

**Title : Design, Synthesis, and Bioactivity of Novel Coumarin-3-carboxylic Acid
Derivatives Containing Thioether Quinoline Moiety**

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1 Spectrogram data of the target compound A1-A39

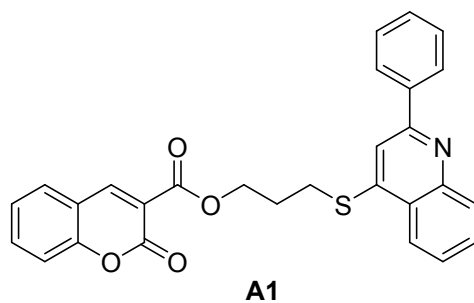


Figure S1

3-((2-phenylquinolin-4-yl)thio)propyl 2-oxo-2H-chromene-3-carboxylate (A1)

White solid, m.p. 123.2-124.0 °C, yield 52%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.49 (s, 1H, Ph-H), 8.16 – 8.11 (m, 2H, Ph-H), 8.10 (dd, *J* = 5.2, 3.4 Hz, 2H, Ph-H), 7.74 – 7.70 (m, 2H, Ph-H), 7.70-7.66 (m, *J* = 8.6, 7.4, 1.6 Hz, 1H, Ph-H), 7.56 – 7.51 (m, 2H, Ph-H), 7.46 (dd, *J* = 10.4, 4.7 Hz, 2H, Ph-H), 7.38 – 7.30 (m, 3H, Ph-H), 4.54 (t, *J* = 6.0 Hz, 2H, -COO-CH₂CH₂CH₂-S-), 3.43 (t, *J* = 7.2 Hz, 2H, -COO-CH₂CH₂CH₂-S-), 2.35 – 2.28 (m, 2H, -COO-CH₂CH₂CH₂-S-). ¹³C NMR (125 MHz, Chloroform-*d*) δ 163.42 (s), 156.76 (s), 155.30 (s), 149.19 (s), 147.69 (s), 147.22 (s), 139.83 (s), 134.63 (s), 130.35 (s), 130.07 (s), 129.70 (s), 128.88 (s), 127.74 (s), 126.25 (s), 125.69 (s), 124.97 (s), 123.49 (s), 117.93 (d, *J* = 18.0 Hz), 116.89 (s), 114.53 (s), 64.25 (s), 27.78 (s). HRMS (ESI) calcd for C₂₈H₂₂NO₄S [M+H]⁺: 468.12641, found 468.12572.

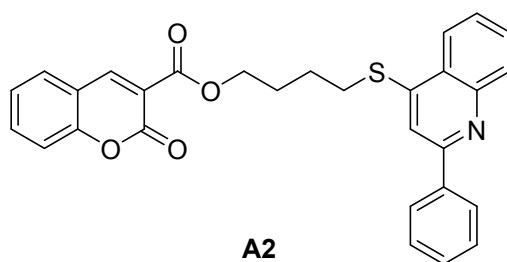
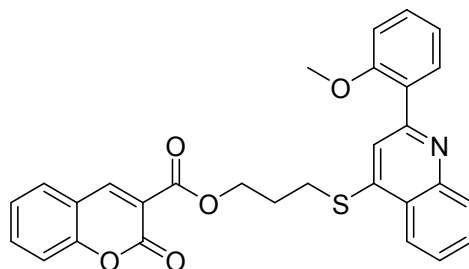


Figure S2

4-((2-phenylquinolin-4-yl)thio)butyl 2-oxo-2H-chromene-3-carboxylate (A2)

White solid, m.p. 113.6-114.6 °C, yield 13%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.44 (s, 1H, Ph-H), 8.15 – 8.08 (m, 4H, Ph-H), 7.72-7.68 (m, *J* = 8.4, 6.9, 1.4 Hz, 1H, Ph-H), 7.66 – 7.61 (m, 2H, Ph-H), 7.54 – 7.49 (m, 4H, Ph-H), 7.46 – 7.42 (m, 1H, Ph-H), 7.34 – 7.28 (m, 2H, Ph-H), 4.44 (t, *J* = 5.9 Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 3.30 (t, *J* = 6.7 Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 2.06 (dt, *J* = 6.5, 3.3 Hz, 4H, -COO-CH₂CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.22 (s), 155.56

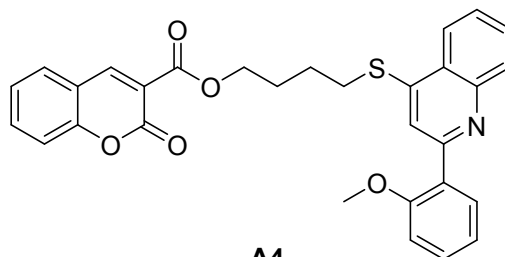
(d, $J = 1.4$ Hz), 154.16 (s), 147.79 (s), 146.56 (d, $J = 3.2$ Hz), 138.77 (s), 133.40 (s), 129.24 (s), 128.89 (s), 128.41 (d, $J = 17.4$ Hz), 127.82 (s), 126.56 (s), 125.06 (s), 124.58 (s), 123.80 (s), 122.38 (s), 117.02 (s), 116.75 (s), 115.76 (s), 113.32 (s), 64.27 (s), 29.91 (s), 26.75 (s), 23.98 (s). HRMS (ESI) calcd for $C_{29}H_{24}NO_4S$ $[M+H]^+$: 482.142055, found 482.14191.



A3

Figure S3

3-((2-(2-methoxyphenyl)quinolin-4-yl)thio)propyl 2-oxo-2H-chromene-3-carboxylate (A3) White solid, m.p. 138.9-139.9 °C, yield 69%; 1H NMR (400 MHz, Chloroform-*d*) δ 8.46 (s, 1H, Ph-H), 8.14 – 8.11 (m, 2H, Ph-H), 7.81 (dd, $J = 7.6, 1.8$ Hz, 1H, Ph-H), 7.76 (s, 1H, Ph-H), 7.72 – 7.68 (m, 1H, Ph-H), 7.66 – 7.62 (m, 1H, Ph-H), 7.54 – 7.50 (m, 2H, Ph-H), 7.35 – 7.28 (m, 3H, Ph-H), 7.08 – 7.04 (m, $J = 7.5, 0.9$ Hz, 1H, Ph-H), 6.96 (d, $J = 8.1$ Hz, 1H, Ph-H), 4.53 (t, $J = 6.0$ Hz, 2H, -COO-CH₂CH₂CH₂-S-), 3.84 (s, 3H, Ph-OCH₃), 3.34 (t, $J = 7.1$ Hz, 2H, -COO-CH₂CH₂CH₂-S-), 2.35 – 2.29 (m, 2H, -COO-CH₂CH₂CH₂-S-). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.15 (s), 156.03 (s), 155.50 (s), 154.98 (s), 154.20 (s), 147.91 (s), 146.64 (s), 144.01 (s), 133.46 (s), 130.35 (s), 129.34 (s), 129.14 (s), 128.68 – 128.42 (m), 125.04 (s), 124.49 (s), 123.81 (s), 122.30 (s), 120.24 (s), 117.64 (s), 116.82 (d, $J = 9.8$ Hz), 115.76 (s), 110.41 (s), 63.08 (s), 54.74 (s), 26.53 (d, $J = 6.8$ Hz). HRMS (ESI) calcd for $C_{29}H_{24}NO_5S$ $[M+H]^+$: 498.13697, found 498.13677.



A4

Figure S4

4-((2-(2-methoxyphenyl)quinolin-4-yl)thio)butyl 2-oxo-2H-chromene-3-

carboxylate (A4) White solid, m.p. 119.1-120.7 °C, yield 82%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.42 (s, 1H, Ph-H), 8.14 – 8.09 (m, 2H, Ph-H), 7.81 (dd, *J* = 7.6, 1.8 Hz, 1H, Ph-H), 7.72 – 7.66 (m, 2H, Ph-H), 7.69-7.61 (m, *J* = 8.6, 7.4, 1.6 Hz, 1H, Ph-H), 7.54 – 7.48 (m, 2H, Ph-H), 7.40-7.37 (m, *J* = 8.3, 7.5, 1.8 Hz, 1H, Ph-H), 7.35 – 7.28 (m, 2H, Ph-H), 7.06 (ddd, *J* = 19.9, 13.2, 4.6 Hz, 2H, Ph-H), 4.42 (t, *J* = 5.9 Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 3.86 (s, 3H, Ph-OCH₃), 3.22 (t, *J* = 6.7 Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 2.03 (dd, *J* = 5.9, 2.5 Hz, 4H, -COO-CH₂CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.13 (s), 156.06 (s), 155.58 (s), 154.93 (s), 154.15 (s), 147.72 (s), 146.59 (s), 144.51 (s), 133.39 (s), 130.38 (s), 129.37 (s), 129.14 (s), 128.52 (t, *J* = 5.2 Hz), 124.96 (s), 124.45 (s), 123.80 (s), 122.30 (s), 120.30 (s), 117.46 (s), 116.97 (s), 116.76 (s), 115.74 (s), 110.54 (s), 64.20 (s), 54.78 (s), 29.66 (s), 26.69 (s), 23.87 (s). HRMS (ESI) calcd for C₃₀H₂₆NO₅S [M+H]⁺: 512.152620, found 512.15216.

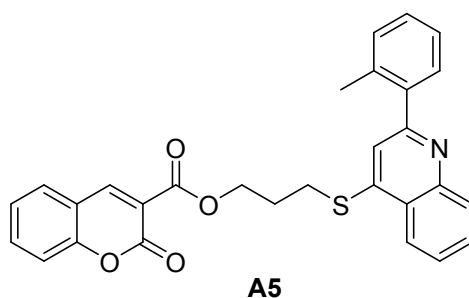
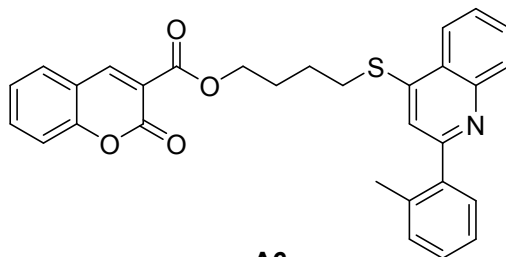


Figure S5

3-((2-(o-tolyl)quinolin-4-yl)thio)propyl 2-oxo-2H-chromene-3-carboxylate (A5)

White solid, m.p. 91.2-92.3 °C, yield 54%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.46 (s, 1H, Ph-H), 8.18 – 8.09 (m, 2H, Ph-H), 7.70-7.64 (m, 2H, Ph-H), 7.57 – 7.53 (m, 2H, Ph-H), 7.45 (d, *J* = 7.6 Hz, 1H, Ph-H), 7.39 (s, 1H, Ph-H), 7.37 – 7.31 (m, 2H, Ph-H), 7.23 – 7.14 (m, 3H, Ph-H), 4.51 (t, *J* = 5.9 Hz, 2H, -COO-CH₂CH₂CH₂-S-), 3.36 (t, *J* = 7.1 Hz, 2H, -COO-CH₂CH₂CH₂-S-), 2.38 (s, 3H, Ph-OCH₃), 2.31 – 2.25 (m, 2H, -COO-CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.25 (s), 158.31 (s), 155.47 (s), 154.25 (s), 147.94 (s), 146.17 (s), 145.61 (s), 139.70 (s), 134.94 (s), 133.46 (s), 129.69 (s), 129.12 (s), 128.89 (s), 128.51 (d, *J* = 7.4 Hz), 127.39 (s), 125.21 (s), 124.87 (s), 124.12 (s), 123.82 (s), 122.32 (s), 116.86 (d, *J* = 8.1

Hz), 116.10 (s), 115.81 (s), 63.02 (s), 26.82 (s), 26.40 (s), 19.30 (s). HRMS (ESI) calcd for C₂₉H₂₄NO₄S [M+H]⁺: 482.14206, found 482.14224.

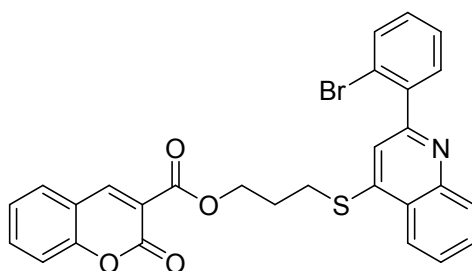


A6

Figure S6

4-((2-(o-tolyl)quinolin-4-yl)thio)butyl 2-oxo-2H-chromene-3-carboxylate (A6)

White solid, m.p. 129.0-130.5 °C, yield 89%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.46 (s, 1H, Ph-H), 8.12 (ddd, *J* = 25.3, 8.4, 0.8 Hz, 2H, Ph-H), 7.71 (ddd, *J* = 8.4, 6.9, 1.4 Hz, 1H, Ph-H), 7.66 – 7.62 (m, 1H, Ph-H), 7.57 – 7.51 (m, 2H, Ph-H), 7.48 – 7.45 (m, 1H, Ph-H), 7.35 – 7.27 (m, 6H, Ph-H), 4.42 (t, *J* = 5.9 Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 3.22 (t, *J* = 6.7 Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 2.39 (s, 3H, Ph-OCH₃), 2.03 (dd, *J* = 6.4, 2.9 Hz, 4H, -COO-CH₂CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.22 (s), 158.25 (s), 155.53 (s), 154.18 (s), 147.80 (s), 146.11 (s), 139.78 (s), 134.91 (s), 133.41 (s), 129.81 (s), 129.10 (s), 128.85 (s), 128.47 (d, *J* = 3.1 Hz), 127.52 (s), 125.07 (d, *J* = 15.5 Hz), 124.07 (s), 123.81 (s), 122.32 (s), 117.02 (s), 116.78 (s), 116.09 (s), 115.78 (s), 64.25 (s), 29.74 (s), 26.72 (s), 23.95 (s), 19.31 (s). HRMS (ESI) calcd for C₃₀H₂₆NO₄S[M+H]⁺: 496.15771, found 496.15711.



A7

Figure S7

3-((2-(2-bromophenyl)quinolin-4-yl)thio)propyl 2-oxo-2H-chromene-3-

carboxylate (A7) White solid, m.p. 110.2-111.9 °C, yield 68%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.49 (s, 1H, Ph-H), 8.16 (dd, *J* = 8.4, 0.9 Hz, 1H, Ph-H), 8.11 (dd, *J* =

8.4, 0.6 Hz, 1H, Ph-H), 7.73 (ddd, $J = 8.4, 6.9, 1.4$ Hz, 1H, Ph-H), 7.68 – 7.62 (m, 2H,

Ph-H), 7.59 – 7.54 (m, 4H, Ph-H), 7.41–7.37 (m, $J = 7.5, 1.2$ Hz, 1H, Ph-H), 7.36 – 7.31 (m, 2H, Ph-H), 7.17 – 7.13 (m, 1H, Ph-H), 4.53 (t, $J = 5.9$ Hz, 2H, -COO-CH₂CH₂CH₂-S-), 3.38 (t, $J = 7.2$ Hz, 2H, -COO-CH₂CH₂CH₂-S-), 2.35 – 2.28 (m, 2H, -COO-CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 163.21 (s), 157.70 (s), 156.52 (s), 155.25 (s), 149.02 (s), 147.24 (s), 146.27 (s), 141.60 (s), 134.53 (s), 133.09 (s), 131.63 (s), 130.23 (s), 130.00 (d, $J = 4.0$ Hz), 129.63 (s), 127.75 (s), 126.62 (s), 125.55 (s), 124.89 (s), 123.44 (s), 121.76 (s), 117.88 (d, $J = 9.0$ Hz), 117.55 (s), 116.84 (s), 64.08 (s), 27.92 (s), 27.43 (s). HRMS (ESI) calcd for C₃₀H₂₆NO₄S[M+H]⁺: 546.03692, found 546.03575.

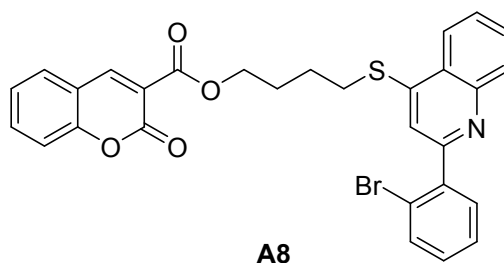
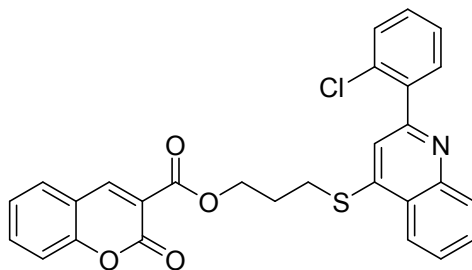


Figure S8

4-((2-(2-bromophenyl)quinolin-4-yl)thio)butyl 2-oxo-2H-chromene-3-carboxylate (A8) White solid, m.p. 108.6-109.4 °C, yield 21%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.46 (s, 1H, Ph-H), 8.16 (dd, $J = 8.4, 0.8$ Hz, 1H, Ph-H), 8.10 (dd, $J = 8.4, 0.5$ Hz, 1H, Ph-H), 7.72 (ddd, $J = 8.4, 6.9, 1.4$ Hz, 1H, Ph-H), 7.67 – 7.62 (m, 3H, Ph-H), 7.59 – 7.55 (m, 1H, Ph-H), 7.52 (dd, $J = 7.8, 1.5$ Hz, 1H, Ph-H), 7.48 (s, 1H, Ph-H), 7.42 (td, $J = 7.5, 1.1$ Hz, 1H, Ph-H), 7.34 (d, $J = 8.3$ Hz, 1H, Ph-H), 7.29 (ddd, $J = 13.7, 7.1, 4.2$ Hz, 3H, Ph-H), 7.26 (s, 1H, Ph-H), 4.42 (t, $J = 5.8$ Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 3.24 (t, $J = 6.7$ Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 2.03 (dd, $J = 6.4, 2.9$ Hz, 4H, -COO-CH₂CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.14 (s), 156.57 (s), 155.59 (s), 154.13 (s), 147.85 (s), 146.12 (s), 145.71 (s), 140.55 (s), 133.43 (s), 132.20 (s), 130.56 (s), 129.32 – 128.79 (m), 128.51 (s), 126.76 (s), 125.51 (s), 124.42 (s), 123.83 (s), 122.39 (s), 120.71 (s), 116.82 (d, $J = 16.2$ Hz), 116.42 (s), 115.76 (s), 64.29 (s), 29.62 (s), 26.71 (s), 24.12 (s). HRMS (ESI) calcd for C₂₉H₂₃BrNO₄S [M+H]⁺: 560.05257, found 560.05251.

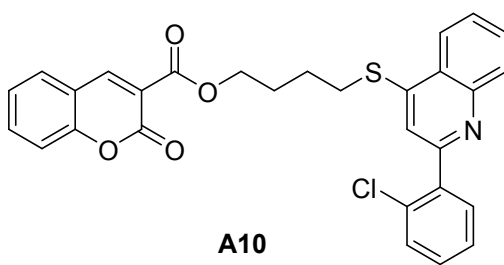


A9

Figure S9

3-((2-(2-chlorophenyl)quinolin-4-yl)thio)propyl 2-oxo-2H-chromene-3-

carboxylate (A9) White solid, m.p. 116.9-118.0 °C, yield 26%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.50 (s, 1H, Ph-H), 8.16 (dd, *J* = 8.4, 0.8 Hz, 1H, Ph-H), 8.12 (dd, *J* = 8.4, 0.5 Hz, 1H, Ph-H), 7.73 (ddd, *J* = 8.4, 6.9, 1.3 Hz, 1H, Ph-H), 7.70 – 7.64 (m, 2H, Ph-H), 7.60 – 7.55 (m, 3H, Ph-H), 7.37–7.32 (m, *J* = 8.6, 4.2 Hz, 4H, Ph-H), 7.26 – 7.18 (m, 1H, Ph-H), 4.53 (t, *J* = 5.9 Hz, 2H, -COO-CH₂CH₂CH₂-S-), 3.38 (t, *J* = 7.2 Hz, 2H, -COO-CH₂CH₂-S-), 2.34 – 2.27 (m, 2H, -COO-CH₂CH₂-S-). ¹³C NMR (125 MHz, Chloroform-*d*) δ 163.26 (s), 156.62 (s), 156.43 (s), 155.30 (s), 149.10 (s), 147.41 (s), 146.37 (s), 139.63 (s), 134.61 (s), 132.25 (s), 131.79 (s), 130.29 (s), 130.17 – 129.77 (m), 129.70 (s), 127.31 (s), 126.69 (s), 125.60 (s), 124.97 (s), 123.50 (s), 117.92 (d, *J* = 9.8 Hz), 117.62 (s), 116.90 (s), 64.16 (s), 27.85 (s), 27.48 (s). HRMS (ESI) calcd for C₂₈H₂₁ClNO₄S [M+H]⁺: 502.08743, found 502.08725.



A10

Figure S10

4-((2-(2-chlorophenyl)quinolin-4-yl)thio)butyl 2-oxo-2H-chromene-3-carboxylate

(A10) White solid, m.p. 122.3-124.0 °C, yield 35%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.46 (s, 1H, Ph-H), 8.15 (dd, *J* = 8.4, 0.9 Hz, 1H, Ph-H), 8.10 (dd, *J* = 8.4, 0.6 Hz, 1H, Ph-H), 7.75 – 7.67 (m, 2H, Ph-H), 7.64 (ddd, *J* = 8.6, 7.4, 1.6 Hz, 1H, Ph-H), 7.57 (ddd, *J* = 8.2, 6.9, 1.2 Hz, 1H, Ph-H), 7.54 – 7.50 (m, 2H, Ph-H), 7.49 – 7.44 (m, 1H, Ph-H), 7.41 – 7.29 (m, 4H, Ph-H), 4.42 (t, *J* = 5.7 Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-),

3.24 (t, $J = 6.6$ Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 2.08 – 1.99 (m, 4H, -COO-CH₂CH₂CH₂CH₂-S-). ¹³C NMR (125 MHz, Chloroform-*d*) (126 MHz,) δ 163.24 (s), 156.71 (s), 156.36 (s), 155.24 (s), 148.93 (s), 147.36 (s), 146.87 (s), 139.64 (s), 134.54 (s), 132.26 (s), 131.76 (s), 130.62 – 129.78 (m), 129.62 (s), 127.34 (s), 126.62 (s), 125.55 (s), 124.94 (s), 123.50 (s), 117.94 (d, $J = 20.7$ Hz), 117.60 (s), 116.86 (s), 65.40 (s), 30.76 (s), 27.83 (s), 25.17 (s). HRMS (ESI) calcd for C₂₉H₂₃ClNO₄S [M+H]⁺: 516.10308, found 516.10234.

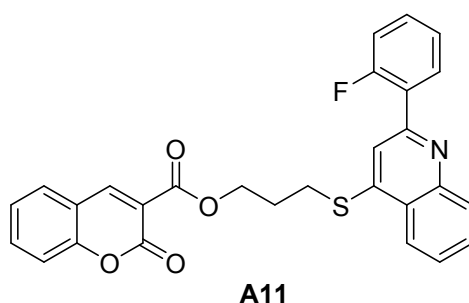
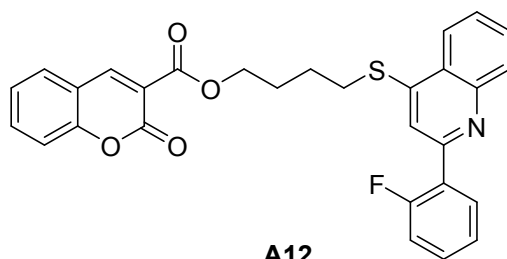


Figure S11

3-((2-(2-fluorophenyl)quinolin-4-yl)thio)propyl 2-oxo-2H-chromene-3-carboxylate (A11) White solid, m.p. 117.8-118.5 °C, yield 24%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.51 (s, 1H, Ph-H), 8.13 (td, $J = 8.5, 0.7$ Hz, 2H, Ph-H), 8.05 (td, $J = 7.8, 1.9$ Hz, 1H, Ph-H), 7.75 – 7.70 (m, 2H, Ph-H), 7.65 (ddd, $J = 8.7, 7.4, 1.6$ Hz, 1H, Ph-H), 7.58 – 7.53 (m, 2H, Ph-H), 7.36 – 7.30 (m, 3H, Ph-H), 7.29–7.25 (m, $J = 7.5, 1.3$ Hz, 1H, Ph-H), 7.08 (ddd, $J = 11.2, 8.1, 1.2$ Hz, 1H, Ph-H), 4.54 (t, $J = 6.0$ Hz, 2H, -COO-CH₂CH₂CH₂-S-), 3.39 (t, $J = 7.1$ Hz, 2H, -COO-CH₂CH₂CH₂-S-), 2.35 – 2.28 (m, 2H, -COO-CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.13 (s), 159.53 (d, $J = 249.2$ Hz), 155.56 (s), 154.18 (s), 152.01 (d, $J = 1.9$ Hz), 147.94 (s), 146.54 (s), 145.58 (s), 133.48 (s), 130.47 (d, $J = 3.0$ Hz), 129.79 (d, $J = 8.5$ Hz), 129.21 (s), 128.92 (s), 128.56 (s), 126.83 (d, $J = 11.9$ Hz), 125.44 (s), 124.55 (s), 123.84 (s), 123.72 (d, $J = 3.5$ Hz), 122.34 (s), 116.83 (d, $J = 14.5$ Hz), 116.23 (d, $J = 8.2$ Hz), 115.78 (s), 115.08 (d, $J = 22.8$ Hz), 63.10 (s), 26.48 (d, $J = 2.4$ Hz). ¹⁹F NMR (377 MHz, Chloroform-*d*) δ -117.11 (s). HRMS (ESI) calcd for C₂₈H₂₁FNO₄S [M+H]⁺: 486.11698, found 486.11649.

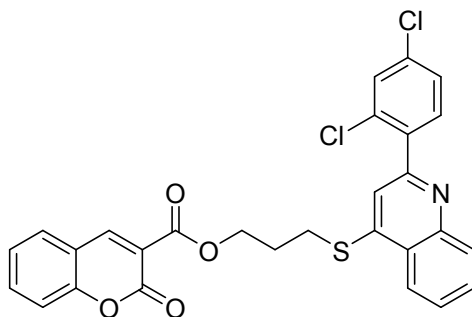


A12

Figure S12

4-((2-(2-fluorophenyl)quinolin-4-yl)thio)butyl 2-oxo-2H-chromene-3-carboxylate

(A12) White solid, m.p. 110.8-112.1 °C, yield 34%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.46 (s, 1H, Ph-H), 8.15 – 8.09 (m, 2H, Ph-H), 8.07–8.03 (m, $J = 7.8, 1.8$ Hz, 1H, Ph-H), 7.72 (ddd, $J = 8.3, 6.9, 1.3$ Hz, 1H, Ph-H), 7.63 (ddd, $J = 9.8, 6.6, 1.9$ Hz, 2H, Ph-H), 7.55 (ddd, $J = 8.2, 7.0, 1.2$ Hz, 1H, Ph-H), 7.50 (dd, $J = 7.8, 1.4$ Hz, 1H, Ph-H), 7.41 (tdd, $J = 7.1, 5.0, 1.8$ Hz, 1H, Ph-H), 7.34 – 7.27 (m, 3H, Ph-H), 7.16 (ddd, $J = 11.3, 8.2, 0.9$ Hz, 1H, Ph-H), 4.43 (t, $J = 5.7$ Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 3.25 (t, $J = 6.6$ Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 2.04 (dt, $J = 6.1, 3.2$ Hz, 4H, -COO-CH₂CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.07 (s), 159.57 (d, $J = 249.1$ Hz), 155.61 (s), 154.11 (s), 151.93 (d, $J = 1.9$ Hz), 147.77 (s), 146.48 (s), 146.09 (s), 133.40 (s), 130.44 (d, $J = 3.0$ Hz), 129.85 (d, $J = 8.5$ Hz), 129.18 (s), 128.87 (s), 128.49 (s), 126.82 (d, $J = 11.9$ Hz), 125.36 (s), 124.49 (s), 123.79 (s), 123.74 (d, $J = 3.4$ Hz), 122.33 (s), 116.81 (d, $J = 18.0$ Hz), 116.07 (d, $J = 8.5$ Hz), 115.74 (s), 115.20 (d, $J = 22.8$ Hz), 64.27 (s), 29.59 (s), 26.74 (s), 23.89 (s). ¹⁹F NMR (471 MHz, Chloroform-*d*) δ -117.00 (s). HRMS (ESI) calcd for C₂₉H₂₃FNO₄S [M+H]⁺: 500.13263, found 500.13254.



A13

Figure S13

3-((2-(2,4-dichlorophenyl)quinolin-4-yl)thio)propyl 2-oxo-2H-chromene-3-

carboxylate (A13) White solid, m.p. 120.4-122.4 °C, yield 43%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.51 (s, 1H, Ph-H), 8.16 (dd, *J* = 8.4, 0.8 Hz, 1H, Ph-H), 8.10 (dd, *J* = 8.4, 0.5 Hz, 1H, Ph-H), 7.74 (ddd, *J* = 8.4, 6.9, 1.3 Hz, 1H, Ph-H), 7.69 – 7.64 (m, 2H, Ph-H), 7.60 – 7.56 (m, 3H, Ph-H), 7.38 – 7.32 (m, 4H, Ph-H), 4.52 (t, *J* = 5.9 Hz, 2H, -COO-CH₂CH₂CH₂-S-), 3.39 (t, *J* = 7.2 Hz, 2H, -COO-CH₂CH₂CH₂-S-), 2.33 – 2.26 (m, 2H, -COO-CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 163.32 (s), 156.52 (s), 155.28 (d, *J* = 6.9 Hz), 149.12 (s), 147.33 (s), 146.65 (s), 138.13 (s), 135.16 (s), 134.64 (s), 132.99 (s), 132.67 (s), 130.16 (d, *J* = 7.5 Hz), 129.65 (d, *J* = 6.3 Hz), 127.57 (s), 126.77 (s), 125.57 (s), 124.95 (s), 123.45 (s), 117.83 (d, *J* = 12.4 Hz), 117.24 (s), 116.91 (s), 64.06 (s), 27.91 (s), 27.38 (s). HRMS (ESI) calcd for C₂₈H₂₀Cl₂NO₄S [M+H]⁺: 536.04846, found 536.04828.

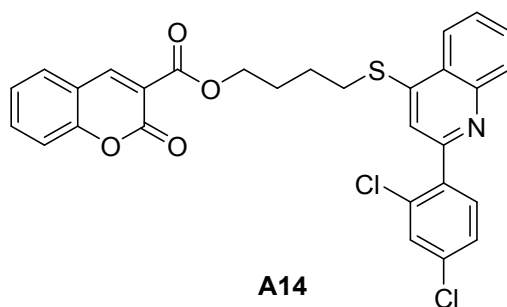
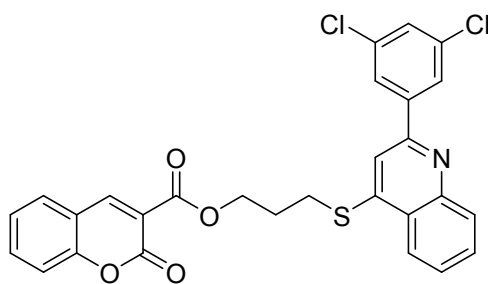


Figure S14

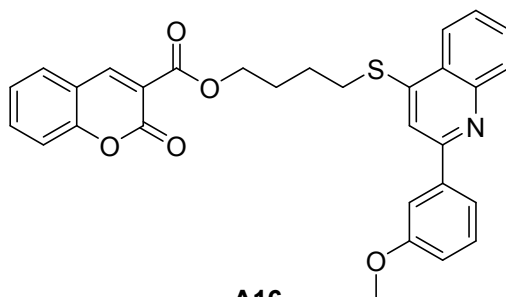
4-((2-(2,4-dichlorophenyl)quinolin-4-yl)thio)butyl 2-oxo-2H-chromene-3-carboxylate (A14) White solid, m.p. 132.9-134.8 °C, yield 17%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.48 (s, 1H, Ph-H), 8.15 (dd, *J* = 8.3, 0.8 Hz, 1H, Ph-H), 8.08 (d, *J* = 8.0 Hz, 1H, Ph-H), 7.72 (ddd, *J* = 8.3, 7.0, 1.3 Hz, 1H, Ph-H), 7.68 – 7.62 (m, 2H, Ph-H), 7.59 – 7.53 (m, 2H, Ph-H), 7.51 – 7.46 (m, 2H, Ph-H), 7.37 – 7.29 (m, 3H, Ph-H), 4.42 (t, *J* = 5.7 Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 3.24 (t, *J* = 6.7 Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 2.09 – 1.97 (m, 4H, -COO-CH₂CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.22 (s), 155.56 (s), 154.13 (d, *J* = 1.4 Hz), 147.93 (s), 146.16 (d, *J* = 9.7 Hz), 137.07 (s), 134.16 (s), 133.48 (s), 131.89 (s), 131.58 (s), 129.07 (d, *J* = 6.7 Hz), 128.80 (s), 128.51 (s), 126.58 (s), 125.66 (s), 124.43 (s), 123.84 (s), 122.39 (s), 116.80 (d, *J* = 14.7 Hz), 116.13 (s), 115.76 (s), 64.33 (s), 29.61 (s), 26.69 (s), 24.09 (s). HRMS (ESI) calcd for C₂₉H₂₂Cl₂NO₄S [M+H]⁺: 550.06411, found 550.06379.



A15

Figure S15

3-((2-(3,5-dichlorophenyl)quinolin-4-yl)thio)propyl 2-oxo-2H-chromene-3-carboxylate (A15) White solid, m.p. 173.5-174.3 °C, yield 22%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.51 (s, 1H, Ph-H), 8.13 (ddd, *J* = 17.8, 8.4, 0.7 Hz, 2H, Ph-H), 8.00 (d, *J* = 1.9 Hz, 2H, Ph-H), 7.76 – 7.71 (m, 2H, Ph-H), 7.69 – 7.64 (m, 1H, Ph-H), 7.58 – 7.53 (m, 2H, Ph-H), 7.33 (dd, *J* = 11.2, 4.4 Hz, 2H, Ph-H), 7.25 (d, *J* = 1.9 Hz, 1H, Ph-H), 4.53 (t, *J* = 5.9 Hz, 2H, -COO-CH₂CH₂CH₂-S-), 3.49 (t, *J* = 7.3 Hz, 2H, -COO-CH₂CH₂CH₂-S-), 2.33 (dt, *J* = 12.7, 6.4 Hz, 2H, -COO-CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.54 (s), 155.68 (s), 154.20 (s), 152.75 (s), 148.24 (s), 147.14 (s), 146.31 (s), 141.66 (s), 134.25 (s), 133.55 (s), 129.29 (s), 128.54 (s), 127.92 (s), 125.72 (s), 125.13 (s), 124.84 (s), 123.87 (s), 122.41 (s), 116.82 (d, *J* = 18.2 Hz), 115.79 (s), 112.68 (s), 63.15 (s), 26.74 (s), 26.49 (s). HRMS (ESI) calcd for C₂₈H₂₀Cl₂NO₄S [M+H]⁺: 536.048461, found 536.04857.



A16

Figure S16

4-((2-(3-methoxyphenyl)quinolin-4-yl)thio)butyl 2-oxo-2H-chromene-3-carboxylate (A16) White solid, m.p. 86.0-87.8 °C, yield 10%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.43 (s, 1H, Ph-H), 8.15 – 8.09 (m, 2H, Ph-H), 7.70 (ddd, *J* = 5.9, 5.4, 1.4 Hz, 2H, Ph-H), 7.65–7.61 (m, *J* = 5.5, 1.6 Hz, 3H, Ph-H), 7.54 – 7.48 (m, 2H, Ph-H), 7.41 (t, *J* = 7.9 Hz, 1H, Ph-H), 7.34 – 7.28 (m, 2H, Ph-H), 6.99 (dd, *J* = 8.0, 2.3 Hz, 1H, Ph-H), 4.44 (t, *J* = 5.7 Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 3.91 (s, 3H,

Ph-OCH₃), 3.29 (t, *J* = 6.6 Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 2.05 (dt, *J* = 6.3, 3.3 Hz, 4H, -COO-CH₂CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.18 (s), 159.04 (s), 155.56 (s), 155.31 (s), 154.15 (s), 147.75 (s), 146.52 (d, *J* = 10.8 Hz), 140.25 (s), 133.37 (s), 129.25 (s), 128.85 (d, *J* = 9.7 Hz), 128.50 (s), 125.11 (s), 124.66 (s), 123.78 (s), 122.38 (s), 118.94 (s), 117.00 (s), 116.75 (s), 115.74 (s), 114.19 (s), 113.38 (s), 111.88 (s), 64.24 (s), 54.40 (s), 29.90 (s), 26.76 (s), 23.97 (s). HRMS (ESI) calcd for C₃₀H₂₆NO₅S [M+H]⁺: 512.15262, found 512.15207.

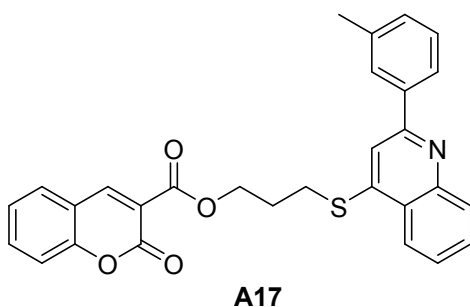
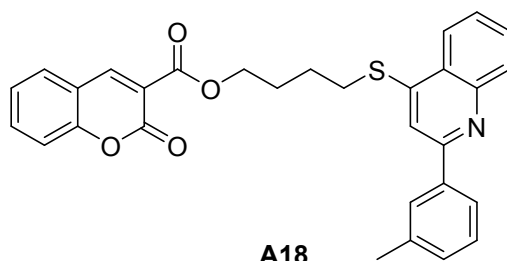


Figure S17

3-((2-(m-tolyl)quinolin-4-yl)thio)propyl 2-oxo-2H-chromene-3-carboxylate (A17)

White solid, m.p. 98.0-100.0 °C, yield 54%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.48 (s, 1H, Ph-H), 8.14 (dd, *J* = 12.2, 4.6 Hz, 2H, Ph-H), 7.93 (s, 1H, Ph-H), 7.84 (d, *J* = 7.7 Hz, 1H, Ph-H), 7.74 – 7.69 (m, 2H, Ph-H), 7.65 (ddd, *J* = 8.6, 7.4, 1.6 Hz, 1H, Ph-H), 7.55 – 7.50 (m, 2H, Ph-H), 7.32 (ddd, *J* = 10.4, 5.3, 2.9 Hz, 3H, Ph-H), 7.17 (d, *J* = 7.5 Hz, 1H, Ph-H), 4.53 (t, *J* = 6.0 Hz, 2H, -COO-CH₂CH₂CH₂-S-), 3.43 (t, *J* = 7.1 Hz, 2H, -COO-CH₂CH₂CH₂-S-), 2.43 (s, 3H, Ph-OCH₃), 2.35 – 2.28 (m, 2H, -COO-CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.29 (s), 155.88 (s), 155.59 (s), 154.19 (s), 148.05 (s), 146.56 (s), 145.99 (s), 138.69 (s), 137.47 (s), 133.49 (s), 129.37 – 128.82 (m), 128.56 (s), 127.62 (s), 127.28 (s), 125.06 (s), 124.58 (s), 123.78 (d, *J* = 10.2 Hz), 122.38 (s), 116.81 (d, *J* = 13.1 Hz), 115.75 (s), 113.66 (s), 63.09 (s), 26.67 (d, *J* = 4.0 Hz), 20.53 (s). HRMS (ESI) calcd for C₂₉H₂₄NO₄S [M+H]⁺: 482.14206, found 482.14151.

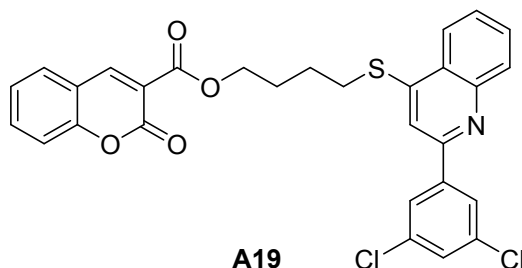


A18

Figure S18

4-((2-(m-tolyl)quinolin-4-yl)thio)butyl 2-oxo-2H-chromene-3-carboxylate (A18)

White solid, m.p. 89.8-90.9 °C, yield 71%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.43 (s, 1H, Ph-H), 8.15 – 8.09 (m, 2H, Ph-H), 7.93 (s, 1H, Ph-H), 7.84 (d, *J* = 7.7 Hz, 1H, Ph-H), 7.70 (ddd, *J* = 8.3, 6.9, 1.4 Hz, 1H, Ph-H), 7.65 – 7.60 (m, 2H, Ph-H), 7.53 – 7.47 (m, 2H, Ph-H), 7.41–7.37 (m, *J* = 7.6 Hz, 1H, Ph-H), 7.33 – 7.24 (m, 3H, Ph-H), 7.26 (s, 1H, Ph-H), 4.44 (t, *J* = 5.8 Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 3.29 (t, *J* = 6.7 Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 2.46 (s, 3H, Ph-OCH₃), 2.05 (dt, *J* = 6.3, 3.2 Hz, 4H, -COO-CH₂CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 163.21 (s), 156.69 (d, *J* = 18.2 Hz), 155.18 (s), 148.79 (s), 147.54 (d, *J* = 7.9 Hz), 139.76 (s), 138.57 (s), 134.41 (s), 130.20 (d, *J* = 7.4 Hz), 129.89 (s), 129.53 (s), 128.74 (s), 128.26 (s), 126.04 (s), 125.61 (s), 124.75 (d, *J* = 13.1 Hz), 123.42 (s), 118.03 (s), 117.78 (s), 116.77 (s), 114.50 (s), 65.28 (s), 30.95 (s), 27.78 (s), 24.99 (s), 21.61 (s). HRMS (ESI) calcd for C₃₀H₂₆NO₄S [M+H]⁺: 496.15771, found 496.15757.



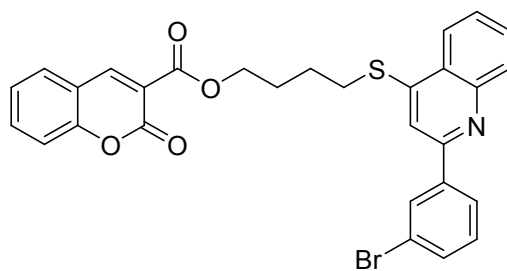
A19

Figure S19

4-((2-(3,5-dichlorophenyl)quinolin-4-yl)thio)butyl 2-oxo-2H-chromene-3-

carboxylate (A19) White solid, m.p. 130.8-132.8 °C, yield 10%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.47 (s, 1H, Ph-H), 8.14 – 8.06 (m, 2H, Ph-H), 8.00 (d, *J* = 1.9 Hz, 1H, Ph-H), 7.72 (ddd, *J* = 8.3, 6.9, 1.3 Hz, 1H, Ph-H), 7.64 (td, *J* = 3.4, 1.7 Hz, 1H, Ph-H), 7.56 – 7.49 (m, 3H, Ph-H), 7.41 – 7.28 (m, 4H, Ph-H), 4.45 (t, *J* = 5.6 Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 3.32 (t, *J* = 6.6 Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-),

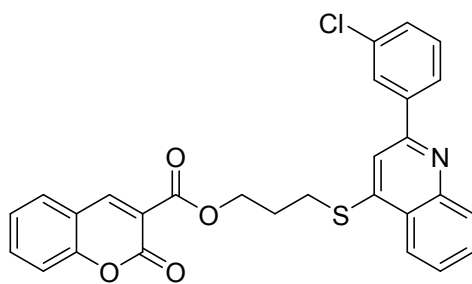
2.09 – 2.03 (m, 4H, -COO-CH₂CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 163.36 (s), 156.65 (s), 155.18 (s), 153.57 (s), 149.01 (s), 148.72 (s), 147.26 (s), 142.65 (s), 135.44 (s), 134.52 (s), 130.33 (s), 129.53 (s), 129.10 (s), 126.75 (s), 126.06 (s), 125.83 (s), 124.88 (s), 123.46 (s), 117.95 (s), 117.75 (s), 116.82 (s), 113.54 (s), 65.39 (s), 30.97 (s), 27.74 (s), 24.97 (s). HRMS (ESI) calcd for C₂₉H₂₂Cl₂NO₄S [M+H]⁺: 550.06411, found 550.06440.



A20

Figure S20

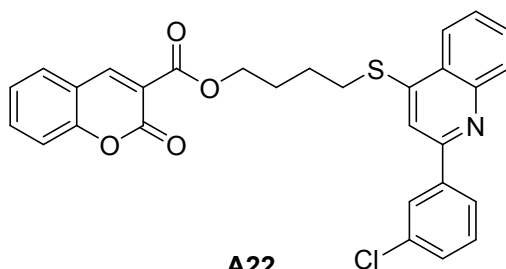
4-((2-(3-bromophenyl)quinolin-4-yl)thio)butyl 2-oxo-2H-chromene-3-carboxylate (A20) White solid, m.p. 132.0-133.8 °C, yield 30%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.45 (s, 1H, Ph-H), 8.28 (t, *J* = 1.8 Hz, 1H, Ph-H), 8.11 (ddd, *J* = 15.8, 8.4, 0.7 Hz, 2H, Ph-H), 8.02 – 7.98 (m, 1H, Ph-H), 7.72 (ddd, *J* = 8.4, 6.9, 1.4 Hz, 1H, Ph-H), 7.63 (ddd, *J* = 8.7, 7.3, 1.6 Hz, 1H, Ph-H), 7.59 (s, 1H, Ph-H), 7.57 – 7.48 (m, 3H, Ph-H), 7.37 (t, *J* = 7.9 Hz, 1H, Ph-H), 7.33 – 7.28 (m, 2H, Ph-H), 4.44 (t, *J* = 5.8 Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 3.30 (t, *J* = 6.7 Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 2.06 (dt, *J* = 6.1, 3.1 Hz, 4H, -COO-CH₂CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.23 (s), 155.59 (s), 154.11 (s), 153.82 (s), 147.90 (s), 147.14 (s), 146.33 (s), 140.73 (s), 133.45 (s), 131.20 (s), 129.58 (s), 129.43 – 129.00 (m), 128.48 (s), 125.39 (s), 125.06 (s), 124.63 (s), 123.82 (s), 122.37 (s), 122.08 (s), 116.79 (d, *J* = 20.0 Hz), 115.75 (s), 112.79 (s), 64.29 (s), 29.86 (s), 26.69 (s), 23.90 (s). HRMS (ESI) calcd for C₂₉H₂₃BrNO₄S [M+H]⁺: 560.05257, found 560.05229.



A21

Figure S21

3-((2-(3-chlorophenyl)quinolin-4-yl)thio)propyl 2-oxo-2H-chromene-3-carboxylate (A21) White solid, m.p. 165.0-165.9 °C, yield 63%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.50 (s, 1H, Ph-H), 8.15 (dd, *J* = 8.4, 0.8 Hz, 1H, Ph-H), 8.13 – 8.10 (m, 2H, Ph-H), 7.99 – 7.96 (m, 1H, Ph-H), 7.75 – 7.70 (m, 2H, Ph-H), 7.66 (ddd, *J* = 8.6, 7.4, 1.6 Hz, 1H, Ph-H), 7.57 – 7.52 (m, 2H, Ph-H), 7.38 – 7.27 (m, 4H, Ph-H), 4.53 (t, *J* = 5.9 Hz, 2H, -COO-CH₂CH₂CH₂-S-), 3.45 (t, *J* = 7.2 Hz, 2H, -COO-CH₂CH₂CH₂-S-), 2.35 – 2.28 (m, 2H, -COO-CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.41 (s), 155.64 (s), 154.15 (d, *J* = 7.6 Hz), 148.16 (s), 146.53 (d, *J* = 19.7 Hz), 140.51 (s), 133.74 (s), 133.53 (s), 129.39 – 128.84 (m), 128.56 (s), 128.18 (s), 126.74 (s), 125.43 (s), 124.73 (d, *J* = 3.9 Hz), 123.86 (s), 122.39 (s), 116.81 (d, *J* = 15.4 Hz), 115.77 (s), 113.03 (s), 63.12 (s), 26.65 (d, *J* = 10.3 Hz). HRMS (ESI) calcd for C₂₈H₂₁ClNO₄S [M+H]⁺: 502.08743, found 502.08754.

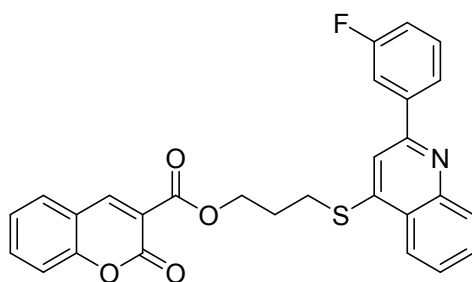


A22

Figure S22

4-((2-(3-chlorophenyl)quinolin-4-yl)thio)butyl 2-oxo-2H-chromene-3-carboxylate (A22) White solid, m.p. 114.0-115.7 °C, yield 57%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.37 (s, 1H, Ph-H), 8.08 – 8.01 (m, 3H, Ph-H), 7.90 (dt, *J* = 7.3, 1.6 Hz, 1H, Ph-H), 7.65 (ddd, *J* = 8.4, 6.9, 1.4 Hz, 1H, Ph-H), 7.59 – 7.54 (m, 2H, Ph-H), 7.48 – 7.42 (m, 2H, Ph-H), 7.39 – 7.31 (m, 2H, Ph-H), 7.24 (ddd, *J* = 8.6, 5.7, 1.9 Hz, 2H, Ph-H), 4.38 (t, *J* = 5.8 Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 3.24 (t, *J* = 6.7 Hz, 2H, -COO-

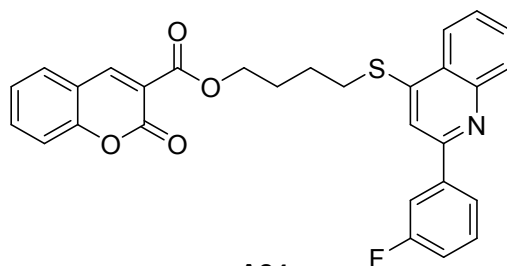
CH₂CH₂CH₂CH₂-S-), 1.99 (dt, *J* = 6.5, 3.3 Hz, 4H, -COO-CH₂CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.27 (s), 155.55 (s), 154.16 (s), 153.95 (s), 147.83 (s), 147.11 (s), 146.41 (s), 140.53 (s), 133.88 (s), 133.42 (s), 129.38 – 128.92 (m), 128.38 (d, *J* = 18.7 Hz), 126.71 (s), 125.39 (s), 124.66 (d, *J* = 9.7 Hz), 123.80 (s), 122.41 (s), 117.01 (s), 116.73 (s), 115.77 (s), 112.93 (s), 64.29 (s), 29.95 (s), 26.73 (s), 23.97 (s). HRMS (ESI) calcd for C₂₉H₂₃ClNO₄S [M+H]⁺: 516.10308, found 516.10302.



A23

Figure S23

3-((2-(3-fluorophenyl)quinolin-4-yl)thio)propyl 2-oxo-2H-chromene-3-carboxylate (A23) White solid, m.p. 155.0-156.1 °C, yield 53%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.50 (s, 1H, Ph-H), 8.13 (ddd, *J* = 12.6, 8.4, 0.7 Hz, 2H, Ph-H), 7.89 – 7.83 (m, 2H, Ph-H), 7.75 – 7.70 (m, 2H, Ph-H), 7.66 (ddd, *J* = 8.7, 7.4, 1.6 Hz, 1H, Ph-H), 7.58 – 7.52 (m, 2H, Ph-H), 7.40 (td, *J* = 8.0, 5.9 Hz, 1H, Ph-H), 7.37 – 7.31 (m, 2H, Ph-H), 7.03 (tdd, *J* = 8.4, 2.6, 0.8 Hz, 1H, Ph-H), 4.54 (t, *J* = 5.9 Hz, 2H, -COO-CH₂CH₂CH₂-S-), 3.45 (t, *J* = 7.2 Hz, 2H, -COO-CH₂CH₂CH₂-S-), 2.35 – 2.28 (m, 2H, -COO-CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.42 (s), 162.11 (d, *J* = 245.6 Hz), 155.65 (s), 154.19 (d, *J* = 2.0 Hz), 148.16 (s), 146.48 (d, *J* = 11.1 Hz), 140.99 (d, *J* = 7.5 Hz), 133.53 (s), 129.26 (s), 129.21 (d, *J* = 8.4 Hz), 129.11 (s), 128.56 (s), 125.40 (s), 124.73 (s), 123.86 (s), 122.38 (s), 122.20 (d, *J* = 2.8 Hz), 116.82 (d, *J* = 16.8 Hz), 115.78 (s), 115.07 (d, *J* = 21.3 Hz), 113.56 (d, *J* = 22.7 Hz), 113.05 (s), 63.14 (s), 26.63 (d, *J* = 8.8 Hz). ¹⁹F NMR (377 MHz, Chloroform-*d*) δ -112.66 (s). HRMS (ESI) calcd for C₂₈H₂₁FNO₄S [M+H]⁺: 486.11698, found 486.11654.

