

Supporting Information

For

Stereoselective One-Pot Synthesis of Spiro-Indenoquinoline– Pyrrolidine Hybrids: Structural Elucidation and Biological Evaluation

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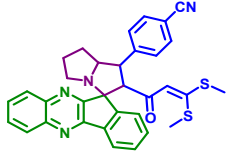
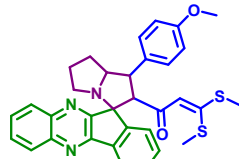
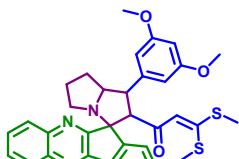
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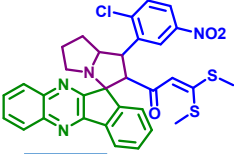
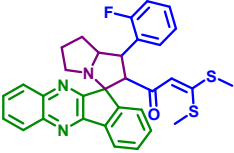
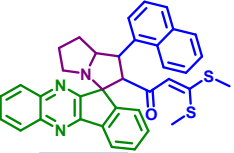
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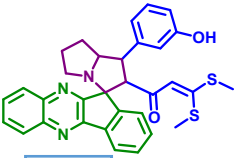
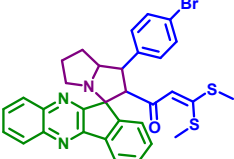
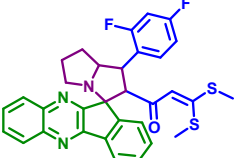
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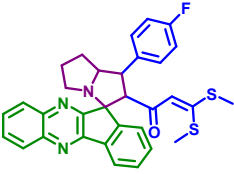
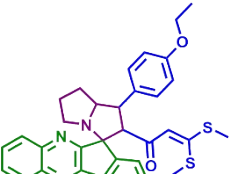
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1. Spectroscopic data of new compounds

 <p style="text-align: center;">6a</p>	<p>Nature: Mild Yellow solid Yield: 69% R_f (30% EtOAc-Hexane): 0.45 Mp: 274-276 °C ¹H NMR (400 MHz, CDCl₃) δ 8.33 – 8.28 (m, 1H), 8.16 – 8.11 (m, 2H), 7.78 – 7.74 (m, 2H), 7.70 (d, <i>J</i> = 8.3 Hz, 2H), 7.66 – 7.60 (m, 3H), 7.57 – 7.49 (m, 2H), 4.65 (d, <i>J</i> = 11.7 Hz, 1H), 4.55 (s, 1H), 4.35 (dt, <i>J</i> = 9.3, 7.1 Hz, 1H), 4.14 (dd, <i>J</i> = 11.7, 9.4 Hz, 1H), 2.66 – 2.40 (m, 3H), 2.12 (s, 3H), 2.02 – 1.91 (m, 2H), 1.86 – 1.73 (m, 2H), 1.13 (s, 3H) ppm. (Fig. S1) ¹³C NMR (100.6 MHz, CDCl₃) δ 188.1, 165.3, 164.7, 153.6, 146.6, 143.8, 142.8, 142.2, 137.4, 132.4, 131.3, 129.9, 129.7, 129.7, 129.1, 129.1, 128.9, 127.7, 122.2, 119.0, 111.1, 110.5, 75.7, 72.7, 69.5, 51.84, 47.69, 31.5, 28.1, 15.6, 14.6 ppm (Fig. S2) DEPT-135 (100.6 MHz, CDCl₃) δ 132.4, 131.4, 129.9, 129.8, 129.7, 129.2, 129.1, 129.0, 127.8, 122.3, 111.2, 72.7, 69.6, 51.8, 47.6, 28.1, 15.6, 14.6 ppm. (Fig. S3) FT-IR (KBr) u_{max} = 1639.53 (C=O), 1494.83 (C=C), 1105.94 (=C-H) cm⁻¹. (Fig. S4) HRMS (ESI): Calcd for C₃₃H₂₈N₄OS₂ (M+H)⁺ <i>m/z</i> = 560.1705; Found 561.1786. (Fig. S5)</p>
 <p style="text-align: center;">6b</p>	<p>Nature: Light Green solid Yield: 70% R_f (30% EtOAc-Hexane): 0.33 Mp: 270-271 °C ¹H NMR (400 MHz, CDCl₃) δ 8.37 – 8.27 (m, 1H), 8.12 (d, <i>J</i> = 7.1 Hz, 2H), 7.73 (ddd, <i>J</i> = 10.1, 4.1, 3.0 Hz, 2H), 7.69 (s, 1H), 7.58 – 7.43 (m, 4H), 6.87 (d, <i>J</i> = 8.7 Hz, 2H), 4.61 (d, <i>J</i> = 4.8 Hz, 1H), 4.34 (dt, <i>J</i> = 9.1, 7.1 Hz, 1H), 4.03 (dd, <i>J</i> = 11.8, 9.4 Hz, 1H), 3.77 (s, 3H), 2.63–2.44 (m, 3H), 2.09 (s, 3H), 2.03–1.74 (m, 5H), 1.12 (s, 3H) ppm. (Fig. S6) ¹³C NMR (100.6 MHz, CDCl₃) δ 188.8, 165.2, 163.9, 158.4, 153.7, 144.3, 142.8, 142.3, 137.4, 132.7, 131.2, 129.8, 129.7, 129.5, 129.4, 129.2, 128.9, 128.9, 127.9, 122.1, 114.0, 112.9, 111.8, 75.9, 73.0, 69.8, 55.2, 51.0, 47.7, 31.6, 28.2, 15.5, 14.6 ppm. (Fig. S7) DEPT-135 (100.6 MHz, CDCl₃) δ 131.3, 129.9, 129.7, 129.5, 129.5, 129.2, 128.9, 128.9, 128.0, 122.1, 114.0, 113.0, 111.8, 73.1, 69.9, 55.3, 51.0, 47.8, 31.7, 28.2, 17.3, 15.6, 14.9, 14.6 ppm. (Fig. S8) FT-IR (KBr) u_{max} = 1644.18 (C=O), 1485.91 (C=C), 1244.62 (=C-H) cm⁻¹. (Fig. S9) HRMS (ESI): Calcd for C₃₃H₃₁N₃O₂S₂ (M+H)⁺ <i>m/z</i> = 565.1858; Found 566.1844. (Fig. S10)</p>
 <p style="text-align: center;">6c</p>	<p>Nature: Sandal yellow solid Yield: 72% R_f (25% EtOAc-Hexane): 0.30 Mp: 255-257 °C ¹H NMR (400 MHz, CDCl₃) δ 8.36 – 8.29 (m, 1H), 8.12 (d, <i>J</i> = 8.3 Hz, 2H), 7.79 – 7.70 (m, 3H), 7.55 (t, <i>J</i> = 7.5 Hz, 1H), 7.48 (t, <i>J</i> = 7.4 Hz, 1H), 7.40 (d, <i>J</i> = 9.0 Hz, 1H), 6.47 (d, <i>J</i> = 6.9 Hz, 2H), 4.97 (d, <i>J</i> = 12.3 Hz, 1H), 4.79 (s, 1H), 4.40 (dd, <i>J</i> = 12.2, 9.4 Hz, 1H), 4.28 – 4.18 (m, 1H), 3.94 (s, 3H), 3.77 (s, 3H), 2.53 – 2.43 (m, 2H), 2.07 (s, 3H), 1.97 – 1.85 (m, 4H), 1.22 (s, 3H) ppm. (Fig. S11) ¹³C NMR (100.6 MHz, CDCl₃) δ 189.4, 165.4, 163.5, 159.4, 158.9, 153.8, 144.7, 142.8, 142.3, 137.5, 131.2, 129.9, 129.5, 129., 128.89, 128.7, 128.7, 127.8, 122.1, 121.0, 111.8, 104.4, 98.9, 75.8, 72.2, 67.1, 55.7, 55.3, 47.6, 45.1, 31.8, 28.2, 15.6, 14.6 ppm. (Fig. S12) DEPT-135 (100.6 MHz, CDCl₃) δ 131.2, 129.9, 129.6, 129.3, 128.9, 128.8, 128.8, 127.9, 122.1, 111.9, 104.4, 98.9, 72.3, 67.1, 55.7, 55.3, 45.1, 15.6, 14.6 ppm. (Fig. S13) FT-IR (KBr) u_{max} = 1638.99 (C=O), 1488.51 (C=C), 1137.06 (=C-H) cm⁻¹. (Fig. S14) HRMS (ESI): Calcd for C₃₄H₃₃N₃O₃S₂ (M+H)⁺ <i>m/z</i> = 595.1963; Found 596.2013. (Fig. S15)</p>

 <p style="text-align: center;">6d</p>	<p>Nature: Sandal yellow solid Yield: 70% R_f (30% EtOAc-Hexane): 0.38 Mp: 242-245 °C ¹H NMR (400 MHz, CDCl₃) δ 8.79 (d, <i>J</i> = 2.7 Hz, 1H), 8.48 – 8.40 (m, 1H), 8.15 (ddd, <i>J</i> = 7.1, 3.5, 2.0 Hz, 2H), 8.03 – 7.99 (m, 1H), 7.81 – 7.76 (m, 2H), 7.72 (d, <i>J</i> = 7.4 Hz, 1H), 7.57 (d, <i>J</i> = 8.7 Hz, 2H), 7.54 – 7.50 (m, 1H), 4.76 (d, <i>J</i> = 11.4 Hz, 1H), 4.68 (s, 1H), 4.30 (dt, <i>J</i> = 9.6, 6.1 Hz, 1H), 2.76 – 2.69 (m, 1H), 2.59 – 2.49 (m, 2H), 2.14 (s, 3H), 2.08 – 2.00 (m, 2H), 2.00 – 1.86 (m, 3H), 1.24 (s, 3H) ppm. (Fig. S16) ¹³C NMR (100.6 MHz, CDCl₃) δ 188.3, 165.3, 164.7, 153.4, 147.0, 143.8, 142.9, 142.1, 142.0, 140.9, 137.6, 131.4, 130.7, 130.0, 129.8, 129.2, 128.9, 127.7, 123.7, 122.5, 122.2, 111.4, 75.3, 73.4, 68.9, 47.8, 46.9, 30.6, 27.6, 15.8, 14.5 ppm. (Fig. S17) DEPT-135 (100.6 MHz, CDCl₃) δ 131.5, 130.7, 130.0, 129.8, 129.3, 128.9, 127.8, 123.7, 122.5, 122.3, 111.4, 73.4, 69.0, 47.8, 46.9, 30.7, 27.7, 15.8, 14.6 ppm. (Fig. S18) FT-IR (KBr) u_{max} = 1517.04 (C=O), 1483.32 (C=C) cm⁻¹. (Fig. S19) HRMS (ESI): Calcd for C₃₂H₂₇ClN₄O₃S₂ (M+H) m/z = 615.1630; Found 615.1249. (Fig. S20)</p>
 <p style="text-align: center;">6e</p>	<p>Nature: Brown solid Yield: 80% R_f (30% EtOAc-Hexane): 0.30 Mp: 277-278 °C ¹H NMR (400 MHz, CDCl₃) δ 8.35 – 8.29 (m, 1H), 8.13 (d, <i>J</i> = 9.1 Hz, 2H), 7.75 – 7.69 (m, 3H), 7.60 – 7.54 (m, 2H), 7.49 (s, 1H), 7.21 – 7.14 (m, 1H), 7.12 – 7.06 (m, 1H), 7.05 (d, <i>J</i> = 8.3 Hz, 1H), 4.90 (d, <i>J</i> = 12.0 Hz, 1H), 4.68 (s, 1H), 4.40 (dd, <i>J</i> = 11.9, 9.4 Hz, 1H), 4.34 – 4.24 (m, 1H), 2.51 (dd, <i>J</i> = 6.7, 4.2 Hz, 1H), 2.45 (s, 1H), 2.08 (s, 3H), 1.94 – 1.80 (m, 4H), 1.17 (s, 3H) ppm. (Fig. S21) ¹³C NMR (100.6 MHz, CDCl₃) δ 188.53, 165.02, 164.40, 153.75, 144.26, 142.84, 142.33, 137.50, 131.40, 129.91, 129.76, 129.55, 129.11, 129.06, 128.95, 128.90, 128.15, 128.06, 127.84, 127.45, 124.33, 122.21, 115.86, 115.64, 111.35, 75.81, 72.22, 67.62, 47.67, 44.87, 31.71, 28.23, 15.59, 14.59 ppm. (Fig. S22) DEPT-135 (100.6 MHz, CDCl₃) δ 131.4, 129.9, 129.8, 129.6, 129.1, 129.1, 129.0, 128.9, 128.1, 128.1, 127.8, 124.3, 122.2, 115.9, 115.6, 111.4, 72.2, 67.6, 47.7, 44.9, 31.7, 28.2, 15.6, 14.6 ppm. (Fig. S23) FT-IR (KBr) u_{max} = 1641.58 (C=O), 1483.32 (C=C), 754.26 (-F) cm⁻¹. (Fig. S24)</p>
 <p style="text-align: center;">6f</p>	<p>Nature: Yellowish solid Yield: 74% R_f (30% EtOAc-Hexane): 0.30 Mp: 277-279 °C ¹H NMR (400 MHz, CDCl₃) δ 8.72 (d, <i>J</i> = 8.5 Hz, 1H), 8.39 – 8.33 (m, 1H), 8.17 (d, <i>J</i> = 5.1 Hz, 1H), 8.16 – 8.14 (m, 1H), 7.94 (d, <i>J</i> = 6.9 Hz, 1H), 7.89 – 7.83 (m, 2H), 7.78 – 7.72 (m, 4H), 7.67 – 7.62 (m, 2H), 7.53 – 7.47 (m, 3H), 5.03 (d, <i>J</i> = 8.5 Hz, 1H), 4.69 (s, 1H), 4.50 – 4.44 (m, 1H), 2.70 – 2.63 (m, 1H), 2.59 – 2.53 (m, 1H), 2.06 (s, 3H), 1.92 (td, <i>J</i> = 9.6, 5.9 Hz, 3H), 1.28 – 1.19 (m, 1H), 1.12 (s, 3H) ppm. (Fig. S25) ¹³C NMR (100.6 MHz, CDCl₃) δ 189.07, 165.25, 164.20, 153.72, 144.56, 142.85, 142.34, 137.61, 137.41, 134.14, 132.56, 131.44, 129.90, 129.75, 129.52, 128.98, 128.94, 128.83, 127.98, 127.22, 126.16, 125.61, 125.52, 123.93, 122.27, 111.78, 76.24, 74.65, 70.13, 47.66, 32.27, 28.31, 15.58, 14.55 ppm. (Fig. S26) DEPT-135 (100.6 MHz, CDCl₃) δ 131.4, 129.9, 129.8, 129.5, 129.0, 128.9, 128.8, 128.0, 127.2, 126.2, 125.6, 125.5, 123.9, 122.3, 111.8, 70.1, 47.7, 32.3, 28.3, 15.6, 14.5 ppm. (Fig. S27) FT-IR (KBr) u_{max} = 1646.77 (C=O), 1478.13 (C=C) cm⁻¹. (Fig. S28) HRMS (ESI): Calcd for C₃₆H₃₁N₃OS₂ (M+H)⁺ m/z = 585.1909; Found 586.1808. (Fig. S29)</p>

 <p style="text-align: center;">6g</p>	<p>Nature: Bright yellow solid Yield: 85% R_f (25% EtOAc-Hexane): 0.35 Mp: 270-271 °C ¹H NMR (400 MHz, CDCl₃) δ 8.14 – 8.02 (m, 2H), 8.02 – 7.95 (m, 1H), 7.73 – 7.65 (m, 2H), 7.61 (td, <i>J</i> = 7.7, 1.5 Hz, 1H), 7.54 (td, <i>J</i> = 7.5, 1.3 Hz, 1H), 7.51 – 7.46 (m, 1H), 7.30 (s, 1H), 7.16 (t, <i>J</i> = 7.7 Hz, 1H), 7.10 (d, <i>J</i> = 7.7 Hz, 1H), 6.73 – 6.66 (m, 1H), 4.79 (d, <i>J</i> = 12.1 Hz, 1H), 4.72 (s, 1H), 4.38 – 4.22 (m, 1H), 4.04 (dd, <i>J</i> = 12.0, 9.5 Hz, 1H), 2.63 – 2.45 (m, 2H), 2.07 (s, 3H), 2.06 – 1.79 (m, 4H), 1.15 (s, 3H) ppm. (Fig. S30) ¹³C NMR (100.6 MHz, CDCl₃) δ 188.6, 164.8, 164.8, 156.7, 153.6, 144.0, 142.6, 141.9, 141.9, 137.4, 131.2, 129.7, 129.6, 129.5, 129.5, 129.0, 128.7, 127.8, 122.3, 120.5, 115.0, 114.3, 111.6, 76.0, 73.0, 69.2, 52.0, 47.8, 31.6, 28.2, 15.7, 14.6 ppm. (Fig. S31) DEPT-135 (100.6 MHz, CDCl₃) δ 131.3, 129.7, 129.7, 129.6, 129.5, 129.1, 128.7, 127.9, 122.3, 120.6, 115.1, 114.4, 111.6, 73.0, 69.3, 52.0, 47.9, 31.7, 28.2, 15.7, 14.6 ppm. (Fig. S32) FT-IR (KBr) u_{max} = 3296.88 (-OH), 1597.47 (C=O), 1485.91 (C=C) cm⁻¹. (Fig. S33) SC-XRD: CCDC (Fig. S67), ¹³C-¹H (Fig. S35), ¹H-¹H COSY (Fig. S36), and HMBC (Fig. S37) HRMS (ESI): Calcd for C₃₂H₂₉N₃O₂S₂ (M+H)⁺ <i>m/z</i> = 551.1701; Found 552.1733. (Fig. S34)</p>
 <p style="text-align: center;">6h</p>	<p>Nature: Dark yellow solid Yield: 84% R_f (15% EtOAc-Hexane): 0.30 Mp: 280-283 °C ¹H NMR (400 MHz, CDCl₃) δ 8.37 – 8.27 (m, 1H), 8.15 – 8.11 (m, 2H), 7.77 – 7.73 (m, 2H), 7.71 – 7.65 (m, 1H), 7.55 (td, <i>J</i> = 7.5, 1.3 Hz, 1H), 7.51 (dd, <i>J</i> = 7.4, 0.9 Hz, 1H), 7.49 – 7.44 (m, 4H), 4.63 (d, <i>J</i> = 11.8 Hz, 1H), 4.58 (s, 1H), 4.33 (dt, <i>J</i> = 9.1, 7.1 Hz, 1H), 4.05 (dd, <i>J</i> = 11.8, 9.4 Hz, 1H), 2.72 – 2.55 (m, 1H), 2.53 – 2.49 (m, 1H), 2.11 (s, 3H), 2.05 – 1.86 (m, 3H), 1.79 (dq, <i>J</i> = 11.8, 7.7 Hz, 1H), 1.13 (s, 3H) ppm. (Fig. S38) ¹³C NMR (100.6 MHz, CDCl₃) δ 188.4, 164.9, 164.6, 153.6, 144.1, 142.8, 142.25, 139.8, 137.4, 131.6, 131.3, 130.6, 130.2, 130.0, 129.8, 129.5, 129.0, 128.9, 127.8, 122.2, 120.5, 111.4, 75.8, 72.8, 69.6, 51.2, 47.7, 31.6, 28.1, 15.5, 14.6 ppm. (Fig. S39) DEPT-135 (100.6 MHz, CDCl₃) δ 131.7, 131.3, 131.1, 130.6, 130.3, 130.1, 129.8, 129.6, 129.0, 128.9, 127.9, 122.2, 113.5, 111.5, 72.9, 69.6, 51.3, 47.7, 31.6, 28.2, 15.6, 14.6 ppm. (Fig. S40) FT-IR (KBr) u_{max} = 1641.58 (C=O), 1488.51 (C=C), 756.85 (-Br) cm⁻¹. (Fig. S41) HRMS (ESI): Calcd for C₃₂H₂₈BrN₃OS₂ (M+H)⁺ <i>m/z</i> = 613.0857; Found 614.0939. (Fig. S42)</p>
 <p style="text-align: center;">6i</p>	<p>Nature: Sandal yellow solid Yield: 76% R_f (30% EtOAc-Hexane): 0.38 Mp: 269-270 °C ¹H NMR (400 MHz, CDCl₃) δ 8.34 – 8.31 (m, 1H), 8.13 – 8.12 (m, 1H), 7.76 – 7.72 (m, 3H), 7.69 (s, 1H), 7.55 (dd, <i>J</i> = 5.3, 2.2 Hz, 2H), 7.49 (d, <i>J</i> = 1.0 Hz, 1H), 6.82 (ddd, <i>J</i> = 10.2, 8.3, 4.6 Hz, 3H), 4.82 (s, 1H), 4.64 (s, 1H), 4.33 (d, <i>J</i> = 9.5 Hz, 1H), 4.27 – 4.23 (m, 1H), 2.53 – 2.49 (m, 2H), 2.09 (s, 3H), 1.91 (d, <i>J</i> = 5.0 Hz, 2H), 1.15 (s, 3H) ppm. (Fig. S43) ¹³C NMR (100.6 MHz, CDCl₃) δ 188.36, 164.90, 164.70, 153.73, 144.11, 142.86, 142.30, 137.48, 131.44, 129.88, 129.82, 129.73, 129.61, 129.01, 128.93, 127.79, 122.23, 111.53, 111.29, 111.21, 104.36, 104.11, 103.84, 75.67, 72.00, 67.59, 47.65, 44.49, 31.65, 28.19, 15.58, 14.59 ppm. (Fig. S44) DEPT-135 (100.6 MHz, CDCl₃) δ 131.4, 129.9, 129.8, 129.7, 129.6, 129.0, 128.9, 127.8, 122.2, 111.5, 111.3, 111.2, 104.4, 104.1, 103.8, 72.0, 67.6, 47.6, 44.5, 31.7, 28.2, 15.6, 14.6 ppm. (Fig. S45) HRMS (ESI): Calcd for C₃₂H₂₇F₂N₃OS₂ (M+H)⁺ <i>m/z</i> = 571.1564; Found 572.1599. (Fig. S46)</p>

