**Supporting Information to the *New Journal of Chemistry***

# Design, synthesis and antifungal mechanism of novel acetophenone derivatives containing 1, 3, 4-thiadiazole-2-thioethers

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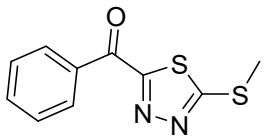
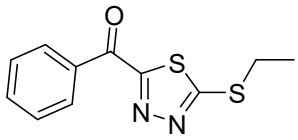
## Contents

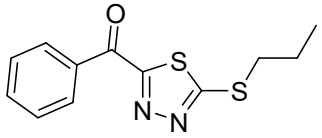
## 1. $^{1}$H NMR, $^{13}$C NMR, $^{19}$F NMR and HRMS data of the title compounds



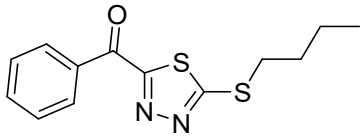
*Date for* **E1**. A yellow solid, yield 95%, m.p. 59-60 $^{o}$C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ: 8.52–8.49 (m, 2H, phenyl H), 7.69–7.64 (m, 1H, phenyl H), 7.55–7.51 (m, 2H, phenyl H), 2.87 (s, 3H, $CH_3$); $^{13}$C NMR (101 MHz, $CDCl_3$) δ: 182.97, 173.53, 169.13, 134.53, 134.51, 131.28, 128.74, 16.63; HRMS (ESI): m/z calcd for $C_{10}H_8N_2OS_2$ $[M+H]^+$ 237.01508, found 237.01466.



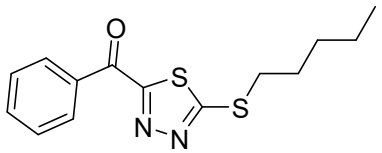
*Date for* **E2**. A yellow solid, yield 89%, m.p. 32-33 $^{o}$C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ: 8.52–8.49 (m, 2H, phenyl H), 7.68–7.63 (m, 1H, phenyl H), 7.54–7.50 (m, 2H, phenyl H), 3.43 (q, $J$ = 8.0 Hz, 2H, $CH_2$), 1.53 (t, $J$ = 8.0 Hz, 3H, $CH_3$); $^{13}$C NMR (101 MHz, $CDCl_3$) δ: 182.94, 172.74, 169.02, 134.57, 134.45, 131.25, 128.71, 28.71, 14.57; HRMS (ESI): m/z calcd for $C_{11}H_{10}N_2OS_2$ $[M+H]^+$ 251.03073, found 251.03006.



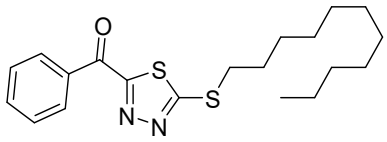
*Date for* **E3**. A yellow liquid, yield 90%. $^{1}$H NMR (400 MHz, $CDCl_3$) δ: 8.52–8.49 (m, 2H, phenyl H), 7.68–7.64 (m, 1H, phenyl H), 7.55–7.51 (m, phenyl H), 3.40 (t, $J$ = 8.0 Hz, 2H, $\underline{CH_2}CH_2CH_3$), 1.95–1.85 (m, 2H, $CH_2\underline{CH_2}CH_3$), 1.09 (t, $J$ = 8.0 Hz, 3H, $CH_2CH_2\underline{CH_3}$); $^{13}$C NMR (101 MHz, $CDCl_3$) δ: 182.97, 173.07, 168.96, 134.59, 134.46, 131.27, 128.72, 36.18, 22.64, 13.46; HRMS (ESI): m/z calcd for $C_{12}H_{12}N_2OS_2$ $[M+H]^+$ 265.04638, found 265.04578.



*Date for* **E4**. A orange-red solid, yield 88%, m.p. 32-33 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ: 8.52–8.49 (m, 2H, phenyl H), 7.68–7.64 (m, 1H, phenyl H), 7.55–7.51 (m, 2H, phenyl H), 3.42 (t, *J* = 8.0 Hz, 2H, $\underline{CH_2}CH_2CH_2CH_3$), 1.88–1.81 (m, 2H, $CH_2\underline{CH_2}CH_2CH_3$), 1.56–1.46 (m, 2H, $CH_2CH_2\underline{CH_2}CH_3$), 0.97 (t, *J* = 8.0 Hz, 3H, $CH_2CH_2CH_2\underline{CH_3}$); $^{13}$C NMR (101 MHz, $CDCl_3$) δ: 182.97, 173.11, 168.96, 134.59, 134.45, 131.27, 128.72, 34.05, 31.13, 22.06, 13.68; HRMS (ESI): m/z calcd for $C_{13}H_{14}N_2OS_2$ $[M+H]^+$ 279.06203, found 279.06174.

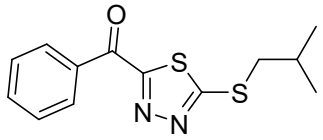


*Date for* **E5**. A orange-red liquid, yield 91%. $^1$H NMR (400 MHz, $CDCl_3$) δ: 8.51 (d, *J* = 8.0 Hz, 2H, phenyl H), 7.69–7.64 (m, 1H, phenyl H), 7.55–7.51 (m, 2H, phenyl H), 3.42 (t, *J* = 8.0 Hz, 2H, $\underline{CH_2}CH_2CH_2CH_2CH_3$), 1.90–1.83 (m, 2H, $CH_2\underline{CH_2}CH_2CH_2CH_3$), 1.50–1.42 (m, 2H, $CH_2CH_2\underline{CH_2}CH_2CH_3$), 1.41–1.33 (m, 2H, $CH_2CH_2CH_2\underline{CH_2}CH_3$), 0.92 (t, *J* = 8.0 Hz, 3H, $CH_2CH_2CH_2CH_2\underline{CH_3}$); $^{13}$C NMR (101 MHz, $CDCl_3$) δ: 183.01, 173.15, 168.96, 134.61, 134.47, 131.28, 128.74, 34.34, 31.02, 28.84, 22.31, 14.07; HRMS (ESI): m/z calcd for $C_{14}H_{16}N_2OS_2$ $[M+H]^+$ 293.07768, found 293.07712.

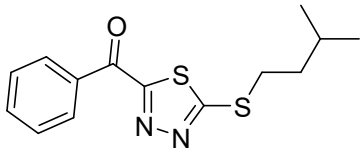


*Date for* **E6**. A yellow solid, yield 76%, m.p. 37-39 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ: 8.52–8.49 (m, 2H, phenyl H), 7.69–7.64 (m, 1H, phenyl H), 7.55–7.51 (m, 2H, phenyl H), 3.41 (t, *J* = 8.0 Hz, 2H, $SCH_2$), 3.28–3.25 (m, 2H, $CH_2\underline{CH_2}(CH_2)_8CH_3$), 1.89–1.82 (m, 2H, $(CH_2)_2\underline{CH_2}(CH_2)_7CH_3$),

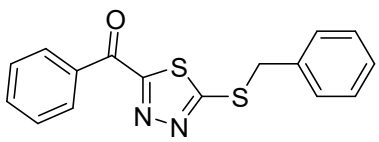
1.81–1.74 (m, 2H, $(CH_2)_3\underline{CH_2}(CH_2)_6CH_3$), 1.51–1.33 (m, 8H, $(CH_2)_3CH_2(\underline{CH_2})_4CH_2CH_2CH_3$), 0.89–0.86 (m, 7H, $(CH_2)_8\underline{CH_2CH_2CH_3}$); $^{13}$C NMR (101 MHz, $CDCl_3$) δ: 182.99, 173.17, 168.94, 165.38, 134.59, 134.46, 131.28, 128.73, 34.41 (d, $J$ = 8.1 Hz) , 32.03, 29.84, 29.71 (d, $J$ = 3.0 Hz), 29.60 (d, $J$ = 1.0 Hz), 29.39 (d, $J$ = 1.4 Hz), 29.16 (d, $J$ = 8.1 Hz), 28.88 (d, $J$ = 5.1 Hz), 22.83, 14.27; HRMS (ESI): m/z calcd for $C_{20}H_{28}N_2OS_2$ $[M+H]^+$ 377.17158, found 377.17194.



*Date for* **E7**. A yellow liquid, yield 93%. $^1$H NMR (400 MHz, $CDCl_3$) δ: 8.52–8.49 (m, 2H, phenyl H), 7.68–7.63 (m, 1H, phenyl H), 7.54–7.50 (m, 2H, phenyl H), 3.33 (d, $J$ = 8.0 Hz, 2H, $CH_2$), 2.14 (m, 1H, CH), 1.09 (d, $J$ = 8.0 Hz, 6H, $CH_3$); $^{13}$C NMR (101 MHz, $CDCl_3$) δ: 182.95, 173.32, 168.91, 134.60, 134.43, 131.25, 128.70, 42.69, 28.55, 21.95; HRMS (ESI): m/z calcd for $C_{13}H_{14}N_2OS_2$ $[M+H]^+$ 279.06203, found 279.06140.

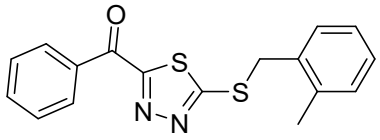


*Date for* **E8**. A yellow liquid, yield 90%. $^1$H NMR (400 MHz, $CDCl_3$) δ: 8.51 (d, $J$ = 8.0 Hz, 2H, phenyl H), 7.69–7.64 (m, 1H, phenyl H), 7.56–7.51 (m, 2H, phenyl H), 3.43 (t, $J$ = 8.0 Hz, 2H, $S\underline{CH_2}$), 1.82–1.70 (m, 3H, $CH_2\underline{CH_2CH}(CH_3)_2$), 0.98 (d, $J$ = 4.0 Hz, 6H, $CH_2CH_2CH(\underline{CH_3})_2$); $^{13}$C NMR (101 MHz, $CDCl_3$) δ: 183.01, 173.10, 168.97, 134.61, 134.47, 131.28, 128.74, 37.80, 32.52, 27.71, 22.31; HRMS (ESI): m/z calcd for $C_{14}H_{16}N_2OS_2$ $[M+H]^+$ 293.07768, found 293.07727.

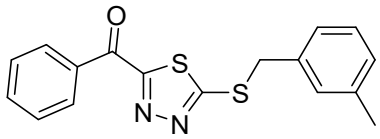


*Date for* **E9**. A yellowish orange solid, yield 88%, m.p. 56-58 $^o$C. $^1$H NMR (400 MHz, DMSO-$d_6$)

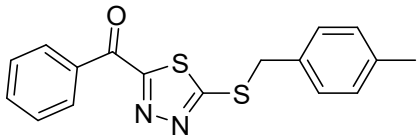
δ: 8.34–8.31 (m, 2H, phenyl H), 7.79–7.75 (m, 1H, phenyl H), 7.65–7.61 (m, 2H, phenyl H), 7.55–7.53 (m, 2H, phenyl H), 7.40–7.36 (m, 2H, phenyl H), 7.34–7.30 (m, 1H, phenyl H), 4.71 (s, 2H, $CH_2$); $^{13}C$ NMR (101 MHz, DMSO-$d_6$) δ: 182.71, 171.95, 168.74, 135.84, 134.45, 134.26, 130.66, 129.22, 128.73, 128.69, 127.89, 37.52; HRMS (ESI): m/z calcd for $C_{16}H_{12}N_2OS_2$ $[M+H]^+$ 313.04638, found 313.04599.



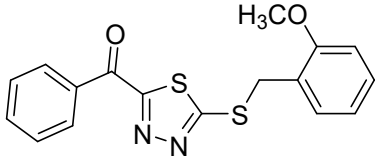
*Date for* **E10**. A yellowish orange solid, yield 90%, m.p. 45-47 °C. $^1H$ NMR (400 MHz, DMSO-$d_6$) δ: 8.34 (d, $J$ = 8.0 Hz, 2H, phenyl H), 7.80–7.76 (m, 1H, phenyl H), 7.65–7.62 (m, 2H, phenyl H), 7.48 (d, $J$ = 8.0 Hz, 1H, phenyl H), 7.26–7.24 (m, 2H, phenyl H), 7.23–7.18 (m, 1H, phenyl H), 4.73 (s, 2H, $CH_2$), 2.42 (s, 3H, $CH_3$); $^{13}C$ NMR (101 MHz, DMSO-$d_6$) δ: 182.75, 171.74, 168.81, 137.06, 134.50, 134.28, 133.18, 130.69, 130.59, 130.20, 128.77, 128.35, 126.26, 36.13, 18.86; HRMS (ESI): m/z calcd for $C_{17}H_{14}N_2OS_2$ $[M+H]^+$ 327.06203, found 327.06158.



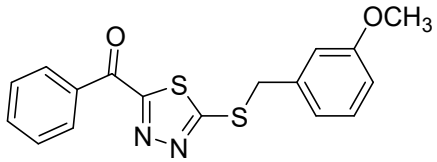
*Date for* **E11**. A greenish-yellow solid, yield 89%, m.p. 58-59 °C. $^1H$ NMR (400 MHz, $CDCl_3$) δ: 8.52–8.49 (m, 2H, phenyl H), 7.70–7.65 (m, 1H, phenyl H), 7.56–7.52 (m, 2H, phenyl H), 7.27–7.22 (m, 3H, phenyl H), 7.13 (d, $J$ = 8.0 Hz, 1H, phenyl H), 4.63 (s, 2H, $CH_2$), 2.36 (s, 3H, $CH_3$); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ: 183.03, 172.14, 169.26, 138.82, 135.12, 134.59, 134.52, 131.28, 130.03, 129.12, 128.91, 128.77, 126.43, 38.28, 21.51; HRMS (ESI): m/z calcd for $C_{17}H_{14}N_2OS_2$ $[M+H]^+$ 327.06203, found 327.06155.



*Date for* **E12**. A yellow solid, yield 86%, m.p. 71-72 °C. $^1$H NMR (400 MHz, DMSO-$d_6$) δ: 8.34–8.31 (m, 2H, phenyl H), 7.79–7.75 (m, 1H, phenyl H), 7.64–7.61 (m, 2H, phenyl H), 7.41 (d, $J$ = 8.0 Hz, 2H, phenyl H), 7.18 (d, $J$ = 8.0 Hz, 2H, phenyl H), 4.66 (s, 2H, $CH_2$), 2.29 (s, 3H, $CH_3$); $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ: 182.70, 172.08, 168.67, 137.23, 134.46, 134.27, 132.64, 130.67, 129.25, 129.16, 128.74, 37.40, 20.74; HRMS (ESI): m/z calcd for $C_{17}H_{14}N_2OS_2$ $[M+H]^+$ 327.06203, found 327.06161.

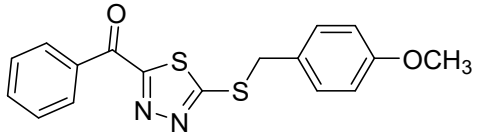


*Date for* **E13**. A white solid, yield 87%, m.p. 85-86 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ: 8.50 (d, $J$ = 8.0 Hz, 2H, phenyl H), 7.68–7.64 (m, 1H, phenyl H), 7.55–7.47 (m, 3H, phenyl H), 7.32–7.24 (m, 1H, phenyl H), 6.94–6.90 (m, 2H, phenyl H), 4.69 (s, 2H, $CH_2$), 3.89 (s, 3H, $CH_3$); $^{13}$C NMR (101 MHz, $CDCl_3$) δ: 183.07, 173.10, 169.05, 157.71, 134.64, 134.44, 131.25, 131.05, 129.83, 128.73, 123.79, 120.71, 110.75, 55.66, 33.36; HRMS (ESI): m/z calcd for $C_{17}H_{14}N_2O_2S_2$ $[M+H]^+$ 343.05695, found 343.05679.

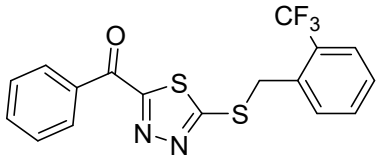


*Date for* **E14**. A white solid, yield 90%, m.p. 71-72 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ: 8.51–8.48 (m, 2H, phenyl H), 7.69–7.65 (m, 1H, phenyl H), 7.56–7.52 (m, 2H, phenyl H), 7.27 (t, $J$ = 8.0 Hz, 1H, phenyl H), 7.06 (d, $J$ = 8.0 Hz, 1H, phenyl H), 7.00 (s, 1H, phenyl H), 6.87–6.84 (m, 1H, phenyl H), 4.63 (s, 2H, $CH_2$), 3.81 (s, 3H, $CH_3$); $^{13}$C NMR (101 MHz, $CDCl_3$) δ: 182.99, 171.96,

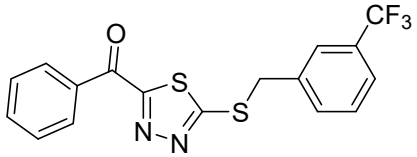
169.30, 159.99, 136.72, 134.54, 134.52, 131.26, 130.04, 128.76, 121.65, 114.83, 113.83, 55.42, 38.22; HRMS (ESI): m/z calcd for $C_{17}H_{14}N_2O_2S_2$ $[M+H]^+$ 343.05695, found 343.05612.




*Date for* **E15**. A white solid, yield 91%, m.p. 89-90 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ: 8.51–8.48 (m, 2H, phenyl H), 7.69–7.65 (m, 1H, phenyl H), 7.56–7.52 (m, 2H, phenyl H), 7.41–7.37 (m, 2H, phenyl H), 6.89–6.86 (m, 2H, phenyl H), 4.61 (s, 2H, $CH_2$), 3.80 (s, 3H, $CH_3$); $^{13}$C NMR (101 MHz, $CDCl_3$) δ: 183.01, 172.15, 169.19, 159.56, 134.57, 134.50, 131.26, 130.65, 128.75, 127.12, 114.35, 55.43, 37.91; HRMS (ESI): m/z calcd for $C_{17}H_{14}N_2O_2S_2$ $[M+H]^+$ 343.05695, found 343.05606.

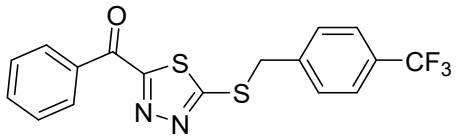



*Date for* **E16**. A yellow solid, yield 90%, m.p. 64-66 °C. $^1$H NMR (400 MHz, DMSO-$d_6$) δ: 8.36–8.33 (m, 2H, phenyl H), 7.86 (d, $J$ = 8.0 Hz, 1H, phenyl H), 7.82–7.76 (m, 2H, phenyl H), 7.72 (t, $J$ = 8.0 Hz, 1H, phenyl H), 7.65–7.61 (m, 2H, phenyl H), 7.58 (t, $J$ = 8.0 Hz, 1H, phenyl H), 4.90 (s, 2H, $CH_2$); $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ: 182.76, 170.74, 169.24, 134.53, 134.23, 133.76 (d, $J$ = 1.0 Hz), 133.18, 132.05, 130.70, 128.83, 128.76, 127.38 (q, $J$ = 30.3 Hz), 126.48 (q, $J$ = 5.1 Hz), 124.28 (q, J = 275.7 Hz), 34.20 (d, $J$ = 2.0 Hz); $^{19}$F NMR (376 MHz, DMSO-$d_6$) δ: -58.09; HRMS (ESI): m/z calcd for $C_{17}H_{11}F_3N_2OS_2$ $[M+H]^+$ 381.03377, found 381.03305.

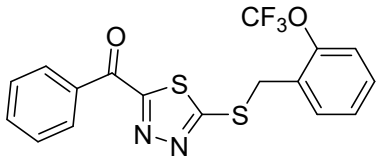



*Date for* **E17**. A yellow solid, yield 90%, m.p. 74-76 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ: 8.51–

8.48 (m, 2H, phenyl H), 7.73 (s, 1H, phenyl H), 7.71–7.65 (m, 2H, phenyl H), 7.58–7.52 (m, 3H, phenyl H), 7.48 (t, $J$ = 8.0 Hz, 1H, phenyl H), 4.72 (s, 2H, $CH_2$); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ: 182.95, 170.92, 169.69, 136.79, 134.61, 134.49, 132.81 (d, $J$ = 1.0 Hz), 131.53, 131.26, 129.47, 128.81, 126.08 (q, $J$ = 4.0 Hz), 125.10 (q, $J$ = 4.0 Hz), 123.96 (q, $J$ = 269.7 Hz), 37.25; $^{19}F$ NMR (376 MHz, $CDCl_3$) δ -62.65; HRMS (ESI): m/z calcd for $C_{17}H_{11}F_3N_2OS_2$ $[M+H]^+$ 381.03377, found 381.03302.

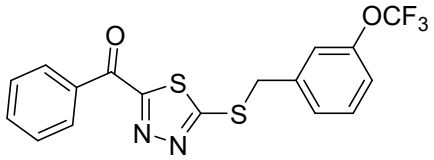



*Date for* **E18**. A yellowish orange solid, yield 89%, m.p. 117-118 °C. $^1H$ NMR (400 MHz, DMSO-$d_6$) δ: 8.32 (d, $J$ = 8.0 Hz, 2H, phenyl H), 7.79–7.73 (m, 5H, phenyl H), 7.64–7.60 (m, 2H, phenyl H), 4.81 (s, 2H, $CH_2$); $^{13}C$ NMR (101 MHz, DMSO-$d_6$) δ: 182.68, 171.35, 169.03, 141.29 (d, $J$ = 1.0 Hz), 134.46, 134.22, 130.65, 130.00, 128.72, 128.25 (q, $J$ = 31.9 Hz), 125.49 (q, $J$ = 4.0 Hz), 124.16 (q, $J$ = 272.7 Hz), 36.57; $^{19}F$ NMR (471 MHz, $CDCl_3$) δ: -62.50; HRMS (ESI): m/z calcd for $C_{17}H_{11}F_3N_2OS_2$ $[M+H]^+$ 381.03377, found 381.03311.

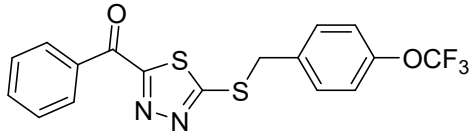



*Date for* **E19**. A yellow solid, yield 92%, m.p. 66-67 °C. $^1H$ NMR (400 MHz, $CDCl_3$) δ: 8.50 (d, $J$ = 8.0 Hz, 2H, phenyl H), 7.70–7.65 (m, 2H, phenyl H), 7.57–7.53 (m, 2H, phenyl H), 7.38–7.34 (m, 1H, phenyl H), 7.31–7.24 (m, 2H, phenyl H), 4.74 (s, 2H, $CH_2$); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ: 182.99, 171.49, 169.59, 147.86 (q, $J$ = 1.4 Hz), 134.57, 134.55, 131.86, 131.26, 129.91, 128.79, 128.22, 127.06, 120.67 (q, $J$ = 259.6 Hz), 120.39 (q, $J$ = 1.6 Hz), 32.08; $^{19}F$ NMR (376 MHz, $CDCl_3$) δ: -56.88; HRMS (ESI): m/z calcd for $C_{17}H_{11}F_3N_2O_2S_2$ $[M+H]^+$ 397.02868, found

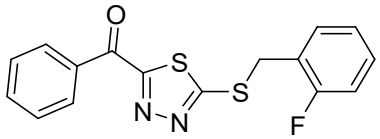
397.02795.



*Date for* **E20**. A yellow solid, yield 93%, m.p. 64-66 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ: 8.51–8.48 (m, 2H, phenyl H), 7.70–7.66 (m, 1H, phenyl H), 7.57–7.52 (m, 2H, phenyl H), 7.44–7.41 (m, 1H, phenyl H), 7.38 (t, *J* = 8.0 Hz, 1H, phenyl H), 7.34 (s, 1H, phenyl H), 7.18–7.15 (m, 1H, phenyl H), 4.67 (s, 2H, $CH_2$); $^{13}$C NMR (101 MHz, $CDCl_3$) δ: 182.95, 171.02, 169.63, 149.53 (q, *J* = 2.0 Hz), 137.97, 134.60, 134.48, 131.26, 130.34, 128.80, 127.78, 121.90, 120.68, 120.52 (q, *J* = 258.6 Hz), 37.19; $^{19}$F NMR (376 MHz, $CDCl_3$) δ: -57.75; HRMS (ESI): m/z calcd for $C_{17}H_{11}F_3N_2O_2S_2$ $[M+H]^+$ 397.02868, found 397.02808.

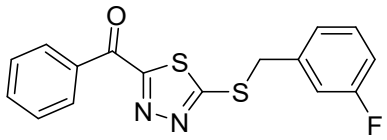


*Date for* **E21**. A yellow solid, yield 87%, m.p. 90-91 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ: 8.51–8.48 (m, 2H, phenyl H), 7.70–7.66 (m, 1H, phenyl H), 7.57–7.50 (m, 4H, phenyl H), 7.19 (d, *J* = 8.0 Hz, 2H, phenyl H), 4.66 (s, 2H, $CH_2$); $^{13}$C NMR (101 MHz, $CDCl_3$) δ: 182.96, 171.23, 169.60, 149.03 (q, *J* = 2.0 Hz), 134.60, 134.6 (d, *J* = 3.9 Hz), 131.26, 130.89, 128.80, 121.41, 120.52 (q, *J* = 258.4 Hz), 119.26 (q, *J* = 2.5 Hz), 37.00; $^{19}$F NMR (376 MHz, $CDCl_3$) δ: -57.83; HRMS (ESI): m/z calcd for $C_{17}H_{11}F_3N_2O_2S_2$ $[M+H]^+$ 397.02868, found 397.02817.

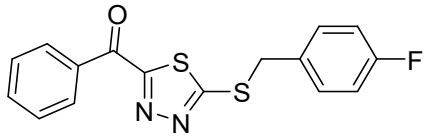


*Date for* **E22**. A yellowish orange solid, yield 91%, m.p. 59-60 °C. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ: 8.34–8.31 (m, 2H, phenyl H), 7.80–7.75 (m, 1H, phenyl H), 7.65–7.61 (m, 3H, phenyl H),

7.42–7.37 (m, 1H, phenyl H), 7.29–7.24 (m, 1H, phenyl H), 7.23–7.20 (m, 1H, phenyl H), 4.75 (s, 2H, $CH_2$); $^{13}C$ NMR (101 MHz, DMSO-$d_6$) δ: 182.74, 171.20, 169.08, 160.57 (d, $J$ = 247.5 Hz), 134.51, 134.25, 131.62 (d, $J$ = 3.0 Hz), 130.70, 130.36 (d, $J$ = 8.1 Hz), 128.76, 124.72 (d, $J$ = 3.0 Hz), 122.94 (d, $J$ = 14.1 Hz), 115.64 (d, $J$ = 20.2 Hz), 31.16 (d, $J$ = 3.0 Hz); $^{19}F$ NMR (471 MHz, $CDCl_3$) δ: -116.31; HRMS (ESI): m/z calcd for $C_{16}H_{11}FN_2OS_2$ $[M+H]^+$ 331.03696, found 331.03632.

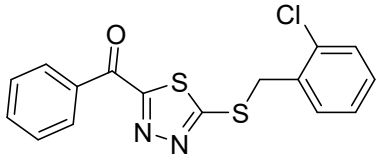



*Date for* **E23**. A greenish-yellow solid, yield 89%, m.p. 66-67 °C. $^1H$ NMR (400 MHz, $CDCl_3$) δ: 8.51–8.48 (m, 2H, phenyl H), 7.69–7.65 (m, 1H, phenyl H), 7.56–7.52 (m, 2H, phenyl H), 7.34–7.29 (m, 1H, phenyl H), 7.24 (s, 1H, phenyl H), 7.22–7.18 (m, 1H, phenyl H), 7.03–6.97 (m, 1H, phenyl H), 4.64 (s, 2H, $CH_2$); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ: 182.93, 171.28, 169.53, 162.93 (d, $J$ = 248.5 Hz), 137.99 (d, $J$ = 7.1 Hz), 134.56, 134.47, 131.24, 130.48 (d, $J$ = 8.1 Hz), 128.77, 125.04 (d, $J$ = 3.0 Hz), 116.30 (d, $J$ = 22.2 Hz), 115.25 (d, $J$ = 21.2 Hz), 37.34 (d, $J$ = 2.0 Hz); $^{19}F$ NMR (376 MHz, $CDCl_3$) δ: -112.17; HRMS (ESI): m/z calcd for $C_{16}H_{11}FN_2OS_2$ $[M+H]^+$ 331.03696, found 331.03647.

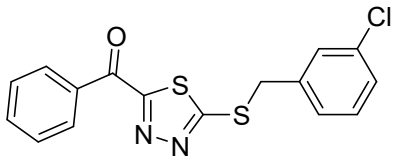



*Date for* **E24**. A yellow solid, yield 90%, m.p. 96-97 °C. $^1H$ NMR (400 MHz, DMSO-$d_6$) δ: 8.33–8.30 (m, 2H, phenyl H), 7.79–7.74 (m, 1H, phenyl H), 7.64–7.55 (m, 4H, phenyl H), 7.23–7.17 (m, 2H, phenyl H), 4.70 (s, 2H, $CH_2$); $^{13}C$ NMR (101 MHz, DMSO-$d_6$) δ: 182.70, 171.71, 168.82, 161.67 (d, $J$ = 245.4 Hz), 134.46, 134.25, 132.26 (d, $J$ = 3.0 Hz), 131.33 (d, $J$ = 8.1 Hz), 130.66,

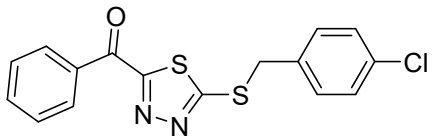
128.73, 115.49 (d, $J$ = 22.2 Hz), 36.61; $^{19}$F NMR (376 MHz, $CDCl_3$) δ: -114.24; HRMS (ESI): m/z calcd for $C_{16}H_{11}FN_2OS_2$ $[M+H]^+$ 331.03696, found 331.03644.




*Date for* **E25**. A yellowish orange solid, yield 87%, m.p. 103-104 °C. $^1$H NMR (400 MHz, DMSO-$d_6$) δ: 8.34–8.31 (m, 2H, phenyl H), 7.79–7.75 (m, 1H, phenyl H), 7.71–7.68 (m, 1H, phenyl H), 7.62 (t, $J$ = 8.0 Hz, 2H, phenyl H), 7.54–7.51 (m, 1H, phenyl H), 7.40–7.34 (m, 2H, phenyl H), 4.80 (s, 2H, $CH_2$); $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ: 182.73, 171.07, 169.09, 134.48, 134.23, 133.50, 133.28, 131.72, 130.67, 130.05, 129.71, 128.74, 127.56, 35.52; HRMS (ESI): m/z calcd for $C_{16}H_{11}ClN_2OS_2$ $[M+H]^+$ 347.00741, found 347.00681.

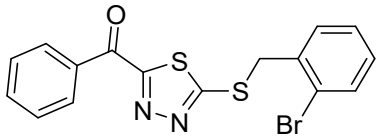



*Date for* **E26**. A greenish-yellow solid, yield 85%, m.p. 77-78 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ: 8.51–8.48 (m, 2H, phenyl H), 7.70–7.65 (m, 1H, phenyl H), 7.56–7.52 (m, 2H, phenyl H), 7.48 (s, 1H, phenyl H), 7.39–7.34 (m, 1H, phenyl H), 7.31–7.28 (m, 2H, phenyl H), 4.63 (s, 2H, $CH_2$); $^{13}$C NMR (101 MHz, $CDCl_3$) δ: 182.97, 171.21, 169.58, 137.61, 134.76, 134.58, 134.51, 131.27, 130.21, 129.39, 128.79, 128.49, 127.57, 37.27; HRMS (ESI): m/z calcd for $C_{16}H_{11}ClN_2OS_2$ $[M+H]^+$ 347.00741, found 347.00677.

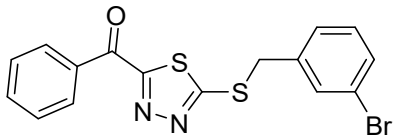



*Date for* **E27**. A yellowish orange solid, yield 90%, m.p. 106-108 °C. $^1$H NMR (400 MHz, DMSO-$d_6$) δ: 8.32 (d, $J$ = 8.0 Hz, 2H, phenyl H), 7.79–7.75 (m, 1H, phenyl H), 7.64–7.61 (m, 2H,

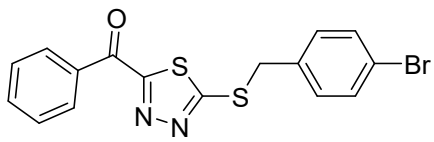
phenyl H), 7.57 (d, *J* = 8.0 Hz, 2H, phenyl H), 7.44 (d, *J* = 8.0 Hz, 2H, phenyl H), 4.71 (s, 2H, $CH_2$); $^{13}C$ NMR (101 MHz, DMSO-$d_6$) δ: 182.69, 171.58, 168.89, 135.23, 134.46, 134.24, 132.45, 131.09, 130.66, 128.72, 128.62, 36.57; HRMS (ESI): m/z calcd for $C_{16}H_{11}ClN_2OS_2$ $[M+H]^+$ 347.00741, found 347.00681.




*Date for* **E28**. A yellowish solid, yield 88%, m.p. 105-106 °C. $^1H$ NMR (400 MHz, DMSO-$d_6$) δ: 8.35–8.32 (m, 2H, phenyl H), 7.80–7.76 (m, 1H, phenyl H), 7.72–7.69 (m, 2H, phenyl H), 7.65–7.61 (m, 2H, phenyl H), 7.43–7.39 (m, 1H, phenyl H), 7.32–7.28 (m, 1H, phenyl H), 4.80 (s, 2H, $CH_2$); $^{13}C$ NMR (101 MHz, DMSO-$d_6$) δ: 182.75, 171.05, 169.12, 134.92, 134.51, 134.25, 133.02, 131.79, 130.70, 130.27, 128.76, 128.16, 124.25, 38.16; HRMS (ESI): m/z calcd for $C_{16}H_{11}BrN_2OS_2$ $[M+H]^+$ 390.95689, found 390.95636.

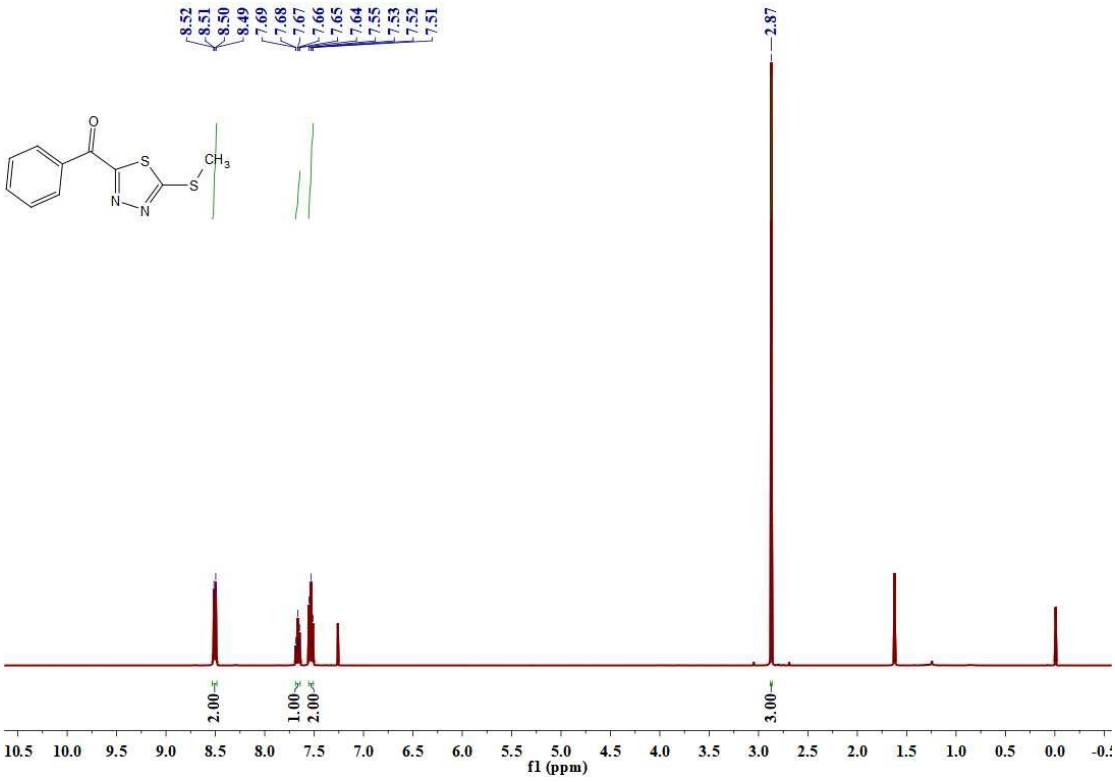


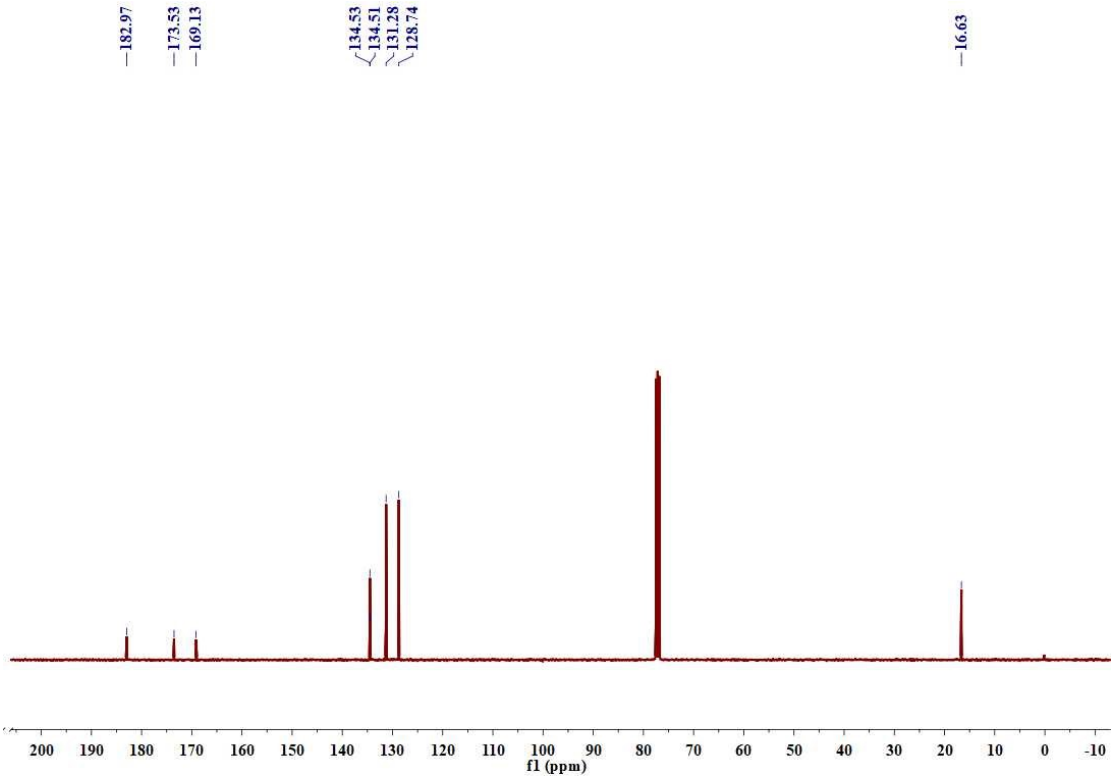

*Date for* **E29**. A yellow solid, yield 84%, m.p. 97-98 °C. $^1H$ NMR (400 MHz, $CDCl_3$) δ: 8.51–8.48 (m, 2H, phenyl H), 7.70–7.65 (m, 1H, phenyl H), 7.63 (s, 1H, phenyl H), 7.56–7.52 (m, 2H, phenyl H), 7.45–7.41 (m, 2H, phenyl H), 7.22 (t, *J* = 8.0 Hz, 1H, phenyl H), 4.62 (s, 2H, $CH_2$); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ: 182.95, 171.17, 169.58, 137.88, 134.57, 134.50, 132.27, 131.40, 131.26, 130.47, 128.79, 128.04, 122.89, 37.19; HRMS (ESI): m/z calcd for $C_{16}H_{11}BrN_2OS_2$ $[M+H]^+$ 390.95689, found 390.95630.



