**Supplementary data**

# Synthesis and biological evaluation of terminal functionalized thiourea-containing dipeptides as antitumor agents

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## spectral data of title compounds

*1-(1-(1-(2,5-dimethoxyphenylamino)-1-oxo-3-phenylpropan-2-ylamino)-3-methyl-1-oxopentan-2-yl)-3-(3-nitrophenyl)thiourea (**I-1**)*. Yield 77.4%. Mp 187.5−190.1 °C. $[\alpha_D]^{20}$ = -29.2 (*c* 0.1, AcOEt). $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 10.15 (s, 1H), 9.06 (s, 1H), 8.84 (s, 1H), 8.61 (d, *J* = 7.9 Hz, 1H), 7.97 (d, *J* = 8.5 Hz, 1H), 7.92 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.83 (dd, *J* = 8.1, 1.2 Hz, 1H),7.73 (d, *J* = 2.7 Hz, 1H), 7.58 (t, *J* = 8.2 Hz, 1H),7.33 (d, *J* = 7.3 Hz, 2H), 7.23 (t, *J* = 7.4 Hz, 2H), 7.16 (d, *J* = 7.3 Hz, 1H), 6.94 (d, *J* = 9.0 Hz, 1H), 6.62 (dd, *J* = 8.9, 3.0 Hz, 1H), 5.00–4.90 (m, 1H), 4.82 (dd, *J* = 13.0, 8.7 Hz, 1H), 3.76 (s, 3H), 3.68 (s 3H), 3.15 and 2.96 (dd, *J* = 13.9, 4.7 Hz, 1H; dd, *J* = 13.8, 9.7 Hz, 1H), 1.90–1.80 (m, 1H), 1.44 and 1.08 (ddd, *J* = 13.1, 7.4, 3.1 Hz, 1H; td, *J* = 13.7, 8.2 Hz, 1H), 0.91–0.73 (m, 6H, 2×$CH_3$). $^{13}$C NMR (100 MHz, DMSO-$d_6$) $\delta$ 180.4, 170.9, 169.7, 152.9, 147.5, 143.1, 141.0, 137.6, 129.7, 129.3, 129.3, 128.0, 128.0, 127.8, 126.2, 117.9, 115.9, 111.8, 108.0, 107.5, 60.9, 56.2, 55.3, 55.3, 54.9, 37.5, 36.7, 24.3, 15.1, 11.3. ESI-HRMS*m*/*z* calcd for $C_{30}H_{35}N_5O_6S$ $[M+H]^+$: 594.2381 found: 594.2355.

*1-(1-(1-(3,5-dimethoxyphenylamino)-1-oxo-3-phenylpropan-2-ylamino)-3-methyl-1-oxopentan-2-yl)-3-(3-nitrophenyl)thiourea (**I-2**)*. Yield 80.7%. Mp 187.5−190.1 °C. $[\alpha_D]^{20}$ = -30.0 (*c* 0.1, AcOEt). $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 10.18 (s, 1H), 9.86 (s, 1H), 8.84 (s, 1H), 8.41 (d, *J* = 7.9 Hz, 1H), 7.94 (dd, *J* = 16.9, 8.2 Hz, 2H), 7.84 (d, *J* = 8.1 Hz, 1H), 7.58 (t, *J* = 8.2 Hz, 1H), 7.30 (d, *J* = 7.2 Hz, 2H), 7.25 (t, *J* = 7.3 Hz, 2H), 7.18 (d, *J* = 7.1 Hz, 1H), 6.82 (d, *J* = 1.9 Hz, 2H), 6.22 (s, 1H), 4.88 (t, *J* = 6.6 Hz, 1H), 4.70 (dd, *J* = 13.5, 8.4 Hz, 1H), 3.70 (s, 6H), 3.09 and 2.94 (dd, *J* = 13.8, 5.0 Hz, 1H; dd, *J* = 13.8, 9.5 Hz, 1H), 1.86 (d, *J* = 6.1 Hz, 1H), 1.46–1.33 and 1.12–1.02 (m, 1H; m, 1H), 0.83 (dd, *J* = 13.9, 6.8 Hz, 6H, 2 × $CH_3$). $^{13}$C NMR (100 MHz, DMSO-$d_6$) $\delta$ 180.4, 170.6, 169.8, 160.5, 147.5, 141.0, 140.3, 137.5, 129.7, 129.2, 129.2, 128.1, 128.1, 127.9, 126.4, 118.0, 115.8, 97.7, 97.6, 95.4, 61.1, 55.1, 55.1, 55.0, 37.5, 37.4, 24.3, 15.23, 14.8, 11.4. ESI-HRMS*m*/*z* calcd for $C_{30}H_{35}N_5O_6S$ $[M-H]^-$:592.2235 found: 592.2240.

*1-(1-(1-(3,5-dimethylphenylamino)-1-oxo-3-phenylpropan-2-ylamino)-3-methyl-1-oxobutan-2-yl)-3-(3-nitrophenyl)thiourea (**I-3**)*. Yield 90.5%. Mp 197.7−200.5 °C. $[\alpha_D]^{20}$ = -24.5 (*c* 0.1, AcOEt). $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 10.19 (s, 1H), 9.76 (s, 1H), 8.86 (s, 1H), 8.41 (d, *J* = 8.0 Hz, 1H), 7.98 (d, *J* = 8.3 Hz, 1H), 7.92 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.86–7.80 (m, 1H), 7.58 (t, *J* = 8.2 Hz, 1H), 7.31 (d, *J* = 7.3 Hz, 2H), 7.24 (t, *J* = 7.4 Hz, 2H), 7.18 (d, *J* = 11.3 Hz, 3H), 6.69 (s, 1H), 4.88 (t, *J* = 7.1 Hz, 1H), 4.71 (dd, *J* = 13.8, 8.5 Hz, 1H), 3.08 and 2.94 (dd, *J* = 13.9, 5.1 Hz, 1H; dd, *J* = 13.8, 9.3 Hz, 1H), 2.22 (s, 6H), 1.89–1.78 (m, 1H), 1.41 and 1.08 (ddd, *J* = 10.0, 6.7, 2.9 Hz, 1H; dd, *J* = 13.7, 8.9 Hz, 1H), 0.83 (dd, *J* = 15.5, 7.6 Hz, 6H, 2×$CH_3$). $^{13}$CNMR (125 MHz, DMSO-$d_6$) $\delta$ 180.4, 170.5, 169.5, 147.5, 141.1, 138.6, 137.6, 137.5, 129.7, 129.2, 129.2, 128.1, 128.1, 127.8, 126.3, 125.0, 118.0, 117.2, 117.2, 115.8, 61.1, 54.9, 37.5, 31.1, 29.8, 24.4, 21.1, 21.1, 15.2, 11.4. ESI-HRMS*m*/*z* calcd for $C_{30}H_{35}N_5O_4S$ $[M-H]^-$: 560.2337 found: 560.2342.

*1-(3-methyl-1-oxo-1-(1-oxo-3-phenyl-1-(3,4,5-trimethoxyphenylamino)propan-2-ylamino)pentan-2-yl)-3-(3-nitrophenyl)thiourea (**I-4**)*. Yield 79.4%. Mp 107.4−123.2 °C. $[\alpha_D]^{20}$ = -

31.1 (*c* 0.1, AcOEt). $^{1}$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 10.19 (s, 1H), 9.82 (s, 1H), 8.84 (s, 1H), 8.39 (d, $J$ = 7.7 Hz, 1H), 7.97 (d, $J$ = 7.8 Hz, 1H), 7.92 (d, $J$ = 7.8 Hz, 1H), 7.84 (d, $J$ = 7.8 Hz, 1H), 7.58 (t, $J$ = 8.1 Hz, 1H), 7.31 (d, $J$ = 6.9 Hz, 2H), 7.25 (t, $J$ = 7.2 Hz, 2H), 7.18 (d, $J$ = 7.0 Hz, 1H), 6.95 (s, 2H), 4.87 (s, 1H), 4.69 (d, $J$ = 4.4 Hz, 1H), 3.72 (s, 6H), 3.62 (s, 3H, $OCH_3$), 3.10 and 3.02–2.90 (dd, $J$ = 13.6, 4.4 Hz, 1H; m, 1H), 1.85 (s, 1H), 1.36 and 1.11–0.99 (d, $J$ = 16.0 Hz, 1H; m, 1H), 0.82 (dd, $J$ = 14.1, 6.8 Hz, 6H, 2 × $CH_3$). $^{13}$C NMR (125 MHz, DMSO-$d_6$) $\delta$180.6, 170.6, 169.6, 152.7, 152.7, 147.5, 141.0, 137.6, 134.8, 133.6, 129.7, 129.2, 129.2, 128.1, 128.1, 127.9, 126.4, 118.1, 115.9, 97.2, 97.2, 61.3, 60.1, 60.1, 55.7, 55.7, 55.0, 37.4, 24.3, 15.3, 11.4. ESI-HRMS *m*/*z* calcd for $C_{31}H_{37}N_5O_7S[M-H]^-$:622.2341 found: 622.2343.

*1-(3-chlorophenyl)-3-(1-(1-(4-methoxyphenylamino)-1-oxo-3-phenylpropan-2-ylamino)-3-methyl-1-oxopentan-2-yl)thiourea (**I-5**)*. Yield 76.5%. Mp 169.9−173.5 °C. $[\alpha_D]^{20}$ = -27.0 (*c* 0.1, AcOEt). $^{1}$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 9.92 (s, 1H), 9.74 (s, 1H), 8.35 (d, $J$ = 8.0 Hz, 1H), 7.96 (s, 1H), 7.83 (d, $J$ = 8.1 Hz, 1H), 7.46 (d, $J$ = 8.9 Hz, 2H), 7.35 (dd, $J$ = 10.3, 8.1 Hz, 2H), 7.29 (d, $J$ = 7.0 Hz, 2H), 7.24 (t, $J$ = 7.4 Hz, 2H), 7.17 (d, $J$ = 7.1 Hz, 1H), 7.13 (d, $J$ = 7.4 Hz, 1H), 6.87 (d, $J$ = 9.0 Hz, 2H), 4.85 (d, $J$ = 6.5 Hz, 1H), 4.70 (dd, $J$ = 13.9, 8.4 Hz, 1H), 3.72 (s, 3H), 3.09 and 2.95 (dd, $J$ = 13.8, 5.2 Hz, 1H; dd, $J$ = 13.7, 9.3 Hz, 1H), 1.83 (d, $J$ = 6.1 Hz, 1H), 1.39 and 1.11–0.97 (dd, $J$ = 11.9, 5.6 Hz, 1H; m, 1H), 0.82 (d, $J$ = 7.8 Hz, 6H, 2×$CH_3$). $^{13}$C NMR(100 MHz, DMSO-$d_6$) $\delta$180.3, 170.5, 169.1, 155.4, 141.2, 137.6, 132.5, 131.8, 130.0, 129.2, 129.2, 128.0, 128.0, 126.3, 123.4, 121.4, 121.4, 121.0, 120.4, 113.8, 113.8, 61.2, 55.1, 54.7, 37.5, 37.4, 24.4, 15.2, 11.4. ESI-HRMS *m*/*z* calcd for $C_{29}H_{33}ClN_4O_3S$ $[M-H]^-$: 551.1889 found: 551.1903.

*1-(3-chloro-4-methylphenyl)-3-(1-(1-(4-methoxyphenylamino)-1-oxo-3-phenylpropan-2-ylamino)-3-methyl-1-oxopentan-2-yl)thiourea (**I-6**)*. Yield 88.1%. Mp 126.7–131.1 °C. $[\alpha_D]^{20}$ = -20.4 (*c* 0.1, AcOEt). $^{1}$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 9.81 (s, 1H), 9.73 (s, 1H), 8.34 (d, $J$ = 8.0 Hz, 1H), 7.86 (s, 1H), 7.73 (d, $J$ = 8.1 Hz, 1H), 7.47 (d, $J$ = 8.9 Hz, 2H), 7.30 (d, $J$ = 7.2 Hz, 2H), 7.27–7.22 (m, 4H), 7.17 (t, $J$ = 7.1 Hz, 1H), 6.87 (d, $J$ = 9.0 Hz, 2H), 4.85 (s, 1H), 4.70 (dd, $J$ = 13.9, 8.5 Hz, 1H), 3.72 (s, 3H), 3.10 and 2.95 (dd, $J$ = 13.8, 5.2 Hz, 1H; dd, $J$ = 13.7, 9.3 Hz, 1H), 2.28 (s, 3H), 1.90–1.75 (m, 1H), 1.42–1.34 and 1.12–1.00 (m, 1H; m, 1H), 0.81 (t, $J$ = 7.6 Hz, 6H, 2×$CH_3$). $^{13}$C NMR (100 MHz, DMSO-$d_6$) $\delta$180.5, 170.6, 169.1, 155.4, 138.7, 137.6, 132.5, 131.8, 130.8, 130.6, 129.2, 128.0, 126.3, 122.4, 121.1, 121.0, 113.8, 61.2, 55.1, 54.7, 37.5, 37.4, 24.4, 18.9, 15.2, 11.4. ESI-HRMS *m*/*z* calcd for $C_{30}H_{35}ClN_4O_3S$ $[M-H]^-$: 565.2046 found: 565.2054.

*1-(2,4-dibromophenyl)-3-(3-methyl-1-oxo-1-(1-oxo-3-phenyl-1-(3,4,5-trimethoxyphenylamino)propan-2-ylamino)pentan-2-yl)thiourea (**I-7**)*. Yield 82.8%. Mp 139.6−143.5 °C. $[\alpha_D]^{20}$ = -16.6 (*c* 0.1, AcOEt). $^{1}$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 9.82 (s, 1H), 9.33 (s, 1H), 8.31 (d, $J$ = 7.8 Hz, 1H), 8.21 (d, $J$ = 8.4 Hz, 1H), 7.87 (d, $J$ = 2.0 Hz, 1H), 7.67 (d, $J$ = 8.6 Hz, 1H), 7.52 (dd, $J$ = 8.6, 1.8 Hz, 1H), 7.28 (dt, $J$ = 14.9, 7.4 Hz, 4H), 7.20 (d, $J$ = 7.0 Hz, 1H), 6.95 (s, 2H), 4.86 (t, $J$ = 6.9 Hz, 1H), 4.68 (dd, $J$ = 13.7, 8.0 Hz, 1H), 3.72 (s, 6H), 3.62 (s, 3H), 3.09 and 2.95 (dd, $J$ = 13.8, 5.2 Hz, 1H; dd, $J$ = 13.8, 9.2 Hz, 1H), 1.86 (d, $J$ = 6.1 Hz, 1H), 1.46-1.35 and 1.17-1.01 (m, 1H; m, 1H), 0.83 (dd, $J$ = 13.6, 6.8 Hz, 6H, 2×$CH_3$). $^{13}$C NMR (101

MHz, DMSO-$d_6$) $\delta$181.68, 170.62, 169.50, 152.67, 152.67, 137.48, 134.77, 134.15, 133.62, 130.81, 130.26, 129.12, 129.12, 128.11, 128.11, 126.37, 120.33, 118.10, 97.26, 97.26, 61.67, 60.09, 60.09, 55.69, 55.69, 54.87, 37.46, 37.36, 24.31, 15.22, 11.35. ESI-HRMS *m*/*z* calcd for $C_{31}H_{36}Br_2N_4O_5S$ $[M-H]^-$: 773.0700 found: 773.0687.

*1-(1-(1-(4-methoxyphenylamino)-1-oxo-3-phenylpropan-2-ylamino)-3-methyl-1-oxopentan-2-yl)-3-(naphthalen-2-yl)thiourea (**I-8**)*. Yield 84.7%. Mp 127.6−131.5 °C. $[\alpha_D]^{20}$ = -13.2 (*c* 0.1, AcOEt). $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 7.97–7.95 (m, 1H), 7.93 (d, *J* = 7.2 Hz, 1H), 7.89 (dd, *J* = 7.0, 2.2 Hz, 1H), 7.57–7.43 (m, 4H), 7.34 (d, *J* = 2.2 Hz, 1H), 7.33 (d, *J* = 2.2 Hz, 1H), 7.28–7.22 (m, 4H), 7.21–7.15 (m, 1H), 6.80 (d, *J* = 9.1 Hz, 2H), 4.84 (d, *J* = 6.8 Hz, 1H), 4.73 (dd, *J* = 8.4, 6.5 Hz, 1H), 3.75 (s, 3H), 3.23 and 3.01 (dd, *J* = 13.7, 6.4 Hz, 1H; dd, *J* = 13.7, 8.5 Hz, 1H), 1.73 (dd, *J* = 6.1, 3.1 Hz, 1H), 1.28–1.18 and 0.93–0.84 (m, 1H; m, 1H), 0.76 (dd, *J* = 8.3, 7.3 Hz, 6H, 2×$CH_3$).$^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$182.3, 170.7, 169.2, 155.3, 137.6, 134.6, 133.9, 131.8, 129.6, 129.2, 128.2, 128.1, 126.4, 126.2, 125.5, 124.9, 122.6, 120.9, 113.8, 61.6, 55.1, 54.8, 37.5, 24.4, 15.2, 11.4. ESI-HRMS *m*/*z* calcd for $C_{33}H_{36}N_4O_3S$ $[M+H]^+$: 569.2581 found: 569.2556.

*N-(3-chloro-4-fluorophenyl)-2-(2-(3-(3-fluorophenyl)thioureido)-3-phenylpropanamido)-3-phenylpropanamide (**I-9**)*. Yield 79.6%. Mp 108.6−121.5 °C. $[\alpha_D]^{20}$ = -29.8 (*c* 0.1, AcOEt). $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 10.31 (s, 1H), 10.05 (s, 1H), 8.76 (d, *J* = 7.7 Hz, 1H), 7.96 (s, 1H), 7.91 (d, *J* = 6.6 Hz, 1H), 7.85 (d, *J* = 7.3 Hz, 1H), 7.51 (d, *J* = 8.7 Hz, 1H), 7.47 (d, *J* = 8.8 Hz, 1H), 7.39 (t, *J* = 9.0 Hz, 1H), 7.28 (dd, *J* = 13.8, 6.3 Hz, 5H), 7.23–7.10 (m, 7H), 5.14 (d, *J* = 5.5 Hz, 1H), 4.69 (dd, *J* = 14.3, 7.6 Hz, 1H), 3.29–3.19 (m, 1H), 3.09 (dd, *J* = 13.7, 5.3 Hz, 1H), 2.97 (dt, *J* = 13.9, 7.1 Hz, 2H).$^{13}$C NMR (125 MHz, DMSO-$d_6$) $\delta$179.6, 170.4, 170.0, 152.3, 139.5, 137.2, 136.9, 135.9, 130.6, 130.3, 129.5, 129.2, 128.2, 128.0, 126.5, 126.4, 125.4, 123.4, 122.3, 120.8, 119.7, 119.2, 119.1, 117.1, 116.9, 57.7, 54.9, 37.5, 37.4.ESI-HRMS *m*/*z* calcd for $C_{31}H_{27}ClF_2N_4O_2S$ $[M+Na]^+$: 615.1404 found: 615.1421.

*2-(3-(3,4-dichlorophenyl)thioureido)-N-(1-oxo-3-phenyl-1-((3-(trifluoromethyl)phenyl)amino)propan-2-yl)-3-phenylpropanamide (**I-10**)*. Yield 82.0%. Mp 113.6−119.0 °C. $[\alpha_D]^{20}$ = -25.3 (*c* 0.1, AcOEt). $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 10.44 (s, 1H), 10.06 (s, 1H), 8.78 (d, *J* = 7.7 Hz, 1H), 8.09 (s, 1H), 7.97 (s, 1H), 7.85 (d, *J* = 7.4 Hz, 1H), 7.79 (d, *J* = 8.1 Hz, 1H), 7.58 (t, *J* = 8.0 Hz, 1H), 7.51 (d, *J* = 8.7 Hz, 1H), 7.44 (d, *J* = 7.7 Hz, 1H), 7.29 (dt, *J* = 15.0, 7.8 Hz, 5H), 7.23–7.06 (m, 6H), 5.16 (d, *J* = 5.2 Hz, 1H), 4.84–4.52 (m, 1H), 3.28–3.17 (m, 1H), 3.12 (dd, *J* = 13.8, 5.5 Hz, 1H), 3.05–2.81 (m, 2H).$^{13}$C NMR (125 MHz, DMSO-$d_6$) $\delta$179.6, 170.4, 170.3, 139.5, 139.5, 137.3, 136.9, 130.6, 130.3, 130.1, 129.5, 129.4, 129.2, 128.2, 127.9, 126.5, 126.3, 125.4, 125.2, 123.4, 123.0, 122.9, 122.3, 119.9, 119.6, 115.5, 57.6, 54.9, 37.4, 37.4. ESI-HRMS *m*/*z* calcd for $C_{32}H_{27}Cl_2F_3N_4O_2S$ $[M+Na]^+$: 681.1076 found: 681.1068.

*N-(1-oxo-3-phenyl-1-((3-(trifluoromethyl)phenyl)amino)propan-2-yl)-3-phenyl-2-(3-(3-(trifluoromethyl)phenyl)thioureido)propanamide (**I-11**)*. Yield 78.3%. Mp 143.8−150.6 °C. $[\alpha_D]^{20}$ = -26.0 (*c* 0.2, AcOEt). $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 10.45 (s, 1H), 10.15 (s, 1H), 8.80 (d, *J* = 7.8 Hz, 1H), 8.10 (s, 2H), 7.85 (d, *J* = 7.5 Hz, 1H), 7.80 (d, *J* = 8.4 Hz, 1H), 7.59 (dd, *J* = 17.8, 9.0

Hz, 2H), 7.50 (t, *J* = 7.9 Hz, 1H), 7.42 (dd, *J* = 15.7, 7.8 Hz, 2H), 7.33 (d, *J* = 7.3 Hz, 2H), 7.28 (t, *J* = 7.5 Hz, 2H), 7.22–7.16 (m, 3H), 7.15–7.10 (m, 3H), 5.18 (dd, *J* = 12.3, 6.8 Hz, 1H), 4.74 (td, *J* = 8.4, 5.9 Hz, 1H), 3.27 (dd, *J* = 13.8, 4.7 Hz, 1H), 3.13 (dd, *J* = 13.9, 5.6 Hz, 1H), 3.00 (ddd, *J* = 13.7, 7.7, 5.9 Hz, 2H). $^{13}$C NMR (125 MHz, DMSO-$d_6$) $\delta$179.8, 170.5, 170.4, 140.3, 139.5, 137.3, 136.9, 130.1, 129.7, 129.6, 129.4, 129.0, 128.2, 127.9, 126.5, 126.3, 125.9, 125.2, 125.1, 123.1, 123.00, 122.9, 120.2, 119.9, 118.4, 115.5, 115.4, 57.5, 55.0, 37.5. ESI-HRMS *m*/*z* calcd for $C_{33}H_{28}F_6N_4O_2S$ $[M+Na]^+$: 681.1729 found: 681.1722.

*2-(3-(3,4-dichlorophenyl)thioureido)-N-(1-oxo-3-phenyl-1-(o-tolylamino)propan-2-yl)-3-phenylpropanamide (**I-12**).* Yield 84.5%. Mp 151.2−157.6 °C. $[\alpha_D]^{20}$ = -43.0 (*c* 0.1, AcOEt). $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 10.09 (s, 1H), 9.44 (s, 1H), 8.75 (d, *J* = 7.9 Hz, 1H), 8.00 (d, *J* = 2.3 Hz, 1H), 7.88 (d, *J* = 7.5 Hz, 1H), 7.52 (d, *J* = 8.7 Hz, 1H), 7.40–7.27 (m, 6H), 7.24–7.14 (m, 8H), 7.10 (td, *J* = 7.4, 1.1 Hz, 1H), 5.16 (dd, *J* = 12.2, 6.8 Hz, 1H), 4.83 (dd, *J* = 14.6, 8.2 Hz, 1H), 3.27 (dd, *J* = 13.8, 4.8 Hz, 1H), 3.13 (dd, *J* = 13.7, 6.2 Hz, 1H), 3.05–2.90 (m, 2H), 2.07 (s, 3H, $CH_3$). $^{13}$C NMR (125 MHz, DMSO-$d_6$) $\delta$179.6, 170.3, 169.7, 139.6, 137.5, 136.9, 135.9, 132.0, 130.6, 130.3, 129.6, 129.3, 128.2, 128.0, 126.5, 126.4, 125.9, 125.4, 125.4, 125.1, 123.3, 122.2, 57.6, 54.5, 37.8, 37.4, 17.7. ESI-HRMS *m*/*z* calcd for $C_{32}H_{30}Cl_2N_4O_2S$ $[M+Na]^+$: 627.1359 found: 627.1354.

*N-(3-fluorophenyl)-3-phenyl-2-(3-phenyl-2-(3-(3-(trifluoromethyl)phenyl)thioureido)propanamido)propanamide (**I-13**).* Yield 86.5%. Mp 132.3−141.2 °C. $[\alpha_D]^{20}$ = -22.1 (*c* 0.1, AcOEt). $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 9.17 (s, 1H), 9.06 (s, 1H), 8.47 (s, 1H), 7.67 (s, 1H), 7.57 (s, 1H), 7.45 (d, *J* = 3.8 Hz,2H), 7.39 (d, *J* = 5.2 Hz, 2H), 7.21 (d, *J* = 7.6 Hz, 1H), 7.16 (d, *J* = 6.3 Hz, 2H), 7.03 (dd, *J* = 13.6, 6.2 Hz, 5H), 6.91 (d, *J* = 4.0 Hz, 1H), 6.85 (d, *J* = 3.3 Hz, 4H), 5.43 (s, 1H), 5.06 (s, 1H), 3.11 (dd, *J* = 21.7, 8.4 Hz, 2H), 2.91 (d, *J* = 7.9 Hz, 1H), 2.78 (s, 1H). $^{13}$C NMR(125 MHz, $CDCl_3$) $\delta$ 180.1, 171.2, 170.8, 138.6, 137.7, 135.8, 135.3, 134.9, 131.5, 131.2, 130.2, 129.6, 129.5, 128.9, 128.8, 128.5, 128.4, 127.5, 126.9, 125.72, 124.9, 122.7, 121.8, 121.5, 119.2, 59.2, 55.9, 39.2, 38.2. ESI-HRMS *m*/*z* calcd for $C_{32}H_{28}F_4N_4O_2S$ $[M+K]^+$: 647.1501 found: 647.1458.

*2-(3-(3,4-dichlorophenyl)thioureido)-N-(1-((3-fluorophenyl)amino)-1-oxo-3-phenylpropan-2-yl)-3-phenylpropanamide (**I-14**).* Yield 80.2%. Mp 118.6−123.2 °C. $[\alpha_D]^{20}$ = -29.4 (*c* 0.1, AcOEt). $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 10.29 (s, 1H), 10.06 (s, 1H), 8.76 (d, *J* = 7.9 Hz, 1H), 7.97 (d, *J* = 2.2 Hz, 1H), 7.90–7.77 (m, 2H), 7.51 (d, *J* = 8.7 Hz, 1H), 7.47–7.43 (m, 1H), 7.36 (t, *J* = 8.1 Hz, 1H), 7.33–7.25 (m, 5H), 7.20 (d, *J* = 7.2 Hz, 1H), 7.18–7.11 (m, 6H), 5.14 (dd, *J* = 12.3, 7.0 Hz, 1H), 4.72 (td, *J* = 8.5, 5.9 Hz, 1H), 3.23 (dd, *J* = 13.9, 4.7 Hz, 1H), 3.10 (dd, *J* = 13.9, 5.6 Hz, 1H), 3.05–2.87 (m, 2H). $^{13}$C NMR (125 MHz, DMSO-$d_6$) $\delta$179.6, 170.4, 170.2, 140.1, 139.5, 137.3, 136.9, 133.1, 130.6, 130.5, 130.3, 129.5, 129.2, 128.2, 128.0, 126.5, 126.4, 125.4, 123.4, 123.3, 122.2, 118.9, 117.8, 57.6, 54.9, 37.5, 37.4. ESI-HRMS *m*/*z* calcd for $C_{31}H_{27}Cl_2FN_4O_2S$ $[M+K]^+$: 647.0847 found: 647.0806.

*N-(3-fluorophenyl)-2-(2-(3-(3-methoxyphenyl)thioureido)-3-phenylpropanamido)-3-phenylpropanamide (**I-15**).* Yield 76.6%. Mp 144.6−149.5 °C. $[\alpha_D]^{20}$ = -46.2 (*c* 0.1, AcOEt). $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 8.59 (s, 1H), 8.34 (s, 1H), 7.58 (s, 1H), 7.28 (s, 1H), 7.23–7.18 (m, 1H), 7.15 (d, *J* = 3.2 Hz, 4H), 7.12–7.06 (m, 3H), 7.05–6.94 (m, 6H), 6.81 (dd, *J* = 8.3, 1.9 Hz, 1H), 6.63 (s, 2H), 6.48 (d, *J* = 7.2 Hz, 1H), 5.14 (q, *J* = 6.3 Hz, 1H), 4.84 (dd, *J* = 14.2, 7.1 Hz, 1H), 3.73 (s, 3H, $OCH_3$), 3.16–2.91 (m, 4H). $^{13}$C NMR(125 MHz, $CDCl_3$) $\delta$ 180.4, 170.9, 169.3, 160.9, 138.6, 136.9, 136.1, 135.5, 134.5, 130.9, 129.9, 129.4, 129.3, 129.2, 128.9, 128.9, 127.4, 127.3, 124.8, 120.8, 118.6, 117.0, 113.0, 110.9, 59.7, 55.5, 55.1, 37.7, 37.5. ESI-HRMS *m*/*z* calcd for $C_{32}H_{31}FN_4O_3S$ $[M+K]^+$: 609.1732 found: 609.1694.

*2-(3-(3-chlorophenyl)thioureido)-N-(1-((3,5-dimethylphenyl)amino)-1-oxo-3-phenylpropan-2-yl)-3-phenylpropanamide (**I-16**).* Yield 83.1%. Mp 139.6−147.2 °C. $[\alpha_D]^{20}$ = -37.0 (*c* 0.2, AcOEt). $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 9.16 (d, *J* = 33.1 Hz, 2H), 8.69 (s, 1H), 7.63 (s, 1H), 7.43 (s, 1H), 7.24 (d, *J* = 6.0 Hz, 2H), 7.15 (s, 3H), 7.07 (s, 2H), 6.96 (s, 3H), 6.85 (s, 1H), 6.78 (d, *J* = 6.8 Hz, 5H), 5.44 (s, 1H), 5.12 (s, 1H), 3.19–2.96 (m, 2H), 2.90 (d, *J* = 23.0 Hz, 1H), 2.76 (s, 1H), 2.07 (s, 6H, 2×$CH_3$). $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 179.8, 171.0, 170.7, 139.7, 140.0, 139.0, 136.4, 136.2, 135.4, 134.3, 129.9, 129.6, 128.7, 128.3, 127.6, 127.2, 126.6, 125.6, 124.6, 122.9, 119.4, 59.1, 56.1, 39.24, 38.1, 21.2. ESI-HRMS *m*/*z* calcd for $C_{33}H_{33}ClN_4O_2S$ $[M+Na]^+$: 607.1905 found: 607.1900.

*2-(3-(4-chlorophenyl)thioureido)-N-(1-((3,5-dimethylphenyl)amino)-1-oxo-3-phenylpropan-2-yl)-3-phenylpropanamide (**I-17**).* Yield 84.4%. Mp 143.6−154.2 °C. $[\alpha_D]^{20}$ = -38.0 (*c* 0.1, AcOEt). $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 9.91 (d, *J* = 12.1 Hz, 2H), 8.63 (d, *J* = 8.0 Hz, 1H), 7.66 (d, *J* = 7.4 Hz, 1H), 7.43 (d, *J* = 8.8 Hz, 2H), 7.35–7.30 (m, 4H), 7.27 (t, *J* = 7.5 Hz, 2H), 7.23 (s, 2H), 7.20 (d, *J* = 7.1 Hz, 1H), 7.15 (d, *J* = 9.8 Hz, 5H), 6.72 (s, 1H), 5.13 (d, *J* = 5.4 Hz, 1H), 4.72 (td, *J* = 8.6, 5.7 Hz, 1H), 3.25–3.18 (m, 1H), 3.09 (dd, *J* = 13.8, 5.3 Hz, 1H), 2.95 (ddd, *J* = 13.7, 7.8, 6.0 Hz, 2H), 2.25 (s, 6H, 2×$CH_3$).$^{13}$C NMR (100 MHz, DMSO-$d_6$) $\delta$179.7, 170.4, 169.6, 138.6, 138.2, 137.7, 137.5, 137.0, 129.5, 129.2, 128.4, 128.1, 128.0, 127.8, 126.4, 126.3, 125.1, 124.1, 117.3, 57.7, 54.8, 37.6, 37.4, 21.1. ESI-HRMS *m*/*z* calcd for $C_{33}H_{33}ClN_4O_2S$ $[M+Na]^+$: 607.1905 found: 607.1900.

*2-(3-(3-chloro-4-fluorophenyl)thioureido)-N-(1-((3,5-dimethylphenyl)amino)-1-oxo-3-phenylpropan-2-yl)-3-phenylpropanamide (**I-18**).* Yield 87.2%. Mp 142.0−149.5 °C. $[\alpha_D]^{20}$ = -30.5 (*c* 0.1, AcOEt). $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 9.93 (d, *J* = 11.2 Hz, 2H), 8.66 (d, *J* = 8.0 Hz, 1H), 7.82–7.77 (m, 1H), 7.73 (d, *J* = 7.5 Hz, 1H), 7.33 (t, *J* = 8.0 Hz, 3H), 7.28 (d, *J* = 7.4 Hz, 1H), 7.27–7.22 (m, 4H), 7.20 (d, *J* = 7.2 Hz, 1H), 7.16 (dd, *J* = 8.1, 3.9 Hz, 5H), 6.72 (s, 1H), 5.13 (dd, *J* = 12.1, 6.9 Hz, 1H), 4.73 (td, *J* = 8.6, 5.6 Hz, 1H), 3.24 (dd, *J* = 13.8, 4.6 Hz, 1H), 3.09 (dd, *J* = 13.8, 5.3 Hz, 1H), 2.96 (dt, *J* = 13.7, 9.2 Hz, 2H), 2.25 (s, 6H, 2×$CH_3$). $^{13}$C NMR(125 MHz, DMSO-$d_6$) $\delta$179.9, 170.4, 169.6, 154.8, 152., 138.6, 137.7, 137.5, 136.9, 136.5, 129.5, 129.2, 128.2, 128.1, 126.4, 126.3, 125.1, 124.5, 123.4, 123.3, 118.9, 118.7, 117.2, 116.7, 116.5, 57.7,

54.8, 37.7, 37.4, 21.1. ESI-HRMS *m*/*z* calcd for $C_{33}H_{32}ClFN_4O_2S$ $[M+Na]^+$: 625.1811 found: 625.1805.

*2-(3-(3-chlorophenyl)thioureido)-N-(1-oxo-3-phenyl-1-((3-(trifluoromethyl)phenyl)amino)propan-2-yl)-3-phenylpropanamide* ***(I-19)***. Yield 85.2%. Mp 144.8−153.5 °C. $[\alpha_D]^{20}$ = -40.1 (*c* 0.1, AcOEt). $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 8.93 (s, 1H), 8.62 (s, 1H), 7.68 (s, 1H), 7.58 (d, *J* = 8.1 Hz, 1H), 7.34 (d, *J* = 7.8 Hz, 1H), 7.26 (dd, *J* = 9.2, 6.7 Hz, 1H), 7.21–7.18 (m, 2H), 7.15 (s, 1H), 7.09 (s, 5H), 7.05–7.00 (m, 2H), 6.99–6.95 (m, 3H), 6.93 (d, *J* = 7.1 Hz, 2H), 5.28 (d, *J* = 6.1 Hz, 1H), 5.05–4.83 (m, 1H), 3.11 (ddd, *J* = 21.4, 13.8, 8.0 Hz, 2H), 2.95 (d, *J* = 5.6 Hz, 2H).$^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 180.2, 171.1, 170.2, 138.1, 137.5, 135.8, 135.4, 135.0, 131.6, 131.3, 130.5, 129.7, 129.5, 129.4, 128.9, 128.7, 127.5, 127.3, 127.0, 125.0, 124.9, 124.0, 123.2, 122.7, 121.8, 117.7, 59.4, 55.6, 38.5, 37.9. ESI-HRMS *m*/*z* calcd for $C_{32}H_{28}ClF_3N_4O_2S$ $[M+Na]^+$: 647.1466 found: 647.1458.

*N-(4-bromophenyl)-2-(2-(3-(3-bromophenyl)thioureido)-3-methylbutanamido)-3-methylpentanamide* ***(I-20)***. Yield 88.2%. Mp 126.7−131.1 °C. $[\alpha_D]^{20}$ = -26.9 (*c* 0.1, AcOEt). $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 10.21 (s, 1H), 9.88 (s, 1H), 8.25 (d, *J* = 7.9 Hz, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.62–7.29 (m, 8H), 4.94 (s, 1H), 4.28 (t, *J* = 8.0 Hz, 1H), 2.12 (dd, *J* = 12.7, 6.4 Hz, 1H), 1.81 (d, *J* = 5.4 Hz, 1H), 1.54 (s, 1H), 1.24–1.06 (m, 1H), 0.85 (dd, *J* = 16.8, 6.6 Hz, 12H, 4×$CH_3$). $^{13}$C NMR (100 MHz, DMSO-$d_6$) $\delta$180.4, 170.7, 170.3, 139.1, 138.2, 131.6, 131.5, 131.2, 131.1, 124.2, 121.2, 115.6, 114.9, 61.2, 58.1, 36.2, 31.2, 24.6, 18.9, 18.2, 15.3, 10.9. ESI-HRMS *m*/*z* calcd for $C_{24}H_{30}Br_2N_4O_2S$ $[M+K]^+$: 635.0088 found: 635.0080.

*N-(4-bromophenyl)-2-(2-(3-(3,4-dichlorophenyl)thioureido)-3-methylbutanamido)-3-methylpentanamide* ***(I-21)***.Yield 88.3%. Mp 126.7−131.1 °C. $[\alpha_D]^{20}$ = -36.8 (*c* 0.1, AcOEt). $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 10.21 (s, 1H), 10.01 (s, 1H), 8.27 (d, *J* = 8.2 Hz, 1H), 8.16 (d, *J* = 2.0 Hz, 1H), 7.98 (d, *J* = 8.3 Hz, 1H), 7.61–7.55 (m, 2H), 7.53 (d, *J* = 8.8 Hz, 1H), 7.48 (d, *J* = 8.9 Hz, 2H), 7.43 (dd, *J* = 8.8, 2.5 Hz, 1H), 5.03–4.81 (m, 1H), 4.29 (t, *J* = 8.2 Hz, 1H), 2.13 (dd, *J* = 12.9, 6.6 Hz, 1H), 1.81 (dd, *J* = 14.2, 6.2 Hz, 1H), 1.62–1.45 (m, 1H), 1.32–1.01 (m, 1H), 0.95–0.40 (m, 12H, 4×$CH_3$). $^{13}$C NMR (100 MHz, DMSO-$d_6$) $\delta$180.3, 170.6, 170.3, 139.9, 138.2, 131.6, 130.4, 130.2, 125.1, 123.1, 122.0, 121.2, 114.9, 61.3, 58.1, 36.3, 31.2, 24.6, 18.9, 18.2, 15.3, 10.9. ESI-HRMS *m*/*z* calcd for $C_{24}H_{29}BrCl_2N_4O_2S$ $[M+Na]^+$: 609.0464 found: 609.0459.

*N-(4-bromophenyl)-2-(2-(3-(2-fluorophenyl)thioureido)-3-methylbutanamido)-3-methylpentanamide* ***(I-22)***. Yield 83.2%. Mp 118.4−126.5 °C. $[\alpha_D]^{20}$ = -30.5 (*c* 0.1, AcOEt). $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 10.15 (s, 1H), 9.73 (s, 1H), 8.17 (d, *J* = 8.1 Hz, 1H), 7.70 (dd, *J* = 26.2, 7.4 Hz, 1H), 7.57–7.51 (m, 2H), 7.51–7.44 (m, 3H), 7.43 (s, 1H), 7.10 (t, *J* = 8.8 Hz, 2H), 4.90 (d, *J* = 5.8 Hz, 1H), 4.23 (t, *J* = 8.1 Hz, 1H), 2.08 (dd, *J* = 12.9, 6.6 Hz, 1H), 1.77 (dd, *J* = 14.5, 6.2 Hz, 1H), 1.50 (ddd, *J* = 13.0, 7.4, 3.1 Hz, 1H), 1.12 (dd, *J* = 14.6, 7.5 Hz, 1H), 0.90–0.71 (m, 12H, 4×$CH_3$). $^{13}$C NMR (100 MHz, DMSO-$d_6$) $\delta$180.9, 170.9, 170.4, 160.0, 157.6, 138.2, 135.8, 131.6, 125.1, 125.0, 121.2, 115.2, 115.0, 61.4, 58.2, 36.3, 31.2, 24.6, 18.9, 18.2, 15.3, 10.9. ESI-HRMS *m*/*z* calcd for $C_{24}H_{30}BrFN_4O_2S$ $[M+Na]^+$: 559.1149 found: 559.1145.

*N-(4-bromophenyl)-2-(2-(3-(4-fluorophenyl)thioureido)-3-methylbutanamido)-3-methylpentanamide (**I-23**)*. Yield 85.5%. Mp 131.8−139.2 °C. $[\alpha_D]^{20}$ = -24.3 (*c* 0.1, AcOEt). $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 10.19 (s, 1H), 9.76 (s, 1H), 8.22 (d, *J* = 8.1 Hz, 1H), 7.71 (d, *J* = 8.3 Hz, 1H), 7.61–7.55 (m, 2H), 7.60–7.53 (m, 3H), 7.47 (s, 1H), 7.14 (ddd, *J* = 12.6, 5.4, 3.0 Hz, 2H), 5.01–4.87 (m, 1H), 4.26 (d, *J* = 8.1 Hz, 1H), 2.12 (dq, *J* = 13.4, 6.7 Hz, 1H), 1.81 (dd, *J* = 14.4, 6.3 Hz, 1H), 1.54 (ddd, *J* = 13.1, 7.4, 3.1 Hz, 1H), 1.25–1.11 (m, 1H), 0.91–0.82 (m, 12H, 4×$CH_3$). $^{13}$C NMR (100 MHz, DMSO-$d_6$) $\delta$180.9, 170.8, 170.3, 159.9, 157.6, 138.2, 135.8, 131.6, 125.0, 124.9, 121.2, 115.1, 114.9, 61.3, 58.1, 36.2, 31.2, 24.6, 18.9, 18.2, 15.3, 14.9, 11.5, 10.9.ESI-HRMS *m*/*z* calcd for $C_{24}H_{30}BrFN_4O_2S$ $[M+Na]^+$: 559.1149 found: 559.1144.

