

Supplementary Material

Solvent-free synthesis and *in vitro* cytotoxicity of fluorinated chalcones against HepG2 cells

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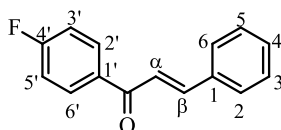
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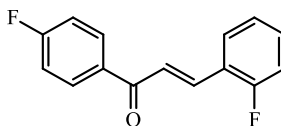
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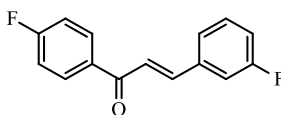
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1. ^1H , ^{13}C NMR and ESIMS data of known compounds **1a-1e**, **1g**, **2a**, **2c**, **3a**, **3e***(E)*-1-(4-Fluorophenyl)-3-phenylprop-2-en-1-one (**1a**)

Yield 50%; white solid; mp 80-81 °C; ^1H NMR (600 MHz, CDCl_3): δ_{H} 7.18 (dd, $J(\text{H,H})$ 8.4 Hz, $J(\text{H,F})$ 9.0 Hz, 2H, H-3',5'), 7.42-7.43 (m, 3H, H-2,4,6), 7.49 (d, $J(\text{H,H})$ 15.6 Hz, 1H, H- α), 7.64-7.65 (m, 2H, H-3,5), 7.80 (d, $J(\text{H,H})$ 15.6 Hz, 1H, H- β), 8.05 (d, $J(\text{H,H})$ 8.4 Hz, 1H, H-2'), 8.06 (d, $J(\text{H,H})$ 8.4 Hz, 1H; H-6'); ^{13}C NMR (150 MHz, CDCl_3): δ_{C} 115.67-115.84 (d, $J(\text{C,F})$ 25.5 Hz, 2C, C-3',5'), 121.67 (1C, C- α), 128.47 (2C, C-3,5), 129.00 (2C, C-2,6), 130.65 (1C, C-4), 131.06 (d, $J(\text{C,F})$ 10.5 Hz, 2C, C-2',6'), 134.81 (1C, C-1'), 145.0 (1 C, C- β), 188.87 (1 C, $>\text{C}=\text{O}$). ESIMS calcd. for $[\text{M} + \text{H}]$: 227.1; found: m/z 226.9 ($\text{M} + \text{H}$) $^+$.

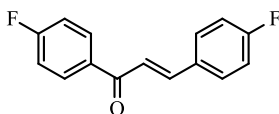
(E)-3-(2-Fluorophenyl)-1-(4-fluorophenyl)prop-2-en-1-one (**1b**)

Yield 72%; yellow powder; mp 77-79 °C; ^1H NMR (600 MHz, CDCl_3): δ_{H} 7.13-7.16 (m, 1H, H-3), 7.20 (dd, $J(\text{H,H})$ 8.4 Hz, $J(\text{H,F})$ 8.4 Hz, 2H, H-3',5'), 7.17-7.22 (m, 1H, H-5), 7.38-7.40 (m, 1H, H-6), 7.61 (d, $J(\text{H,H})$ 16.2 Hz, 1H, H- α), 7.62-7.65 (m, 1H, H-4), 7.88 (d, $J(\text{H,H})$ 15.6 Hz, 1H; H- β), 8.05 (d, $J(\text{H,H})$ 9.0 Hz, 1H, H-2'), 8.06 (d, $J(\text{H,H})$ 9.0 Hz, 1H, H-6'). ^{13}C NMR (150 MHz, CDCl_3): δ_{C} 115.9 (d, $J(\text{C,F})$ 22.5 Hz, 2C, C-3',5'), 116.3 (d, $J(\text{C,F})$ 22.5 Hz, 1C- C-3), 122.9 (d, $J(\text{C,F})$ 12.0 Hz, 1C, C-1), 124.26 (1C, C- α), 124.5 (d, $J(\text{C,F})$ 5.5 Hz, 1C, C-5), 129.9 (d, $J(\text{C,F})$ 3.0 Hz, 1C, C-4), 131.1 (d, $J(\text{C,F})$ 9.0 Hz, 2C, C-2',6'), 131.9 (d, $J(\text{C,F})$ 9.0 Hz, 2C, C-6), 134.4 (1C, C-1'), 137.8 (1C, C- β), 162.6 (d, $J(\text{C,F})$ 246.0 Hz, 1C, C-2), 164.9 (d, $J(\text{C,F})$ 252.0 Hz, 1C, C-4'), 188.8 (1C, $>\text{C}=\text{O}$). ESIMS calcd. for $[\text{M} + \text{H}]$: 245.1; found: m/z 244.9 ($[\text{M} + \text{H}]^+$).

(E)-3-(3-Fluorophenyl)-1-(4-fluorophenyl)prop-2-en-1-one (**1c**)

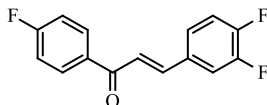
Yield 43%; white solid; mp 80-81 °C; ^1H NMR (600 MHz, CDCl_3): δ_{H} 7.11-7.14 (m, 1H, H-2), 7.19 (dd, $J(\text{H,H})$ 8.4 Hz, $J(\text{H,F})$ 8.4 Hz, 2H, H-3',5'), 7.33-7.34 (m, 1H, H-4), 7.34-7.41 (m, 2H, H-5,6), 7.47 (d, $J(\text{H,H})$ 15.6 Hz, 1H, H- α), 7.75 (d, $J(\text{H,H})$ 15.6 Hz, 1H, H- β), 8.05 (d, $J(\text{H,H})$ 9.0 Hz, 2H, H-2'), 8.06 (d, $J(\text{H,H})$ 9.0 Hz, 2H, H-6'). ^{13}C -NMR (150 MHz, CDCl_3): δ_{C} 114.40 (d, $J(\text{C,F})$ 27.0 Hz, 1C, C-4), 115.77-115.95 (d, $J(\text{C,F})$ 27.0 Hz, 2C, C3',5'), 117.49 (d, $J(\text{C,F})$ 27.0 Hz, 1C, C-2), 121.54 (1C, C-1), 122.76 (1C, C- α), 124.60 (d, $J(\text{C,F})$ 3.0 Hz, 1C, C-6), 130.53 (d, $J(\text{C,F})$ 10.5 Hz, 1C, C-5), 131.11-131.19 (d, $J(\text{C,F})$ 12.0 Hz, 2C, C-2',6'), 134.29 (1C, C-1'), 143.52 (1C, C- β), 162.10 (d, $J(\text{C,F})$ 294.0 Hz, 1C, C-3), 172.66 (1C, C-4'), 188.49 (1C, $>\text{C}=\text{O}$). ESIMS calcd. for $[\text{M} + 4\text{H}_2\text{O}]$: 316.1; found: m/z 316.1 ($[\text{M} + 4\text{H}_2\text{O}]^+$).

(*E*)-1,3-Bis(4-fluorophenyl)prop-2-en-1-one (**1d**)



Yield 67%; white solid; mp 102-104 °C; ^1H NMR (600 MHz, CDCl_3): δ_{H} 7.12 (dd, $J(\text{H,H})$ 8.4 Hz, $J(\text{H,F})$ 9.0 Hz, 2H, H-3',5'), 7.18 (dd, $J(\text{H,H})$ 8.4 Hz, $J(\text{H,F})$ 8.4 Hz, 2H, H-3,5), 7.41 (d, $J(\text{H,H})$ 15.6 Hz, 1H, H- α), 7.62 (d, $J(\text{H,H})$ 9.0 Hz, 1H, H-2), 7.63 (d, $J(\text{H,H})$ 9.0 Hz, 1H, H-6), 7.76 (d, $J(\text{H,H})$ 15.6 Hz, 1H, H- β), 8.04 (d, $J(\text{H,H})$ 9.0 Hz, 1H, H-2'), 8.05 (d, $J(\text{H,H})$ 9.0 Hz, 1H, H-6'). ^{13}C NMR (150 MHz, CDCl_3): δ_{C} 115.71-115.88 (d, $J(\text{C,F})$ 25.5 Hz, 2C, C-3',5'), 116.11-116.28 (d, $J(\text{C,F})$ 25.5 Hz, 2C, C-3,5), 121.32 (1C, C- α), 130.35-130.42 (d, $J(\text{C,F})$ 10.5 Hz, 2C, C-2,6), 131.04-131.11 (d, $J(\text{C,F})$ 10.5 Hz, 2C, C-2',6'), 134.46 (1C, C-1'), 143.74 (1C, C- β), 164.65 (1C, C-4), 165.15 (1C, C-4'), 188.63 (1C, $>\text{C}=\text{O}$) ppm. ESIMS calcd. for $[\text{M} + \text{H}]$: 245.1; found: m/z 244.9 ($[\text{M} + \text{H}]^+$).

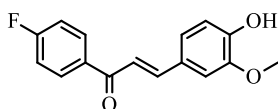
(*E*)-3-(3,4-Difluorophenyl)-1-(4-fluorophenyl)prop-2-en-1-one (**1e**)



Yield 49%; white solid; mp 117-119 °C; ^1H NMR (600 MHz, CDCl_3): δ_{H} 7.20 (dd, $J(\text{H,H})$ 8.4 Hz, $J(\text{H,F})$ 9.0 Hz, 2H, H-3',5'), 7.20-7.24 (m, 1H, H-5), 7.36 (m, 1H, H-2), 7.40 (d, $J(\text{H,H})$ 15.6 Hz, 1H, H- α), 7.45-7.50 (m, 1H, H-6), 7.70 (d, $J(\text{H,H})$ 15.6 Hz, 1H, H- β), 8.04 (d, $J(\text{H,H})$ 9.0 Hz, 1H, H-2'), 8.05 (d, $J(\text{H,H})$ 9.0 Hz, 1H, H-6'). ^{13}C NMR (150 MHz, CDCl_3): δ_{C} 115.80-116.59 (d, $^2J(\text{C,F})$ 27.0 Hz, 2C, C-3',5'), 116.45 (d, $J(\text{C,F})$ 21.0 Hz, 1C, C-6), 117.90 (d, $J(\text{C,F})$ 21.0 Hz, 1C, C-5), 122.42 (C-1), 122.44

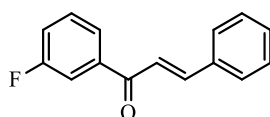
(C- α), 125.36 (dd, $J(\text{C},\text{F})$ 7.5 Hz, $J(\text{C},\text{F})$ 4.5 Hz, 2C; C-2), 131.09-131.17 (d, $J(\text{C},\text{F})$ 12.0 Hz, 2C, C-5',6'), 134.22 (d, $J(\text{C},\text{F})$ 3.0 Hz, 1C, C-1'), 142.54 (1C, C- β), 149.76 (1C, C-3), 150.66 (1C, C-4), 164.76 (d, $J(\text{C},\text{F})$ 304.5 Hz, 1C, C-4'), 188.23 (1C, >C=O). ESIMS calcd. for $[\text{M} + 3\text{H}_2\text{O}]$: 316.1; found: m/z 316.1 ($\text{M} + 3\text{H}_2\text{O}$)⁺).

(*E*)-1-(4-Fluorophenyl)-3-(4-hydroxy-3-methoxyphenyl)prop-2-en-1-one (**1g**)

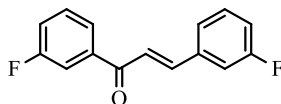


Yield 41%; yellow solid; mp 102-104 °C; ¹H NMR (600 MHz, CDCl₃): δ_{H} 3.99 (s, 3H, -OCH₃), 5.97 (s, 1H, -OH), 6.99 (d, $J(\text{H},\text{H})$ 8.4 Hz, 1H, H-5), 7.15 (d, $J(\text{H},\text{H})$ 1.8 Hz, 1H, H-2), 7.18 (dd, $J(\text{H},\text{H})$ 8.4 Hz, $J(\text{H},\text{F})$ 8.4 Hz, 2H, H-3',5'), 7.24 (dd, $J(\text{H},\text{H})$ 8.4 Hz, $J(\text{H},\text{F})$ 1.8 Hz, 1H, H-6), 7.35 (d, $J(\text{H},\text{H})$ 15.6 Hz, 1H, H- α), 7.76 (d, $J(\text{H},\text{H})$ 15.6 Hz, 1H, H- β), 8.05 (d, $J(\text{H},\text{H})$ 9.0 Hz, 1H, H-2'), 8.06 (d, $J(\text{H},\text{H})$ 7.8 Hz, 1H, H-6'); ¹³C NMR (150 MHz, CDCl₃): δ_{C} 56.05 (1C, -OCH₃), 110.11 (1C, C-2), 114.93 (1C, C-5), 115.59 (d, $J(\text{C},\text{F})$ 21.0 Hz, 2C; C-3',5'), 119.34 (1C, C- α), 123.41 (1C, C-6), 127.40 (1C, C-1), 130.95 (d, $J(\text{C},\text{F})$ 9.0 Hz, 2C, C-2',6'), 134.83 (1C, C-1'), 145.41 (1C, C- β), 146.85 (1C, C-3), 148.42 (1C, C-4), 166.41 (1C, C-4'), 188.94 (1C, >C=O) ppm. ESI MS calcd. for $[\text{M} - \text{H}]$: 271.1; found: m/z 270.8 ($\text{M} - \text{H}$)⁻).

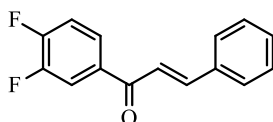
(*E*)-1-(3-Fluorophenyl)-3-phenylprop-2-en-1-one (**2a**)



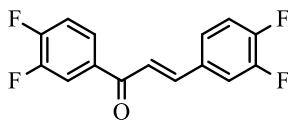
Yield 58%; white solid; mp 62-64 °C; ¹H NMR (600 MHz, CDCl₃): δ_{H} 7.29 (m, 1H, H-4'), 7.43-7.44 (m, 3H, H-2,4,6), 7.46 (d, $J(\text{H},\text{H})$ 15.6 Hz, 1H, H- α), 7.47-7.51 (m, 1H, H-3'), 7.64-7.66 (m, 2H, H-3,5), 7.69-7.71 (m, 1H, H-6'), 7.80 (d, $J(\text{H},\text{H})$ 7.8 Hz, 1H, H-2'), 7.82 (d, $J(\text{H},\text{H})$ 16.2 Hz, 1H, H- β); ¹³C NMR (150 MHz, CDCl₃): δ_{C} 115.30 (d, $J(\text{C},\text{F})$ 22.5 Hz, 1C, C-6'), 119.76 (d, $J(\text{C},\text{F})$ 22.5 Hz, 1C, C-4'), 121.61 (1C, C- α), 124.17 (1C, C-2), 128.55 (2C, C-2,6), 129.04 (2C, C-3,5), 130.30 (d, $J(\text{C},\text{F})$ 7.5 Hz, 1C, C-3'), 130.81 (1C, C-4), 134.71 (1C, C-1), 140.39 (d, $J(\text{C},\text{F})$ 6.0 Hz, 1C, C-1'), 145.60 (1C, C- β), 162.11 (d, $J(\text{C},\text{F})$ 246.0 Hz, 1C, C-5'), 189.19 (1C, >C=O). ESIMS calcd. for $[\text{M} + \text{H}]$: 227.1; found m/z 226.9 ($[\text{M} + \text{H}]$)⁺).

(E)-1,3-Bis(3-fluorophenyl)prop-2-en-1-one (2c)

Yield 58%; white solid; mp 83-84 °C; ^1H NMR (600 MHz, CDCl_3): δ_{H} 7.11-7.15 (m, 1H, H-2), 7.29-7.32 (m, 1H, H-4'), 7.33-7.34 (m, 1H, H-4), 7.38 (m, 2H, H-5,6), 7.45 (d, $J(\text{H,H})$ 15.6 Hz, 1H, H- α), 7.48 (m, 1H, H-3'), 7.69-7.71 (m, 1H, H-6'), 7.76 (d, $J(\text{H,H})$ 15.6 Hz, 1H, H- β), 7.79 (m, 1H, H-2') ppm. ^{13}C NMR (150 MHz, CDCl_3): δ_{C} 114.50 (d, $J(\text{C,F})$ 25.5 Hz, 1C, C-4), 115.25 (d, $J(\text{C,F})$ 27.0 Hz, 1C, C-6'), 117.60 (d, $J(\text{C,F})$ 25.5 Hz, 1C, C-2), 119.94 (d, $J(\text{C,F})$ 25.5 Hz, 1C, C-4'), 122.72 (1C, C- α), 124.19 (d, $J(\text{C,F})$ 3.0 Hz, 1C, C-2'), 124.63 (d, $J(\text{C,F})$ 3.0 Hz, 1C, C-6), 130.35 (d, $J(\text{C,F})$ 9.0 Hz, 1C, C-3'), 130.56 (d, $J(\text{C,F})$ 10.5 Hz, 1C, C-5), 136.94 (d, $J(\text{C,F})$ 9.0 Hz, 1C, C-1), 140.05 (d, $J(\text{C,F})$ 7.5 Hz, 1C, C-1'), 144.03 (1C; C- β), 162.0 (d, $J(\text{C,F})$ 295.5 Hz, 1C, C-3), 162.12 (d, $J(\text{C,F})$ 294.0 Hz, 1C, C-5'), 188.84 (1C, $>\text{C}=\text{O}$). ESIMS calcd. for $[\text{M}]$: 244.1; found: m/z 243.9 ($[\text{M}]^+$).

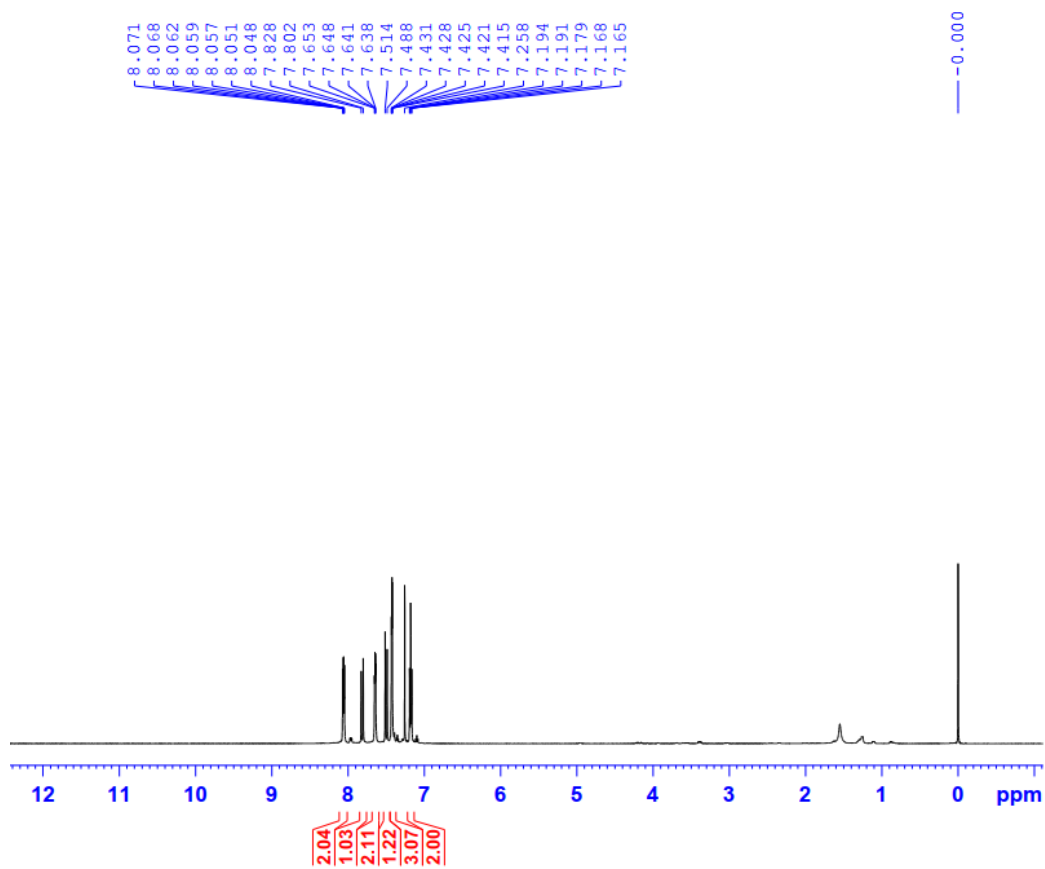
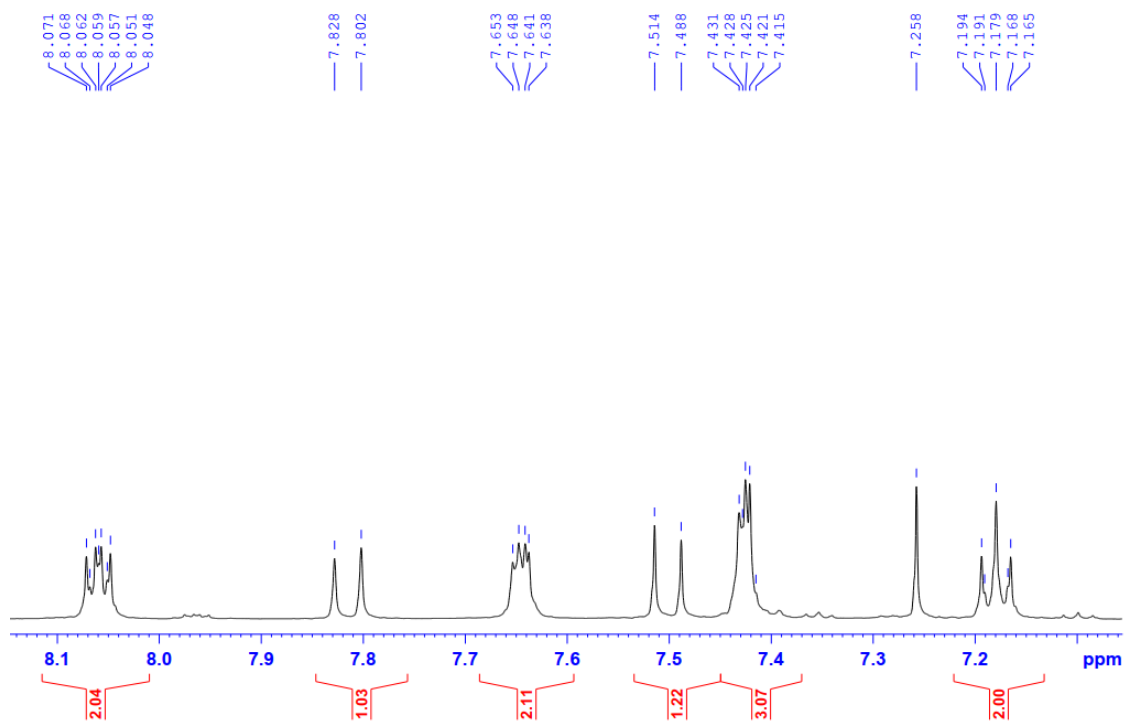
(E)-1-(3,4-Difluorophenyl)-3-phenylprop-2-en-1-one (3a)

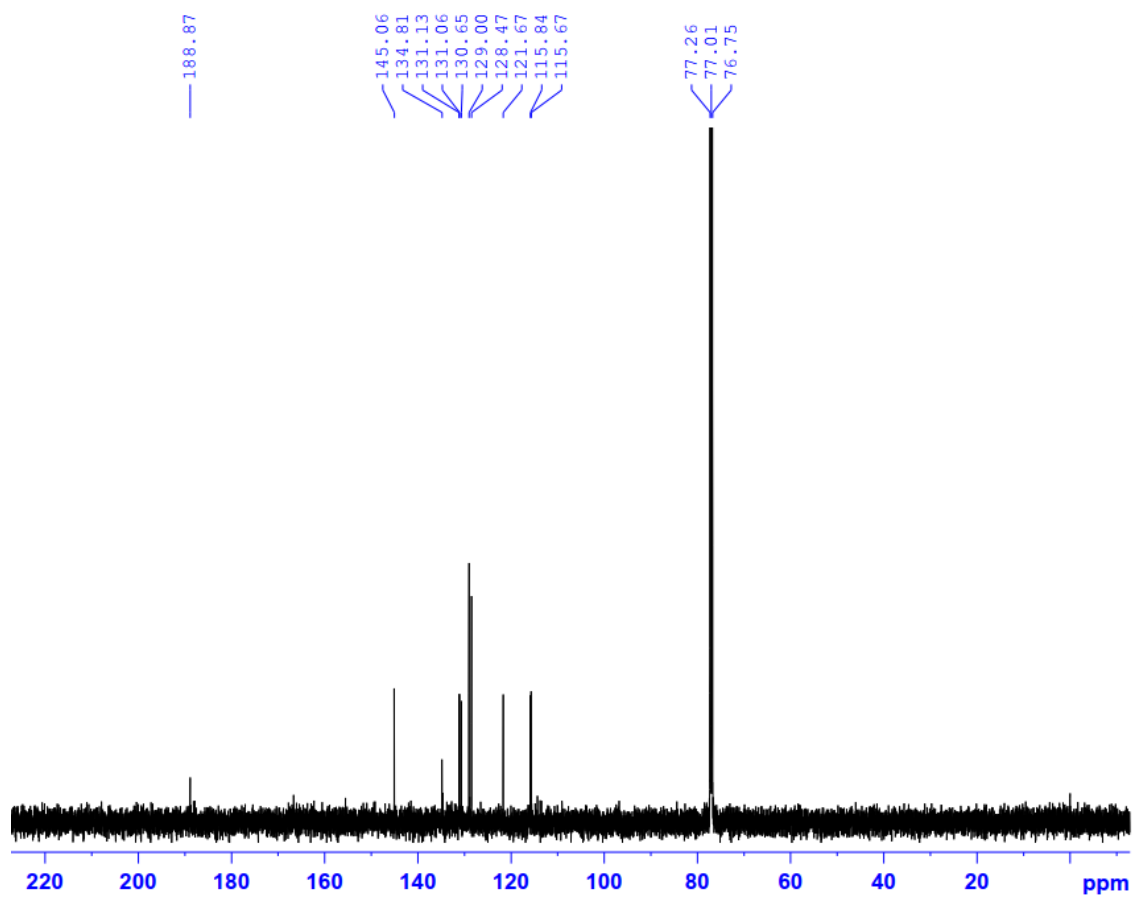
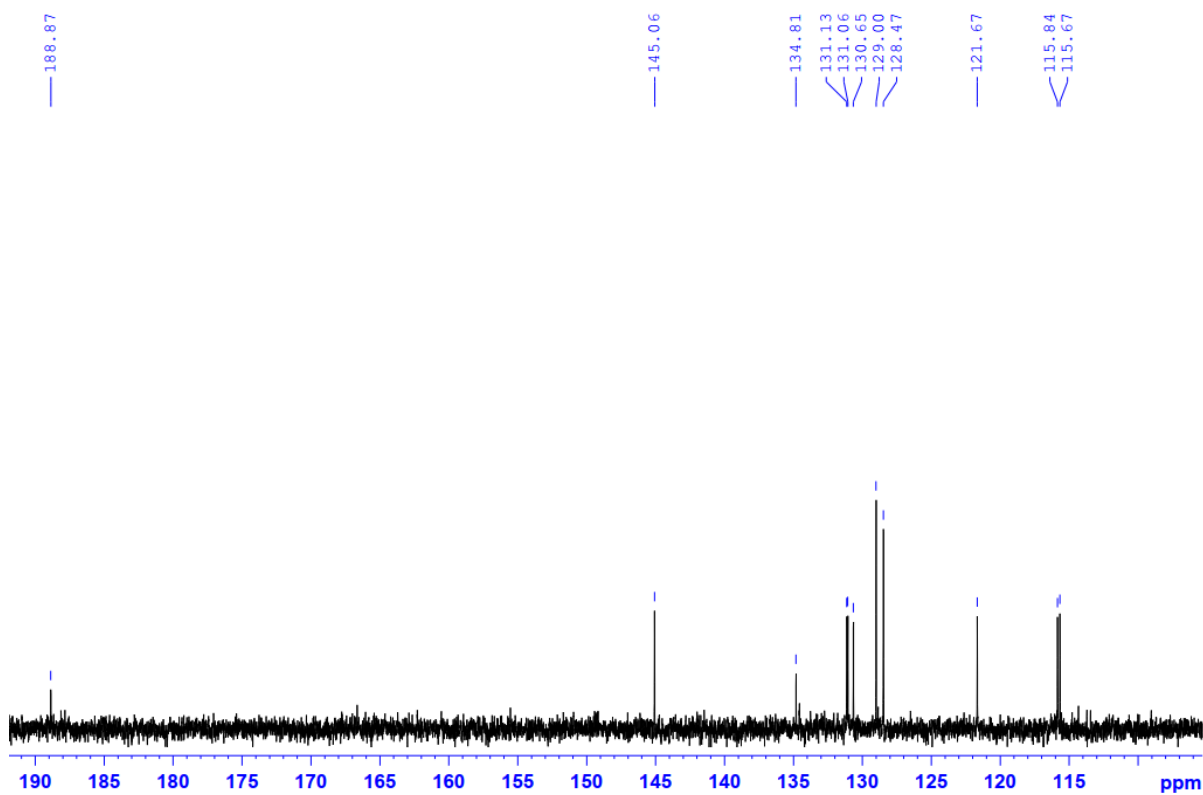
Yield 51%; white solid; mp 81-82 °C; ^1H NMR (600 MHz, CDCl_3): δ_{H} 7.27-7.31 (m, 1H, H-3'), 7.43-7.45 (m, 3H, H-2,4,6), 7.44 (d, $J(\text{H,H})$ 15.6 Hz, 1H, H- β), 7.64-7.66 (m, 2H, H-3,5), 7.80-7.81 (m, 1H, H-2'), 7.82 (d, $J(\text{H,H})$ 15.6 Hz, 1H, H- α), 7.85-7.89 (m, 1H, H-6'). ^{13}C NMR (150 MHz, CDCl_3): δ_{C} 117.48 (d, $J(\text{C,F})$ 18.0 Hz, 1C, C-3'), 117.81 (d, $J(\text{C,F})$ 18.0 Hz, 1C, C-6'), 120.96 (1C, C- α), 125.31 (d, $J(\text{C,F})$ 7.5 Hz, 1C, C-2'), 128.57 (2C, C-3,5), 129.06 (2C, C-2,6), 130.91 (1C, C-4), 134.59 (1C, C-1), 135.26 (1C, C-1'), 145.80 (1C, C- β), 187.71 (1C, $>\text{C}=\text{O}$). ESIMS calcd. for $[\text{M} + \text{H}]$: 245.1; found: m/z 244.9 ($[\text{M} + \text{H}]^+$).

(E)-1,3-Bis(3,4-Difluorophenyl)prop-2-en-1-one (3e)

Yield 32%; white solid; mp 132-133 °C; ^1H NMR (600 MHz, CDCl_3): δ_{H} 7.21-7.25 (m, 1H, H-5), 7.28-7.32 (m, 1H, H-6), 7.35 (d, $J(\text{H,H})$ 15.6 Hz, 1H, H- α), 7.36-7.39 (m, 1H, H-2); 7.46-7.49 (m, 1H, H-

3'), 7.72 (d, $J(\text{H,H})$ 15.6 Hz, 1H, H- β), 7.79-7.82 (m, 1H, H-2'), 7.85-7.88 (m, 1H; H-6'). ^{13}C NMR (150 MHz, CDCl_3): δ_{C} 116.56 (d, $J(\text{C,F})$ 21.0 Hz, 1C, C-3'), 117.59 (d, $J(\text{C,F})$ 21.0 Hz, 1C, C-6), 117.82 (d, $J(\text{C,F})$ 25.5 Hz, 1C, C-6'), 117.97 (d, $J(\text{C,F})$ 22.5 Hz, 1C, C-5), 121.74 (1C, C- α), 125.34-125.53 (m, C-2,2'), 131.78 (1C, C-1), 134.93 (1C, C-1'), 143.26 (1C, C- β), 149.52-152.66 (4C, C-3,4,4',5'), 187.13 (1 C, $>\text{C}=\text{O}$). ESIMS calcd. for $[\text{2M} - \text{H}]^-$: 559.1; found: m/z 559.0 ($[\text{2M} - \text{H}]^-$).

2. ^1H , ^{13}C NMR, HSQC and HRESIMS/ESIMS spectra of all fluorinated chalconoidsFigure S1a. ^1H -NMR spectrum of **1a**.Figure S1b. ^1H -NMR spectrum of **1a**.

Figure S1c. ^{13}C -NMR spectrum of 1a.Figure S1d. ^{13}C -NMR spectrum of 1a.

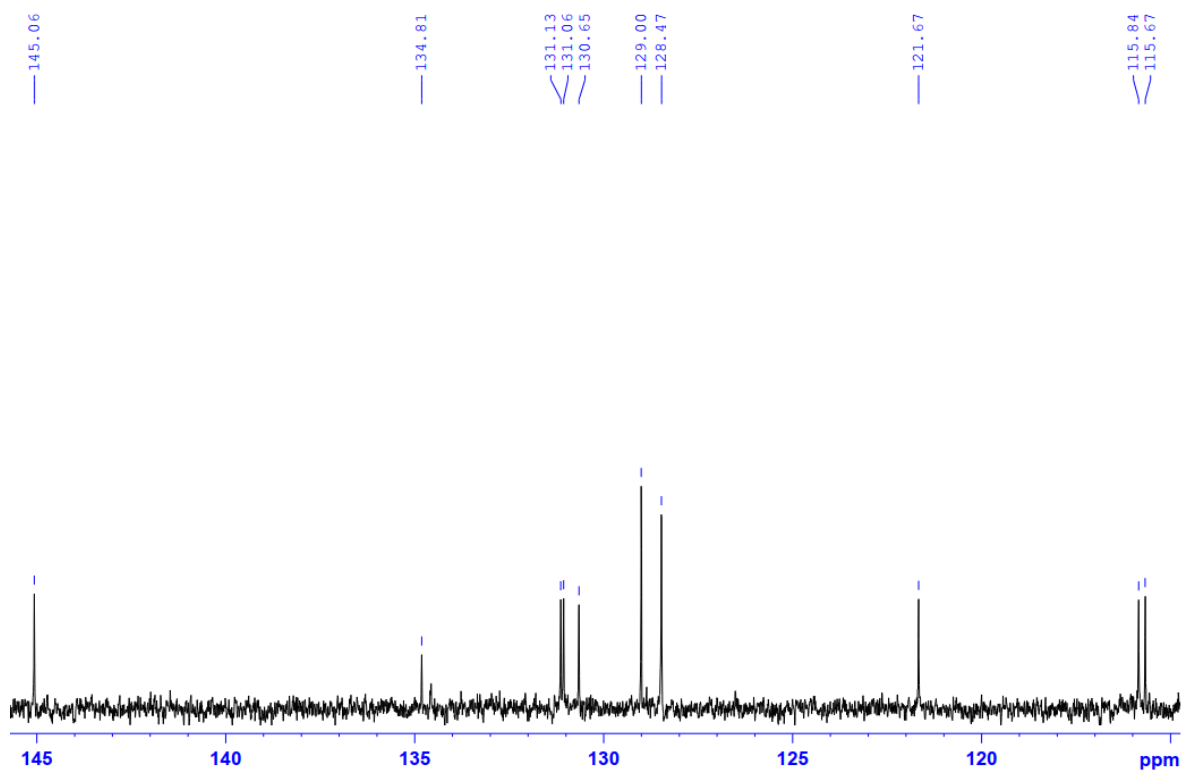
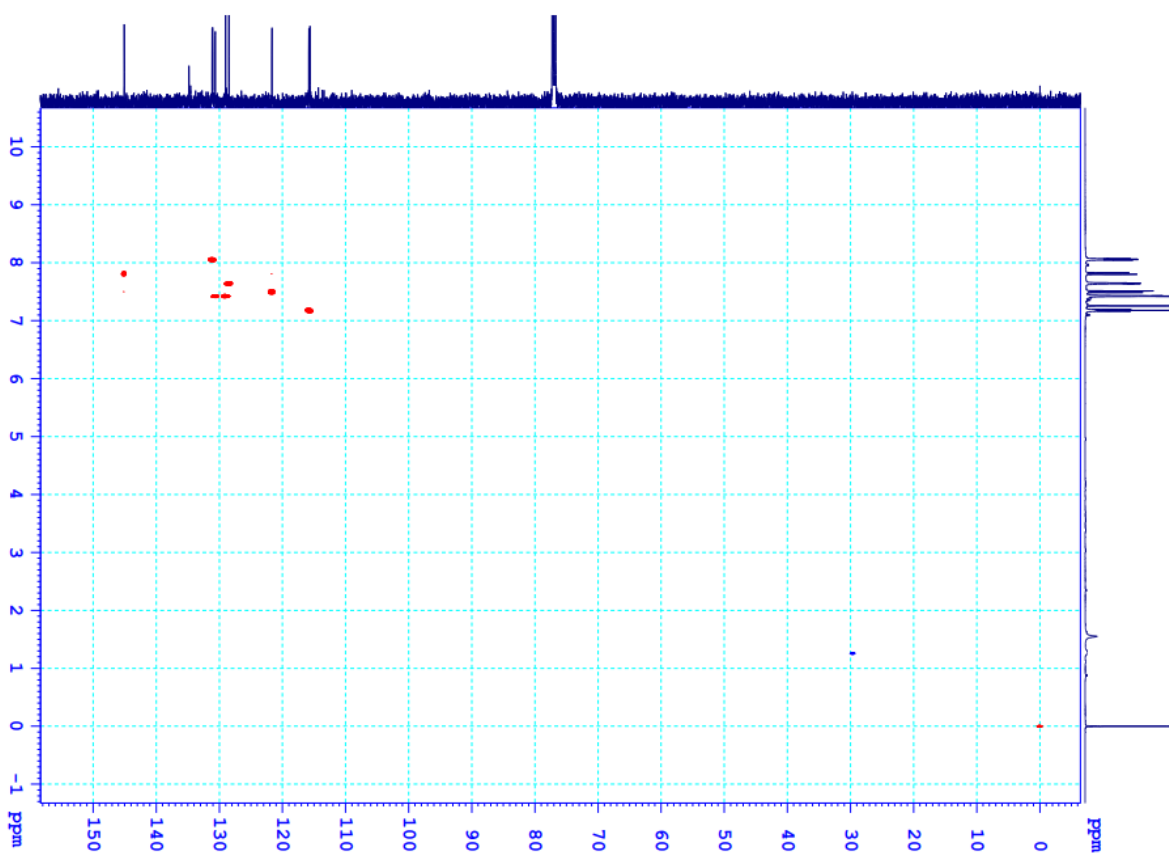
Figure S1e. ^{13}C -NMR spectrum of 1a.

Figure S1f. HSQC spectrum of 1a.

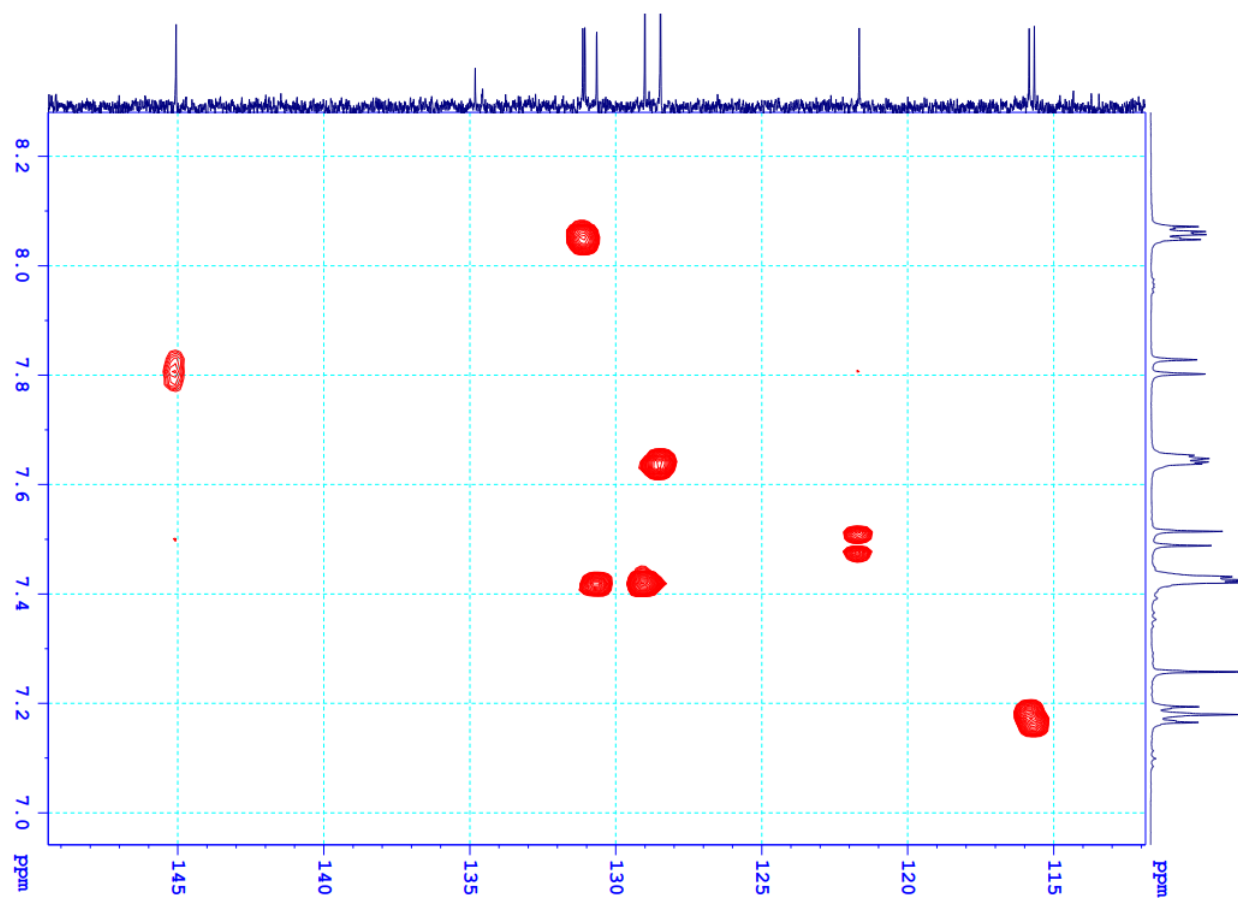


Figure S1g. HSQC spectrum of 1a.

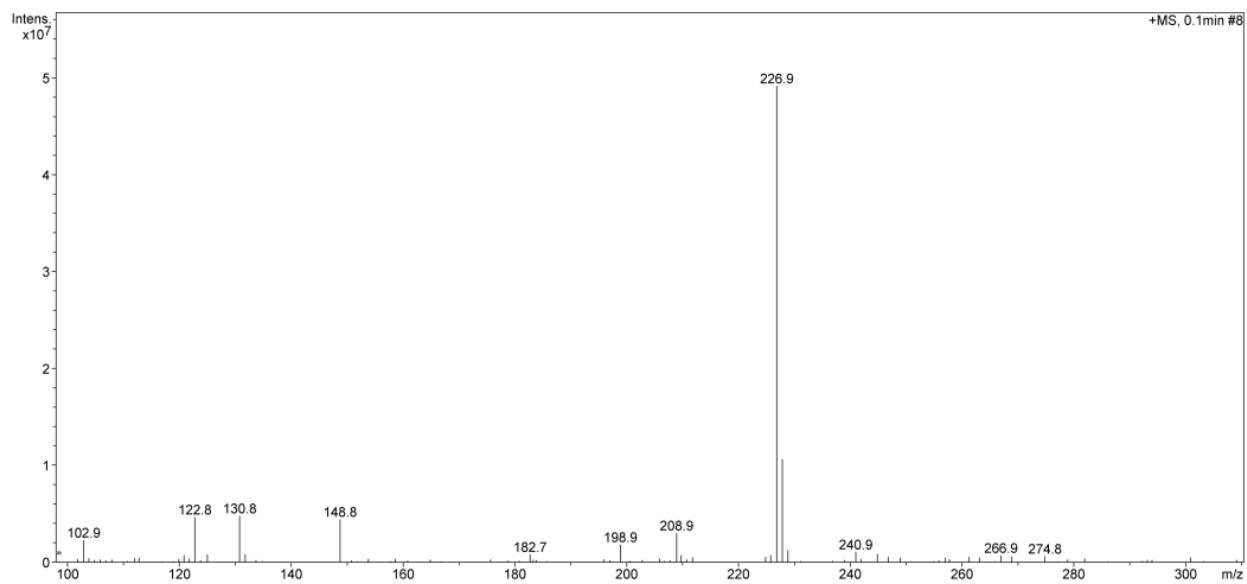
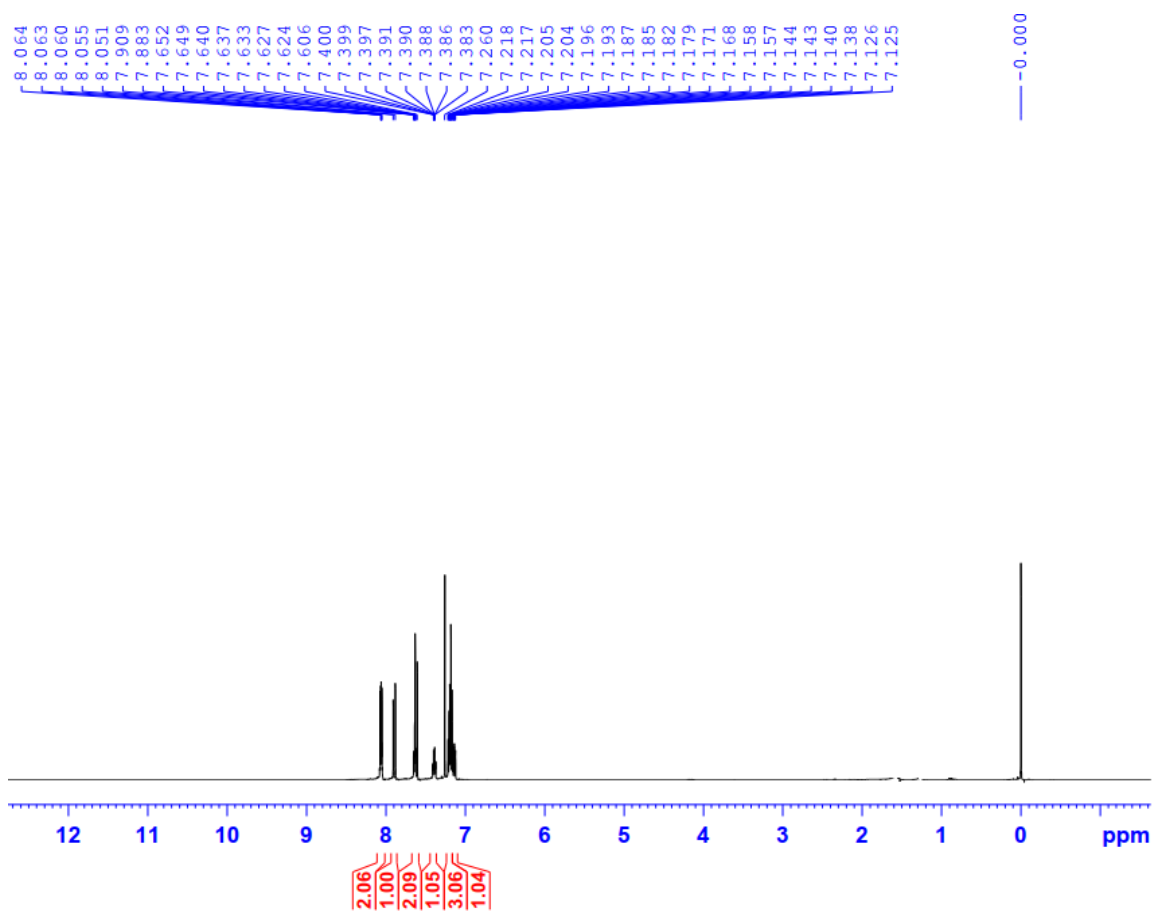
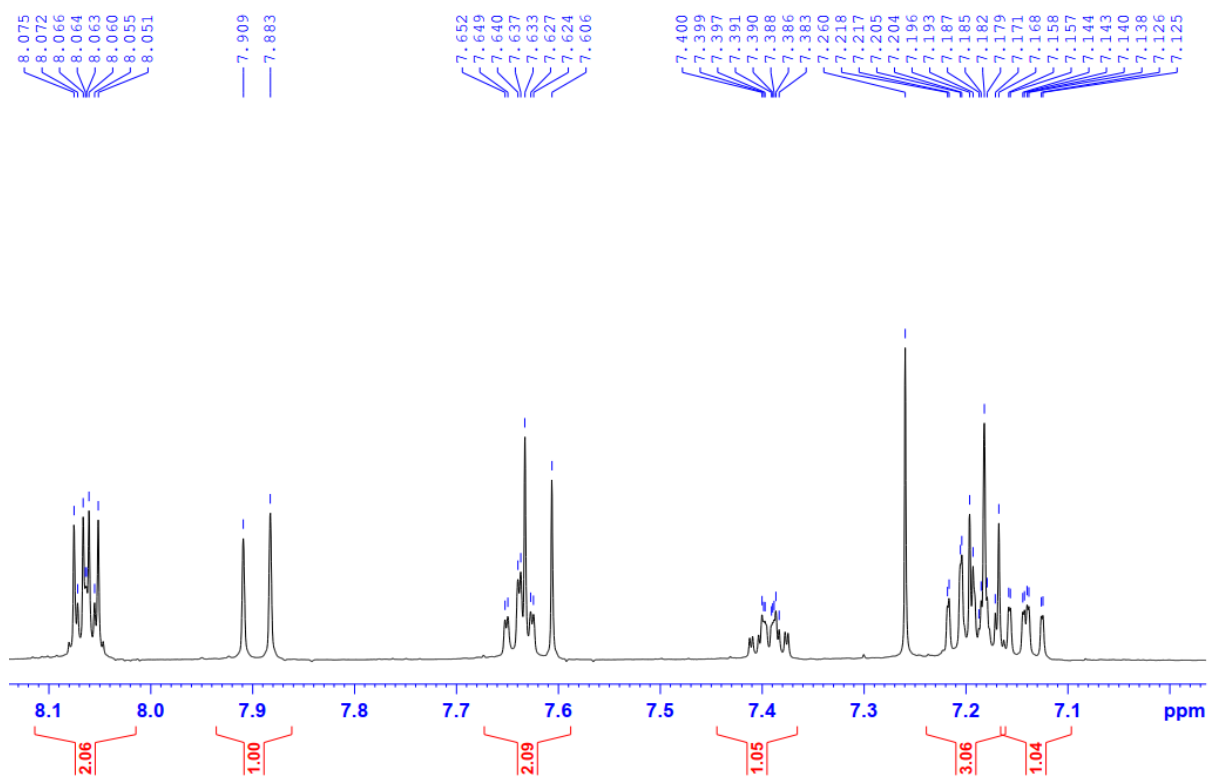
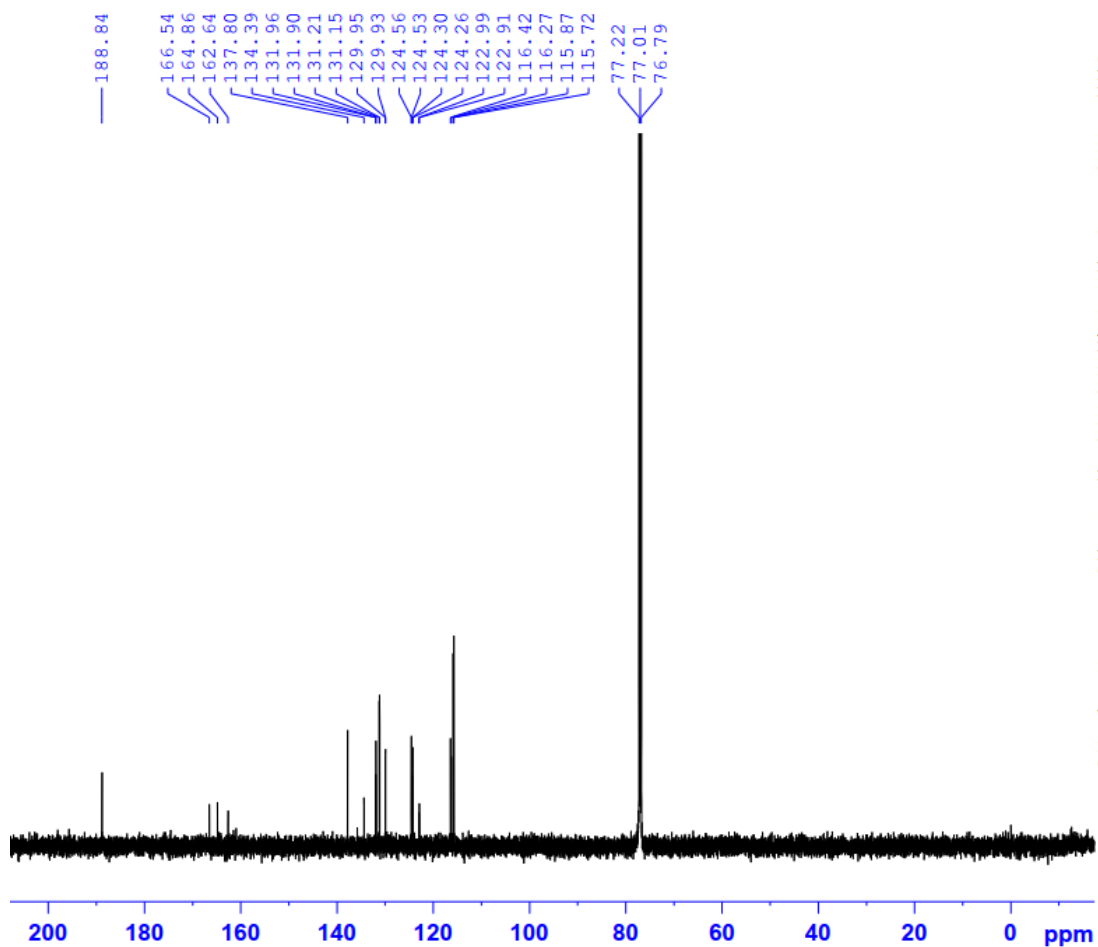
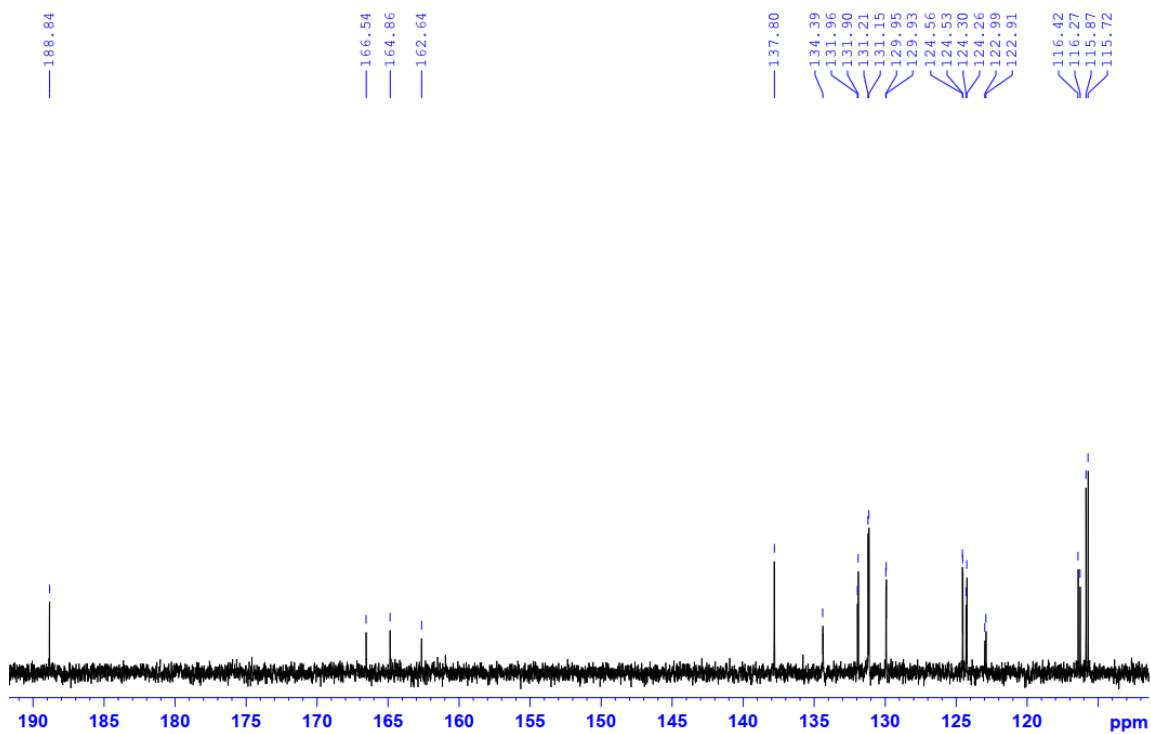
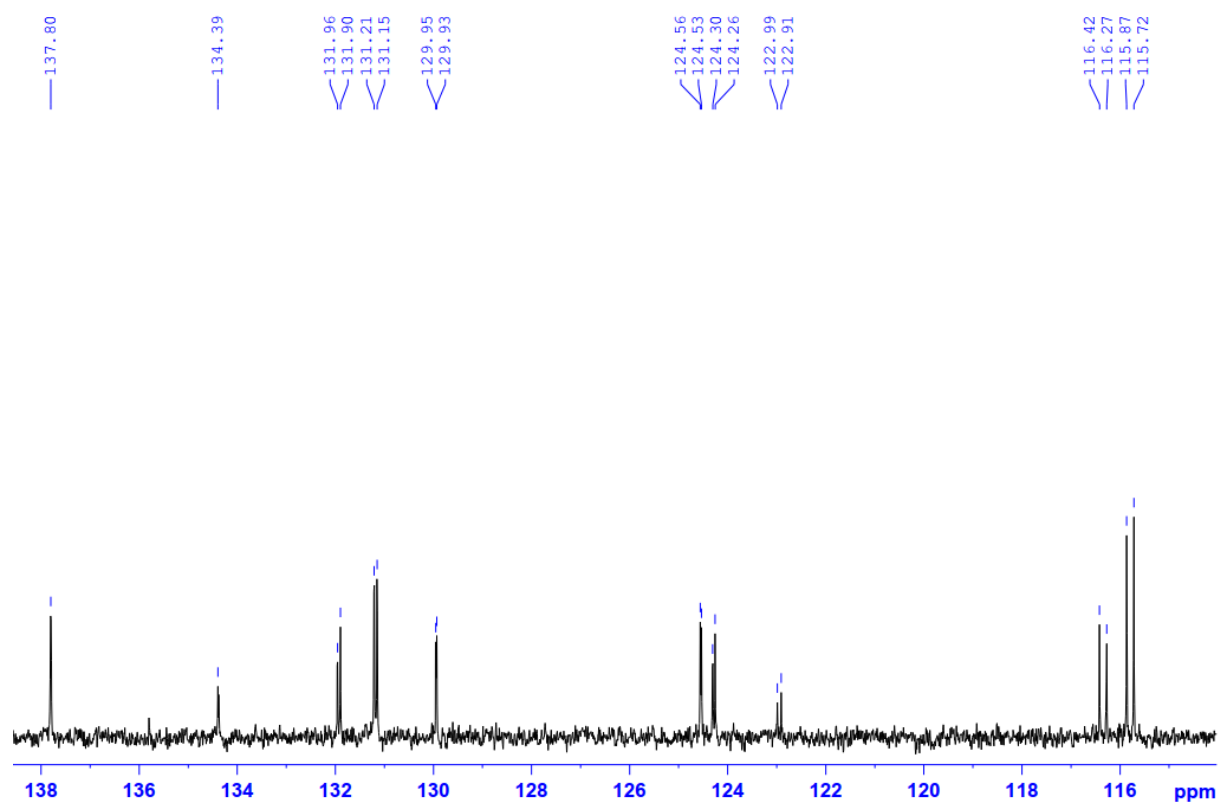
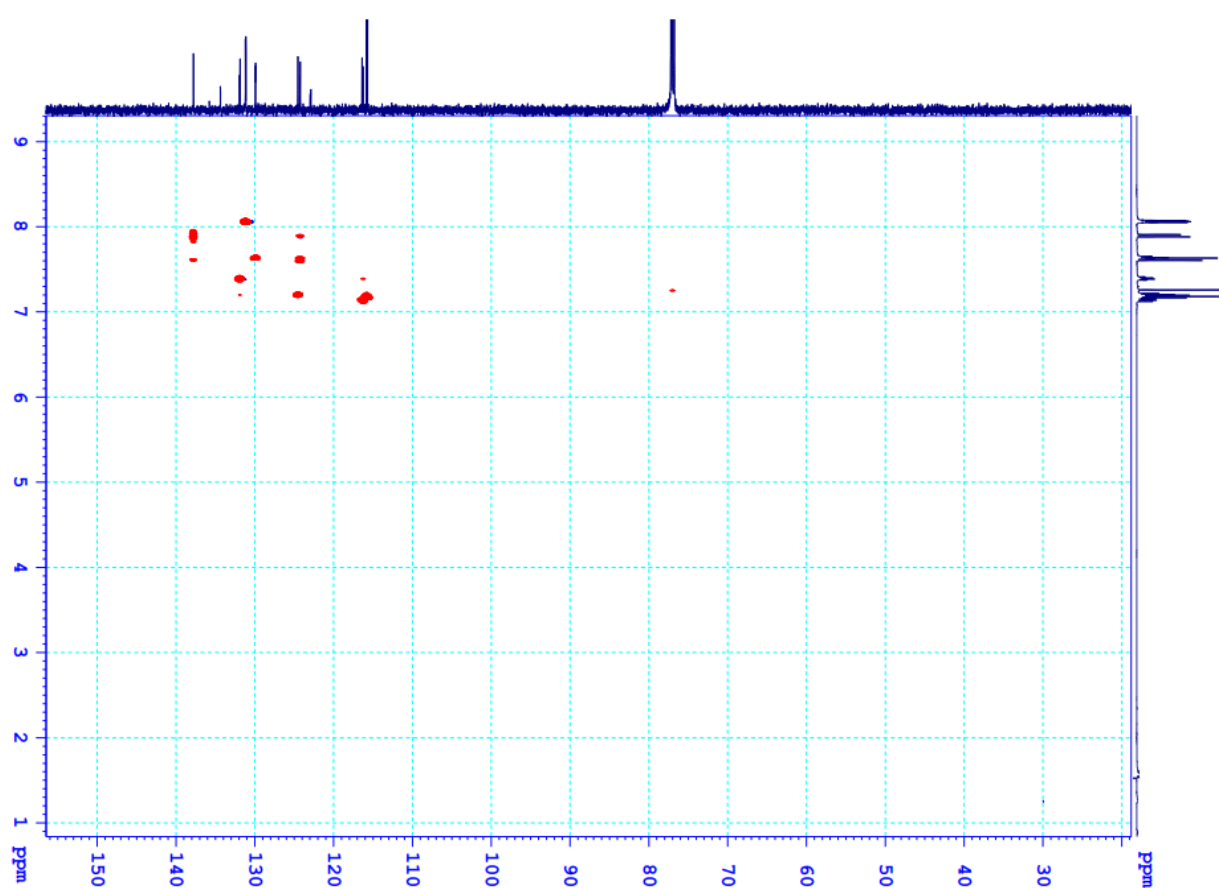
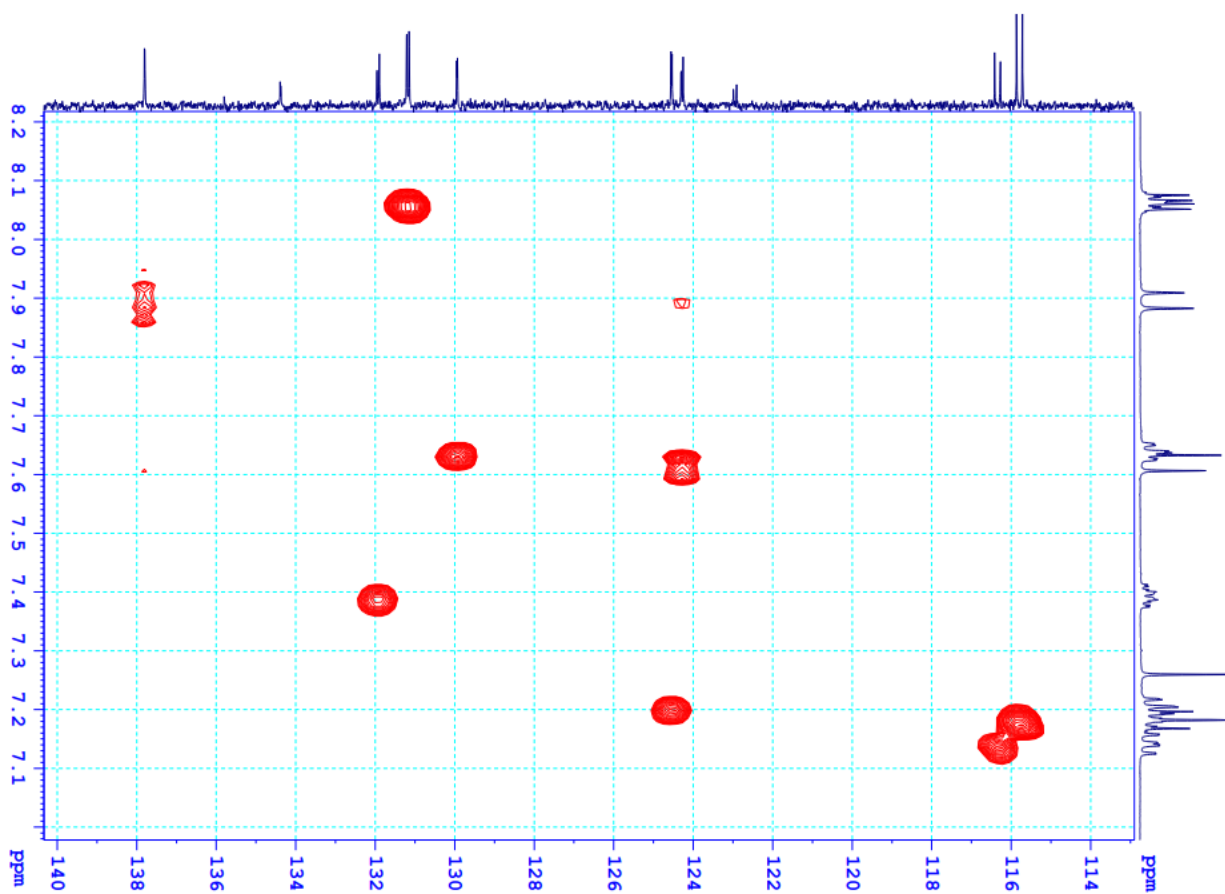
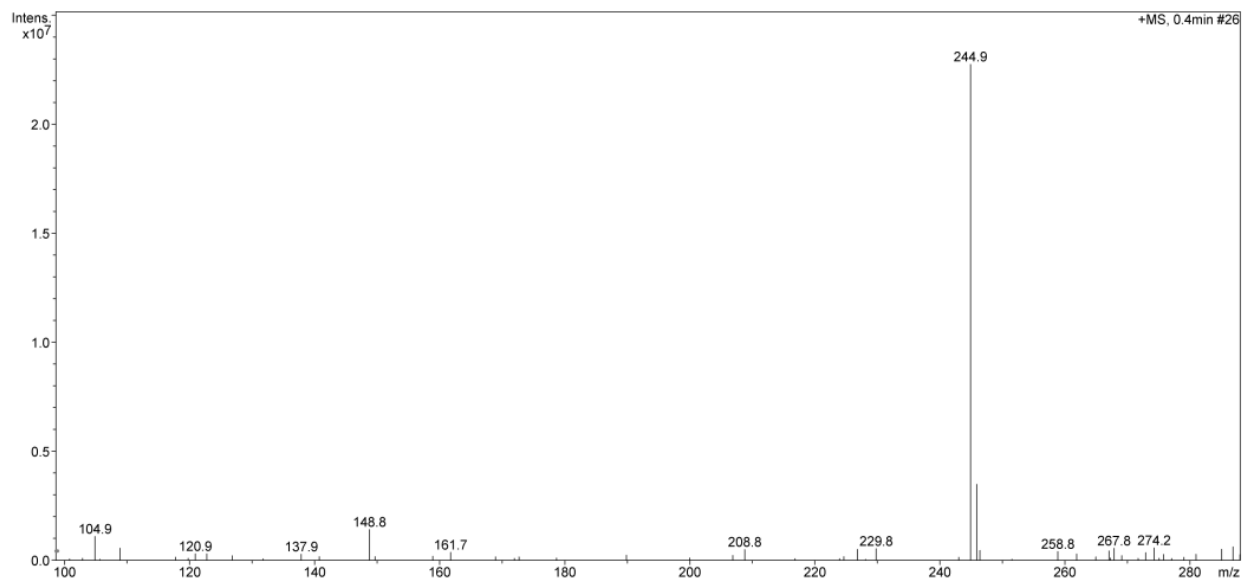


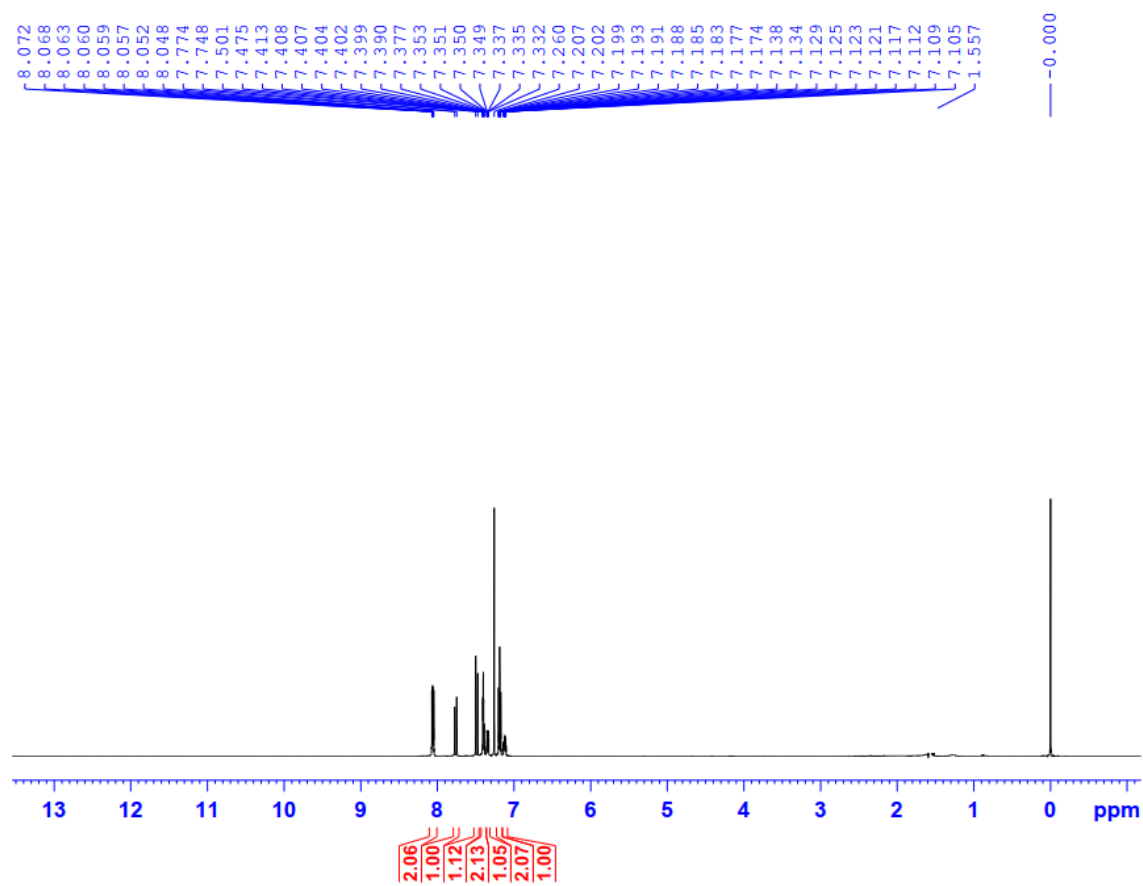
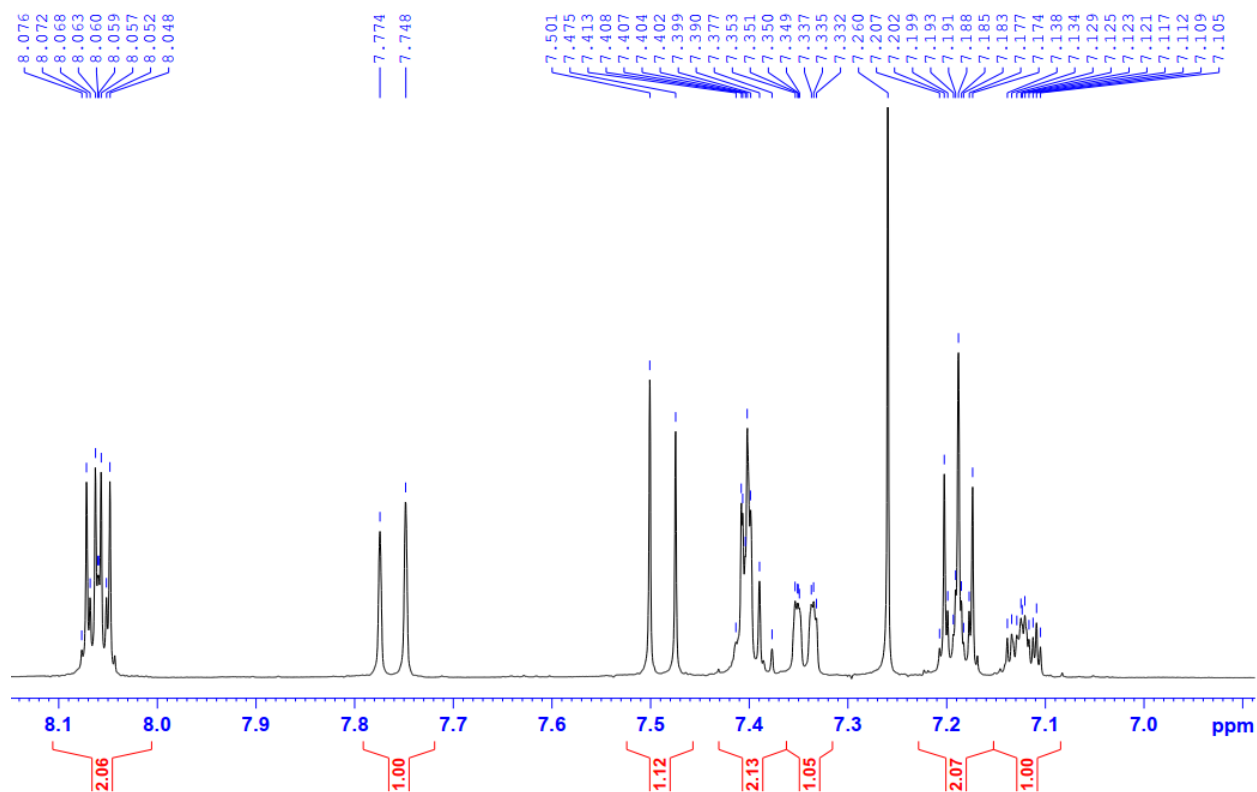
Figure S1h. MS of 1a.

