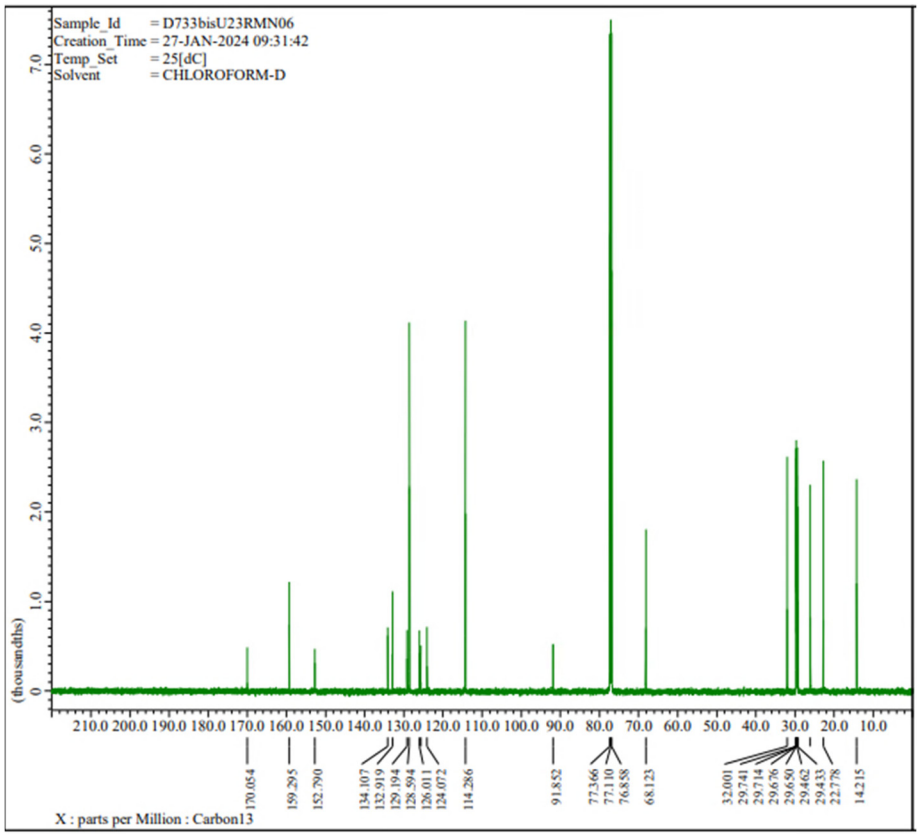
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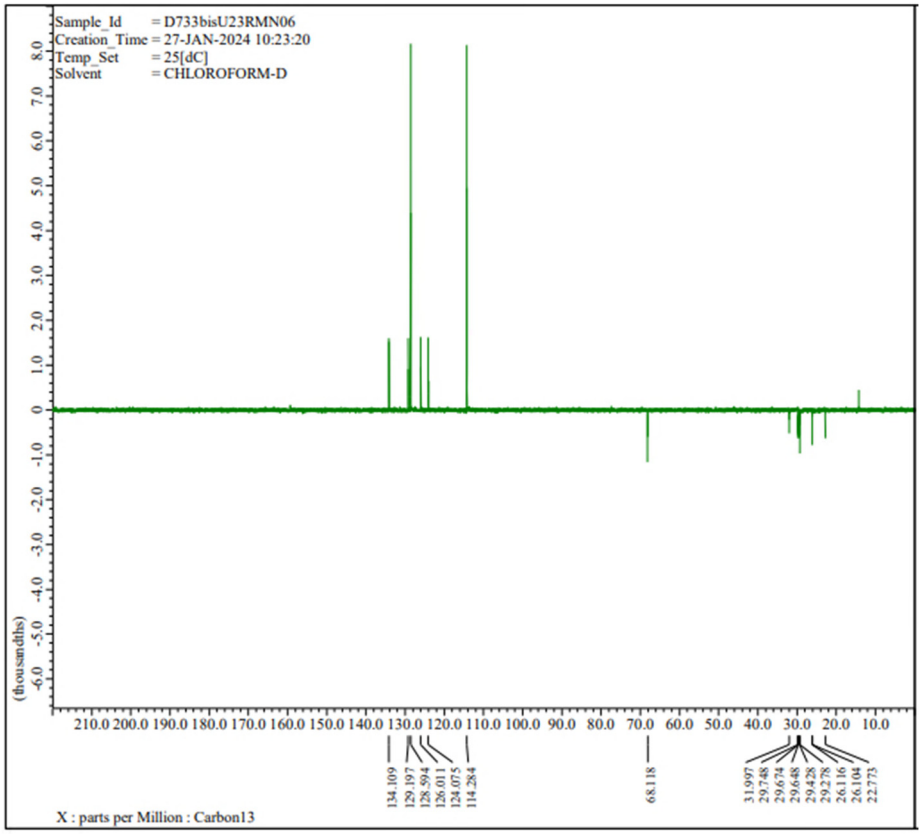
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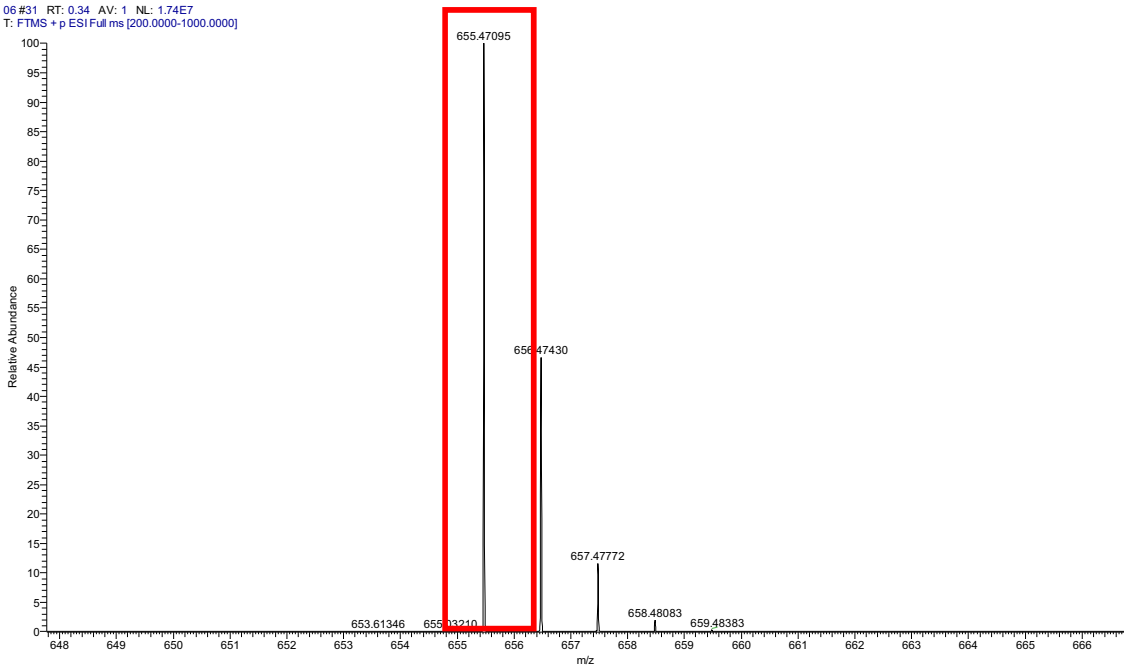

References

[1] Dennington R, Keith TA, Millam JM. GaussView, version 6.0. 16. Semichem Inc Shawnee Mission KS. 2016.
[2] Frisch MJ, Trucks GW, Schlegel HB, Scuseria GE, Robb MA, Cheeseman JR, et al. Gaussian 09, Revision D. 01. Wallingford CT: Gaussian, Inc.; 2009. p. 620. See Also URL. Httpwww Gaussian Com.
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