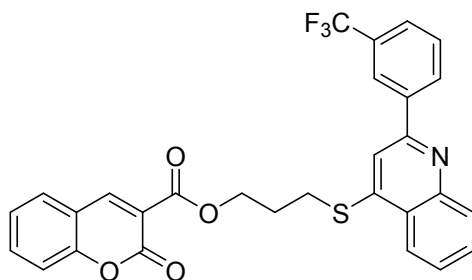


A24

Figure S24

4-((2-(3-fluorophenyl)quinolin-4-yl)thio)butyl 2-oxo-2H-chromene-3-carboxylate

(A24) White solid, m.p. 128.8-130.8 °C, yield 57%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.45 (s, 1H, Ph-H), 8.15 – 8.08 (m, 2H, Ph-H), 7.89 – 7.84 (m, 2H, Ph-H), 7.71 (ddd, *J* = 8.4, 6.9, 1.3 Hz, 1H, Ph-H), 7.66 – 7.61 (m, 2H, Ph-H), 7.55 – 7.44 (m, 3H, Ph-H), 7.33 – 7.28 (m, 2H, Ph-H), 7.15 – 7.10 (m, 1H, Ph-H), 4.44 (t, *J* = 5.8 Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 3.30 (t, *J* = 6.7 Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 2.06 (dt, *J* = 6.4, 3.3 Hz, 4H, -COO-CH₂CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.27 (s), 162.24 (d, *J* = 245.8 Hz), 155.56 (s), 154.16 (s), 154.06 (d, *J* = 2.7 Hz), 147.84 (s), 147.04 (s), 146.40 (s), 141.05 (d, *J* = 7.5 Hz), 133.42 (s), 129.29 (d, *J* = 8.0 Hz), 129.28 (s), 128.48 (s), 125.36 (s), 124.72 (s), 123.80 (s), 122.40 (s), 122.08 (d, *J* = 2.8 Hz), 117.01 (s), 116.74 (s), 115.76 (s), 115.17 (d, *J* = 21.4 Hz), 113.53 (d, *J* = 22.7 Hz), 112.97 (s), 64.30 (s), 29.93 (s), 26.73 (s), 23.97 (s). ¹⁹F NMR (377 MHz, Chloroform-*d*) δ -112.60 (s). HRMS (ESI) calcd for C₂₉H₂₃FNO₄S [M+H]⁺: 500.13263, found 500.13261.



A25

Figure S25

3-((2-(3-(trifluoromethyl)phenyl)quinolin-4-yl)thio)propyl 2-oxo-2H-chromene-3-

carboxylate (A25) White solid, m.p. 117.5-119.5 °C, yield 18%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.49 (s, 1H, Ph-H), 8.43 (s, 1H, Ph-H), 8.29 (d, *J* = 7.5 Hz, 1H, Ph-H), 8.16 (ddd, *J* = 13.8, 8.4, 0.7 Hz, 2H, Ph-H), 7.77 – 7.72 (m, 2H, Ph-H), 7.66 (ddd,

$J = 8.6, 7.3, 1.6$ Hz, 1H, Ph-H), 7.63 – 7.54 (m, 4H, Ph-H), 7.36 – 7.31 (m, 2H, Ph-H), 4.54 (t, $J = 6.0$ Hz, 2H, -COO-CH₂CH₂CH₂-S-), 3.47 (t, $J = 7.2$ Hz, 2H, -COO-CH₂CH₂CH₂-S-), 2.36 – 2.29 (m, 2H, -COO-CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.46 (s), 155.59 (s), 154.23 (s), 154.00 (s), 148.11 (s), 146.83 (s), 146.52 (s), 139.50 (s), 133.52 (s), 130.14 (d, $J = 32.3$ Hz), 129.84 (s), 129.27 (d, $J = 13.9$ Hz), 128.55 (s), 128.17 (s), 125.56 (s), 124.82 (s), 124.78 (d, $J = 3.8$ Hz), 123.87 (s), 123.58 (d, $J = 3.9$ Hz), 123.25 (d, $J = 298.6$ Hz), 122.47 (s), 117.02 (s), 116.76 (s), 115.78 (s), 113.14 (s), 63.09 (s), 26.75 (d, $J = 5.2$ Hz). ¹⁹F NMR (377 MHz, Chloroform-*d*) δ -62.47 (s). HRMS (ESI) calcd for C₂₉H₂₁F₃NO₄S [M+H]⁺: 536.11379, found 536.11369.

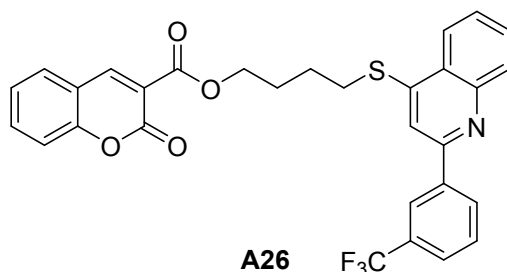


Figure S26

4-((2-(3-(trifluoromethyl)phenyl)quinolin-4-yl)thio)butyl 2-oxo-2H-chromene-3-carboxylate (A26) White solid, m.p. 117.0-118.7 °C, yield 23%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.45 (s, 1H, Ph-H), 8.29 (d, $J = 7.7$ Hz, 1H, Ph-H), 8.18 – 8.09 (m, 2H, Ph-H), 7.73 (ddd, $J = 15.0, 8.0, 4.6$ Hz, 2H, Ph-H), 7.63 (dd, $J = 13.1, 5.6$ Hz, 3H, Ph-H), 7.57 – 7.50 (m, 2H, Ph-H), 7.30 (dd, $J = 11.4, 4.3$ Hz, 2H, Ph-H), 4.45 (t, $J = 5.5$ Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 3.33 (t, $J = 6.5$ Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 2.10 – 2.04 (m, 4H, -COO-CH₂CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.31 (s), 155.55 (s), 154.16 (s), 153.84 (s), 147.86 (s), 147.34 (s), 146.44 (s), 139.50 (s), 133.43 (s), 130.53 (d, $J = 32.2$ Hz), 129.73 (s), 129.25 (d, $J = 15.8$ Hz), 128.47 (s), 128.27 (s), 125.51 (s), 124.87 (d, $J = 3.9$ Hz), 124.75 (s), 123.81 (s), 123.48 (d, $J = 3.7$ Hz), 123.27 (d, $J = 298.2$ Hz), 122.44 (s), 117.03 (s), 116.74 (s), 115.76 (s), 112.87 (s), 64.32 (s), 30.00 (s), 26.72 (s), 24.00 (s). ¹⁹F NMR (377 MHz, Chloroform-*d*) δ -62.47 (s). HRMS (ESI) calcd for C₃₀H₂₃F₃NO₄S [M+H]⁺: 550.12944, found 550.12937.

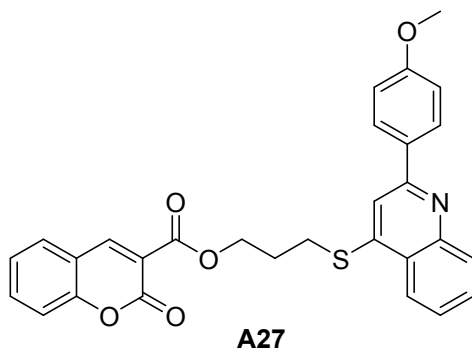


Figure S27

3-((2-(4-methoxyphenyl)quinolin-4-yl)thio)propyl 2-oxo-2H-chromene-3-carboxylate (A27) White solid, m.p. 131.0-131.5 °C, yield 9%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.48 (s, 1H, Ph-H), 8.14 – 8.06 (m, 4H, Ph-H), 7.71 – 7.63 (m, 3H, Ph-H), 7.55 – 7.47 (m, 2H, Ph-H), 7.33 (dd, *J* = 12.2, 4.6 Hz, 2H, Ph-H), 6.98 – 6.94 (m, 2H, Ph-H), 4.53 (t, *J* = 6.0 Hz, 2H, -COO-CH₂CH₂CH₂-S-), 3.80 (s, 3H, Ph-OCH₃), 3.42 (t, *J* = 7.2 Hz, 2H, -COO-CH₂CH₂CH₂-S-), 2.34 – 2.28 (m, 2H, -COO-CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 163.31 (s), 160.77 (s), 156.58 (s), 156.11 (s), 155.21 (s), 149.00 (s), 134.46 (s), 129.93 (d, *J* = 2.6 Hz), 129.57 (s), 128.98 (s), 125.80 (s), 125.41 (s), 124.84 (s), 123.39 (s), 118.00 (s), 117.77 (s), 116.77 (s), 114.16 (d, *J* = 5.7 Hz), 64.14 (s), 55.27 (s), 27.78 (s), 1.00 (s). HRMS (ESI) calcd for C₂₉H₂₄NO₅S [M+H]⁺: 498.13697, found 498.13656.

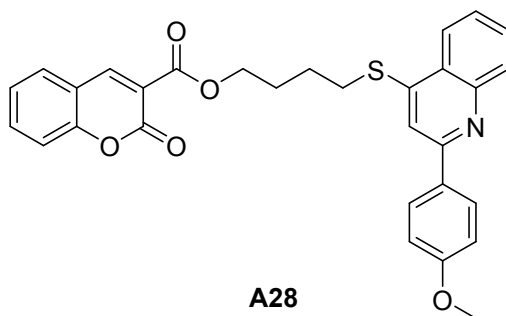
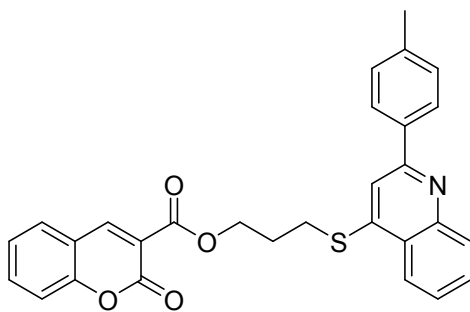


Figure S28

4-((2-(4-methoxyphenyl)quinolin-4-yl)thio)butyl 2-oxo-2H-chromene-3-carboxylate (A28) White solid, m.p. 138.0-139.8 °C, yield 10%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.43 (s, 1H, Ph-H), 8.13 – 8.10 (m, 1H, Ph-H), 8.07 (dd, *J* = 7.0, 1.9 Hz, 3H, Ph-H), 7.71 – 7.62 (m, 3H, Ph-H), 7.51 – 7.47 (m, 2H, Ph-H), 7.31 (dd, *J* = 14.3, 7.7 Hz, 2H, Ph-H), 7.04 – 7.00 (m, 2H, Ph-H), 4.44 (t, *J* = 5.7 Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 3.87 (s, 3H, Ph-OCH₃), 3.29 (t, *J* = 6.6 Hz, 2H, -COO-

CH₂CH₂CH₂CH₂-S-), 2.06 (dd, $J = 6.2, 2.9$ Hz, 4H, -COO-CH₂CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.21 (s), 159.80 (s), 155.58 (s), 155.05 (s), 154.16 (s), 147.78 (s), 133.40 (s), 128.92 (d, $J = 16.0$ Hz), 128.51 (s), 127.87 (s), 124.73 (s), 124.36 (s), 123.80 (s), 122.38 (s), 117.01 (s), 116.76 (s), 115.75 (s), 113.21 (s), 112.95 (s), 64.27 (s), 54.39 (s), 29.91 (s), 26.76 (s), 24.01 (s). HRMS (ESI) calcd for C₃₀H₂₆NO₅S [M+H]⁺: 512.15262, found 512.15283.

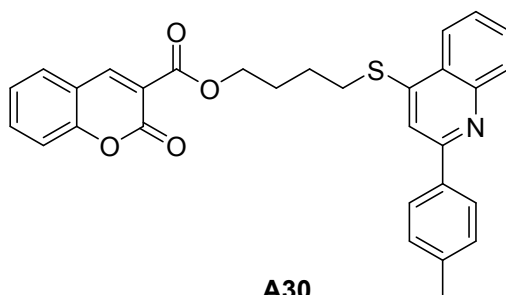


A29

Figure S29

3-((2-(p-tolyl)quinolin-4-yl)thio)propyl 2-oxo-2H-chromene-3-carboxylate (29)

White solid, m.p. 103.5-104.3 °C, yield 30%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.47 (s, 1H, Ph-H), 8.12 (ddd, $J = 12.5, 8.4, 0.7$ Hz, 2H, Ph-H), 8.00 (d, $J = 8.2$ Hz, 2H, Ph-H), 7.73 – 7.63 (m, 3H, Ph-H), 7.55 – 7.49 (m, 2H, Ph-H), 7.37 – 7.30 (m, 2H, Ph-H), 7.24 (d, $J = 7.9$ Hz, 2H, Ph-H), 4.53 (t, $J = 6.0$ Hz, 2H, -COO-CH₂CH₂CH₂-S-), 3.43 (t, $J = 7.2$ Hz, 2H, -COO-CH₂CH₂CH₂-S-), 2.33 – 2.29 (m, 5H, Ph-OCH₃, -COO-CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.29 (s), 155.60 (s), 154.18 (s), 148.02 (s), 146.60 (s), 145.85 (s), 138.35 (s), 135.86 (s), 133.48 (s), 129.13 (s), 128.87 (s), 128.51 (d, $J = 12.1$ Hz), 126.45 (d, $J = 5.5$ Hz), 124.93 (s), 124.52 (s), 123.84 (s), 122.36 (s), 116.84 (d, $J = 18.8$ Hz), 115.76 (s), 113.32 (s), 63.14 (s), 26.69 (d, $J = 11.6$ Hz), 20.22 (s). HRMS (ESI) calcd for C₂₉H₂₄NO₅S [M+H]⁺: 482.14206, found 482.14212.



A30

Figure S30

4-((2-(p-tolyl)quinolin-4-yl)thio)butyl 2-oxo-2H-chromene-3-carboxylate (A30)

White solid, m.p. 80.2-82.0 °C, yield 45%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.43 (s, 1H, Ph-H), 8.11 (ddd, *J* = 14.3, 8.4, 0.8 Hz, 2H, Ph-H), 8.01 – 7.98 (m, 2H, Ph-H), 7.69 (ddd, *J* = 8.4, 6.9, 1.4 Hz, 1H, Ph-H), 7.66 – 7.61 (m, 2H, Ph-H), 7.52 – 7.48 (m, 2H, Ph-H), 7.34 – 7.28 (m, 4H, Ph-H), 4.44 (t, *J* = 5.9 Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 3.29 (t, *J* = 6.7 Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 2.41 (s, 3H, Ph-OCH₃), 2.05 (dt, *J* = 6.5, 3.2 Hz, 4H, -COO-CH₂CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.15 (s), 155.52 (d, *J* = 15.0 Hz), 154.11 (s), 147.81 (s), 146.43 (d, *J* = 18.3 Hz), 138.43 (s), 135.86 (s), 133.41 (s), 129.12 (s), 128.83 (s), 128.52 (d, *J* = 3.3 Hz), 126.40 (d, *J* = 4.0 Hz), 124.87 (s), 124.45 (s), 123.79 (s), 122.33 (s), 116.81 (d, *J* = 19.5 Hz), 115.72 (s), 113.07 (s), 64.24 (s), 29.80 (s), 26.72 (s), 23.93 (s), 20.32 (s). HRMS (ESI) calcd for C₃₀H₂₆NO₄S [M+H]⁺: 496.15771, found 496.15737.

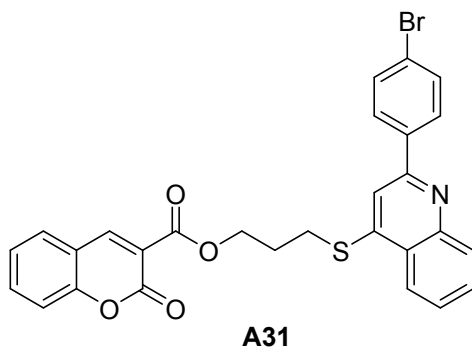


Figure S31

3-((2-(4-bromophenyl)quinolin-4-yl)thio)propyl 2-oxo-2H-chromene-3-

carboxylate (A31) White solid, m.p. 142.1-143.5 °C, yield 16%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.51 (s, 1H, Ph-H), 8.13 (ddd, *J* = 18.5, 8.4, 0.7 Hz, 2H, Ph-H), 8.04 – 7.95 (m, 2H, Ph-H), 7.75 – 7.64 (m, 3H, Ph-H), 7.62 – 7.47 (m, 4H, Ph-H), 7.40 – 7.32 (m, 2H, Ph-H), 4.53 (t, *J* = 5.9 Hz, 2H, -COO-CH₂CH₂CH₂-S-), 3.45 (t, *J* = 7.2 Hz, 2H, -COO-CH₂CH₂CH₂-S-), 2.31 (dt, *J* = 12.9, 6.3 Hz, 2H, -COO-CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.49 (s), 154.42 (s), 154.21 (s), 148.22 (s), 146.50 (s), 133.65 (s), 130.85 (s), 129.15 (d, *J* = 7.2 Hz), 128.58 (s), 128.23 (s), 125.32 (s), 124.74 (d, *J* = 18.5 Hz), 124.16 (s), 123.95 (s), 122.85 (s), 122.42 (s),

115.88 (s), 63.13 (s), 28.68 (s), 26.61 (s). HRMS (ESI) calcd for C₂₈H₂₁BrNO₄S [M+H]⁺: 546.03692, found 546.03701.

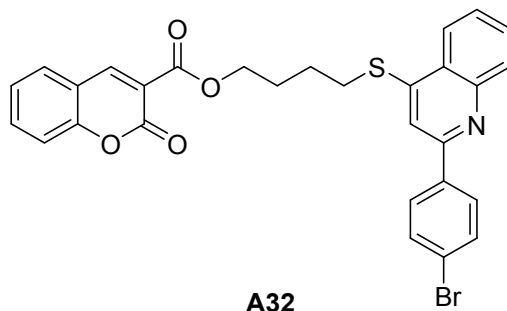


Figure S32

4-((2-(4-bromophenyl)quinolin-4-yl)thio)butyl 2-oxo-2H-chromene-3-carboxylate

(A32) White solid, m.p. 106.7-108.6 °C, yield 29%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.46 (s, 1H, Ph-H), 8.11 (ddd, *J* = 20.8, 8.4, 0.7 Hz, 2H, Ph-H), 8.02 – 7.99 (m, 2H, Ph-H), 7.71 (ddd, *J* = 8.4, 6.9, 1.4 Hz, 1H, Ph-H), 7.63 (ddd, *J* = 5.6, 3.3, 1.5 Hz, 4H, Ph-H), 7.53 (ddd, *J* = 8.1, 5.8, 1.4 Hz, 2H, Ph-H), 7.34 – 7.31 (m, 2H, Ph-H), 4.44 (d, *J* = 3.9 Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 3.31 (t, *J* = 6.6 Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 2.06 (dd, *J* = 5.9, 3.1 Hz, 4H, -COO-CH₂CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.36 (s), 155.55 (s), 154.17 (s), 147.85 (d, *J* = 13.4 Hz), 147.02 (s), 146.45 (s), 137.59 (s), 133.46 (s), 130.94 (s), 129.13 (d, *J* = 14.9 Hz), 128.50 (s), 128.13 (s), 125.27 (s), 124.62 (s), 123.83 (s), 122.89 (s), 122.42 (s), 116.75 (s), 115.78 (s), 112.80 (s), 64.36 (s), 29.94 (s), 26.73 (s), 24.07 (s). HRMS (ESI) calcd for C₂₉H₂₃BrNO₄S [M+H]⁺: 560.05257, found 560.05231.

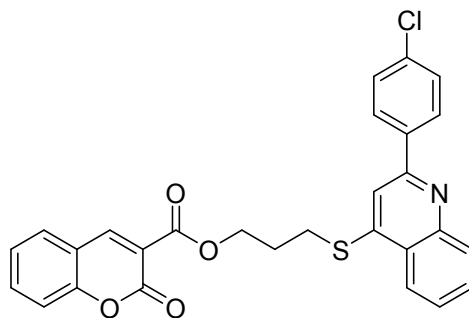


Figure S33

3-((2-(4-chlorophenyl)quinolin-4-yl)thio)propyl 2-oxo-2H-chromene-3-

carboxylate (A33) White solid, m.p. 139.9-140.9 °C, yield 21%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.50 (s, 1H, Ph-H), 8.16 – 8.13 (m, 1H, Ph-H), 8.10 (d, *J* = 8.3 Hz,

1H, Ph-H), 8.08 – 8.04 (m, 2H, Ph-H), 7.74 – 7.70 (m, 2H, Ph-H), 7.67 (ddd, $J = 7.5$, 5.3, 1.5 Hz, 1H, Ph-H), 7.58 – 7.51 (m, 2H, Ph-H), 7.42 – 7.38 (m, 2H, Ph-H), 7.38 – 7.31 (m, 2H, Ph-H), 4.52 (t, $J = 5.9$ Hz, 2H, -COO-CH₂CH₂CH₂-S-), 3.45 (t, $J = 7.2$ Hz, 2H, -COO-CH₂CH₂CH₂-S-), 2.34 – 2.27 (m, 2H, -COO-CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.45 (s), 155.64 (s), 154.26 (d, $J = 16.4$ Hz), 148.18 (s), 146.46 (d, $J = 3.2$ Hz), 137.07 (s), 134.43 (s), 133.62 (s), 129.13 (d, $J = 9.0$ Hz), 128.56 (s), 127.91 (d, $J = 5.2$ Hz), 125.28 (s), 124.60 (s), 123.92 (s), 122.39 (s), 116.91 (s), 116.70 (s), 115.83 (s), 112.94 (s), 63.12 (s), 26.69 (d, $J = 16.7$ Hz). HRMS (ESI) calcd for C₂₈H₂₁ClNO₄S [M+H]⁺: 502.08743, found 502.08685.

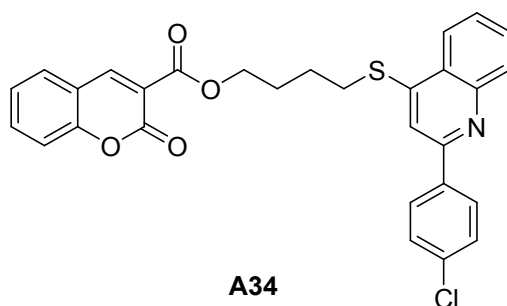
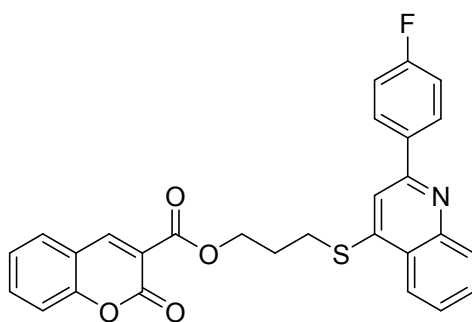


Figure S34

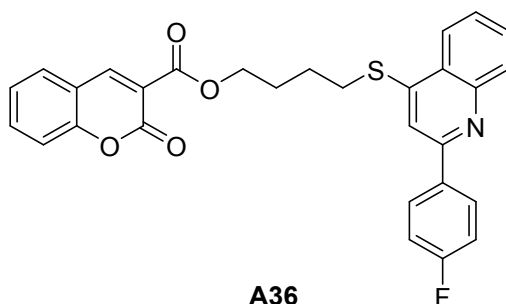
4-((2-(4-chlorophenyl)quinolin-4-yl)thio)butyl 2-oxo-2H-chromene-3-carboxylate (A34) White solid, m.p. 126.1-127.6 °C, yield 13%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.46 (s, 1H, Ph-H), 8.13 (dd, $J = 8.4$, 0.9 Hz, 1H, Ph-H), 8.10 – 8.05 (m, 3H, Ph-H), 7.71 (ddd, $J = 8.4$, 6.9, 1.4 Hz, 1H, Ph-H), 7.66 – 7.62 (m, 2H, Ph-H), 7.52 (ddd, $J = 7.2$, 6.3, 1.3 Hz, 2H, Ph-H), 7.49 – 7.45 (m, 2H, Ph-H), 7.31 (ddd, $J = 8.6$, 6.5, 2.7 Hz, 2H, Ph-H), 4.44 (t, $J = 5.7$ Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 3.30 (t, $J = 6.7$ Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 2.09 – 2.03 (m, 4H, -COO-CH₂CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.34 (s), 155.55 (s), 154.19 (d, $J = 5.2$ Hz), 147.90 (s), 146.98 (s), 146.44 (s), 137.14 (s), 134.50 (s), 133.45 (s), 129.11 (d, $J = 15.9$ Hz), 128.50 (s), 127.91 (d, $J = 12.9$ Hz), 125.24 (s), 124.59 (s), 123.82 (s), 122.40 (s), 117.02 (s), 116.75 (s), 115.76 (s), 112.84 (s), 64.35 (s), 29.93 (s), 26.73 (s), 24.05 (s). HRMS (ESI) calcd for C₂₉H₂₃ClNO₄S [M+H]⁺: 516.10308, found 516.10239.



A35

Figure S35

3-((2-(4-fluorophenyl)quinolin-4-yl)thio)propyl 2-oxo-2H-chromene-3-carboxylate (A35) White solid, m.p. 135.6-136.5 °C, yield 26%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.50 (s, 1H, Ph-H), 8.15 – 8.08 (m, 4H, Ph-H), 7.74 – 7.69 (m, 2H, Ph-H), 7.69 – 7.65 (m, 1H, Ph-H), 7.58 – 7.50 (m, 2H, Ph-H), 7.38 – 7.31 (m, 2H, Ph-H), 7.15 – 7.10 (m, 2H, Ph-H), 4.53 (t, *J* = 5.9 Hz, 2H, -COO-CH₂CH₂CH₂-S-), 3.44 (t, *J* = 7.2 Hz, 2H, -COO-CH₂CH₂CH₂-S-), 2.30 (dd, *J* = 13.0, 6.7 Hz, 2H, -COO-CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.66 (d, *J* = 249.1 Hz), 162.43 (s), 155.62 (s), 154.55 (s), 154.18 (s), 148.17 (s), 146.40 (d, *J* = 17.6 Hz), 134.82 (d, *J* = 3.1 Hz), 133.60 (s), 129.08 (d, *J* = 8.2 Hz), 128.51 (d, *J* = 8.1 Hz), 125.15 (s), 124.48 (s), 123.91 (s), 122.39 (s), 116.91 (s), 116.71 (s), 115.80 (s), 114.66 (d, *J* = 21.6 Hz), 113.03 (s), 63.12 (s), 26.68 (d, *J* = 8.9 Hz). ¹⁹F NMR (376 MHz, Chloroform-*d*) δ -112.38 (s). HRMS (ESI) calcd for C₂₈H₂₁FNO₄S [M+H]⁺: 486.11698, found 486.11685.



A36

Figure S36

4-((2-(4-fluorophenyl)quinolin-4-yl)thio)butyl 2-oxo-2H-chromene-3-carboxylate (A36) White solid, m.p. 117.4-118.9 °C, yield 9%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.46 (s, 1H, Ph-H), 8.15 – 8.07 (m, 4H, Ph-H), 7.70 (ddd, *J* = 8.4, 6.9, 1.3 Hz, 1H, Ph-H), 7.67 – 7.61 (m, 2H, Ph-H), 7.54 – 7.50 (m, 2H, Ph-H), 7.34 – 7.29 (m, 2H,

Ph-H), 7.21 – 7.16 (m, 2H, Ph-H), 4.45 (t, $J = 5.8$ Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 3.30 (t, $J = 6.7$ Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 2.06 (dt, $J = 6.6, 3.4$ Hz, 4H, -COO-CH₂CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.75 (d, $J = 249.1$ Hz), 162.34 (s), 161.93 (d, $J = 83.4$ Hz), 155.57 (s), 154.46 (s), 154.18 (s), 147.89 (s), 146.84 (s), 146.46 (s), 133.45 (s), 129.26 (d, $J = 3.2$ Hz), 129.15 (s), 129.00 (s), 128.45 (d, $J = 9.5$ Hz), 125.11 (s), 124.48 (s), 123.83 (s), 122.40 (s), 117.04 (s), 116.76 (s), 115.77 (s), 114.75 (d, $J = 21.5$ Hz), 112.96 (s), 64.34 (s), 29.94 (s), 26.73 (s), 24.02 (s). ¹⁹F NMR (377 MHz, Chloroform-*d*) δ -112.38 (s). HRMS (ESI) calcd for C₂₉H₂₃FNO₄S [M+H]⁺: 500.13263, found 500.13193.

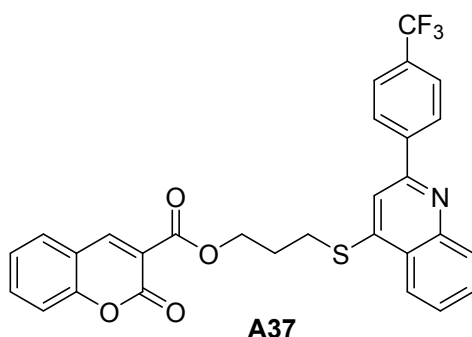


Figure S37

3-((2-(4-(trifluoromethyl)phenyl)quinolin-4-yl)thio)propyl 2-oxo-2H-chromene-3-carboxylate (A37) White solid, m.p. 156.3-158.2 °C, yield 9%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.51 (s, 1H, Ph-H), 8.26 (d, $J = 8.2$ Hz, 2H, Ph-H), 8.15 (dd, $J = 15.8, 8.4$ Hz, 2H, Ph-H), 7.79 (s, 1H, Ph-H), 7.76 – 7.65 (m, 4H, Ph-H), 7.56 (t, $J = 8.2$ Hz, 2H, Ph-H), 7.37 – 7.32 (m, 2H, Ph-H), 4.54 (t, $J = 5.9$ Hz, 2H, -COO-CH₂CH₂CH₂-S-), 3.47 (t, $J = 7.3$ Hz, 2H, -COO-CH₂CH₂CH₂-S-), 2.35 – 2.28 (m, 2H, -COO-CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.55 (s), 155.63 (s), 154.14 (d, $J = 15.6$ Hz), 148.19 (s), 146.78 (s), 146.54 (s), 142.04 (s), 133.62 (s), 129.97 (d, $J = 32.3$ Hz), 129.29 (d, $J = 18.9$ Hz), 128.54 (s), 127.02 (s), 125.60 (s), 124.85 (s), 124.62 (d, $J = 3.7$ Hz), 123.94 (s), 123.11 (d, $J = 271.8$ Hz), 122.45 (s), 117.06 (s), 116.74 (s), 115.81 (s), 113.17 (s), 63.15 (s), 26.76 (d, $J = 14.5$ Hz). ¹⁹F NMR (377 MHz, Chloroform-*d*) δ -62.61 (s). HRMS (ESI) calcd for C₂₉H₂₁F₃NO₄S [M+H]⁺: 536.11379, found 536.11363.

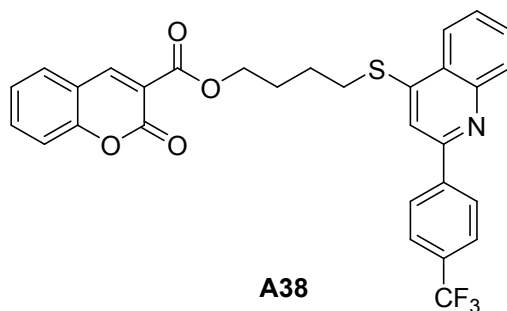


Figure S38

4-((2-(4-(trifluoromethyl)phenyl)quinolin-4-yl)thio)butyl 2-oxo-2H-chromene-3-carboxylate (A38) White solid, m.p. 91.2-92.5 °C, yield 25%; ¹H NMR (400 MHz, Chloroform-*d*) δ 8.46 (s, 1H, Ph-H), 8.24 (d, *J* = 8.2 Hz, 2H, Ph-H), 8.16 – 8.09 (m, 2H, Ph-H), 7.73 (ddd, *J* = 10.0, 9.5, 4.8 Hz, 3H, Ph-H), 7.67 – 7.61 (m, 2H, Ph-H), 7.53 (ddd, *J* = 9.1, 8.2, 1.1 Hz, 2H, Ph-H), 7.30 (t, *J* = 7.7 Hz, 2H, Ph-H), 4.44 (t, *J* = 5.7 Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 3.32 (t, *J* = 6.7 Hz, 2H, -COO-CH₂CH₂CH₂CH₂-S-), 2.09 – 2.04 (m, 4H, -COO-CH₂CH₂CH₂CH₂-S-). ¹³C NMR (101 MHz, Chloroform-*d*) δ 162.39 (s), 155.59 (s), 154.04 (d, *J* = 18.1 Hz), 148.04 (s), 147.35 (s), 146.37 (s), 142.08 (d, *J* = 0.9 Hz), 133.50 (s), 130.00 (d, *J* = 32.5 Hz), 129.24 (d, *J* = 15.2 Hz), 128.49 (s), 126.91 (s), 125.55 (s), 124.71 (d, *J* = 4.1 Hz), 123.84 (s), 123.14 (d, *J* = 272.3 Hz), 122.39 (s), 116.92 (s), 116.70 (s), 115.74 (s), 112.91 (s), 64.40 (s), 29.87 (s), 26.69 (s), 24.02 (s). ¹⁹F NMR (377 MHz, Chloroform-*d*) δ -62.53 (s). HRMS (ESI) calcd for C₃₀H₂₃F₃NO₄S [M+H]⁺: 550.12944, found 550.12864.

2 ^1H , ^{13}C , ^{19}F NMR, HRMS spectra of target compounds

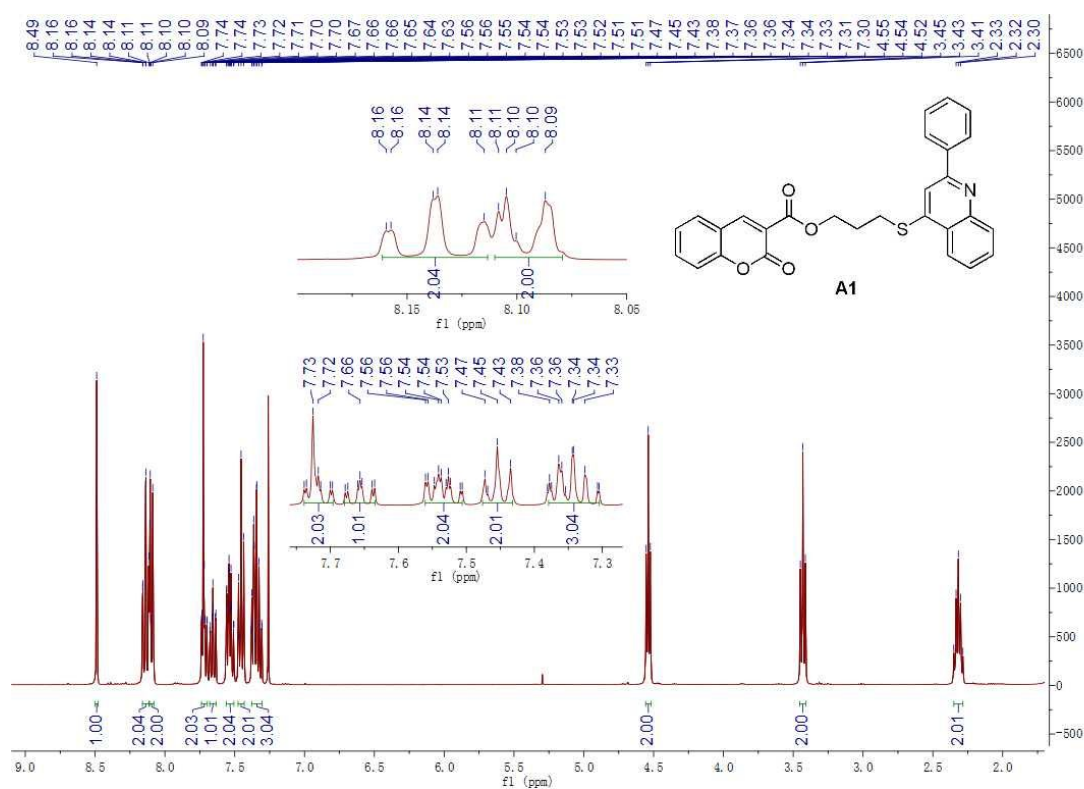


Figure S39 ^1H NMR spectra of compound A1

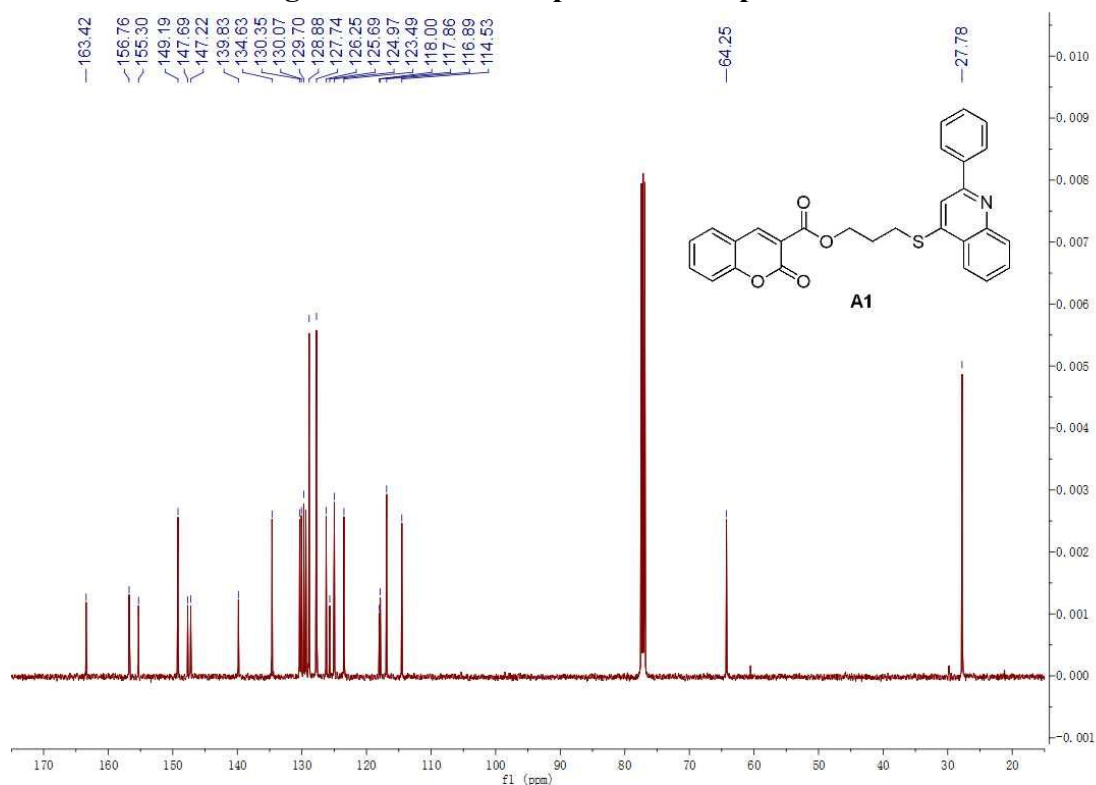


Figure S40 ^{13}C NMR spectra of compound

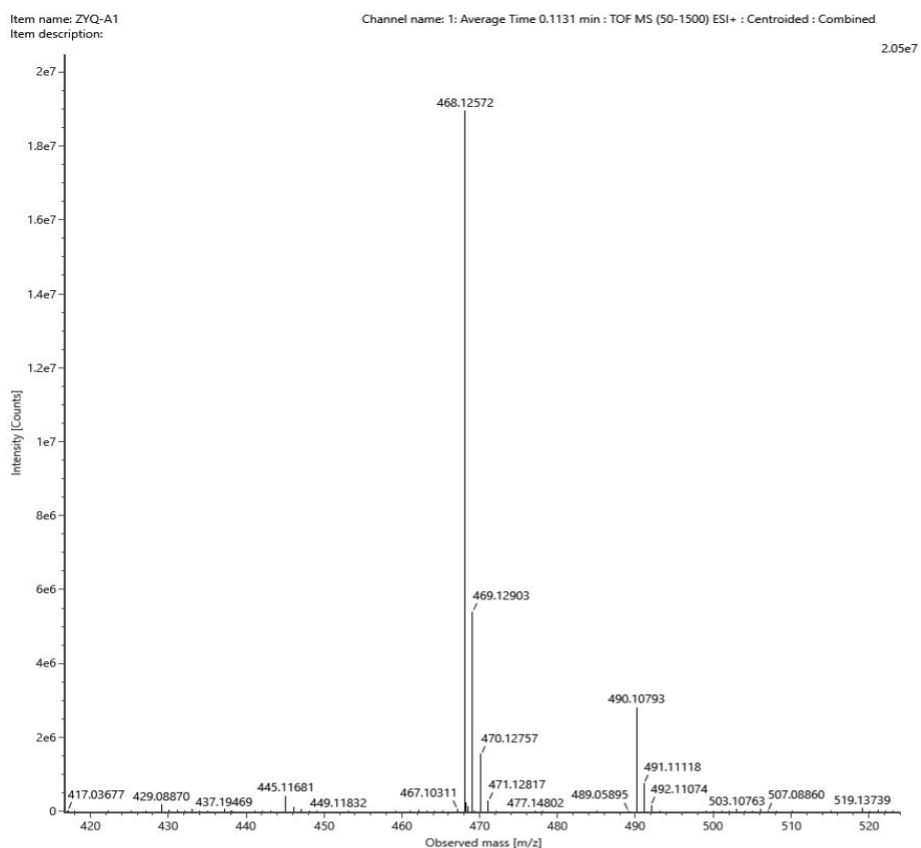


Figure S41 HRMS spectra of compound A1

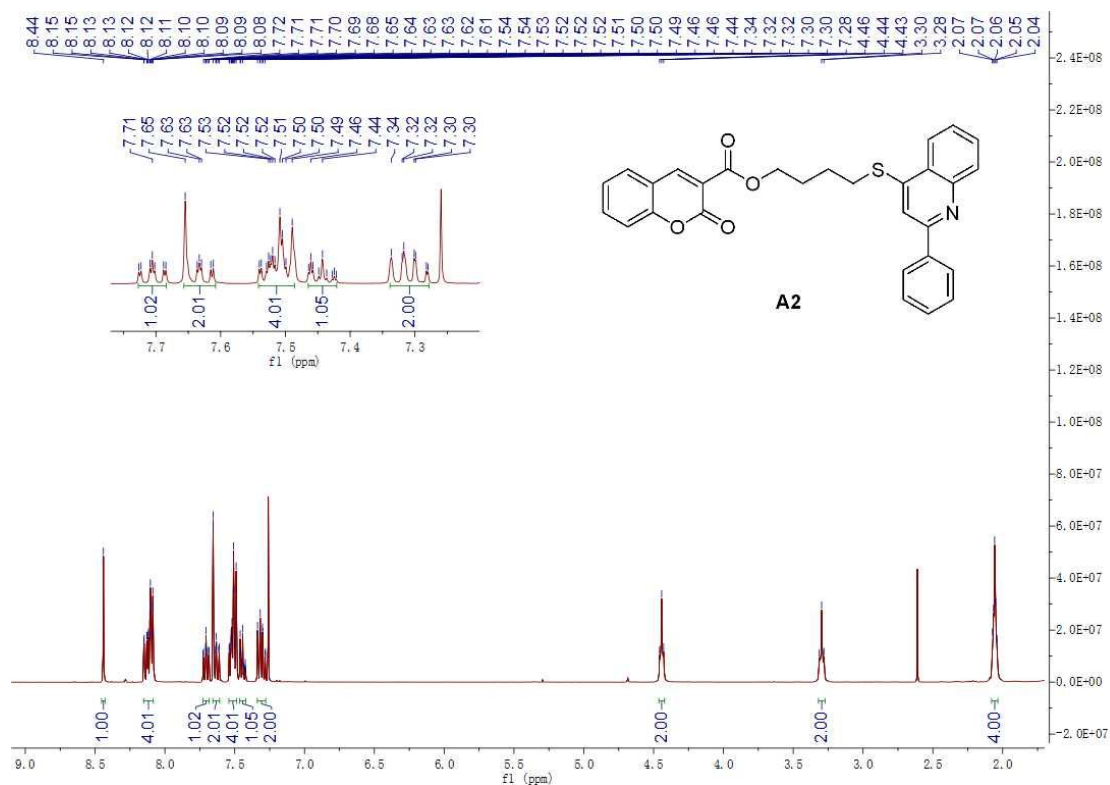
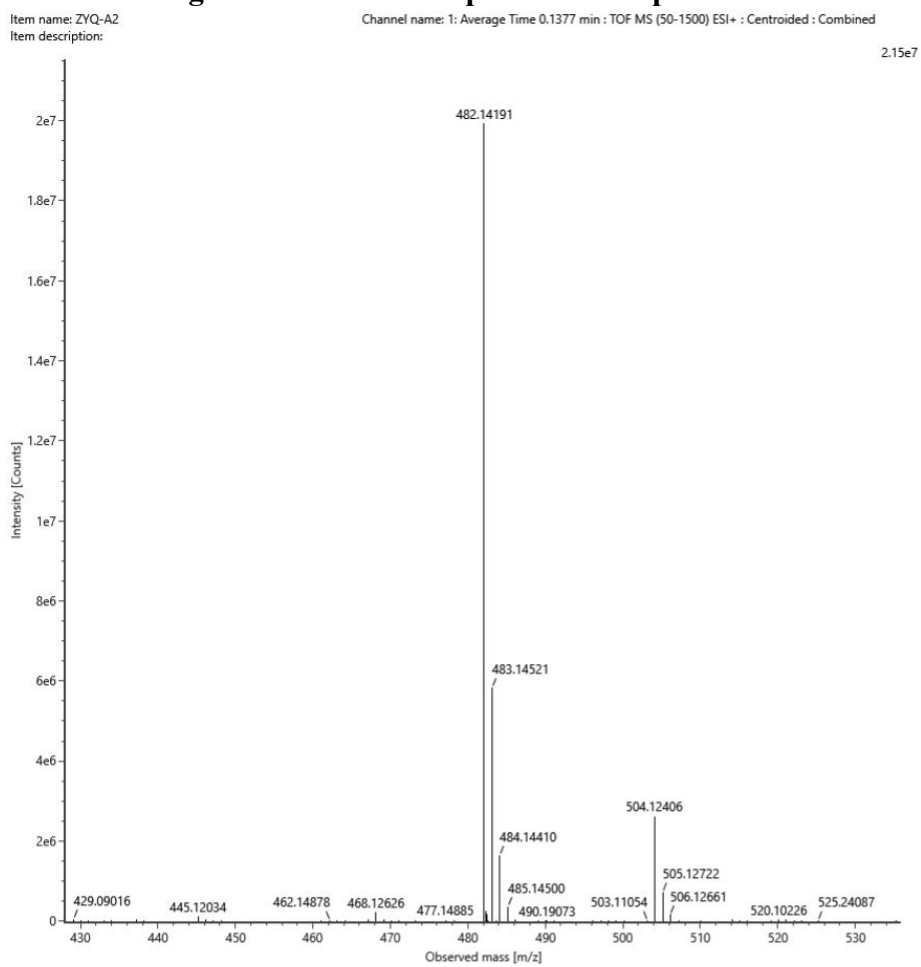
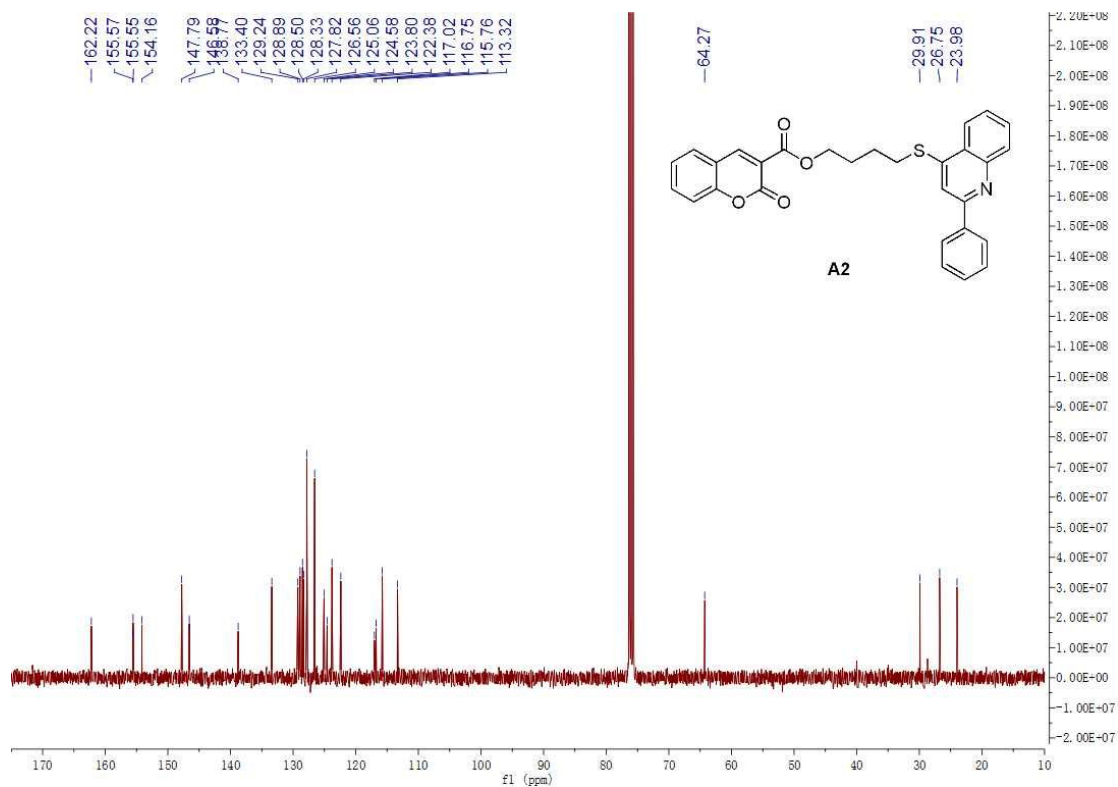