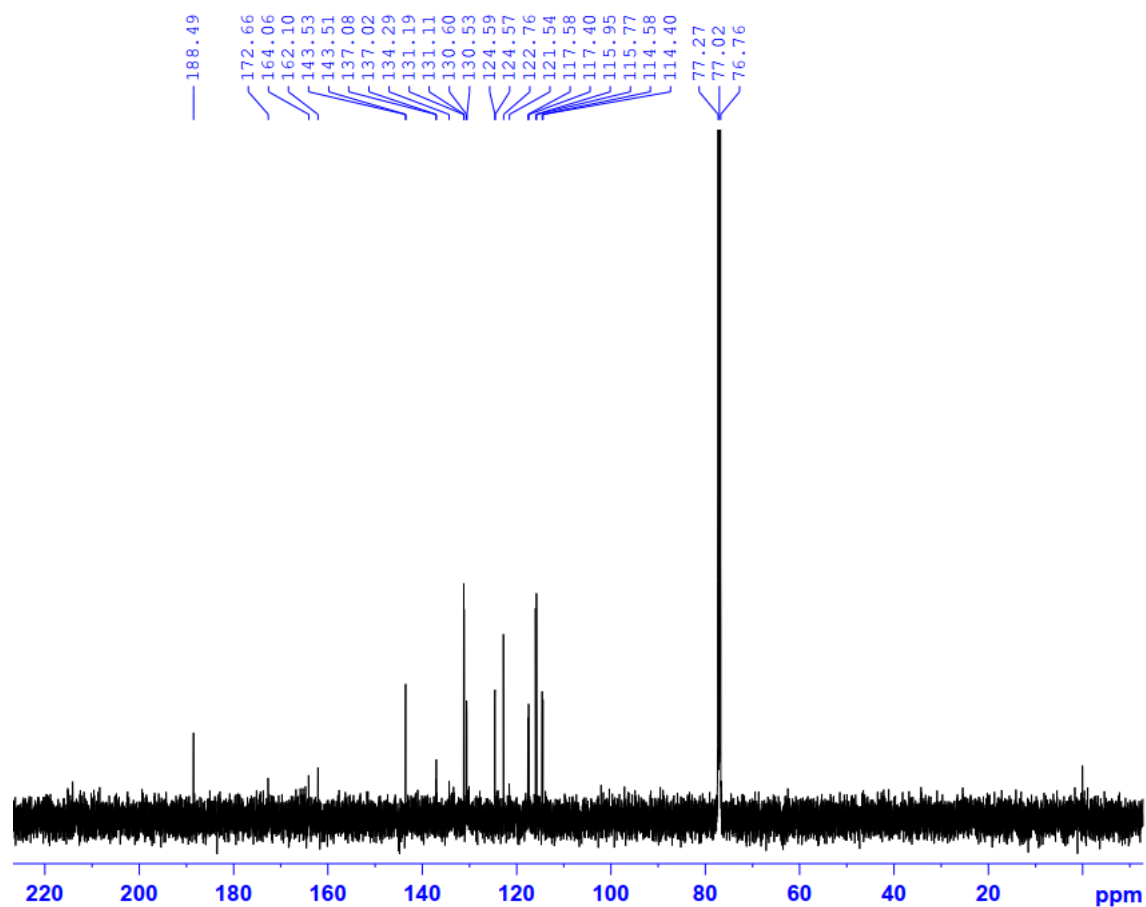
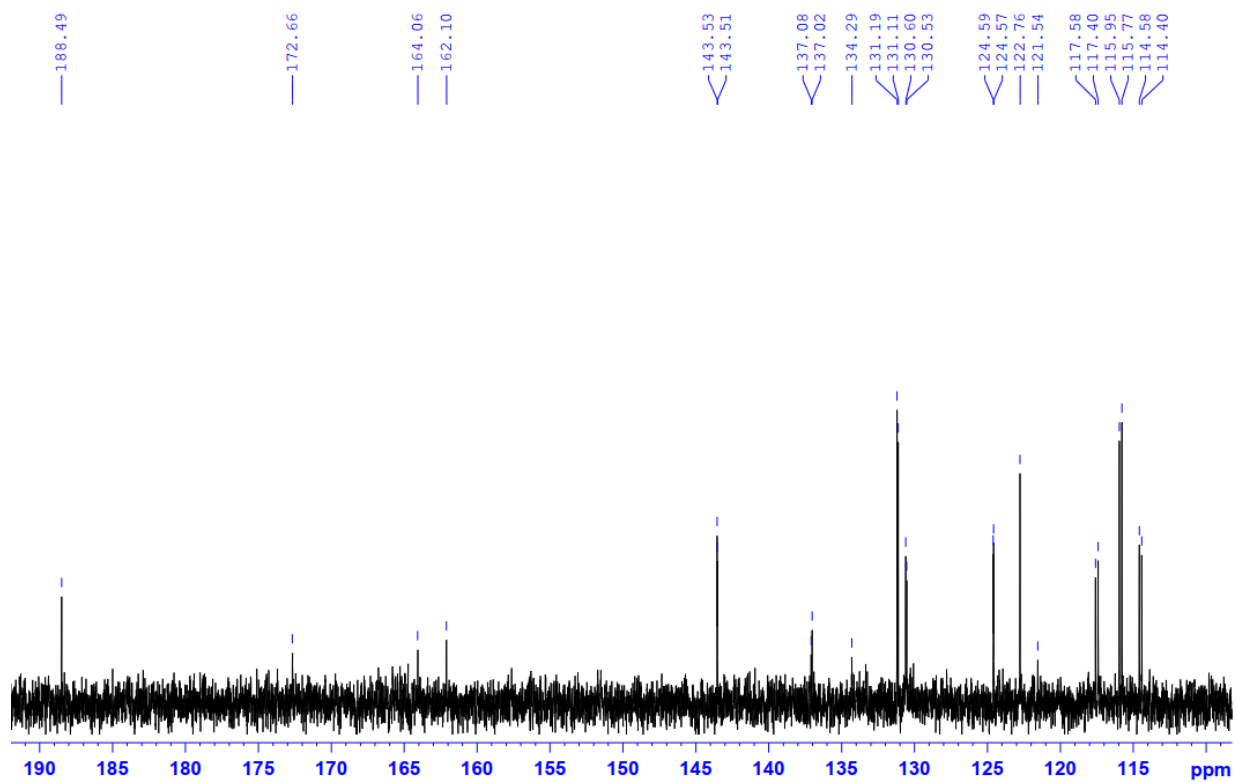
Figure S2a. $^1\text{H-NMR}$ spectrum of **1b**.Figure S2b. $^1\text{H-NMR}$ spectrum of **1b**.

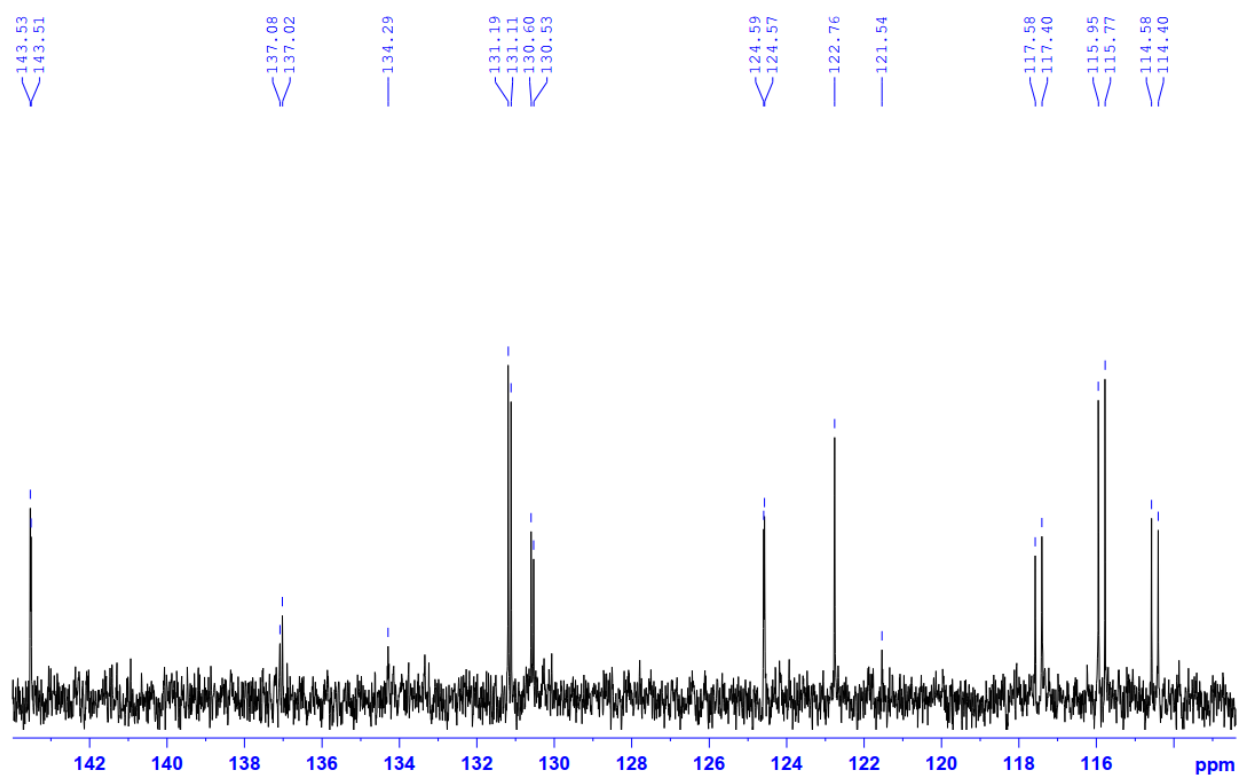
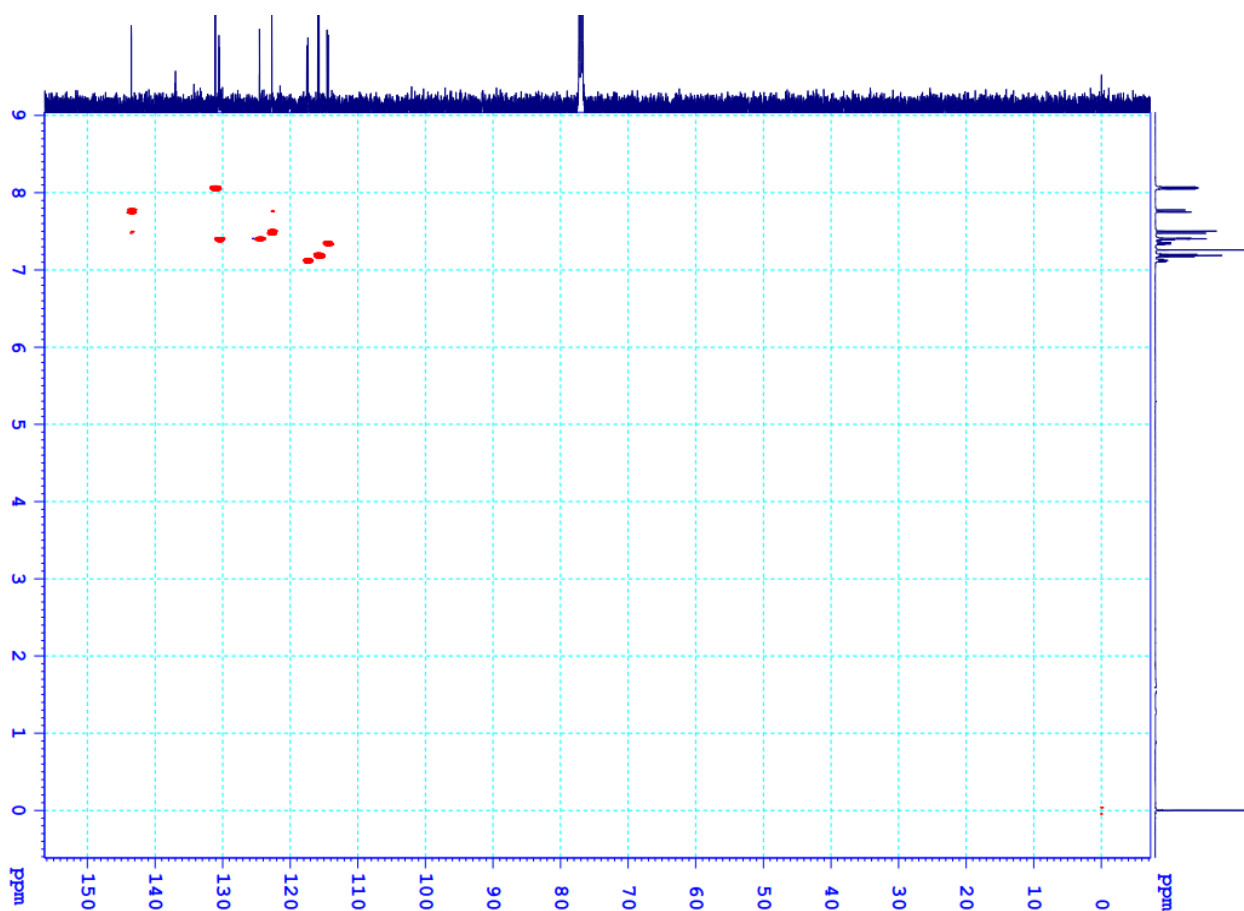
Figure S2c. ^{13}C -NMR spectrum of **1b**.Figure S2d. ^{13}C -NMR spectrum of **1b**.

Figure S2e. ^{13}C -NMR spectrum of **1b**.Figure S2f. HSQC spectrum of **1b**.

Figure S2g. HSQC spectrum of **1b**.Figure S2h. MS of **1b**.

Figure S3a. ¹H-NMR spectrum of **1c**.Figure S3b. ¹H-NMR spectrum of **1c**.

Figure S3c. ¹³C-NMR spectrum of 1c.Figure S3d. ¹³C-NMR spectrum of 1c.

Figure S3e. ^{13}C -NMR spectrum of **1c**.Figure S3f. HSQC spectrum of **1c**.

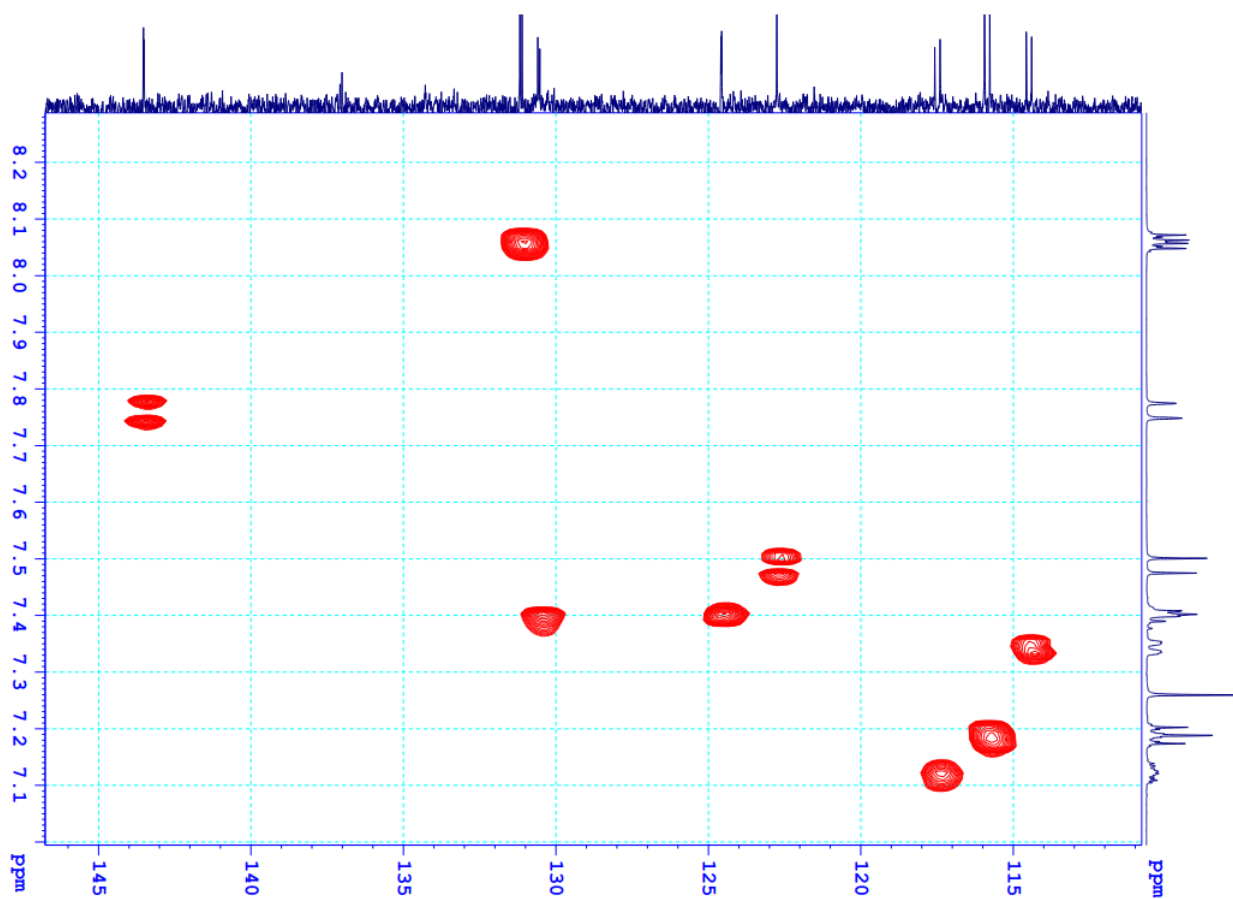


Figure S3g. HSQC spectrum of 1c.

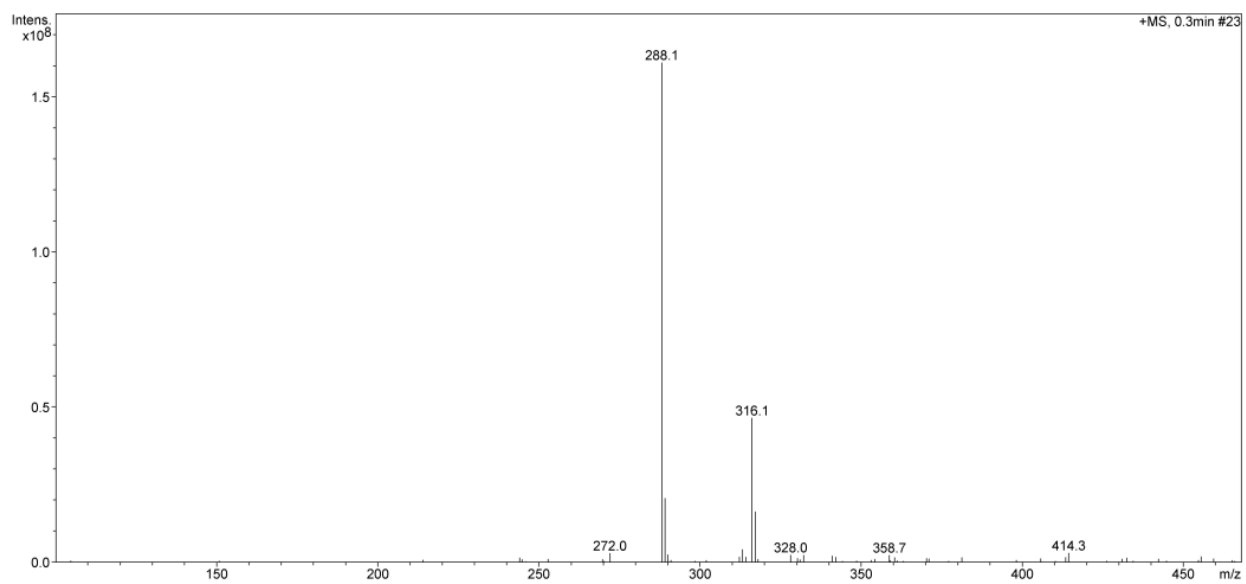
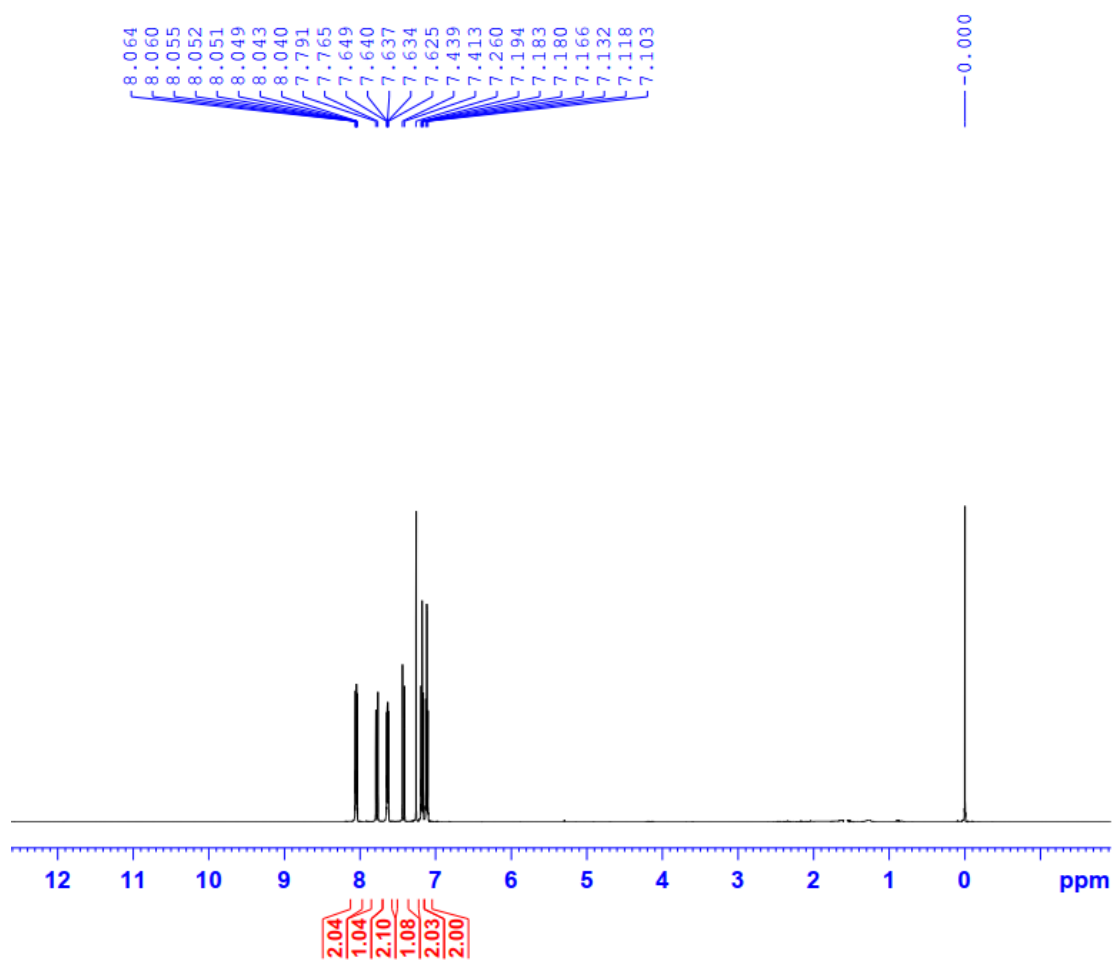
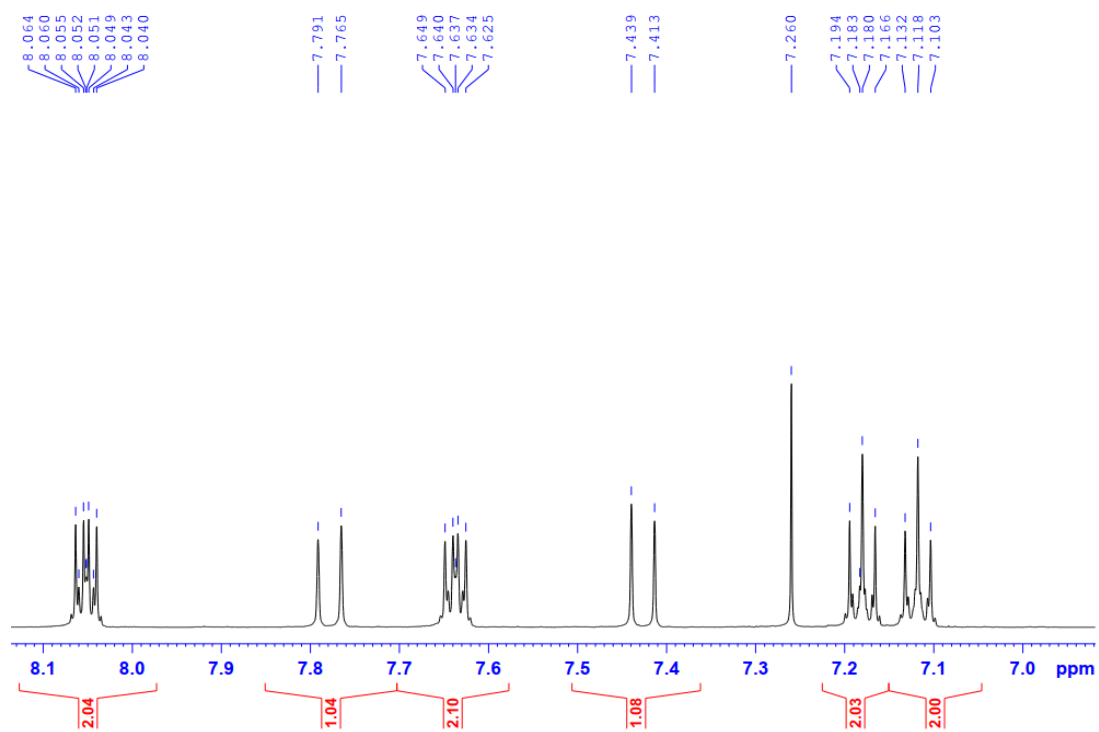
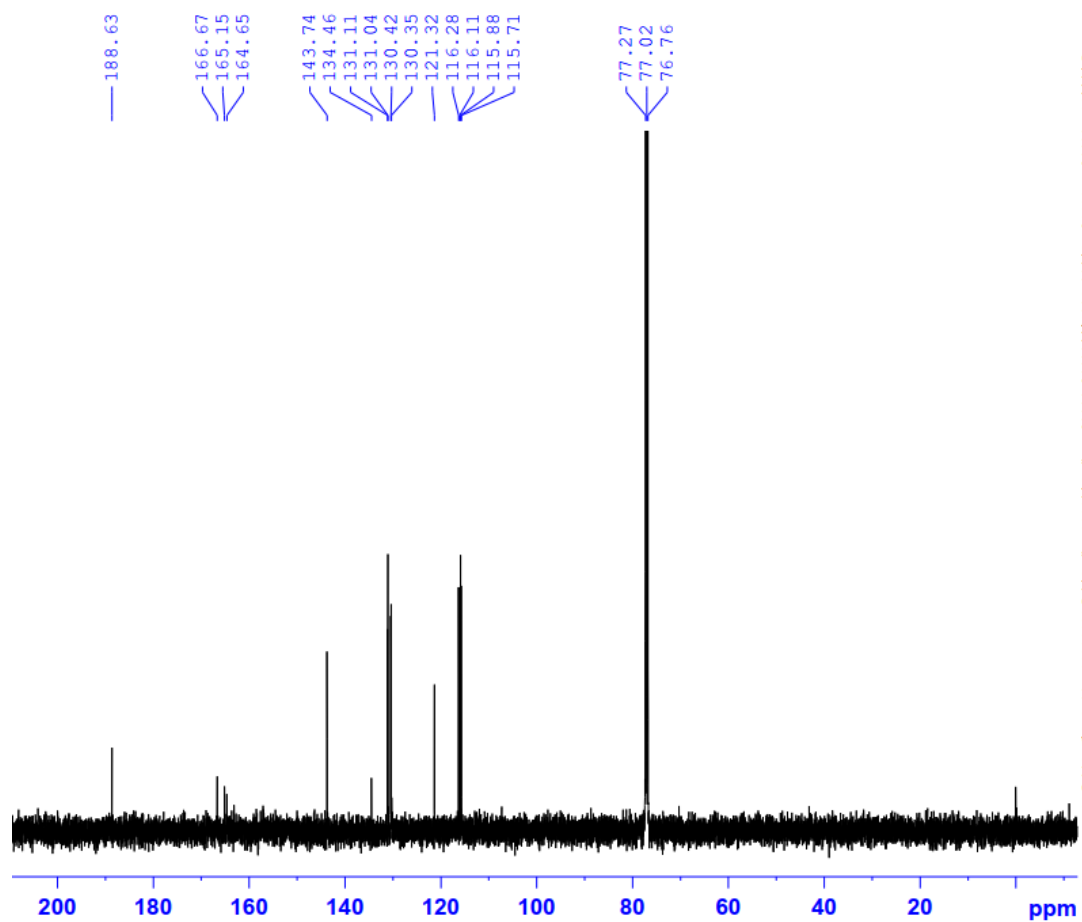
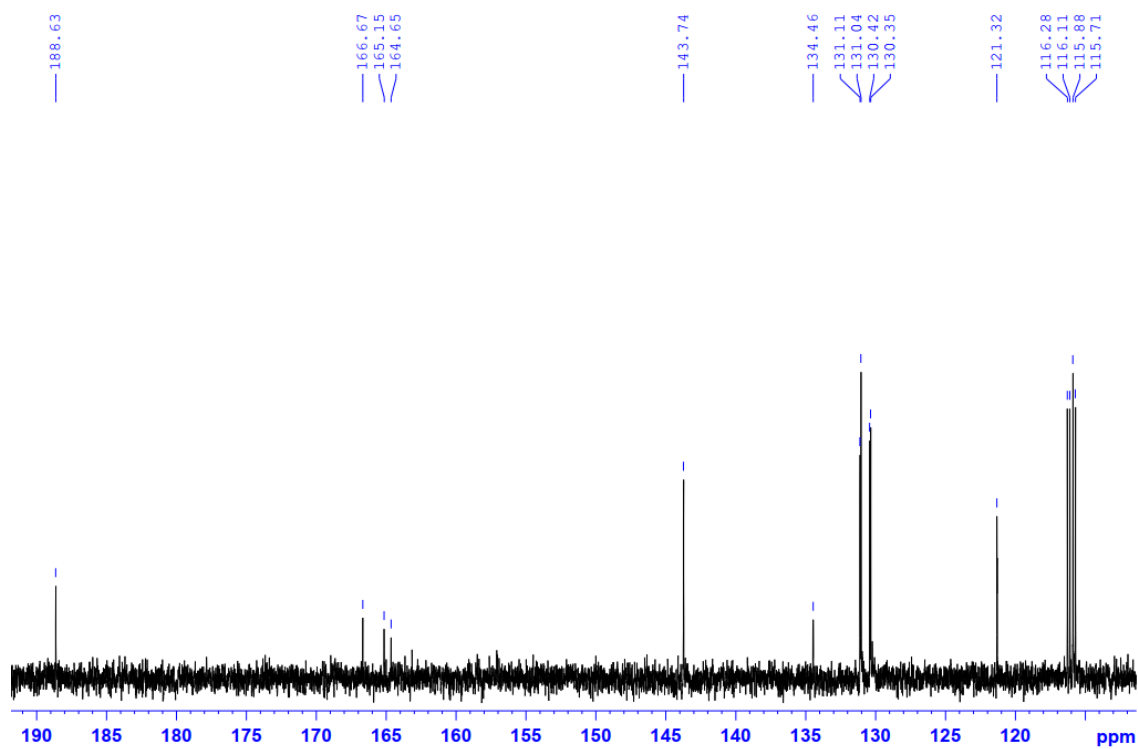


Figure S3h. MS of 1c.

Figure S4a. ¹H-NMR spectrum of 1d.Figure S4b. ¹H-NMR spectrum of 1d.

Figure S4c. ¹³C-NMR spectrum of 1d.Figure S4d. ¹³C-NMR spectrum of 1d.

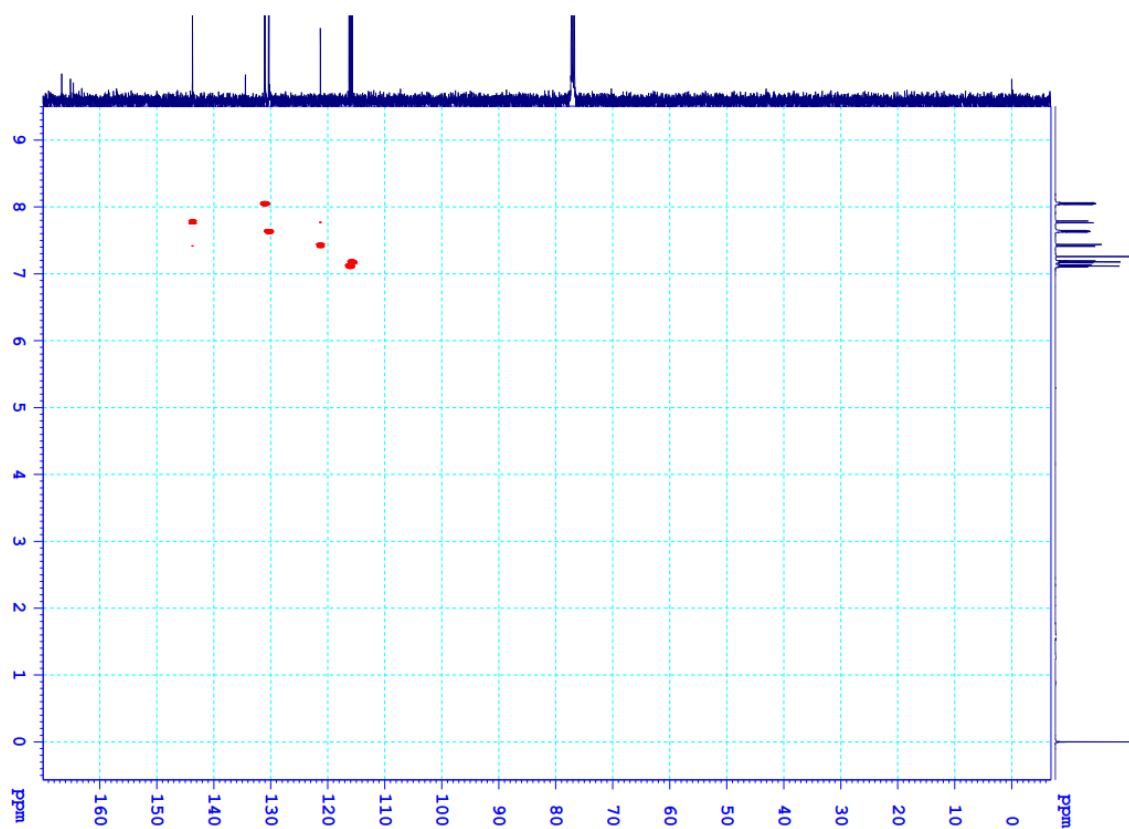


Figure S4e. HSQC spectrum of 1d.

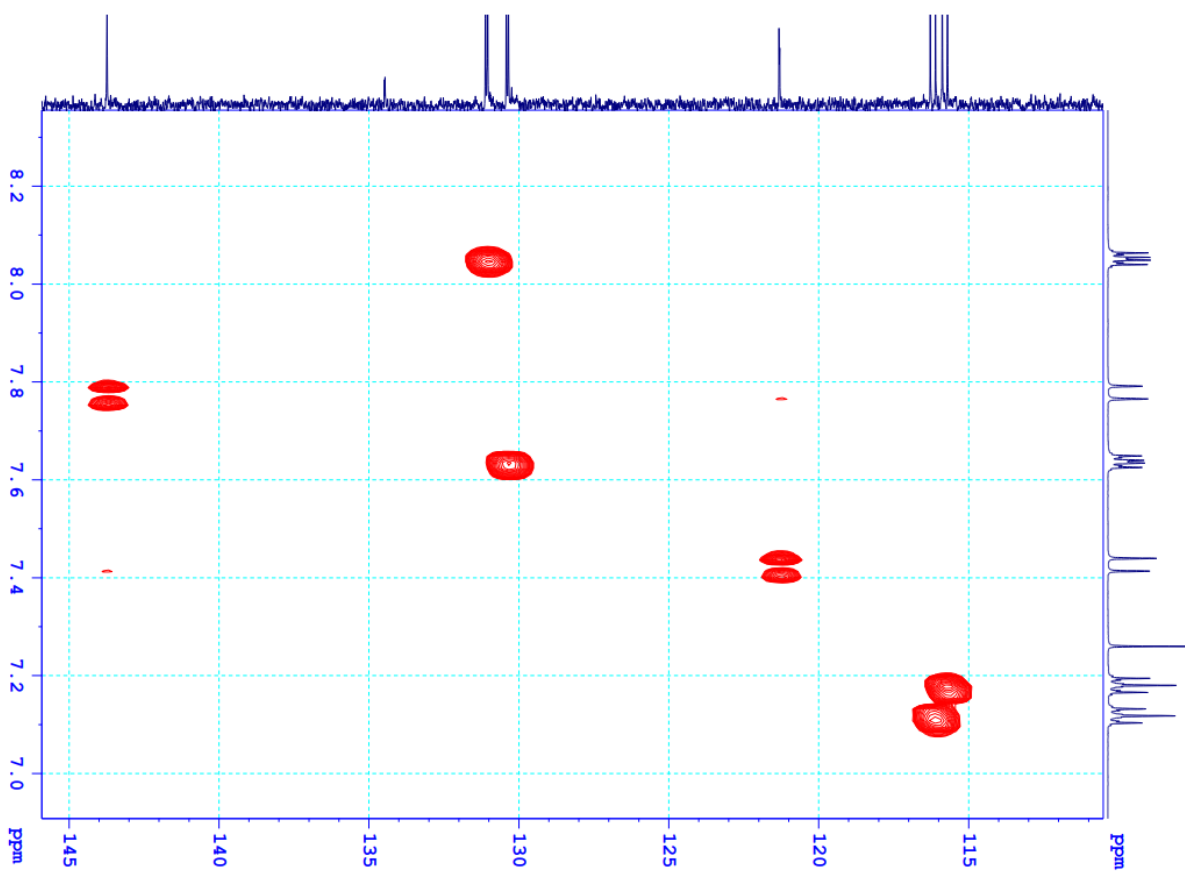


Figure S4f. HSQC spectrum of 1d.

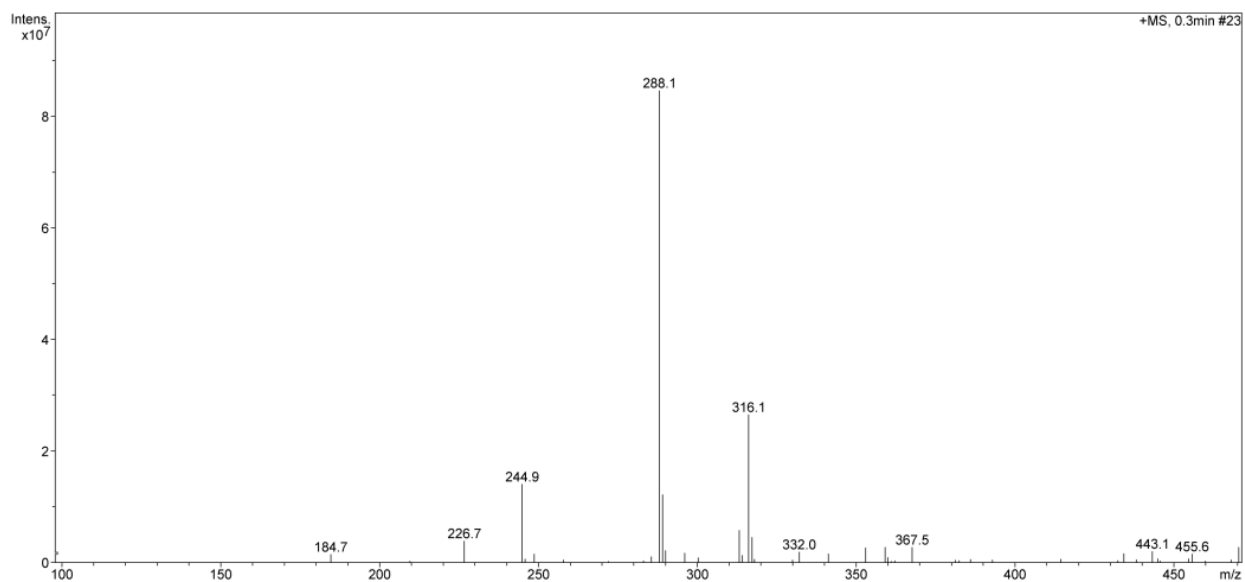
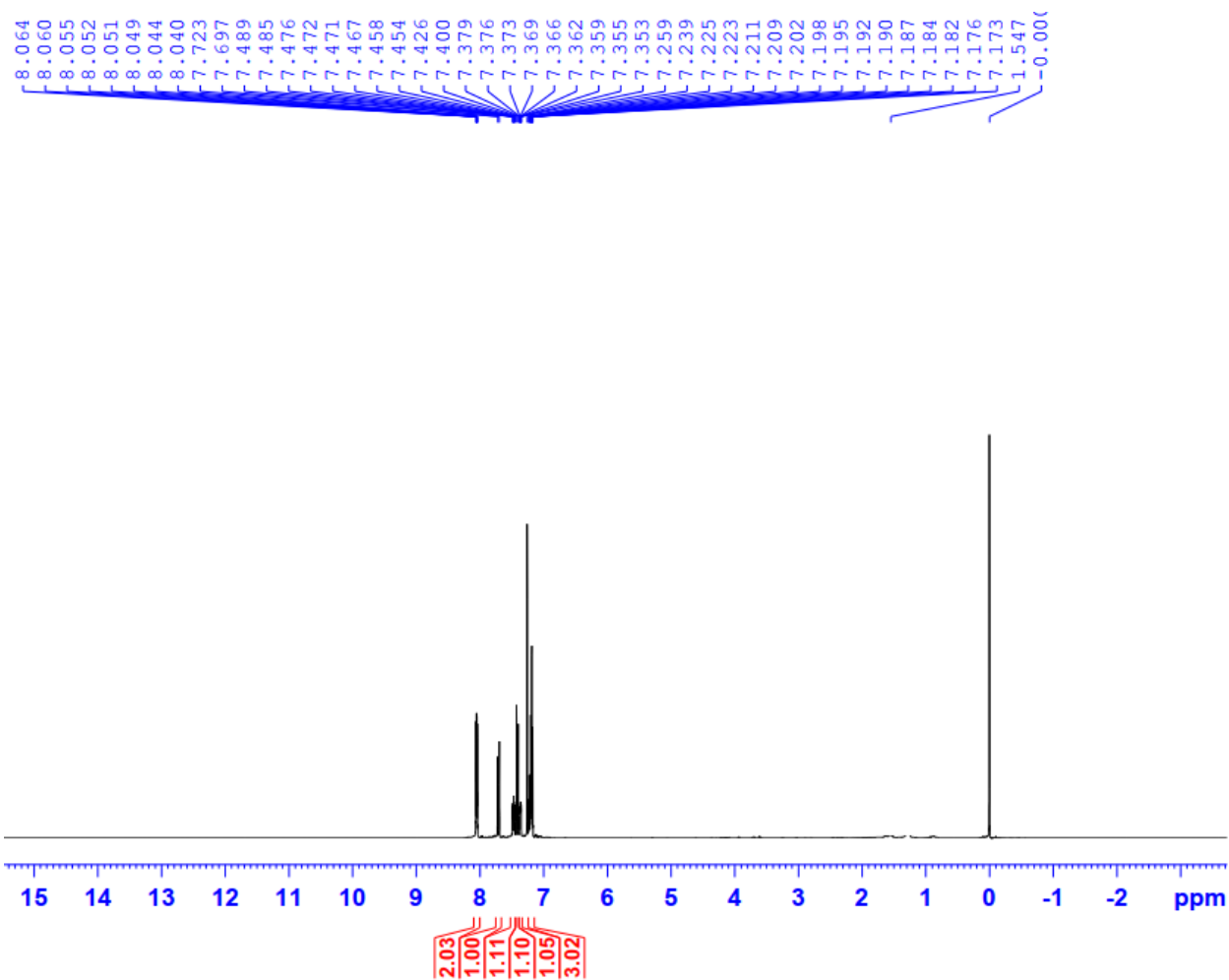
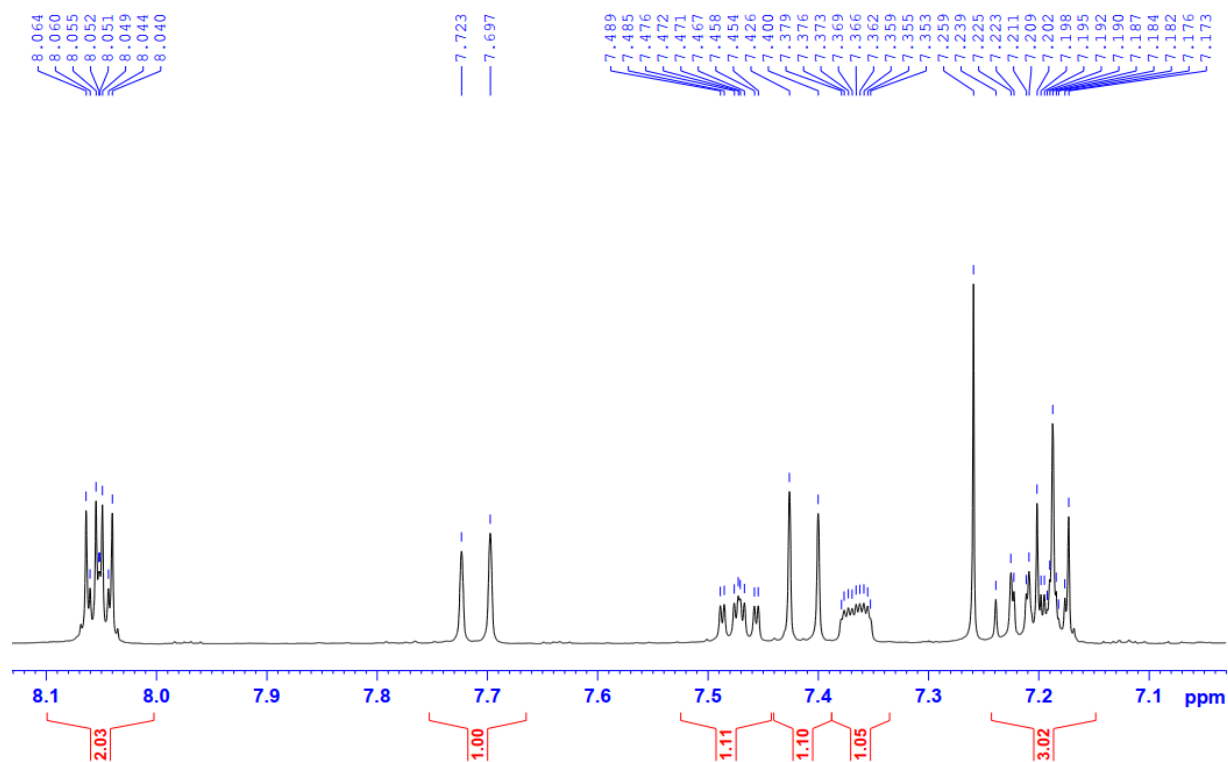
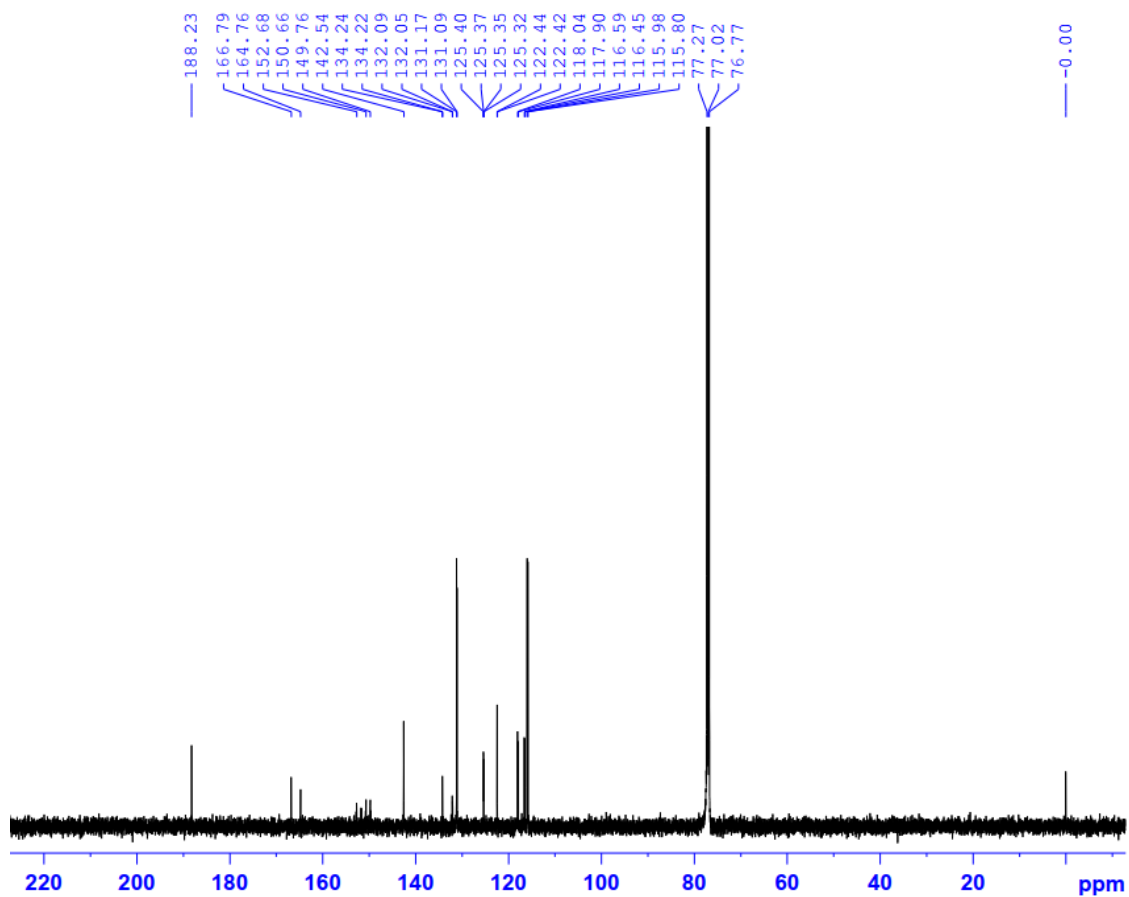


Figure S4g. MS of 1d.

Figure S5a. ¹H-NMR spectrum of 1e.

Figure S5b. ¹H-NMR spectrum of 1e.Figure S5c. ¹³C-NMR spectrum of 1e.

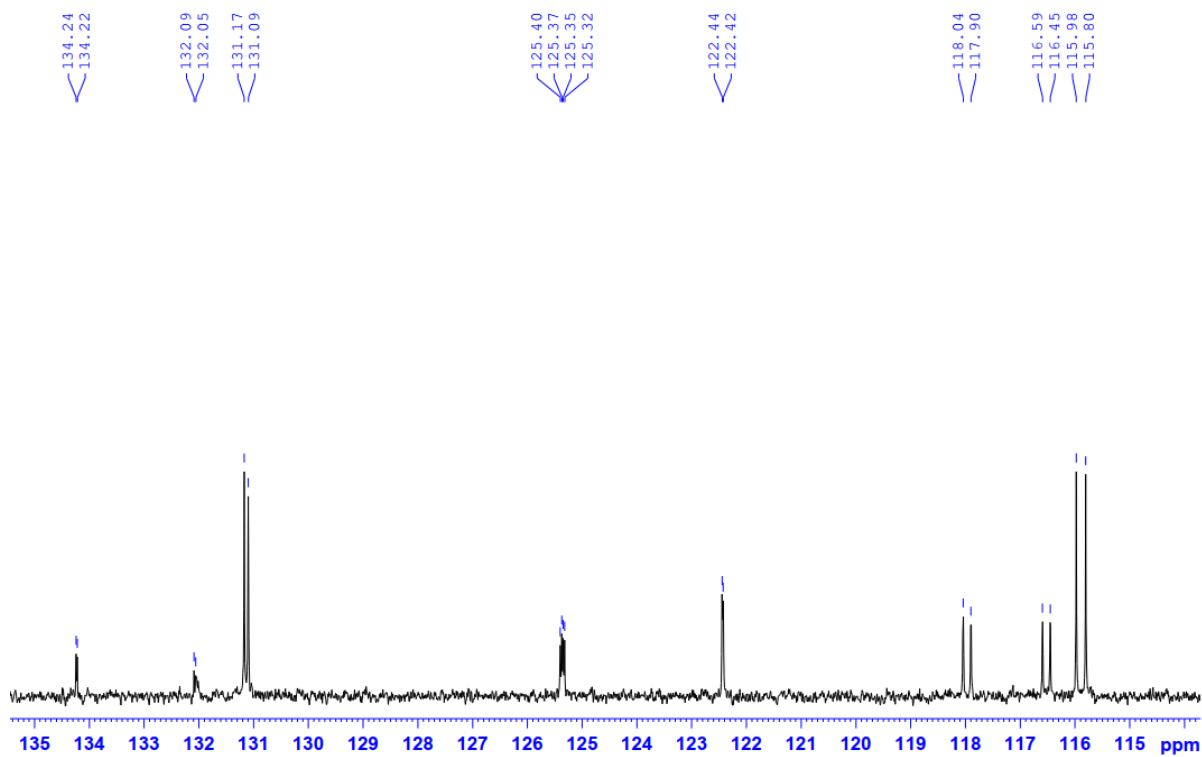
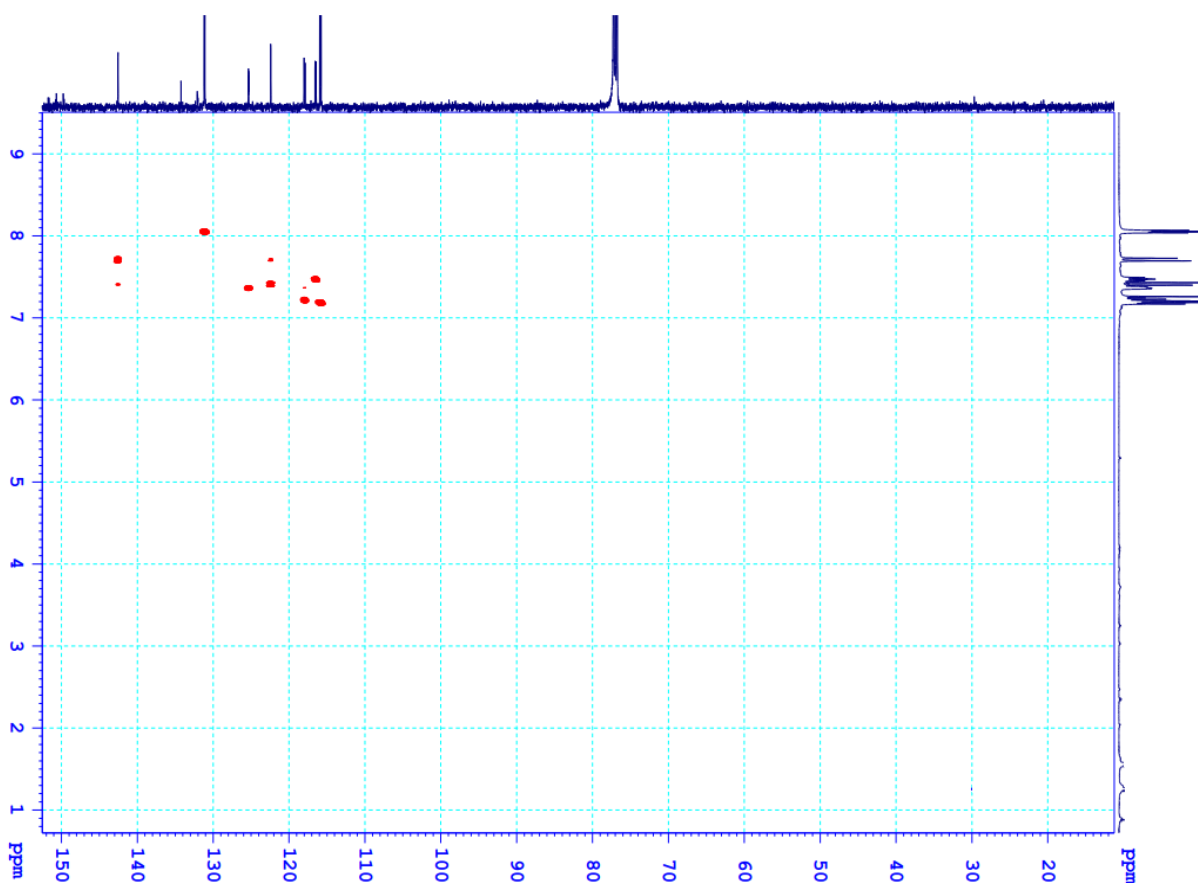
Figure S5d. ¹³C-NMR spectrum of 1e.

Figure S5e. HSQC spectrum of 1e.