*Date for* **E30**. A yellowish orange solid, yield 89%, m.p. 103-104 °C. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ: 8.33–8.31 (m, 2H, phenyl H), 7.79–7.75 (m, 1H, phenyl H), 7.65–7.61 (m, 2H, phenyl H), 7.59–7.56 (m, 2H, phenyl H), 7.52–7.48 (m, 2H, phenyl H), 4.69 (s, 2H, $CH_2$); $^{13}$C NMR (101 MHz, DMSO-$d_6$) δ: 183.16, 172.04, 169.37, 136.14, 134.93, 134.71, 132.01, 131.89, 131.13, 129.20, 121.48, 37.09; HRMS (ESI): m/z calcd for $C_{16}H_{11}BrN_2OS_2$ $[M+H]^+$ 390.95689, found 390.95618.

**2. Copies of $^{1}$H NMR, $^{13}$C NMR, $^{19}$F NMR and HRMS of the title compounds**






23 #39 RT: 0.39 AV: 1 NL: 5.01E+008
T: FTMS + p ESI Full ms [120.0000-1800.0000]

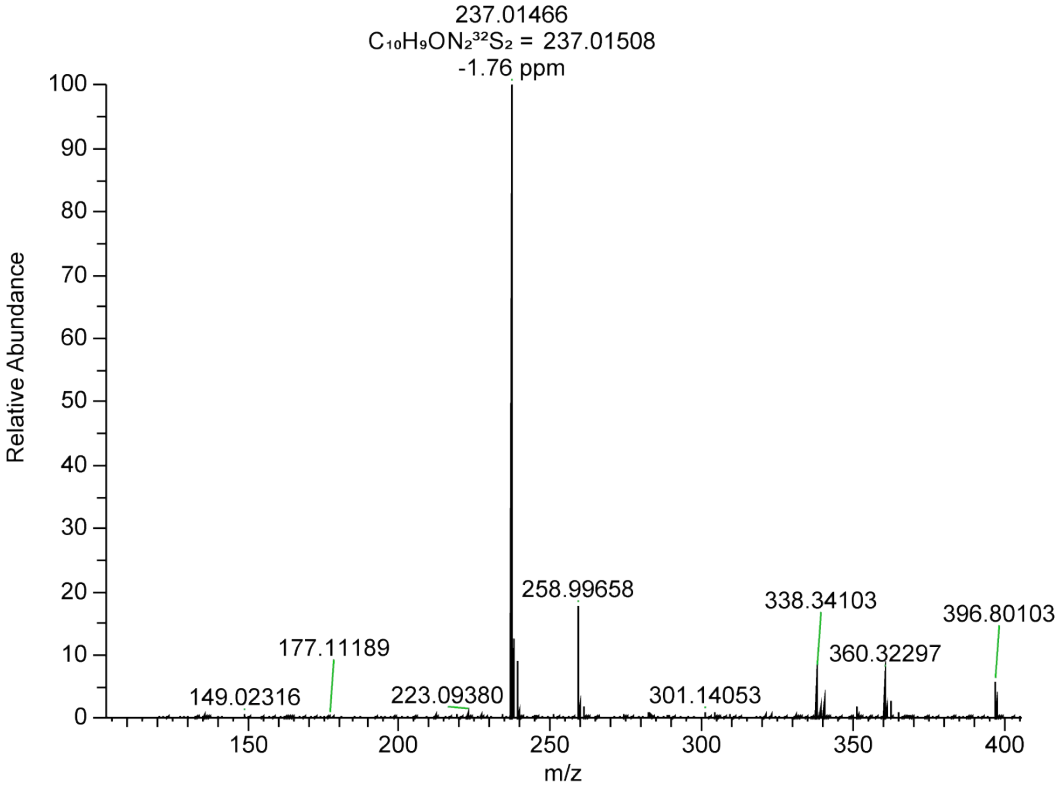
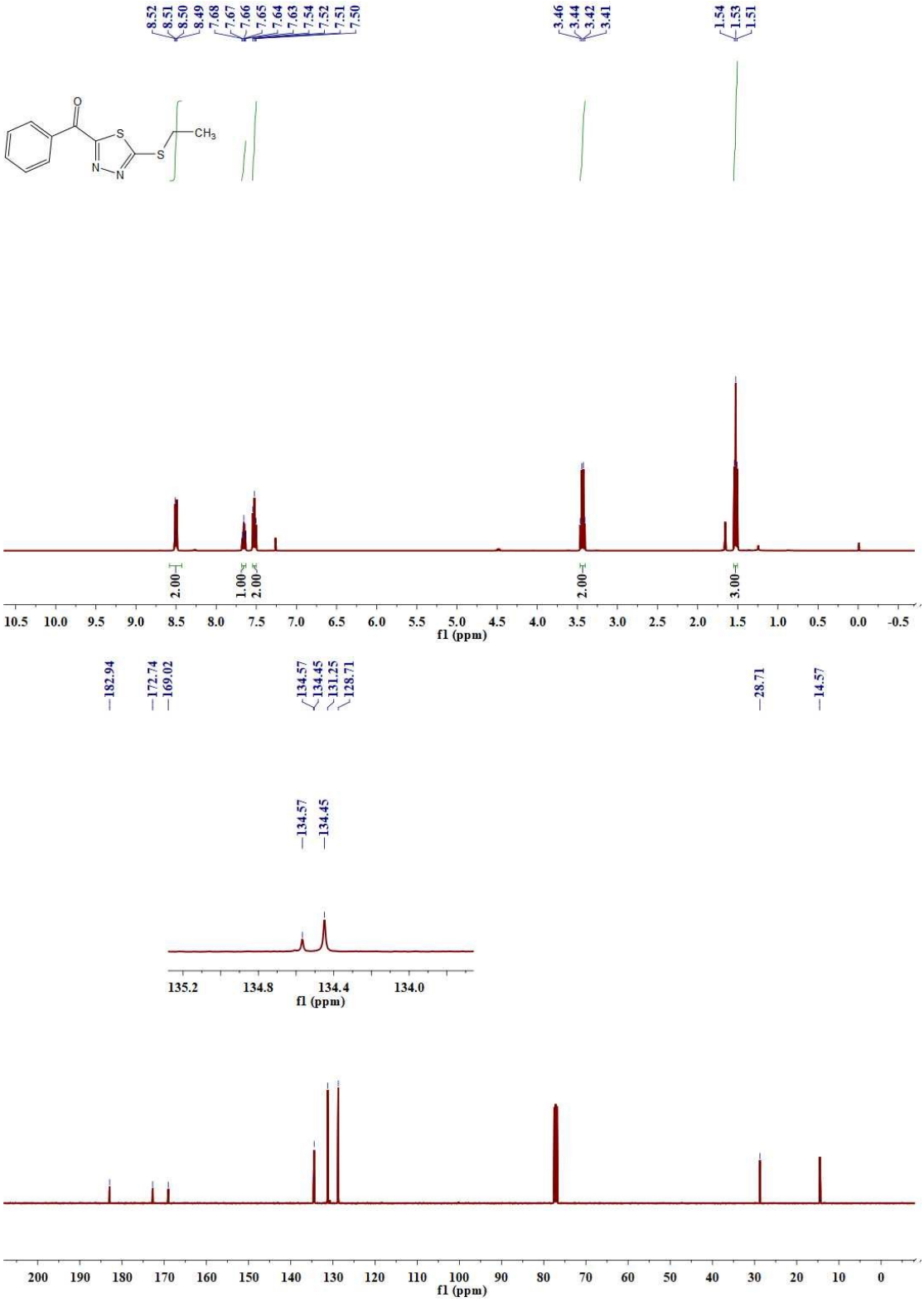



**Figure S1.** $^{1}$H NMR, $^{13}$C NMR and HRMS for **E1**.


8.52
8.51
8.50
8.49
7.68
7.67
7.66
7.65
7.64
7.63
7.54
7.52
7.51
7.50
3.46
3.44
3.42
3.41
1.54
1.53
1.51
O
S
N
N
S
CH3
2.00
1.00
2.00
2.00
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
182.94
172.74
169.02
134.57
134.45
131.25
128.71
28.71
14.57
134.57
134.45
135.2 134.8 134.4 134.0
f1 (ppm)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

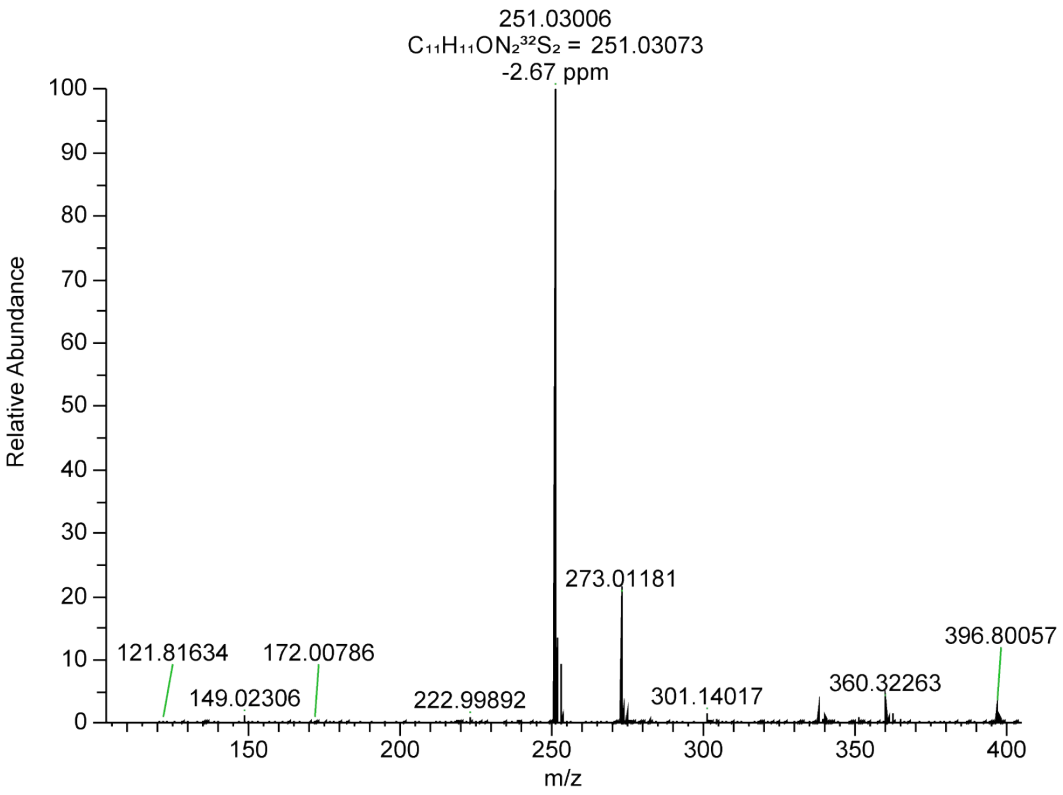
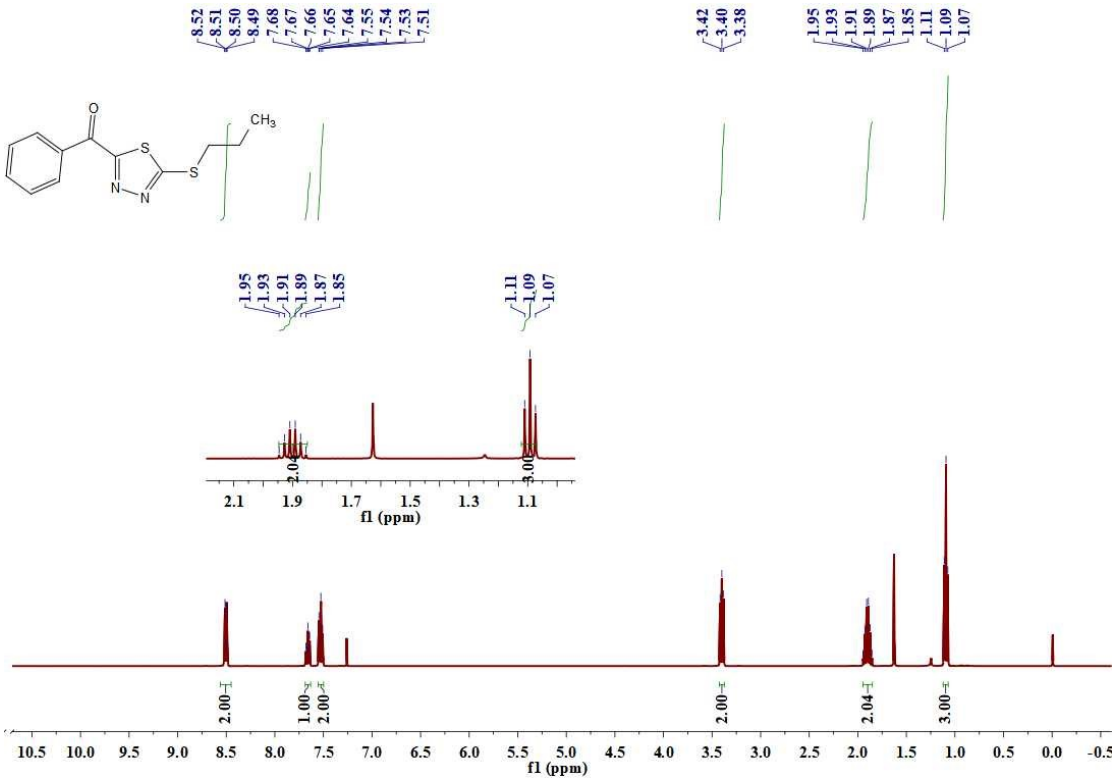
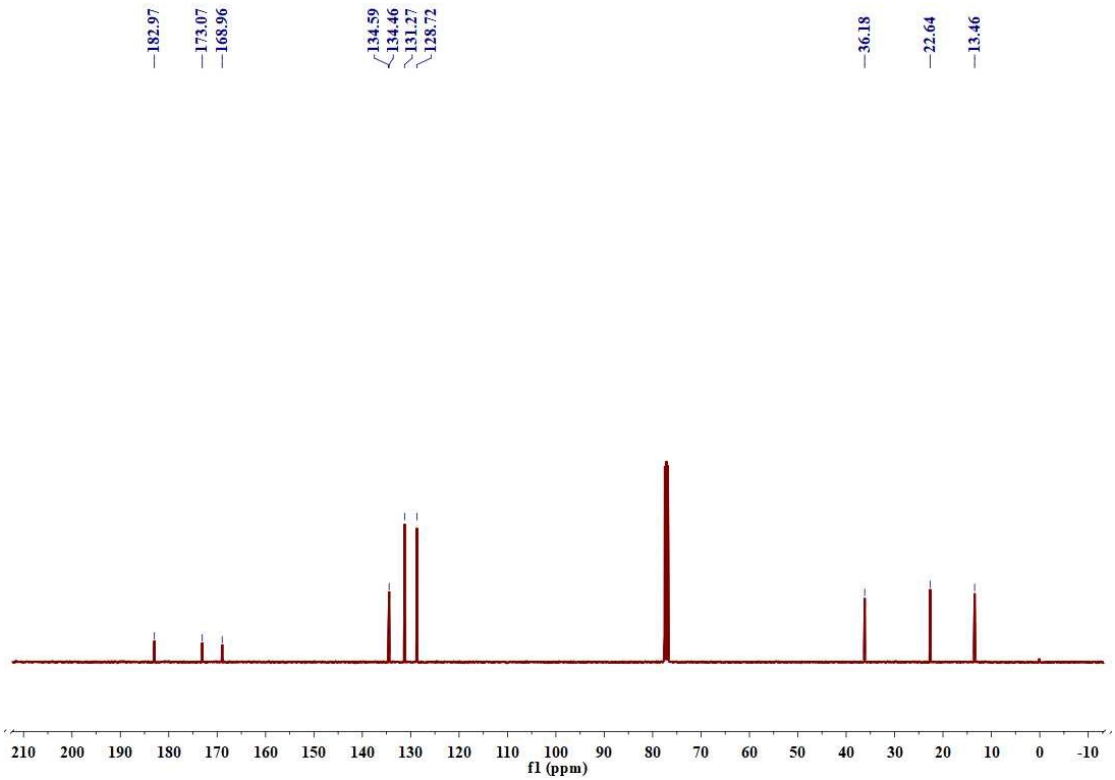



**Figure S2.** $^{1}$H NMR, $^{13}$C NMR and HRMS for **E2**.






25 #57 RT: 0.56 AV: 1 NL: 1.24E+009
T: FTMS + p ESI Full ms [120.0000-1800.0000]

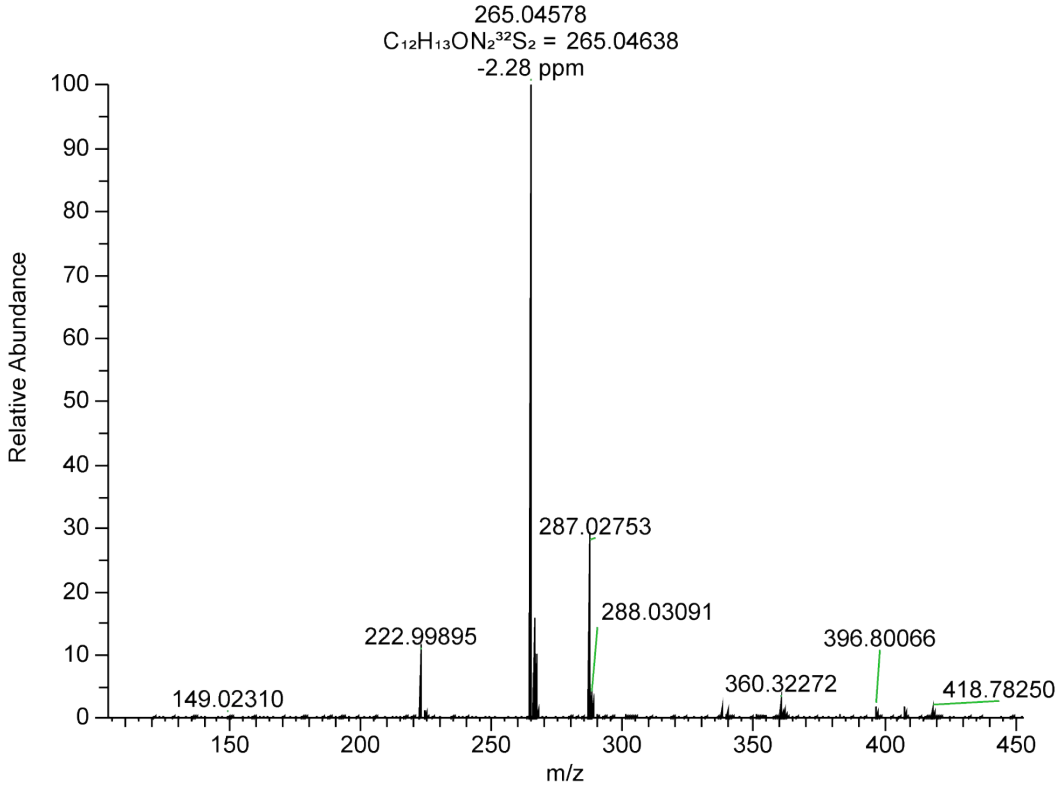
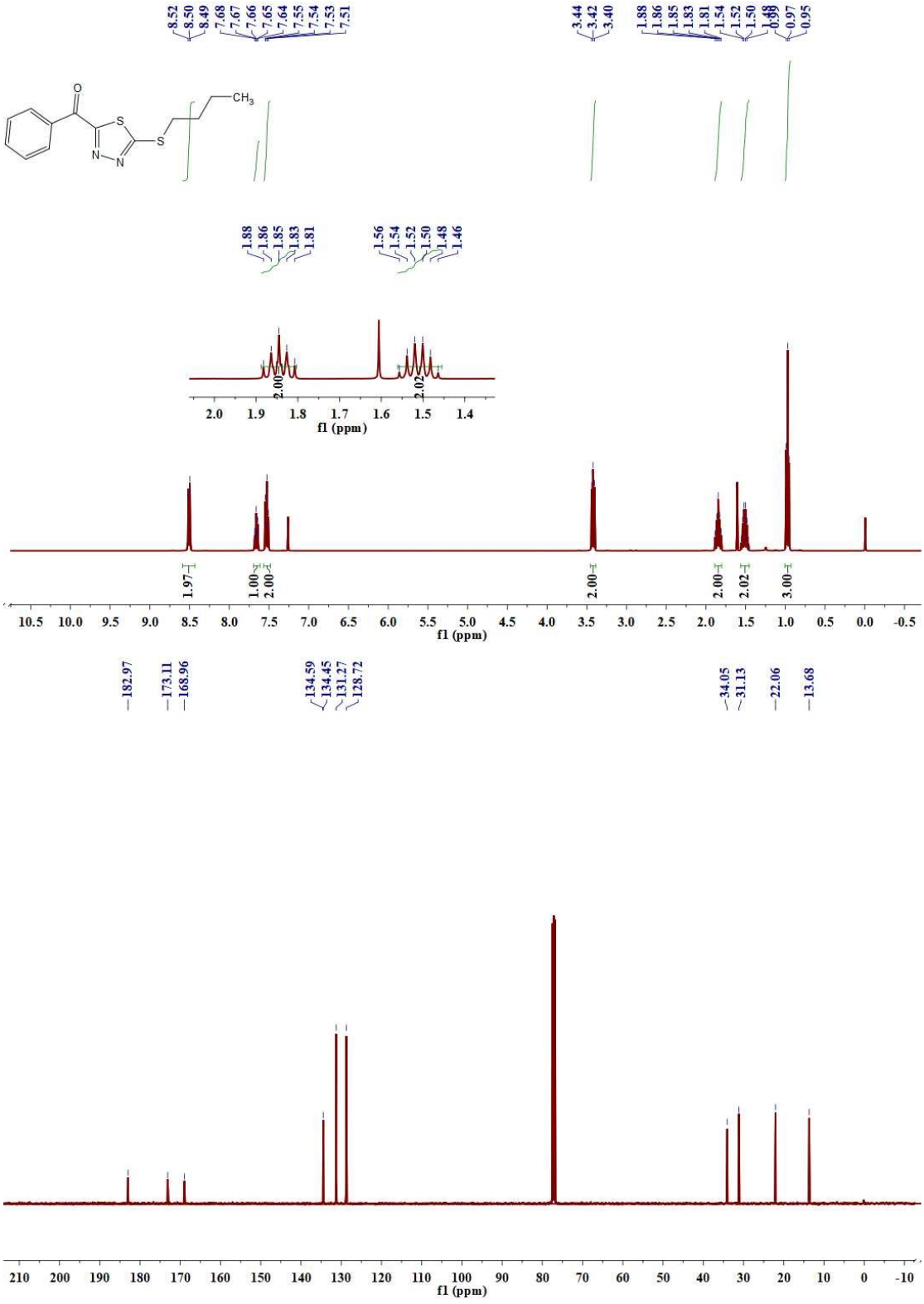



**Figure S3.** $^{1}$H NMR, $^{13}$C NMR and HRMS for **E3**.


8.52
8.50
8.49
7.68
7.67
7.66
7.65
7.64
7.55
7.54
7.53
7.51
3.44
3.42
3.40
1.88
1.86
1.85
1.83
1.81
1.54
1.52
1.50
0.97
0.95
O
S
N
N
S
CH3
1.88
1.86
1.85
1.83
1.81
1.56
1.54
1.52
1.50
1.48
1.46
2.00
2.02
2.0 1.9 1.8 1.7 1.6 1.5 1.4
f1 (ppm)
1.97
1.00
2.00
2.00
2.00
2.02
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
182.97
173.11
168.96
134.59
134.45
131.27
128.72
34.05
31.13
22.06
13.68
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

33 #81 RT: 0.80 AV: 1 NL: 1.04E+008
T: FTMS + p ESI Full ms [120.0000-1800.0000]

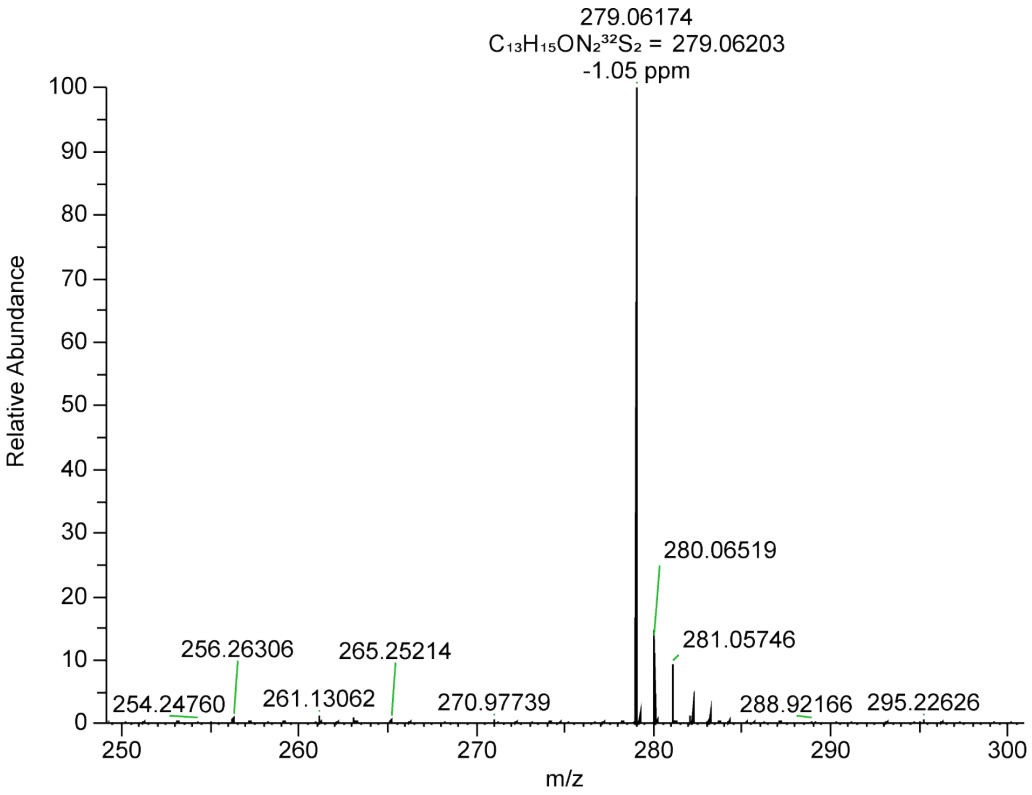
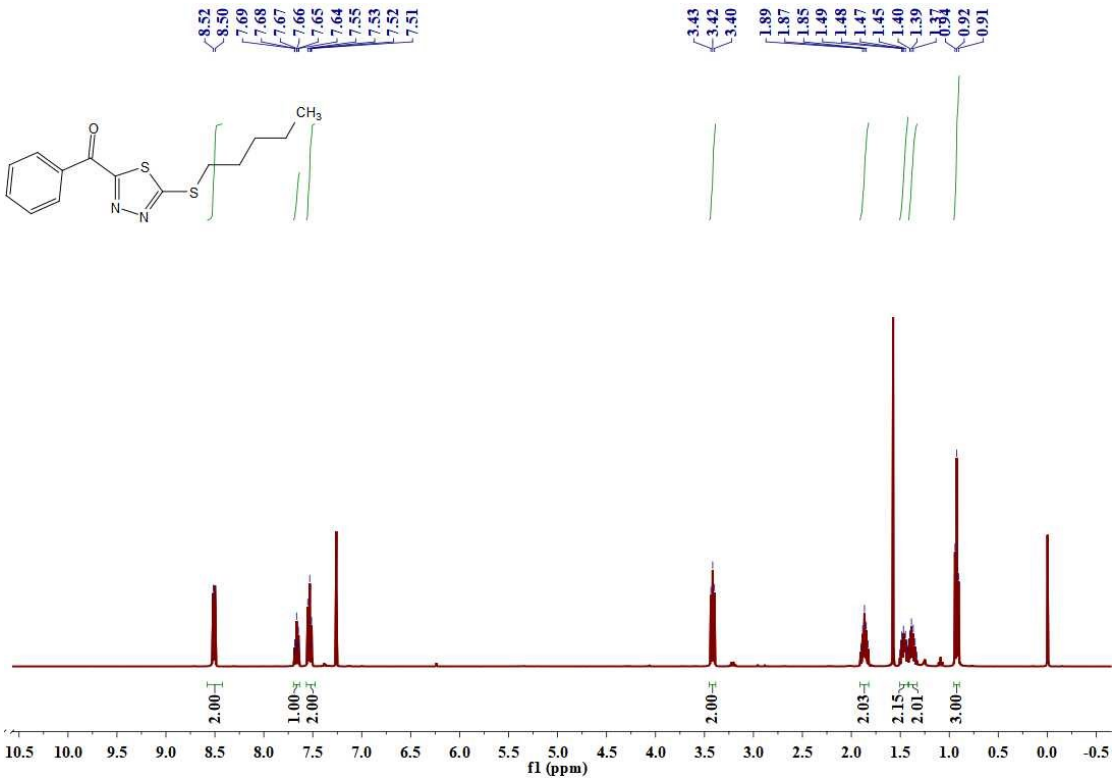
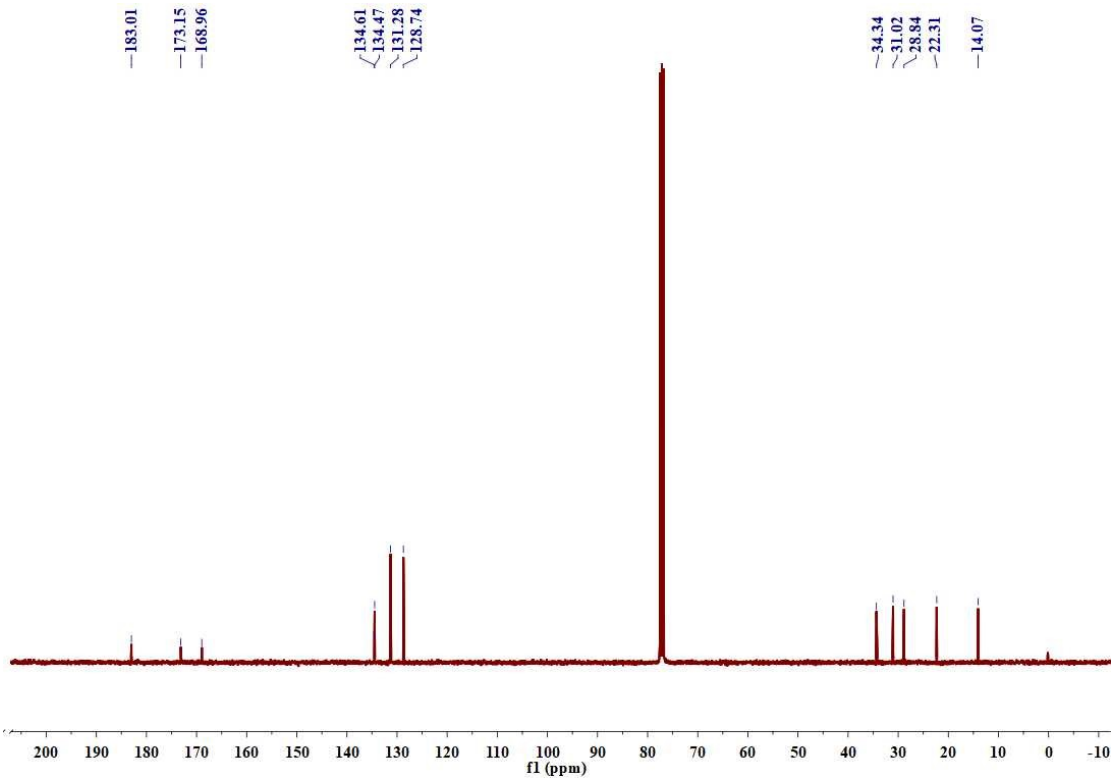



**Figure S4.** $^{1}$H NMR, $^{13}$C NMR and HRMS for **E4**.






34 #45 RT: 0.45 AV: 1 NL: 4.77E+007
T: FTMS + p ESI Full ms [120.0000-1800.0000]

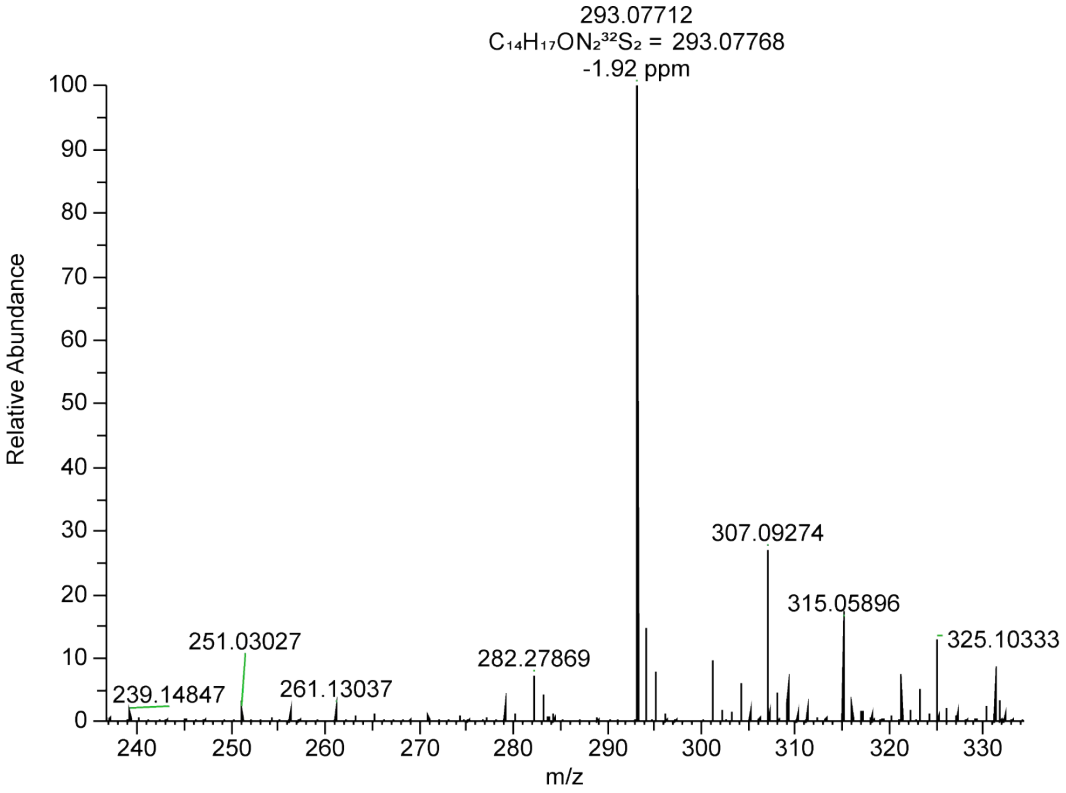
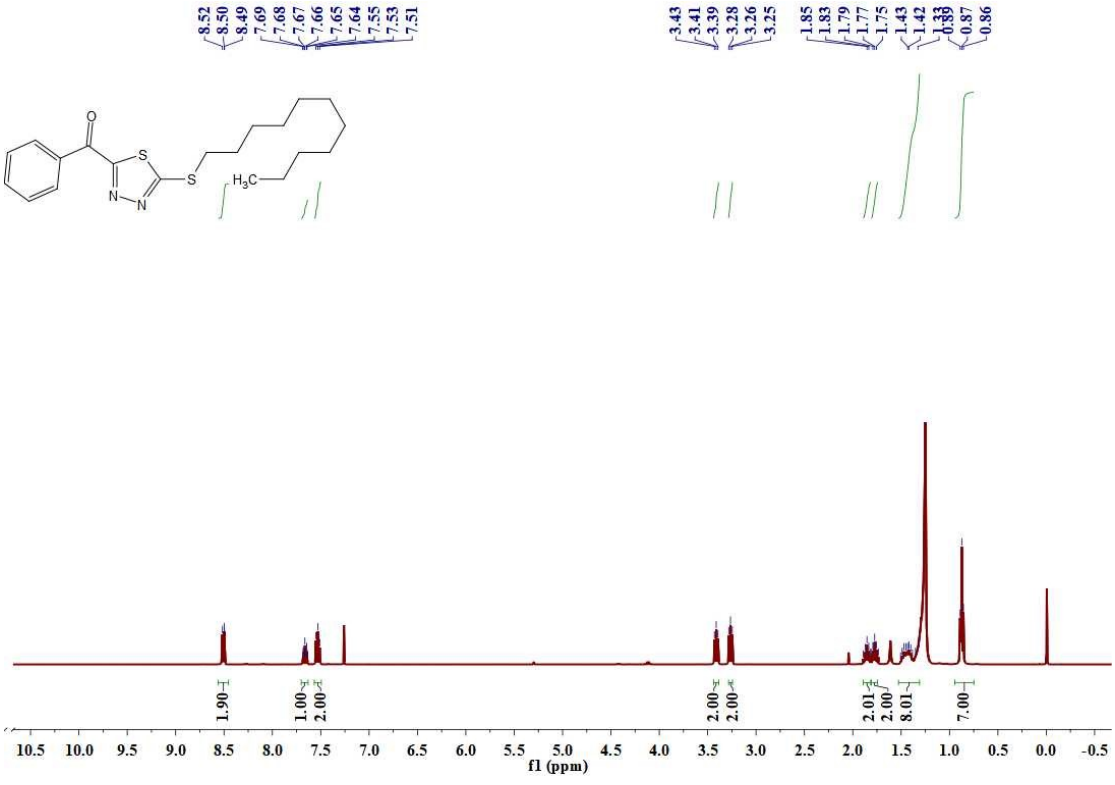