Figure S42 ¹H NMR spectra of compound A2



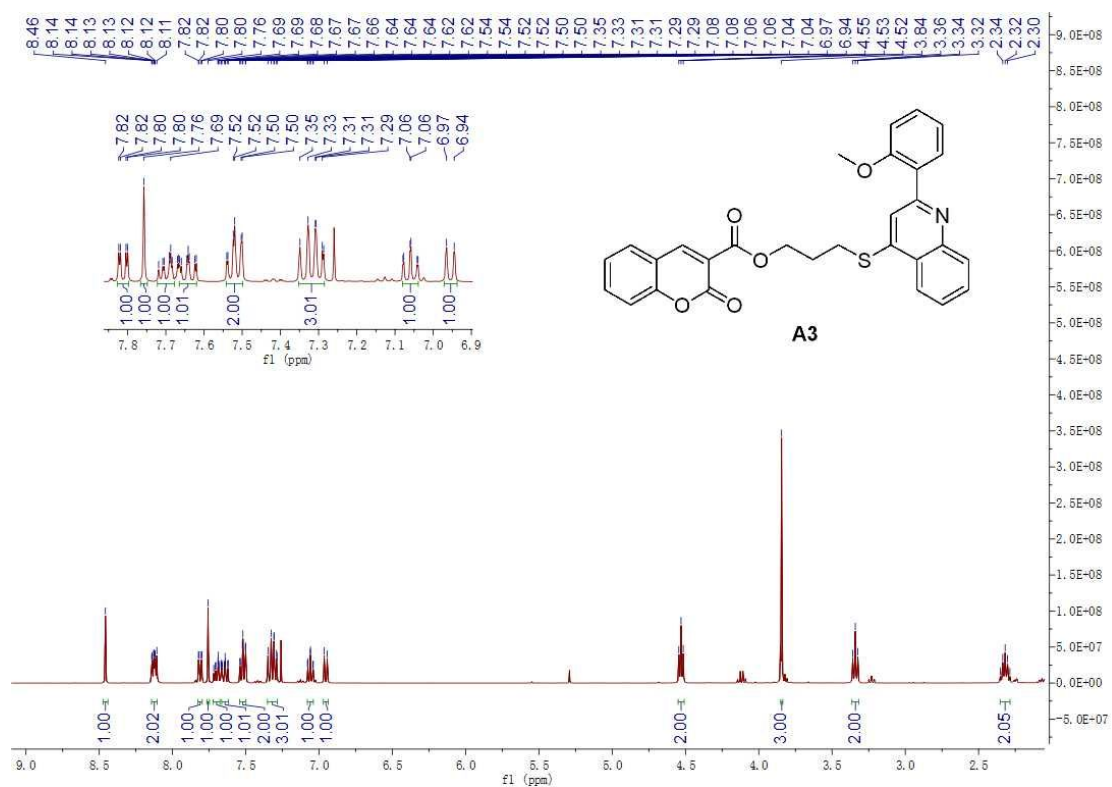


Figure S45 ^1H NMR spectra of compound A3

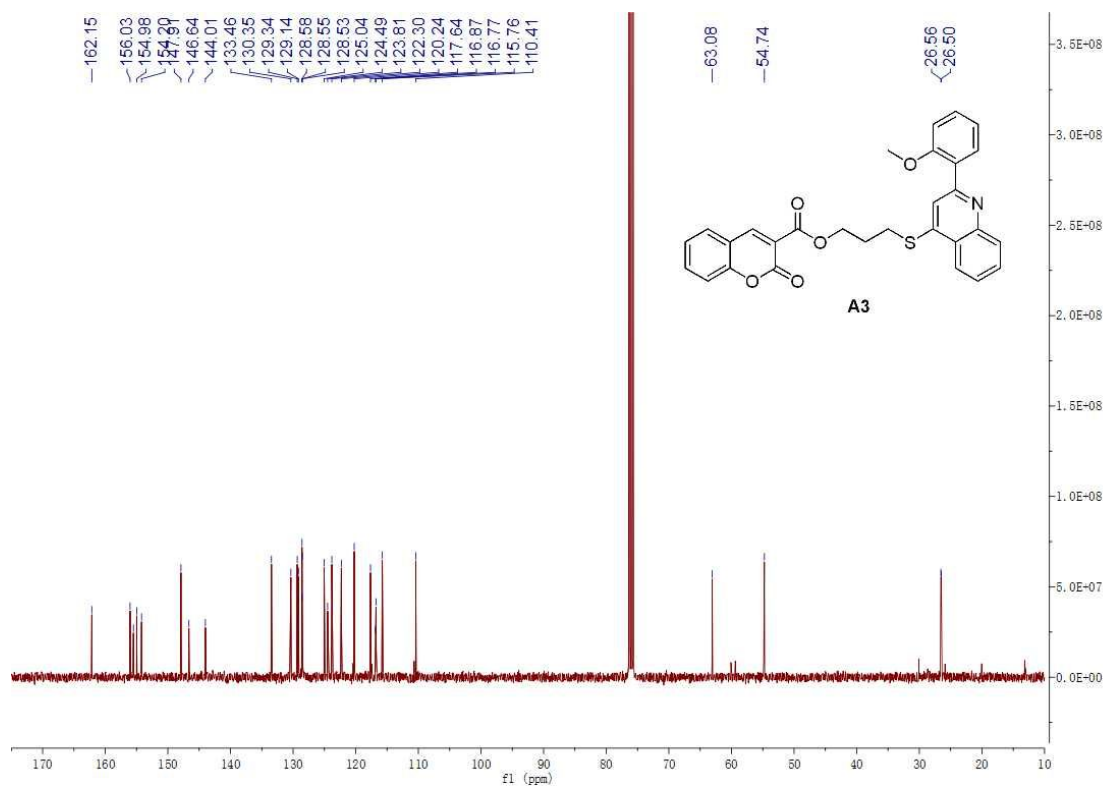


Figure S46 ^{13}C NMR spectra of compound A3

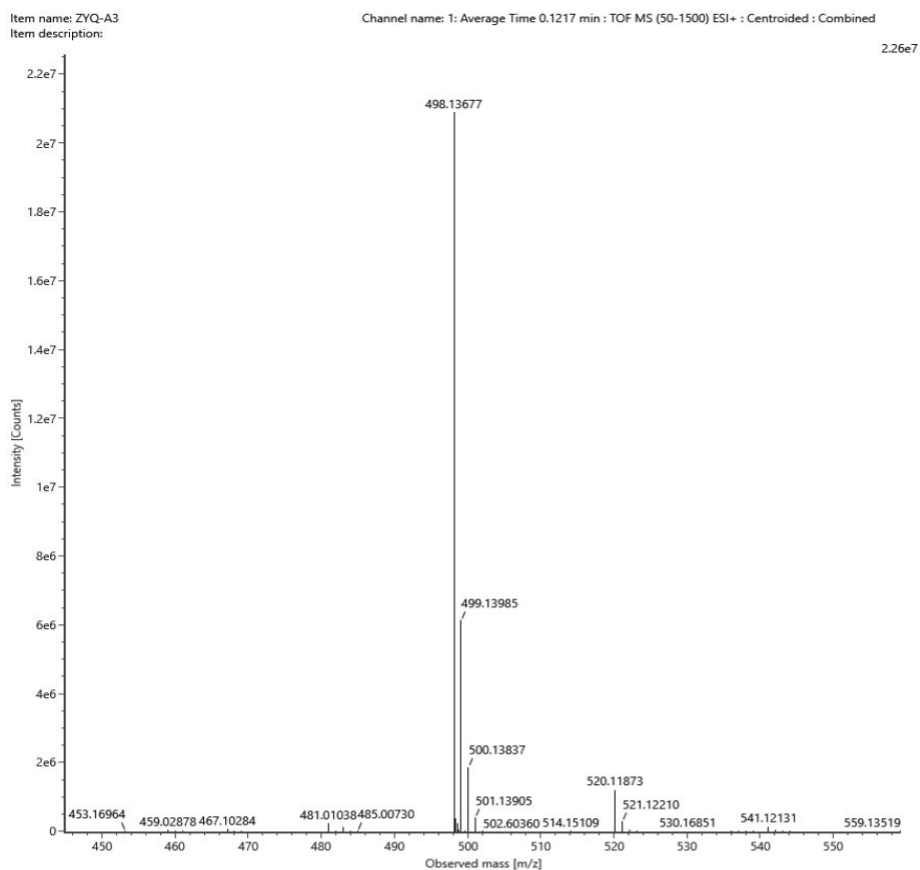


Figure S47 HRMS spectra of compound A3

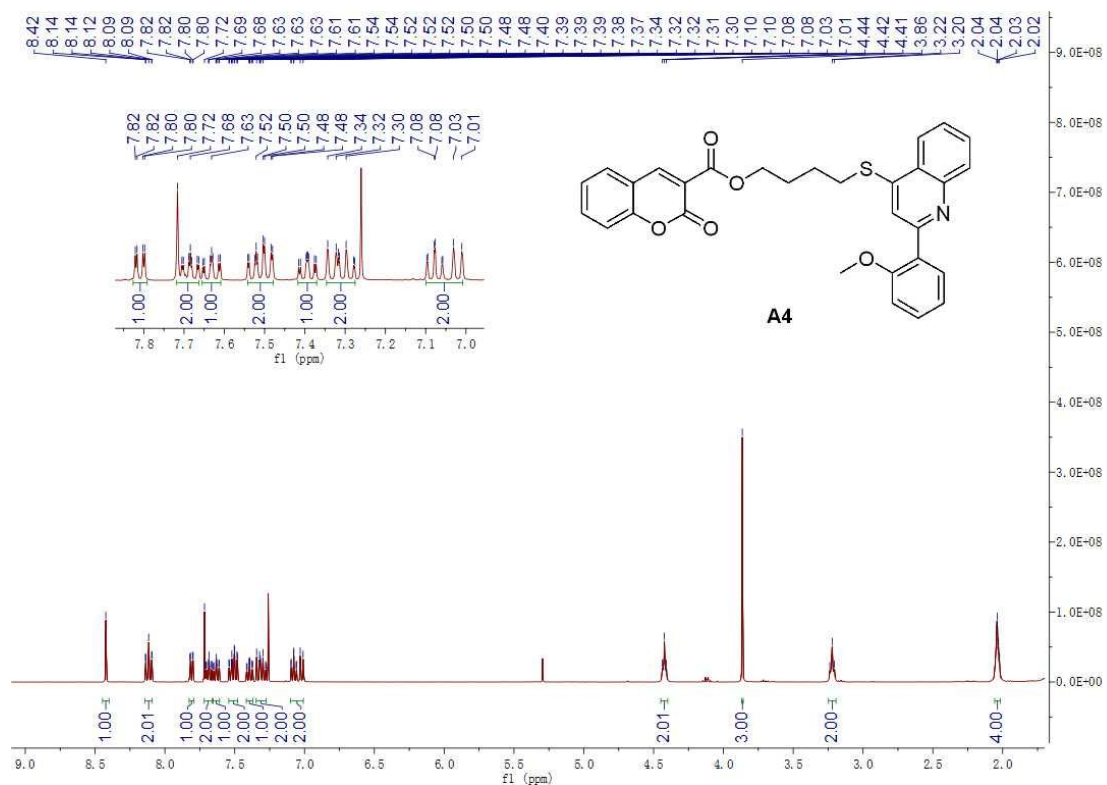


Figure S48 ¹H NMR spectra of compound A4

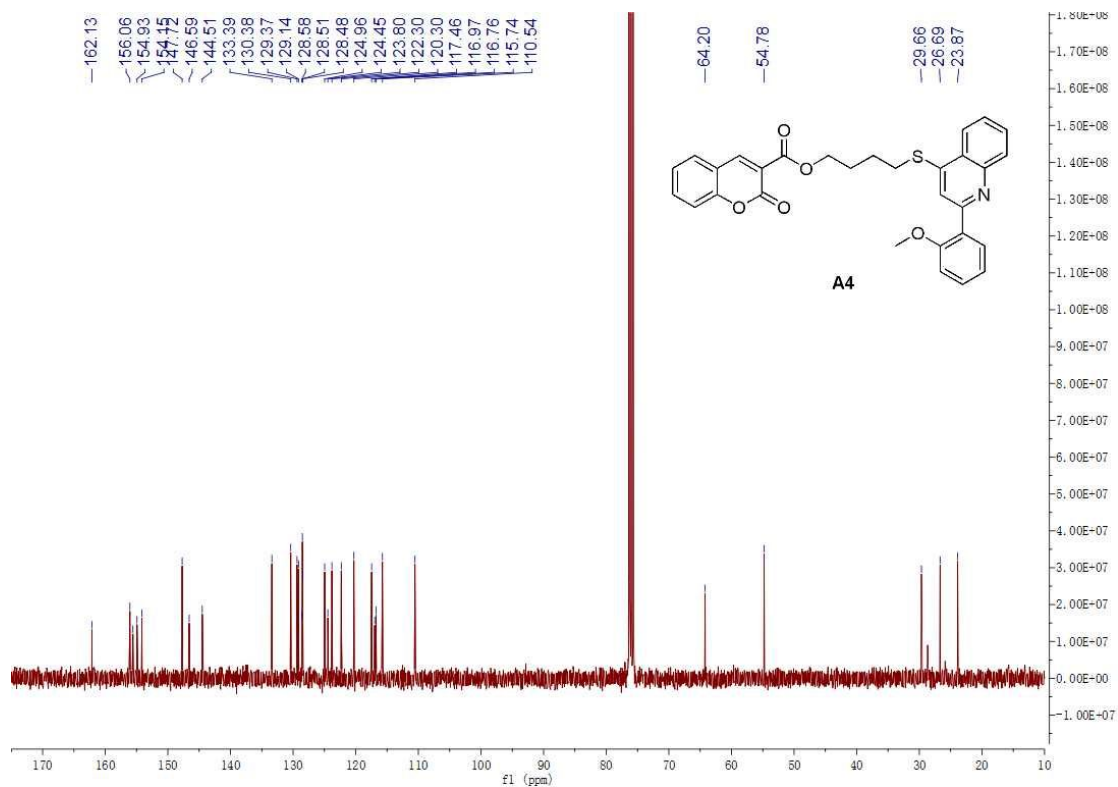


Figure S49 ¹³C NMR spectra of compound A4

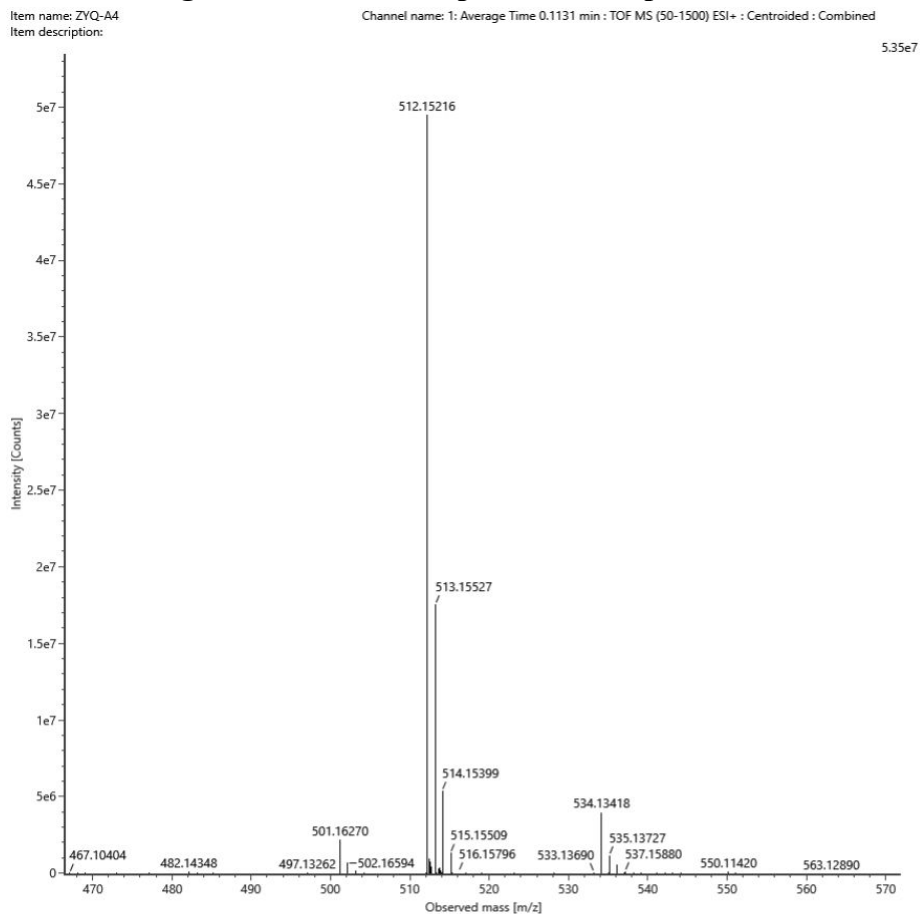


Figure S50 HRMS spectra of compound A4

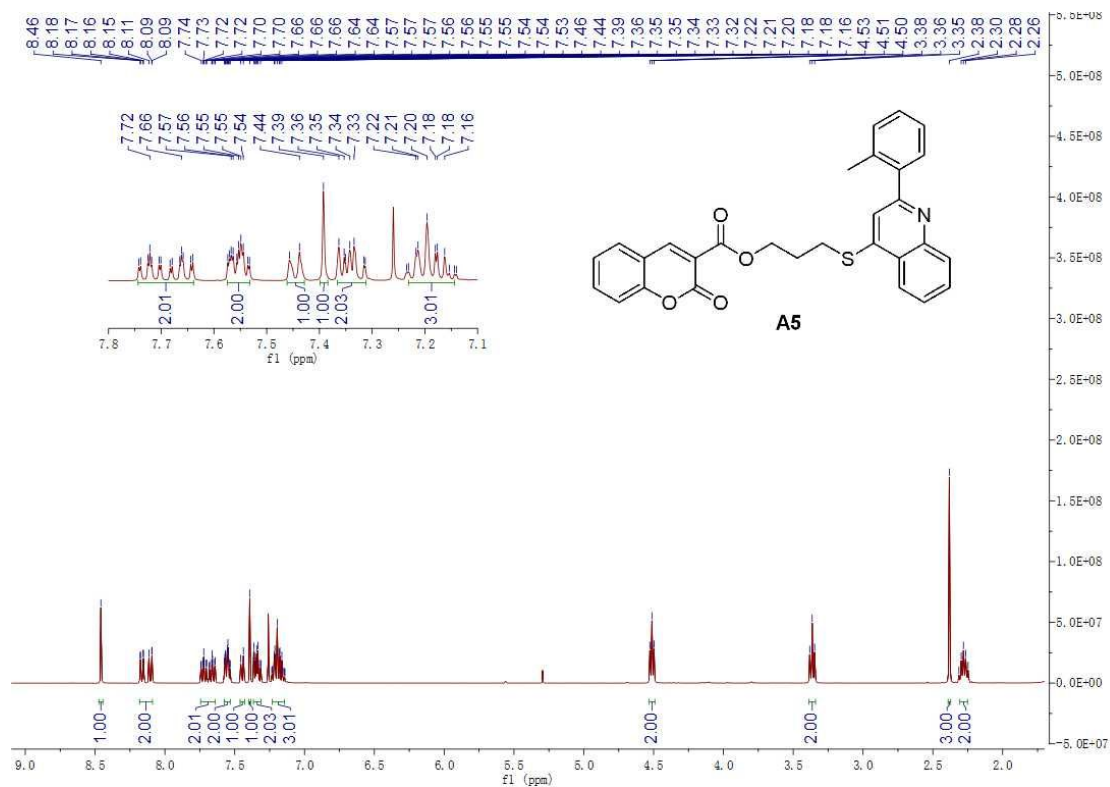


Figure S51 ¹H NMR spectra of compound A5

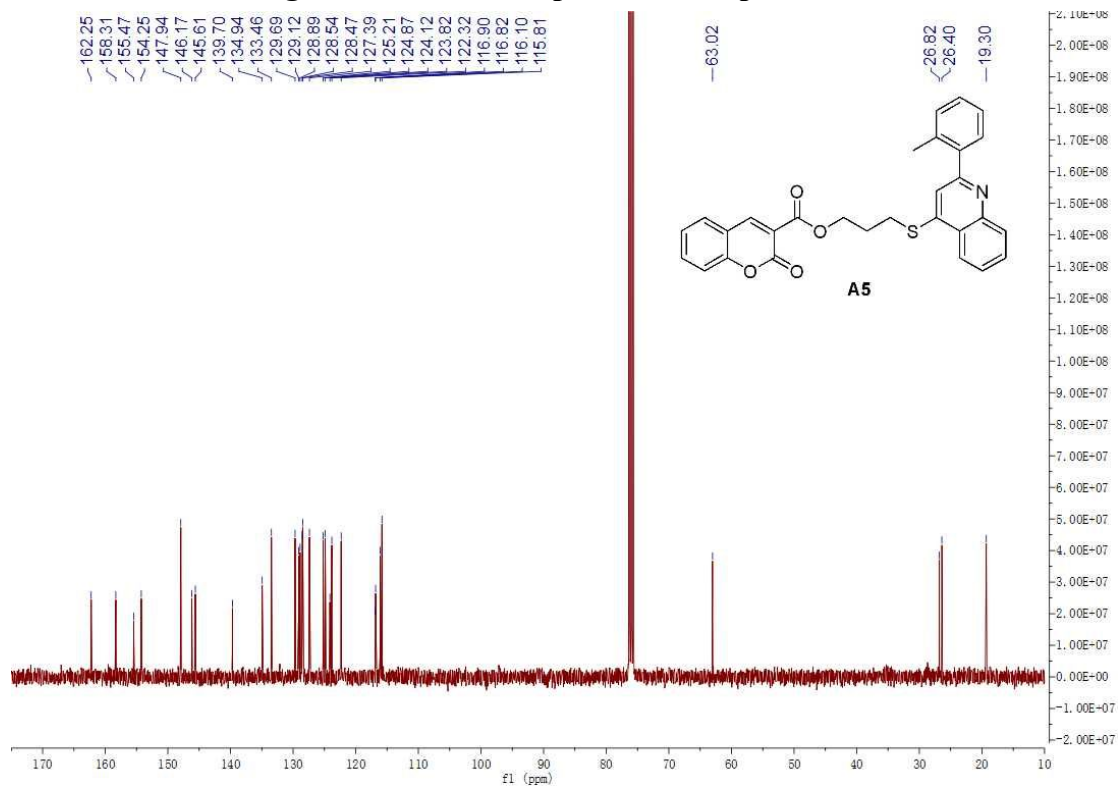


Figure S52 ¹³C NMR spectra of compound A5

Item name: ZYQ-A5
Item description:

Channel name: 1: Average Time 0.1334 min : TOF MS (50-1500) ESI+ : Centroided : Combined

7.97e6

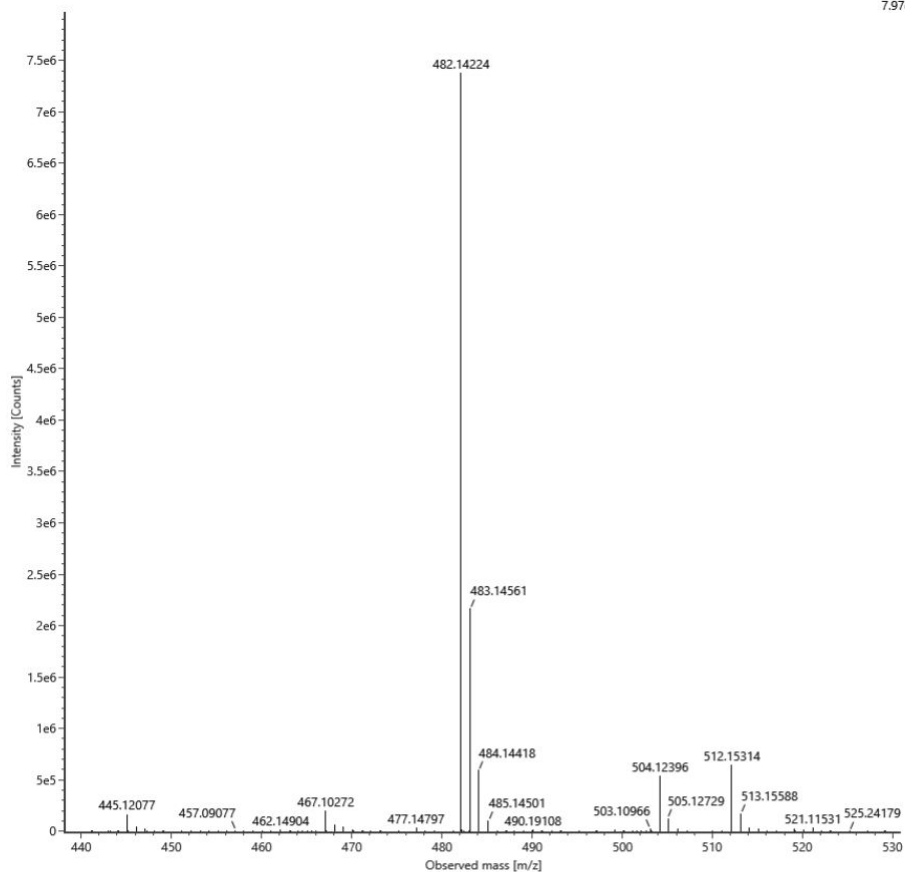


Figure S53 HRMS spectra of compound A5

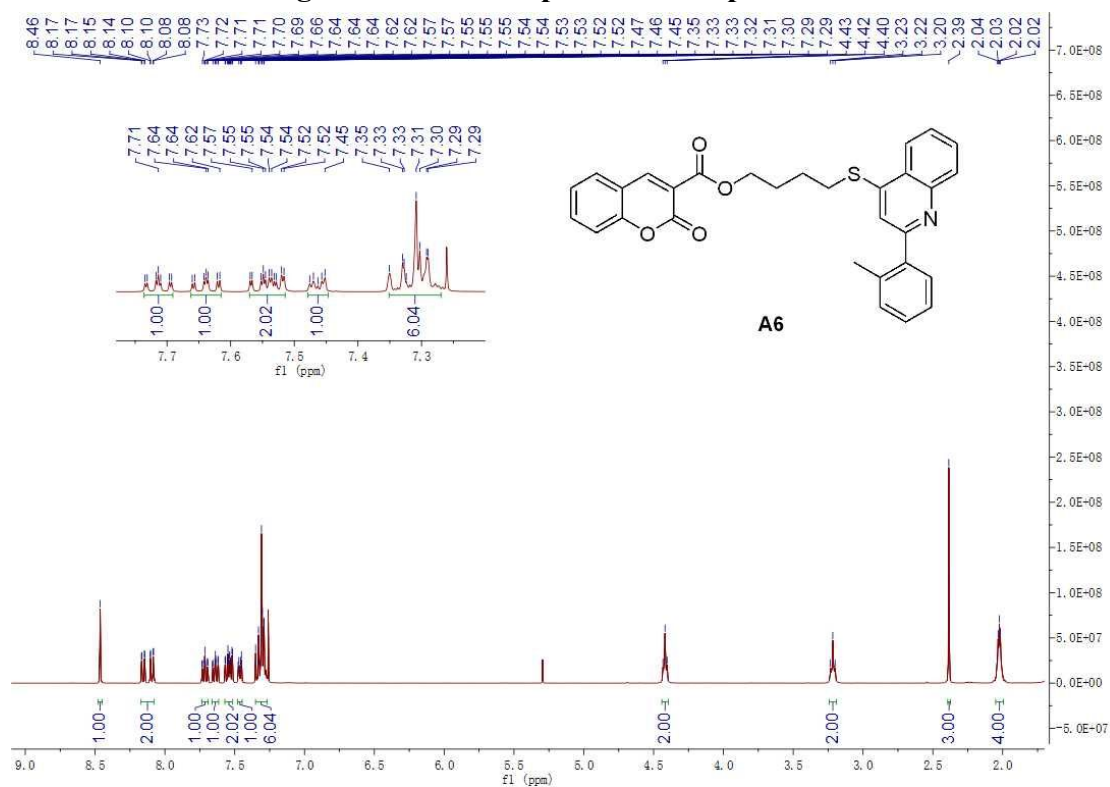
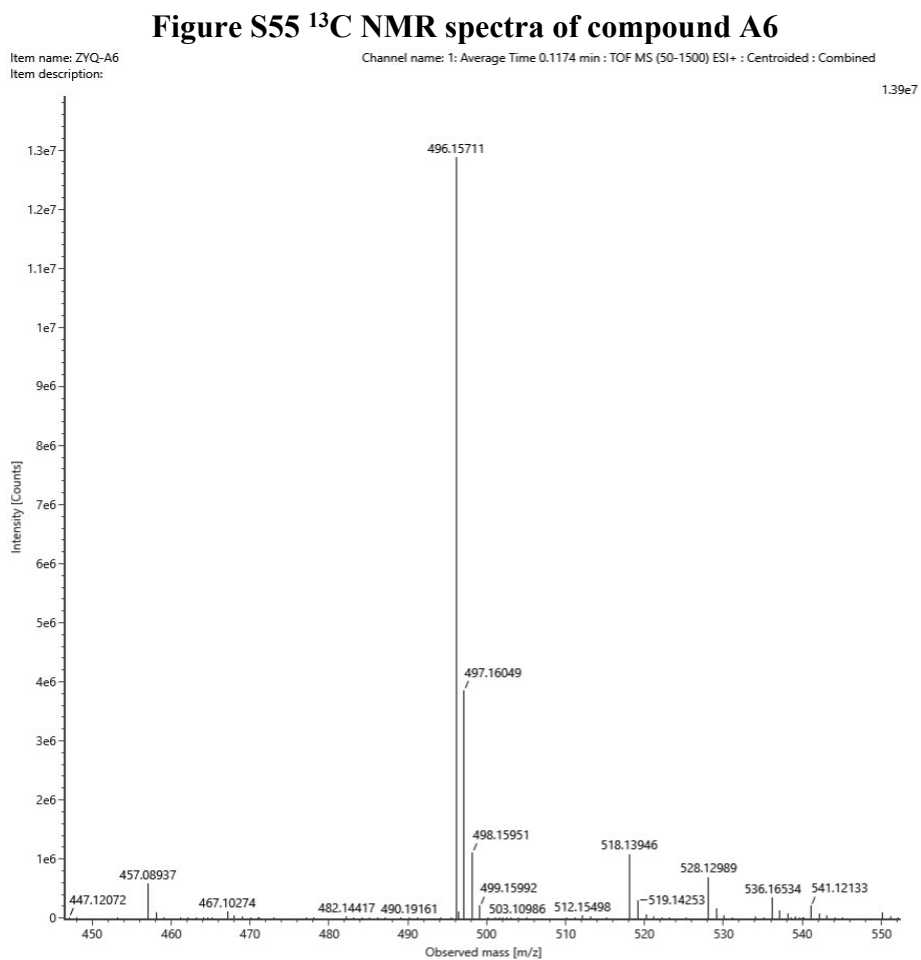
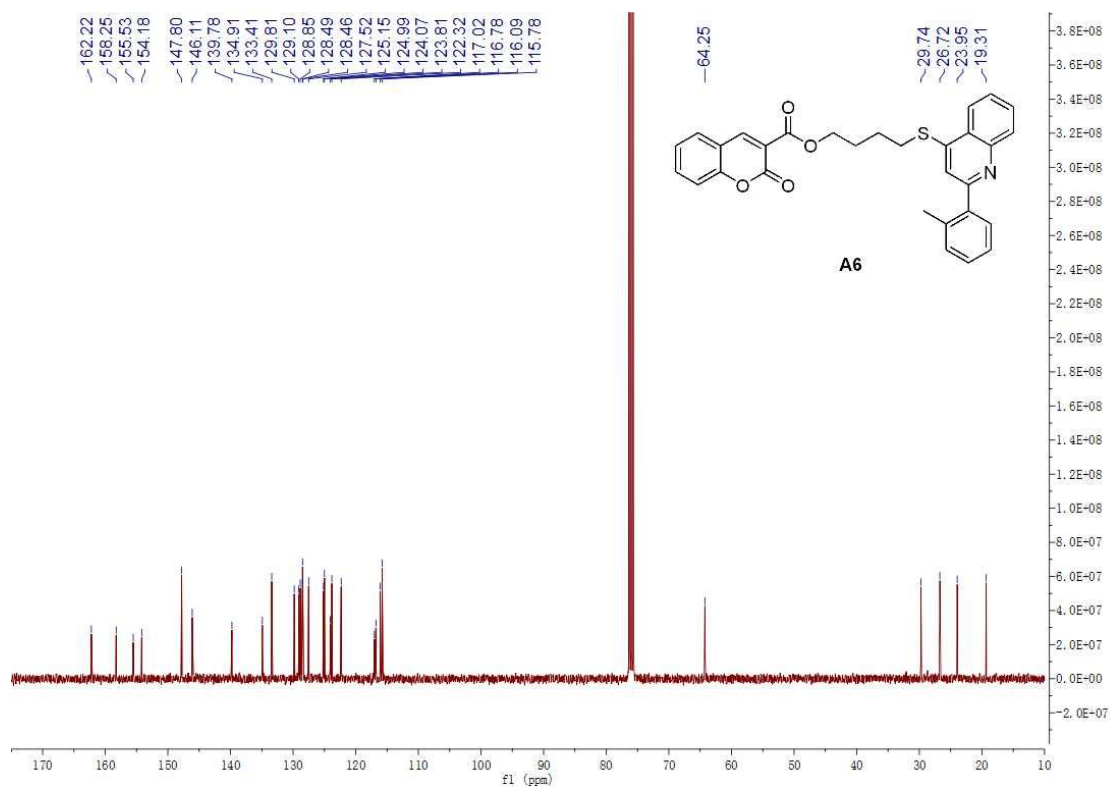


Figure S54 ¹H NMR spectra of compound A6



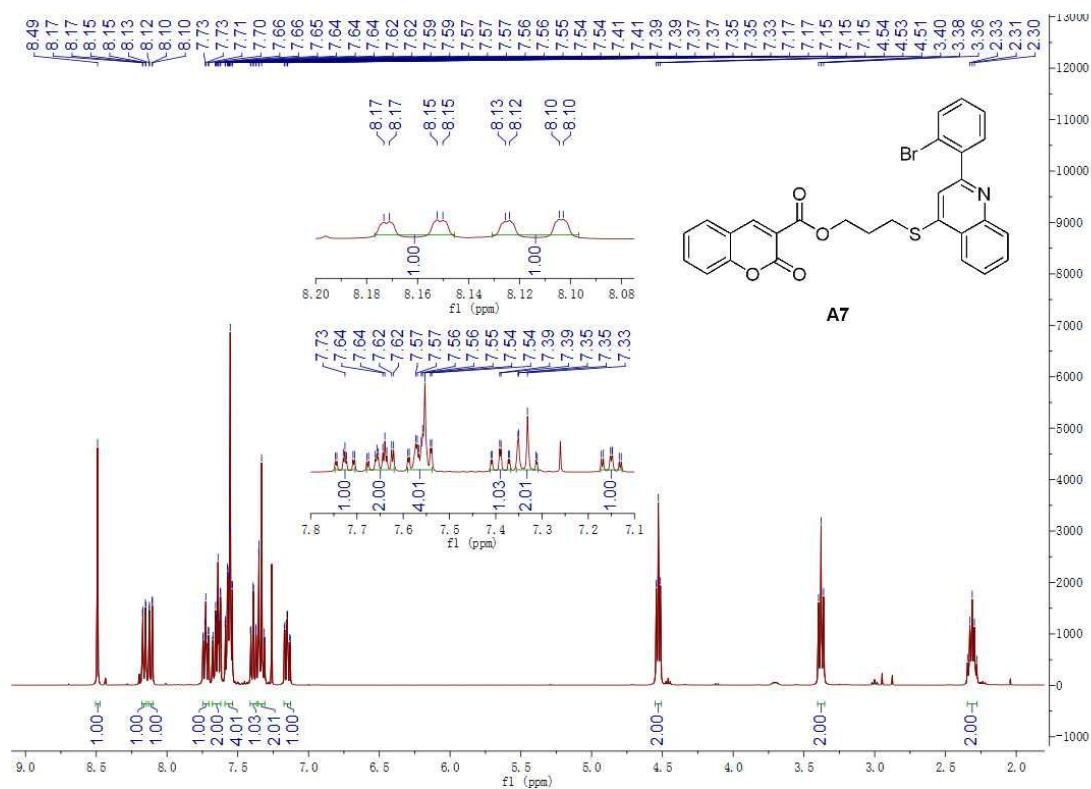


Figure S57 ^1H NMR spectra of compound A7

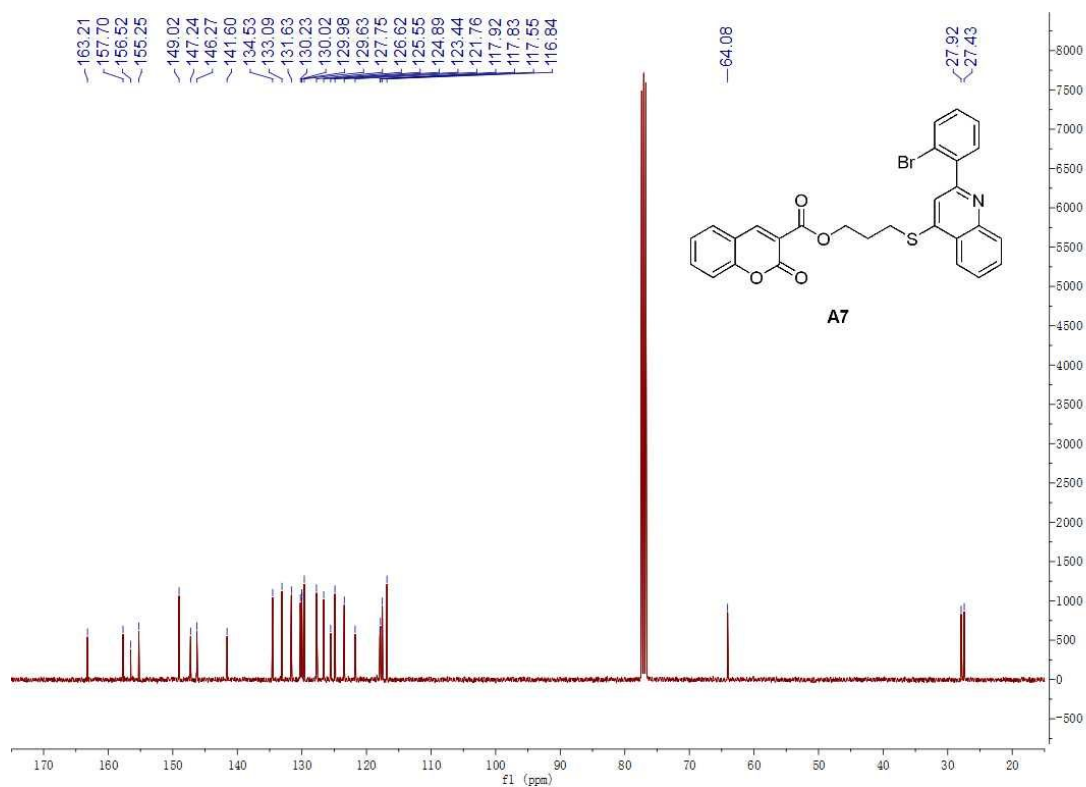


Figure S58 ^{13}C NMR spectra of compound A7

Item name: ZYQ-A7
Item description:

Channel name: 1: Average Time 0.1174 min : TOF MS (50-1500) ESI+ : Centroided : Combined

7.55e6

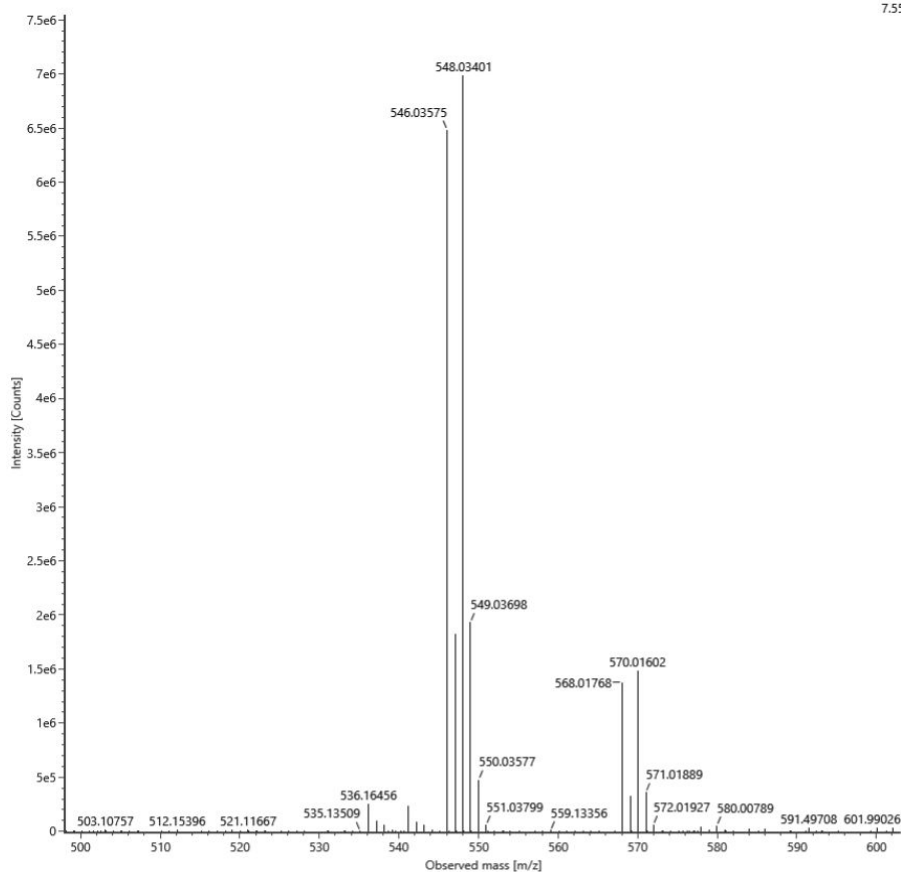


Figure S59 HRMS spectra of compound A7

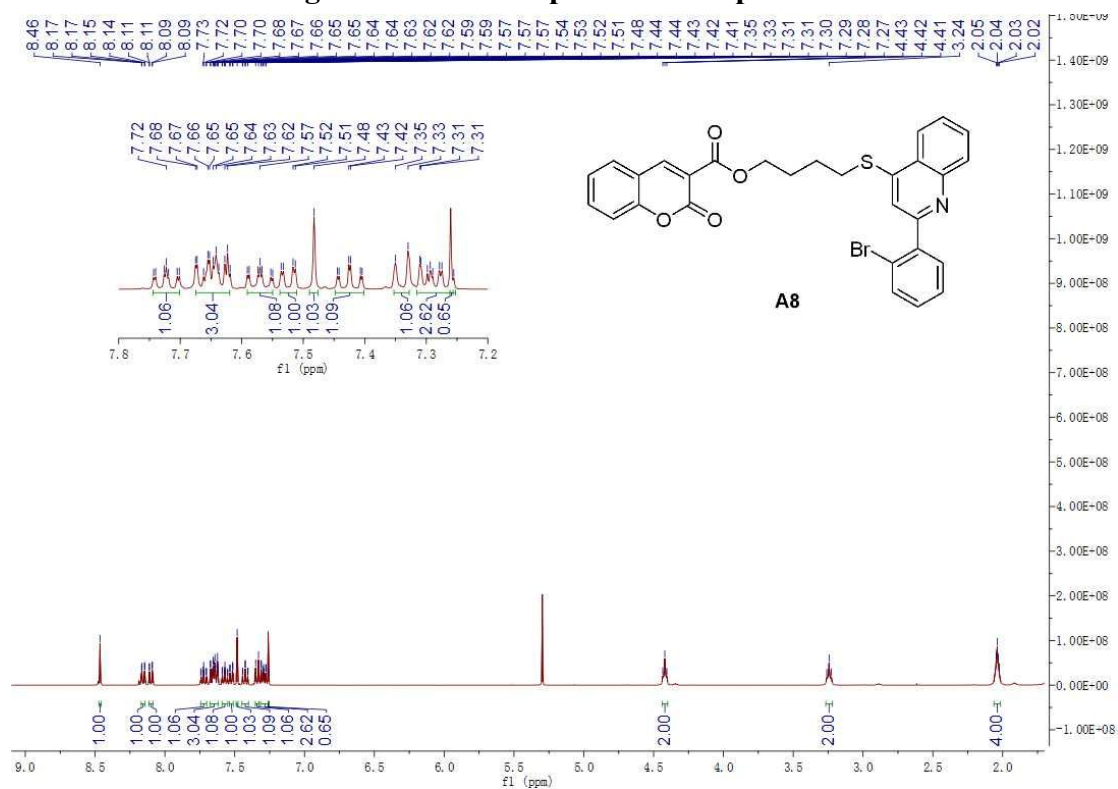
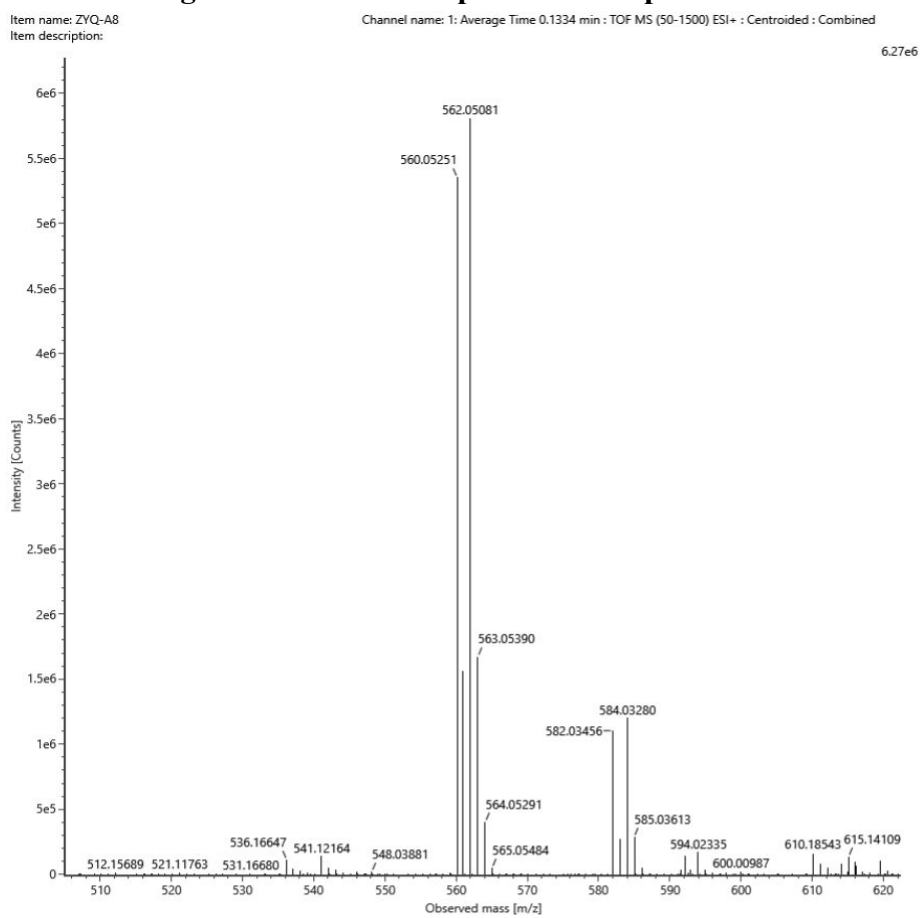
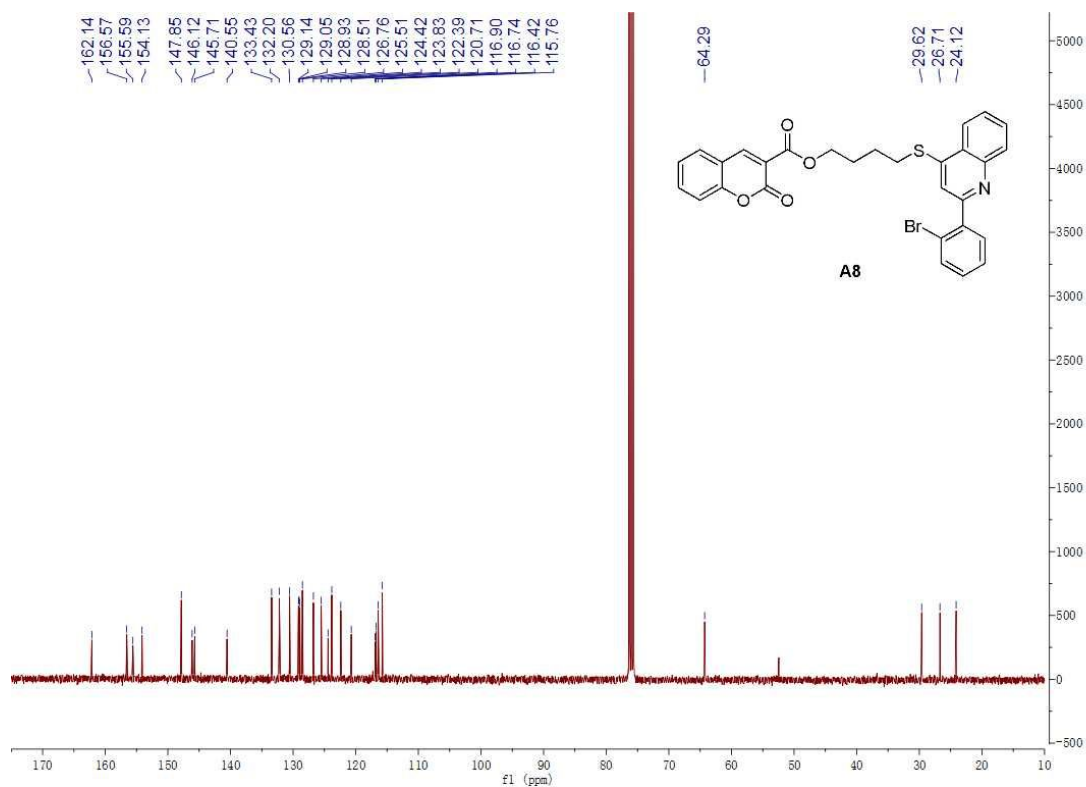
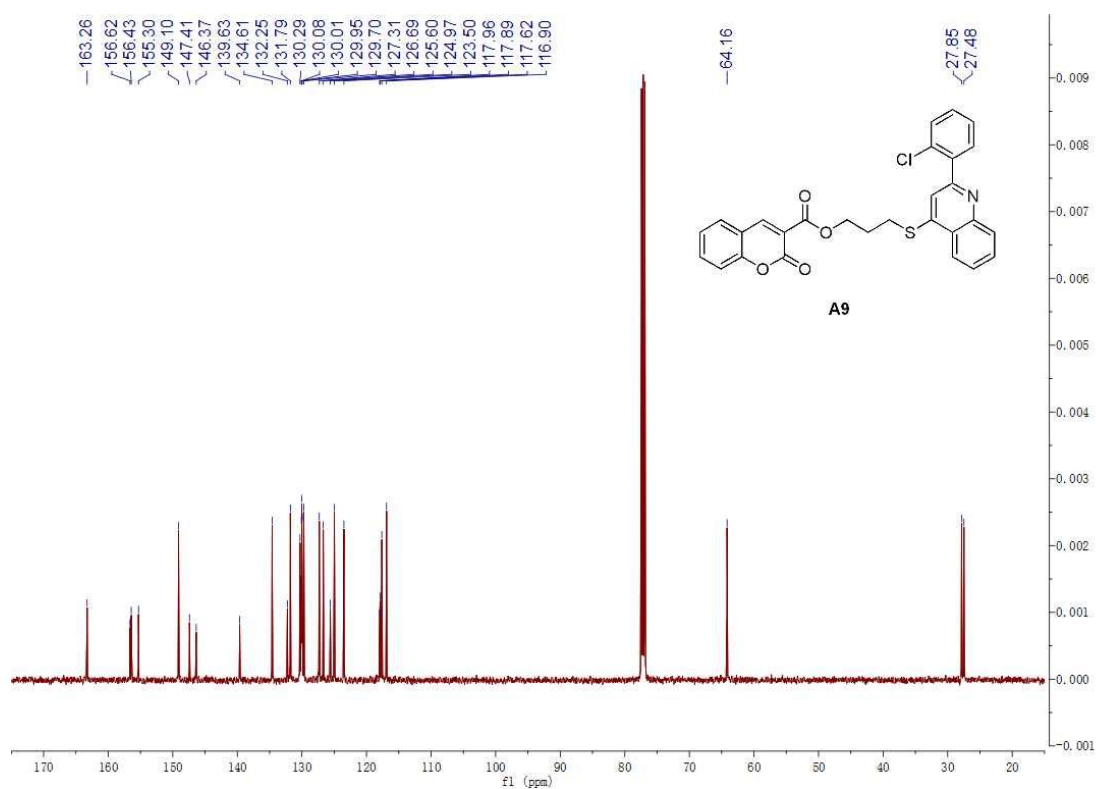
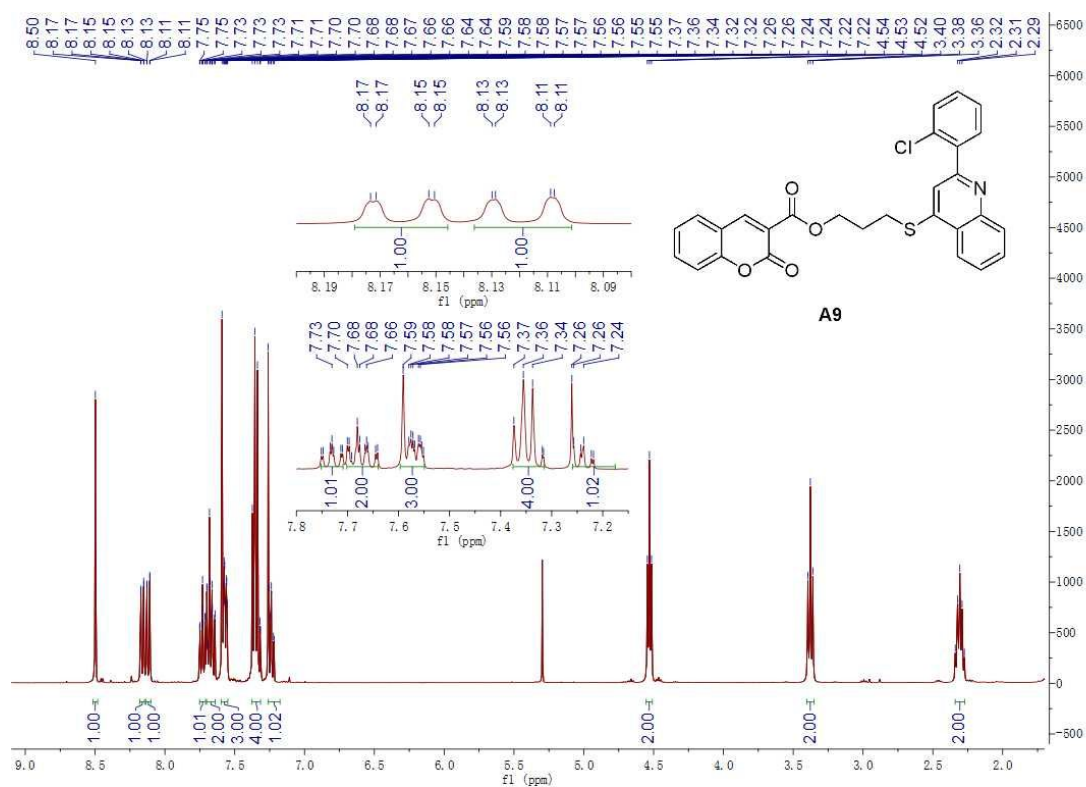


Figure S60 ¹H NMR spectra of compound A8





Item name: ZYQ-A9
Item description:

Channel name: 1: Average Time 0.1217 min : TOF MS (50-1500) ESI+ : Centroided : Combined