*N-(3-chloro-4-fluorophenyl)-3-methyl-2-(3-methyl-2-(3-(naphthalen-2-yl)thioureido)butanamido)pentanamide (**I-24**)*. Yield 81.7%. Mp 116.3−124.2 °C. $[\alpha_D]^{20}$ = -20.4 (*c* 0.1, AcOEt). $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 10.29 (s, 1H), 9.85 (s, 1H), 8.24 (d, *J* = 7.8 Hz, 1H), 7.94 (dt, *J* = 8.4, 5.7 Hz, 3H), 7.84 (d, *J* = 8.2 Hz, 1H), 7.68 (d, *J* = 7.9 Hz, 1H), 7.60 (d, *J* = 7.1 Hz, 1H), 7.57–7.43 (m, 4H), 7.36 (t, *J* = 9.1 Hz, 1H), 5.07–4.86 (m, 1H), 4.24 (t, *J* = 7.8 Hz, 1H), 2.15 (dd, *J* = 12.8, 6.4 Hz, 1H), 1.82 (d, *J* = 6.5 Hz, 1H), 1.61–1.47 (m, 1H), 1.20 (dd, *J* = 13.6, 6.7 Hz, 1H), 0.96–0.59 (m, 12H, 4×$CH_3$).$^{13}$C NMR (100 MHz, DMSO-$d_6$) $\delta$183.0, 171.5, 171.0, 154.9, 152.6, 136.7, 134.5, 130.3, 128.8, 127.1, 126.8, 126.2, 125.6, 123.3, 121.1, 120.1, 119.7, 117.7, 117.5, 62.3, 58.8, 36.8, 31.8, 25.2, 19.6, 18.8, 15.9, 11.5. ESI-HRMS *m*/*z* calcd for $C_{28}H_{32}ClFN_4O_2S$ $[M+Na]^+$: 565.1811 found: 565.1808.

*N-(3-chloro-4-fluorophenyl)-2-(2-(3-(3,4-dichlorophenyl)thioureido)-3-methylbutanamido)-3-methylpentanamide (**I-25**)*. Yield 80.5%. Mp 129.5−133.2 °C. $[\alpha_D]^{20}$ = -21.8 (*c* 0.1, AcOEt). $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 10.31 (s, 1H), 10.01 (s, 1H), 8.28 (d, *J* = 8.0 Hz, 1H), 8.16 (s, 1H), 7.98 (d, *J* = 8.2 Hz, 1H), 7.92 (dd, *J* = 6.8, 2.3 Hz, 1H), 7.53 (d, *J* = 8.7 Hz, 1H), 7.50–7.45 (m, 1H), 7.43 (dd, *J* = 8.8, 2.3 Hz, 1H), 7.35 (t, *J* = 9.1 Hz, 1H), 5.04–4.73 (m, 1H), 4.26 (t, *J* = 8.1 Hz, 1H), 2.13 (dd, *J* = 12.8, 6.5 Hz, 1H), 1.82 (d, *J* = 6.2 Hz, 1H), 1.53 (d, *J* = 7.2 Hz, 1H), 1.20–1.12 (m, 1H), 0.87 (dd, *J* = 15.8, 8.4 Hz, 12H, 4×$CH_3$). $^{13}$C NMR (100 MHz, DMSO-$d_6$) $\delta$ 180.7, 171.1, 170.8, 154.8, 152.4, 140.4, 136.4, 130.8, 130.6, 125.5, 123.5, 122.4, 120.9, 117.5, 117.3, 61.7, 58.5, 36.6, 31.6, 25.0, 19.3, 18.6, 15.7, 11.2.ESI-HRMS *m*/*z* calcd for $C_{24}H_{28}Cl_3FN_4O_2S$ $[M+Na]^+$: 583.0875 found: 583.0870.

*N-(3-chloro-4-fluorophenyl)-2-(2-(3-(3-chloro-4-methylphenyl)thioureido)-3-methylbutanamido)-3-methylpentanamide (**I-26**)*. Yield 84.6%. Mp 132.8−137.5 °C. $[\alpha_D]^{20}$ = -19.7 (*c* 0.1, AcOEt). $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 10.31 (s, 1H), 9.84 (s, 1H), 8.27 (d, *J* = 8.0 Hz, 1H), 7.93 (dd, *J* = 6.9, 2.5 Hz, 1H), 7.85 (s, 1H), 7.81 (d, *J* = 8.4 Hz, 1H), 7.48 (ddd, *J* = 9.0, 4.3, 2.6 Hz, 1H), 7.36 (t, *J* = 9.1 Hz, 1H), 7.26 (d, *J* = 0.9 Hz, 2H), 5.10–4.75 (m, 1H), 4.26 (t, *J* = 8.1 Hz, 1H), 2.28 (s, 3H,$CH_3$), 2.13 (dd, *J* = 12.9, 6.6 Hz, 1H), 1.82 (dd, *J* = 14.6, 6.1 Hz, 1H), 1.55 (ddd, *J* = 13.1, 7.5, 3.1 Hz, 1H), 1.25–1.08 (m, 1H), 0.93–0.50 (m, 12H, 4×$CH_3$). $^{13}$C NMR(100 MHz, DMSO-$d_6$) $\delta$ 180.5, 170.8, 170.4, 154.3, 151.9, 138.8, 136.0, 132.5, 130.8, 122.4, 121.1,

120.5, 117.1, 116.9, 61.2, 58.1, 36.2, 31.2, 24.6, 19.0, 18.9, 18.2, 15.3, 10.8.ESI-HRMS *m/z* calcd for $C_{25}H_{31}Cl_2FN_4O_2S$ $[M+Na]^+$: 563.1421 found: 563.1418.

*N-(3-chloro-4-fluorophenyl)-2-(2-(3-(4-methoxyphenyl)thioureido)-3-methylbutanamido)-3-methylpentanamide (**I-27**).* Yield 85.8%. Mp 125.2−132.5 °C. $[\alpha_D]^{20}$ = -20.6 (*c* 0.1, AcOEt). $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 9.37 (s, 1H), 8.50 (s, 1H), 8.22 (s, 1H), 7.56 (dd, *J* = 6.4, 2.0 Hz, 1H), 7.32 (dd, *J* = 5.2, 3.1 Hz, 1H), 7.13 (d, *J* = 8.8 Hz, 3H), 6.87 (t, *J* = 8.7 Hz, 1H), 6.81 (d, *J* = 8.9 Hz, 2H), 5.10 (s, 1H), 4.52 (t, *J* = 8.3 Hz, 1H), 3.76 (s, 3H), 2.16–2.06 (m, 1H), 1.98 (d, *J* = 8.3 Hz, 1H), 1.63 (dd, *J* = 10.8, 7.4 Hz, 1H), 1.22–1.05 (m, 1H), 0.95 (d, *J* = 6.5 Hz, 3H), 0.89 (d, *J* = 6.3 Hz, 6H, 2×$CH_3$), 0.78 (t, *J* = 7.2 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 181.2, 172.5, 171.1, 156.2, 153.8, 134.1, 134.1, 127.0, 122.5, 121.1, 120.9, 120.1, 120.0, 116.7, 116.4, 114.7, 63.3, 59.6, 55.5, 36.4, 25.5, 19.1, 18.9, 15.7, 11.0.ESI-HRMS *m/z* calcd for $C_{25}H_{32}ClFN_4O_3S$ $[M+Na]^+$: 545.1760 found: 545.1758.

*1-(1-(1-(2,5-dimethoxyphenylamino)-3-methyl-1-oxopentan-2-ylamino)-3-methyl-1-oxobutan-2-yl)-3-(3-nitrophenyl)thiourea (**I-28**).* Yield 96.5%. Mp 128.4−133.6 °C. $[\alpha_D]^{20}$ = -25.5 (*c* 0.1, AcOEt). $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 10.21 (s, 1H), 9.00 (s, 1H), 8.86 (s, 1H), 8.37 (d, *J* = 8.1 Hz, 1H), 8.08 (d, *J* = 8.3 Hz, 1H), 7.91 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.85 (d, *J* = 8.1 Hz, 1H), 7.73 (d, *J* = 2.6 Hz, 1H), 7.58 (t, *J* = 8.2 Hz, 1H), 6.95 (d, *J* = 9.0 Hz, 1H), 6.62 (dd, *J* = 8.9, 3.0 Hz, 1H), 5.05–4.95 (m, 1H), 4.43 (t, *J* = 7.7 Hz, 1H), 3.77 (s, 3H), 3.68 (s, 3H), 2.22 (d, *J* = 6.5 Hz, 1H), 1.91 (d, *J* = 6.0 Hz, 1H), 1.56–1.47 and 1.22 (m, 1H; s, 1H), 0.95 (d, *J* = 6.8 Hz, 3H), 0.92-0.88 (m, 6H, 2×$CH_3$), 0.85 (t, *J* = 7.3 Hz, 3H, $CH_3$). $^{13}$C NMR (100 MHz, DMSO-$d_6$) $\delta$ 180.5, 171.0, 169.9, 153.0, 147.5, 143.3, 141.1, 129.6, 127.8, 127.8, 117.9, 115.9, 111.8, 107.9, 107.6, 61.3, 58.1, 56.2, 55.3, 36.1, 31.1, 24.4, 19.0, 17.9, 15.4, 11.0. ESI-HRMS *m/z* calcd for $C_{26}H_{35}N_5O_6S$ $[M-H]^-$:544.2235 found: 544.2236.

*1-(1-(1-(3-chloro-4-methylphenylamino)-3-methyl-1-oxopentan-2-ylamino)-3-methyl-1-oxobutan-2-yl)-3-(3-nitrophenyl)thiourea (**I-29**).* Yield 74.5%. Mp 183.4−188.6 °C. $[\alpha_D]^{20}$ = -28.2 (*c* 0.1, AcOEt). $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 10.21 (s, 1H), 10.14 (s, 1H), 8.85 (s, 1H), 8.24 (d, *J* = 8.1 Hz, 1H), 8.05 (d, *J* = 8.2 Hz, 1H), 7.90 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.79 (d, *J* = 1.8 Hz, 1H), 7.57 (t, *J* = 8.1 Hz, 1H), 7.37–7.34 (m, 1H), 7.25 (d, *J* = 8.3 Hz, 1H), 5.00–4.92 (m, 1H), 4.29 (t, *J* = 8.1 Hz, 1H), 2.25 (s, 3H), 2.16 (dd, *J* = 12.9, 6.6 Hz, 1H), 1.82 (d, *J* = 6.1 Hz, 1H), 1.54 and 1.22–1.17 (d, *J* = 7.4 Hz, 1H; m, 1H), 0.93–0.88 (m, 6H, 2×$CH_3$), 0.87 (s, 3H, $CH_3$), 0.84 (d, *J* = 7.1 Hz, 3H, $CH_3$). $^{13}$C NMR (100 MHz, DMSO-$d_6$) $\delta$ 180.5, 170.5, 170.2, 147.5, 141.1, 137.9, 133.0, 131.1, 130.0, 129.6, 127.8, 119.2, 117.9, 115.8, 61.3, 58.1, 36.3, 31.1, 29.8, 24.6, 18.9, 18.9, 18.1, 15.3, 10.8. ESI-HRMS *m/z* calcd for $C_{25}H_{32}ClN_5O_4S$ $[M-H]^-$: 532.1791 found: 532.1795.

*N-(1-((3-chlorophenyl)amino)-3-methyl-1-oxobutan-2-yl)-3-methyl-2-(3-(3,4,5-trimethylphenyl)thioureido)pentanamide (**I-30**).* Yield 83.6%. Mp148.6−152.3 °C. $[\alpha_D]^{20}$ = -11.7

(*c* 0.1, AcOEt). $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.72 (s, 1H), 8.26 (s, 1H), 7.59 (t, *J* = 1.8 Hz, 1H), 7.45 (s, 1H), 7.34 (d, *J* = 8.2 Hz, 1H), 7.13 (t, *J* = 8.1 Hz, 1H), 7.07–6.98 (m, 2H), 6.50 (s, 2H), 5.01 (t, *J* = 7.7 Hz, 1H), 4.43 (t, *J* = 8.0 Hz, 1H), 3.82 (s, 3H, $CH_3$), 3.74 (s, 6H, 2×$CH_3$), 2.31–2.11 (m, 1H), 1.95–1.89 (m, 1H), 1.60–1.51 (m, 1H), 1.17–1.06 (m, 1H), 0.99 (dd, *J* = 6.7, 2.9 Hz, 6H, 2×$CH_3$), 0.91–0.74 (m, 6H, 2×$CH_3$). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 180.7, 172.1, 170.1, 153.9, 153.2, 138.6, 134.7, 130.1, 124.8, 120.3, 118.3, 103.6, 102.5, 63.1, 61.0, 60.2, 56.3, 56.2, 37.6, 30.5, 25.6, 19.5, 18.6, 15.4, 12.8, 11.4.ESI-HRMS *m*/*z* calcd for $C_{27}H_{37}ClN_4O_2S$ $[M+K]^+$: 555.1957 found: 555.2003.

*N-(1-((3-chlorophenyl)amino)-3-methyl-1-oxobutan-2-yl)-2-(3-(3,4-dichlorophenyl)thioureido)-3-methylpentanamide* ***(I-31)***. Yield 81.8%. Mp129.4−135.6 °C. $[\alpha_D]^{20}$ = -31.6 (*c* 0.1, AcOEt). $^{1}$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 10.25 (s, 1H), 9.96 (s, 1H), 8.24 (d, *J* = 8.2 Hz, 1H), 8.15 (d, *J* = 2.1 Hz, 1H), 8.01 (d, *J* = 8.3 Hz, 1H), 7.82 (t, *J* = 2.0 Hz, 1H), 7.54 (d, *J* = 8.7 Hz, 1H), 7.48–7.40 (m, 2H), 7.34 (t, *J* = 8.1 Hz, 1H), 7.11 (dd, *J* = 7.9, 1.3 Hz, 1H), 4.92 (dd, *J* = 20.8, 13.4 Hz, 1H), 4.26 (t, *J* = 7.9 Hz, 1H), 2.05 (dd, *J* = 13.9, 6.9 Hz, 1H), 1.92–1.78 (m, 1H), 1.50 (ddd, *J* = 13.3, 7.5, 3.4 Hz, 1H), 1.15 (d, *J* = 7.5 Hz, 1H), 0.88 (ddd, *J* = 21.1, 15.2, 8.1 Hz, 12H, 4×$CH_3$). $^{13}$C NMR (100 MHz, DMSO-$d_6$) $\delta$ 180.6, 171.2, 170.7, 140.6, 140.4, 133.5, 130.9, 130.8, 130.6, 125.5, 123.5, 122.4, 119.1, 118.0, 61.3, 59.6, 37.8, 30.7, 25.0, 19.6, 19.0, 15.6, 11.7.ESI-HRMS *m*/*z* calcd for $C_{24}H_{29}Cl_3N_4O_2S$ $[M+Na]^+$: 565.0969 found: 565.0964.

*N-(1-((3-chlorophenyl)amino)-3-methyl-1-oxobutan-2-yl)-2-(3-(4-fluoro-3-(trifluoromethyl)phenyl)thioureido)-3-methylpentanamide* ***(I-32)***. Yield 86.8%. Mp127.3−133.6 °C. $[\alpha_D]^{20}$ = -33.4 (*c* 0.1, AcOEt). $^{1}$HNMR (400 MHz, $CDCl_3$) $\delta$ 9.30 (s, 1H), 8.93 (s, 2H), 7.99 (s, 1H), 7.66 (s, 1H), 7.55 (s, 1H), 7.48 (d, *J* = 7.0 Hz, 1H), 7.38 (d, *J* = 7.7 Hz, 1H), 7.31 (dd, *J* = 14.3, 6.7 Hz, 2H), 7.06 (d, *J* = 6.3 Hz, 2H), 5.27 (s, 1H), 4.67 (s, 1H), 2.25 (s, 1H), 1.89 (s, 1H), 1.65 (s, 1H), 1.26 (s, 1H), 1.10–0.97 (m, 6H, 2×$CH_3$), 0.88 (d, *J* = 6.0 Hz, 3H,$CH_3$), 0.79 (t, *J* = 7.1 Hz, 3H, $CH_3$). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 181.2, 172.9, 172.1, 139.2, 138.3, 135.1, 131.6, 131.3, 130.5, 129.6, 128.2, 125.8, 125.5, 122.8, 122.7, 121.5, 121.4, 119.3, 62.9, 61.1, 39.3, 26.2, 19.7, 19.5, 15.4, 12.1.ESI-HRMS *m*/*z* calcd for $C_{25}H_{29}ClF_4N_4O_2S$ $[M+Na]^+$: 583.1528 found: 583.1329.

*2-(3-(3,4-dimethylphenyl)thioureido)-3-methyl-N-(3-methyl-1-oxo-1-(m-tolylamino)butan-2-yl)pentanamide* ***(I-33)***. Yield 90.7%. Mp127.5−132.6 °C. $[\alpha_D]^{20}$ = -19.8 (*c* 0.1, AcOEt). $^{1}$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 9.91 (s, 1H), 9.62 (s, 1H), 8.11 (d, *J* = 8.3 Hz, 1H), 7.57 (d, *J* = 8.3 Hz, 1H), 7.44 (s, 1H), 7.37 (d, *J* = 8.2 Hz, 1H), 7.25–7.13 (m, 3H), 7.08 (d, *J* = 8.1 Hz, 1H), 6.87 (d, *J* = 7.5 Hz, 1H), 4.96 (t, *J* = 7.1 Hz, 1H), 4.27 (t, *J* = 7.8 Hz, 1H), 2.27 (s, 3H, *CH*$_3$), 2.19 (d, *J* = 3.8 Hz, 6H, 2×$CH_3$), 2.05 (dd, *J* = 13.8, 6.9 Hz, 1H), 1.90–1.80 (m, 1H), 1.56–1.44 (m, 1H), 1.15–1.05 (m, 1H), 0.93 (t, *J* = 6.6 Hz, 6H, 2×$CH_3$), 0.90–0.81 (m, 6H, 2×$CH_3$). $^{13}$C NMR (100 MHz, DMSO-$d_6$) $\delta$ 180.4, 170.9, 169.8, 138.7, 137.9, 136.8, 136.4, 132.3, 129.5, 128.6, 124.3, 124.0,

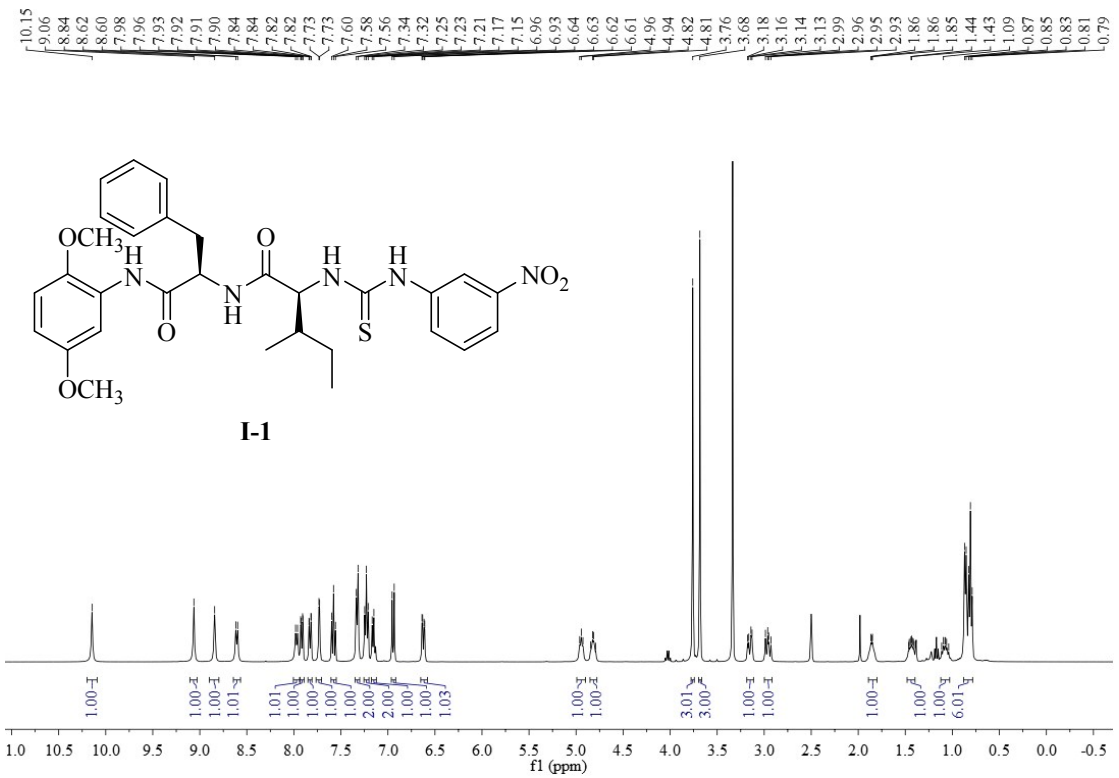
120.6, 119.7, 116.5, 60.9, 59.0, 37.4, 30.4, 24.6, 21.2, 19.5, 19.2 18.8, 18.6, 15.3, 11.3.ESI-HRMS *m*/*z* calcd for $C_{27}H_{38}N_4O_2S$ $[M+Na]^+$: 505.2608 found: 505.2606.

*2-(3-(3-methoxyphenyl)thioureido)-3-methyl-N-(3-methyl-1-oxo-1-(m-tolylamino)butan-2-yl)pentanamide (**I-34**).* Yield 92.8%. Mp126.6−131.8 °C. $[\alpha_D]^{20}$ = -29.9 (*c* 0.1, AcOEt). $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.97 (s, 1H), 8.65 (s, 1H), 8.24 (s, 1H), 7.57 (s, 1H), 7.32 (s, 1H), 7.28 (d, *J* = 8.3 Hz, 1H), 7.13 (t, *J* = 8.1 Hz, 1H), 7.05 (t, *J* = 7.8 Hz, 1H), 7.00 (s, 1H), 6.87 (d, *J* = 7.6 Hz, 1H), 6.80 (d, *J* = 8.1 Hz, 1H), 6.69 (dd, *J* = 8.4, 2.2 Hz, 1H), 5.20 (t, *J* = 7.9 Hz, 1H), 4.62 (t, *J* = 8.6 Hz, 1H), 3.67 (s, 3H, $OCH_3$), 2.25 (dd, *J* = 14.8, 6.9 Hz, 1H), 2.13 (s, 3H, $CH_3$), 1.97–1.84 (m, 1H), 1.68–1.47 (m, 1H), 1.18–1.06 (m, 1H), 1.02 (t, *J* = 6.7 Hz, 6H, 2×$CH_3$), 0.88 (d, *J* = 6.7 Hz, 3H, $CH_3$), 0.80 (t, *J* = 7.3 Hz, 3H, $CH_3$). $^{13}$C NMR(100 MHz, $CDCl_3$) $\delta$ 180.5, 172.3, 170.9, 160.4, 139.1, 139.0, 137.4, 130.1, 129.0, 125.8, 121.4, 117.9, 116.7, 110.2, 62.8, 60.6, 55.5, 38.6, 30.8, 25.9, 21.5, 19.5, 19.2, 15.3, 11.8.ESI-HRMS *m*/*z* calcd for $C_{26}H_{36}N_4O_3S$ $[M+Na]^+$: 507.2400 found: 507.2399.

*2-(3-(4-chlorophenyl)thioureido)-3-methyl-N-(3-methyl-1-oxo-1-(m-tolylamino)butan-2-yl)pentanamide (**I-35**).* Yield 89.0%. Mp118.8−124.5 °C. $[\alpha_D]^{20}$ = -31.3 (*c* 0.1, AcOEt). $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 9.22 (s, 1H), 8.96 (s, 2H), 8.06 (s, 1H), 7.45 (s, 1H), 7.30 (s, 2H), 7.19 (d, *J* = 7.7 Hz, 1H), 7.09 (ddd, *J* = 23.8, 16.0, 7.8 Hz, 3H), 6.90 (d, *J* = 7.9 Hz, 1H), 5.32 (s, 1H), 4.74 (s, 1H), 2.29 (s, 1H), 2.10 (s, 3H, $CH_3$), 1.92 (s, 1H), 1.67 (s, 1H), 1.10 (s, 1H), 1.12–1.01 (m, 6H, 2×$CH_3$), 0.89 (d, *J* = 5.9 Hz, 3H, $CH_3$), 0.80 (d, *J* = 7.1 Hz, 3H, $CH_3$). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 180.7, 172.5, 171.6, 139.9, 139.2, 137.0, 134.3, 129.7, 129.1, 126.3, 125.6, 124.5, 122.7, 121.9, 118.5, 62.7, 60.8, 39.3, 30.8, 26.0, 21.5, 19.5, 19.4, 15.2, 12.1.ESI-HRMS *m*/*z* calcd for $C_{25}H_{33}ClN_4O_2S$ $[M+Na]^+$: 511.1905 found: 511.1905.

*1-(1-(1-(3,4-dimethylphenylamino)-3-methyl-1-oxobutan-2-ylamino)-3-methyl-1-oxopentan-2-yl)-3-(3-nitrophenyl)thiourea (**I-36**).* Yield 80.4%. Mp 194.5−195.4 °C. $[\alpha_D]^{20}$ = -22.7 (*c* 0.1, AcOEt). $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 10.17 (s, 1H), 9.83 (d, *J* = 20.0 Hz, 1H), 8.85 (s, 1H), 8.14 (d, *J* = 8.5 Hz, 1H), 8.09 (d, *J* = 8.4 Hz, 1H), 7.90 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.83 (d, *J* = 7.4 Hz, 1H), 7.57 (t, *J* = 8.2 Hz, 1H), 7.35 (s, 1H), 7.29 (dd, *J* = 8.1, 1.9 Hz, 1H), 7.03 (d, *J* = 8.2 Hz, 1H), 4.95 (t, *J* = 7.4 Hz, 1H), 4.27 (t, *J* = 8.0 Hz, 1H), 2.15 (d, *J* = 10.6 Hz, 6H), 2.04 (dd, *J* = 14.2, 7.1 Hz, 1H), 1.92–1.87 (m, 1H), 1.55–1.50 and 1.16–1.10 (m, 1H; m, 1H), 0.95–0.87 (m, 9H, 3 × $CH_3$), 0.85 (t, *J* = 7.4 Hz, 3H, $CH_3$). $^{13}$C NMR (125 MHz, DMSO-$d_6$) $\delta$ 180.4, 170.7, 169.55, 147.5, 141.1, 136.5, 136.3, 131.1, 129.7, 129.6, 127.9, 120.6, 118.0, 116.9, 115.9, 61.0, 59.0, 37.4, 30.5, 24.6, 19.6, 19.2, 18.8, 18.6, 15.3, 11.3. ESI-HRMS *m*/*z* calcd for $C_{26}H_{35}N_5O_4S$ $[M-H]^-$: 512.2337 found: 512.2338.

$^1$H NMR, $^{13}$CNMR and HRMS of compounds ***I-1*−*I-36***:


OCH3
H
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OCH3

**I-1**


10.15
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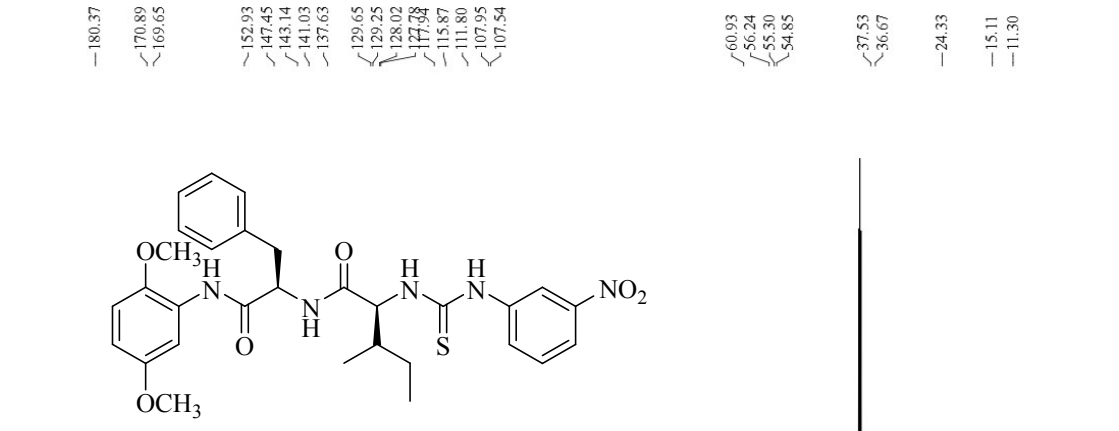
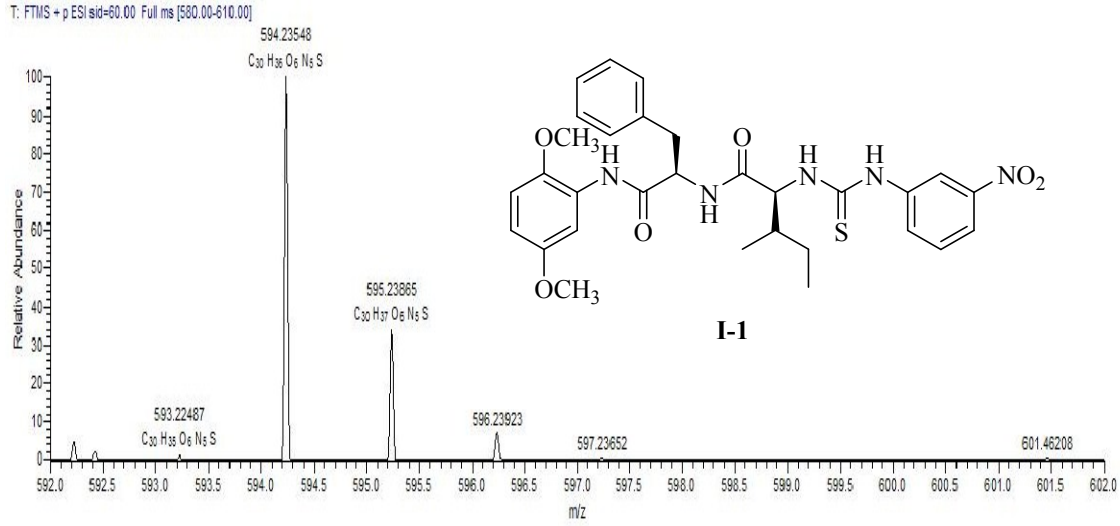
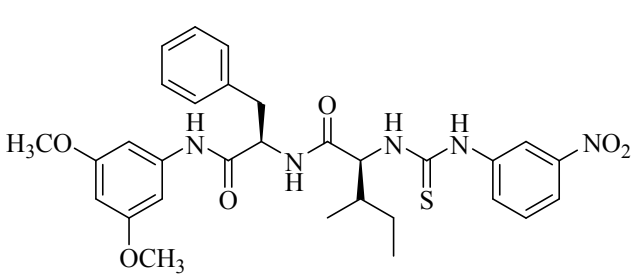
1.01
1.00
1.00
1.00
1.00
2.00
2.00
1.00
1.03
1.00
1.00
3.01
3.00
1.00
1.00
1.00
1.00
1.00
6.01
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


180.37
170.89
169.65
152.93
147.45
143.14
141.03
137.63
129.65
129.25
128.02
127.78
117.94
115.87
111.80
107.95
107.54
60.93
56.24
55.30
54.85
37.53
36.67
24.33
15.11
11.30
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


OCH3
H
N
O
N
H
O
H
N
S
H
N
NO2
OCH3

**I-1**

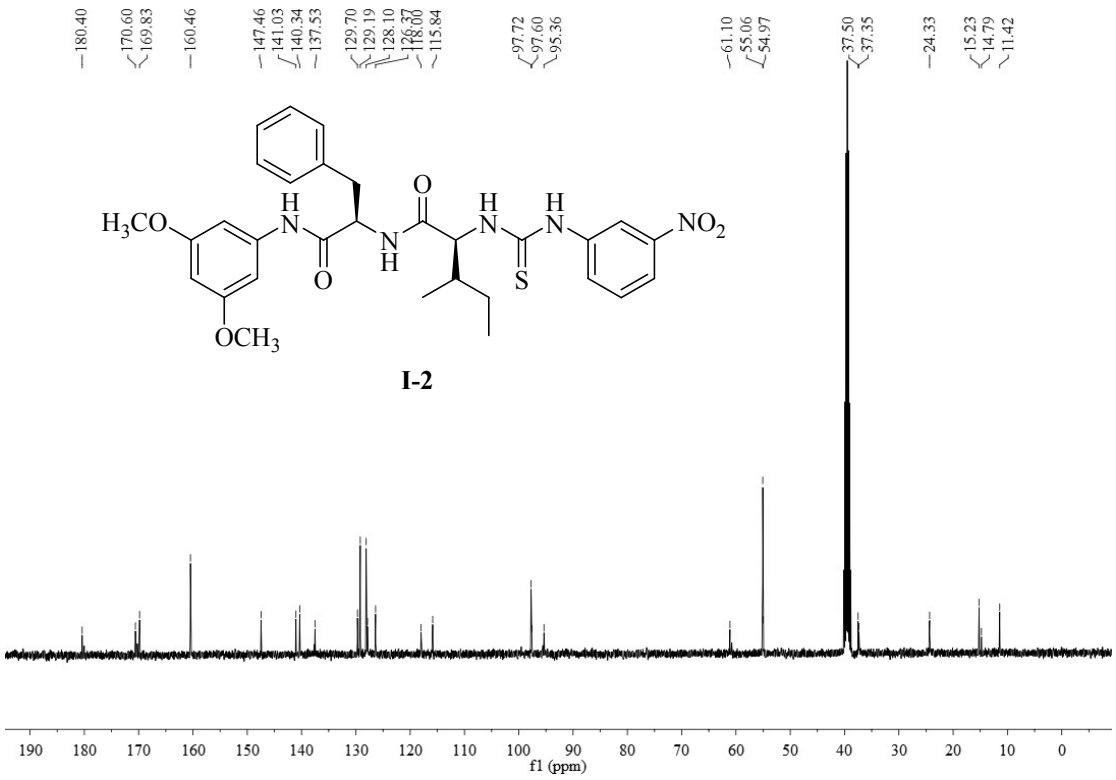

T: FTMS + p ESI sid=60.00 Full ms [580.00-610.00]
594.23548
C30 H36 O6 N5 S
595.23865
C30 H37 O6 N5 S
593.22487
C30 H35 O6 N5 S
596.23923
597.23652
601.46208
Relative Abundance
m/z



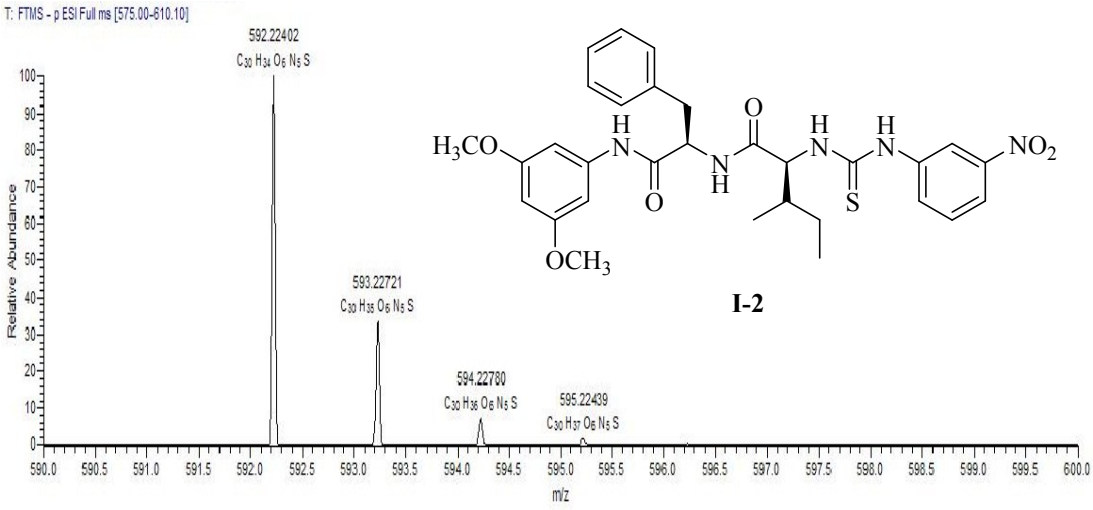
**I-1**



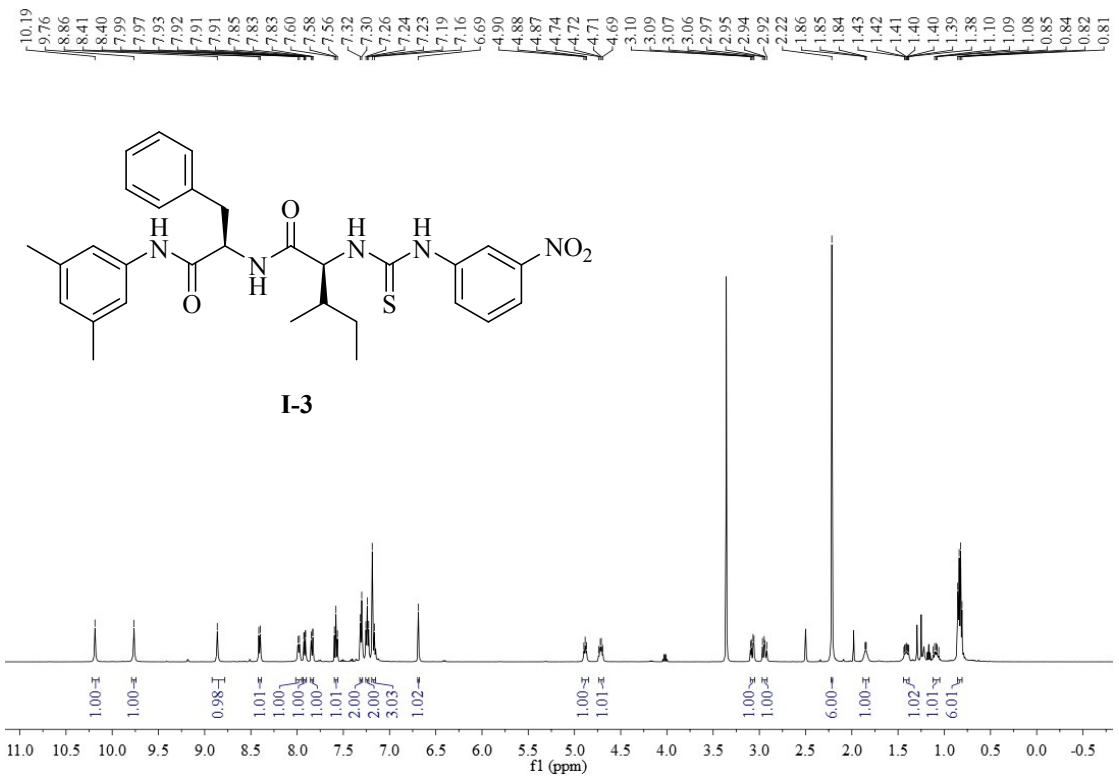
**I-2**


180.40
170.60
169.83
160.46
147.46
141.03
140.34
137.53
129.70
129.19
128.10
118.37
118.00
115.84
97.72
97.60
95.36
61.10
55.06
54.97
37.50
37.35
24.33
15.23
14.79
11.42
H3CO
OCH3
NO2
f1 (ppm)

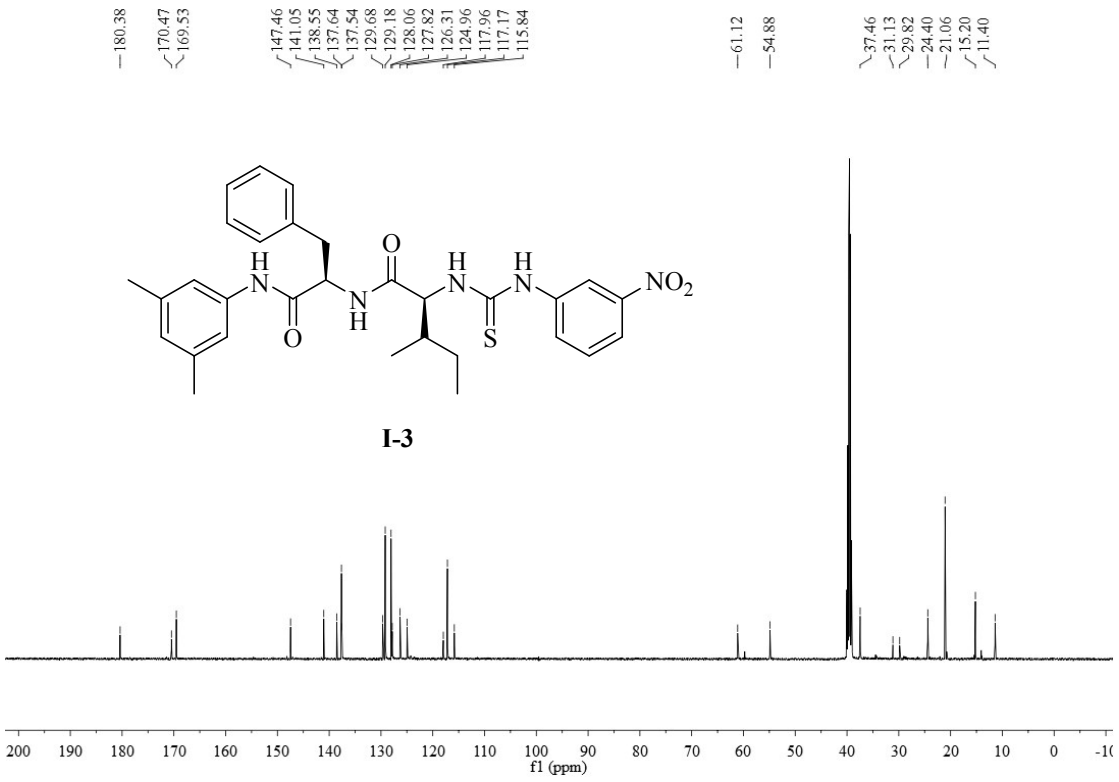
**I-2**


T: FTMS - p ESI Full ms [575.00-610.10]
592.22402
C30 H34 O6 N5 S
593.22721
C30 H35 O6 N5 S
594.22780
C30 H36 O6 N5 S
595.22439
C30 H37 O6 N5 S
Relative Abundance
m/z
H3CO
OCH3
NO2