 <p style="text-align: center;">6j</p>	<p>Nature: Mild brown solid Yield: 78% R_f (30% EtOAc-Hexane): 0.40 Mp: 276-278 °C ¹H NMR (400 MHz, CDCl₃) δ 8.35 – 8.28 (m, 1H), 8.13 (d, <i>J</i> = 7.1 Hz, 2H), 7.78 – 7.72 (m, 2H), 7.69 (d, <i>J</i> = 7.6 Hz, 1H), 7.58 – 7.52 (m, 3H), 7.52 – 7.47 (m, 1H), 7.02 (t, <i>J</i> = 8.7 Hz, 2H), 4.63 (d, <i>J</i> = 11.8 Hz, 1H), 4.59 (s, 1H), 4.39 – 4.29 (m, 1H), 4.07 (dd, <i>J</i> = 11.8, 9.4 Hz, 1H), 2.61 – 2.45 (m, 3H), 2.11 (s, 3H), 2.01 – 1.87 (m, 3H), 1.79 (dd, <i>J</i> = 8.3, 3.7 Hz, 1H), 1.13 (s, 3H). (Fig. S47) ¹³C NMR (100.6 MHz, CDCl₃) δ 188.65, 165.08, 164.46, 153.69, 144.20, 142.83, 142.27, 137.40, 136.47, 136.44, 131.30, 129.83, 129.80, 129.73, 129.66, 129.55, 129.00, 128.92, 127.93, 122.18, 115.48, 115.27, 111.63, 75.88, 73.03, 69.83, 51.02, 47.74, 31.65, 28.19, 15.57, 14.61 ppm. (Fig. S48) DEPT-135 (100.6 MHz, CDCl₃) δ 131.3, 129.8, 129.8, 129.7, 129.7, 129.6, 129.0, 128.9, 127.9, 122.2, 115.5, 115.3, 111.6, 73.0, 69.8, 51.0, 47.7, 31.6, 28.2, 15.6, 14.6 ppm. (Fig. S49) FT-IR (KBr) u_{max} = 1643.58 (C=O), 1494.14 (C=C), 756.25 (-F) cm⁻¹. (Fig. S50) HRMS (ESI): Calcd for C₃₂H₂₈FN₃OS₂ (M+H)⁺ <i>m/z</i> = 553.7144; Found 554.1945. (Fig. S51)</p>
 <p style="text-align: center;">6k</p>	<p>Nature: Brown solid Yield: 80% R_f (30% EtOAc-Hexane): 0.35 Mp: 260-270 °C ¹H NMR (400 MHz, CDCl₃) δ 8.38 – 8.29 (m, 1H), 8.13 (d, <i>J</i> = 7.2 Hz, 1H), 8.06 – 7.98 (m, 1H), 7.85 – 7.70 (m, 3H), 7.60 (d, <i>J</i> = 15.9 Hz, 1H), 7.50 (dd, <i>J</i> = 8.3, 2.5 Hz, 2H), 7.23 (d, <i>J</i> = 8.2 Hz, 1H), 7.19 (d, <i>J</i> = 8.1 Hz, 1H), 6.79 (d, <i>J</i> = 15.8 Hz, 1H), 2.91 (ddd, <i>J</i> = 20.7, 13.8, 7.3 Hz, 1H), 2.51 (d, <i>J</i> = 3.3 Hz, 3H), 2.25 – 2.04 (m, 3H), 1.98 – 1.74 (m, 4H), 1.22 (s, 3H), 1.13 (s, 2H). ppm. (Fig. S52) ¹³C NMR (100.6 MHz, CDCl₃) δ 189.0, 165.1, 153.7, 151.2, 147.1, 144.4, 142.8, 141.3, 138.1, 137.4, 128.9, 128.3, 128.2, 128.0, 127.0, 126.6, 126.4, 122.1, 121.4, 113.4, 111.9, 76.1, 73.1, 69.9, 61.1, 51.4, 47.8, 34.1, 33.7, 23.8, 17.3, 15.1 ppm. (Fig. S53) DEPT-135 (100.6 MHz, CDCl₃) δ 141.3, 128.9, 128.3, 128.2, 128.0, 127.0, 126.6, 126.4, 122.1, 121.4, 113.4, 111.9, 73.1, 69.9, 51.4, 47.8, 34.1, 33.7, 31.8, 28.2, 23.8, 17.3, 15.1, 14.6 ppm. (Fig. S54) FT-IR (KBr) u_{max} = 1587.54 (C=O), 1475.46 (C=C), 1123.20 (=C-H) cm⁻¹. (Fig. S55) HRMS (ESI): Calcd for C₃₄H₃₃N₃O₂S₂ (M+H)⁺ <i>m/z</i> = 579.2014; Found 580.2083. (Fig. S56)</p>

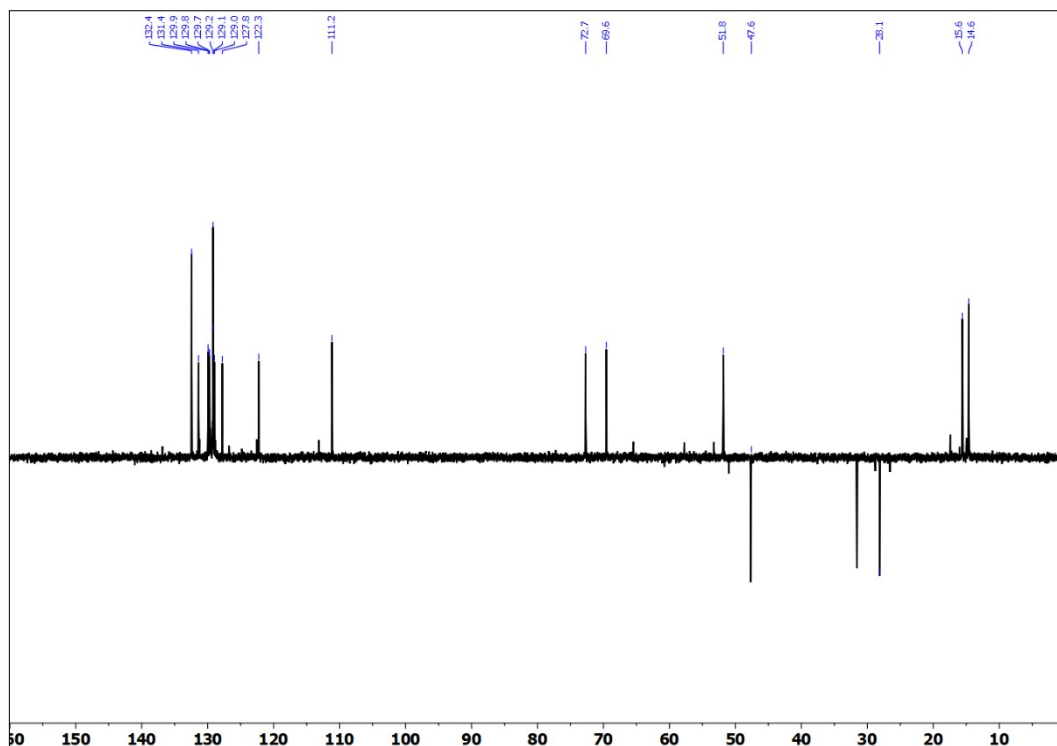


Fig S3: DEPT-135 NMR Spectrum of compound 6a

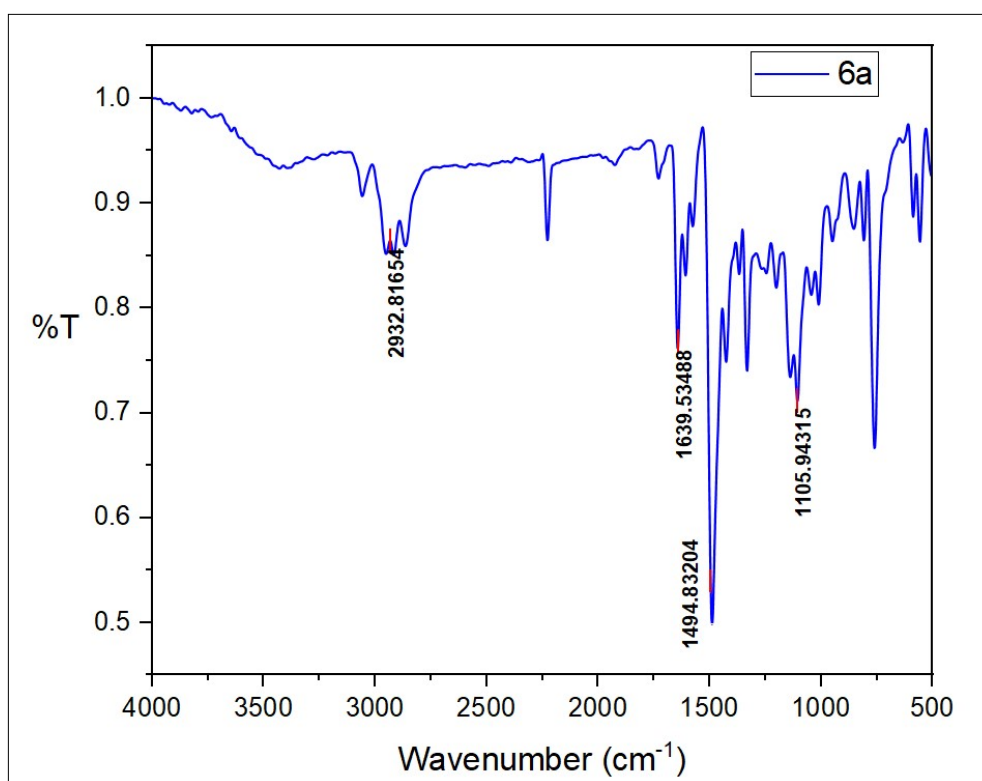


Fig S4: FT-IR Spectrum of compound 6a

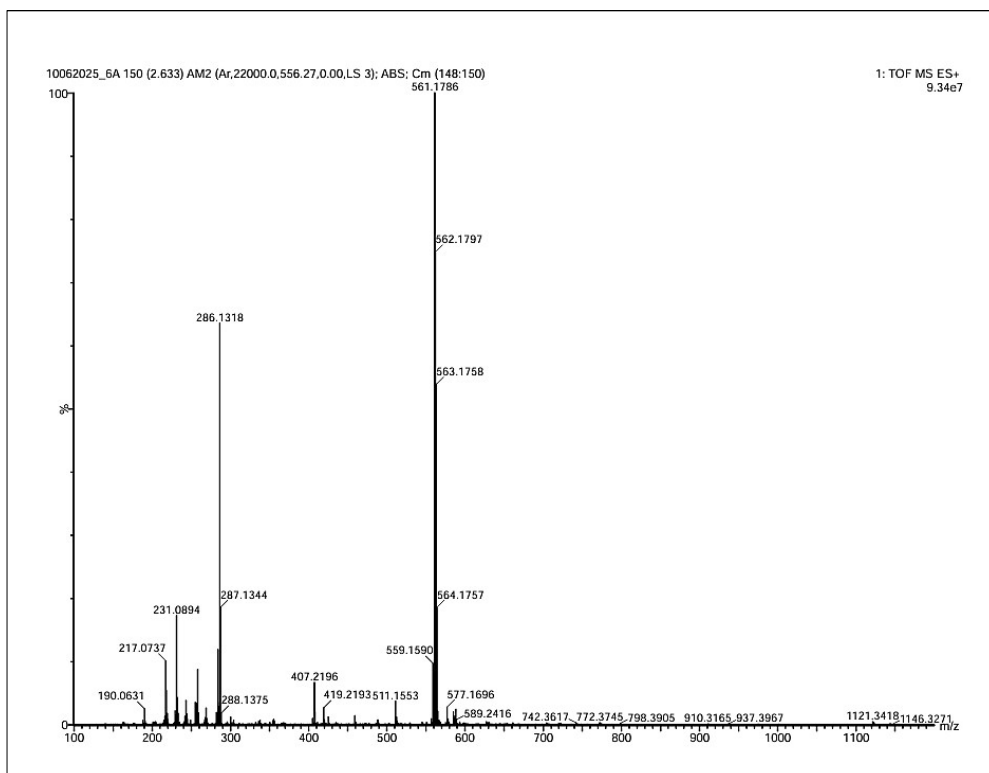
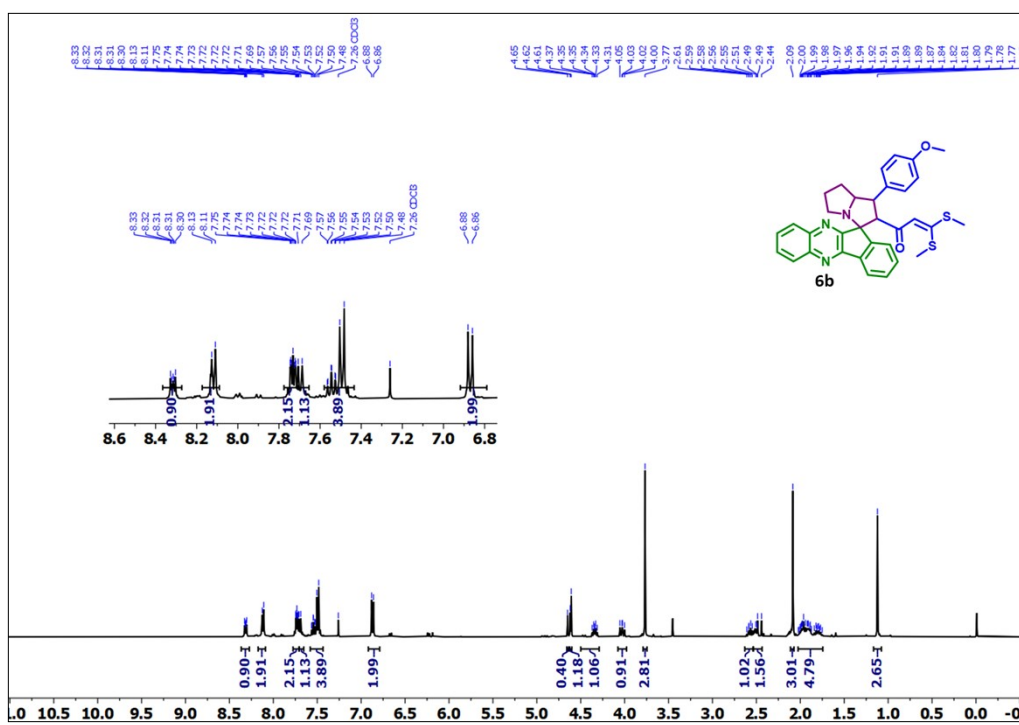