1.44e7

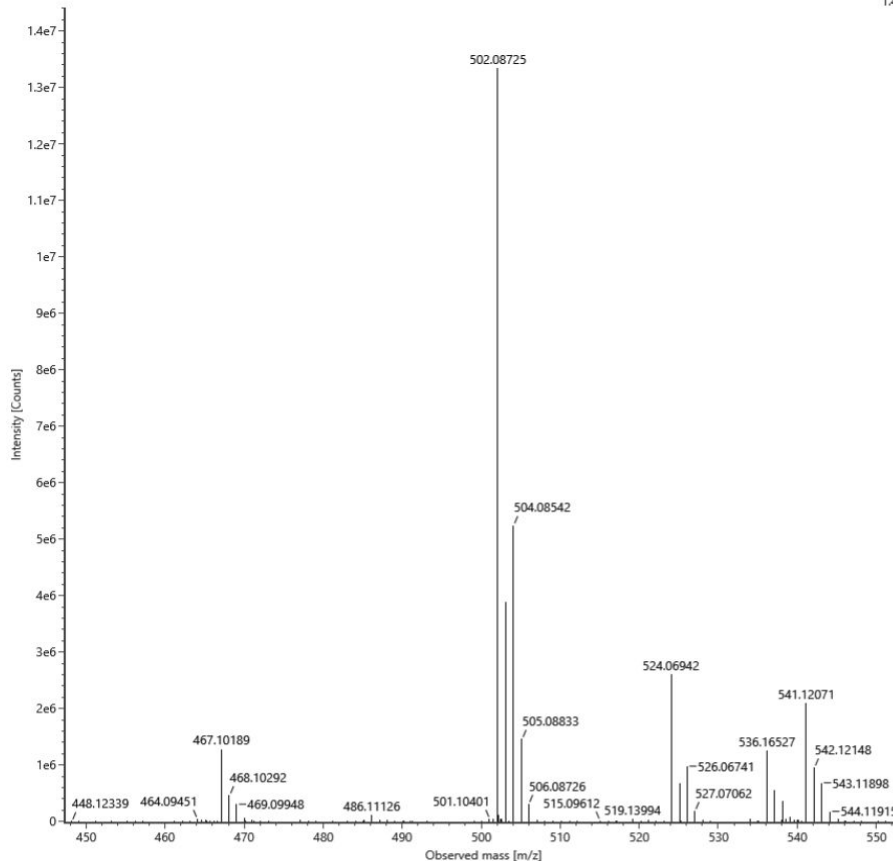


Figure S65 HRMS spectra of compound A9

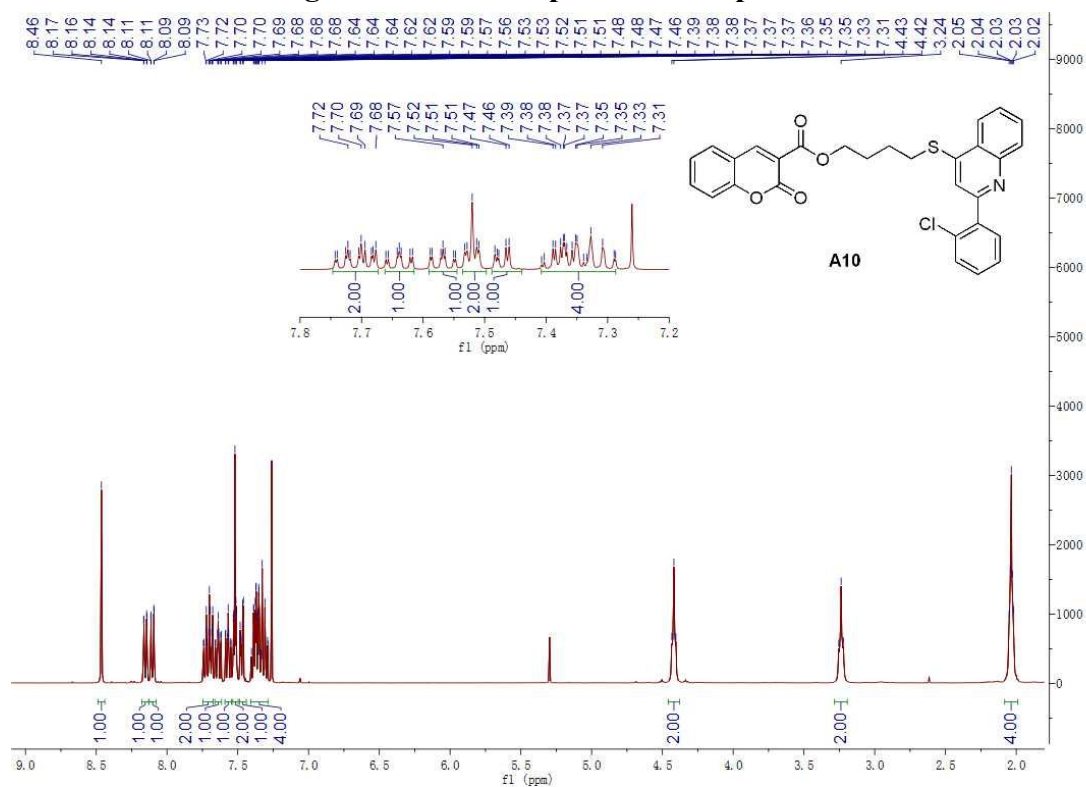


Figure S66 ¹H NMR spectra of compound A10

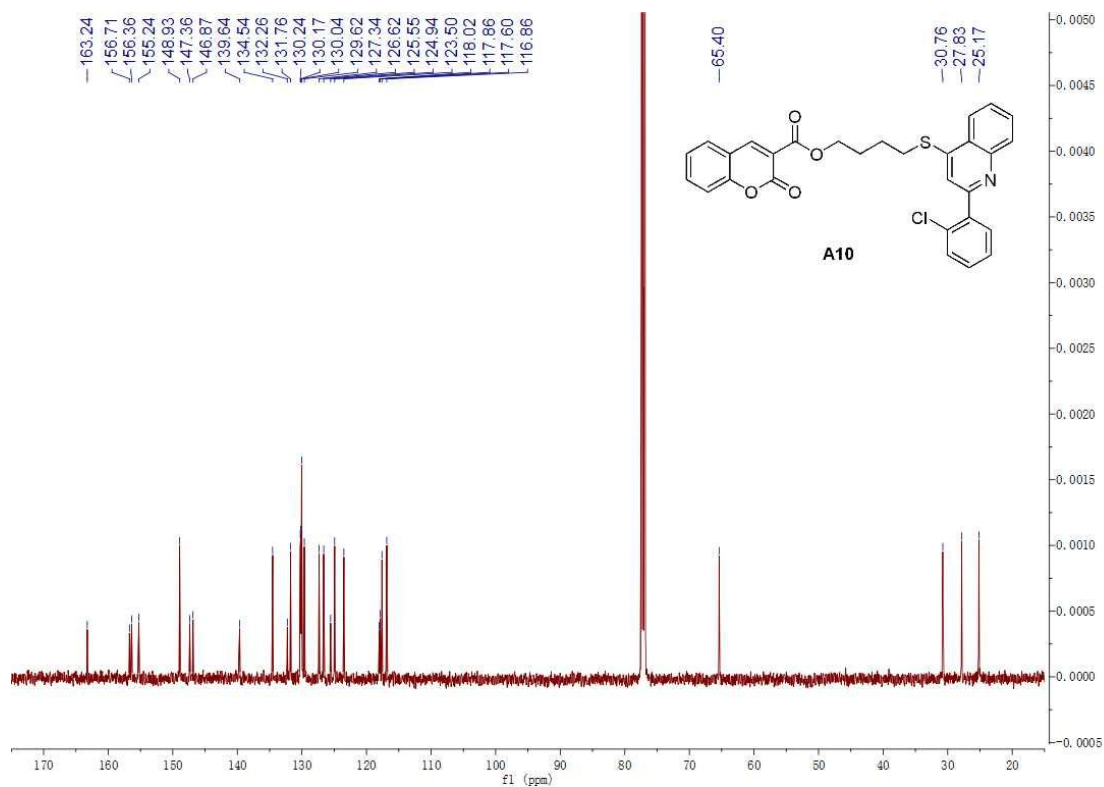


Figure S67 ¹³C NMR spectra of compound A10

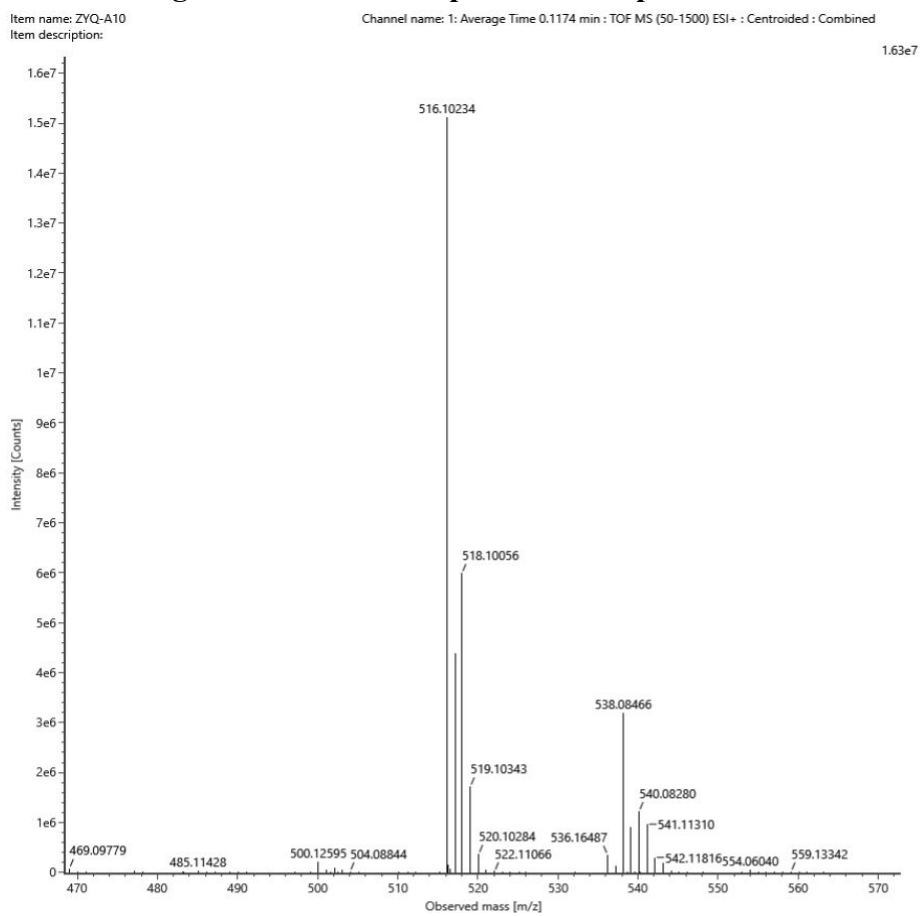


Figure S68 HRMS spectra of compound A10

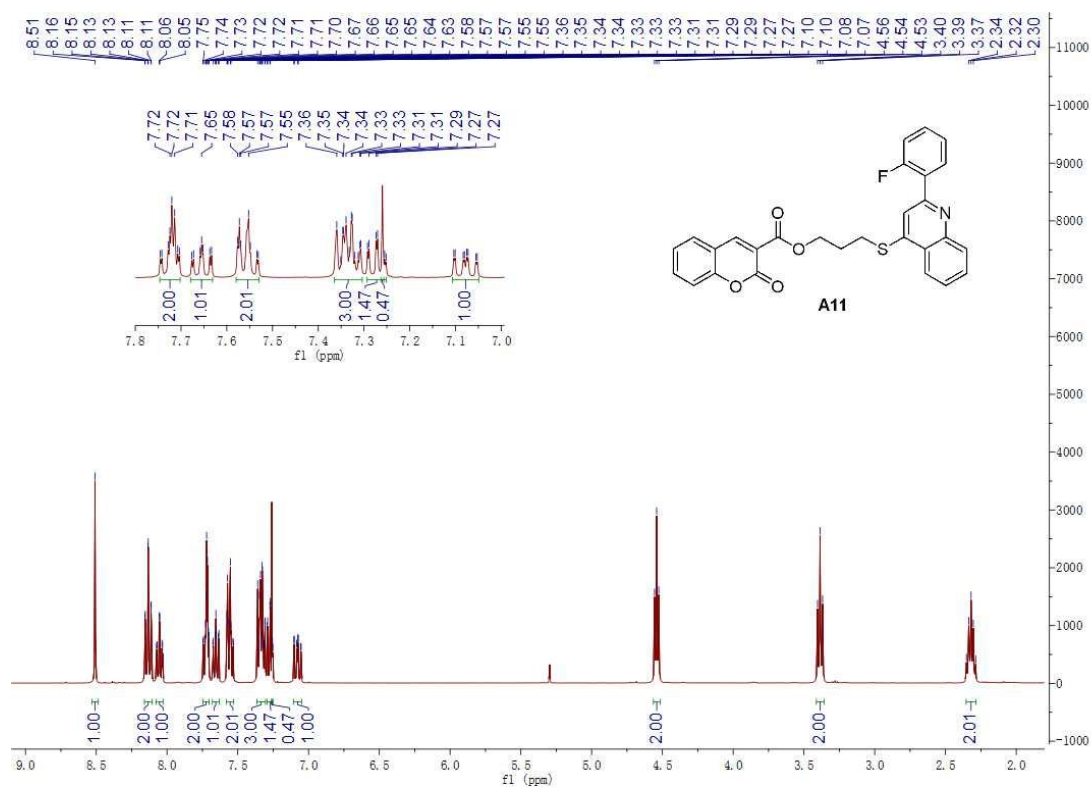


Figure S69 ^1H NMR spectra of compound A11

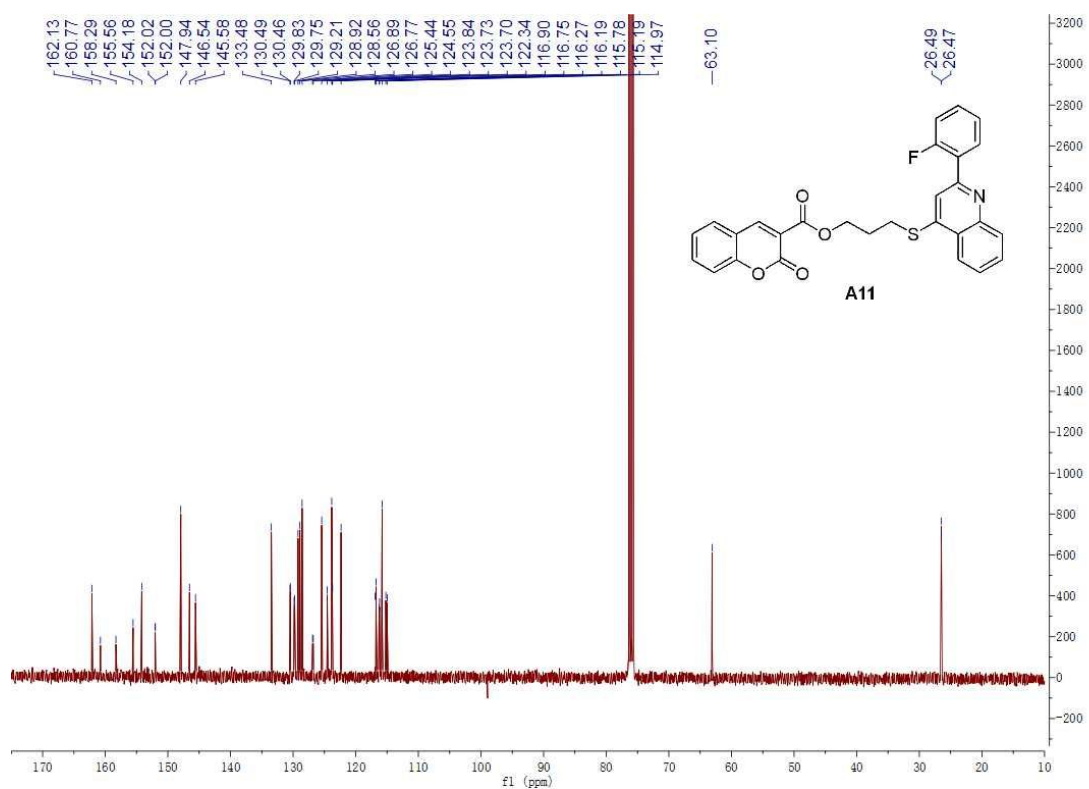


Figure S70 ^{13}C NMR spectra of compound A11

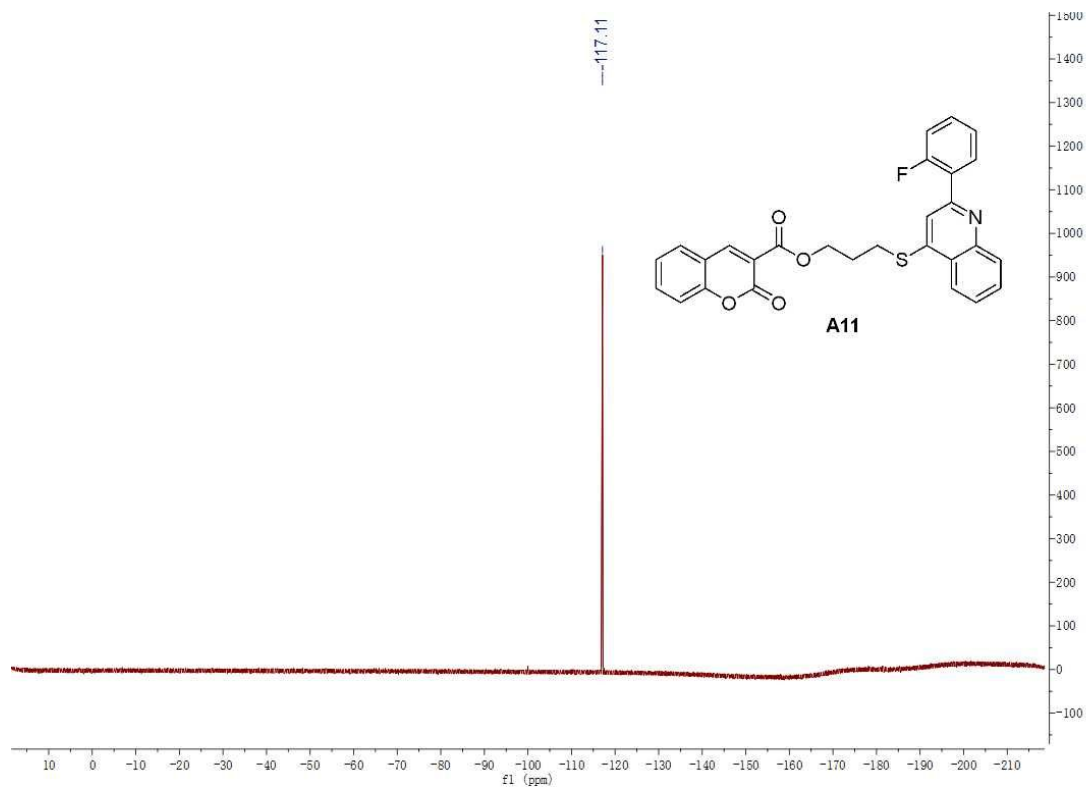


Figure S71 ¹⁹F NMR spectra of compound A11

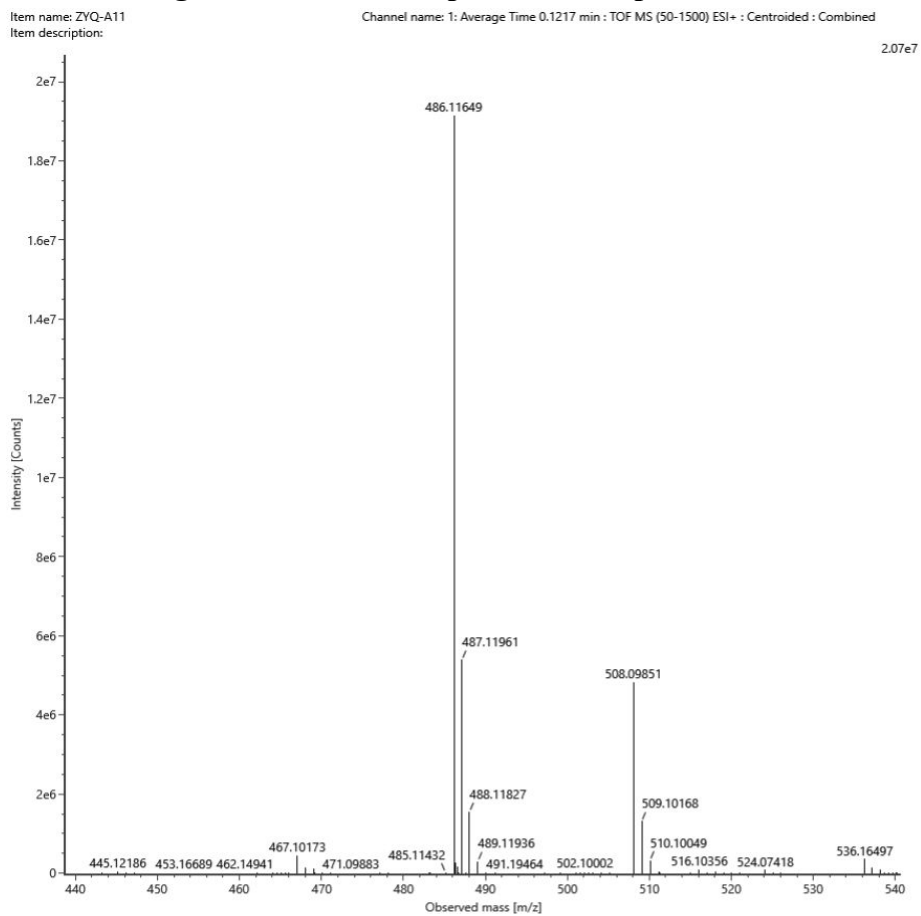
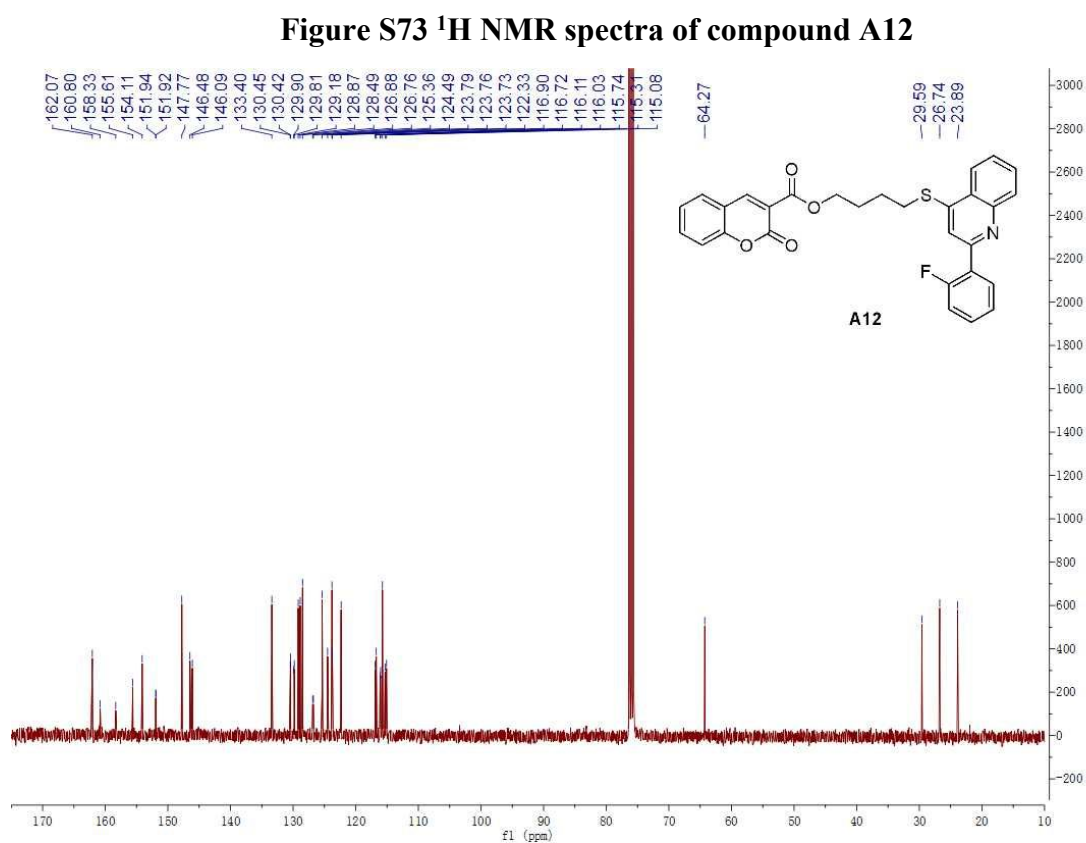
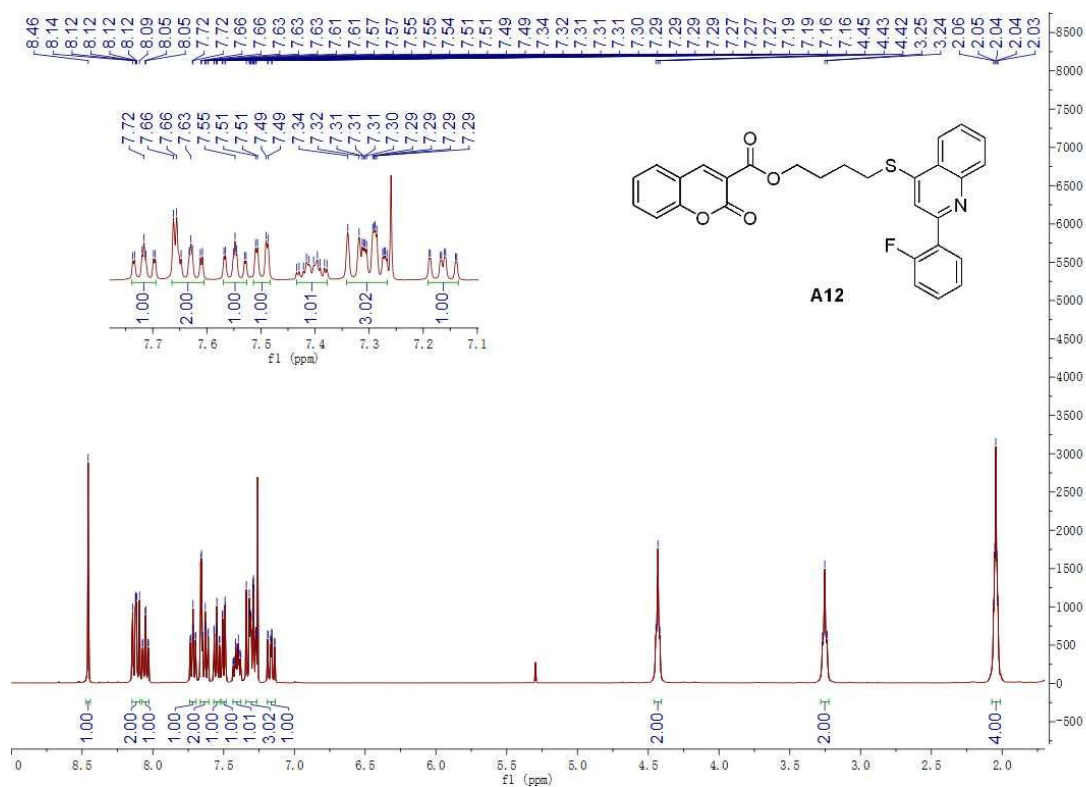


Figure S72 HRMS spectra of compound A11



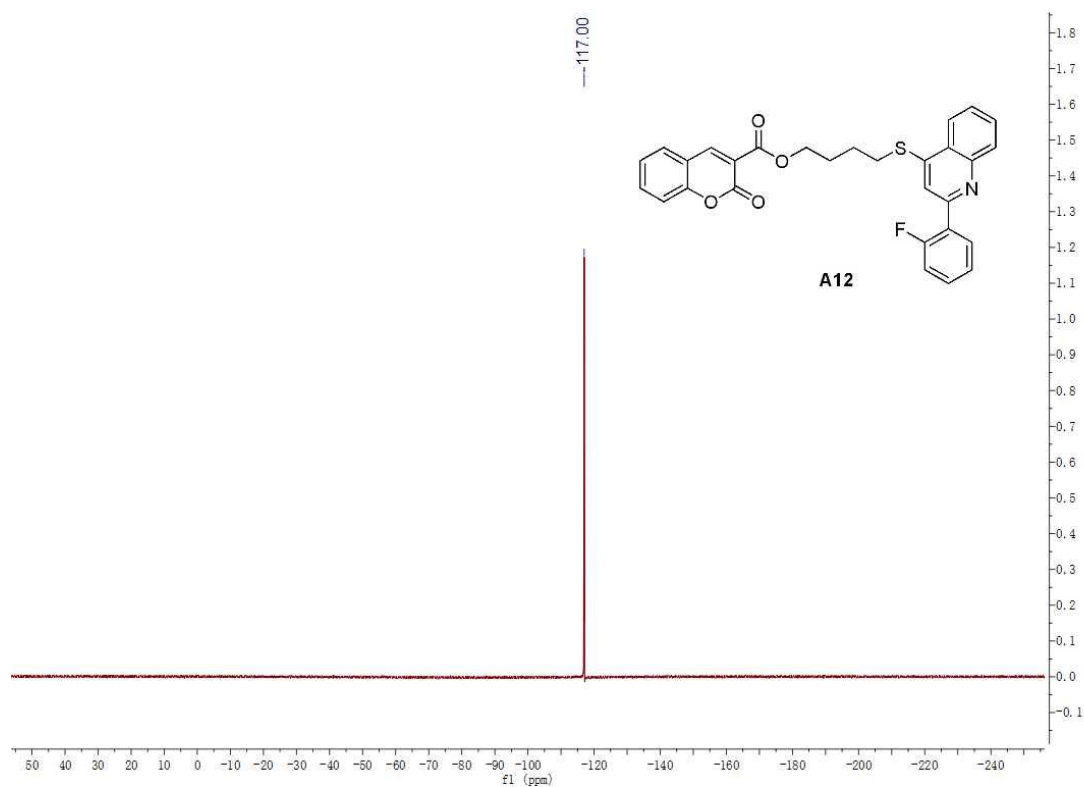


Figure S75 ¹⁹F NMR spectra of compound A12

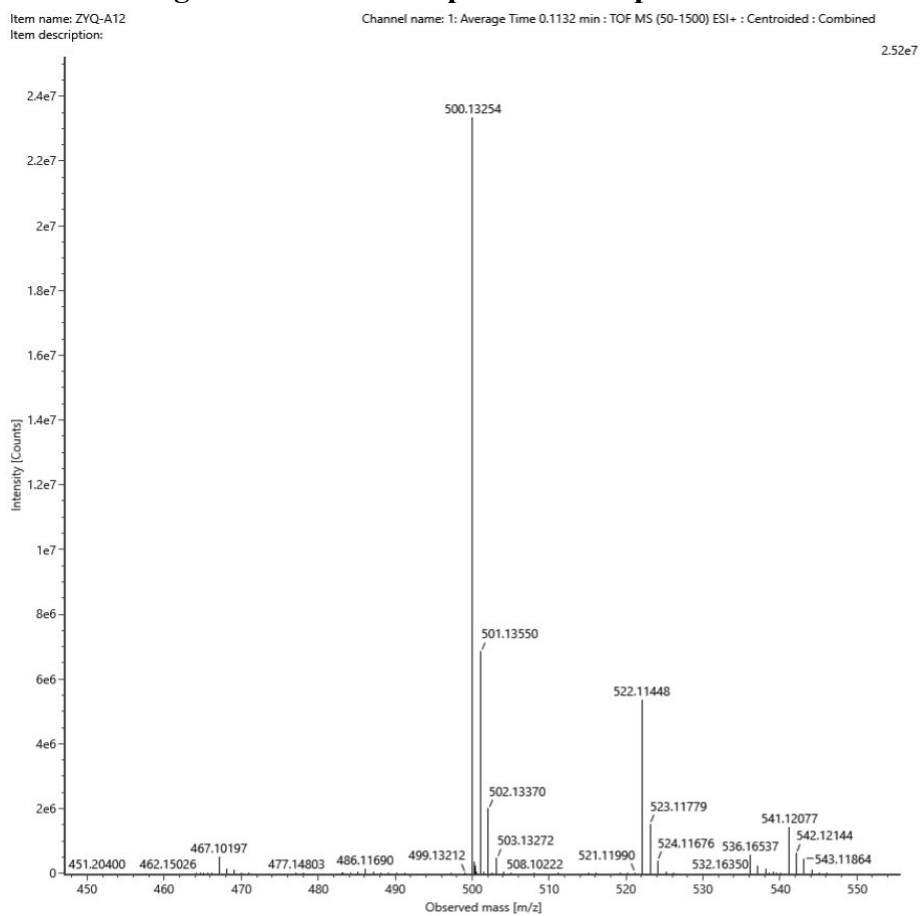


Figure S76 HRMS spectra of compound A12

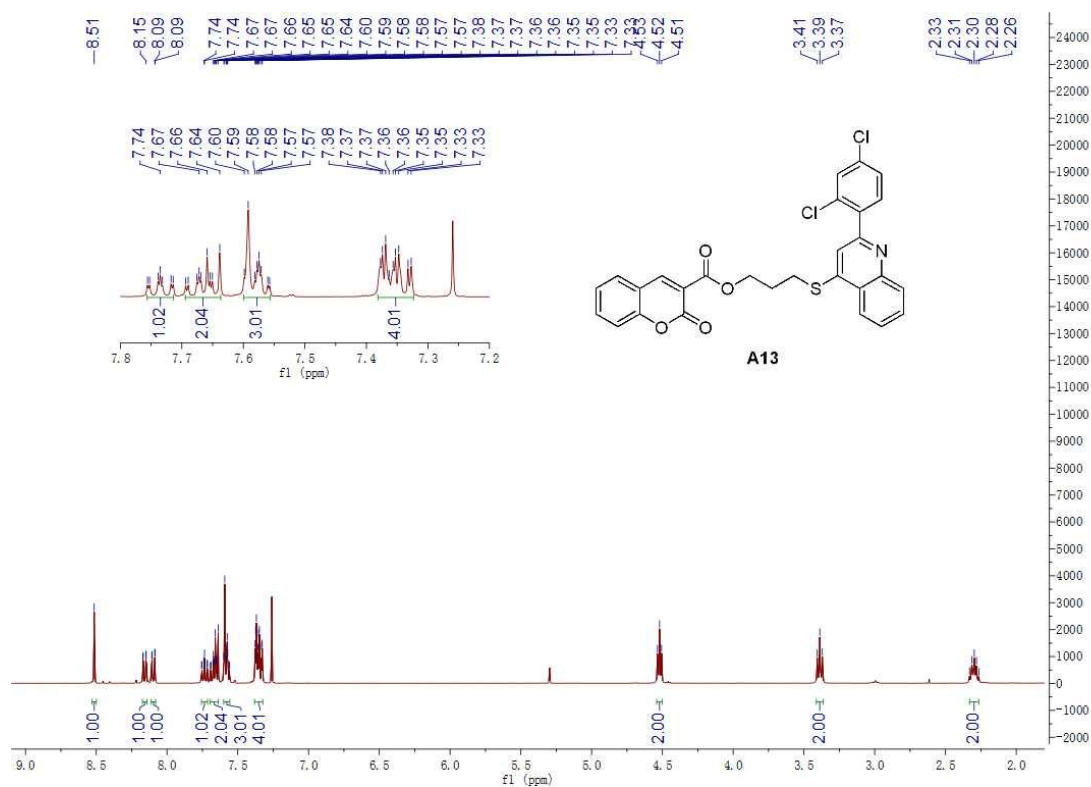


Figure S77 ¹H NMR spectra of compound A13

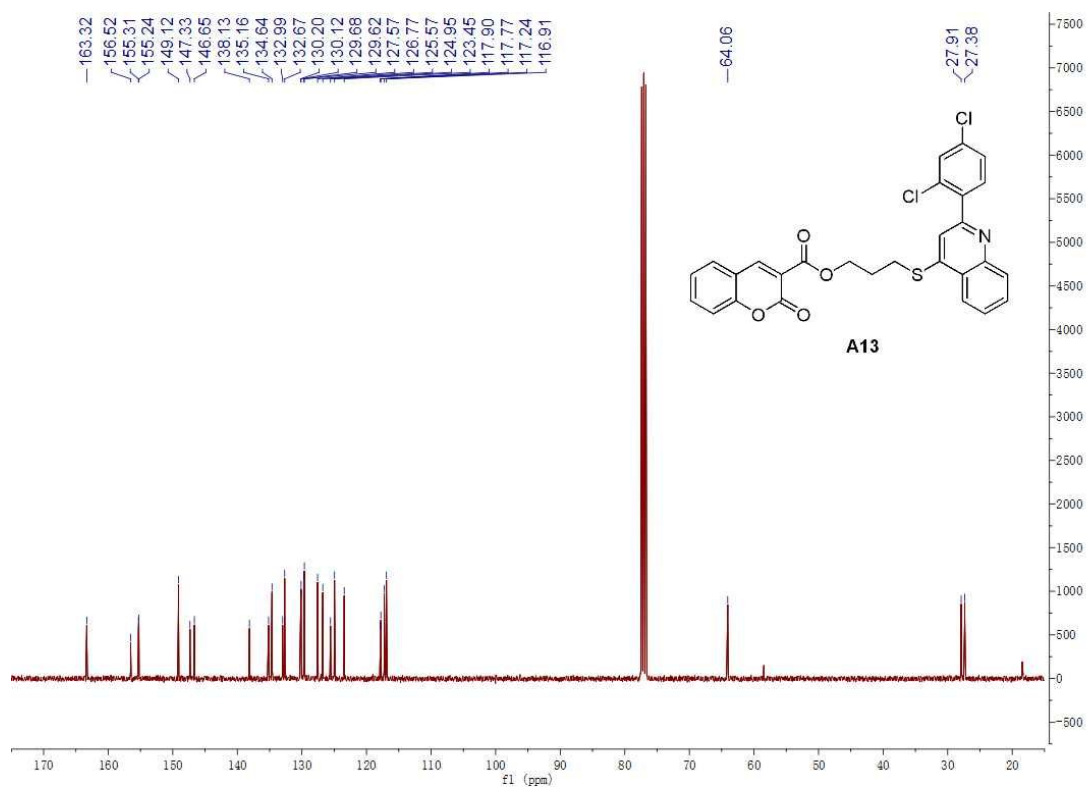


Figure S78 ¹³C NMR spectra of compound A13

Item name: ZYQ-A39
Item description:

Channel name: 1: Average Time 0.1174 min : TOF MS (50-1500) ESI+ : Centroided : Combined

1.67e7

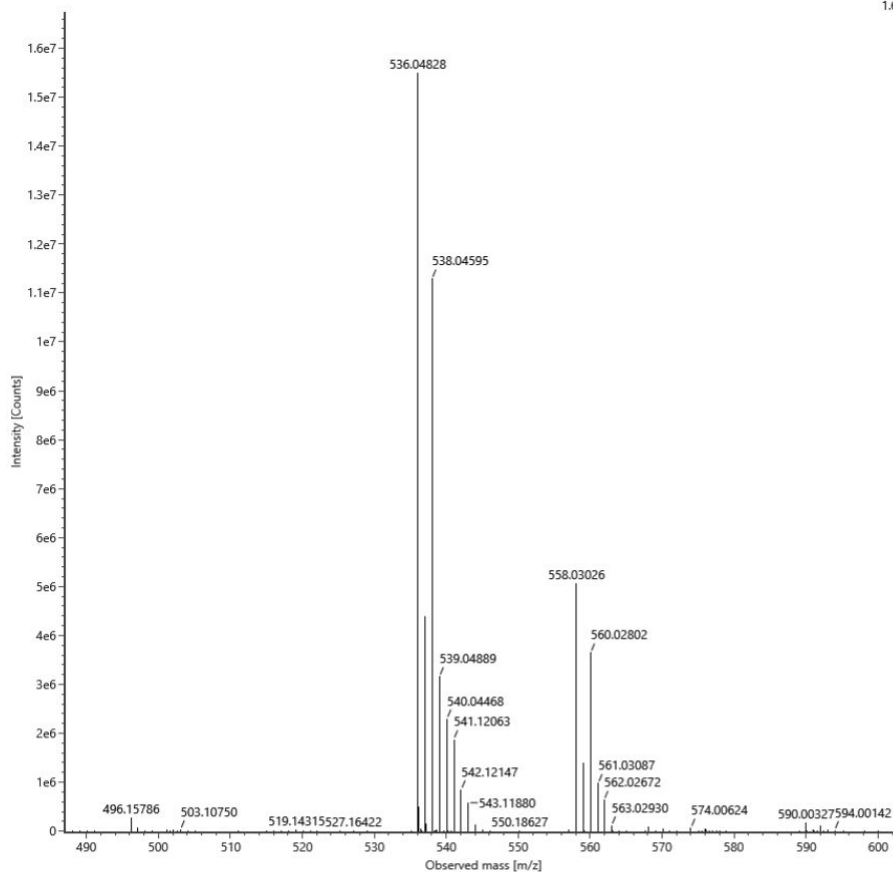


Figure S79 HRMS spectra of compound A13

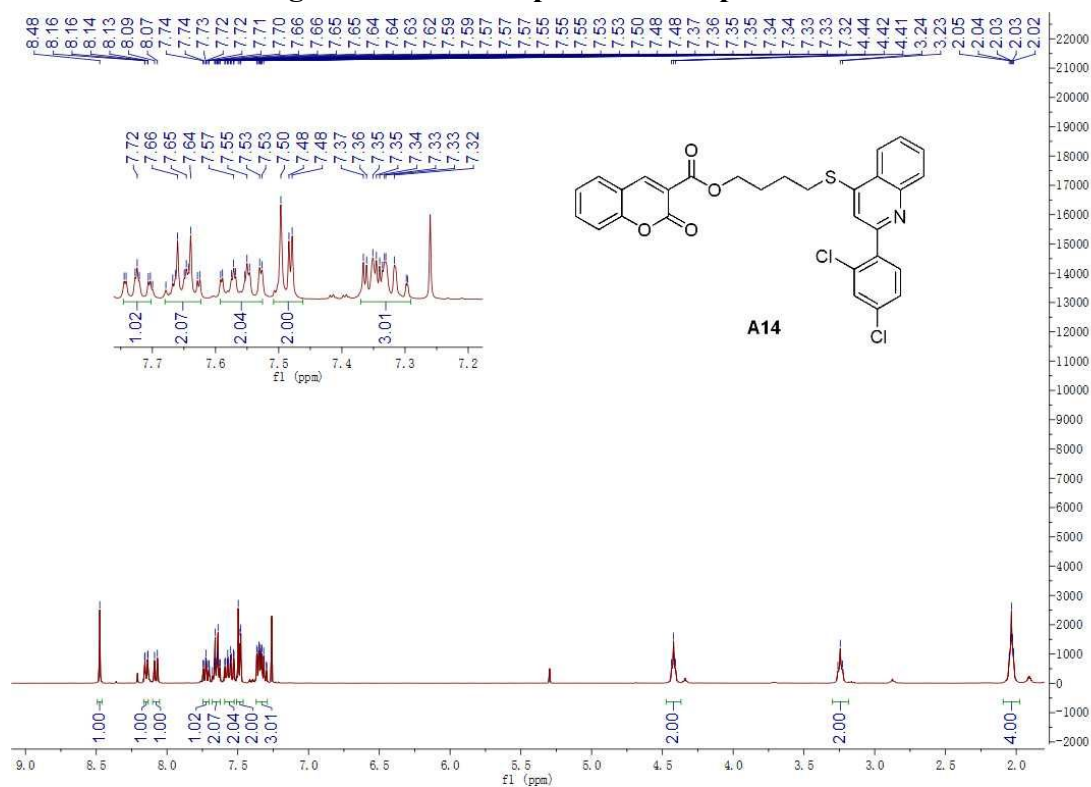
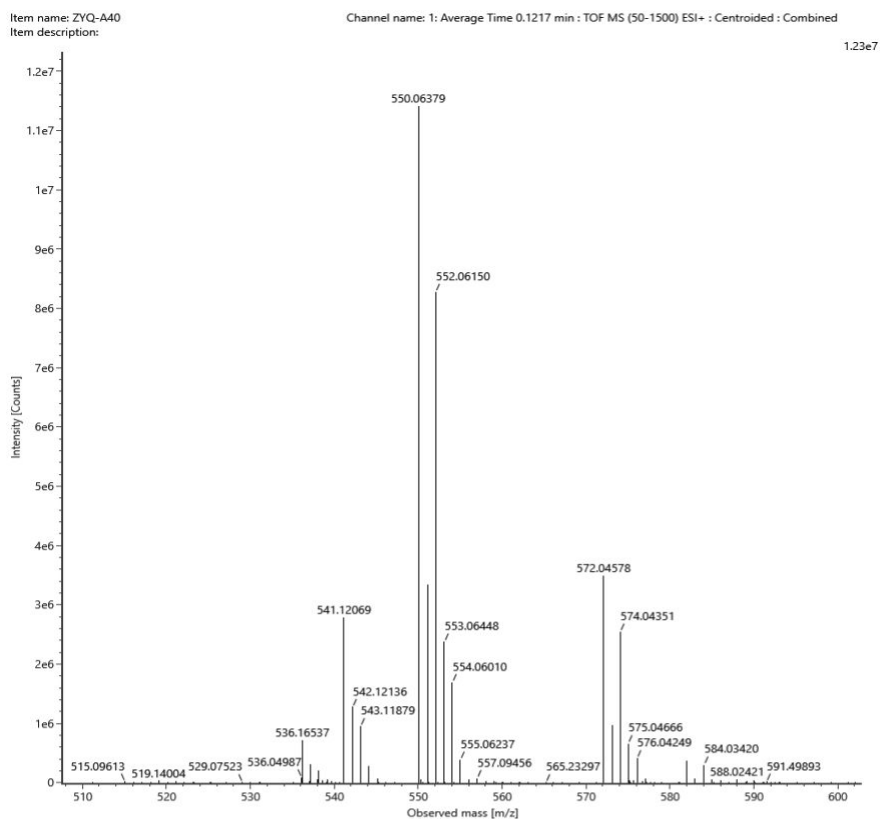
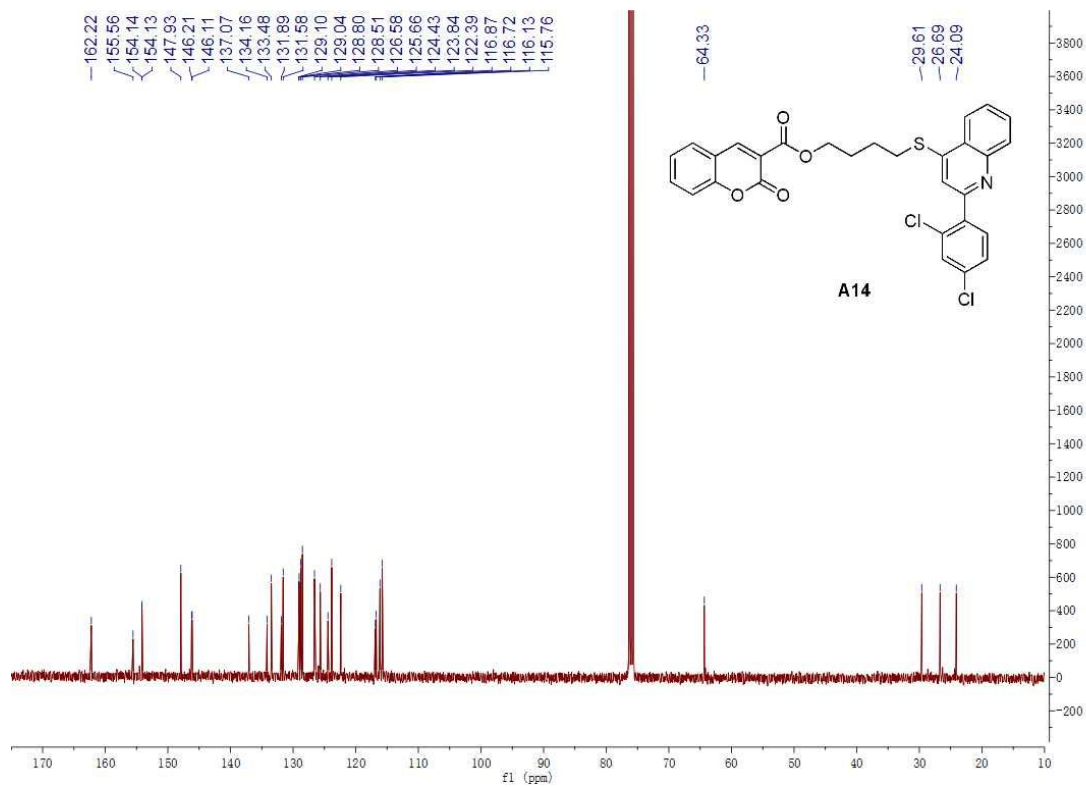
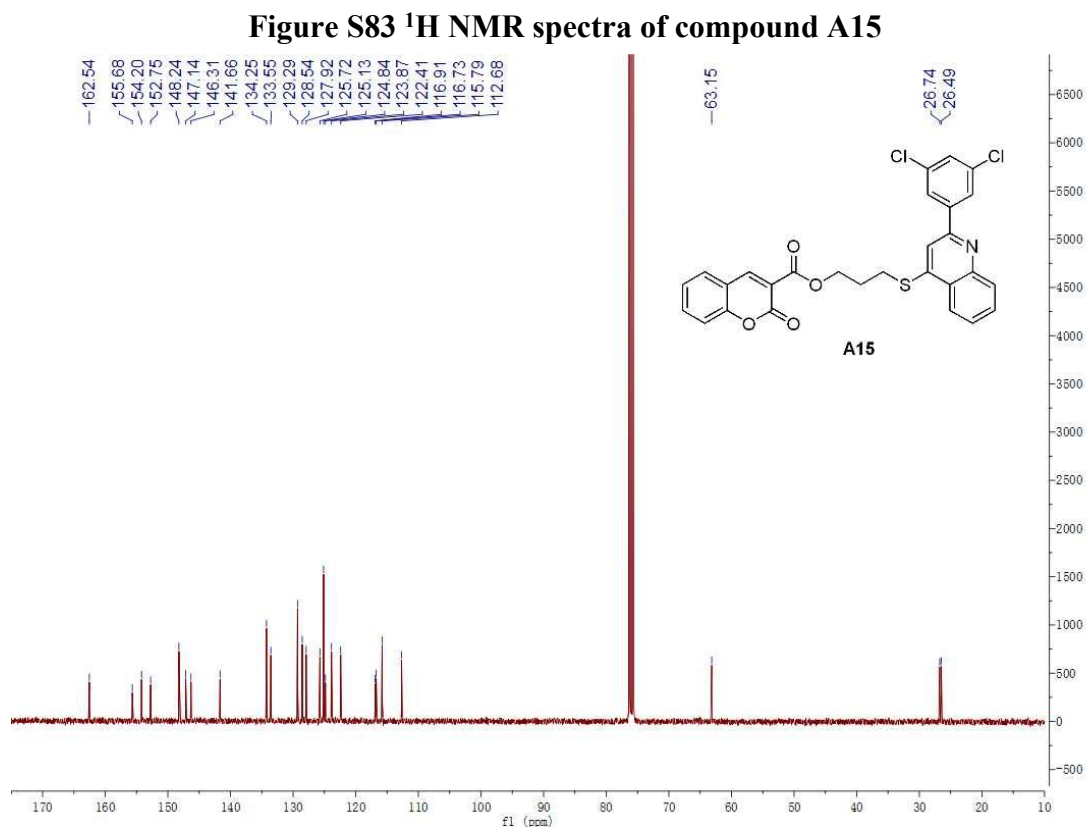
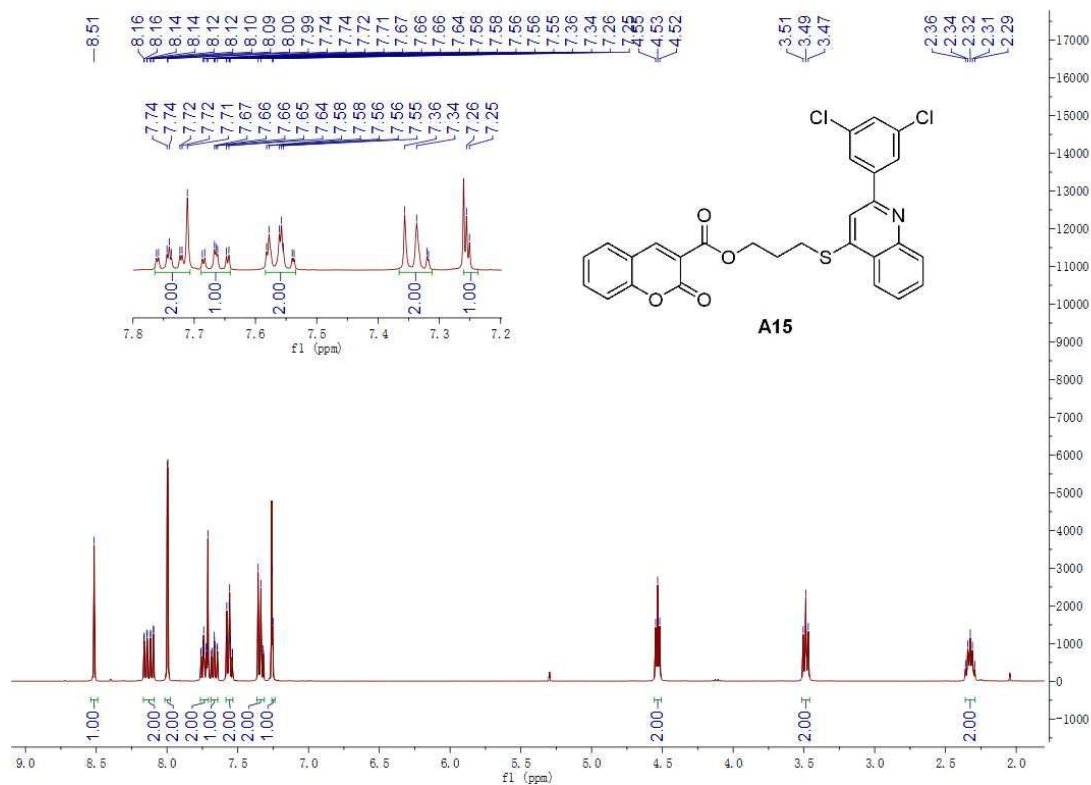