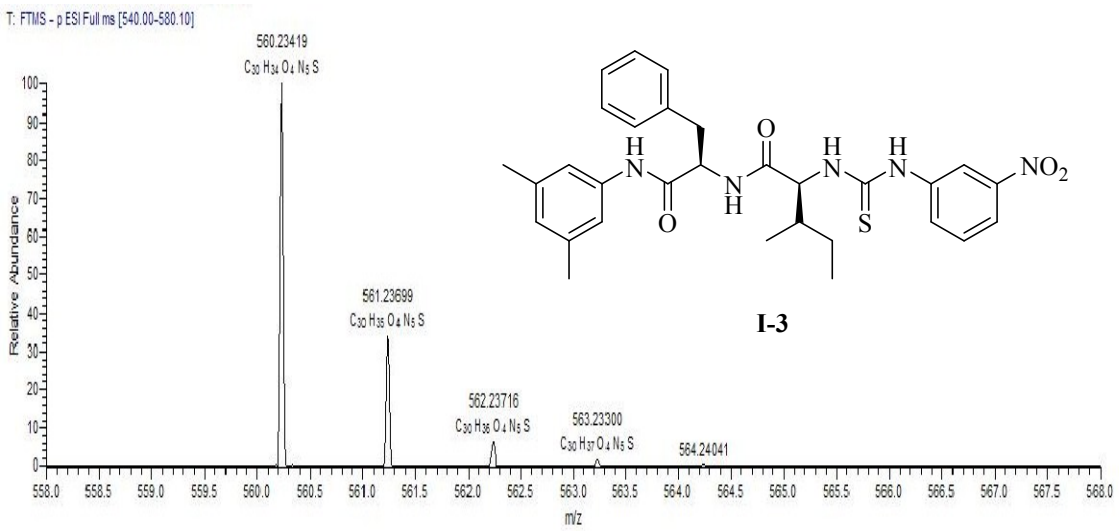
**I-2**


10.19
9.76
8.86
8.41
8.40
7.99
7.97
7.93
7.92
7.91
7.91
7.85
7.83
7.83
7.60
7.58
7.56
7.32
7.30
7.26
7.24
7.23
7.19
7.16
6.69
4.90
4.88
4.87
4.74
4.72
4.71
4.69
3.10
3.09
3.07
3.06
2.97
2.95
2.94
2.92
2.22
1.86
1.85
1.84
1.43
1.42
1.41
1.40
1.40
1.39
1.38
1.10
1.09
1.08
0.85
0.84
0.82
0.81
O
H
N
N
H
O
H
N
S
H
N
NO2
1.00
1.00
0.98
1.01
1.00
1.00
1.01
2.00
2.00
3.03
1.02
1.00
1.01
1.00
1.00
6.00
1.00
1.02
1.01
6.01
11.0
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)

**I-3**

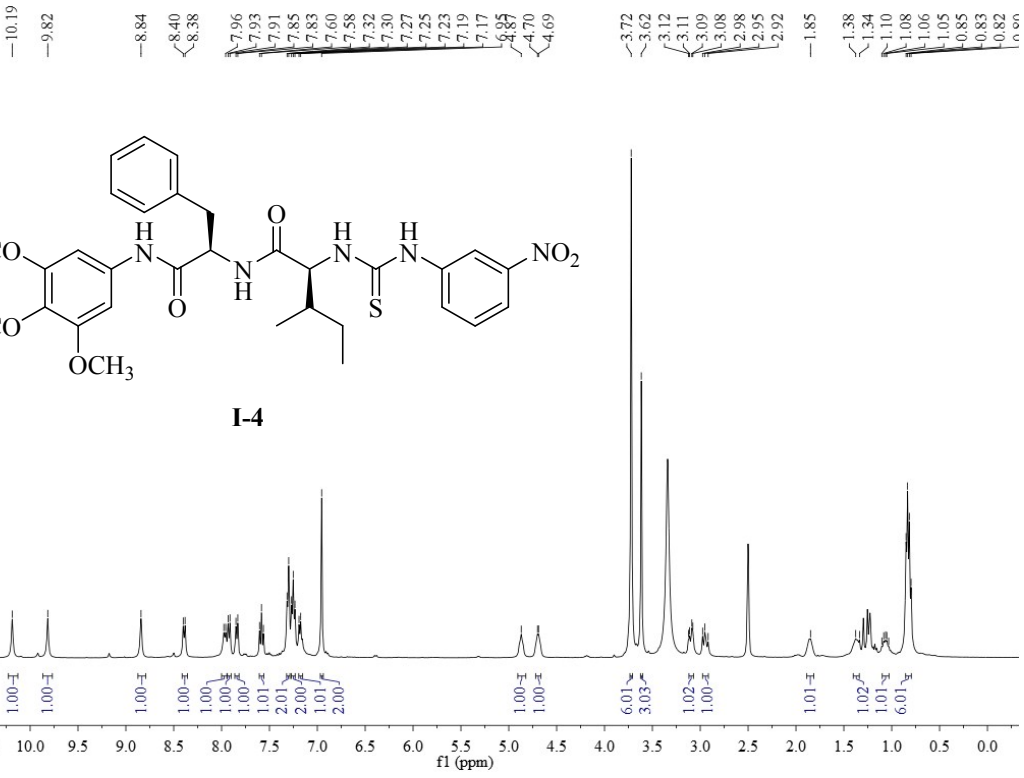

180.38
170.47
169.53
147.46
141.05
138.55
137.64
137.54
129.68
129.18
128.06
127.82
126.31
124.96
117.96
117.17
115.84
61.12
54.88
37.46
31.13
29.82
24.40
21.06
15.20
11.40
O
H
N
N
H
O
H
N
S
H
N
NO2
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

**I-3**


T: FTMS - p ESI Full ms [540.00-580.10]
560.23419
C30 H34 O4 N5 S
561.23699
C30 H35 O4 N5 S
562.23716
C30 H36 O4 N5 S
563.23300
C30 H37 O4 N5 S
564.24041
Relative Abundance
m/z

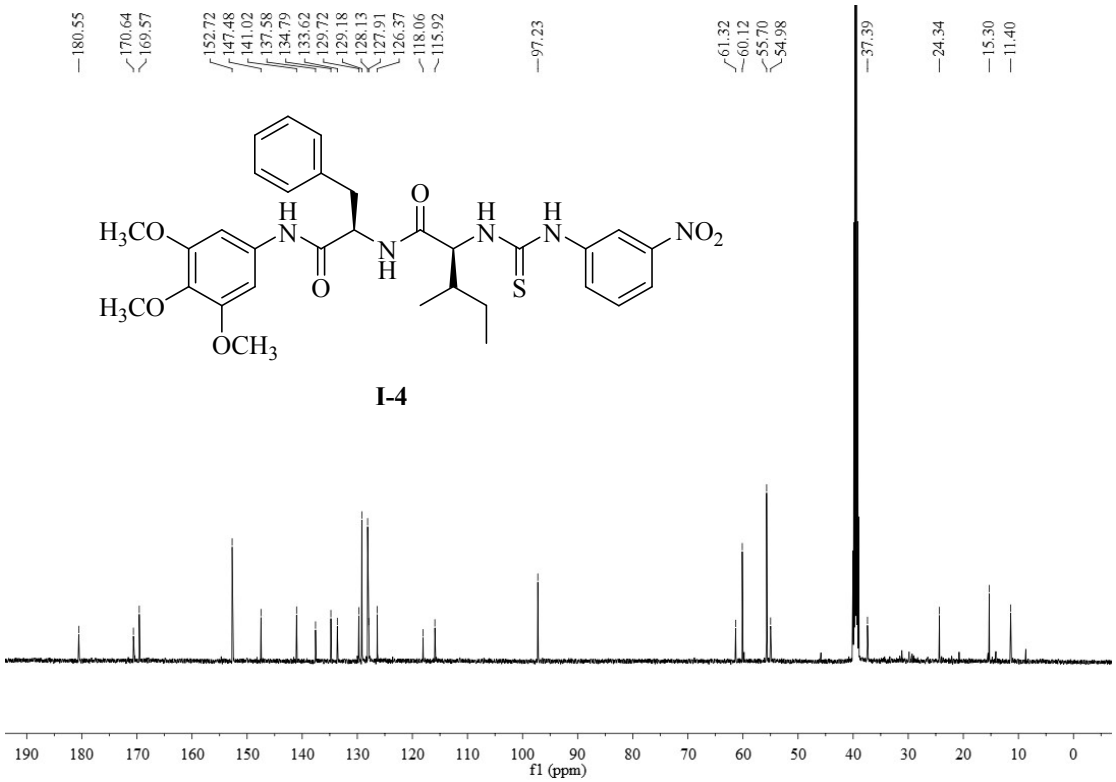


**I-3**

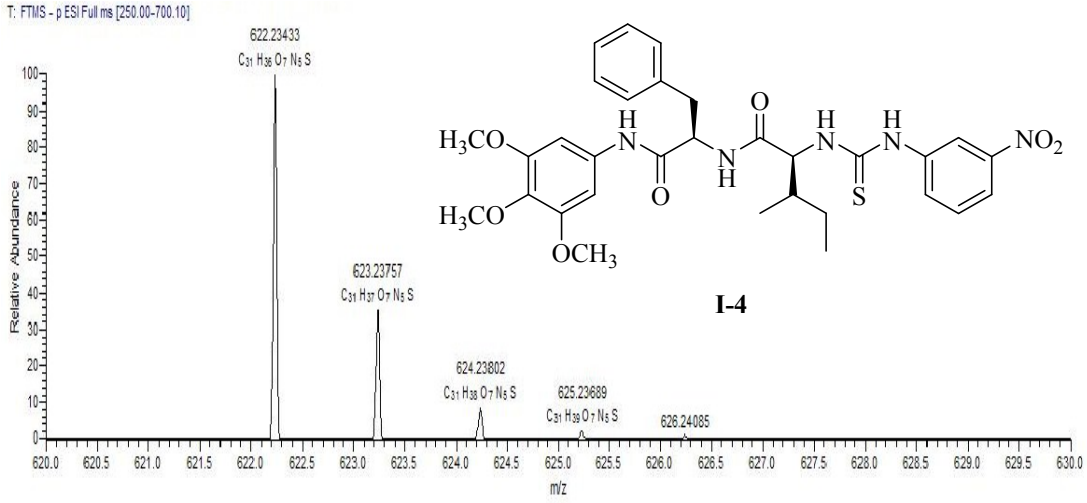

10.19
9.82
8.84
8.40
8.38
7.96
7.93
7.91
7.85
7.83
7.60
7.58
7.32
7.30
7.27
7.25
7.23
7.19
7.17
6.85
4.87
4.70
4.69
3.72
3.62
3.12
3.11
3.09
3.08
2.98
2.95
2.92
1.85
1.38
1.34
1.10
1.08
1.06
1.05
0.85
0.83
0.82
1.00
1.00
1.00
1.00
1.00
1.01
2.01
2.00
1.01
2.00
1.00
1.00
6.01
3.03
1.02
1.00
1.01
1.02
1.01
6.01
f1 (ppm)



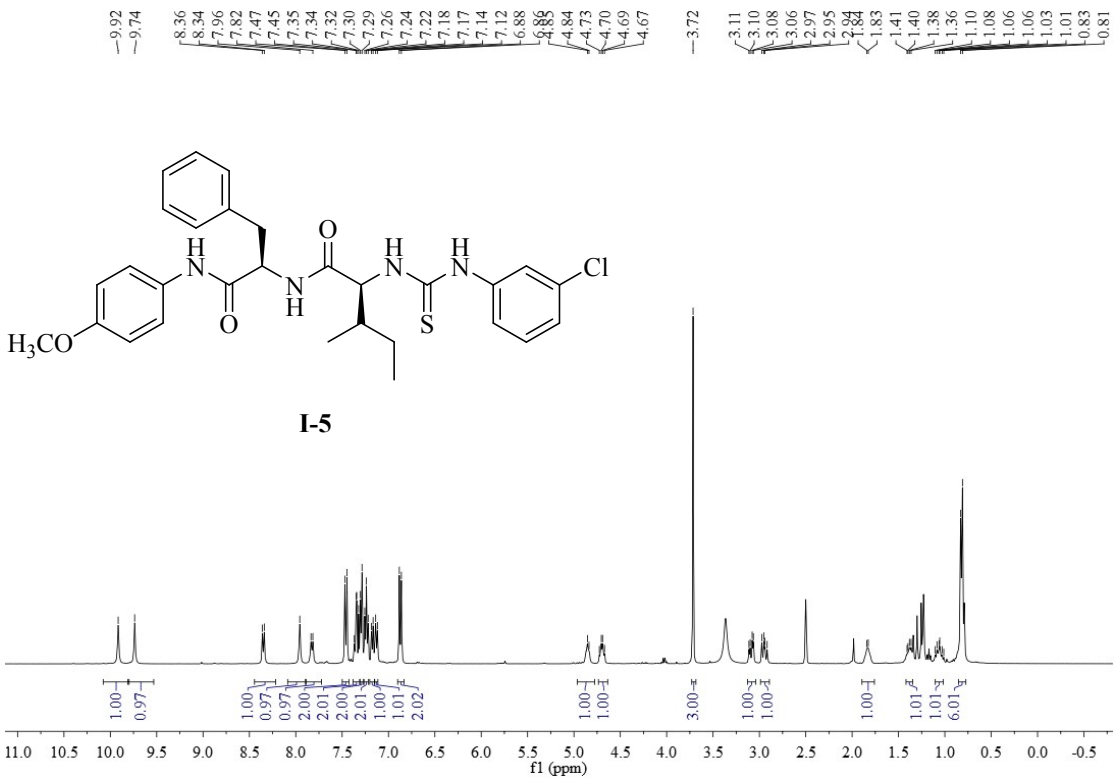
**I-4**


180.55
170.64
169.57
152.72
147.48
141.02
137.58
134.79
133.62
129.72
129.18
128.13
127.91
126.37
118.06
115.92
97.23
61.32
60.12
55.70
54.98
37.39
24.34
15.30
11.40
H3CO
H3CO
OCH3
NO2
f1 (ppm)

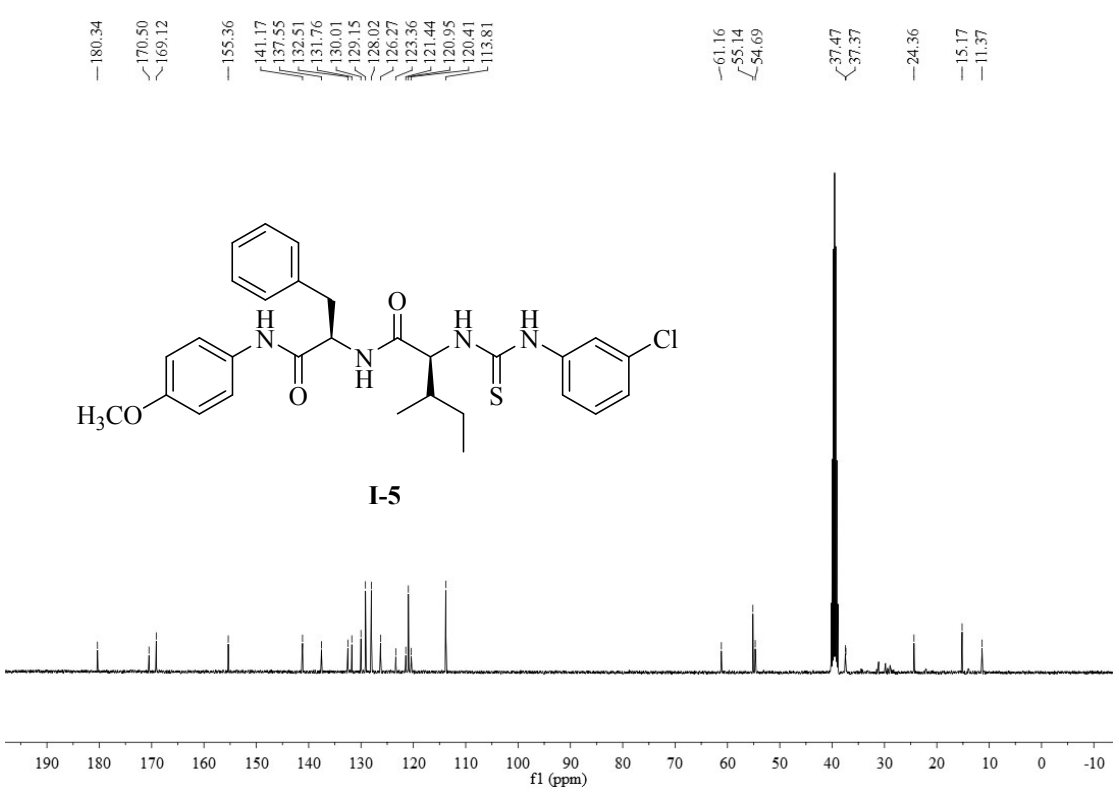
**I-4**


T: FTMS - p ESI Full ms [250.00-700.10]
622.23433
C31 H36 O7 N5 S
623.23757
C31 H37 O7 N5 S
624.23602
C31 H38 O7 N5 S
625.23689
C31 H39 O7 N5 S
626.24085
Relative Abundance
m/z
H3CO
H3CO
OCH3
NO2

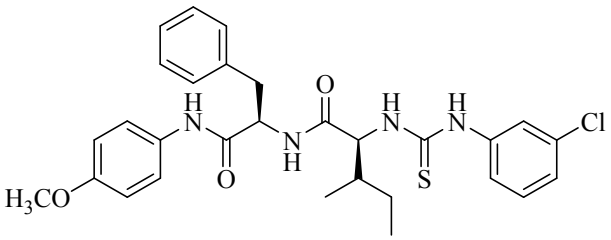
**I-4**


9.92
9.74
8.36
8.34
7.96
7.82
7.47
7.45
7.35
7.34
7.32
7.30
7.29
7.26
7.24
7.22
7.18
7.17
7.14
7.12
6.88
6.86
6.85
4.84
4.73
4.70
4.69
4.67
3.72
3.11
3.10
3.08
3.06
2.97
2.95
2.94
1.84
1.83
1.41
1.40
1.38
1.36
1.10
1.08
1.06
1.06
1.03
1.01
0.83
0.81
H3CO
Cl
1.00
0.97
1.00
0.97
0.97
2.00
2.01
2.00
2.01
1.00
1.01
2.02
1.00
1.00
3.00
1.00
1.00
1.00
1.01
1.01
6.01
11.0 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)

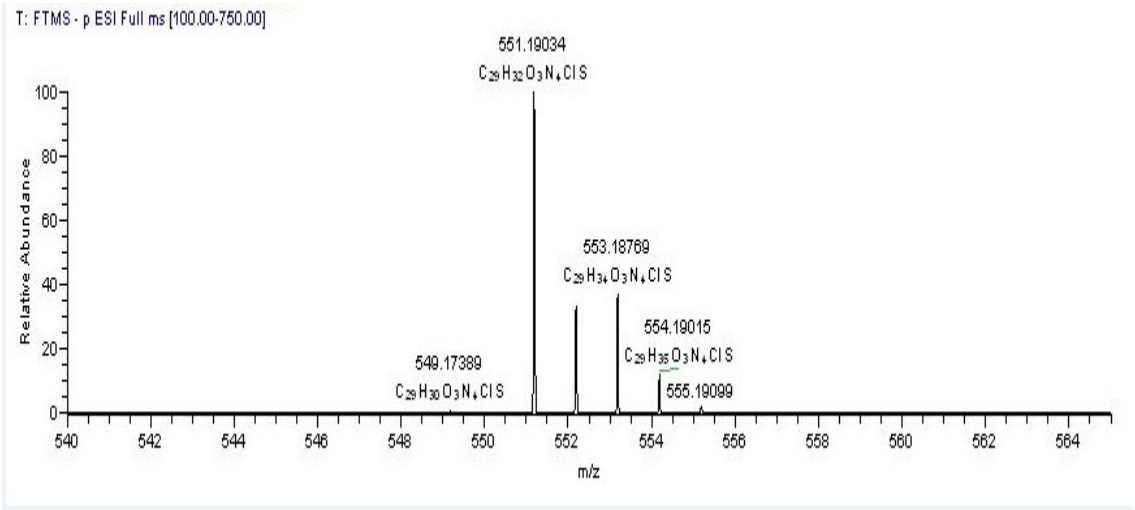
**I-5**

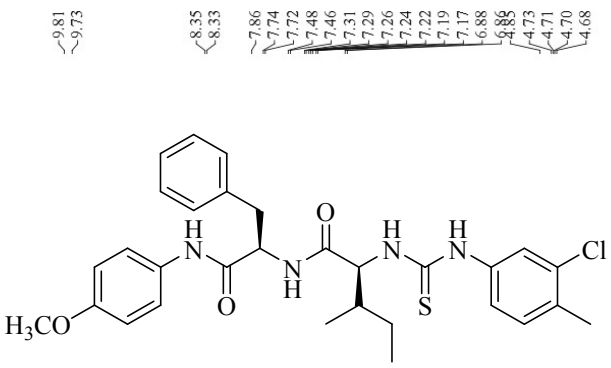

180.34
170.50
169.12
155.36
141.17
137.55
132.51
131.76
130.01
129.15
128.02
126.27
123.36
121.44
120.95
120.41
113.81
61.16
55.14
54.69
37.47
37.37
24.36
15.17
11.37
H3CO
Cl
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

**I-5**


H3CO
Cl

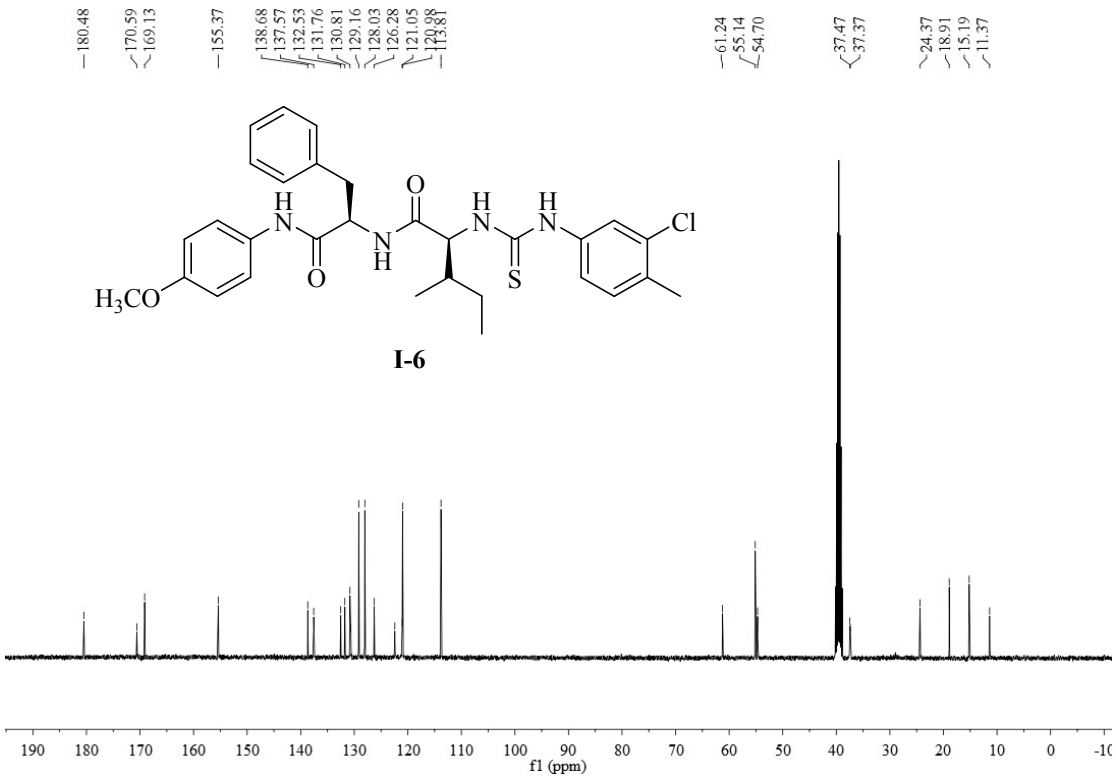
**I-5**


T: FTMS - p ESI Full ms [100.00-750.00]
551.19034
C29H32O3N4ClS
553.18769
C29H34O3N4ClS
554.19015
C29H35O3N4ClS
549.17389
C29H30O3N4ClS
555.19099
Relative Abundance
m/z

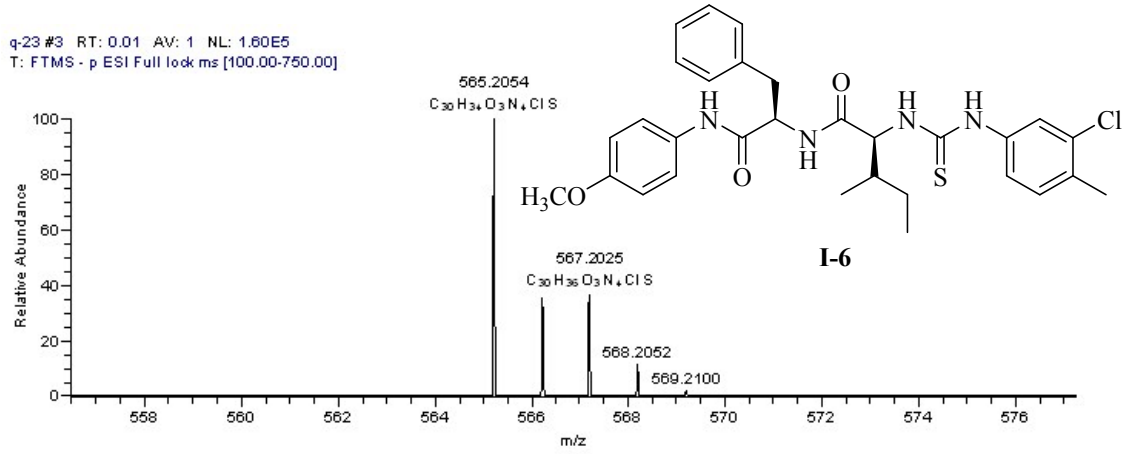

H3CO
Cl

**I-6**

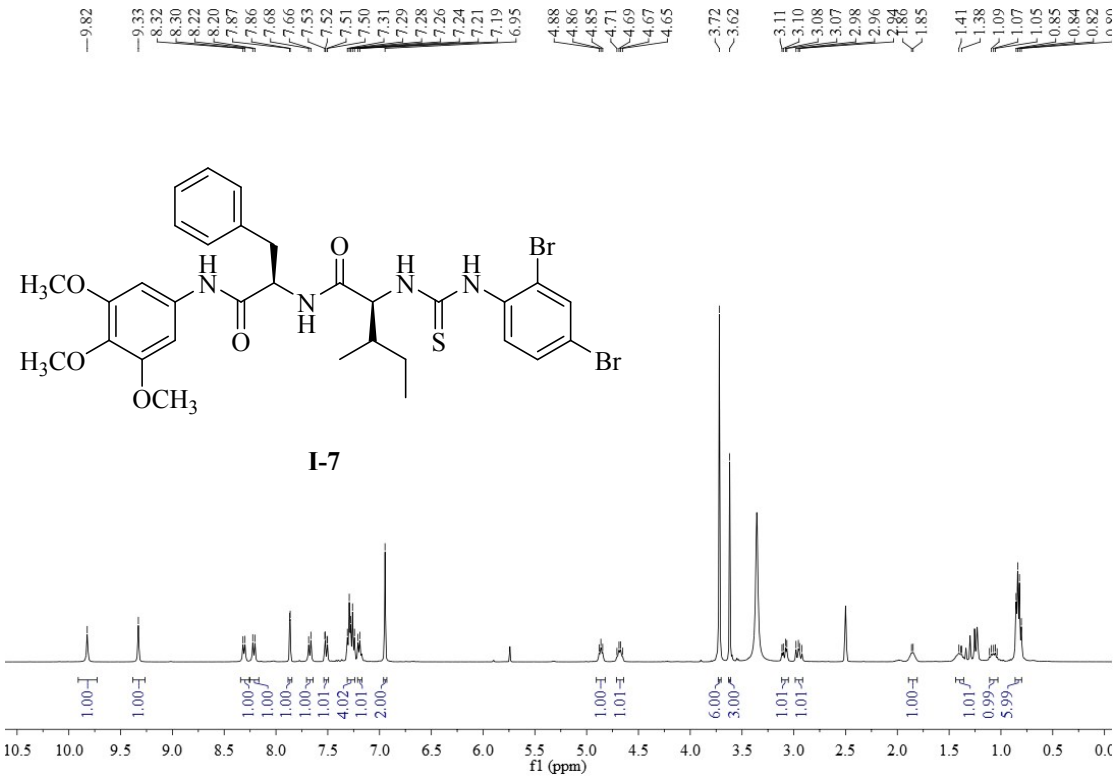

f1 (ppm)


180.48
170.59
169.13
155.37
138.68
137.57
132.53
131.76
130.81
129.16
128.03
126.28
121.05
120.98
113.81
61.24
55.14
54.70
37.47
37.37
24.37
18.91
15.19
11.37
H3CO
Cl
f1 (ppm)

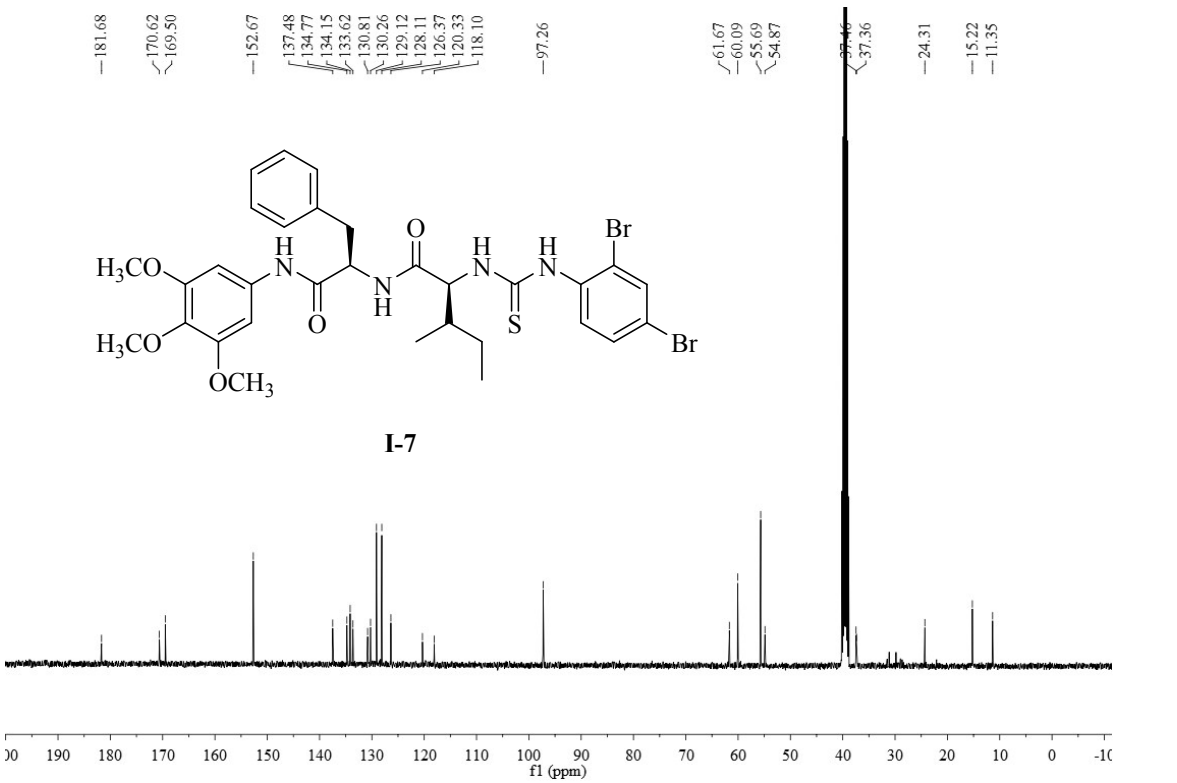
**I-6**


q-23 #3 RT: 0.01 AV: 1 NL: 1.60E5
T: FTMS - p ESI Full lock ms [100.00-750.00]
565.2054
C30H34O3N4ClS
567.2025
C30H36O3N4ClS
568.2052
569.2100
Relative Abundance
m/z
H3CO
Cl

**I-6**

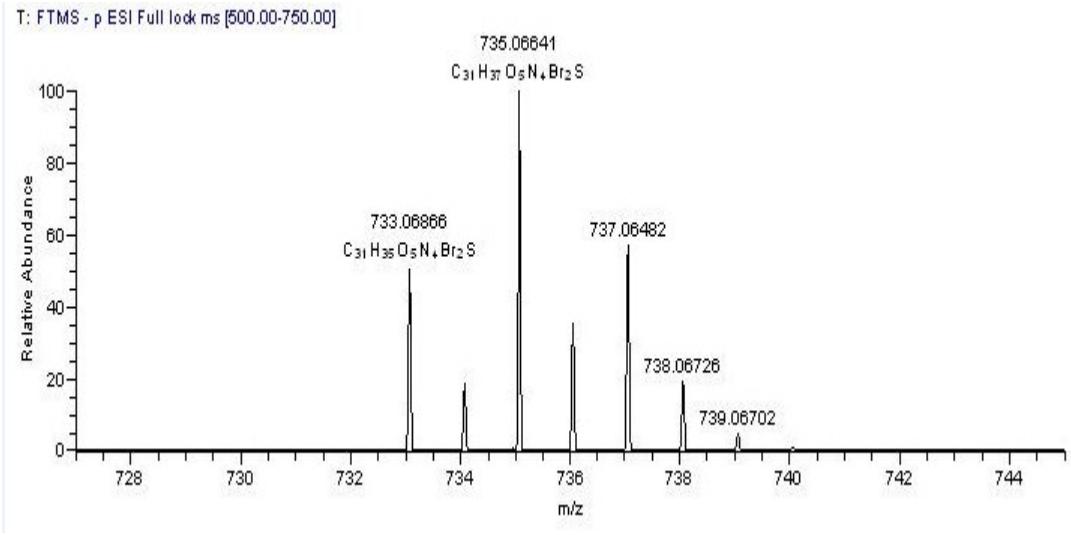

9.82
9.33
8.32
8.30
8.22
8.20
7.87
7.86
7.68
7.66
7.53
7.52
7.51
7.50
7.31
7.29
7.28
7.26
7.24
7.21
7.19
6.95
4.88
4.86
4.85
4.71
4.69
4.67
4.65
3.72
3.62
3.11
3.10
3.08
3.07
2.98
2.96
2.94
1.88
1.85
1.41
1.38
1.09
1.07
1.05
0.85
0.84
0.82
1.00
1.00
1.00
1.00
1.00
1.01
4.02
1.01
2.00
1.00
1.01
6.00
3.00
1.01
1.01
1.00
1.01
0.99
5.99
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
f1 (ppm)

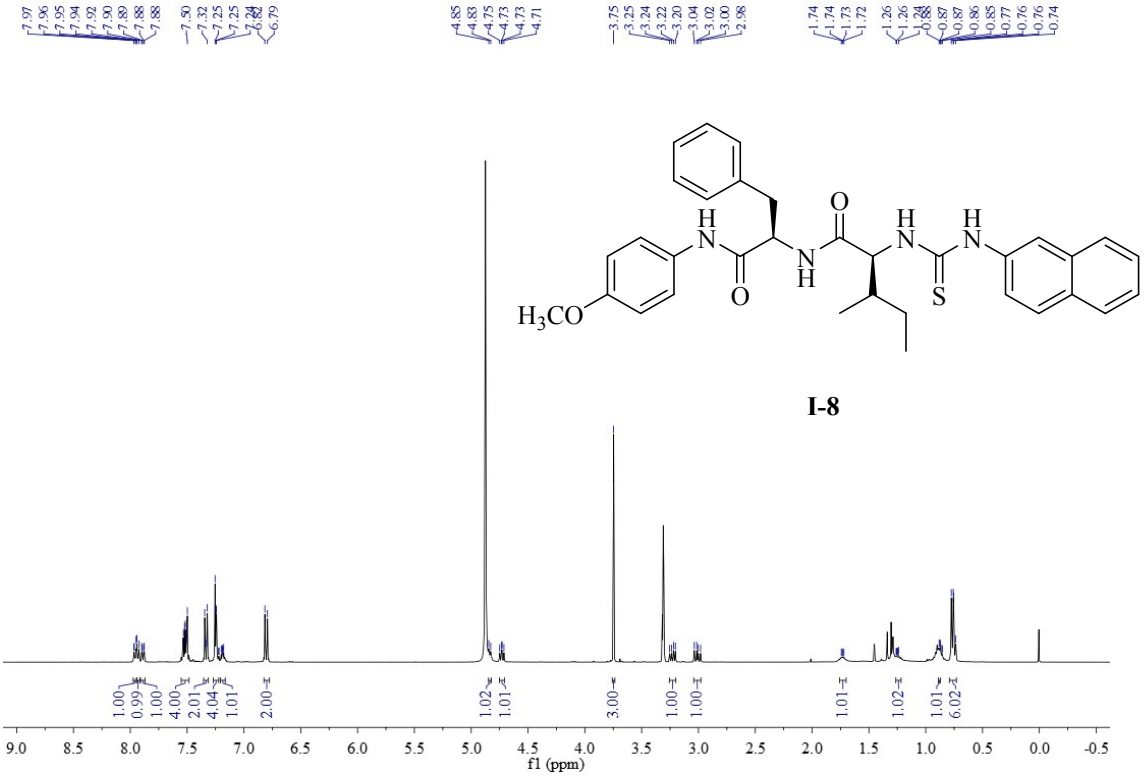
**I-7**

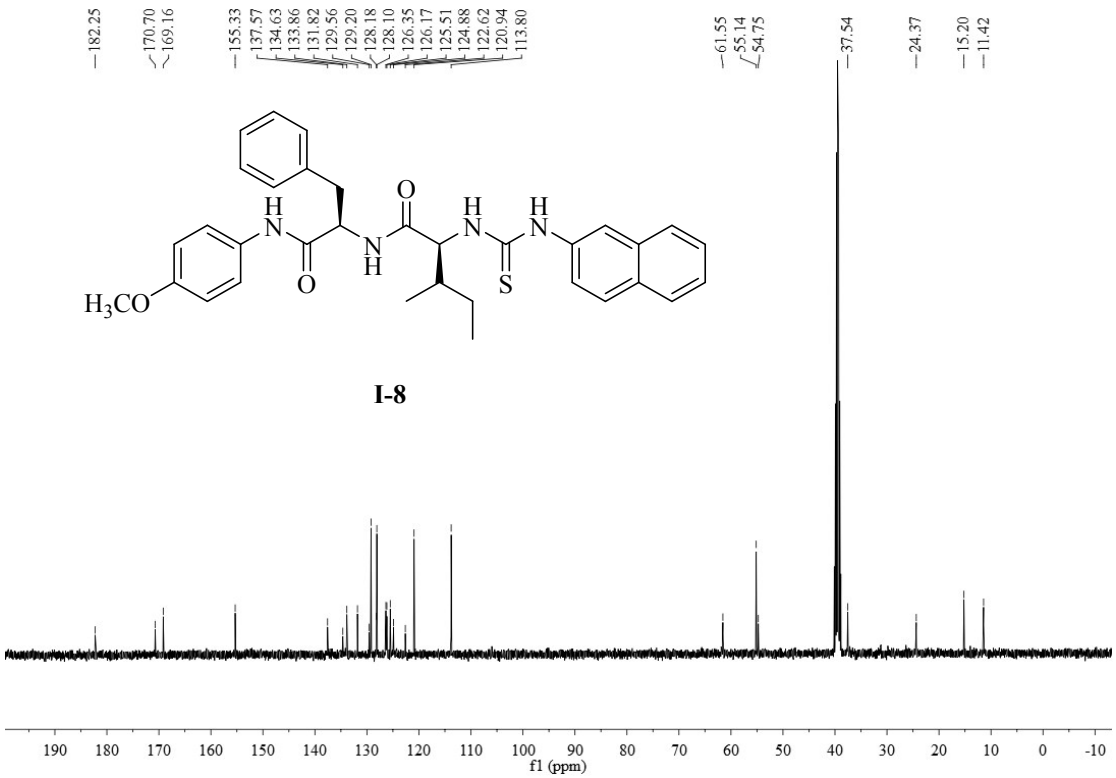

181.68
170.62
169.50
152.67
137.48
134.77
134.15
133.62
130.81
130.26
129.12
128.11
126.37
120.33
118.10
97.26
61.67
60.09
55.69
54.87
37.46
37.36
24.31
15.22
11.35
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