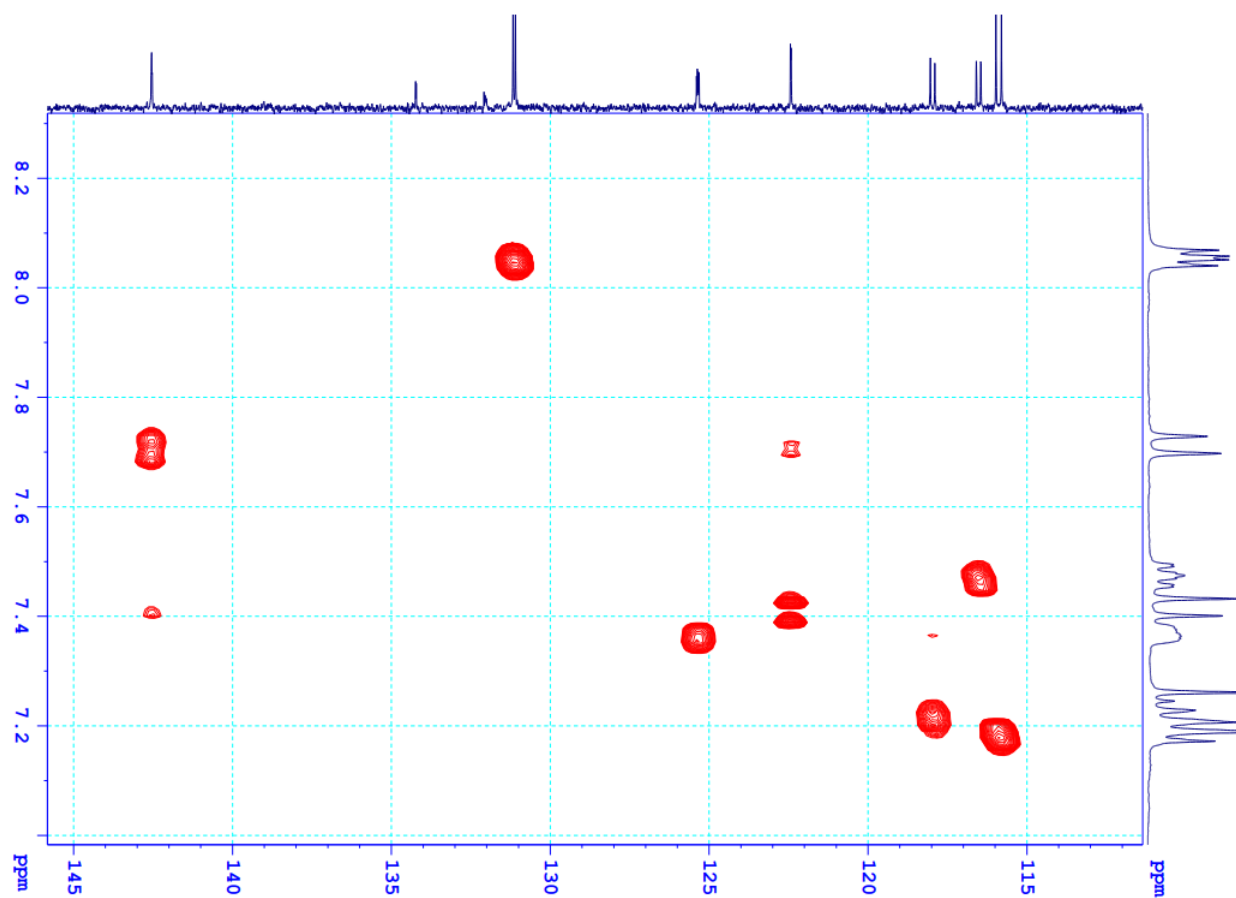


Figure S5f. HSQC spectrum of 1e.

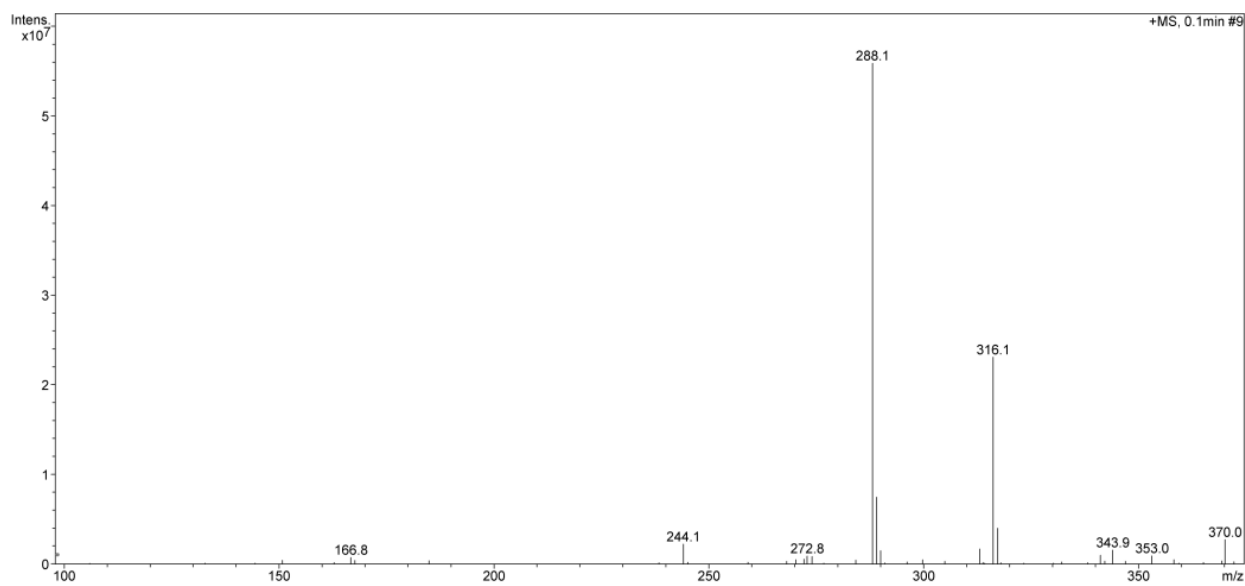
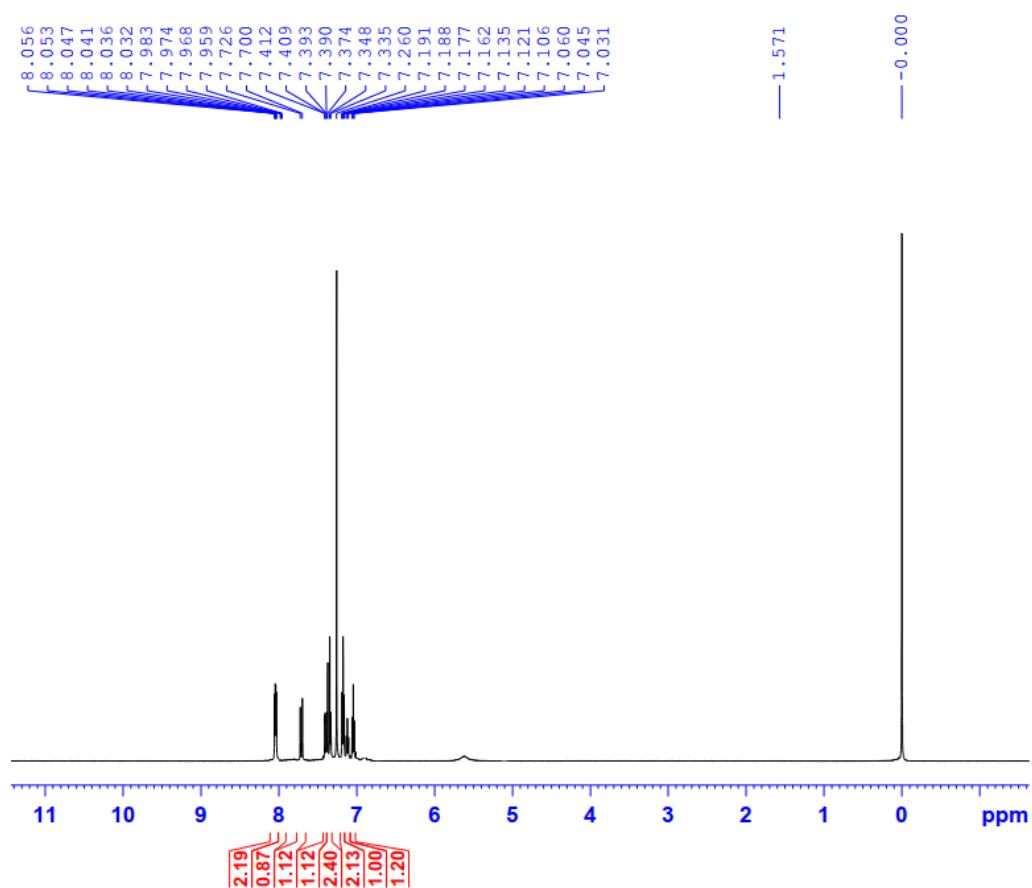
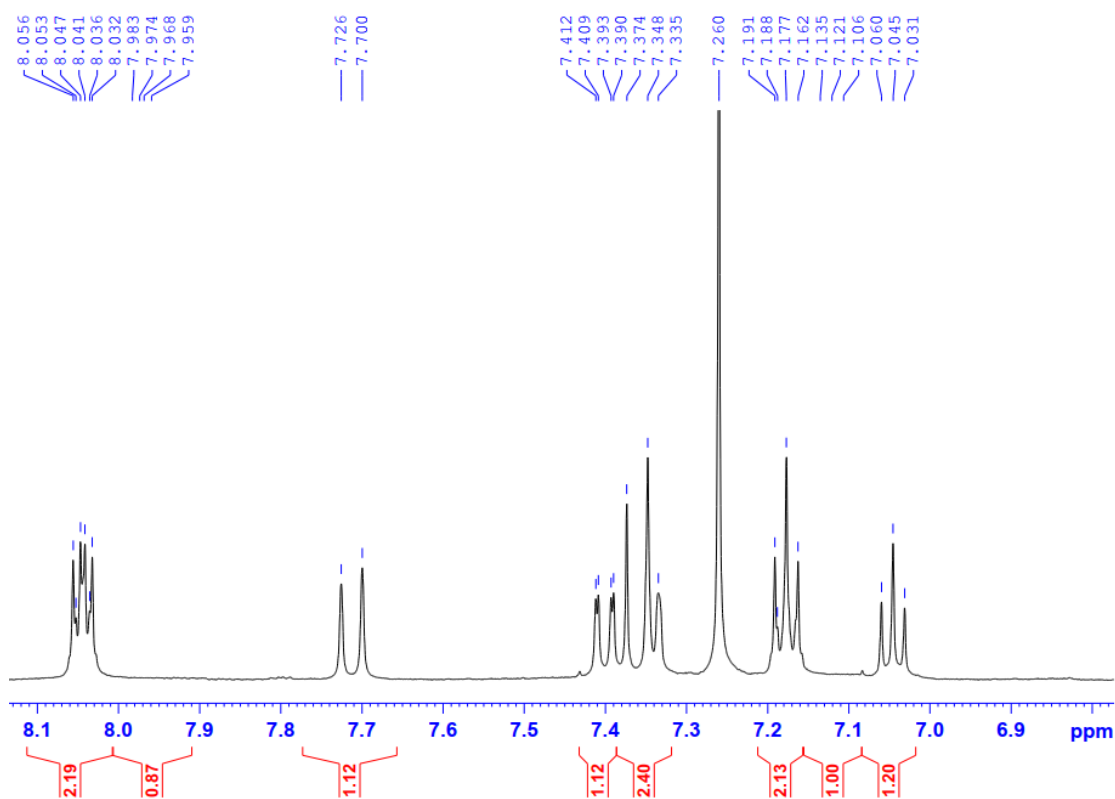
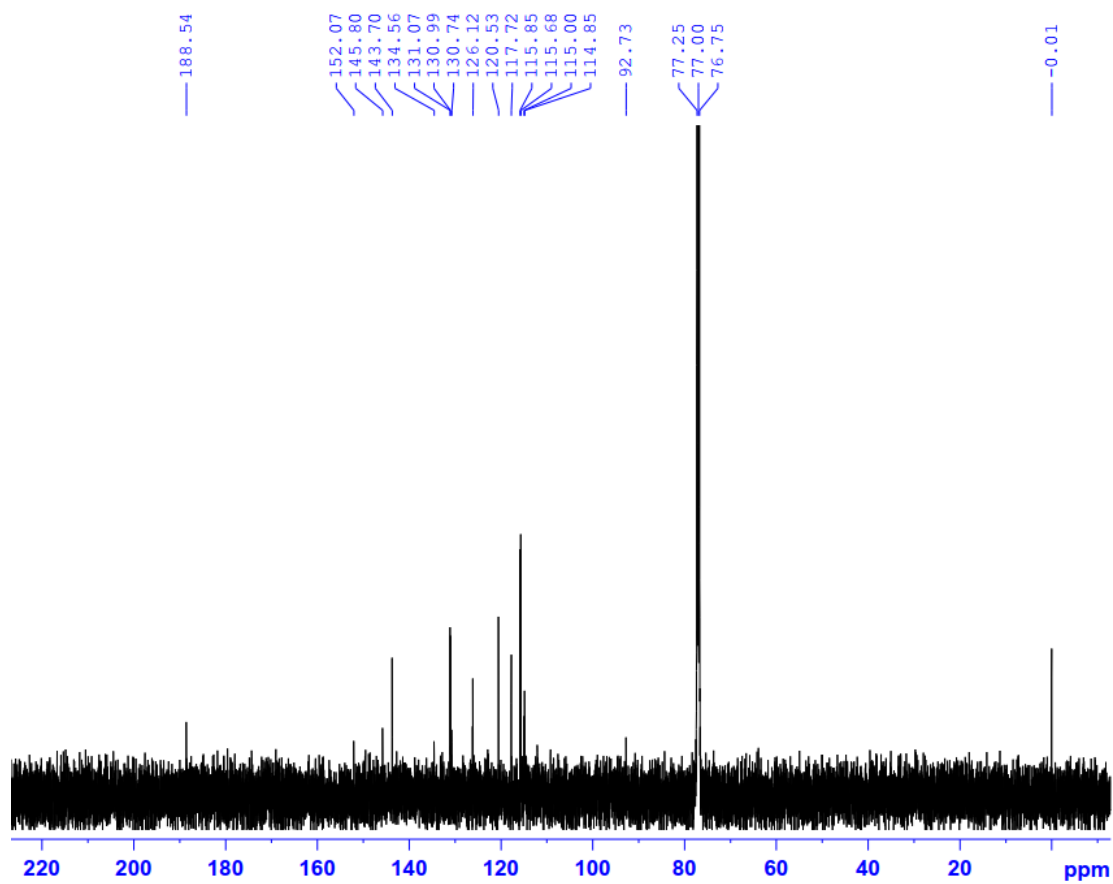
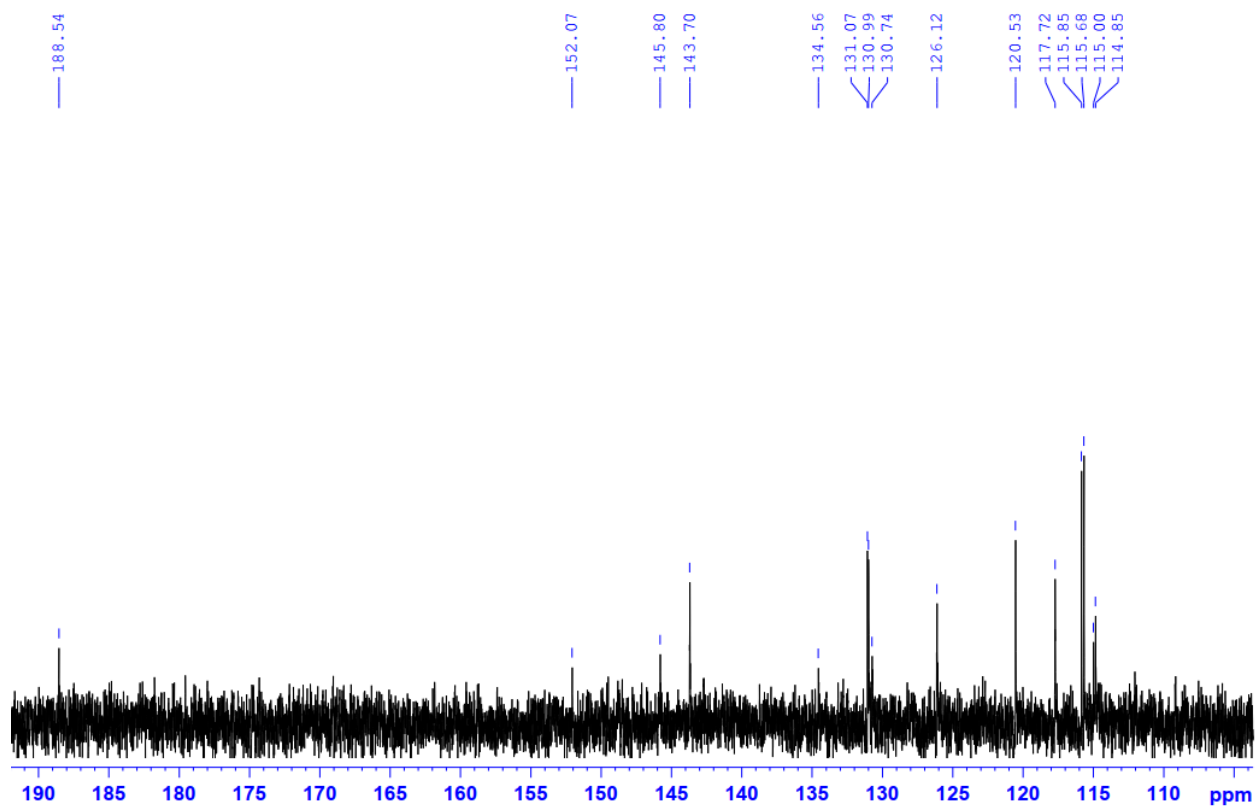


Figure S5g. MS of 1e.

Figure S6a. ¹H-NMR spectrum of 1f.Figure S6b. ¹H-NMR spectrum of 1f.

Figure S6c. ¹³C-NMR spectrum of 1f.Figure S6d. ¹³C-NMR spectrum of 1f.

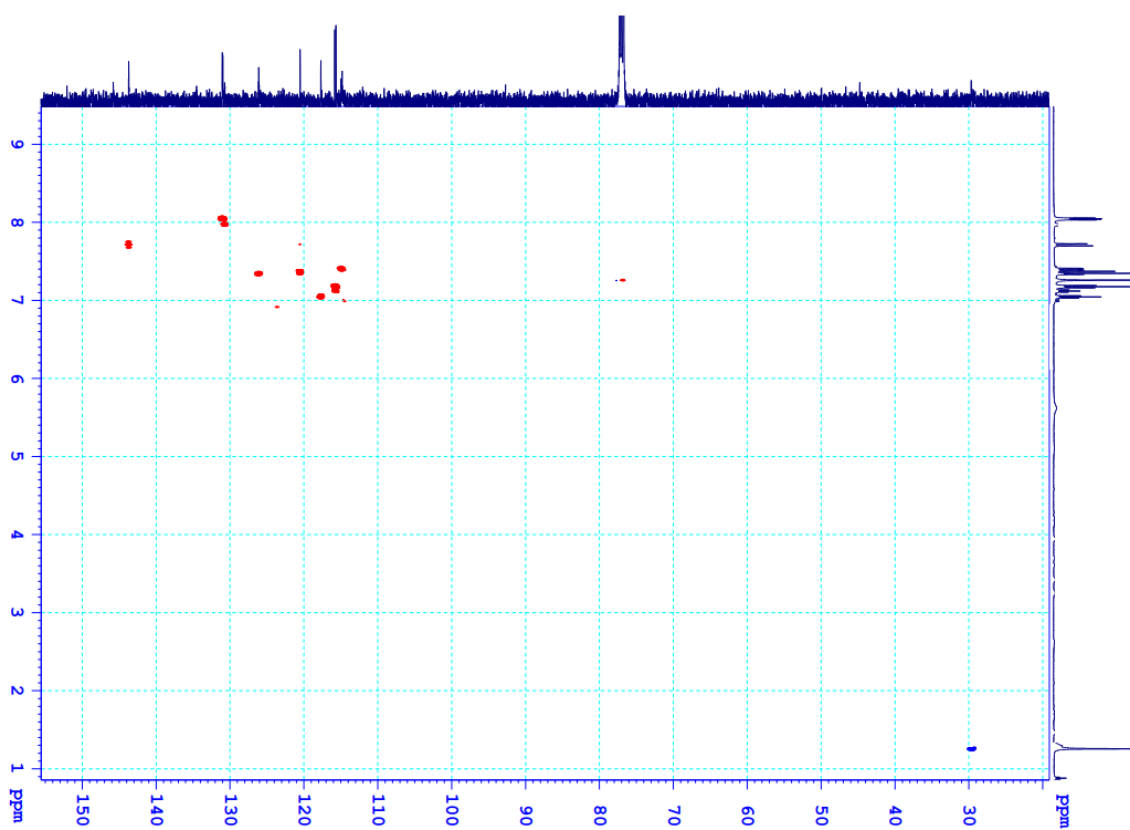


Figure S6e. HSQC spectrum of 1f.

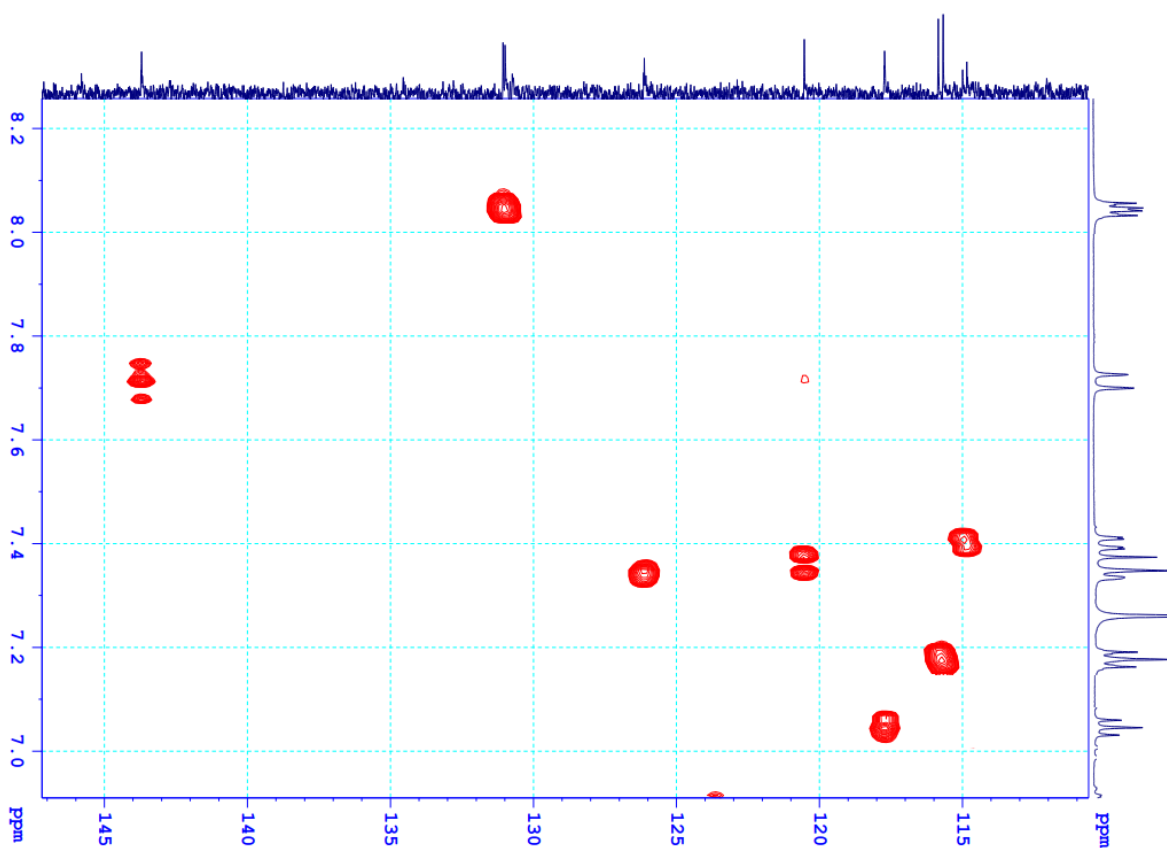


Figure S6f. HSQC spectrum of 1f.

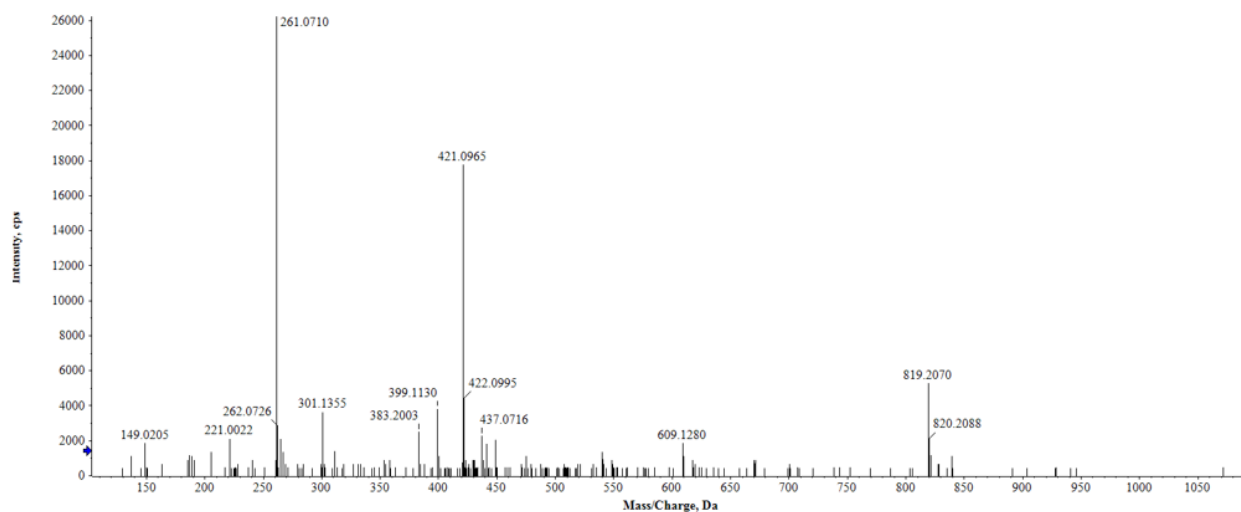
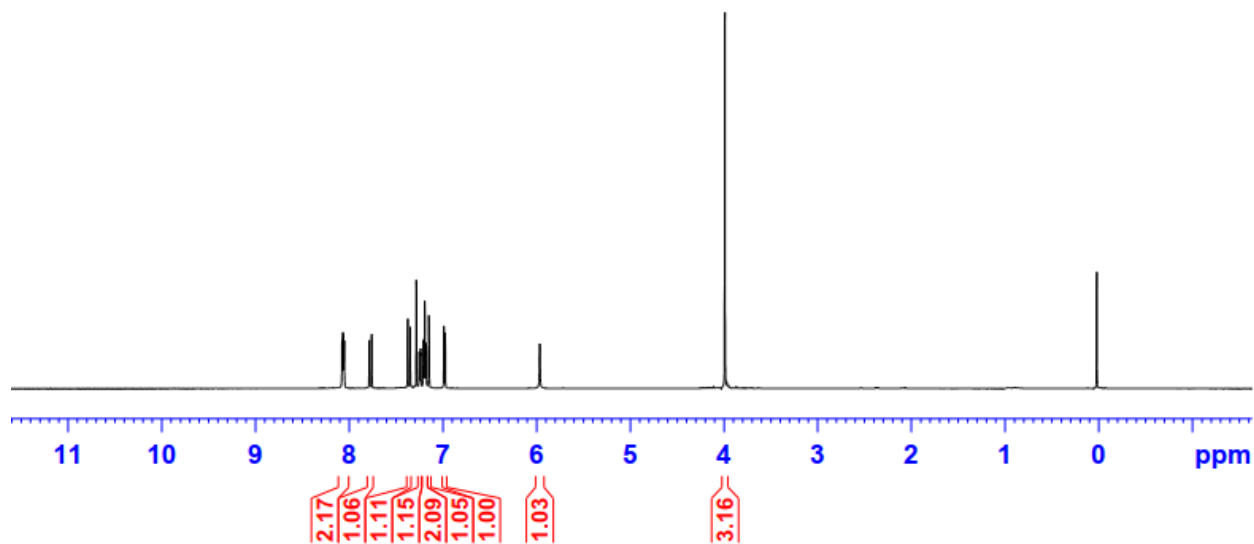
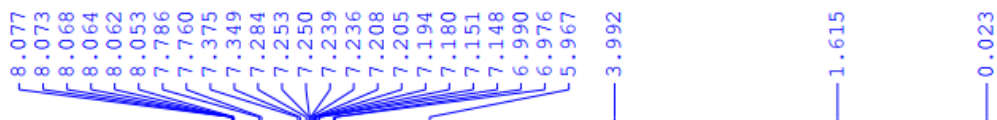
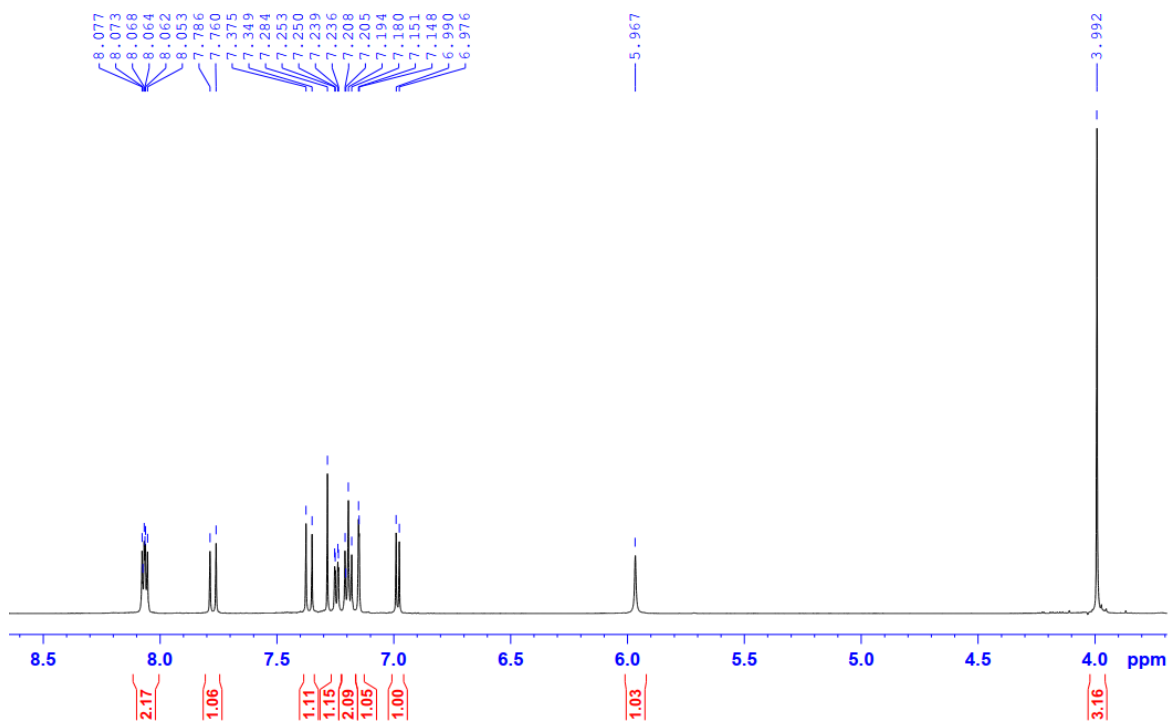
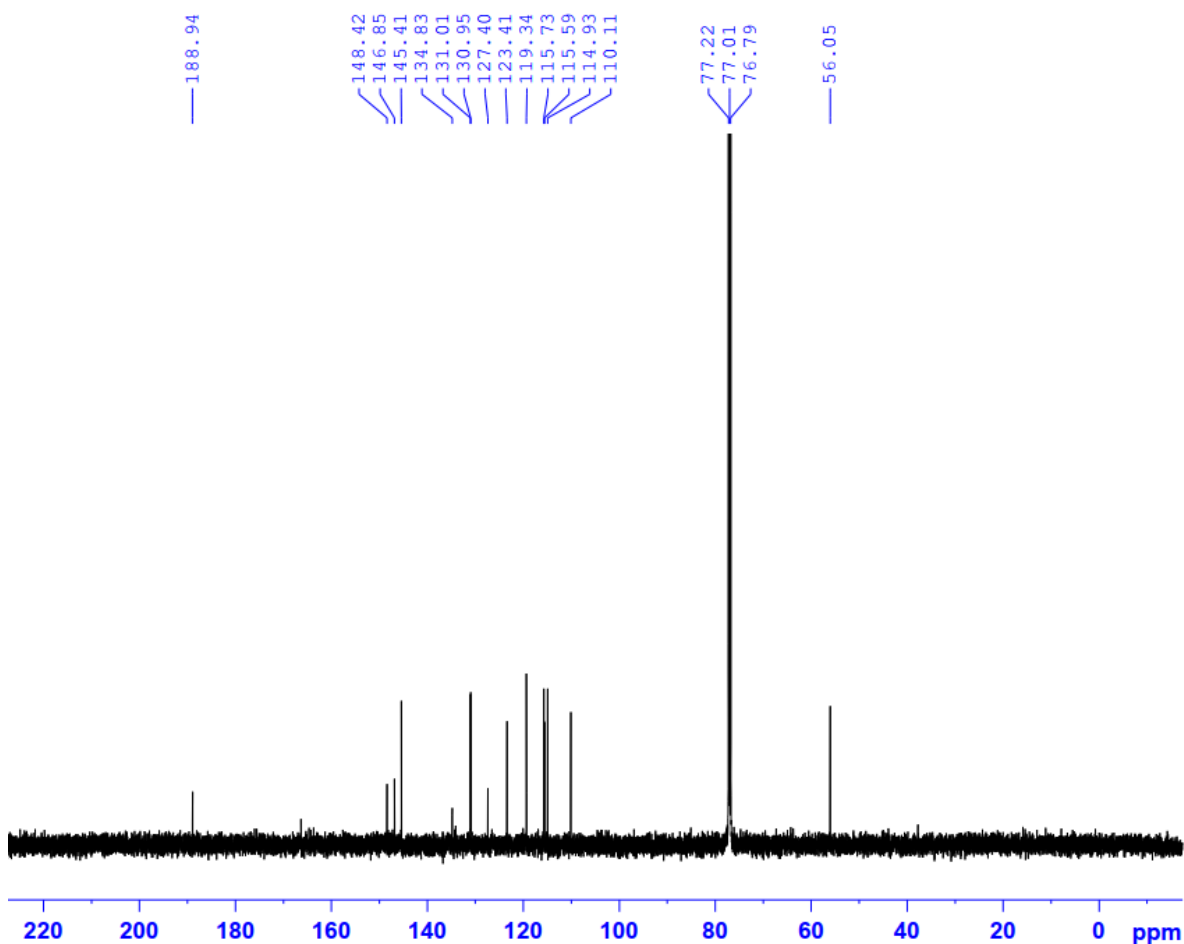
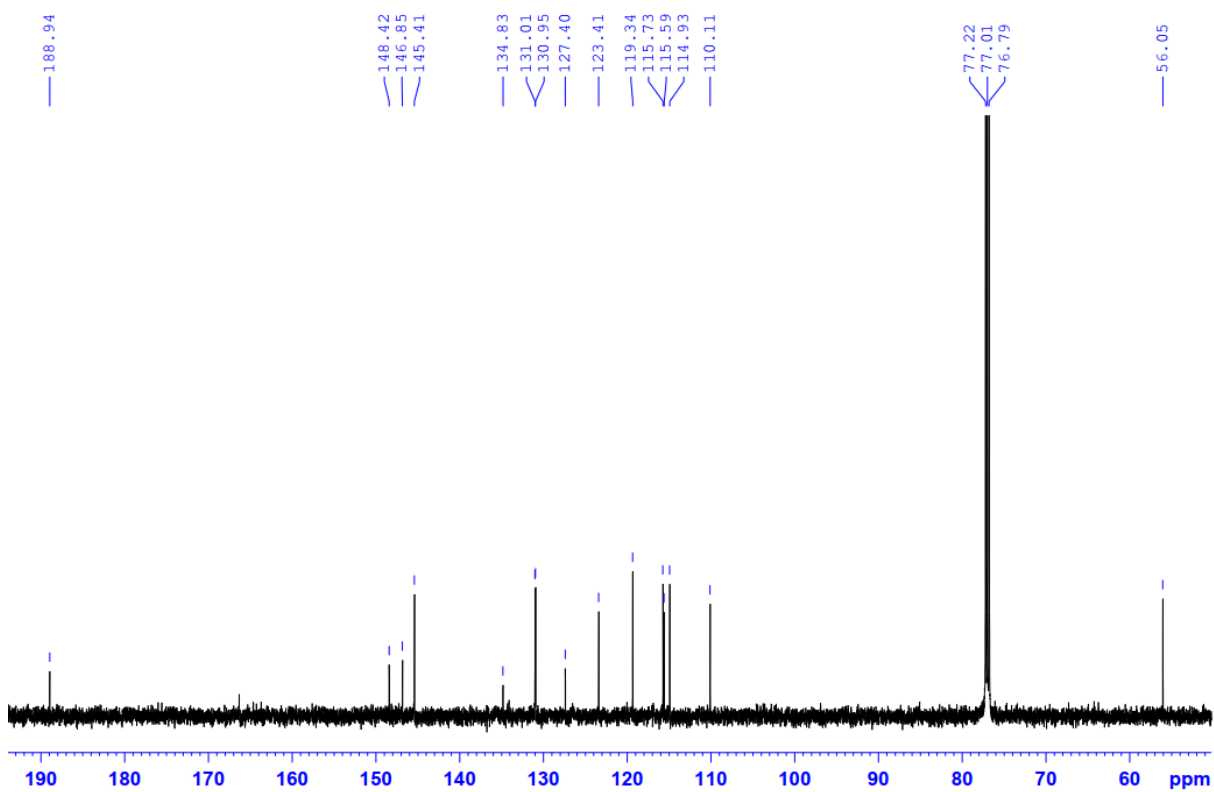
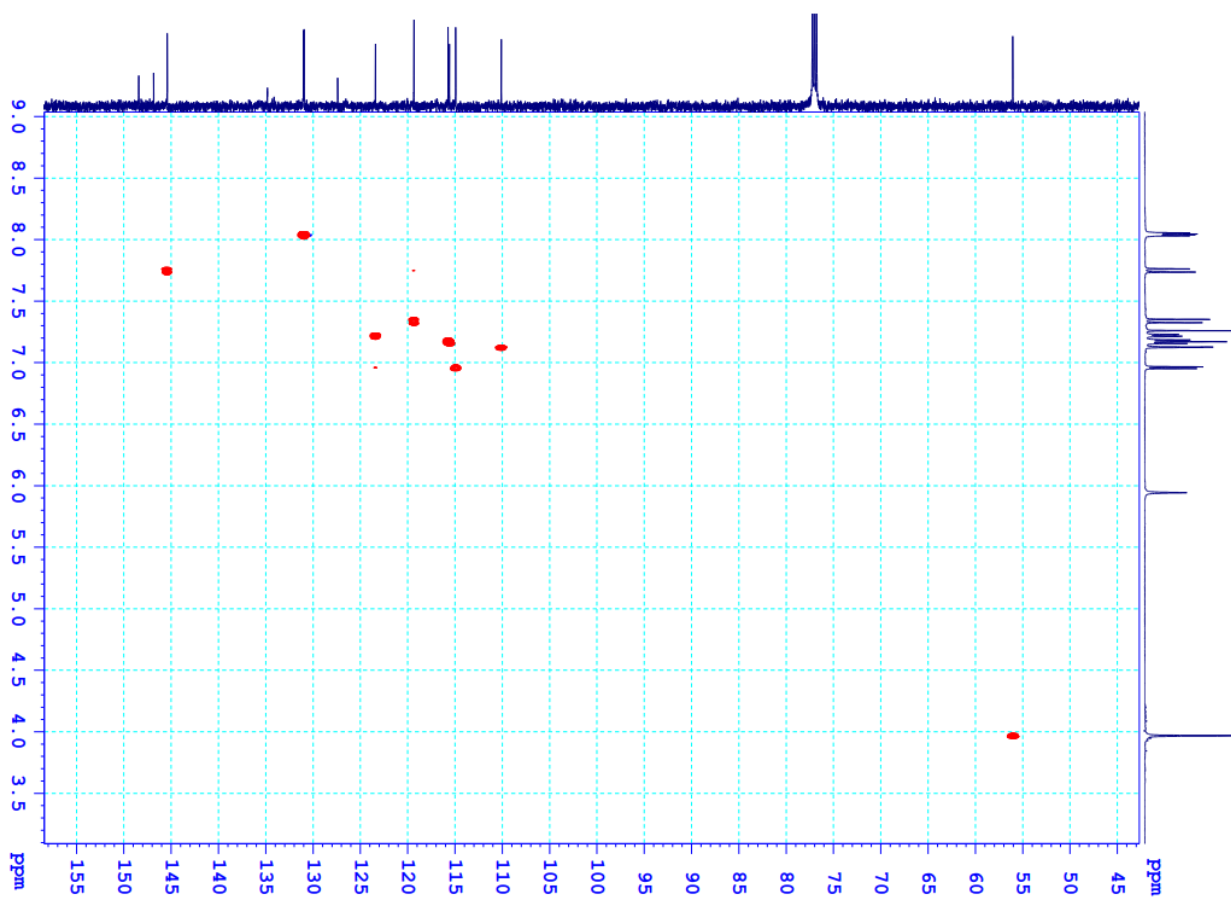
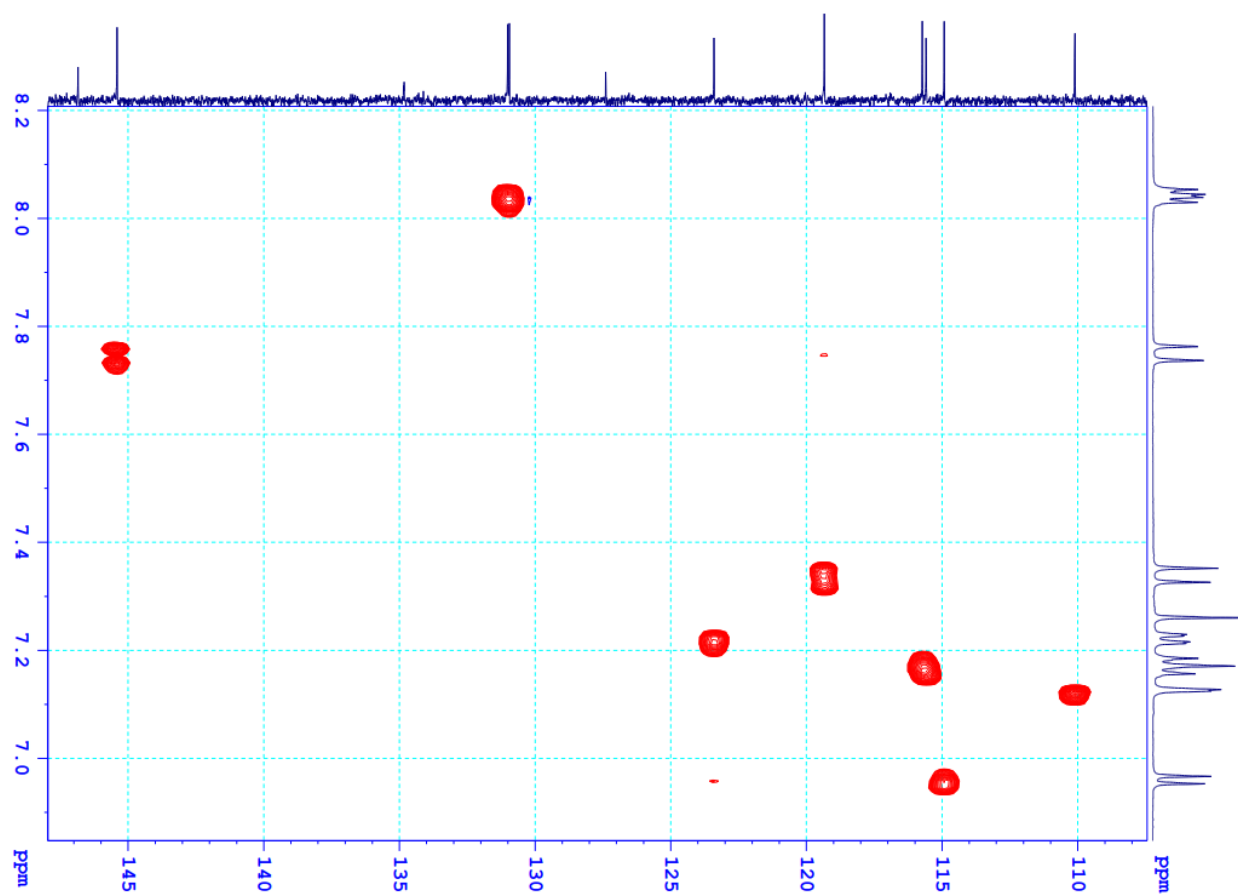
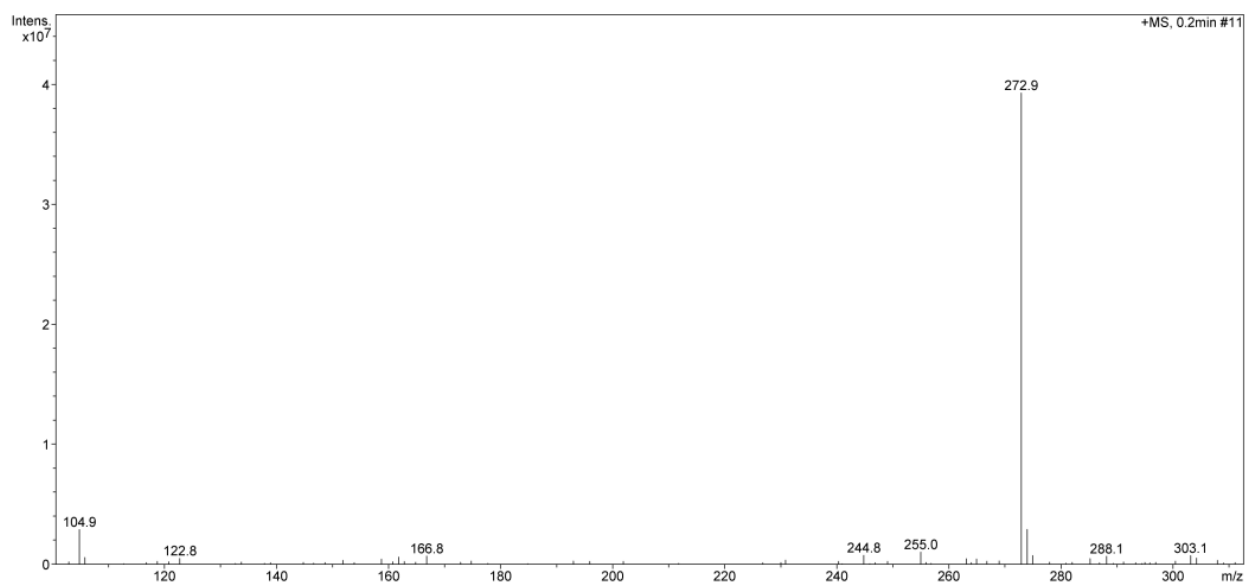


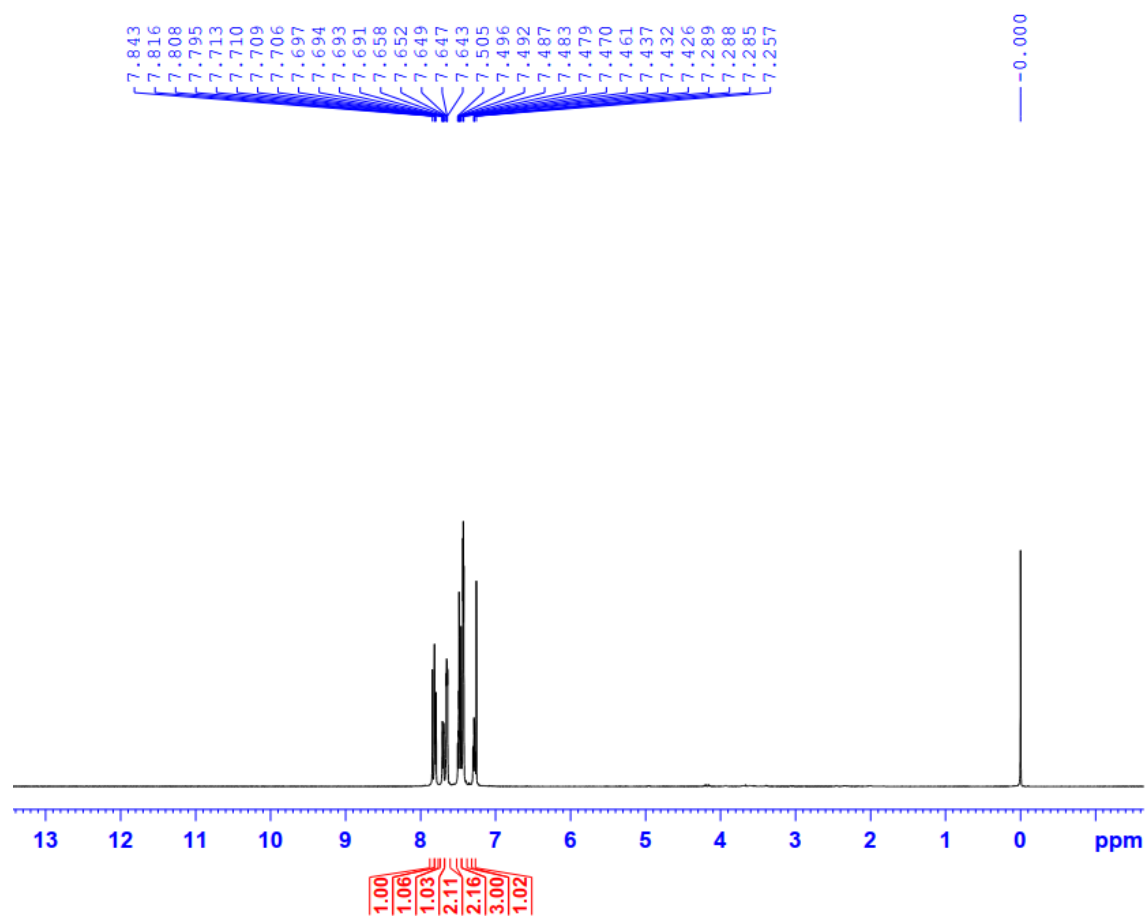
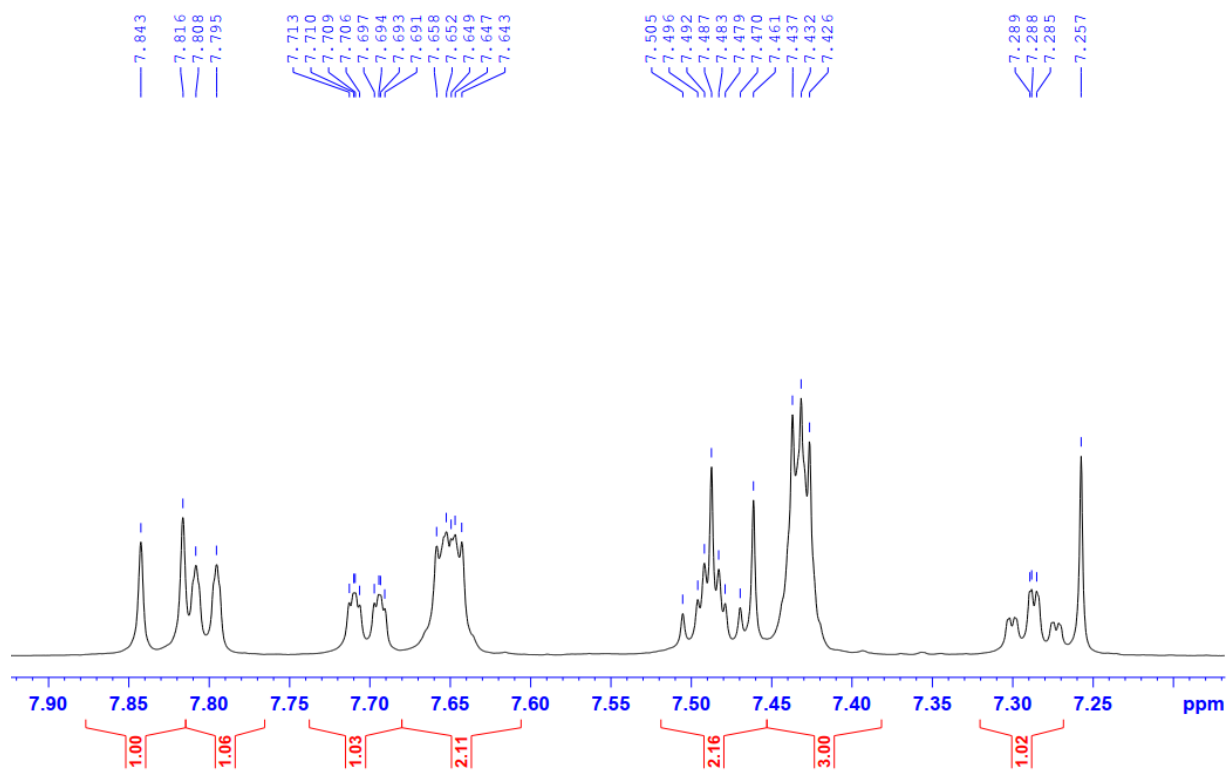
Figure S6g. HRMS of 1f.

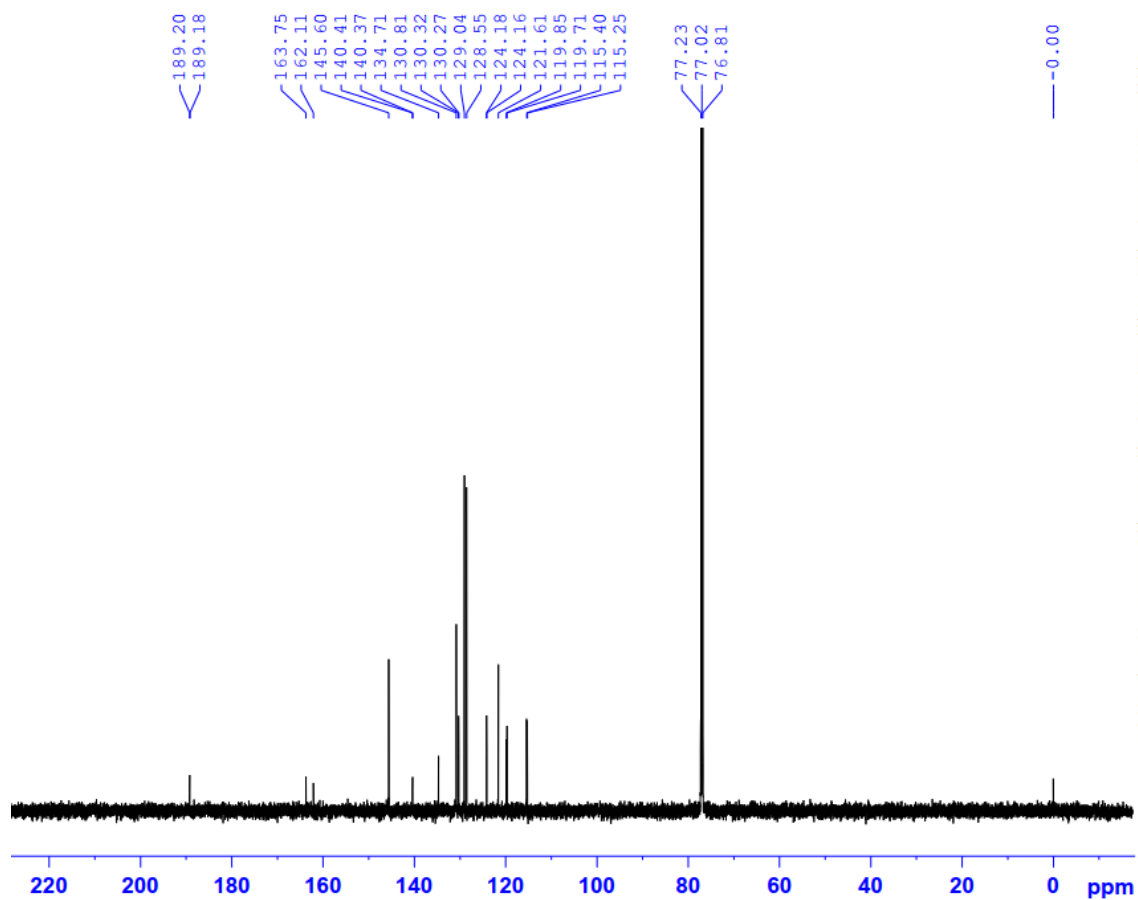
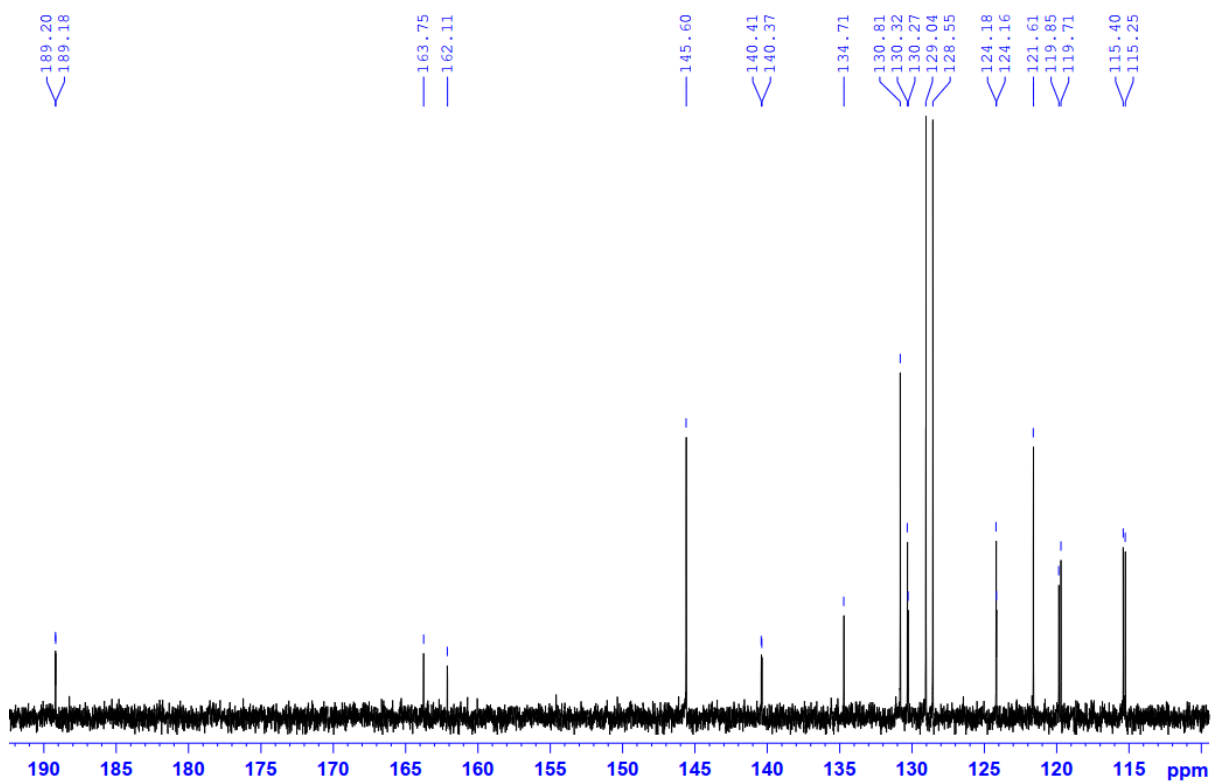
Figure S7a. ¹H-NMR spectrum of 1g.

Figure S7b. $^1\text{H-NMR}$ spectrum of **1g**.Figure S7c. $^{13}\text{C-NMR}$ spectrum of **1g**.

Figure S7d. ^{13}C -NMR spectrum of **1g**.Figure S7e. HSQC spectrum of **1g**.

Figure S7f. HSQC spectrum of **1g**.Figure S7g. MS of **1g**.

Figure S8a. ¹H-NMR spectrum of 2a.Figure S8b. ¹H-NMR spectrum of 2a.

Figure S8c. ¹³C-NMR spectrum of 2a.Figure S8d. ¹³C-NMR spectrum of 2a.

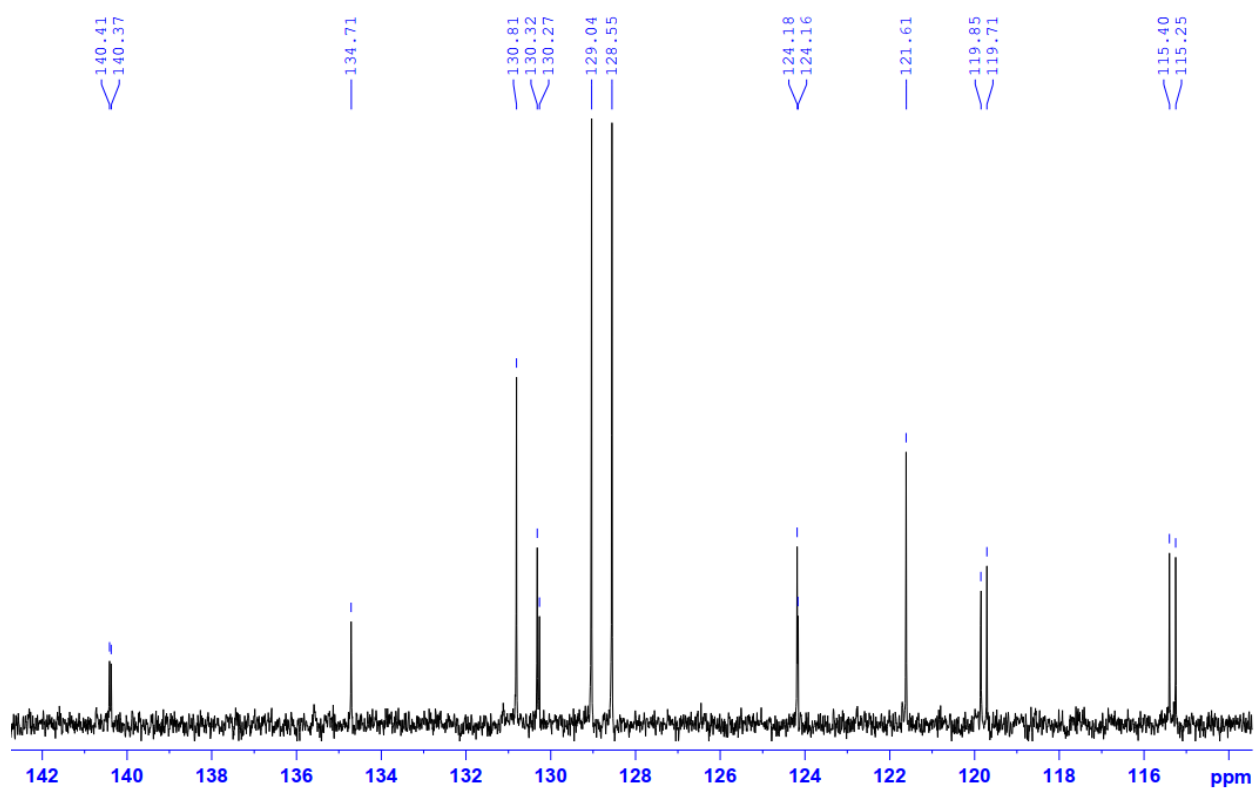
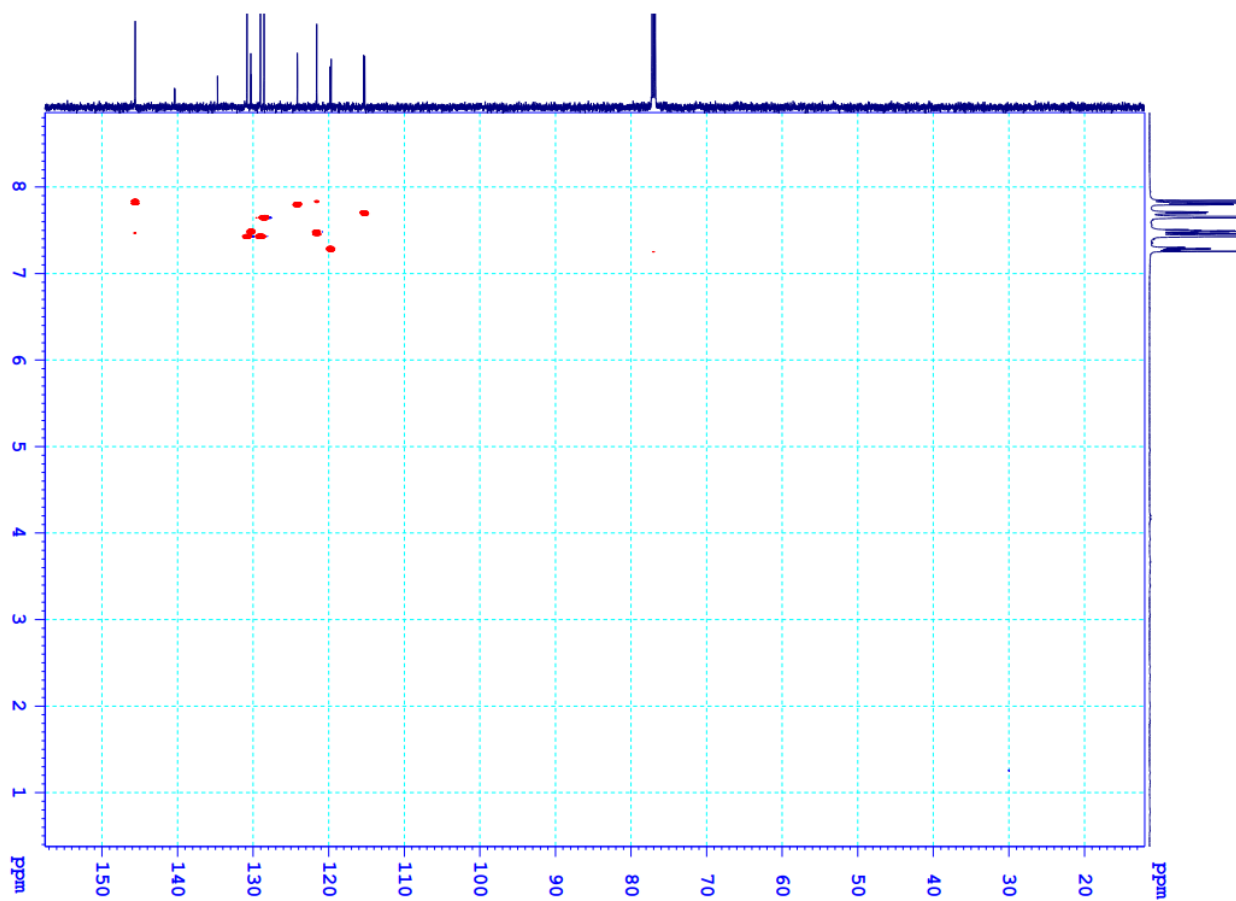
Figure S8e. ^{13}C -NMR spectrum of 2a.

Figure S8f. HSQC spectrum of 2a.