**Figure S5.** $^{1}$H NMR, $^{13}$C NMR and HRMS for **E5**.


8.52
8.50
8.49
7.69
7.68
7.67
7.66
7.65
7.64
7.55
7.53
7.51
3.43
3.41
3.39
3.28
3.26
3.25
1.85
1.83
1.79
1.77
1.75
1.43
1.42
1.33
0.88
0.87
0.86
O
S
N
N
S
H3C
1.90
1.00
2.00
2.00
2.00
2.01
2.00
8.01
7.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
182.99
173.17
168.94
165.38
134.59
134.46
131.28
128.73
34.45
34.37
32.03
29.84
29.72
29.69
29.60
29.59
29.46
29.32
29.20
29.12
28.90
28.85
22.83
14.27
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

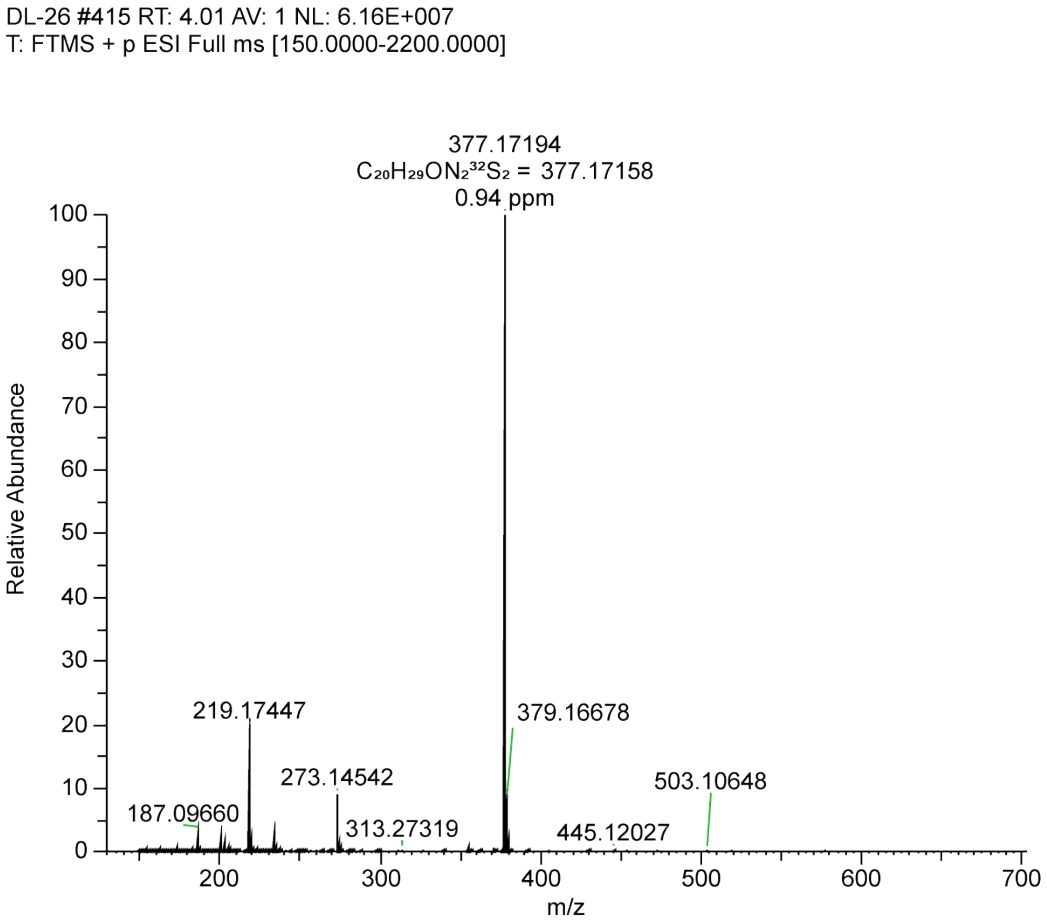
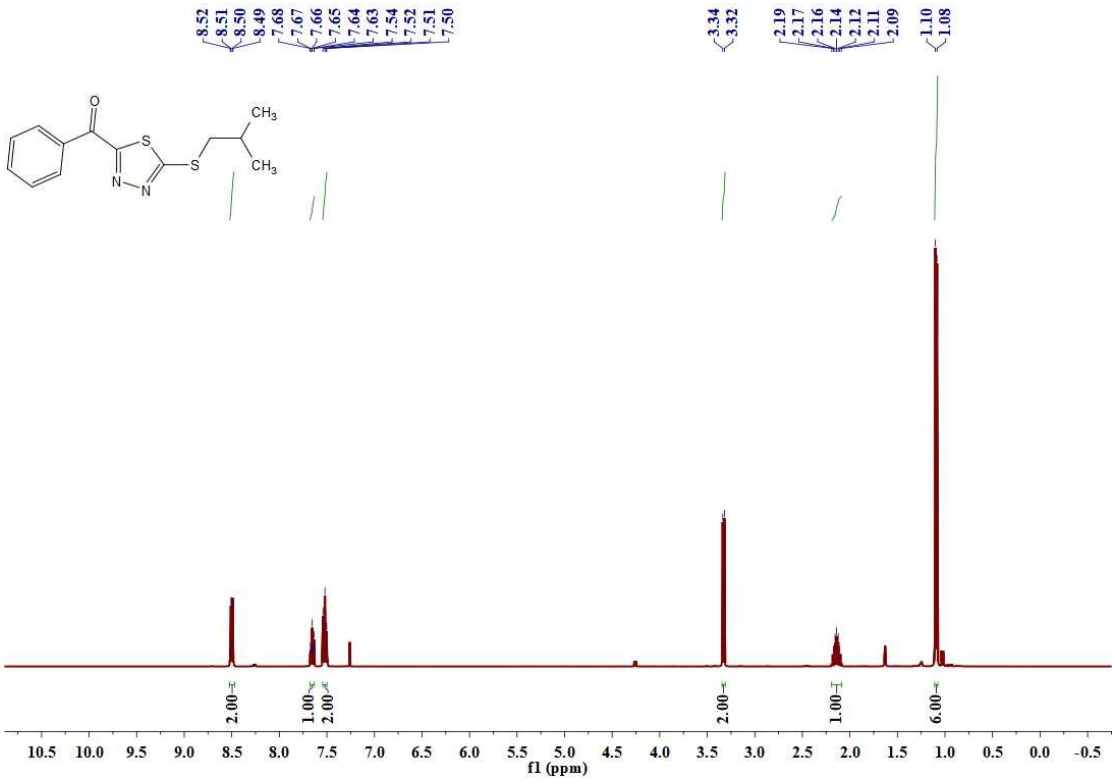
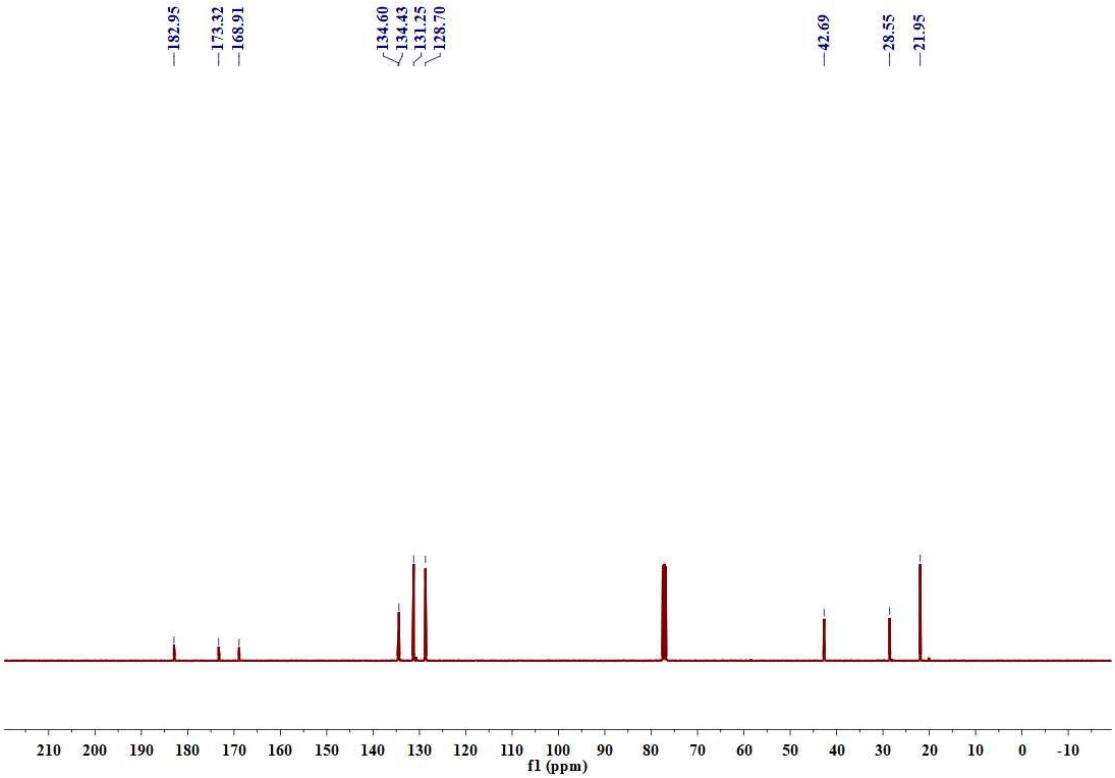



**Figure S6.** $^{1}$H NMR, $^{13}$C NMR and HRMS for **E6**.






27 #59 RT: 0.58 AV: 1 NL: 4.74E+008
T: FTMS + p ESI Full ms [120.0000-1800.0000]

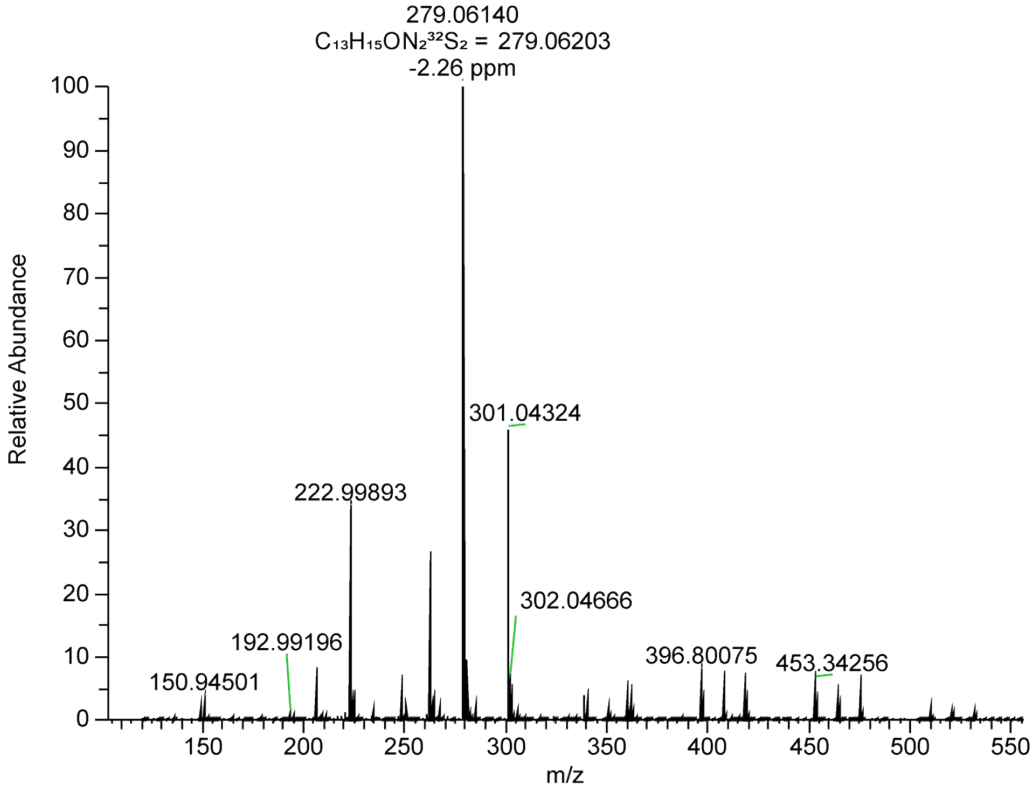
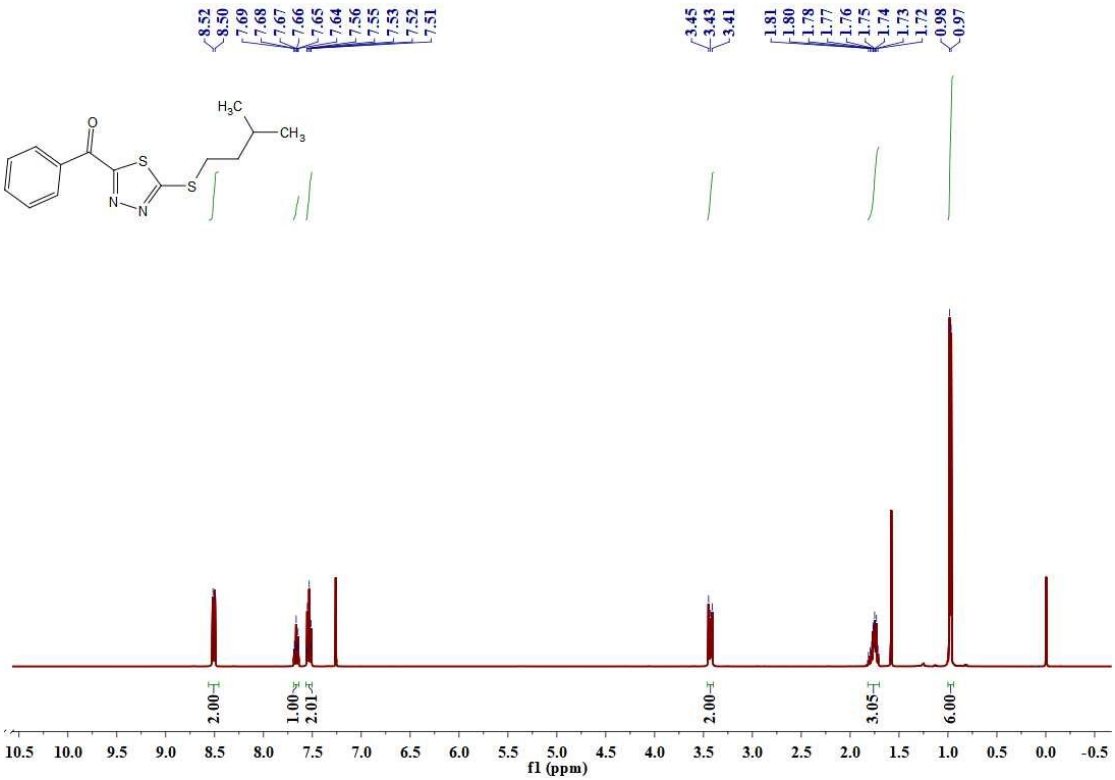
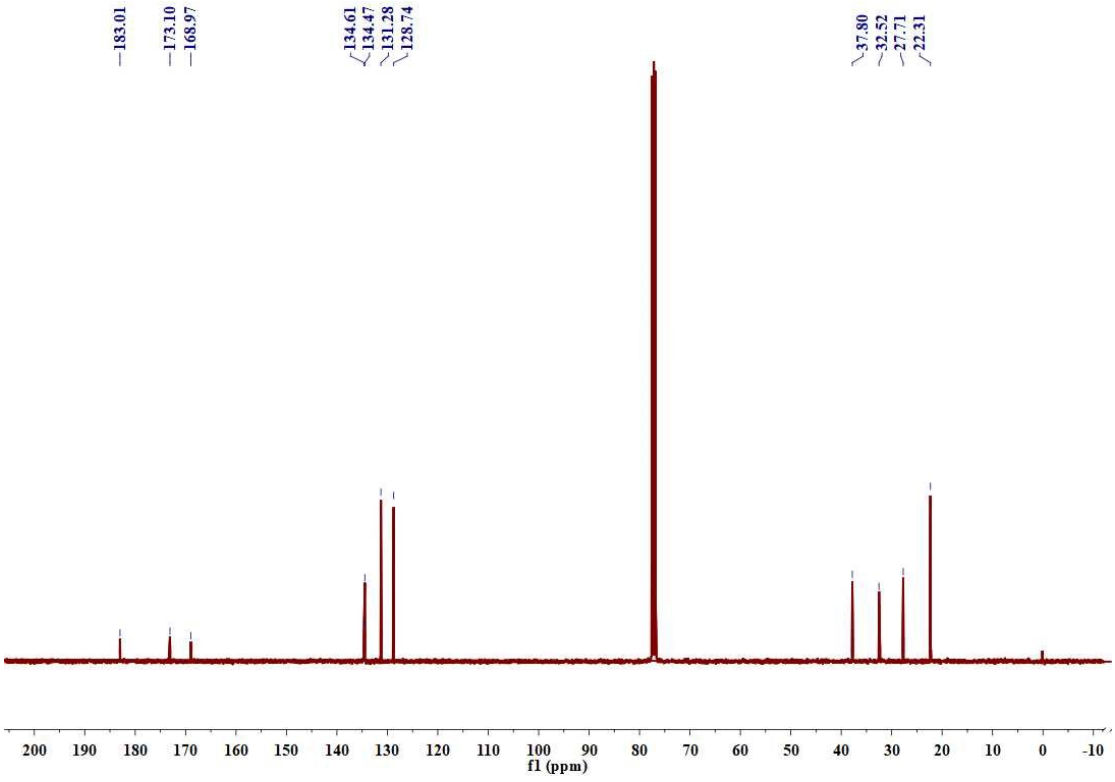



**Figure S7.** $^{1}$H NMR, $^{13}$C NMR and HRMS for **E7**.


8.52
8.50
7.69
7.68
7.67
7.66
7.65
7.64
7.56
7.55
7.53
7.52
7.51
3.45
3.43
3.41
1.81
1.80
1.78
1.77
1.76
1.75
1.74
1.73
1.72
0.98
0.97
O
S
N
N
S
H3C
CH3
2.00
1.00
2.01
2.00
3.05
6.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


183.01
173.10
168.97
134.61
134.47
131.28
128.74
37.80
32.52
27.71
22.31
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

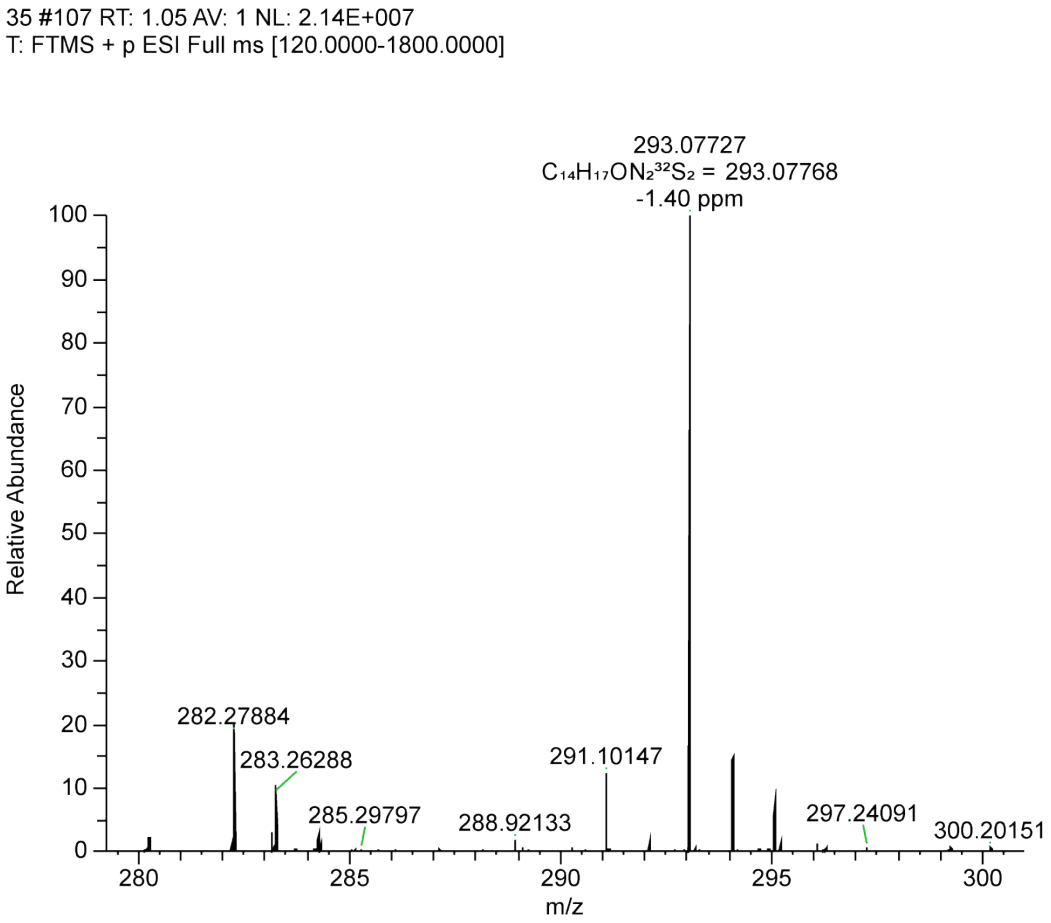
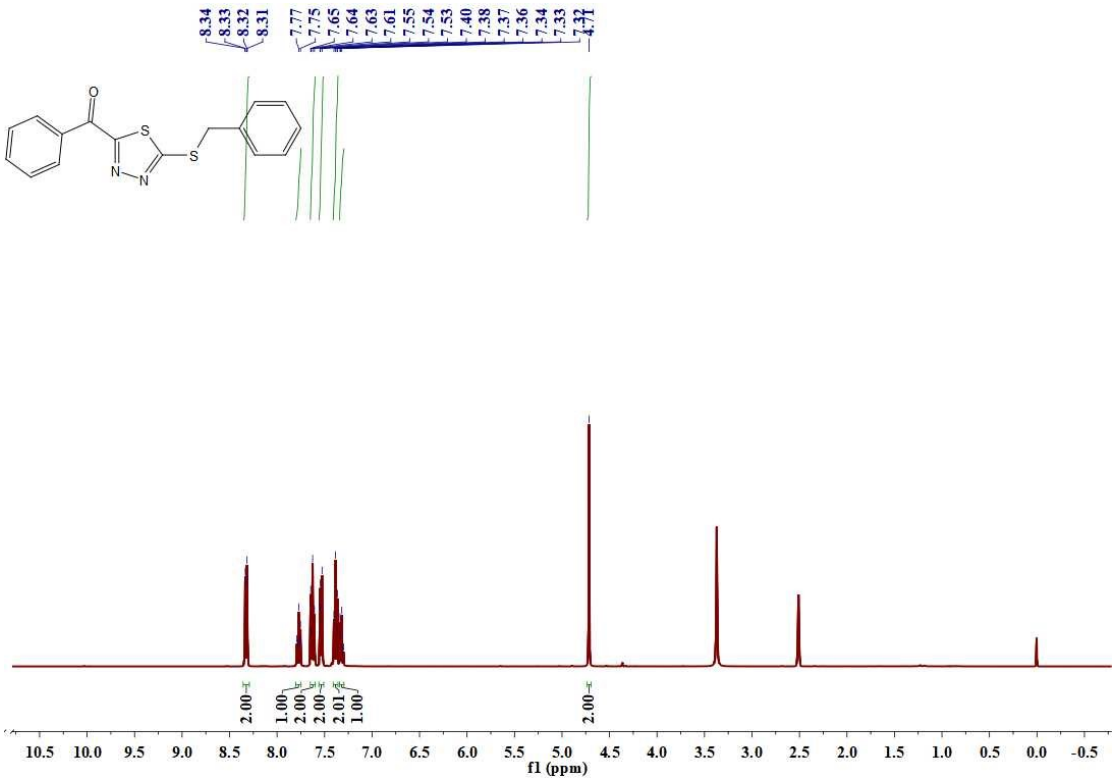
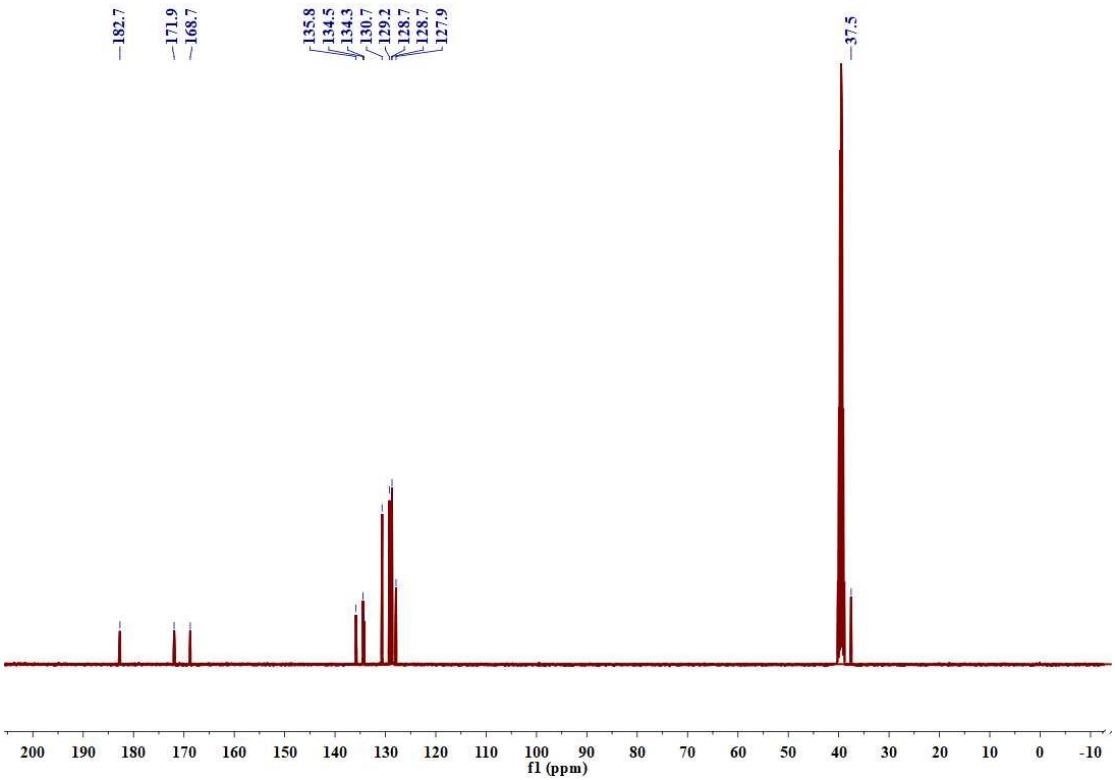



**Figure S8.** $^{1}$H NMR, $^{13}$C NMR and HRMS for **E8**.






23 #69 RT: 0.72 AV: 1 NL: 2.35E+007
T: FTMS + p ESI Full ms [120.0000-1800.0000]

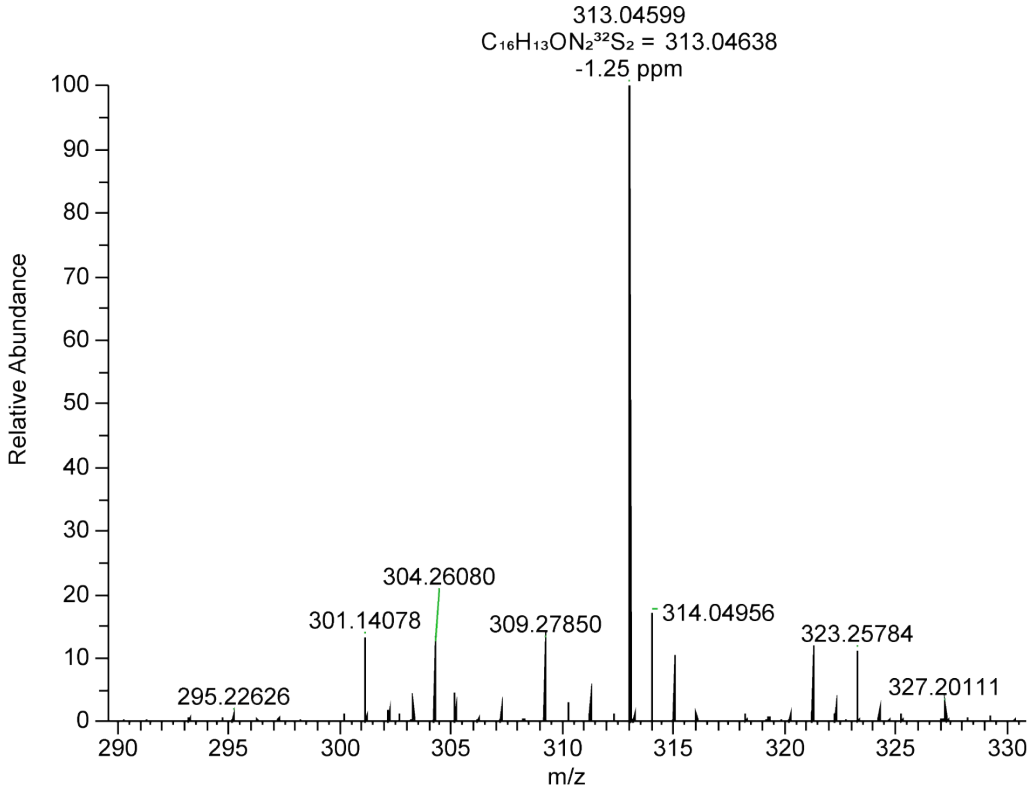
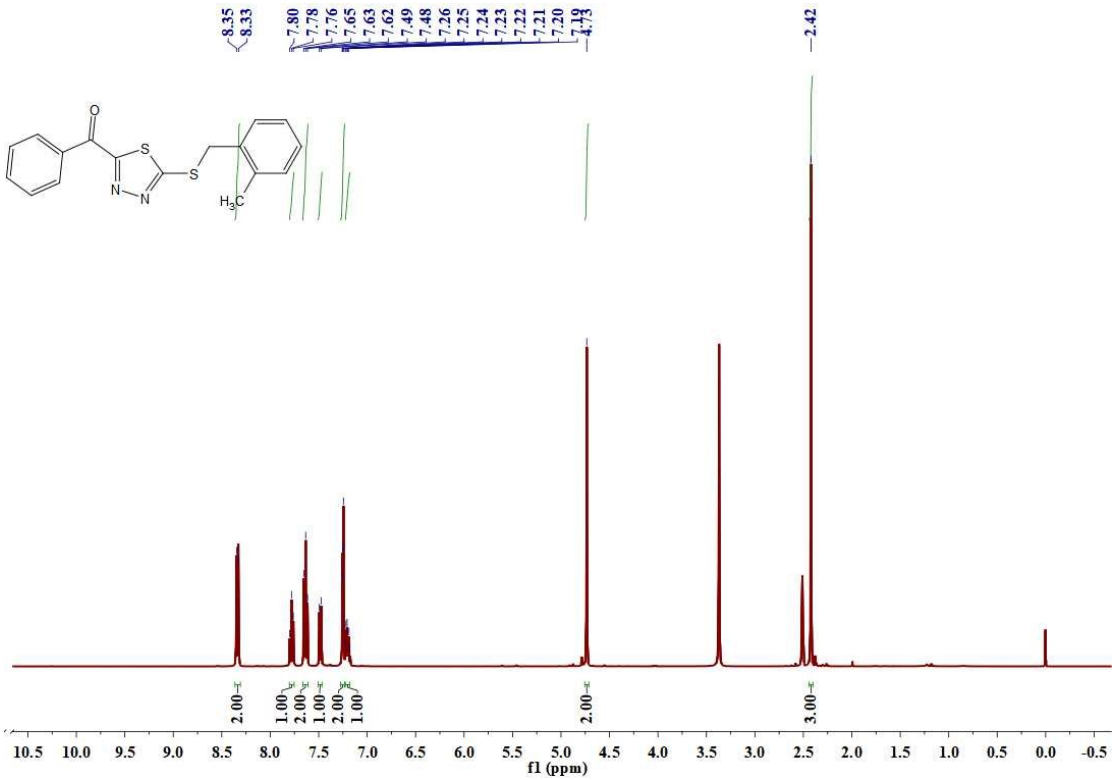
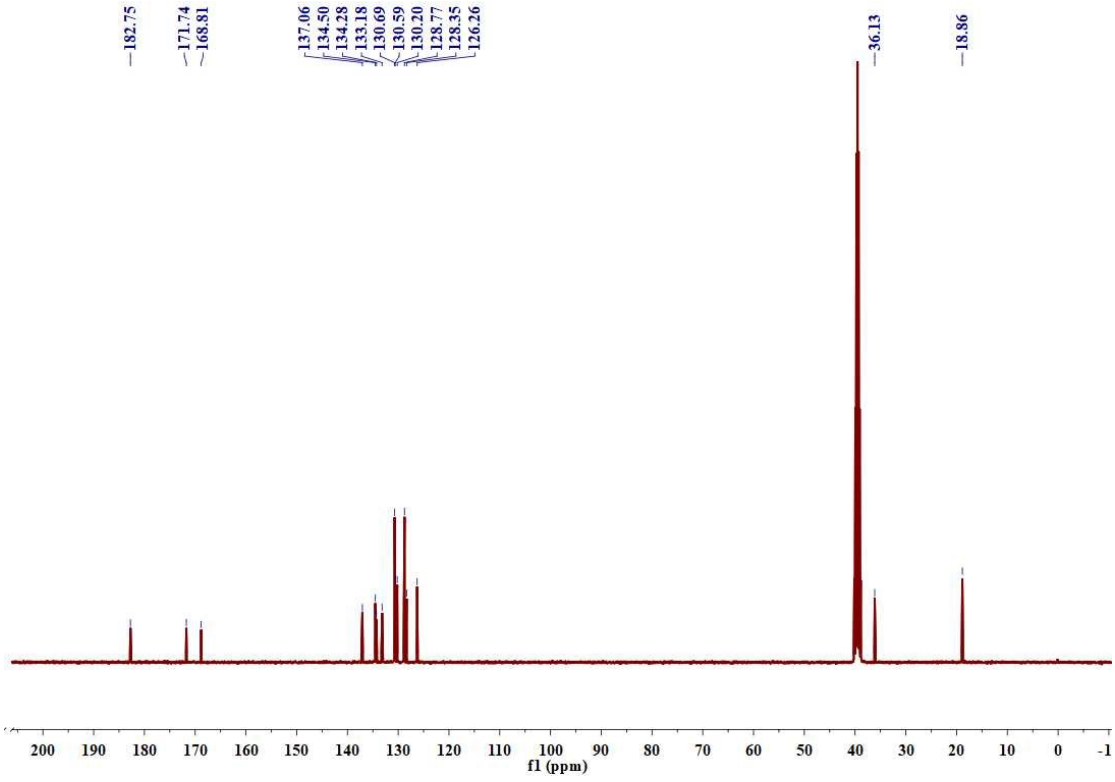



**Figure S9.** $^{1}$H NMR, $^{13}$C NMR and HRMS for **E9**.


8.35
8.33
7.80
7.78
7.76
7.65
7.63
7.62
7.49
7.48
7.26
7.25
7.24
7.23
7.22
7.21
7.20
7.13
4.73
2.42
O
S
N
N
S
H3C
2.00
1.00
2.00
1.00
2.00
1.00
2.00
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


182.75
171.74
168.81
137.06
134.50
134.28
133.18
130.69
130.59
130.20
128.77
128.35
126.26
36.13
18.86
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

27 #41 RT: 0.42 AV: 1 NL: 2.43E+007
T: FTMS + p ESI Full ms [120.0000-1800.0000]