**I-7**

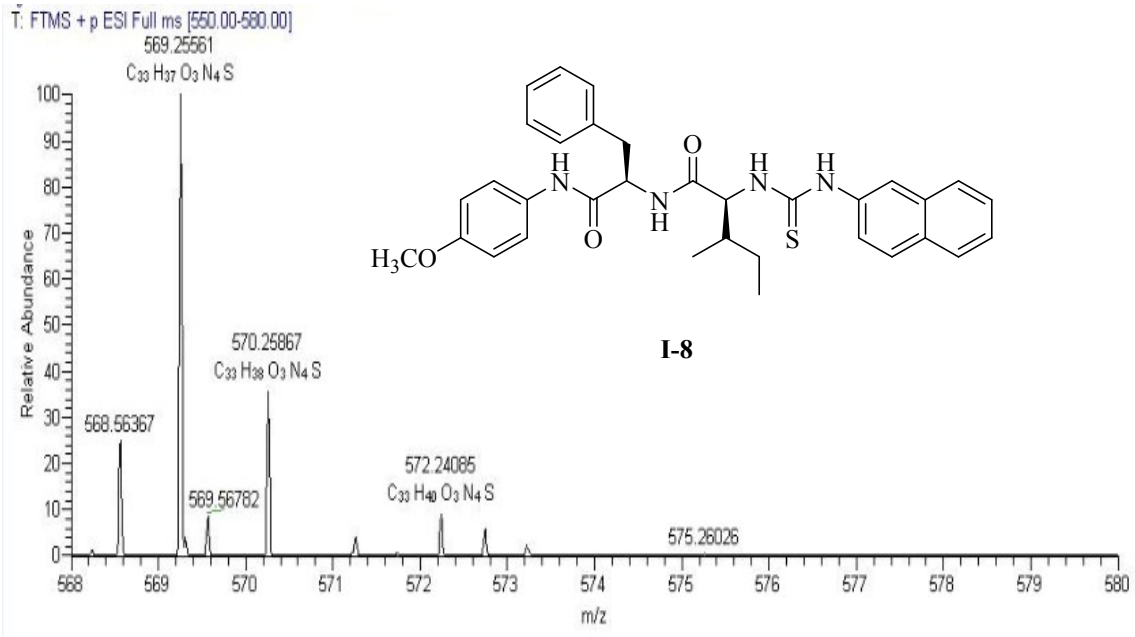
**I-7**


T: FTMS - p ESI Full lock ms [500.00-750.00]
735.06641
C31 H37 O5 N4 Br2 S
733.06866
C31 H35 O5 N4 Br2 S
737.06482
738.06726
739.06702
Relative Abundance
m/z

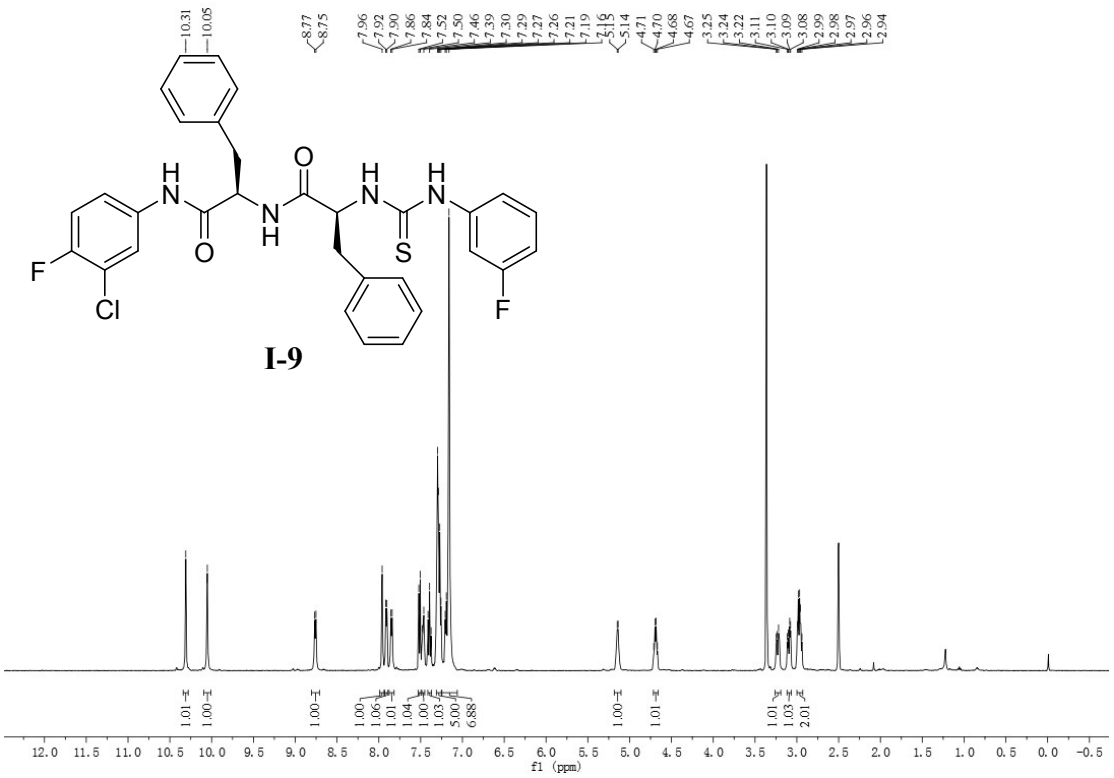

H3CO
I-8
f1 (ppm)


182.25
170.70
169.16
155.33
137.57
134.63
133.86
131.82
129.56
129.20
128.18
128.10
126.35
126.17
125.51
124.88
122.62
120.94
113.80
61.55
55.14
54.75
37.54
24.37
15.20
11.42
H3CO
f1 (ppm)

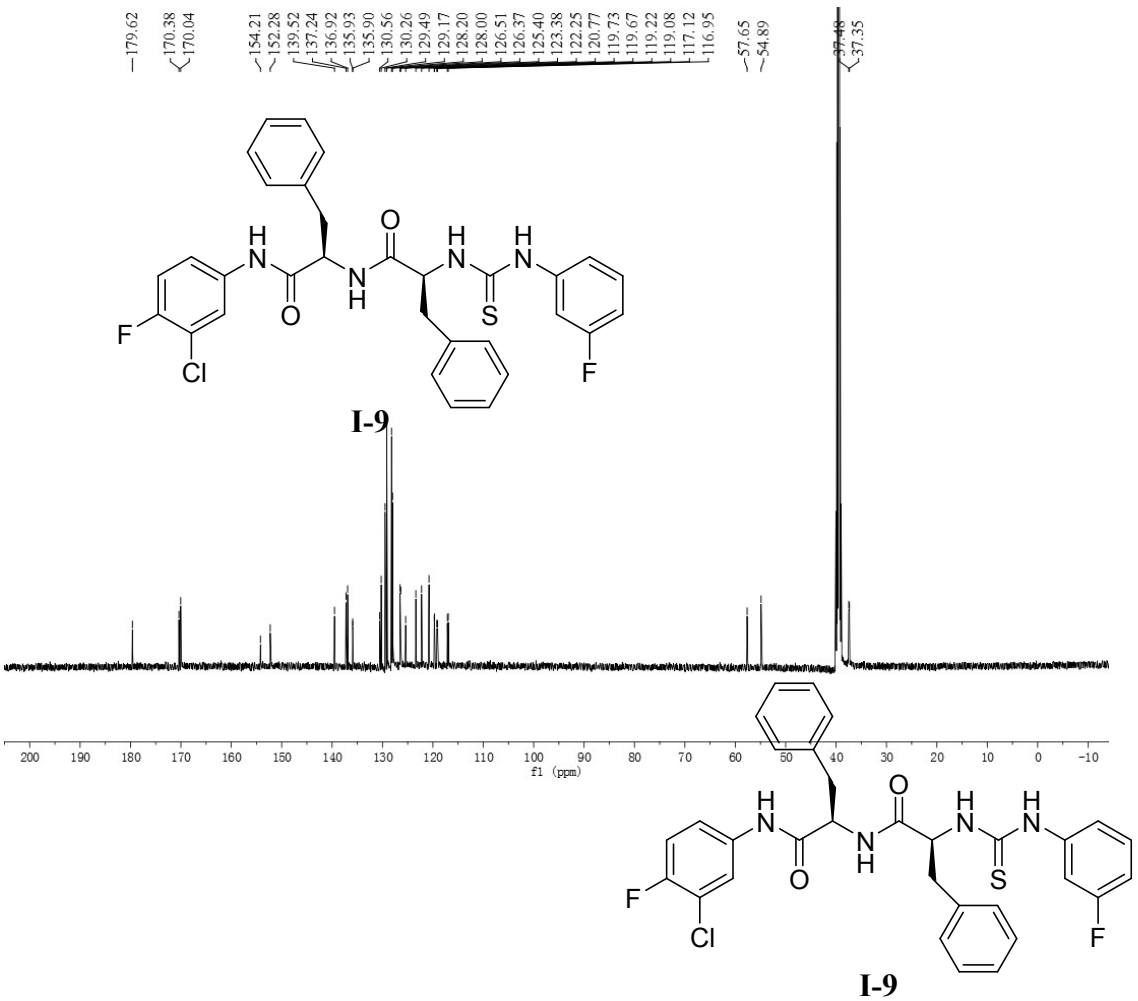
**I-8**


T: FTMS + p ESI Full ms [550.00-580.00]
569.25561
C33 H37 O3 N4 S
570.25867
C33 H38 O3 N4 S
568.56367
569.56782
572.24085
C33 H40 O3 N4 S
575.26026
Relative Abundance
m/z

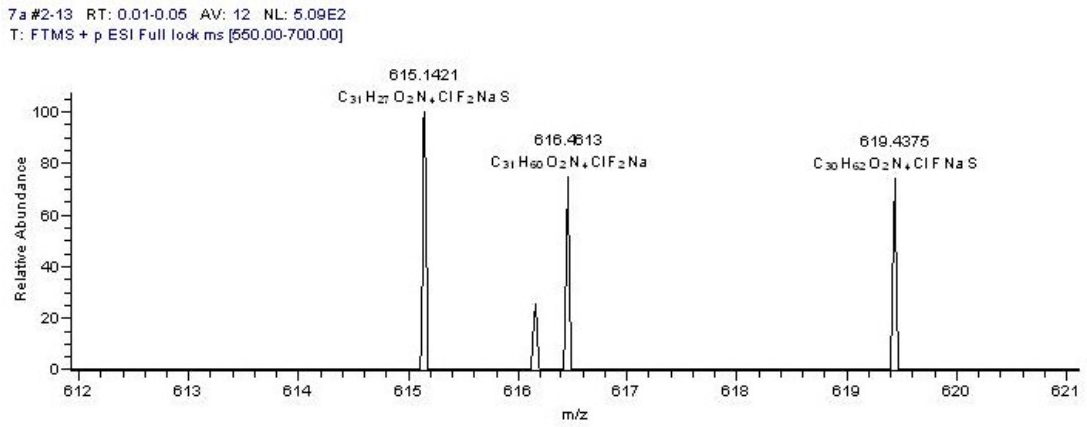
**I-8**

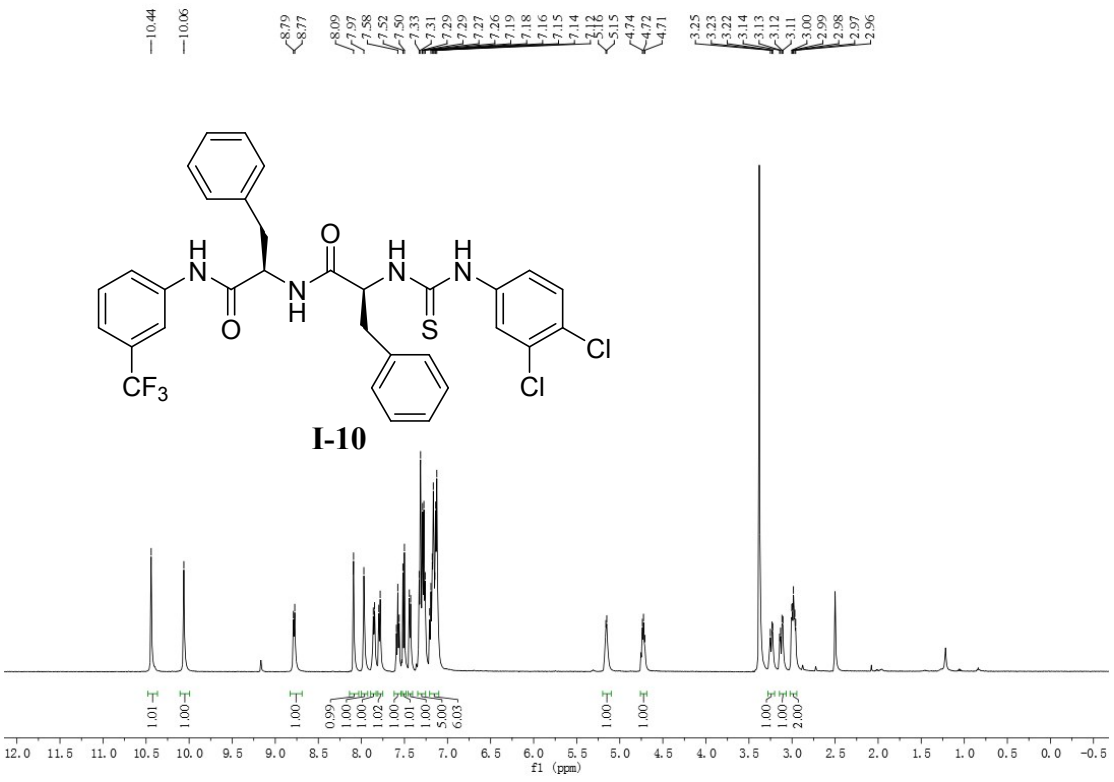

10.31
10.05
8.77
8.75
7.96
7.92
7.90
7.86
7.84
7.52
7.50
7.46
7.39
7.30
7.29
7.27
7.26
7.21
7.19
7.16
5.15
5.14
4.71
4.70
4.68
4.67
3.25
3.24
3.22
3.11
3.10
3.09
3.08
2.99
2.98
2.97
2.96
2.94
1.01
1.00
1.00
1.00
1.06
1.01
1.04
1.00
1.03
5.00
6.88
1.00
1.01
1.01
1.03
2.01
f1 (ppm)

**I-9**

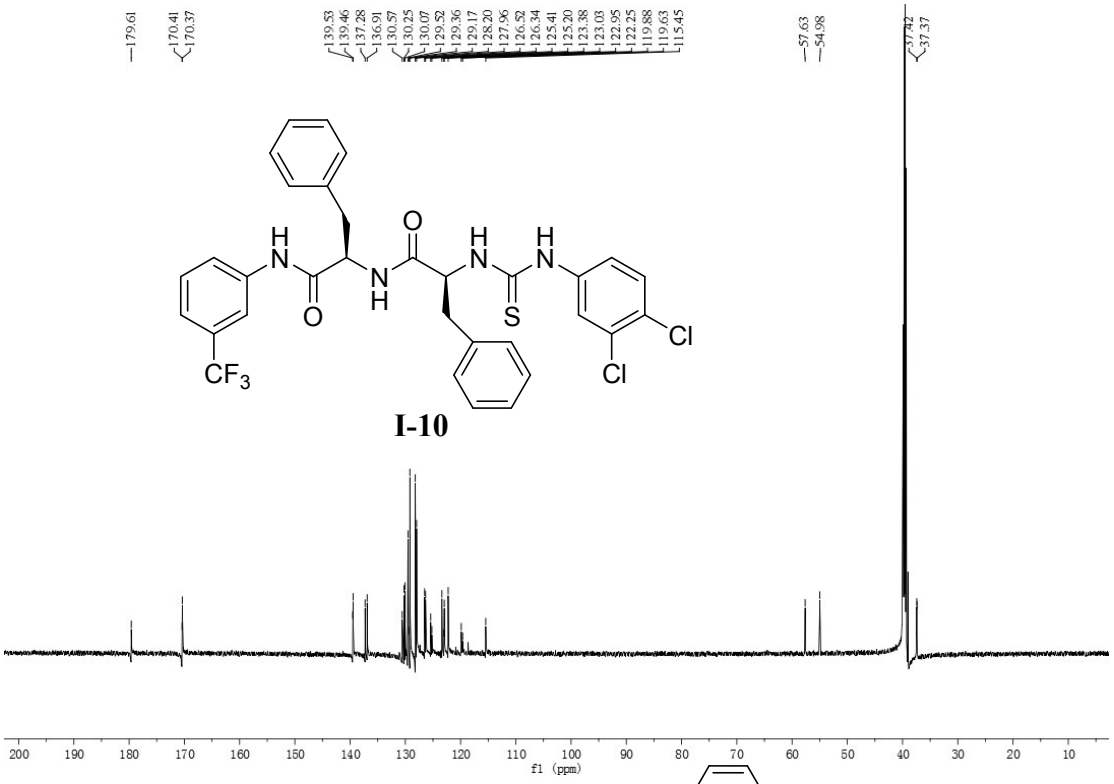

179.62
170.38
170.04
154.21
152.28
139.52
137.24
136.92
135.93
135.90
130.56
130.26
129.49
129.17
128.20
128.00
126.51
126.37
125.40
123.38
122.25
120.77
119.73
119.67
119.22
119.08
117.12
116.95
57.65
54.89
37.48
37.35
f1 (ppm)

**I-9**


7a #2-13 RT: 0.01-0.05 AV: 12 NL: 5.09E2
T: FTMS + p ESI Full lock ms [550.00-700.00]
615.1421
C31H27O2N4ClF2NaS
616.4613
C31H60O2N4ClF2Na
619.4375
C30H62O2N4ClFNaS
Relative Abundance
m/z

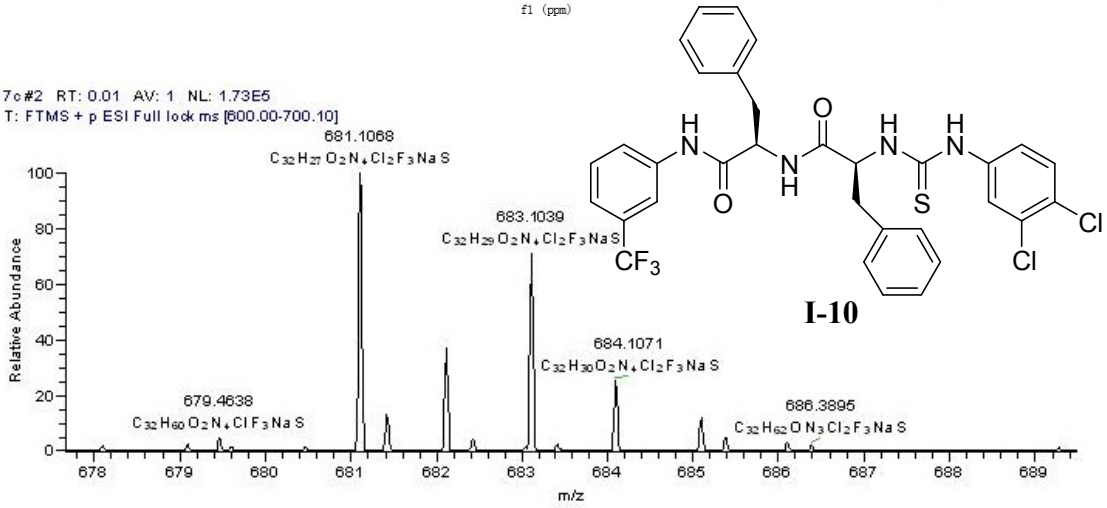

10.44
10.06
8.79
8.77
8.09
7.97
7.58
7.52
7.50
7.33
7.31
7.29
7.29
7.27
7.26
7.19
7.18
7.16
7.15
7.14
7.12
5.18
5.15
4.74
4.72
4.71
3.25
3.23
3.22
3.14
3.13
3.12
3.11
3.00
2.99
2.98
2.97
2.96
CF3
Cl
Cl
f1 (ppm)

**I-10**


179.61
170.41
170.37
139.53
139.46
137.28
136.91
130.57
130.25
130.07
129.52
129.36
129.17
128.20
127.96
126.52
126.34
125.41
125.20
123.38
123.03
122.95
122.25
119.88
119.63
115.45
57.63
54.98
37.42
37.37
f1 (ppm)

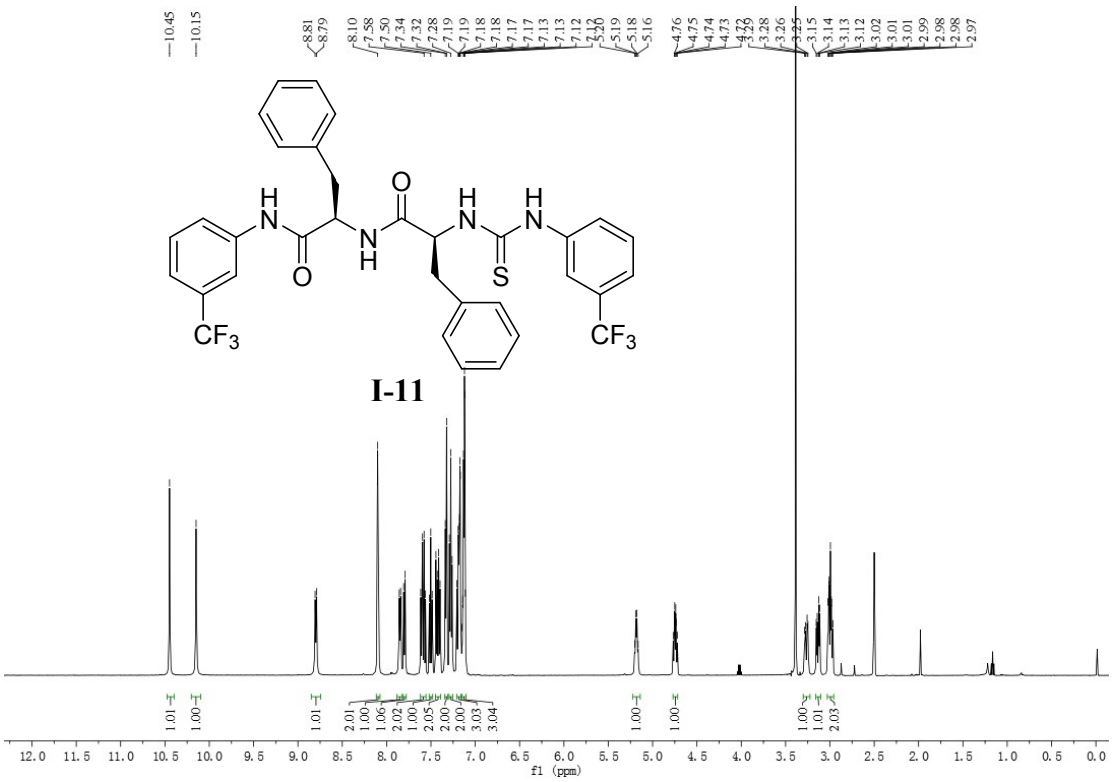

H
N
O
N
H
H
N
O
H
N
S
Cl
Cl
CF3

**I-10**

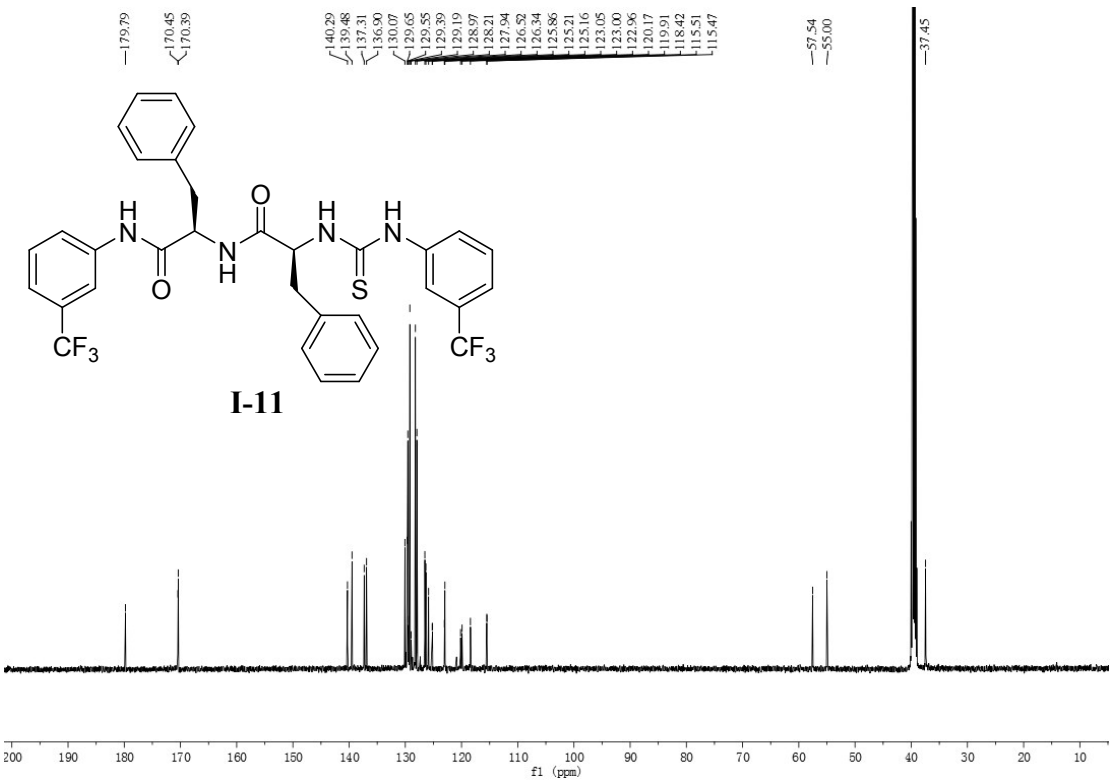

7c #2 RT: 0.01 AV: 1 NL: 1.73E5
T: FTMS + p ESI Full lock ms [600.00-700.10]
681.1068
C32H27O2N4Cl2F3NaS
683.1039
C32H29O2N4Cl2F3NaS
684.1071
C32H30O2N4Cl2F3NaS
679.4638
C32H60O2N4ClF3NaS
686.3895
C32H62ON3Cl2F3NaS
Relative Abundance
m/z


H
N
O
N
H
H
N
O
H
N
S
Cl
Cl
CF3

**I-10**

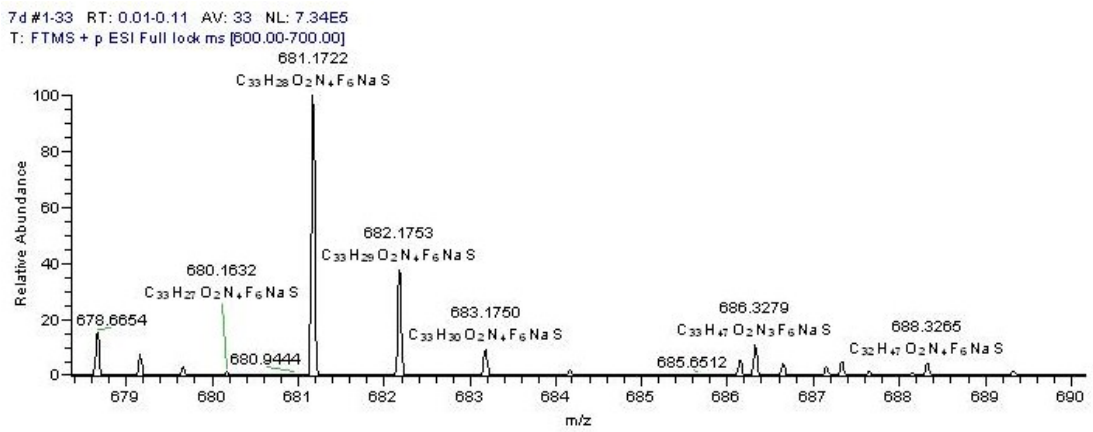

10.45
10.15
8.81
8.79
8.10
7.58
7.50
7.34
7.32
7.28
7.19
7.19
7.18
7.18
7.17
7.17
7.13
7.13
7.12
5.20
5.19
5.18
5.16
4.76
4.75
4.74
4.73
3.29
3.28
3.26
3.25
3.15
3.14
3.13
3.12
3.02
3.01
3.01
2.99
2.98
2.98
2.97
1.01
1.00
1.01
2.01
1.00
1.06
2.02
1.00
2.05
2.00
2.00
3.03
3.04
1.00
1.00
1.00
1.01
2.03
f1 (ppm)

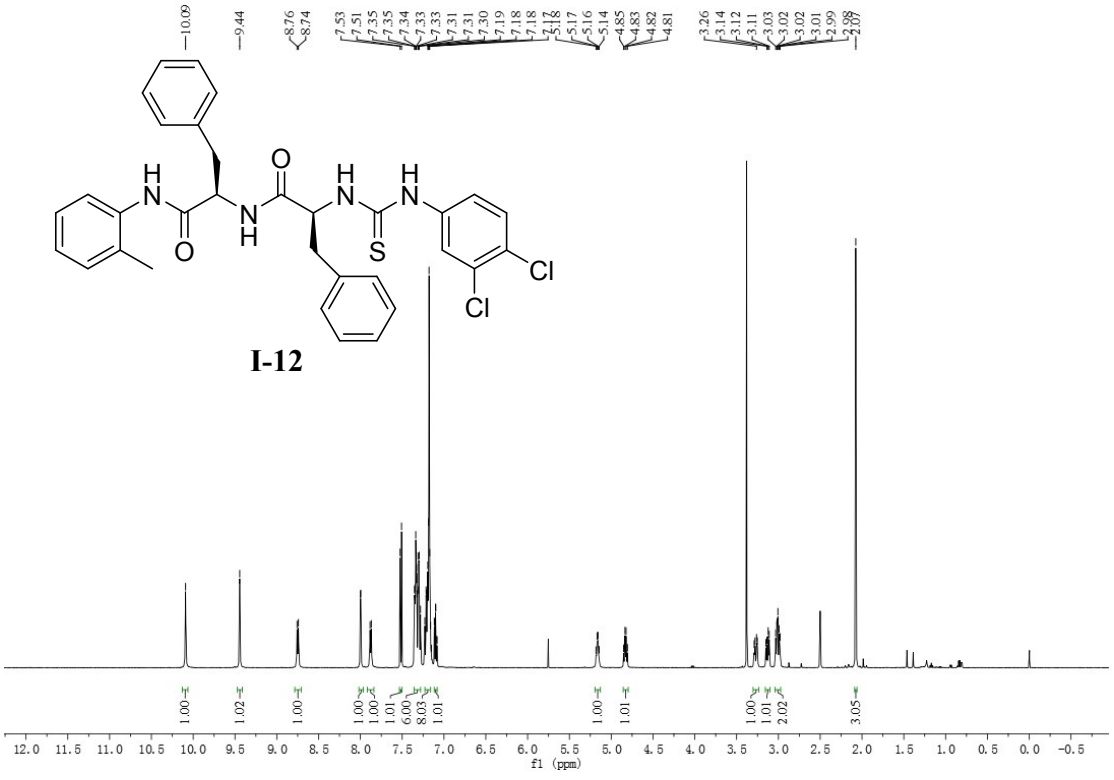
**I-11**

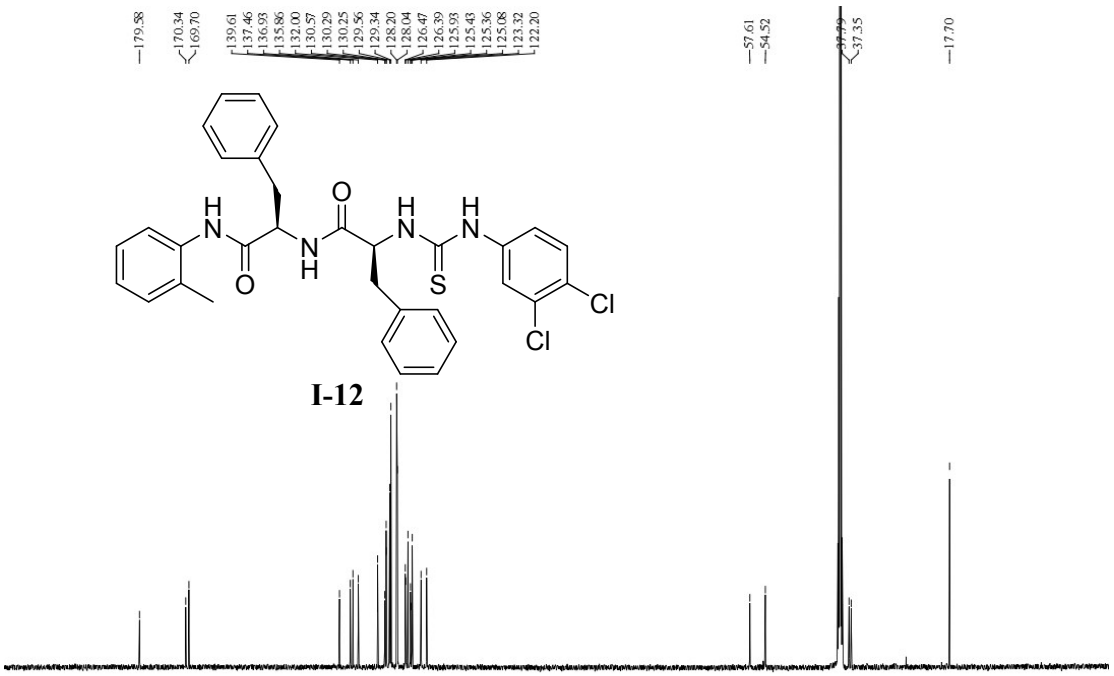

179.79
170.45
170.39
140.29
139.48
137.31
136.90
130.07
129.65
129.55
129.39
129.19
128.97
128.21
127.94
126.52
126.34
125.86
125.21
125.16
123.05
123.00
122.96
120.17
119.91
118.42
115.51
115.47
57.54
55.00
37.45
f1 (ppm)

**I-11**

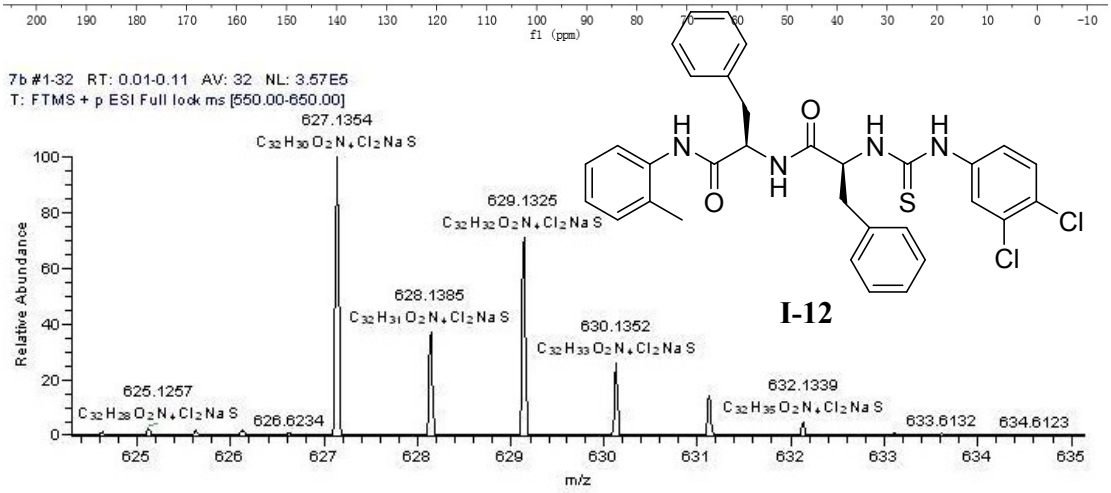
**I-11**


7d #1-33 RT: 0.01-0.11 AV: 33 NL: 7.34E5
T: FTMS + p ESI Full lock ms [600.00-700.00]
681.1722
C33H28O2N4F6NaS
682.1753
C33H29O2N4F6NaS
680.1632
C33H27O2N4F6NaS
683.1750
C33H30O2N4F6NaS
678.6654
680.9444
685.6512
686.3279
C33H47O2N3F6NaS
688.3265
C32H47O2N4F6NaS
Relative Abundance
m/z

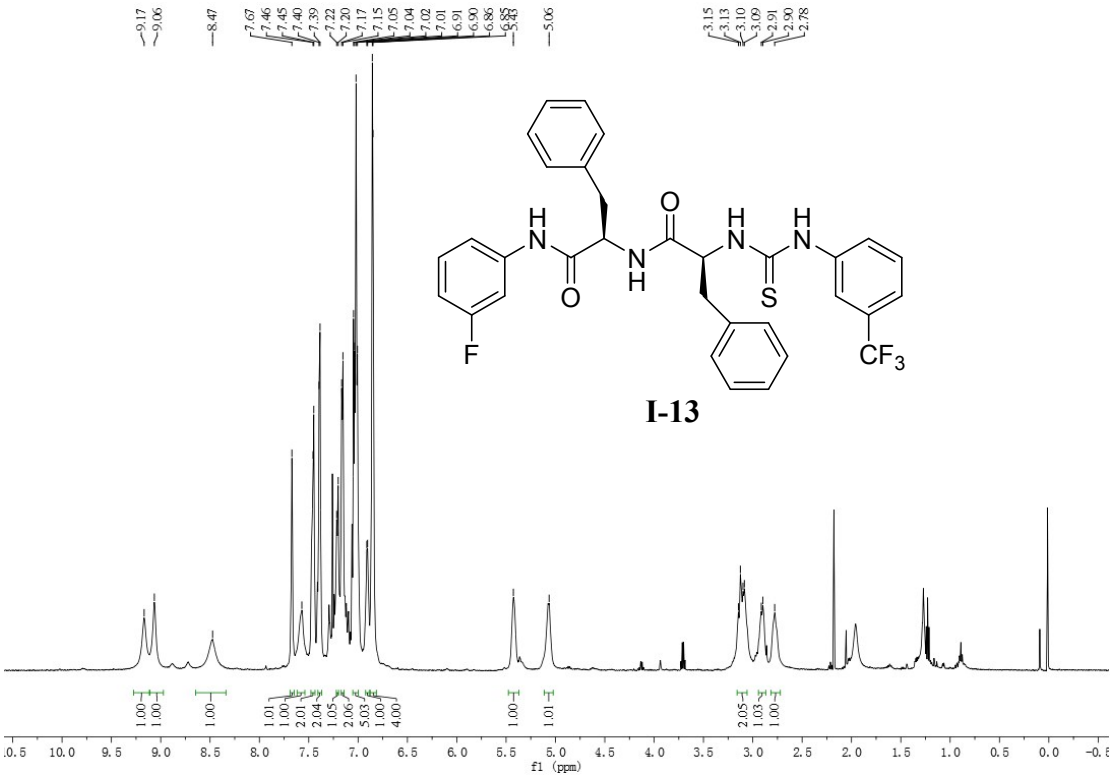

I-12


179.58
170.34
169.70
139.61
137.46
136.93
135.86
132.00
130.57
130.29
130.25
129.56
129.34
128.20
128.04
126.47
126.39
125.93
125.43
125.36
125.08
123.32
122.20
57.61
54.52
37.70
37.35
17.70
H
N
O
N
H
O
H
N
S
H
N
Cl
Cl
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

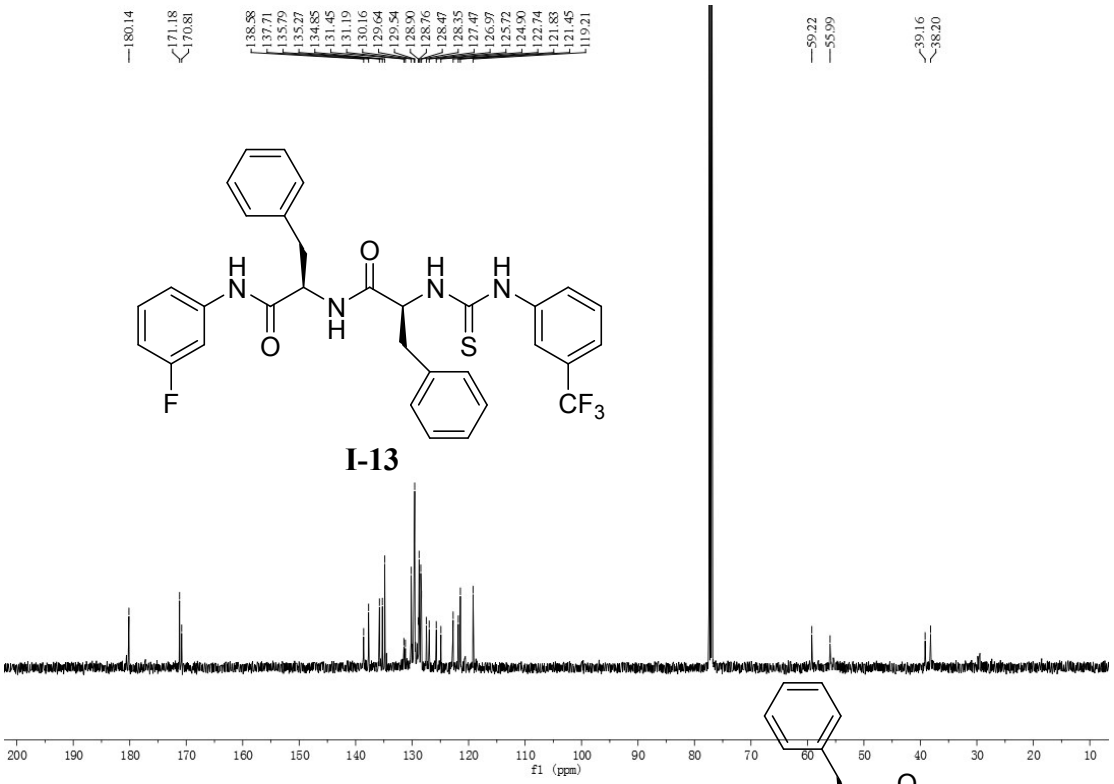
**I-12**


7b #1-32 RT: 0.01-0.11 AV: 32 NL: 3.57E5
T: FTMS + p ESI Full lock ms [550.00-650.00]
627.1354
C32H30O2N4Cl2NaS
629.1325
C32H32O2N4Cl2NaS
628.1385
C32H31O2N4Cl2NaS
630.1352
C32H33O2N4Cl2NaS
625.1257
C32H28O2N4Cl2NaS
626.6234
632.1339
C32H35O2N4Cl2NaS
633.6132
634.6123
Relative Abundance
m/z
100
80
60
40
20
0
625
626
627
628
629
630
631
632
633
634
635
H
N
O
N
H
O
H
N
S
H
N
Cl
Cl