Fig S5: HRMS Spectrum of compound 6a



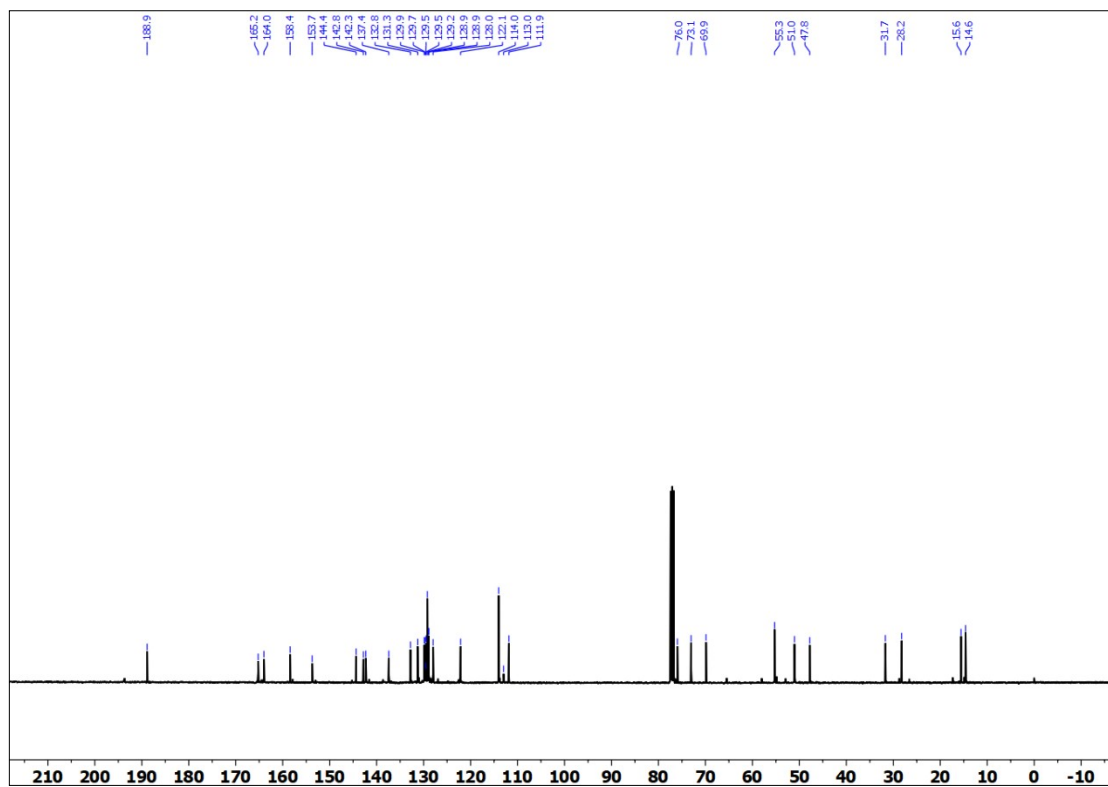


Fig S7: ¹³C NMR Spectrum of compound **6b**

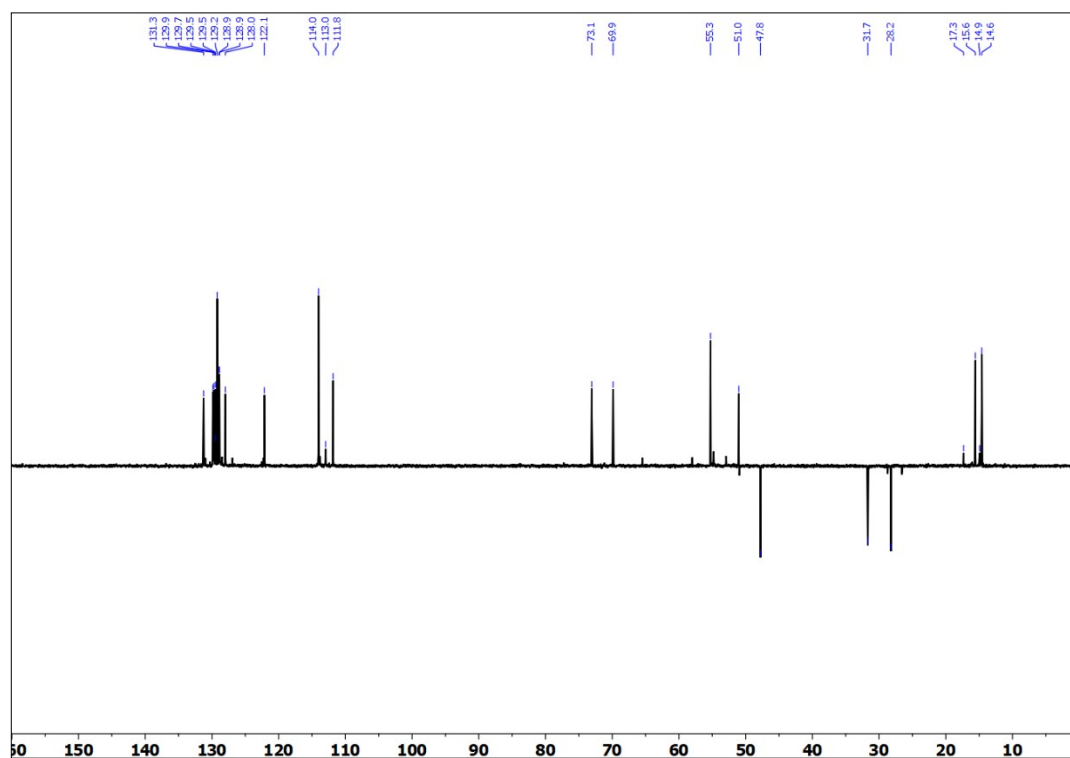


Fig S8: DEPT-135 NMR Spectrum of compound **6b**

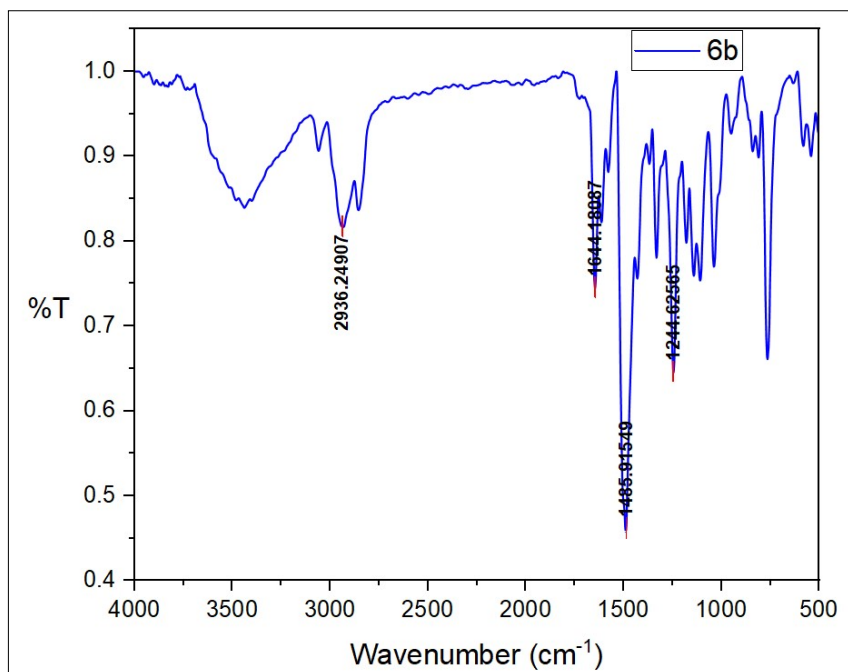


Fig S9: FT-IR Spectrum of compound 6b

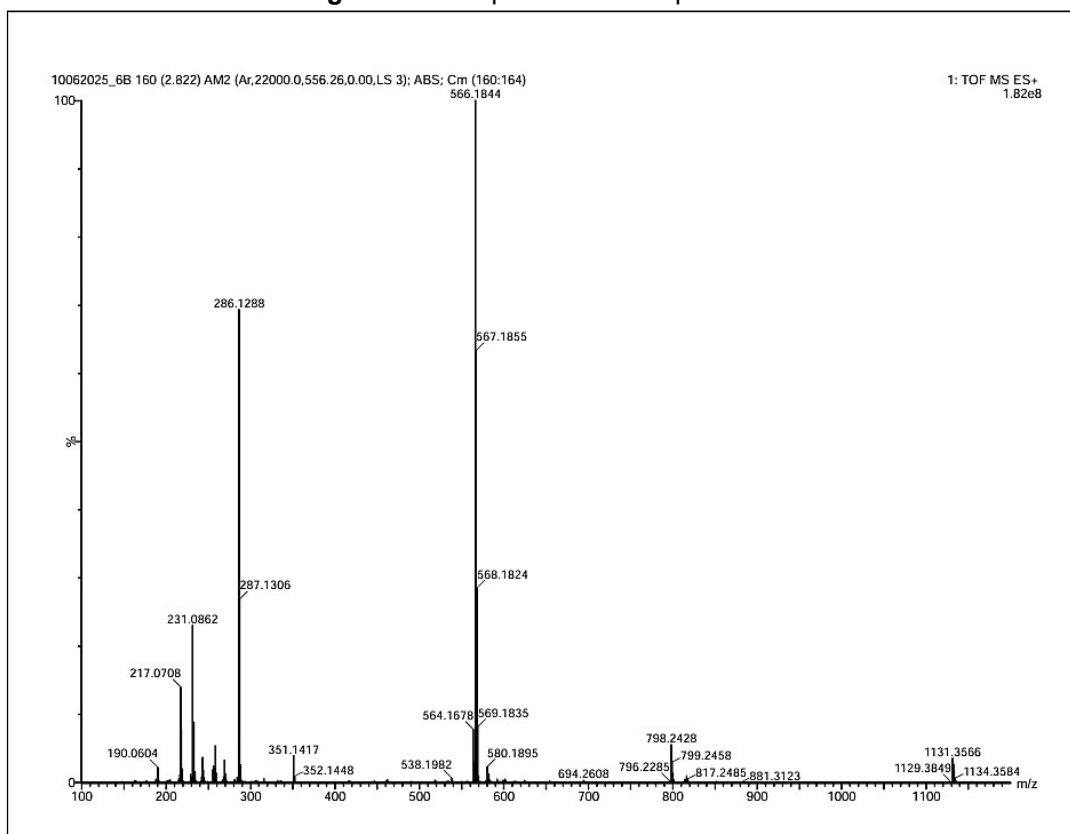
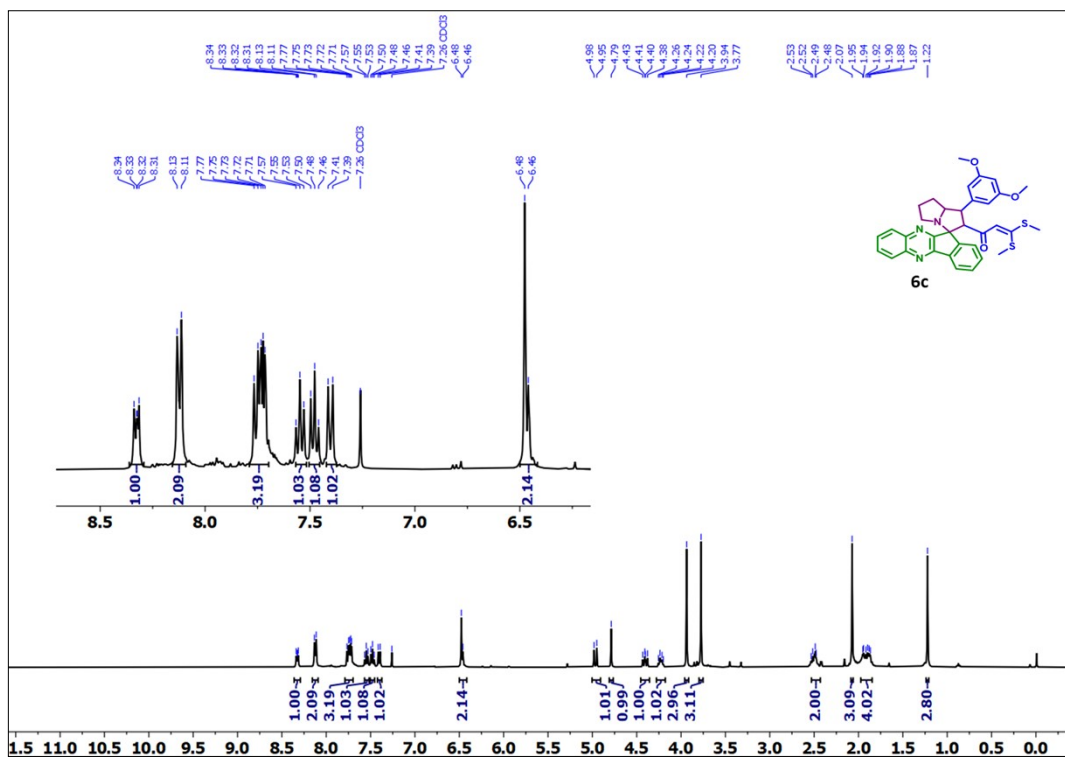
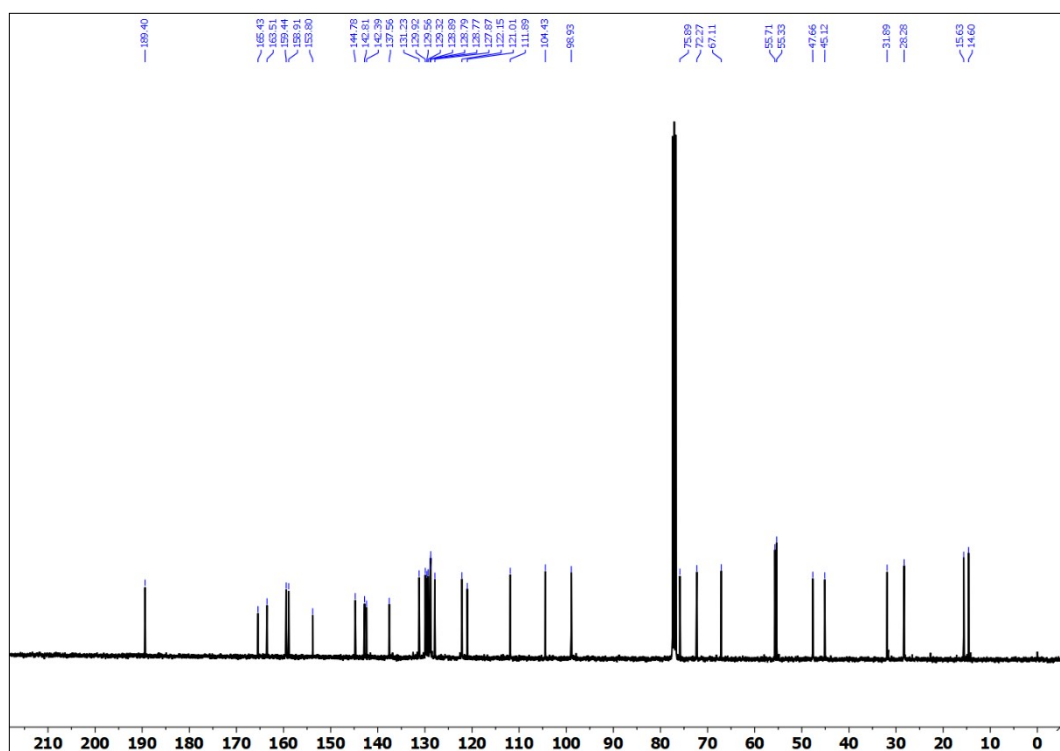


Fig S10: HRMS Spectrum of compound 6b

**Fig S11: ¹H NMR Spectrum of compound 6c****Fig S12: ¹³C NMR Spectrum of compound 6c**

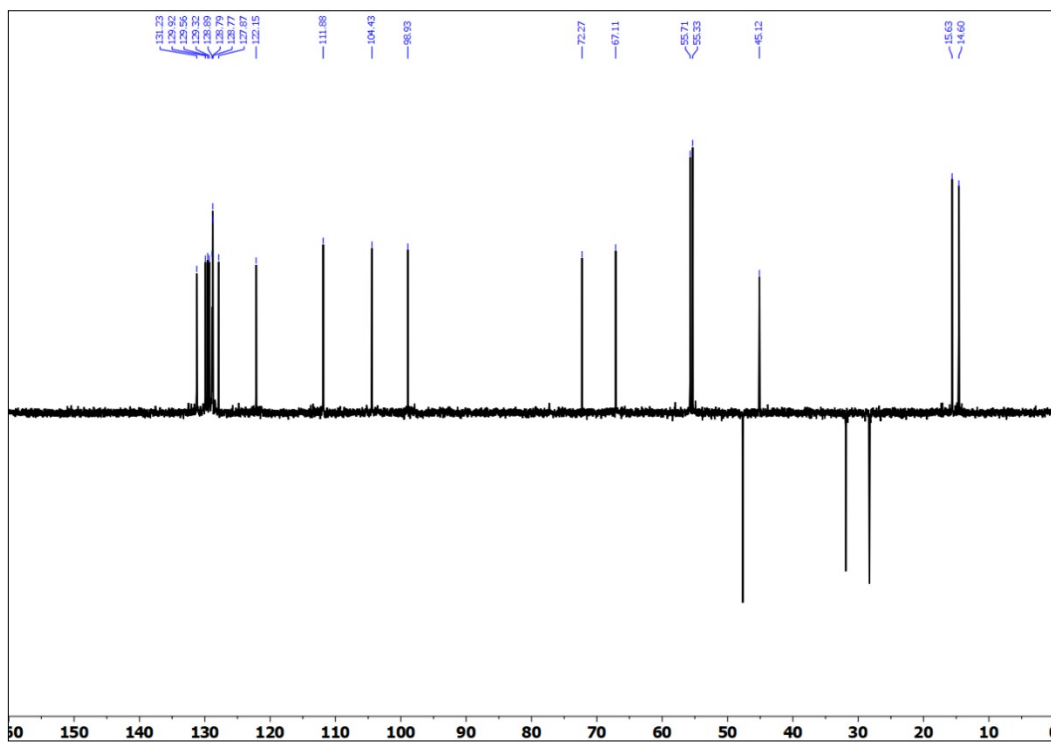


Fig S13: DEPT-135 NMR Spectrum of compound 6c

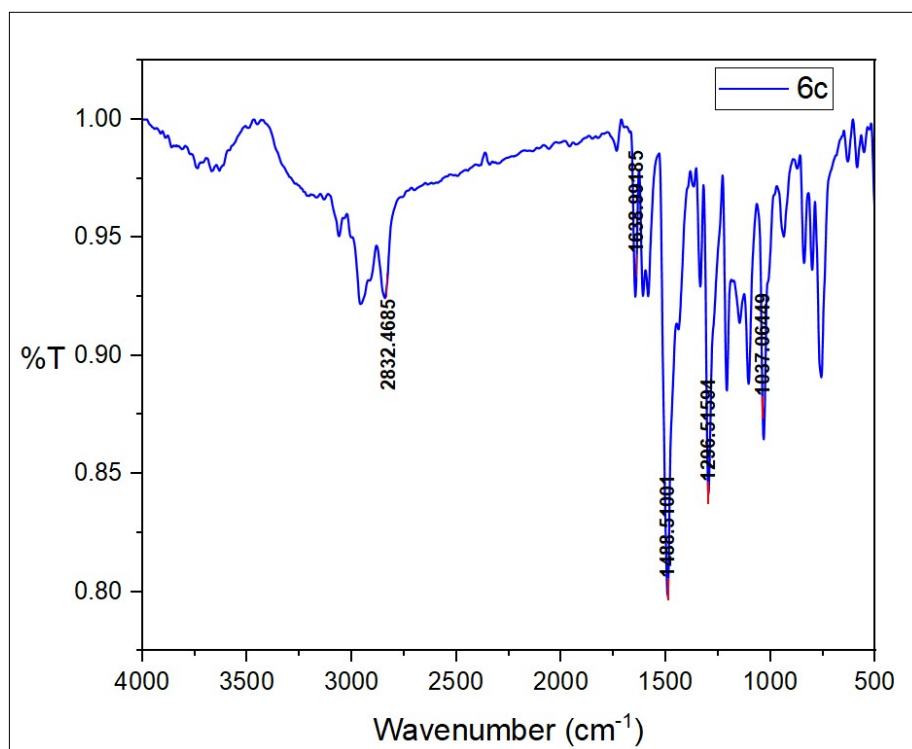


Fig S14: FT-IR Spectrum of compound 6c

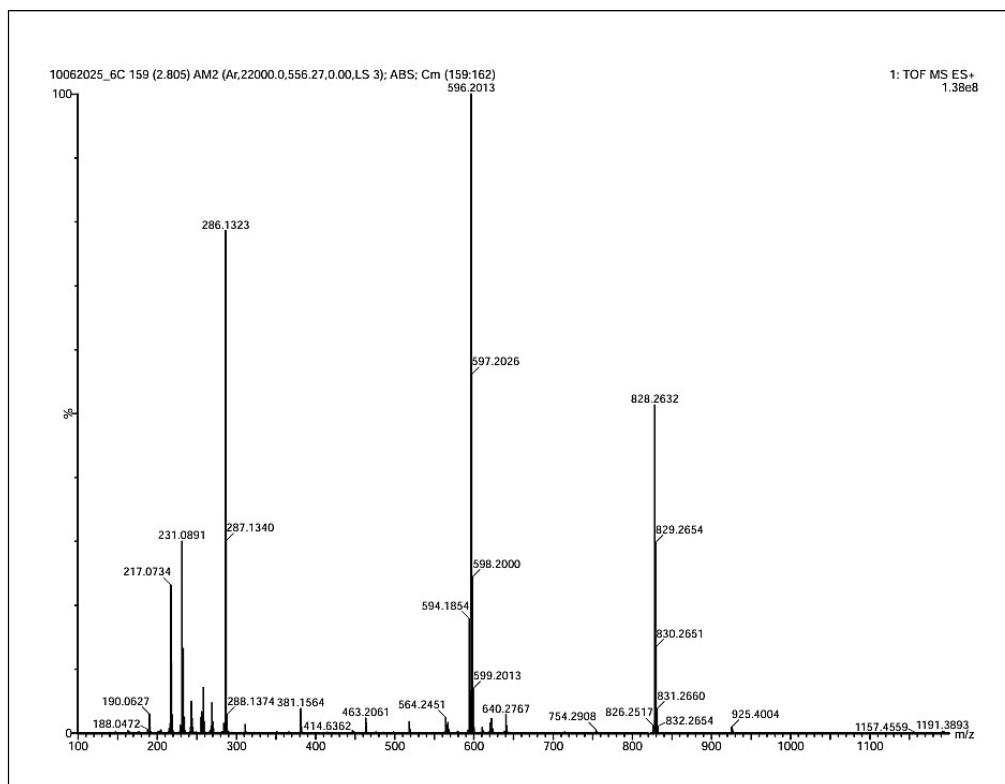
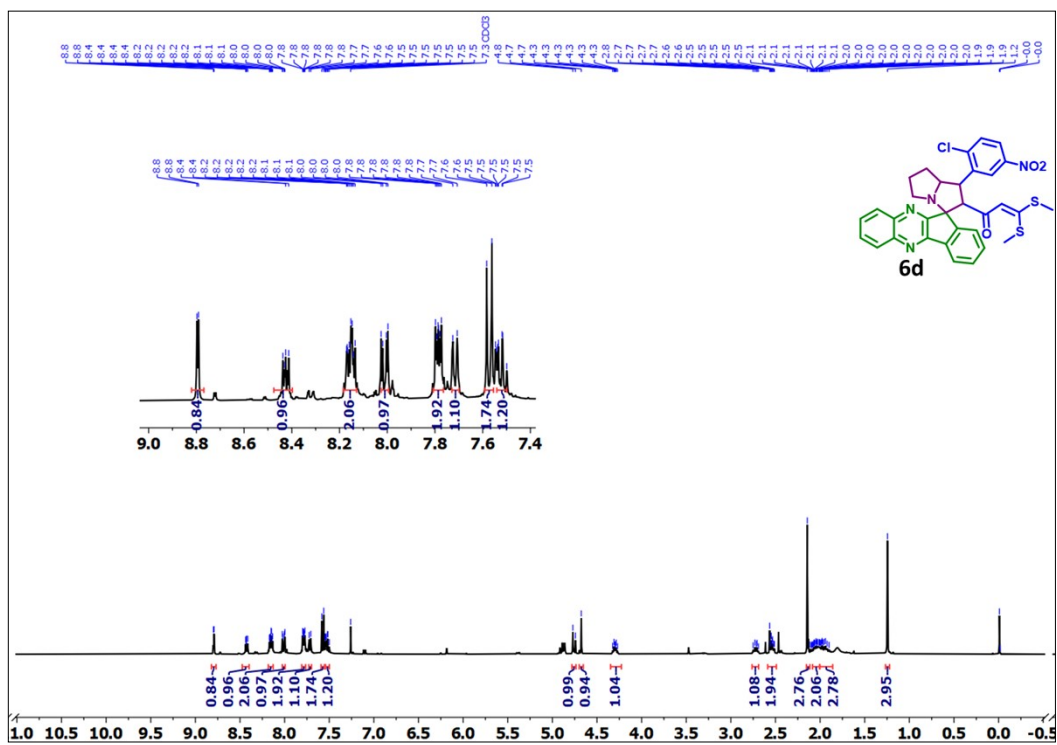