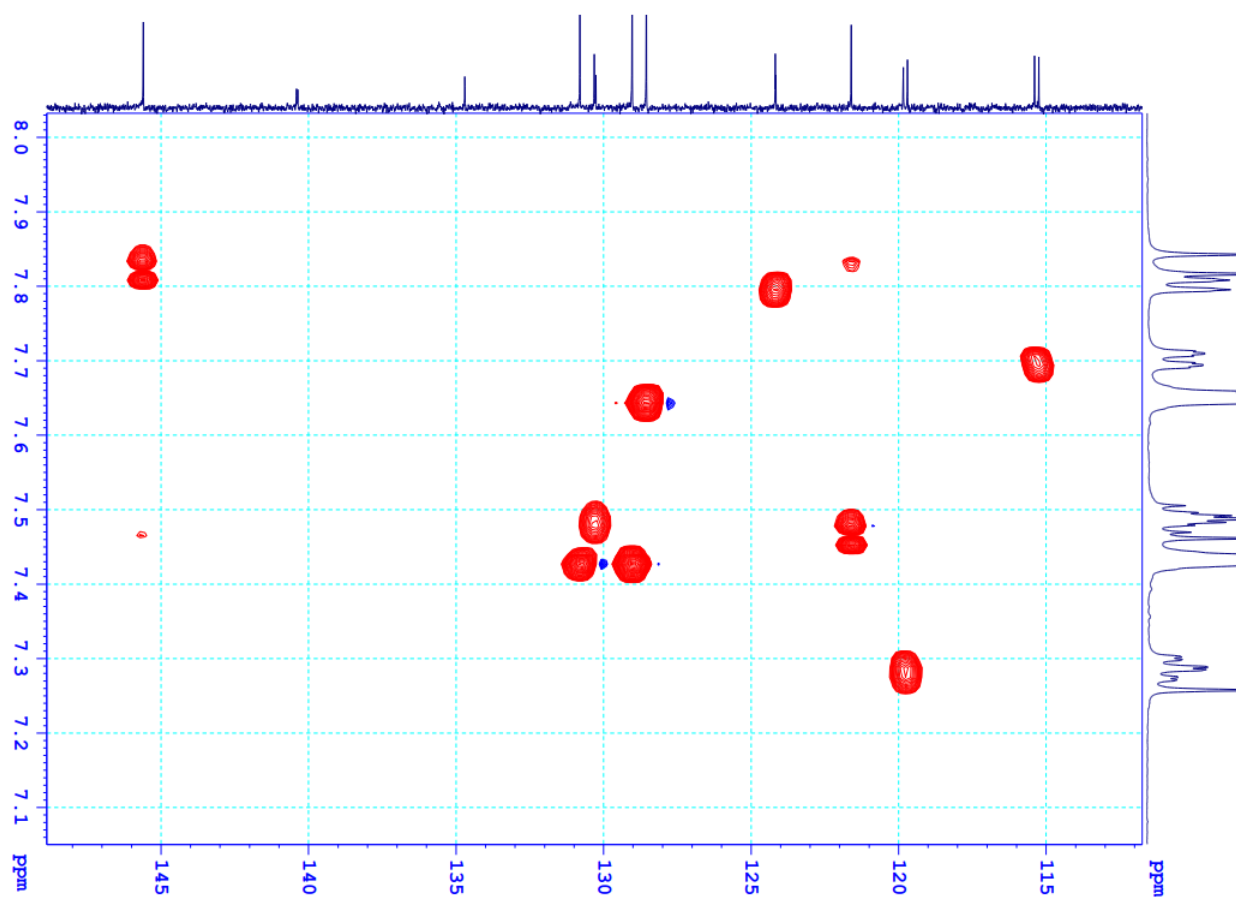


Figure S8g. HSQC spectrum of 2a.

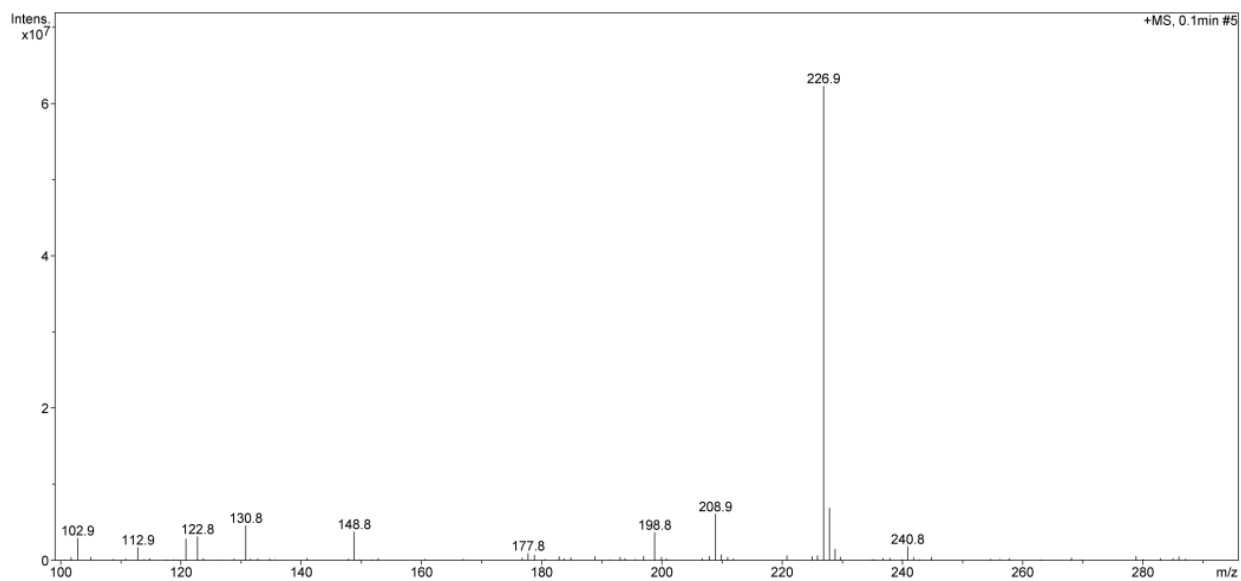
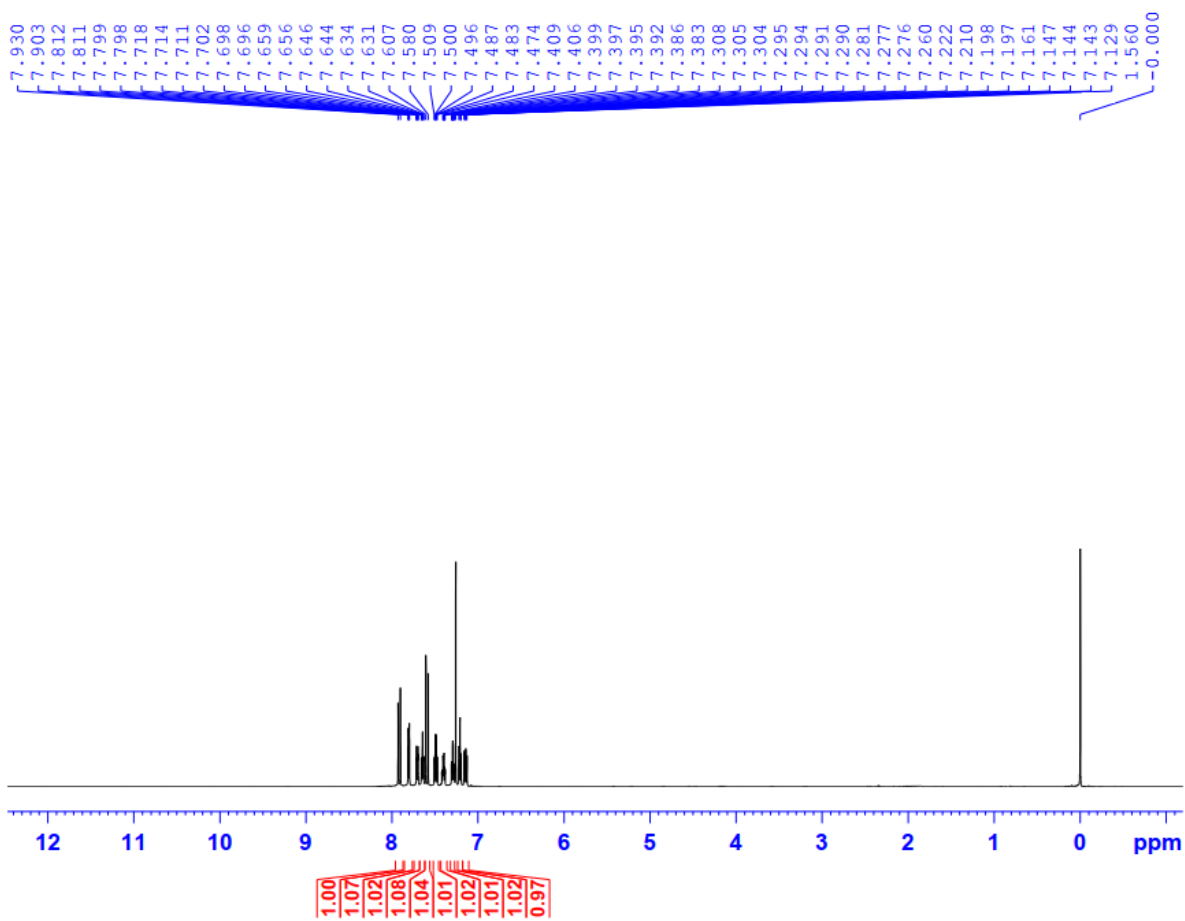
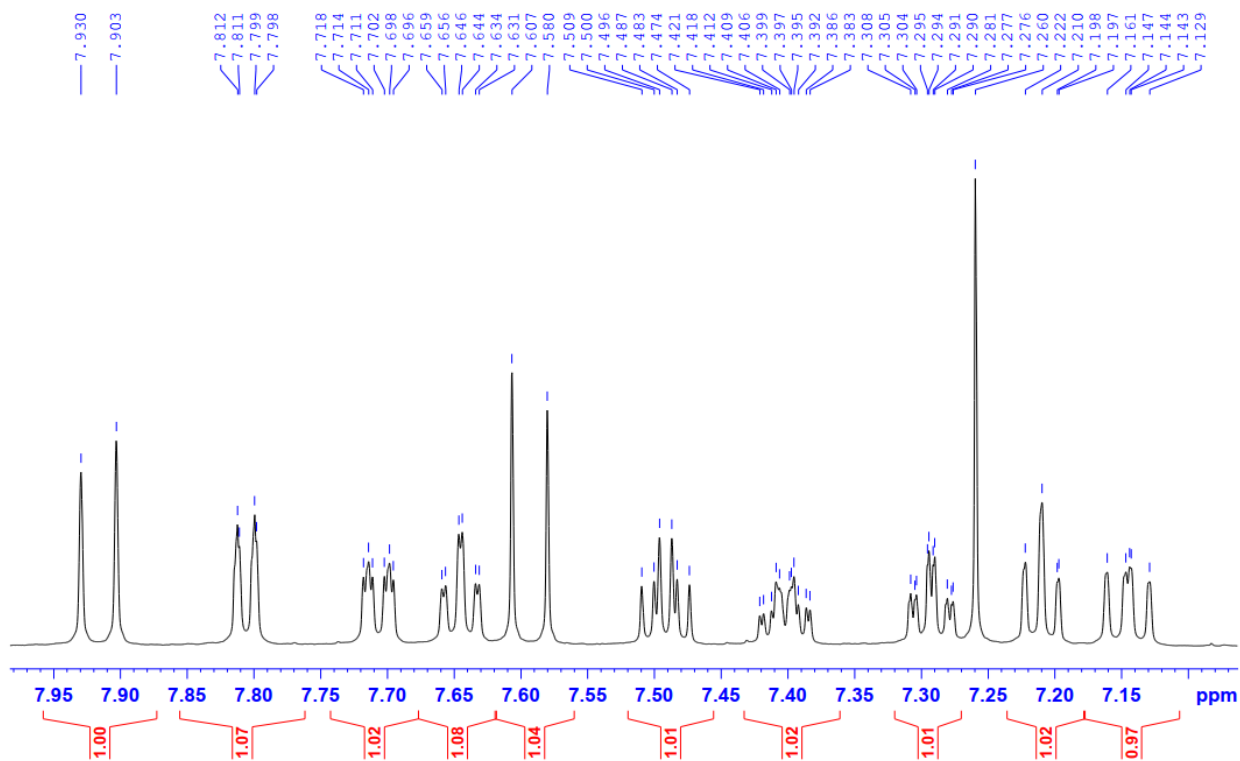
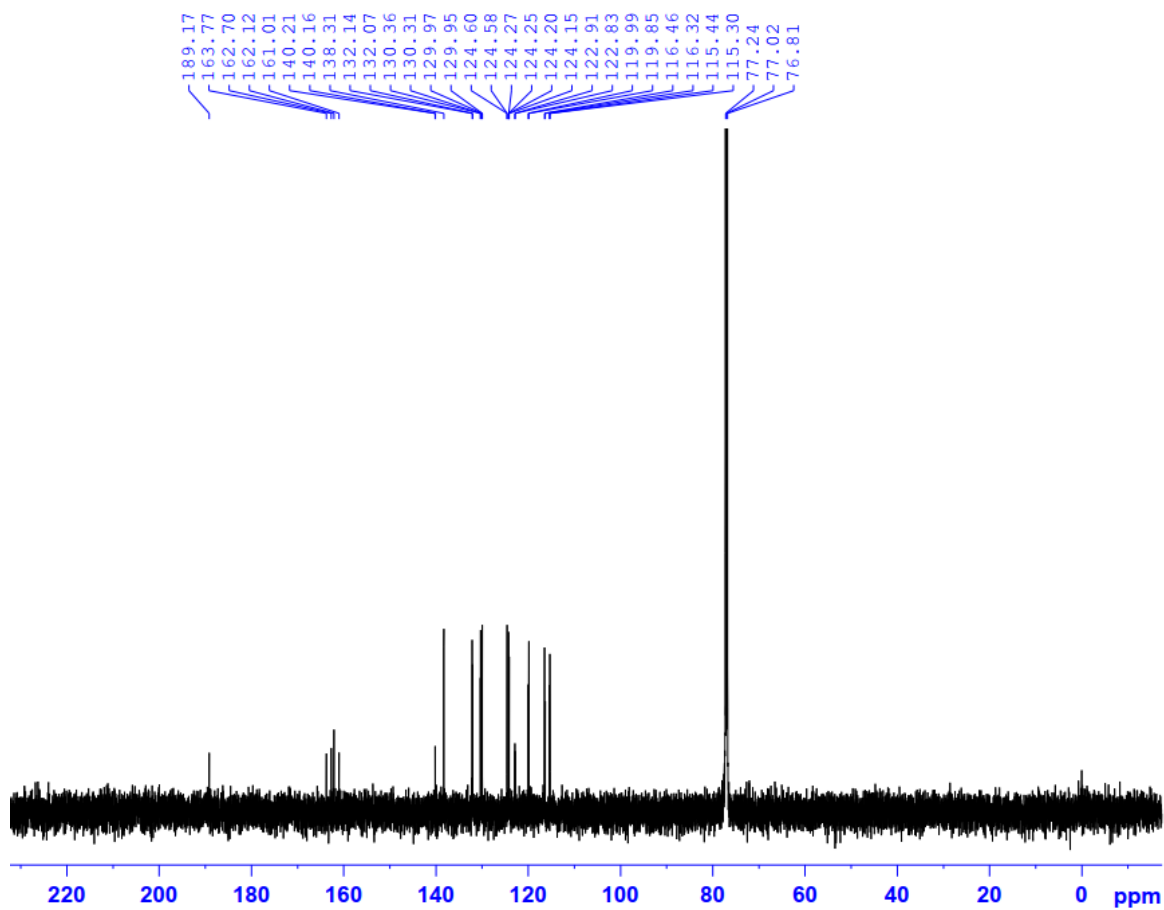
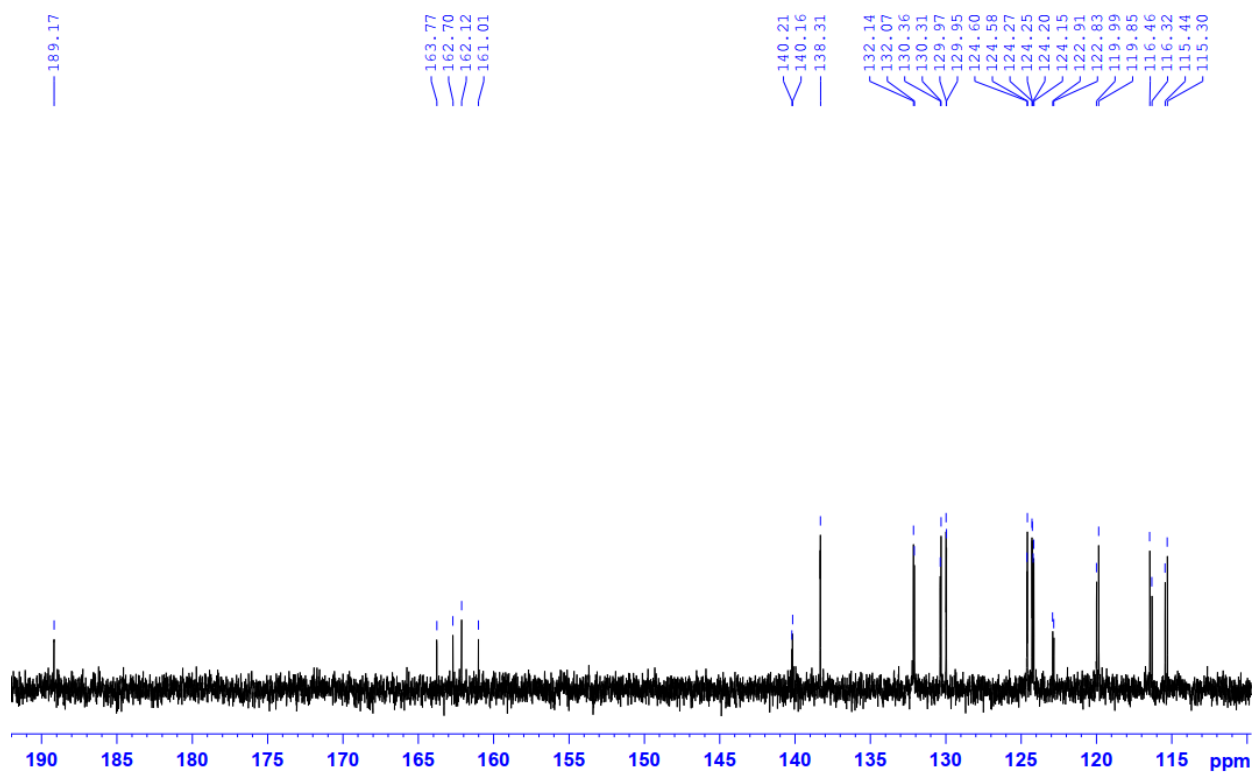


Figure S8h. MS of 2a.

Figure S9a. ¹H-NMR spectrum of 2b.Figure S9b. ¹H-NMR spectrum of 2b.

Figure S9c. ^{13}C -NMR spectrum of 2b.Figure S9d. ^{13}C -NMR spectrum of 2b.

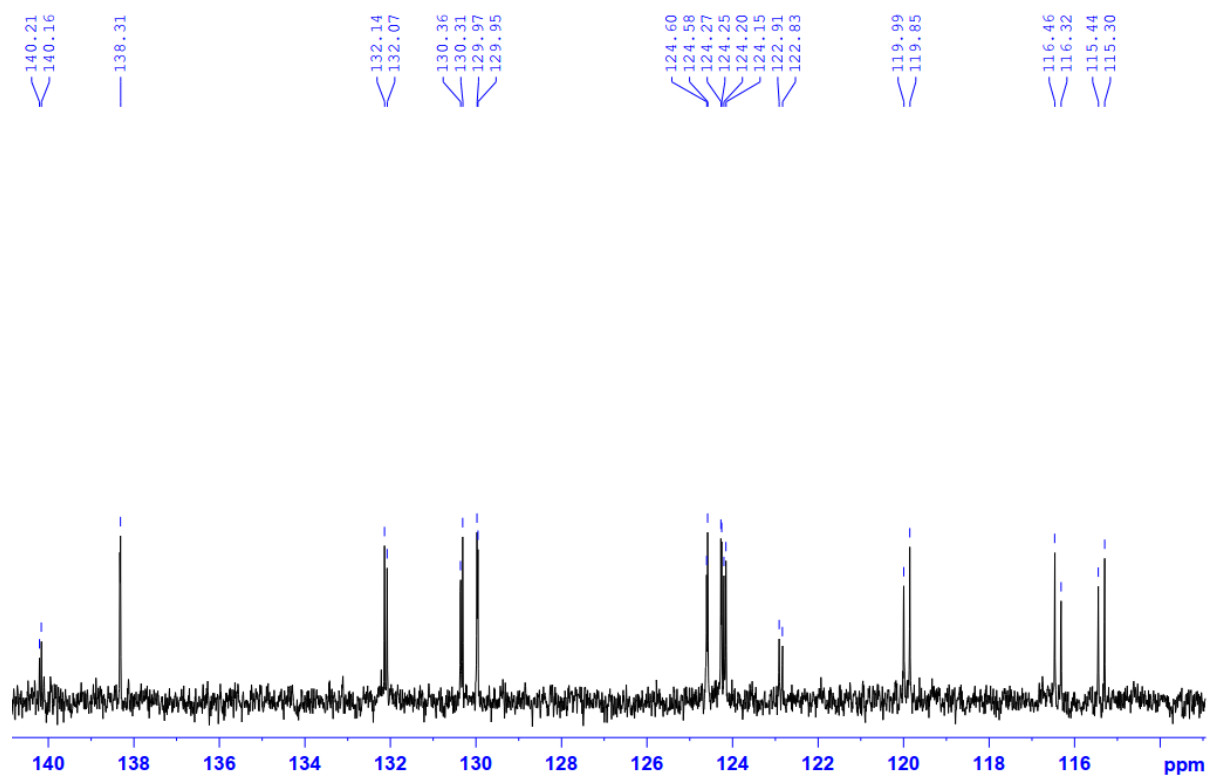
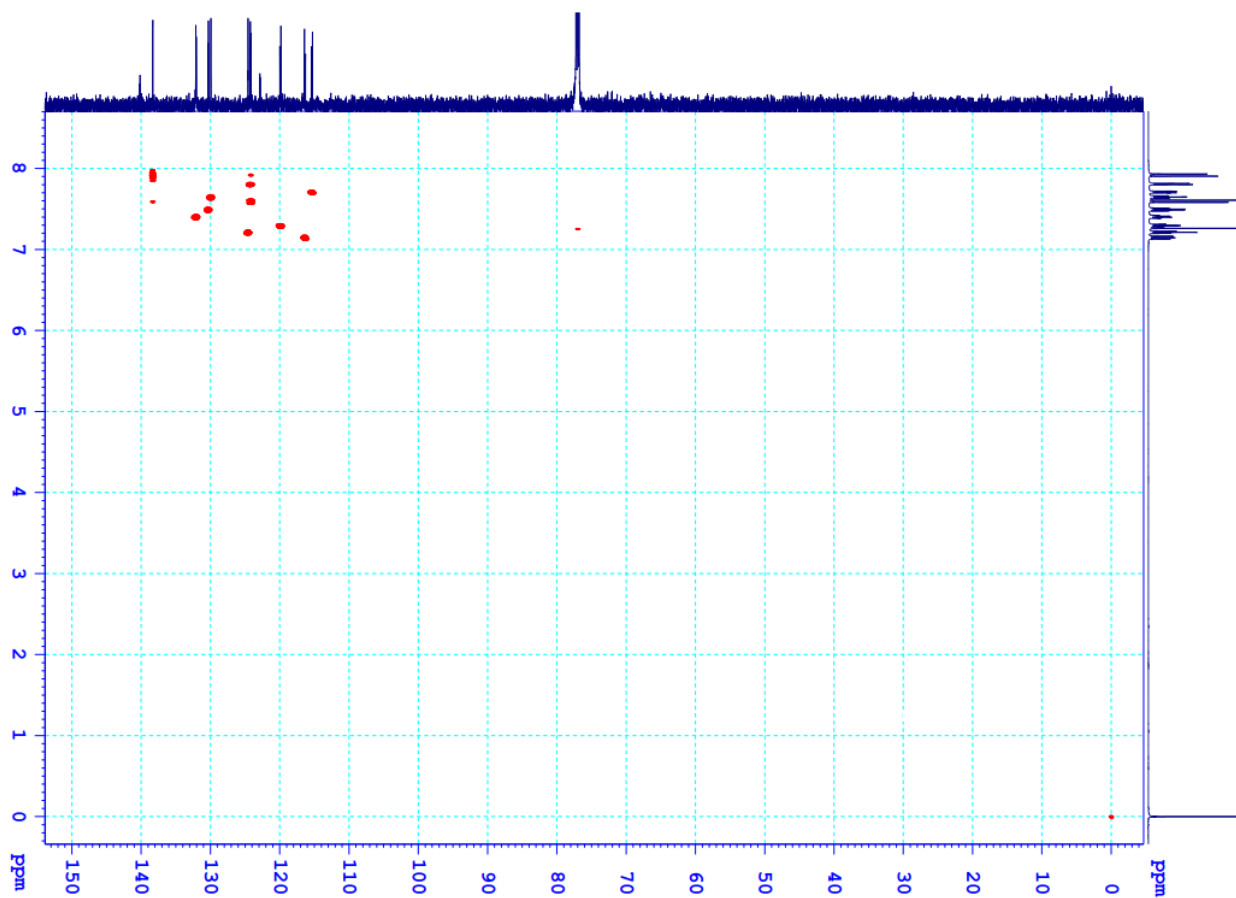
Figure S9e. ^{13}C -NMR spectrum of 2b.

Figure S9f. HSQC spectrum of 2b.

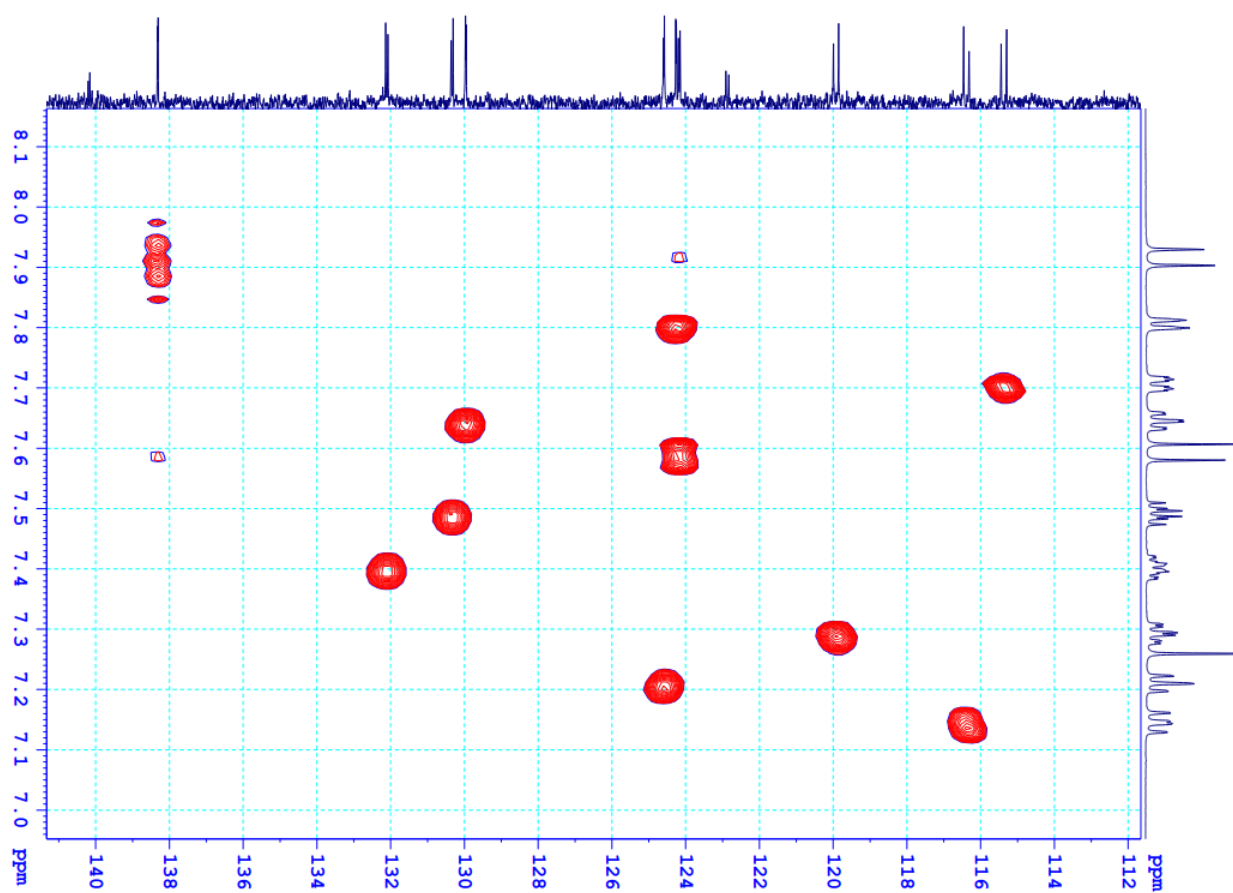


Figure S9g. HSQC spectrum of 2b.

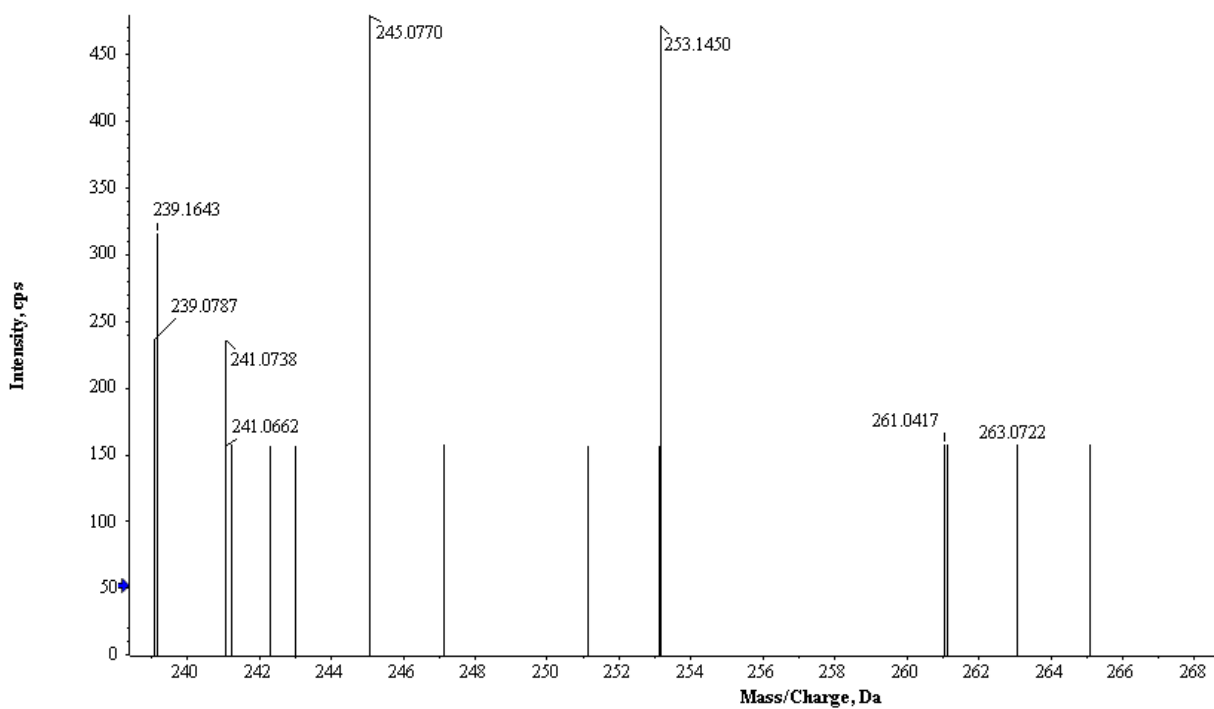
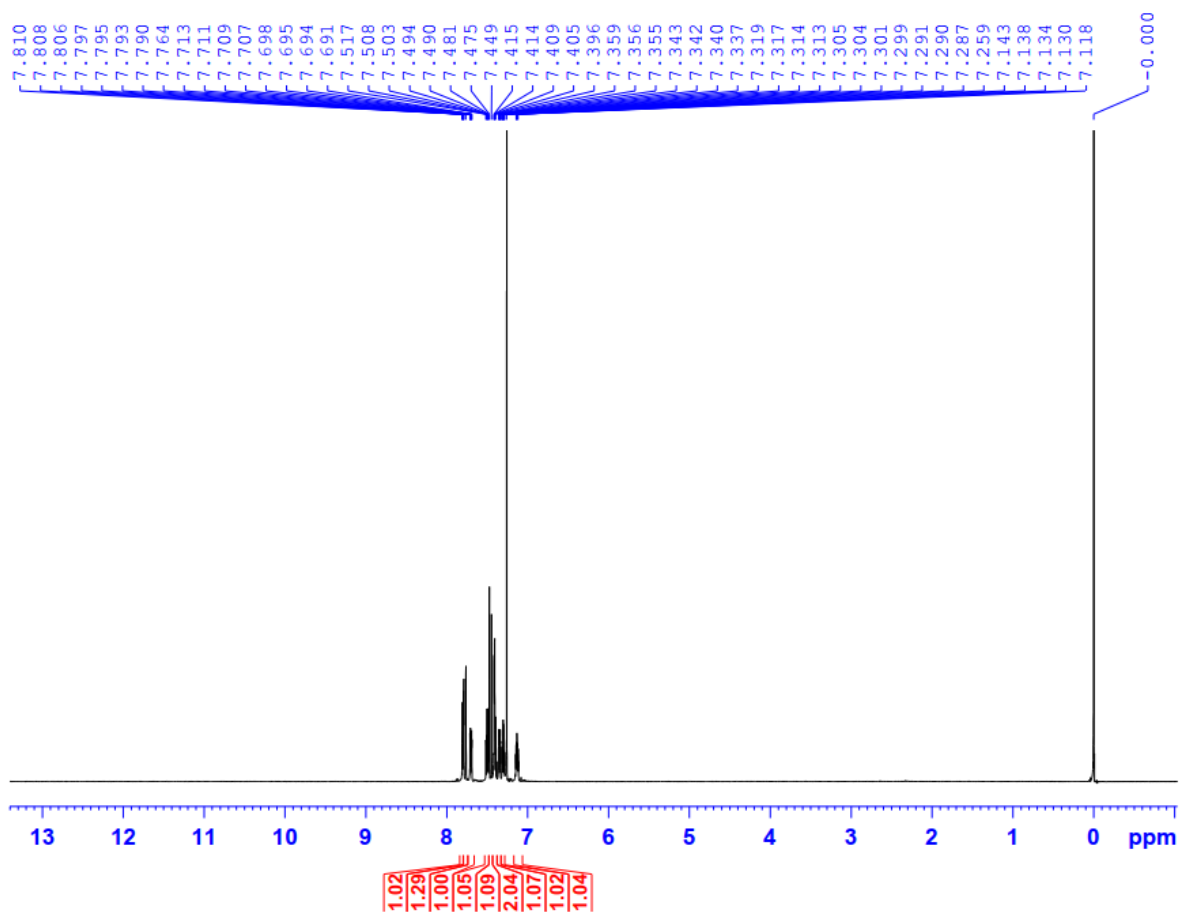
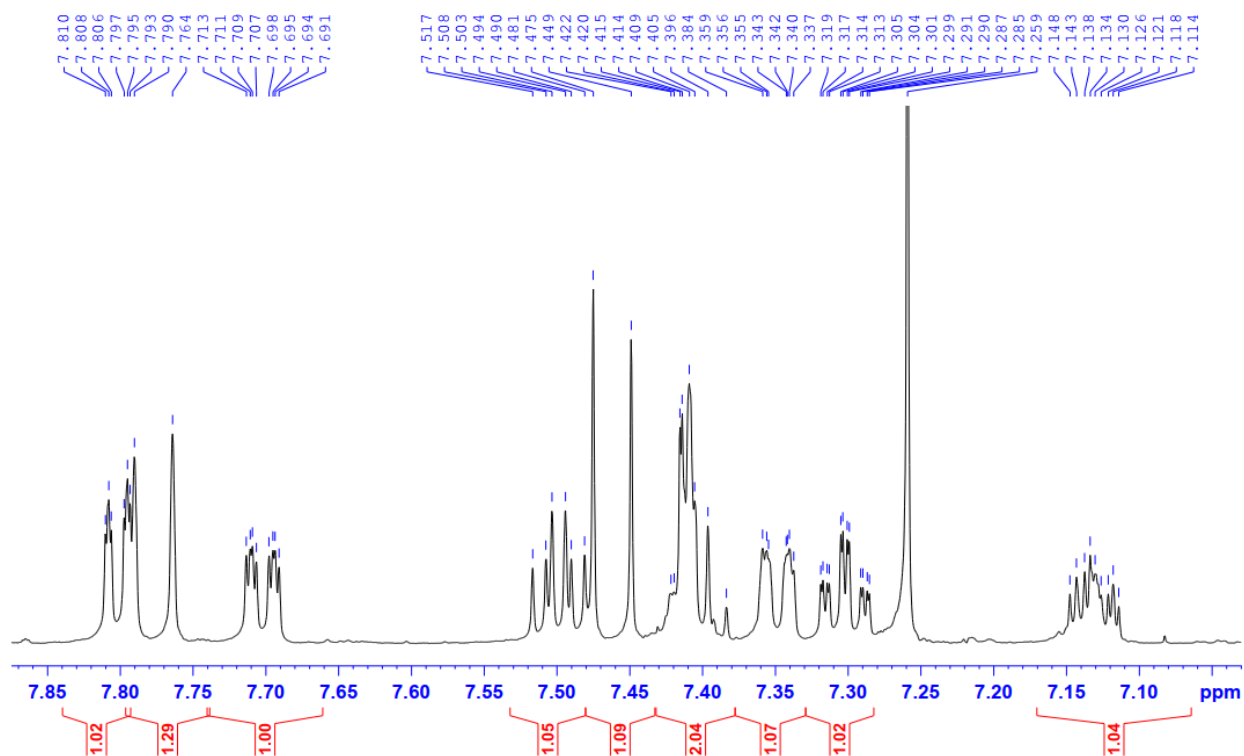
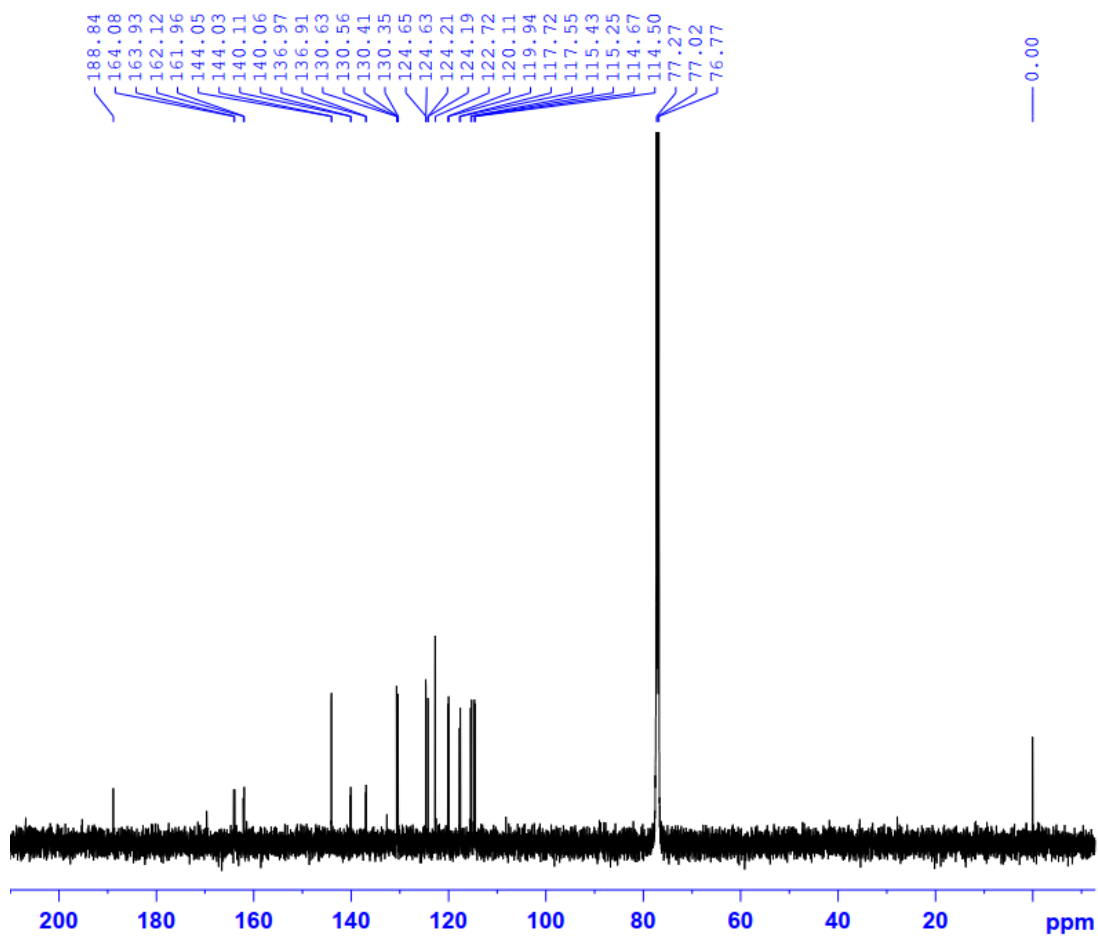
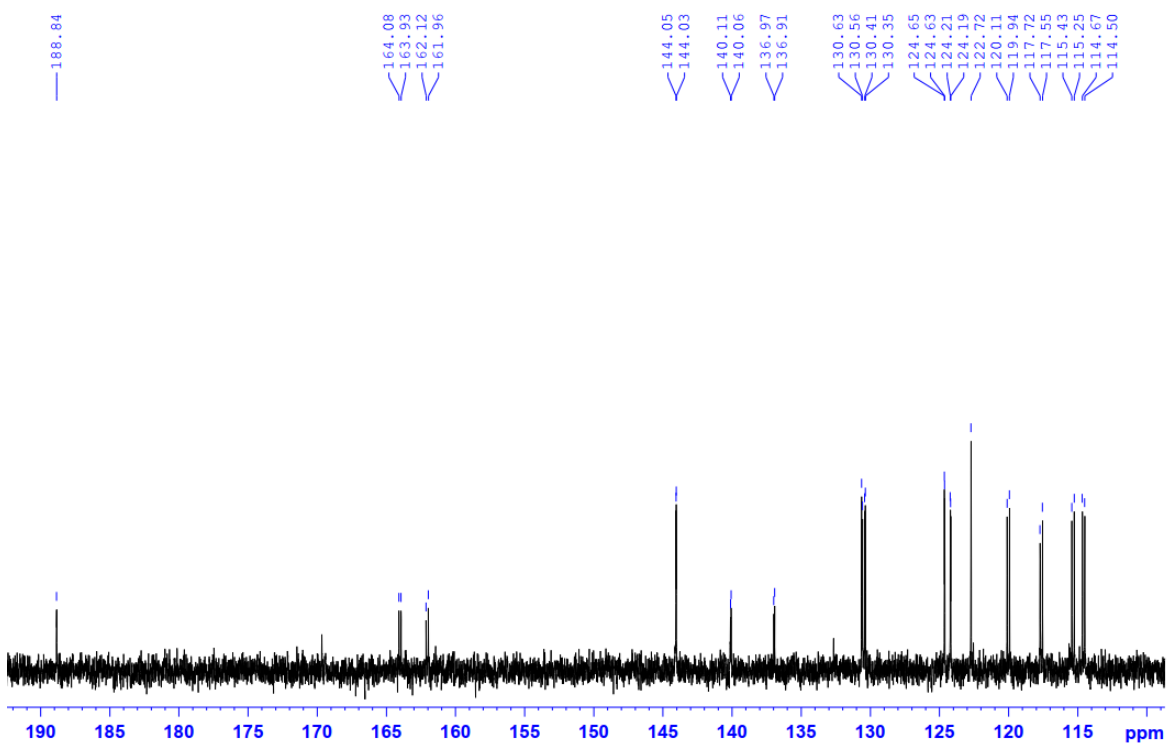


Figure S9h. HRMS of 2b.

Figure S10a. ¹H-NMR spectrum of 2c.Figure S10b. ¹H-NMR spectrum of 2c.

Figure S10c. ¹³C-NMR spectrum of 2c.Figure S10d. ¹³C-NMR spectrum of 2c.

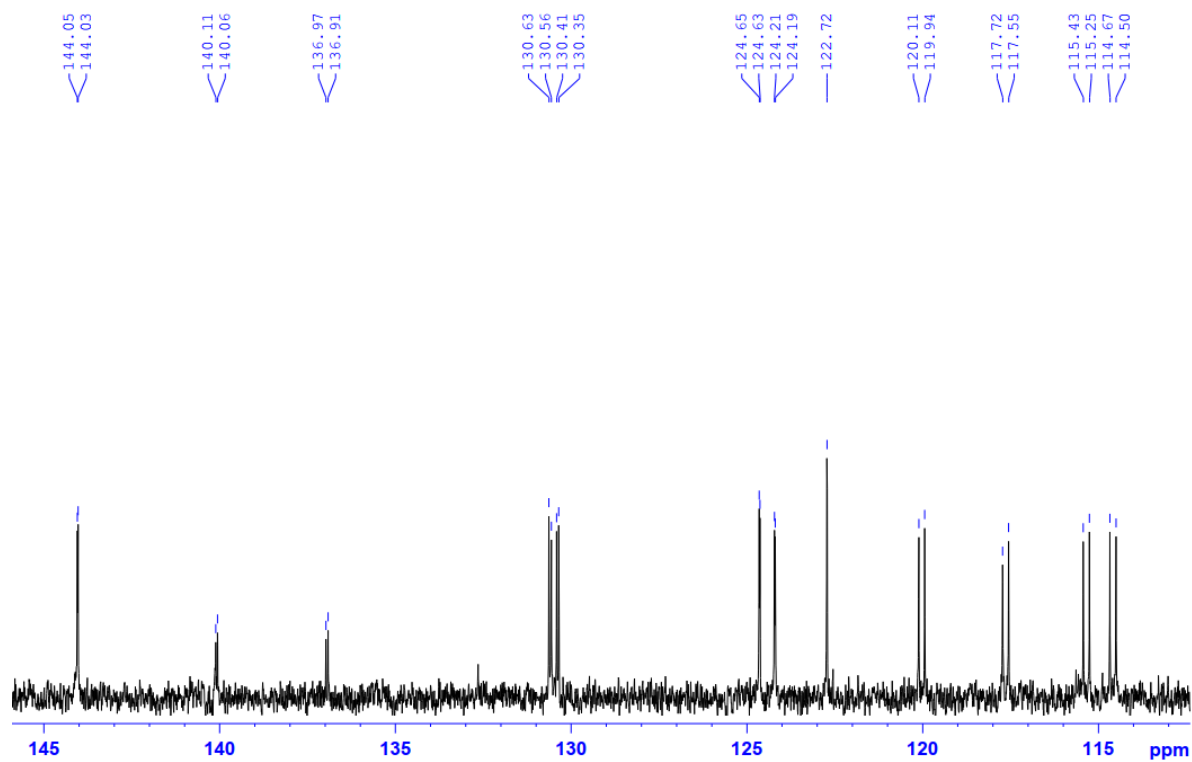
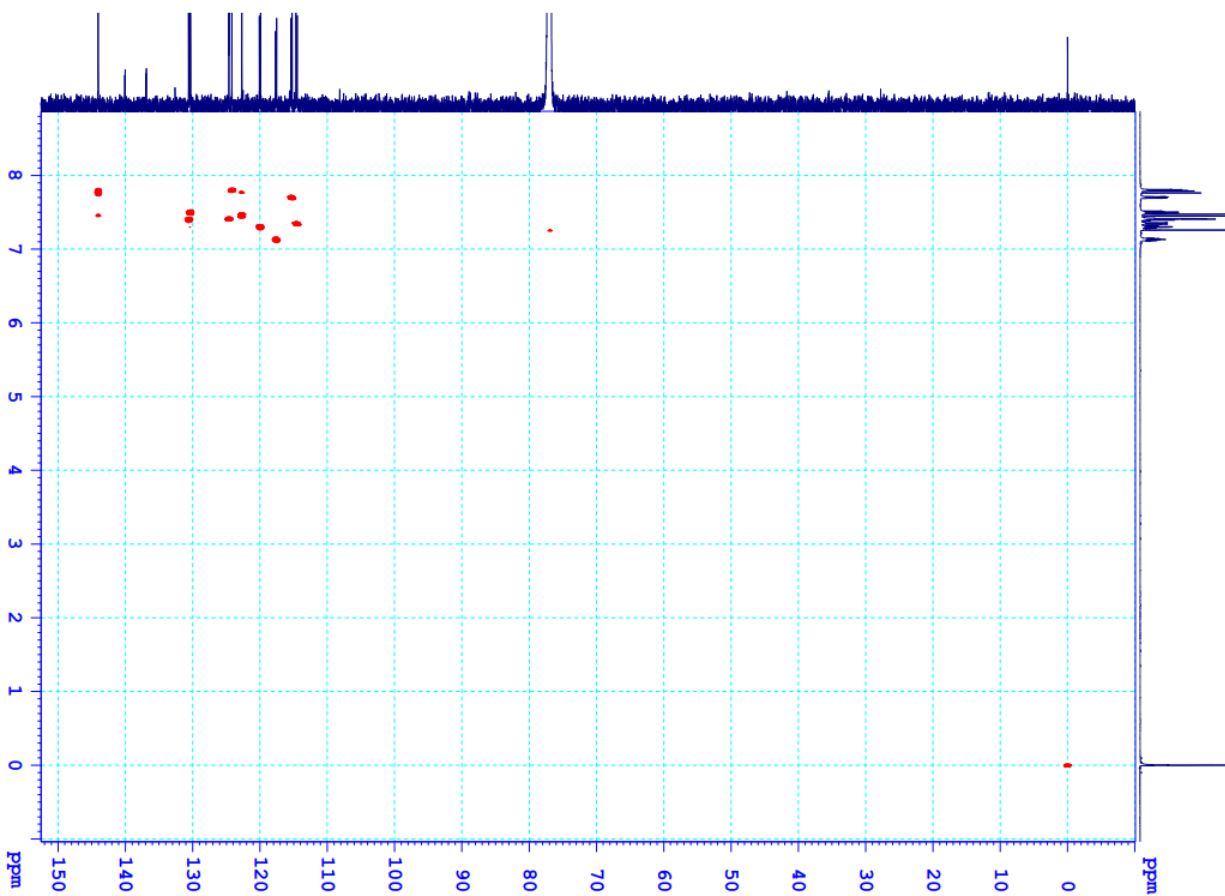
Figure S10e. ^{13}C -NMR spectrum of 2c.

Figure S10f. HSQC spectrum of 2c.

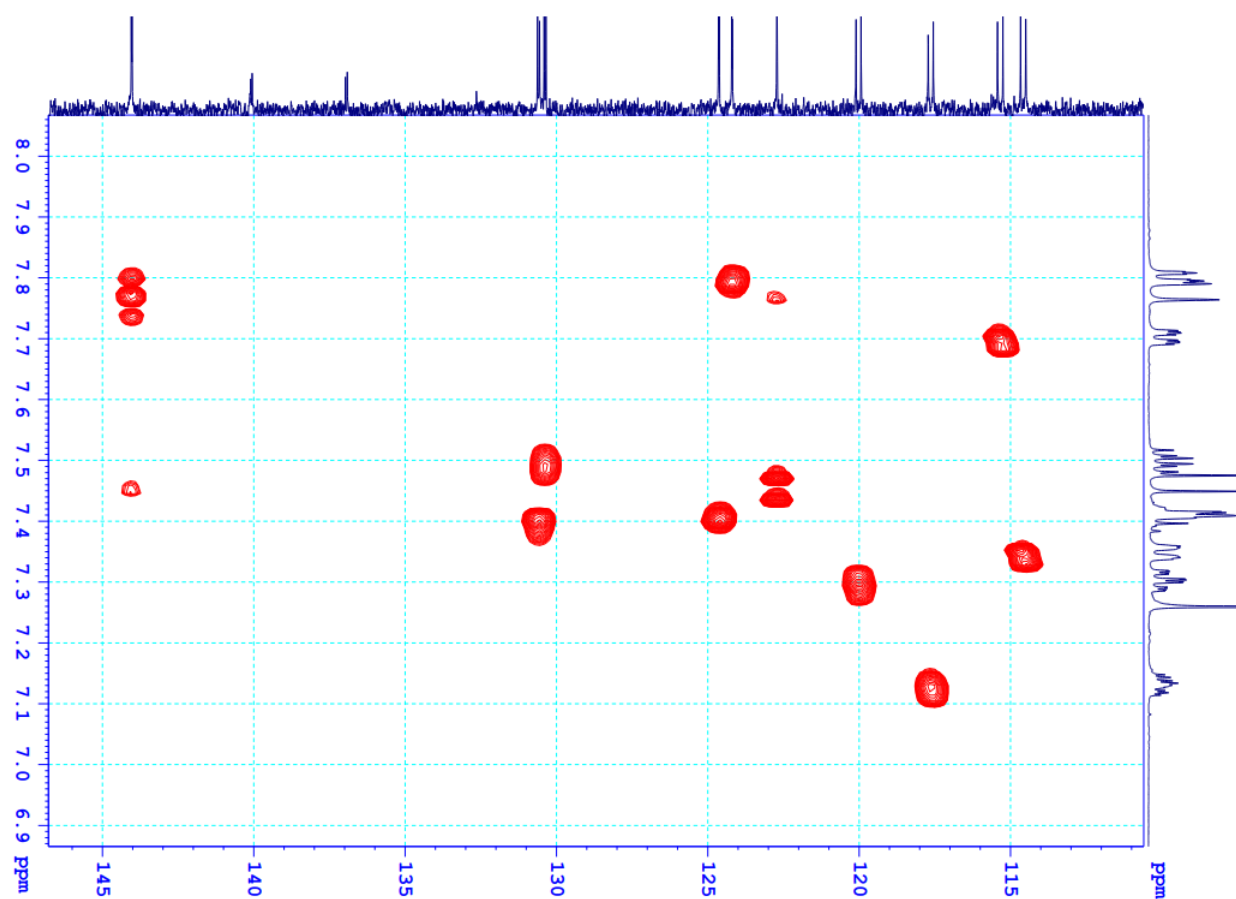


Figure S10g. HSQC spectrum of 2c.

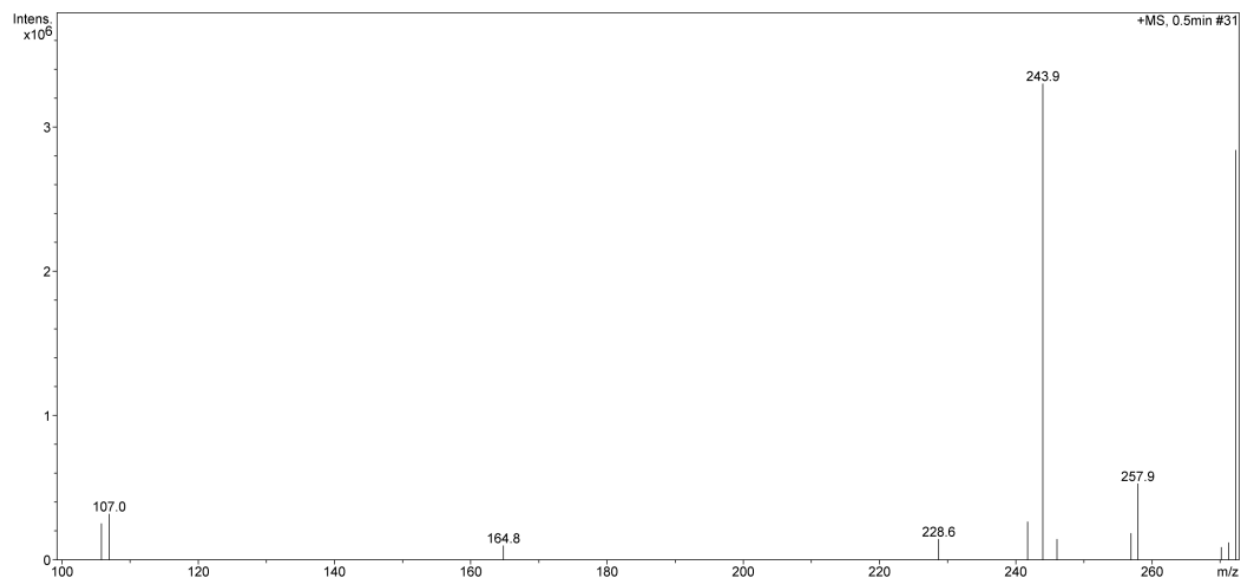
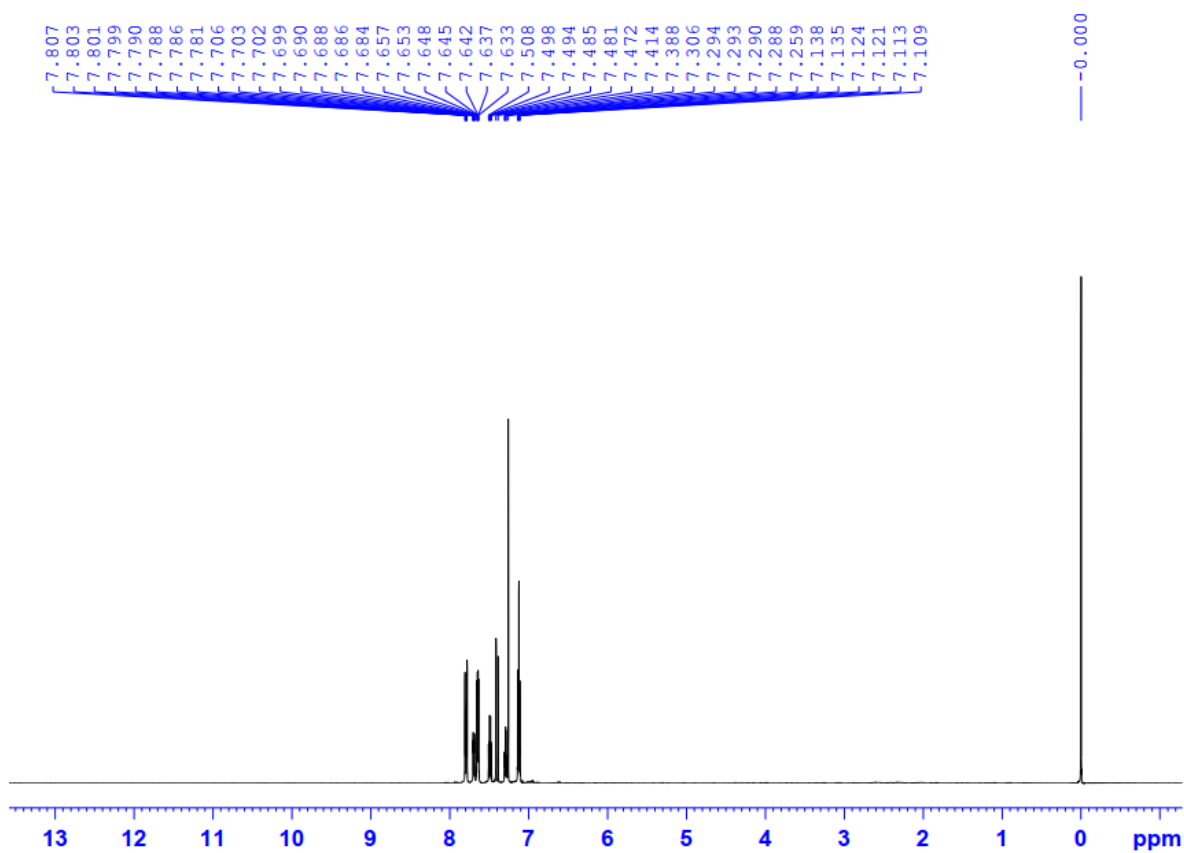
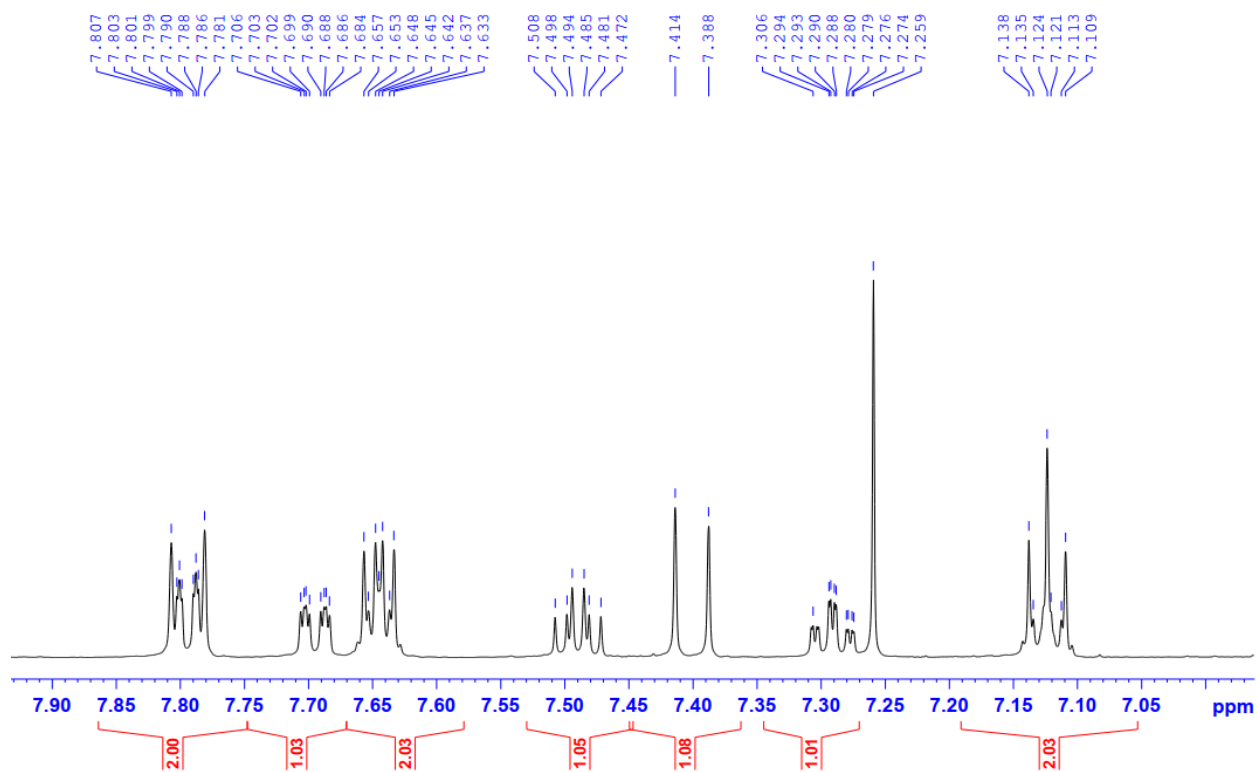
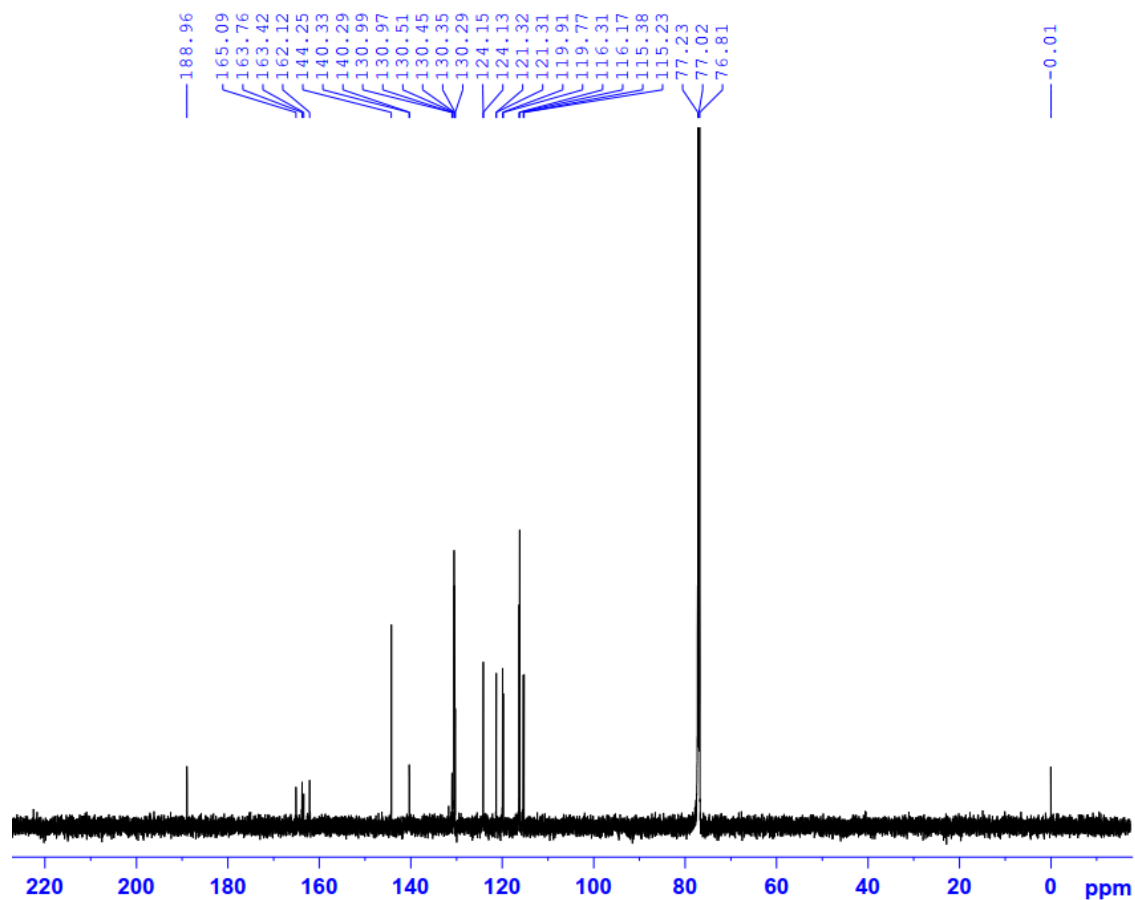
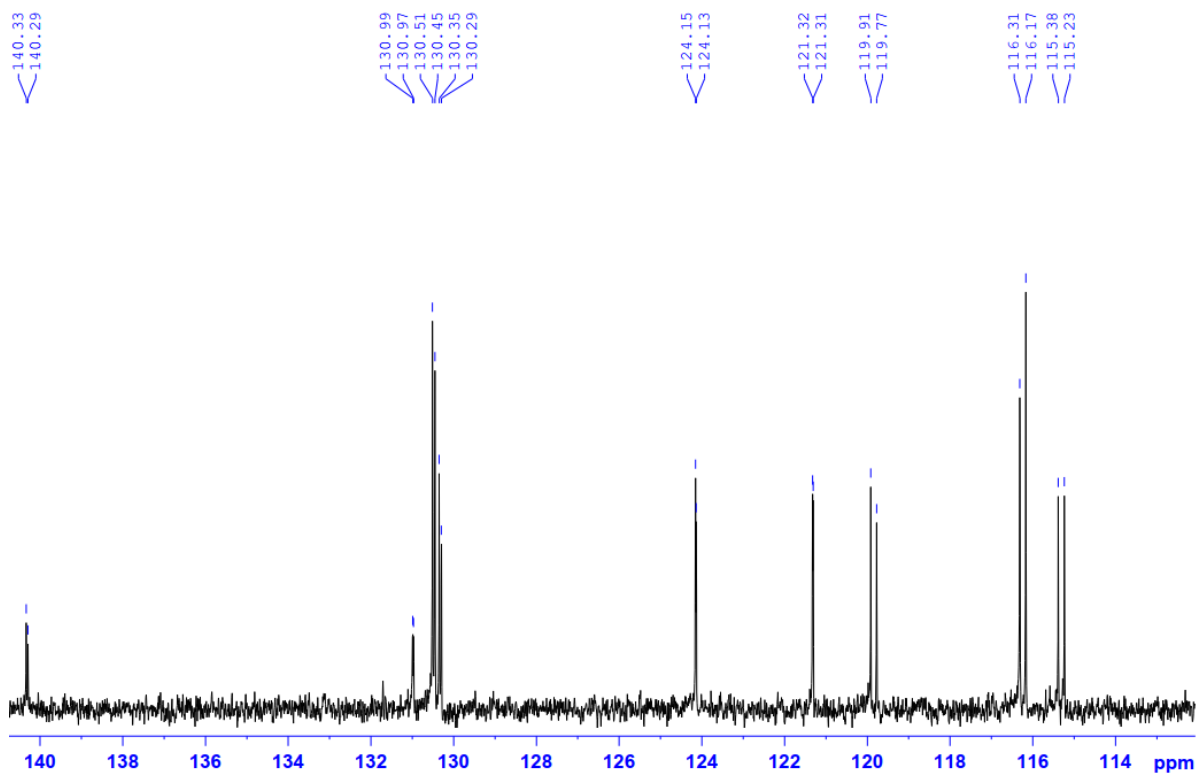


Figure S10h. MS of 2c.