Figure S80 ¹H NMR spectra of compound A14





Item name: ZYQ-A41
Item description:

Channel name: 1: Average Time 0.1377 min : TOF MS (50-1500) ESI+ : Centroided : Combined

2.03e6

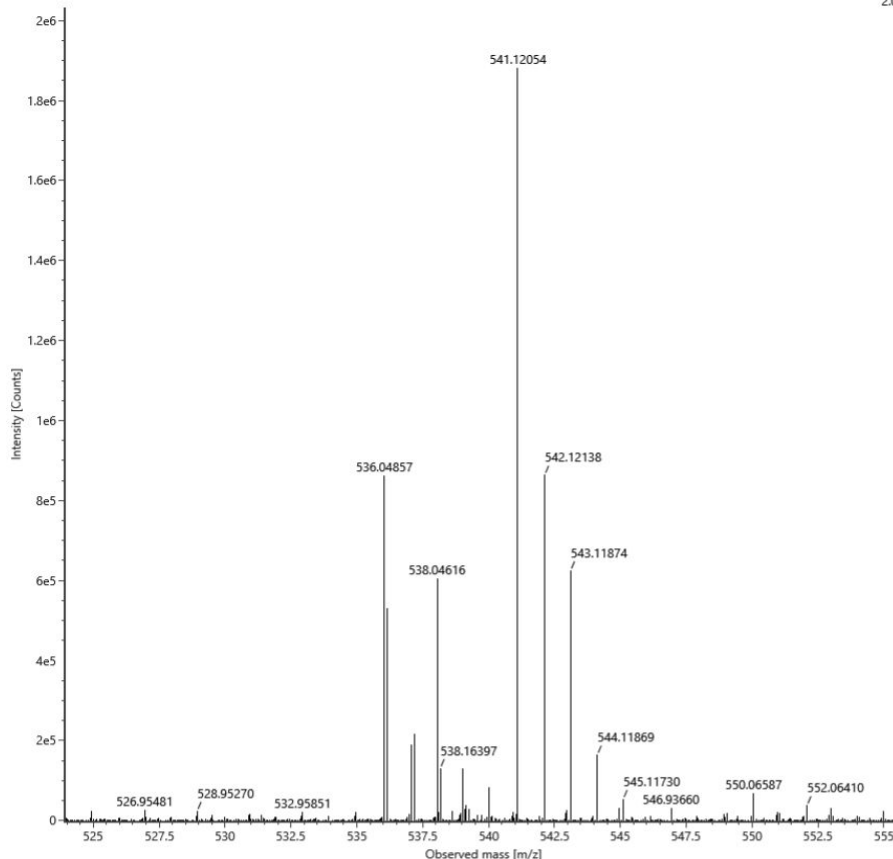


Figure S85 HRMS spectra of compound A15

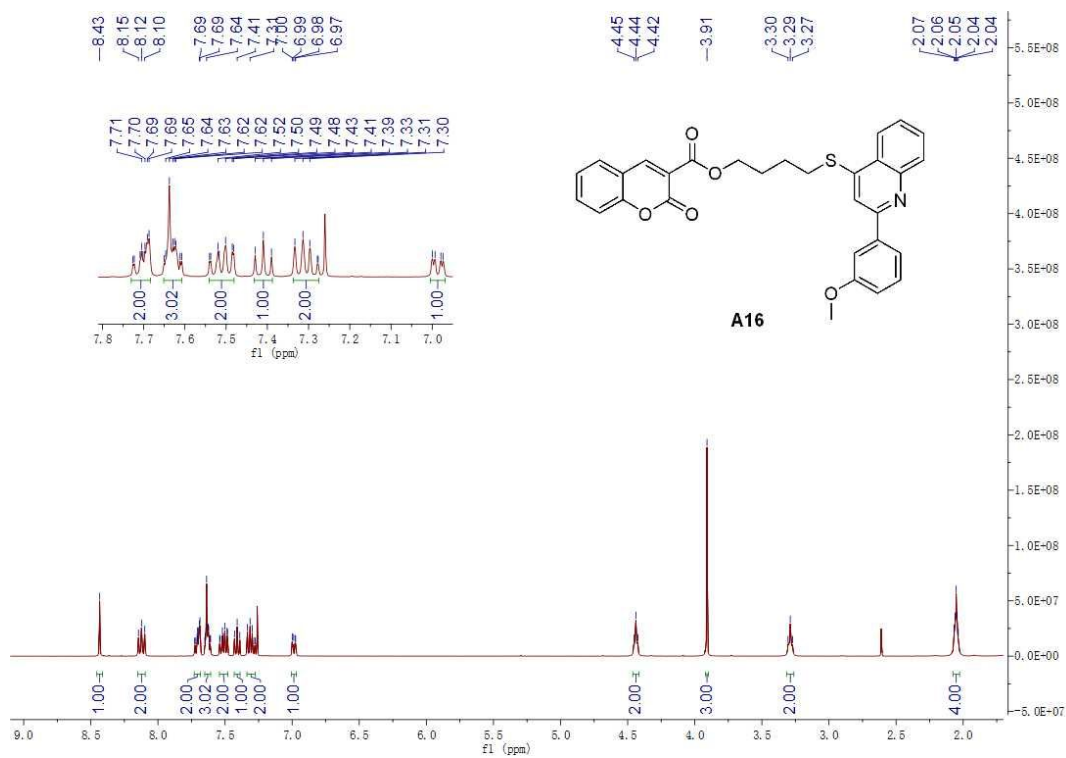


Figure S86 ¹H NMR spectra of compound A16

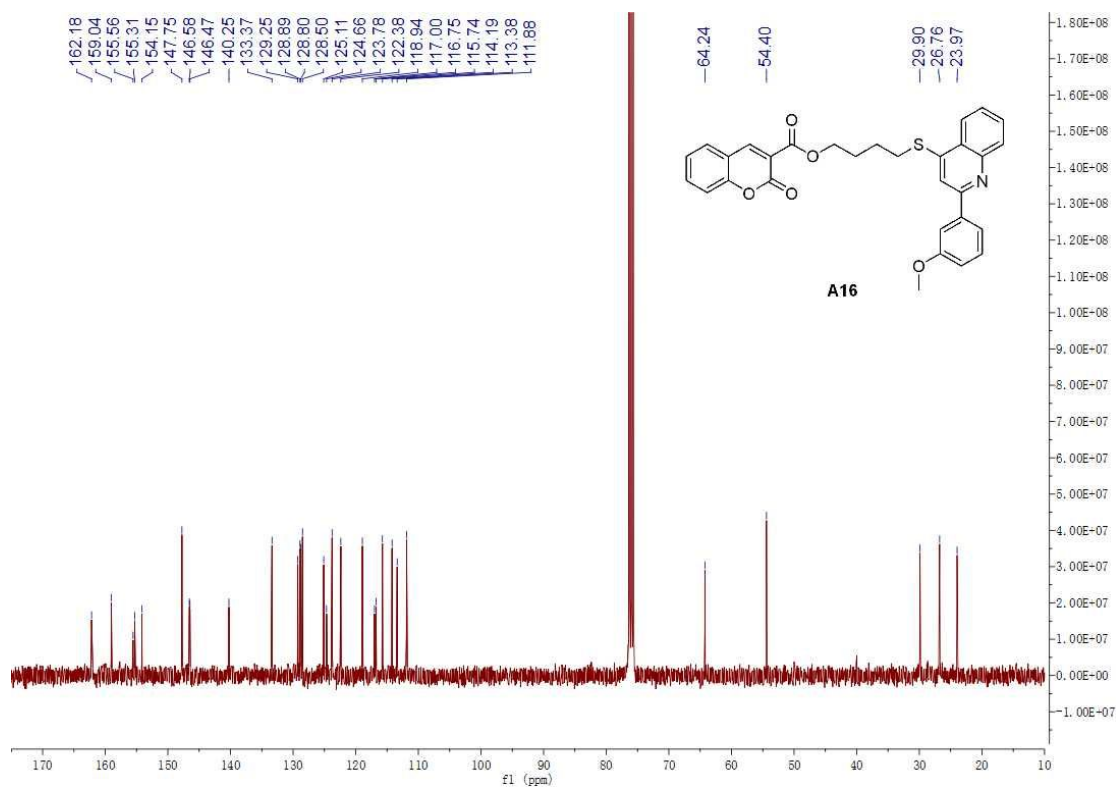


Figure S87 ¹³C NMR spectra of compound A16

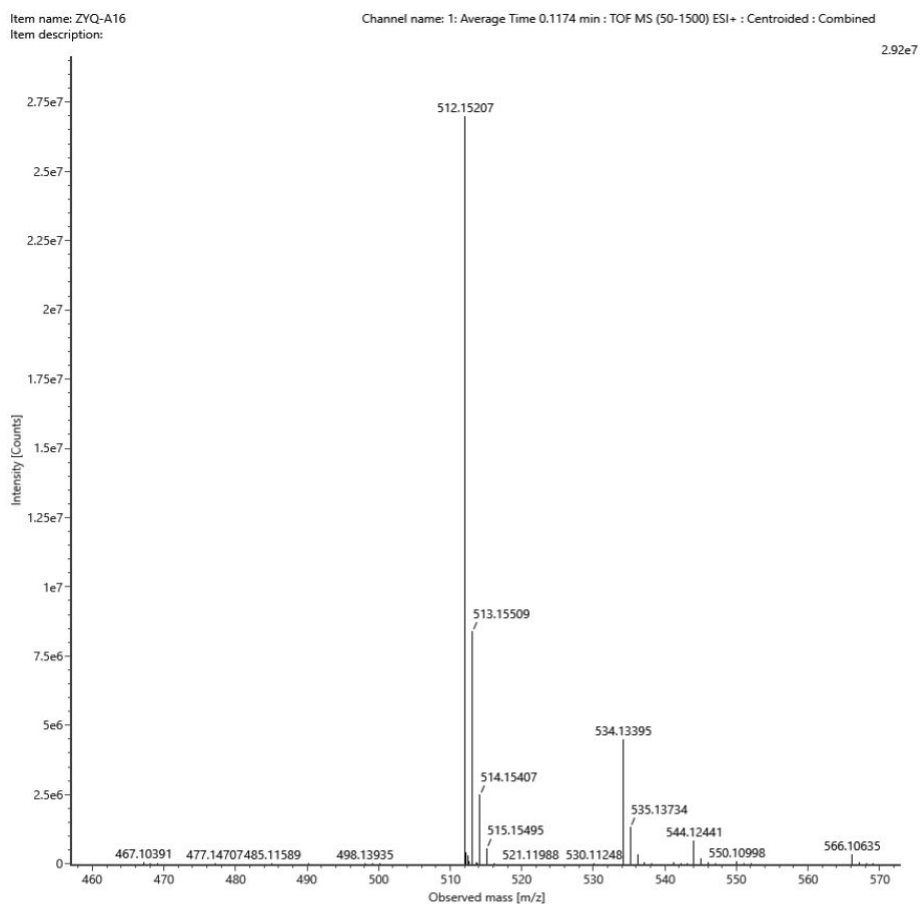


Figure S88 HRMS spectra of compound A16

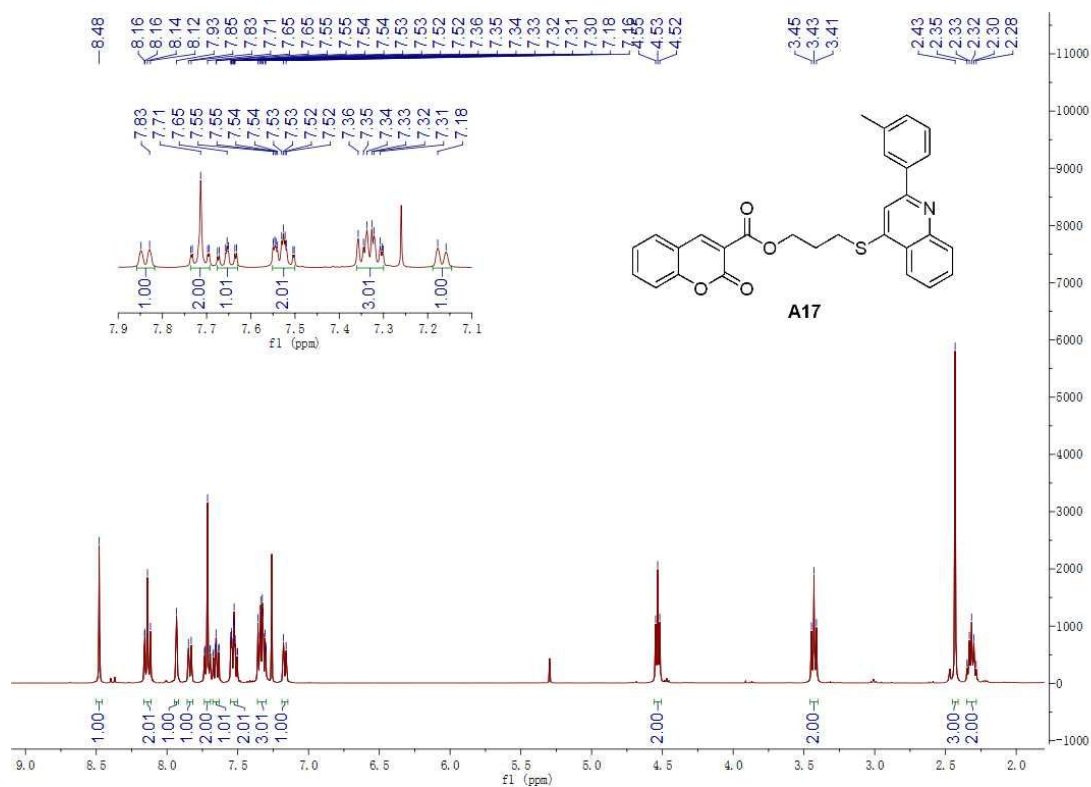


Figure S89 ^1H NMR spectra of compound A17

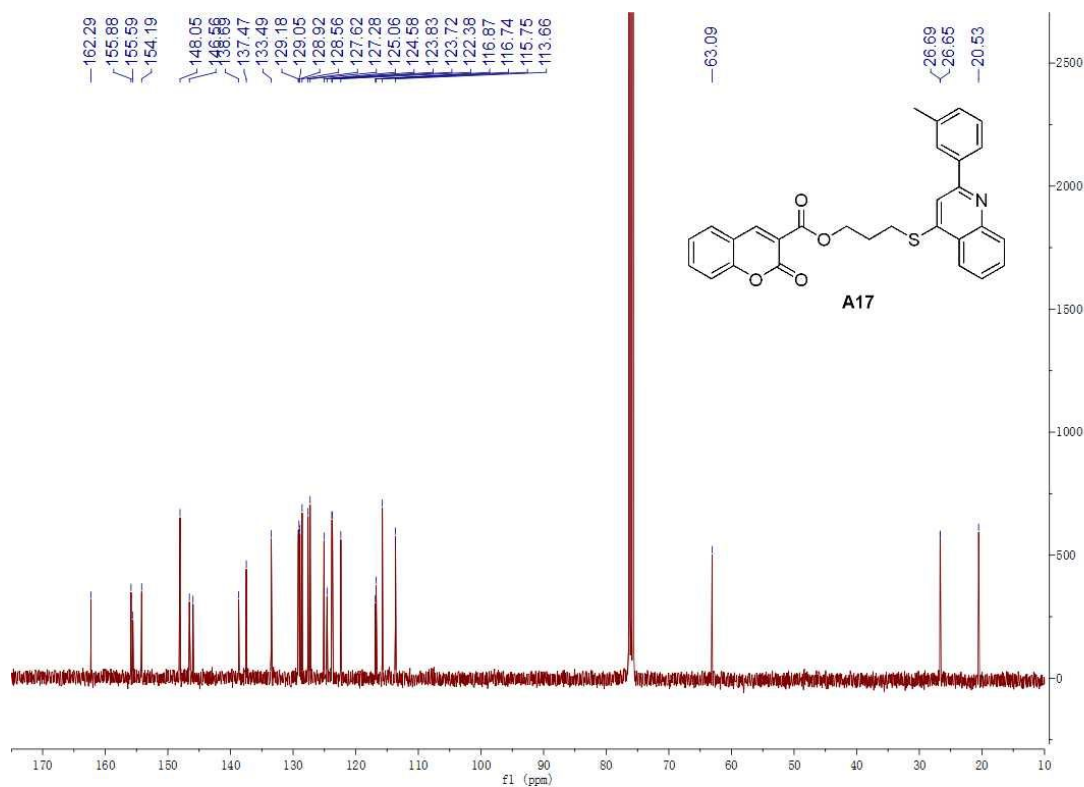


Figure S90 ^{13}C NMR spectra of compound A17

Item name: ZYQ-A17
Item description:

Channel name: 1: Average Time 0.1217 min : TOF MS (50-1500) ESI+ : Centroided : Combined

4.28e7

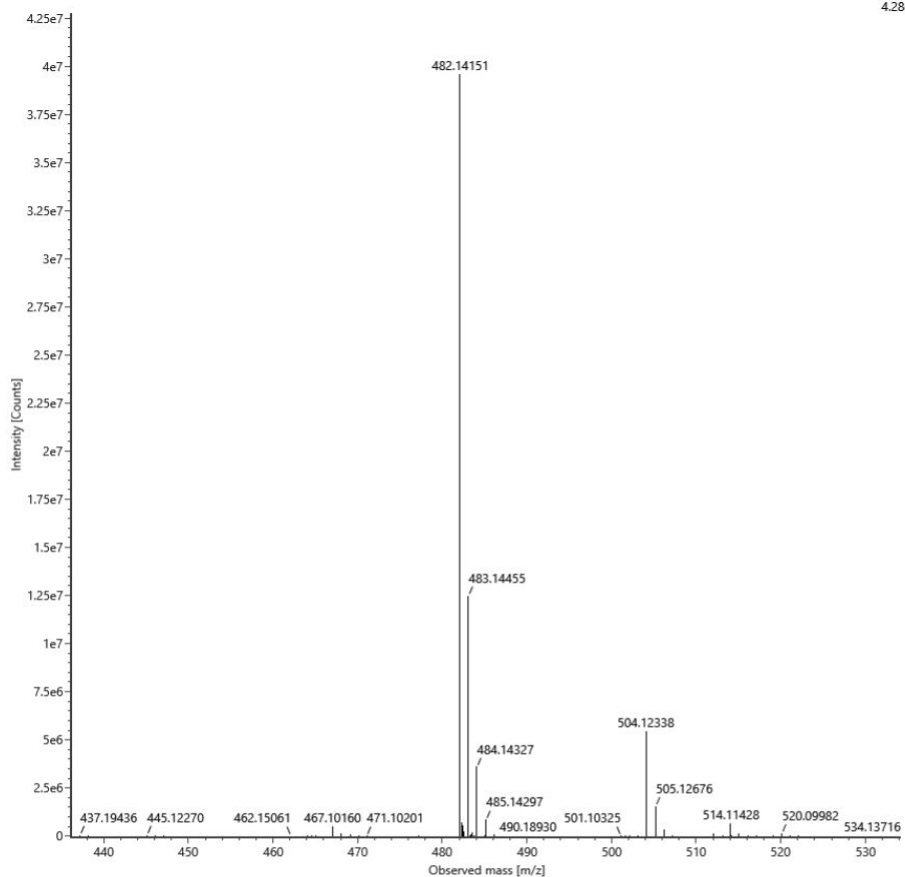


Figure S91 HRMS spectra of compound A17

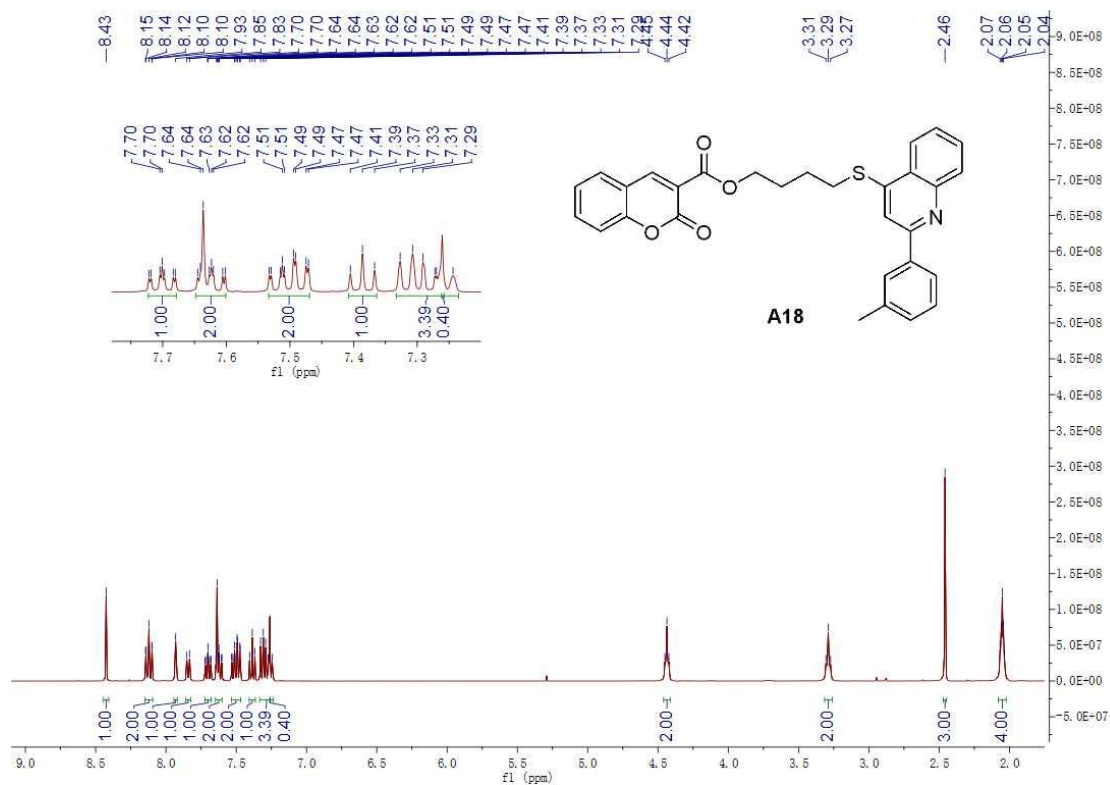
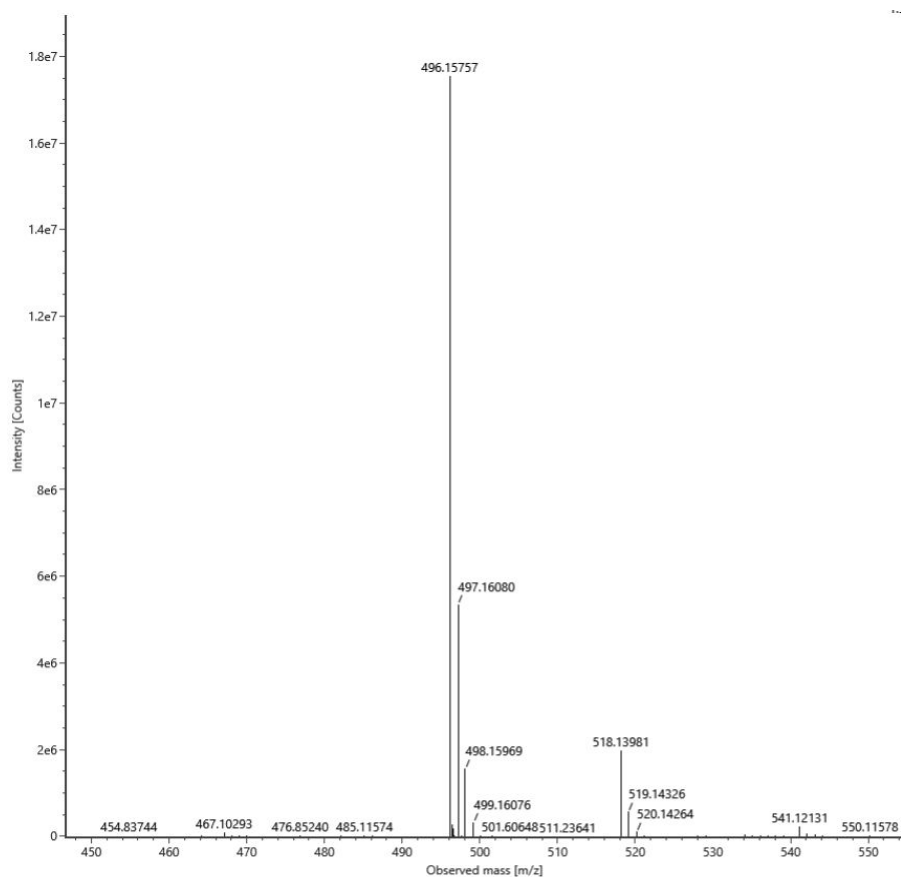
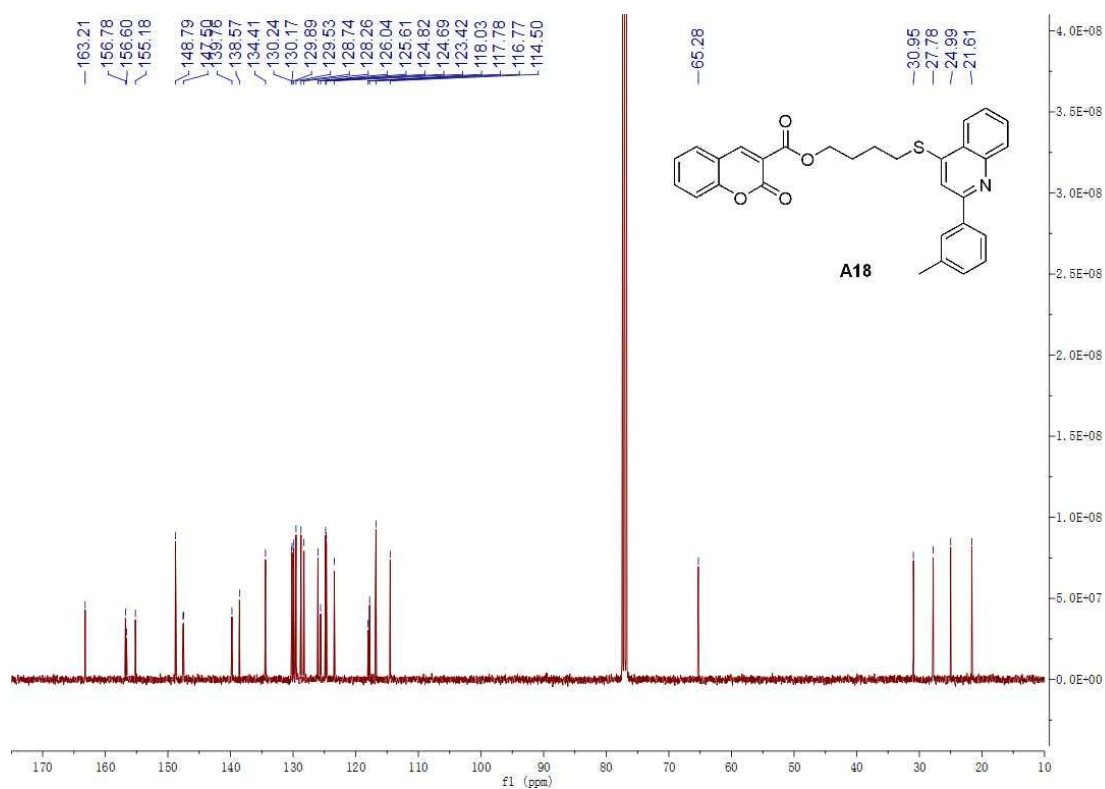


Figure S92 ¹H NMR spectra of compound A18



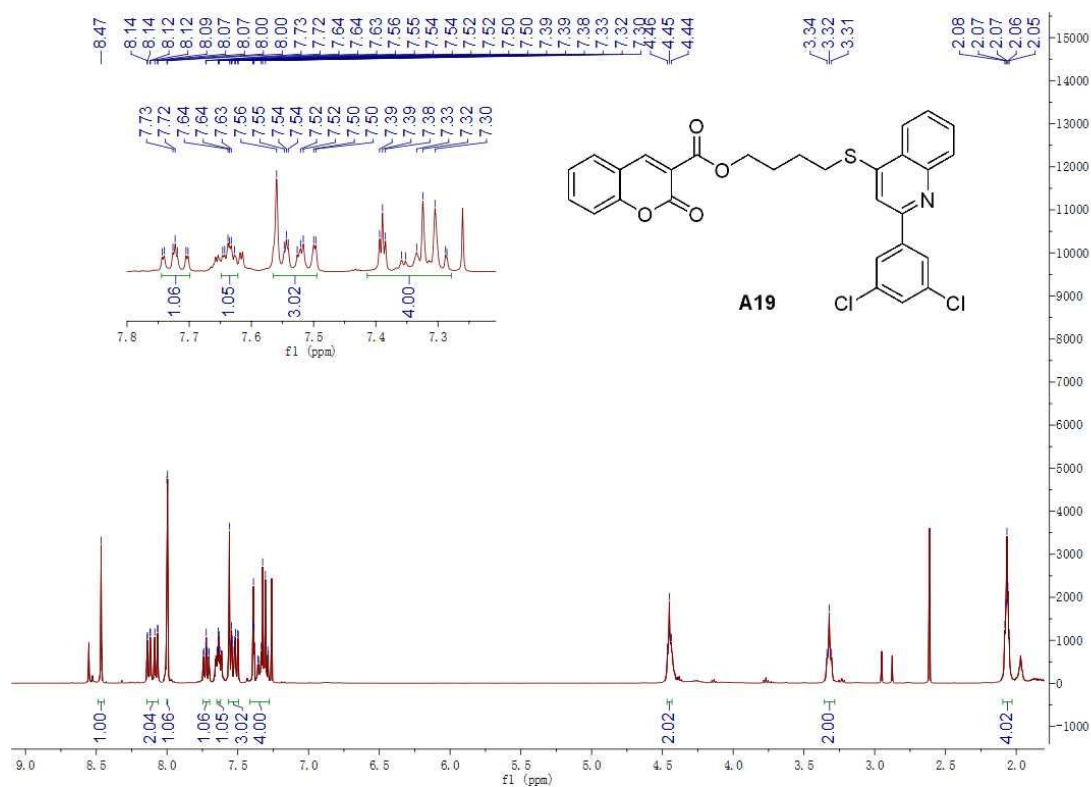


Figure S95 ^1H NMR spectra of compound A19

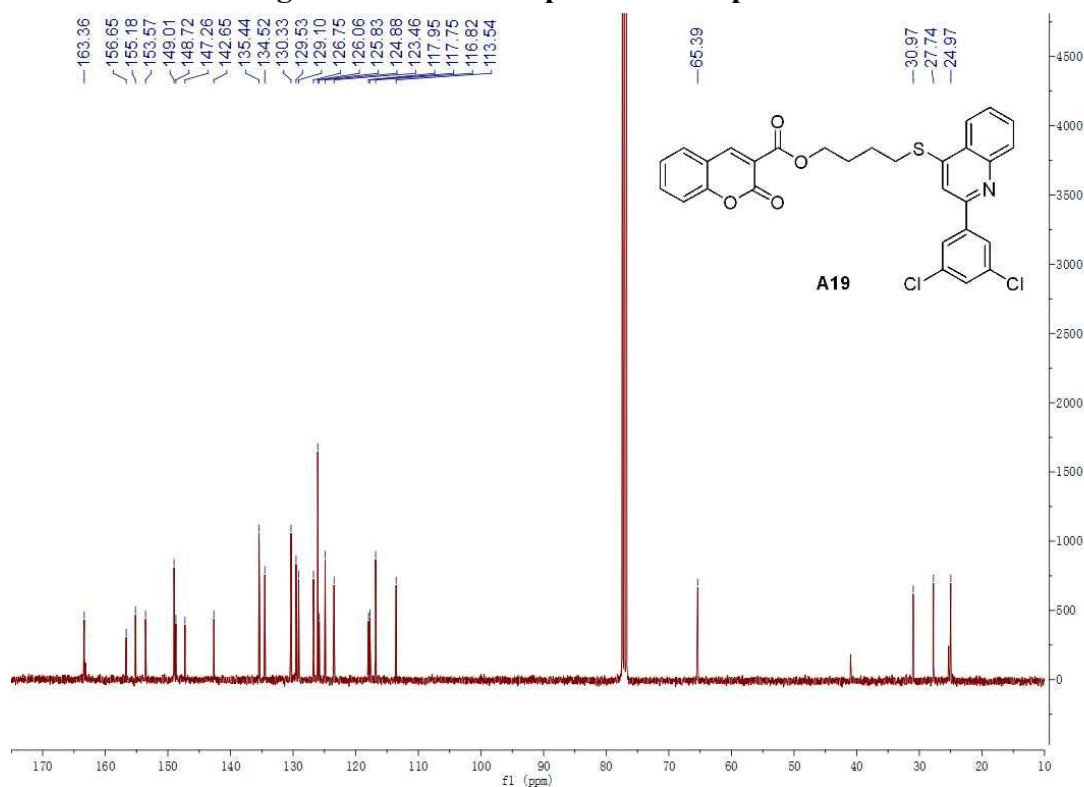


Figure S96 ^{13}C NMR spectra of compound A19

Item name: ZYQ-A42
Item description:

Channel name: 1: Average Time 0.1132 min : TOF MS (50-1500) ESI+ : Centroided : Combined

1.04e6

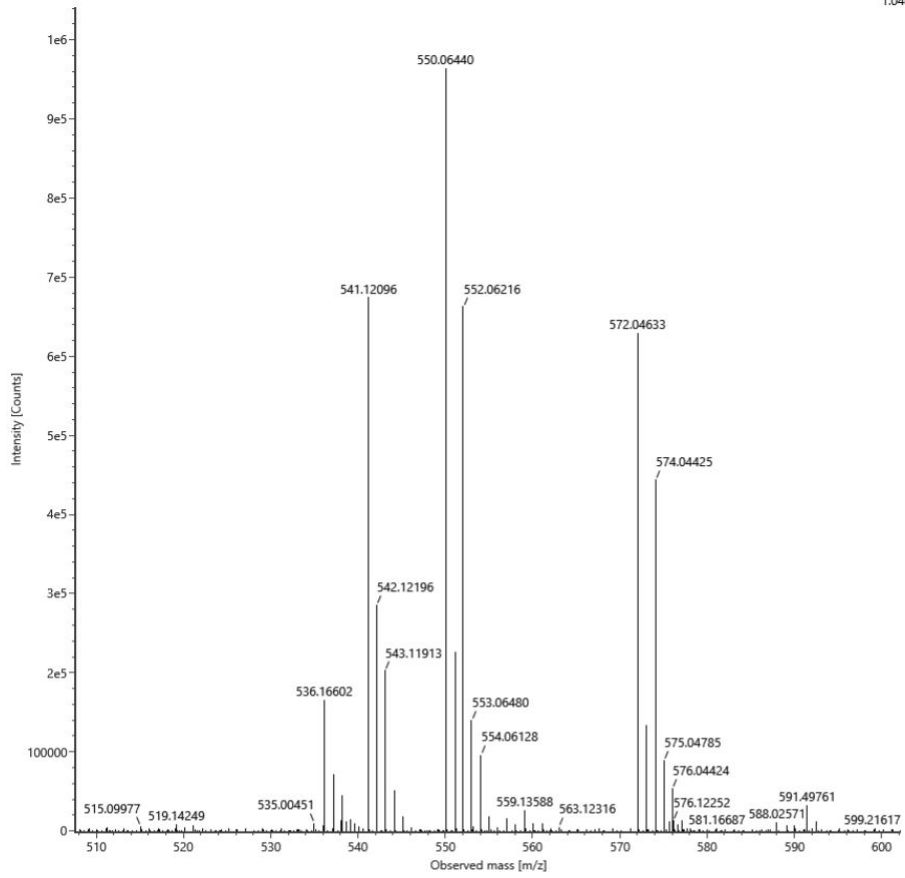


Figure S97 HRMS spectra of compound A19

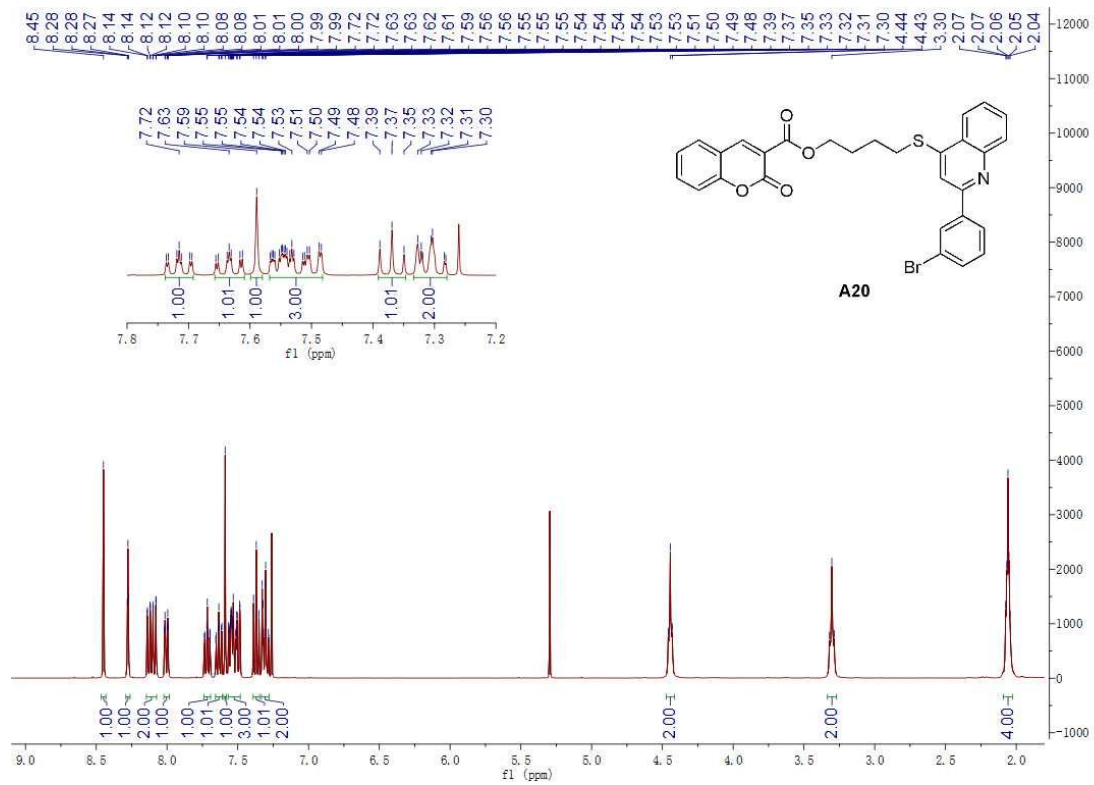


Figure S98 ¹H NMR spectra of compound A20

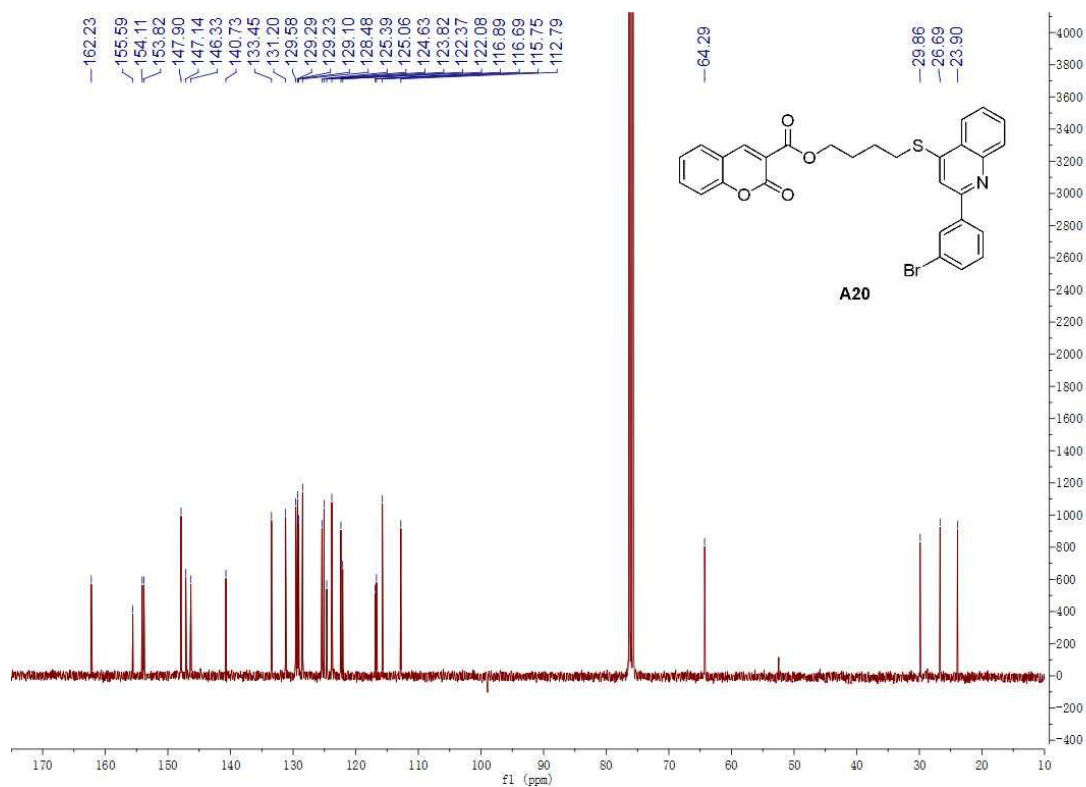


Figure S99 ¹³C NMR spectra of compound A20

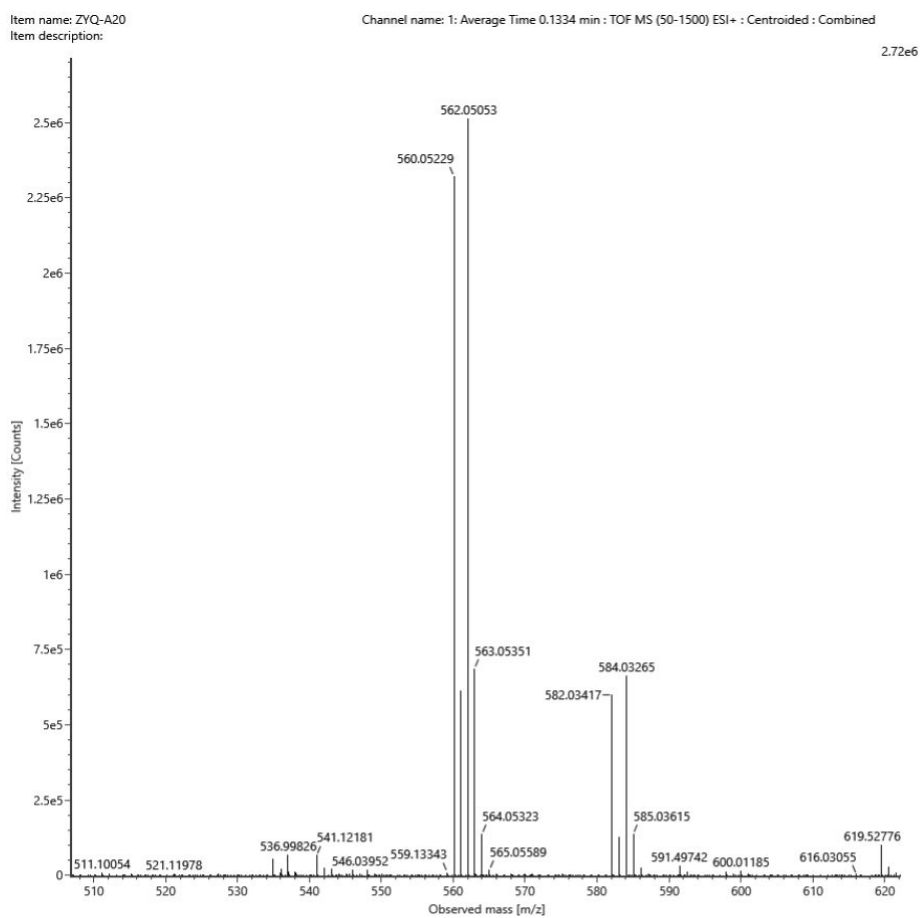


Figure S100 HRMS spectra of compound A20

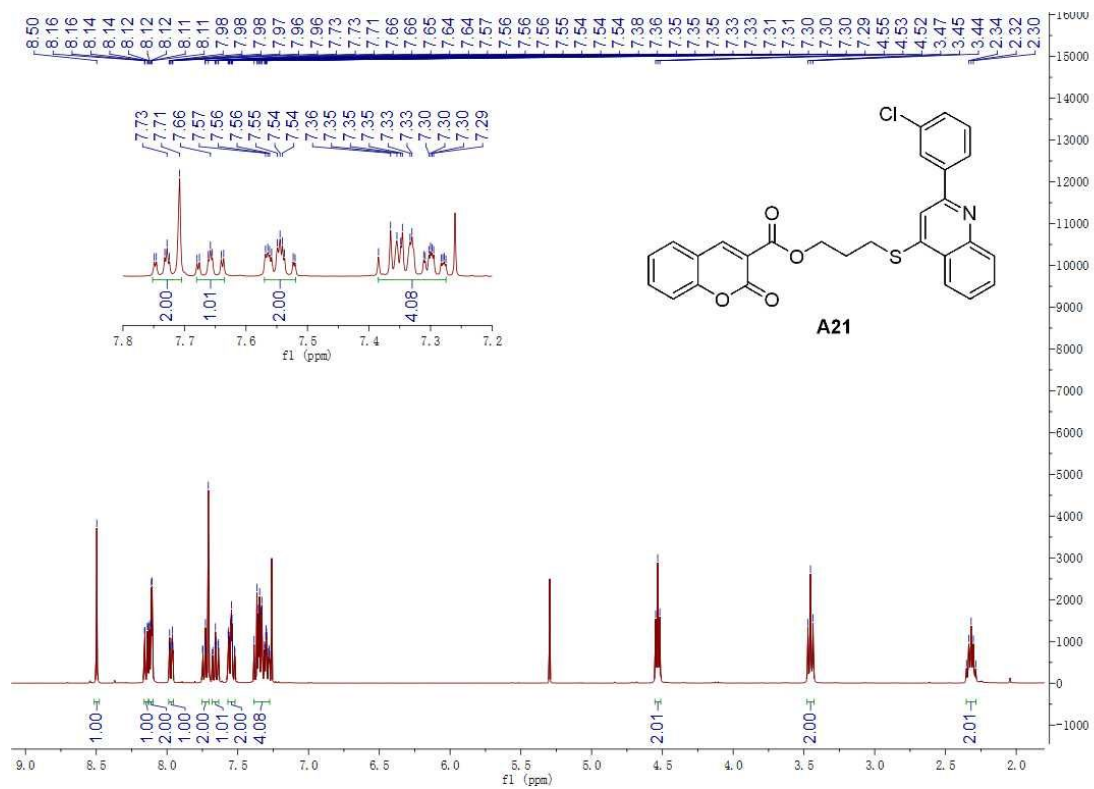


Figure S101 ¹H NMR spectra of compound A21

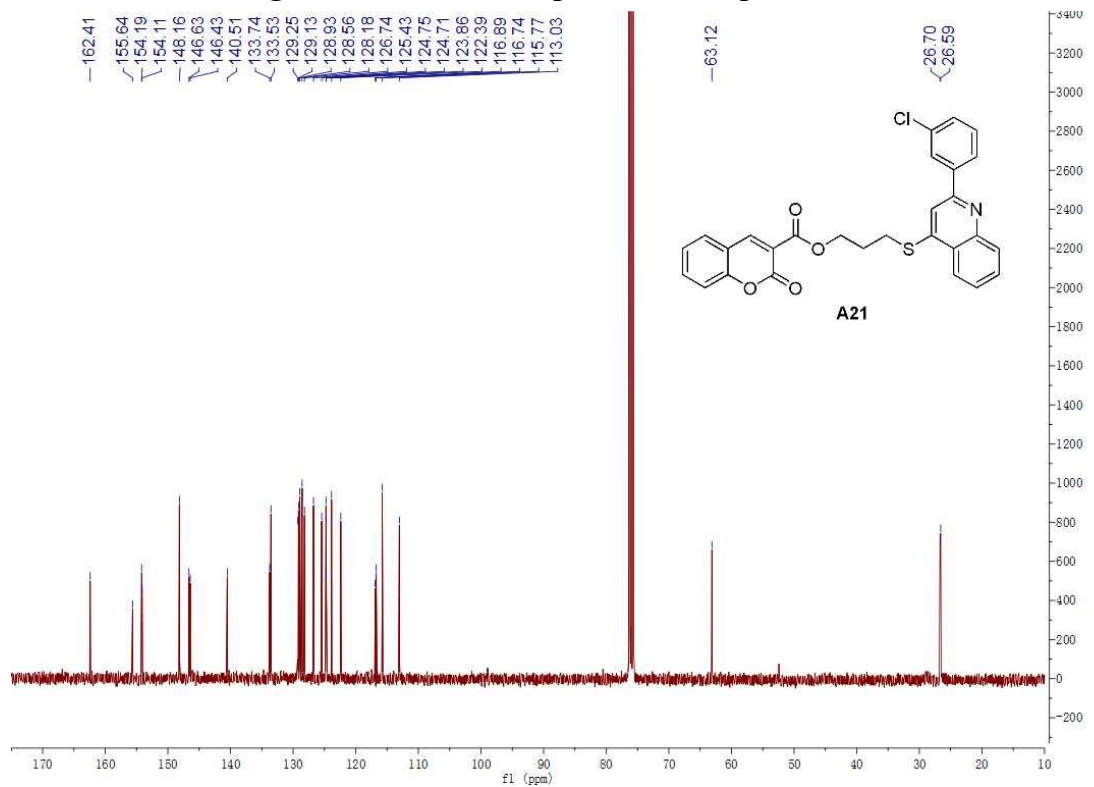


Figure S102 ¹³C NMR spectra of compound A21

Item name: ZYQ-A21
Item description:

Channel name: 1: Average Time 0.1505 min : TOF MS (50-1500) ESI+ : Centroided : Combined