Fig S15: HRMS Spectrum of compound 6c

Fig S16: ¹H NMR Spectrum of compound 6d

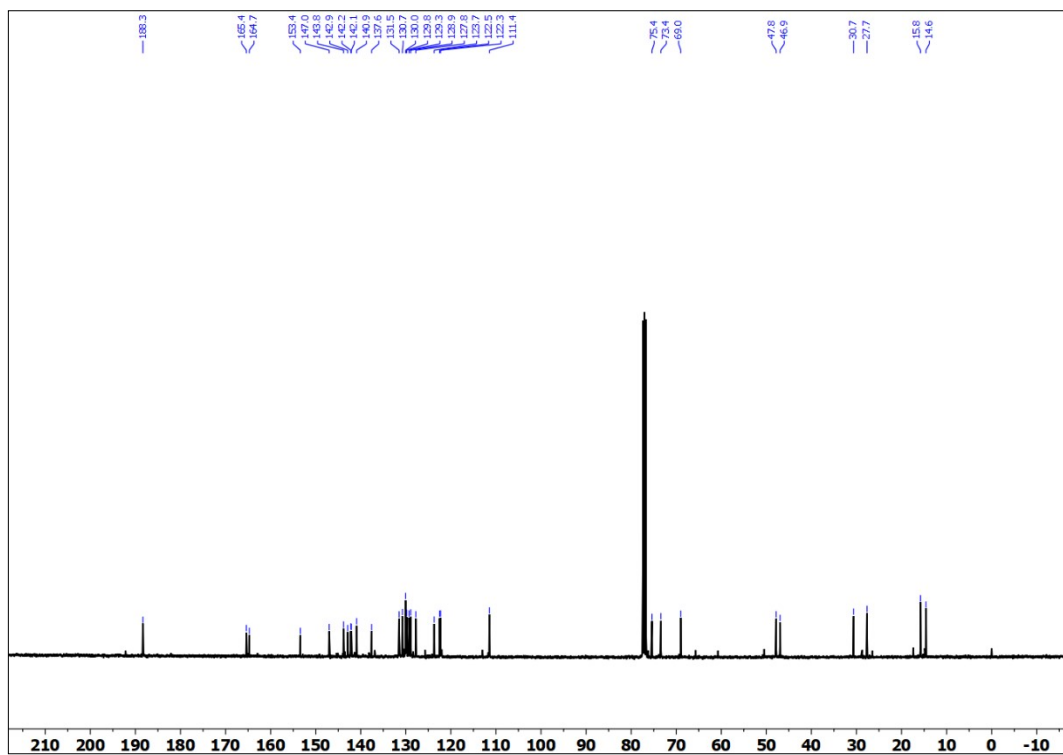
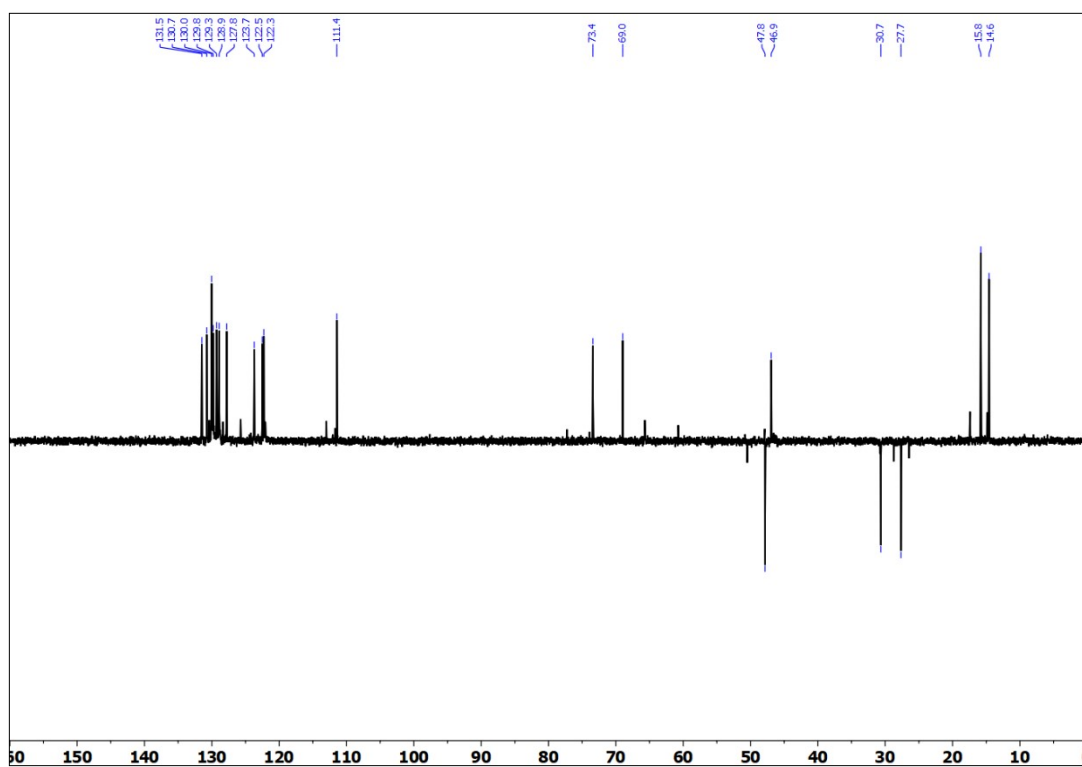
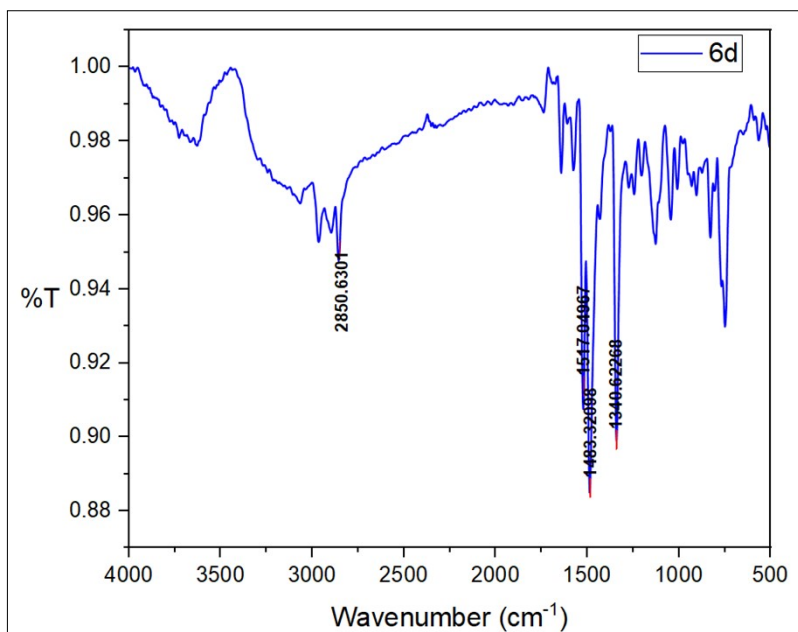
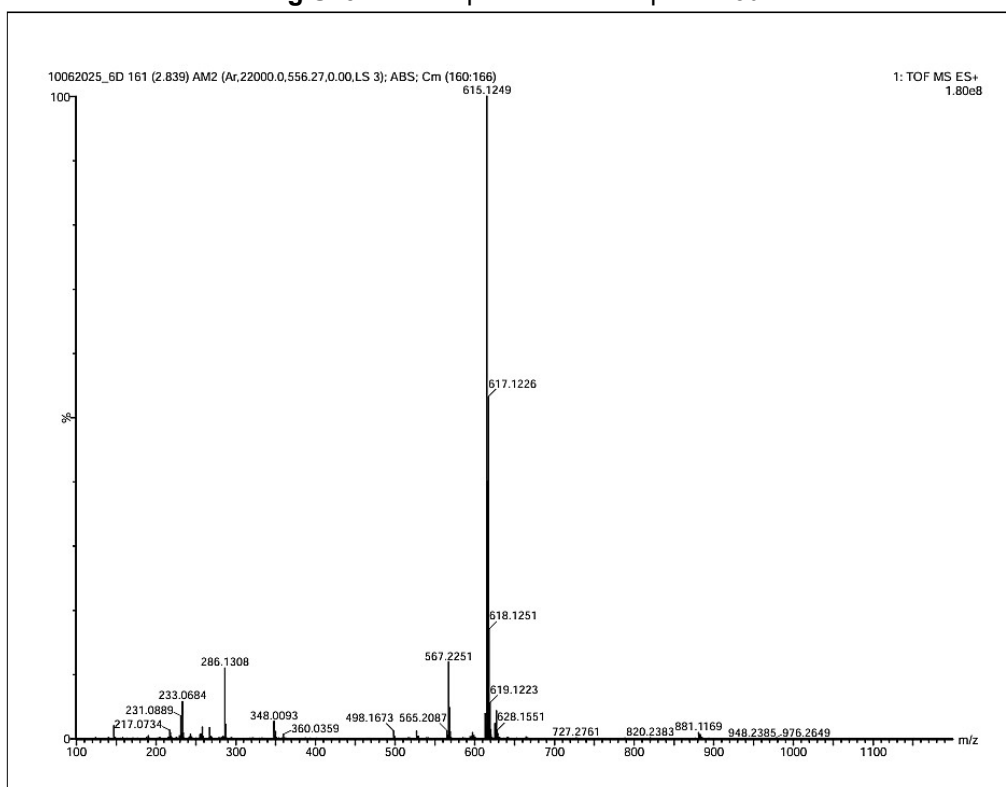
Fig S17: ^{13}C NMR Spectrum of compound 6d

Fig S18: DEPT-135 NMR Spectrum of compound 6d

**Fig S19: FT-IR Spectrum of compound 6d****Fig S20: HRMS Spectrum of compound 6d**

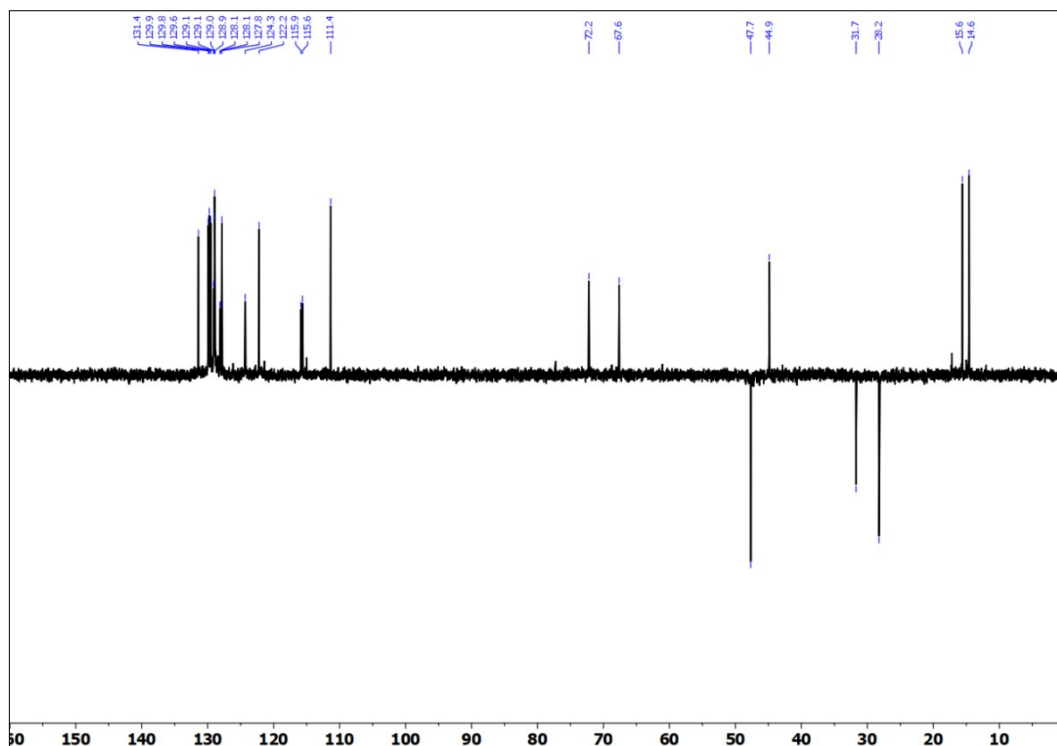


Fig S23: DEPT-135 NMR Spectrum of compound 6e

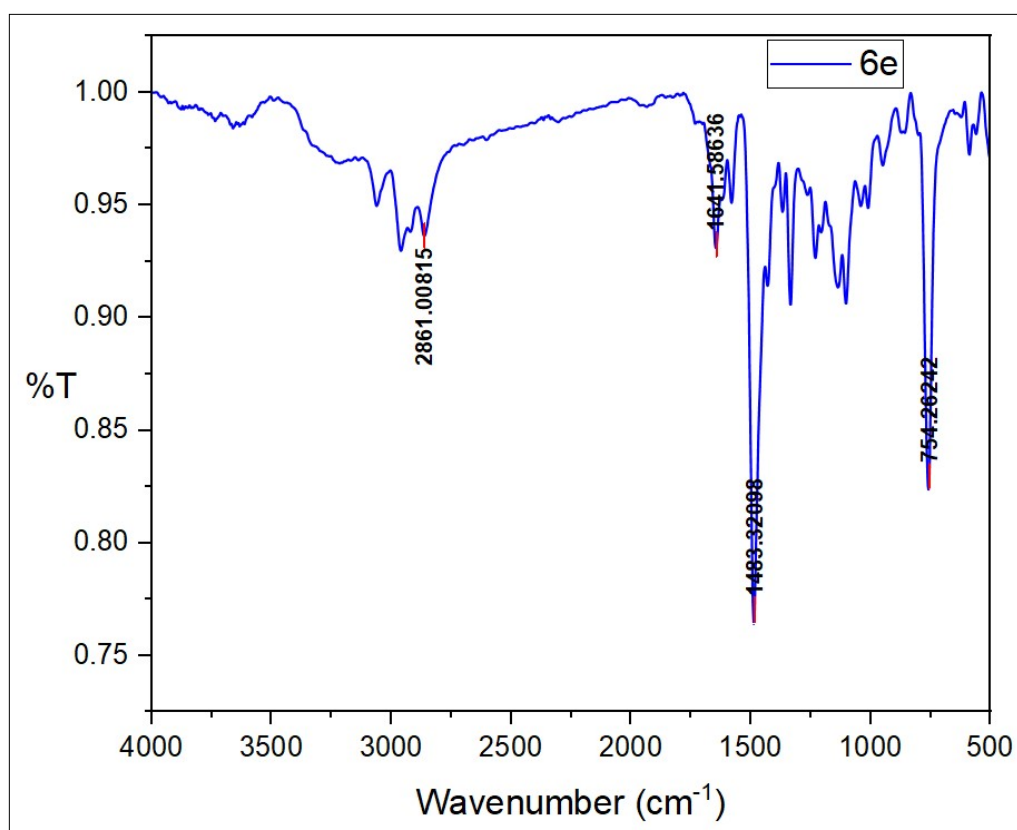
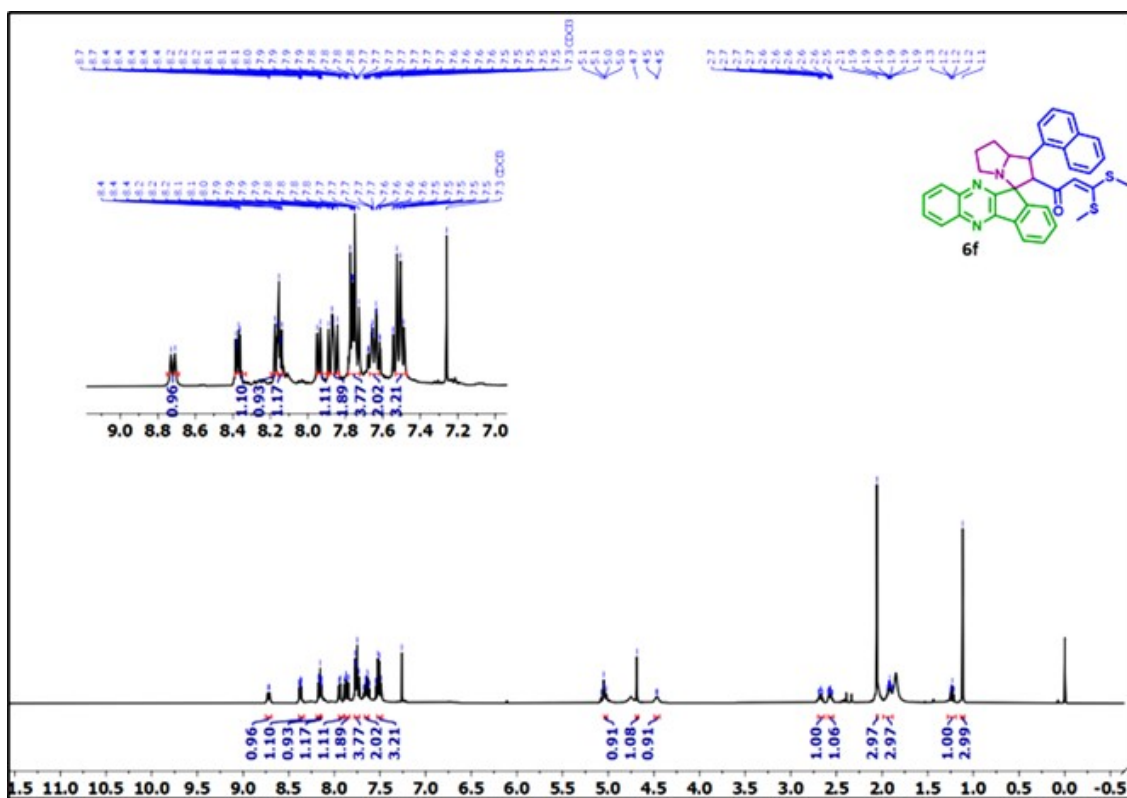
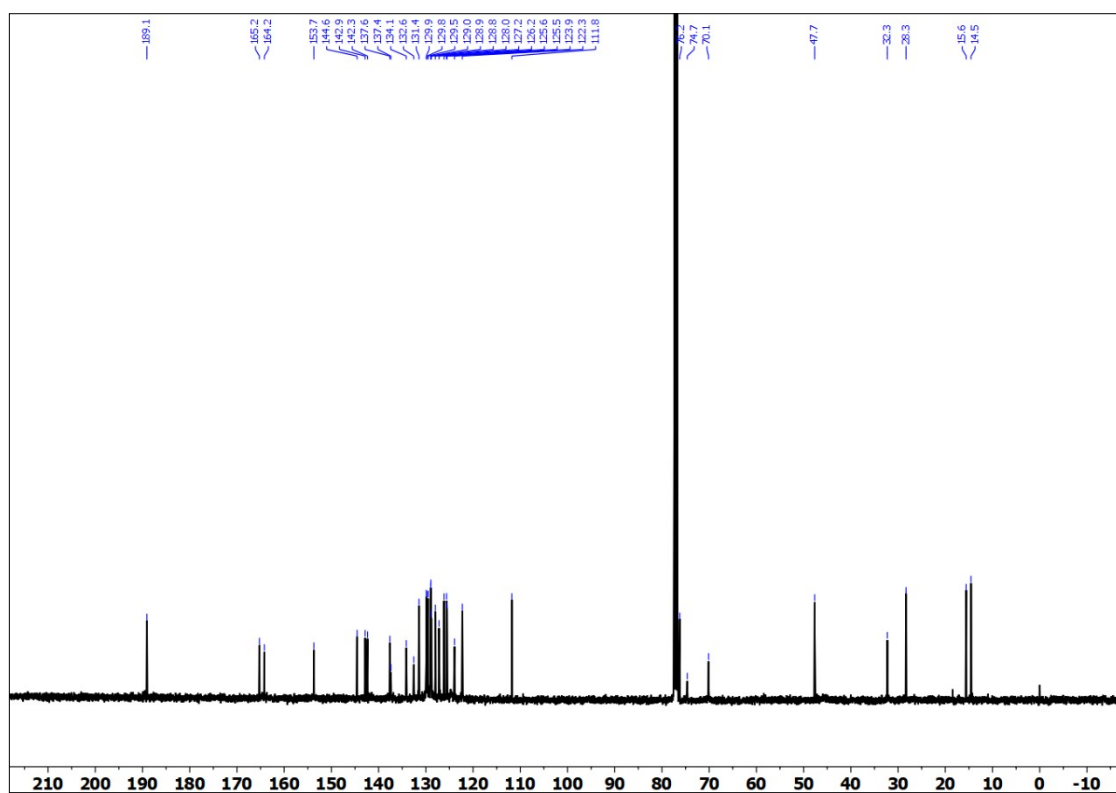


Fig S24: FT-IR Spectrum of compound 6e

Fig S25: ¹H NMR Spectrum of compound **6f**Fig S26: ¹³C NMR Spectrum of compound **6f**