**I-12**

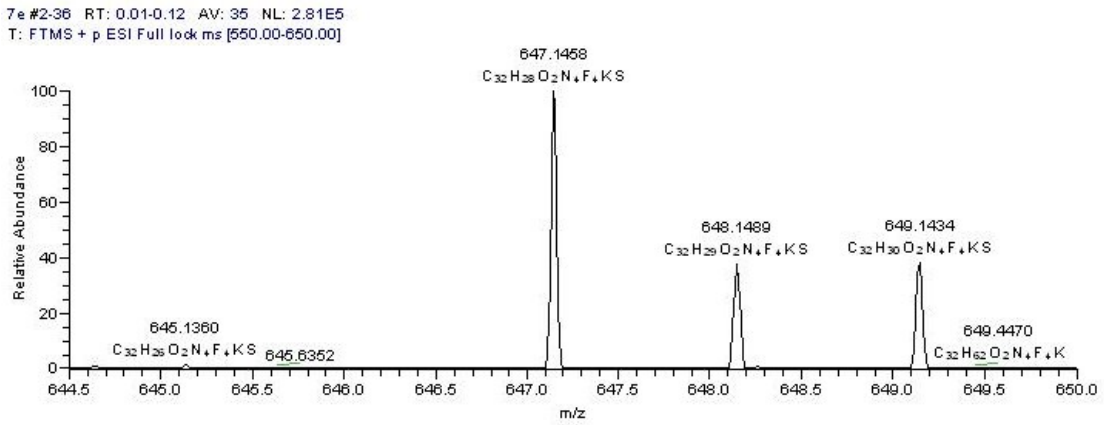

9.17
9.06
8.47
7.67
7.46
7.45
7.40
7.39
7.22
7.20
7.17
7.15
7.05
7.04
7.02
7.01
6.91
6.90
6.86
6.85
5.43
5.06
3.15
3.13
3.10
3.09
2.91
2.90
2.78
1.00
1.00
1.00
1.01
1.00
2.01
2.04
1.05
2.06
5.03
1.00
4.00
1.00
1.01
2.05
1.03
1.00
f1 (ppm)

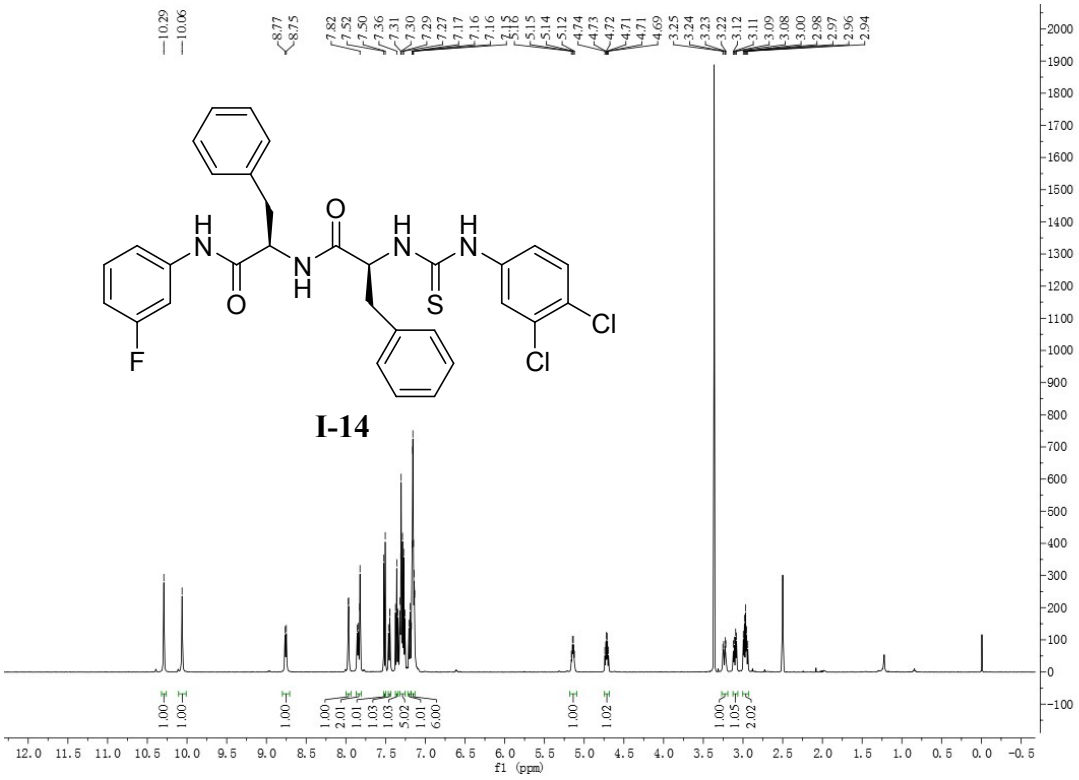
**I-13**

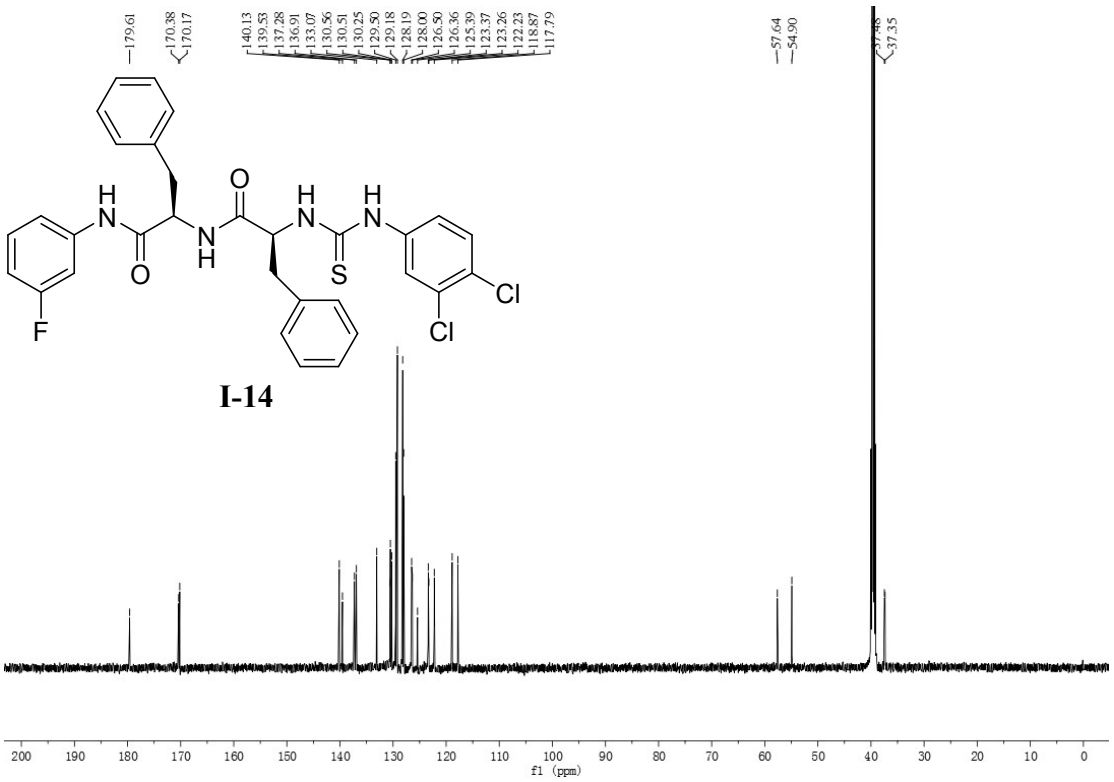

180.14
171.18
170.81
138.58
137.71
135.79
135.27
134.85
131.45
131.19
130.16
129.64
129.54
128.90
128.76
128.47
128.35
127.47
126.97
125.72
124.90
122.74
121.83
121.45
119.21
59.22
55.99
39.16
38.20
f1 (ppm)

**I-13**

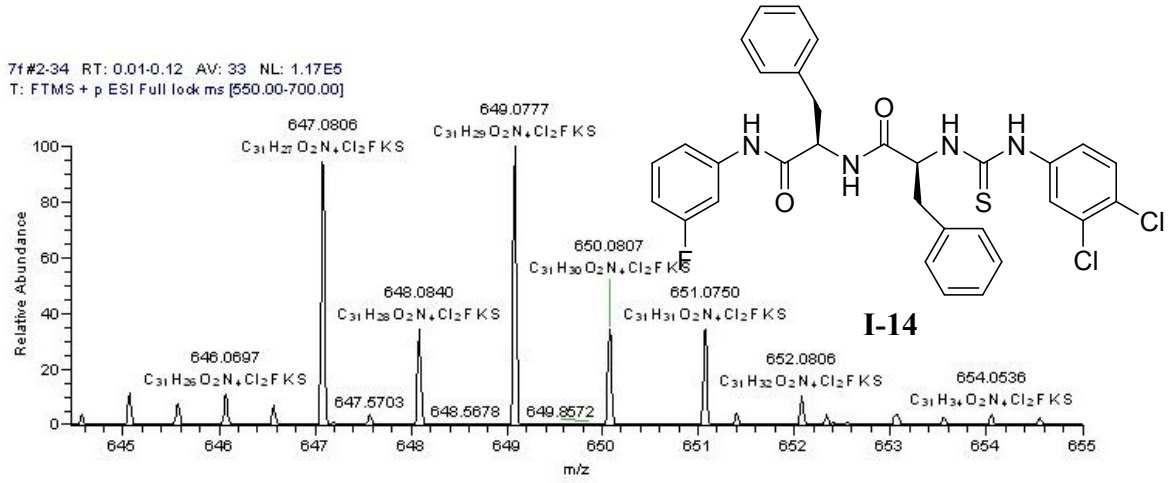
**I-13**


7e #2-36 RT: 0.01-0.12 AV: 35 NL: 2.81E5
T: FTMS + p ESI Full lock ms [550.00-650.00]
647.1458
C32H28O2N4F4KS
648.1489
C32H29O2N4F4KS
649.1434
C32H30O2N4F4KS
645.1360
C32H26O2N4F4KS
645.6352
649.4470
C32H62O2N4F4K
Relative Abundance
m/z

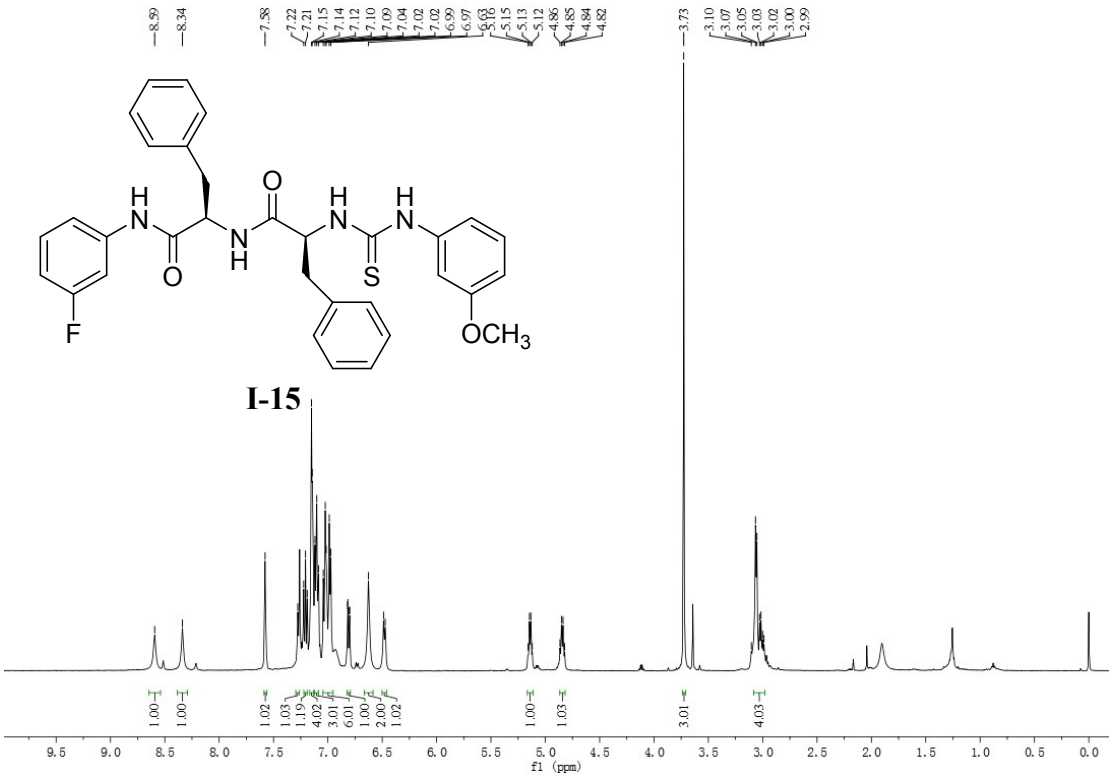

I-14
f1 (ppm)


179.61
170.38
170.17
140.13
139.53
137.28
136.91
133.07
130.56
130.51
130.25
129.50
129.18
128.19
128.00
126.50
126.36
125.39
123.37
123.26
122.23
118.87
117.79
57.64
54.90
37.48
37.35
H
N
O
N
H
H
N
S
H
N
Cl
Cl
F
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

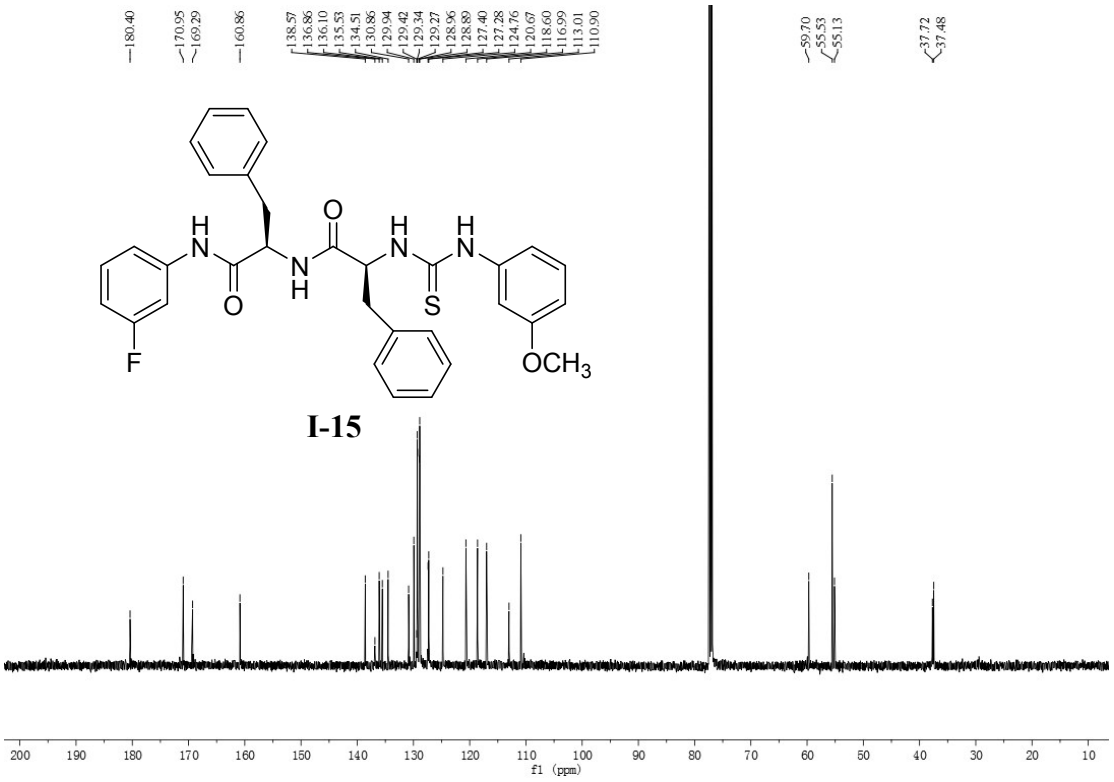
**I-14**


7f #2-34 RT: 0.01-0.12 AV: 33 NL: 1.17E5
T: FTMS + p ESI Full lock ms [550.00-700.00]
647.0806
C31H27O2N4Cl2FKS
649.0777
C31H29O2N4Cl2FKS
650.0807
C31H30O2N4Cl2FKS
648.0840
C31H28O2N4Cl2FKS
651.0750
C31H31O2N4Cl2FKS
646.0697
C31H26O2N4Cl2FKS
652.0806
C31H32O2N4Cl2FKS
654.0536
C31H34O2N4Cl2FKS
647.5703
648.5678
649.8572
Relative Abundance
m/z
645
646
647
648
649
650
651
652
653
654
655
H
N
O
N
H
H
N
S
H
N
Cl
Cl
F

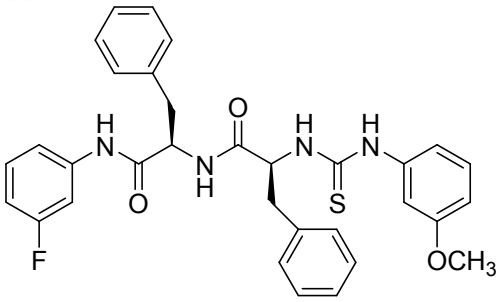
**I-14**


8.99
8.34
7.58
7.22
7.21
7.15
7.14
7.12
7.10
7.09
7.04
7.02
7.02
6.99
6.97
5.16
5.15
5.13
5.12
4.86
4.85
4.84
4.82
3.73
3.10
3.07
3.05
3.03
3.02
3.00
2.99
H
N
O
N
H
H
N
O
S
H
N
F
OCH3
1.00
1.00
1.02
1.03
1.19
4.02
3.01
1.00
2.00
1.02
1.00
1.03
3.01
4.03
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)

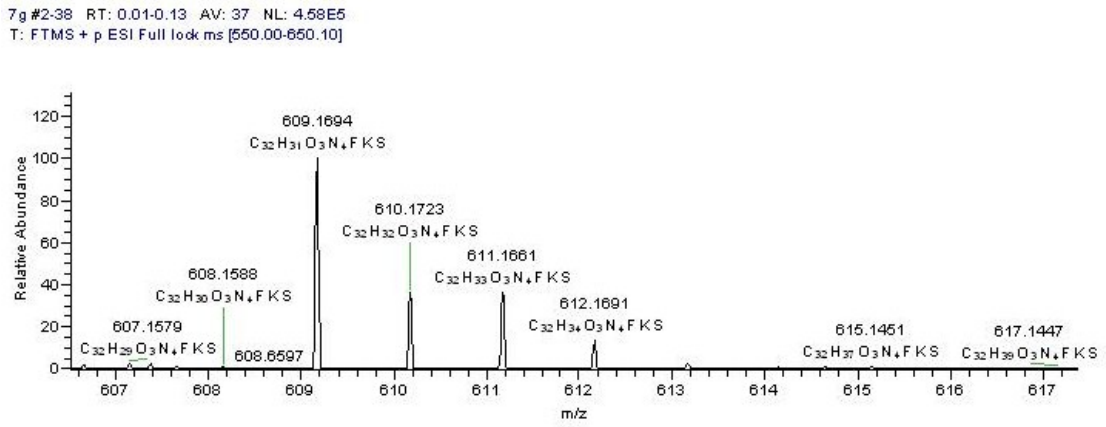
**I-15**

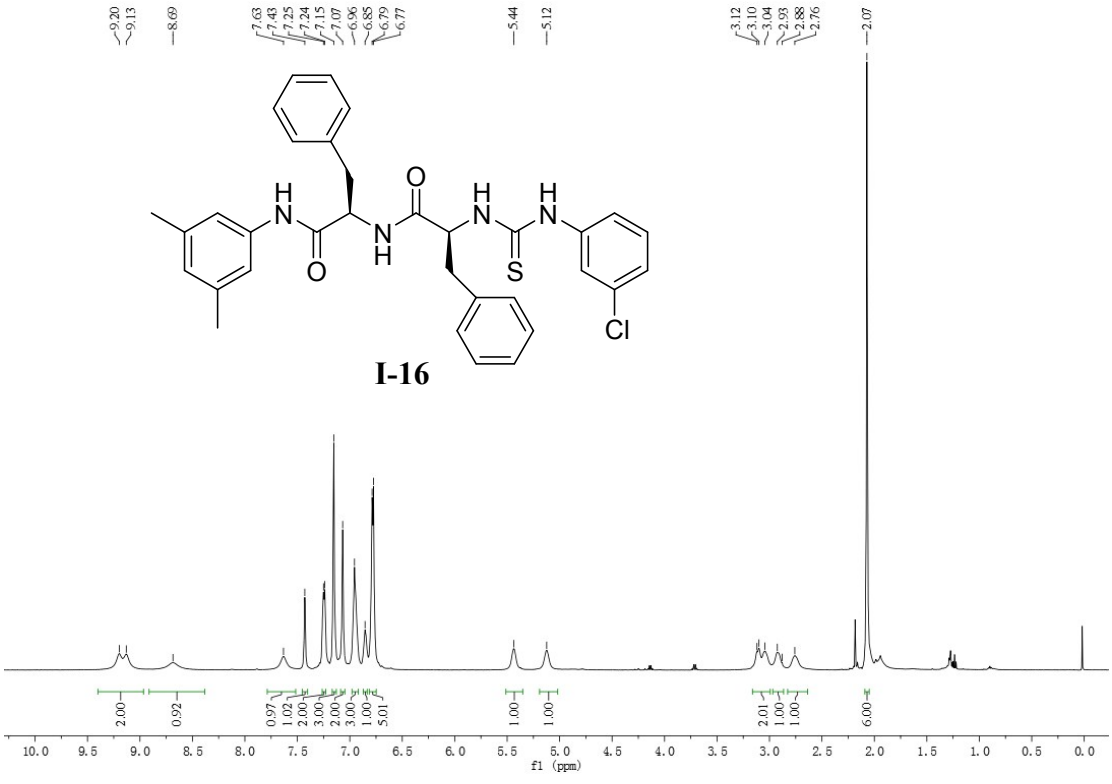

180.40
170.95
169.29
160.86
138.57
136.86
136.10
135.53
134.51
130.86
129.94
129.42
129.34
129.27
128.96
128.89
127.40
127.28
124.76
120.67
118.60
116.99
113.01
110.90
59.70
55.53
55.13
37.72
37.48
H
N
O
N
H
H
N
O
S
H
N
F
OCH3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

**I-15**

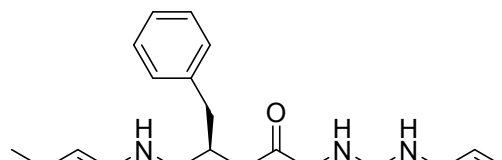

H
N
O
N
H
H
N
O
S
H
N
F
OCH3

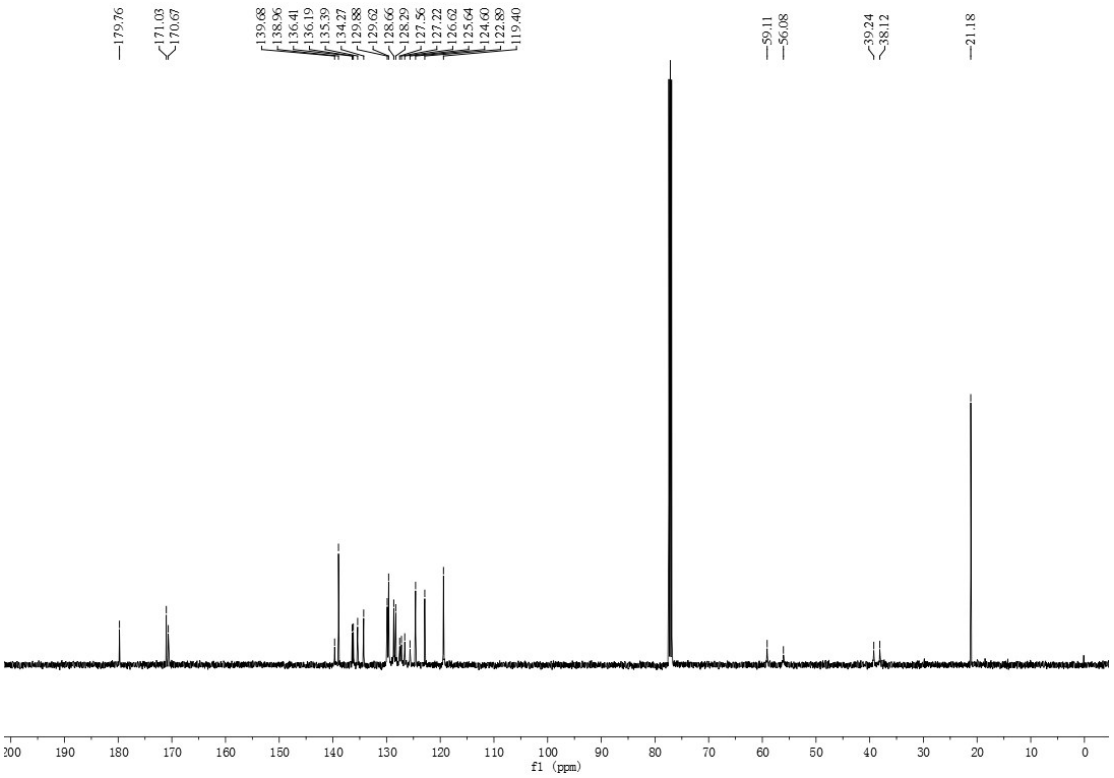
**I-15**

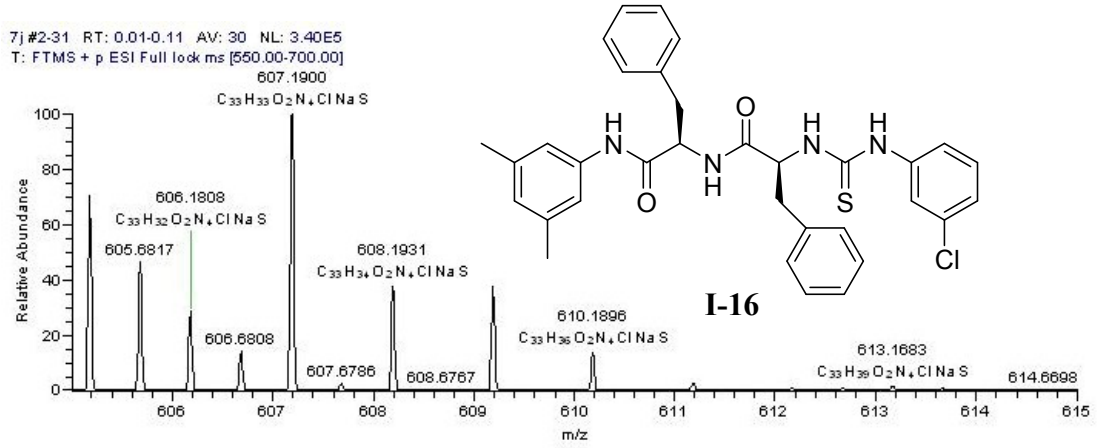

7g #2-38 RT: 0.01-0.13 AV: 37 NL: 4.58E5
T: FTMS + p ESI Full lock ms [550.00-650.10]
609.1694
C32H31O3N4FKS
610.1723
C32H32O3N4FKS
611.1661
C32H33O3N4FKS
608.1588
C32H30O3N4FKS
612.1691
C32H34O3N4FKS
607.1579
C32H29O3N4FKS
608.6597
615.1451
C32H37O3N4FKS
617.1447
C32H39O3N4FKS
Relative Abundance
m/z


9.20
9.13
8.69
7.63
7.43
7.25
7.24
7.15
7.07
6.96
6.85
6.79
6.77
5.44
5.12
3.12
3.10
3.04
2.93
2.88
2.76
2.07
2.00
0.92
0.97
1.02
2.00
3.00
2.00
3.00
1.00
5.01
1.00
1.00
2.01
1.00
1.00
6.00
f1 (ppm)

**I-16**

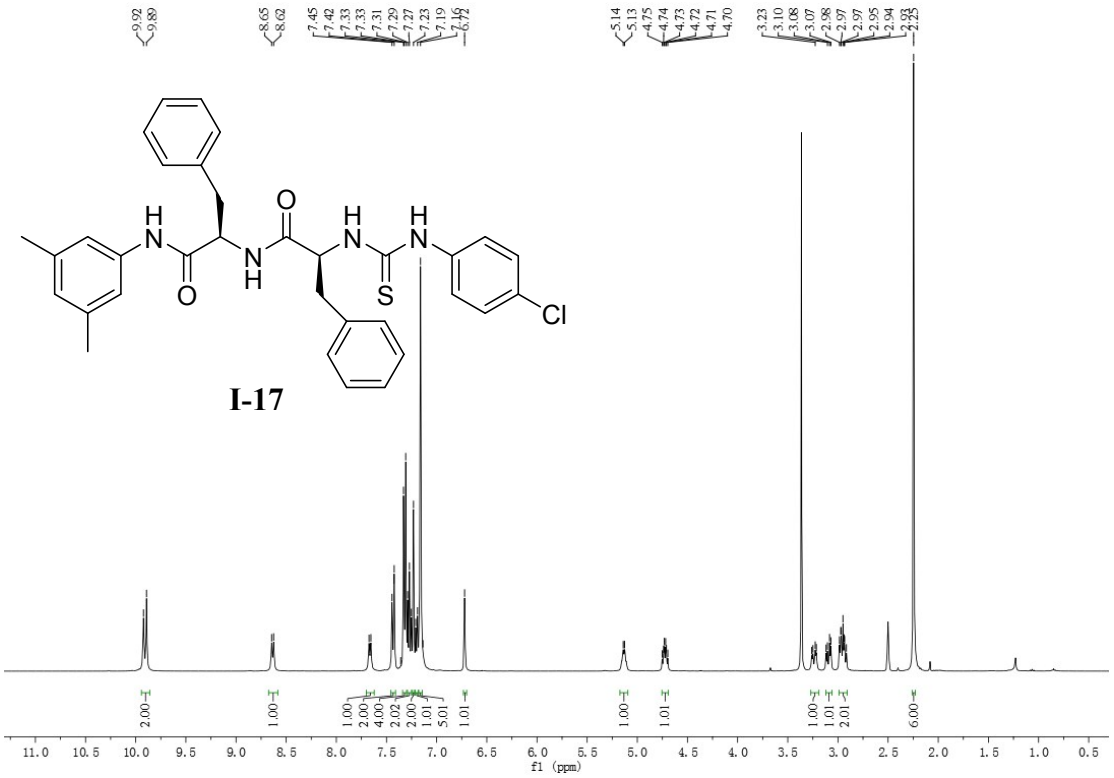



179.76
171.03
170.67
139.68
138.96
136.41
136.19
135.39
134.27
129.88
129.62
128.66
128.29
127.56
127.22
126.62
125.64
124.60
122.89
119.40
59.11
56.08
39.24
38.12
21.18
f1 (ppm)

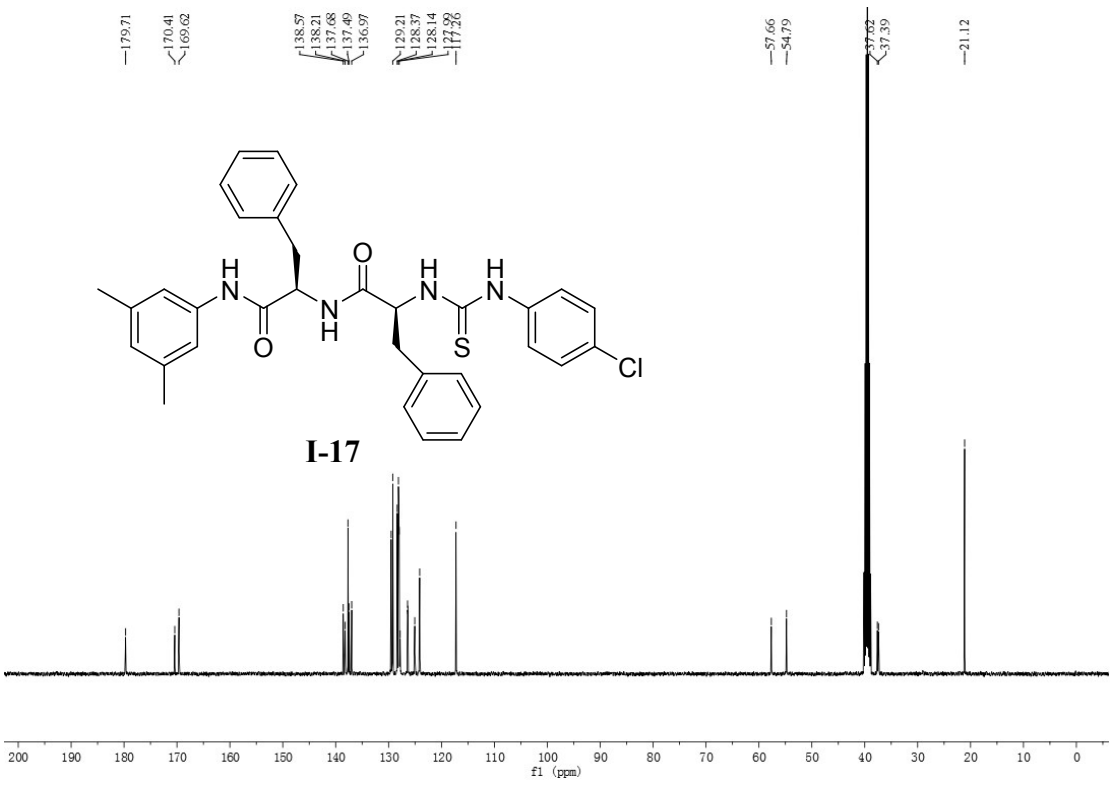

7j #2-31 RT: 0.01-0.11 AV: 30 NL: 3.40E5
T: FTMS + p ESI Full lock ms [550.00-700.00]
607.1900
C33H33O2N4ClNaS
606.1808
C33H32O2N4ClNaS
605.6817
606.6808
607.6786
608.1931
C33H34O2N4ClNaS
608.6767
610.1896
C33H36O2N4ClNaS
613.1683
C33H39O2N4ClNaS
614.6698
Relative Abundance
m/z



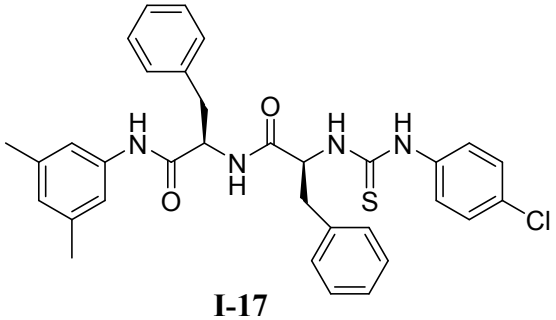
**I-16**


9.92
9.80
8.65
8.62
7.45
7.42
7.33
7.31
7.29
7.27
7.23
7.19
7.16
6.72
5.14
5.13
4.75
4.74
4.73
4.72
4.71
4.70
3.23
3.10
3.08
3.07
2.98
2.97
2.95
2.94
2.93
2.25
H
N
O
N
H
H
N
S
N
Cl
2.00
1.00
1.00
2.00
4.00
2.02
2.00
1.01
5.01
1.01
1.00
1.01
1.00
1.01
2.01
6.00
11.0
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
f1 (ppm)

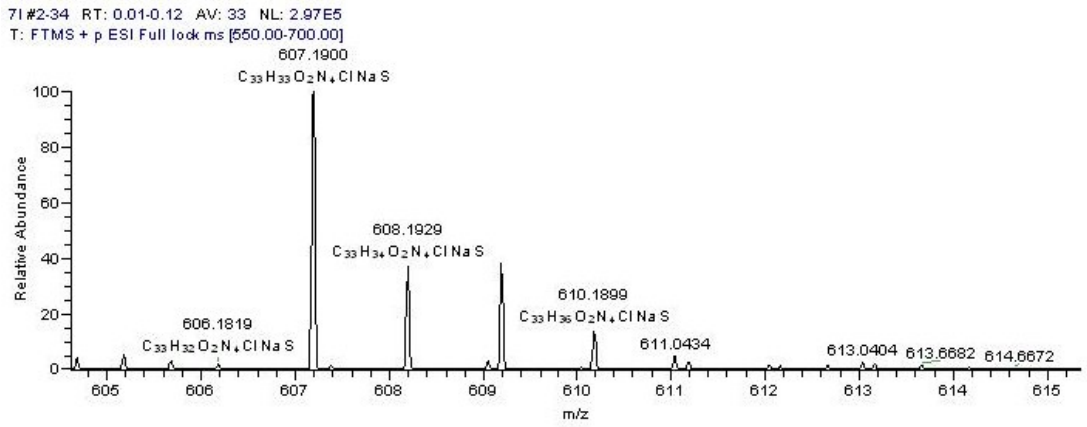
**I-17**

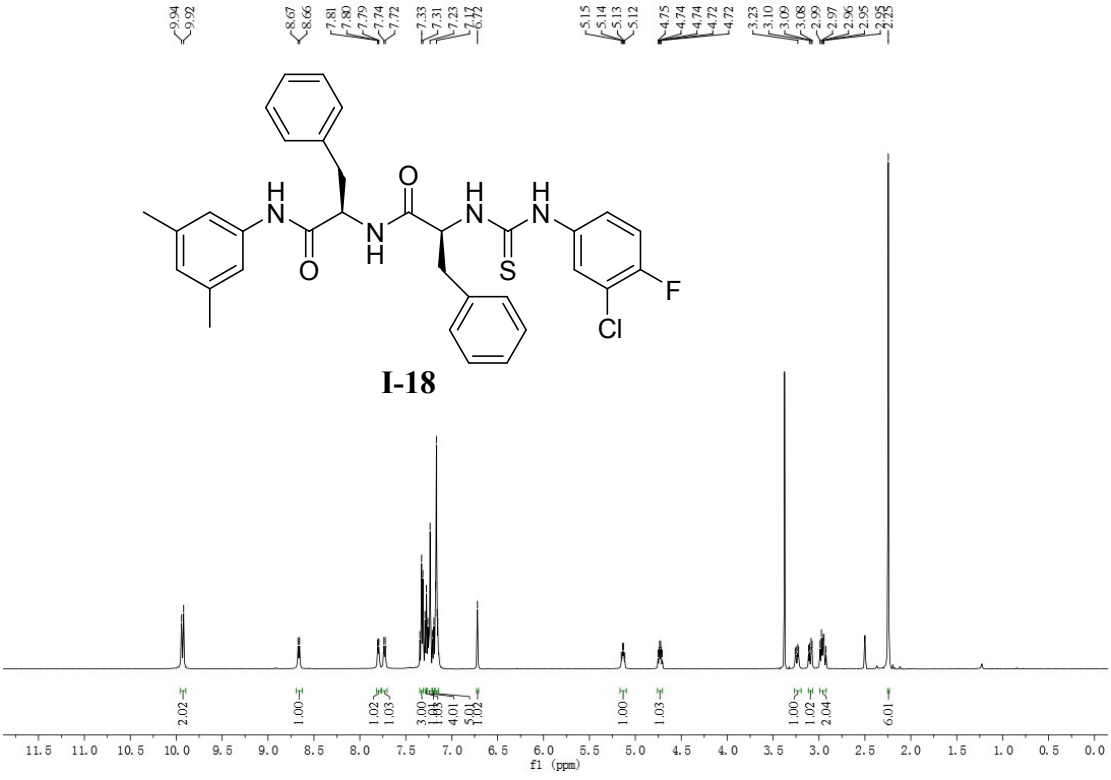

179.71
170.41
169.62
138.57
138.21
137.68
137.49
136.97
129.21
128.37
128.14
127.99
127.26
57.66
54.79
37.62
37.39
21.12
H
N
O
N
H
H
N
S
N
Cl
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

**I-17**

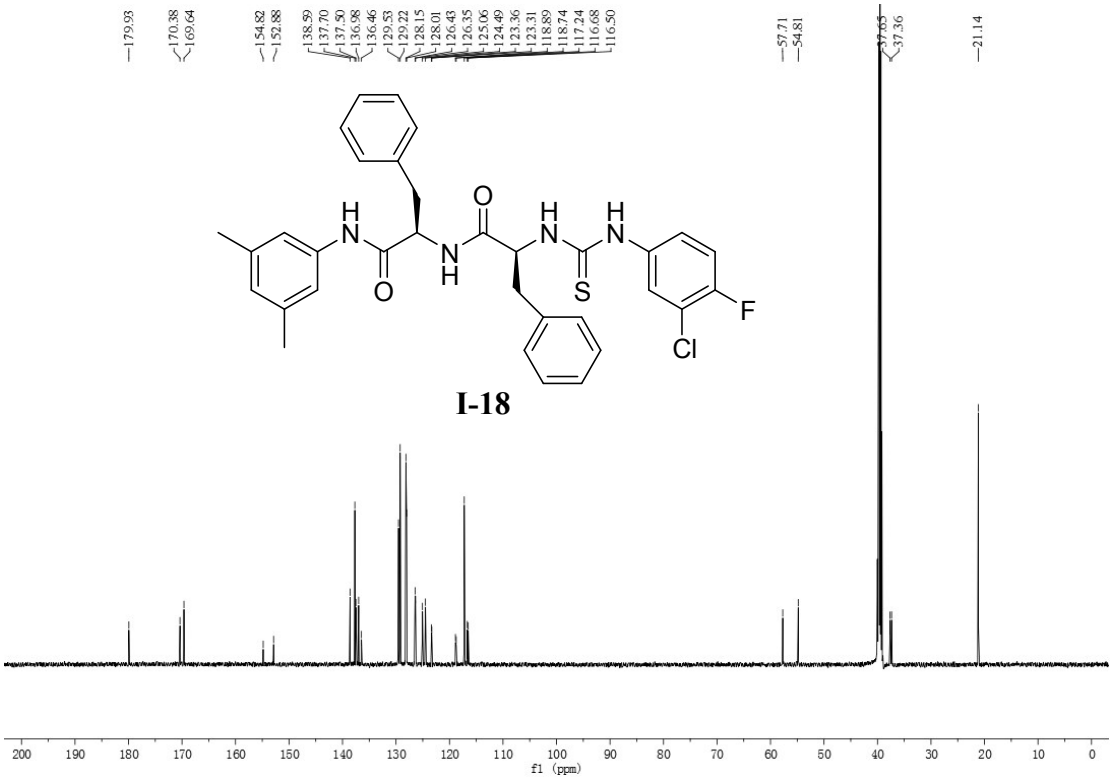

H
N
O
N
H
H
N
S
N
Cl

**I-17**

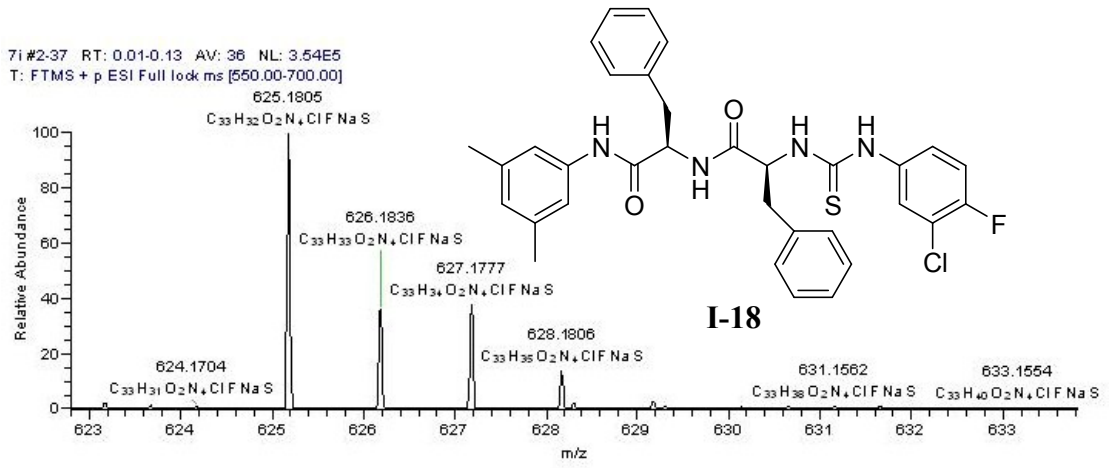

7I #2-34 RT: 0.01-0.12 AV: 33 NL: 2.97E5
T: FTMS + p ESI Full lock ms [550.00-700.00]
607.1900
C33H33O2N4ClNaS
608.1929
C33H34O2N4ClNaS
610.1899
C33H36O2N4ClNaS
606.1819
C33H32O2N4ClNaS
611.0434
613.0404
613.6682
614.6672
Relative Abundance
m/z