4.65e6

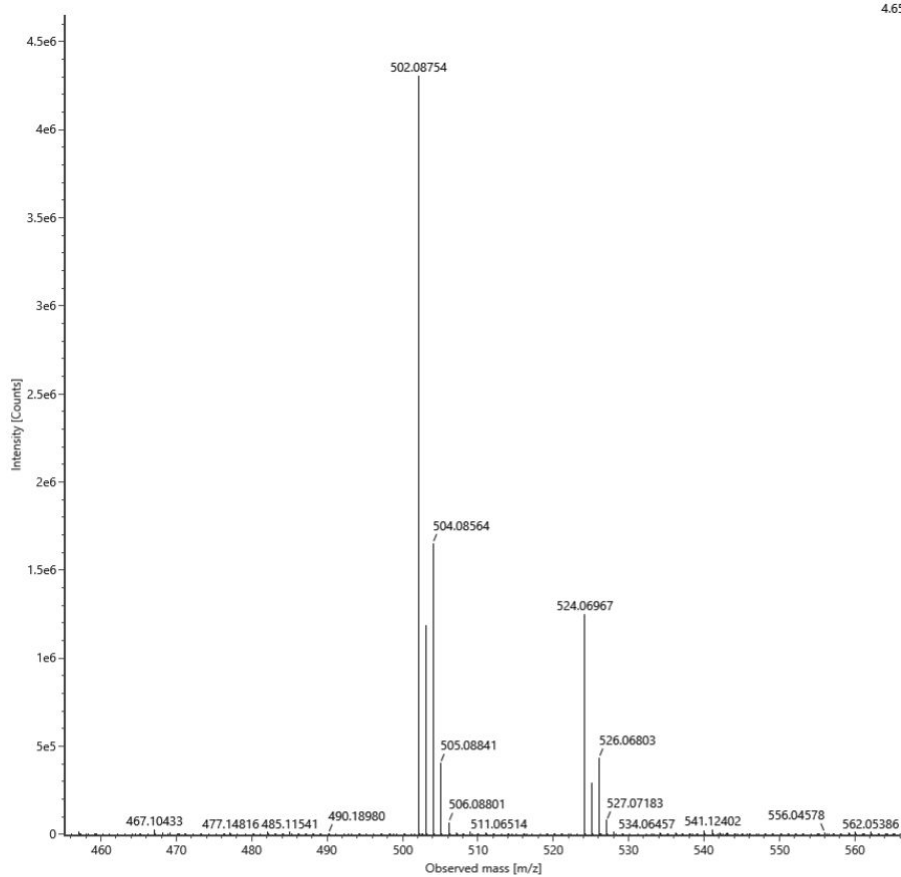


Figure S103 HRMS spectra of compound A21

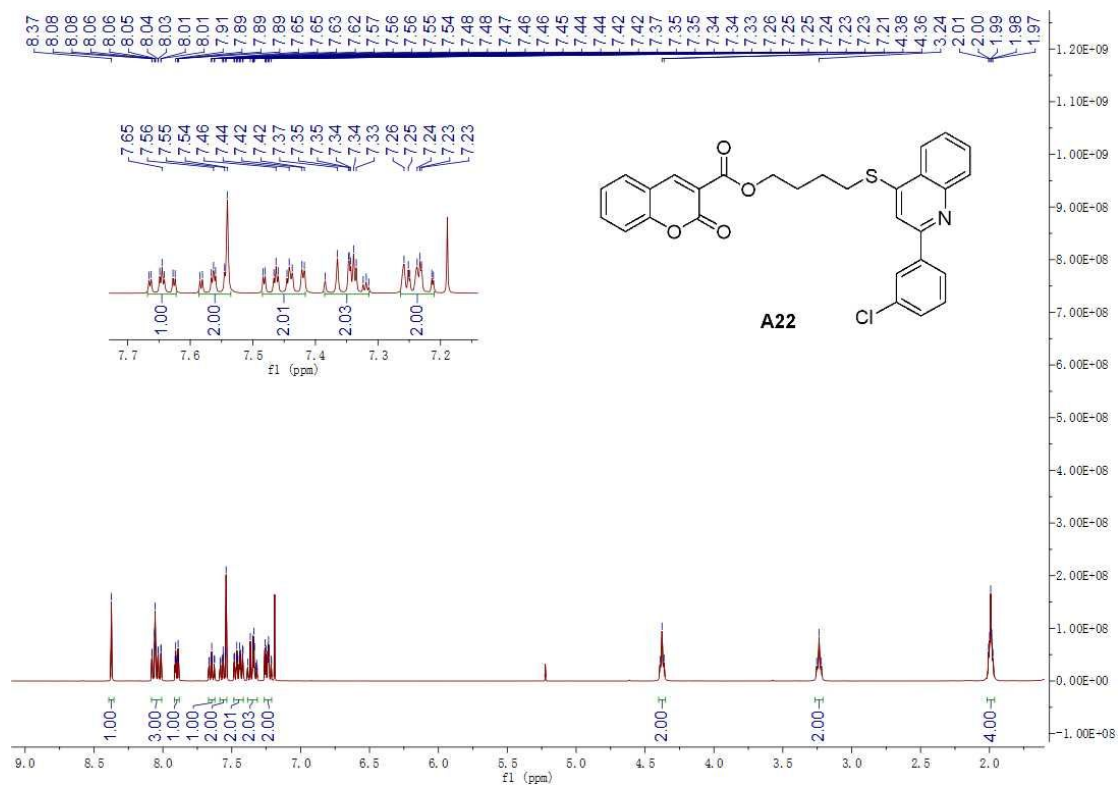
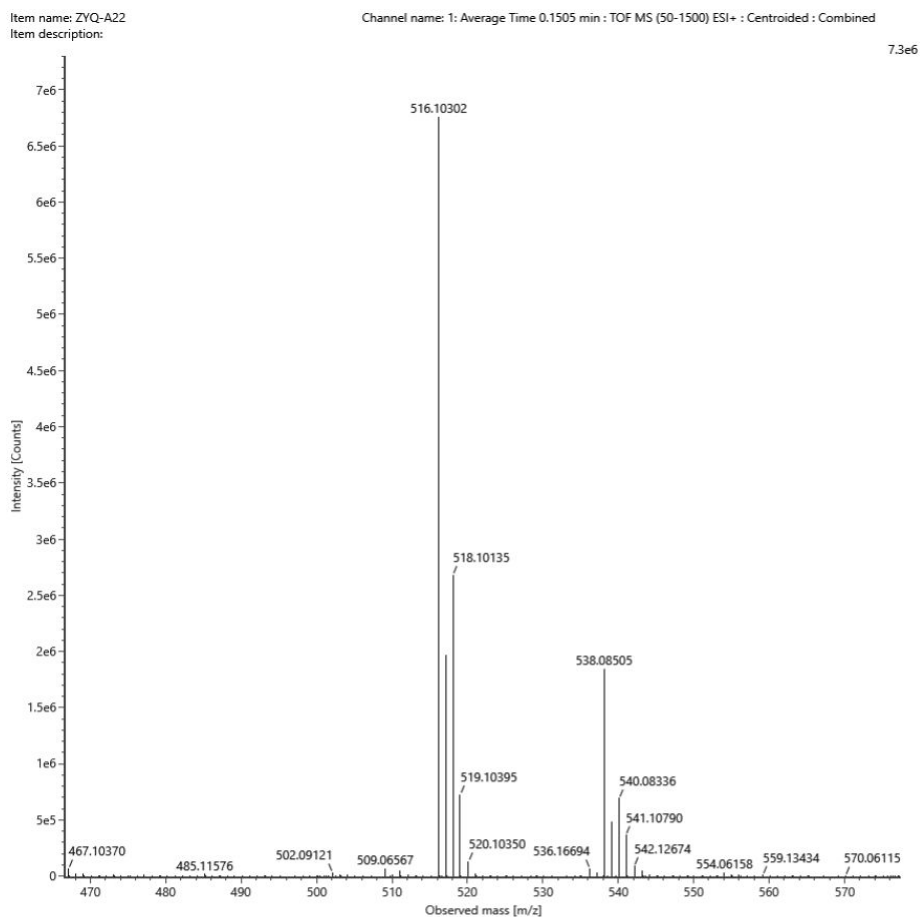
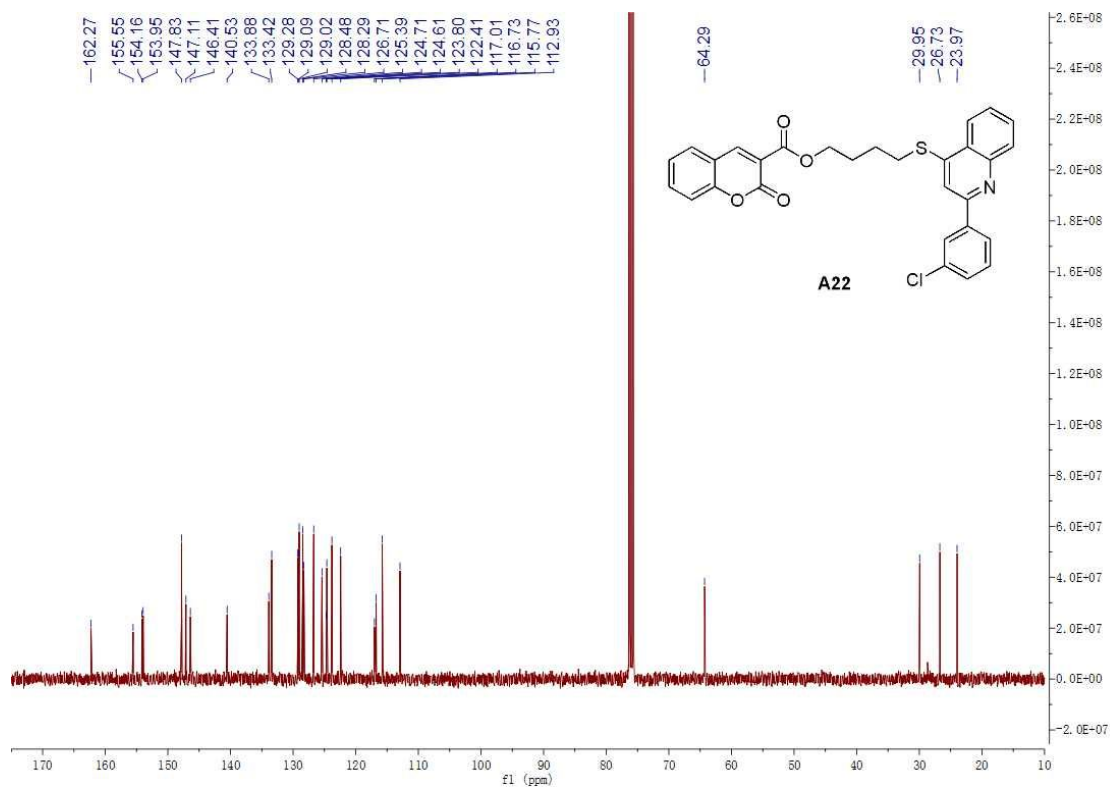


Figure S104 ¹H NMR spectra of compound A22



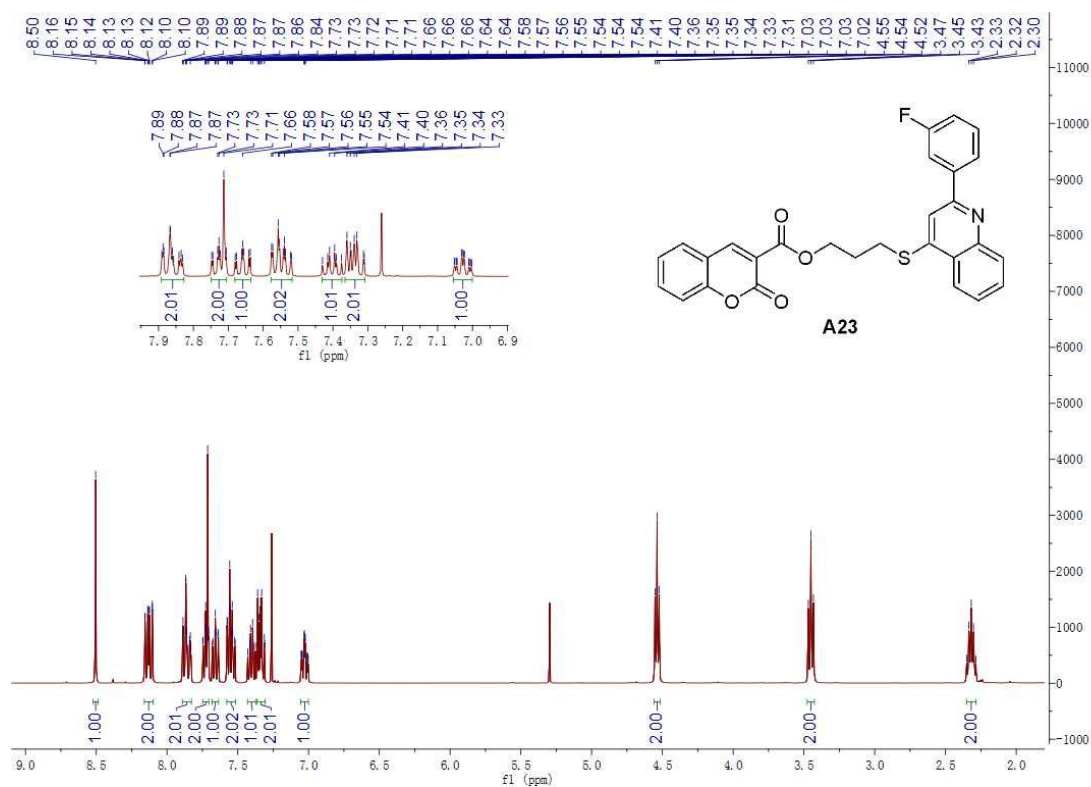


Figure S107 ^1H NMR spectra of compound A23

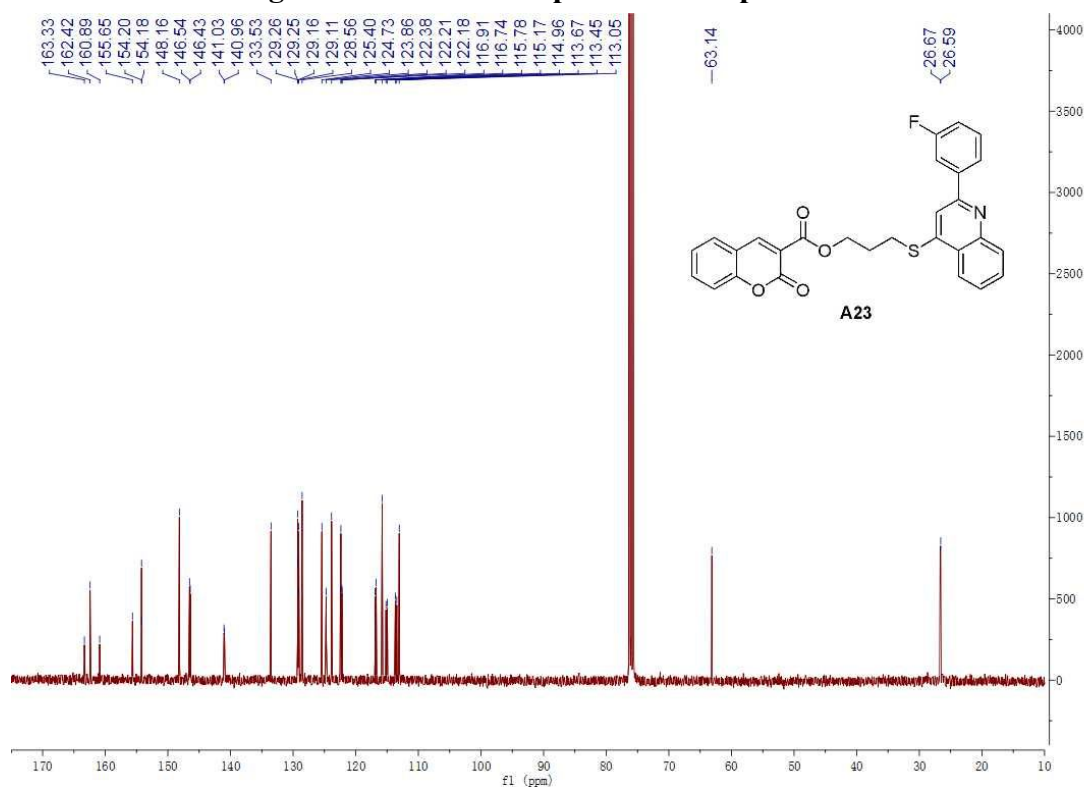


Figure S108 ^{13}C NMR spectra of compound A23

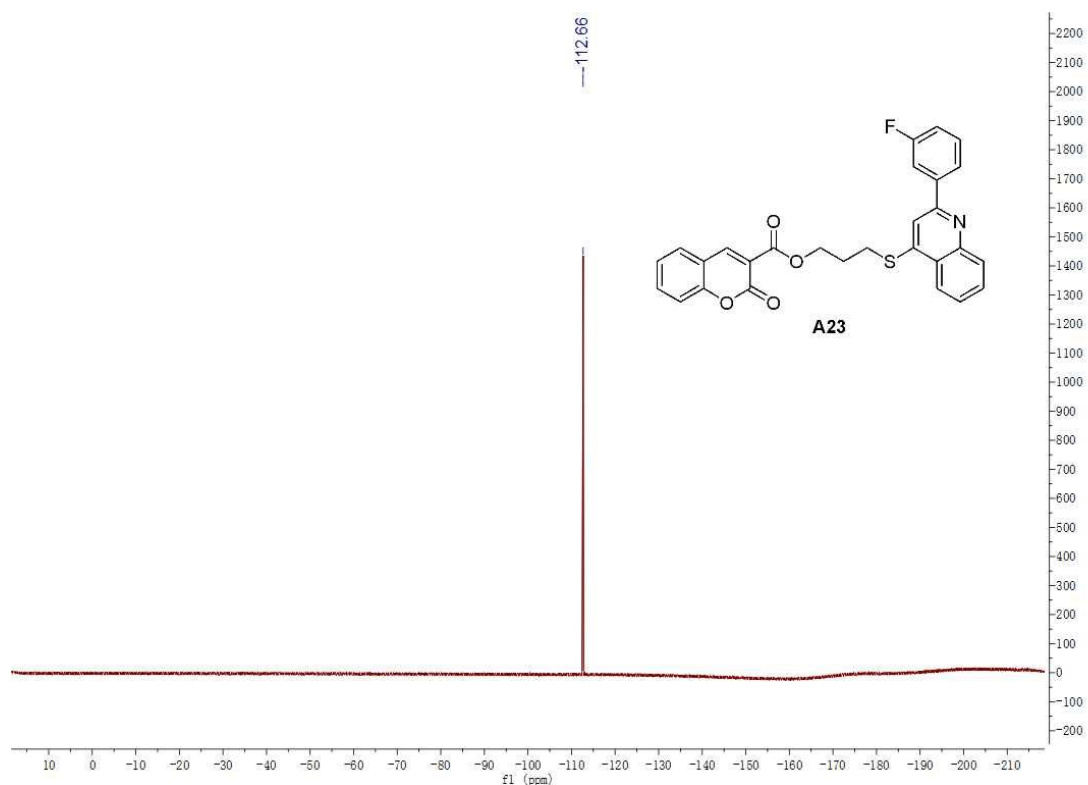


Figure S109 ¹⁹F NMR spectra of compound A23

Item name: ZYQ-A23
Item description:

Channel name: 1: Average Time 0.1377 min : TOF MS (50-1500) ESI+ : Centroided : Combined

1.19e7

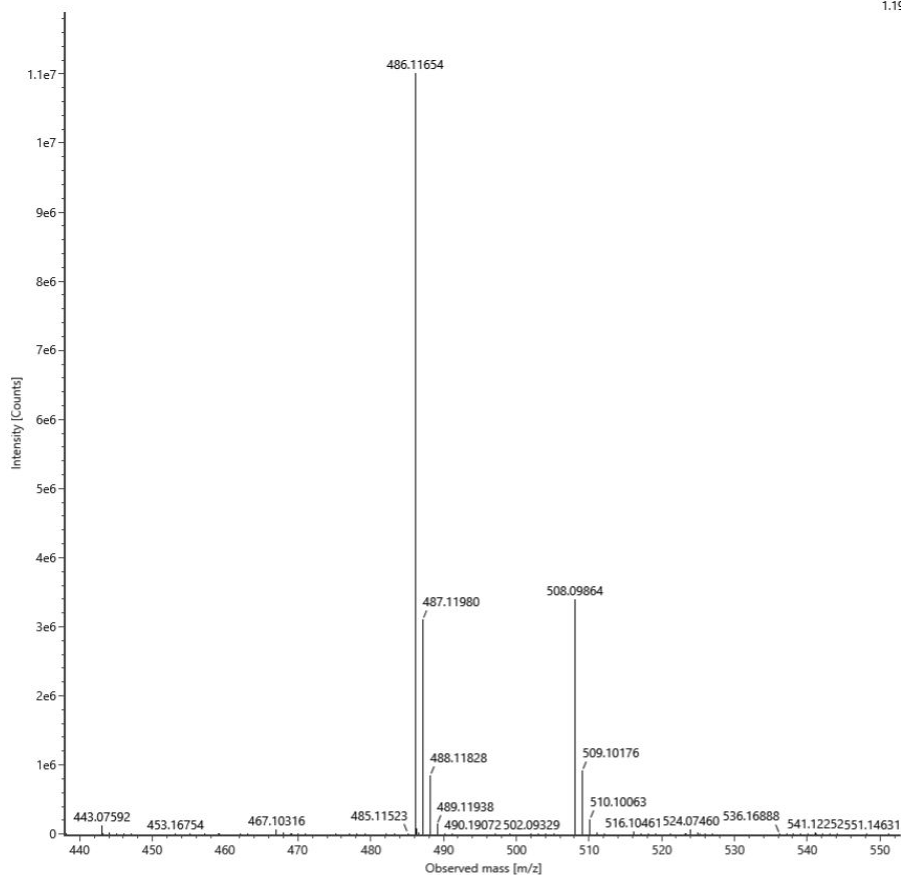


Figure S110 HRMS spectra of compound A23

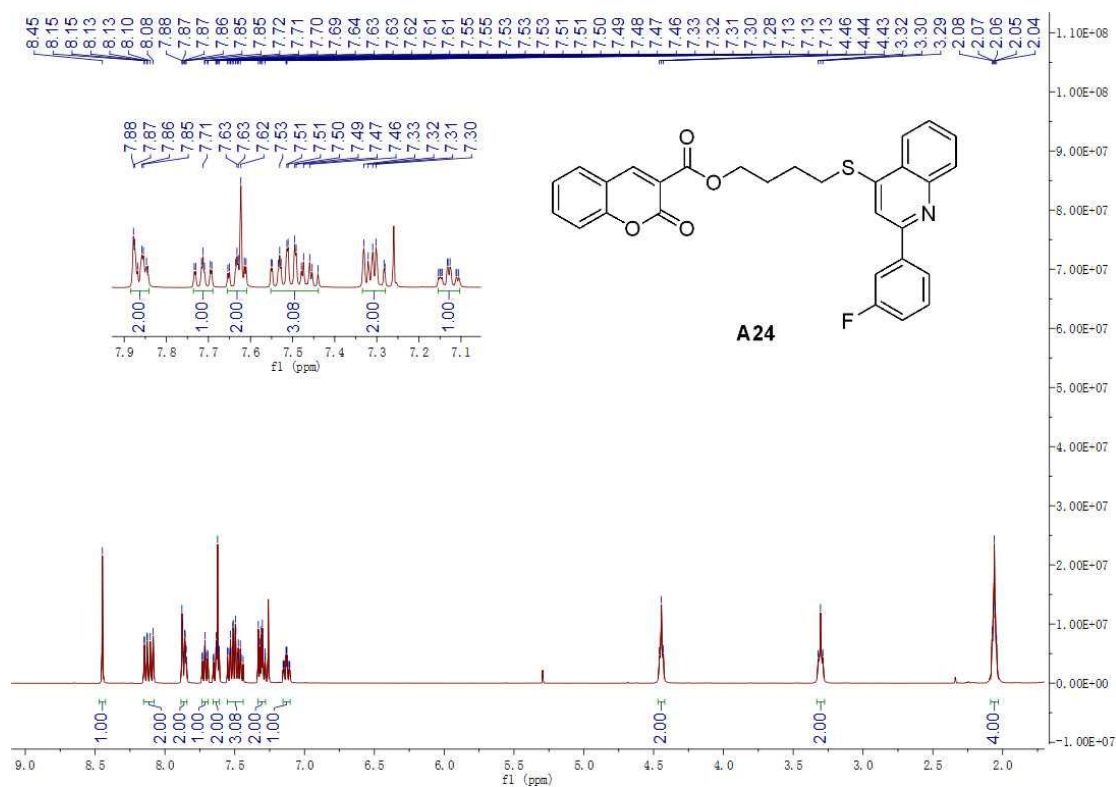


Figure S111 ¹H NMR spectra of compound A24

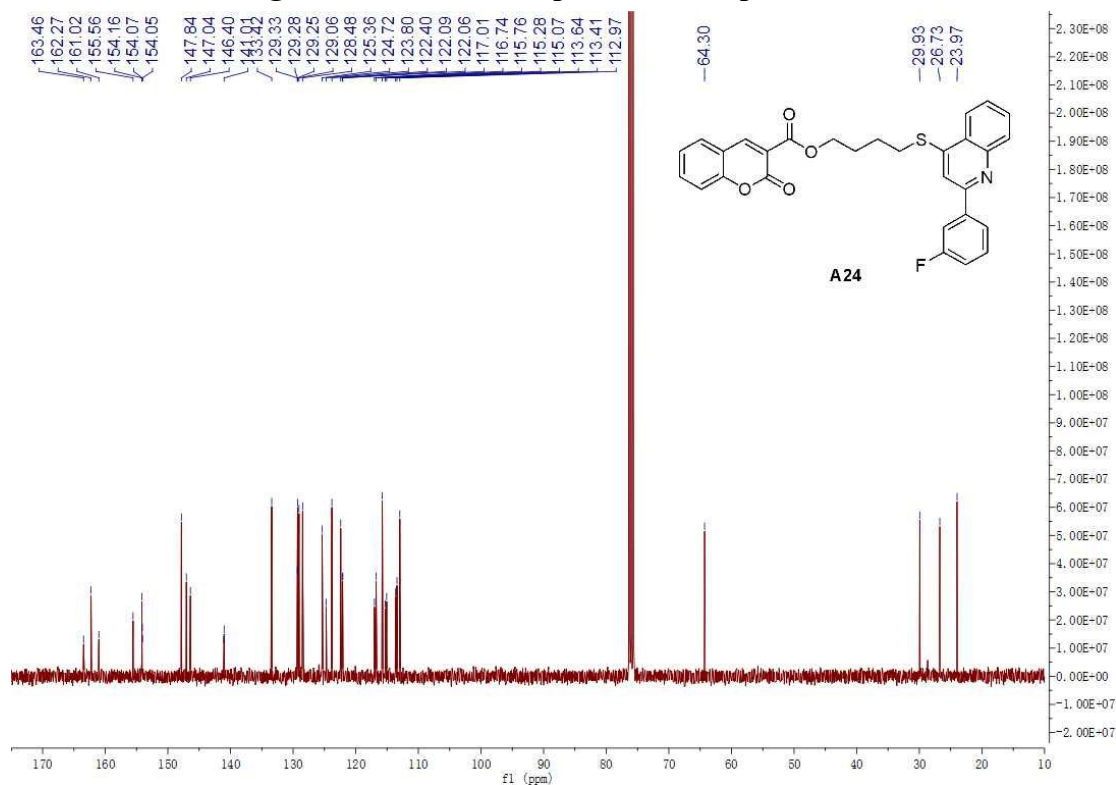


Figure S112 ¹³C NMR spectra of compound A24

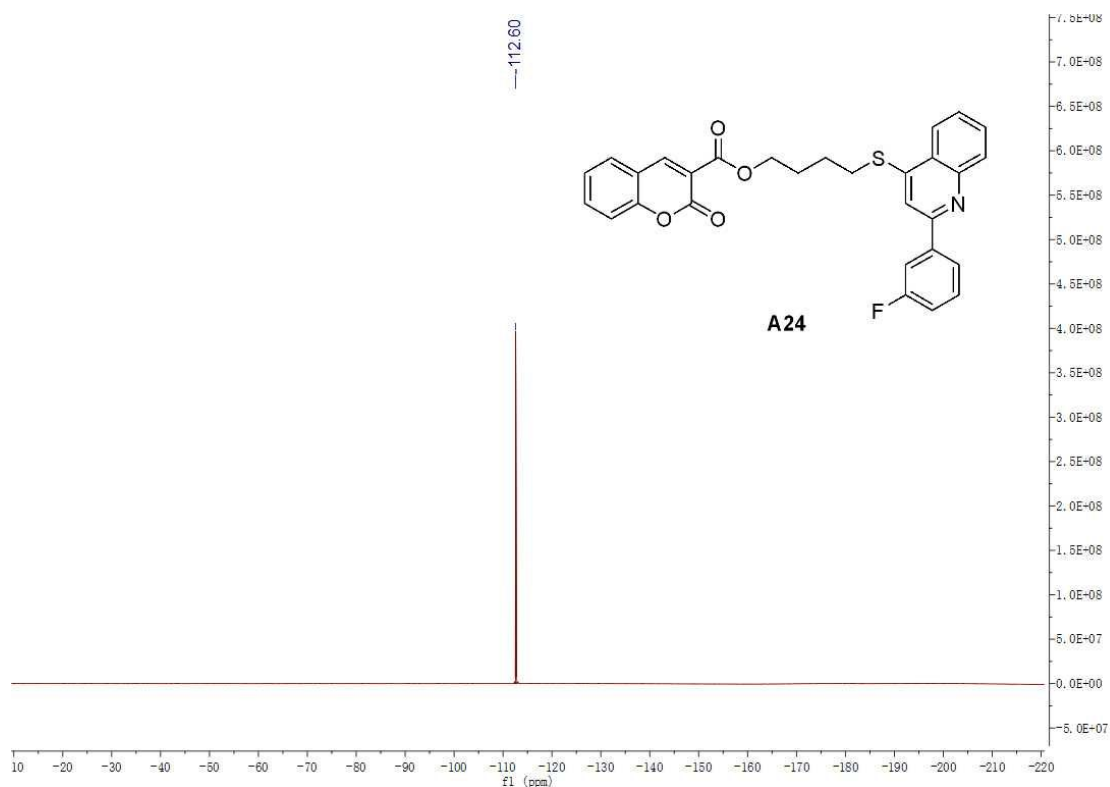


Figure S113 ¹⁹F NMR spectra of compound A24

Item name: ZYQ-A24
Item description:

Channel name: 1: Average Time 0.1174 min : TOF MS (50-1500) ESI+ : Centroided : Combined

1.32e7

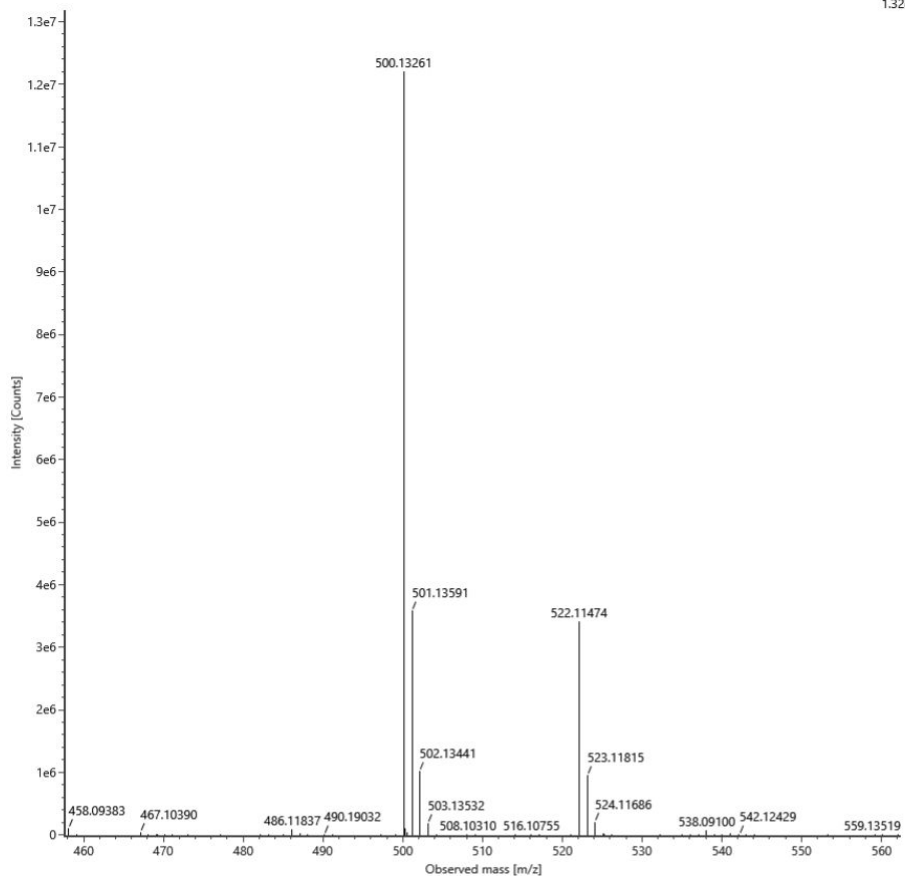


Figure S114 HRMS spectra of compound A24

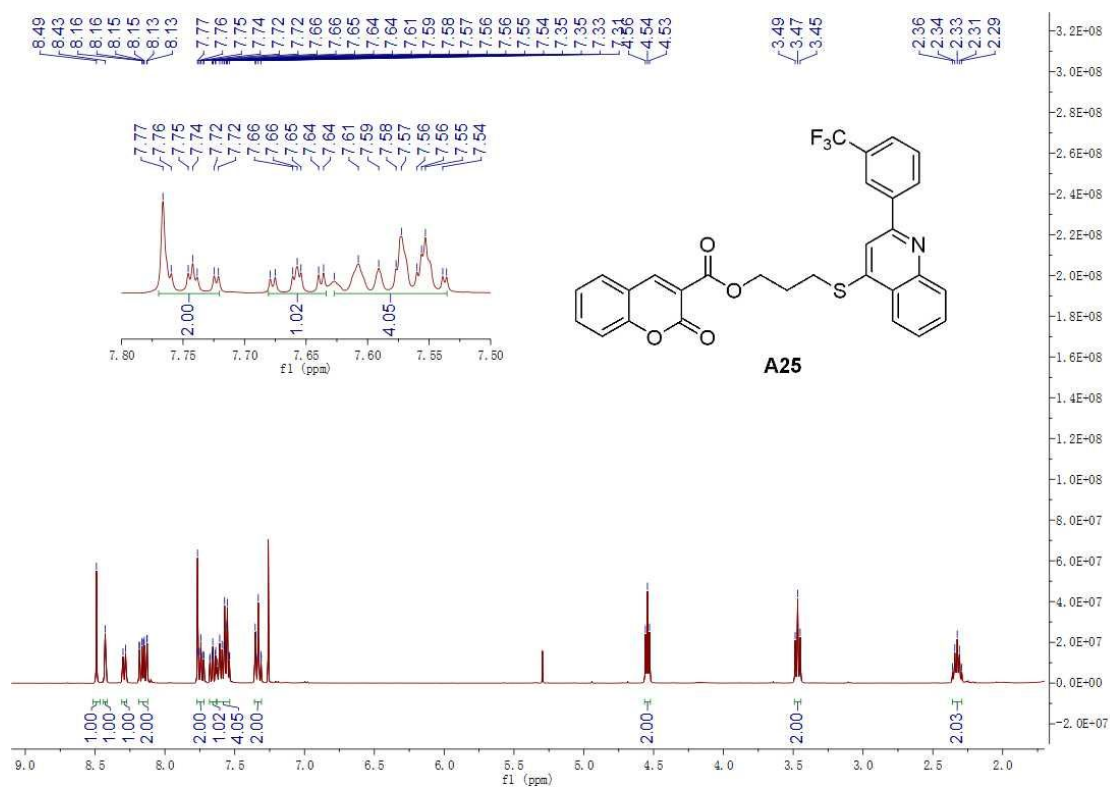


Figure S115 ^1H NMR spectra of compound A25

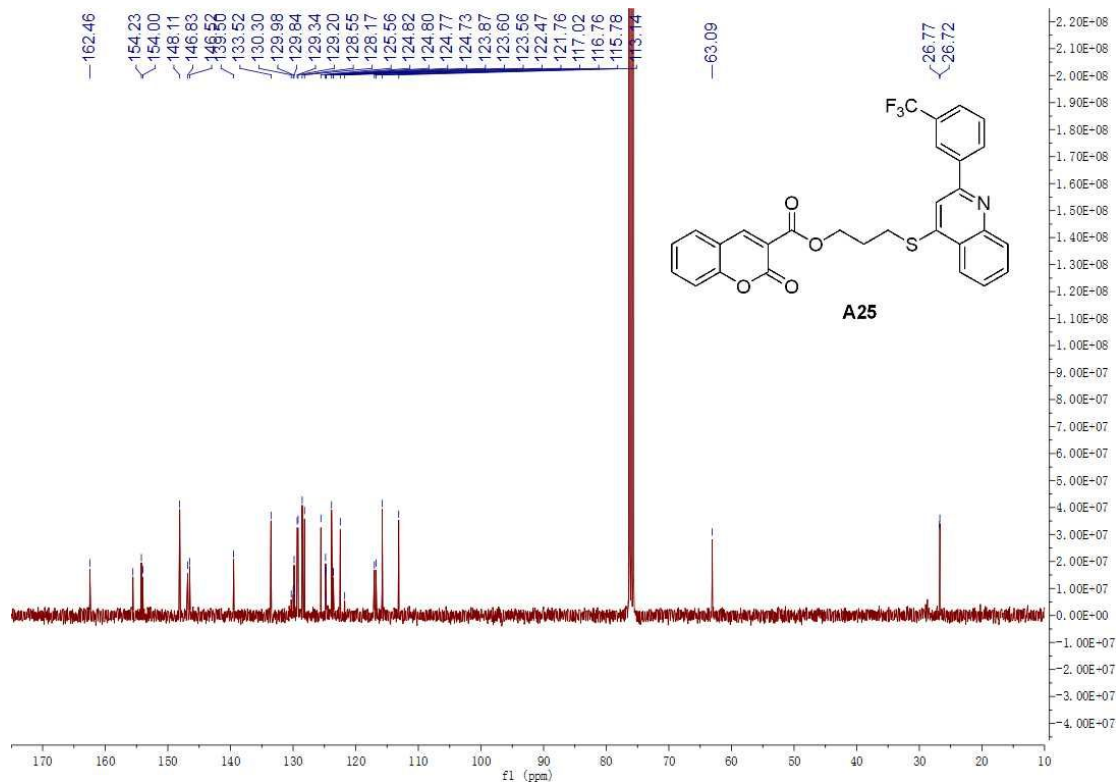


Figure S116 ^{13}C NMR spectra of compound A25

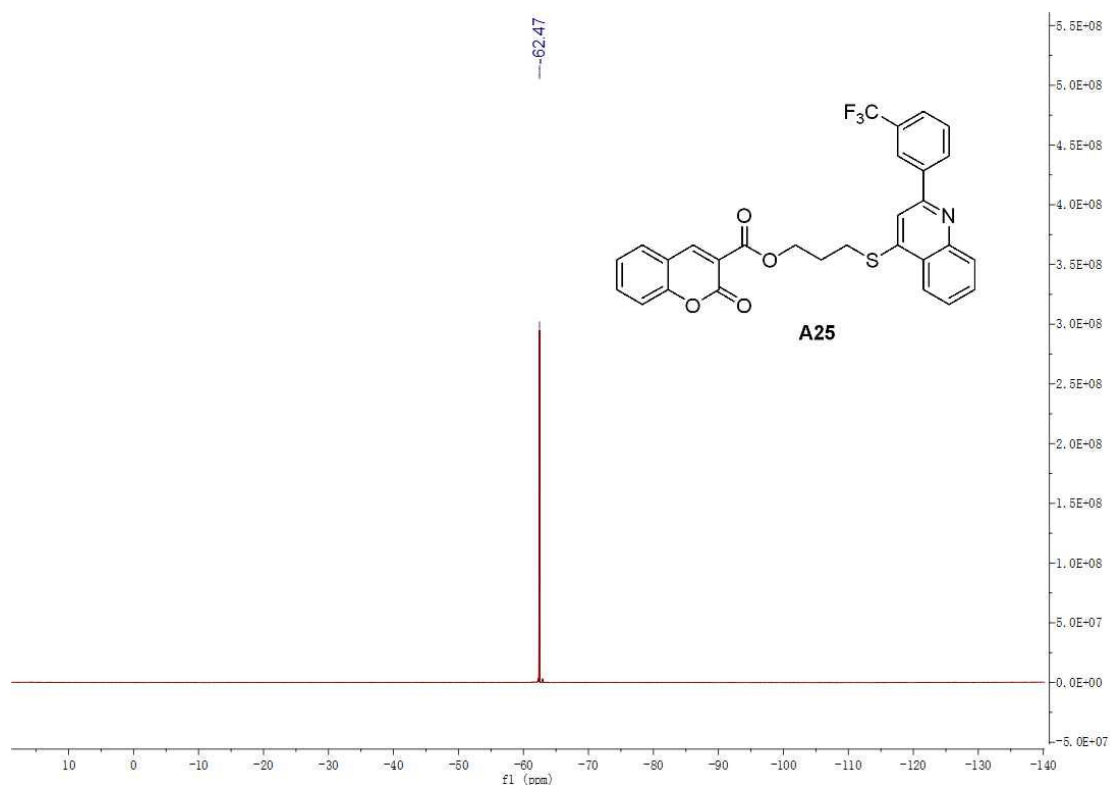


Figure S117 ^{19}F NMR spectra of compound A25

Item name: ZYQ-A25
Item description:

Channel name: 1: Average Time 0.1334 min : TOF MS (50-1500) ESI+ : Centroided : Combined

7.7e6

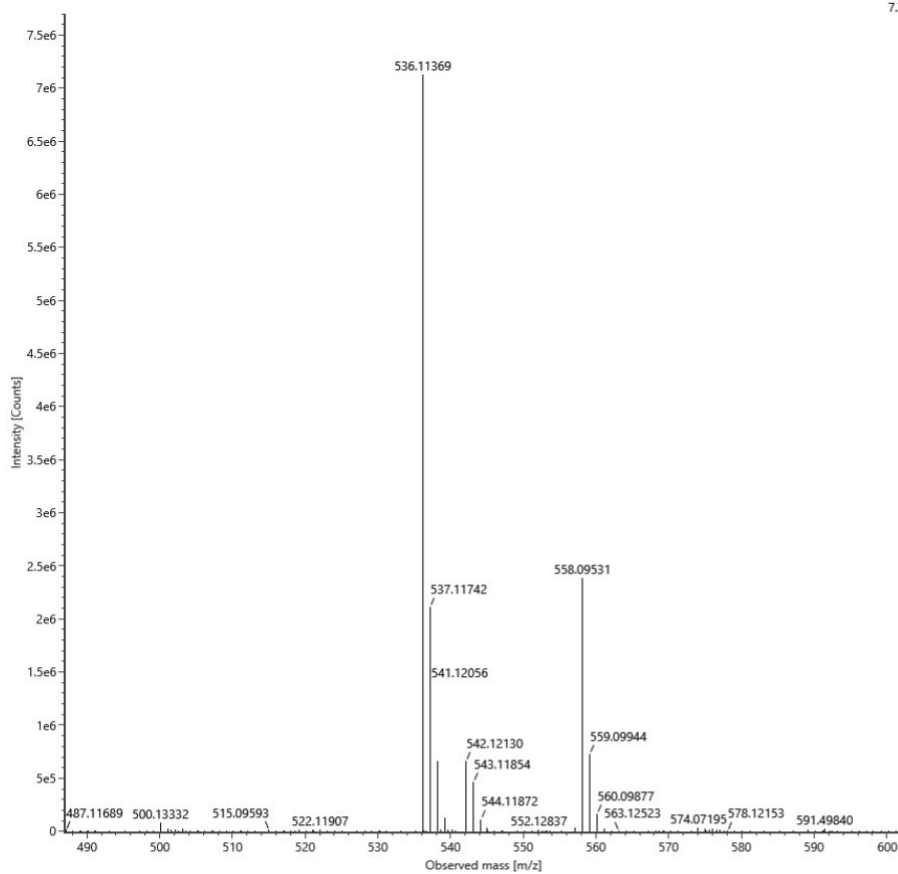


Figure S118 HRMS spectra of compound A25

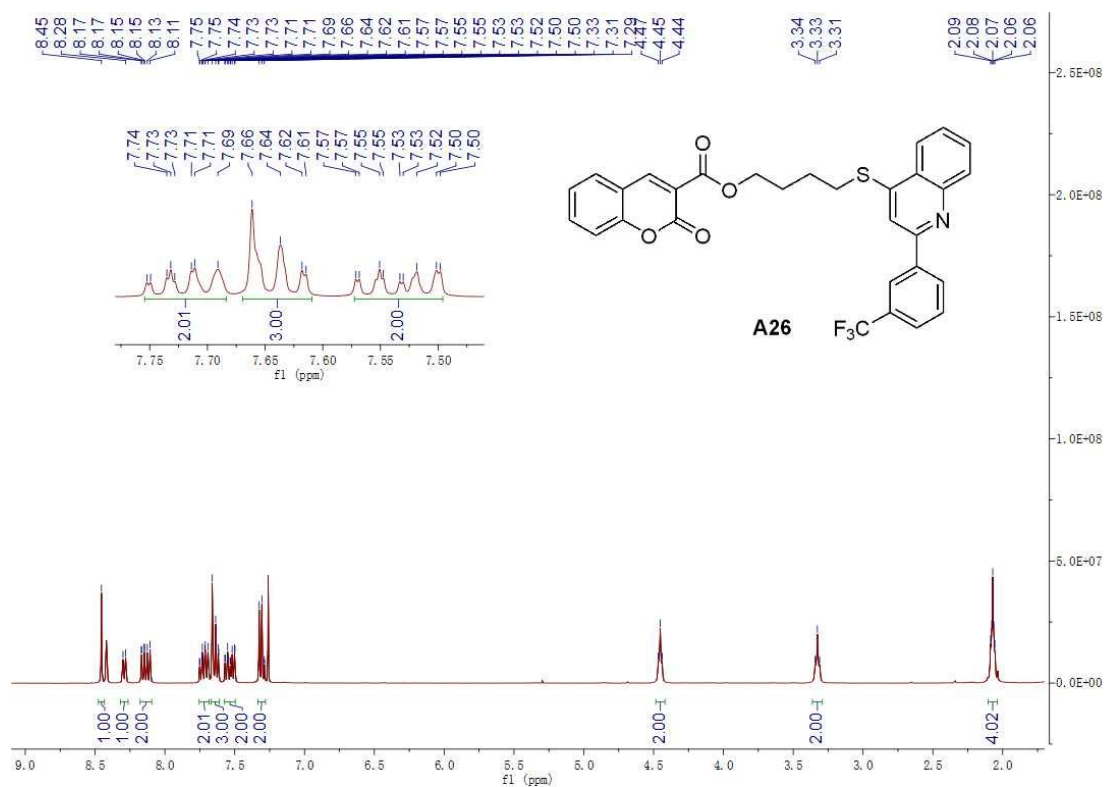


Figure S119 ^1H NMR spectra of compound A26

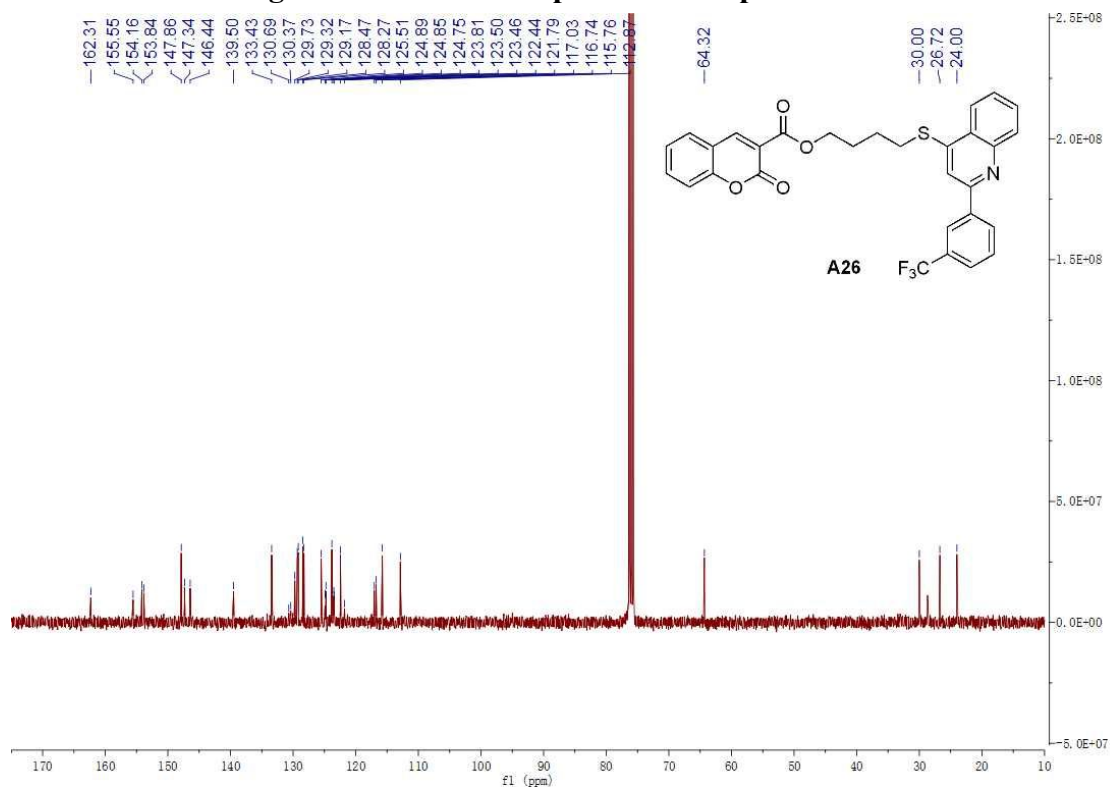


Figure S120 ^{13}C NMR spectra of compound A26

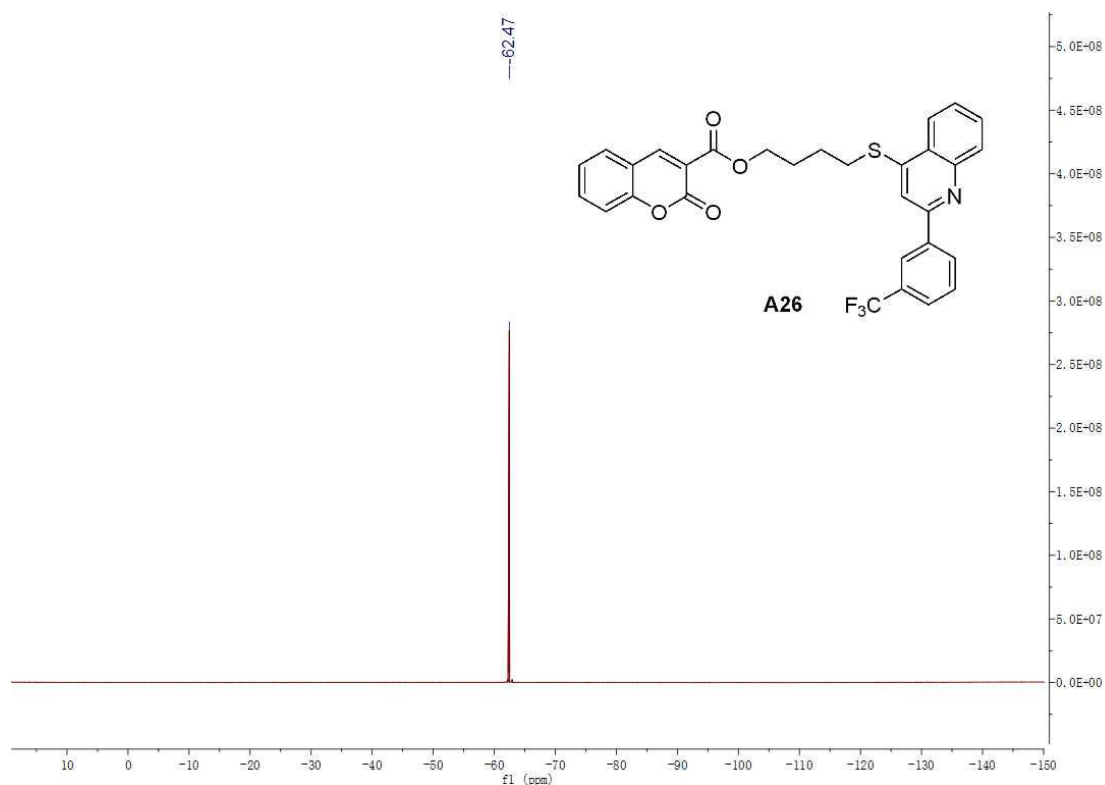


Figure S121 ¹⁹F NMR spectra of compound A26

Item name: ZYQ-A26
Item description:

Channel name: 1: Average Time 0.1377 min : TOF MS (50-1500) ESI+ : Centroided : Combined