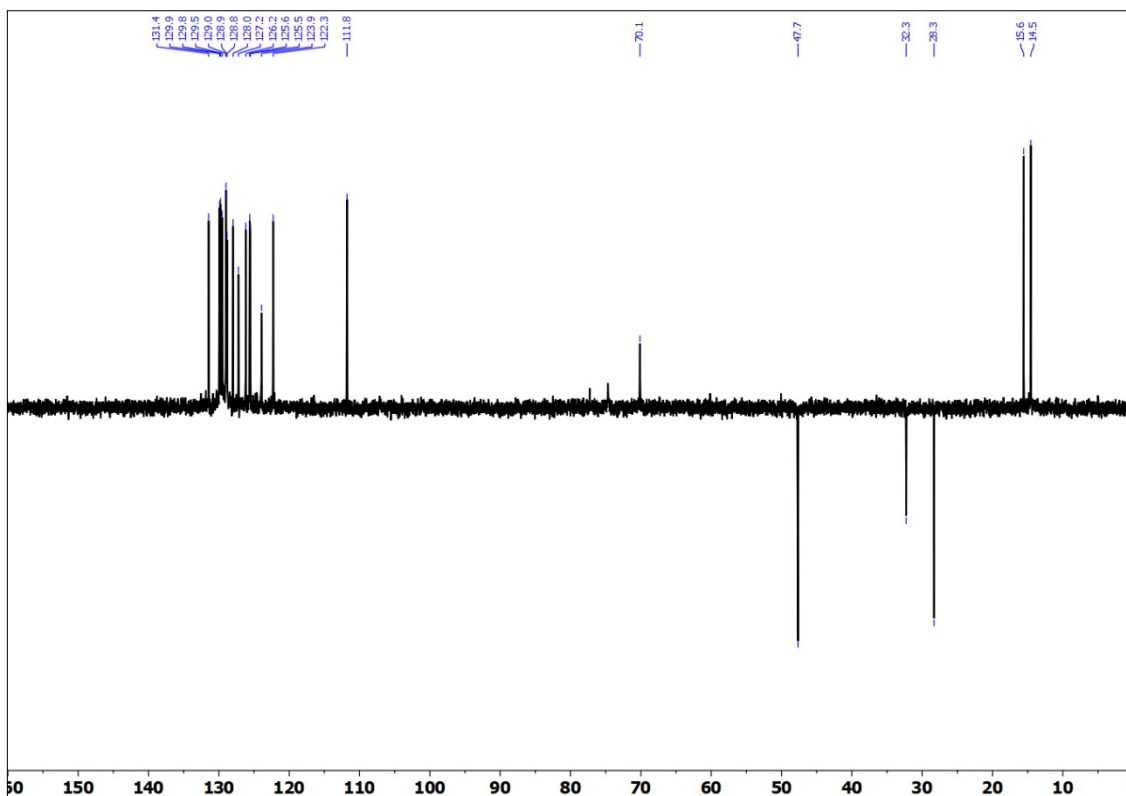


Fig S27: DEPT-135 NMR Spectrum of compound 6f

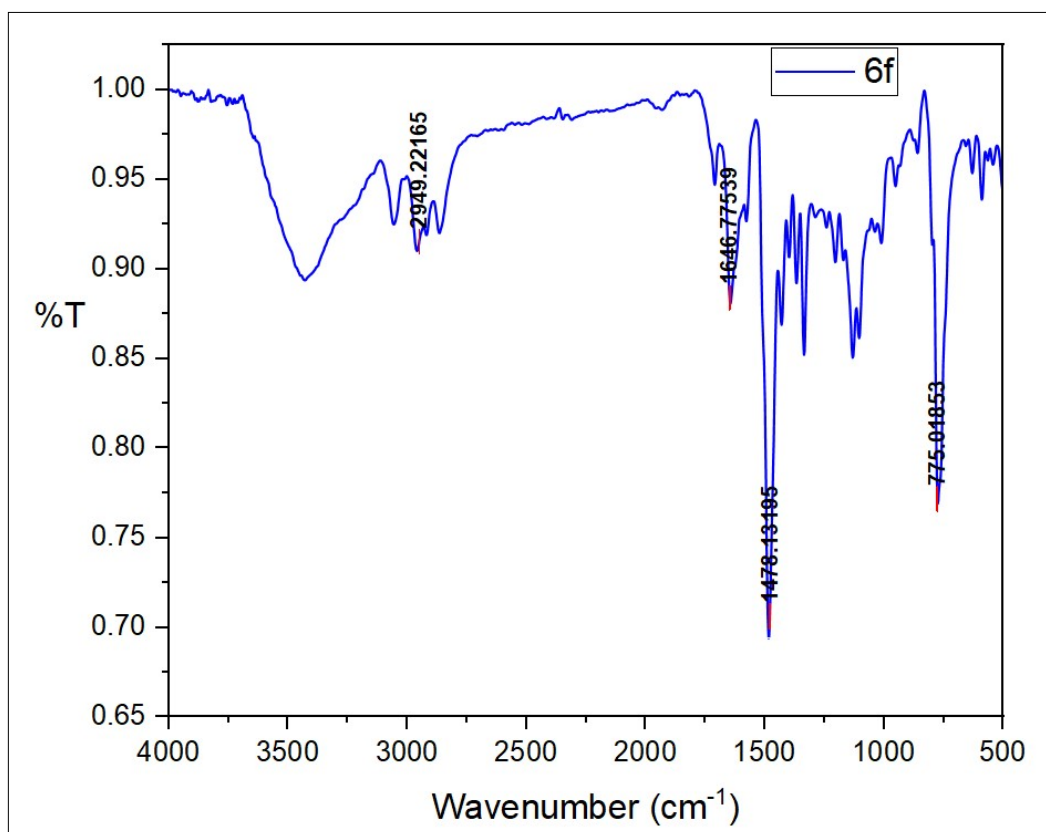
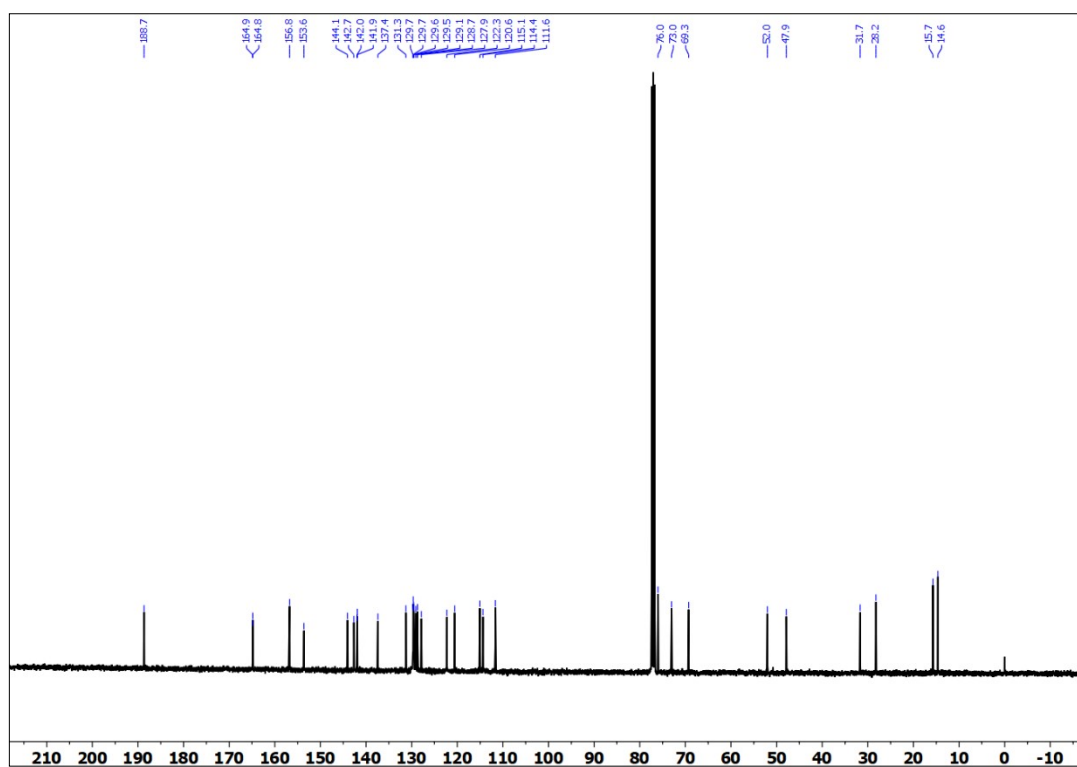
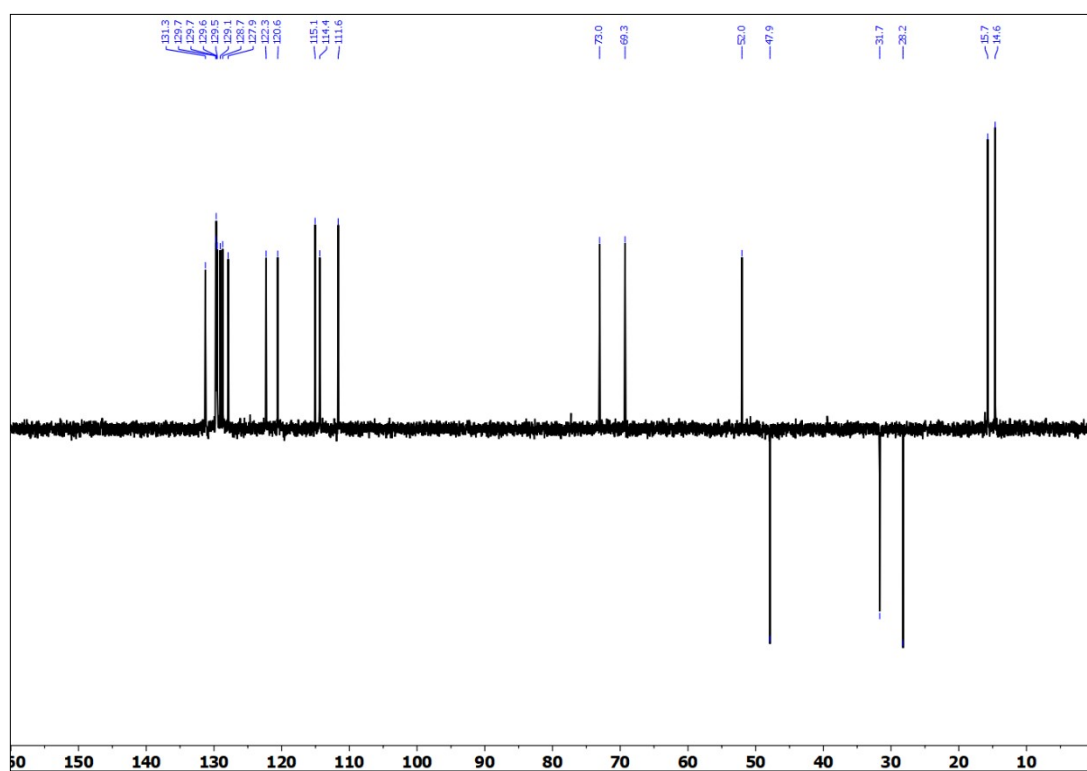


Fig S28: FT-IR Spectrum of compound 6f

Fig S31: ¹³C NMR Spectrum of compound **6g**Fig S32: DEPT-135 NMR Spectrum of compound **6g**

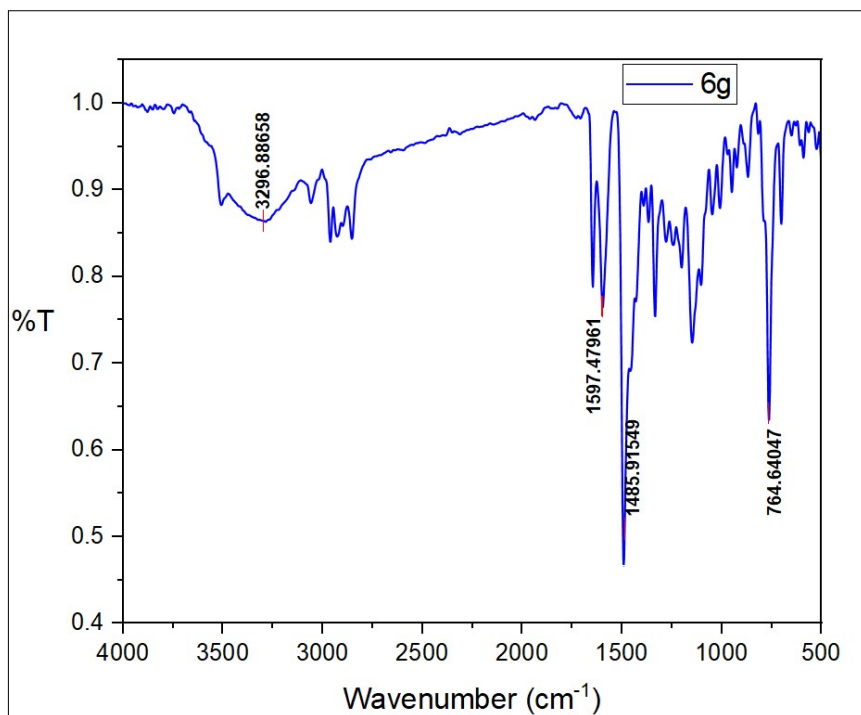


Fig S33: FT-IR Spectrum of compound 6g

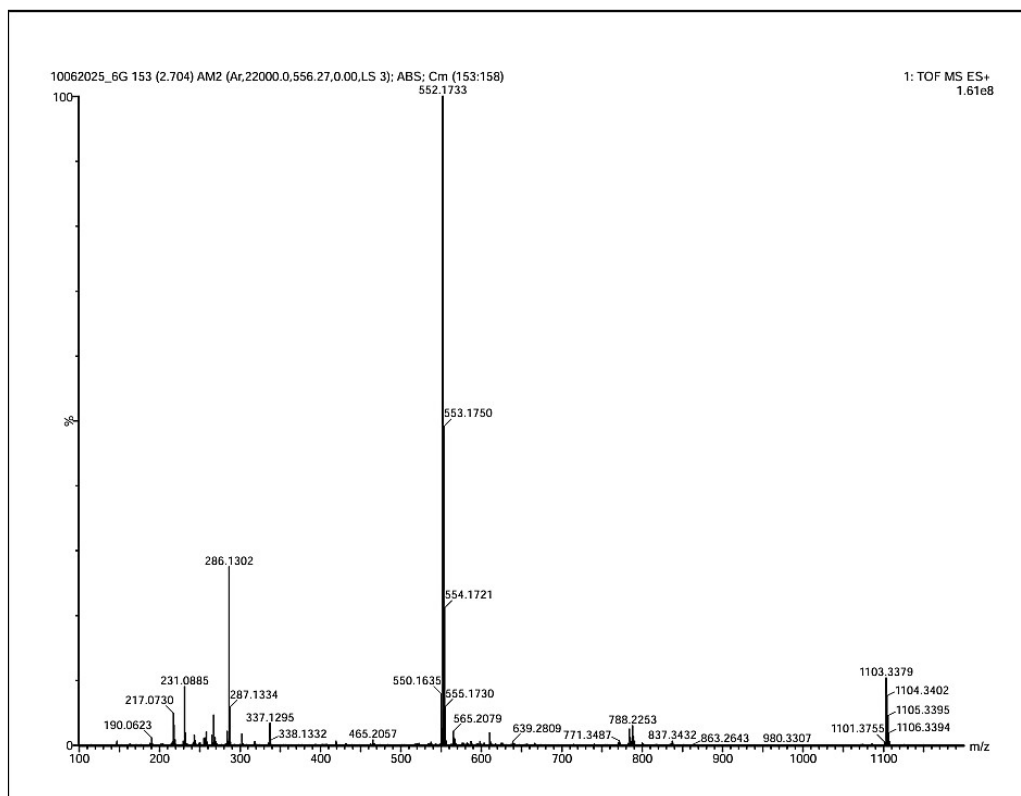
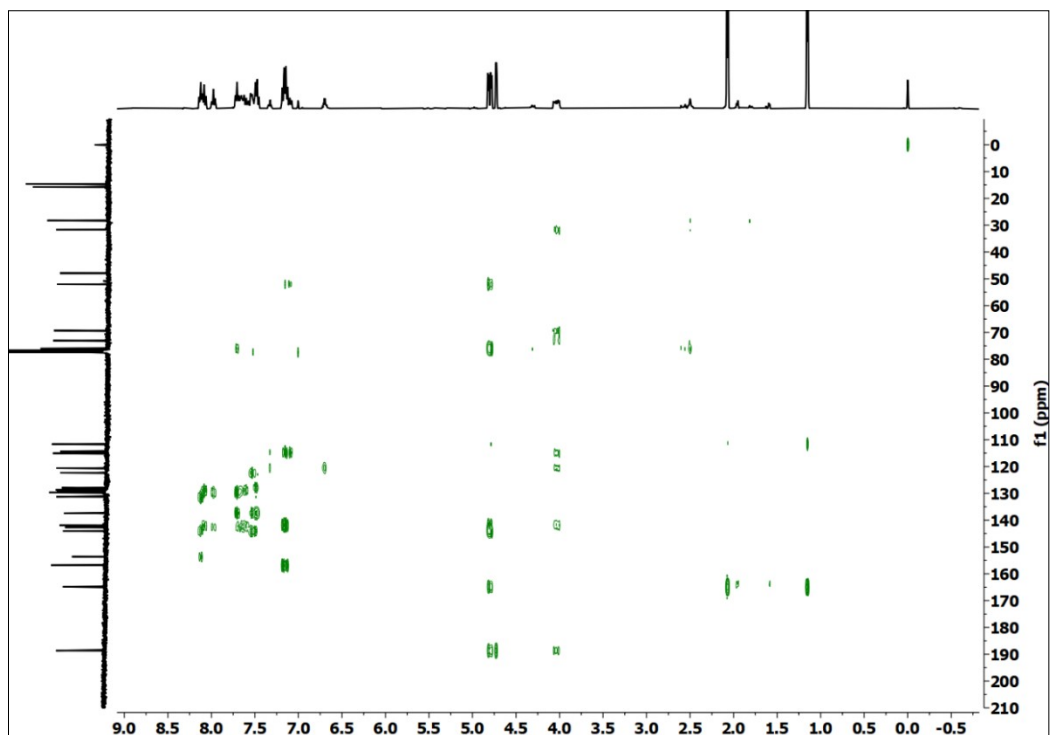
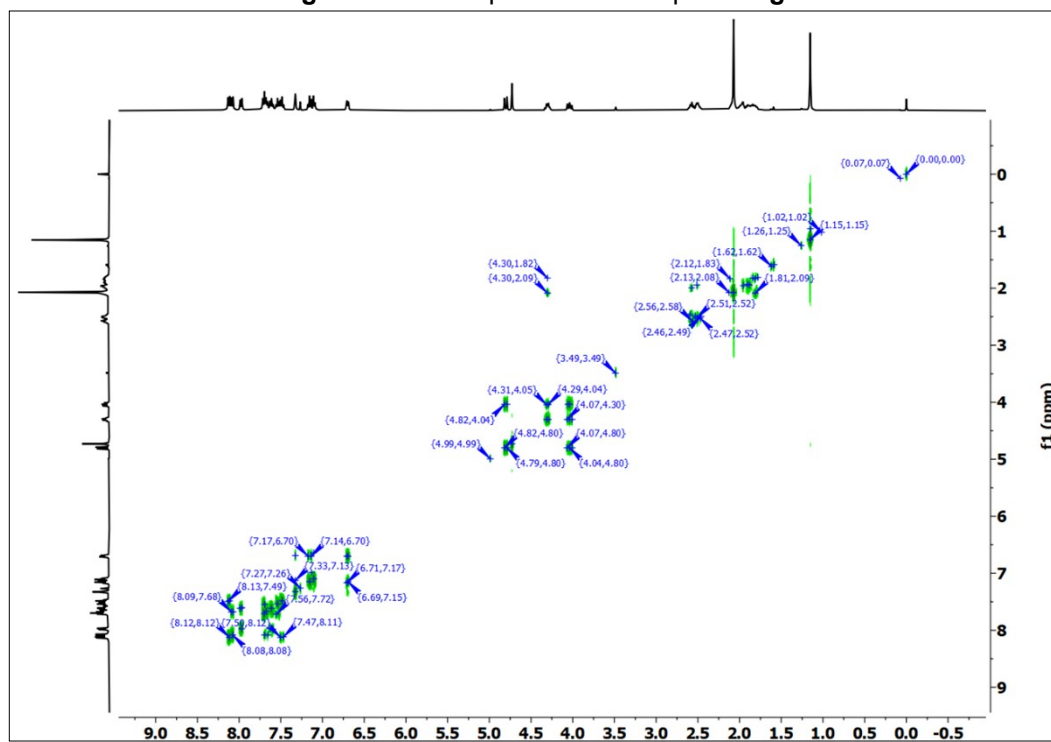


Fig S34: HRMS Spectrum of compound 6g

Fig S35: ^{13}C - ^1H Spectrum of compound 6gFig S36: ^1H - ^1H Spectrum of compound 6g

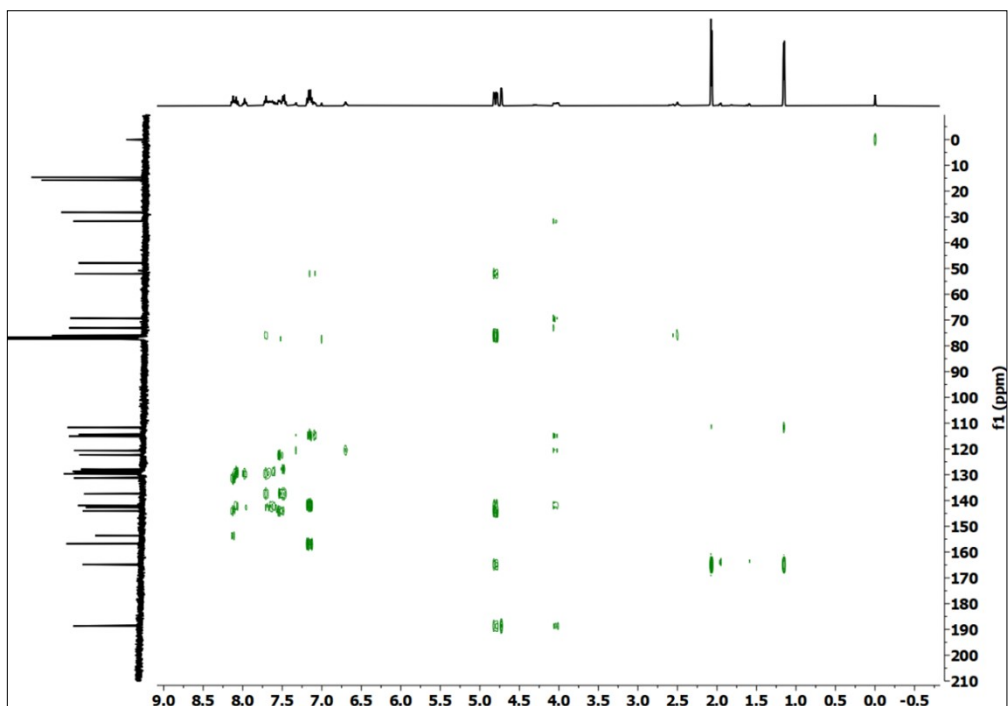
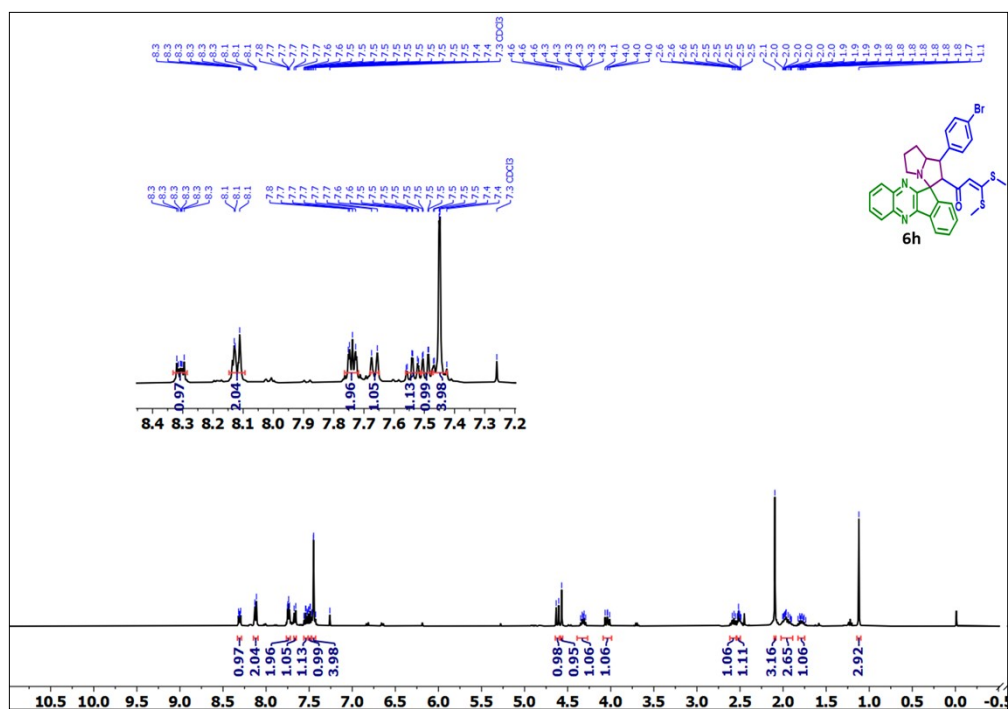