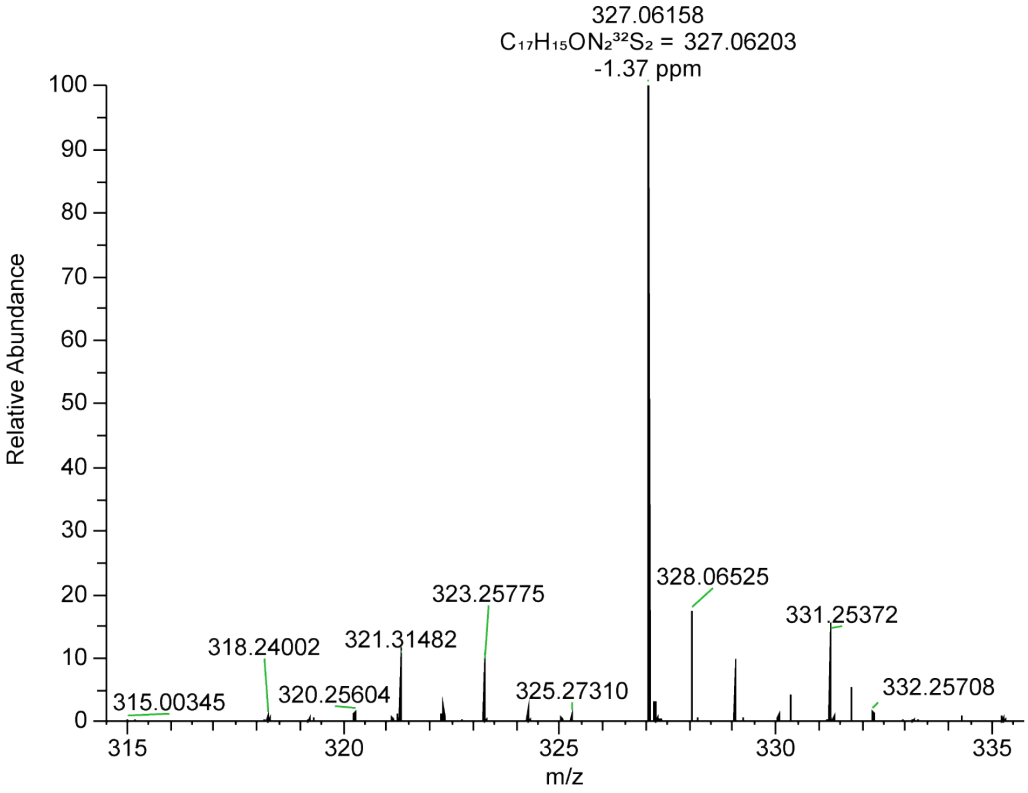
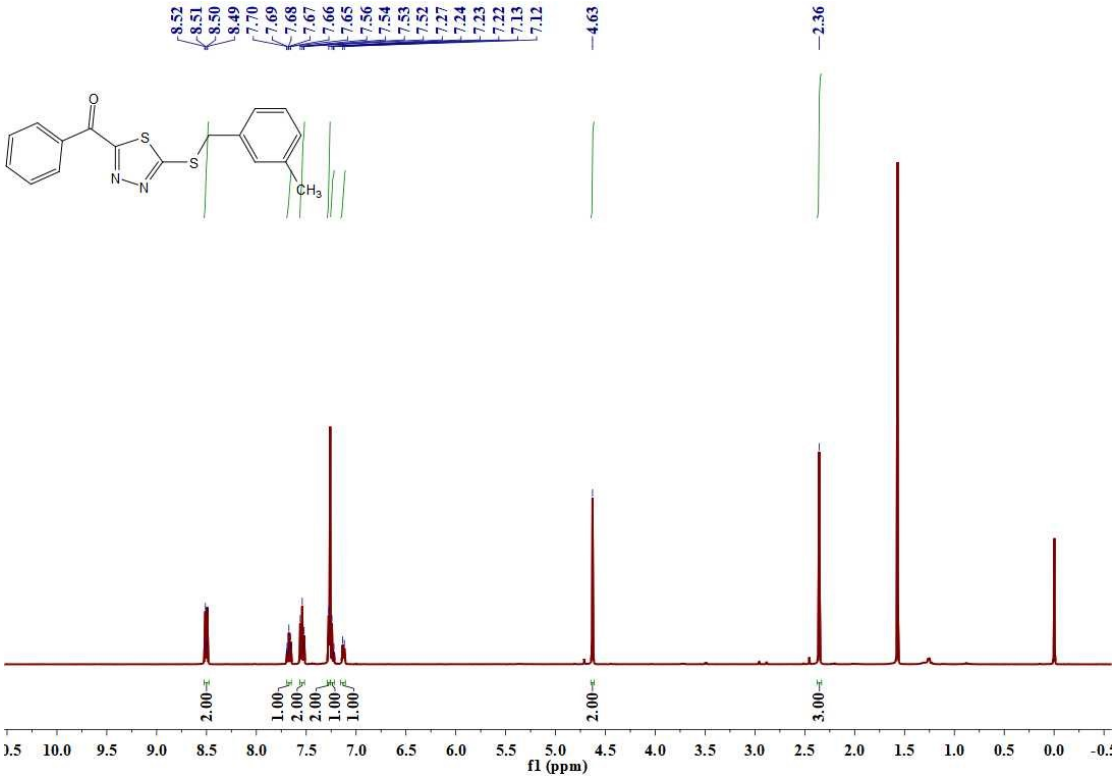
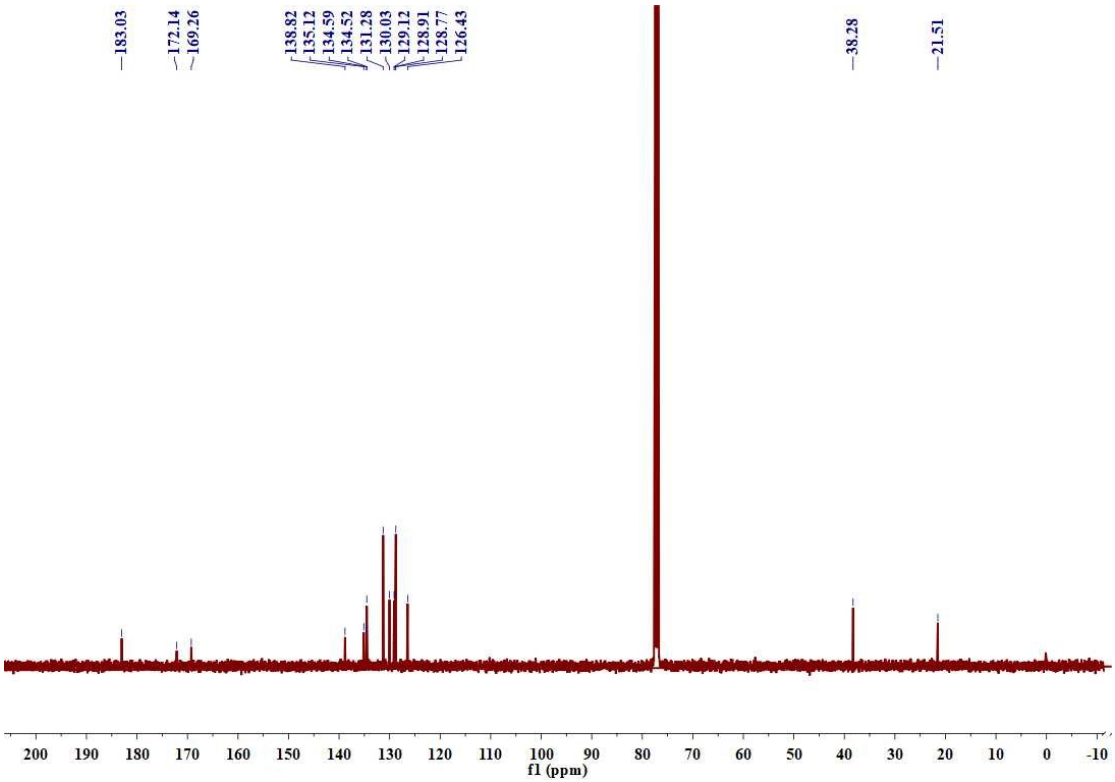



**Figure S10.** $^{1}$H NMR, $^{13}$C NMR and HRMS for **E10**.






28 #77 RT: 0.78 AV: 1 NL: 3.40E+007
T: FTMS + p ESI Full ms [120.0000-1800.0000]

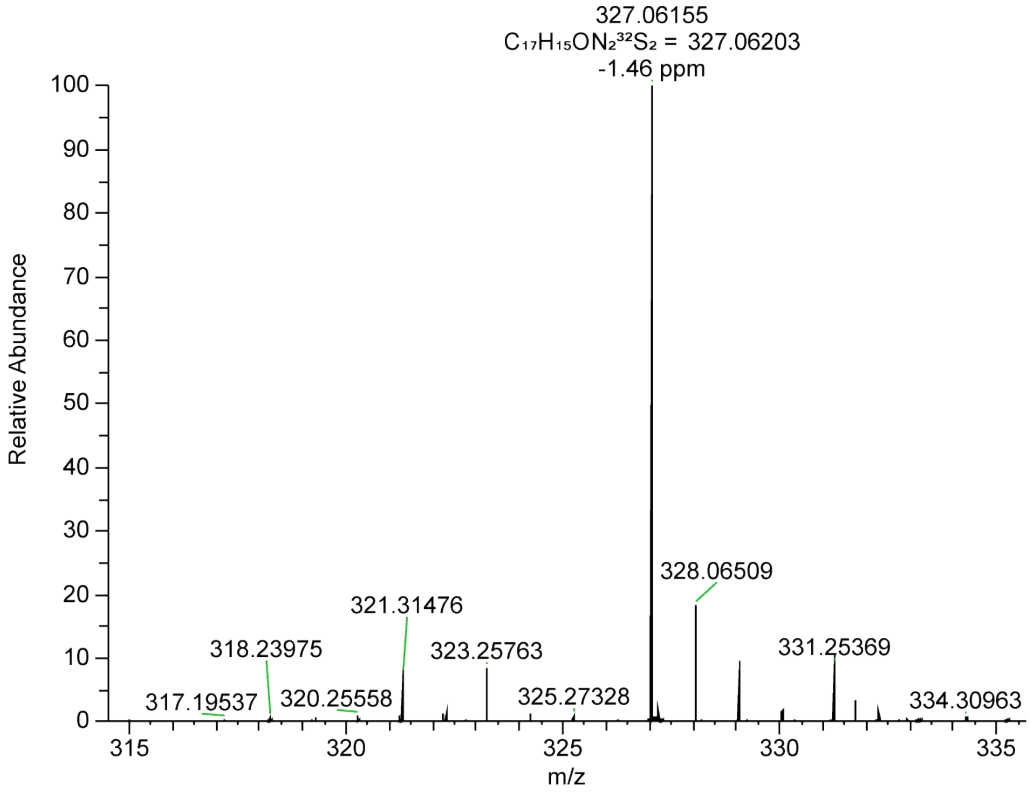
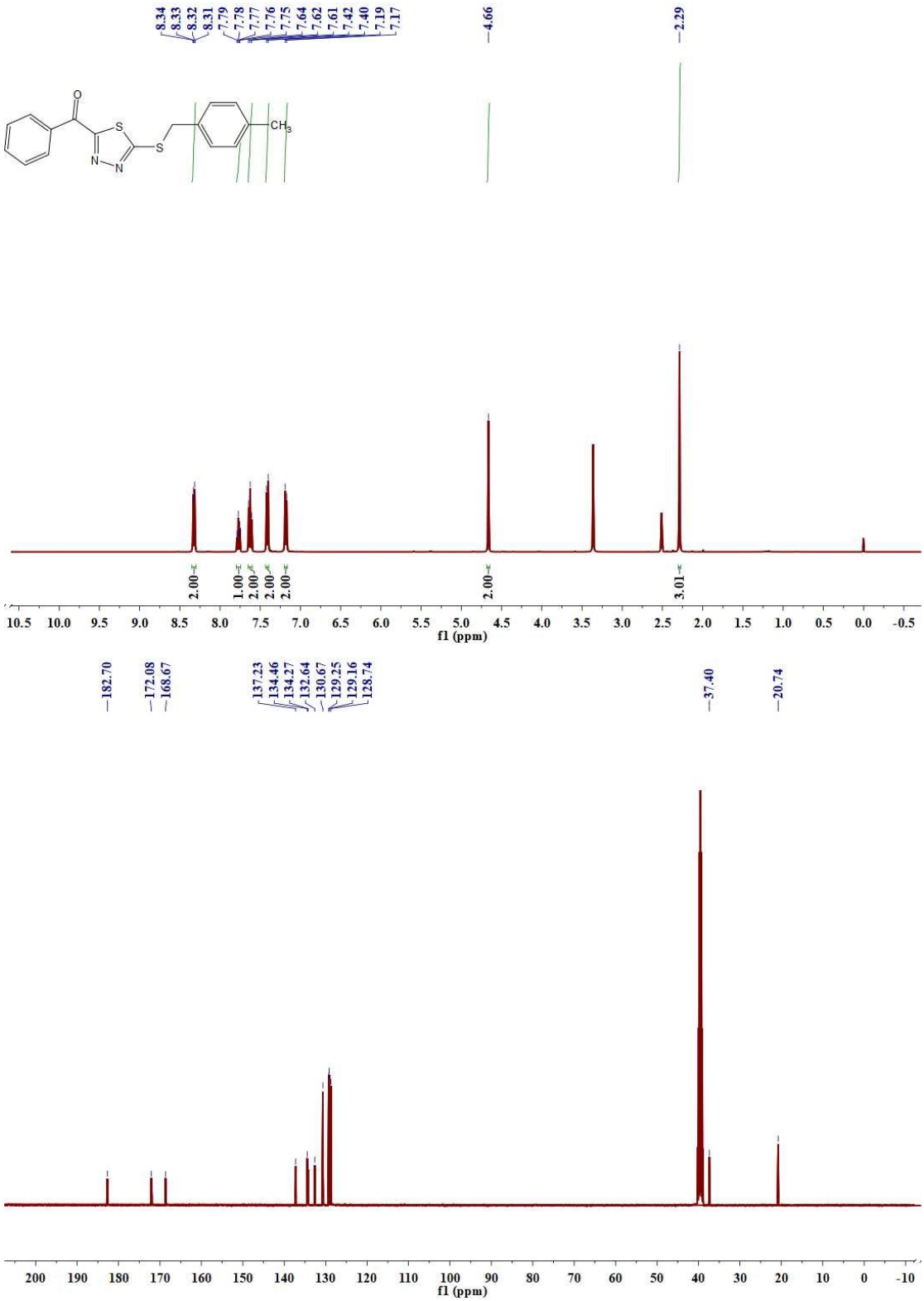



**Figure S11.** $^{1}$H NMR, $^{13}$C NMR and HRMS for **E11**.


8.34
8.33
8.32
8.31
7.79
7.78
7.77
7.76
7.75
7.64
7.62
7.61
7.42
7.40
7.19
7.17
4.66
2.29
O
S
N
N
S
CH3
2.00
1.00
2.00
2.00
2.00
3.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
182.70
172.08
168.67
137.23
134.46
134.27
132.64
130.67
129.25
129.16
128.74
37.40
20.74
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

29 #41 RT: 0.41 AV: 1 NL: 1.75E+007
T: FTMS + p ESI Full ms [120.0000-1800.0000]

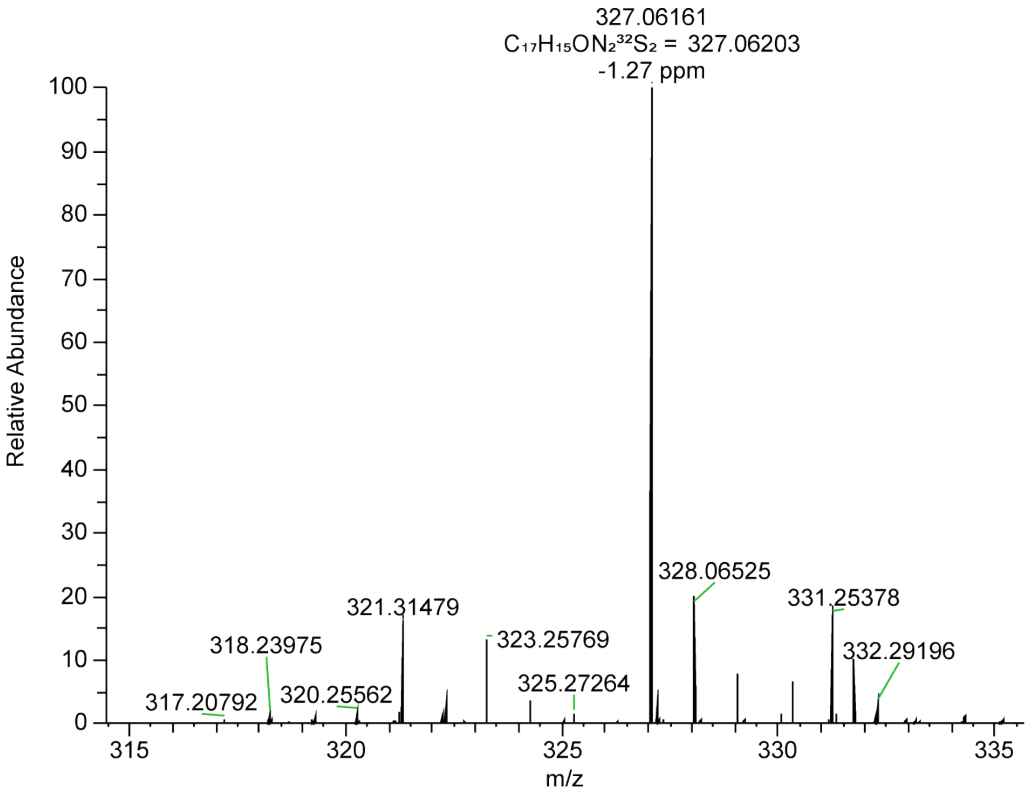
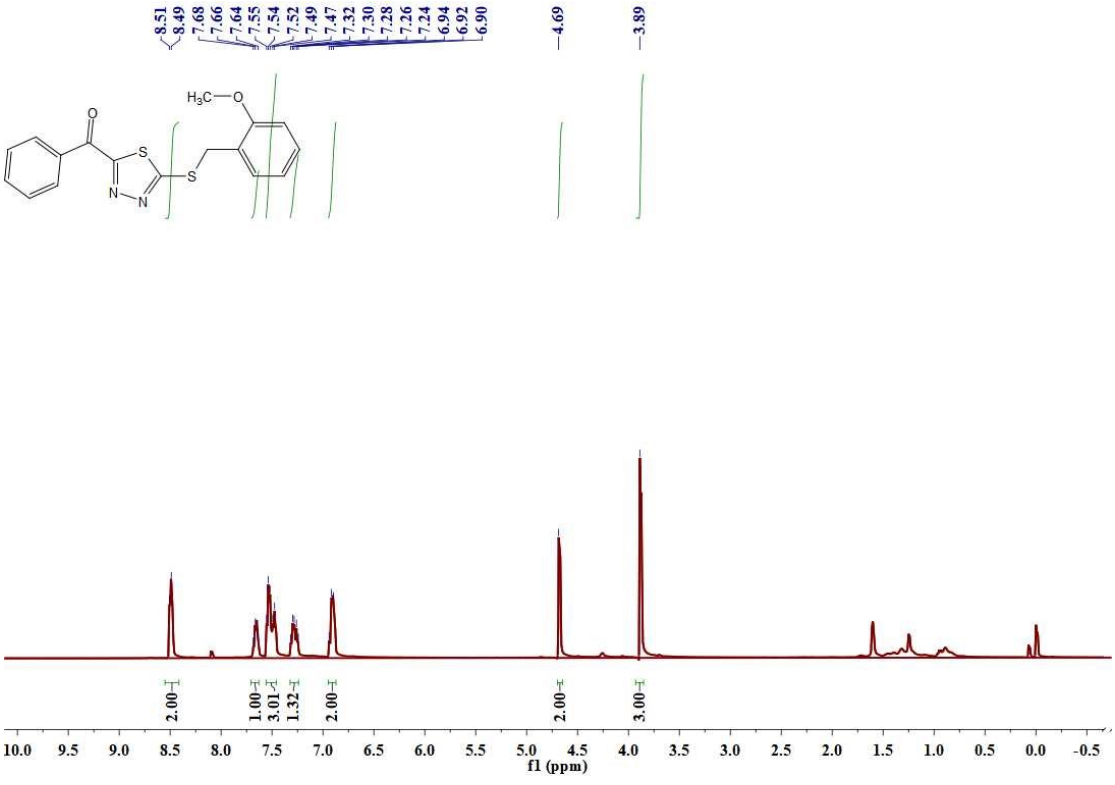
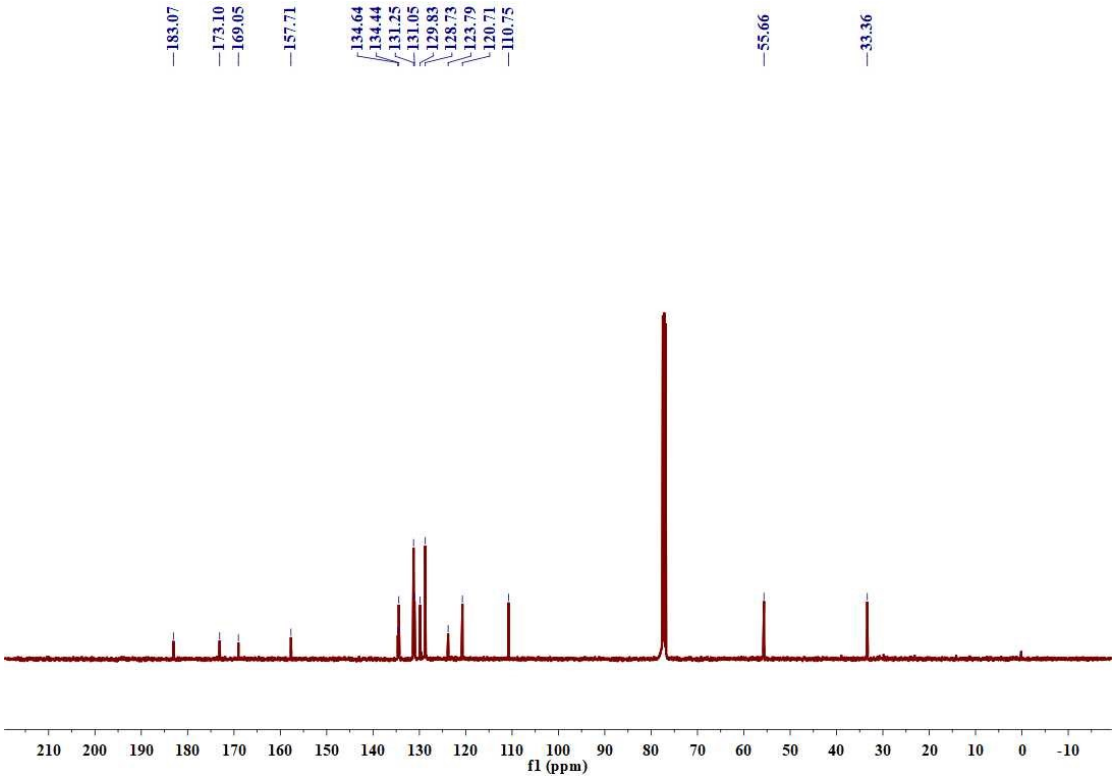



**Figure S12.** $^{1}$H NMR, $^{13}$C NMR and HRMS for **E12**.





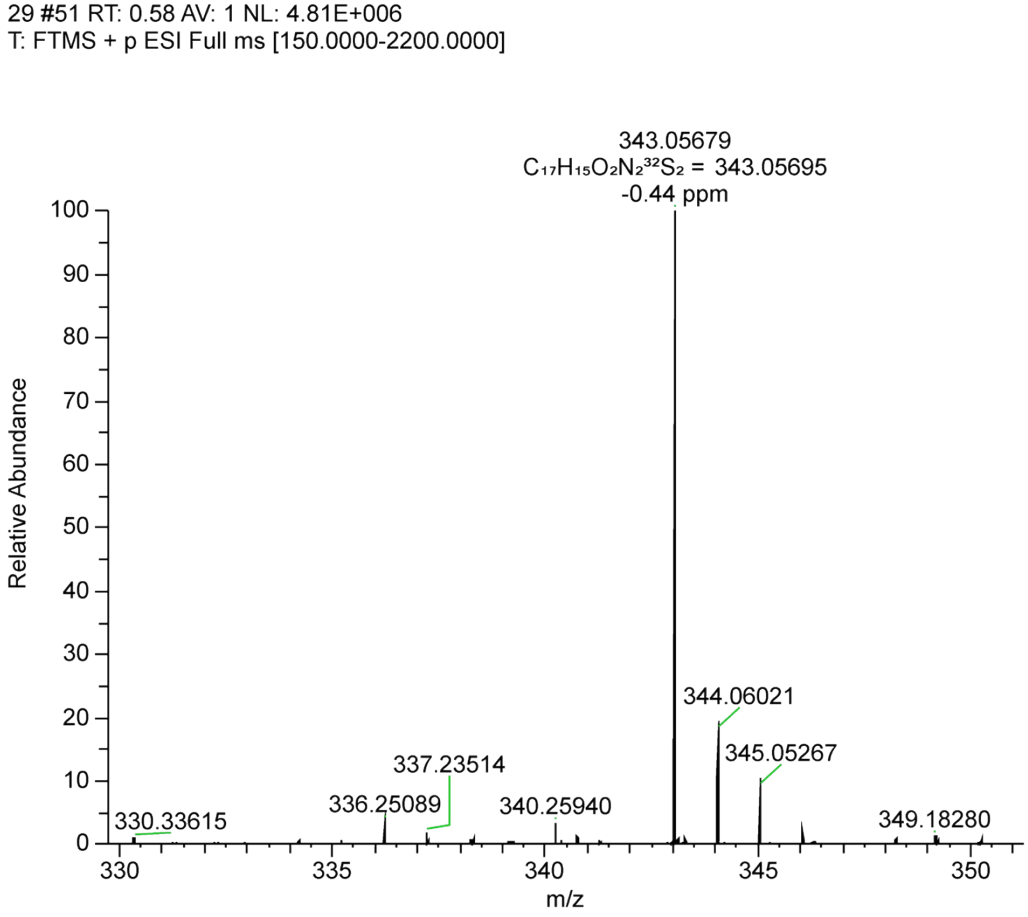
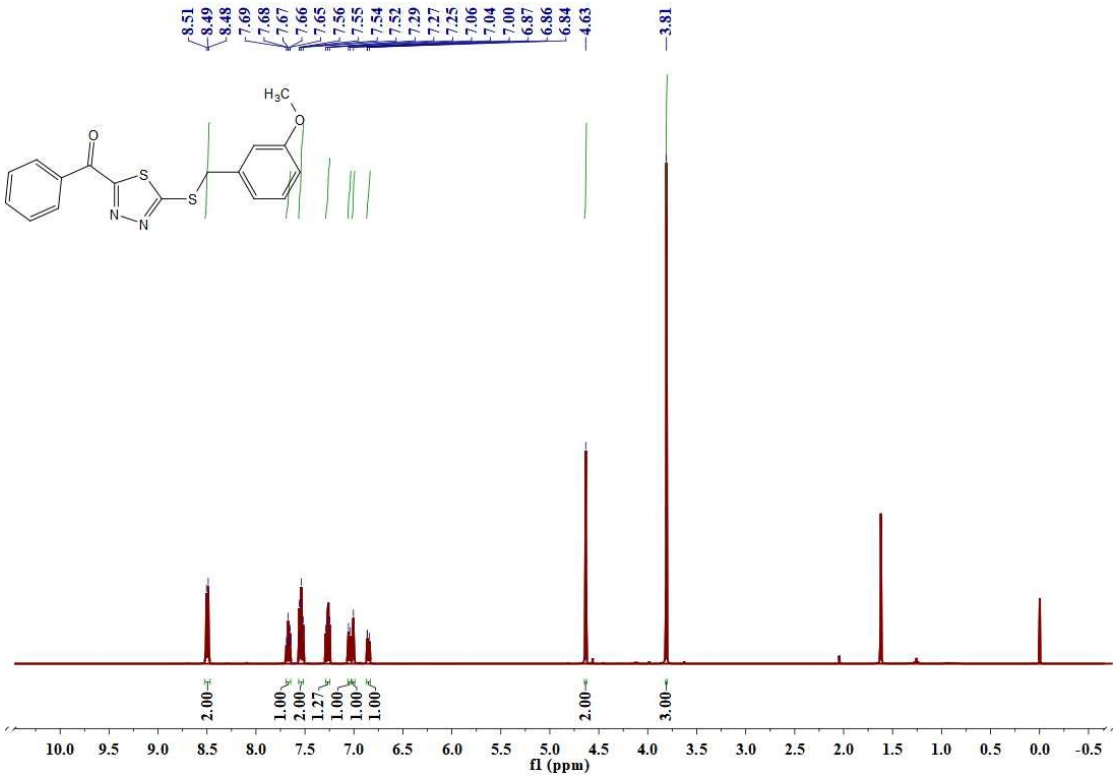
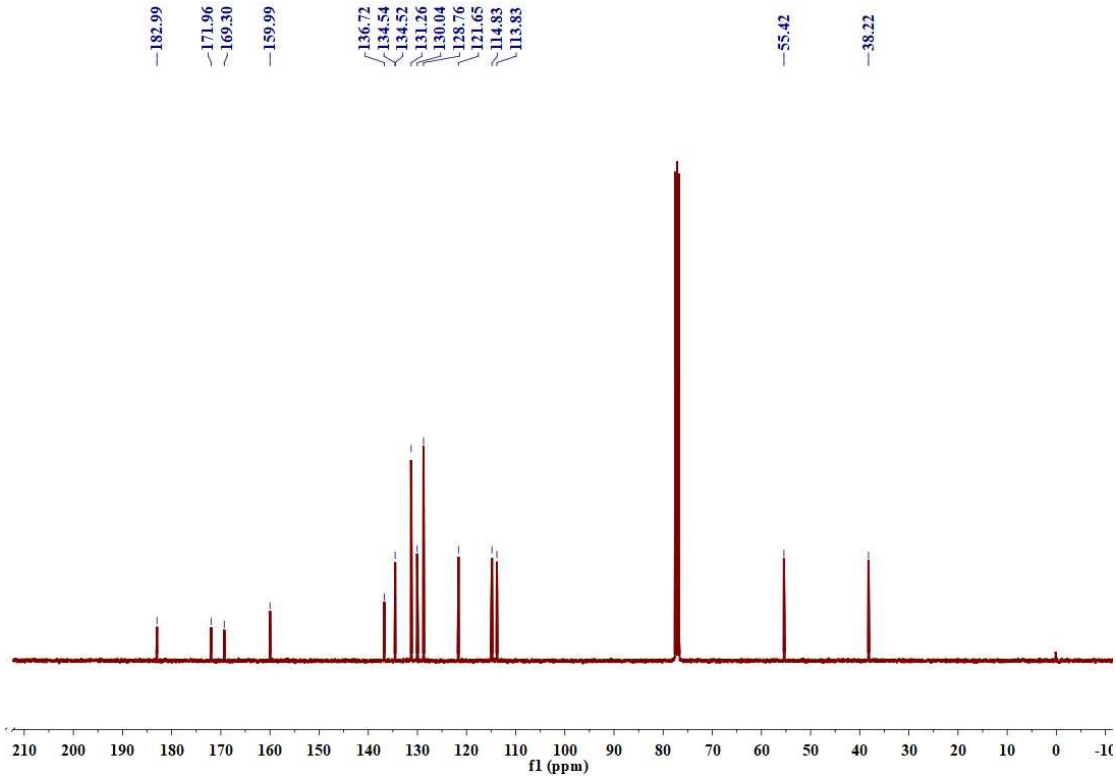




**Figure S13.** $^{1}$H NMR, $^{13}$C NMR and HRMS for **E13**.


8.51
8.49
8.48
7.69
7.68
7.67
7.66
7.65
7.56
7.55
7.54
7.52
7.29
7.27
7.25
7.06
7.04
7.00
6.87
6.86
6.84
4.63
3.81
H3C
O
O
S
S
N
N
2.00
1.00
2.00
1.27
1.00
1.00
1.00
2.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


182.99
171.96
169.30
159.99
136.72
134.54
134.52
131.26
130.04
128.76
121.65
114.83
113.83
55.42
38.22
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

28 #55 RT: 0.54 AV: 1 NL: 1.43E+008
T: FTMS + p ESI Full ms [120.0000-1800.0000]

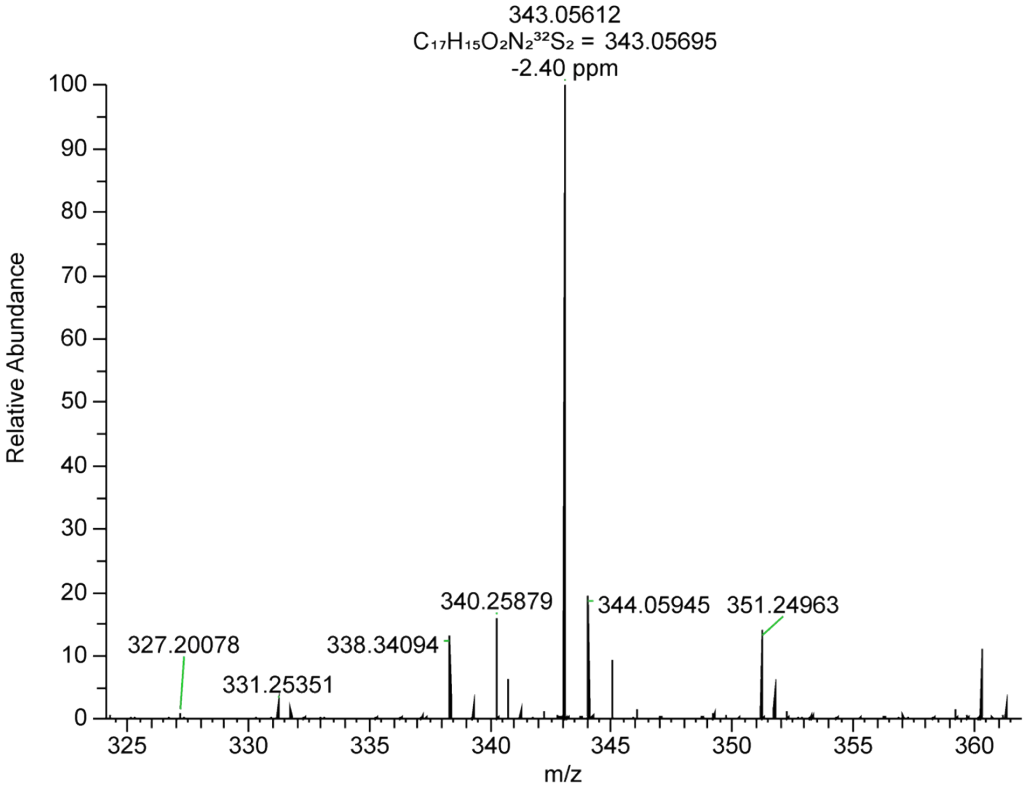
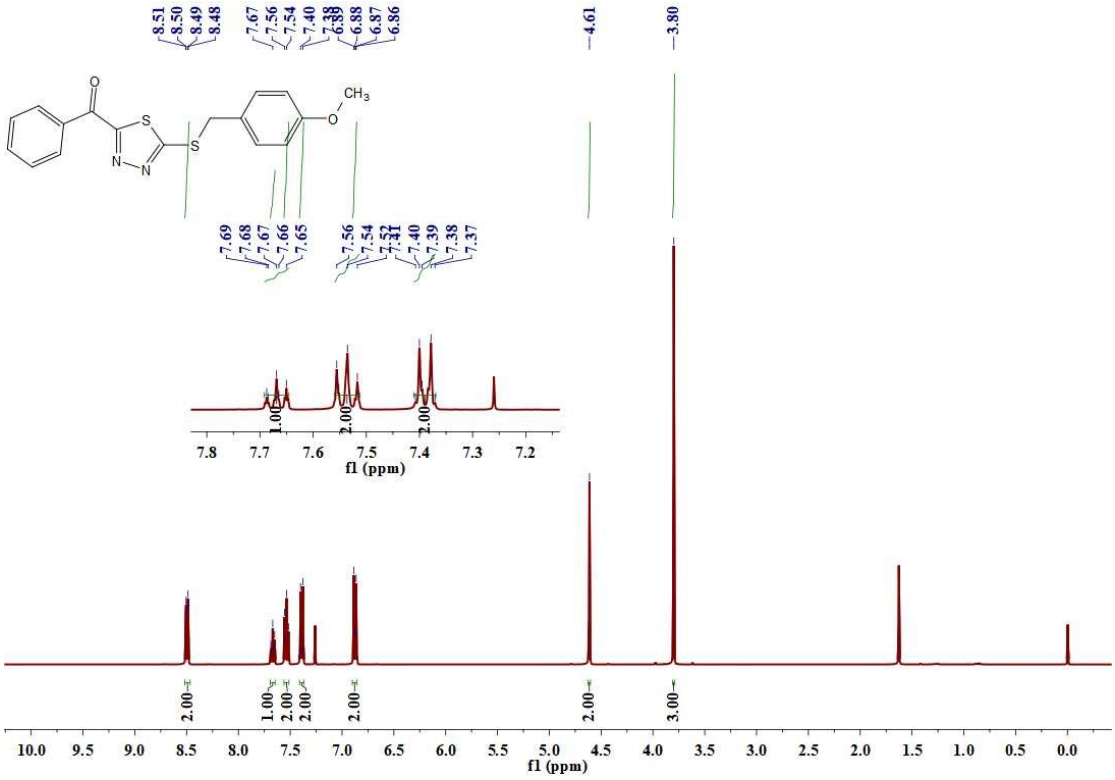
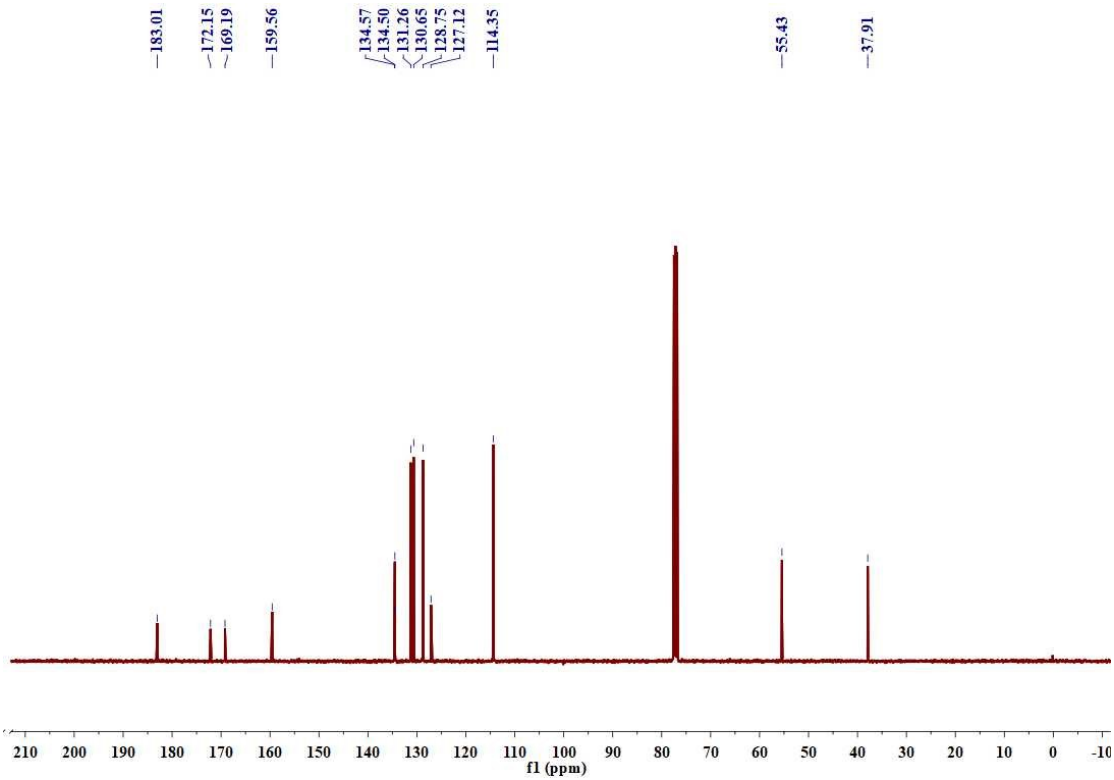



**Figure S14.** $^{1}$H NMR, $^{13}$C NMR and HRMS for **E14**.






30 #5 RT: 0.05 AV: 1 NL: 3.63E+005
T: FTMS + p ESI Full ms [120.0000-1800.0000]