Figure S11a. ¹H-NMR spectrum of 2d.Figure S11b. ¹H-NMR spectrum of 2d.

Figure S11c. ^{13}C -NMR spectrum of 2d.Figure S11d. ^{13}C -NMR spectrum of 2d.

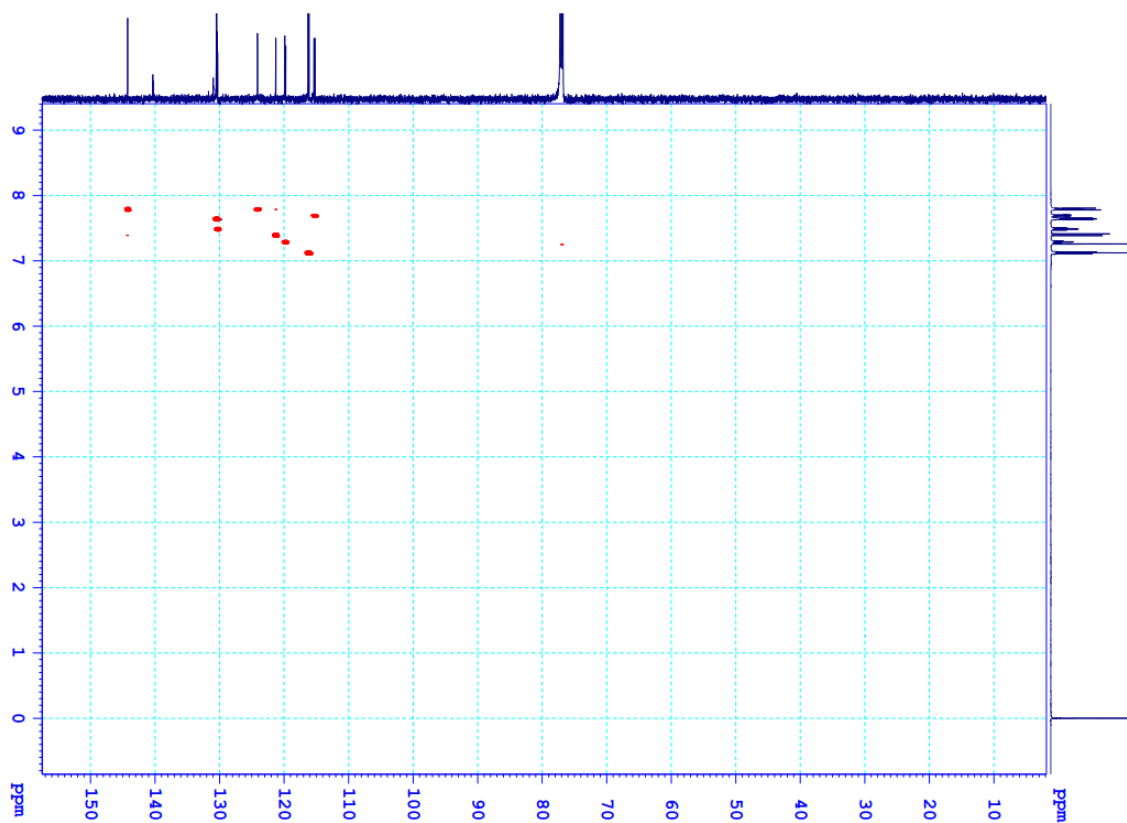


Figure S11e. HSQC spectrum of 2d.

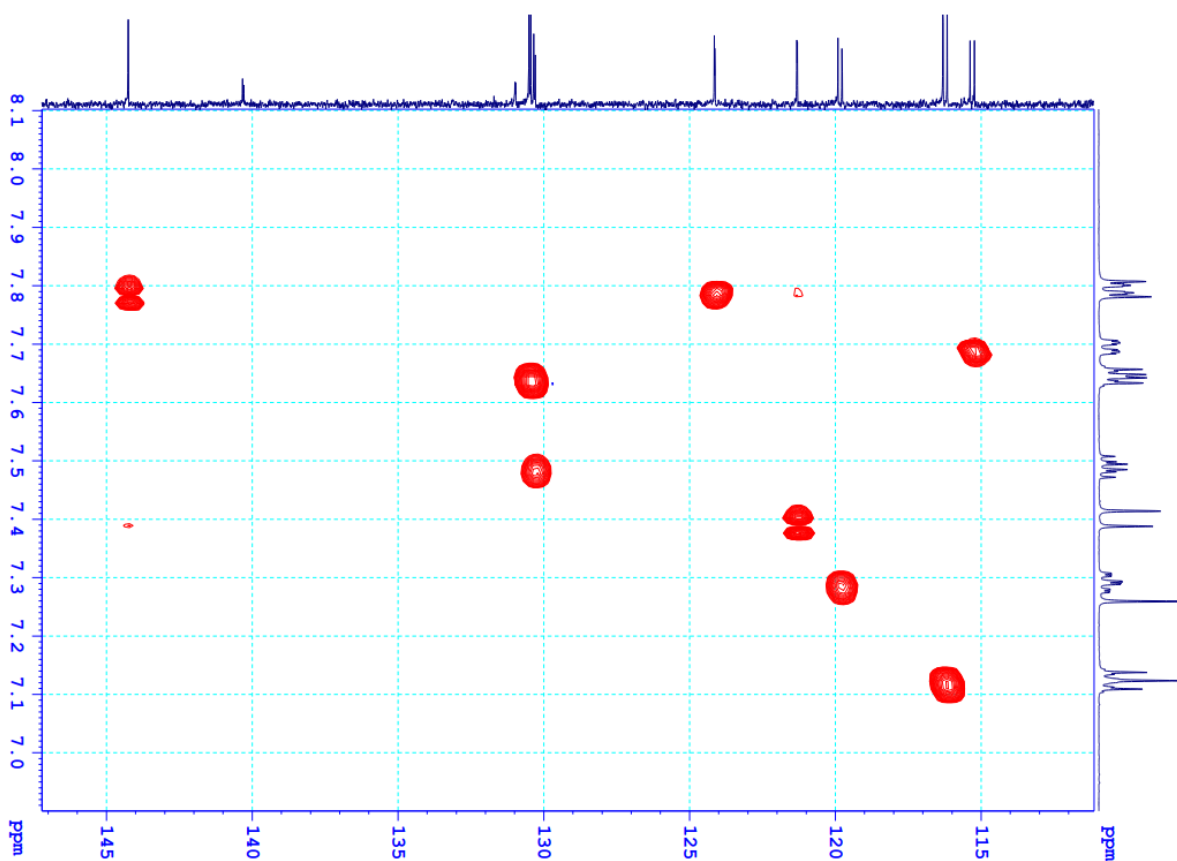


Figure S11f. HSQC spectrum of 2d.

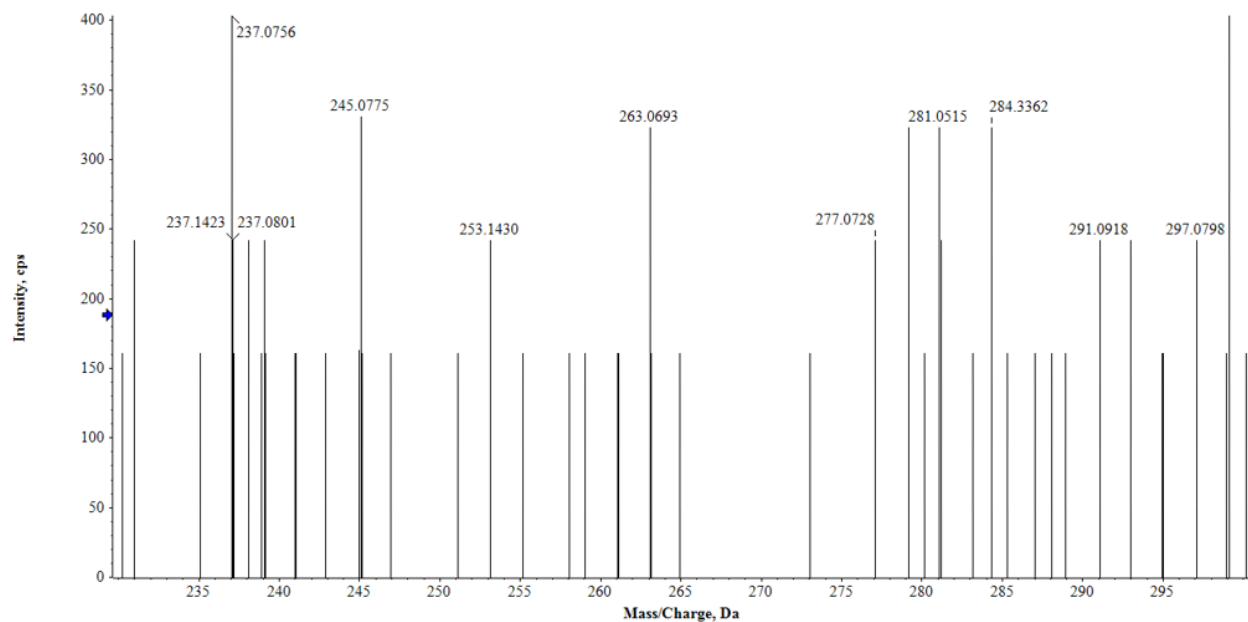
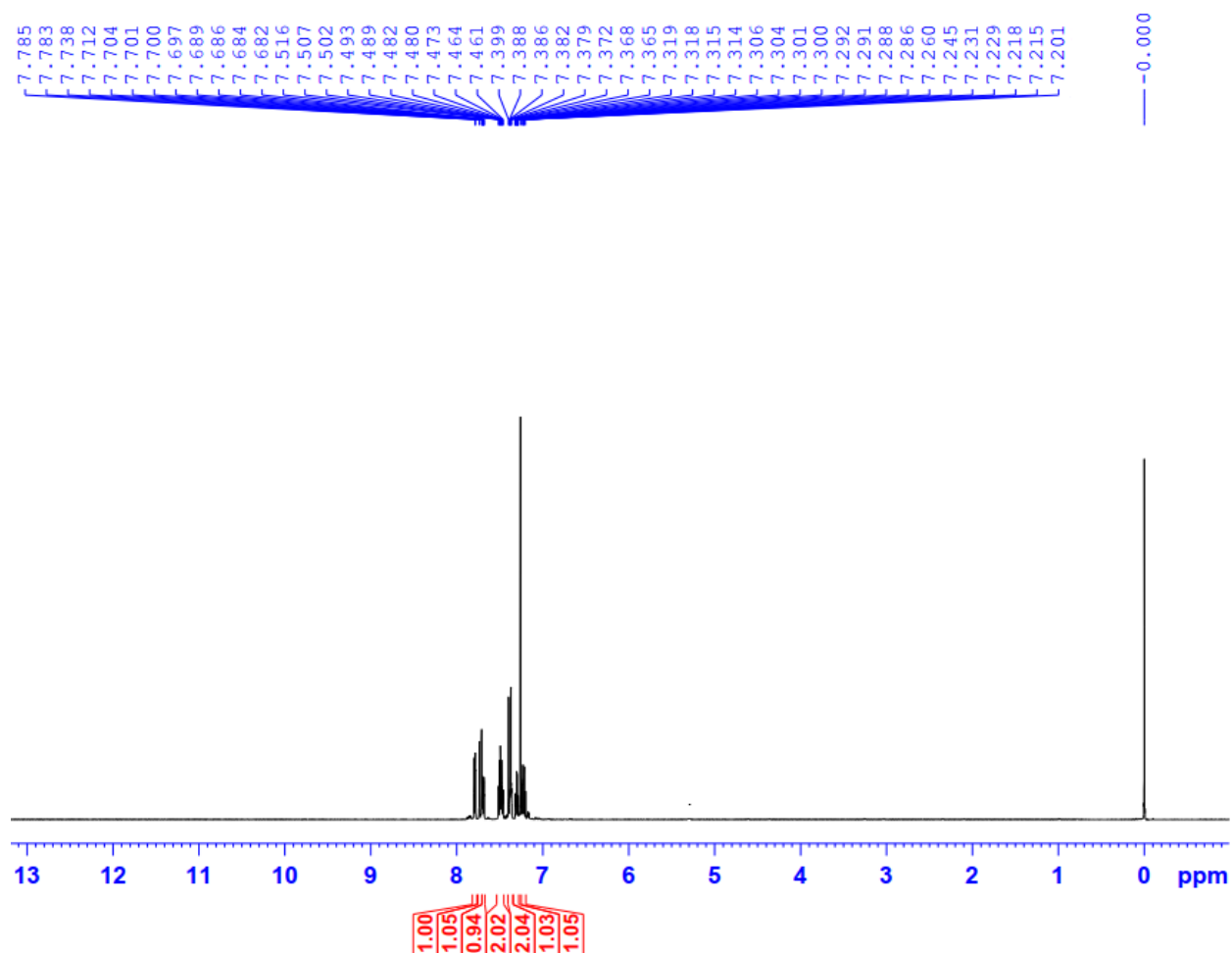
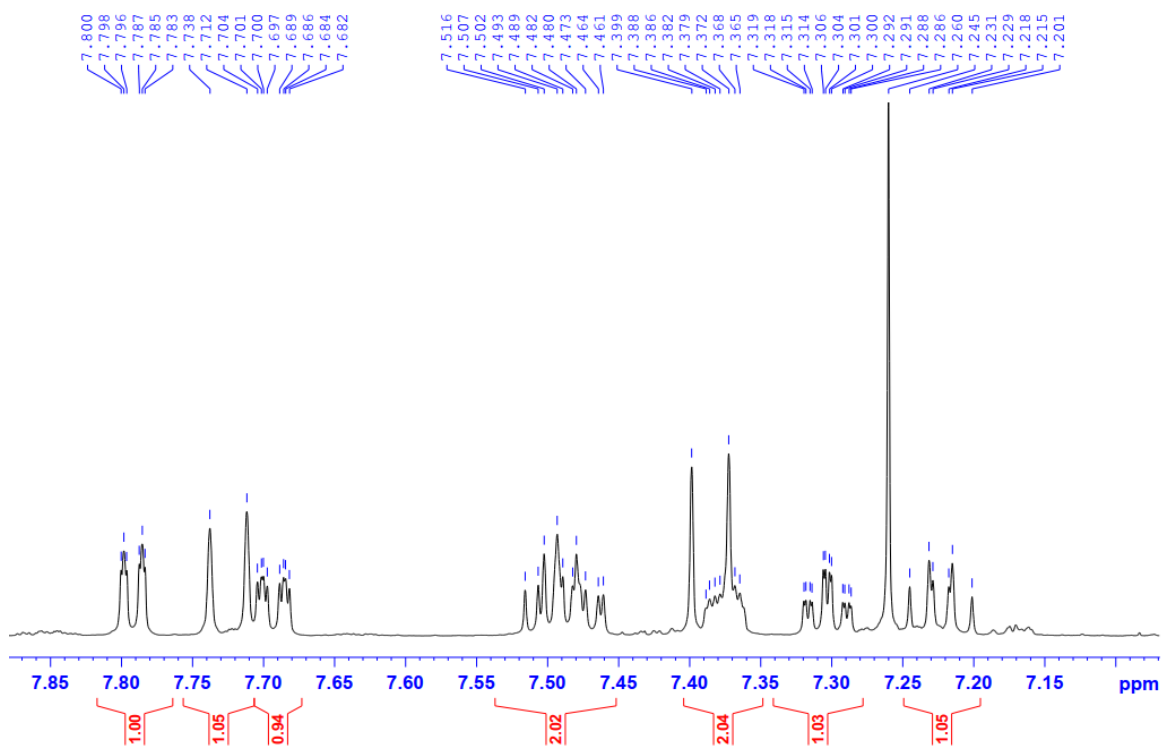
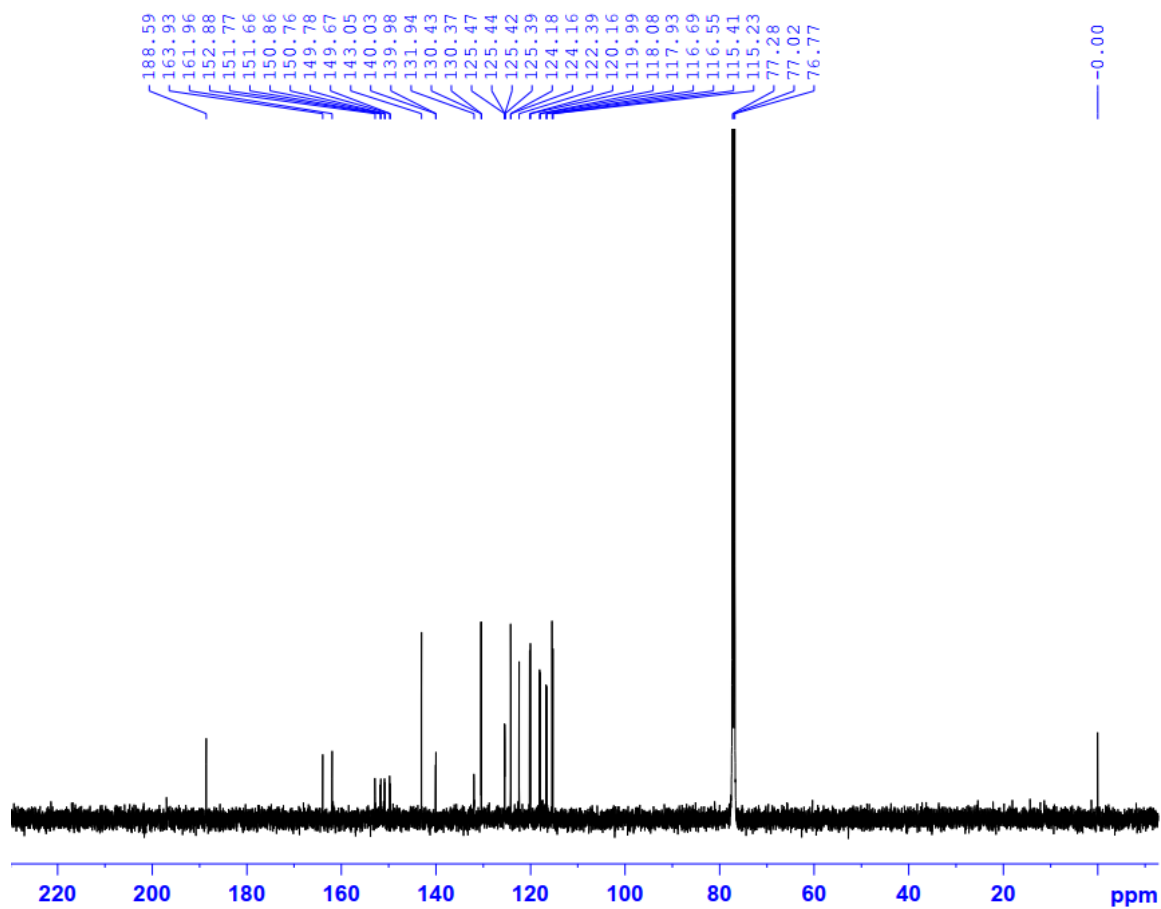
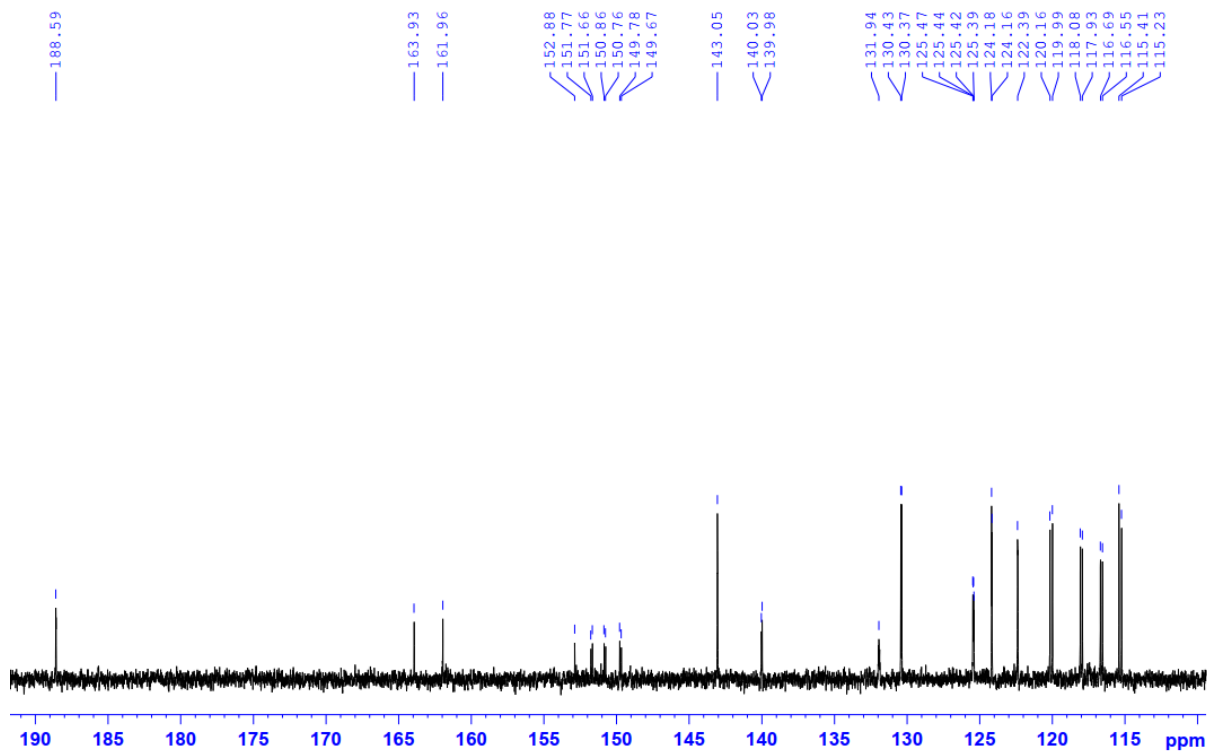
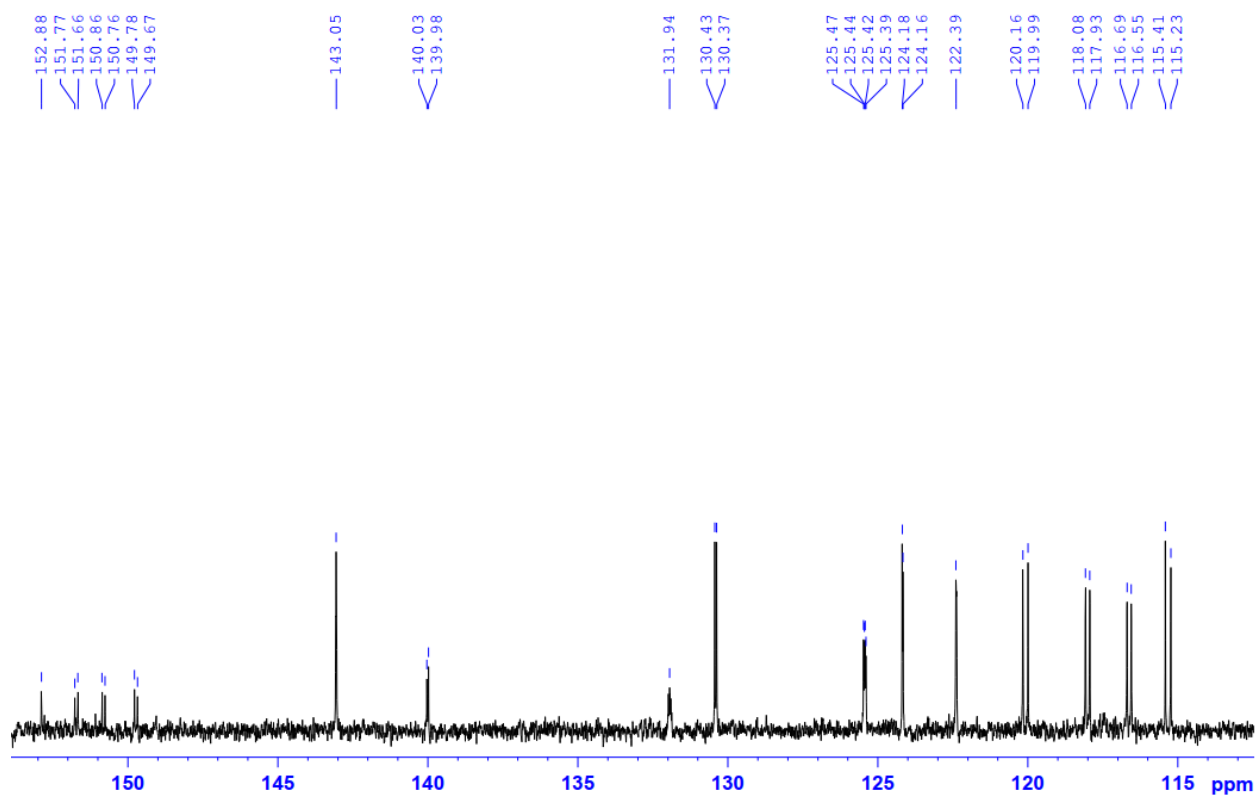


Figure S11g. HRMS of 2d.

Figure S12a. ¹H-NMR spectrum of 2e.

Figure S12b. ¹H-NMR spectrum of 2e.Figure S12c. ¹³C-NMR spectrum of 2e.

Figure S12d. ¹³C-NMR spectrum of 2e.Figure S12e. ¹³C-NMR spectrum of 2e.

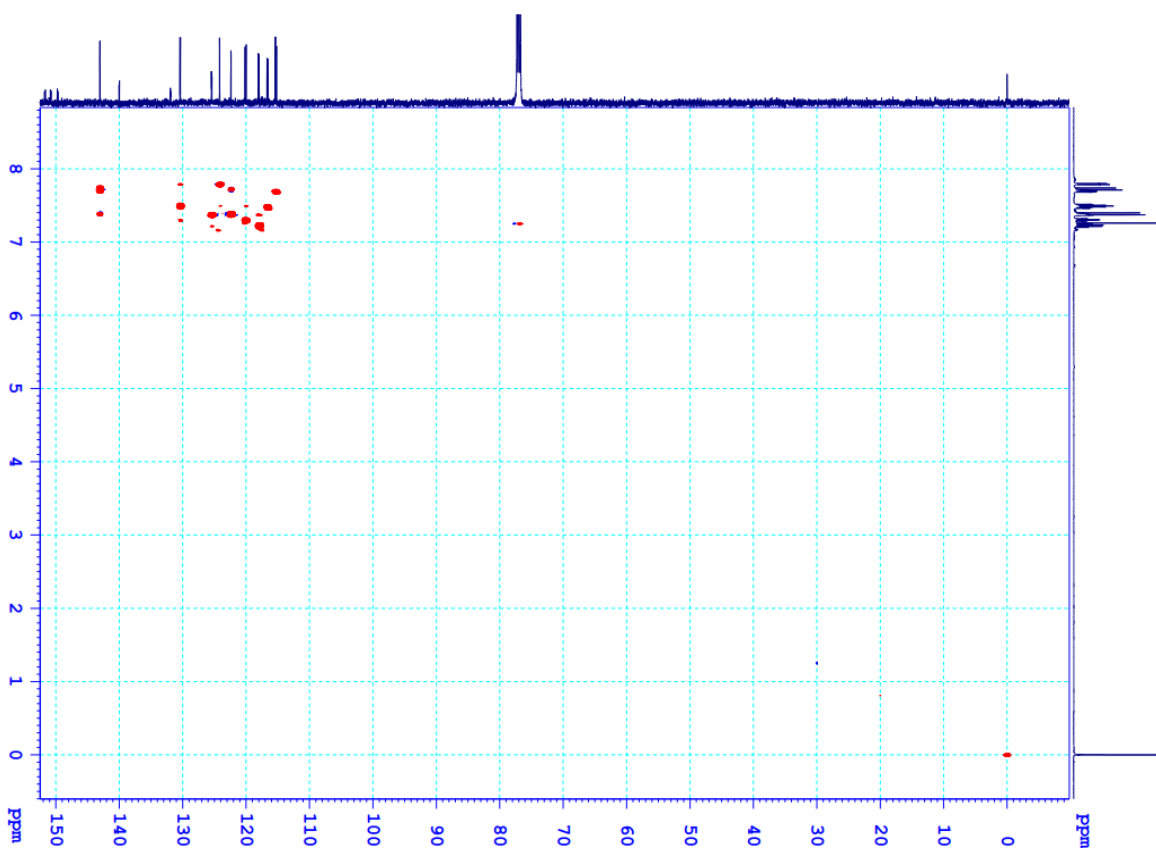


Figure S12f. HSQC spectrum of 2e.

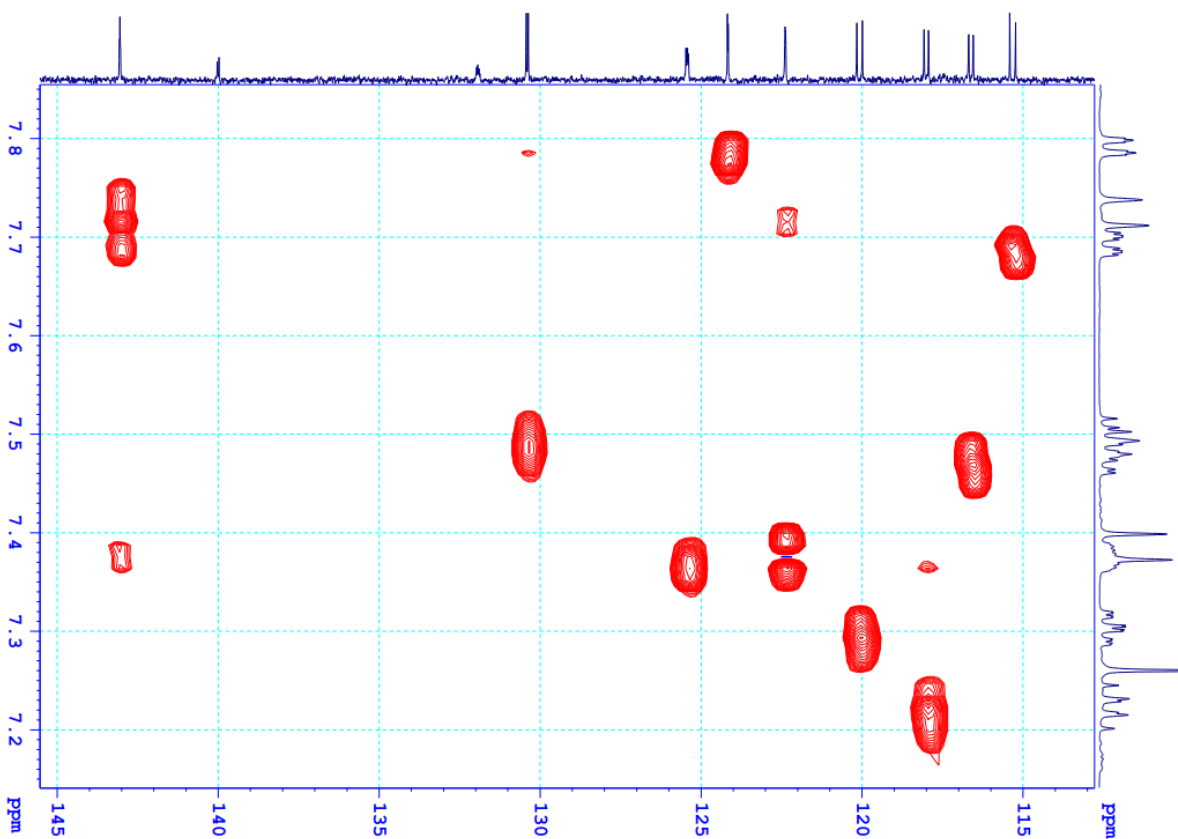


Figure S12g. HSQC spectrum of 2e.

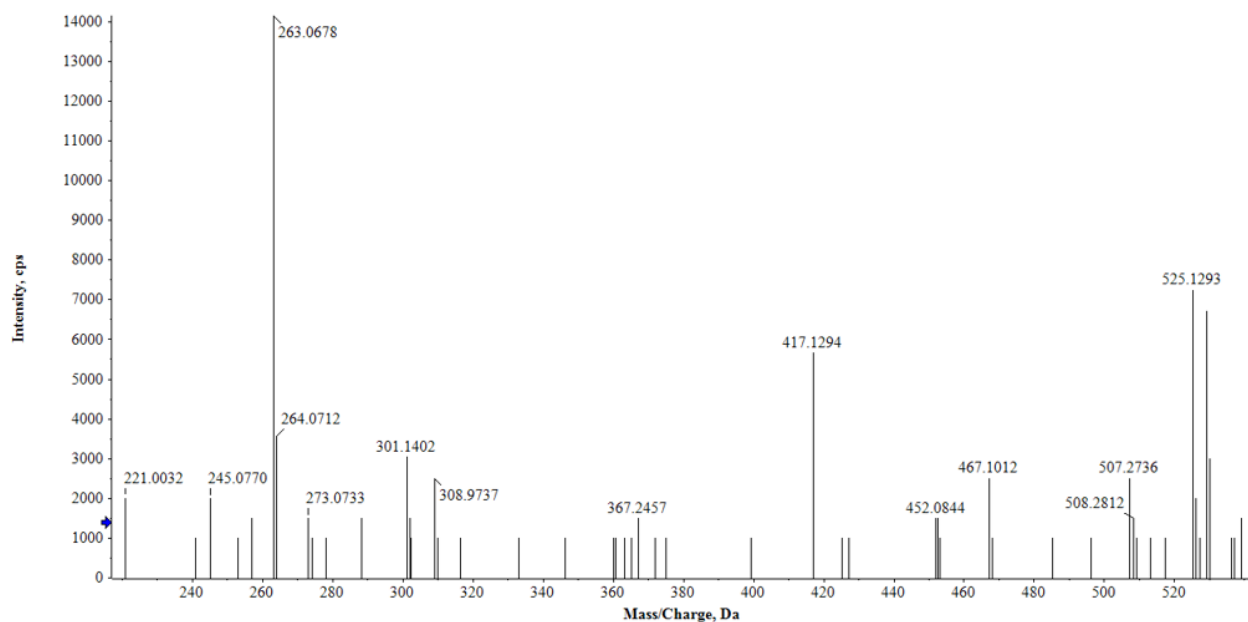
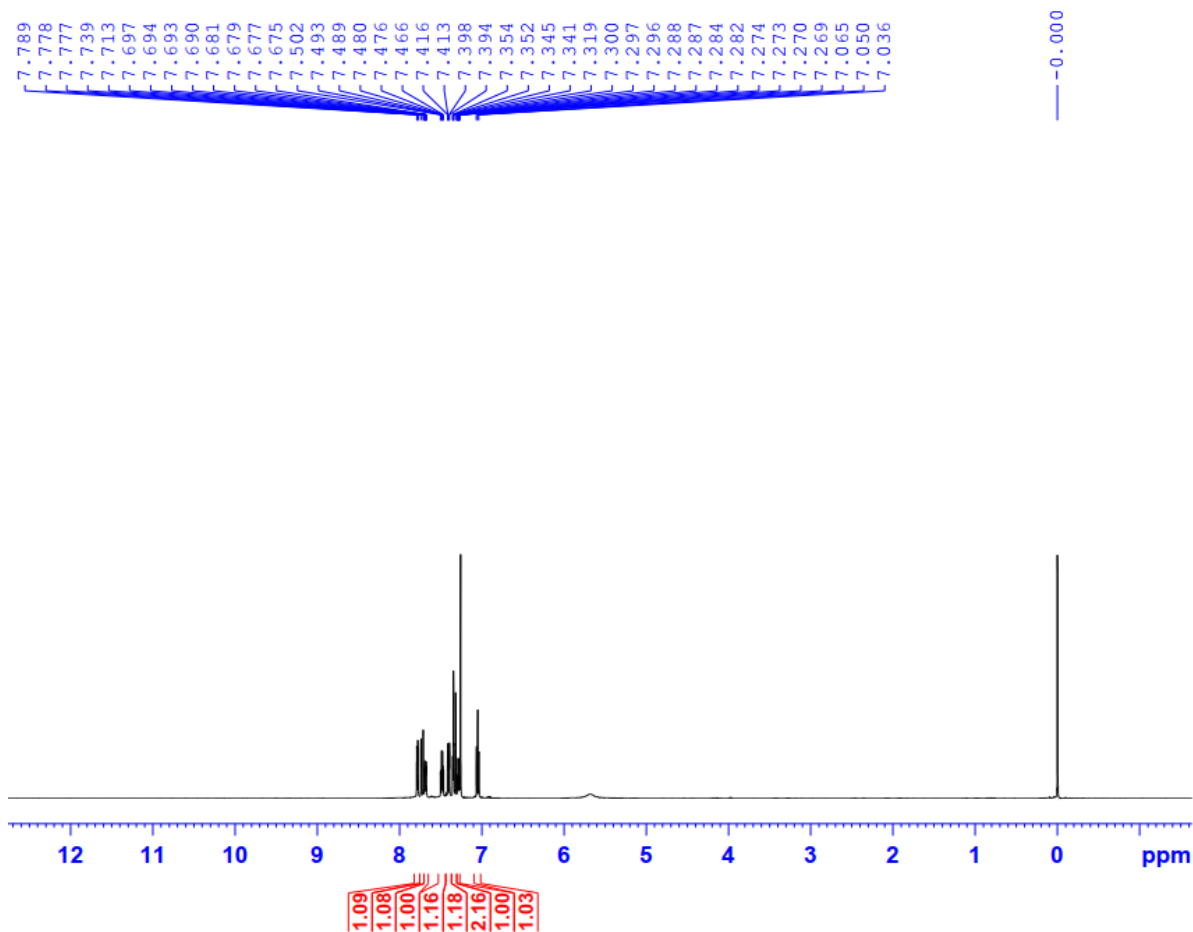
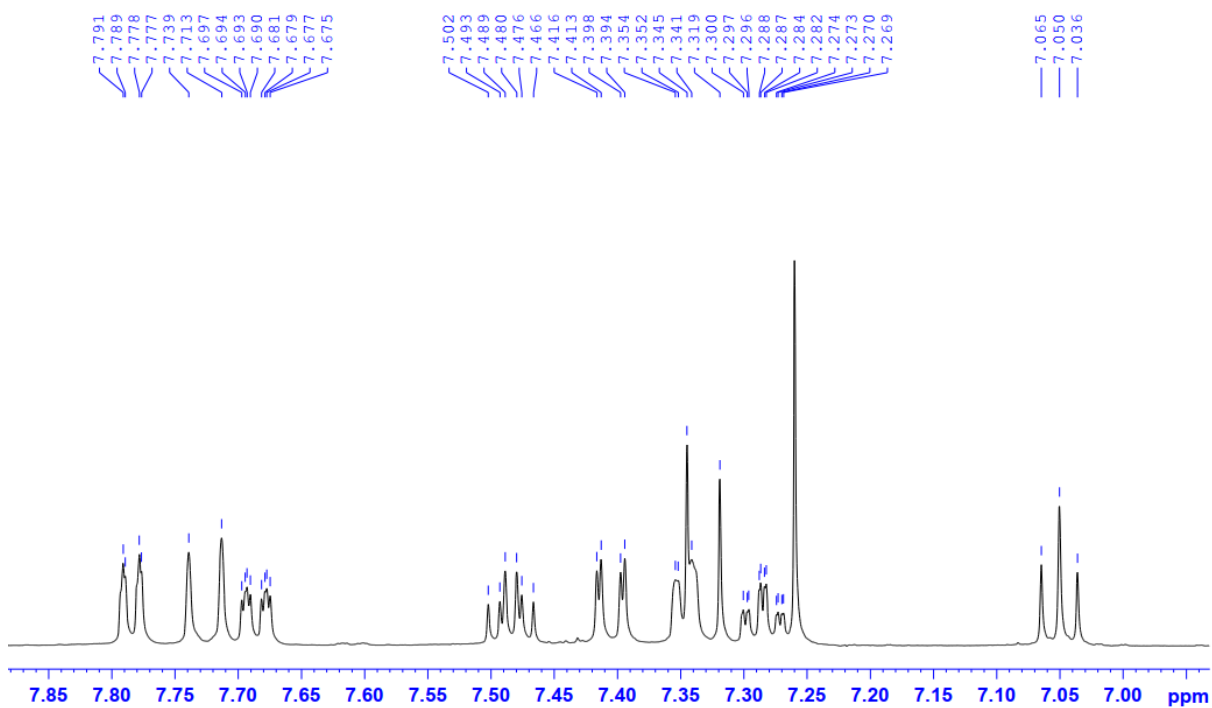
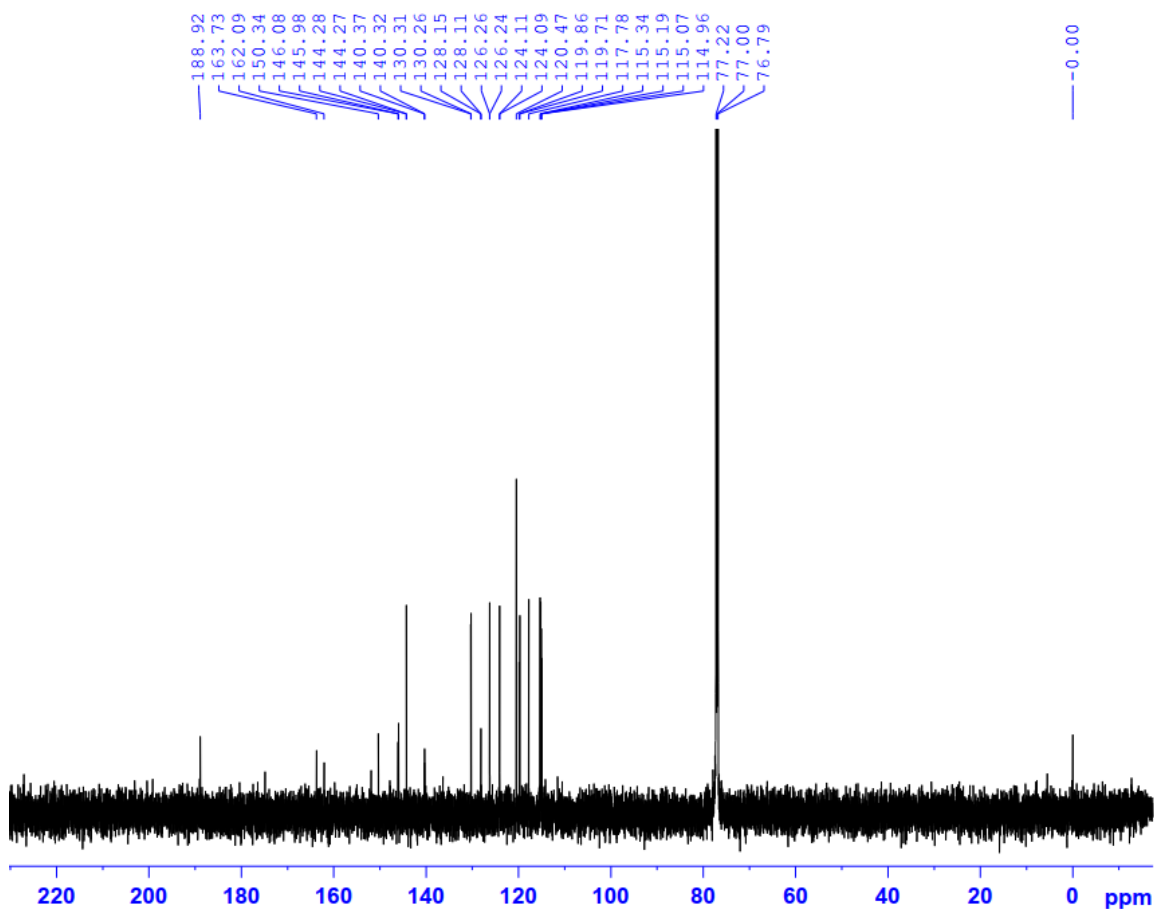
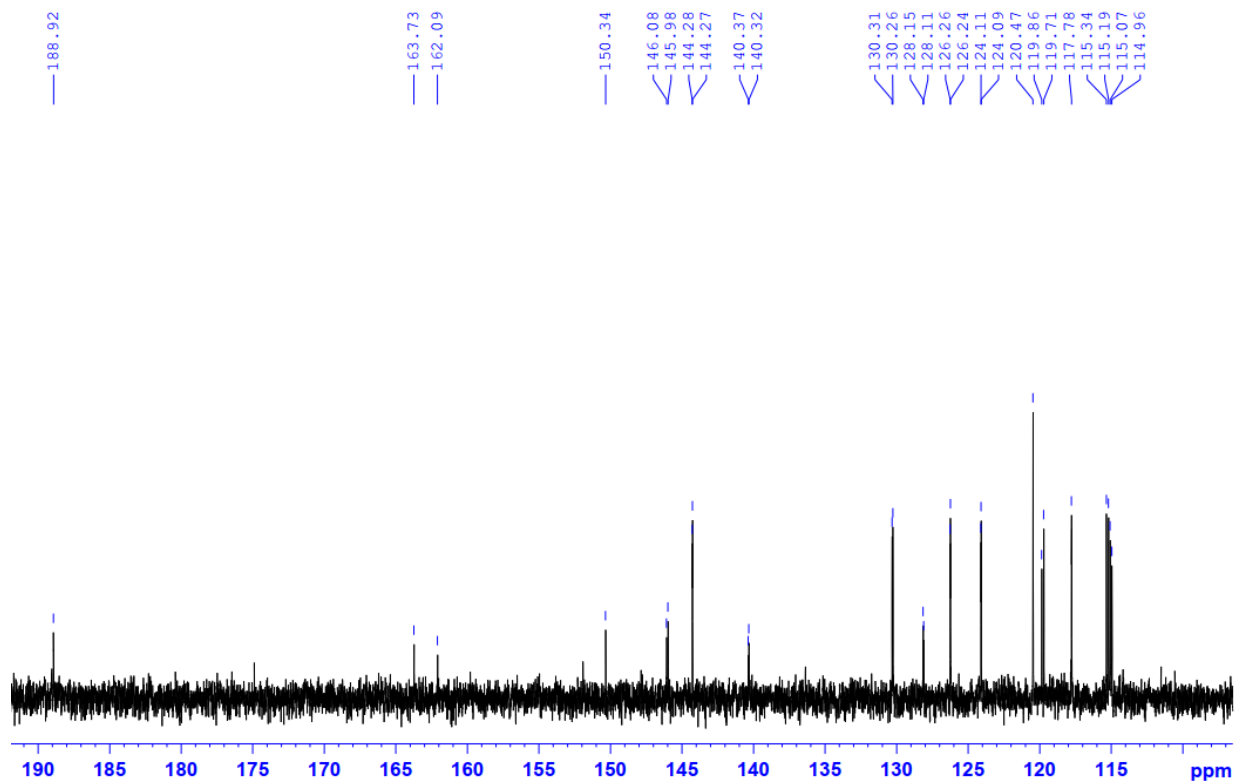
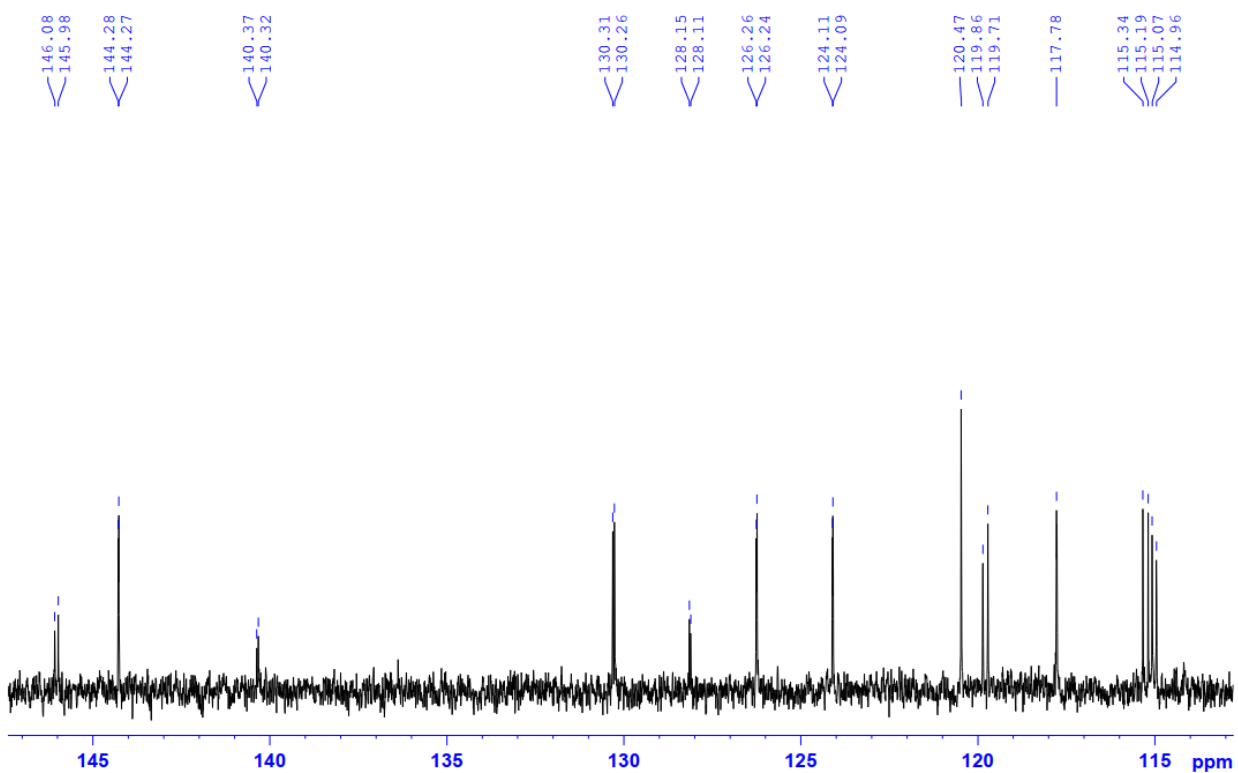


Figure S12h. HRMS of 2e.

Figure S13a. ¹H-NMR spectrum of 2f.

Figure S13b. ¹H-NMR spectrum of 2f.Figure S13c. ¹³C-NMR spectrum of 2f.

Figure S13d. ^{13}C -NMR spectrum of 2f.Figure S13e. ^{13}C -NMR spectrum of 2f.

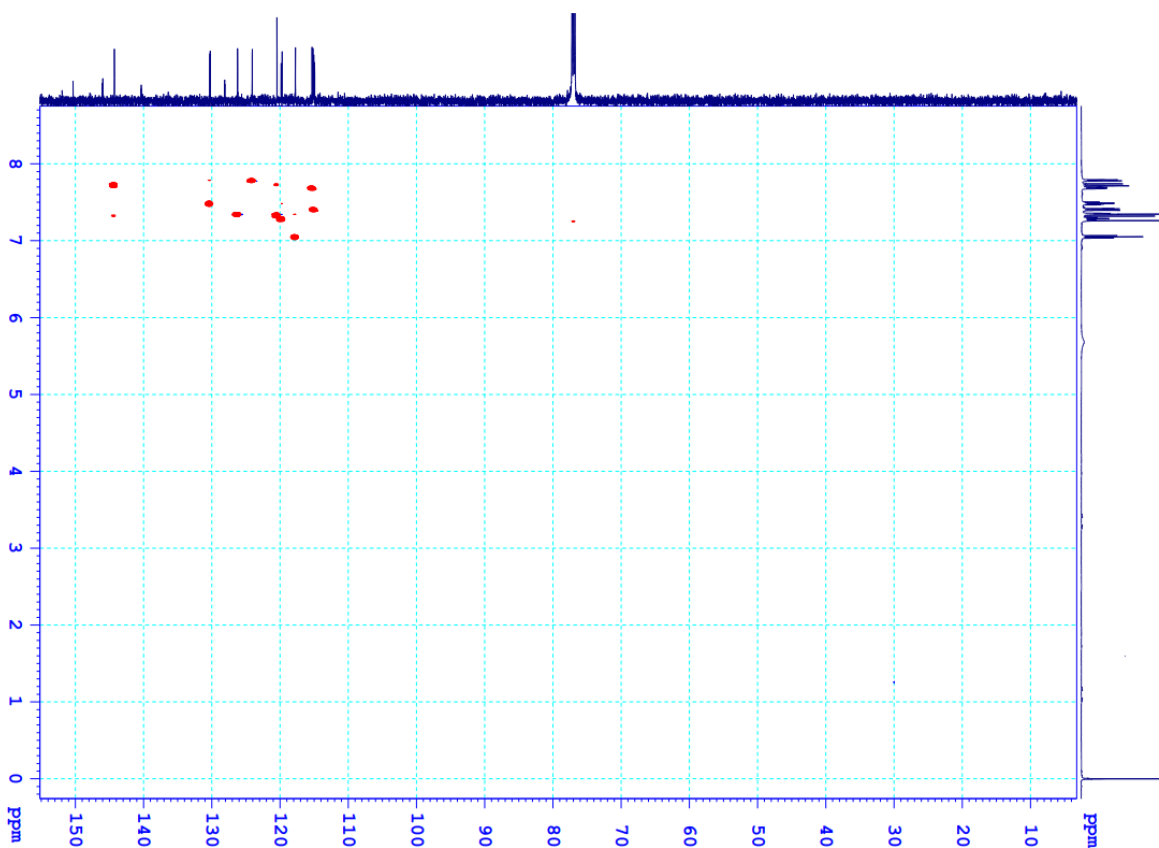


Figure S13f. HSQC spectrum of 2f.

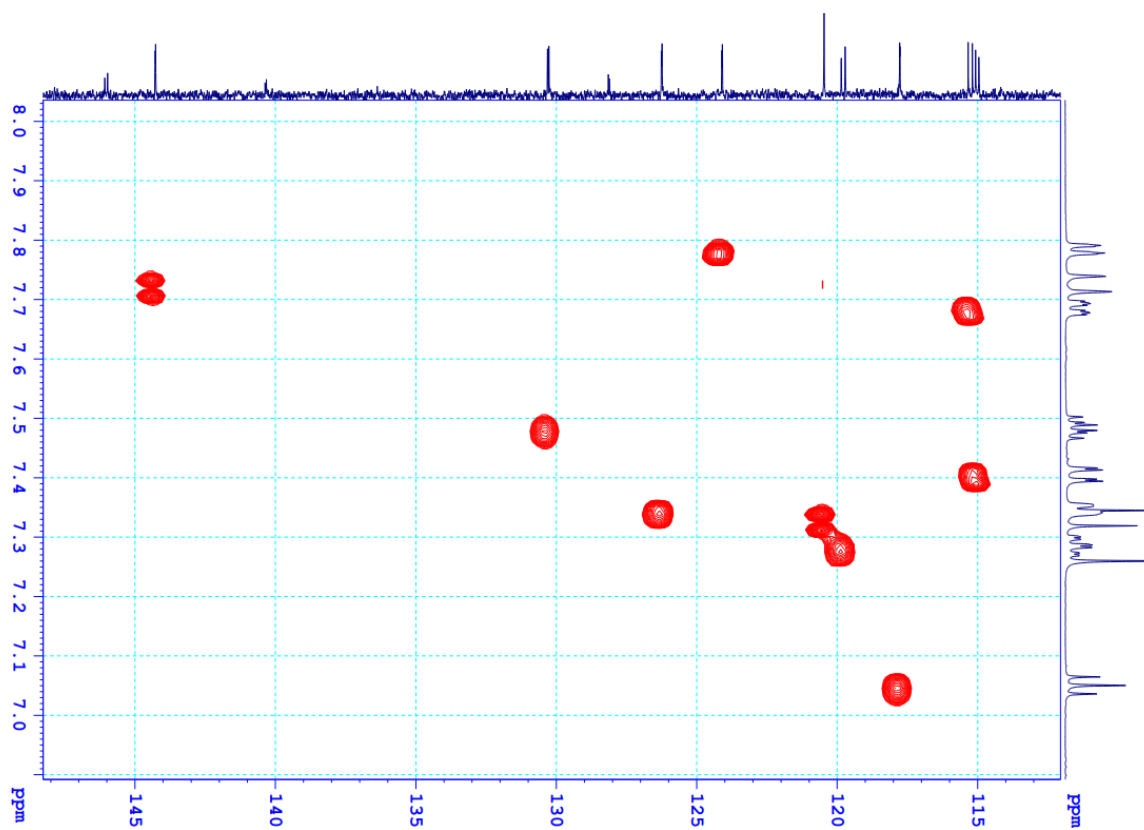


Figure S13g. HSQC spectrum of 2f.