Fig S37: HMBC Spectrum of compound 6g

Fig S38: ^1H NMR Spectrum of compound 6h

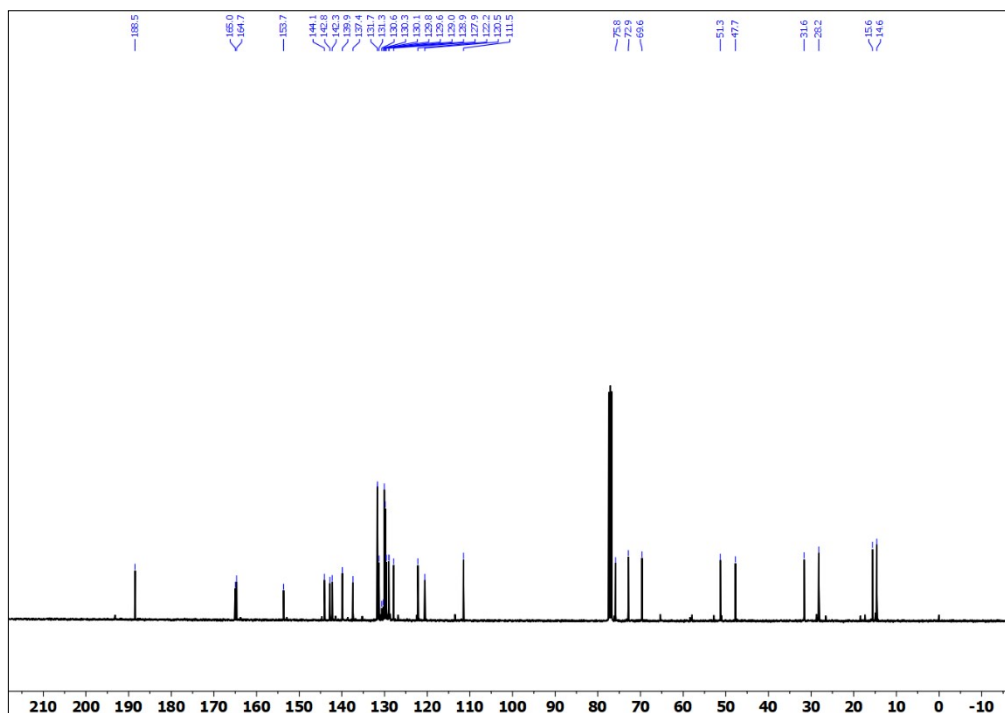
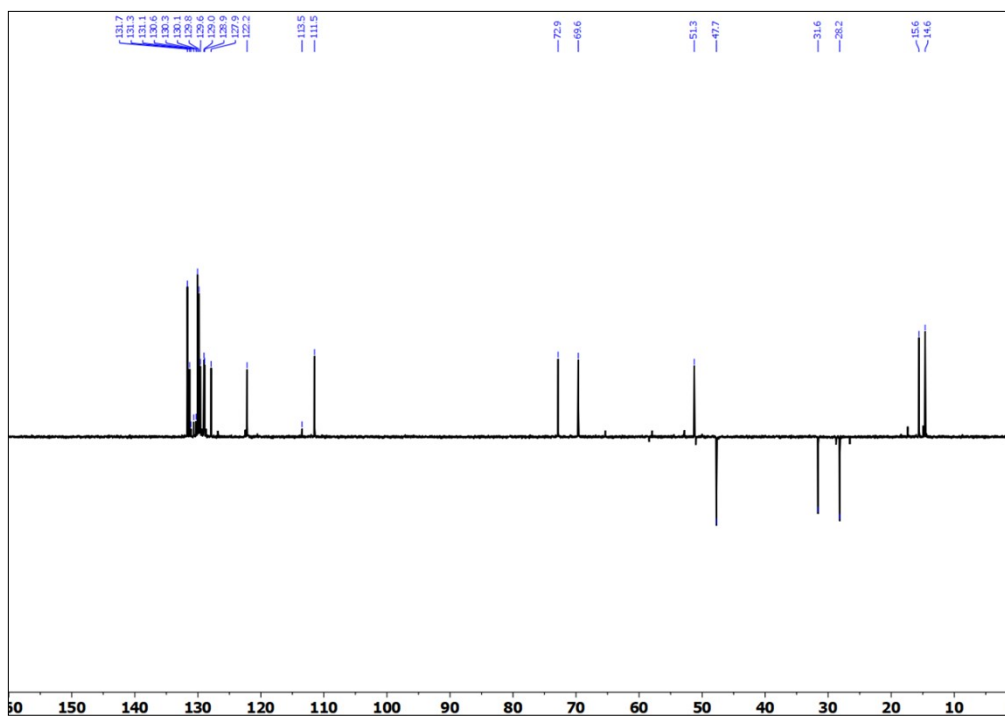
Fig S39: ¹³C NMR Spectrum of compound 6h

Fig S40: DEPT-135 NMR Spectrum of compound 6h

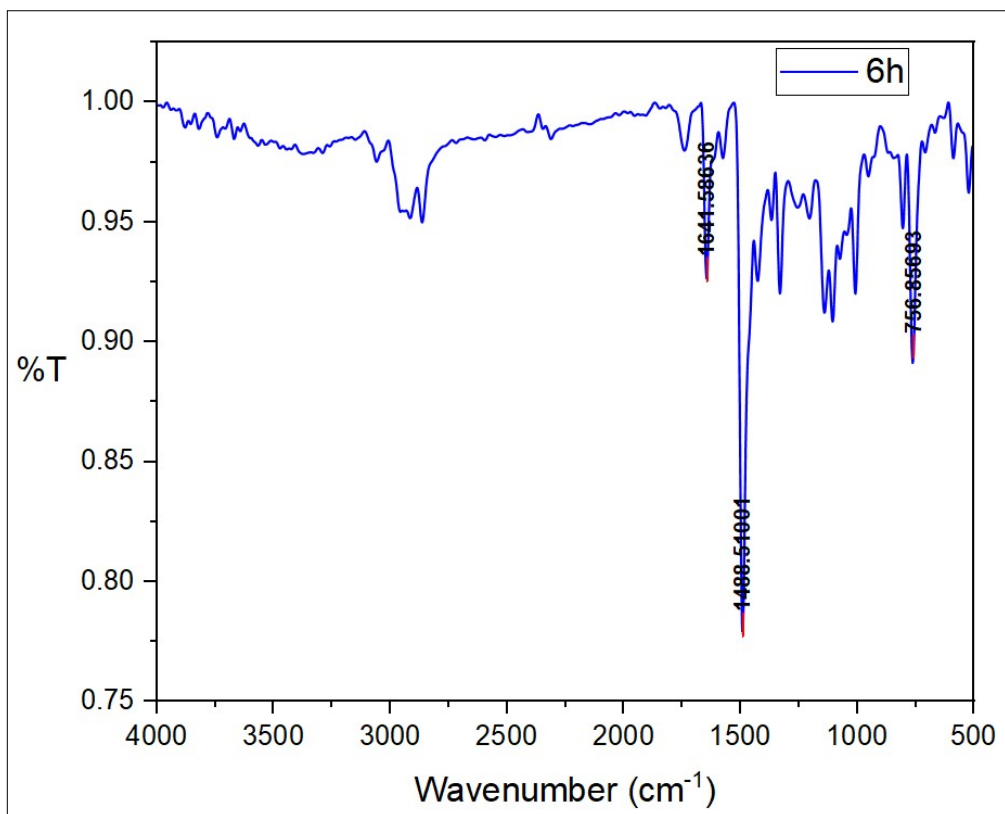


Fig S41: FT-IR Spectrum of compound 6h

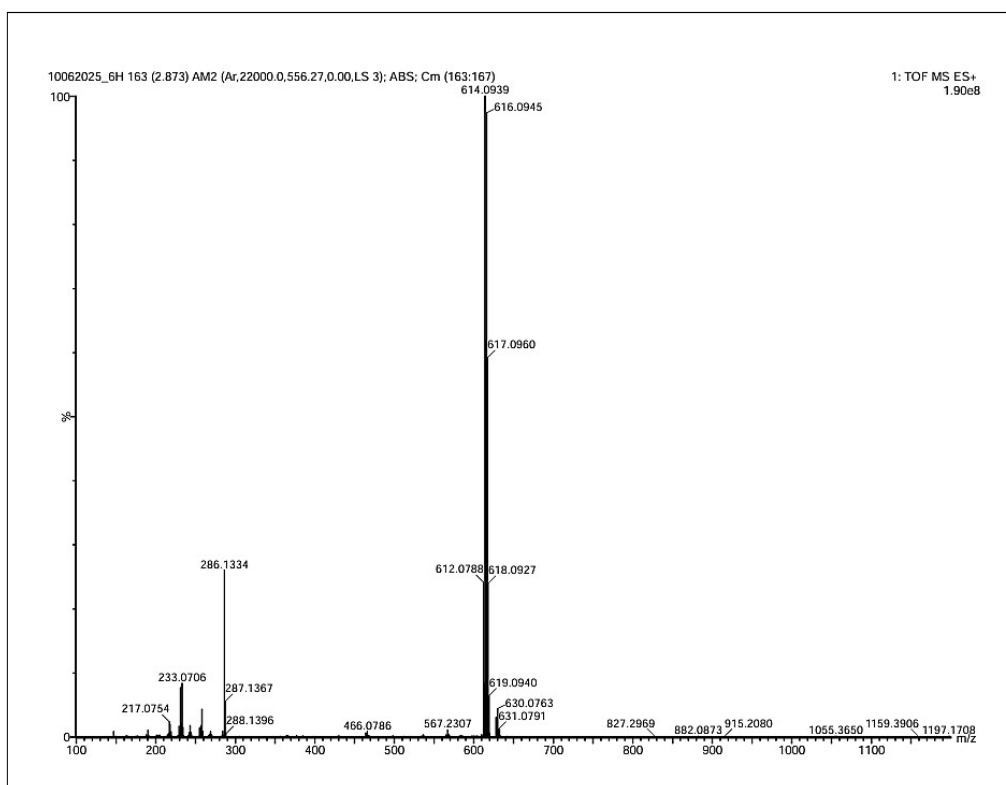


Fig S42: HRMS Spectrum of compound 6h

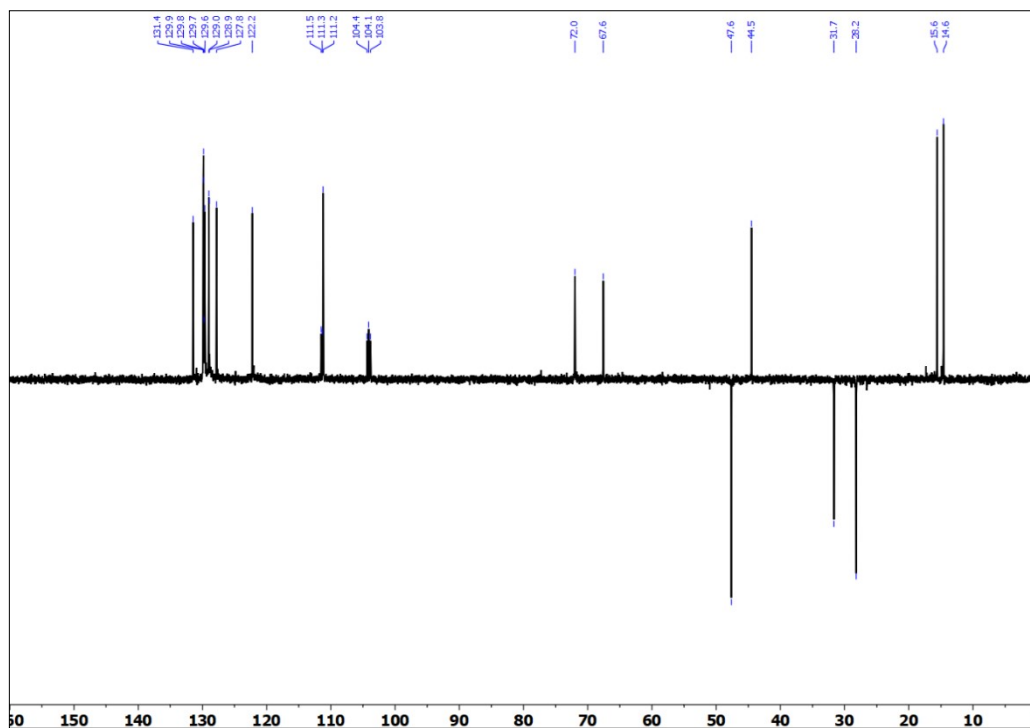


Fig S45: DEPT-135 NMR Spectrum of compound 6i

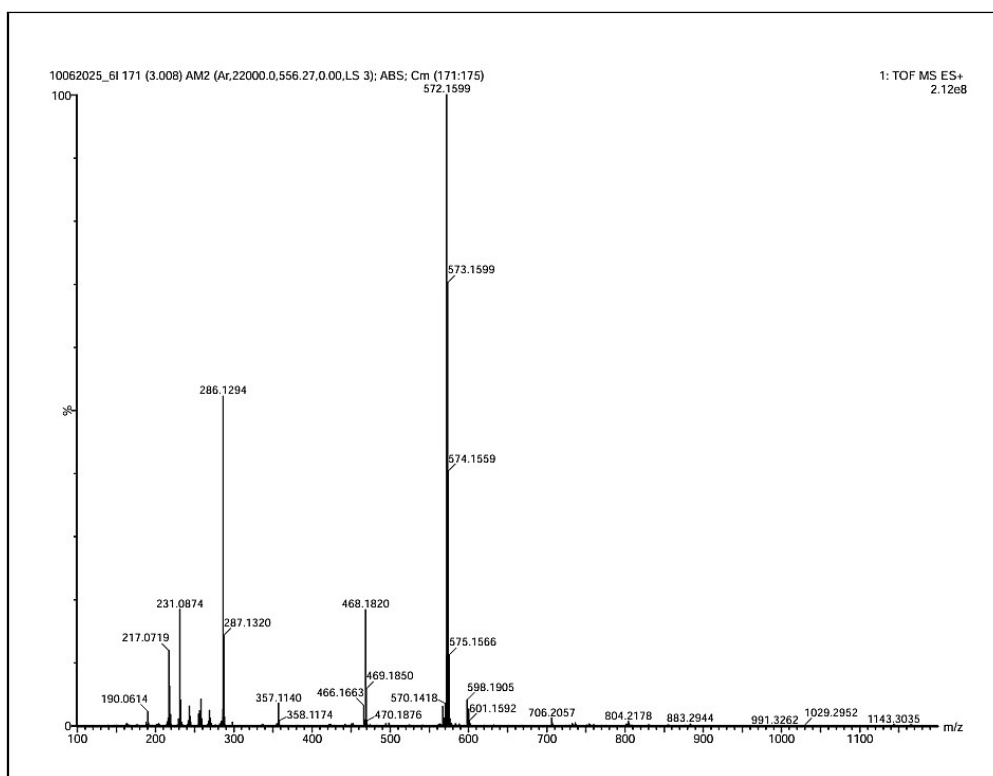
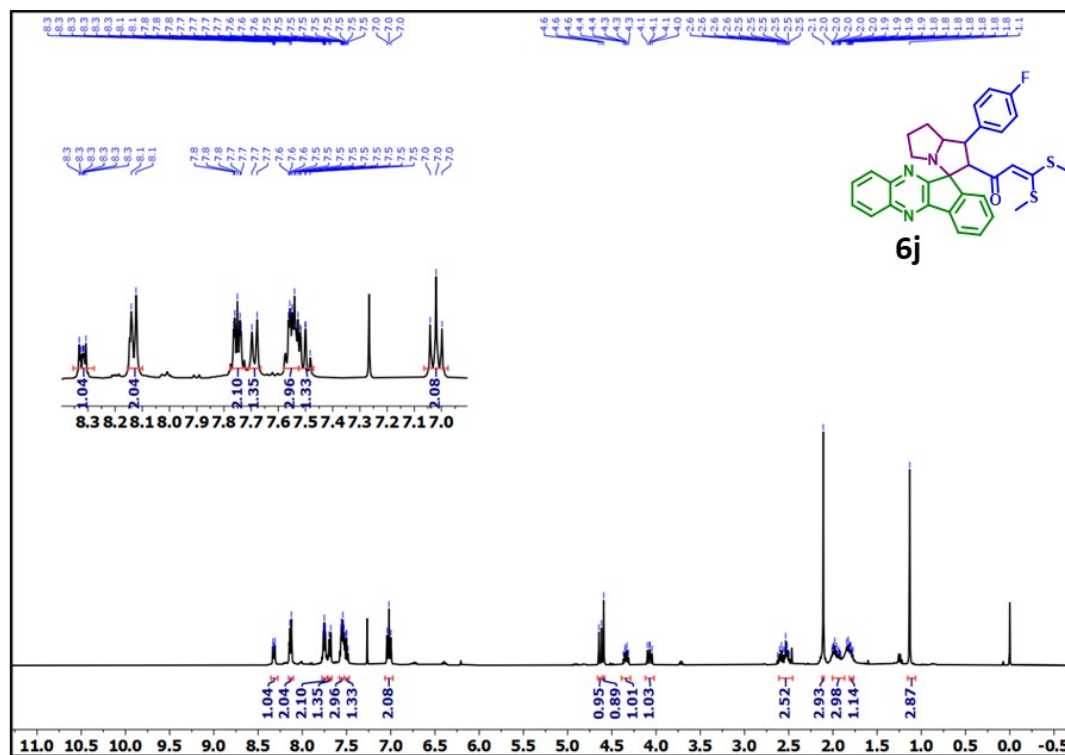
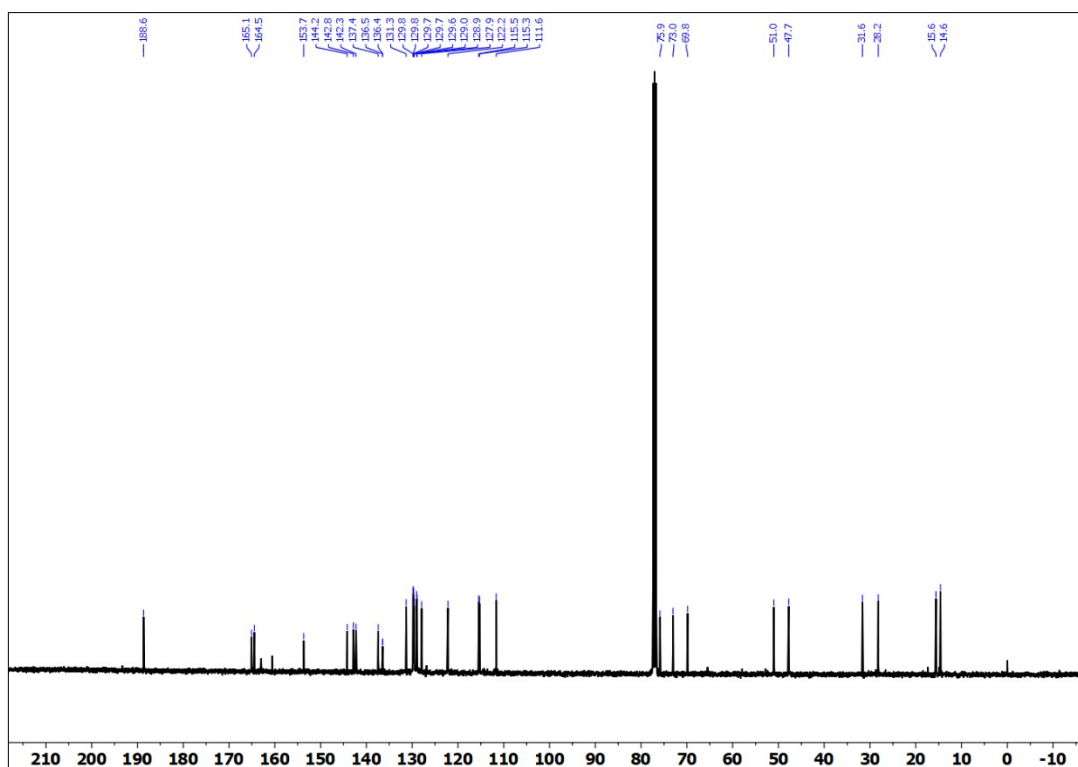


Fig S46: HRMS Spectrum of compound 6i

Fig S47: ¹H NMR Spectrum of compound **6j**Fig S48: ¹³C NMR Spectrum of compound **6j**