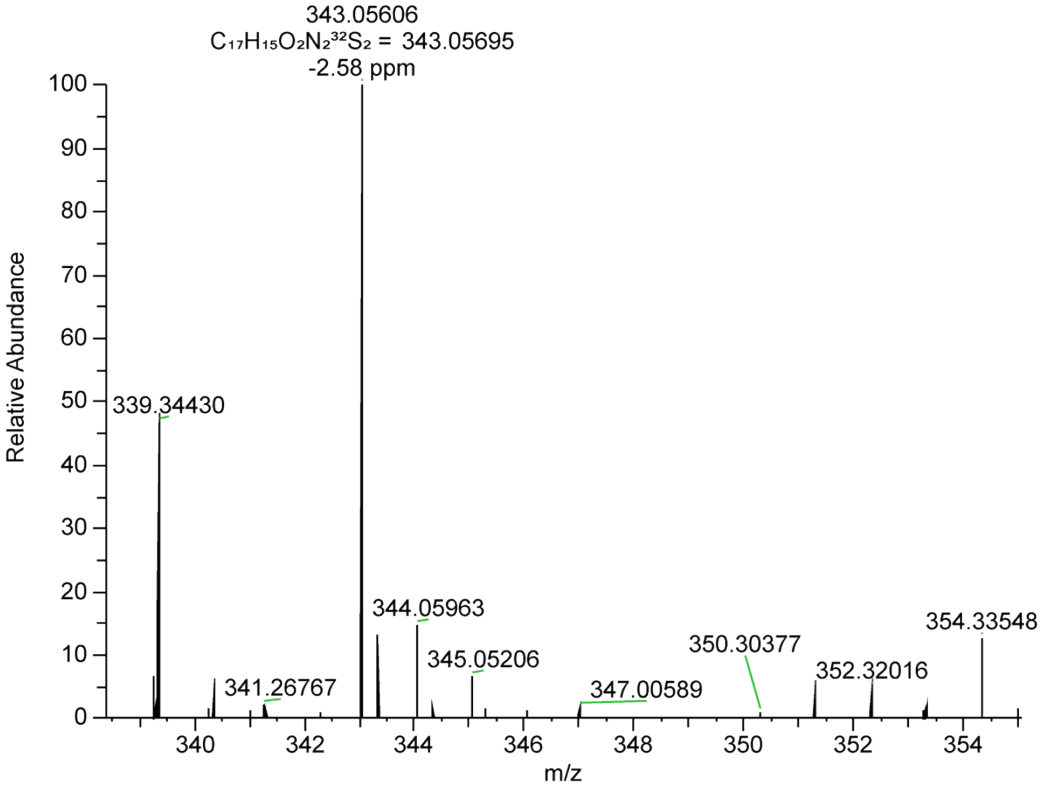
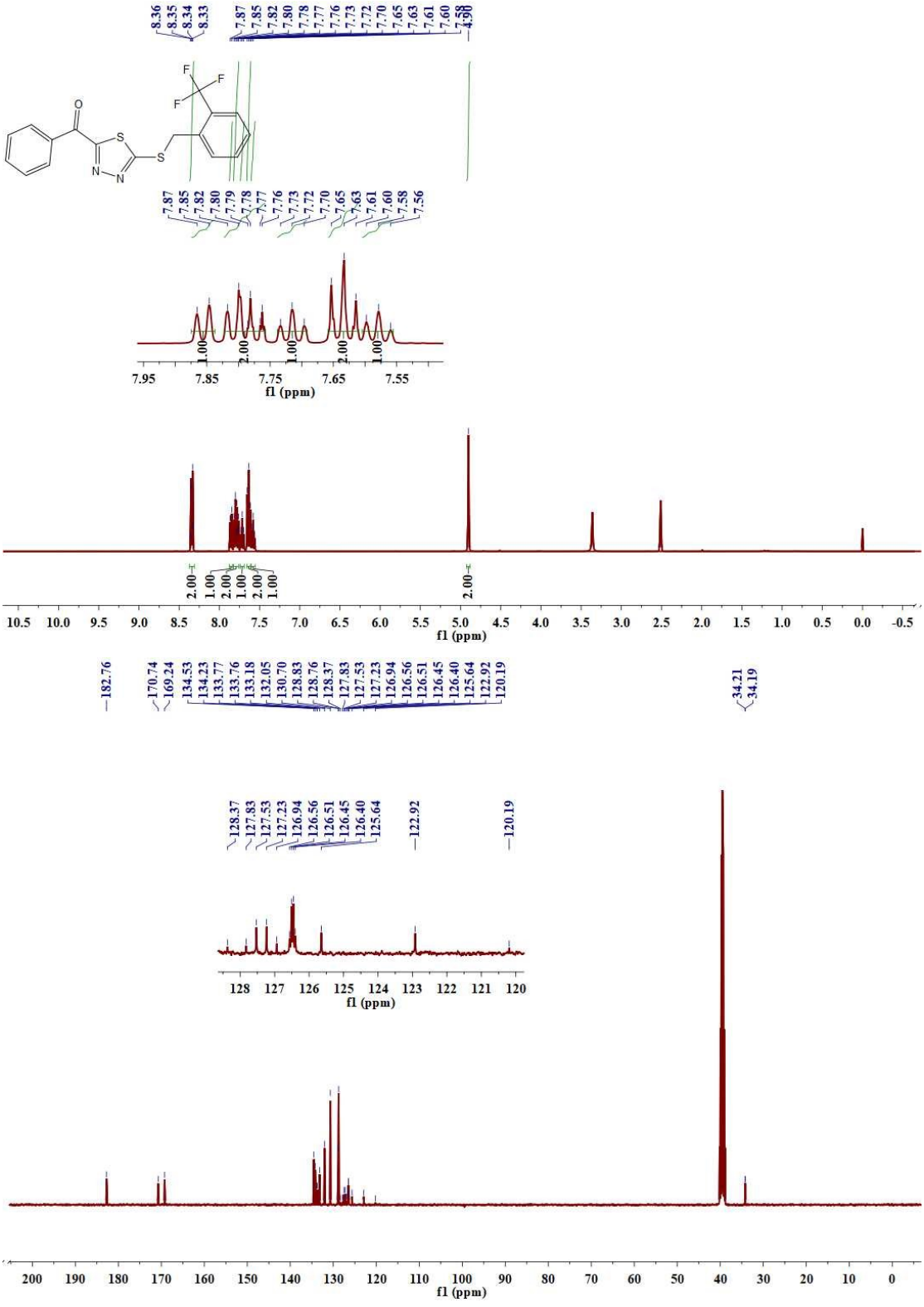
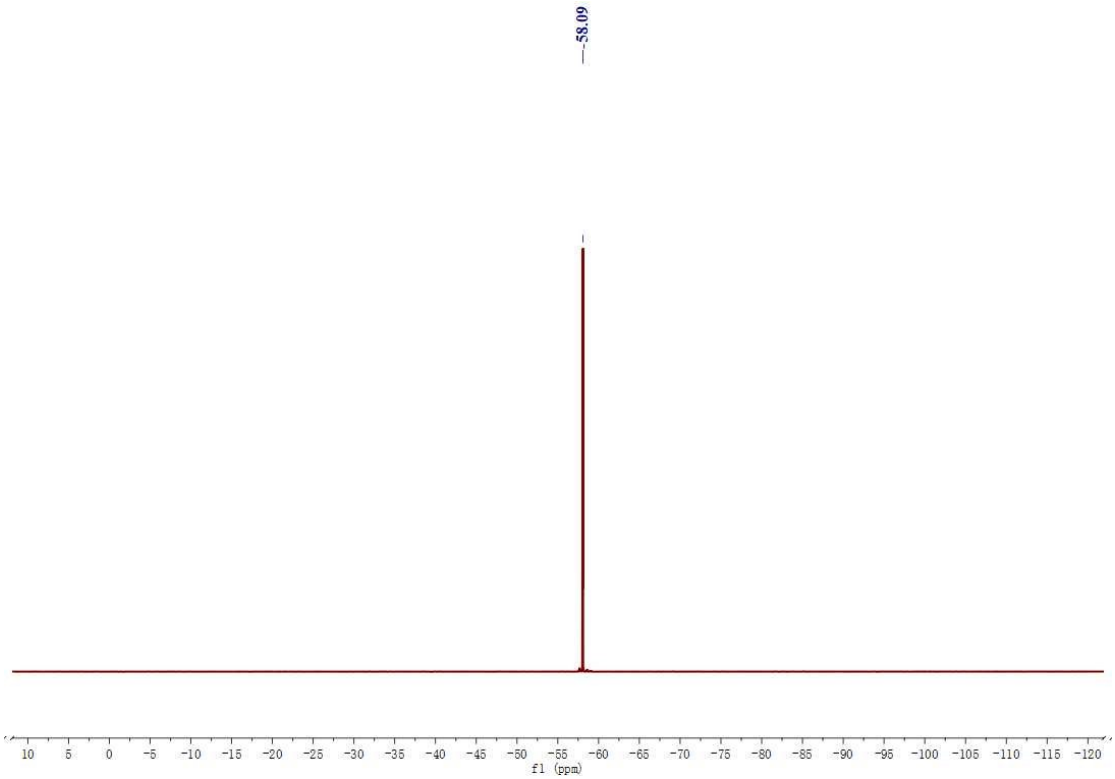



**Figure S15.** $^{1}$H NMR, $^{13}$C NMR and HRMS for **E15**.


8.36
8.35
8.34
8.33
7.87
7.85
7.82
7.80
7.79
7.78
7.77
7.76
7.73
7.72
7.70
7.65
7.63
7.61
7.60
7.58
7.56
4.90
F
F
F
O
S
N
N
S
1.00
2.00
1.00
2.00
1.00
7.95
7.85
7.75
7.65
7.55
f1 (ppm)
2.00
1.00
2.00
1.00
2.00
1.00
2.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)
182.76
170.74
169.24
134.53
134.23
133.77
133.76
133.18
132.05
130.70
128.83
128.76
128.37
127.83
127.53
127.23
126.94
126.56
126.51
126.45
126.40
125.64
122.92
120.19
34.21
34.19
128
127
126
125
124
123
122
121
120
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)




20 #57 RT: 0.65 AV: 1 NL: 2.00E+008
T: FTMS + p ESI Full ms [120.0000-1800.0000]

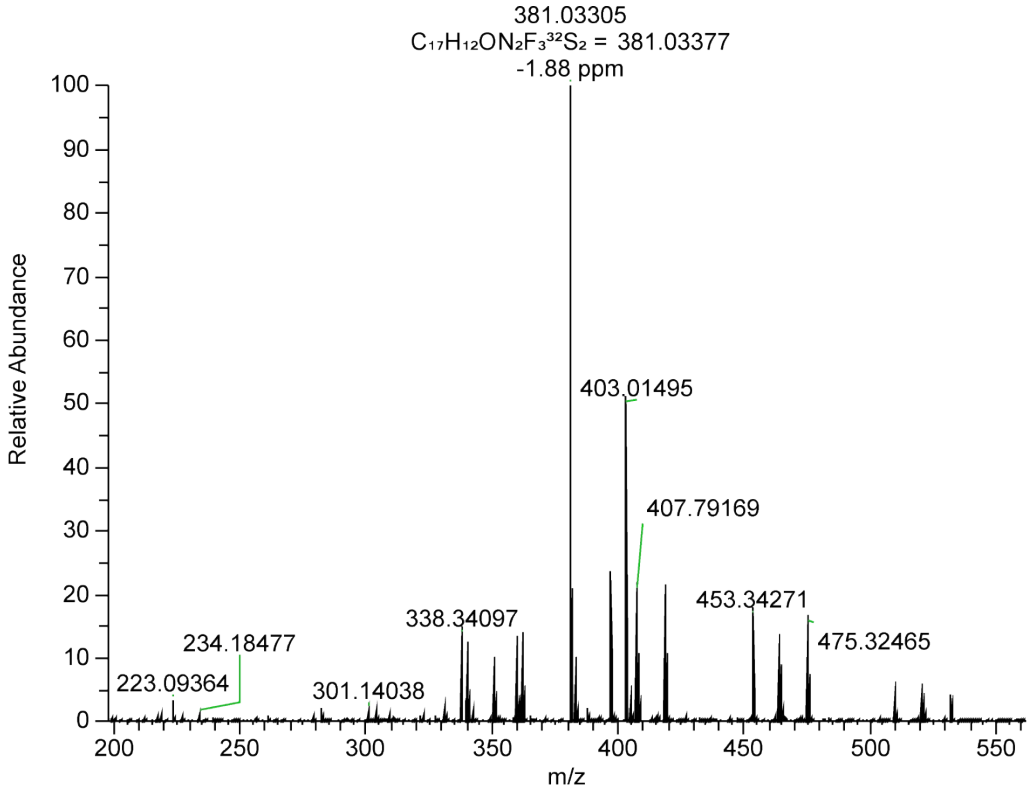
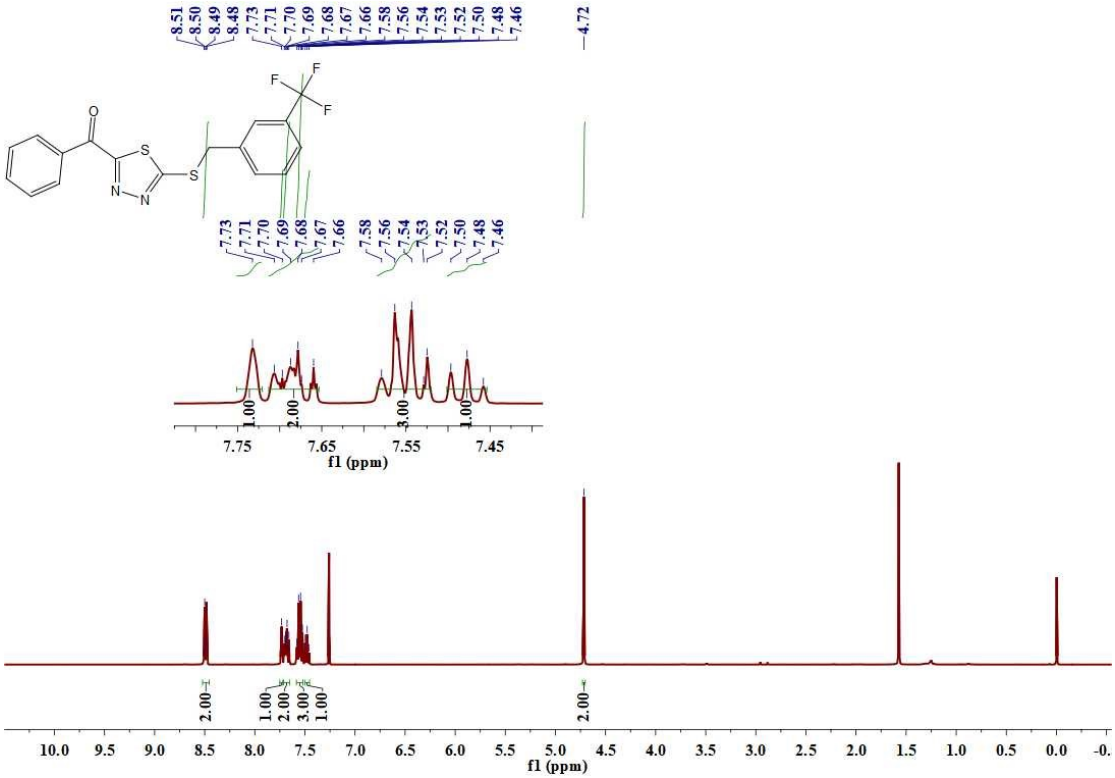
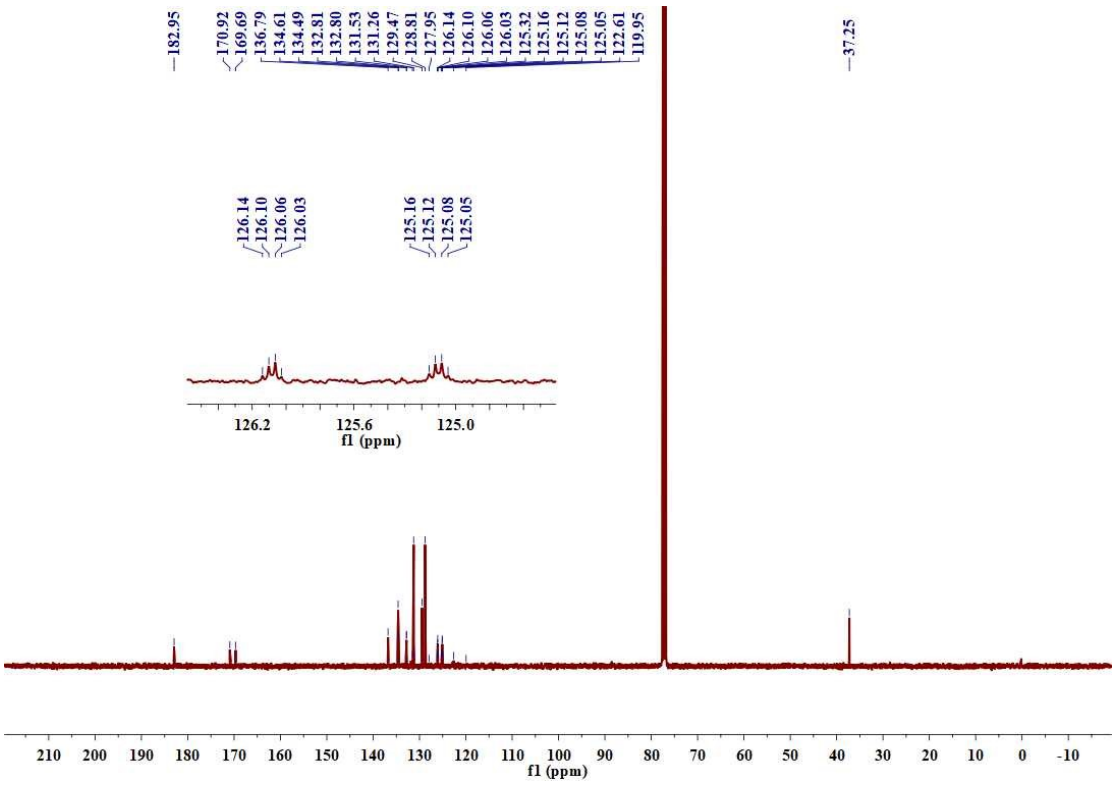
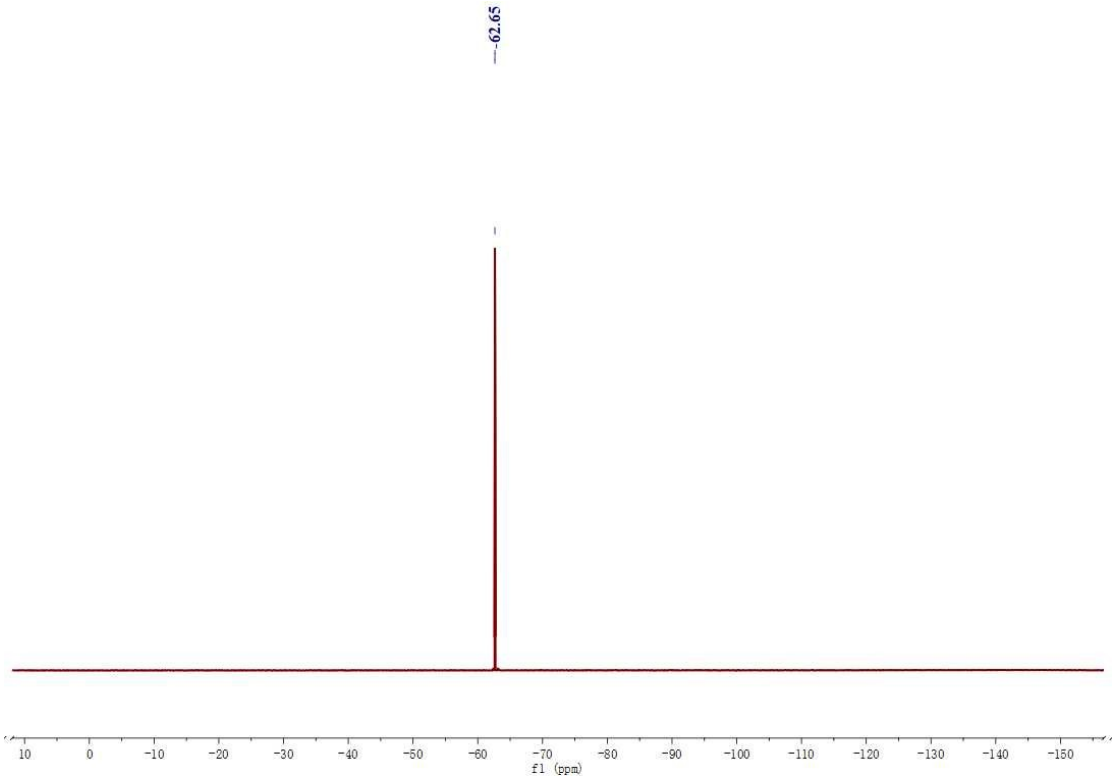



**Figure S16.** $^{1}$H NMR, $^{13}$C NMR, $^{19}$F NMR and HRMS for **E16**.


8.51
8.50
8.49
8.48
7.73
7.71
7.70
7.69
7.68
7.67
7.66
7.58
7.56
7.54
7.53
7.52
7.50
7.48
7.46
4.72
F
F
F
O
S
N
N
S
1.00
2.00
3.00
1.00
7.75
7.65
7.55
7.45
f1 (ppm)
2.00
1.00
2.00
3.00
1.00
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


182.95
170.92
169.69
136.79
134.61
134.49
132.81
132.80
131.53
131.26
129.47
128.81
127.95
126.14
126.10
126.06
126.03
125.32
125.16
125.12
125.08
125.05
122.61
119.95
37.25
126.14
126.10
126.06
126.03
125.16
125.12
125.08
125.05
126.2
125.6
125.0
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)




21 #51 RT: 0.55 AV: 1 NL: 1.63E+008
T: FTMS + p ESI Full ms [120.0000-1800.0000]

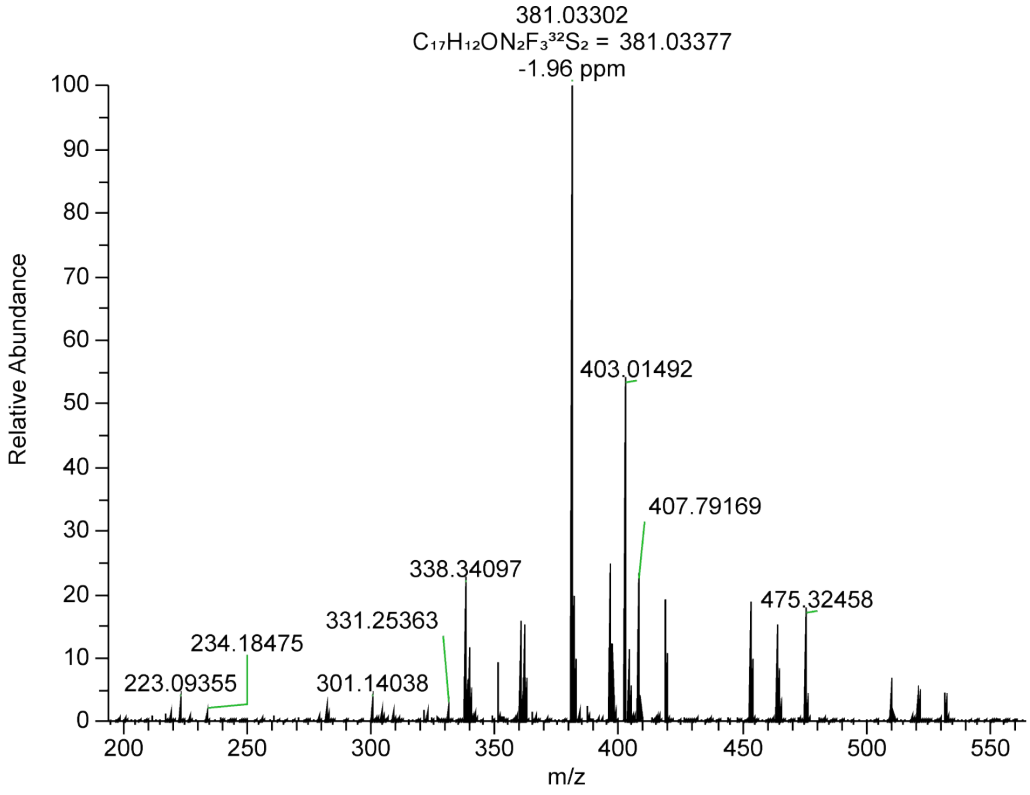
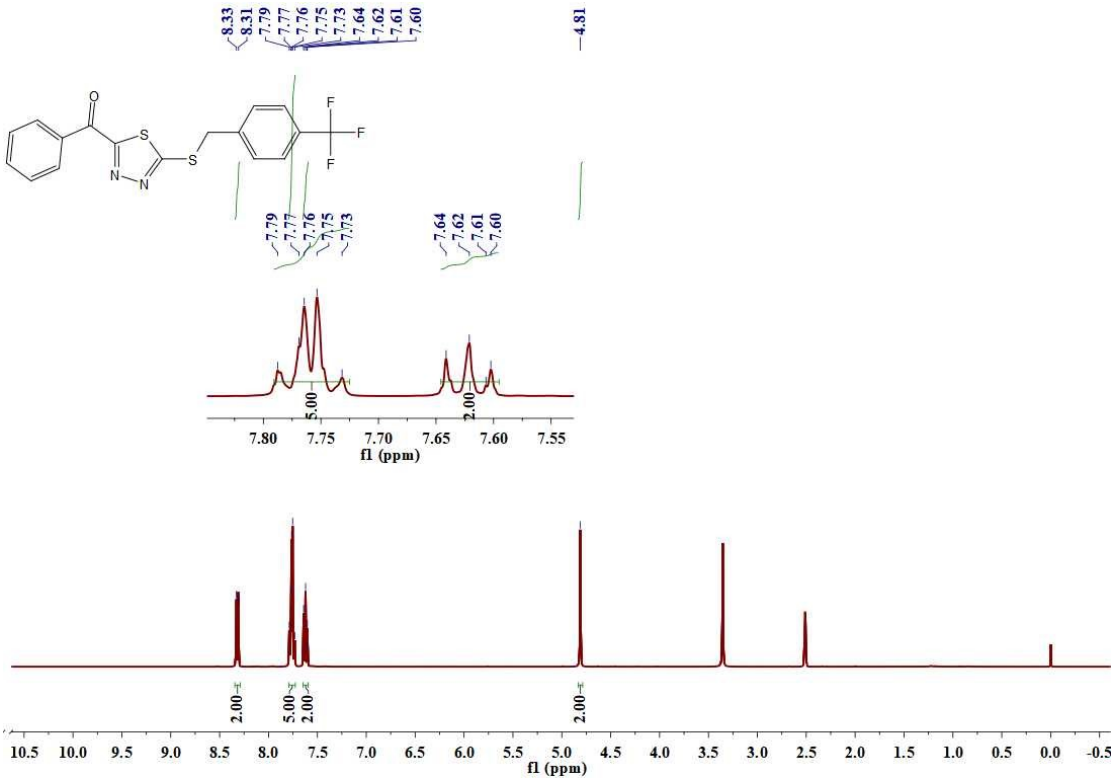
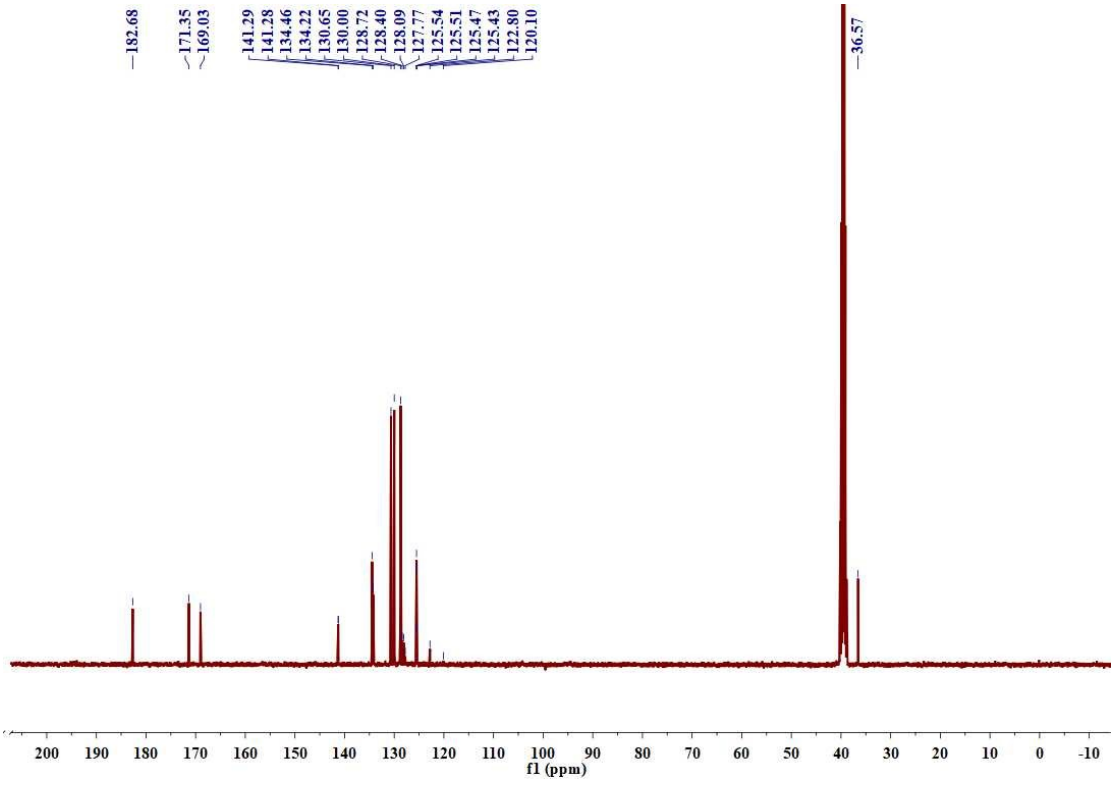
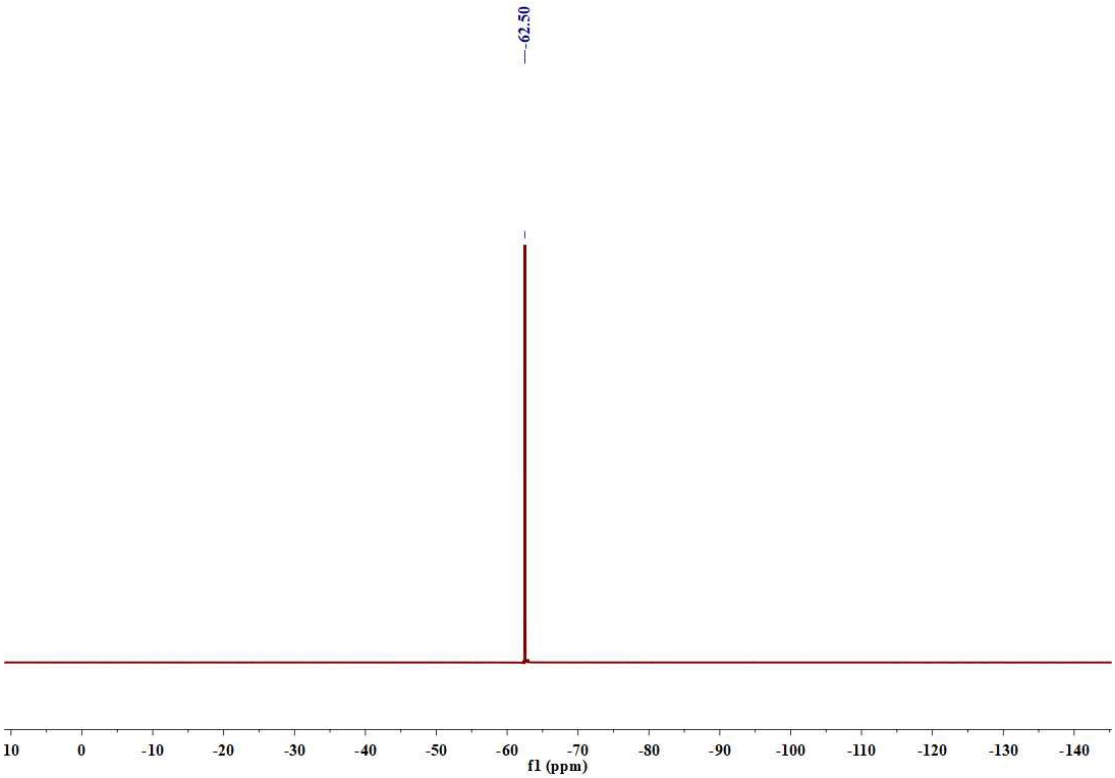



**Figure S17.** $^{1}$H NMR, $^{13}$C NMR, $^{19}$F NMR and HRMS for **E17**.


8.33
8.31
7.79
7.77
7.76
7.75
7.73
7.64
7.62
7.61
7.60
4.81
O
S
N
N
S
F
F
F
5.00
2.00
7.80
7.75
7.70
7.65
7.60
7.55
f1 (ppm)
2.00
5.00
2.00
2.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


182.68
171.35
169.03
141.29
141.28
134.46
134.22
130.65
130.00
128.72
128.40
128.09
127.77
125.54
125.51
125.47
125.43
122.80
120.10
36.57
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)




22 #55 RT: 0.57 AV: 1 NL: 1.30E+008
T: FTMS + p ESI Full ms [120.0000-1800.0000]

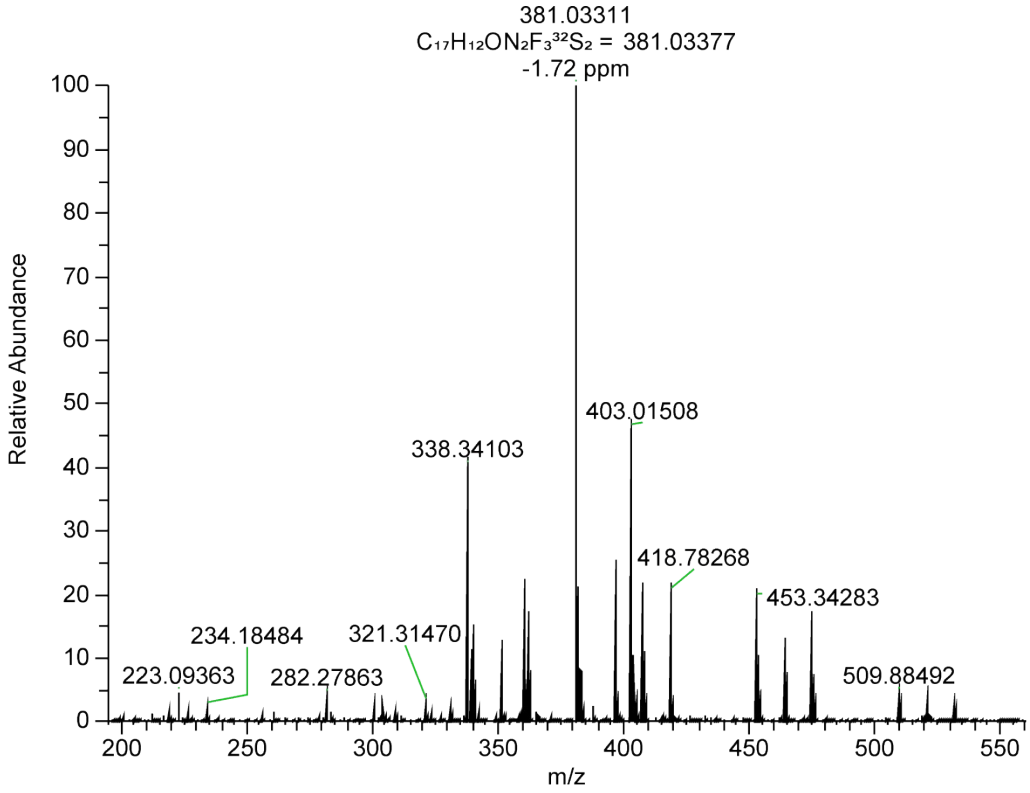
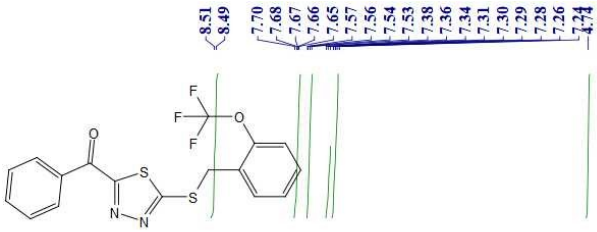
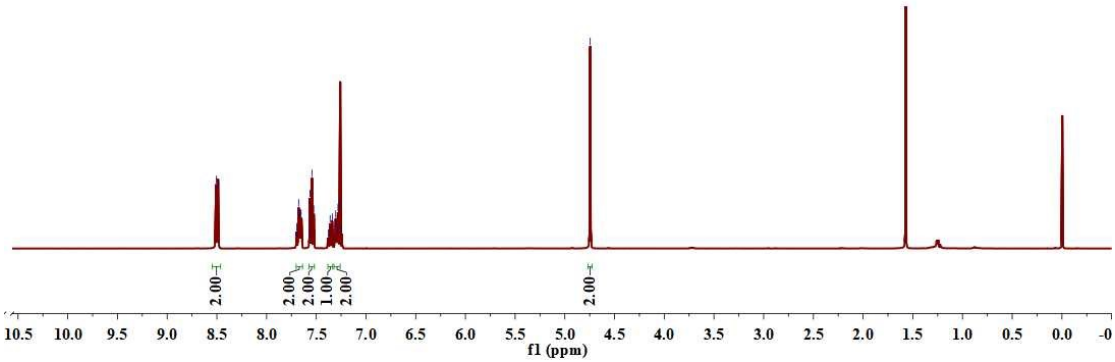
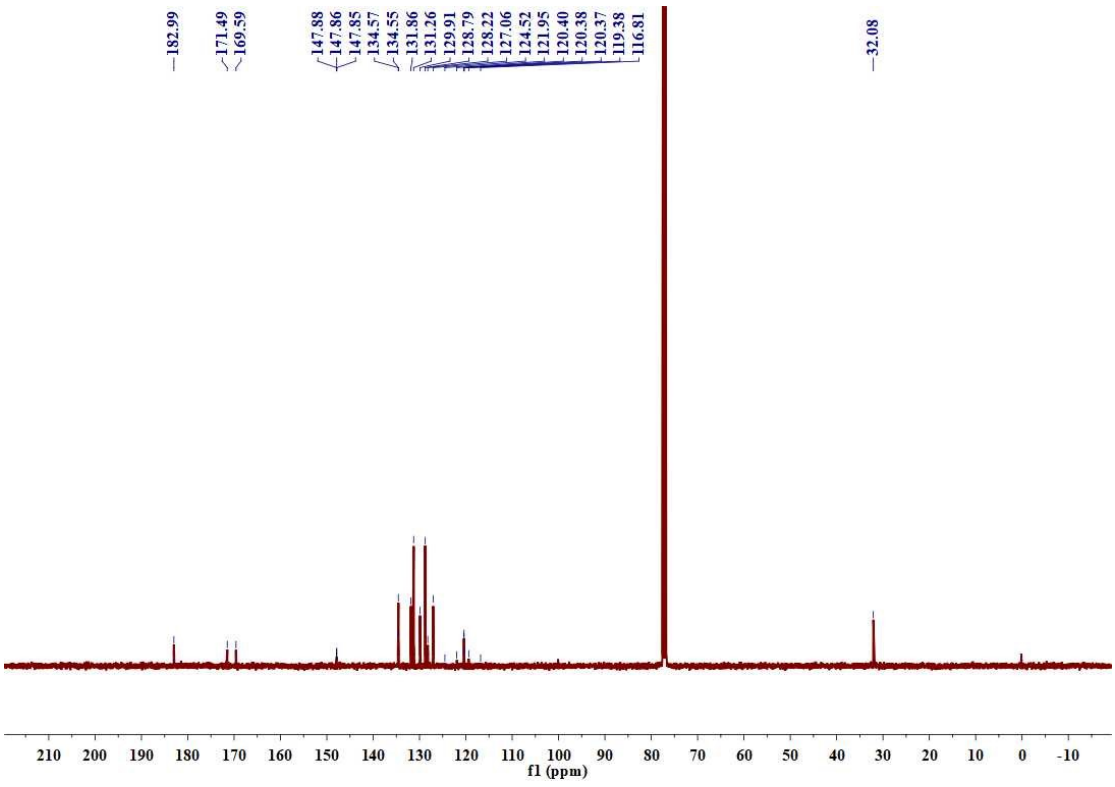
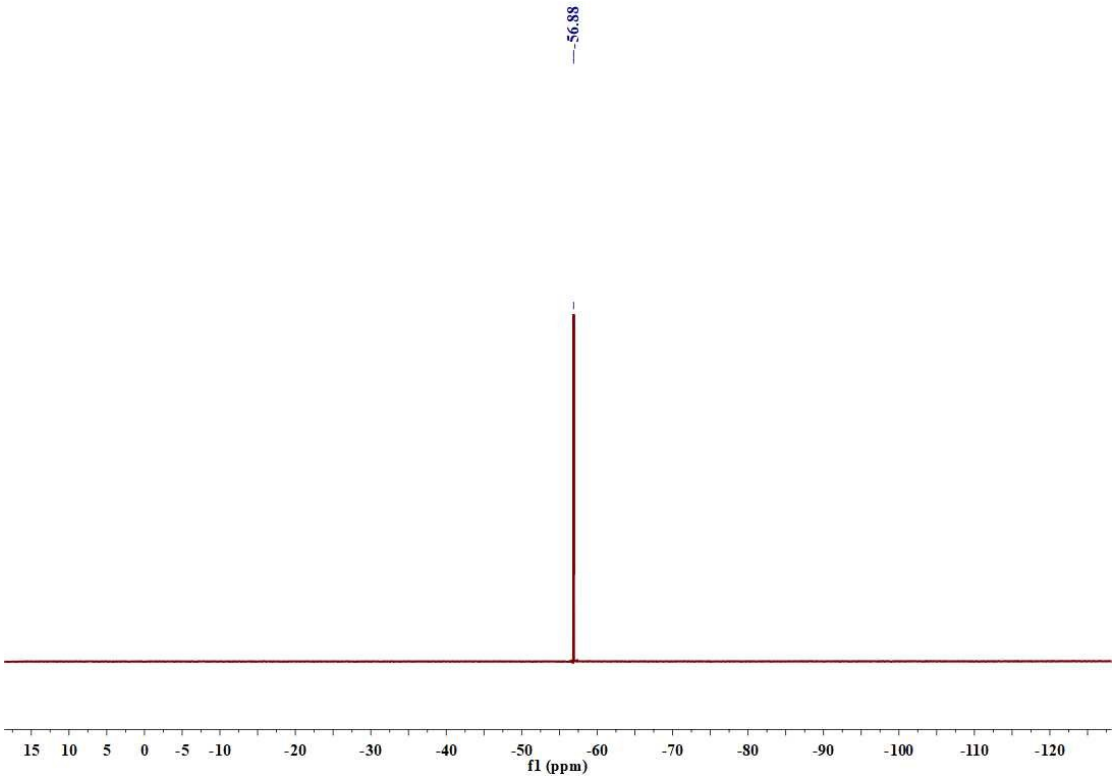