1.34e6

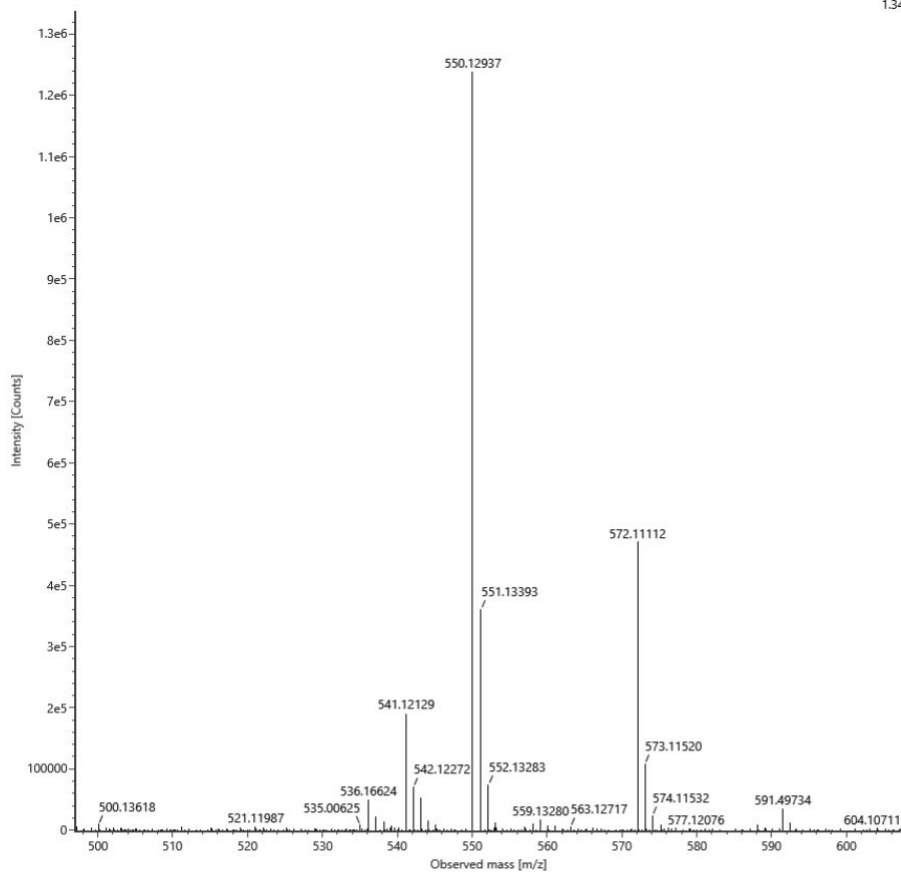
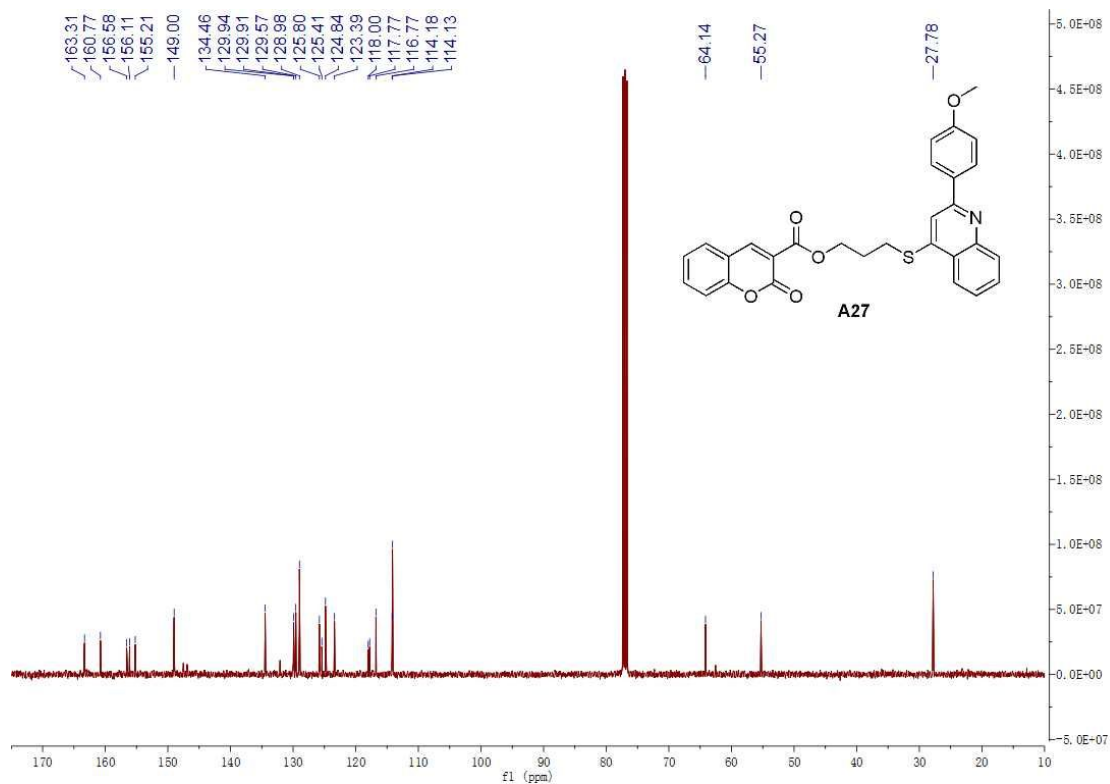
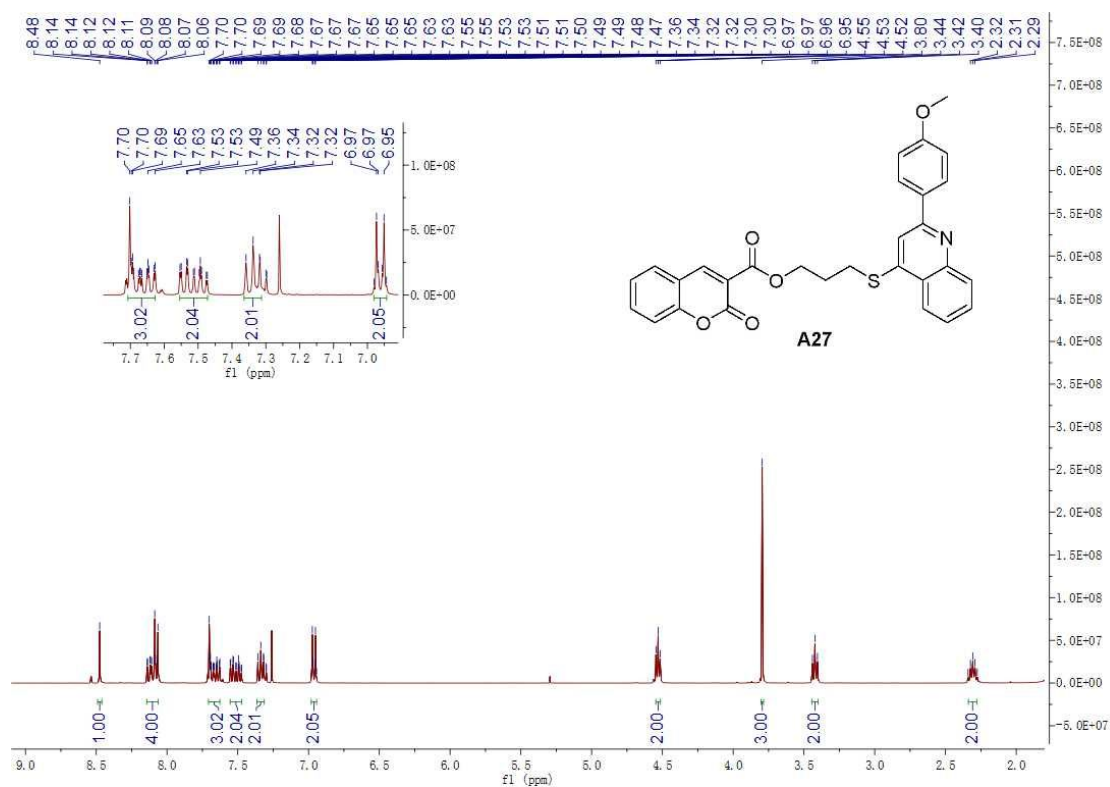


Figure S122 HRMS spectra of compound A26



Item name: ZYQ-A27
Item description:

Channel name: 1: Average Time 0.1131 min : TOF MS (50-1500) ESI+ : Centroided : Combined

1.52e7

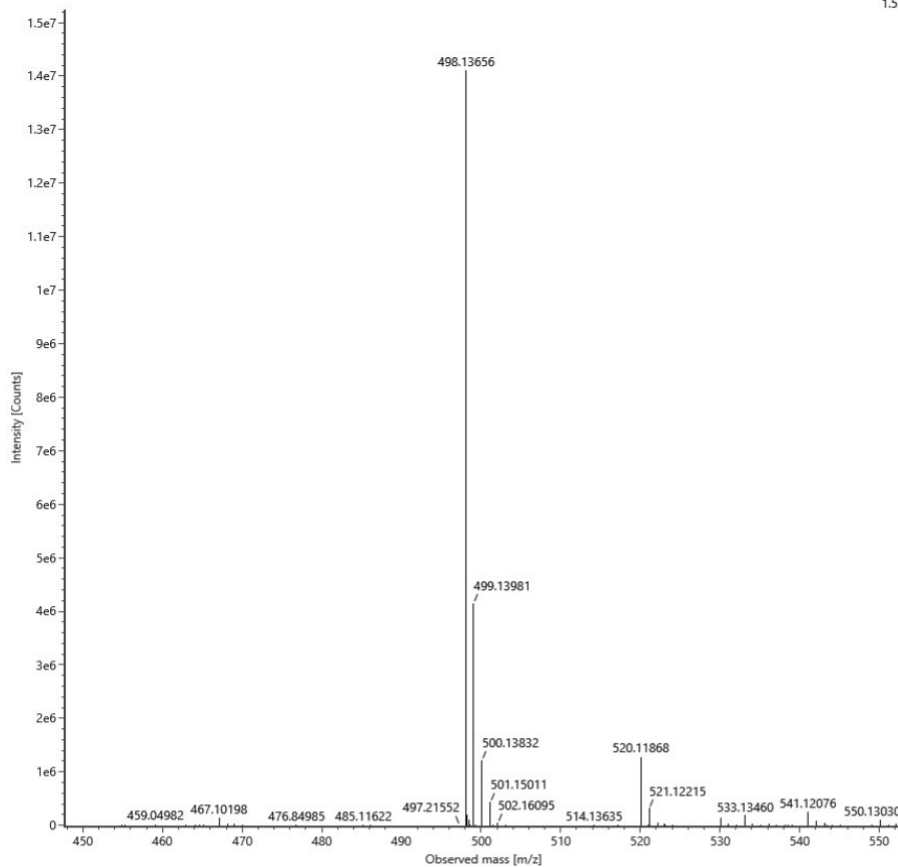


Figure S125 HRMS spectra of compound A27

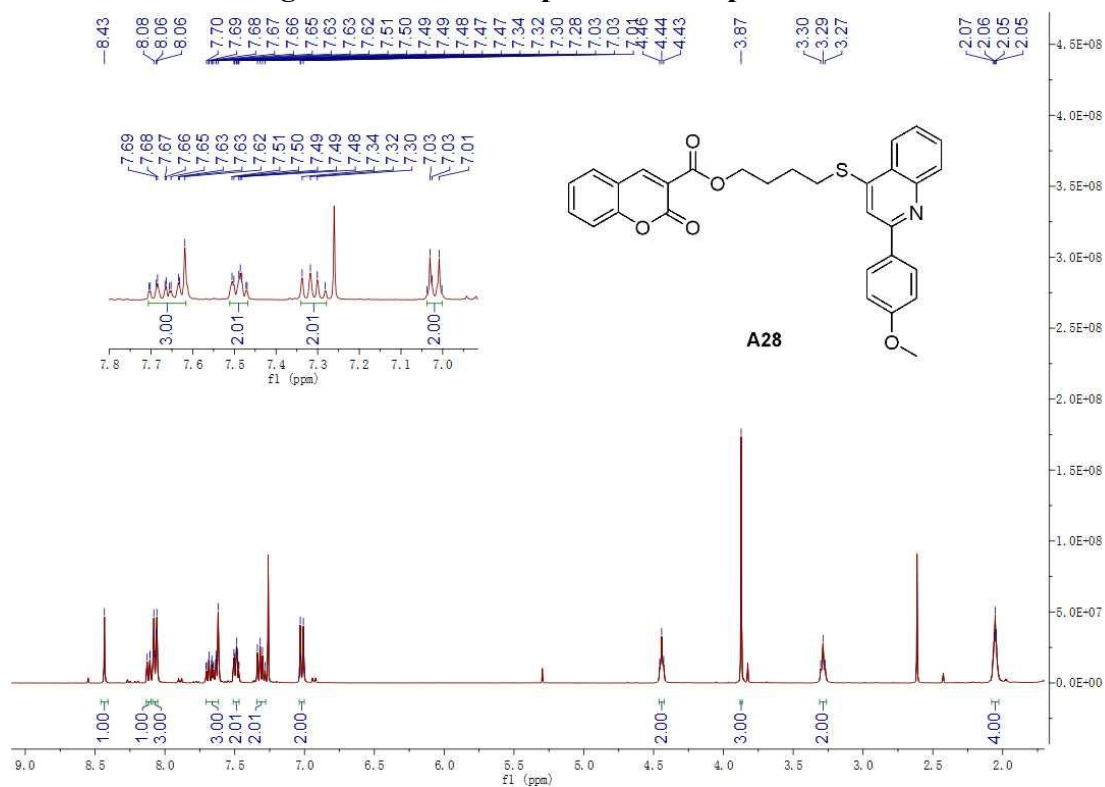


Figure S126 ¹H NMR spectra of compound A28

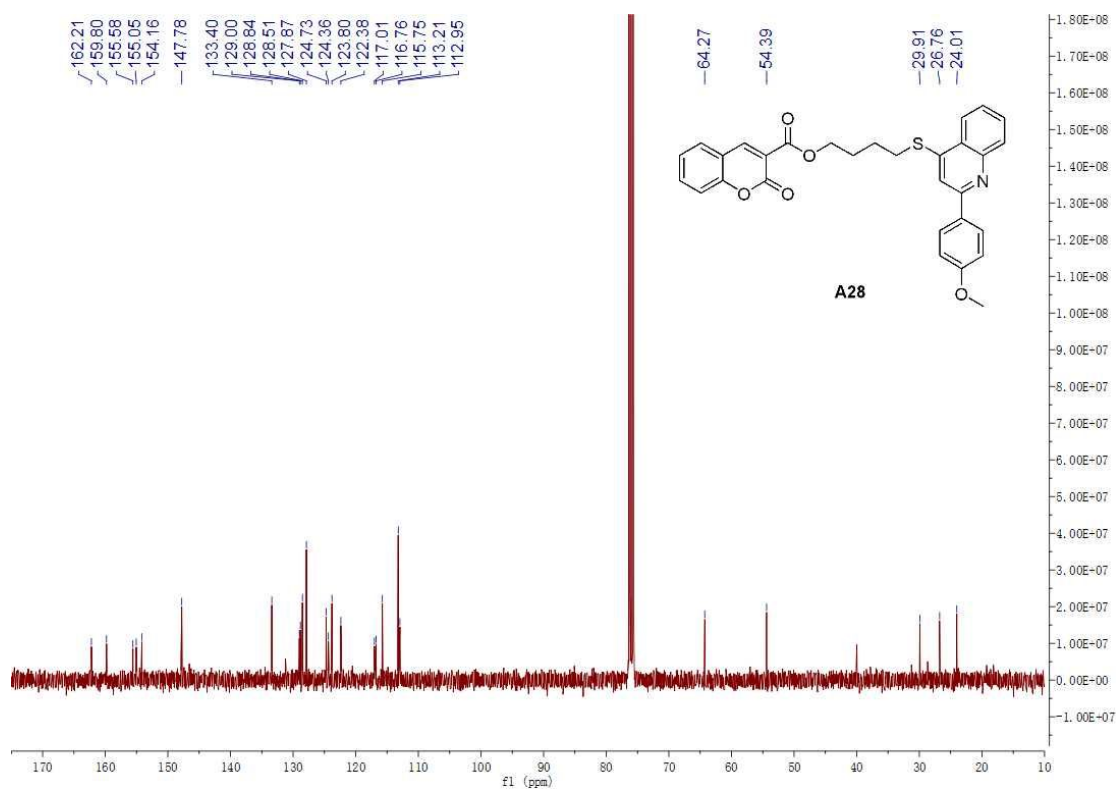
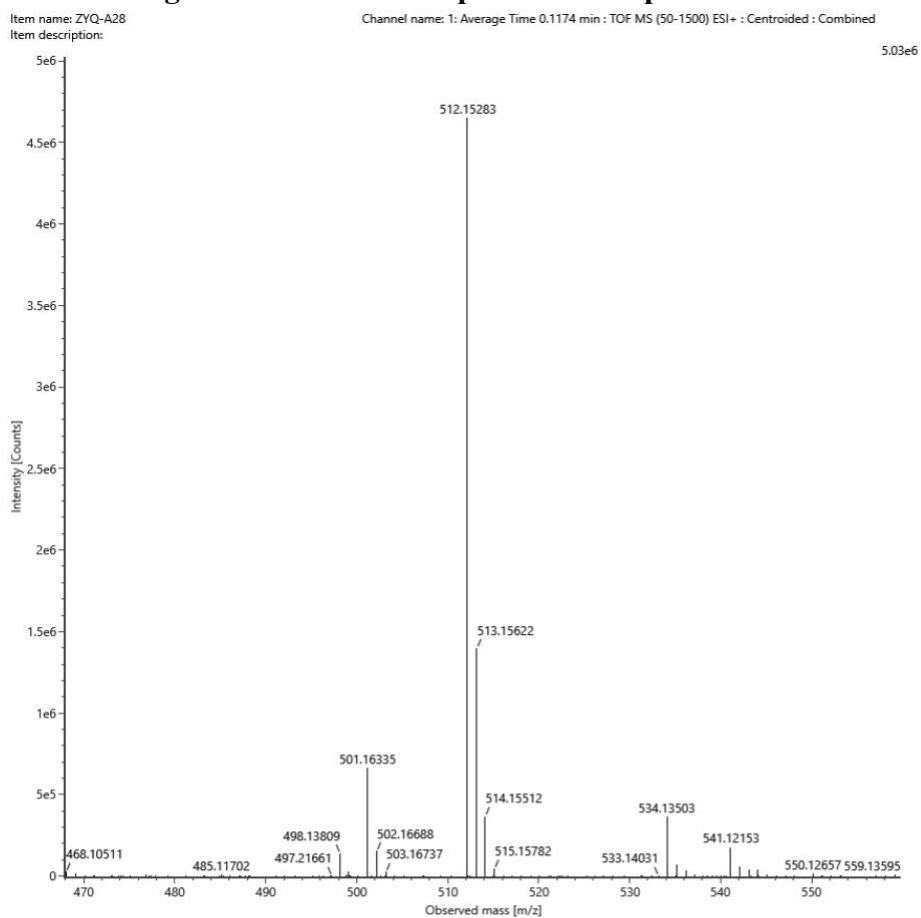


Figure S127 ¹³C NMR spectra of compound A28



Item name: ZYQ-A29
Item description:

Channel name: 1: Average Time 0.1174 min : TOF MS (50-1500) ESI+ : Centroided : Combined

2.94e7

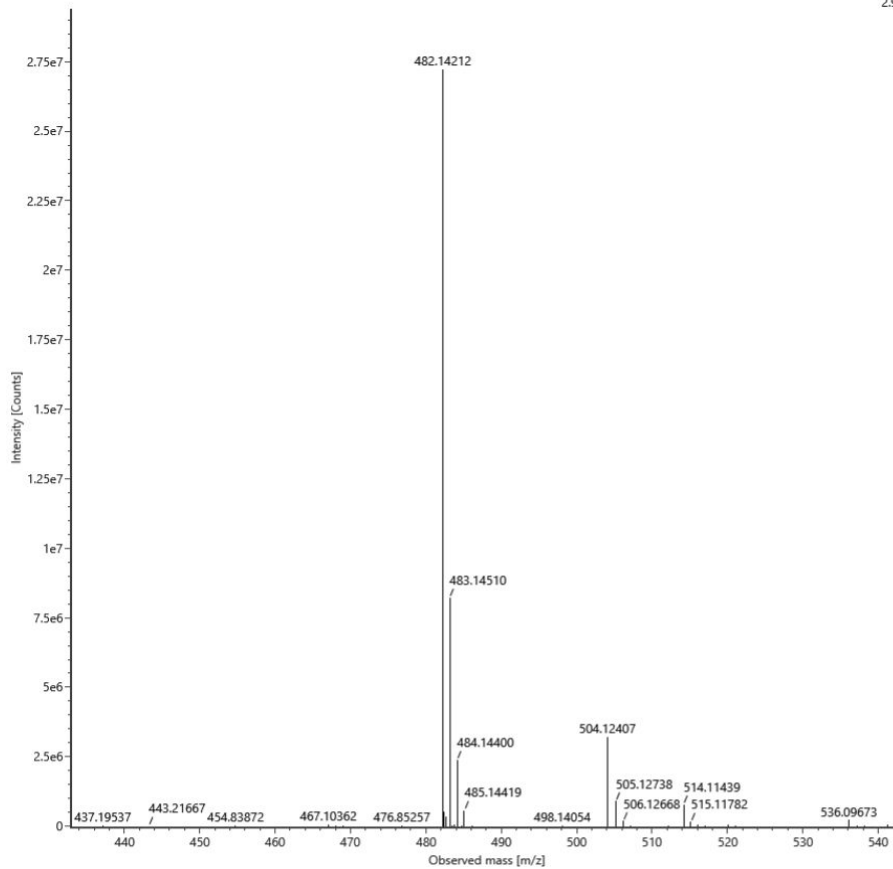


Figure S131 HRMS spectra of compound A29

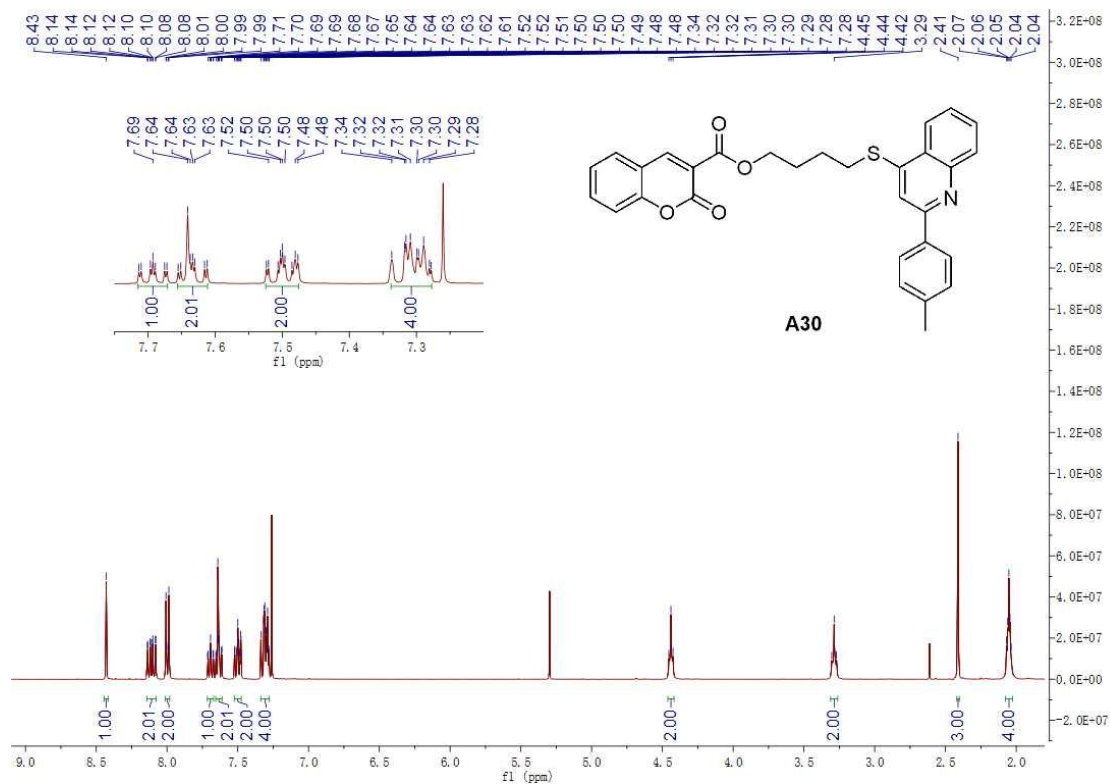


Figure S132 ¹H NMR spectra of compound A30

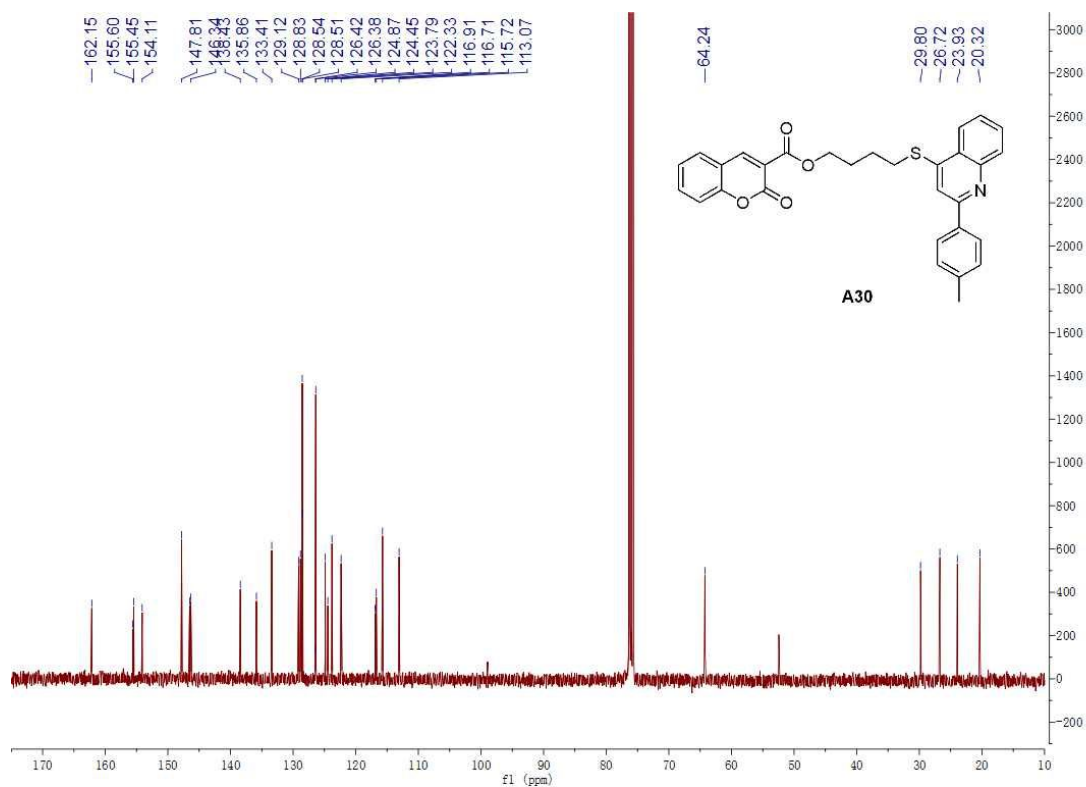


Figure S133 ¹³C NMR spectra of compound A30

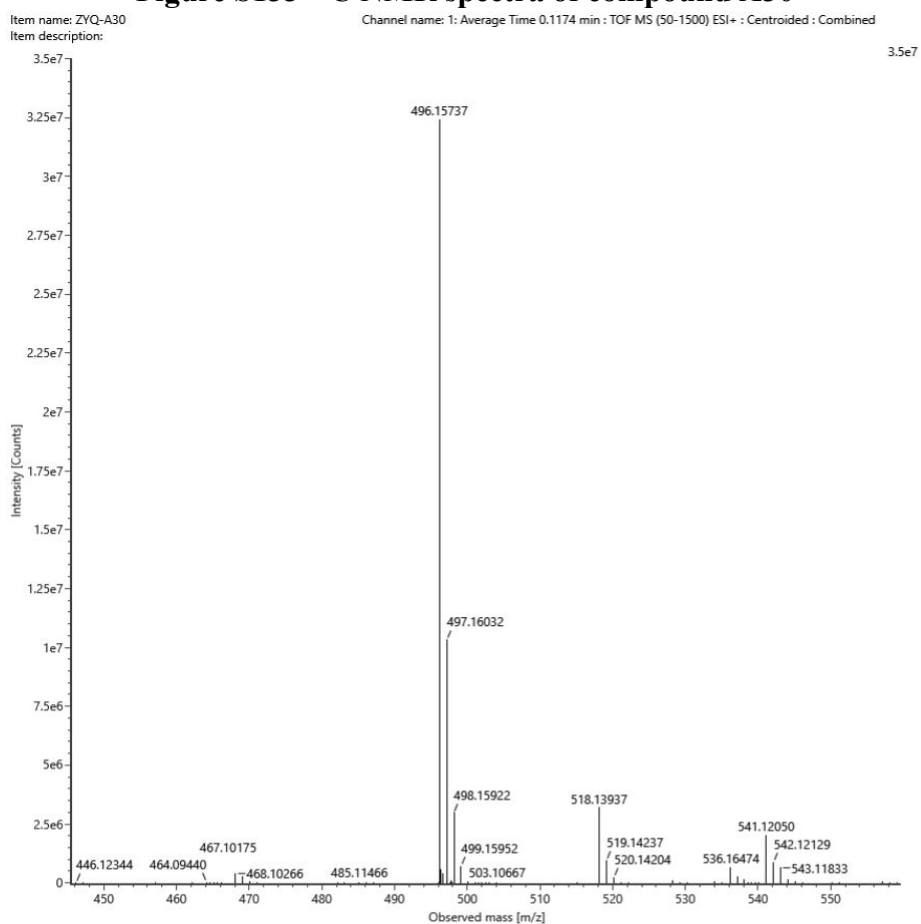


Figure S134 HRMS spectra of compound A30

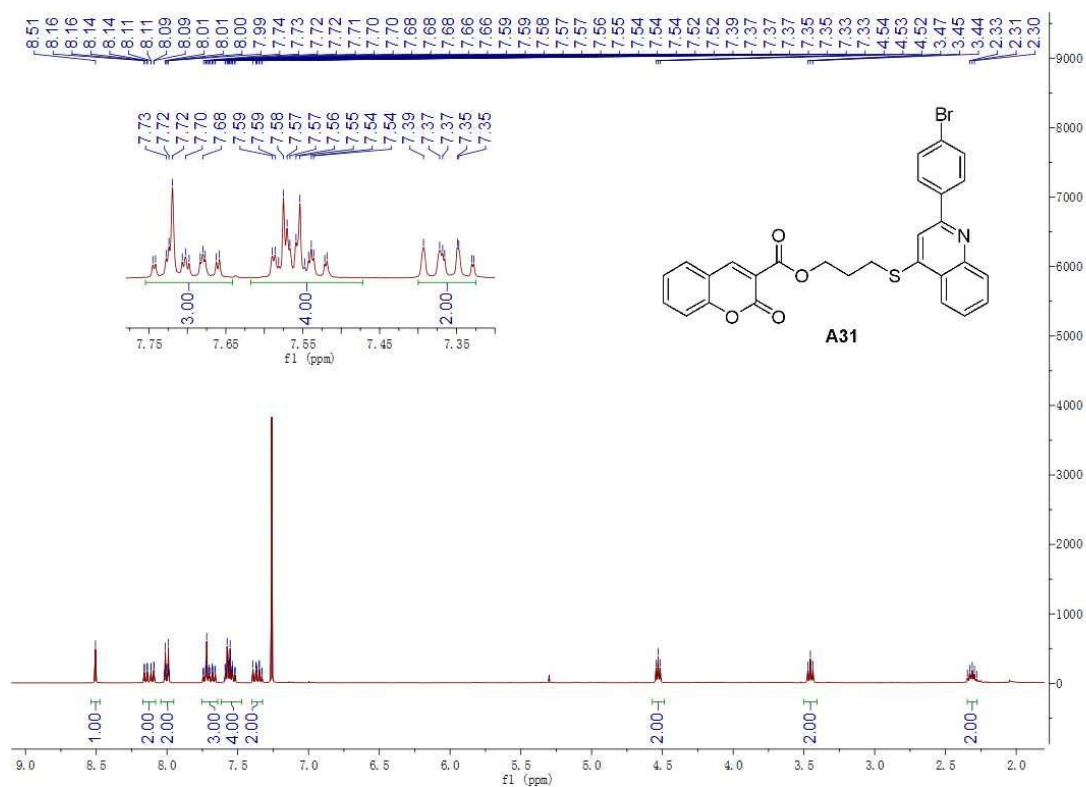


Figure S135 ¹H NMR spectra of compound A31

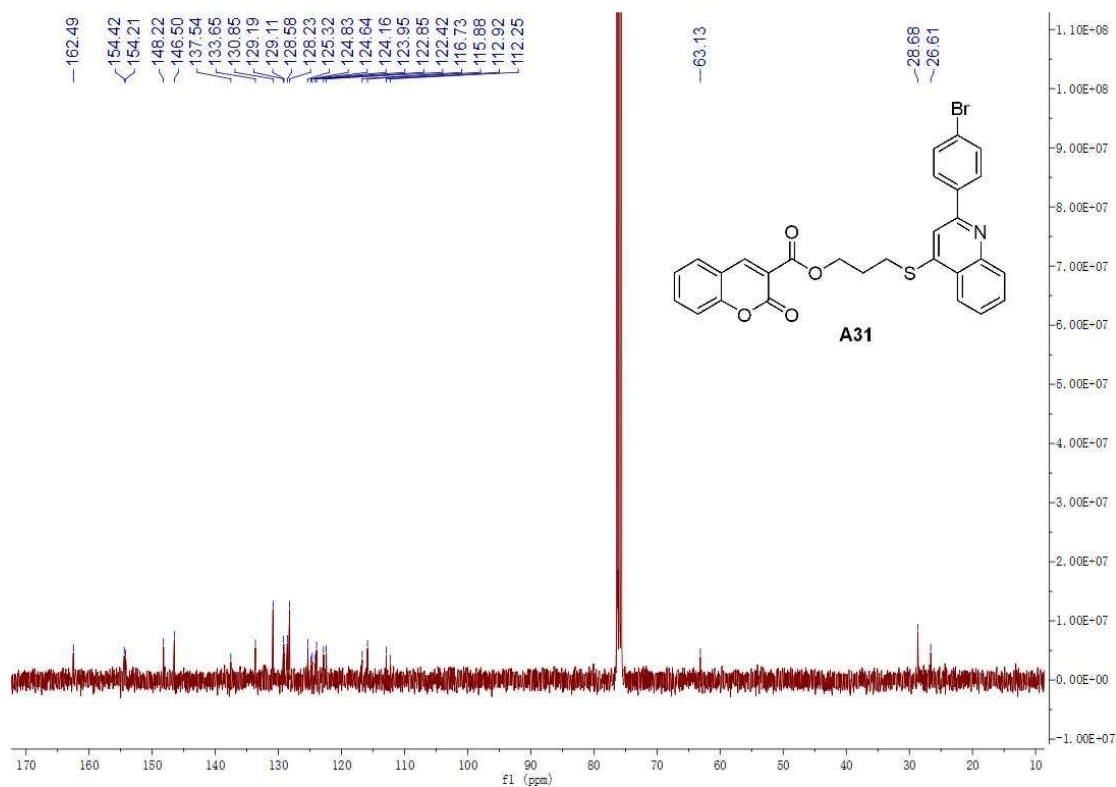


Figure S136 ¹³C NMR spectra of compound A31

Item name: ZYQ-A31
Item description:

Channel name: 1: Average Time 0.1174 min : TOF MS (50-1500) ESI+ : Centroided : Combined

3.49e6

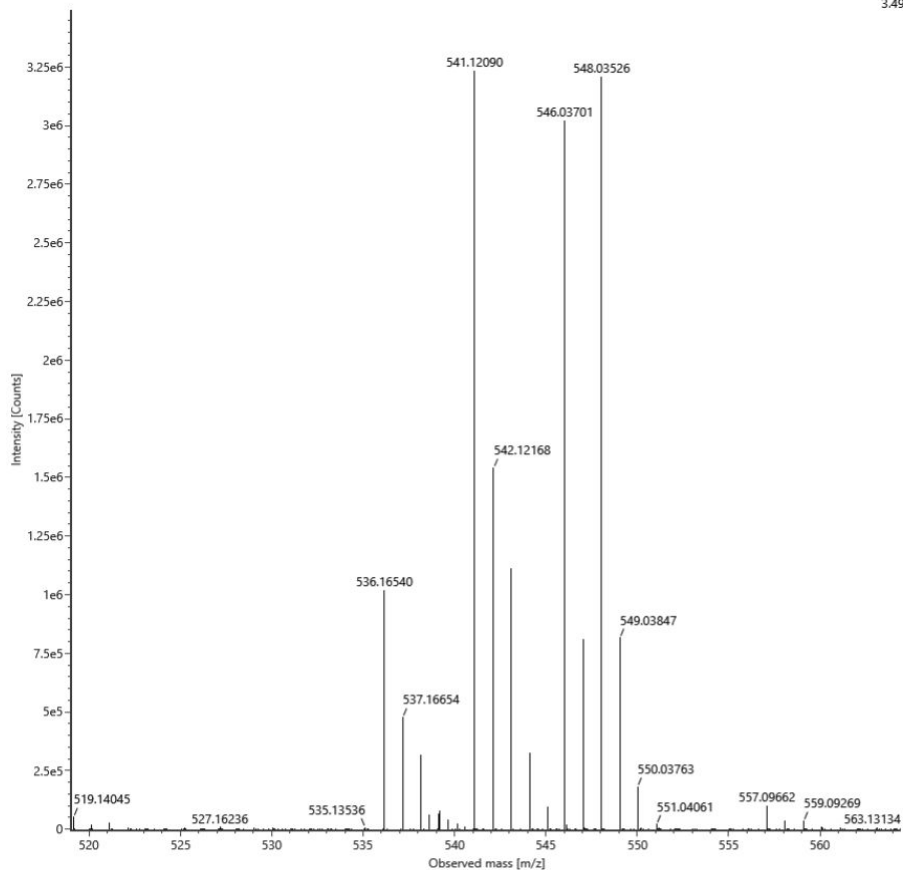


Figure S137 HRMS spectra of compound A31

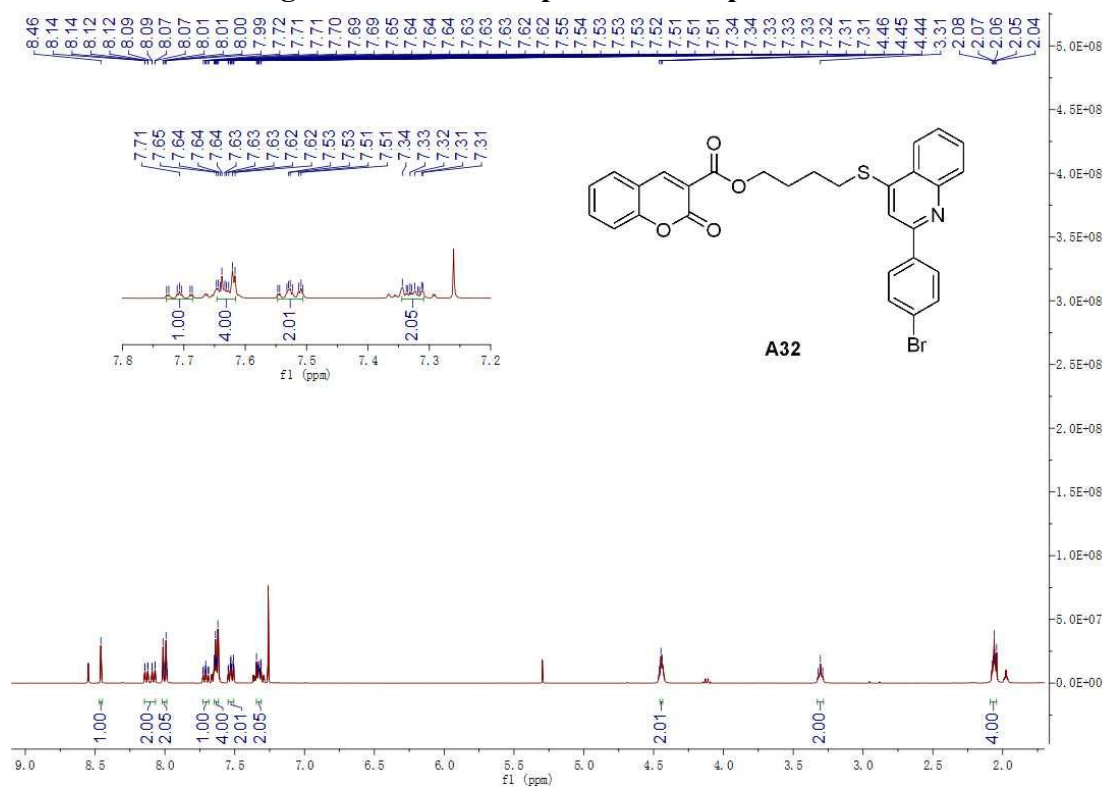


Figure S138 ¹H NMR spectra of compound A32

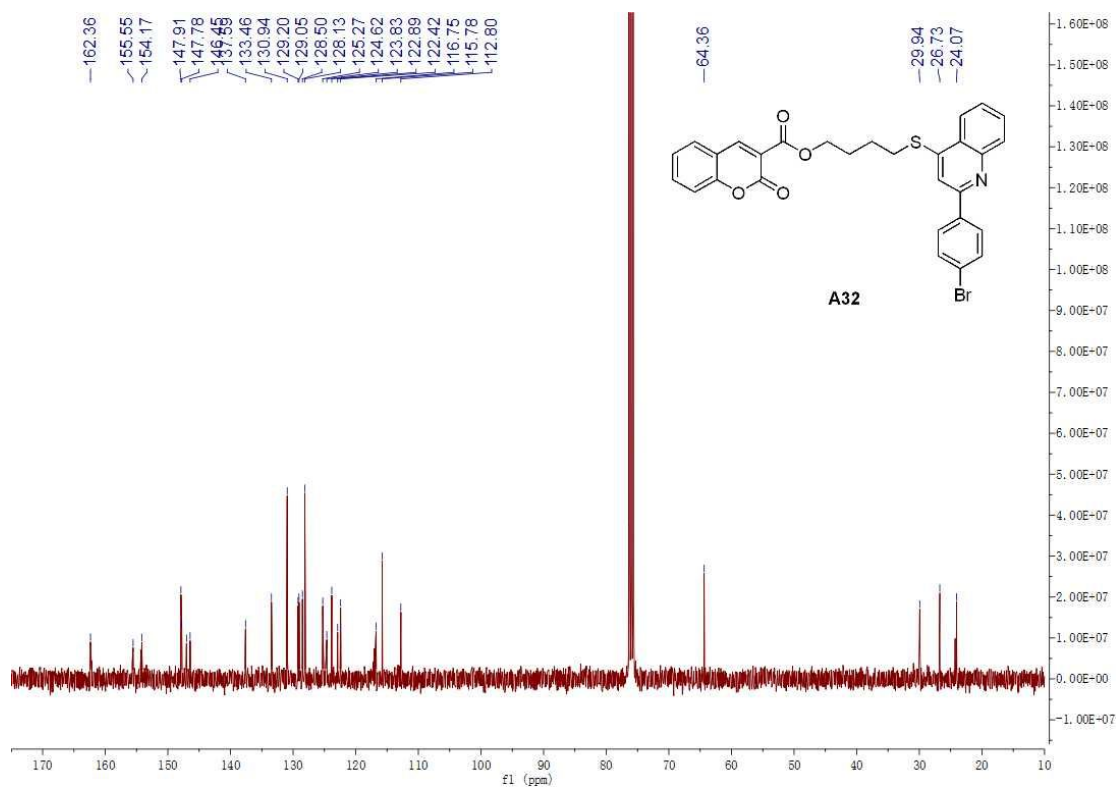


Figure S139 ^{13}C NMR spectra of compound A32

Item name: ZYQ-A32
Item description:

Channel name: 1: Average Time 0.1291 min : TOF MS (50-1500) ESI+ : Centroided : Combined

2.12e6

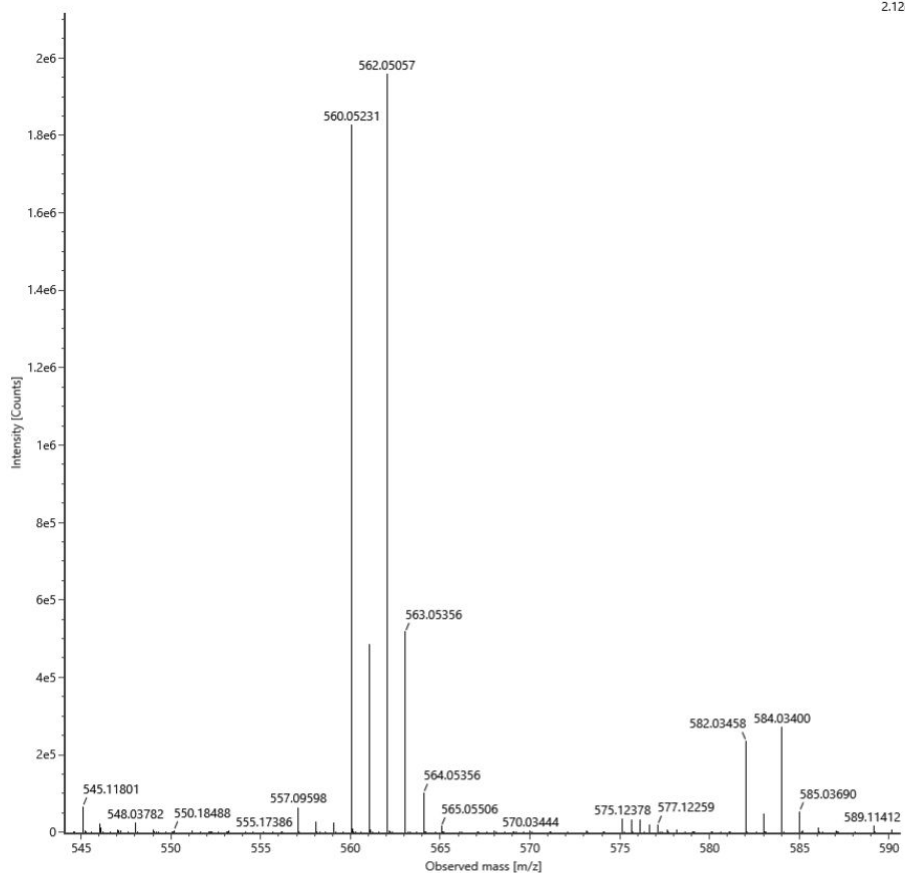


Figure S140 HRMS spectra of compound A32

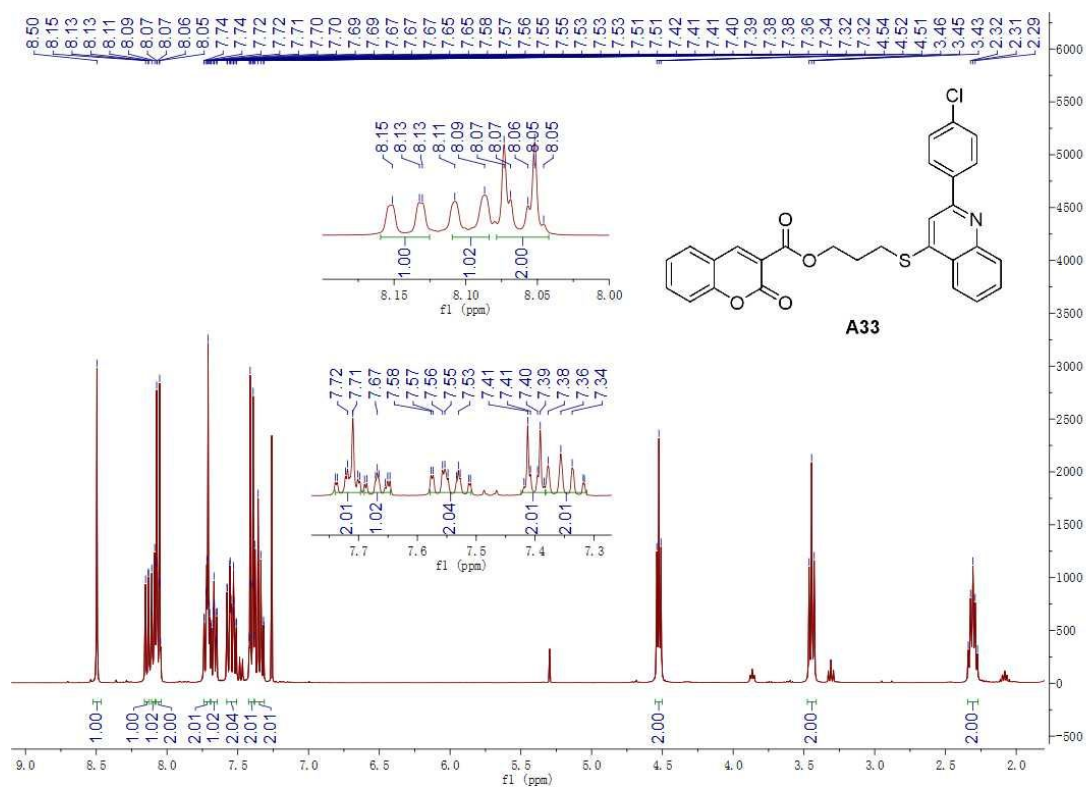


Figure S141 ^1H NMR spectra of compound A33

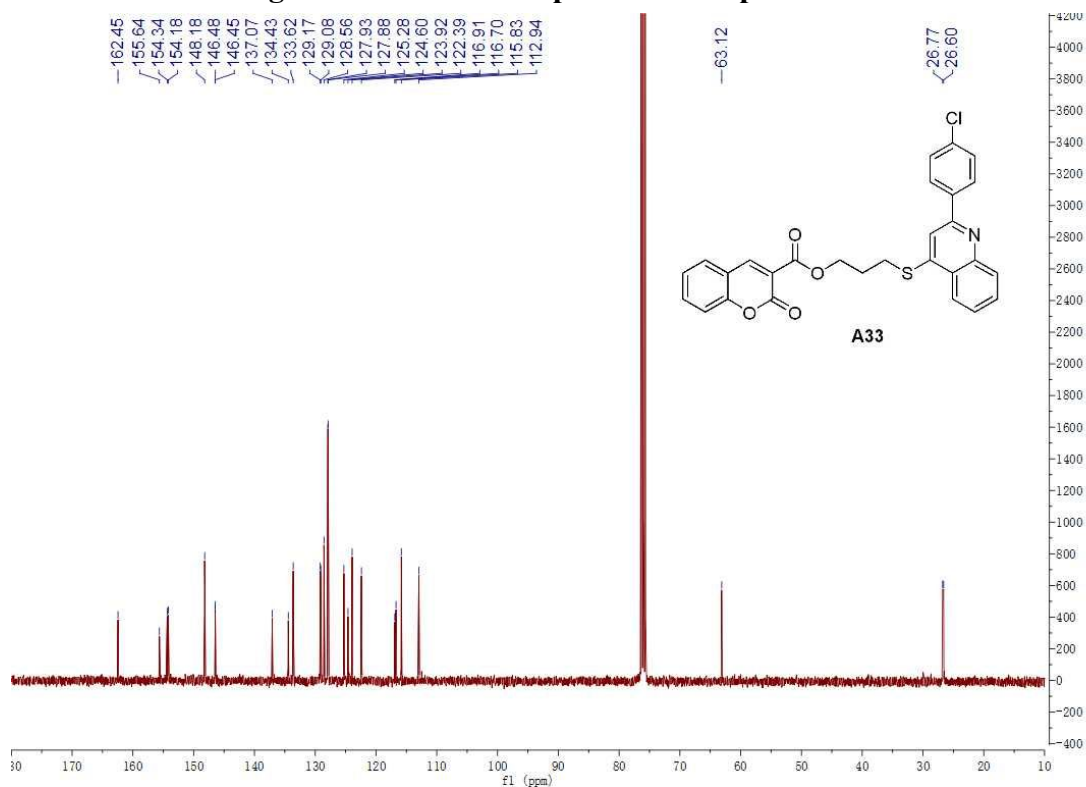


Figure S142 ^{13}C NMR spectra of compound A33

Item name: ZYQ-A33
Item description:

Channel name: 1: Average Time 0.1291 min : TOF MS (50-1500) ESI+ : Centroided : Combined