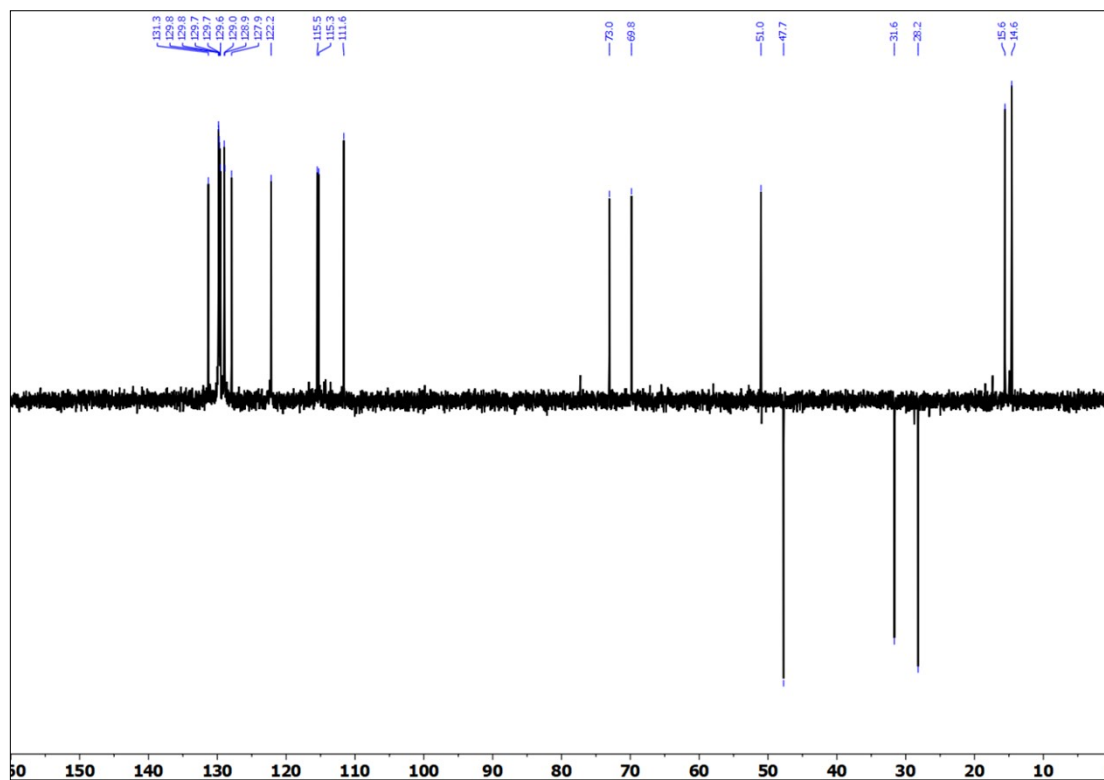


Fig S49: DEPT-135 NMR Spectrum of compound 6j

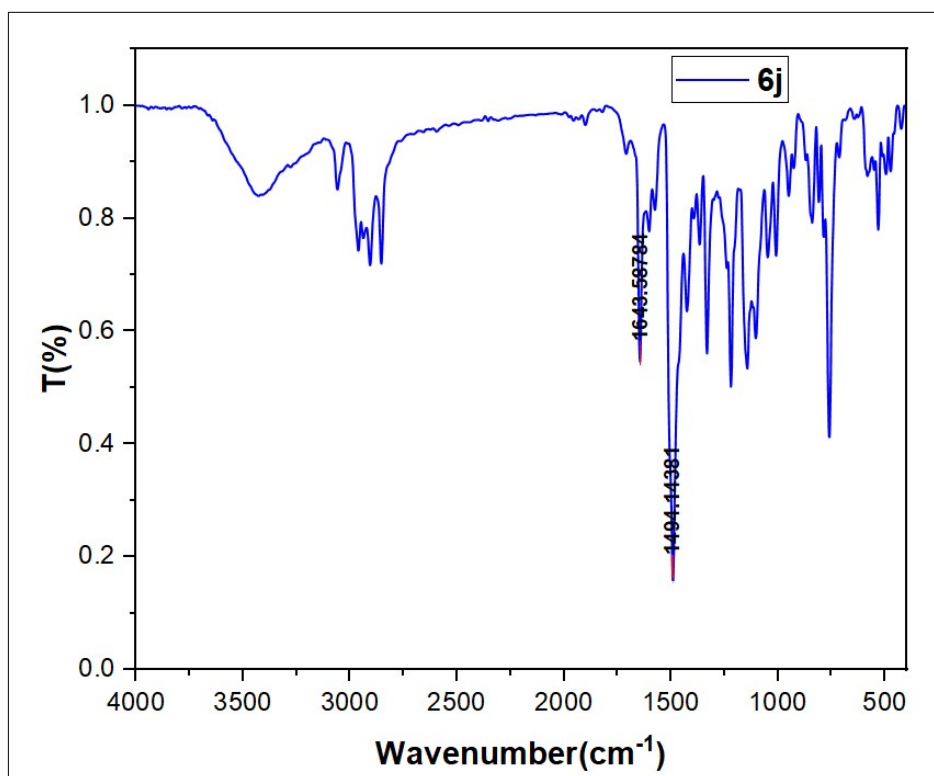


Fig S50: FT-IR Spectrum of compound 6j

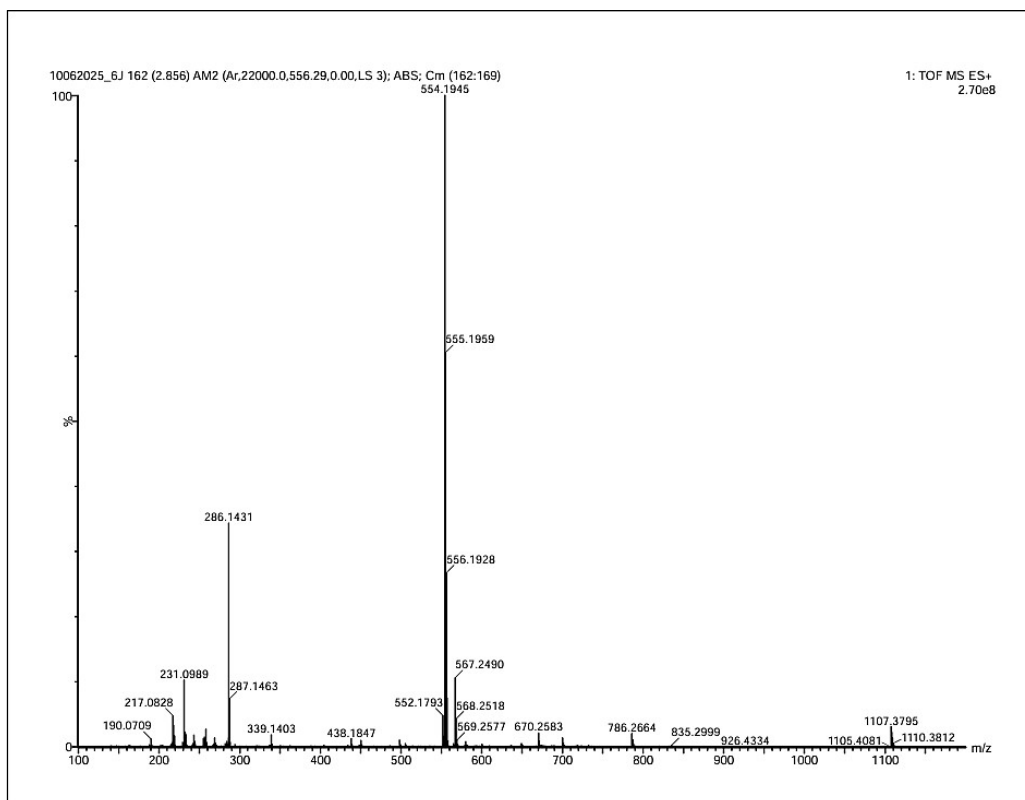
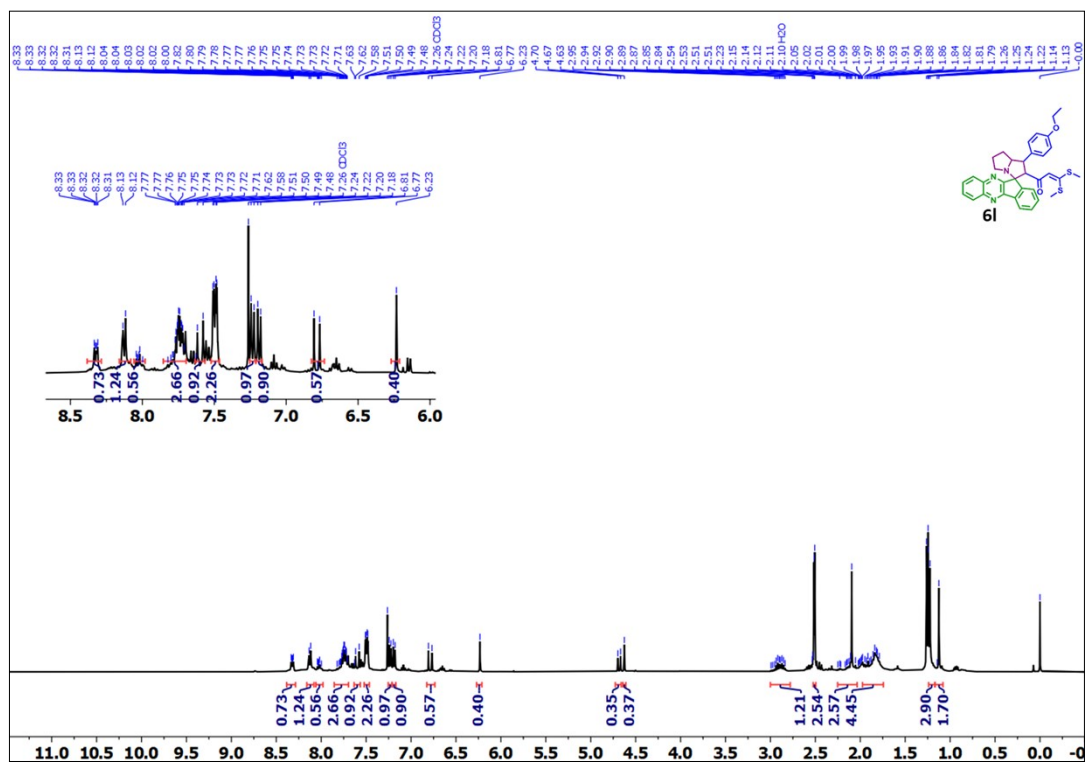


Fig S51: HRMS Spectrum of compound 6j

Fig S52: ¹H NMR Spectrum of compound 6k

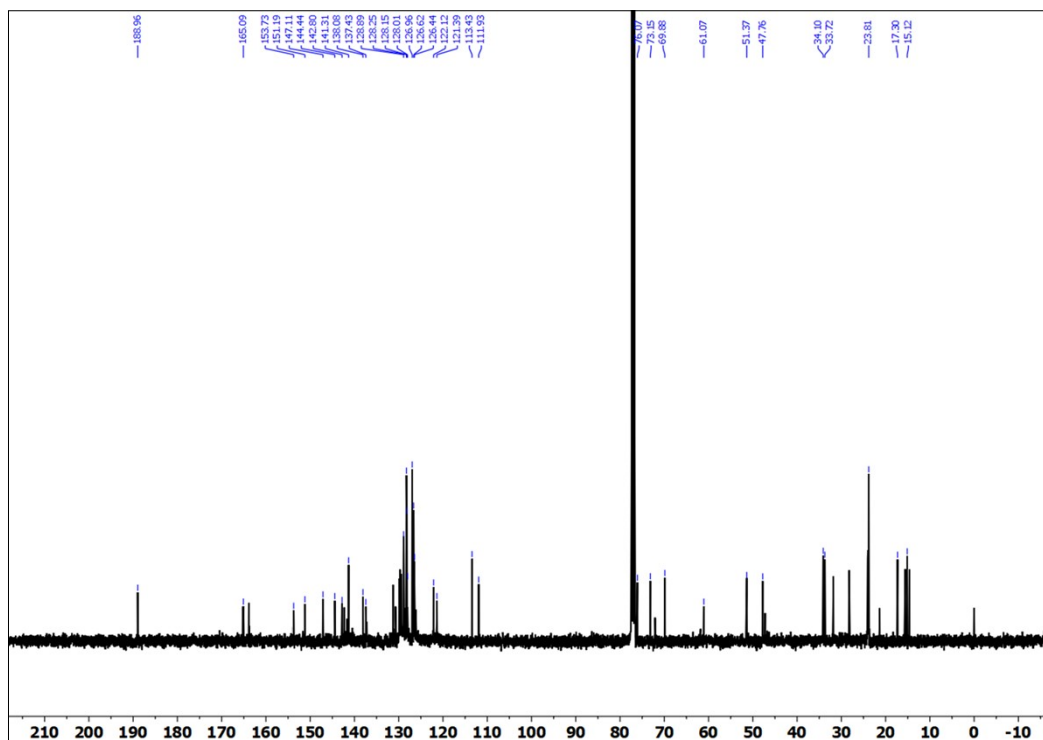


Fig S53: ^{13}C NMR Spectrum of compound 6k

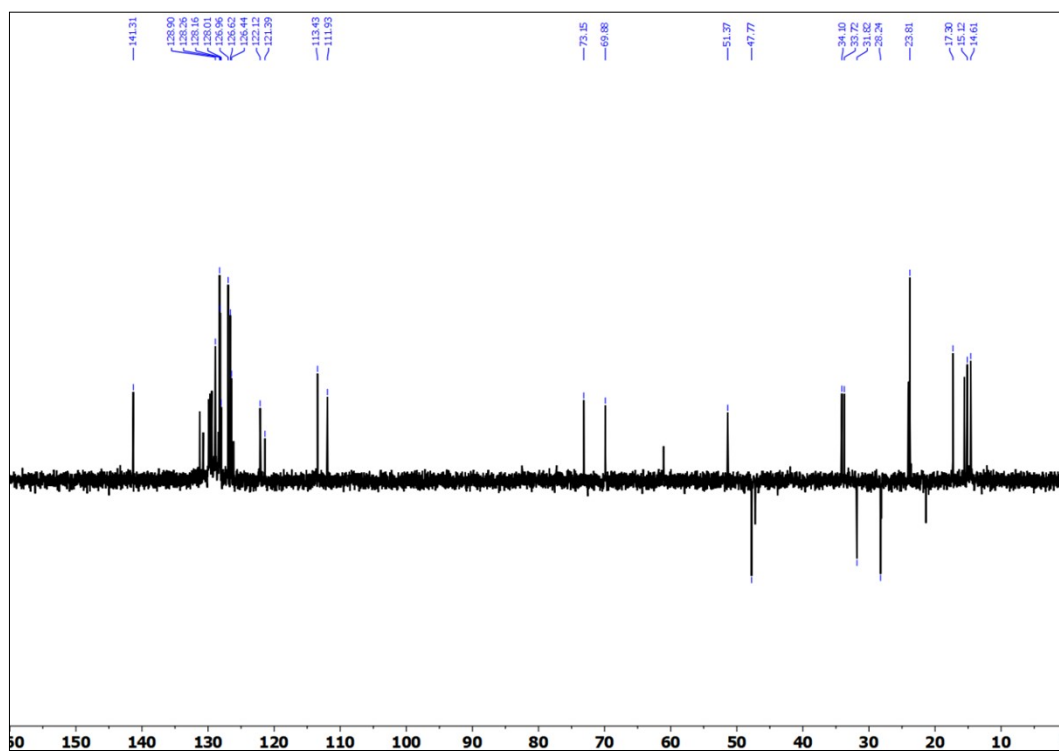


Fig S54: DEPT-135 NMR Spectrum of compound 6k

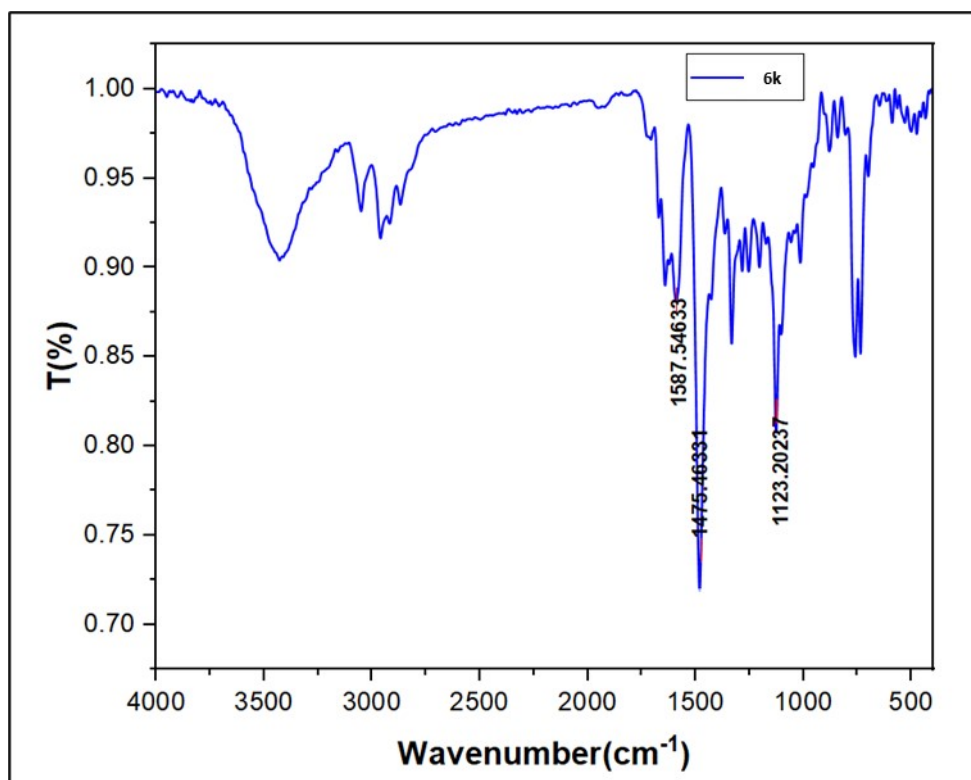


Fig S55: FT-IR Spectrum of compound 6k

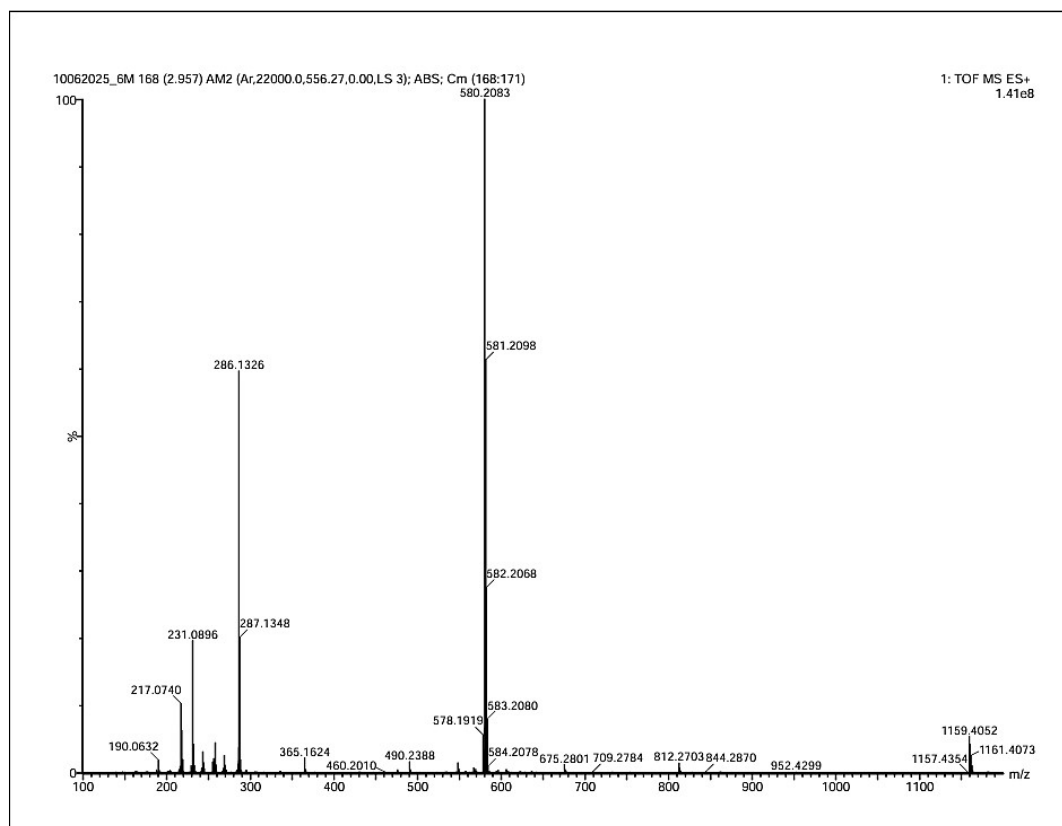


Fig S56: HRMS Spectrum of compound 6k

2. Biological Data Table of Compound 6f, g, and h.

Compounds	Pathogen	125 µg/mL	100 µg/mL	75 µg/mL	50 µg/mL	25 µg/mL
6h	<i>S. agalactiae</i>	99.1 ± 2.2	97.0 ± 2.1	89.5 ± 2.3	62.6 ± 2.0	58.4 ± 1.9
	<i>S. pyogenes</i>	95.8 ± 2.0	93.0 ± 2.0	50.2 ± 2.0	41.8 ± 1.8	37.9 ± 1.6
	<i>P. aeruginosa</i>	94.4 ± 1.9	94.0 ± 2.1	62.0 ± 2.0	40.2 ± 1.7	24.3 ± 1.5
6f	<i>S. agalactiae</i>	96.9 ± 2.0	94.1 ± 1.8	91.6 ± 2.5	66.7 ± 3.5	34.7 ± 4.0
	<i>S. pyogenes</i>	99.1 ± 3.0	86.6 ± 3.0	48.9 ± 4.0	45.1 ± 2.5	16.5 ± 2.0
	<i>P. aeruginosa</i>	94.5 ± 2.5	90.9 ± 2.0	72.2 ± 3.0	19.1 ± 2.5	12.1 ± 2.0
6g	<i>S. agalactiae</i>	95.0 ± 2.0	93.7 ± 1.9	84.8 ± 2.5	66.1 ± 2.2	-
	<i>S. pyogenes</i>	99.6 ± 2.1	93.6 ± 2.0	77.5 ± 2.4	69.5 ± 2.1	56.7 ± 1.7
	<i>P. aeruginosa</i>	98.8 ± 2.0	96.9 ± 2.1	91.7 ± 2.3	49.9 ± 1.8	27.4 ± 1.5

Table S1: Minimum inhibitory concentration (MIC) values of compounds **6f**, **6g**, and **6h** at concentrations against multidrug-resistant pathogens (*Streptococcus agalactiae*, *Streptococcus pyogenes*, and *Pseudomonas aeruginosa*). Results are expressed as percentage inhibition at concentrations ranging from 25-125 µg/mL (mean ± SD, n=3).