**Figure S18.** $^{1}$H NMR, $^{13}$C NMR, $^{19}$F NMR and HRMS for **E18**.


8.51
8.49
7.70
7.68
7.67
7.66
7.65
7.57
7.56
7.54
7.53
7.38
7.36
7.34
7.31
7.30
7.29
7.28
7.26
7.24
7.24
F
F
F
O
O
S
S
N
N


2.00
2.00
2.00
1.00
2.00
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)


182.99
171.49
169.59
147.88
147.86
147.85
134.57
134.55
131.86
131.26
129.91
128.79
128.22
127.06
124.52
121.95
120.40
120.38
120.37
119.38
116.81
32.08
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)




36 #63 RT: 0.62 AV: 1 NL: 2.40E+008
T: FTMS + p ESI Full ms [120.0000-1800.0000]

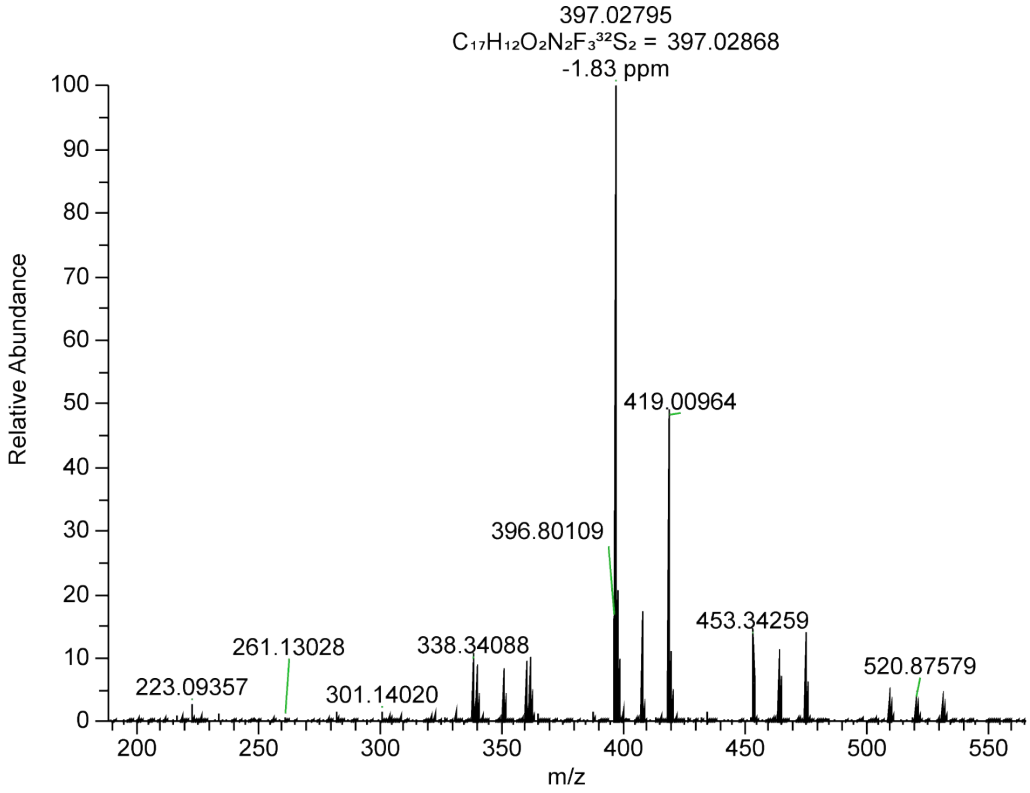
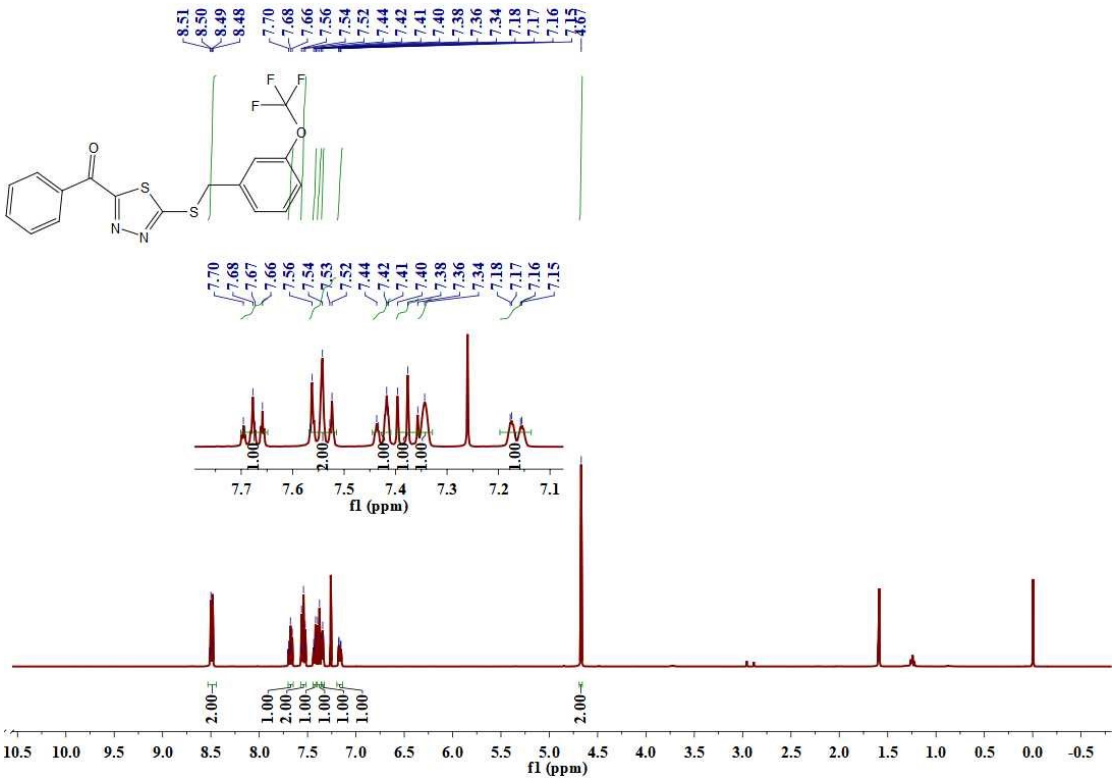
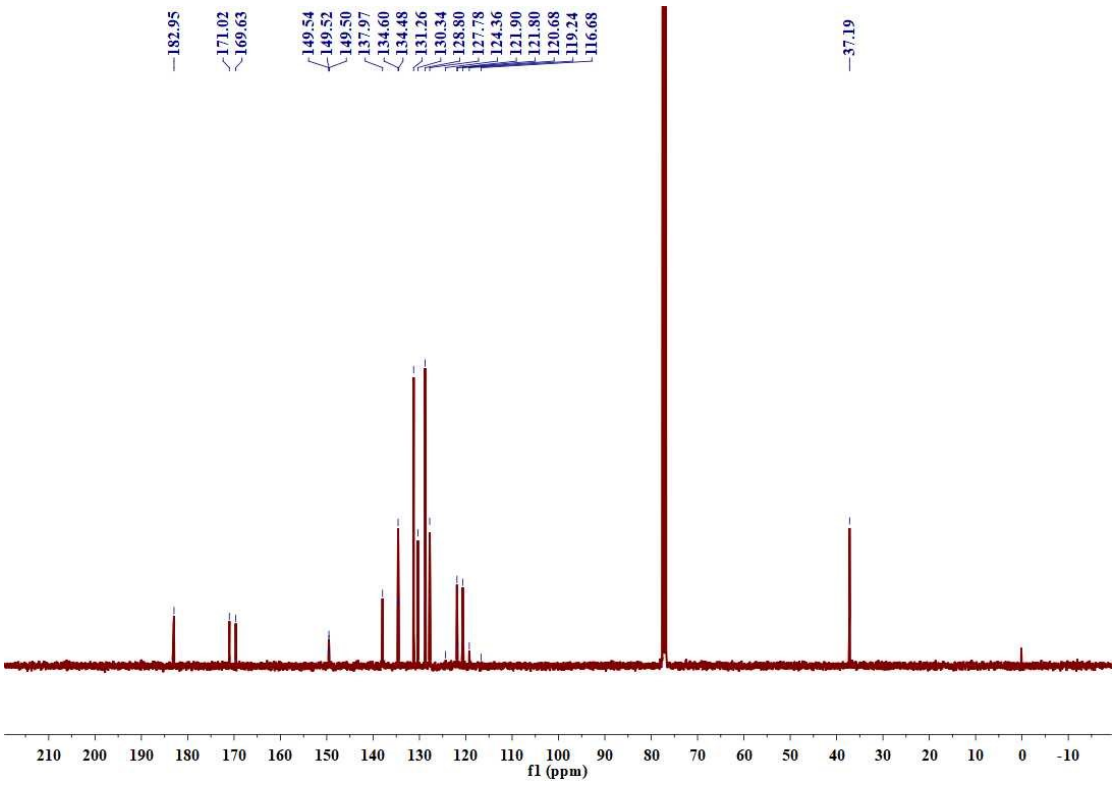
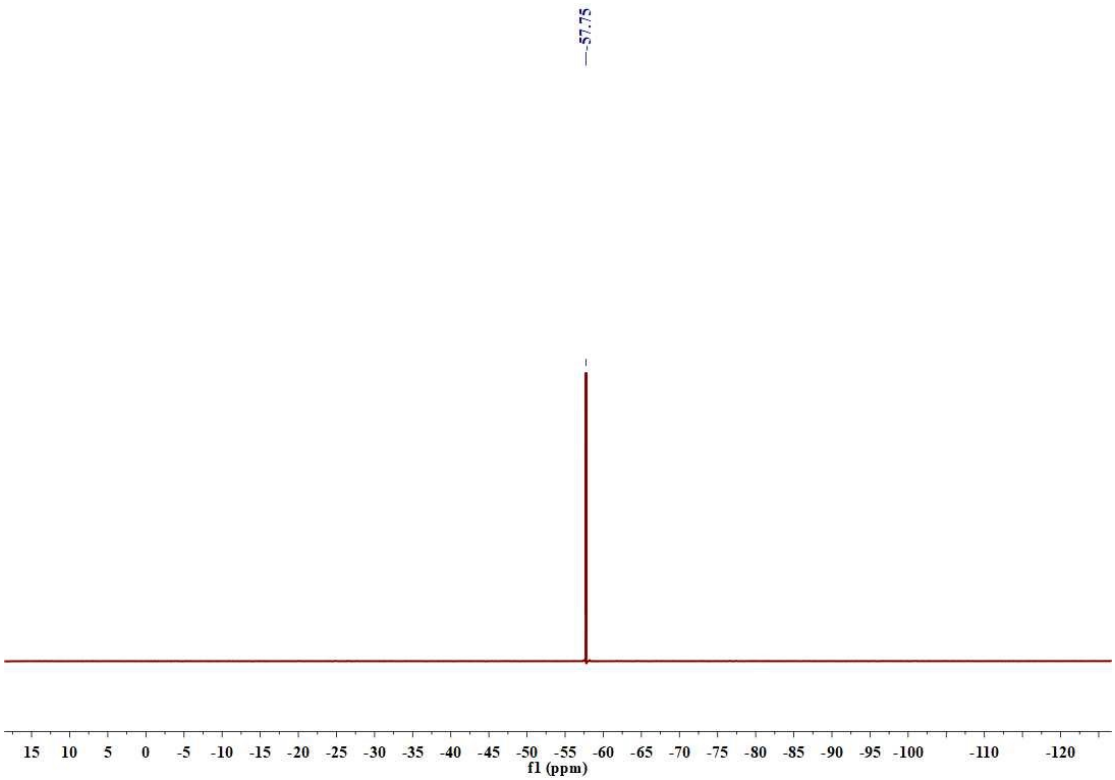



**Figure S19.** $^{1}$H NMR, $^{13}$C NMR, $^{19}$F NMR and HRMS for **E19**.


8.51
8.50
8.49
8.48
7.70
7.68
7.66
7.56
7.54
7.52
7.44
7.42
7.41
7.40
7.38
7.36
7.34
7.18
7.17
7.16
7.15
4.67
F
F
F
O
O
S
S
N
N
7.70
7.68
7.67
7.66
7.56
7.54
7.53
7.52
7.44
7.42
7.41
7.40
7.38
7.36
7.34
7.18
7.17
7.16
7.15
1.00
2.00
1.00
1.00
1.00
1.00
7.7
7.6
7.5
7.4
7.3
7.2
7.1
f1 (ppm)
2.00
1.00
2.00
1.00
1.00
1.00
2.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


182.95
171.02
169.63
149.54
149.52
149.50
137.97
134.60
134.48
131.26
130.34
128.80
127.78
124.36
121.90
121.80
120.68
119.24
116.68
37.19
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)




37 #61 RT: 0.60 AV: 1 NL: 2.02E+008
T: FTMS + p ESI Full ms [120.0000-1800.0000]

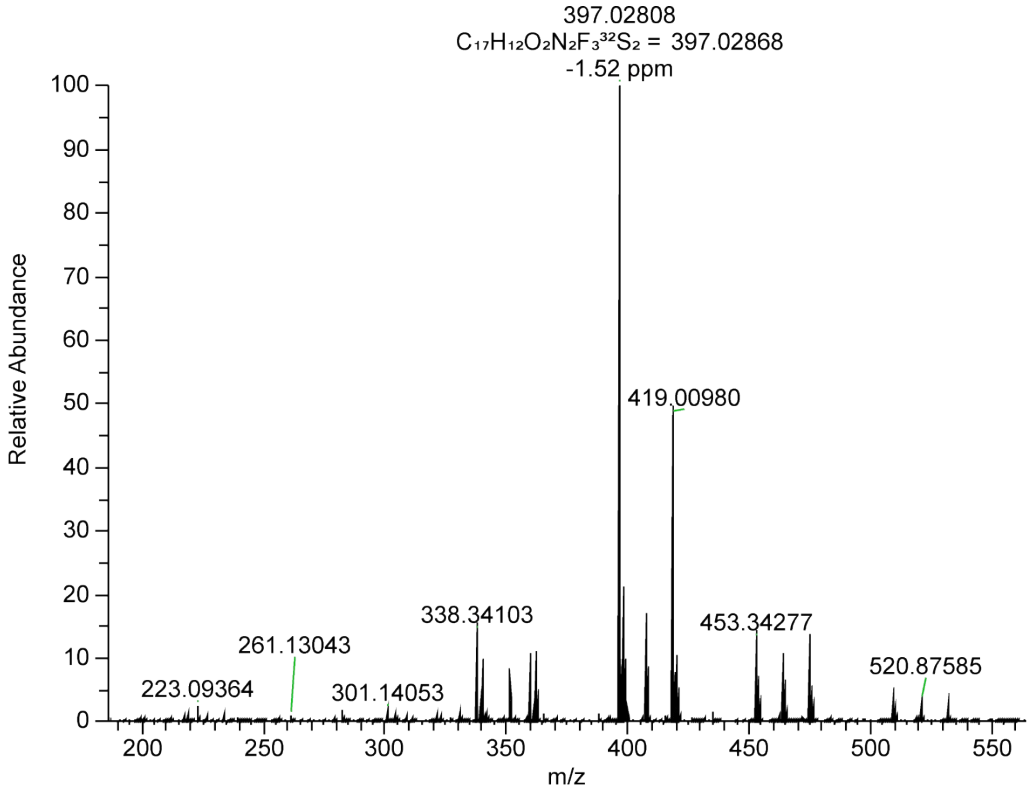
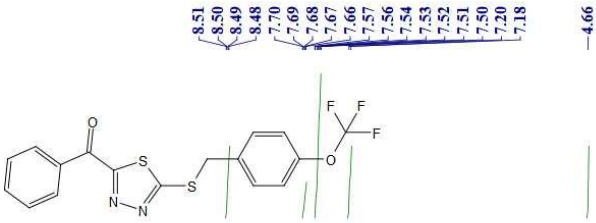
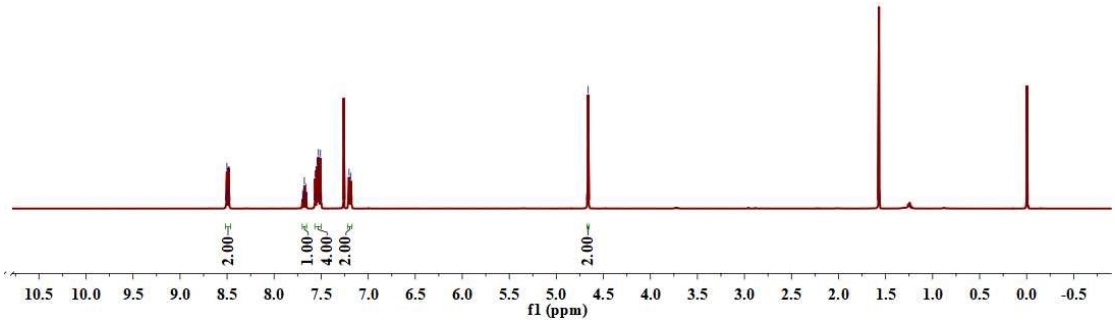
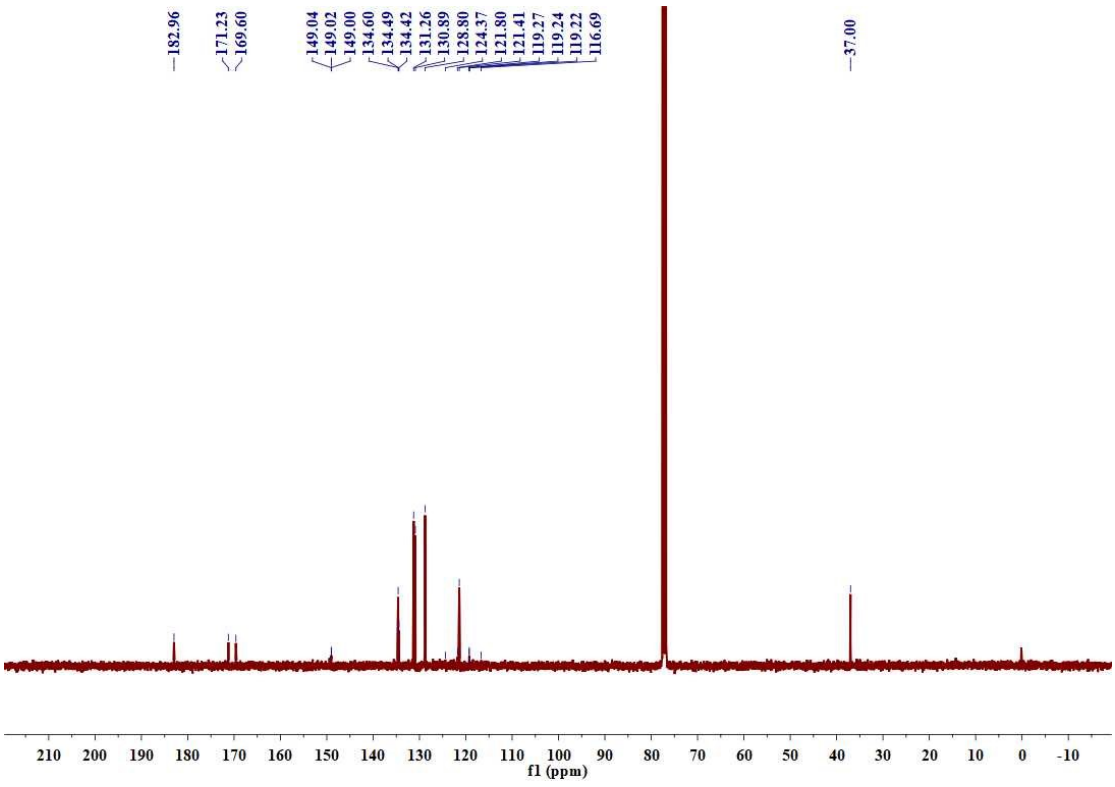
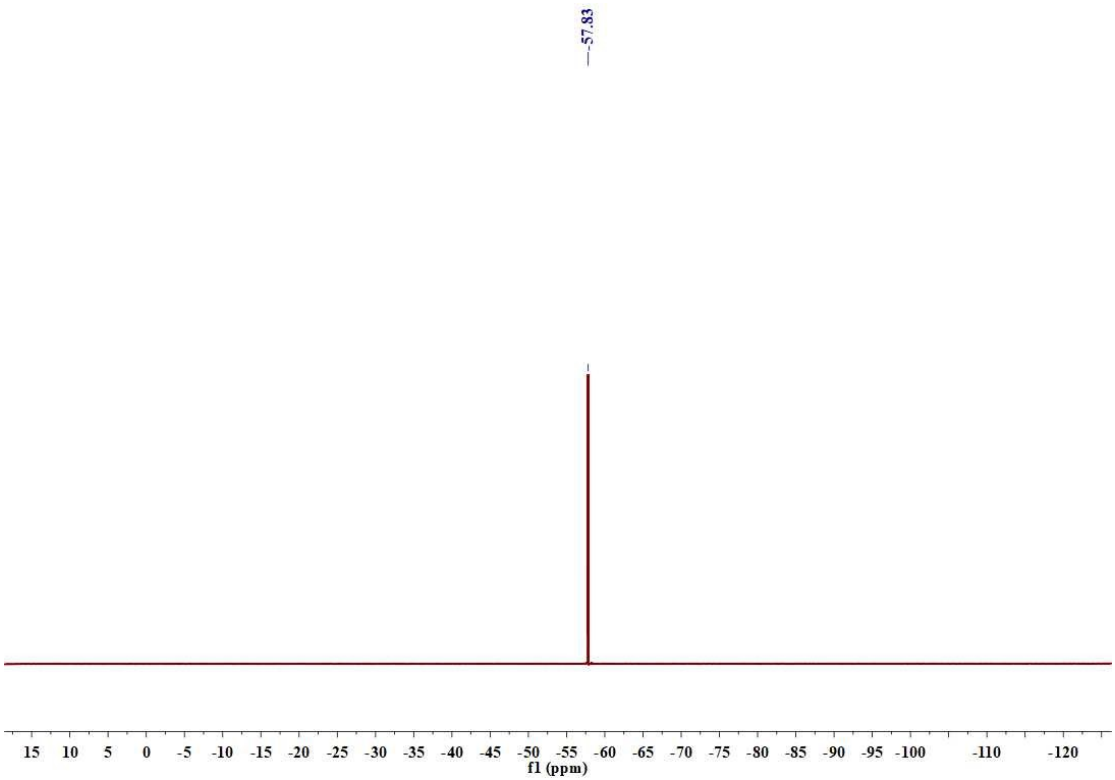



**Figure S20.** $^{1}$H NMR, $^{13}$C NMR, $^{19}$F NMR and HRMS for **E20**.


8.51
8.50
8.49
8.48
7.70
7.69
7.68
7.67
7.66
7.57
7.56
7.54
7.53
7.52
7.51
7.50
7.20
7.18
4.66
O
S
N
N
S
F
F
F
O


2.00
1.00
4.00
2.00
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


182.96
171.23
169.60
149.04
149.02
149.00
134.60
134.49
134.42
131.26
130.89
128.80
124.37
121.80
121.41
119.27
119.24
119.22
116.69
37.00
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)




38 #63 RT: 0.62 AV: 1 NL: 7.31E+007
T: FTMS + p ESI Full ms [120.0000-1800.0000]

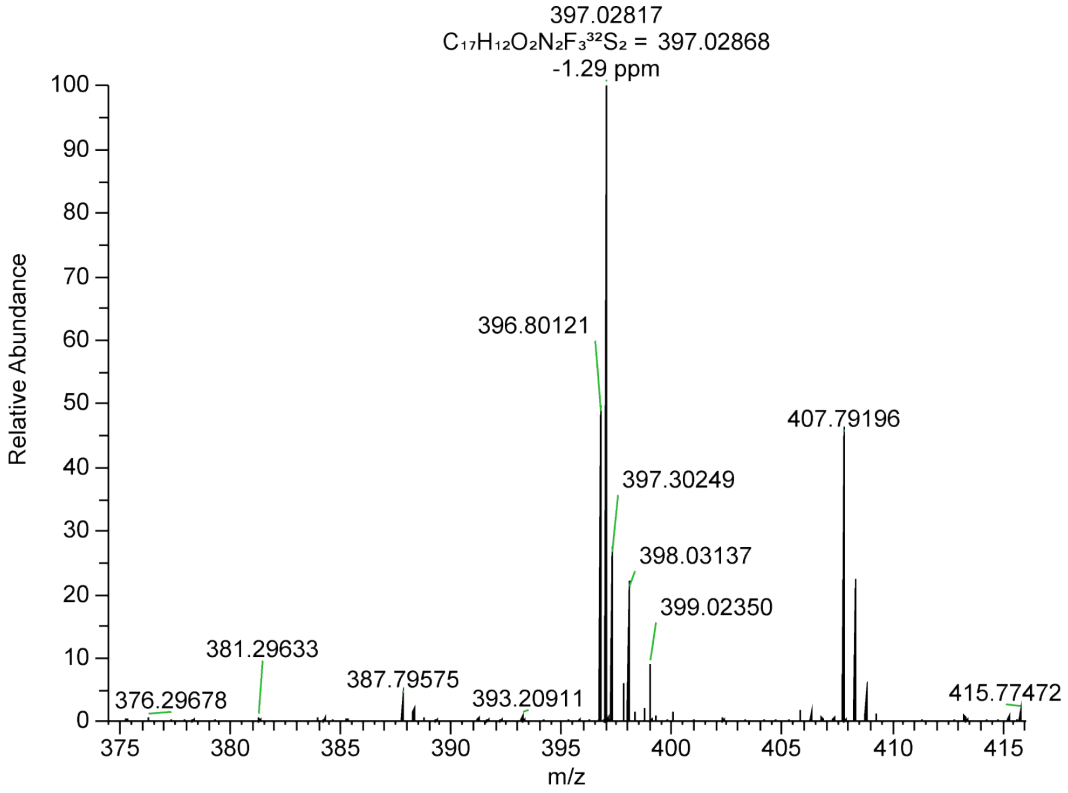
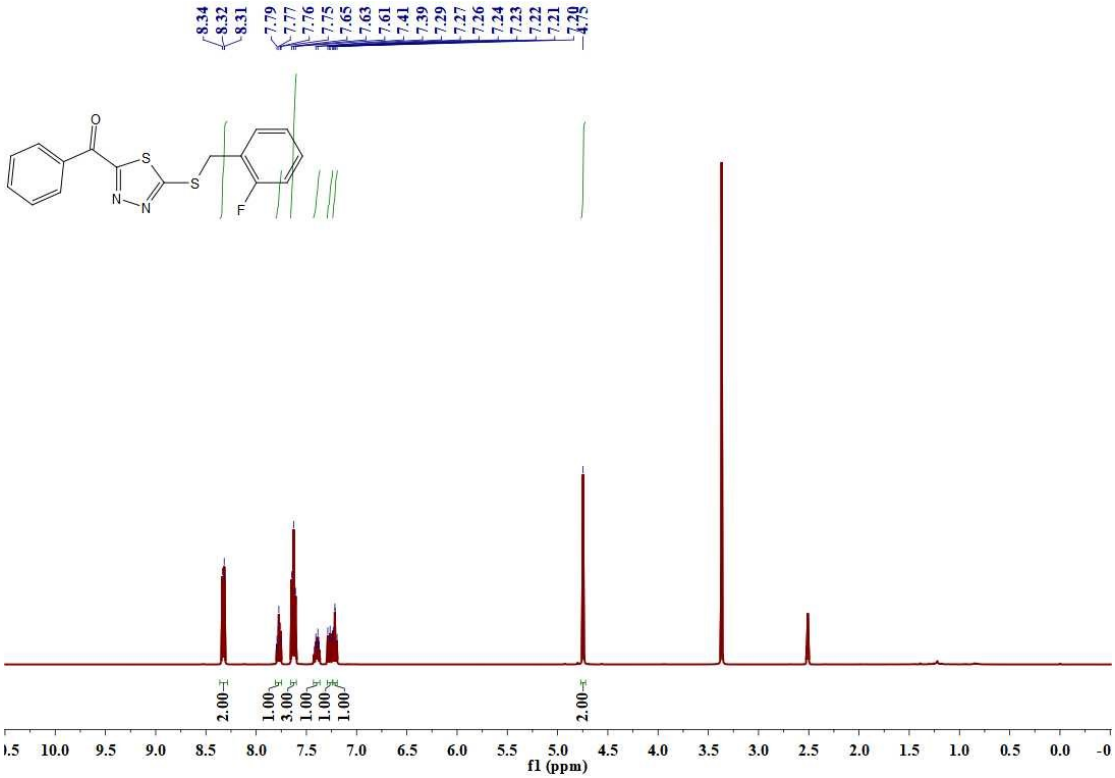
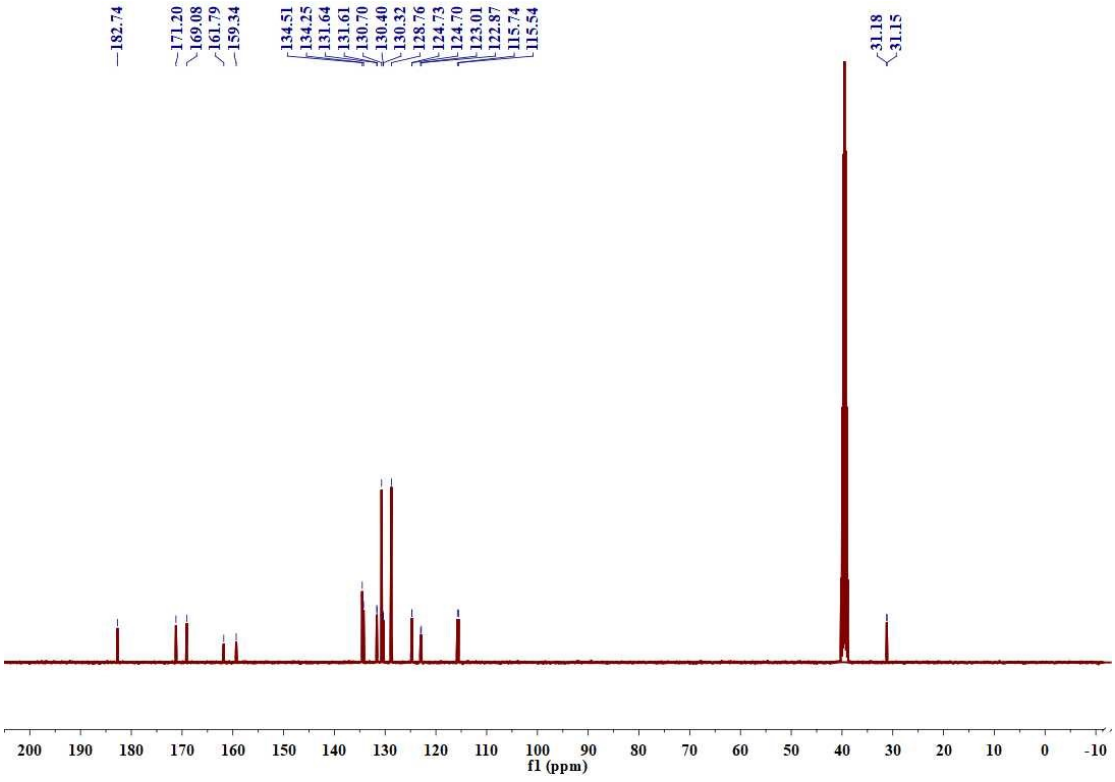
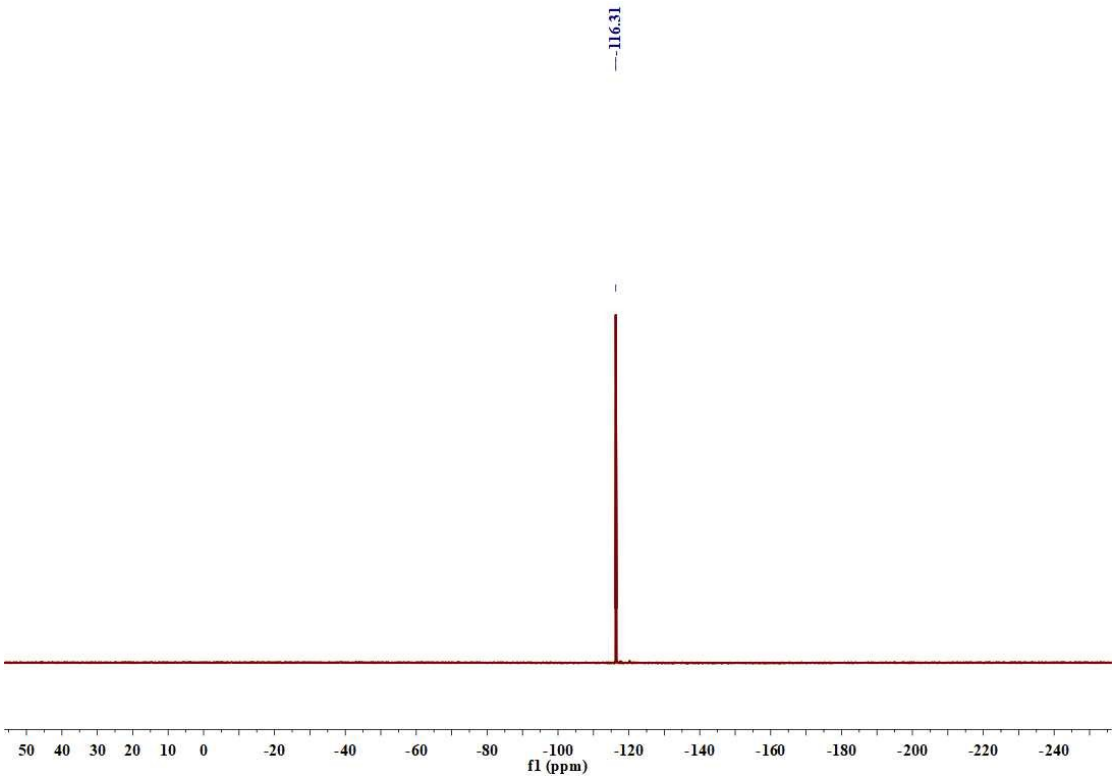



**Figure S21.** $^{1}$H NMR, $^{13}$C NMR, $^{19}$F NMR and HRMS for **E21**.


8.34
8.32
8.31
7.79
7.77
7.76
7.75
7.65
7.63
7.61
7.41
7.39
7.29
7.27
7.26
7.24
7.23
7.22
7.21
7.20
4.73
O
S
N
N
S
F
2.00
1.00
3.00
1.00
1.00
1.00
2.00
f1 (ppm)