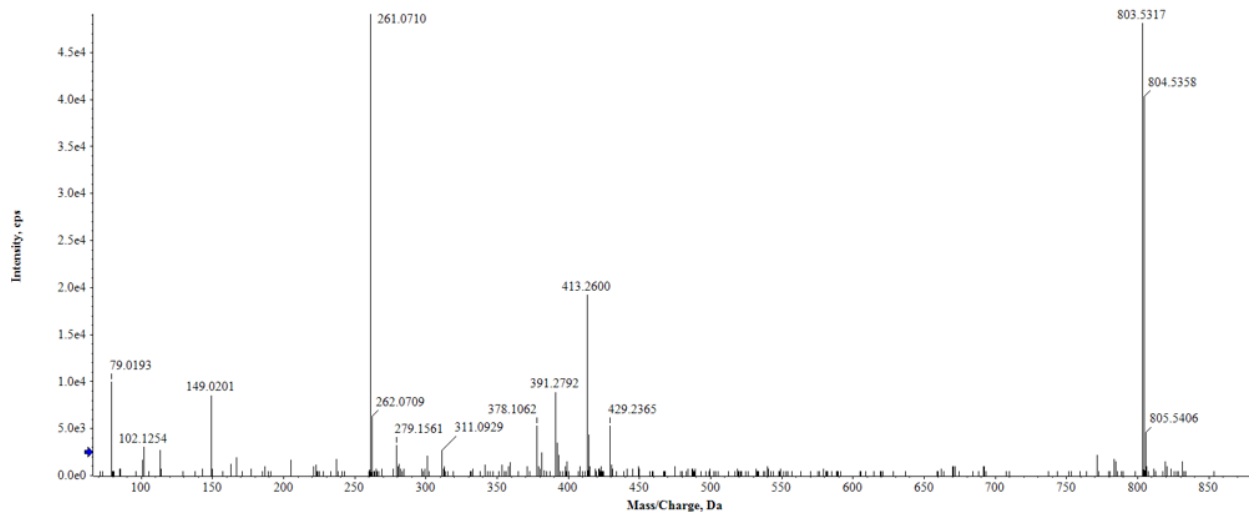
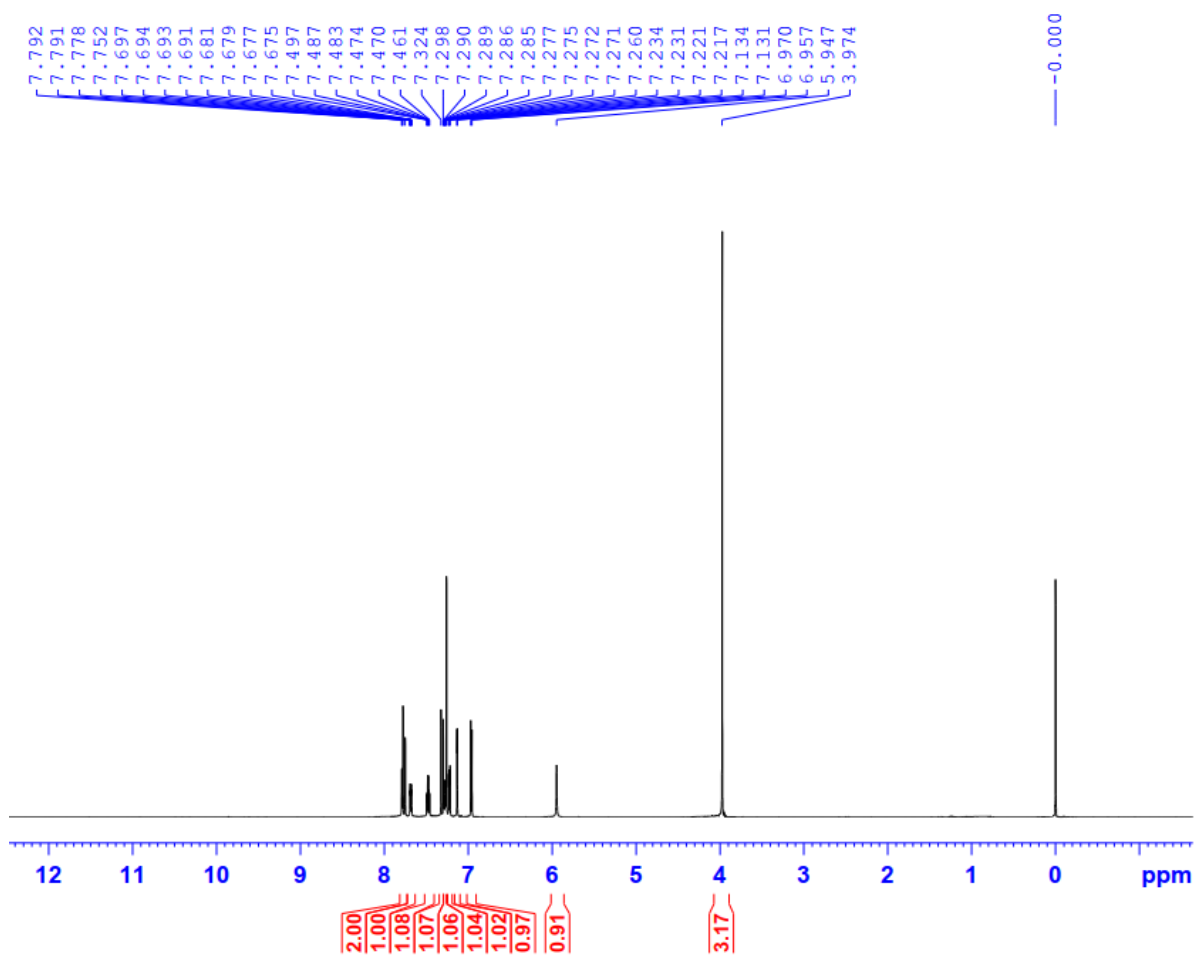
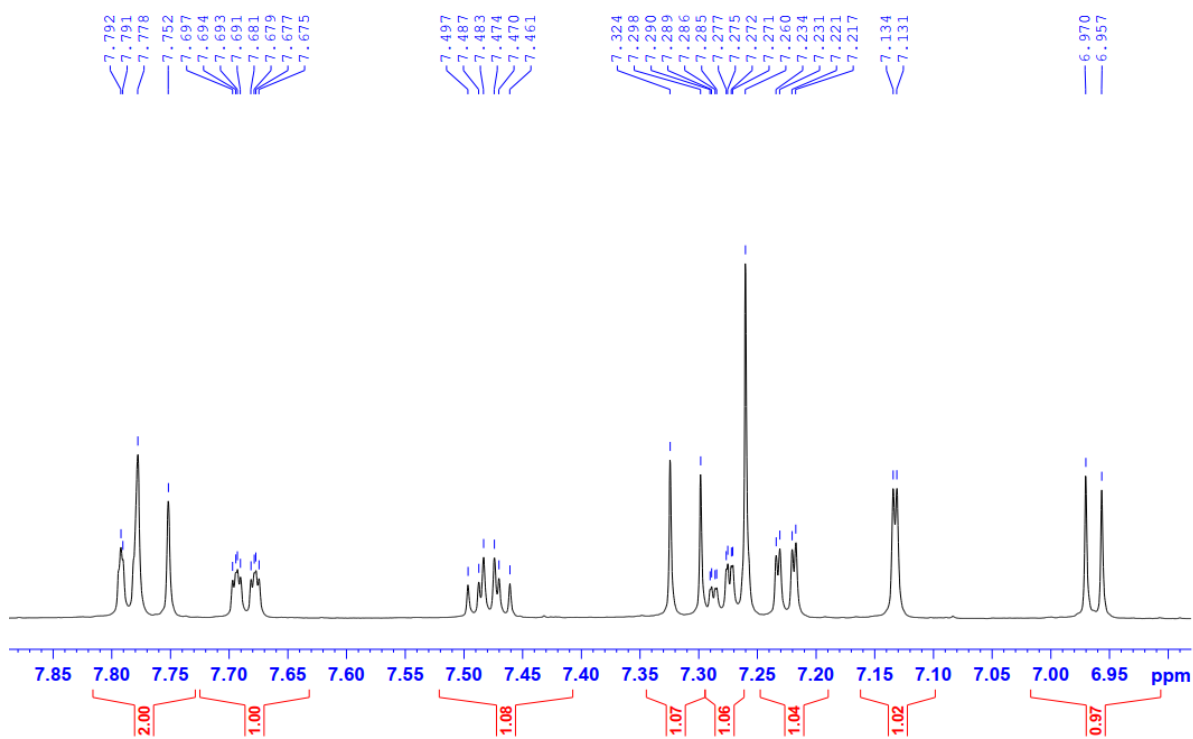
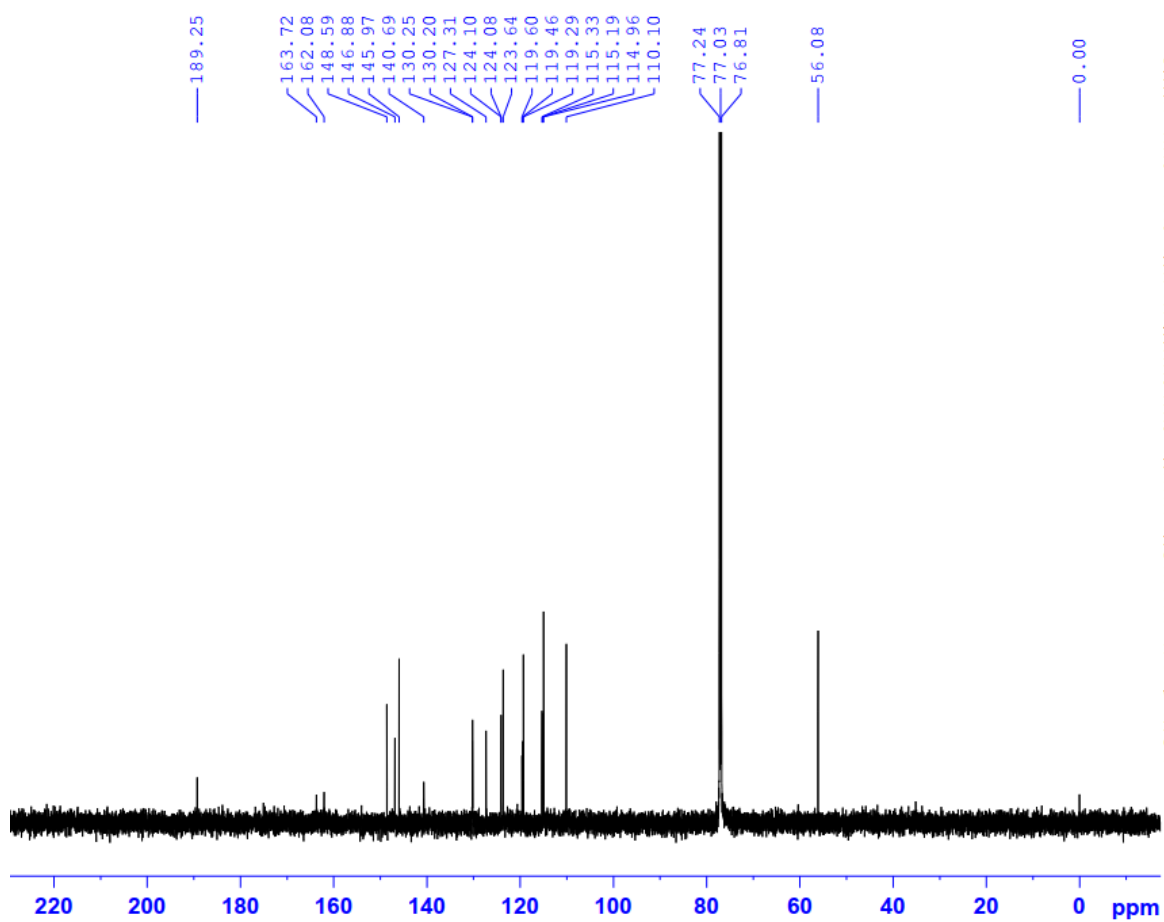
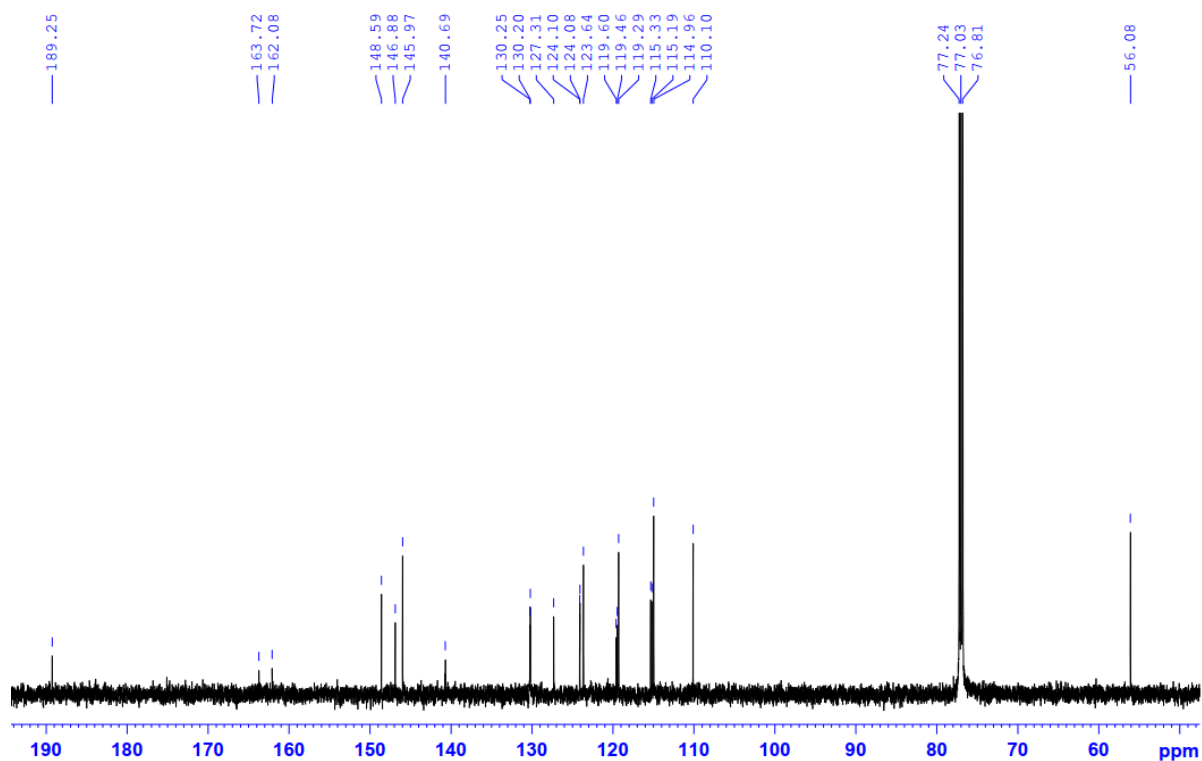
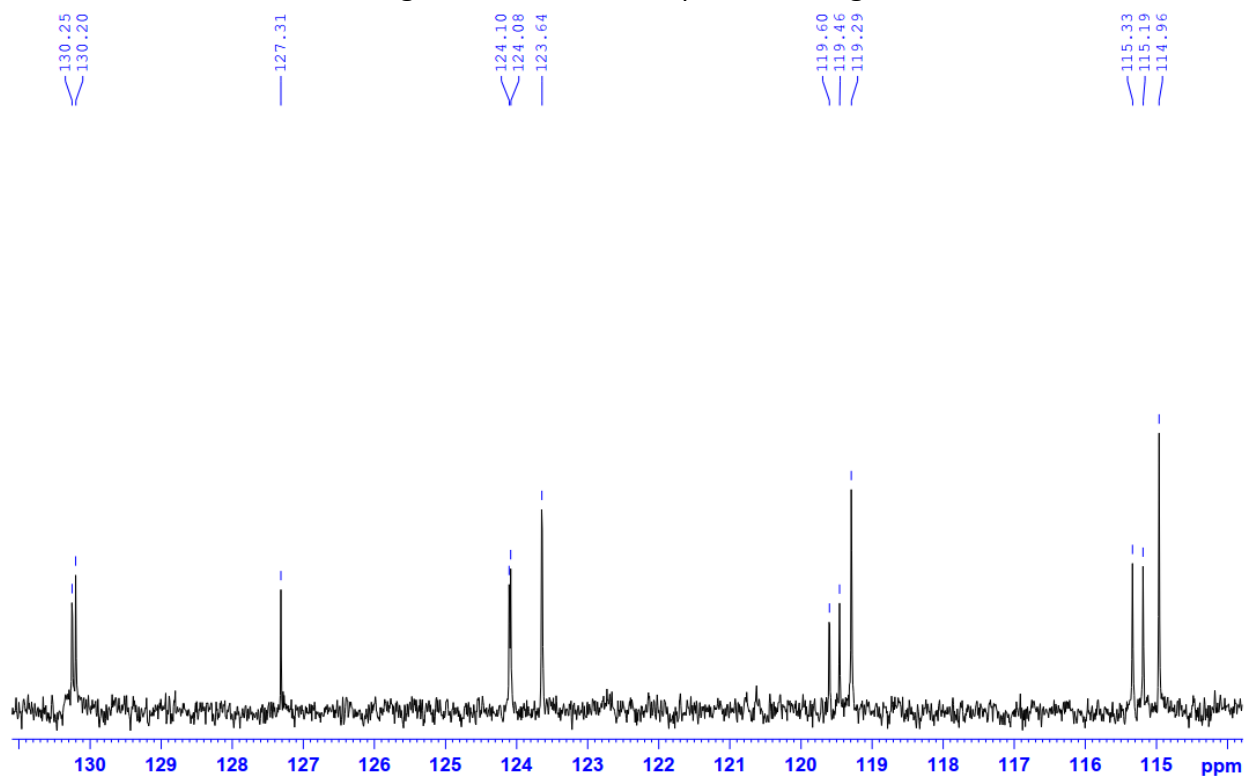


Figure S13h. HRMS of 2f.

Figure S14a. ¹H-NMR spectrum of 2g.

Figure S14b. $^1\text{H-NMR}$ spectrum of **2g**.Figure S14c. $^{13}\text{C-NMR}$ spectrum of **2g**.

Figure S14d. ^{13}C -NMR spectrum of 2g.Figure S14e. ^{13}C -NMR spectrum of 2g.

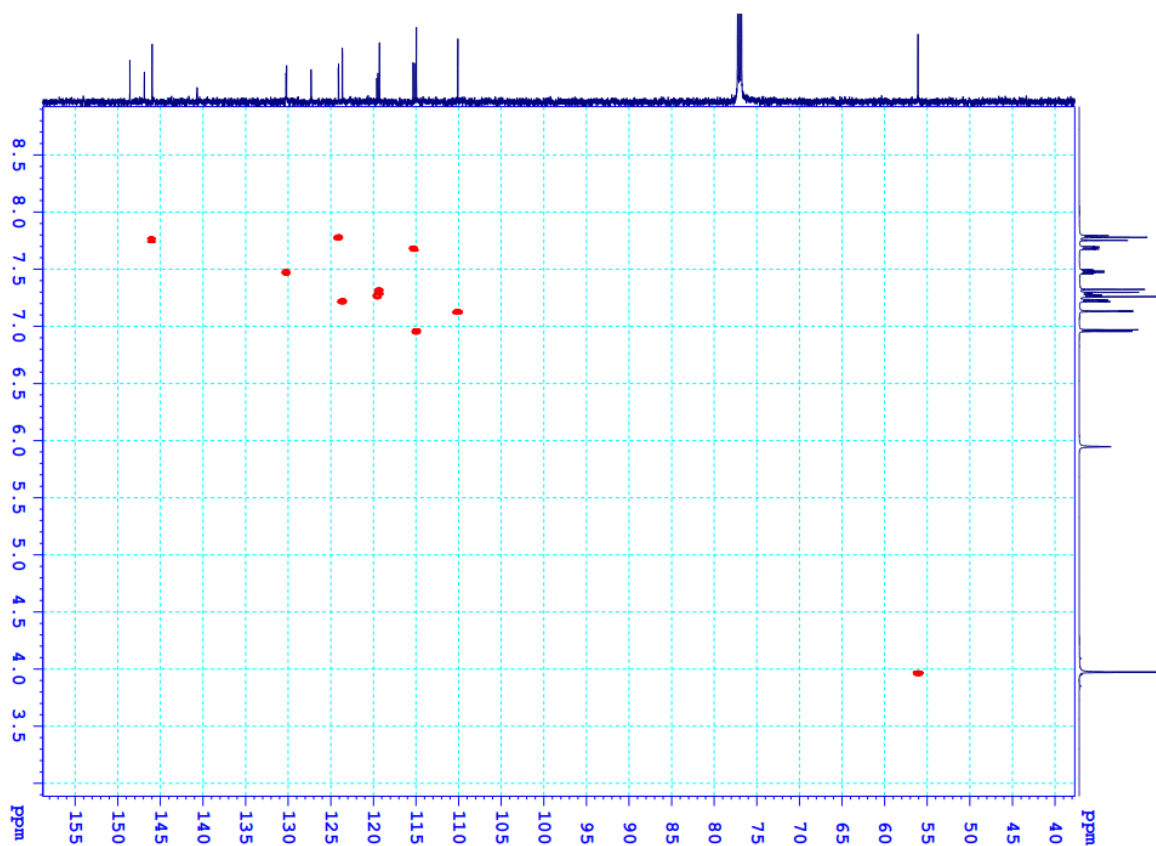


Figure S14f. HSQC spectrum of 2g.

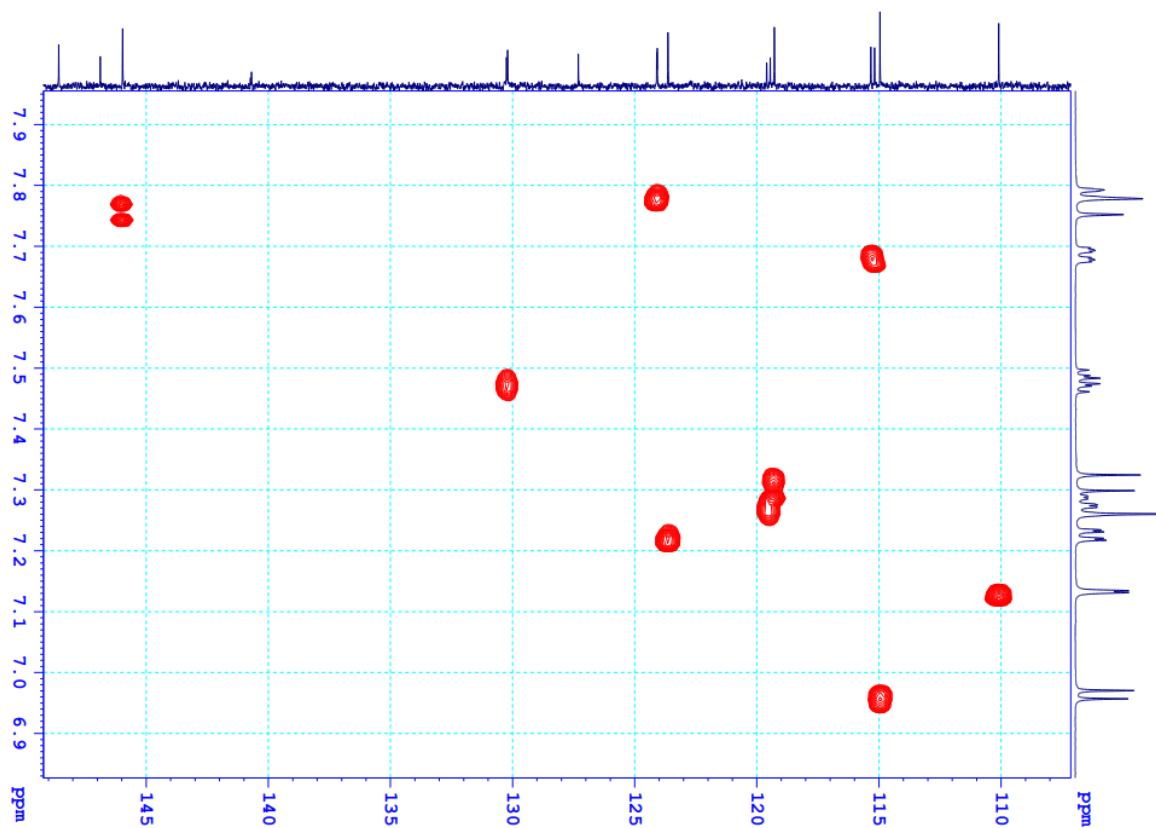


Figure S14g. HSQC spectrum of 2g.

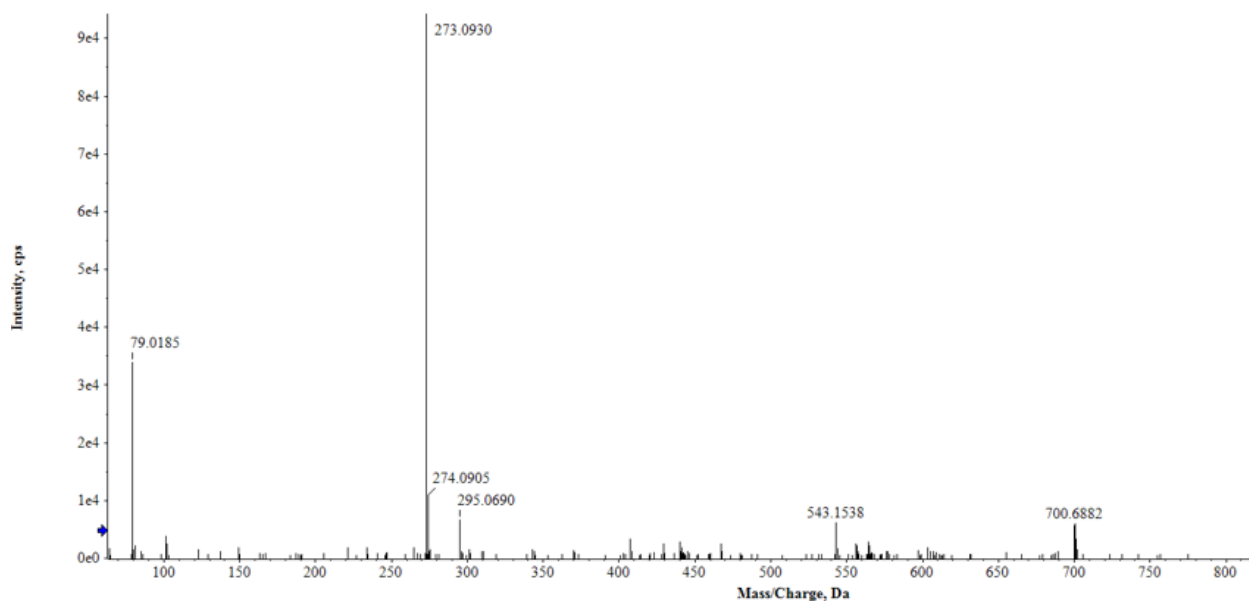
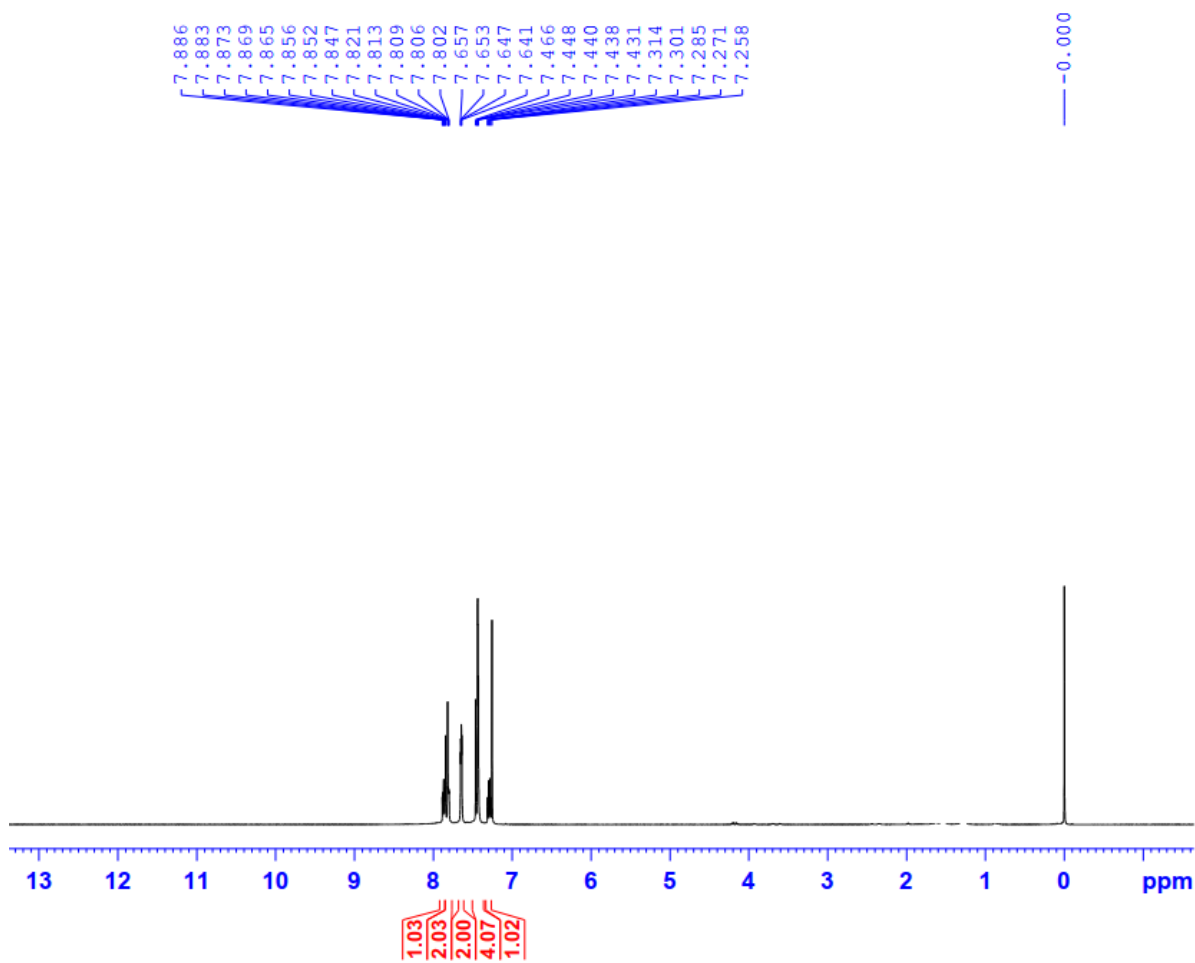
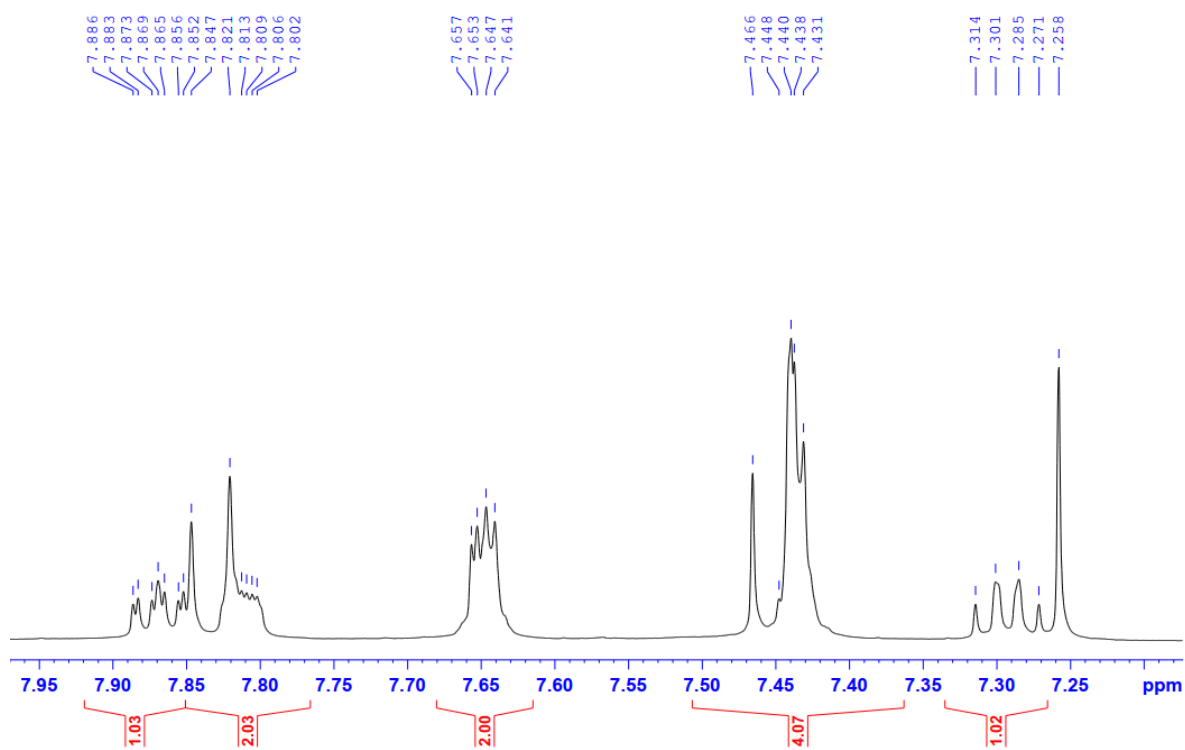
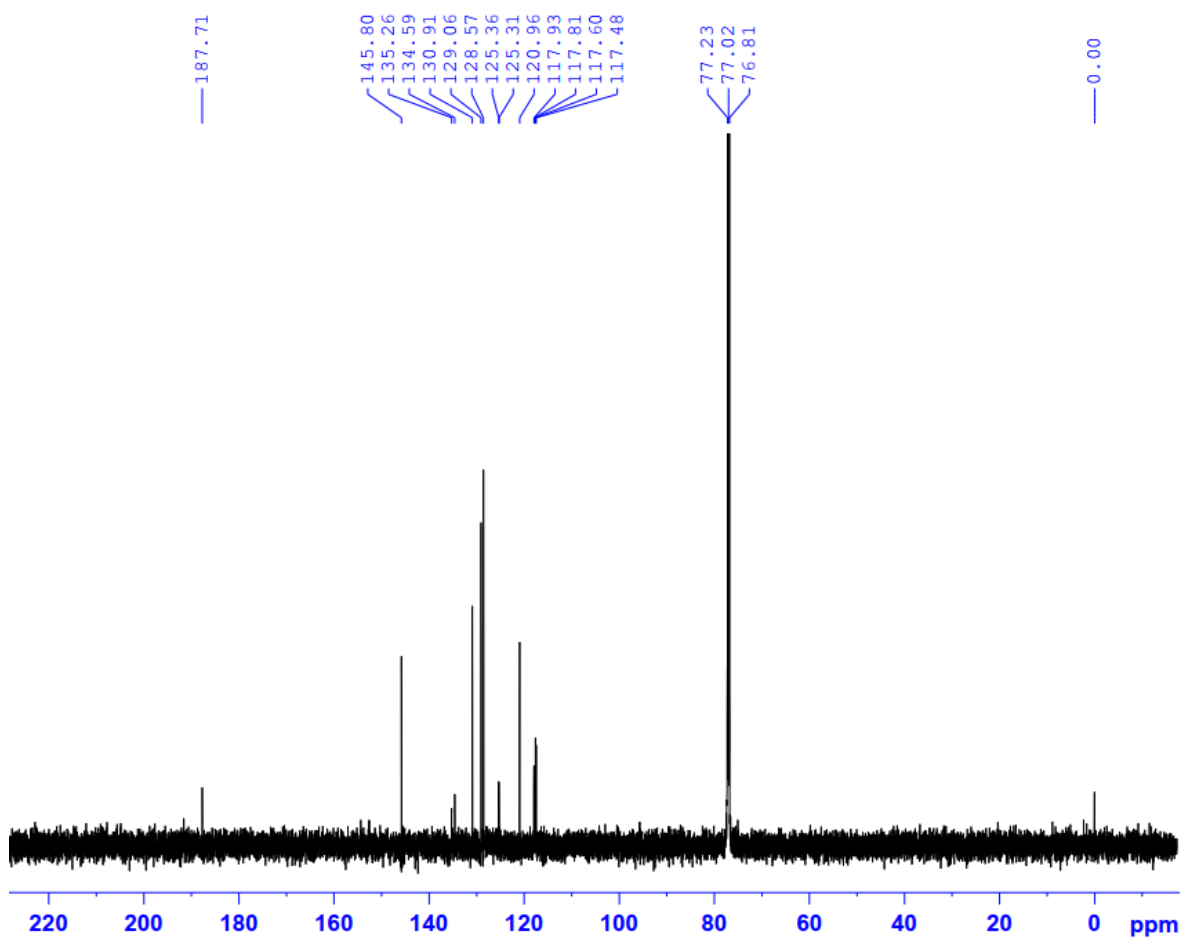
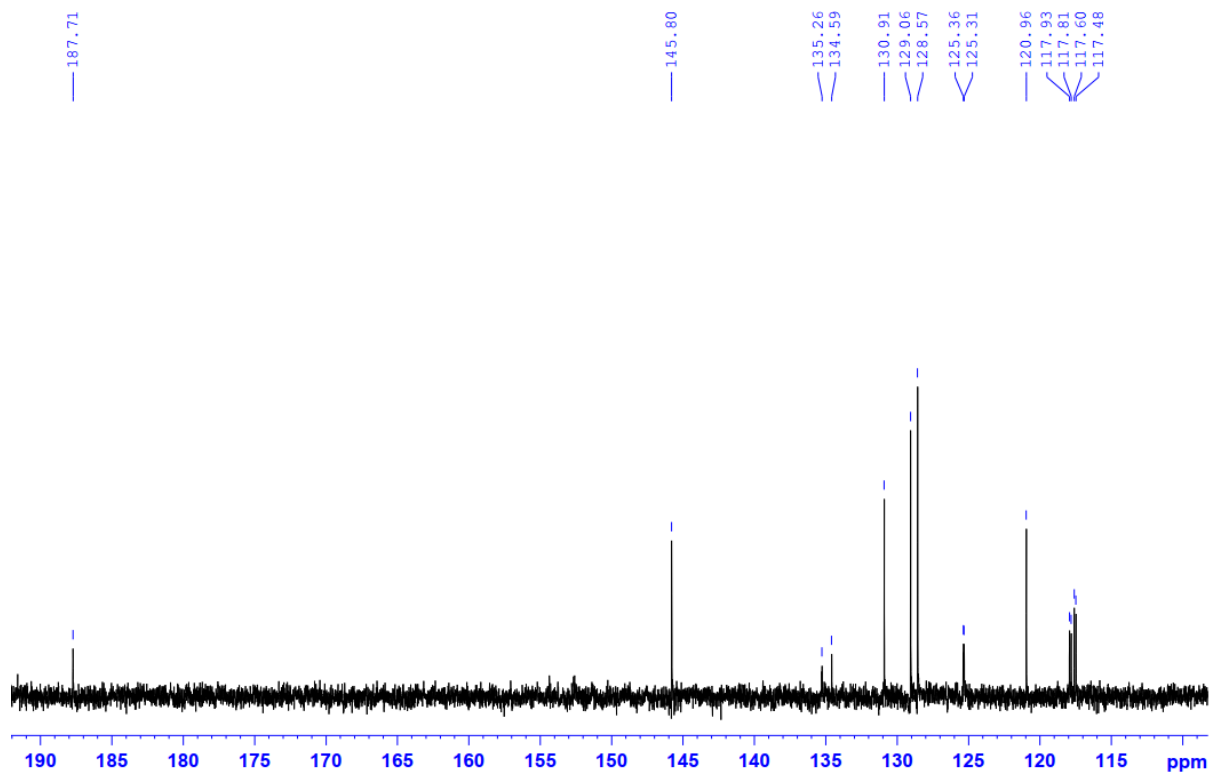
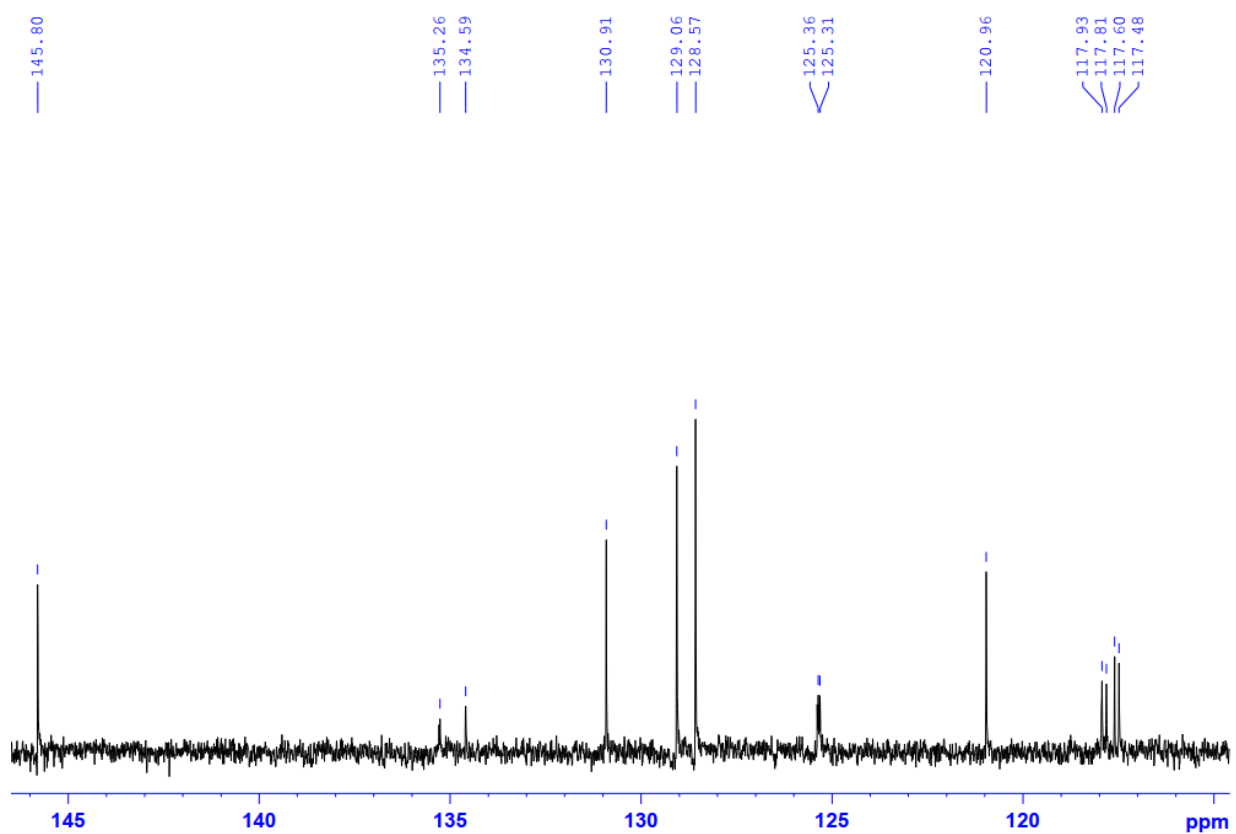


Figure S14h. HRMS of 2g.

Figure S15a. ¹H-NMR spectrum of 3a.

Figure S15b. ¹H-NMR spectrum of 3a.Figure S15c. ¹³C-NMR spectrum of 3a.

Figure S15d. ^{13}C -NMR spectrum of 3a.Figure S15e. ^{13}C -NMR spectrum of 3a.

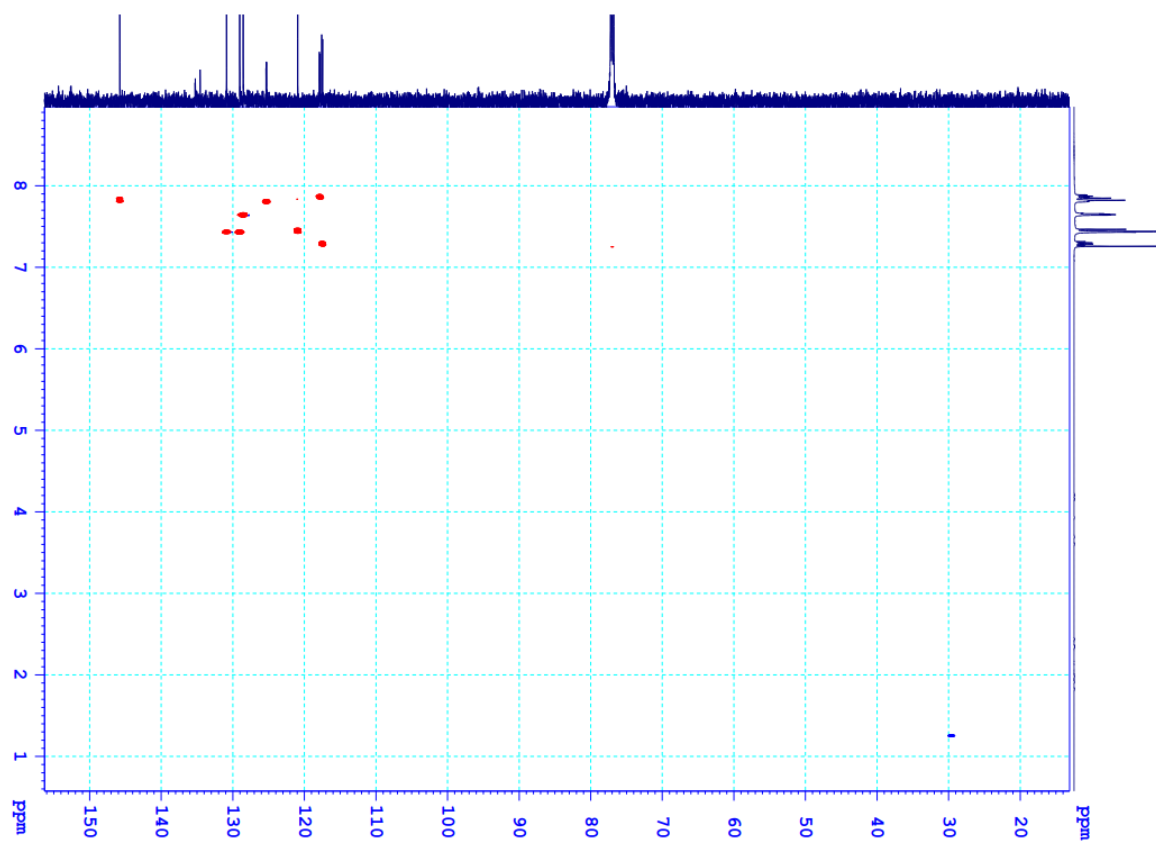


Figure S15f. HSQC spectrum of 3a.

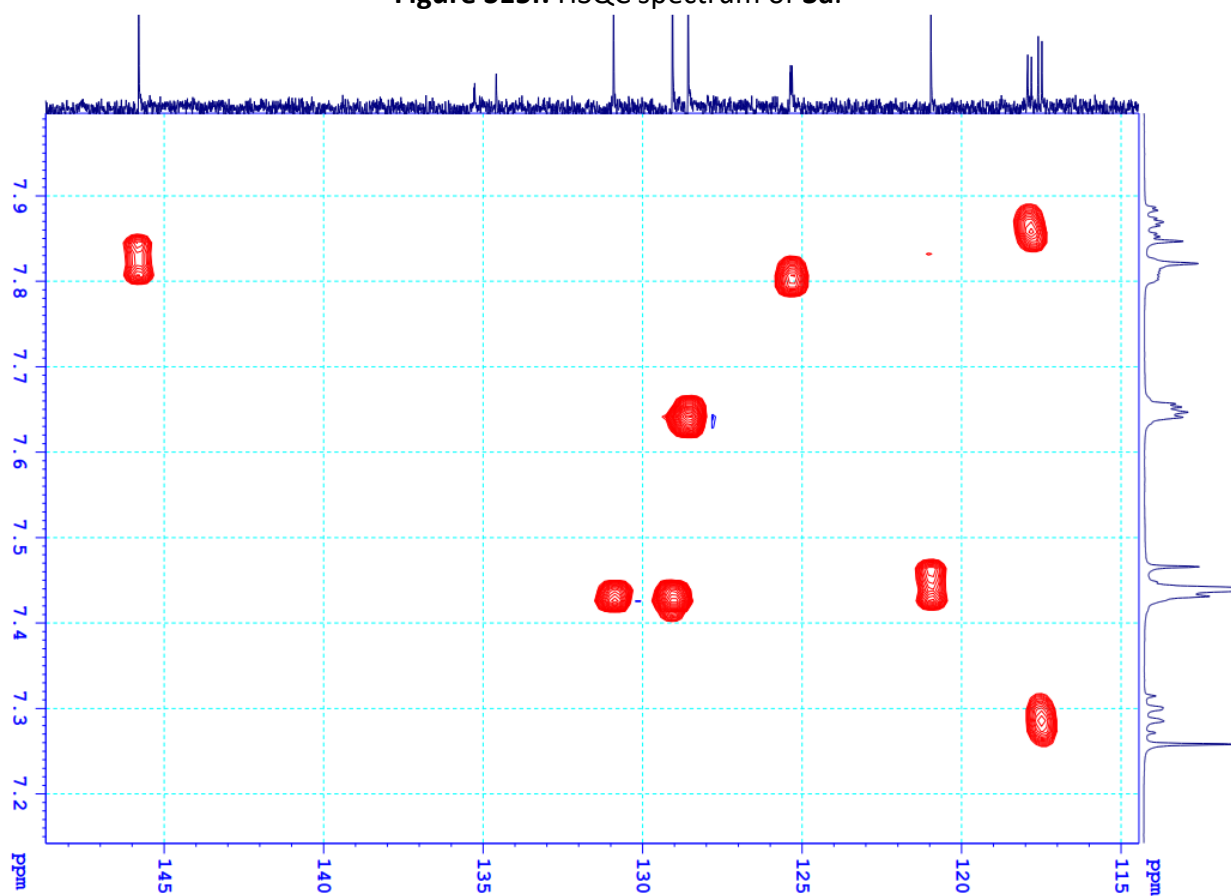


Figure S15g. HSQC spectrum of 3a.

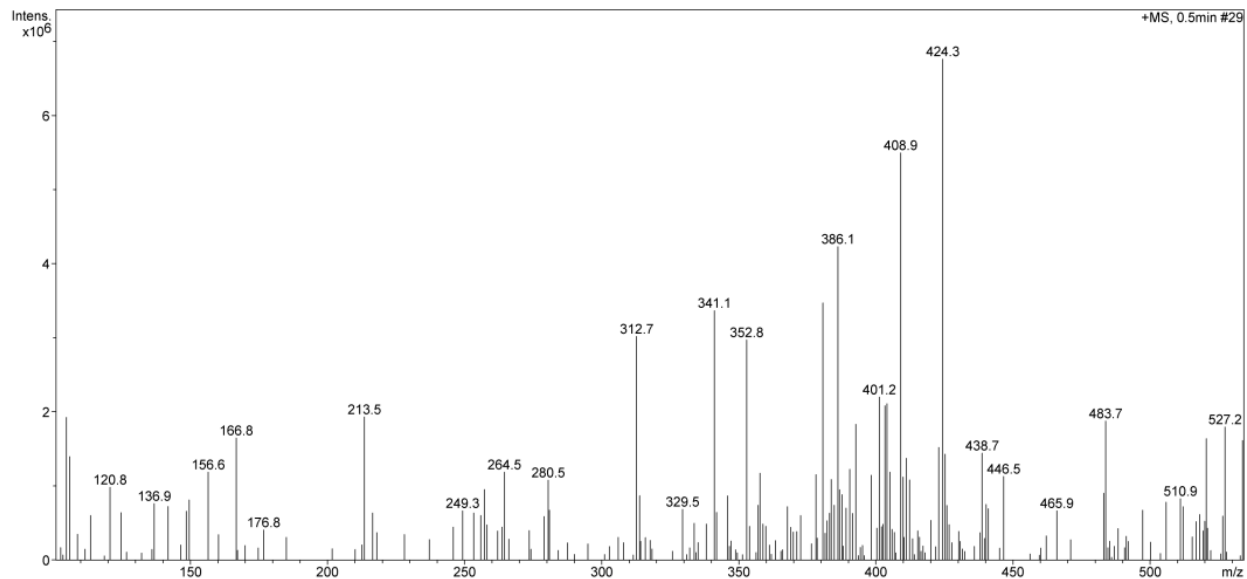
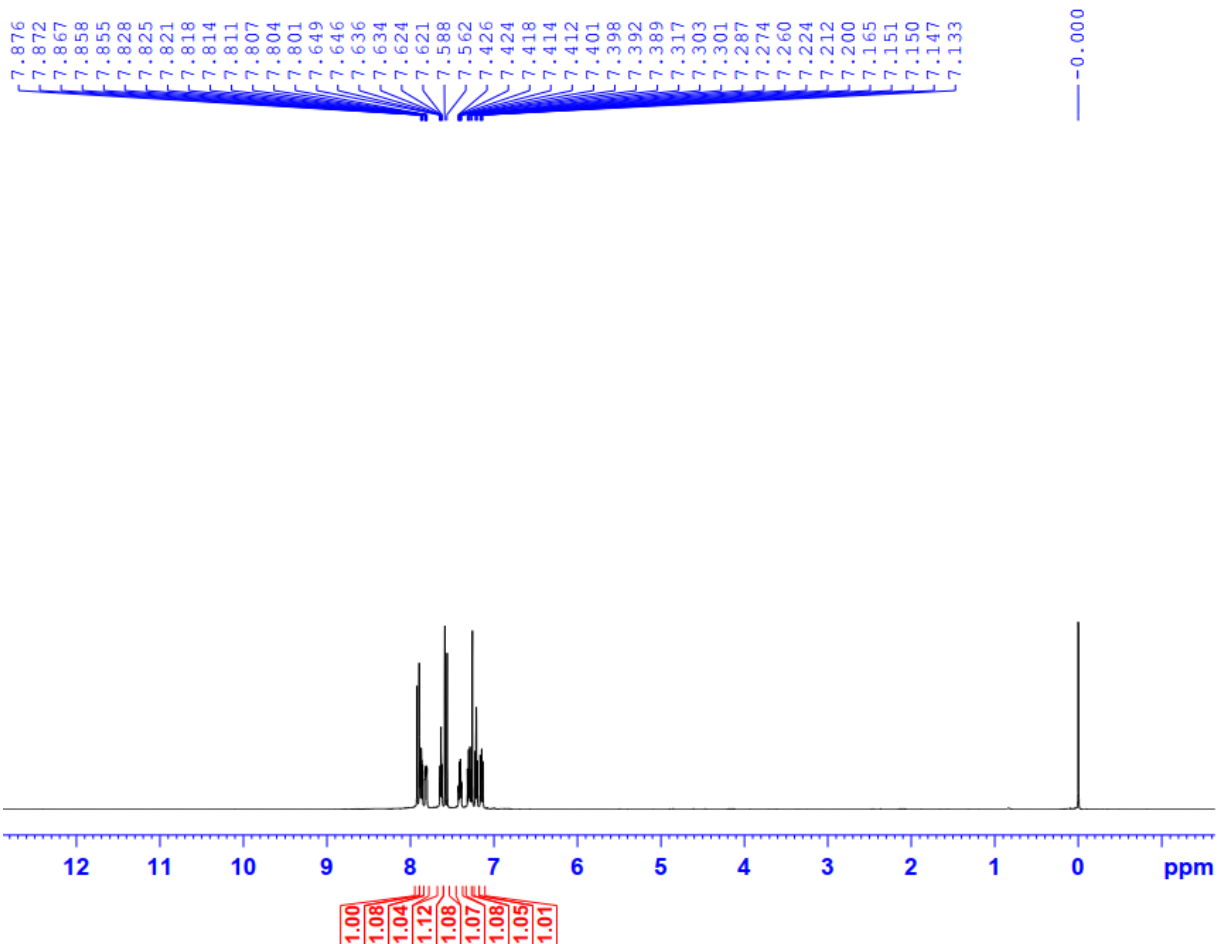
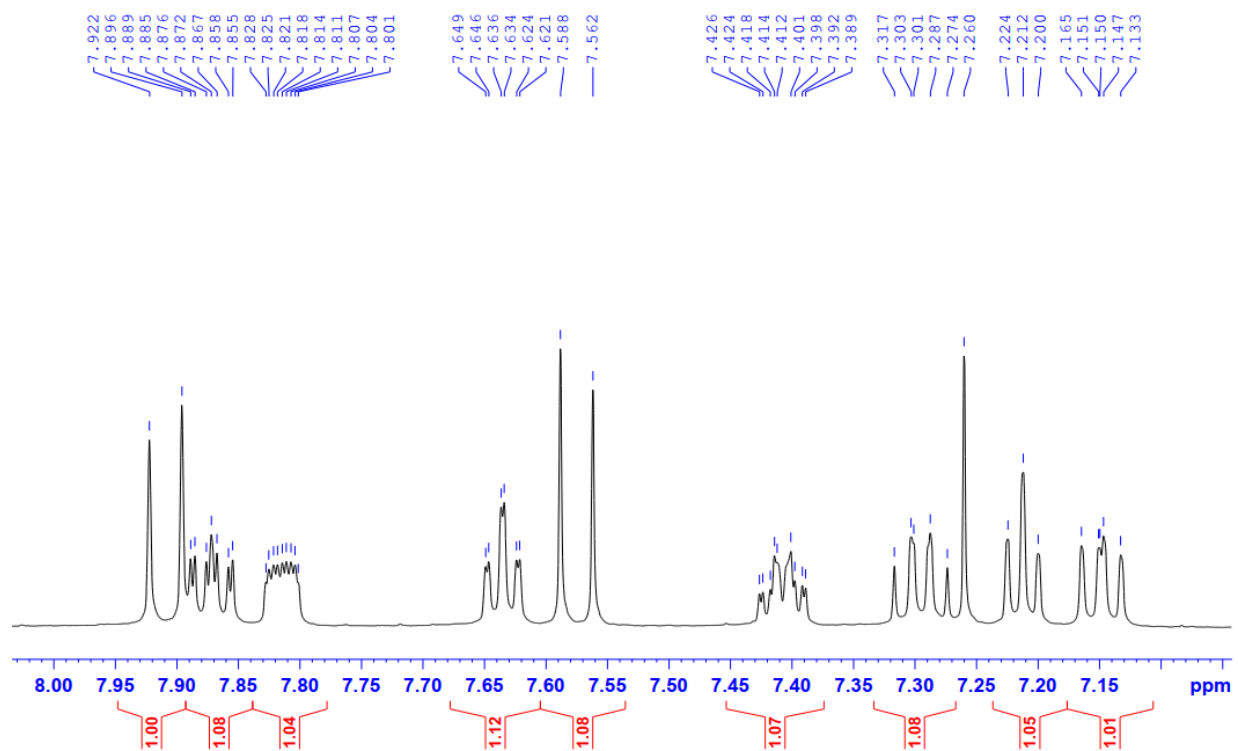
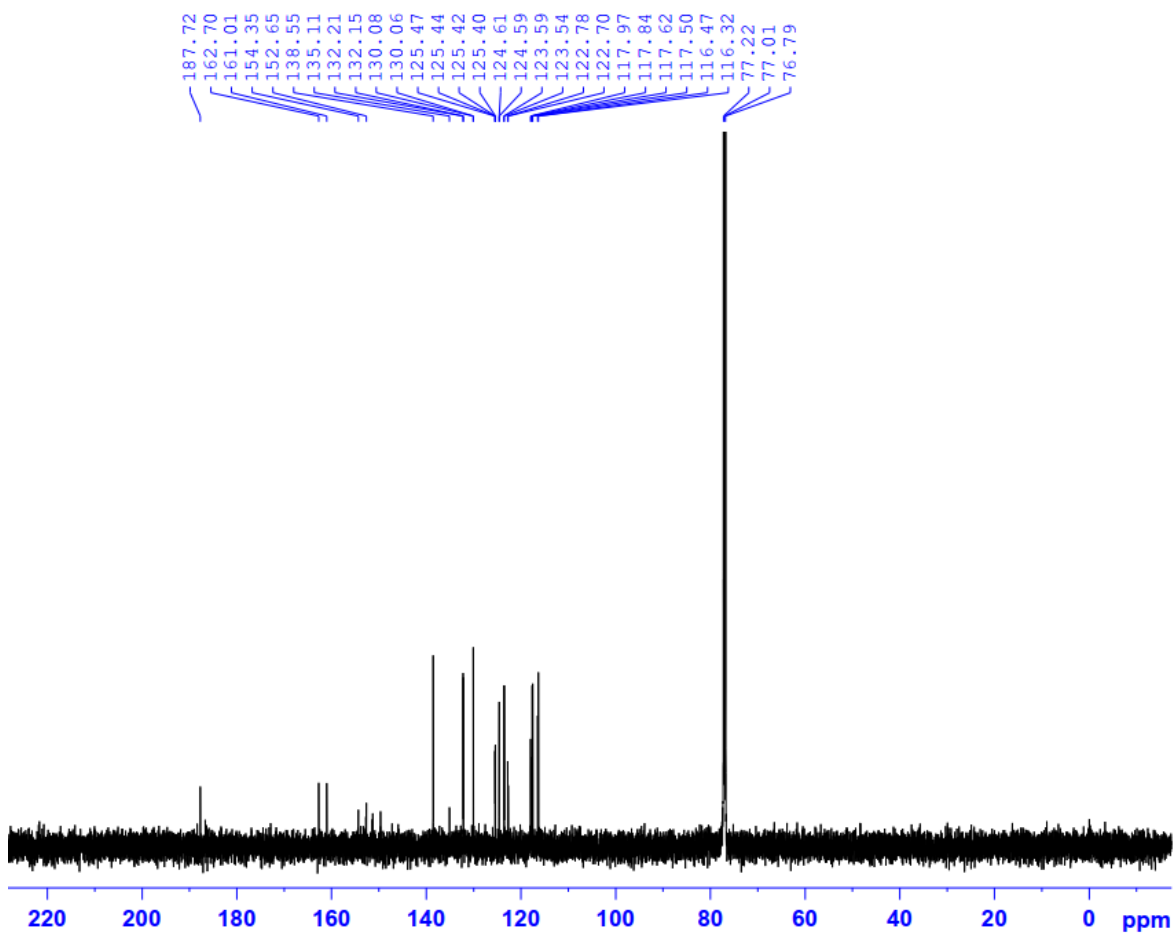
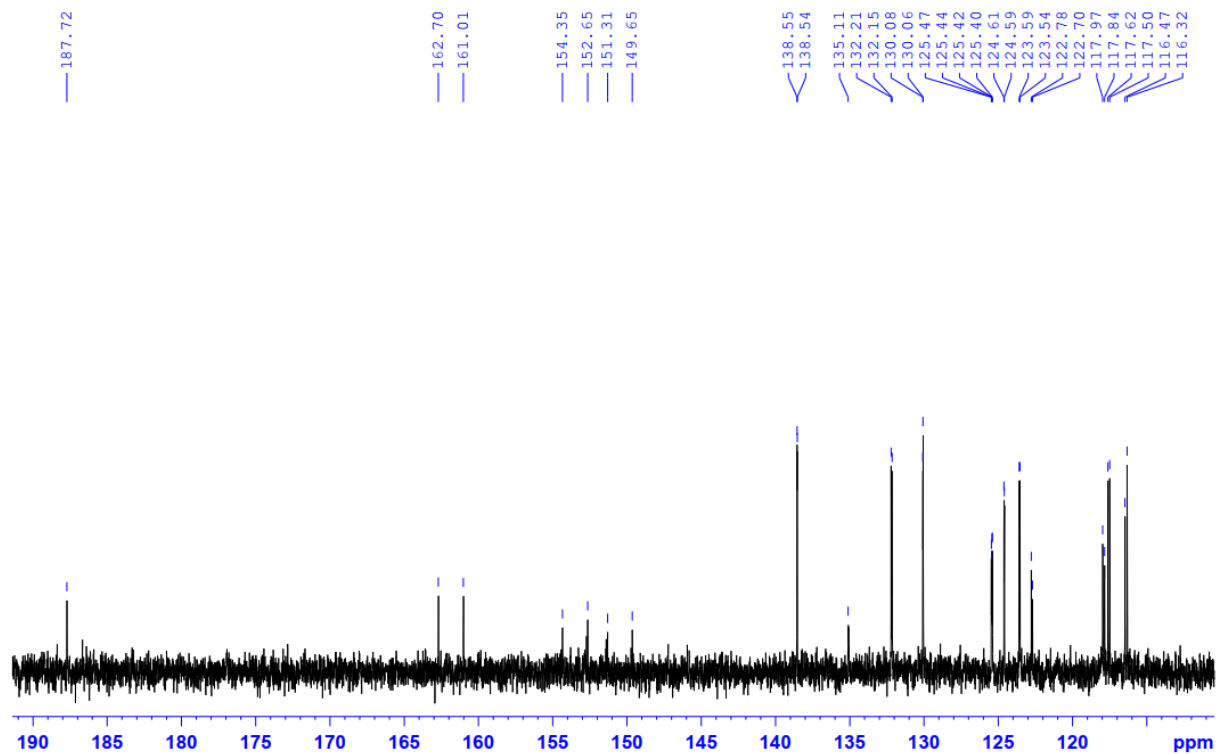
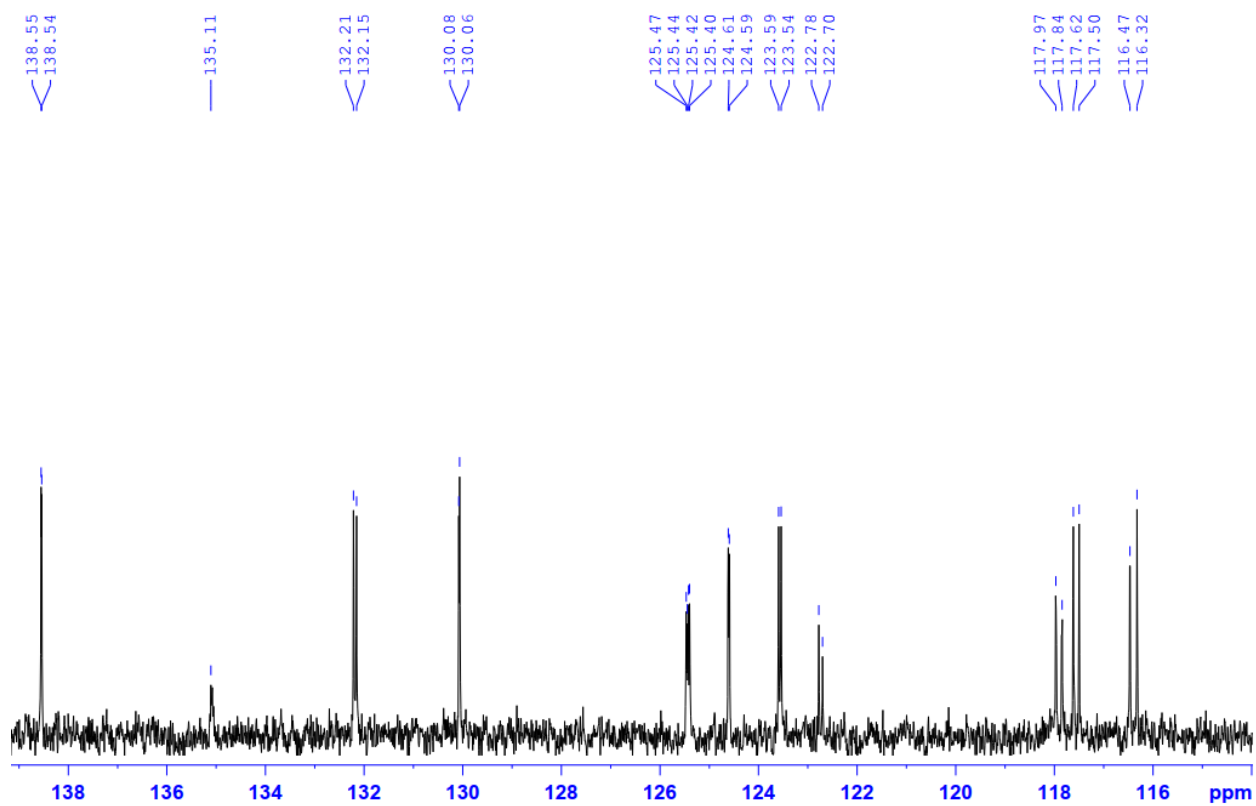


Figure S15h. MS of 3a.

Figure S16a. ¹H-NMR spectrum of 3b.

Figure S16b. ¹H-NMR spectrum of 3b.Figure S16c. ¹³C-NMR spectrum of 3b.

Figure S16d. ¹³C-NMR spectrum of 3b.Figure S16e. ¹³C-NMR spectrum of 3b.

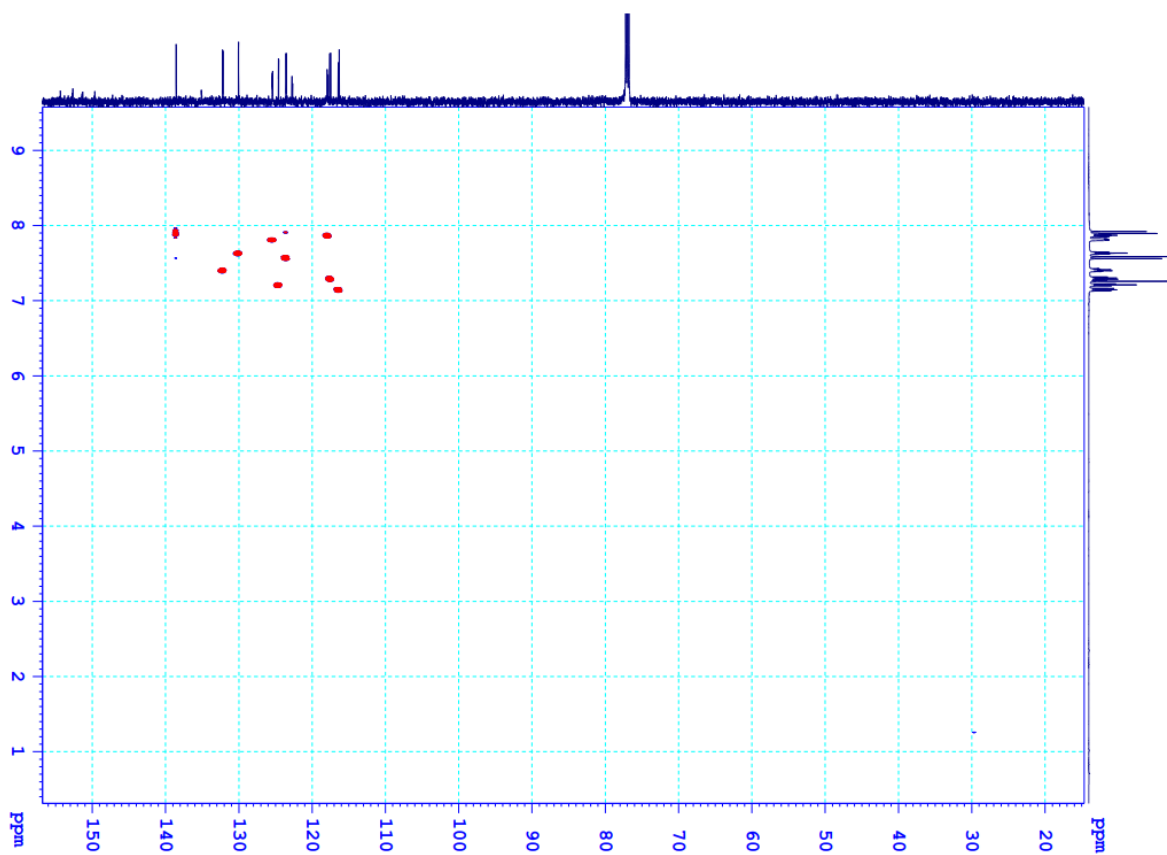


Figure S16f. HSQC spectrum of 3b.

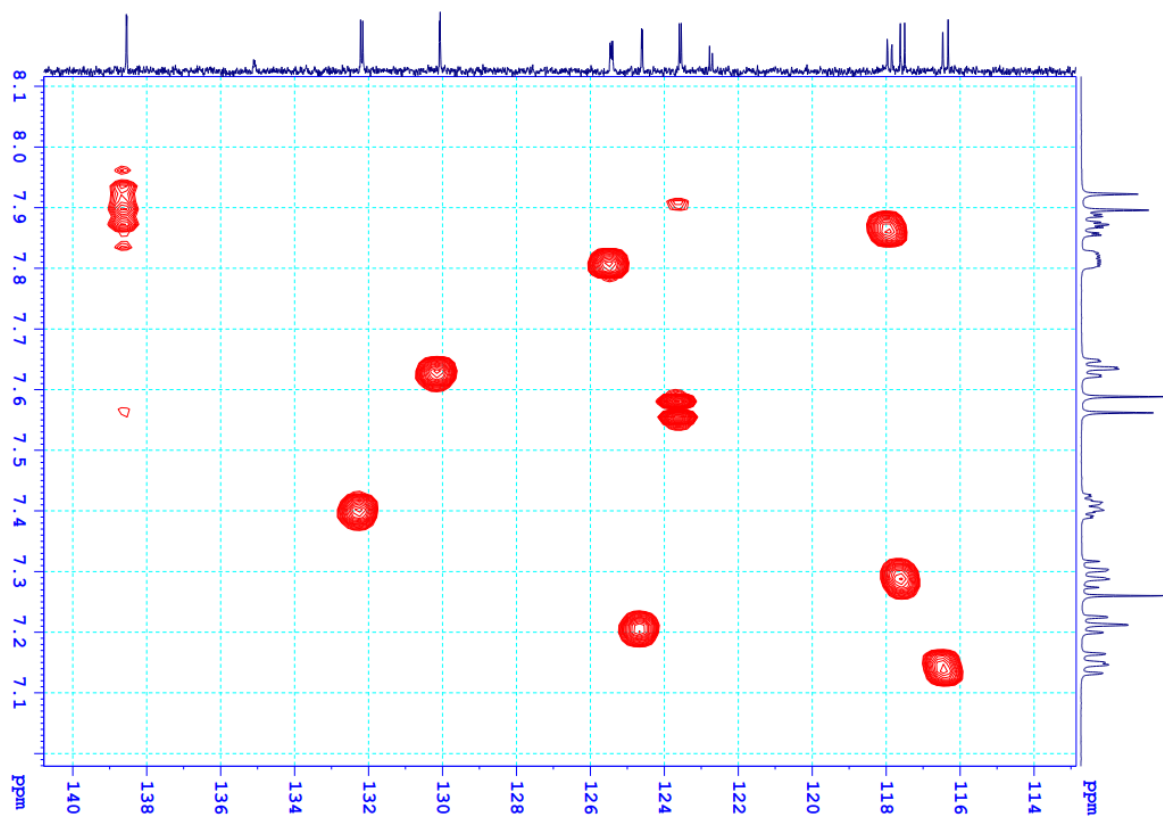


Figure S16g. HSQC spectrum of 3b.