Concentration (µg/mL)	Compound 6f (% Inhibition, mean ± SD)	Compound 6g (% Inhibition, mean ± SD)	Compound 6h (% Inhibition, mean ± SD)
5	10.0 ± 1.2	8.8 ± 0.8	11.2 ± 1.0
10	12.4 ± 1.0	14.4 ± 1.2	14.4 ± 1.1
25	18.0 ± 1.5	11.2 ± 1.1	15.6 ± 1.4
50	30.0 ± 2.0	14.0 ± 1.3	18.8 ± 1.6
100	31.6 ± 2.1	32.8 ± 2.2	24.4 ± 1.9

Table S2. DPPH Radical Scavenging Activity of Compounds **6f**, **6g**, and **6h** at concentrations of 5-100 µg/mL. Results are expressed as percentage inhibition relative to negative control (mean ± SD, n=3).

4. Docking results of Compound 6g.

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	12B	ARG	3.76	3057	84
2	181B	TYR	3.58	3073	1642
3	185B	GLN	3.56	3074	1677
4	187B	ILE	3.24	3077	1699
5	187B	ILE	3.86	3066	1698

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	187B	ILE	2.03	2.93	154.54	×	×	3078 [O3]	1697 [O2]
2	204B	ALA	1.73	2.65	147.18	✓	×	1858 [N am]	3078 [O3]

Table S3. Summary of the **hydrogen bonding, hydrophobic contacts, and π-stacking interactions** between the **6g** and the **A-GAPDH (6IEP) Binding Pocket**.

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	152A	PRO	3.10	4340	1421
2	153A	PHE	3.17	4338	1431

3	326A	ILE	3.84	4333	2936
4	379A	PHE	3.77	4339	3427

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	231A	SER	2.43	3.36	156.17	✓	✓	2101 [O3]	4366 [O3]
2	231A	SER	2.00	2.94	151.57	✓	×	2096 [Nam]	4353 [O2]

Index	Residue	AA	Distance	Angle	Offset	Stacking Type	Ligand Atoms
1	379A	PHE	4.75	20.84	1.03	P	4342, 4343, 4344, 4346, 4350, 4351

Table S4. Summary of the **hydrogen bonding, hydrophobic contacts, and π -stacking interactions** between the **6g** and the **B-npGAPDH (7PKJ) Binding Pocket**.

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	122B	PRO	3.68	4440	744
2	230B	ASN	3.91	4449	1706
3	300B	VAL	3.18	4419	2366
4	301B	PHE	3.55	4440	2378
5	301B	PHE	3.46	4424	2376
6	342B	ALA	3.96	4425	2741
7	532B	HIS	3.57	4434	4362
8	533B	ASP	3.13	4435	4375

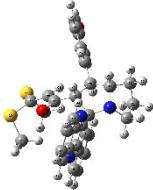
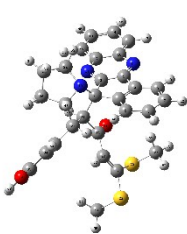
Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	148B	SER	2.86	3.57	132.25	✓	✓	989 [O3]	4436 [N ar]
2	230B	ASN	2.03	2.71	126.81	×	✓	4452 [O3]	1708 [O2]

Index	Residue	AA	Distance	Offset	Protein charged?	Ligand Group	Ligand Atoms
1	532B	HIS	5.52	1.66	✓	Aromatic	4446, 4447, 4448, 4449, 4450, 4451

Index	Residue	AA	Distance	Protein positive?	Ligand Group	Ligand Atoms
1	302B	GLU	5.01	×	Tertamine	4421

Table S5. Summary of the **hydrogen bonding, hydrophobic contacts, and π -stacking interactions** between the **6g** and the **C-Aminopeptidase (8AC7) Binding Pocket**.

5. DFT results of Compound 6g

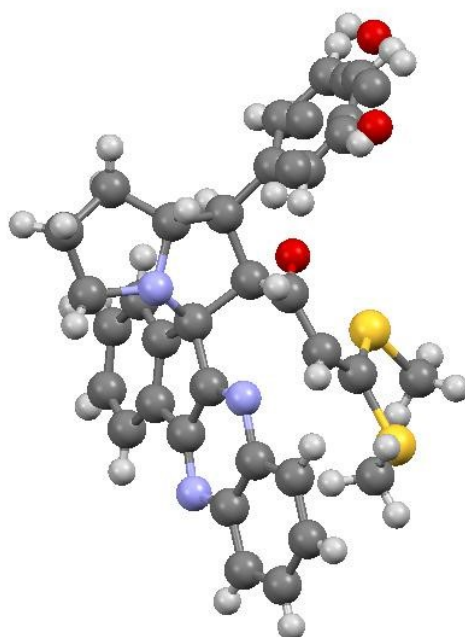
6g endo 4797.4608409484 Hartrees (12,595,204.09 kJ/mol)	6g exo 4846.7105360983 Hartrees (12,725,038.5125 kJ/mol)
	
Stoichiometry C32H29N3O2S2 Framework group C1[X(C32H29N3O2S2)] Deg. of freedom 198	Stoichiometry C32H29N3O2S2 Framework group C1[X(C32H29N3O2S2)] Deg. of freedom 198

Full point group C1 NOp 1						Full point group C1 NOp 1					
Largest Abelian subgroup C1 NOp 1						Largest Abelian subgroup C1 NOp 1					
Largest concise Abelian subgroup C1 NOp 1						Largest concise Abelian subgroup C1 NOp 1					
Standard orientation:						Standard orientation:					
Center	Atomic	Atomic	Coordinates			Center	Atomic	Atomic	Coordinates		
Number	Number	Type	X	Y	Z	Number	Number	Type	X	Y	Z
		(Angstroms)						(Angstroms)			
1	6	0	3.070582	0.642994	0.520125	1	6	0	-2.922790	0.210034	0.862730
2	6	0	2.355081	-0.531150	0.116050	2	6	0	-2.182098	-0.747458	0.215522
3	6	0	1.017831	-0.642771	0.857010	3	6	0	-0.811527	-0.942449	0.862107
4	6	0	1.060920	0.642322	1.716265	4	6	0	-0.946743	0.066368	2.021083
5	6	0	0.116517	1.129755	2.618911	5	6	0	-0.053605	0.375743	3.063767
6	6	0	0.373801	2.331790	3.298229	6	6	0	-0.412203	1.348023	4.011627
7	6	0	1.566270	3.039537	3.079340	7	6	0	-1.652013	2.002891	3.930840
8	6	0	2.521711	2.556915	2.176926	8	6	0	-2.550795	1.683549	2.906917
9	6	0	2.260617	1.361395	1.503990	9	6	0	-2.176049	0.715468	1.977225
10	7	0	2.814617	-1.377998	-0.775437	10	7	0	-2.677763	-1.349458	-0.897973
11	7	0	4.258069	0.971346	0.038159	11	7	0	-4.161588	0.568892	0.444614
12	6	0	4.630693	-1.941450	-2.272545	12	6	0	-4.450610	-1.636872	-2.487686
13	6	0	5.871541	-1.655926	-2.813961	13	6	0	-5.727435	-1.287367	-2.940563
14	6	0	6.584715	-0.498051	-2.409020	14	6	0	-6.477975	-0.320346	-2.261189
15	6	0	6.050027	0.363077	-1.467933	15	6	0	-5.958134	0.306067	-1.123183
16	6	0	4.781851	0.094323	-0.898308	16	6	0	-4.683127	-0.035406	-0.660786
17	6	0	4.062074	-1.078262	-1.307200	17	6	0	-3.921084	-1.018300	-1.350894
18	7	0	0.870011	-1.895036	1.608987	18	7	0	-0.517537	-2.281285	1.440544
19	6	0	-0.341730	-2.657148	1.243199	19	6	0	0.916427	-2.552544	1.161714
20	6	0	-0.852778	-3.274374	2.572387	20	6	0	0.942274	-3.791204	0.256050
21	6	0	-0.112075	-2.494497	3.688896	21	6	0	-0.215629	-4.564474	0.834019
22	6	0	1.222844	-2.081075	3.023932	22	6	0	-1.242524	-3.450006	0.894900
23	6	0	0.010429	4.010936	-0.656066	23	6	0	-0.286845	4.381451	0.238035
24	6	0	-4.625630	4.286471	-0.474657	24	6	0	4.100805	3.329546	-1.769978
25	16	0	-4.262976	2.478952	-0.906923	25	16	0	3.318587	3.772509	-0.188175
26	16	0	-1.597993	3.812770	-1.633950	26	16	0	0.481994	3.955735	-1.356028
27	6	0	-2.424046	2.363160	-0.925066	27	6	0	1.770846	2.953469	-0.592881
28	6	0	-2.327216	-2.210569	-0.332860	28	6	0	2.815170	-1.522307	-0.241645
29	6	0	-1.249211	-1.602208	0.545606	29	6	0	1.540436	-1.280416	0.555586
30	8	0	0.320527	1.240114	-1.409636	30	8	0	-0.533610	1.290417	-1.147043
31	6	0	-0.189505	-0.727350	-0.173254	31	6	0	0.331809	-0.655686	-0.147067
32	6	0	-0.561916	0.643664	-0.738845	32	6	0	0.427398	0.806546	-0.569600
33	6	0	-1.900831	1.175345	-0.507423	33	6	0	1.636290	1.643349	-0.302136
34	6	0	-3.666730	-2.153214	0.076831	34	6	0	3.930310	-2.068140	0.419899
35	6	0	-4.672700	-2.747504	-0.692636	35	6	0	5.125813	-2.305696	-0.266952
36	6	0	-4.359944	-3.408930	-1.884354	36	6	0	5.217290	-1.995789	-1.630192
37	6	0	-3.023405	-3.470741	-2.294401	37	6	0	4.119191	-1.452197	-2.298465
38	6	0	-2.012440	-2.882338	-1.531057	38	6	0	2.924770	-1.215394	-1.613346
39	8	0	-5.972979	-2.643007	-0.205145	39	8	0	6.177777	-2.830402	0.393472
40	1	0	-0.808375	0.593100	2.802025	40	1	0	0.896721	-0.114021	3.179965
41	1	0	-0.357078	2.715520	4.003221	41	1	0	0.270790	1.591877	4.815047
42	1	0	1.748806	3.964629	3.616861	42	1	0	-1.917578	2.749253	4.668168
43	1	0	3.448663	3.090279	1.996754	43	1	0	-3.513469	2.174316	2.843470
44	1	0	4.063324	-2.818293	-2.563503	44	1	0	-3.877484	-2.386107	-3.019808
45	1	0	6.306058	-2.319052	-3.554863	45	1	0	-6.136787	-1.766982	-3.820311
46	1	0	7.556387	-0.289625	-2.844882	46	1	0	-7.464718	-0.055692	-2.618364
47	1	0	6.571502	1.255918	-1.141819	47	1	0	-6.545949	1.053772	-0.605179
48	1	0	-0.113774	-3.450250	0.517079	48	1	0	1.429507	-2.834522	2.109197
49	1	0	-0.588739	-4.337162	2.614320	49	1	0	1.914196	-4.328860	0.251571
50	1	0	-1.942432	-3.206848	2.658730	50	1	0	0.687664	-3.520074	-0.794138
51	1	0	-0.676759	-1.597272	3.971961	51	1	0	-0.532701	-5.440738	0.229142
52	1	0	0.031386	-3.094661	4.593247	52	1	0	0.036019	-4.900774	1.866004

53	1	0	1.975271	-2.875136	3.139182	53	1	0	-2.134209	-3.711298	1.502163
54	1	0	1.640880	-1.163896	3.448604	54	1	0	-1.552882	-3.285377	-0.154365
55	1	0	0.335251	5.030763	-0.868231	55	1	0	-1.167826	5.025590	0.040642
56	1	0	-0.195701	3.888835	0.407495	56	1	0	-0.645277	3.466838	0.755890
57	1	0	0.721425	3.266054	-1.003810	57	1	0	0.422810	4.957055	0.868206
58	1	0	-5.705280	4.318519	-0.316920	58	1	0	5.124968	3.755104	-1.785025
59	1	0	-4.102344	4.562389	0.440512	59	1	0	4.187945	2.226582	-1.864372
60	1	0	-4.340864	4.941114	-1.295219	60	1	0	3.536907	3.771431	-2.617864
61	1	0	-1.735338	-1.011826	1.335106	61	1	0	1.809000	-0.609050	1.383993
62	1	0	0.209674	-1.298708	-1.021352	62	1	0	0.131745	-1.271675	-1.052484
63	1	0	-2.600769	0.501571	-0.027171	63	1	0	2.488532	1.171677	0.169738
64	1	0	-3.952191	-1.647592	0.993138	64	1	0	3.870263	-2.309177	1.474454
65	1	0	-5.142136	-3.866793	-2.483958	65	1	0	6.137411	-2.174814	-2.171954
66	1	0	-2.772632	-3.982076	-3.218296	66	1	0	4.193512	-1.213018	-3.351532
67	1	0	-0.983865	-2.946293	-1.869343	67	1	0	2.098205	-0.793003	-2.165735
68	1	0	-6.618173	-3.060542	-0.807271	68	1	0	7.022427	-3.010109	-0.043754
-----						-----					
Rotational constants (GHZ): 0.1077542 0.0683967 0.0575012						Rotational constants (GHZ): 0.1107755 0.0711261 0.0580189					
Standard basis: 6-31G (6D, 7F)						Standard basis: 6-31G (6D, 7F)					
Filename = Endo-6g						Filename = Exo-6g					
Calculation Type = SP						Calculation Type = SP					
Calculation Method = RB3LYP						Calculation Method = RB3LYP					
Basis Set = 6-31G						Basis Set = 6-31G					
Charge = 0						Charge = 0					
Spin = Singlet						Spin = Singlet					
Solvation = None						Solvation = None					
E(RB+HF-LYP) = -2347.451 Hartree						E(RB+HF-LYP) = -2347.3904 Hartree					
Dipole Moment = 3.057454 Debye						Dipole Moment = 4.2068615 Debye					
Nuclear repulsion energy = 4797.4608409484 Hartrees						Nuclear repulsion energy = 4846.7105360983 Hartrees					
Point Group = C1						Point Group = C1					
Job CPU time: 0 days 0 hours 6 minutes 12.0 seconds.						Job CPU time: 0 days 0 hours 6 minutes 3.0 seconds.					

Table S6. DFT calculation table of Endo and Exo 6g.

6. Basic Crystallographic data of Compound 6g



(CCDC: 2504757)

Fig S57. SC-XRD 3D view data of Compound 6g.

Bond precision:	C-C = 0.0094 Å	Wavelength=0.71073	
Cell:	a=22.317(5) alpha=90	b=22.317(5) beta=90	c=11.022(4) gamma=90
Temperature:	300 K		
	Calculated	Reported	
Volume	5490(3)	5490(3)	
Space group	I -4	I -4	
Hall group	I -4	I -4	
Moiety formula	C32 H28.45 N3 O2 S2 [+ solvent]	C32 H28.452 N3 O2 S2, 0.2[H2O]	
Sum formula	C32 H28.45 N3 O2 S2 [+ solvent]	C32 H28.85 N3 O2.20 S2	
Mr	551.14	554.75	
Dx, g cm ⁻³	1.334	1.342	
Z	8	8	
Mu (mm ⁻¹)	0.229	0.230	
F000	2315.6	2332.0	
F000'	2318.37		
h, k, lmax	29, 29, 14	29, 29, 14	
Nref	6842 [3598]	6834	
Tmin, Tmax	0.930, 0.964		
Tmin'	0.930		
Correction method=	Not given		
Data completeness=	1.90/1.00	Theta(max)= 28.291	
		wR2(reflections)= 0.2367(
R(reflections)=	0.0648(4194)	6834)	
S =	1.162	Npar= 374	

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level**.
Click on the hyperlinks for more details of the test.

Alert level C

[PLAT220_ALERT_2_C](#) NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.4 Ratio
[PLAT222_ALERT_3_C](#) NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.2 Ratio
[PLAT242_ALERT_2_C](#) Low 'MainMol' Ueq as Compared to Neighbors of S002 Check [PLAT309_ALERT_2_C](#) Single Bonded Oxygen (C-O > 1.3 Ang) O011 Check [PLAT340_ALERT_3_C](#) Low Bond Precision on C-C Bonds 0.00942 Ang.
[PLAT905_ALERT_3_C](#) Negative K value in the Analysis of Variance ... -4.534 Report
And 2 other PLAT905 Alerts [More](#)
 ...

Alert level G

[FORMU01_ALERT_2_G](#) There is a discrepancy between the atom counts in the _chemical_formula_sum and the formula from the _atom_site* data. Atom count from _chemical_formula_sum: C32 H28.85 N3 O2.2 S2 Atom count from the _atom_site data: C32 H28.44699 N3 O2 S2
[CELLZ01_ALERT_1_G](#) Difference between formula and atom_site contents detected.
[CELLZ01_ALERT_1_G](#) ALERT: Large difference may be due to a symmetry error - see SYMMG tests
 From the CIF: _cell_formula_units_Z 8

From the CIF: `_chemical_formula_sum` C32 H28.85 N3 O2.20 S2 TEST:
Compare cell contents of formula and `atom_site` data

atom	Z*formula	cif sites	diff	C
256.00	256.00	0.00		
H	230.80	227.58	3.22	
N	24.00	24.00	0.00	
O	17.60	16.00	1.60	
S	16.00	16.00	0.00	

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 14 Note

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 1 Report
H0A

PLAT041_ALERT_1_G Calc. and Reported SumFormula Strings Differ Please Check
Calc: C32 H28.45 N3 O2 S2
Rep.: C32 H28.85 N3 O2.20 S2

PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: C32 H28.45 N3 O2 S2
Rep.: C32 H28.452 N3 O2 S2, 0.2[H2O]

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.11 Report

PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 6 Report

PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 17 Report

PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report

And 9 other PLAT191 Alerts [More](#)

...

PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 15% Note

PLAT304_ALERT_4_G Non-Integer Number of Atoms in. (Resd 1) 67.45 Check

PLAT410_ALERT_2_G Short Intra H...H Contact H00K ..H1 1.98 Ang.

x,y,z = 1_555 Check

PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 25 A**3

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 71 Note

S001 S002 O003 N004 N005 N006 C007 C008
C009 C00A H00A C00B H00B C00C C00D C00E
C00F C00G C00H H00H C00I C00J H00J C00K
H00K C00L H00L C00M H00C H00D C00N H00N
C00O H00E H00F C00P H00P C00Q C00R H00R
C00S H00G H00I C00T H00T C00U H00U C00V
H00V C00W C00X H00X C00Y H00Y C00Z H00Z
C010 H01A H01B H01C O011 C012 H012 C014
H01D H01E H01F C0 H0 O0 H0A

PLAT792_ALERT_1_G Model has Chirality at C008 (Polar SpGr) R Verify

And 3 other PLAT792 Alerts [More](#)

...

PLAT860_ALERT_3_G Number of Least-Squares Restraints 17 Note

PLAT868_ALERT_4_G ALERTS Due to the Use of `_smtbx_masks` Suppressed ! Info

PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min)[Deg]= 2.06 Note

1 1 0, 0 2 0,

PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 2 Note

0 2 0, 3 3 0,

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 8.506 Note

Predicted wR2: Based on SigI**2 2.78 or SHELX Weight 20.37

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

35 **ALERT level G** = General information/check it is not something unexpected

8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

9 ALERT type 2 Indicator that the structure model may be wrong or deficient

18 ALERT type 3 Indicator that the structure quality may be low

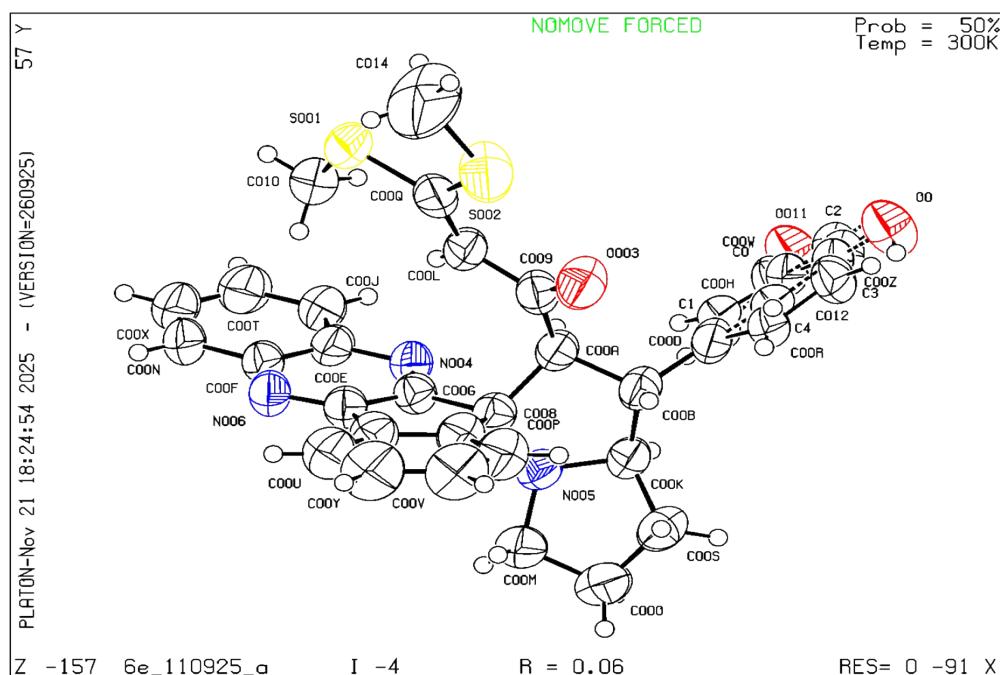
6 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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Table S7. Single Crystal XRD data of Compound **6g**.



The single crystal X-ray diffraction data for **6g** (CCDC 2504757) showed an extra oxygen atom, which was identified as a disordered lattice water molecule. Including this solvent molecule in the final refinement significantly improved the data quality (*R*-factor), which is not a serious threat.

Fig S58. SC-XRD data of Compound **6g**.

7. References

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