182.74
171.20
169.08
161.79
159.34
134.51
134.25
131.64
131.61
130.70
130.40
130.32
128.76
124.73
124.70
123.01
122.87
115.74
115.54
31.18
31.15
f1 (ppm)




30 #61 RT: 0.61 AV: 1 NL: 1.33E+008
T: FTMS + p ESI Full ms [120.0000-1800.0000]

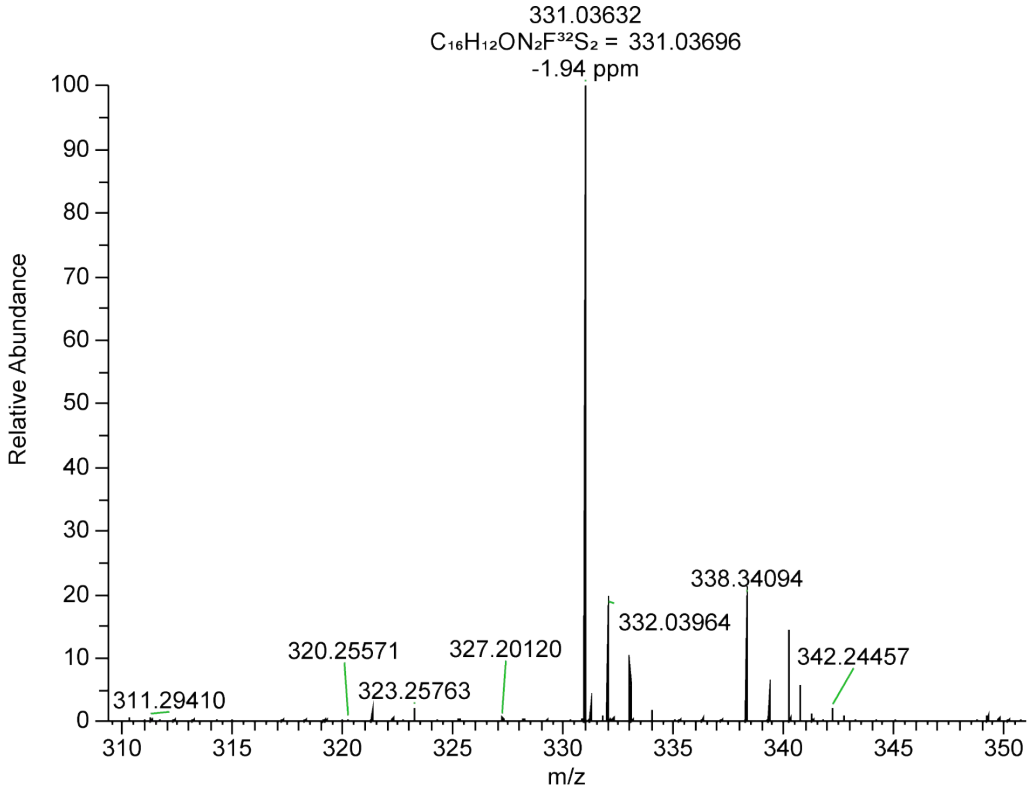
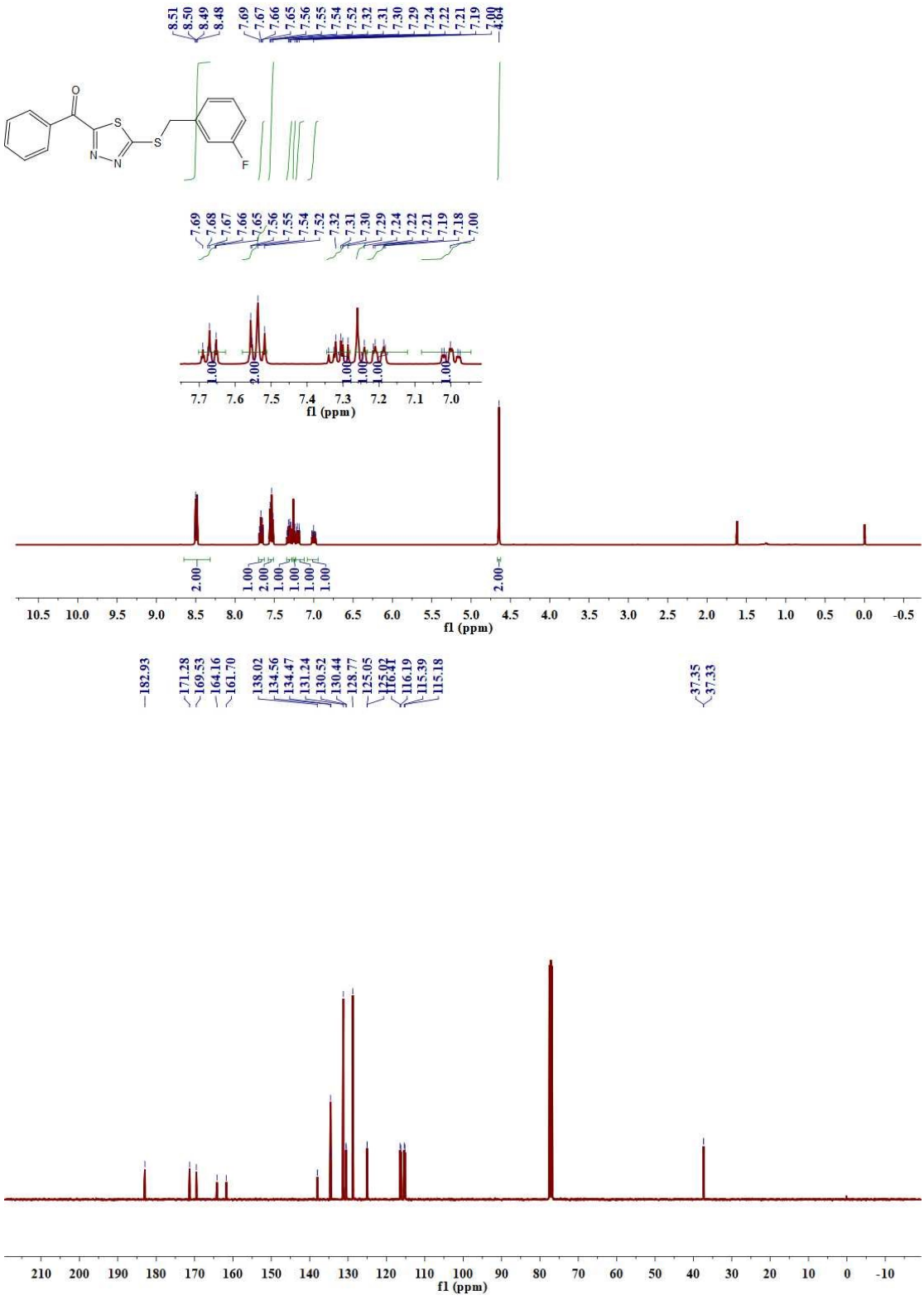
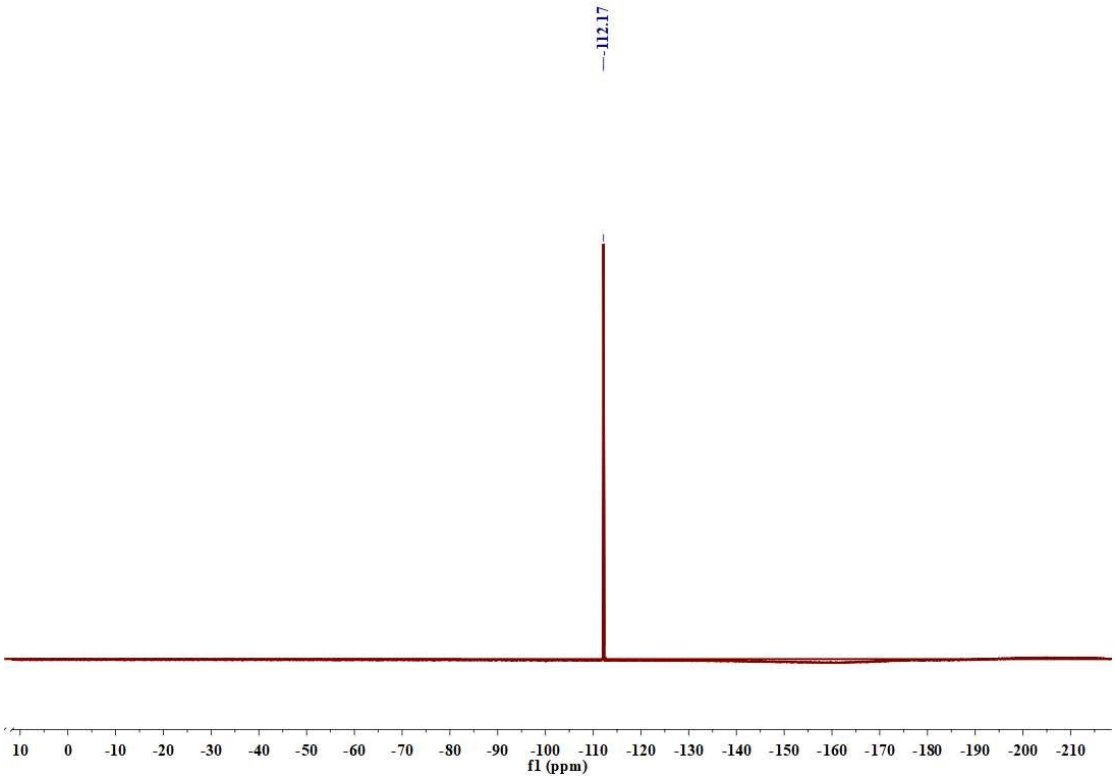



**Figure S22.** $^{1}$H NMR, $^{13}$C NMR, $^{19}$F NMR and HRMS for **E22**.


8.51
8.50
8.49
8.48
7.69
7.67
7.66
7.65
7.56
7.55
7.54
7.52
7.32
7.31
7.30
7.29
7.24
7.22
7.21
7.19
7.00
4.04
O
S
N
N
S
F
7.69
7.68
7.67
7.66
7.65
7.56
7.55
7.54
7.52
7.32
7.31
7.30
7.29
7.24
7.22
7.21
7.19
7.18
7.00
1.00
2.00
1.00
1.00
1.00
1.00
1.00
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
f1 (ppm)
2.00
1.00
2.00
1.00
1.00
1.00
2.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)
182.93
171.28
169.53
164.16
161.70
138.02
134.56
134.47
131.24
130.52
130.44
128.77
125.05
125.02
116.41
116.19
115.39
115.18
37.35
37.33
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)




31 #63 RT: 0.63 AV: 1 NL: 7.14E+007
T: FTMS + p ESI Full ms [120.0000-1800.0000]

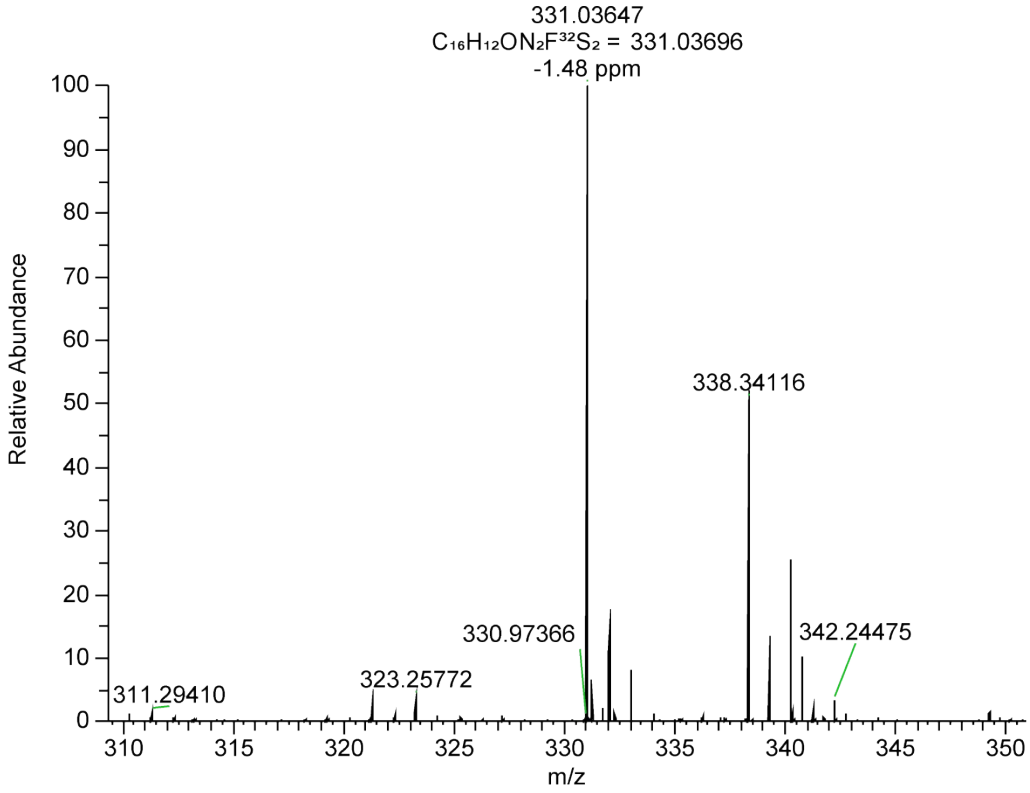
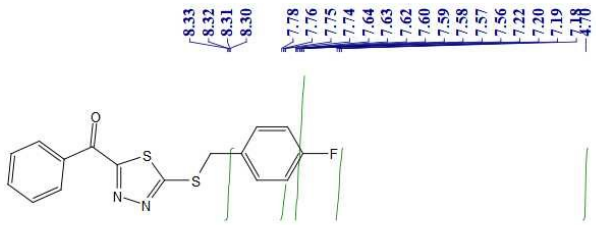
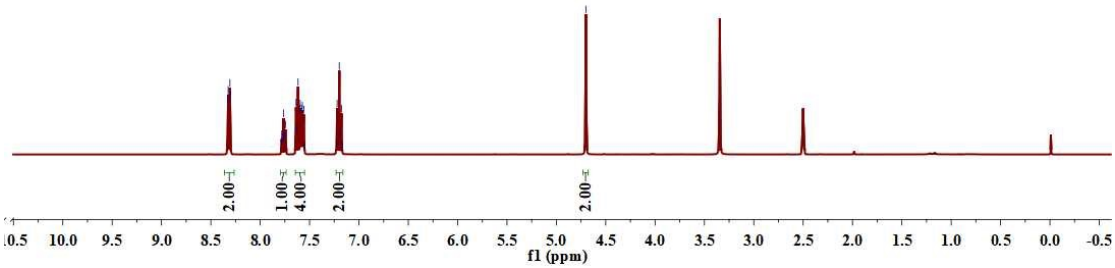
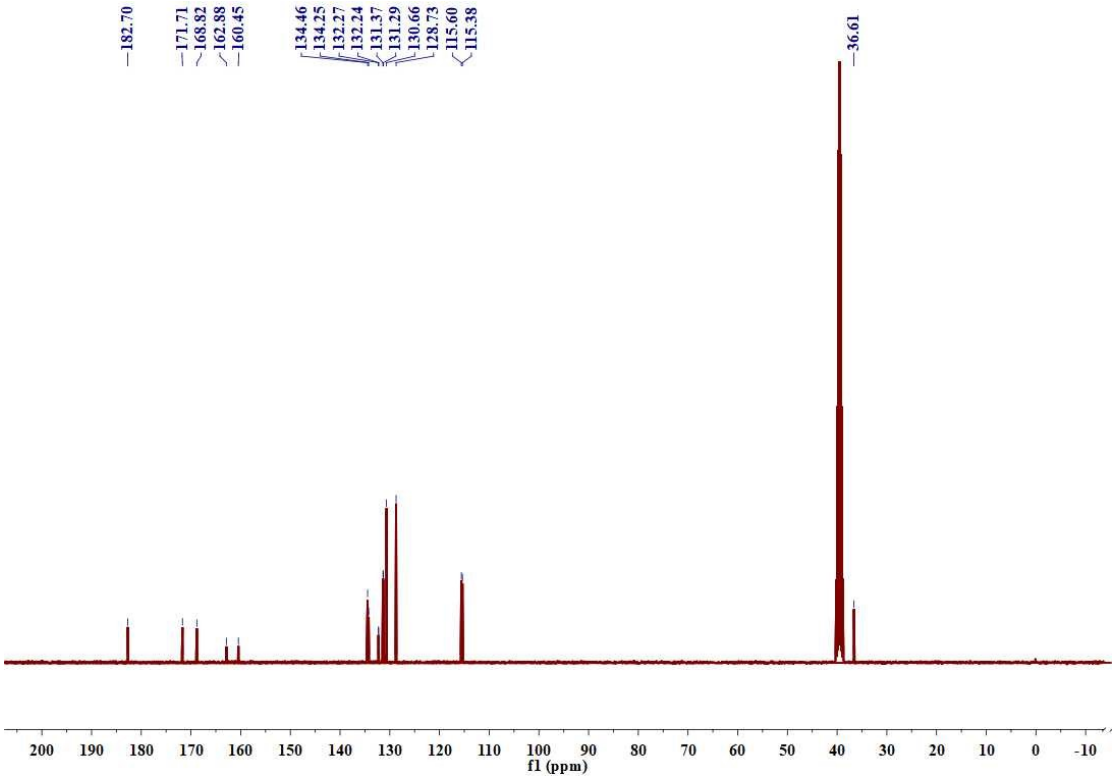
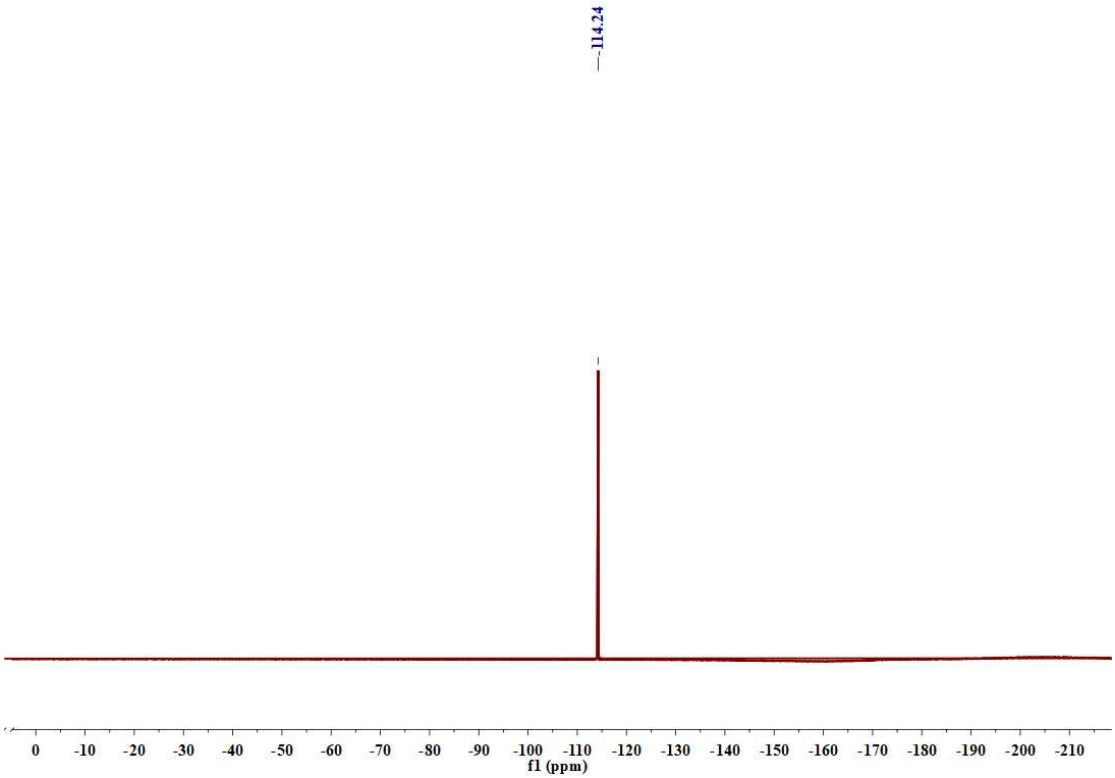



**Figure S23.** $^{1}$H NMR, $^{13}$C NMR, $^{19}$F NMR and HRMS for **E23**.


8.33
8.32
8.31
8.30
7.78
7.76
7.75
7.74
7.64
7.63
7.62
7.60
7.59
7.58
7.57
7.56
7.22
7.20
7.19
O
S
N
N
S
F


2.00
1.00
4.00
2.00
2.00
f1 (ppm)


182.70
171.71
168.82
162.88
160.45
134.46
134.25
132.27
132.24
131.37
131.29
130.66
128.73
115.60
115.38
36.61
f1 (ppm)




32 #55 RT: 0.55 AV: 1 NL: 5.64E+007
T: FTMS + p ESI Full ms [120.0000-1800.0000]

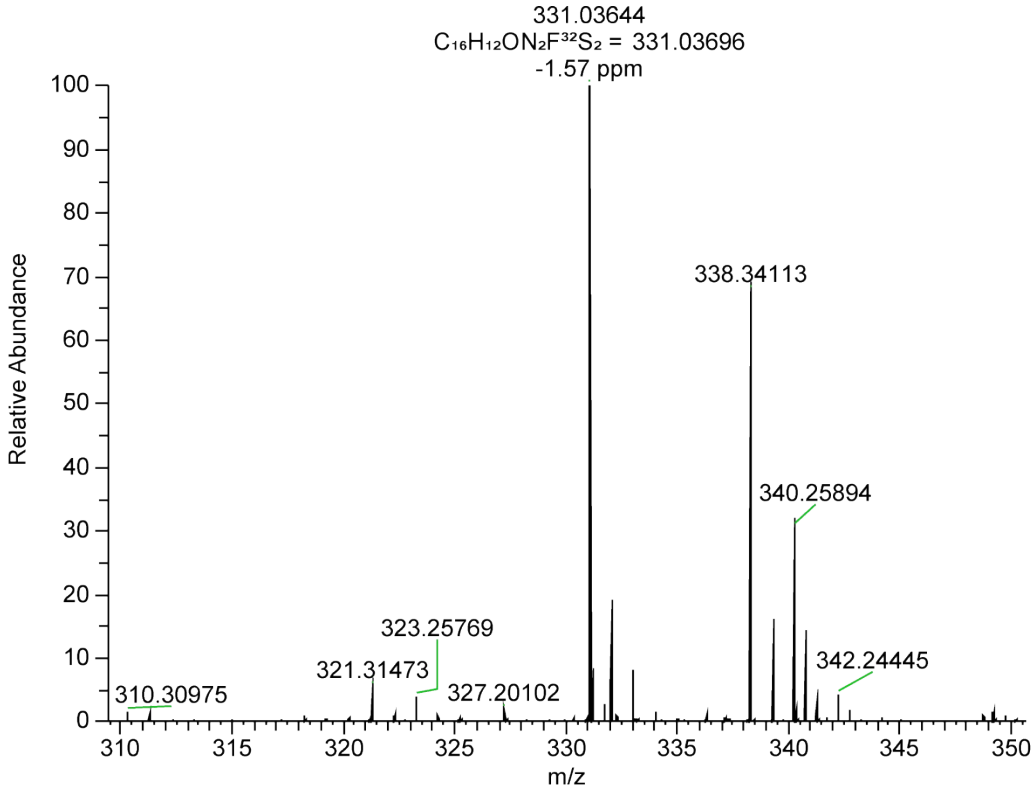
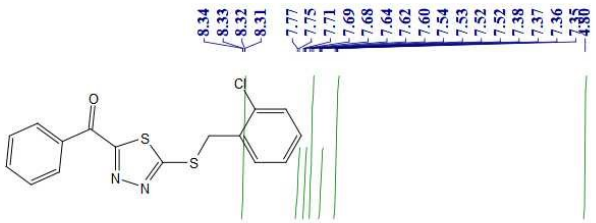
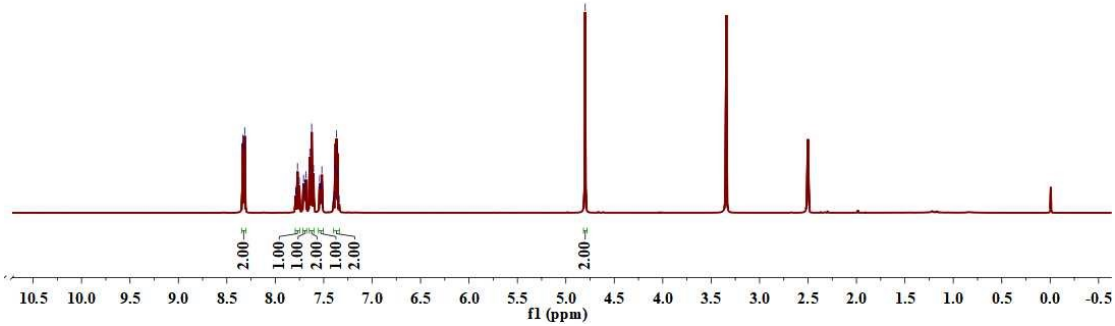
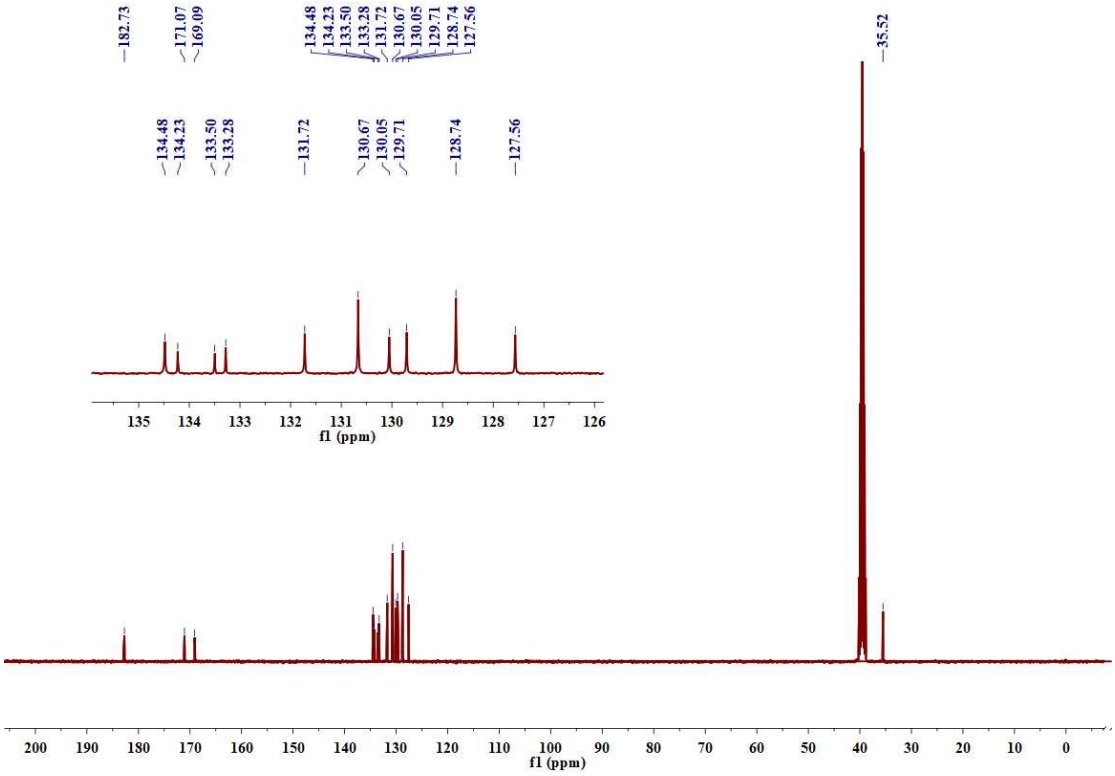



**Figure S24.** $^{1}$H NMR, $^{13}$C NMR, $^{19}$F NMR and HRMS for **E24**.


8.34
8.33
8.32
8.31
7.77
7.75
7.71
7.69
7.68
7.64
7.62
7.60
7.54
7.53
7.52
7.52
7.38
7.37
7.36
7.35
4.30
O
S
N
N
S
Cl


2.00
1.00
1.00
2.00
1.00
2.00
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


182.73
171.07
169.09
134.48
134.23
133.50
133.28
131.72
130.67
130.05
129.71
128.74
127.56
35.52
135 134 133 132 131 130 129 128 127 126
f1 (ppm)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

17 #67 RT: 0.77 AV: 1 NL: 4.74E+007
T: FTMS + p ESI Full ms [120.0000-1800.0000]

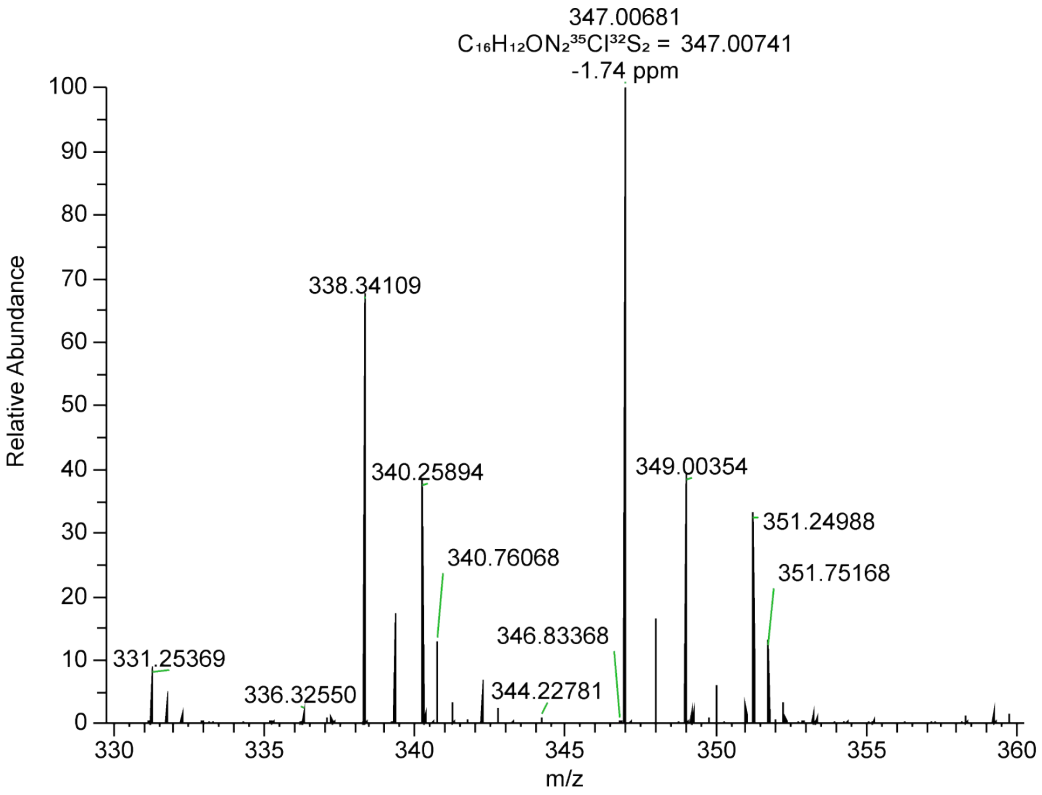
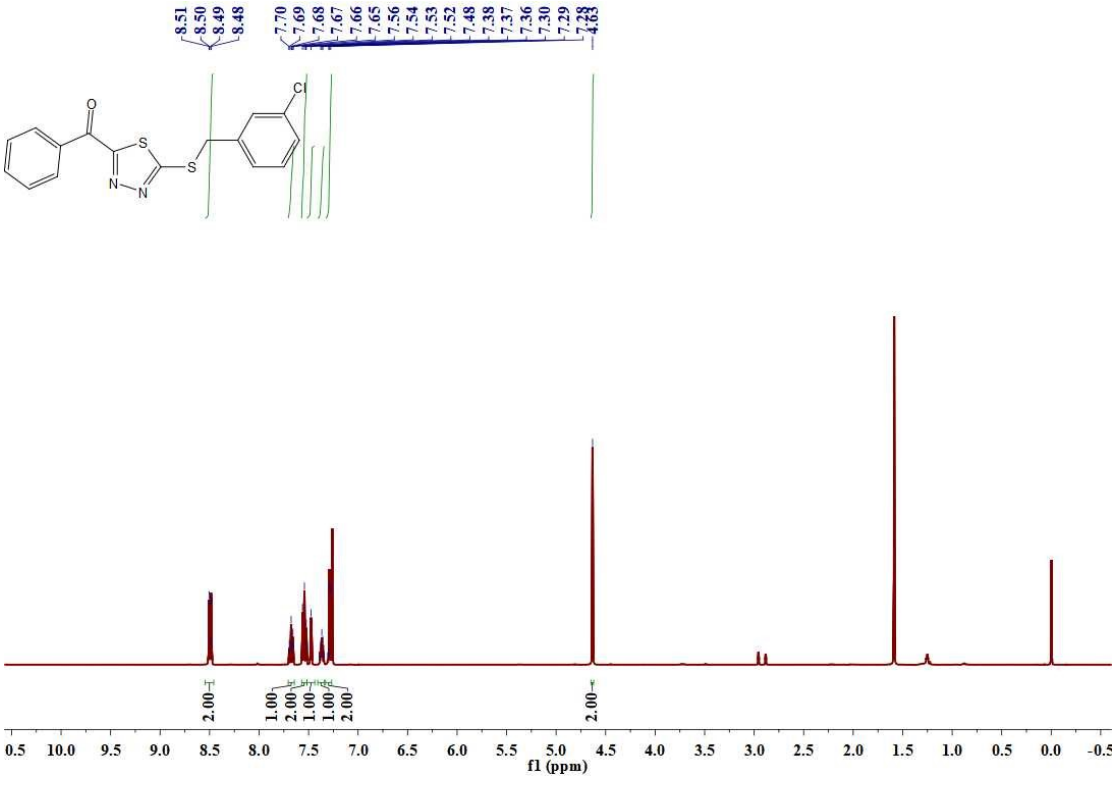
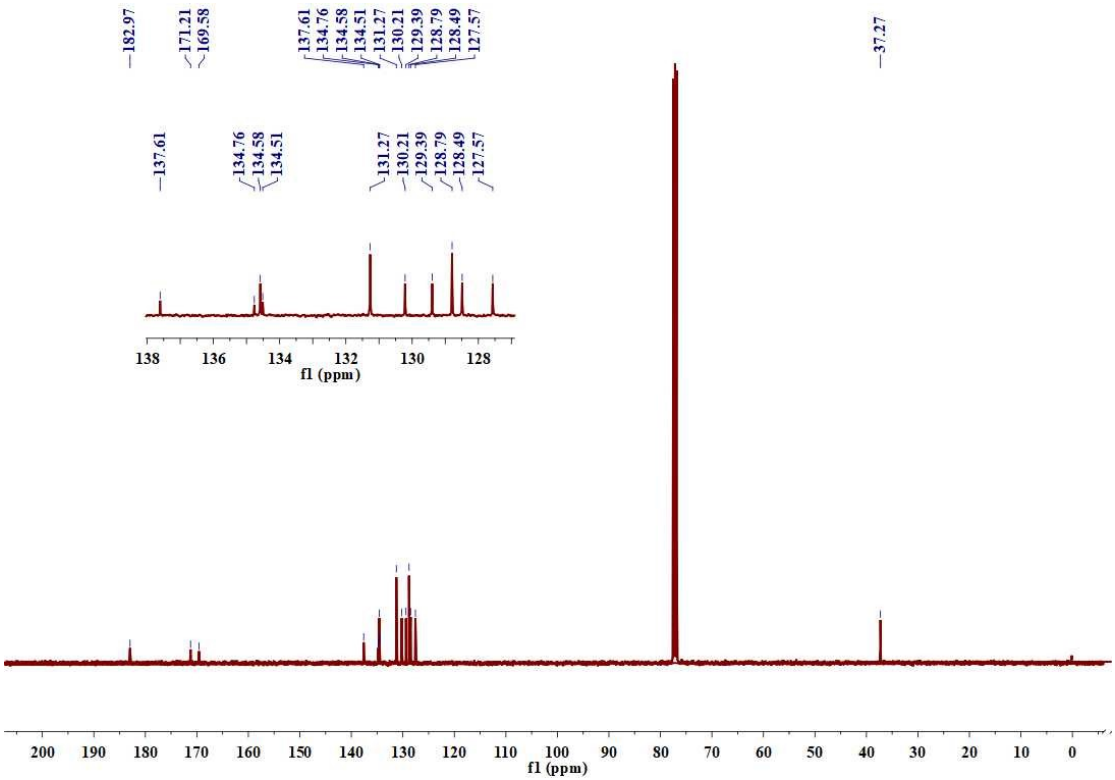



**Figure S25.** [1]H NMR, [13]C NMR and HRMS for **E25**.






18 #55 RT: 0.63 AV: 1 NL: 4.33E+007
T: FTMS + p ESI Full ms [120.0000-1800.0000]