H
N
O
N
H
O
H
N
S
H
N
F
Cl
f1 (ppm)

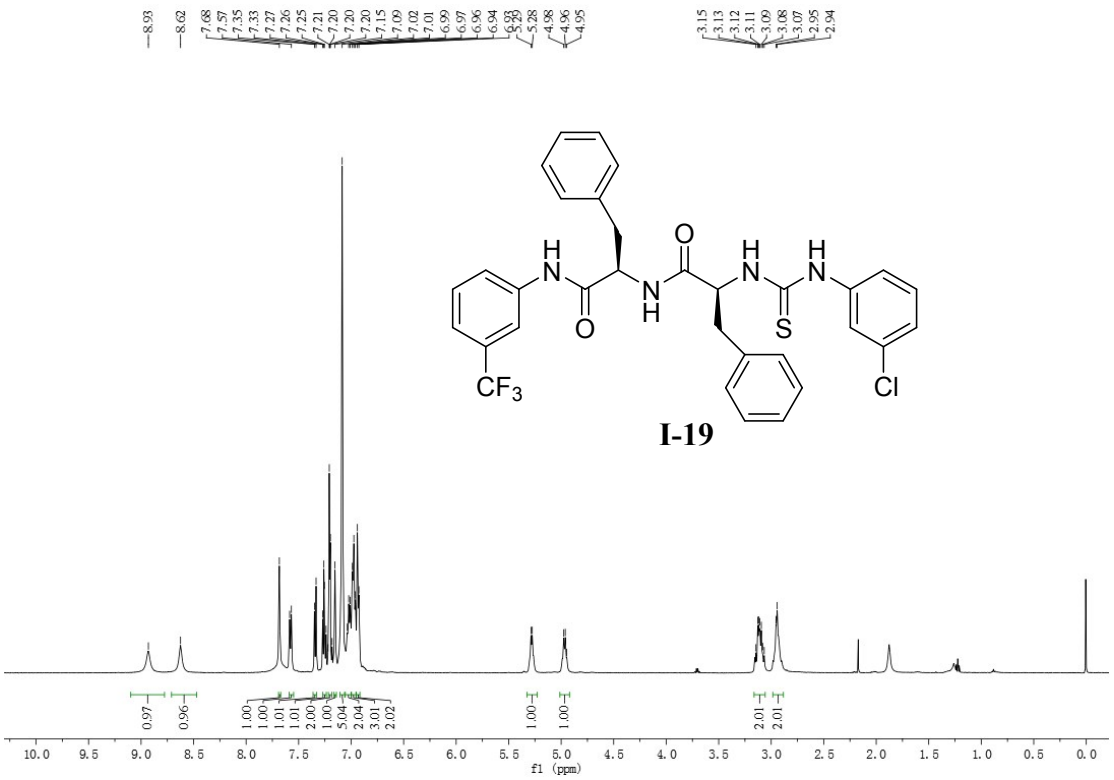
**I-18**


179.93
170.38
169.64
154.82
152.88
138.59
137.70
137.50
136.98
136.46
129.53
129.22
128.15
128.01
126.43
126.35
125.06
124.49
123.36
123.31
118.89
118.74
117.24
116.68
116.50
57.71
54.81
37.65
37.36
21.14
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

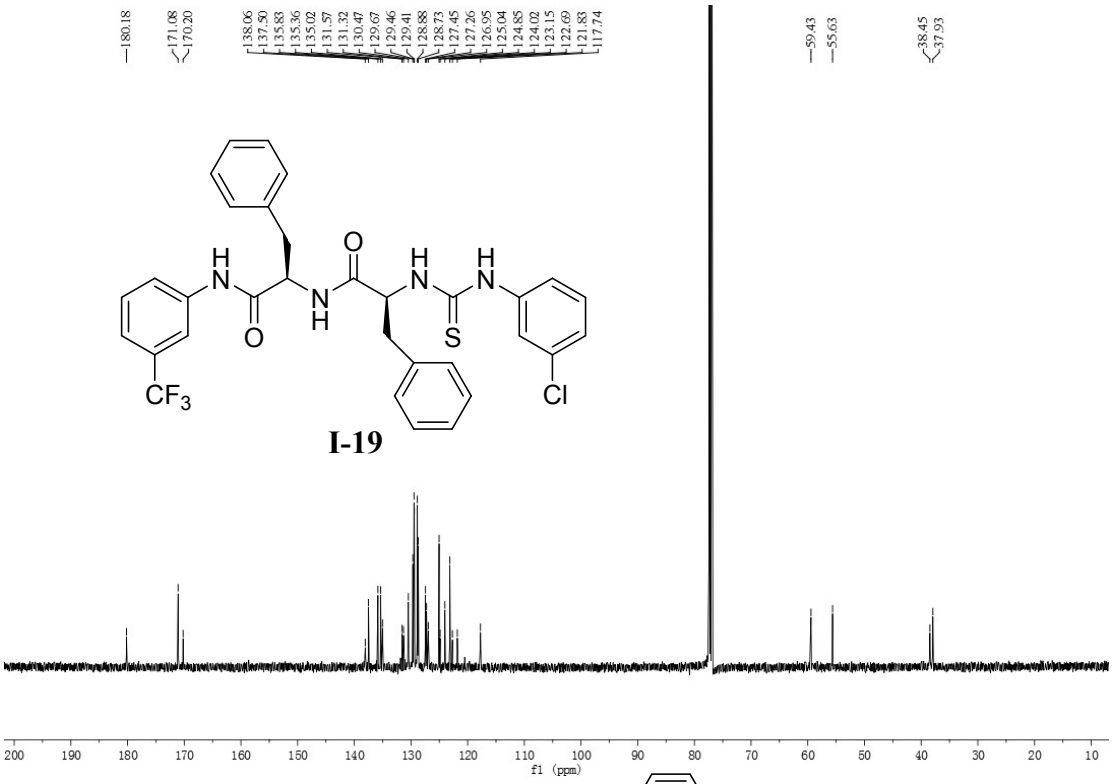
**I-18**


7i #2-37 RT: 0.01-0.13 AV: 36 NL: 3.54E5
T: FTMS + p ESI Full lock ms [550.00-700.00]
625.1805
C33H32O2N4ClFNaS
626.1836
C33H33O2N4ClFNaS
627.1777
C33H34O2N4ClFNaS
628.1806
C33H35O2N4ClFNaS
624.1704
C33H31O2N4ClFNaS
631.1562
C33H38O2N4ClFNaS
633.1554
C33H40O2N4ClFNaS
Relative Abundance
m/z

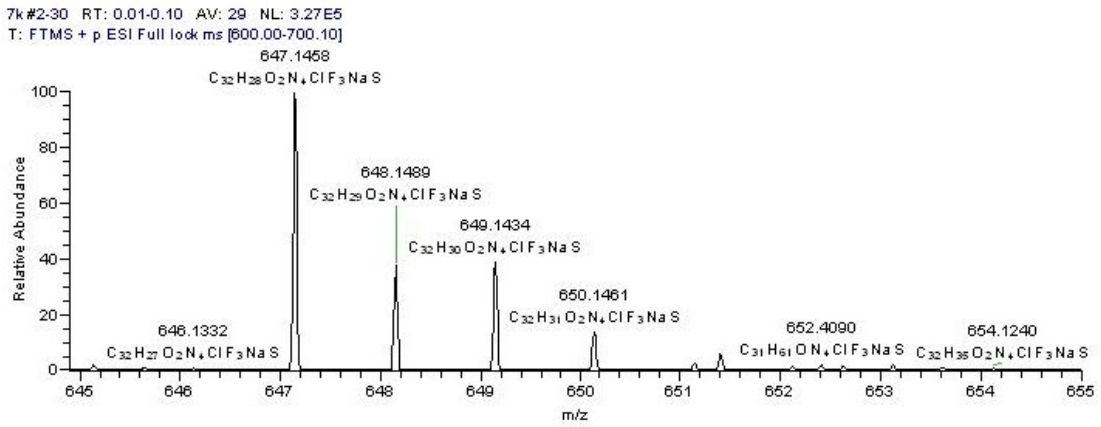
**I-18**

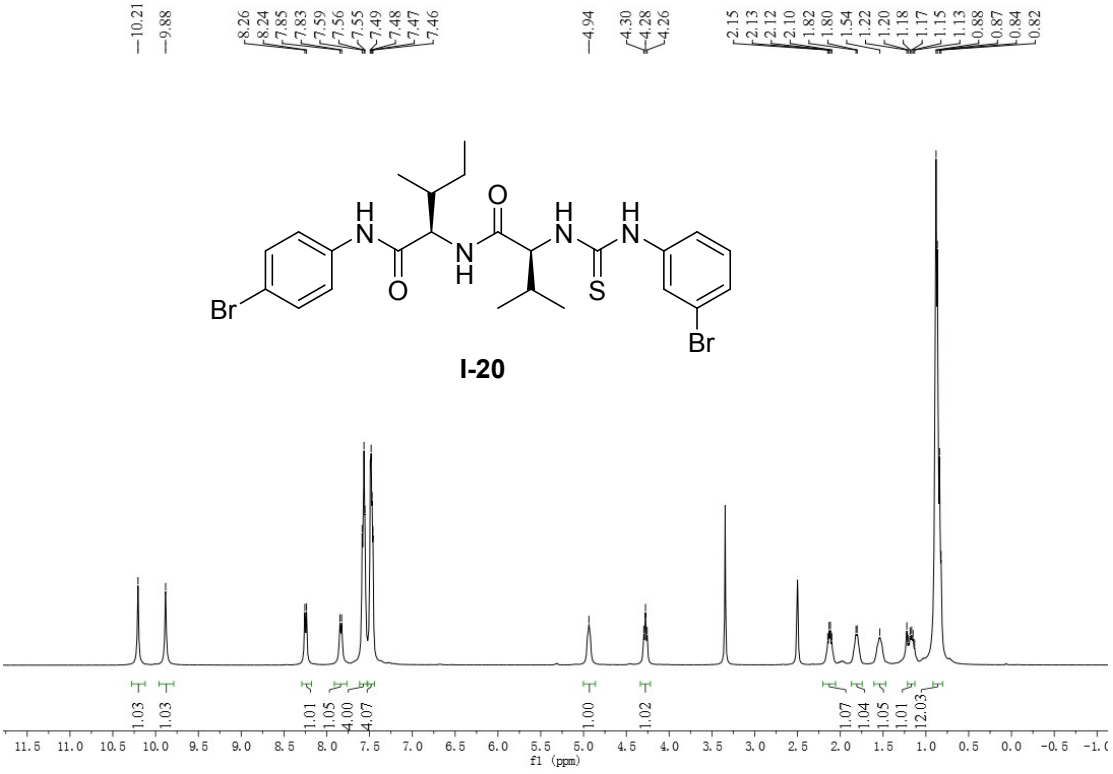

8.93
8.62
7.68
7.57
7.35
7.33
7.27
7.26
7.25
7.21
7.20
7.20
7.20
7.15
7.09
7.02
7.01
6.99
6.97
6.96
6.94
5.28
4.98
4.96
4.95
3.15
3.13
3.12
3.11
3.09
3.08
3.07
2.95
2.94
0.97
0.96
1.00
1.00
1.01
1.01
2.00
1.00
5.04
2.04
3.01
2.02
1.00
1.00
2.01
2.01
f1 (ppm)

**I-19**

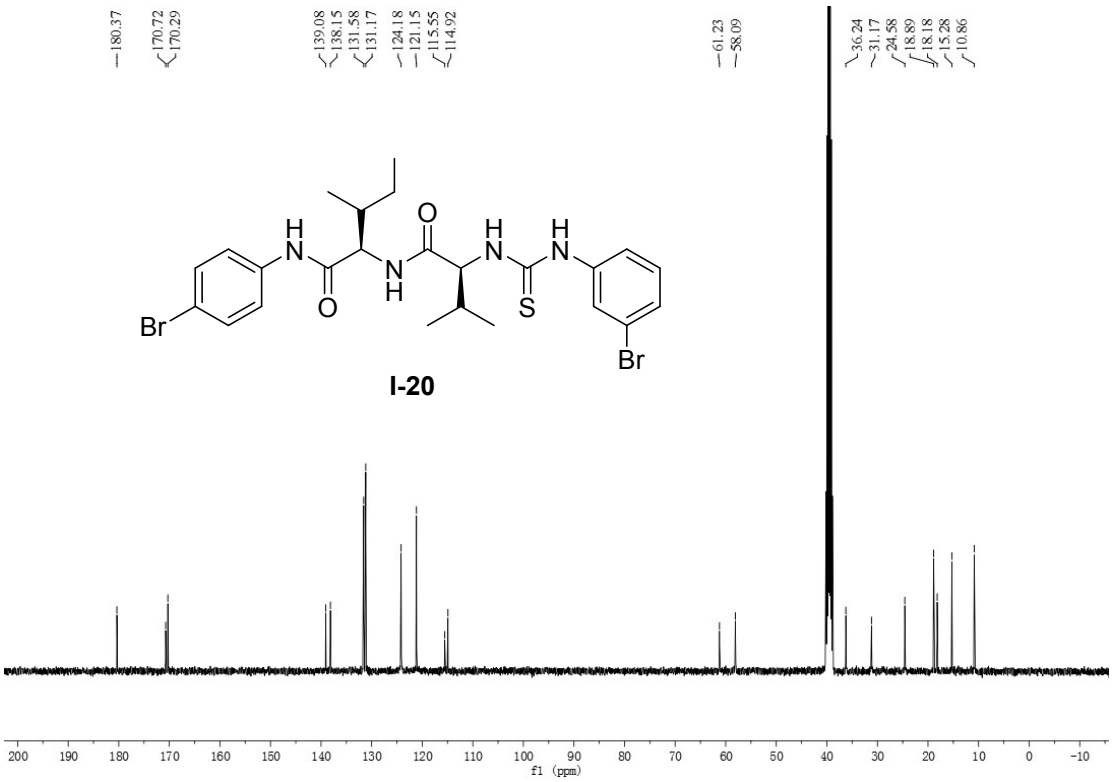

180.18
171.08
170.20
138.06
137.50
135.83
135.36
135.02
131.57
131.32
130.47
129.67
129.46
129.41
128.88
128.73
127.45
127.26
126.95
125.04
124.85
124.02
123.15
122.69
121.83
117.74
59.43
55.63
38.45
37.93
f1 (ppm)

**I-19**

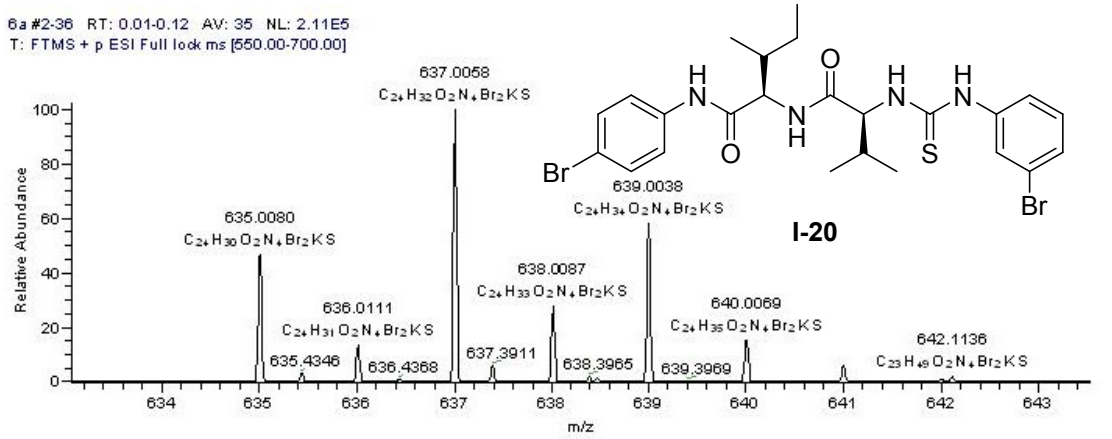

7k #2-30 RT: 0.01-0.10 AV: 29 NL: 3.27E5
T: FTMS + p ESI Full lock ms [600.00-700.10]
647.1458
C32H28O2N4ClF3NaS
648.1489
C32H29O2N4ClF3NaS
649.1434
C32H30O2N4ClF3NaS
650.1461
C32H31O2N4ClF3NaS
646.1332
C32H27O2N4ClF3NaS
652.4090
C31H61ON4ClF3NaS
654.1240
C32H35O2N4ClF3NaS
Relative Abundance
m/z


10.21
9.88
8.26
8.24
7.85
7.83
7.59
7.56
7.55
7.49
7.48
7.47
7.46
4.94
4.30
4.28
4.26
2.15
2.13
2.12
2.10
1.82
1.80
1.54
1.22
1.20
1.18
1.17
1.15
1.13
0.88
0.87
0.84
0.82
Br
Br
1.03
1.03
1.01
1.05
4.00
4.07
1.00
1.02
1.07
1.04
1.05
1.01
12.03
f1 (ppm)

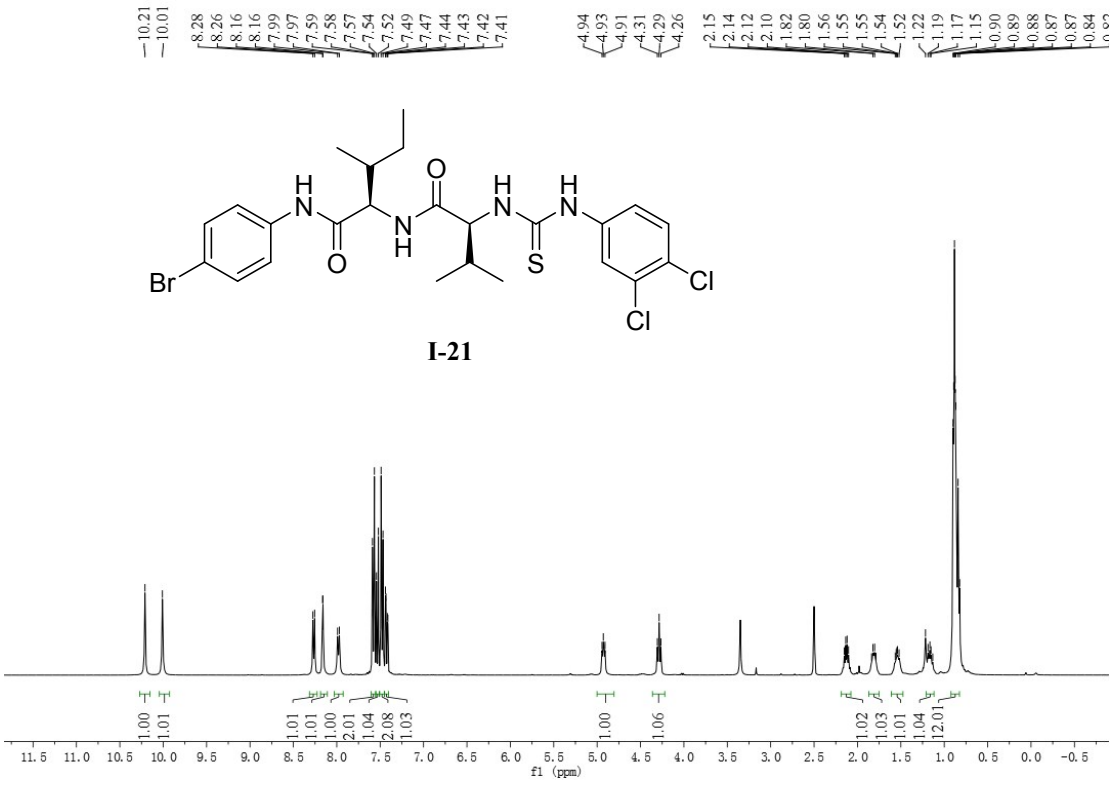
**I-20**


180.37
170.72
170.29
139.08
138.15
131.58
131.17
124.18
121.15
115.55
114.92
61.23
58.09
36.24
31.17
24.58
18.89
18.18
15.28
10.86
Br
Br
f1 (ppm)

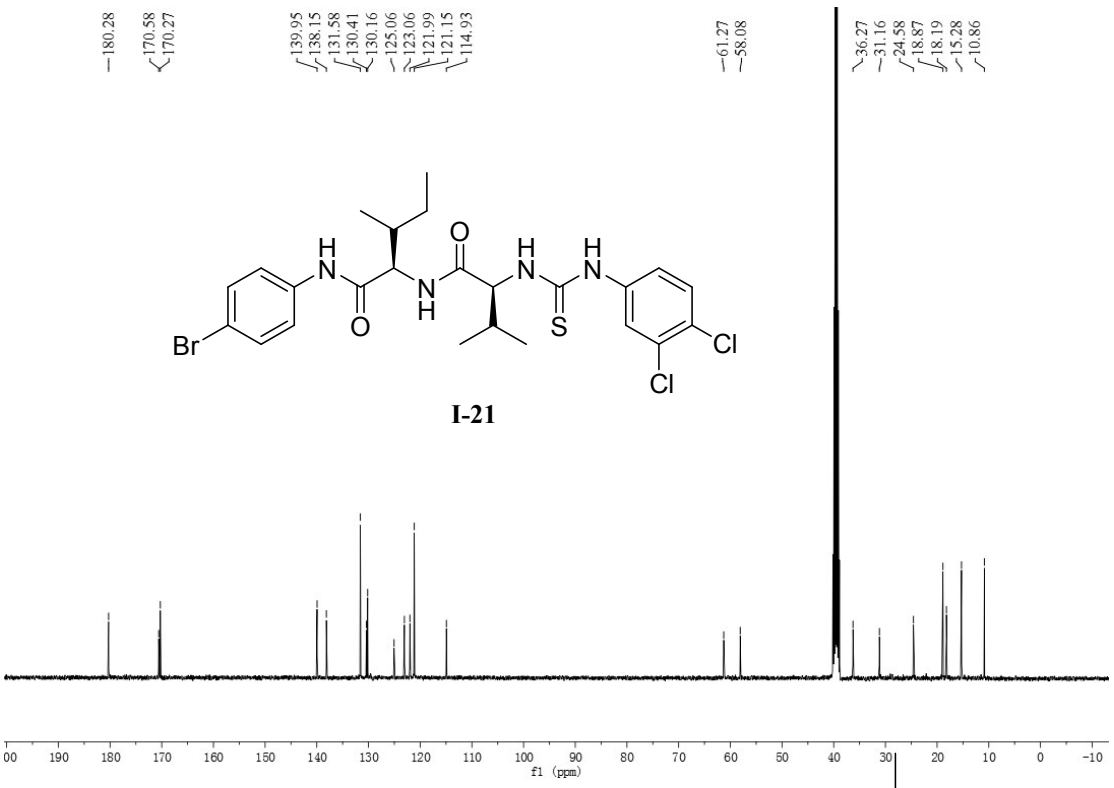
**I-20**


6a #2-36 RT: 0.01-0.12 AV: 35 NL: 2.11E5
T: FTMS + p ESI Full lock ms [550.00-700.00]
637.0058
C24H32O2N4Br2KS
635.0080
C24H30O2N4Br2KS
636.0111
C24H31O2N4Br2KS
638.0087
C24H33O2N4Br2KS
639.0038
C24H34O2N4Br2KS
640.0069
C24H35O2N4Br2KS
642.1136
C23H49O2N4Br2KS
635.4346
636.4368
637.3911
638.3965
639.3969
Relative Abundance
m/z
Br
Br

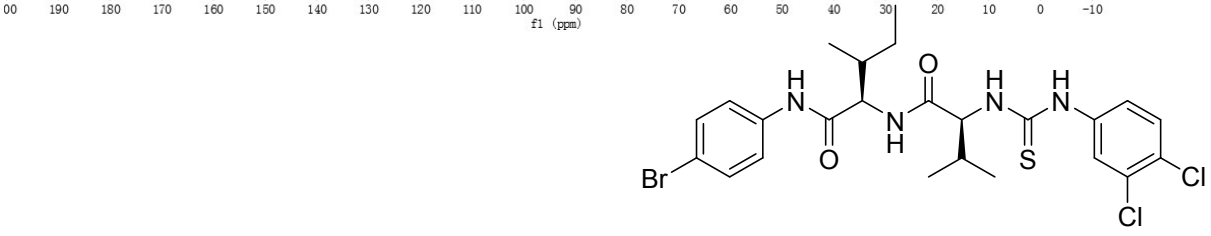
**I-20**



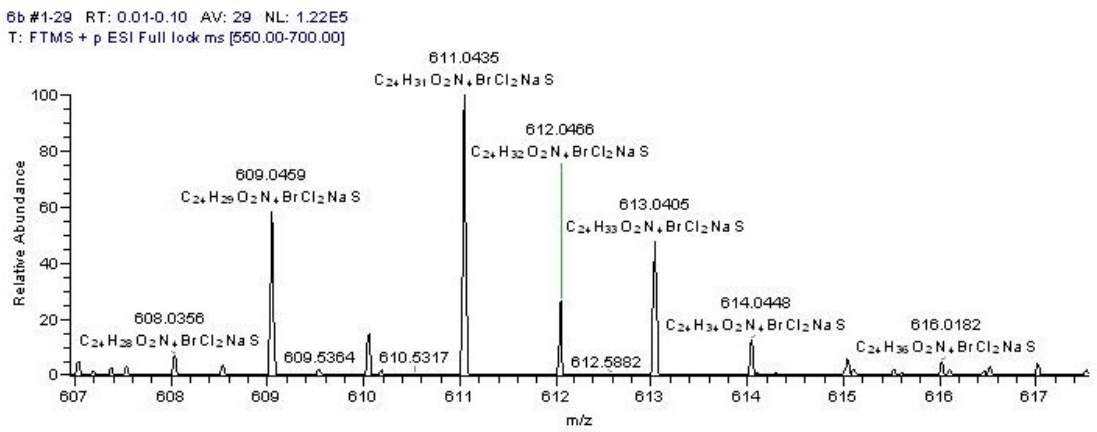
**I-21**

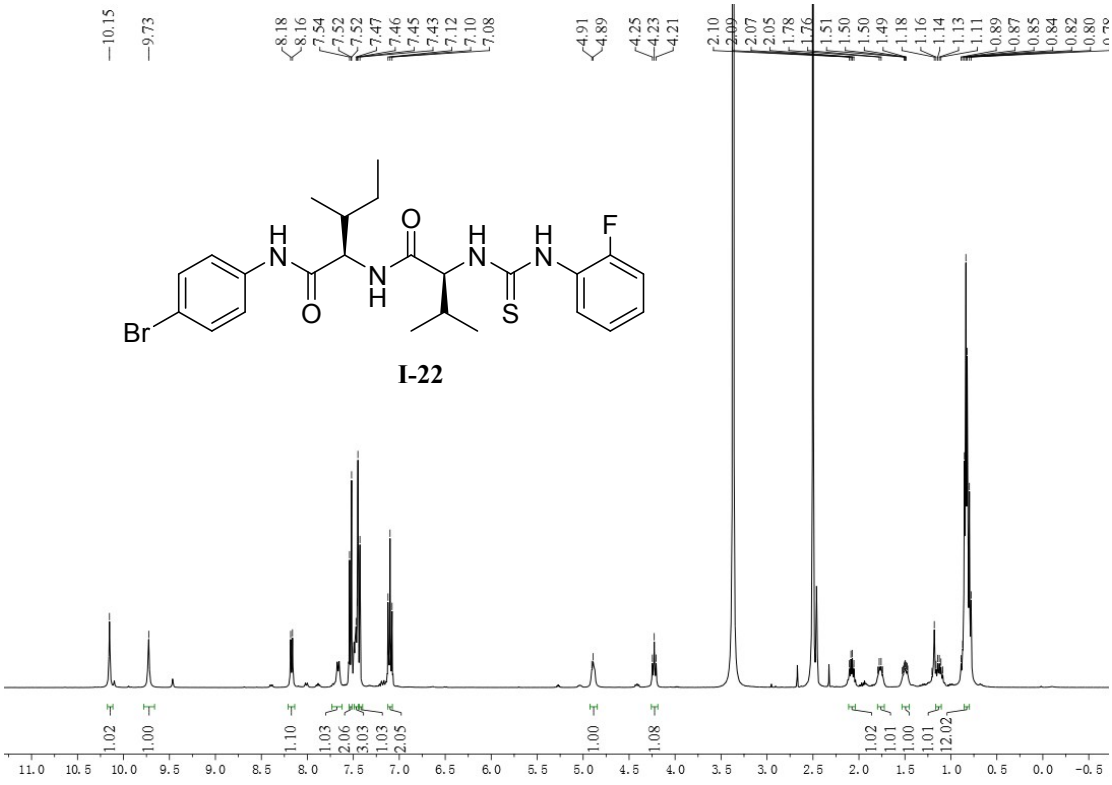


**I-21**

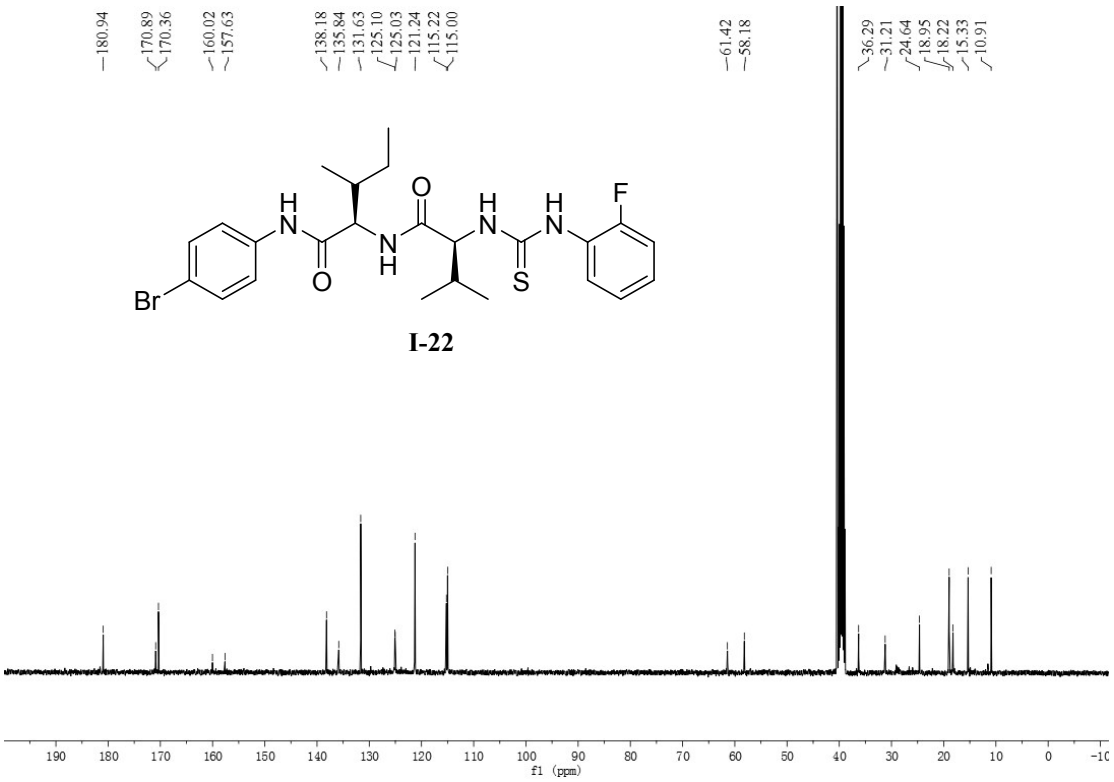


**I-21**

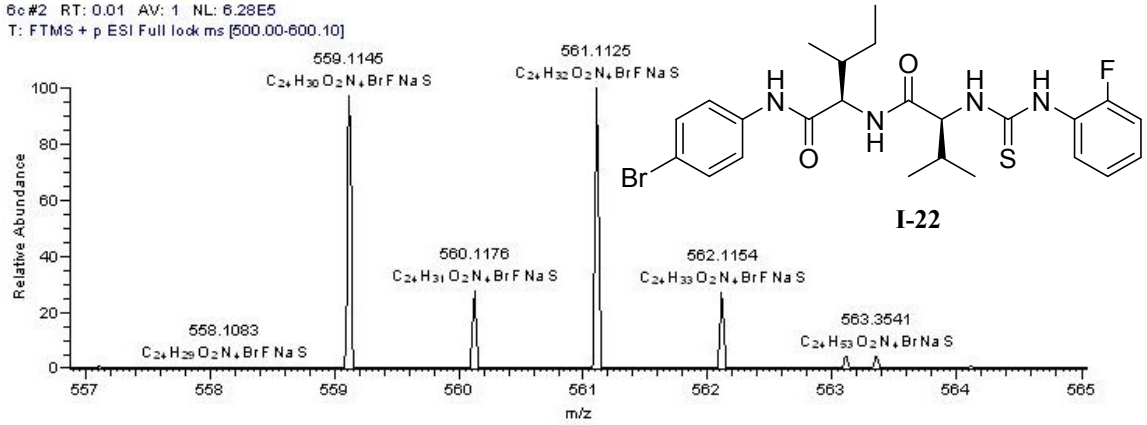

6b #1-29 RT: 0.01-0.10 AV: 29 NL: 1.22E5
T: FTMS + p ESI Full lock ms [550.00-700.00]
611.0435
C24H31O2N4BrCl2NaS
612.0466
C24H32O2N4BrCl2NaS
609.0459
C24H29O2N4BrCl2NaS
613.0405
C24H33O2N4BrCl2NaS
614.0448
C24H34O2N4BrCl2NaS
608.0356
C24H28O2N4BrCl2NaS
616.0182
C24H36O2N4BrCl2NaS
609.5364
610.5317
612.5882
Relative Abundance
m/z


10.15
9.73
8.18
8.16
7.54
7.52
7.52
7.47
7.46
7.45
7.43
7.12
7.10
7.08
4.91
4.89
4.25
4.23
4.21
2.10
2.09
2.07
2.05
1.78
1.76
1.51
1.50
1.50
1.49
1.18
1.16
1.14
1.13
1.11
0.89
0.87
0.85
0.84
0.82
0.80
Br
O
H
N
O
H
N
H
N
S
F

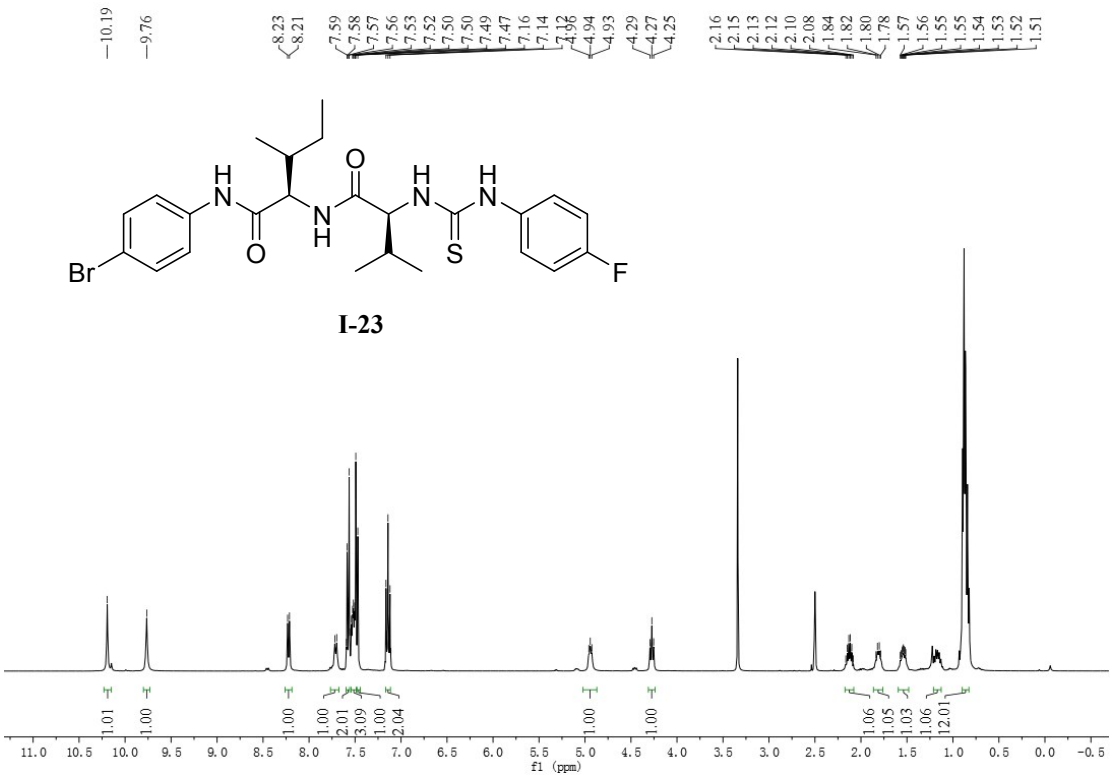
**I-22**


180.94
170.89
170.36
160.02
157.63
138.18
135.84
131.63
125.10
125.03
121.24
115.22
115.00
61.42
58.18
36.29
31.21
24.64
18.95
18.22
15.33
10.91
Br
F
f1 (ppm)

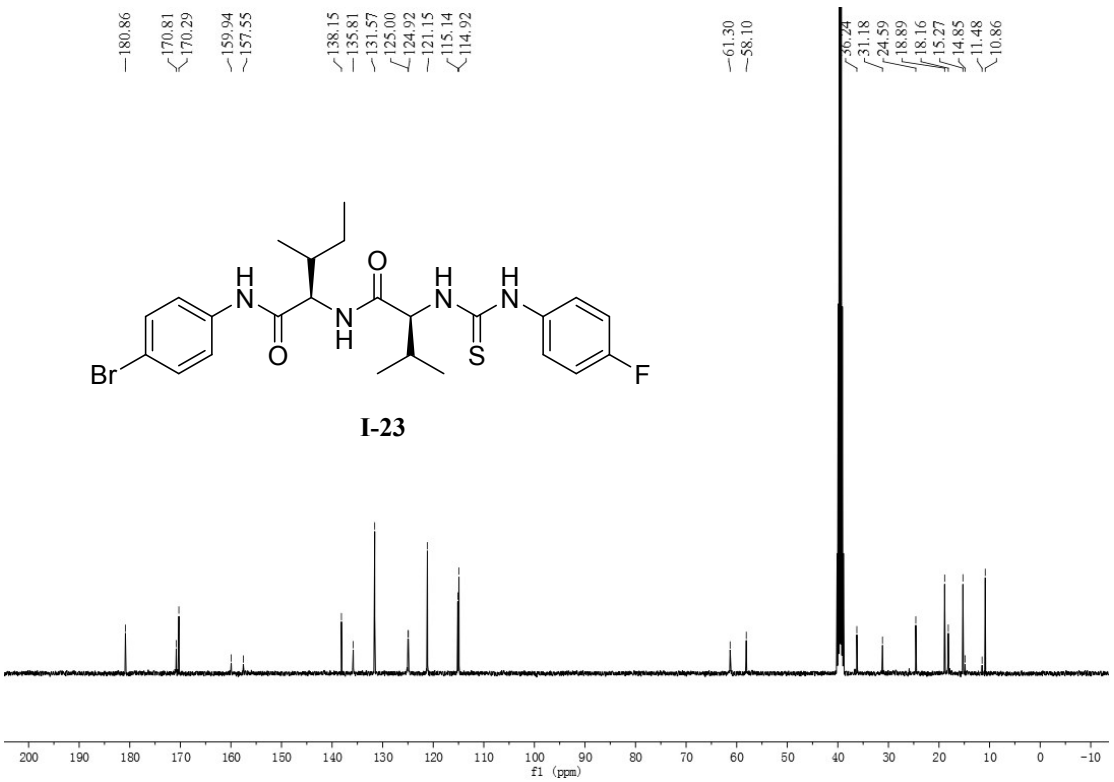
**I-22**


6c#2 RT: 0.01 AV: 1 NL: 6.28E5
T: FTMS + p ESI Full lock ms [500.00-600.10]
559.1145
C24H30O2N4BrFNaS
561.1125
C24H32O2N4BrFNaS
560.1176
C24H31O2N4BrFNaS
562.1154
C24H33O2N4BrFNaS
558.1083
C24H29O2N4BrFNaS
563.3541
C24H53O2N4BrNaS
Relative Abundance
m/z
Br
F

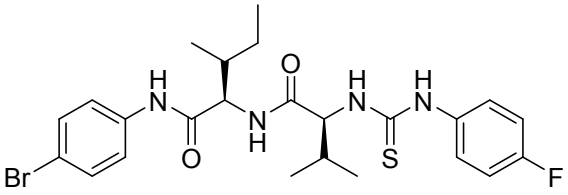
**I-22**


10.19
9.76
8.23
8.21
7.59
7.58
7.57
7.56
7.53
7.52
7.50
7.50
7.49
7.47
7.16
7.14
7.12
4.96
4.94
4.93
4.29
4.27
4.25
2.16
2.15
2.13
2.12
2.10
2.08
1.84
1.82
1.80
1.78
1.57
1.56
1.55
1.55
1.54
1.53
1.52
1.51
Br
F
1.01
1.00
1.00
1.00
2.01
3.09
1.00
2.04
1.00
1.00
1.06
1.05
1.03
1.06
12.01
f1 (ppm)