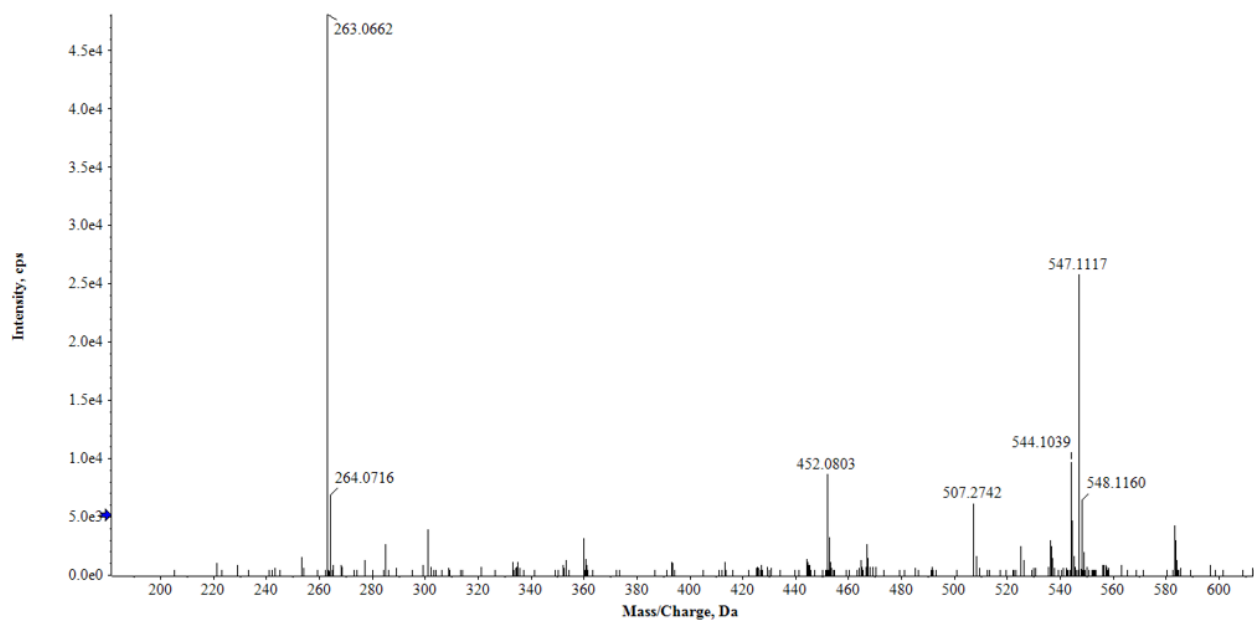
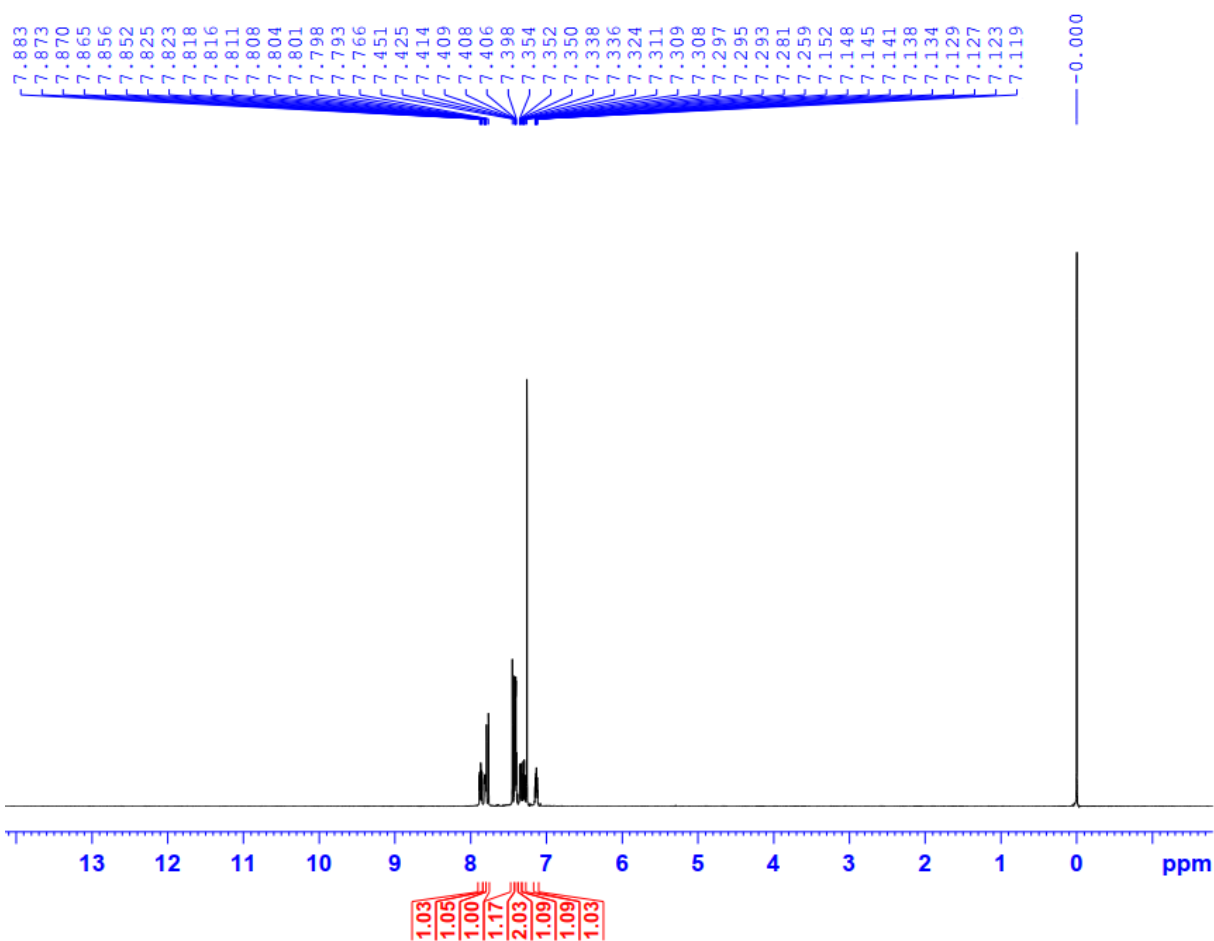
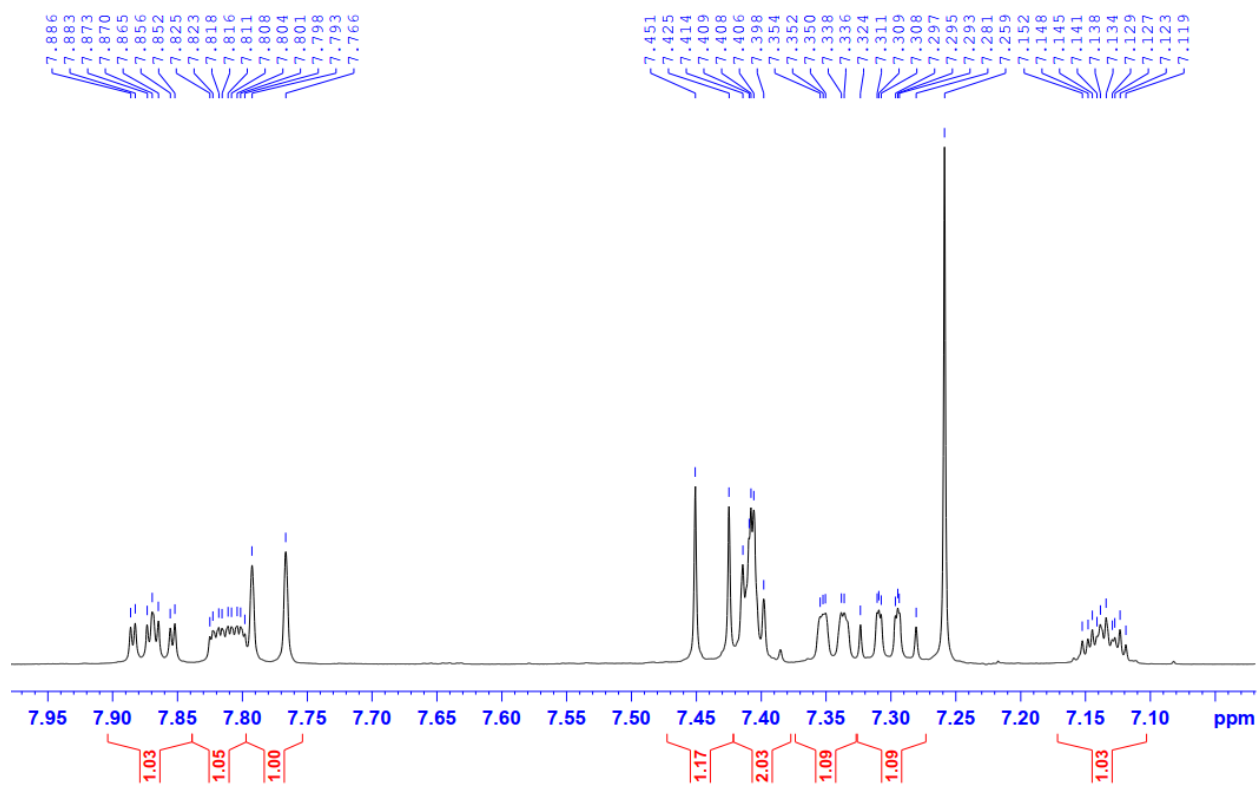
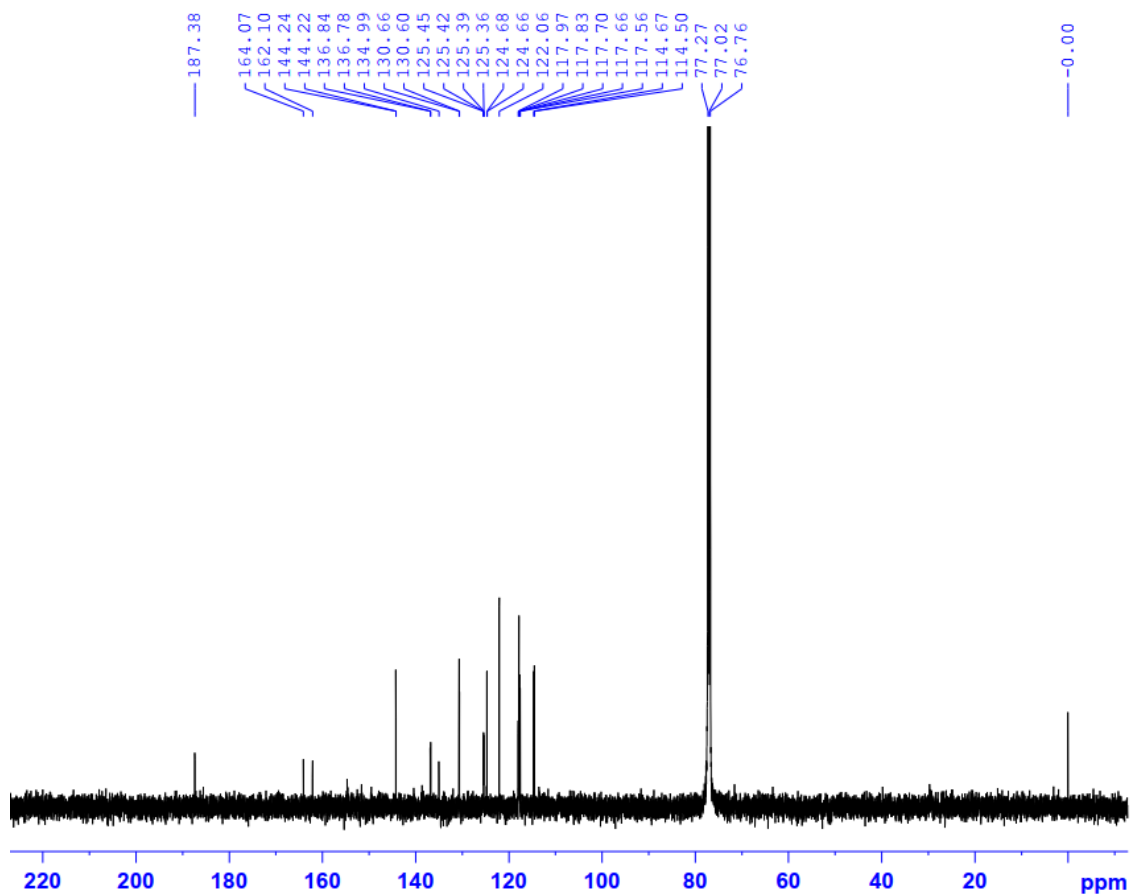
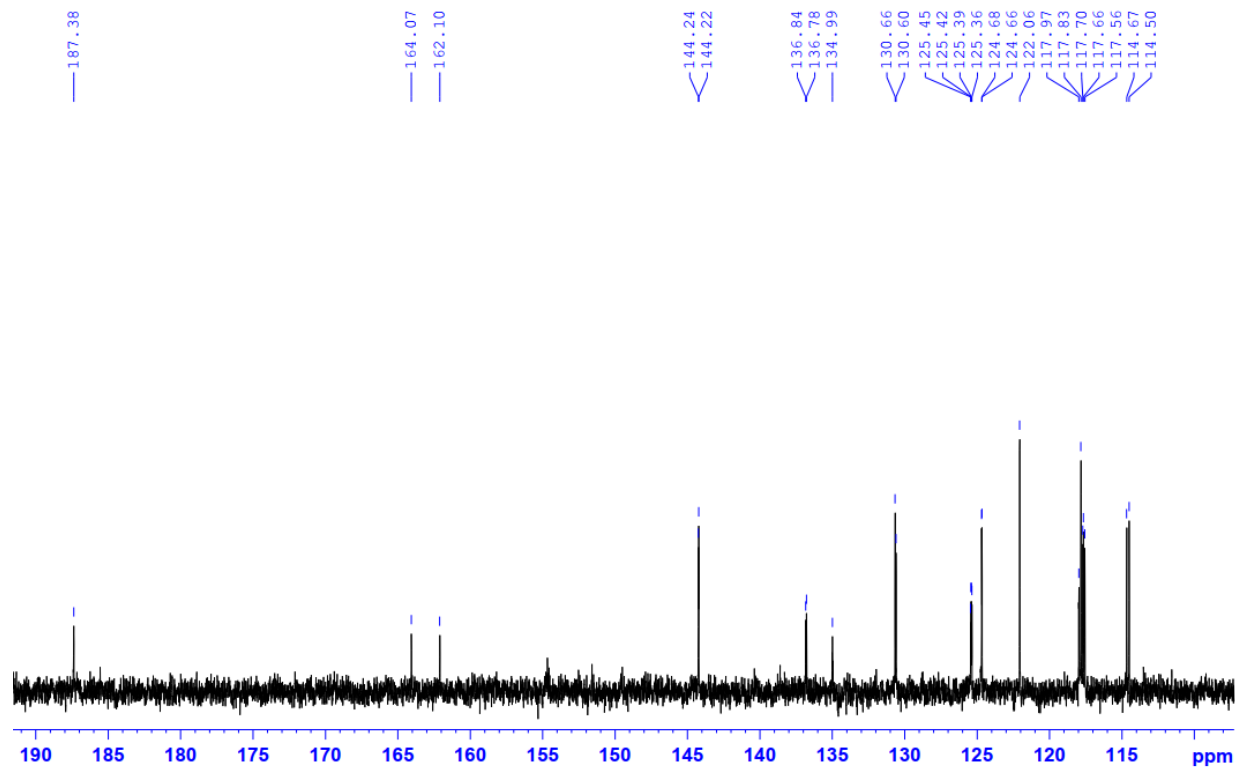
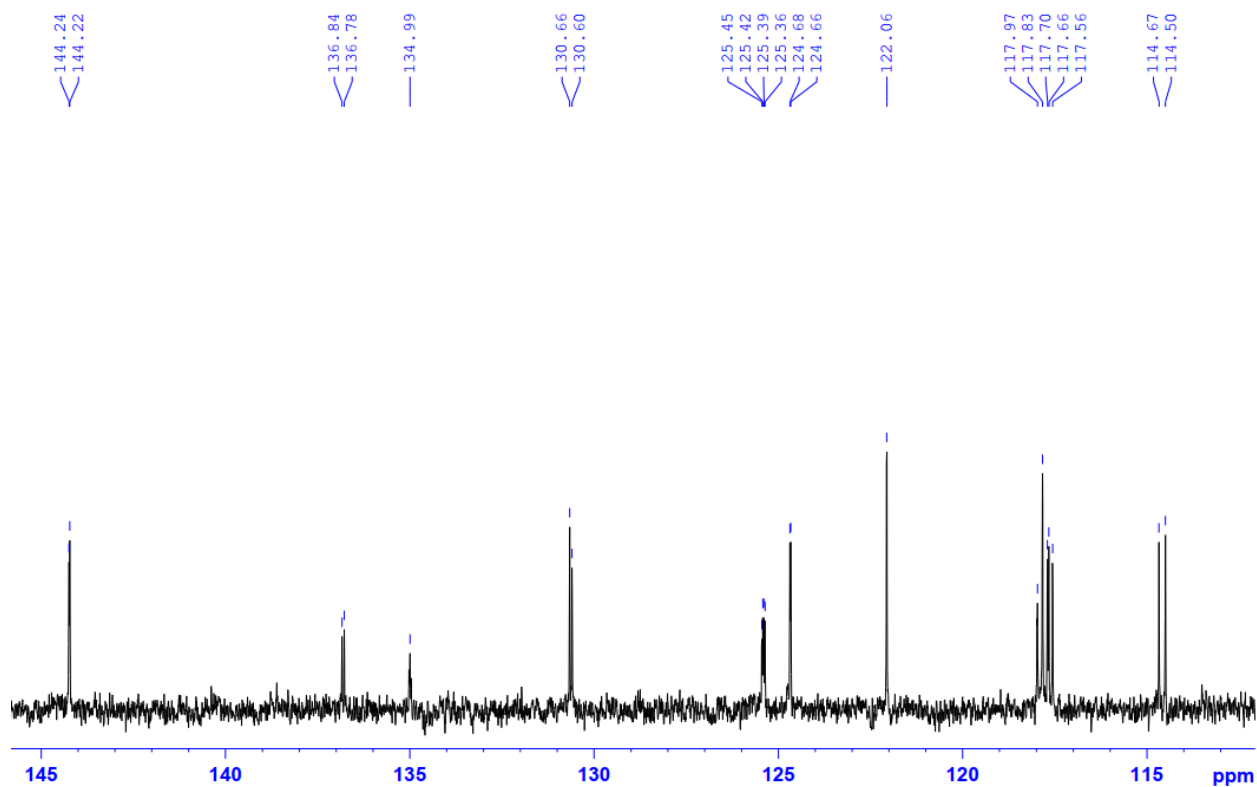


Figure S16h. HRMS of 3b.

Figure S17a. ¹H-NMR spectrum of 3c.

Figure S17b. $^1\text{H-NMR}$ spectrum of **3c**.Figure S17c. $^{13}\text{C-NMR}$ spectrum of **3c**.

Figure S17d. ^{13}C -NMR spectrum of 3c.Figure S17e. ^{13}C -NMR spectrum of 3c.

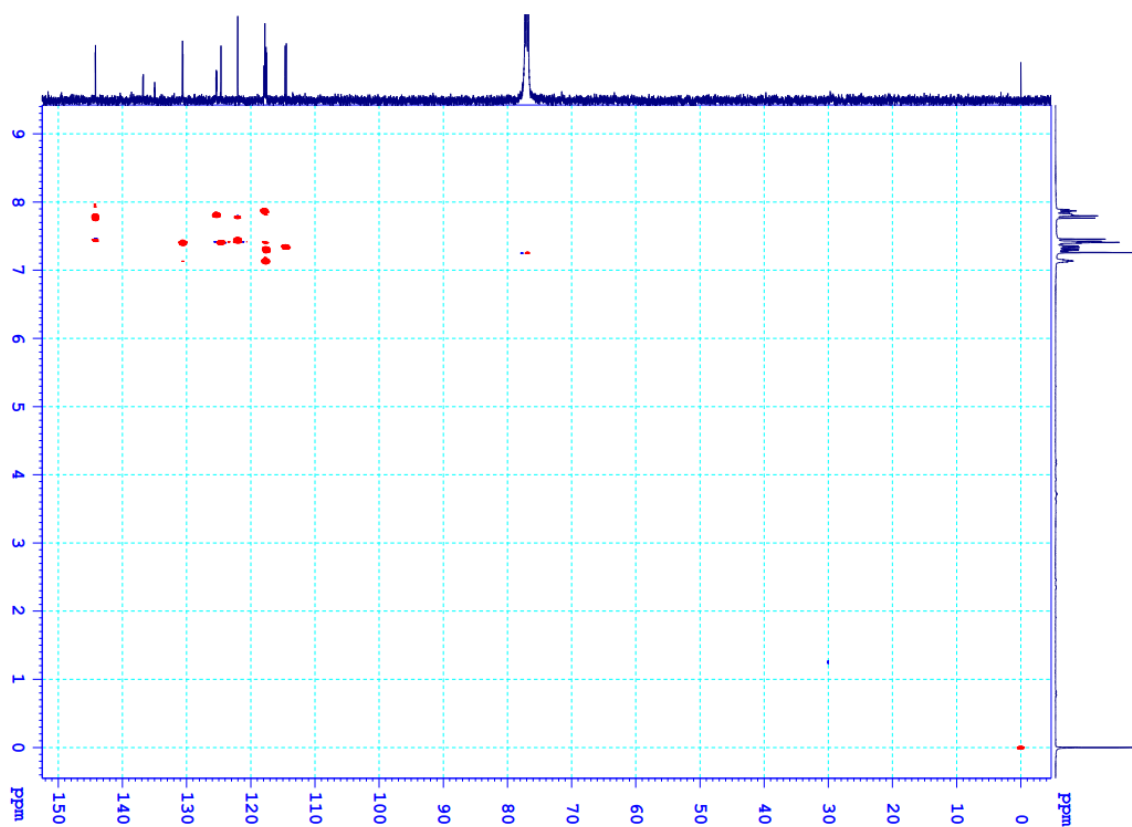


Figure S17f. HSQC spectrum of 3c.

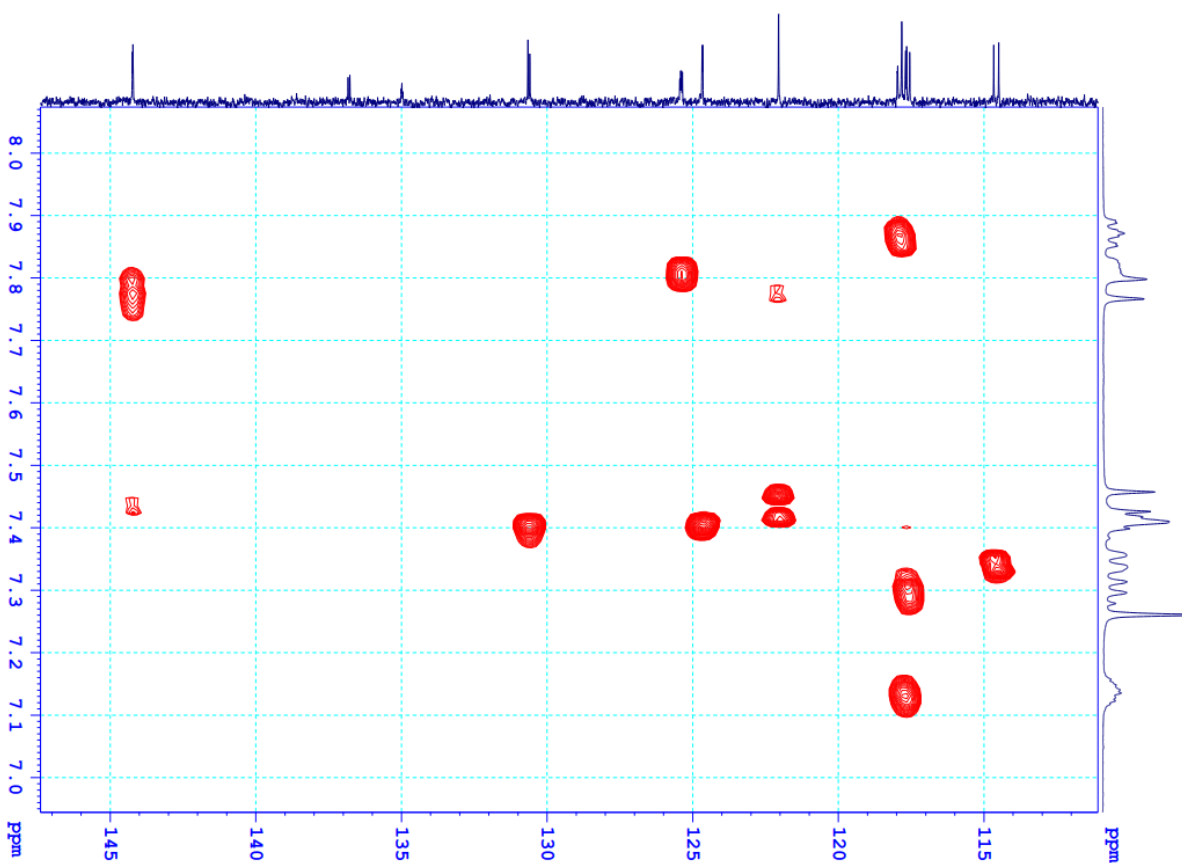


Figure S17g. HSQC spectrum of 3c.

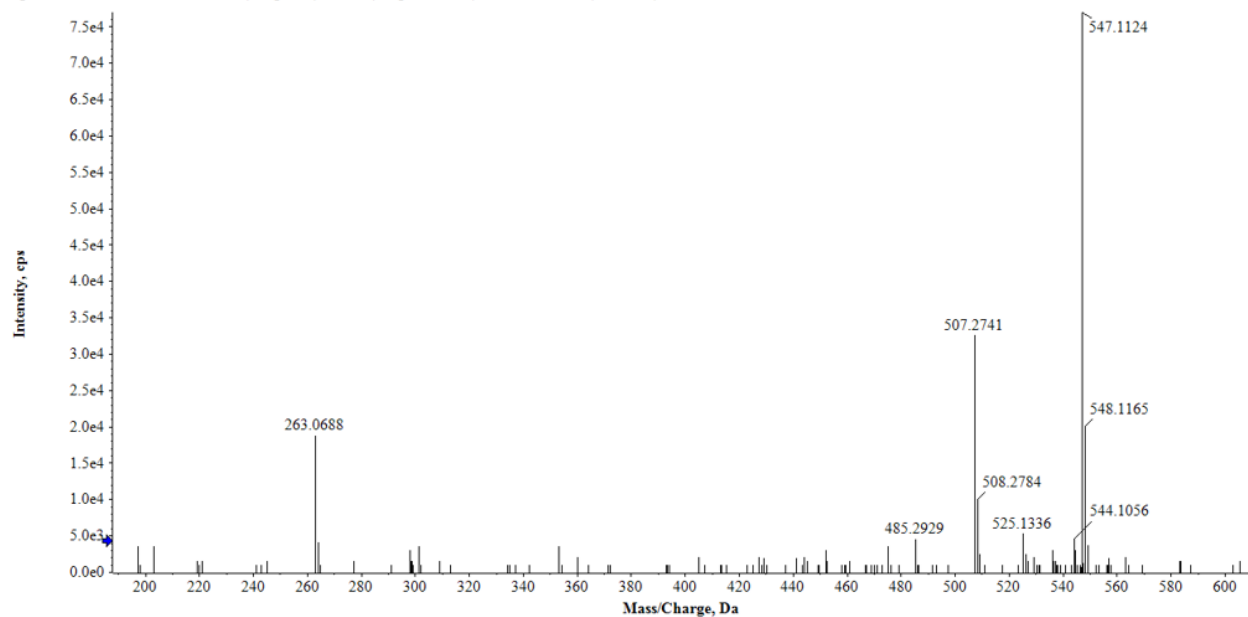
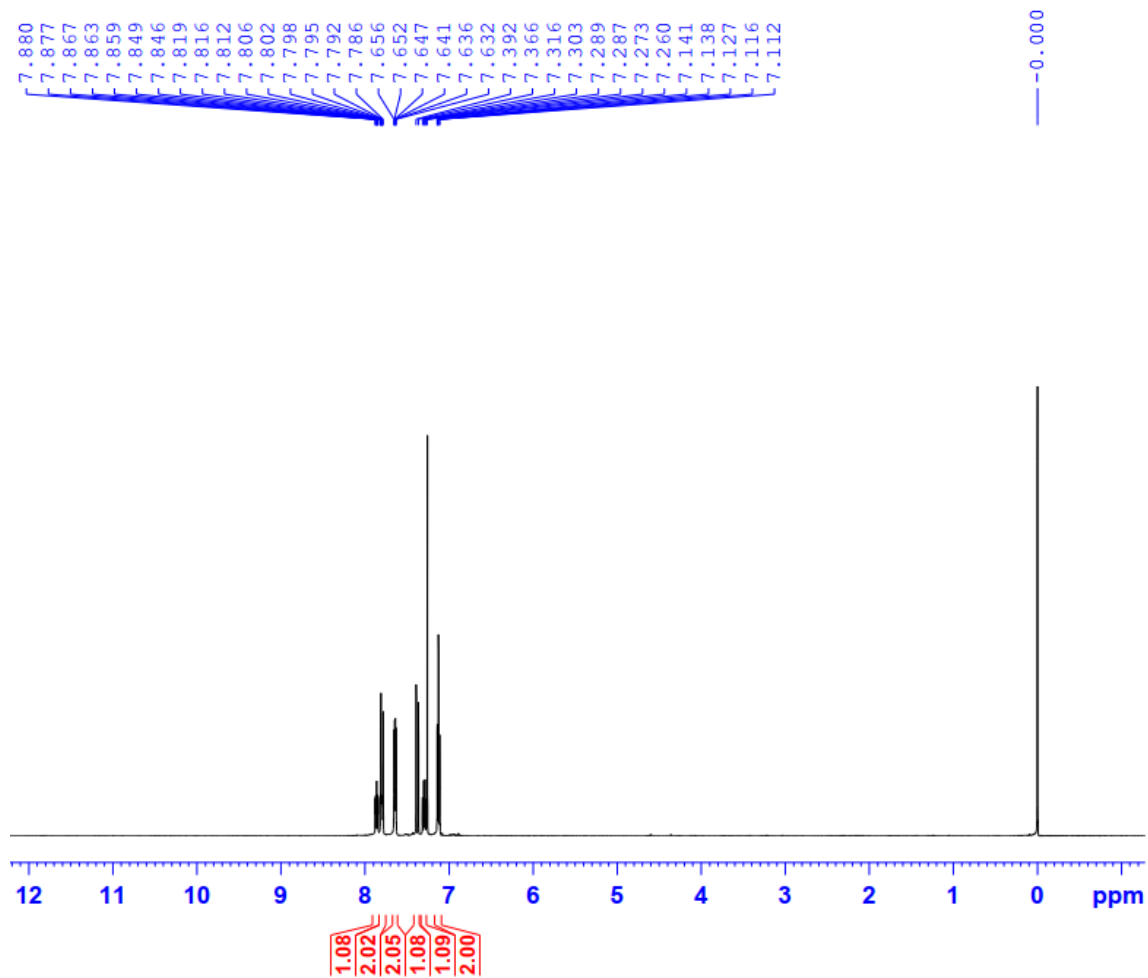
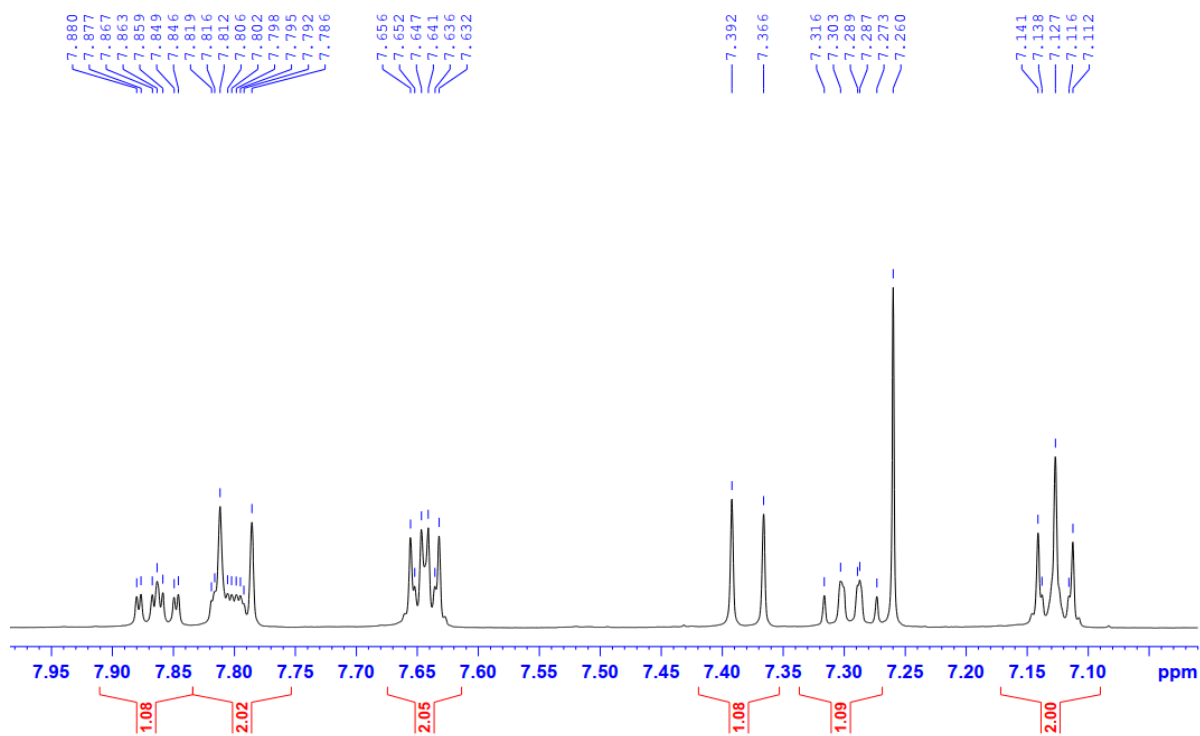
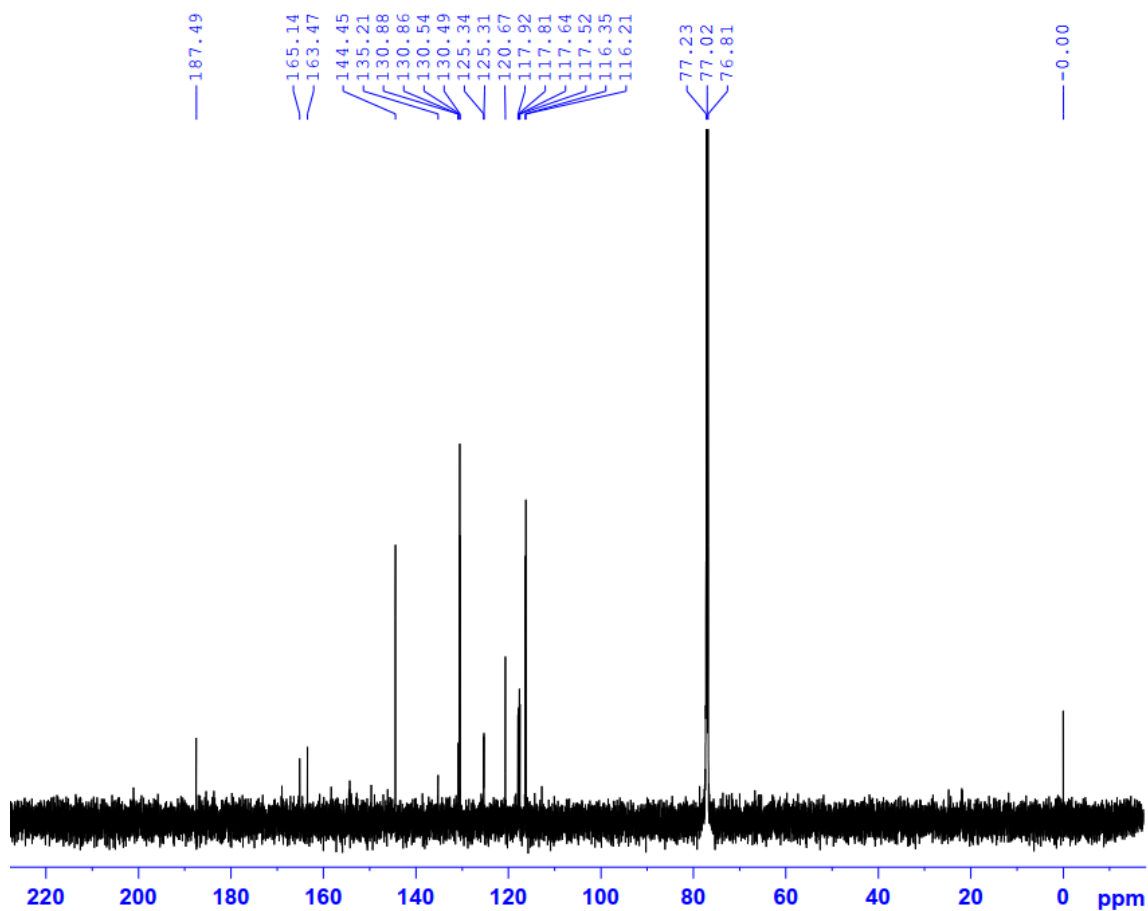
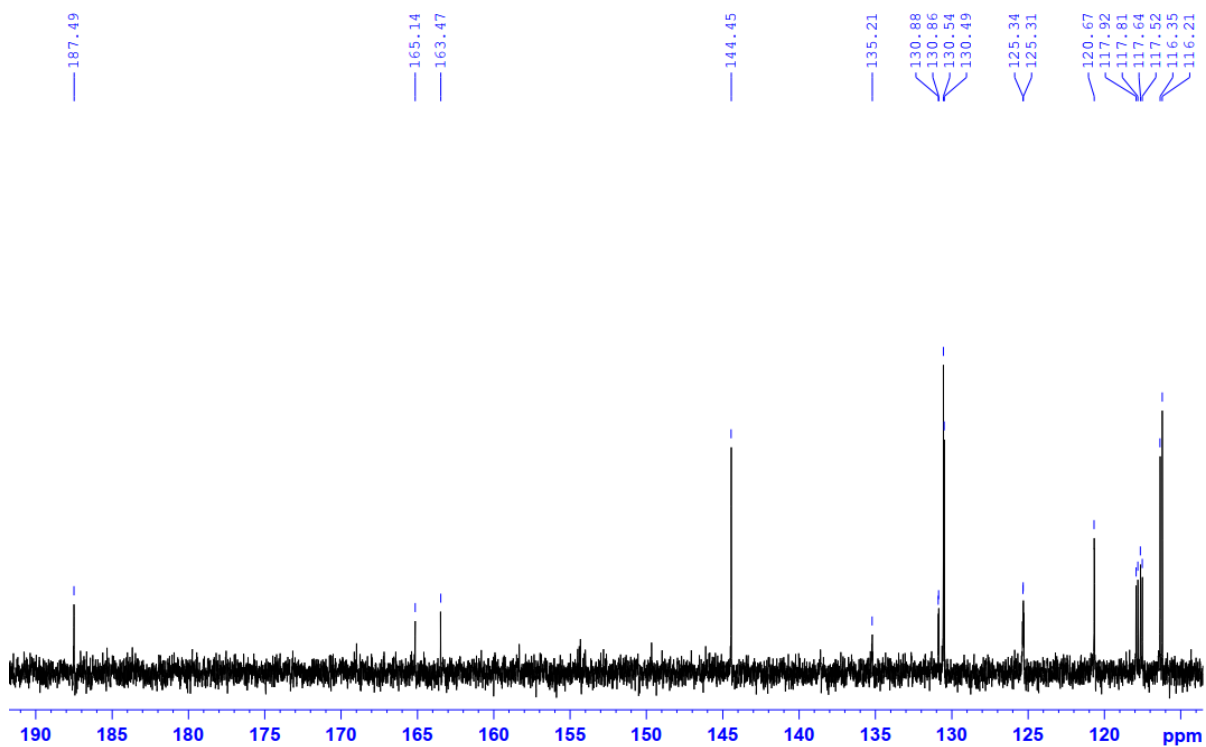
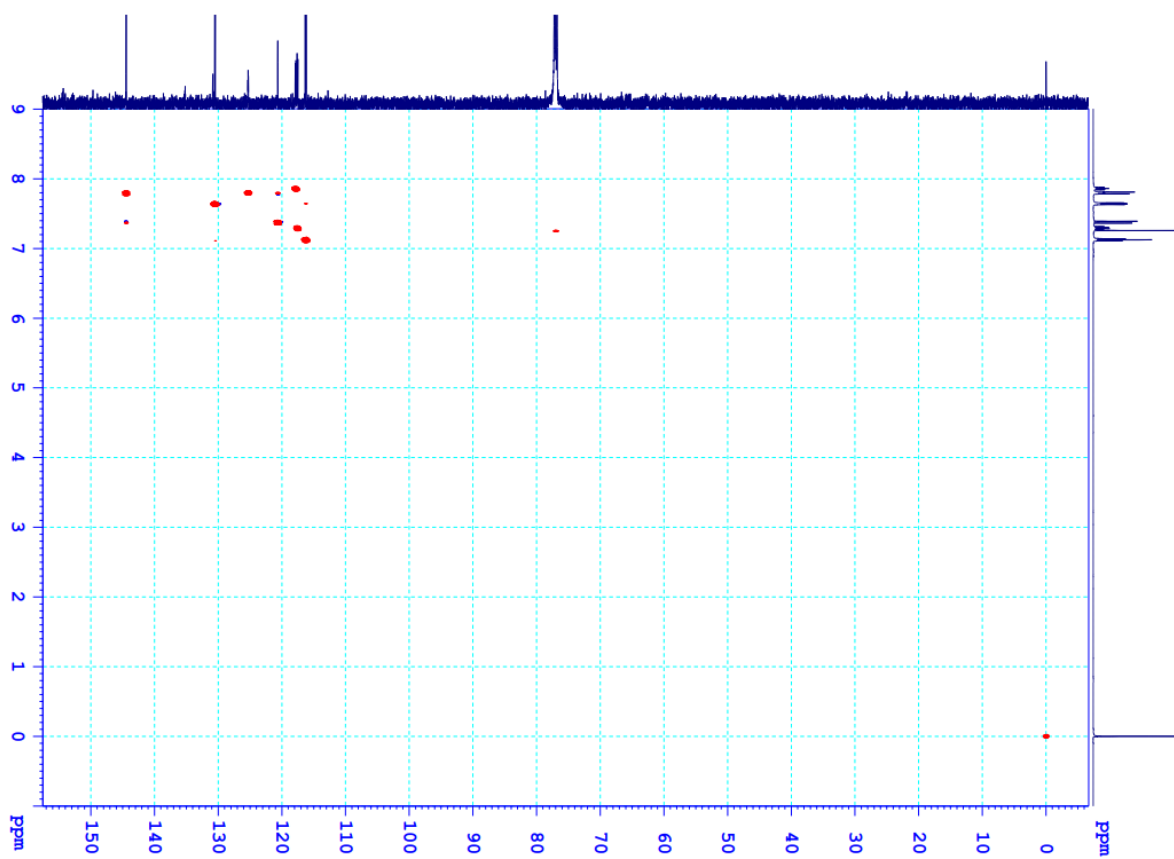


Figure S17h. HRMS of 3c.

Figure S18a. ¹H-NMR spectrum of 3d.

Figure S18b. $^1\text{H-NMR}$ spectrum of **3d**.Figure S18c. $^{13}\text{C-NMR}$ spectrum of **3d**.

Figure S18d. ^{13}C -NMR spectrum of **3d**.Figure S18e. HSQC spectrum of **3d**.

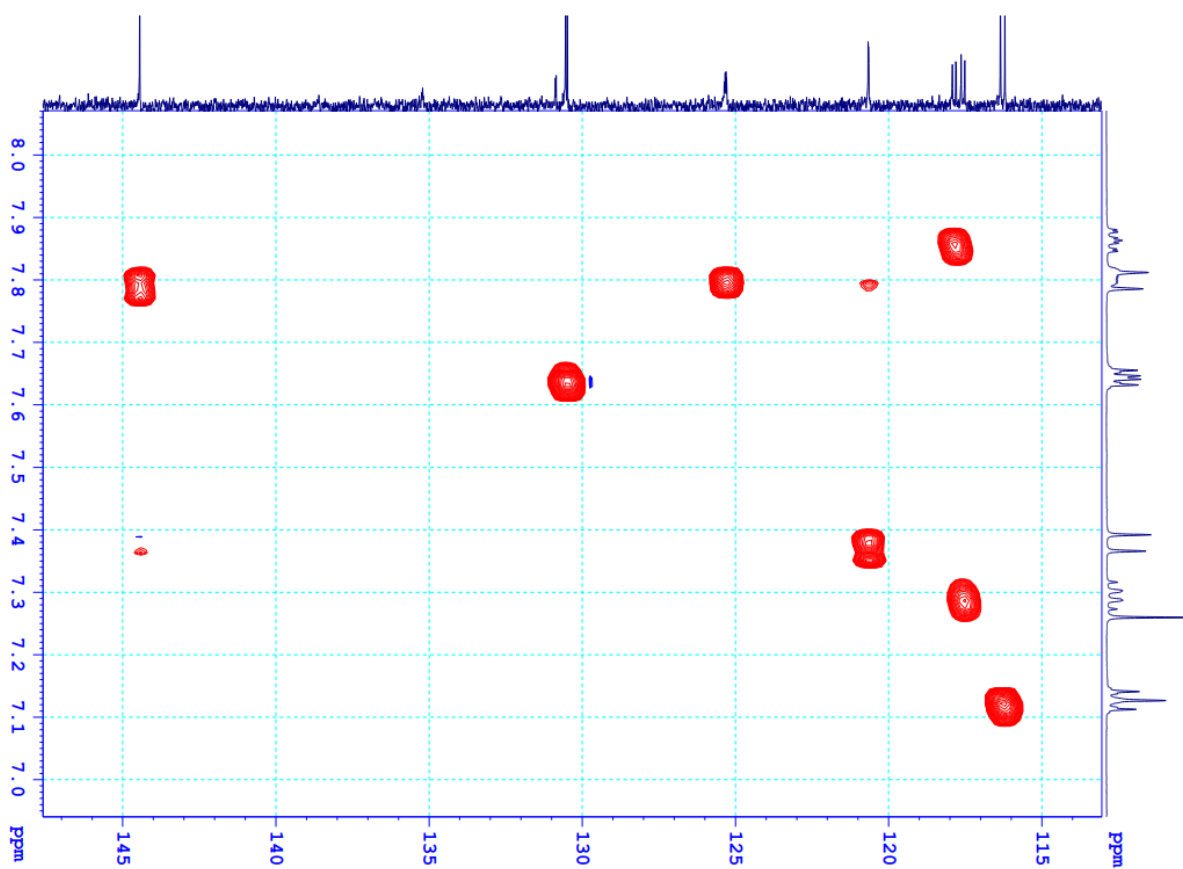


Figure S18f. HSQC spectrum of 3d.

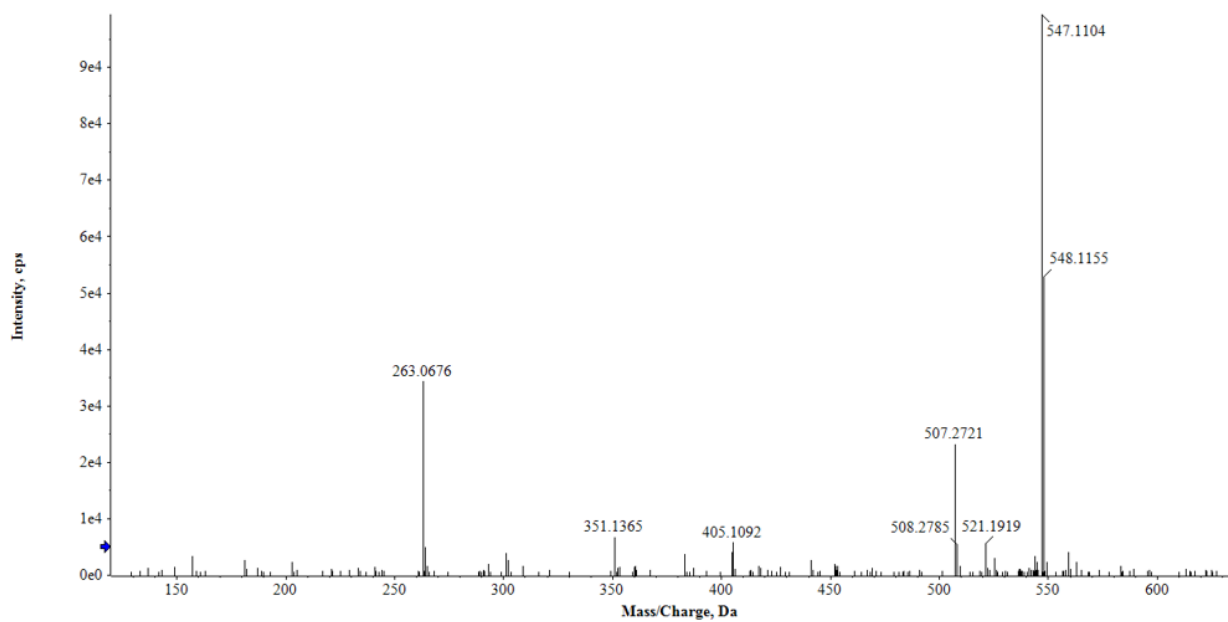
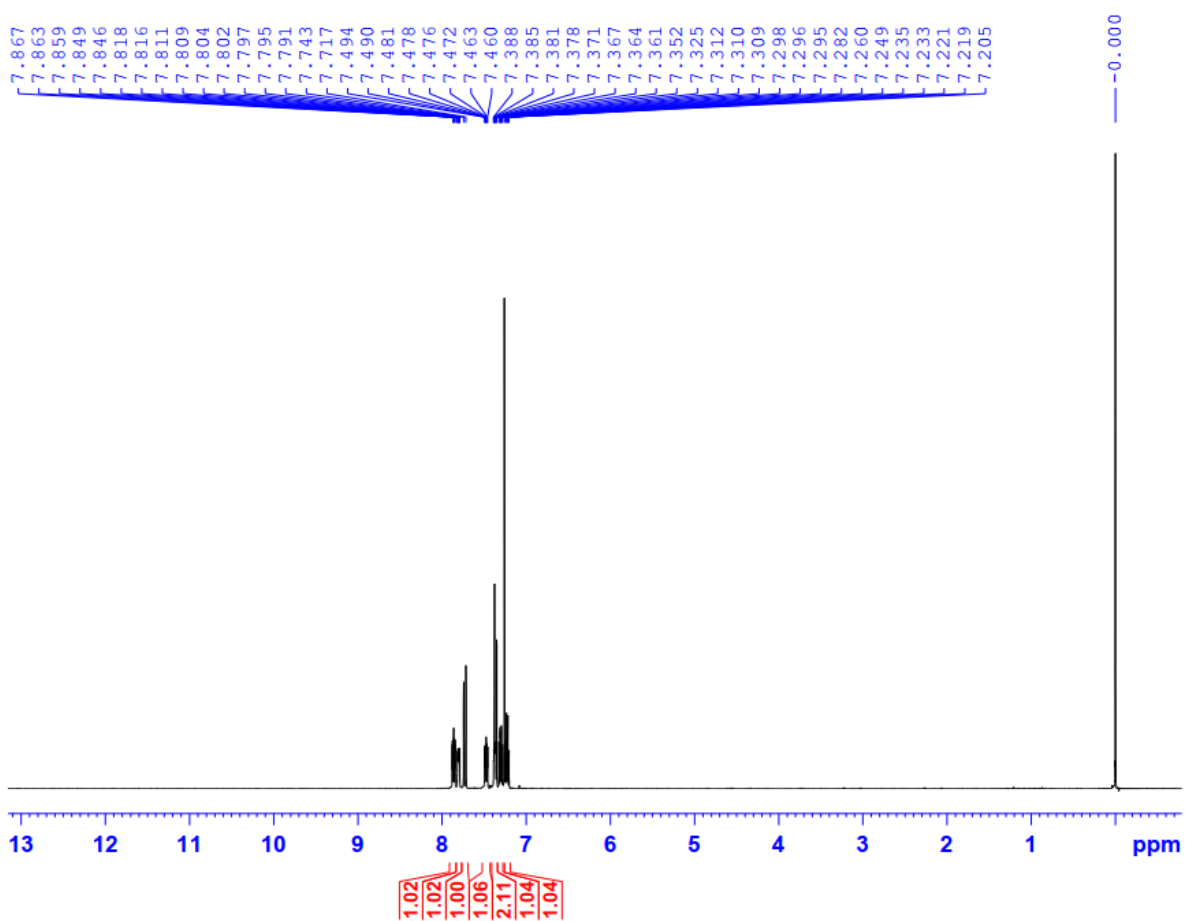
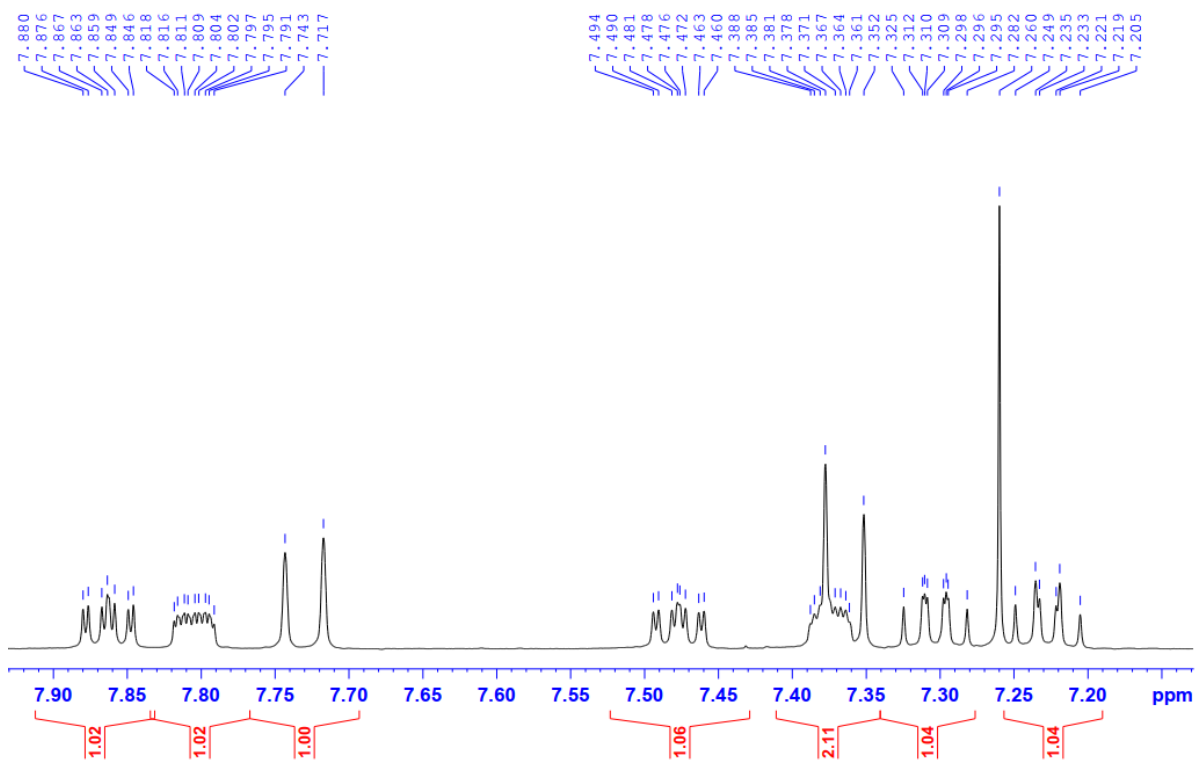
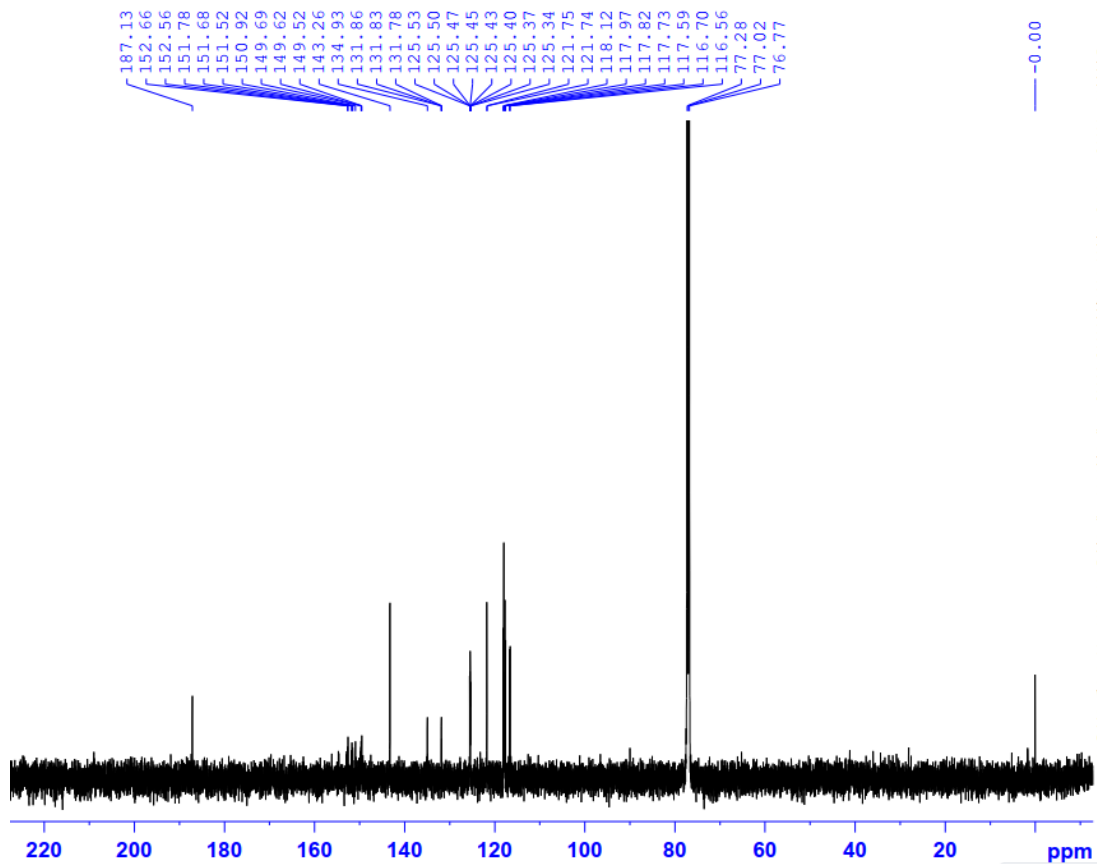
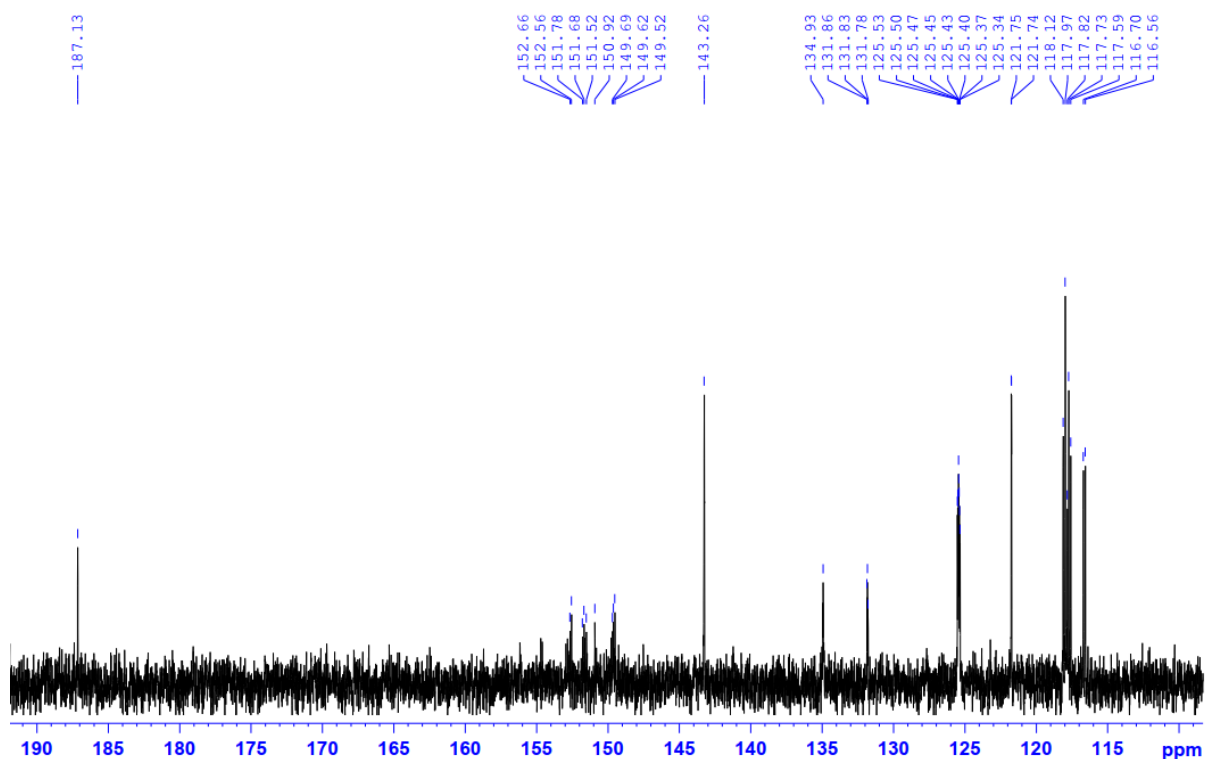
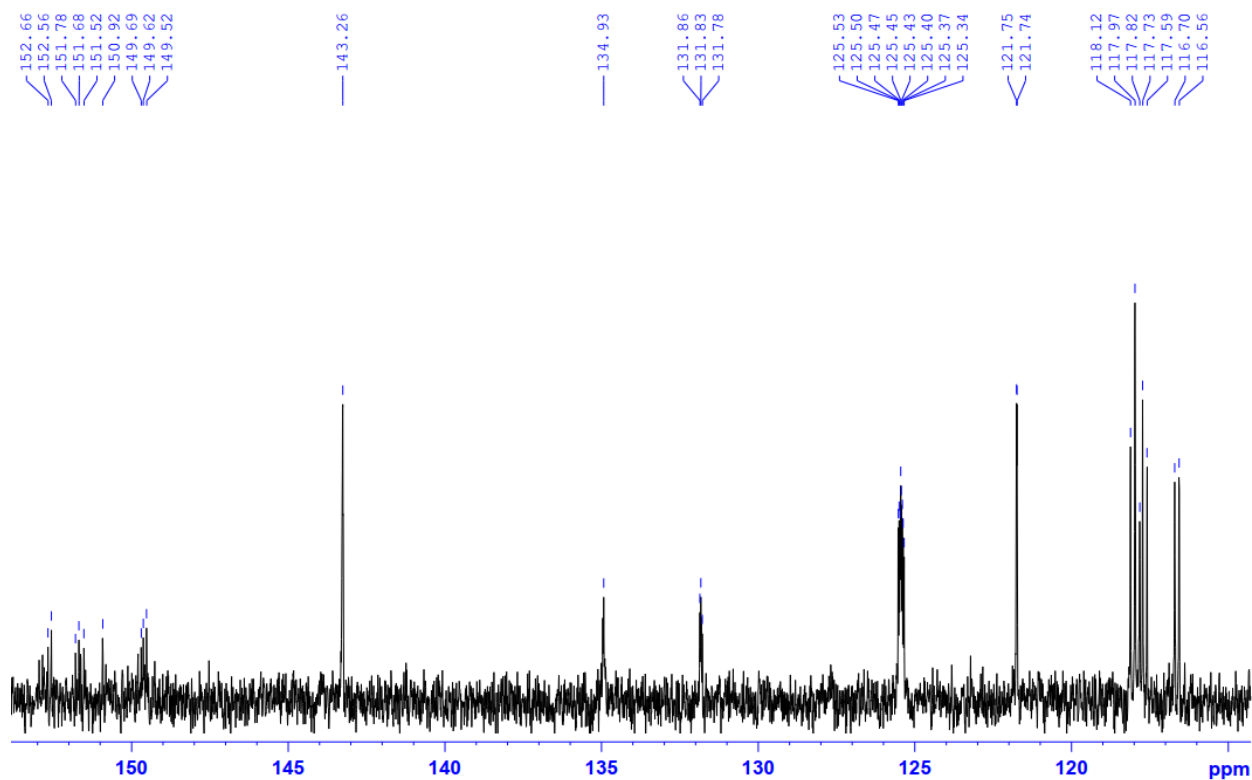
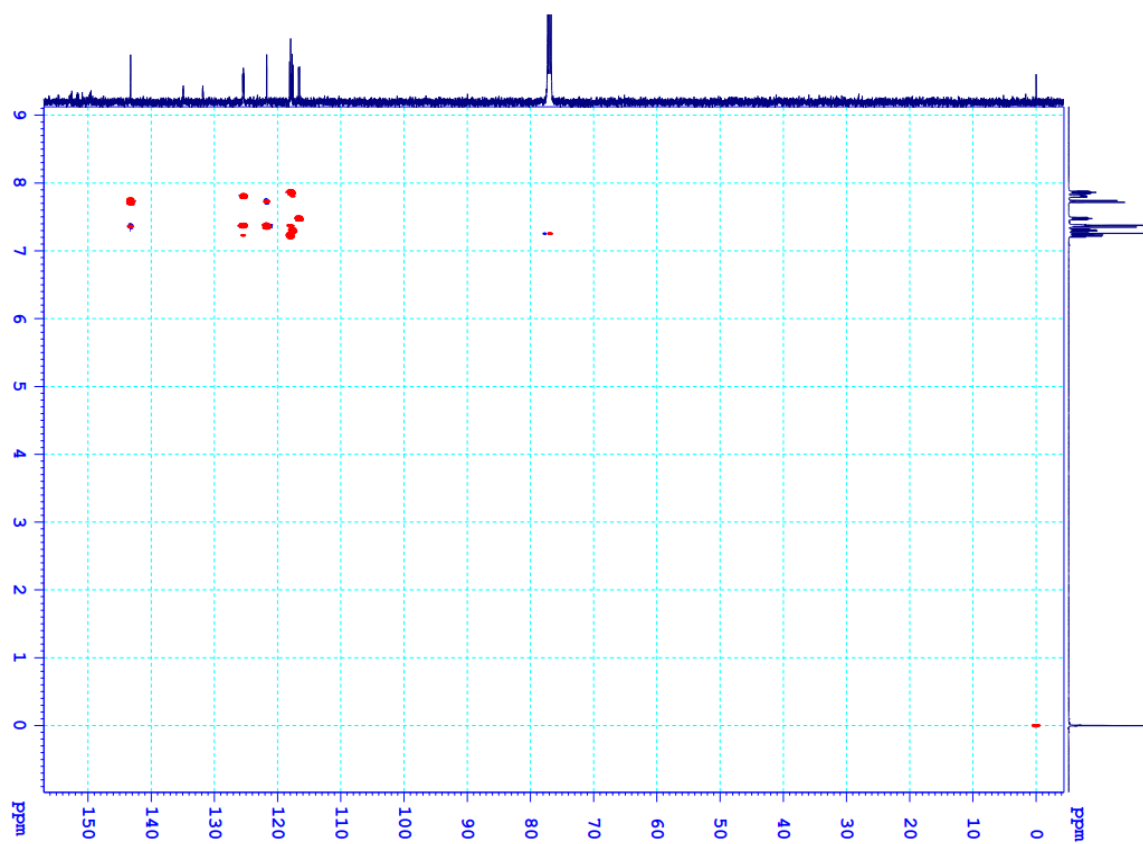


Figure S18g. HRMS of 3d.