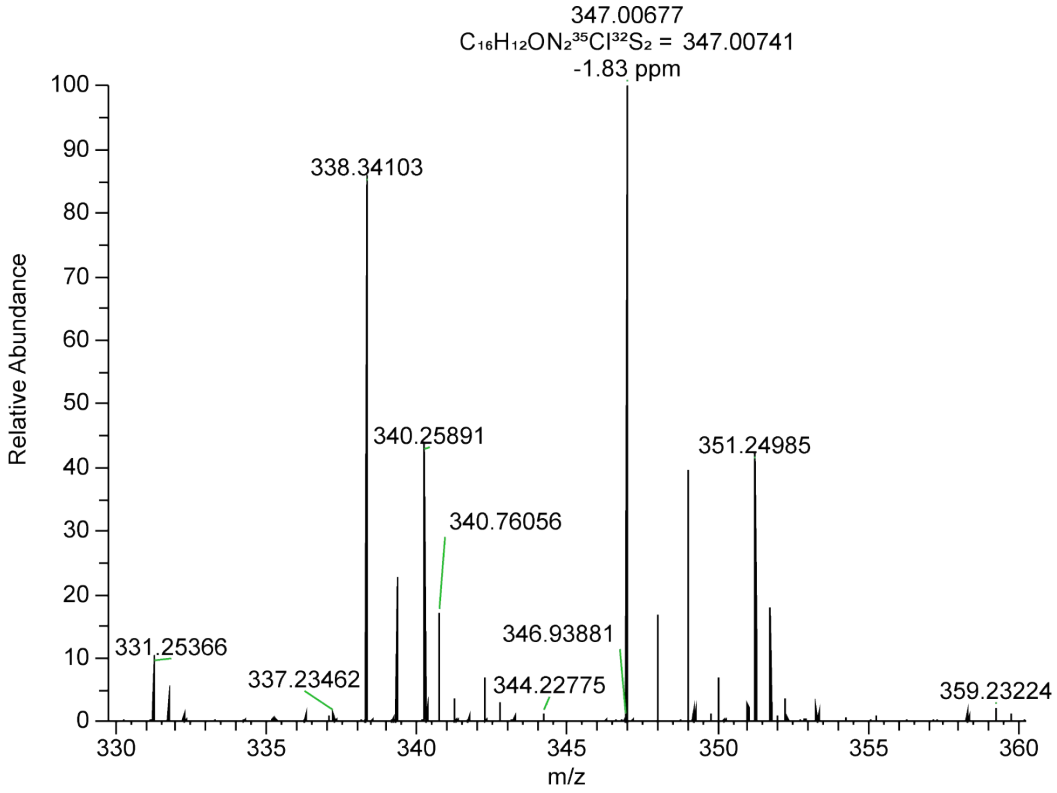
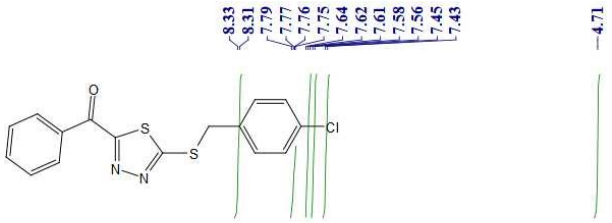
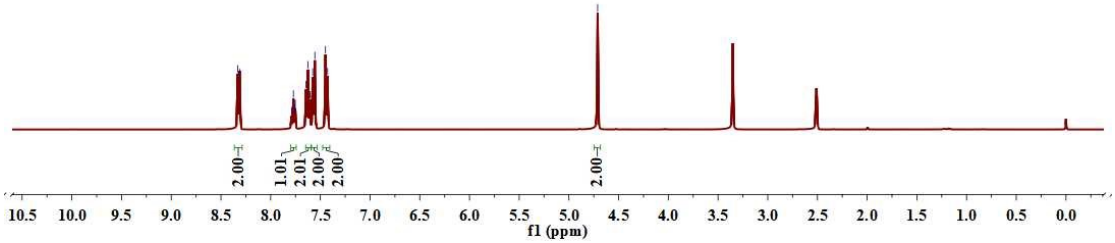
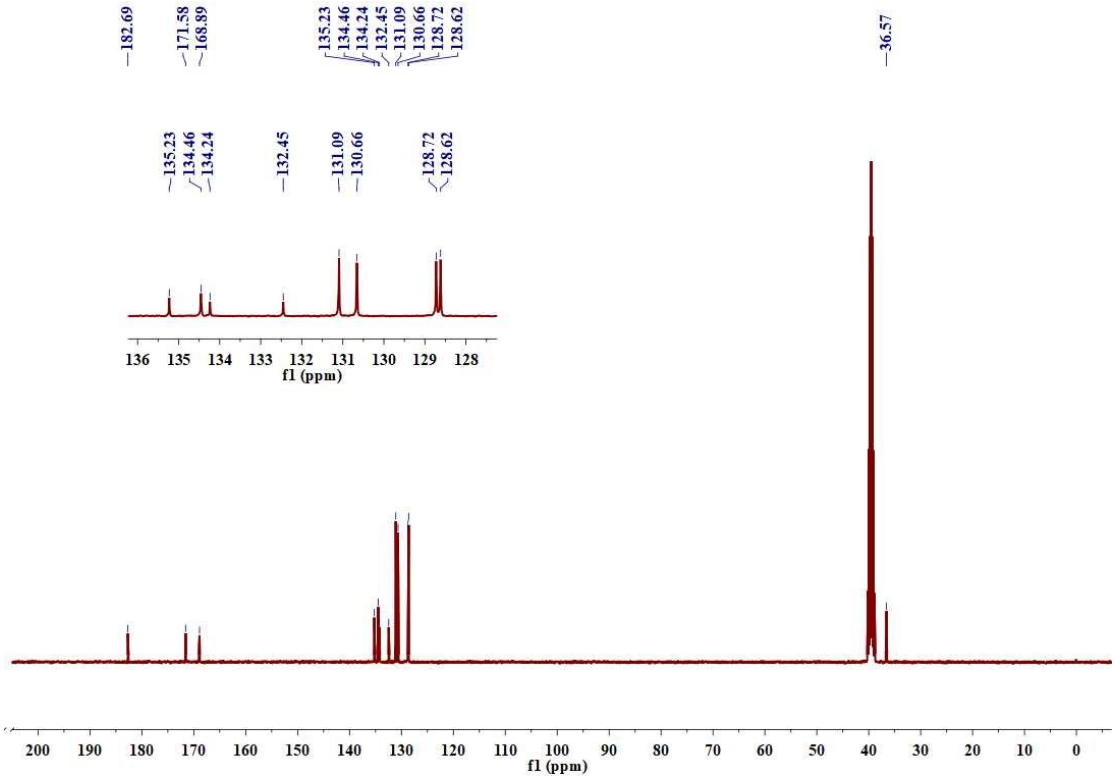



**Figure S26.** $^{1}$H NMR, $^{13}$C NMR and HRMS for **E26**.


8.33
8.31
7.79
7.77
7.76
7.75
7.64
7.62
7.61
7.58
7.56
7.45
7.43
4.71
O
S
N
N
S
Cl


2.00
1.01
2.01
2.00
2.00
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


182.69
171.58
168.89
135.23
134.46
134.24
132.45
131.09
130.66
128.72
128.62
36.57
135.23
134.46
134.24
132.45
131.09
130.66
128.72
128.62
136 135 134 133 132 131 130 129 128
f1 (ppm)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

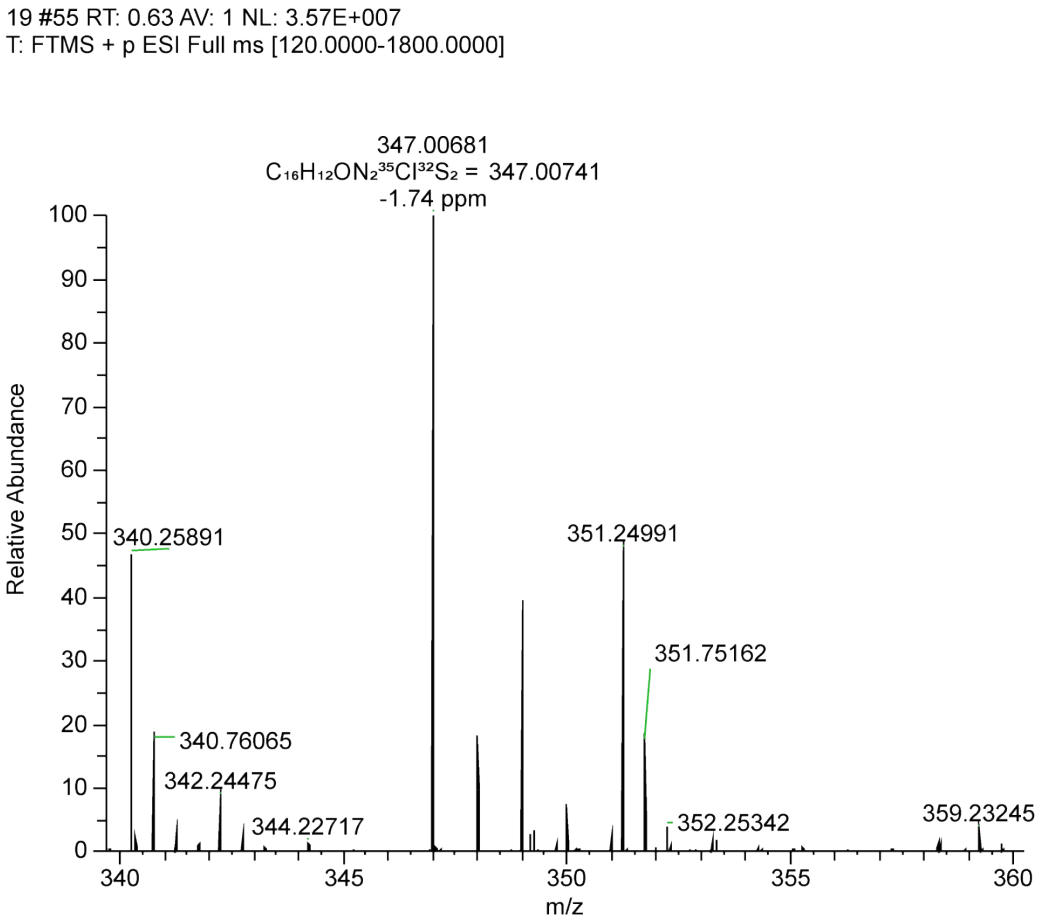
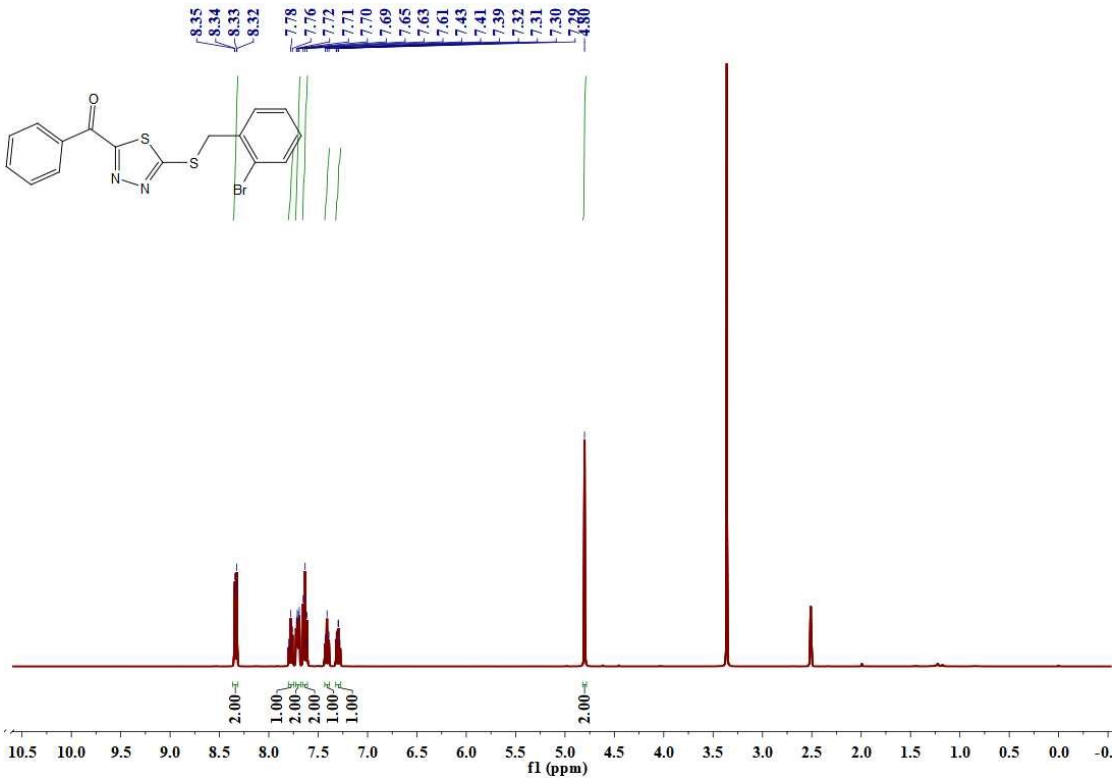
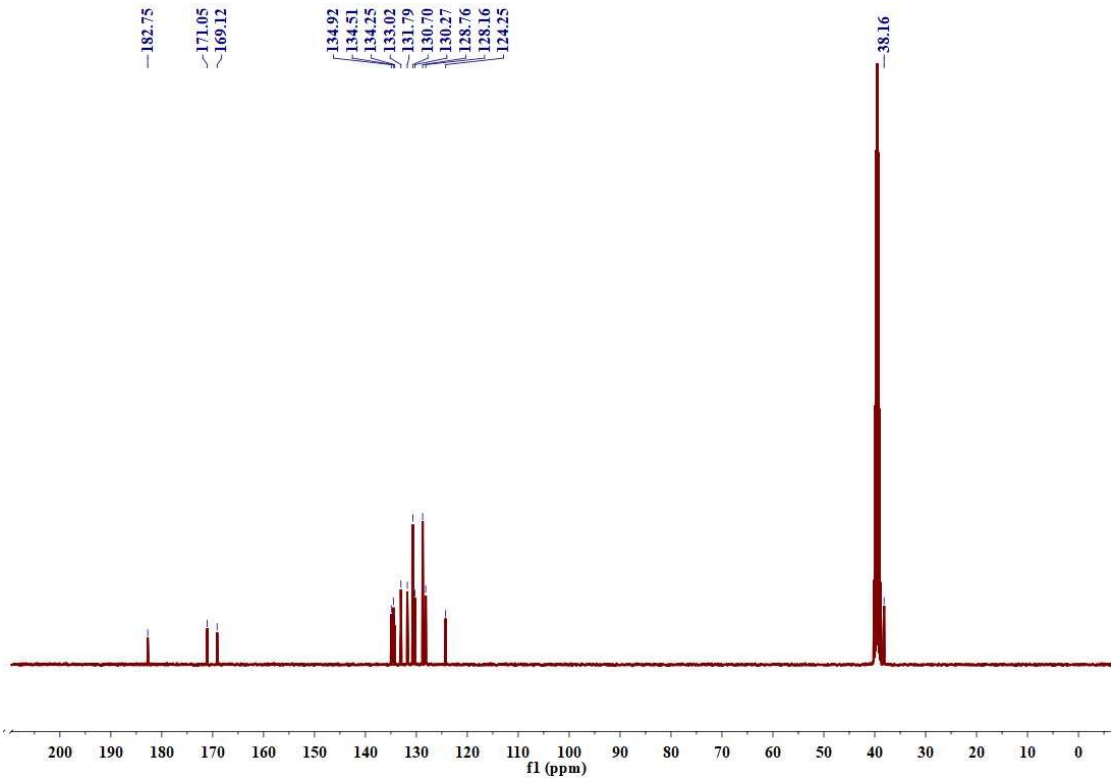



**Figure S27.** $^{1}$H NMR, $^{13}$C NMR and HRMS for **E27**.






24 #77 RT: 0.80 AV: 1 NL: 2.69E+007
T: FTMS + p ESI Full ms [120.0000-1800.0000]

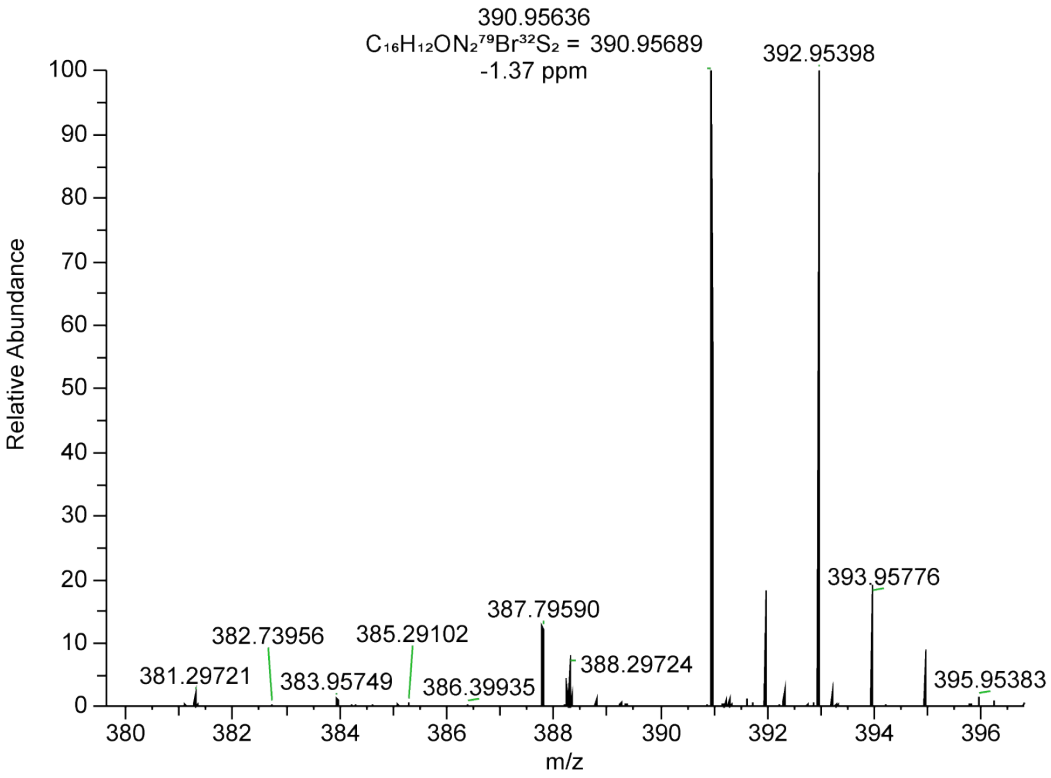
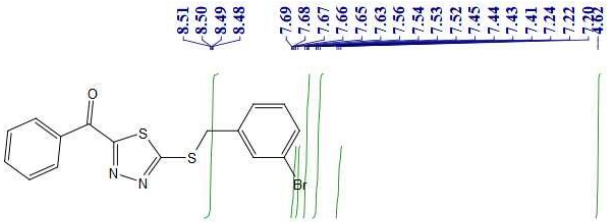
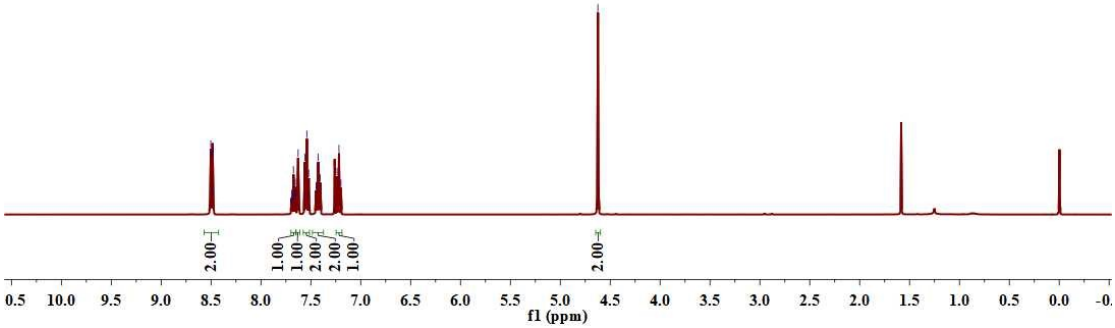
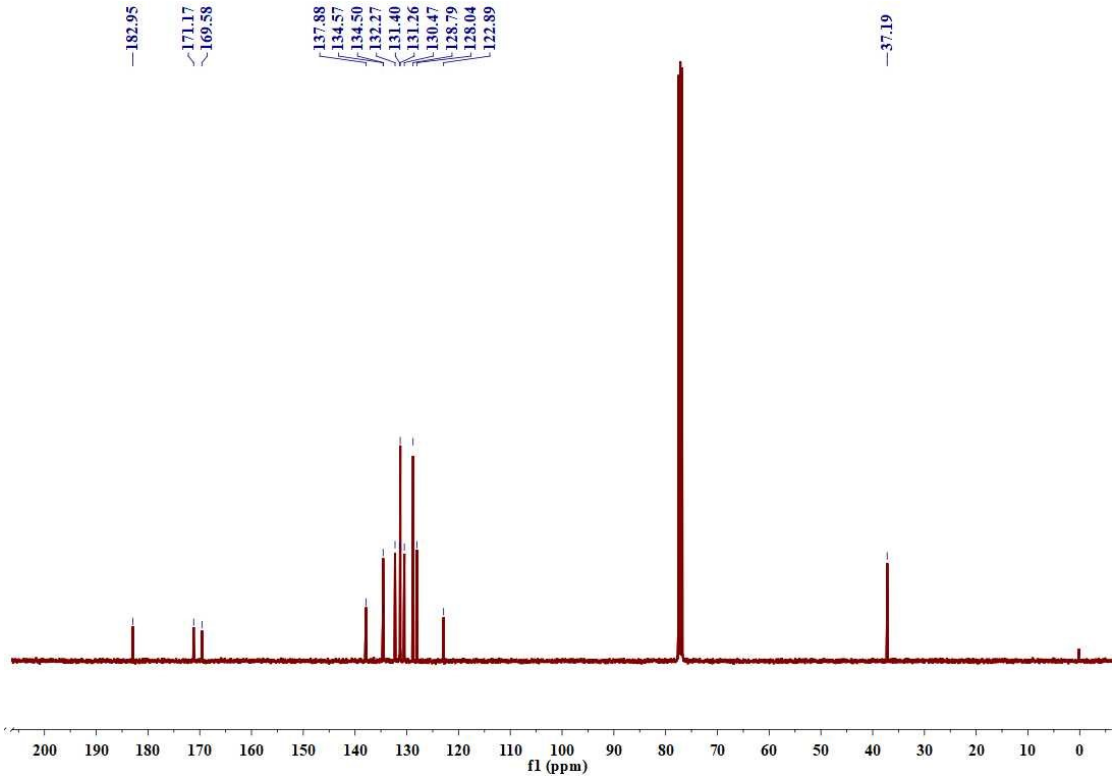



**Figure S28.** $^{1}$H NMR, $^{13}$C NMR and HRMS for **E28**.


8.51
8.50
8.49
8.48
7.69
7.68
7.67
7.66
7.65
7.63
7.56
7.54
7.53
7.52
7.45
7.44
7.43
7.41
7.24
7.22
7.20
4.62
O
S
S
N
N
Br


2.00
1.00
1.00
2.00
2.00
1.00
2.00
f1 (ppm)


182.95
171.17
169.58
137.88
134.57
134.50
132.27
131.40
131.26
130.47
128.79
128.04
122.89
37.19
f1 (ppm)

25 #63 RT: 0.65 AV: 1 NL: 4.38E+007
T: FTMS + p ESI Full ms [120.0000-1800.0000]

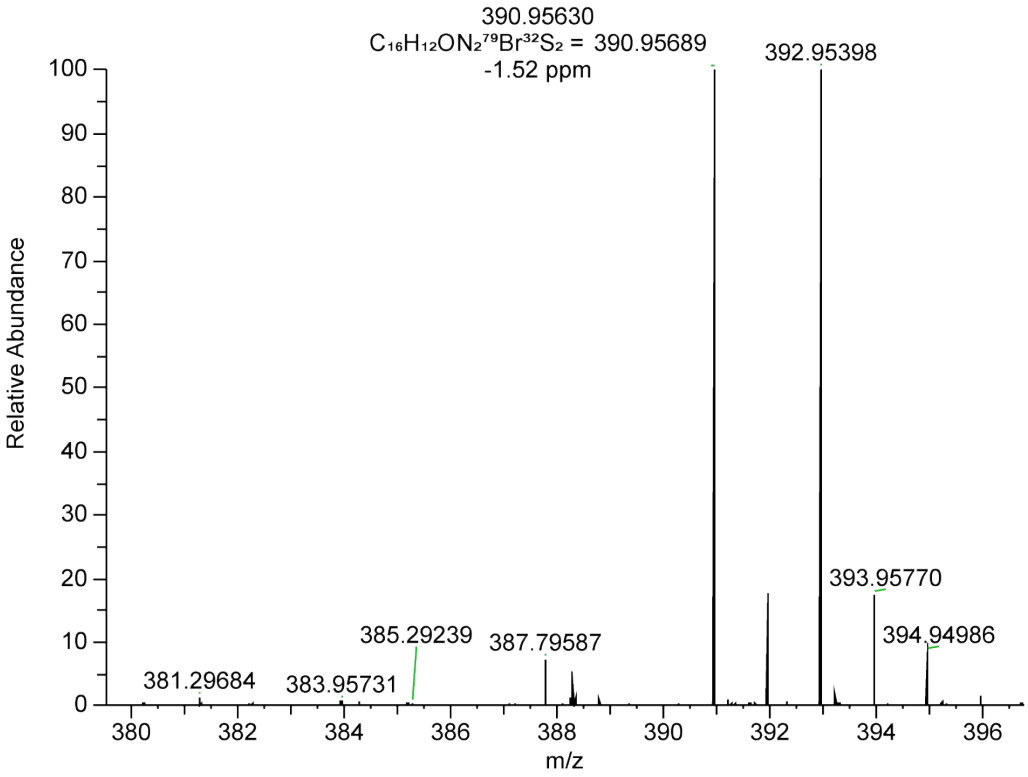
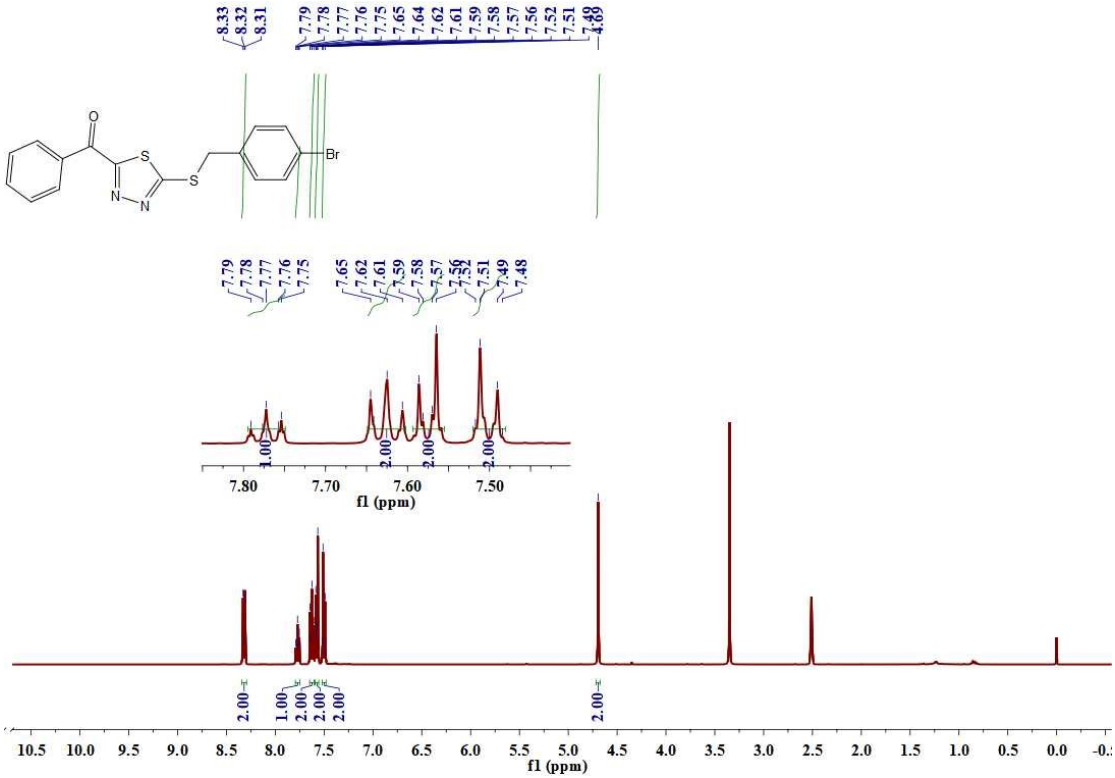
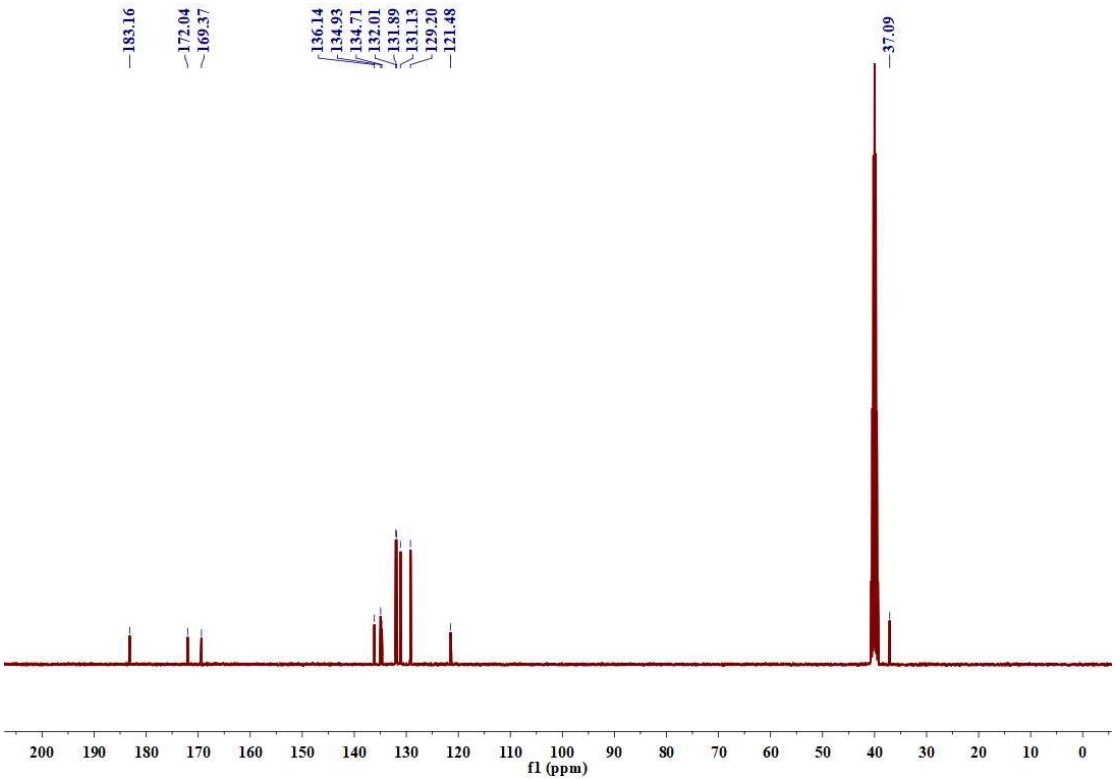



**Figure S29.** $^{1}$H NMR, $^{13}$C NMR and HRMS for **29**.






26 #71 RT: 0.72 AV: 1 NL: 2.14E+007
T: FTMS + p ESI Full ms [120.0000-1800.0000]

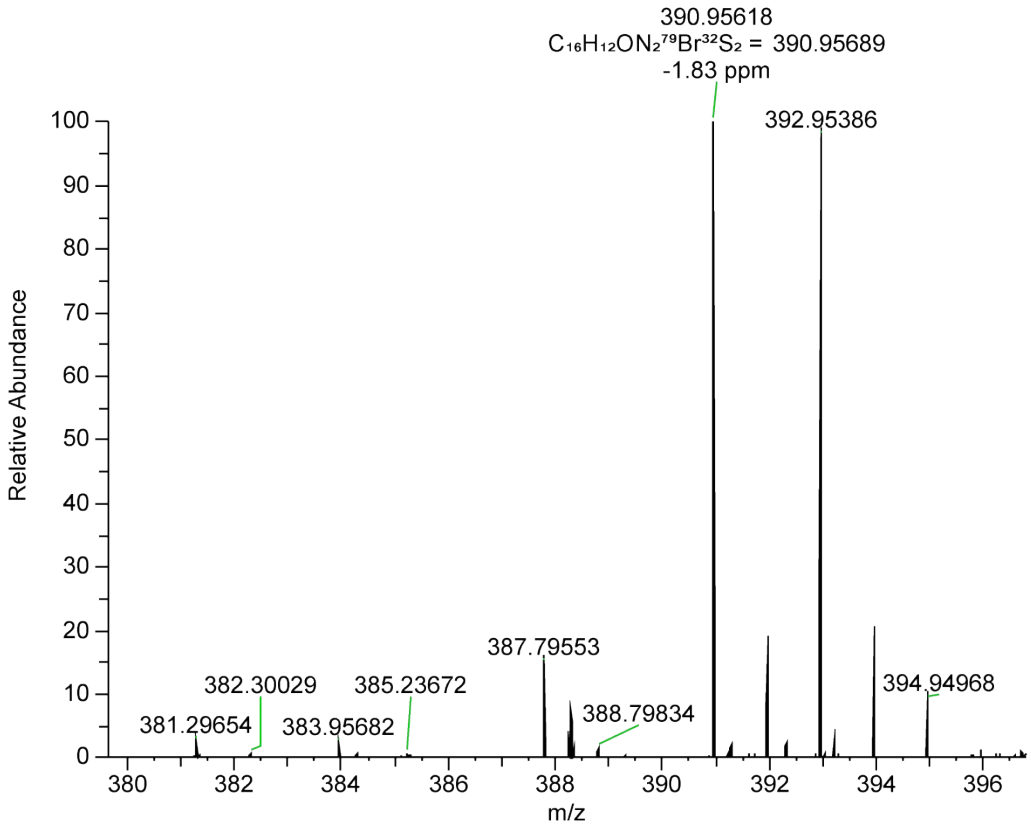



**Figure S30.** $^{1}$H NMR, $^{13}$C NMR and HRMS for **E30**.

## 3. Crystallographic data of compound E27

**Table S1**

Crystallographic data of compound **E27**

| | |
|---|---|
| Empirical formula | $C_{16}H_{11}ClN_2OS_2$ |
| Formula weight | 346.84 |
| Temperature/K | 273.15 |
| Crystal system | triclinic |
| Space group | P-1 |
| a/Å | 8.1736(4) |
| b/Å | 8.9413(4) |
| c/Å | 12.3309(6) |
| α/° | 105.112(2) |
| β/° | 93.310(2) |
| γ/° | 111.564(2) |
| Volume/Å$^3$ | 797.19(7) |
| Z | 2 |
| $\rho_{calc}$g/cm$^3$ | 1.445 |
| μ/mm$^{-1}$ | 4.585 |
| F(000) | 356.0 |
| Crystal size/mm$^3$ | 0.26 × 0.25 × 0.22 |
| Radiation | CuKα (λ = 1.54178) |

| | |
|---|---|
| 2Θ range for data collection/° | 7.536 to 145.138 |
| Index ranges | $-10 \leq h \leq 10, -11 \leq k \leq 11, -15 \leq l \leq 15$ |
| Reflections collected | 20086 |
| Independent reflections | 3126 [$R_{int}$ = 0.0672, $R_{sigma}$ = 0.0427] |
| Data/restraints/parameters | 3126/0/199 |
| Goodness-of-fit on $F^2$ | 1.119 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0953, $wR_2$ = 0.2294 |
| Final R indexes [all data] | $R_1$ = 0.0984, $wR_2$ = 0.2356 |
| Largest diff. peak/hole / e $Å^{-3}$ | 0.81/-1.25 |

## 4. The regression equation of the title compounds with $EC_{50}$ values

**Table S2**

The regression equation of the partial title compounds, triadimefon and tebuconazole with $EC_{50}$ values against *Gibberella saubinetii in vitro* [a]

| Compound no. | *G. saubinetii* | | |
|---|---|---|---|
| | $EC_{50}$ (μg/mL) | Regression equation | $R^2$ |
| **E1** | 30.5±1.4 | y = 1.2451x + 3.152 | 0.970 |
| **E2** | 21.9±1.3 | y = 1.0181x + 3.6357 | 0.988 |
| **E3** | 21.5±0.8 | y = 1.1504x + 3.4666 | 0.892 |
| **triadimefon** | 14.8±0.5 | y = 1.3542x + 3.4166 | 0.986 |
| **tebuconazole** | 0.4±0.0 | y = 1.1883x + 5.4399 | 0.9022 |

[a] Values are means ± SD of three replicates.

**Table S3**

The regression equation of the partial title compounds, triadimefon and tebuconazole with $EC_{50}$ values against *Verticillium dahliae in vitro* [a]

| Compound no. | *V. dahliae* | | |
|---|---|---|---|
| | $EC_{50}$ (μg/mL) | Regression equation | $R^2$ |
| **E1** | 48.1±0.9 | y = 2.2908x + 1.1459 | 0.987 |
| **E2** | 45.4±0.9 | y = 2.1678x + 1.4084 | 0.997 |
| **E3** | 41.6±0.9 | y = 2.04x + 1.6964 | 0.896 |
| **triadimefon** | 2.9±0.2 | y = 0.9237x + 4.567 | 0.834 |
| **tebuconazole** | 0.1±0.0 | y = 1.3375x + 6.1905 | 0.9784 |

[a] Values are means ± SD of three replicates.

**Table S4**

The regression equation of the partial title compounds, triadimefon and tebuconazole with $EC_{50}$ values against *Alternaria solani in vitro* [a]

| Compound no. | *A. solani* | | |
|---|---|---|---|
| | $EC_{50}$ (μg/mL) | Regression equation | $R^2$ |
| **E1** | 61.7±2.0 | y = 2.1879x + 1.0828 | 0.977 |
| **E2** | 67.5±1.1 | y = 2.369x + 0.6663 | 0.921 |
| **E3** | 63.4±0.5 | y = 1.4069x + 2.4651 | 0.978 |
| **triadimefon** | 45.3±0.6 | y = 0.8472x + 3.5972 | 0.992 |
| **tebuconazole** | 1.3±0.0 | y = 1.4719x + 4.8591 | 0.9746 |

[a] Values are means ± SD of three replicates.

**Table S5**

The regression equation of the partial title compounds, triadimefon and tebuconazole with $EC_{50}$ values against *Gibberella zeae in vitro* [a]

| Compound no. | *G. zeae* | | |
|---|---|---|---|
| | $EC_{50}$ (μg/mL) | Regression equation | $R^2$ |
| **E1** | 59.8±0.5 | y = 2.2502x + 1.0022 | 0.972 |
| **E2** | 42.8±0.4 | y = 1.4554x + 2.6256 | 0.969 |
| **E3** | 37.3±0.9 | y = 1.144x + 3.2018 | 0.938 |
| **triadimefon** | 16.9±0.1 | y = 1.0026x + 3.7695 | 0.988 |
| **tebuconazole** | 0.4±0.0 | y = 1.6445x + 5.5957 | 0.9966 |

[a] Values are means ± SD of three replicates.

**Table S6**

The regression equation of the partial title compounds, triadimefon and tebuconazole with $EC_{50}$ values against *Thanatephorus cucumeris in vitro* [a]

| Compound no. | *T. cucumeris* | | |
|---|---|---|---|
| | $EC_{50}$ (μg/mL) | Regression equation | $R^2$ |
| **E1** | 32.8±1.3 | y = 2.176x + 1.7021 | 0.975 |
| **E2** | 22.2±0.7 | y = 1.9322x + 2.3989 | 0.971 |
| **E3** | 39.6±1.3 | y = 1.6096x + 2.4282 | 0.994 |
| **triadimefon** | 11.0±0.7 | y = 0.8934x + 4.0703 | 0.990 |
| **tebuconazole** | 0.6±0.1 | y = 1.184x + 5.2672 | 0.9941 |

[a] Values are means ± SD of three replicates.