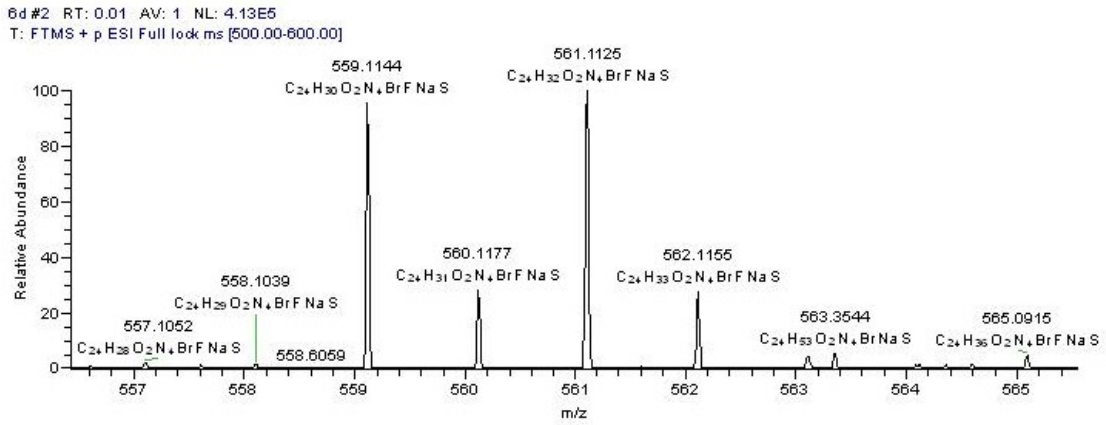
**I-23**

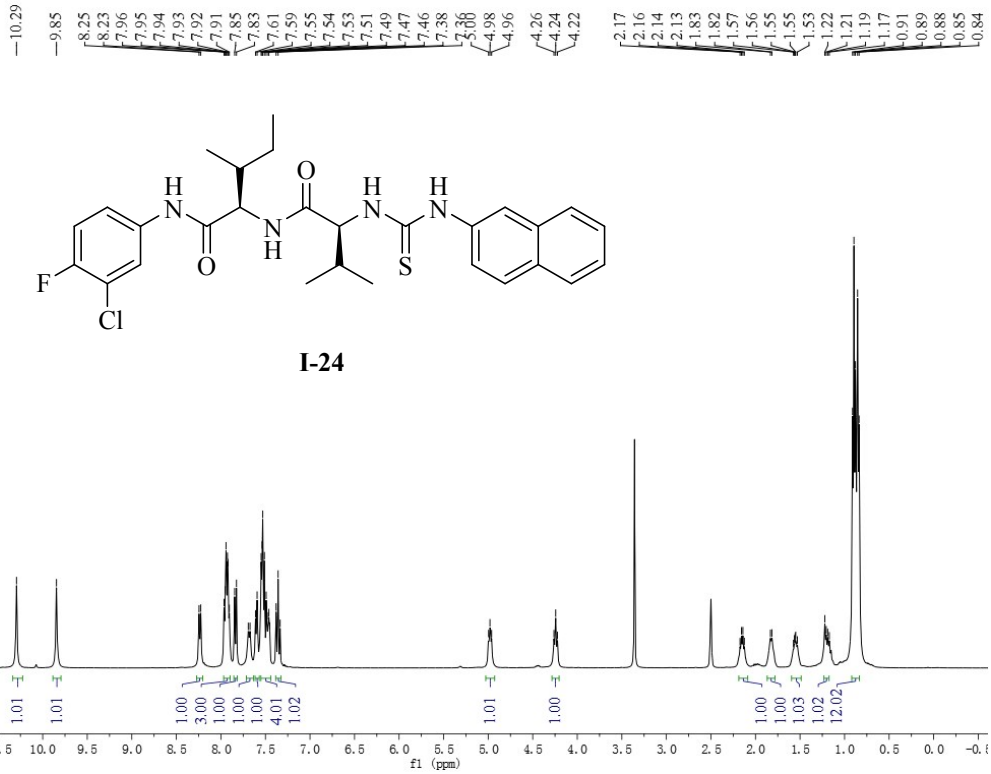

180.86
170.81
170.29
159.94
157.55
138.15
135.81
131.57
125.00
124.92
121.15
115.14
114.92
61.30
58.10
36.24
31.18
24.59
18.89
18.16
15.27
14.85
11.48
10.86
Br
F
f1 (ppm)

**I-23**

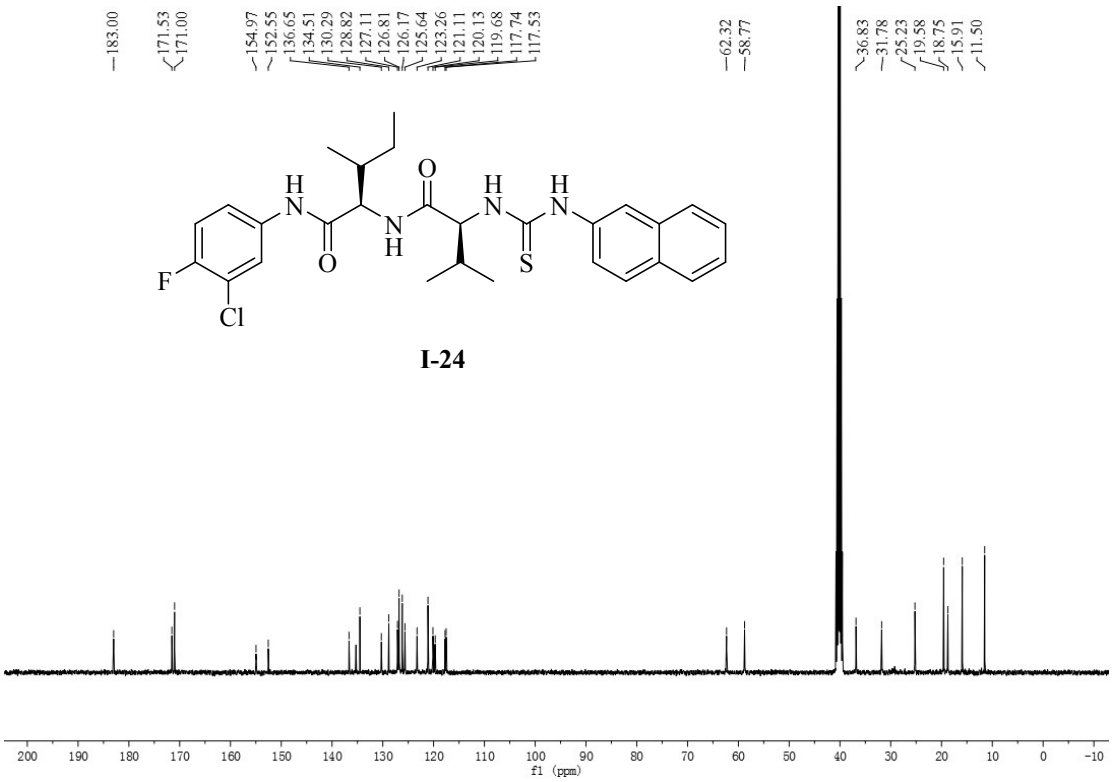

Br
F

**I-23**

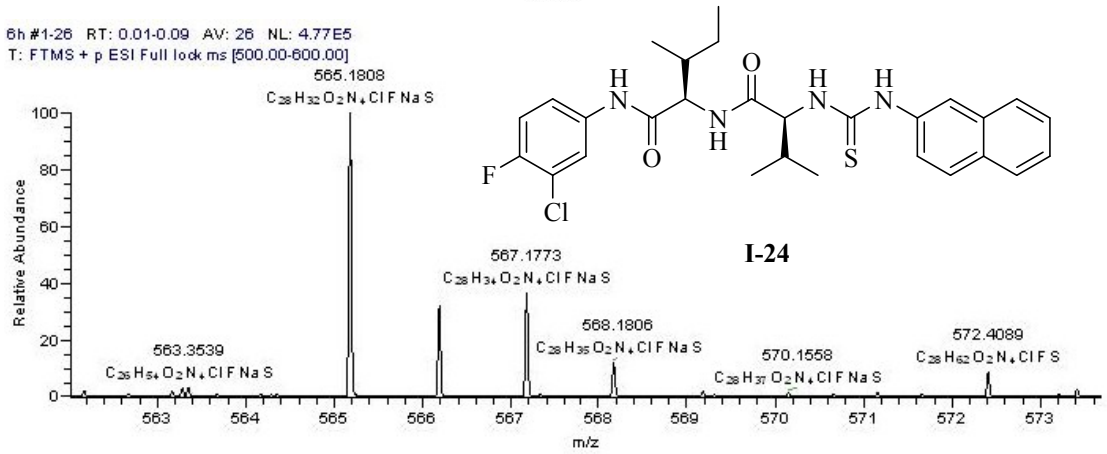

6d #2 RT: 0.01 AV: 1 NL: 4.13E5
T: FTMS + p ESI Full lock ms [500.00-600.00]
559.1144
C24H30O2N4BrF Na S
561.1125
C24H32O2N4BrF Na S
560.1177
C24H31O2N4BrF Na S
562.1155
C24H33O2N4BrF Na S
558.1039
C24H29O2N4BrF Na S
557.1052
C24H28O2N4BrF Na S
558.6059
563.3544
C24H53O2N4BrNa S
565.0915
C24H36O2N4BrF Na S
Relative Abundance
m/z


F
Cl
H
N
O
N
H
O
H
N
H
N
S
f1 (ppm)

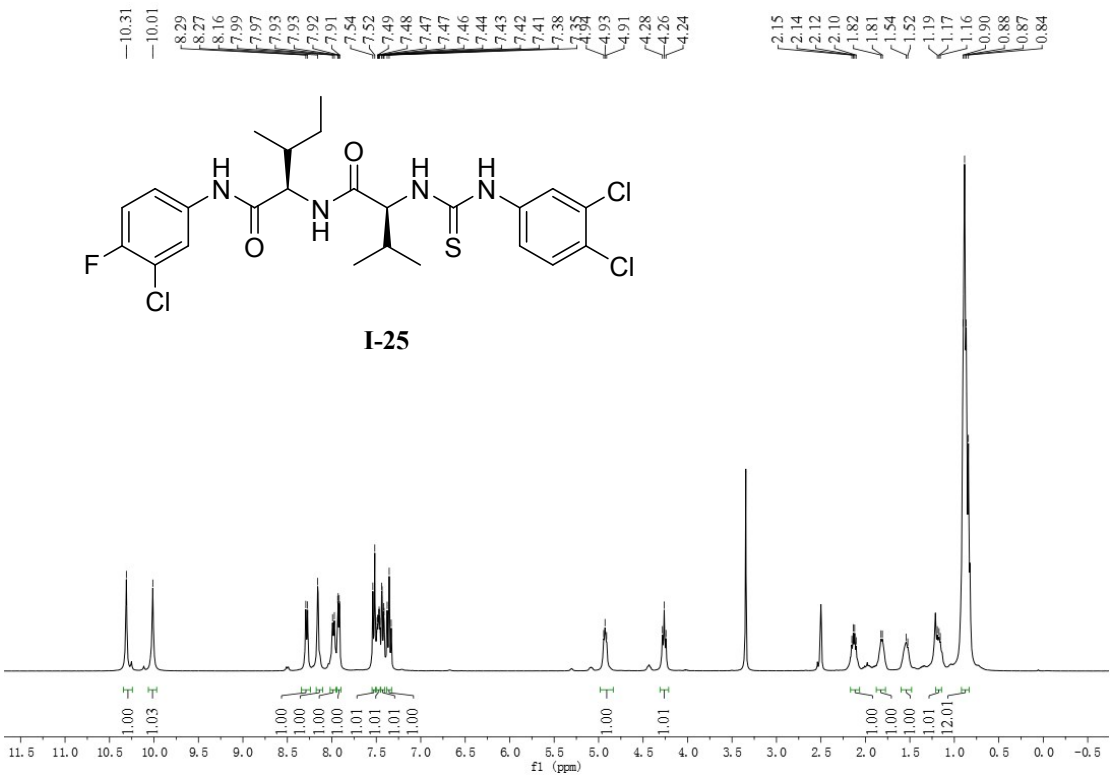
**I-24**


183.00
171.53
171.00
154.97
152.55
136.65
134.51
130.29
128.82
127.11
126.81
126.17
125.64
123.26
121.11
120.13
119.68
117.74
117.53
62.32
58.77
36.83
31.78
25.23
19.58
18.75
15.91
11.50
f1 (ppm)

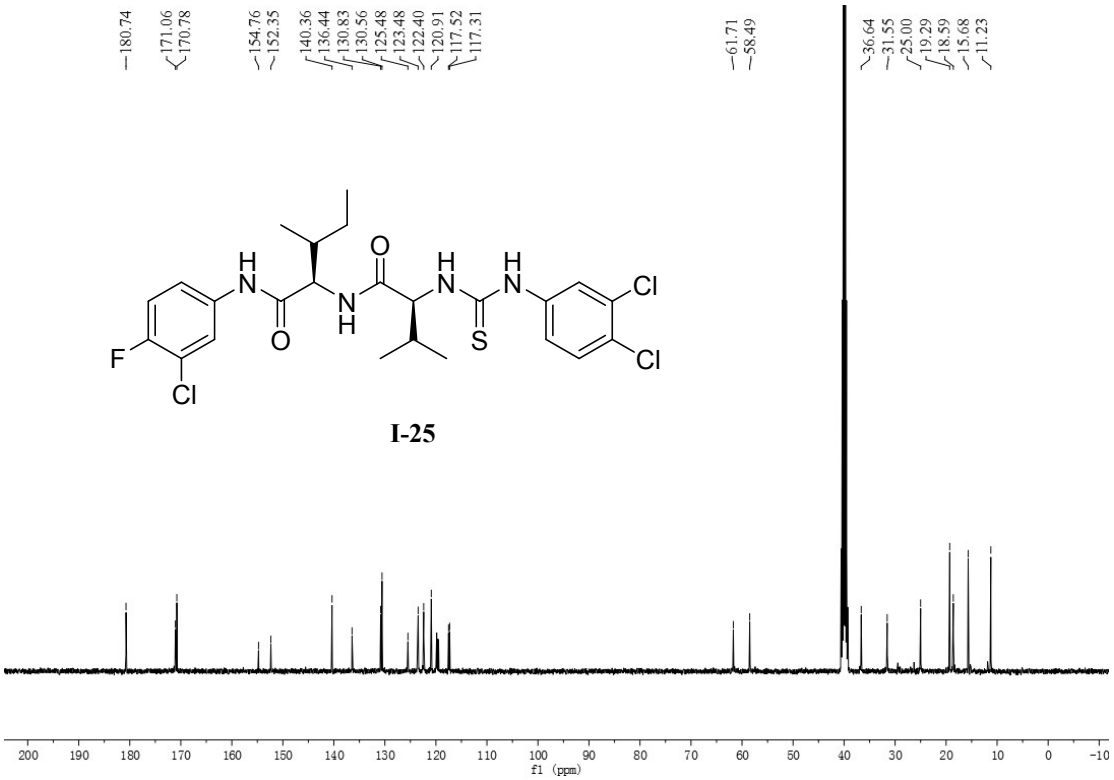
**I-24**


6h #1-26 RT: 0.01-0.09 AV: 26 NL: 4.77E5
T: FTMS + p ESI Full lock ms [500.00-600.00]
565.1808
C28H32O2N4ClFNaS
567.1773
C28H34O2N4ClFNaS
568.1806
C28H35O2N4ClFNaS
563.3539
C26H54O2N4ClFNaS
570.1558
C28H37O2N4ClFNaS
572.4089
C28H62O2N4ClFS
Relative Abundance
m/z

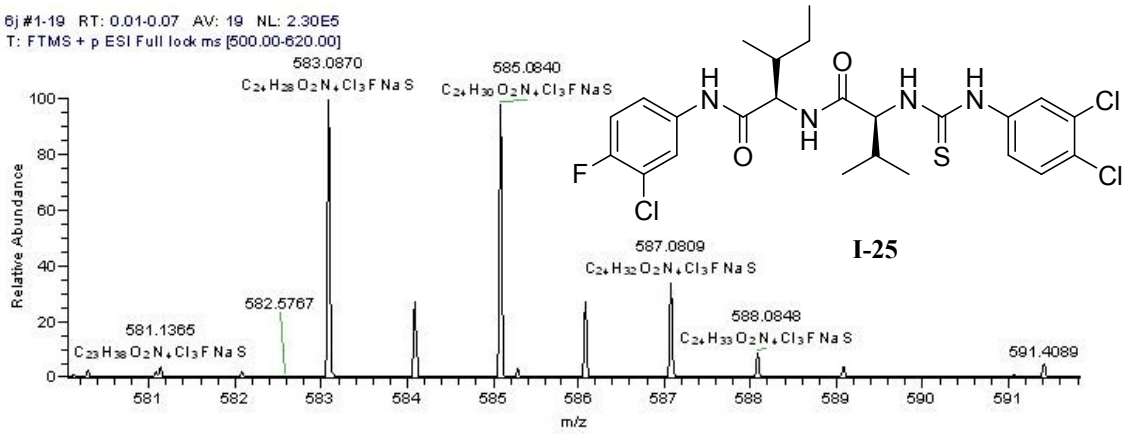
**I-24**


10.31
10.01
8.29
8.27
8.16
7.99
7.97
7.93
7.93
7.92
7.91
7.54
7.52
7.49
7.48
7.47
7.47
7.46
7.44
7.43
7.42
7.41
7.38
7.35
4.93
4.91
4.28
4.26
4.24
2.15
2.14
2.12
2.10
1.82
1.81
1.54
1.52
1.19
1.17
1.16
0.90
0.88
0.87
0.84
H
N
O
N
H
H
N
S
H
N
Cl
Cl
F
Cl
1.00
1.03
1.00
1.00
1.00
1.00
1.01
1.01
1.01
1.00
1.00
1.01
1.00
1.00
1.01
12.01
11.5
11.0
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)

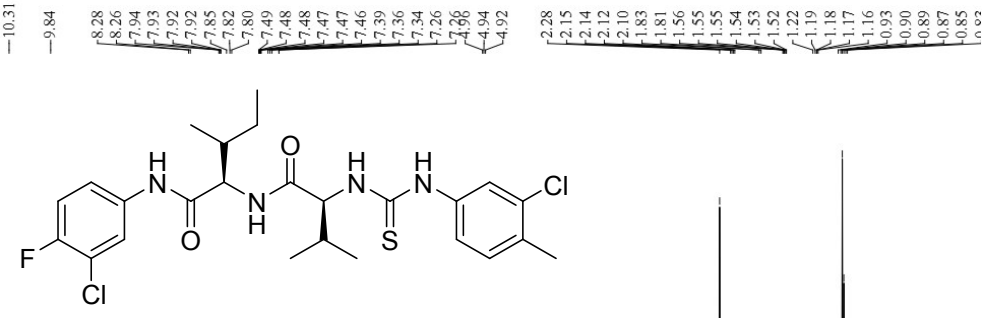
**I-25**


180.74
171.06
170.78
154.76
152.35
140.36
136.44
130.83
130.56
125.48
123.48
122.40
120.91
117.52
117.31
61.71
58.49
36.64
31.55
25.00
19.29
18.59
15.68
11.23
H
N
O
N
H
H
N
S
H
N
Cl
Cl
F
Cl
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

**I-25**

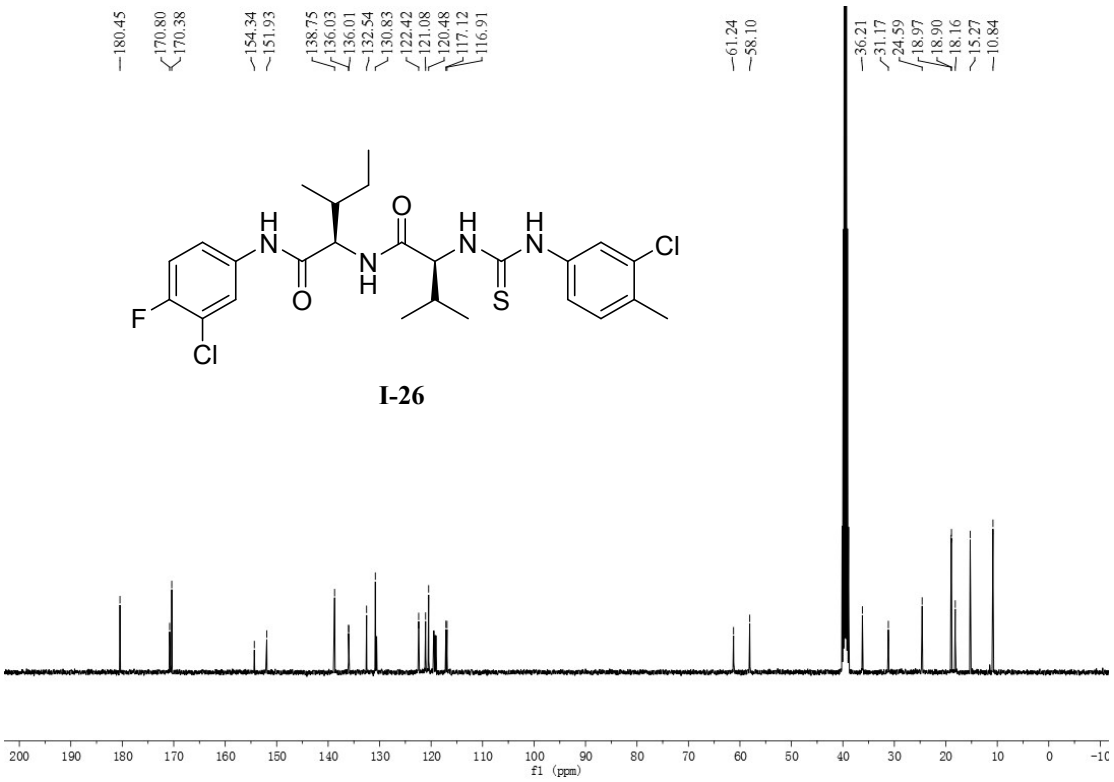

6j #1-19 RT: 0.01-0.07 AV: 19 NL: 2.30E5
T: FTMS + p ESI Full lock ms [500.00-620.00]
583.0870
C24H28O2N4Cl3F Na S
585.0840
C24H30O2N4Cl3F Na S
587.0809
C24H32O2N4Cl3F Na S
582.5767
581.1365
C23H38O2N4Cl3F Na S
588.0848
C24H33O2N4Cl3F Na S
591.4089
Relative Abundance
m/z

**I-25**

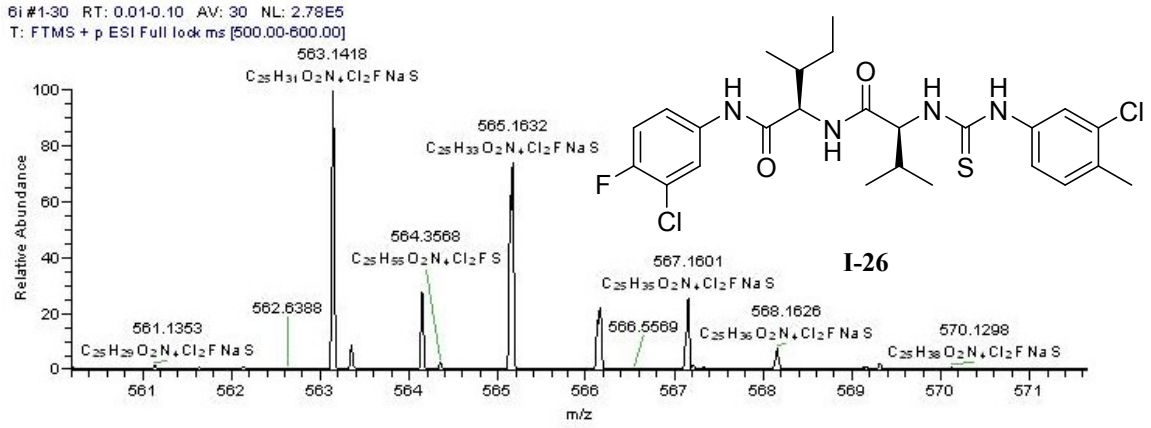


**I-26**


f1 (ppm)

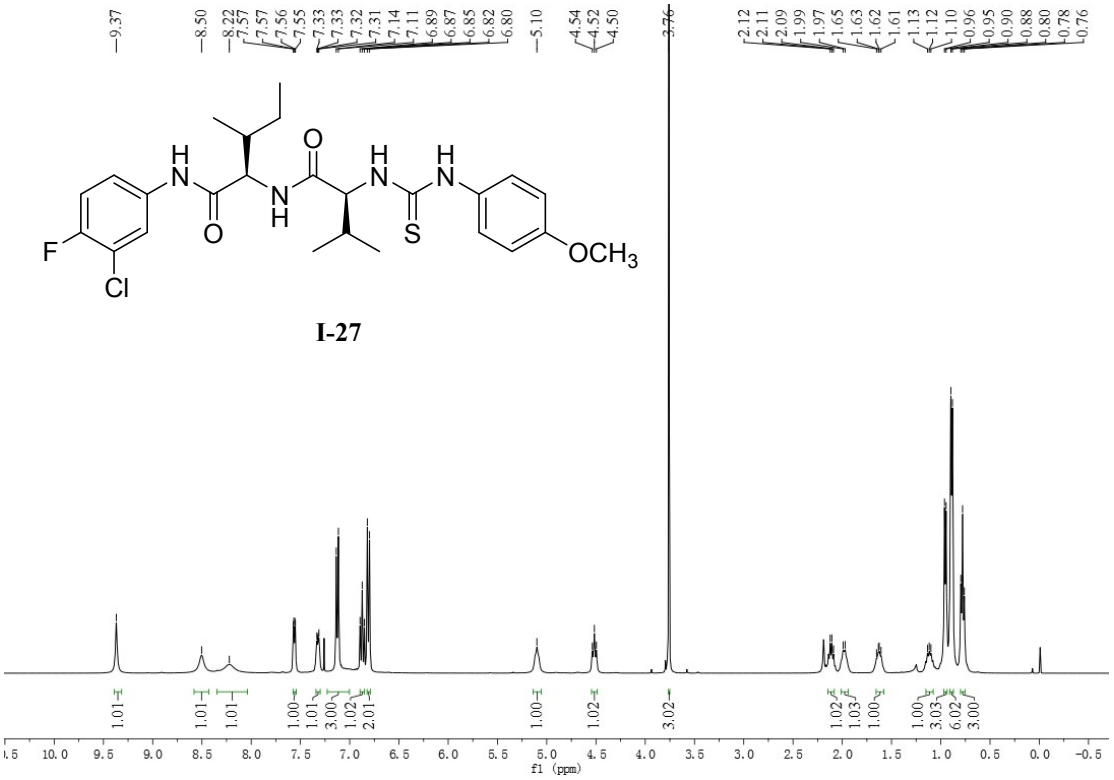

180.45
170.80
170.38
154.34
151.93
138.75
136.03
136.01
132.54
130.83
122.42
121.08
120.48
117.12
116.91
61.24
58.10
36.21
31.17
24.59
18.97
18.90
18.16
15.27
10.84
f1 (ppm)

**I-26**

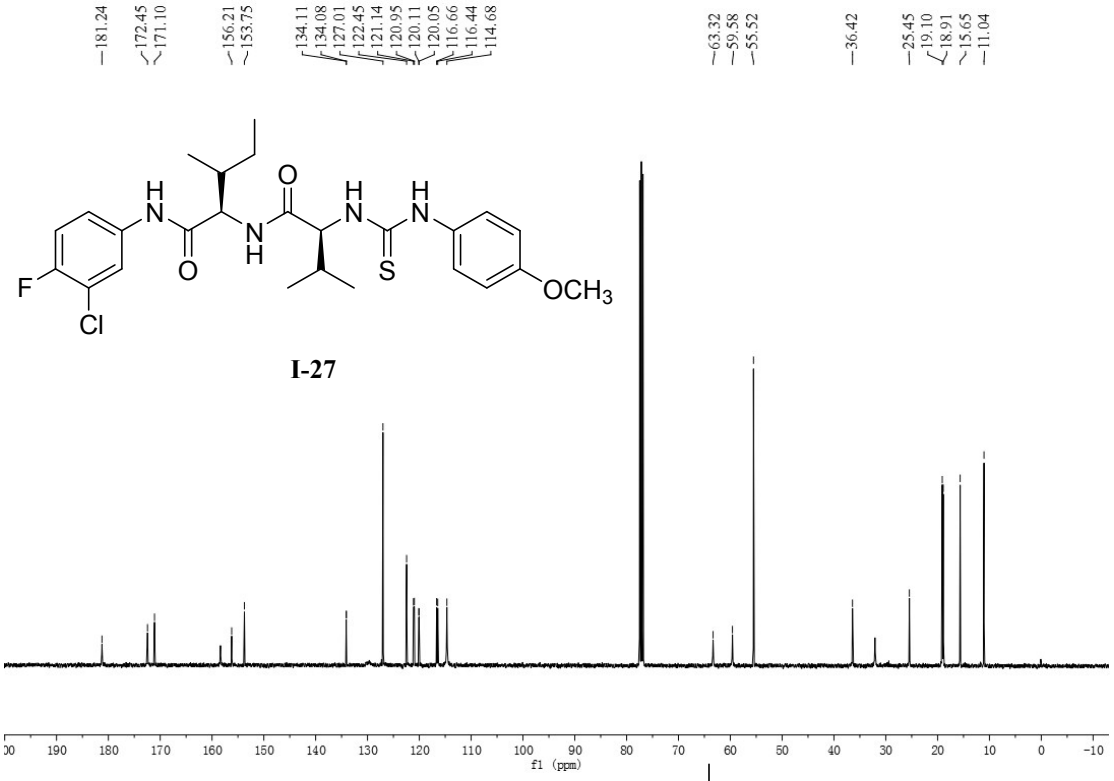

6i #1-30 RT: 0.01-0.10 AV: 30 NL: 2.78E5
T: FTMS + p ESI Full lock ms [500.00-600.00]
563.1418
C25H31O2N4Cl2F Na S
565.1632
C25H33O2N4Cl2F Na S
564.3568
C25H55O2N4Cl2F S
567.1601
C25H35O2N4Cl2F Na S
562.6388
561.1353
C25H29O2N4Cl2F Na S
566.5569
568.1626
C25H36O2N4Cl2F Na S
570.1298
C25H38O2N4Cl2F Na S
Relative Abundance
m/z



**I-26**

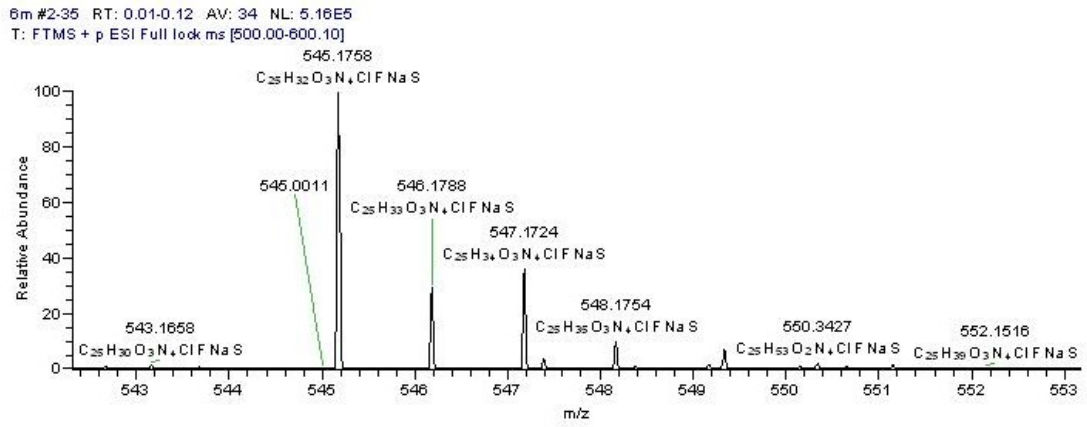

9.37
8.50
8.22
7.57
7.57
7.56
7.55
7.33
7.33
7.32
7.31
7.14
7.11
6.89
6.87
6.85
6.82
6.80
5.10
4.54
4.52
4.50
3.76
2.12
2.11
2.09
1.99
1.97
1.65
1.63
1.62
1.61
1.13
1.12
1.10
0.96
0.95
0.90
0.88
0.80
0.78
0.76
1.01
1.01
1.01
1.00
1.01
3.00
1.02
2.01
1.00
1.02
3.02
1.02
1.03
1.00
1.00
3.03
6.02
3.00
f1 (ppm)

**I-27**

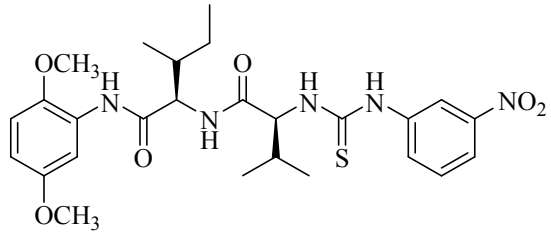

181.24
172.45
171.10
156.21
153.75
134.11
134.08
127.01
122.45
121.14
120.95
120.11
120.05
116.66
116.44
114.68
63.32
59.58
55.52
36.42
25.45
19.10
18.91
15.65
11.04
f1 (ppm)

**I-27**

**I-27**

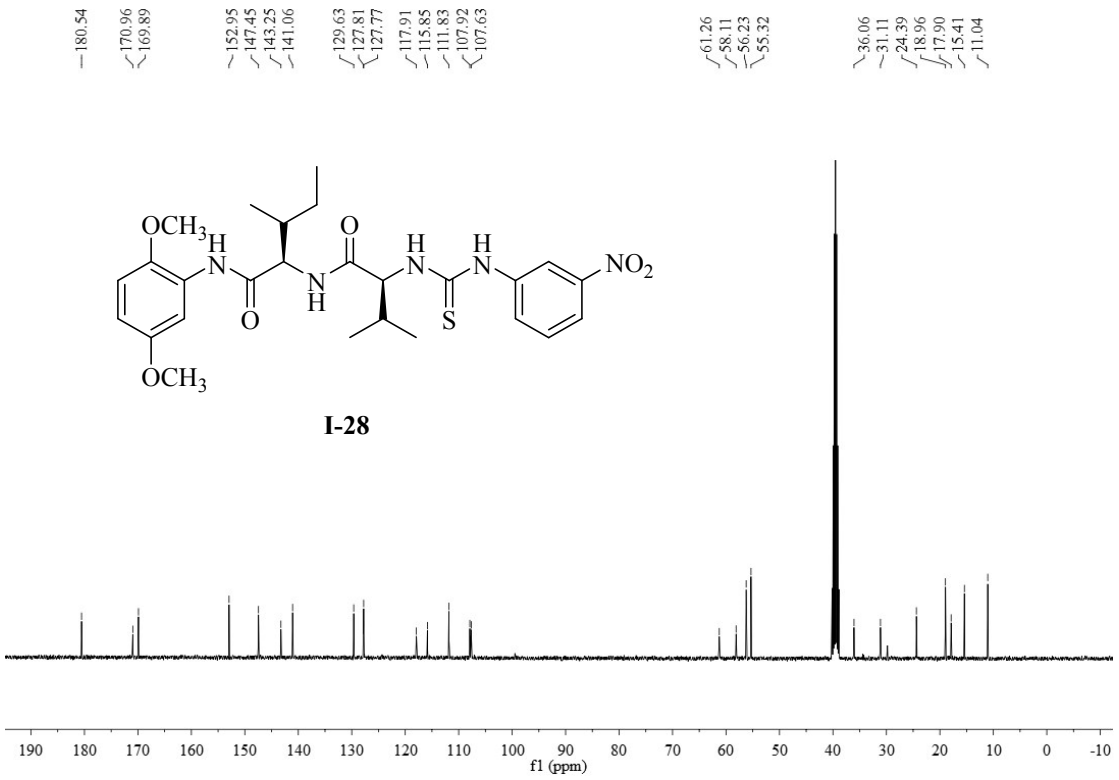

6m #2-35 RT: 0.01-0.12 AV: 34 NL: 5.16E5
T: FTMS + p ESI Full lock ms [500.00-600.10]
545.1758
C25H32O3N4ClFNaS
545.0011
546.1788
C25H33O3N4ClFNaS
547.1724
C25H34O3N4ClFNaS
548.1754
C25H35O3N4ClFNaS
543.1658
C25H30O3N4ClFNaS
550.3427
C25H53O2N4ClFNaS
552.1516
C25H39O3N4ClFNaS
Relative Abundance
m/z


10.21
9.00
8.86
7.90
7.90
7.84
7.73
7.72
7.60
7.58
6.98
6.94
6.64
6.63
6.62
6.61
5.02
5.01
4.99
4.45
4.43
4.41
3.77
3.75
3.68
2.22
2.21
1.92
1.90
1.54
1.53
1.52
1.51
1.50
1.22
0.96
0.94
0.92
0.92
0.90
0.87
0.85
0.83

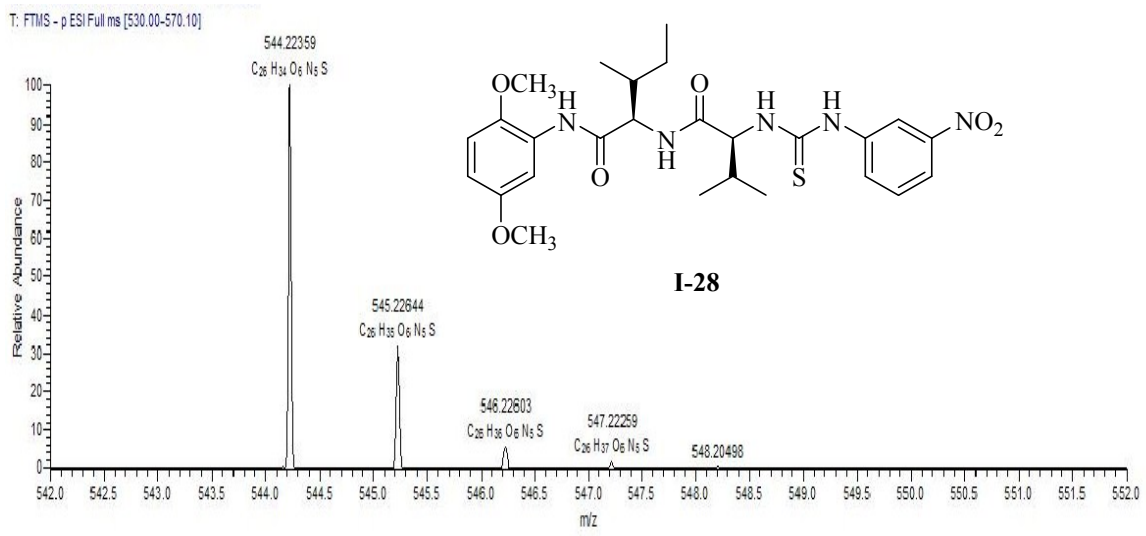

OCH3
H
N
O
N
H
O
H
N
O
H
N
S
NO2
OCH3

**I-28**


1.00
1.00
1.00
1.00
1.01
1.00
1.01
1.17
1.12
1.00
1.00
3.00
3.01
1.00
1.01
1.01
1.02
3.01
6.00
3.01
f1 (ppm)

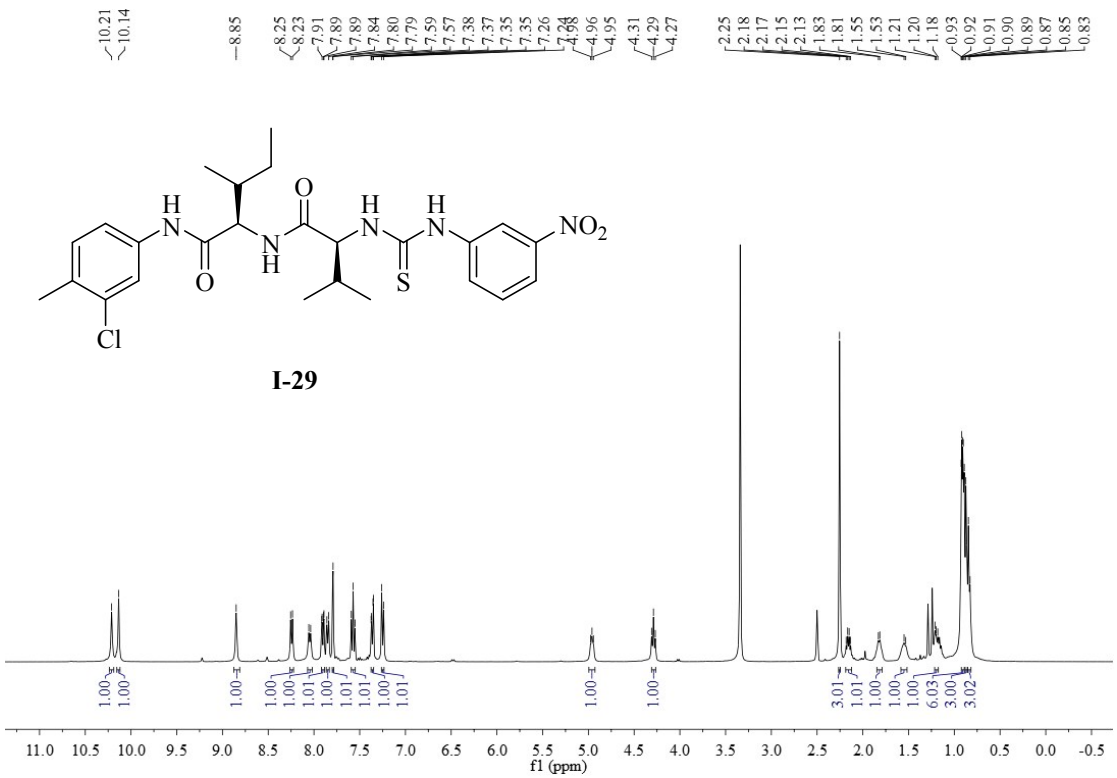

180.54
170.96
169.89
152.95
147.45
143.25
141.06
129.63
127.81
127.77
117.91
115.85
111.83
107.92
107.63
61.26
58.11
56.23
55.32
36.06
31.11
24.39
18.96
17.90
15.41
11.04
OCH3
H
N
O
N
H
O
H
N
S
H
N
NO2
OCH3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