1.07e7

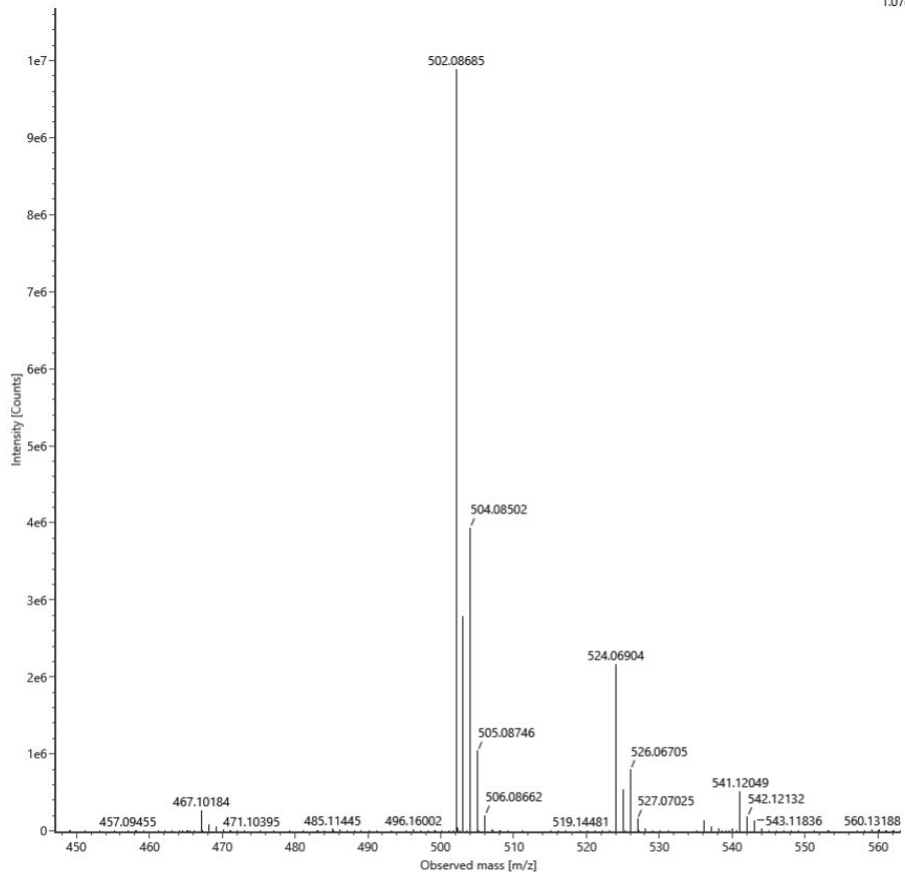


Figure S143 HRMS spectra of compound A33

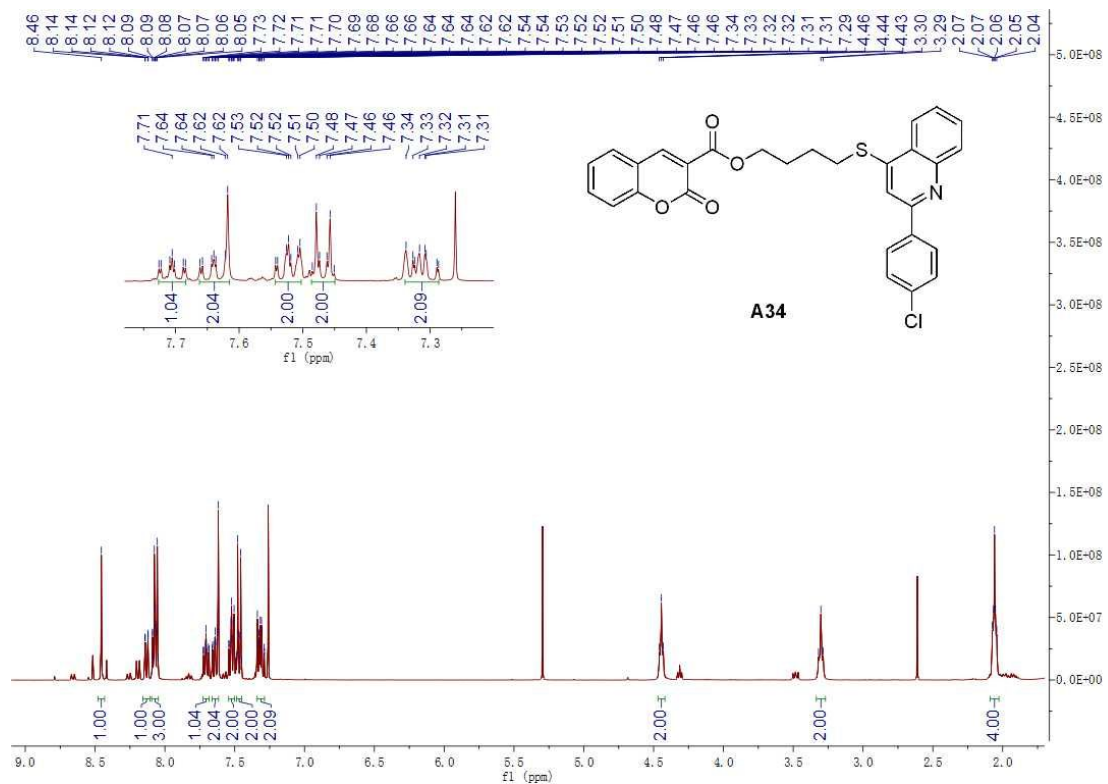
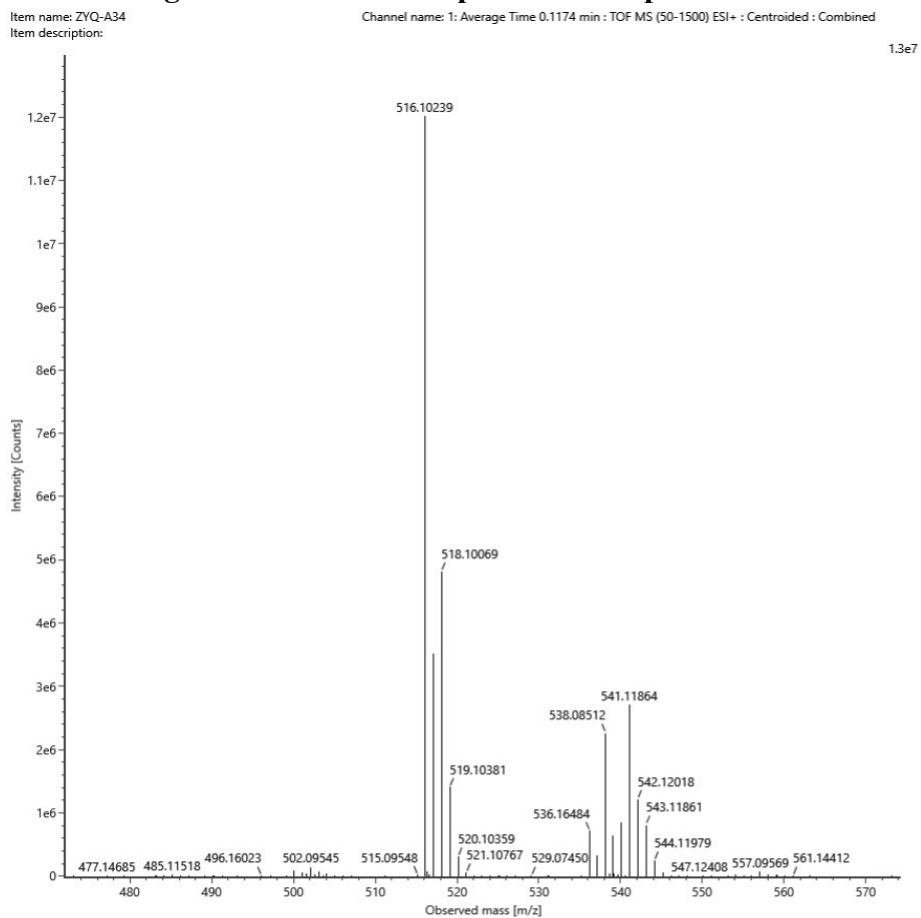
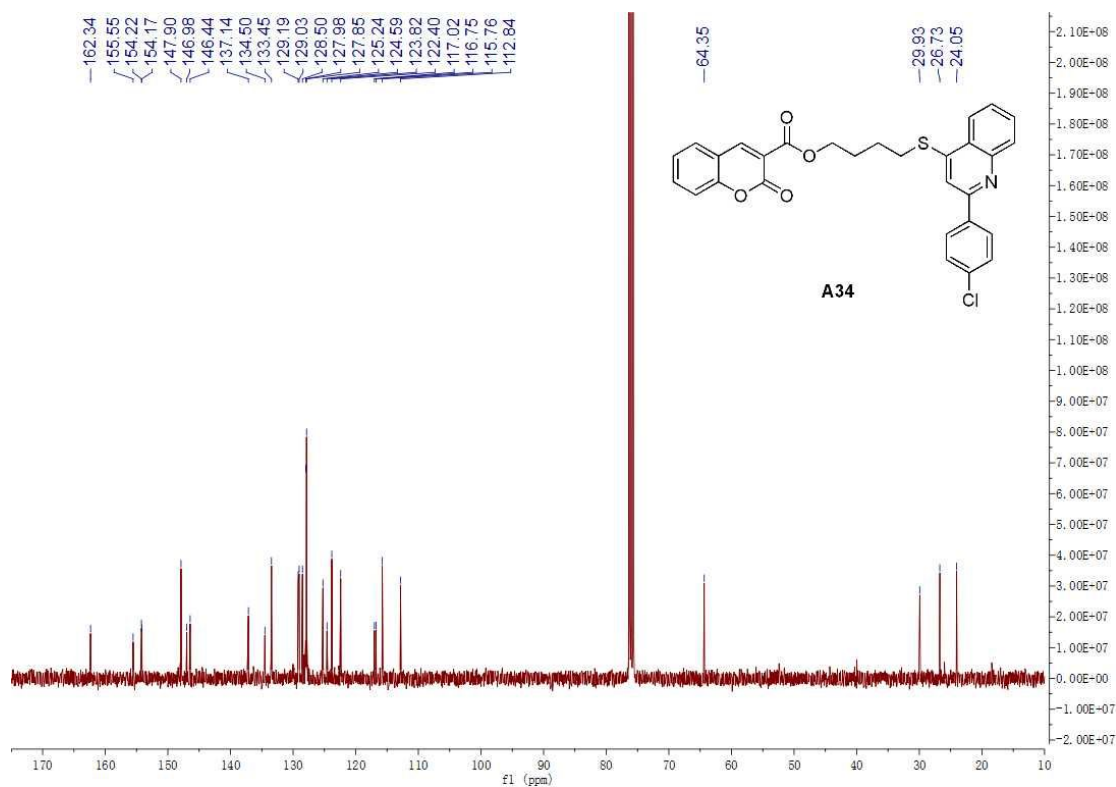


Figure S144 ¹H NMR spectra of compound A34



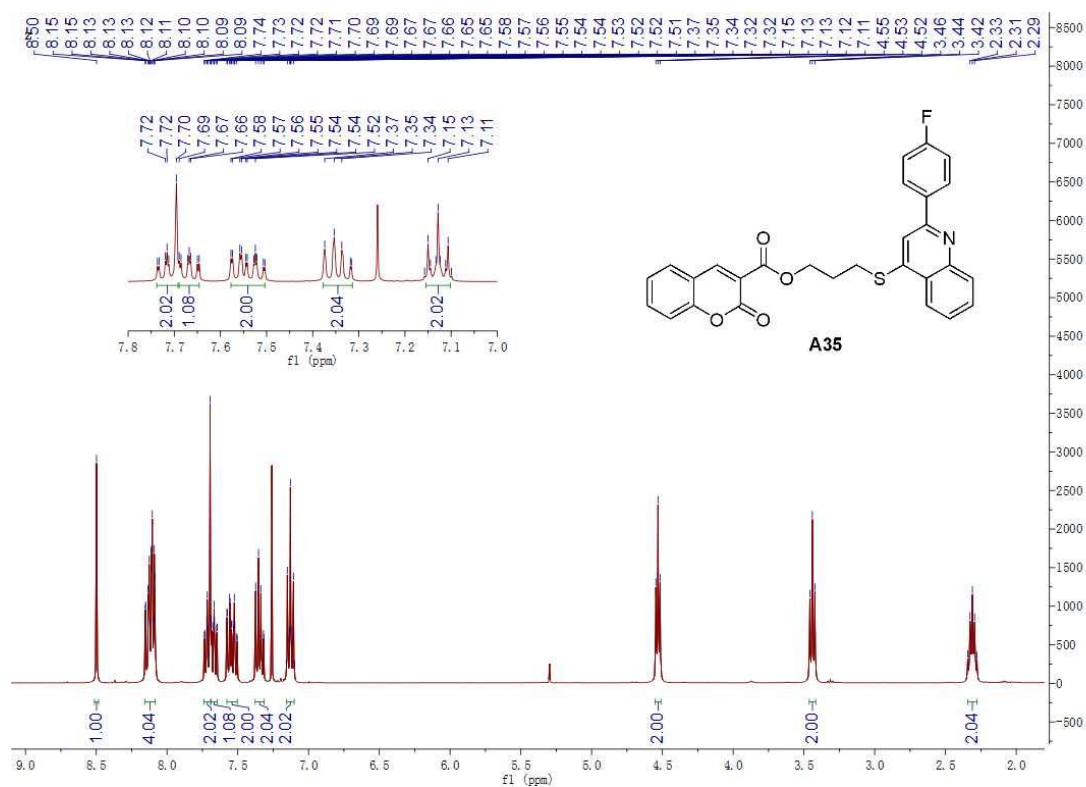


Figure S147 ¹H NMR spectra of compound A35

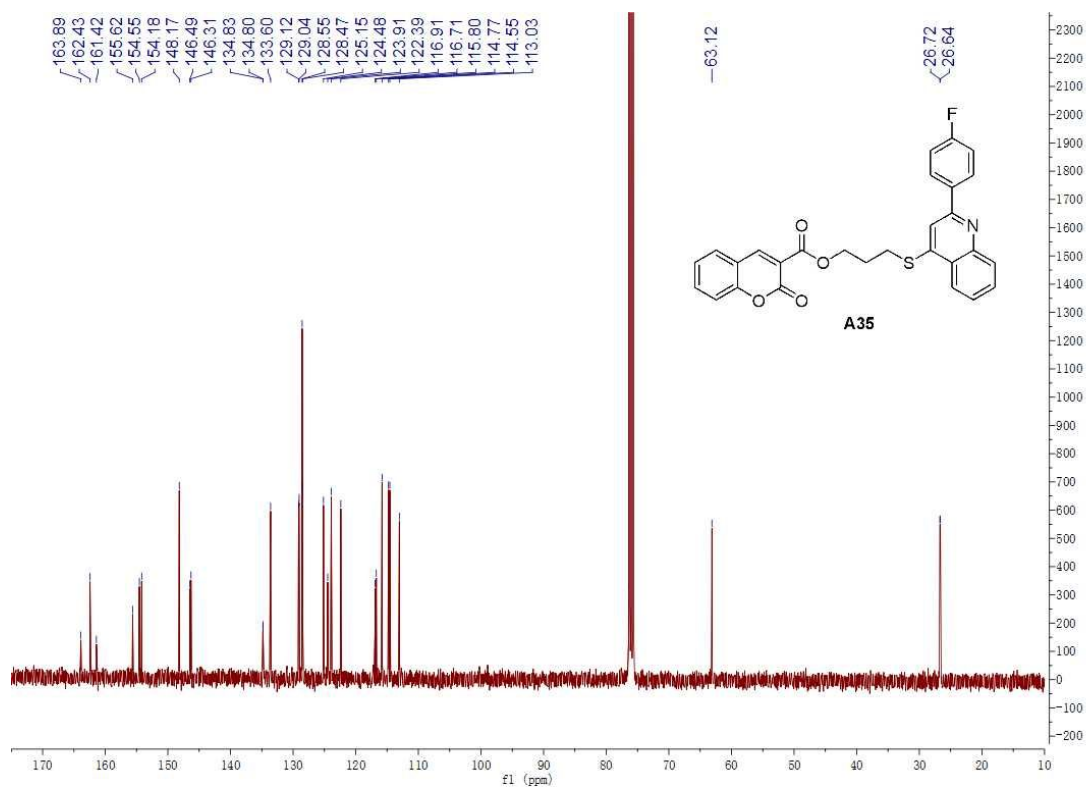
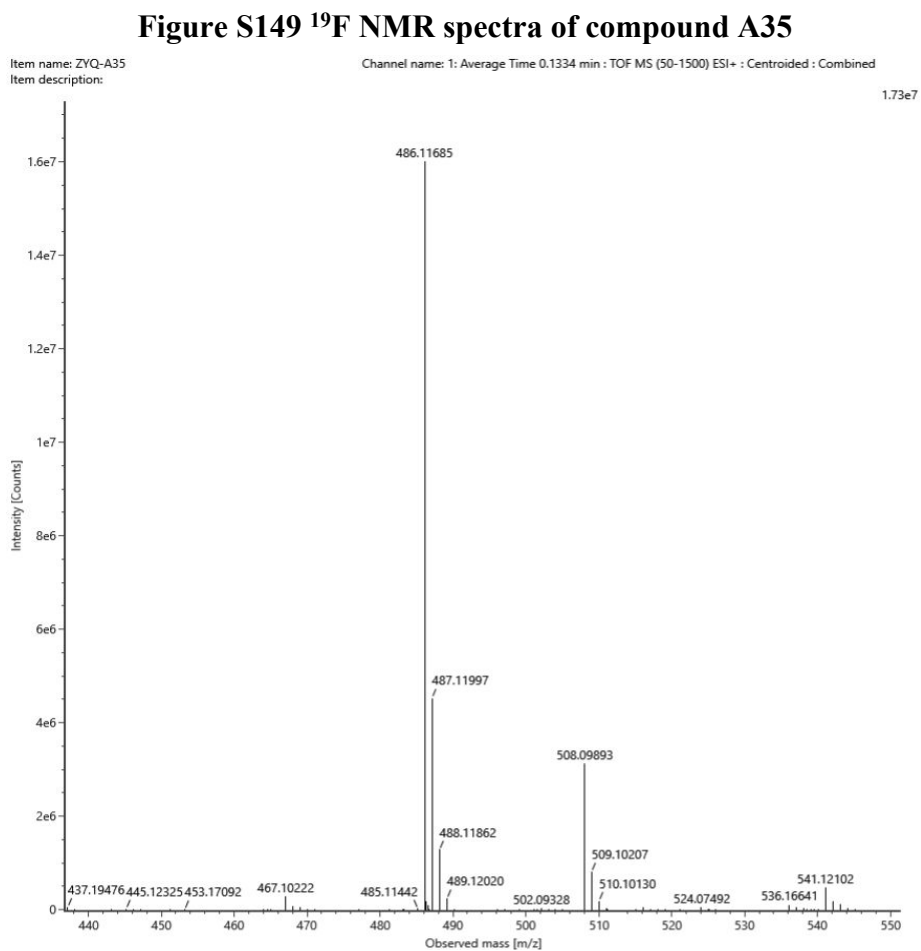
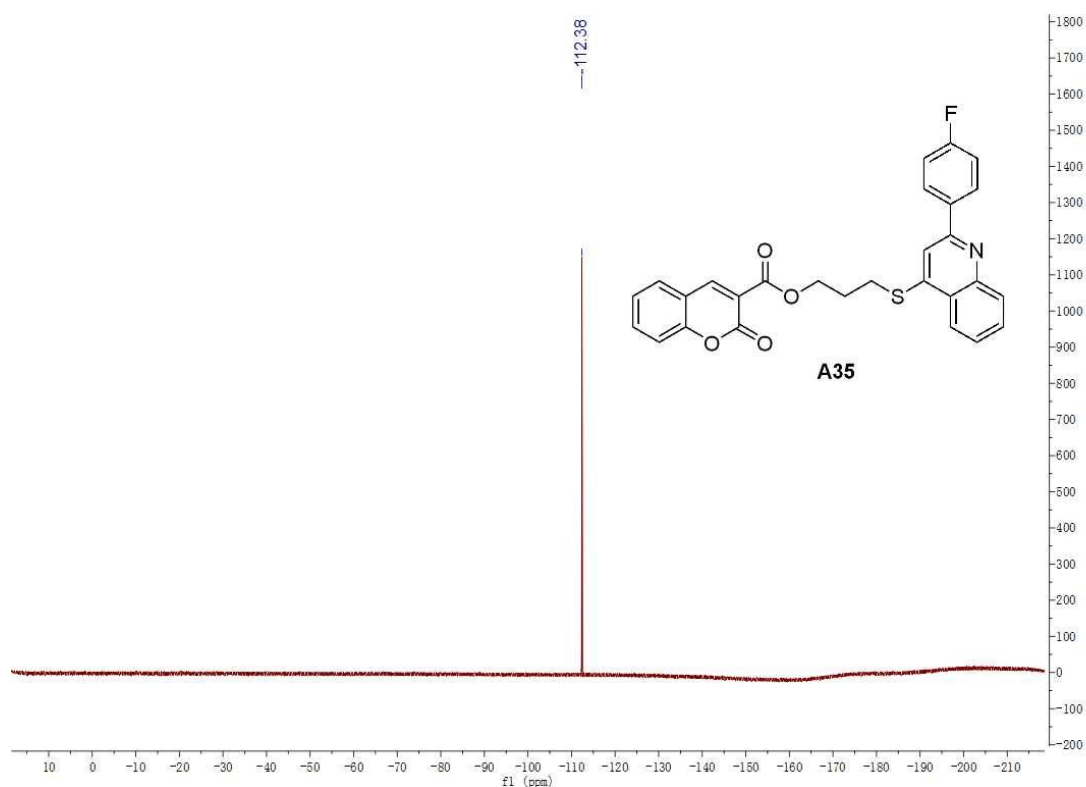


Figure S148 ¹³C NMR spectra of compound A35



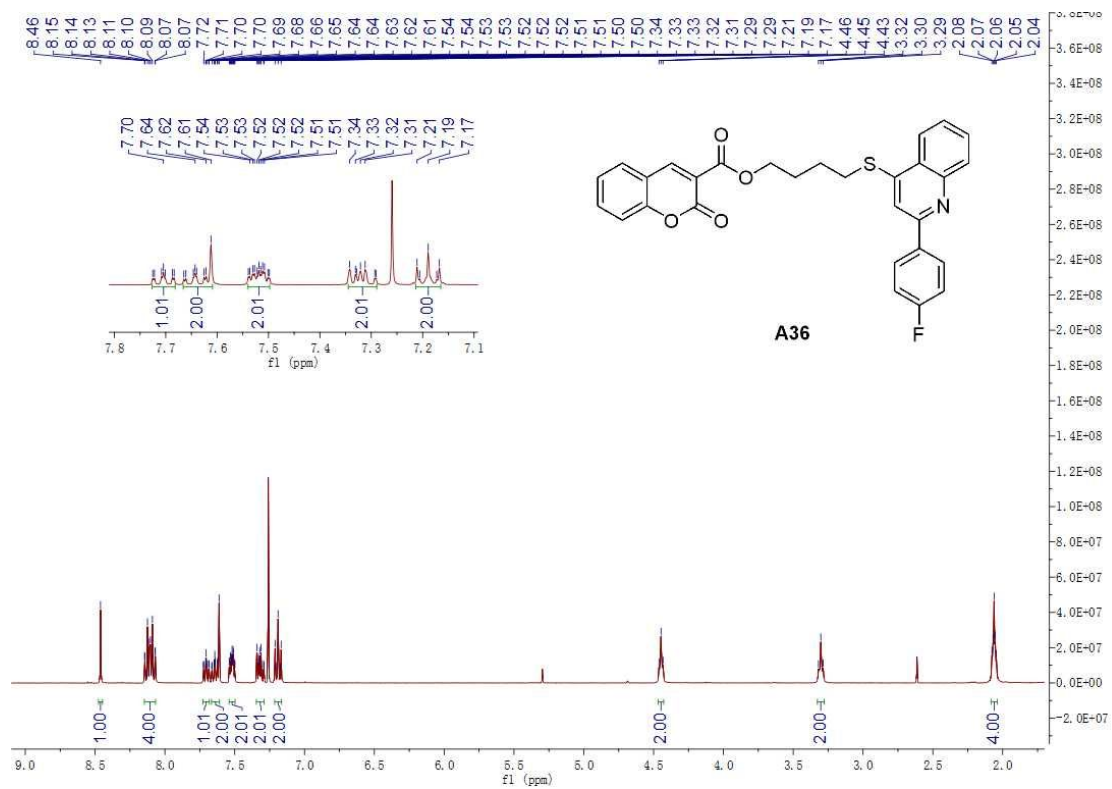


Figure S151 ¹H NMR spectra of compound A36

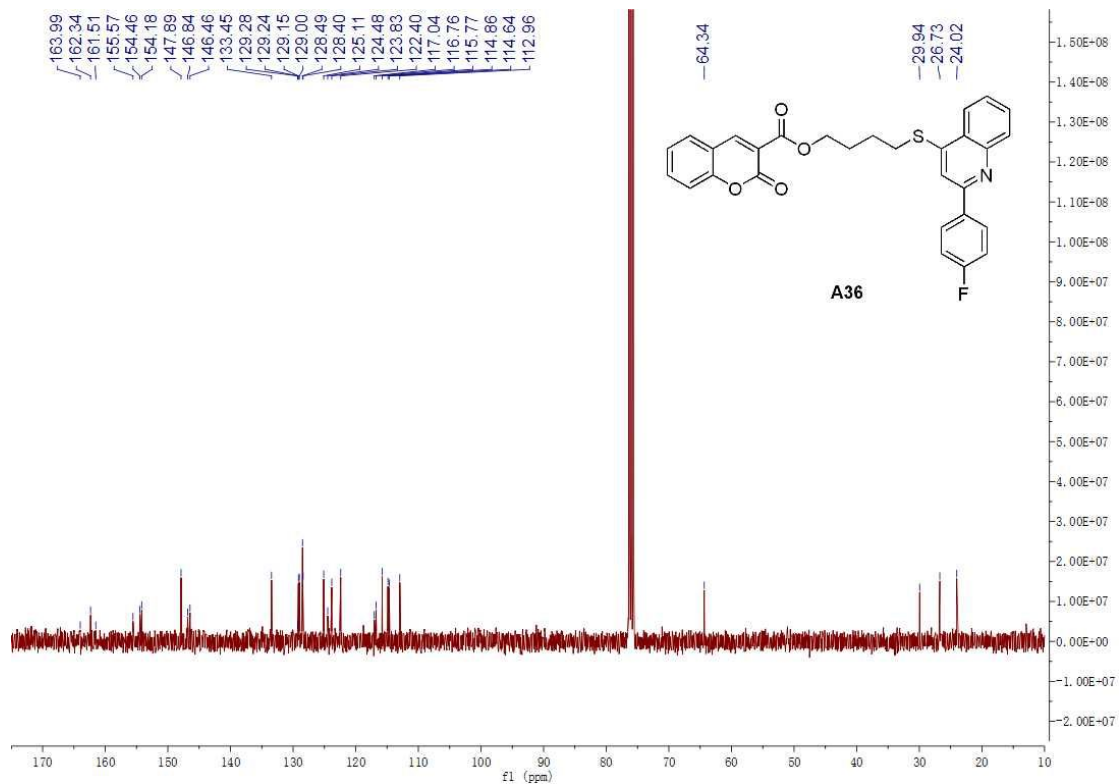


Figure S152 ¹³C NMR spectra of compound A36

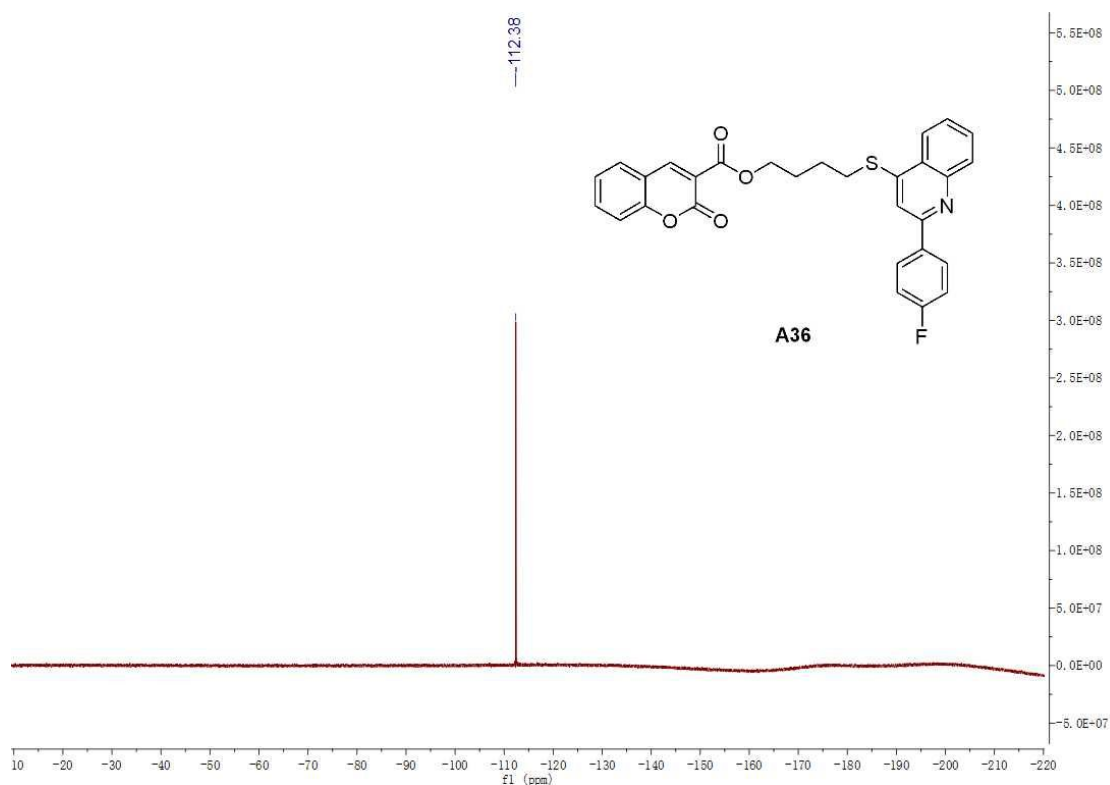


Figure S153 ¹⁹F NMR spectra of compound A36

Item name: ZYQ-A36
Item description:

Channel name: 1: Average Time 0.1217 min : TOF MS (50-1500) ESI+ : Centroided : Combined

6.98e6

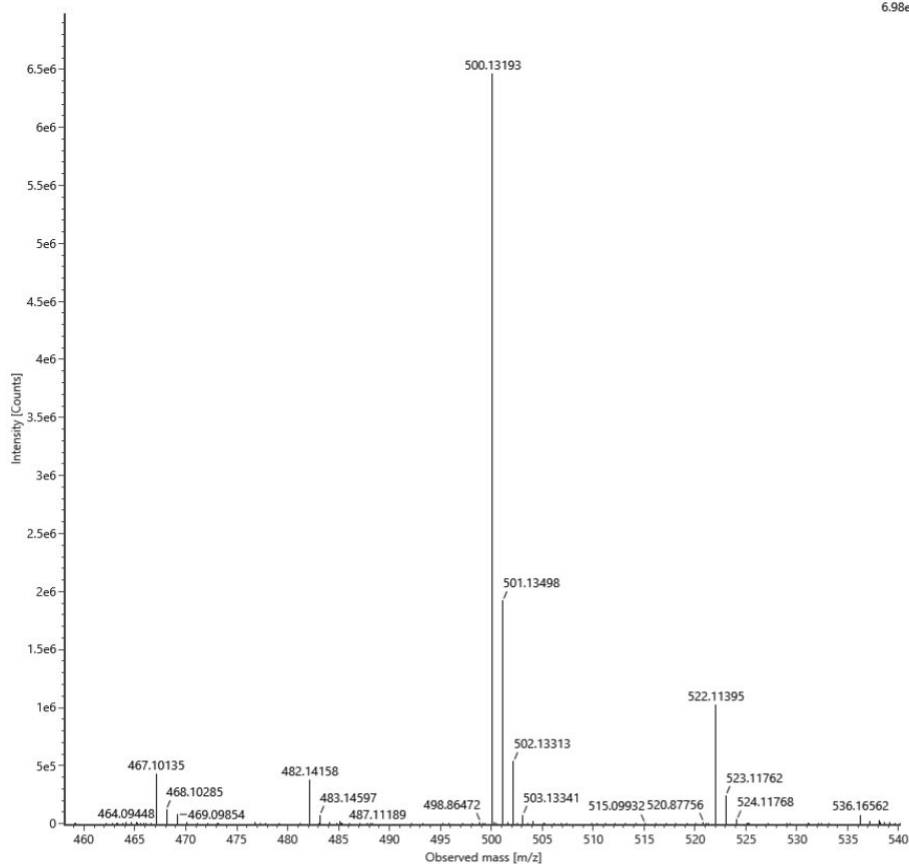


Figure S154 HRMS spectra of compound A36

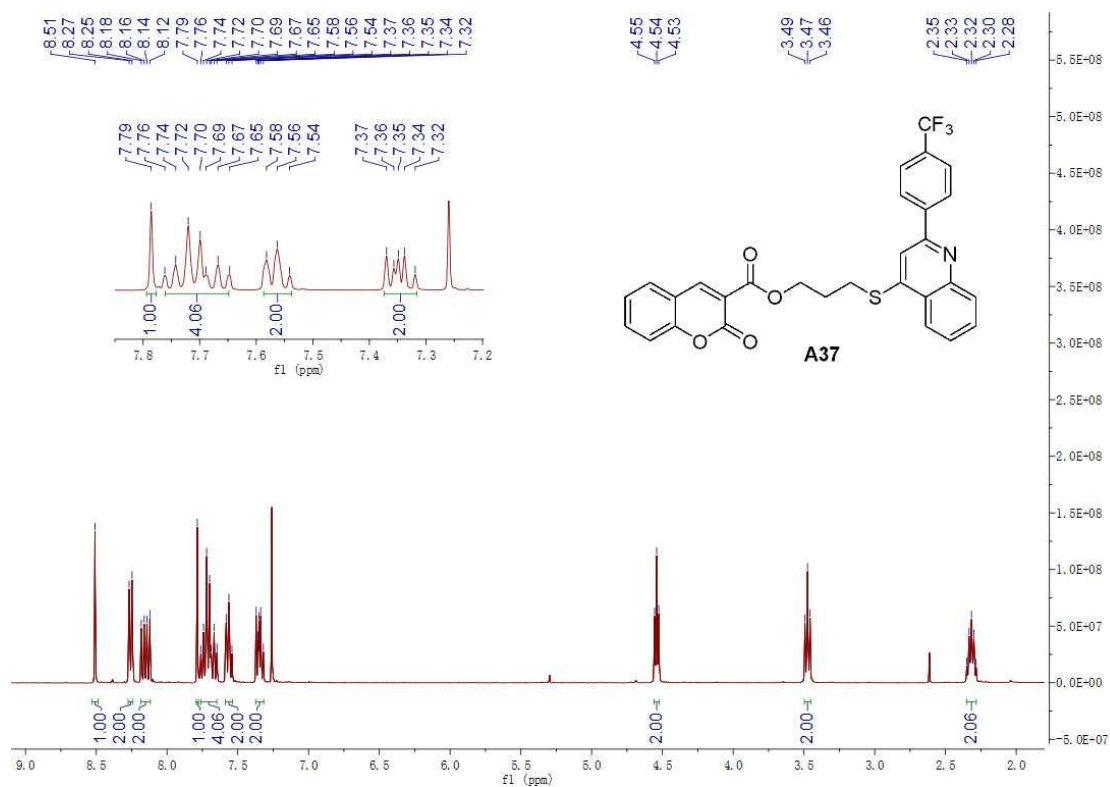


Figure S155 ^1H NMR spectra of compound A37

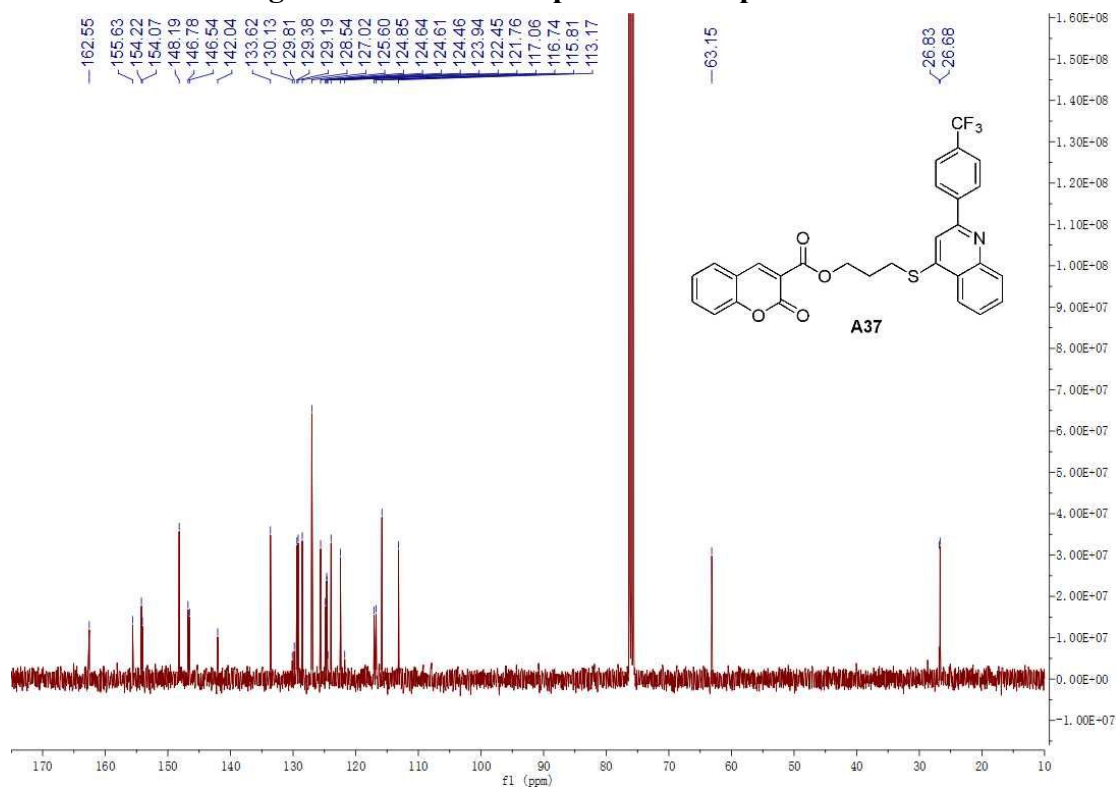


Figure S156 ^{13}C NMR spectra of compound A37

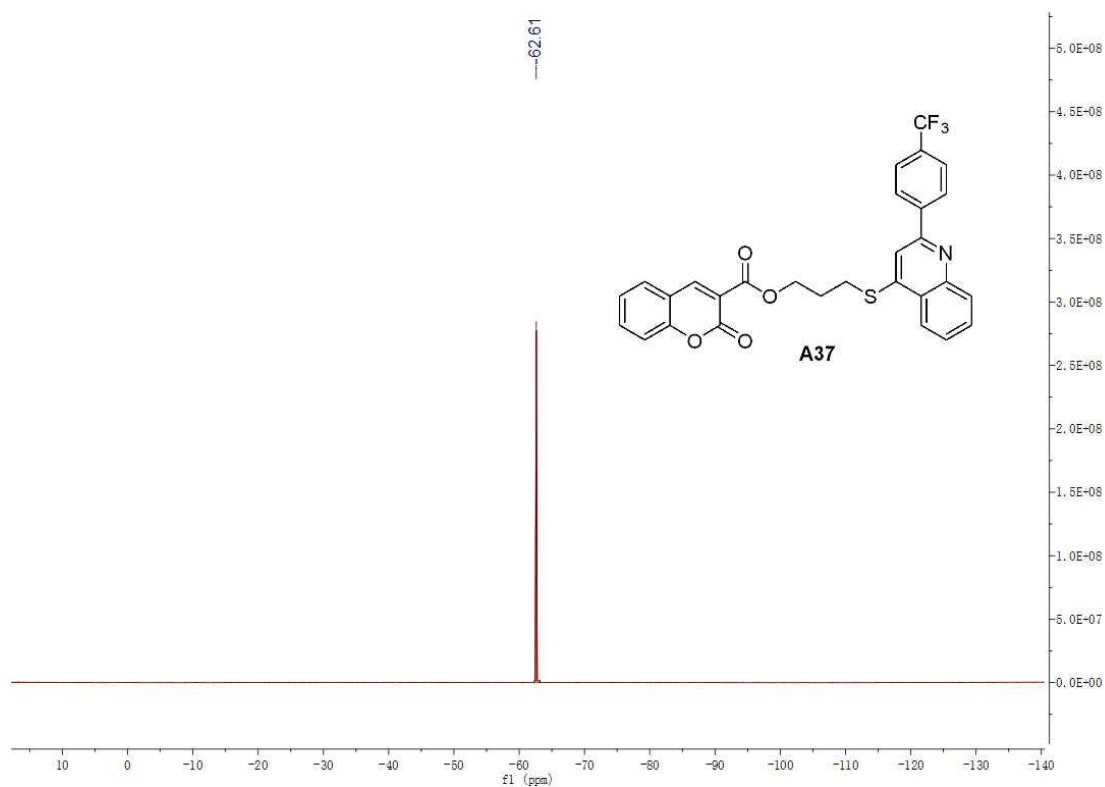


Figure S157 ^{19}F NMR spectra of compound A37

Item name: ZYQ-A37
Item description:

Channel name: 1: Average Time 0.1334 min : TOF MS (50-1500) ESI+ : Centroided : Combined

6.87e6

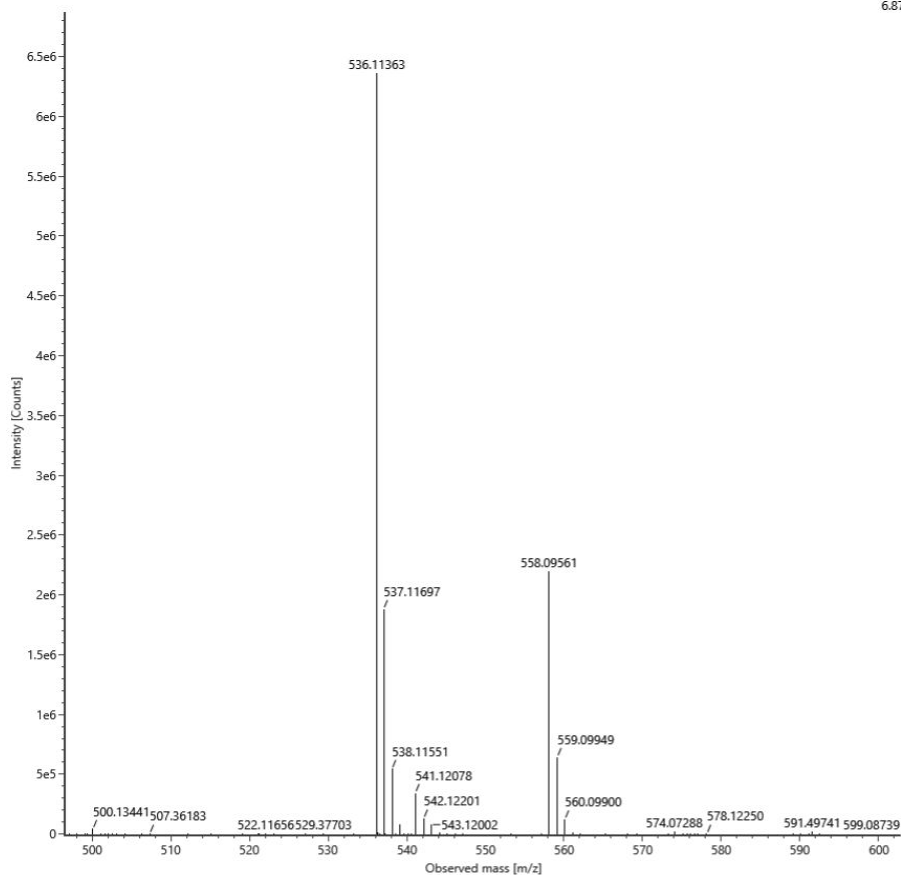


Figure S158 HRMS spectra of compound A37

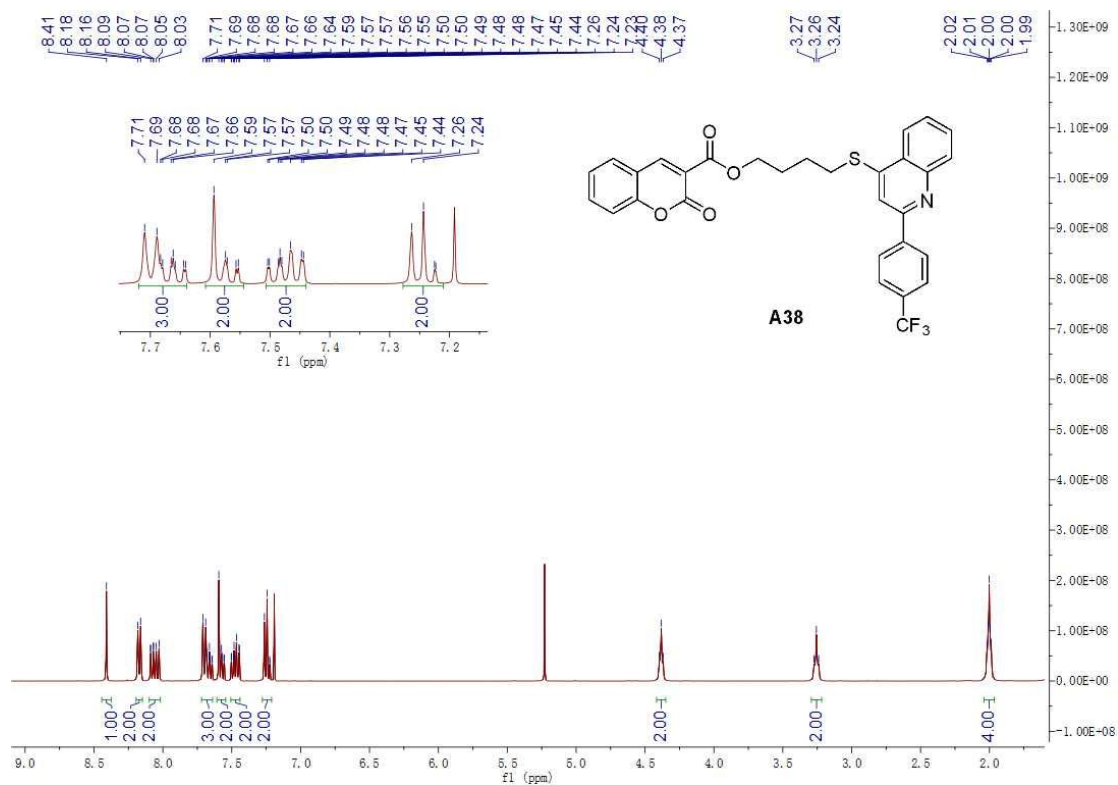


Figure S159 ^1H NMR spectra of compound **A38**

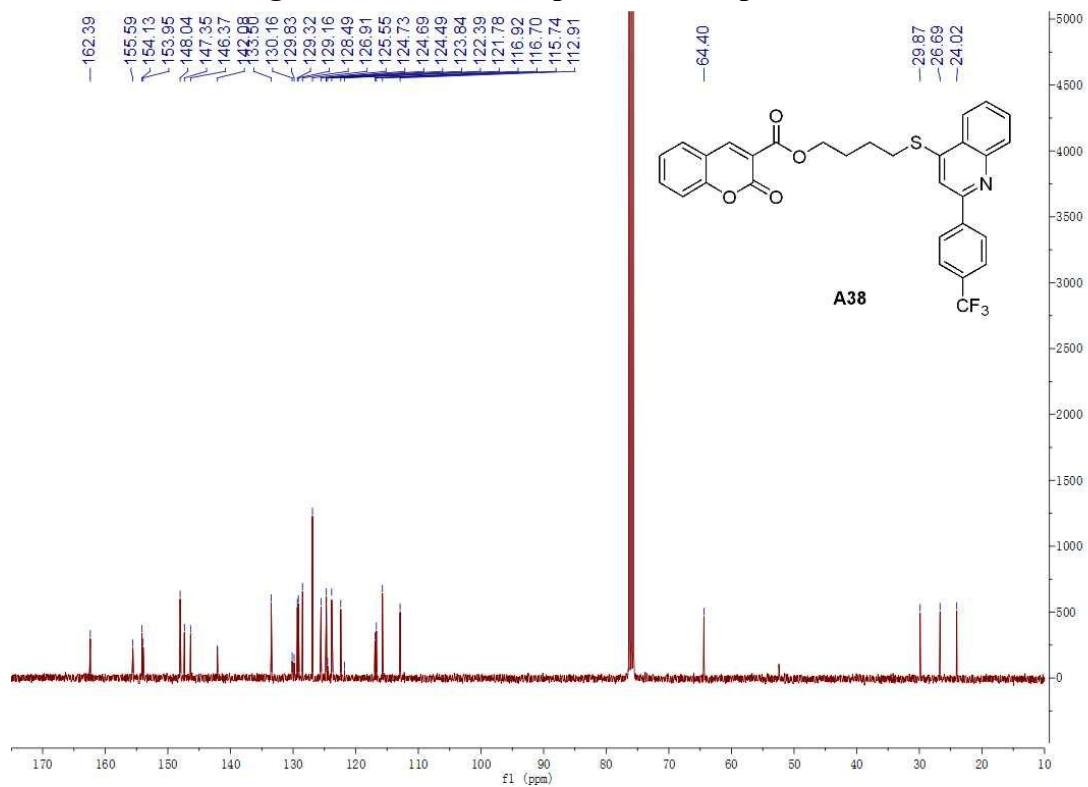


Figure S160 ^{13}C NMR spectra of compound **A38**

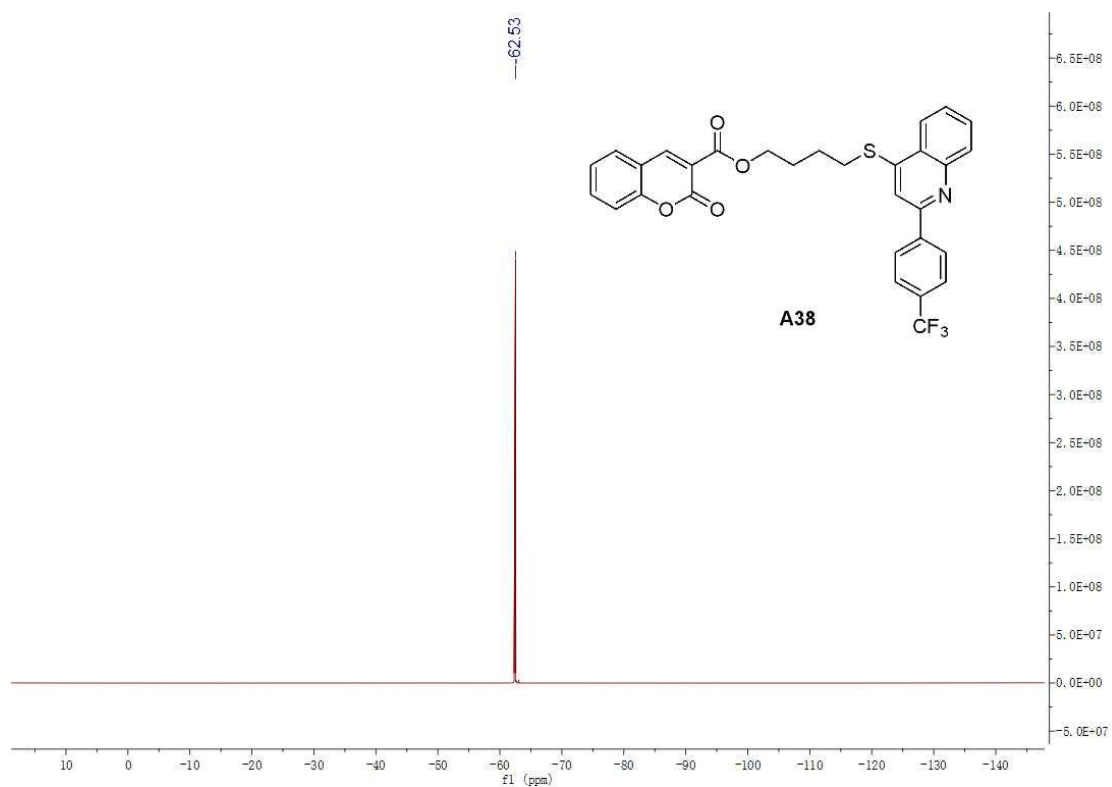


Figure S161 ^{19}F NMR spectra of compound A38

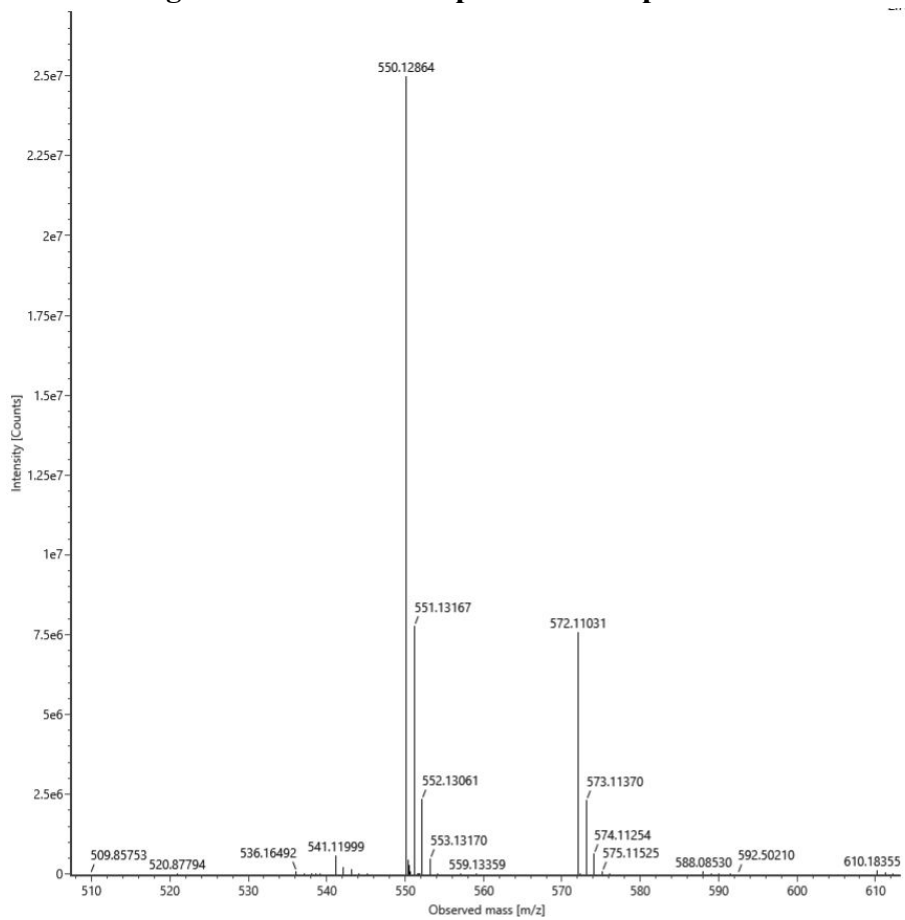


Figure S162 HRMS spectra of compound A38