Figure S19a. ¹H-NMR spectrum of 3e.Figure S19b. ¹H-NMR spectrum of 3e.

Figure S19c. ¹³C-NMR spectrum of 3e.Figure S19d. ¹³C-NMR spectrum of 3e.

Figure S19e. ^{13}C -NMR spectrum of **3e**.Figure S19f. HSQC spectrum of **3e**.

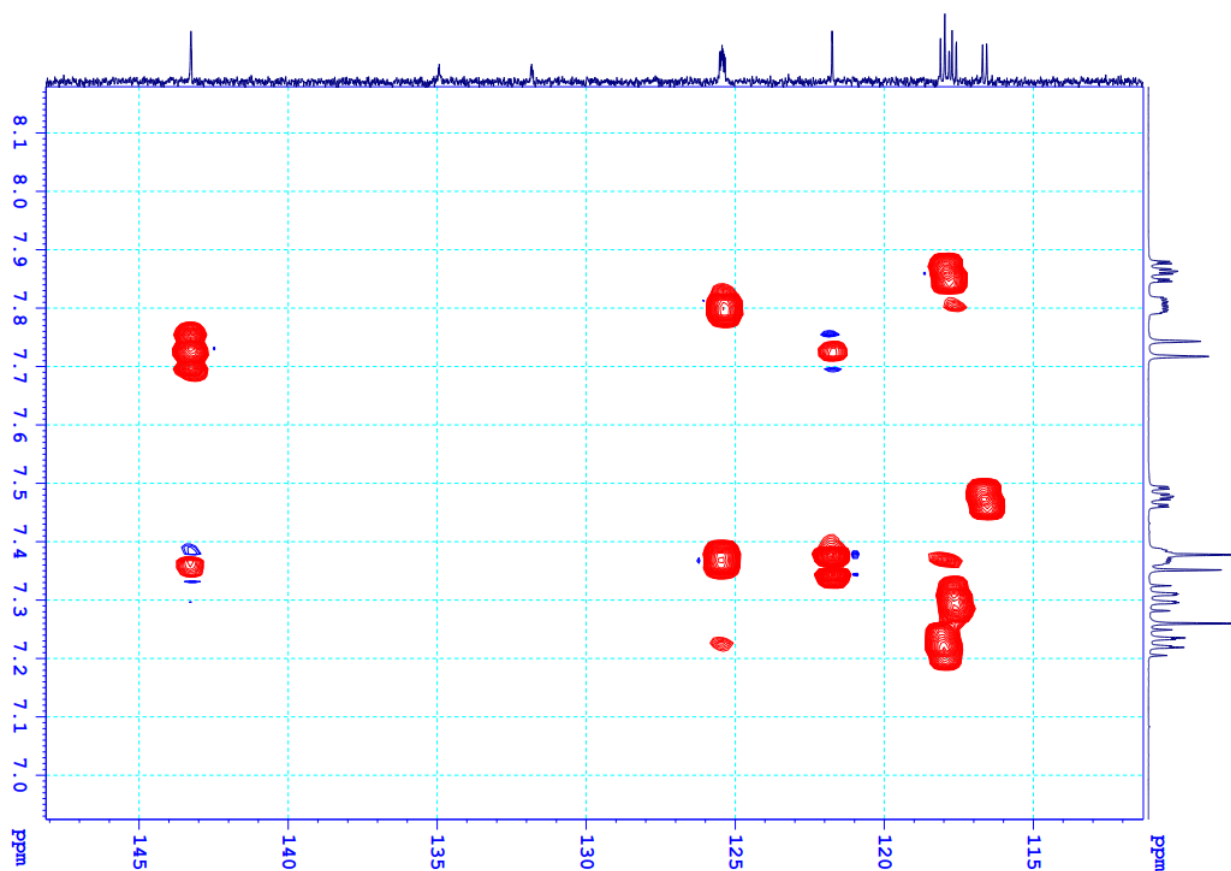


Figure S19g. HSQC spectrum of 3e.

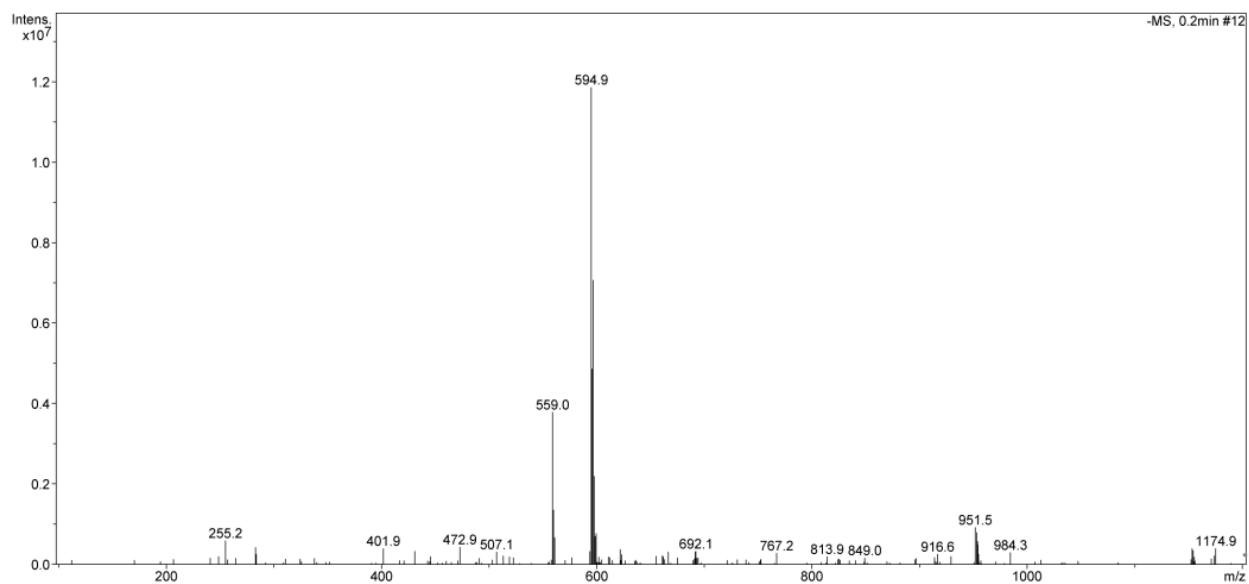
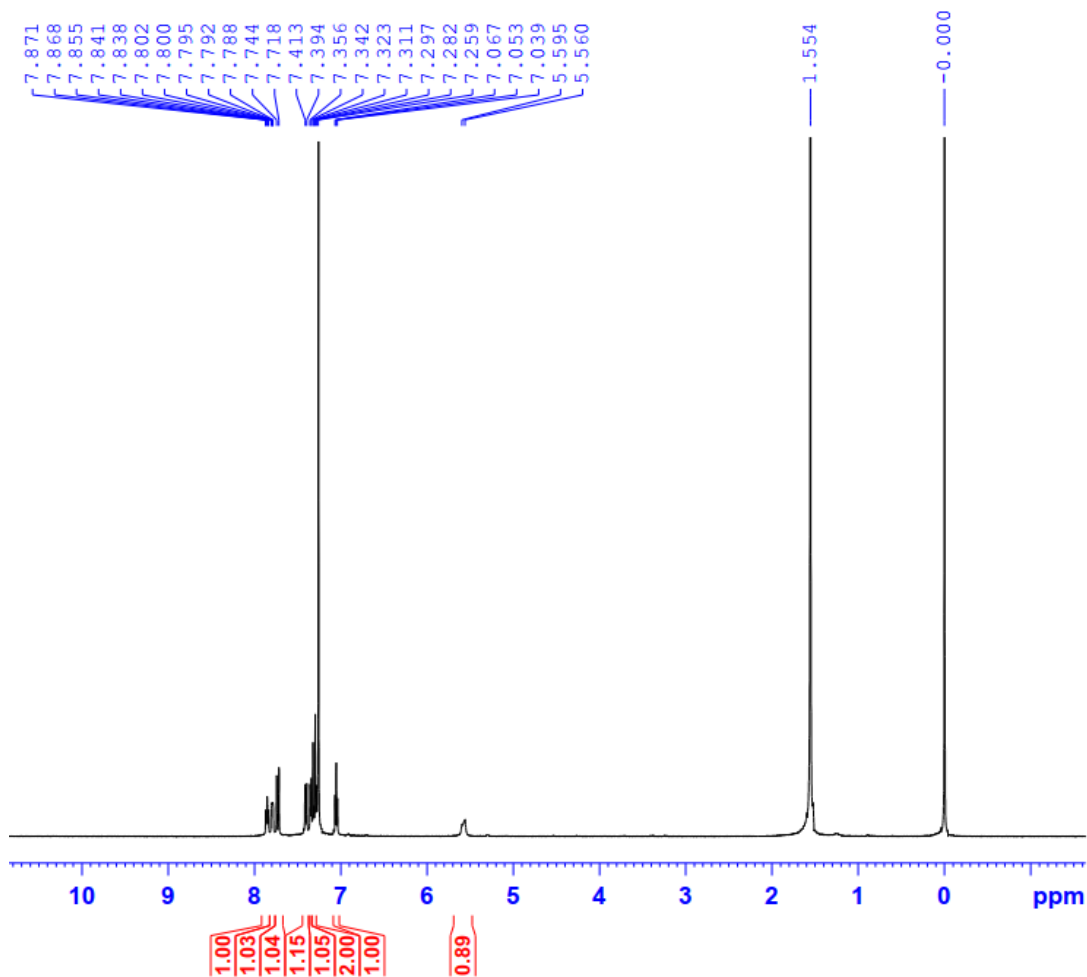
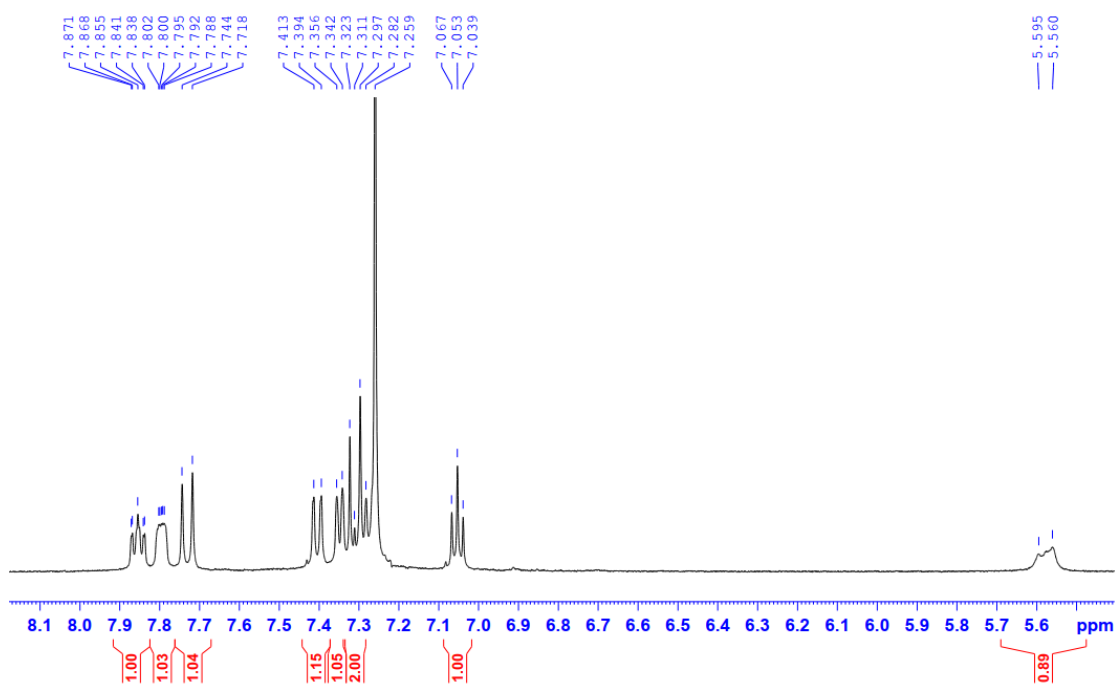
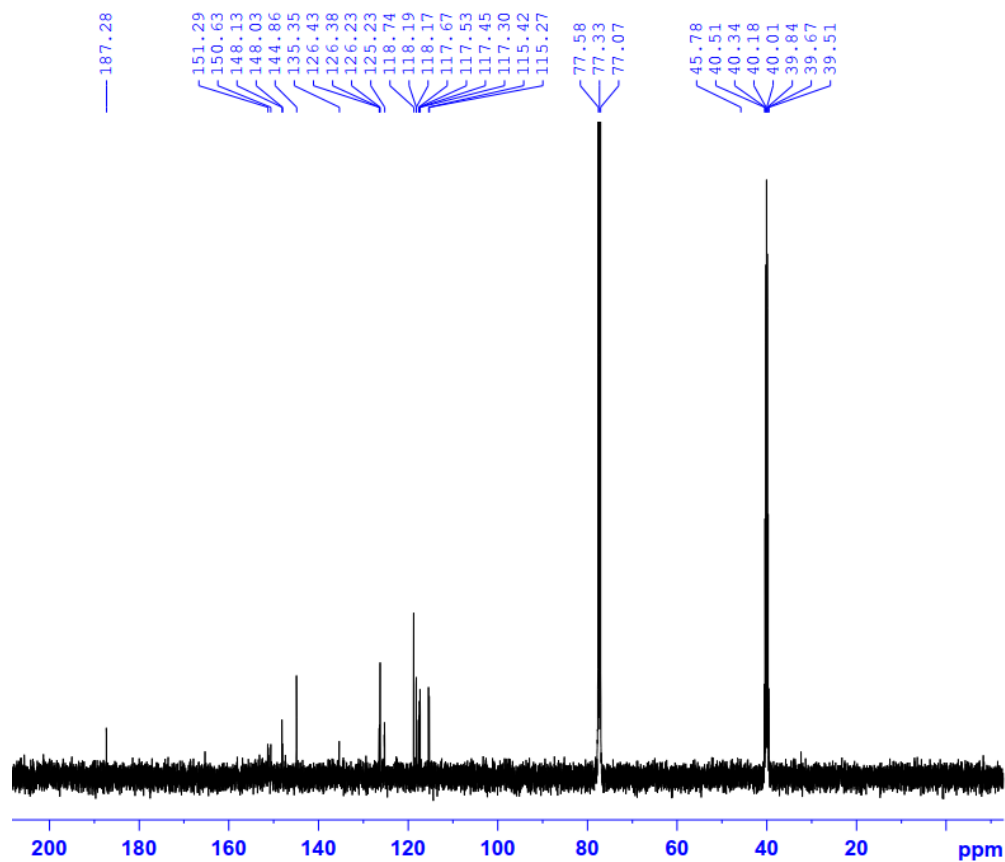
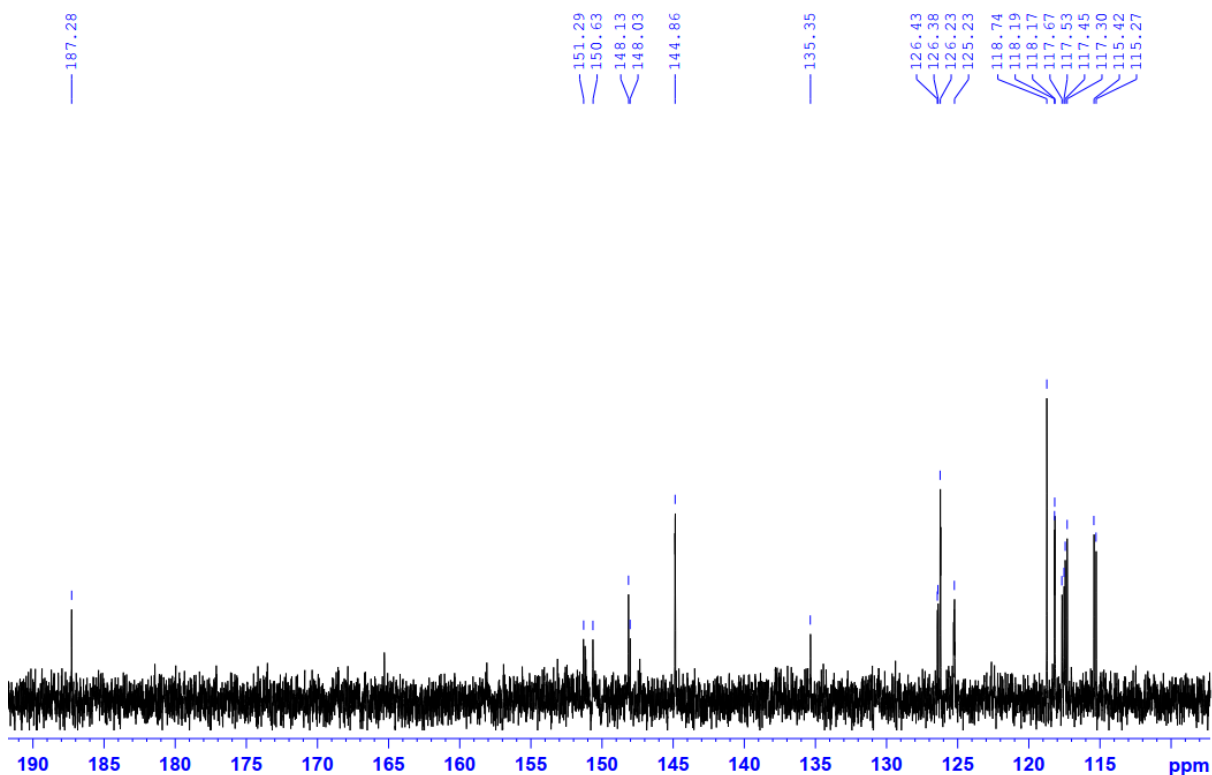
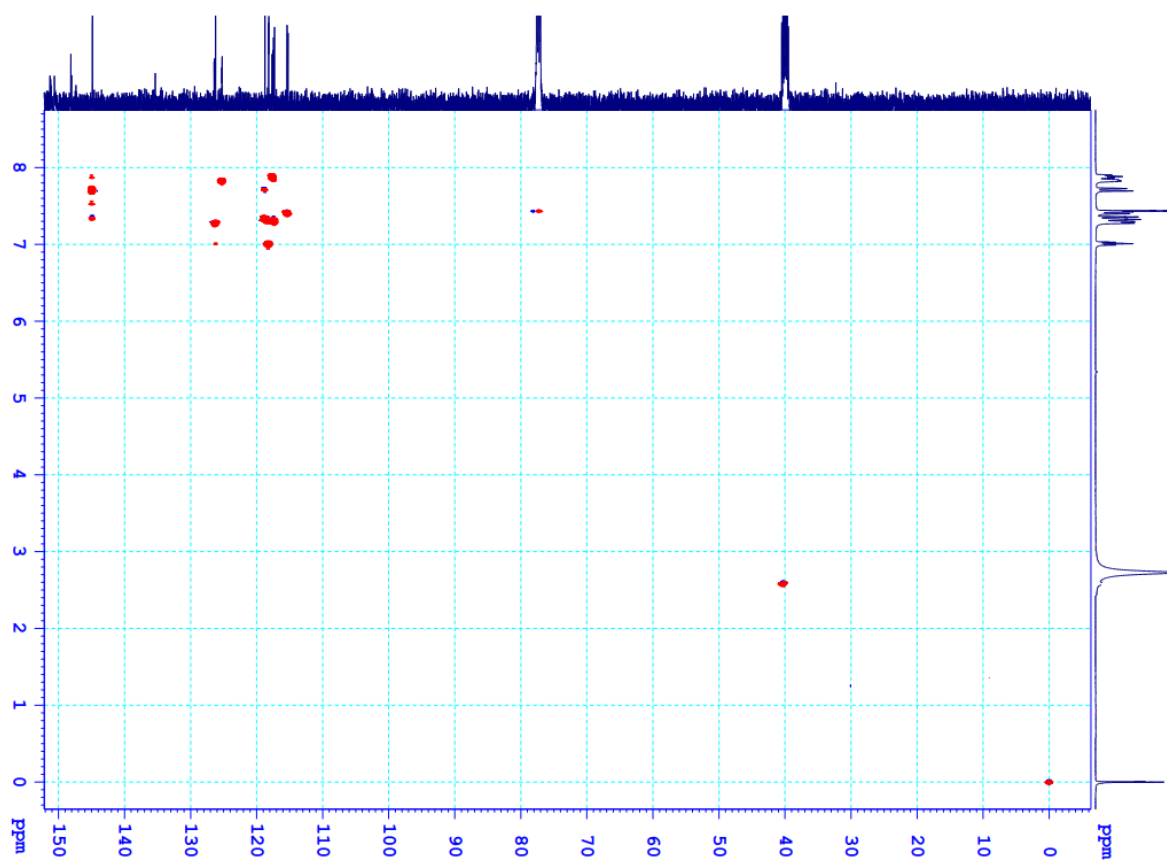
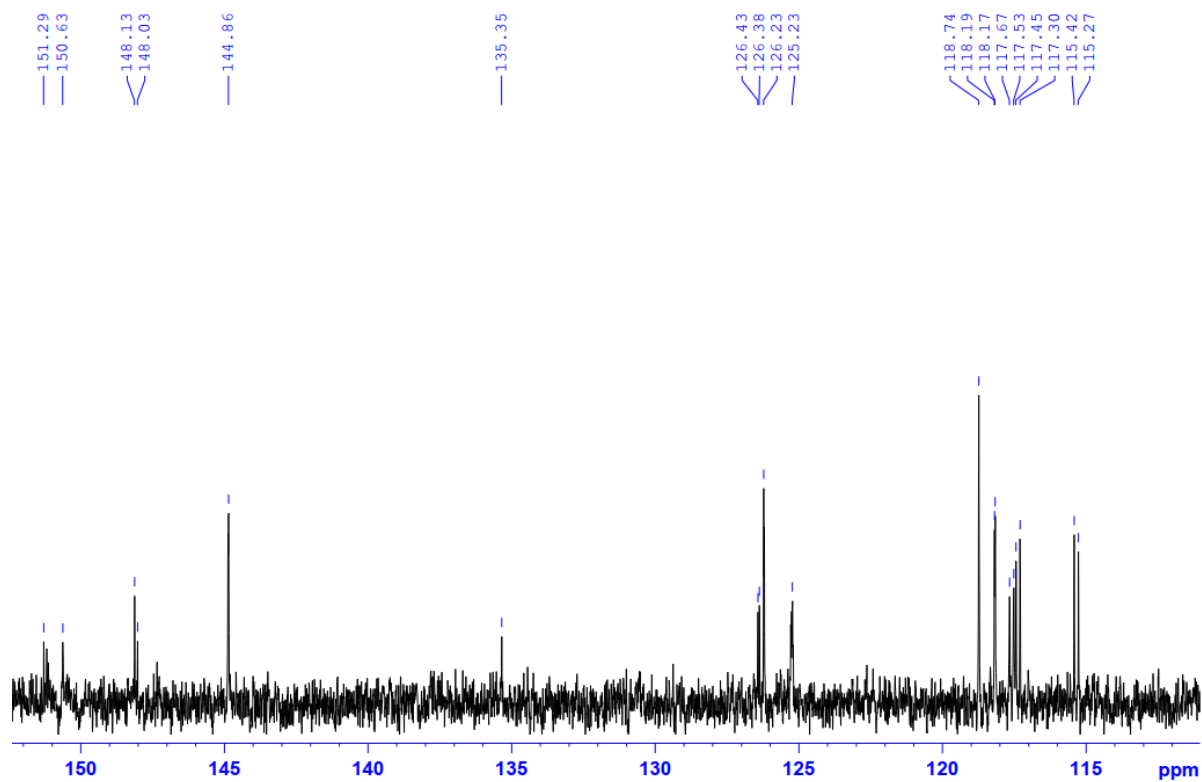


Figure S19h. MS of 3e.

Figure S20a. ¹H-NMR spectrum of **3f**.Figure S20b. ¹H-NMR spectrum of **3f**.

Figure S20c. ^{13}C -NMR spectrum of **3f**.Figure S20d. ^{13}C -NMR spectrum of **3f**.



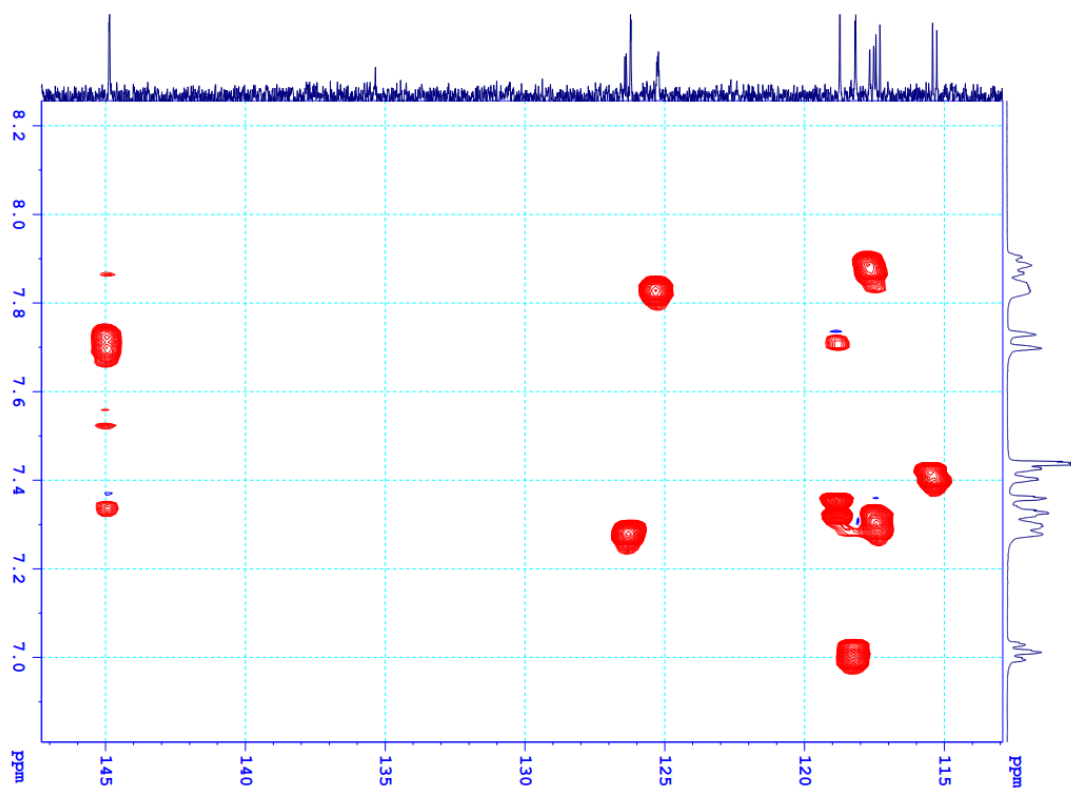


Figure S20g. HSQC spectrum of 3f.

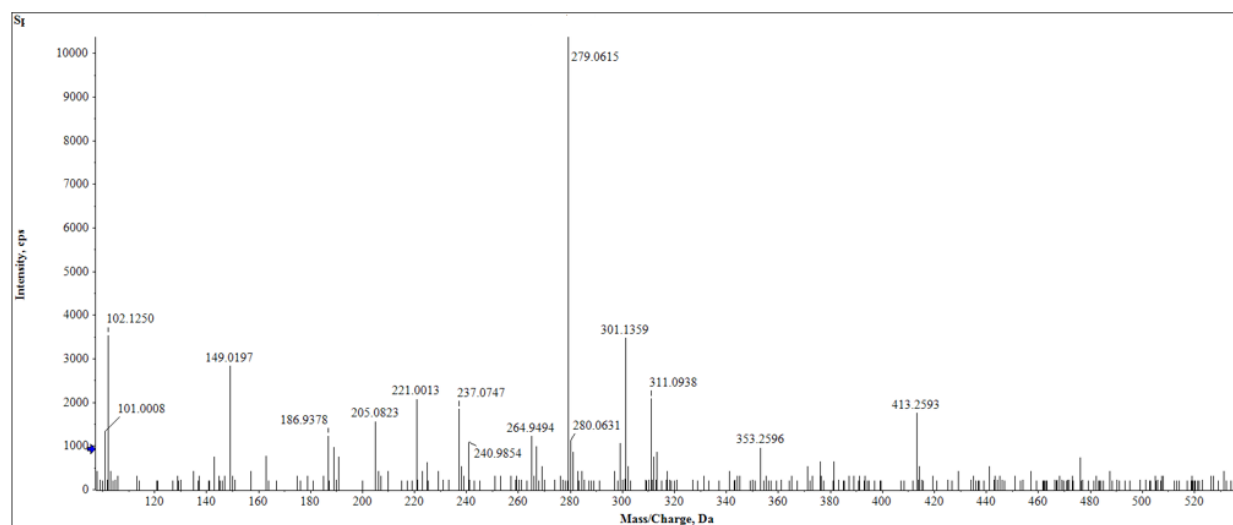
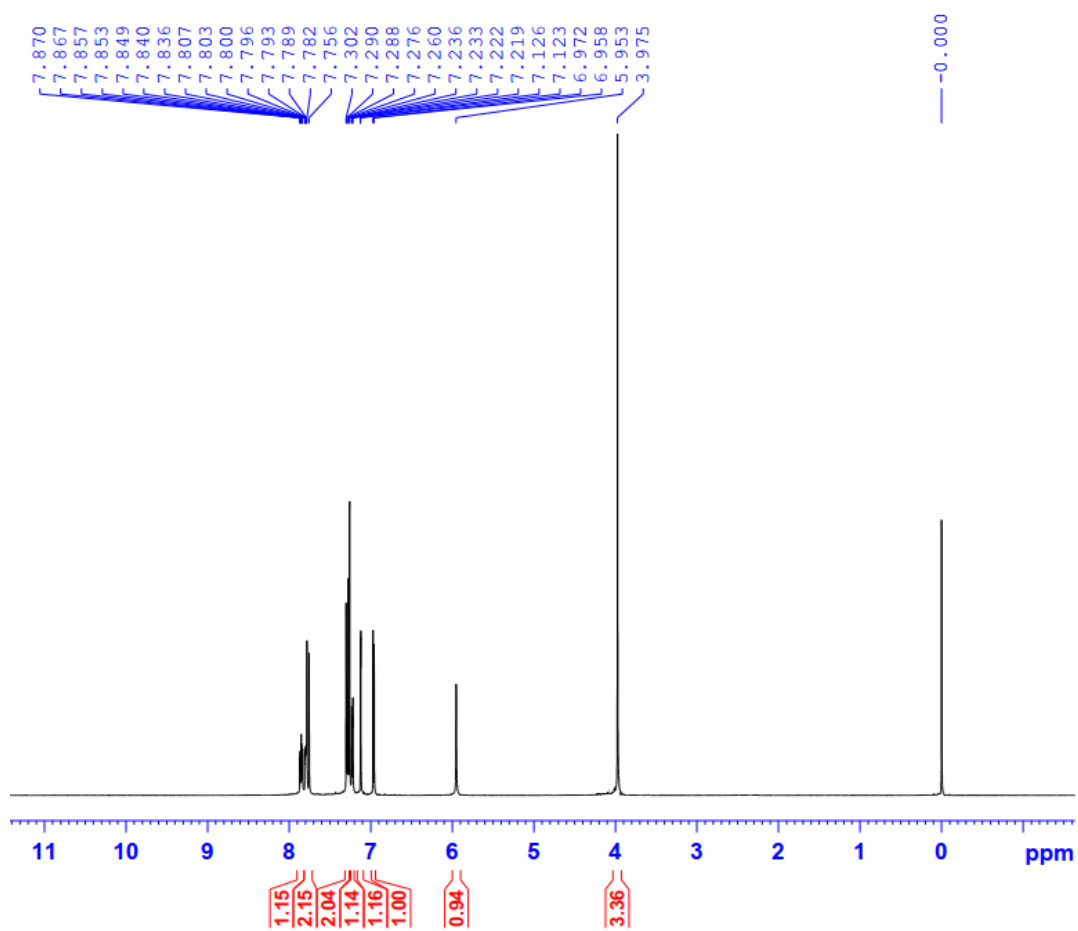
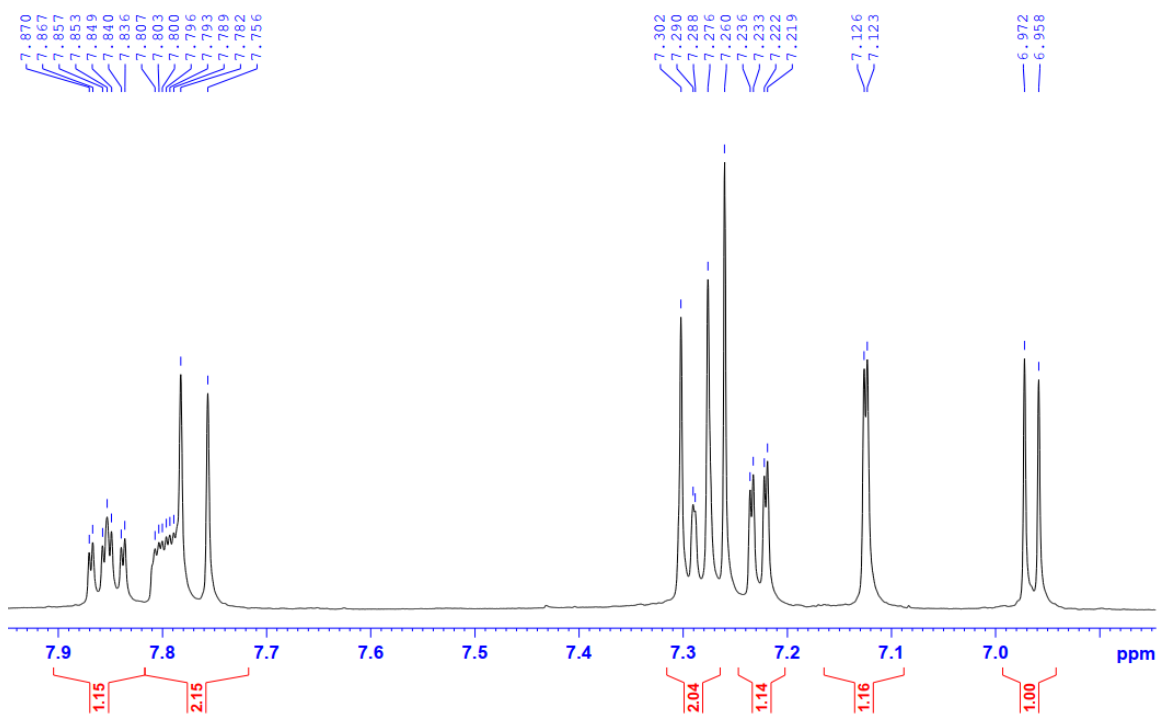
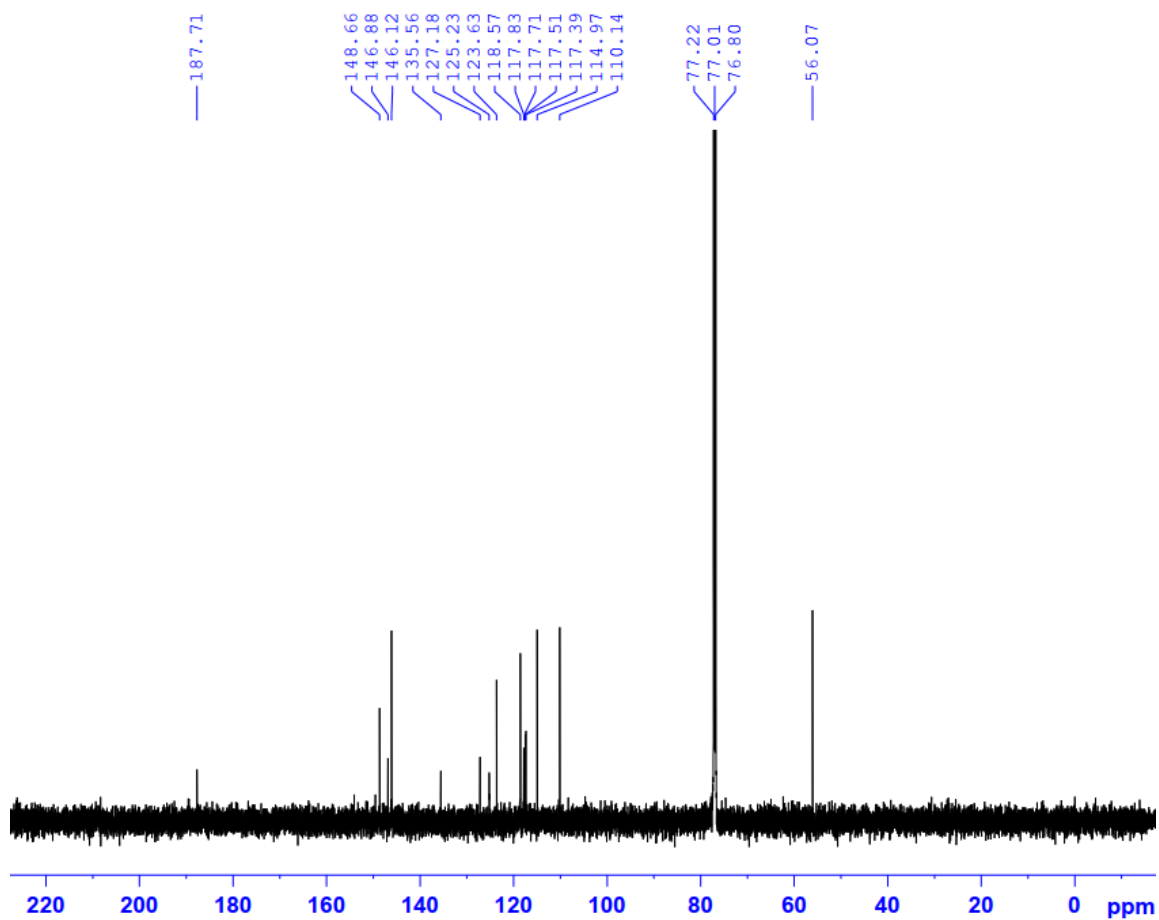
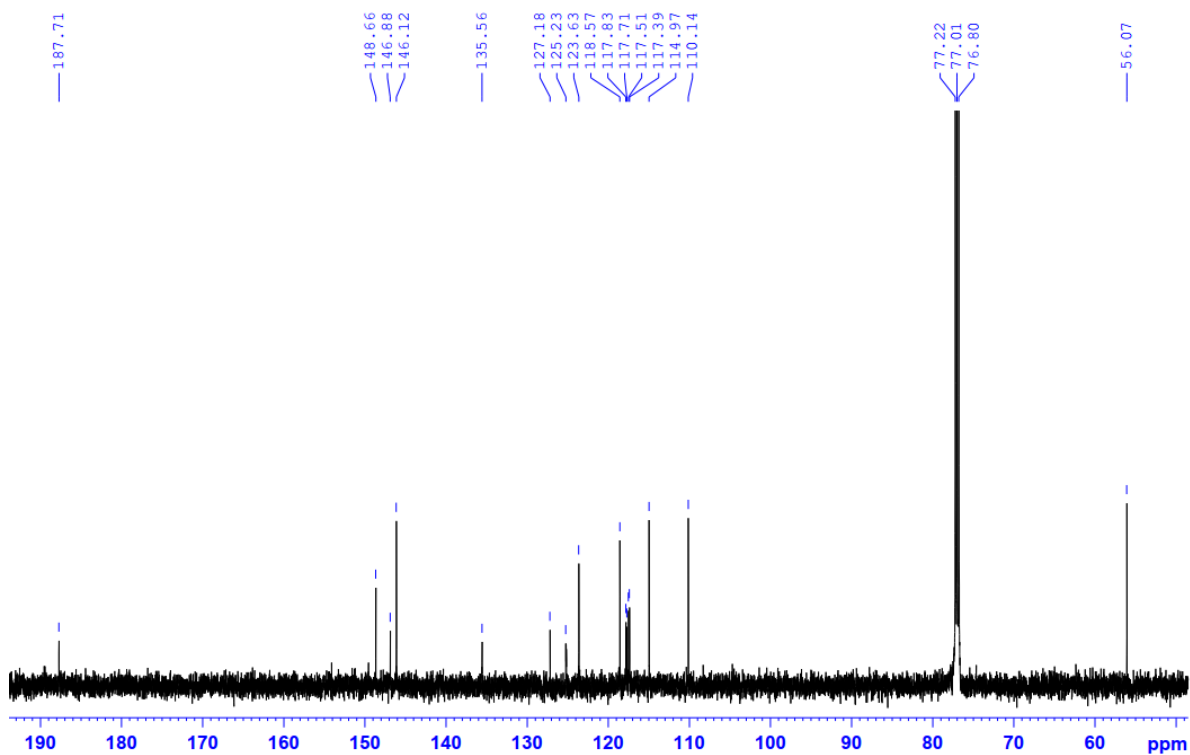
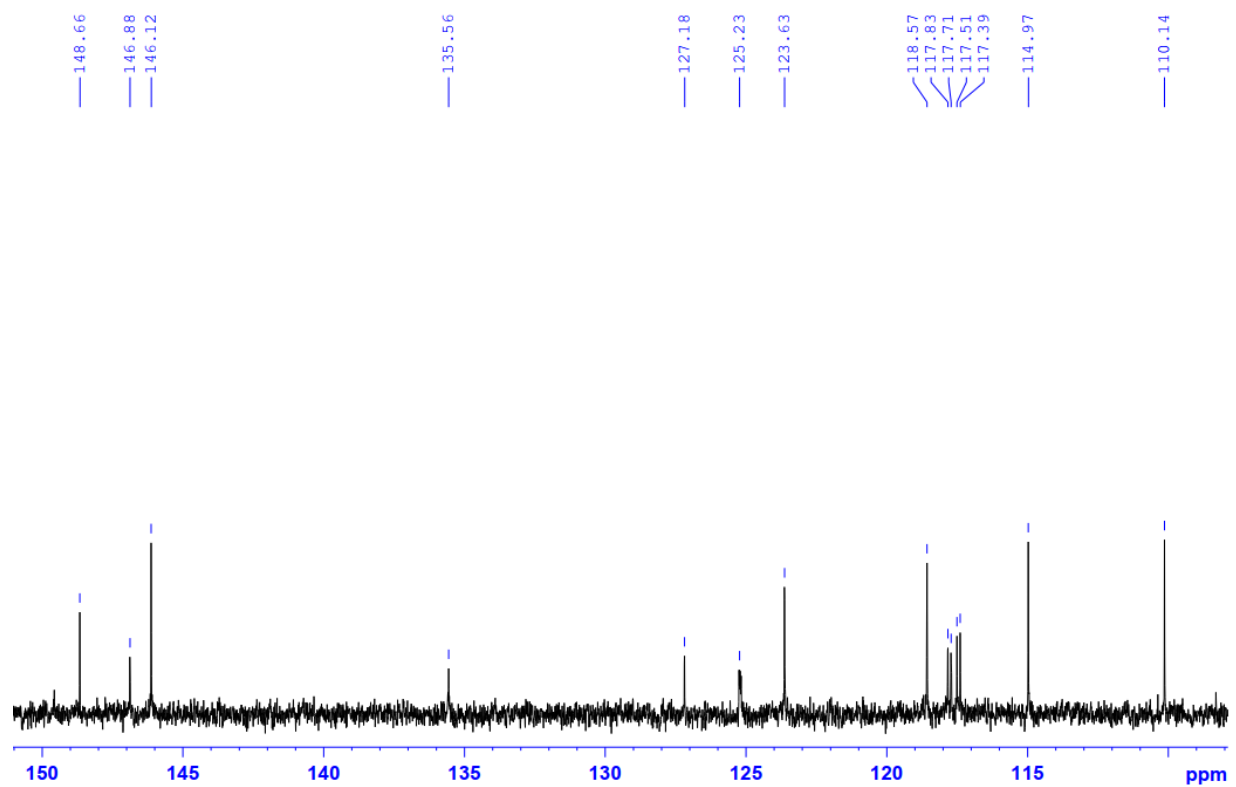
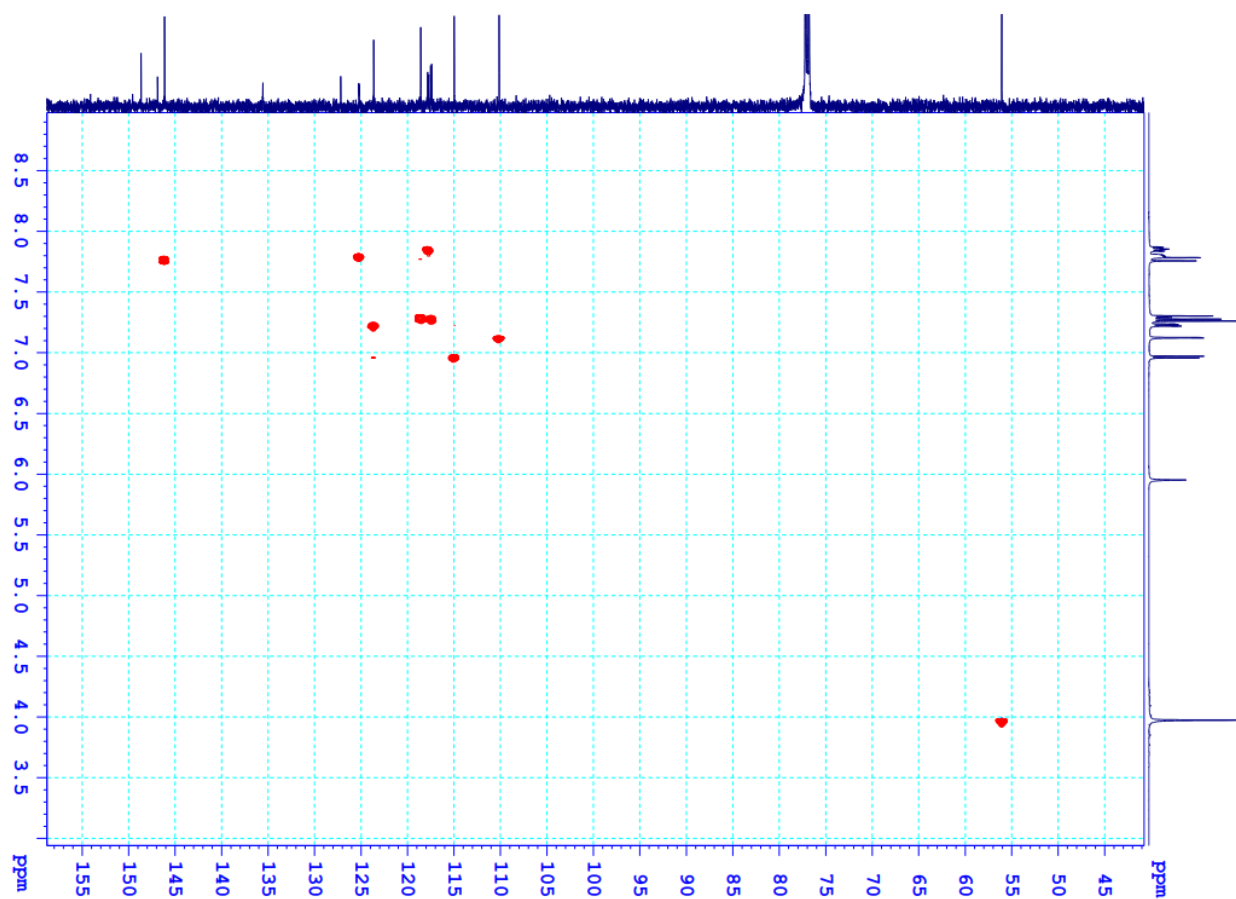


Figure S20h. HRMS of 3f.

Figure S21a. ¹H-NMR spectrum of 3g.Figure S21b. ¹H-NMR spectrum of 3g.

Figure S21c. ^{13}C -NMR spectrum of **3g**.Figure S21d. ^{13}C -NMR spectrum of **3g**.

Figure S21e. ^{13}C -NMR spectrum of **3g**.Figure S21f. HSQC spectrum of **3g**.

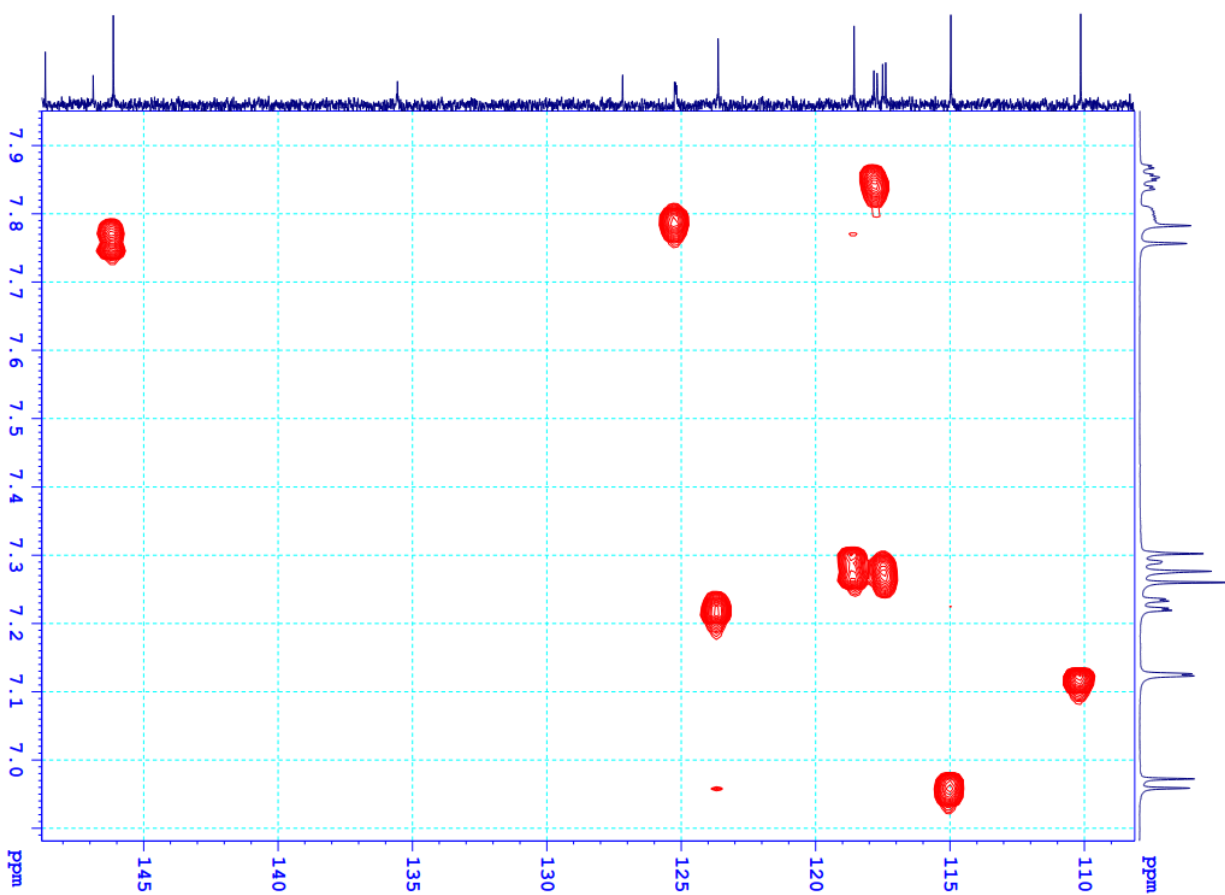


Figure S21g. HSQC spectrum of 3g.

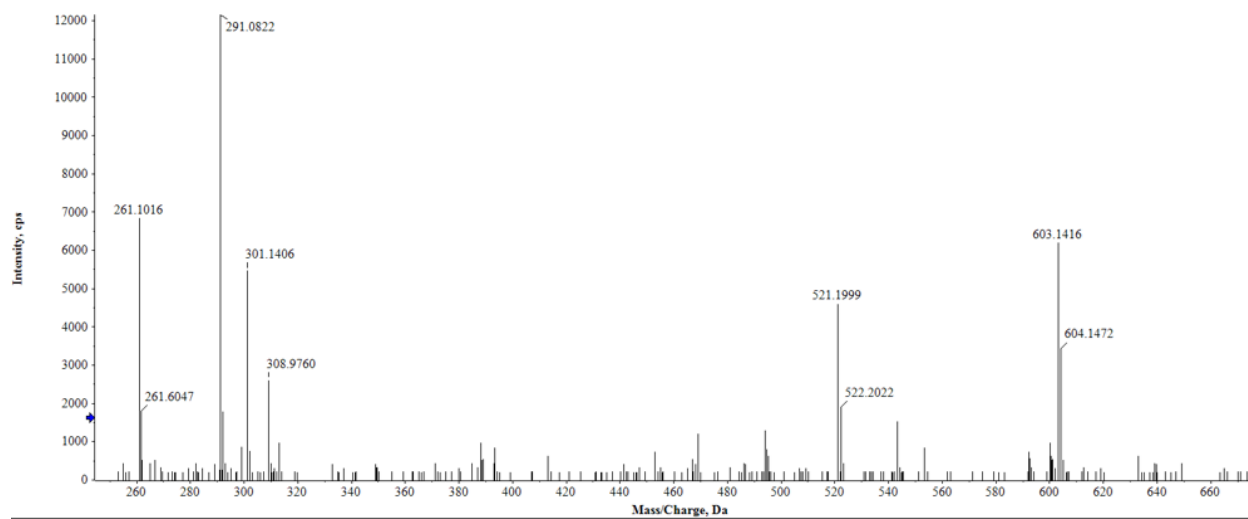


Figure S21h. HRMS of 3g.

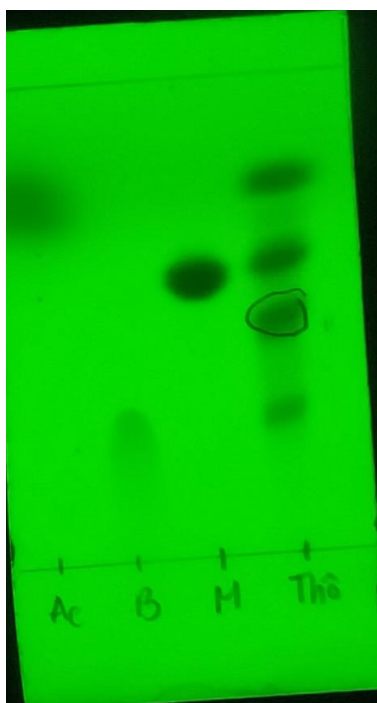


Figure S22. TLC result of the base-catalyzed reaction between acetophenone and benzaldehyde after stirring in ethanol for 24 h at reflux condition. Eluent: *n*-hexane/EA (9/1). Ac: acetophenone. B: benzaldehyde. M: Michael addition product. Thô: crude mixture. Spots were visualized at 254 nm.

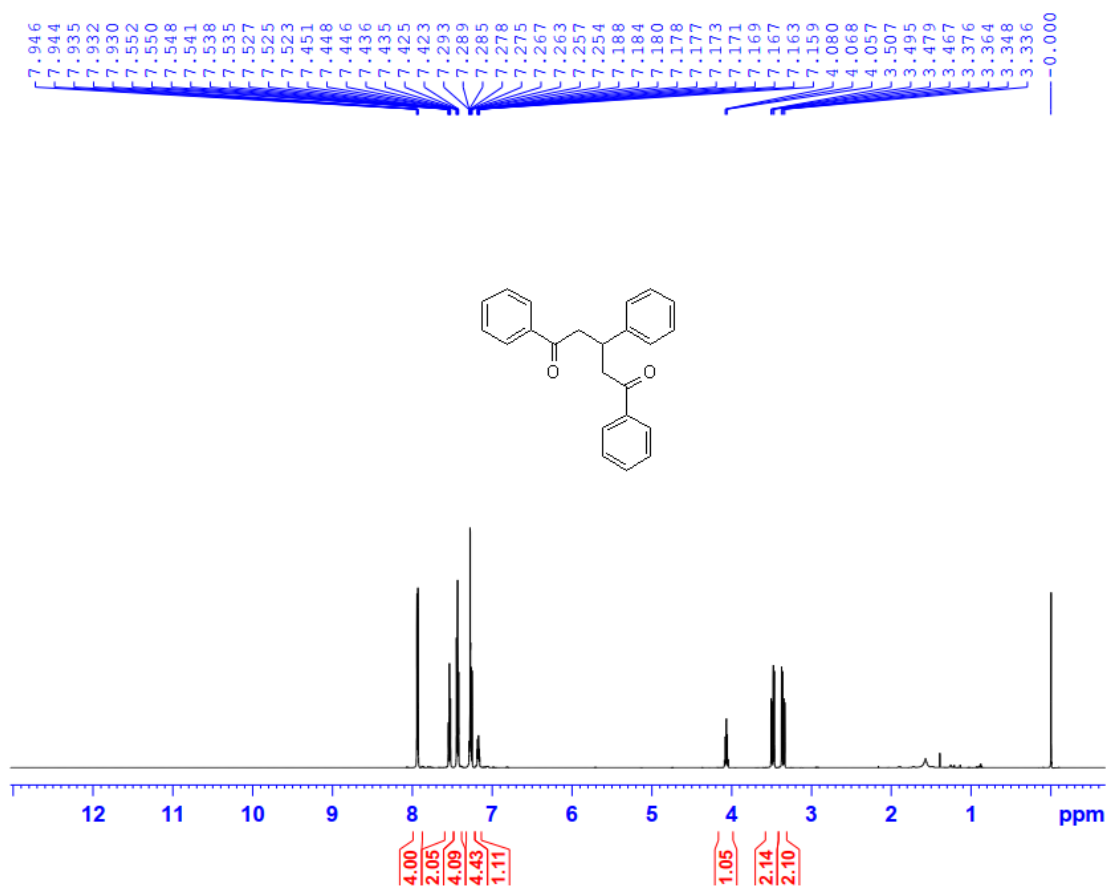


Figure S23a. ¹H-NMR spectrum of Michael addition product.

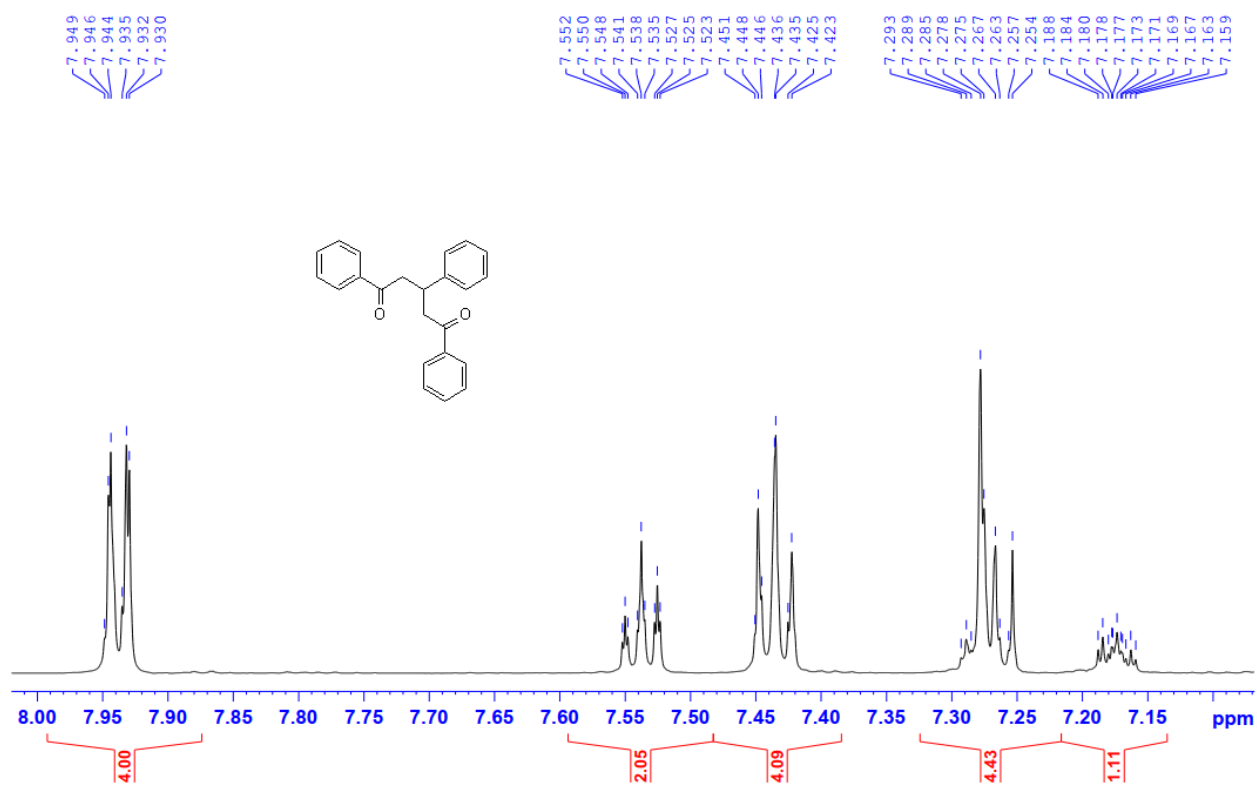


Figure S23b. ¹H-NMR spectrum of Michael addition product (expanded).

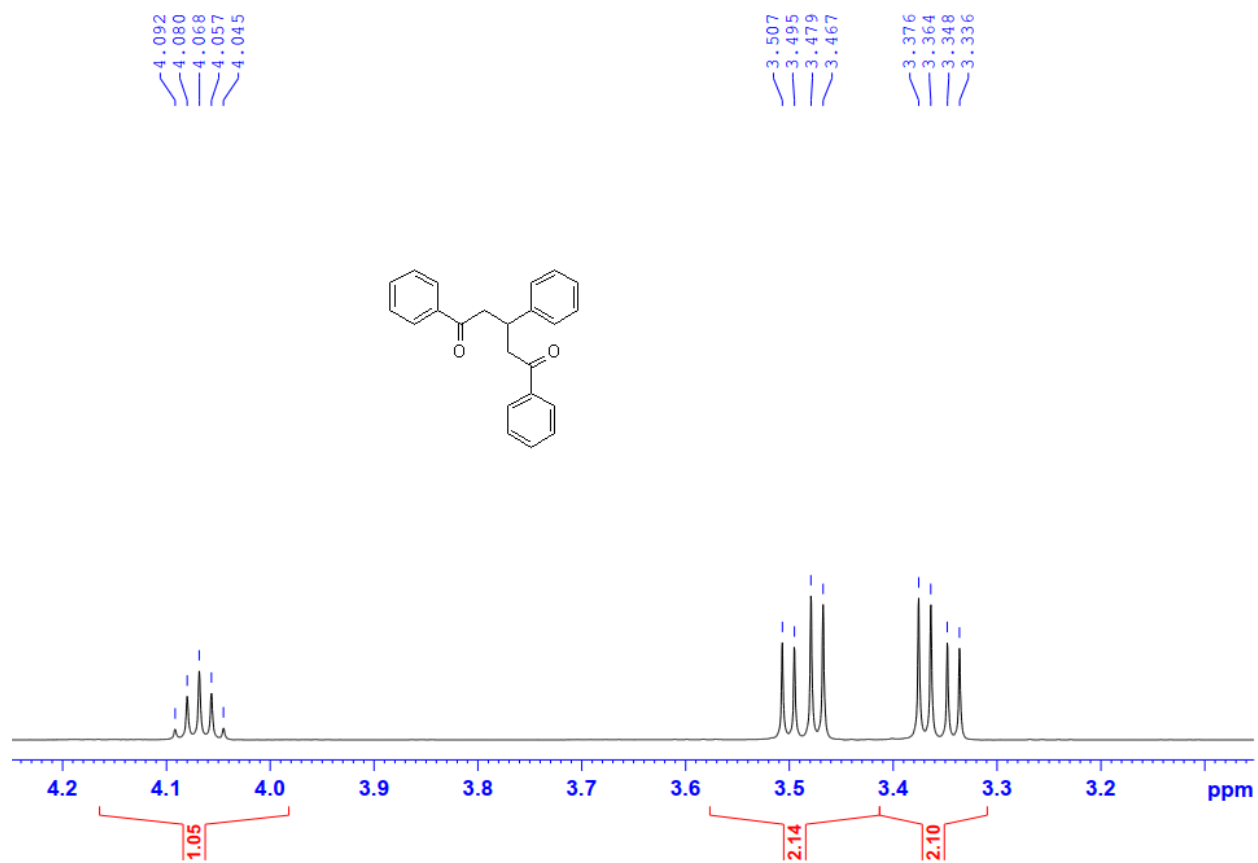


Figure S23c. ¹H-NMR spectrum of Michael addition product (expanded).