**I-28**

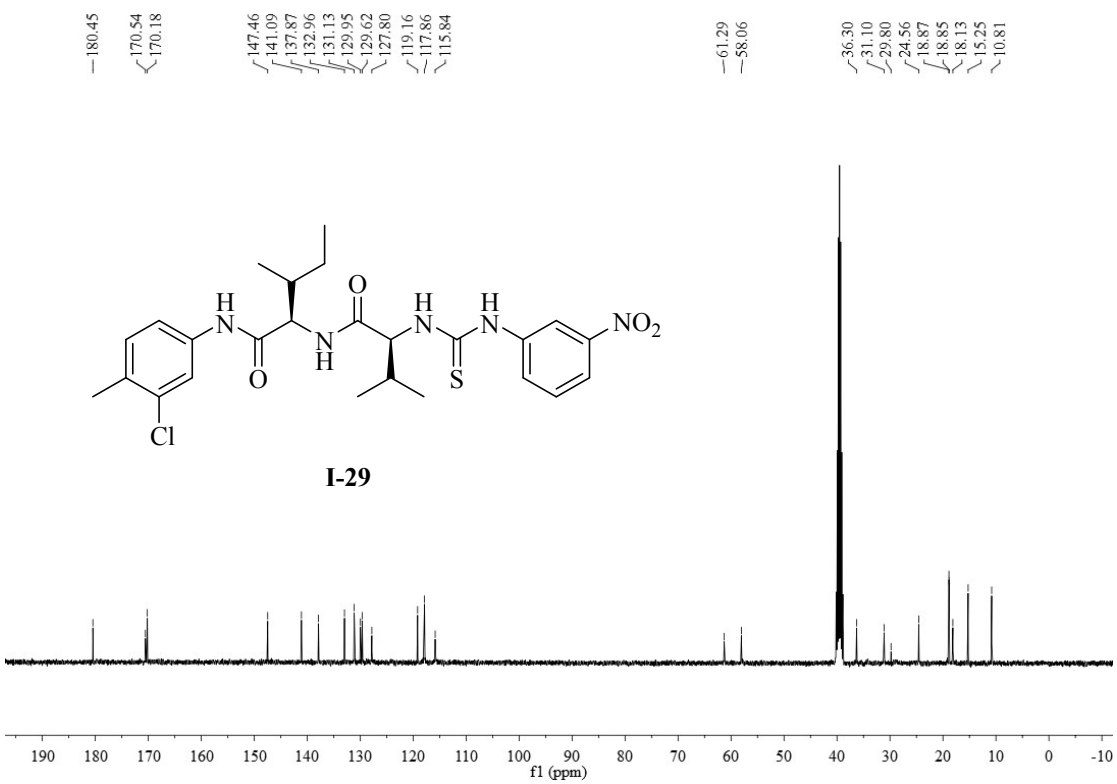

T: FTMS - p ESI Full ms [530.00-570.10]
544.22359
C26 H34 O6 N5 S
545.22644
C26 H35 O6 N5 S
546.22603
C26 H36 O6 N5 S
547.22259
C26 H37 O6 N5 S
548.20498
Relative Abundance
m/z
542.0 542.5 543.0 543.5 544.0 544.5 545.0 545.5 546.0 546.5 547.0 547.5 548.0 548.5 549.0 549.5 550.0 550.5 551.0 551.5 552.0


OCH3
H
N
O
N
H
O
H
N
S
H
N
NO2
OCH3

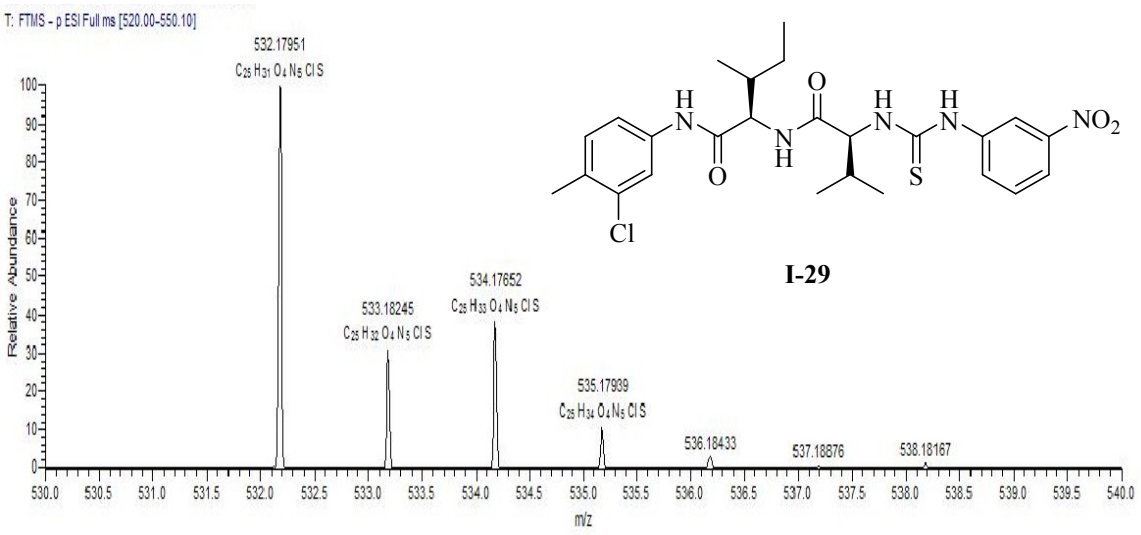
**I-28**


10.21
10.14
8.85
8.25
8.23
7.91
7.89
7.89
7.84
7.80
7.79
7.59
7.57
7.38
7.37
7.35
7.35
7.26
4.98
4.96
4.95
4.31
4.29
4.27
2.25
2.18
2.17
2.15
2.13
1.83
1.81
1.55
1.53
1.21
1.20
1.18
0.93
0.92
0.91
0.90
0.89
0.87
0.85
0.83
H
N
O
N
H
O
H
N
H
N
S
NO2
Cl
1.00
1.00
1.00
1.00
1.00
1.01
1.00
1.01
1.01
1.00
1.01
1.00
1.00
3.01
1.01
1.00
1.00
1.00
6.03
3.00
3.02
11.0
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)

**I-29**

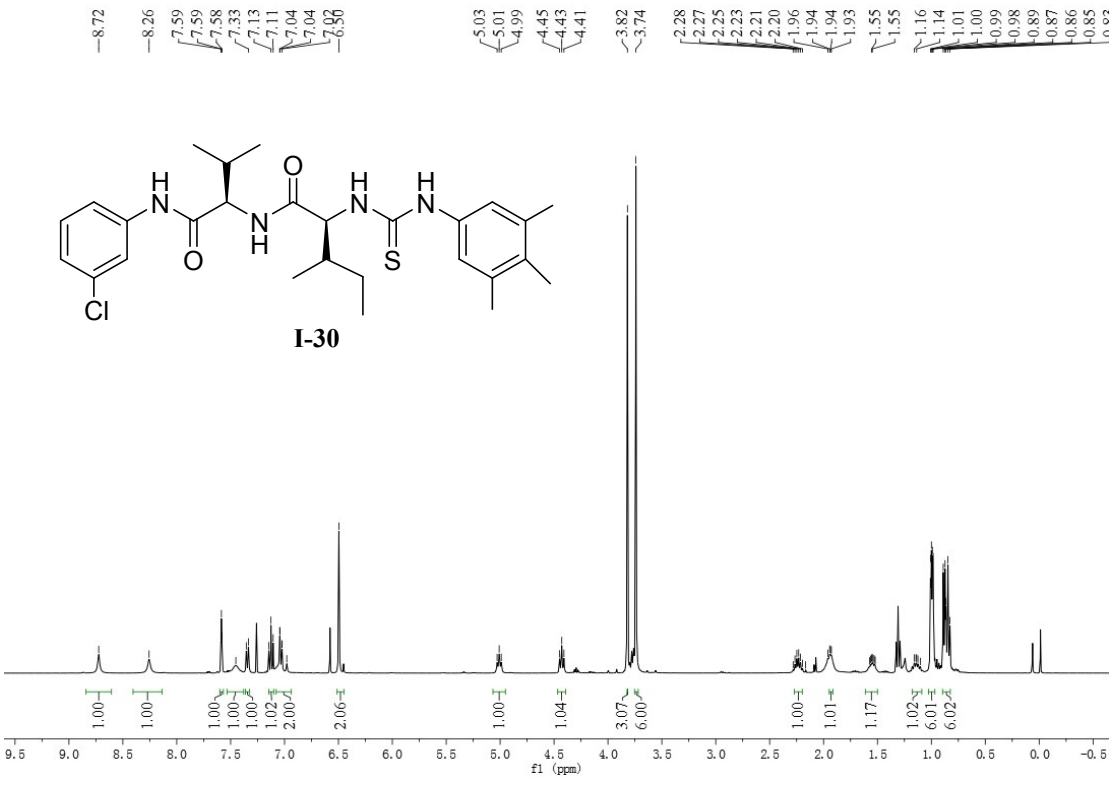

180.45
170.54
170.18
147.46
141.09
137.87
132.96
131.13
129.95
129.62
127.80
119.16
117.86
115.84
61.29
58.06
36.30
31.10
29.80
24.56
18.87
18.85
18.13
15.25
10.81
H
N
O
N
H
O
H
N
H
N
S
NO2
Cl
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

**I-29**


T: FTMS - p ESI Full ms [520.00-550.10]
532.17951
C25 H31 O4 N5 Cl S
533.18245
C25 H32 O4 N5 Cl S
534.17652
C25 H33 O4 N5 Cl S
535.17909
C25 H34 O4 N5 Cl S
536.18433
537.18876
538.18167
Relative Abundance
m/z

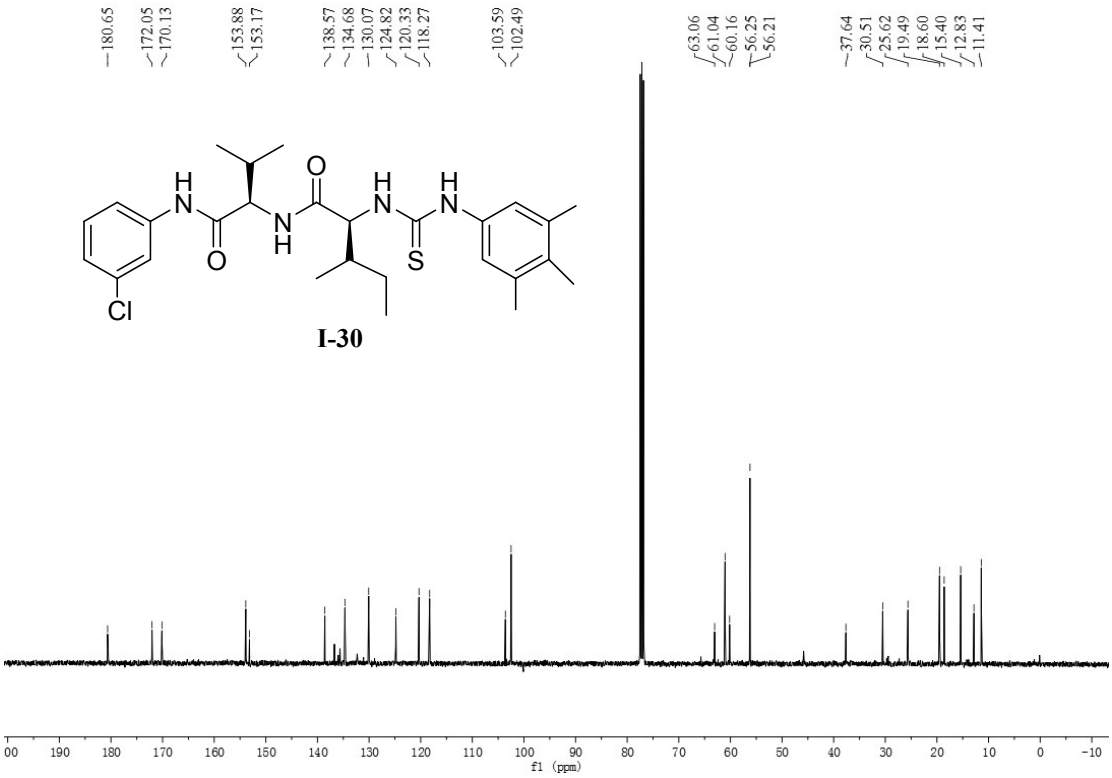


**I-29**

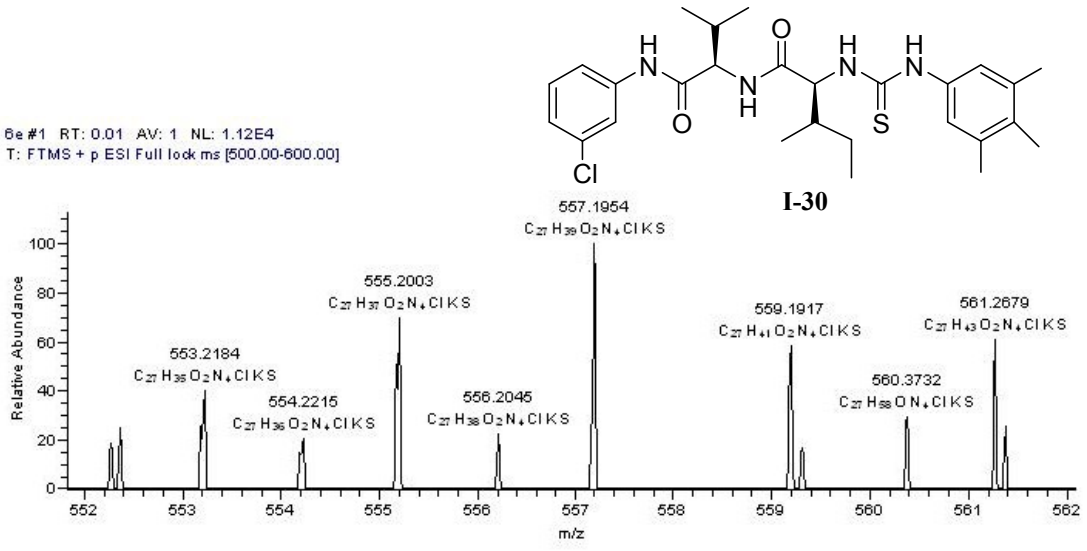




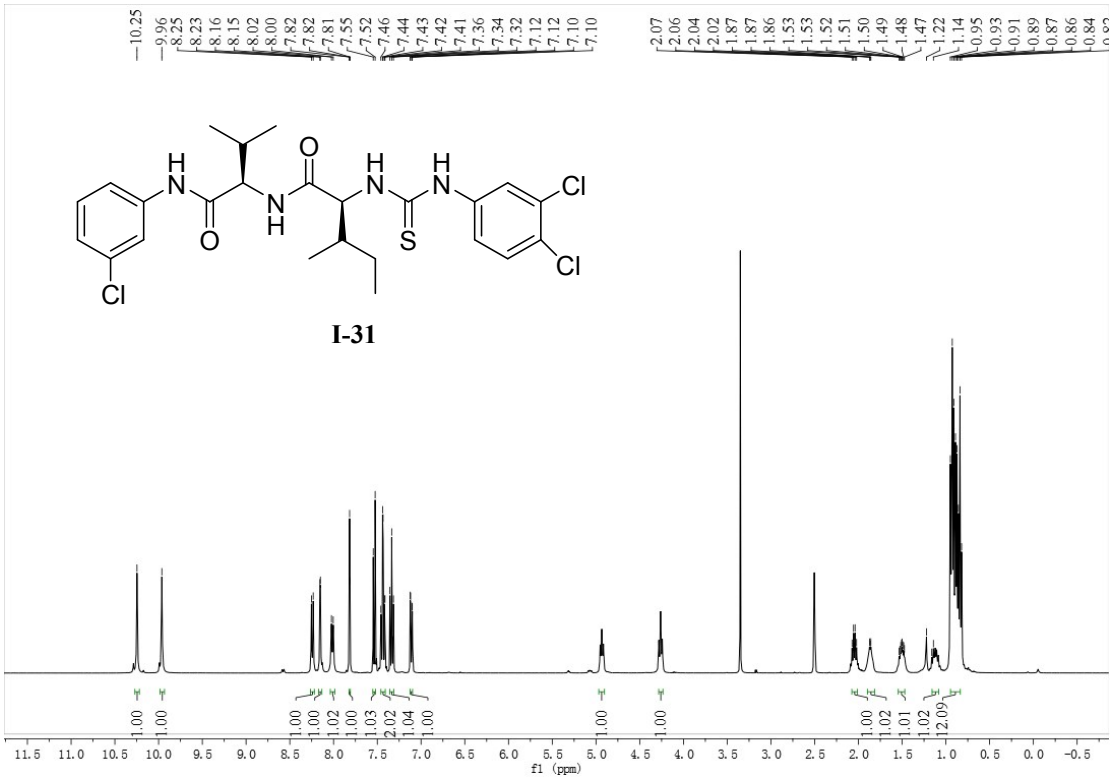
**I-30**


180.65
172.05
170.13
153.88
153.17
138.57
134.68
130.07
124.82
120.33
118.27
103.59
102.49
63.06
61.04
60.16
56.25
56.21
37.64
30.51
25.62
19.49
18.60
15.40
12.83
11.41
f1 (ppm)

**I-30**

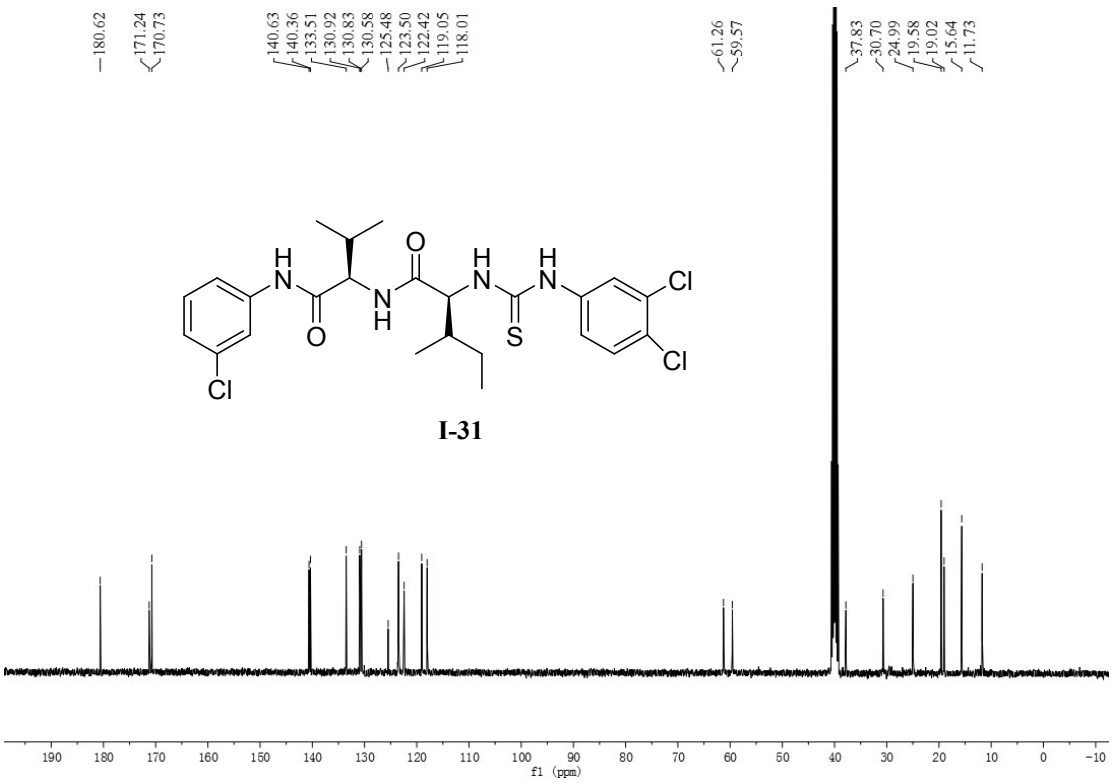

6e #1 RT: 0.01 AV: 1 NL: 1.12E4
T: FTMS + p ESI Full lock ms [500.00-600.00]
553.2184
C27H35O2N4ClKS
554.2215
C27H36O2N4ClKS
555.2003
C27H37O2N4ClKS
556.2045
C27H38O2N4ClKS
557.1954
C27H39O2N4ClKS
559.1917
C27H41O2N4ClKS
560.3732
C27H58ON4ClKS
561.2679
C27H43O2N4ClKS
Relative Abundance
m/z

**I-30**


10.25
9.96
8.25
8.23
8.16
8.15
8.02
8.00
7.82
7.82
7.81
7.55
7.52
7.46
7.44
7.43
7.42
7.41
7.36
7.34
7.32
7.12
7.12
7.10
7.10
2.07
2.06
2.04
2.02
1.87
1.87
1.86
1.53
1.53
1.52
1.51
1.50
1.49
1.48
1.47
1.22
1.14
0.95
0.93
0.91
0.89
0.87
0.86
0.84
1.00
1.00
1.00
1.00
1.02
1.00
1.03
2.02
1.04
1.00
1.00
1.00
1.00
1.02
1.01
1.02
12.09
11.5 11.0 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)

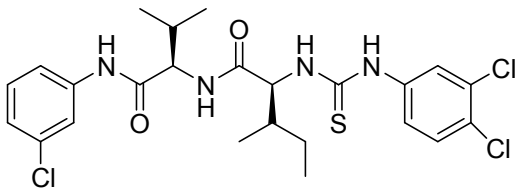

H
N
O
N
H
H
N
H
N
S
Cl
Cl
Cl

**I-31**

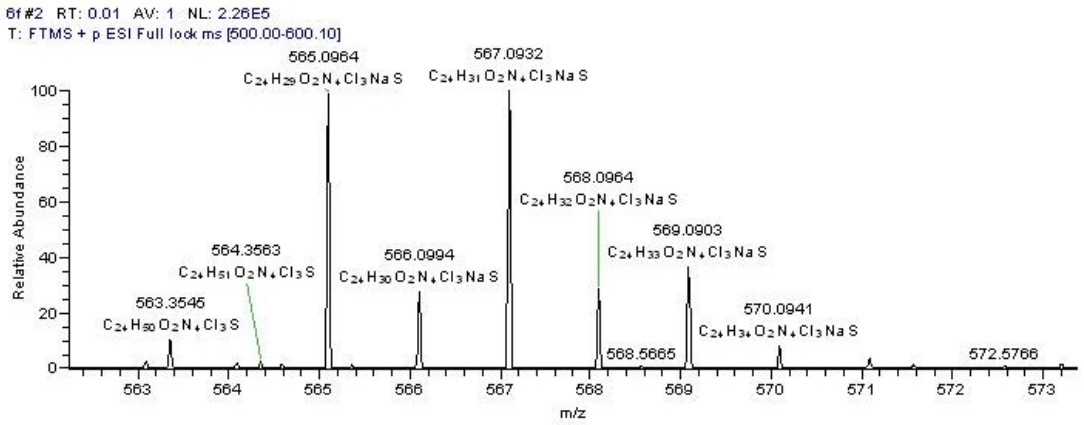

180.62
171.24
170.73
140.63
140.36
133.51
130.92
130.83
130.58
125.48
123.50
122.42
119.05
118.01
61.26
59.57
37.83
30.70
24.99
19.58
19.02
15.64
11.73
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

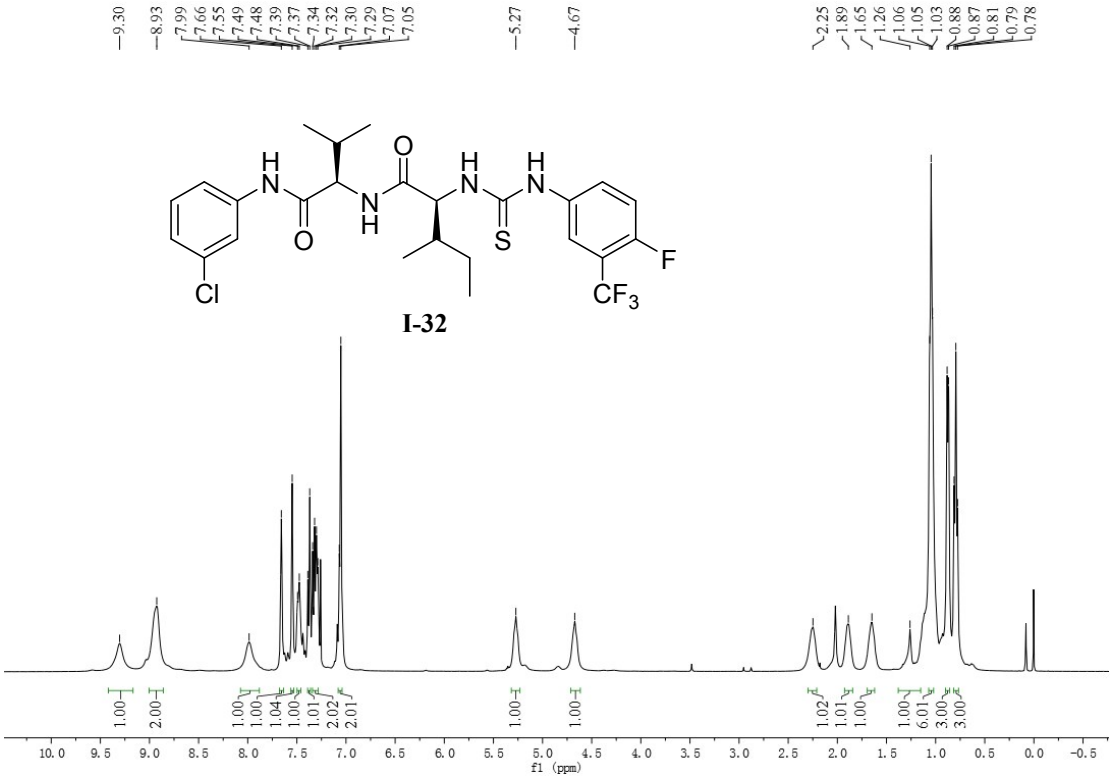

H
N
O
N
H
H
N
H
N
S
Cl
Cl
Cl

**I-31**

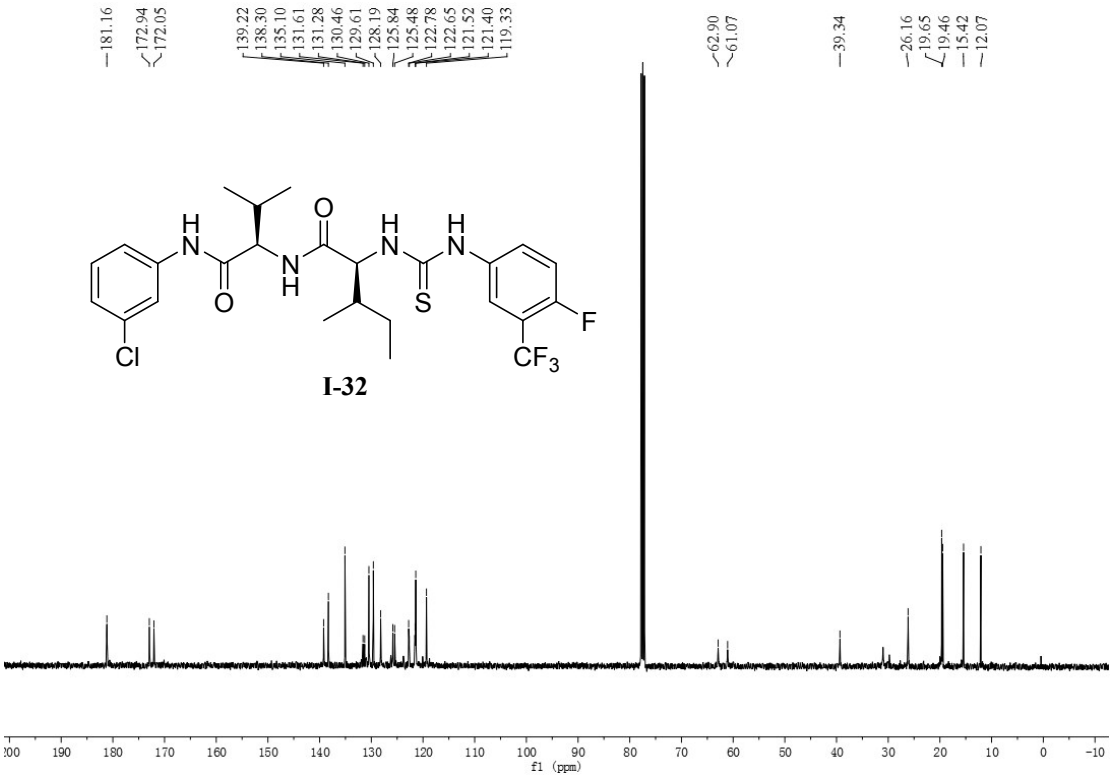

H
N
O
N
H
H
N
H
N
S
Cl
Cl
Cl

**I-31**

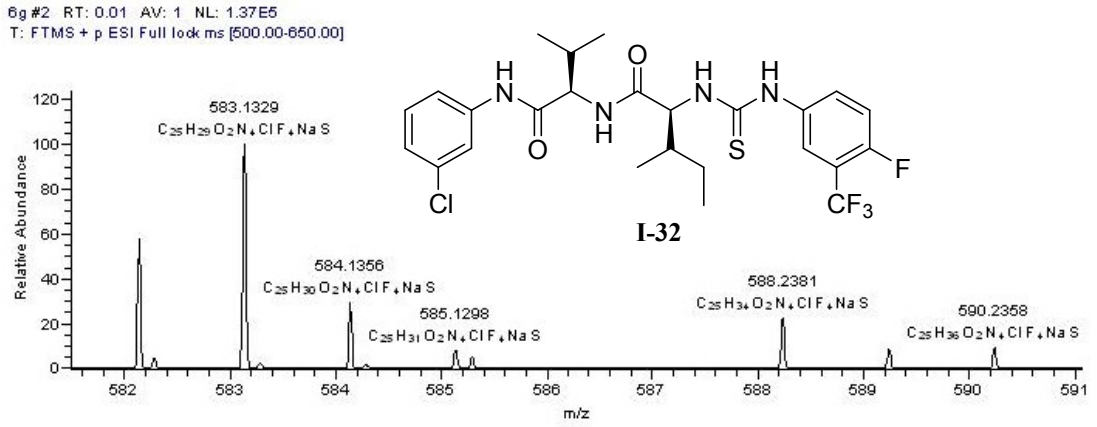

6f #2 RT: 0.01 AV: 1 NL: 2.26E5
T: FTMS + p ESI Full lock ms [500.00-600.10]
565.0964
C24H29O2N4Cl3NaS
567.0932
C24H31O2N4Cl3NaS
568.0964
C24H32O2N4Cl3NaS
569.0903
C24H33O2N4Cl3NaS
564.3563
C24H51O2N4Cl3S
566.0994
C24H30O2N4Cl3NaS
563.3545
C24H50O2N4Cl3S
570.0941
C24H34O2N4Cl3NaS
568.5665
572.5766
Relative Abundance
m/z


9.30
8.93
7.99
7.66
7.55
7.49
7.48
7.39
7.37
7.34
7.32
7.30
7.29
7.07
7.05
5.27
4.67
2.25
1.89
1.65
1.26
1.06
1.05
1.03
0.88
0.87
0.81
0.79
0.78
Cl
F
CF3
f1 (ppm)

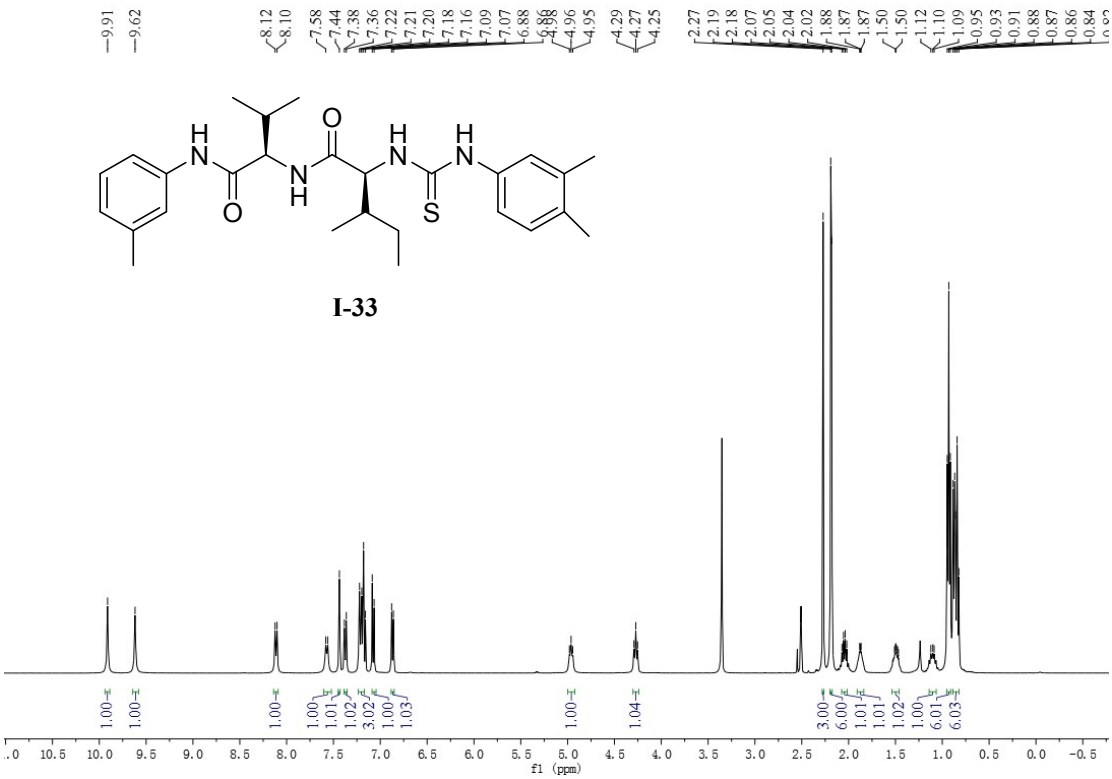
**I-32**


181.16
172.94
172.05
139.22
138.30
135.10
131.61
131.28
130.46
129.61
128.19
125.84
125.48
122.78
122.65
121.52
121.40
119.33
62.90
61.07
39.34
26.16
19.65
19.46
15.42
12.07
f1 (ppm)

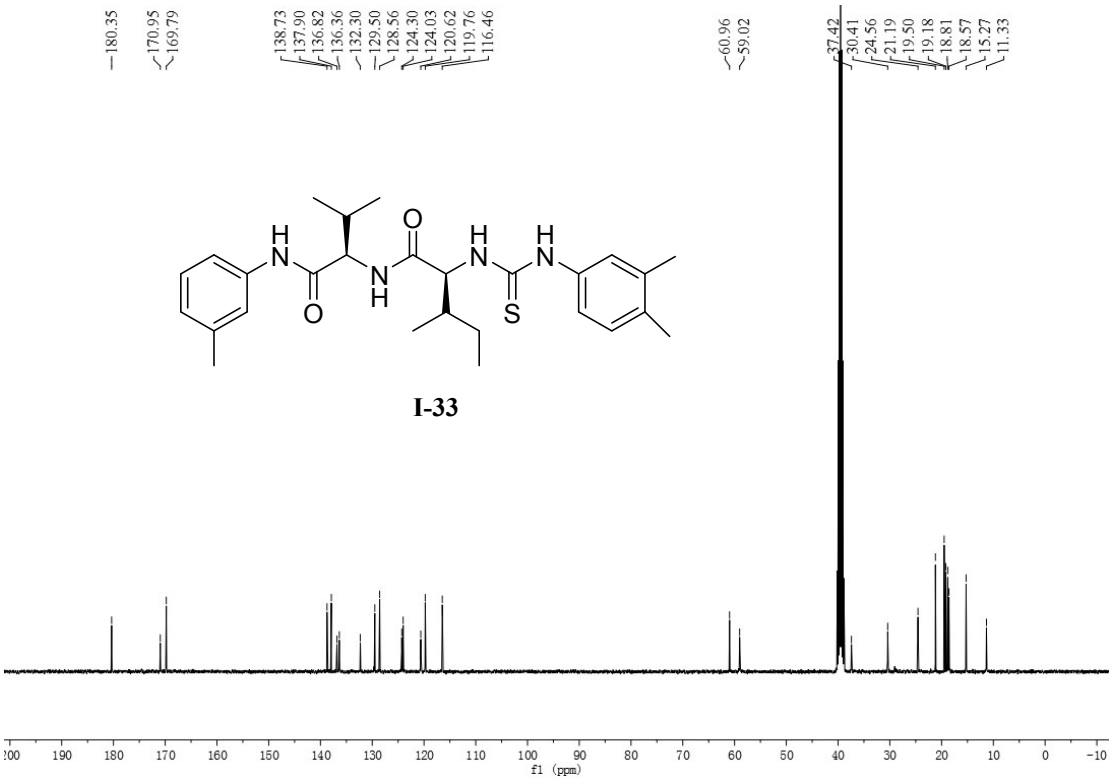
**I-32**


6g #2 RT: 0.01 AV: 1 NL: 1.37E5
T: FTMS + p ESI Full lock ms [500.00-650.00]
583.1329
C25H29O2N4ClF4NaS
584.1356
C25H30O2N4ClF4NaS
585.1298
C25H31O2N4ClF4NaS
588.2381
C25H34O2N4ClF4NaS
590.2358
C25H36O2N4ClF4NaS
Relative Abundance
m/z

**I-32**

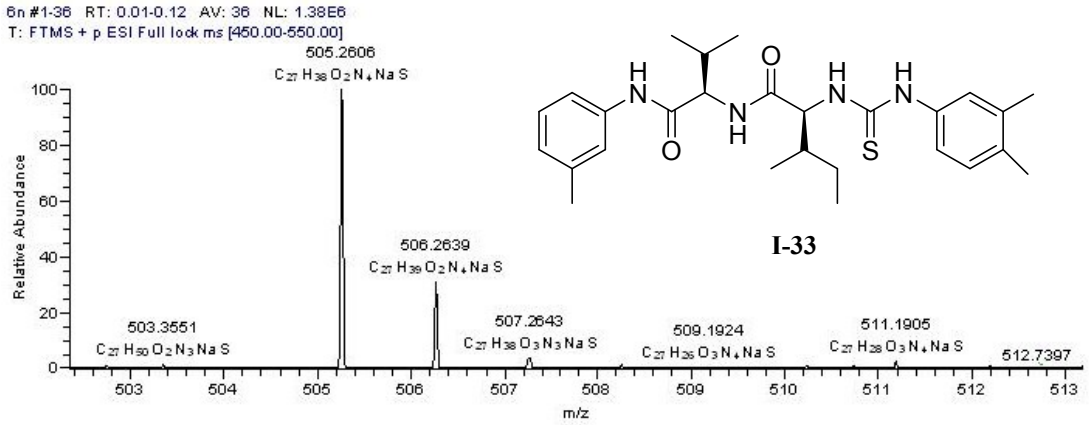


**I-33**



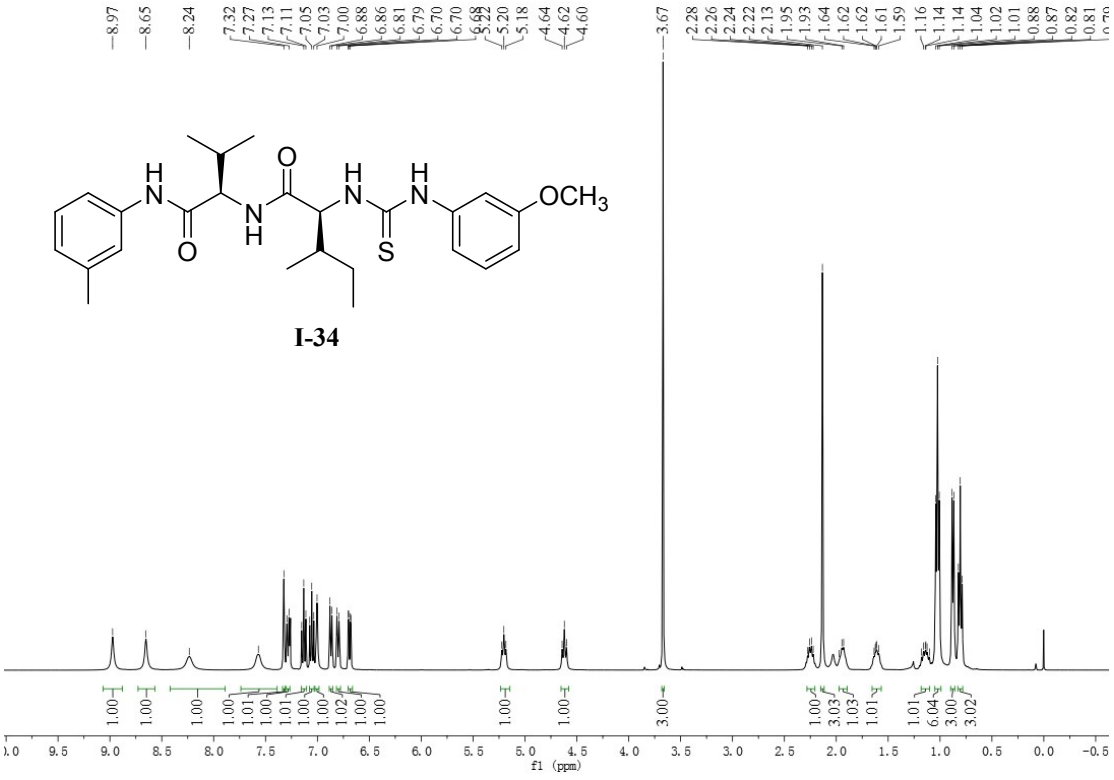


**I-33**


6n #1-36 RT: 0.01-0.12 AV: 36 NL: 1.38E6
T: FTMS + p ESI Full lock ms [450.00-550.00]
505.2606
C27 H38 O2 N4 Na S
506.2639
C27 H39 O2 N4 Na S
503.3551
C27 H50 O2 N3 Na S
507.2643
C27 H38 O3 N3 Na S
509.1924
C27 H35 O3 N4 Na S
511.1905
C27 H28 O3 N4 Na S
512.7397
Relative Abundance
m/z

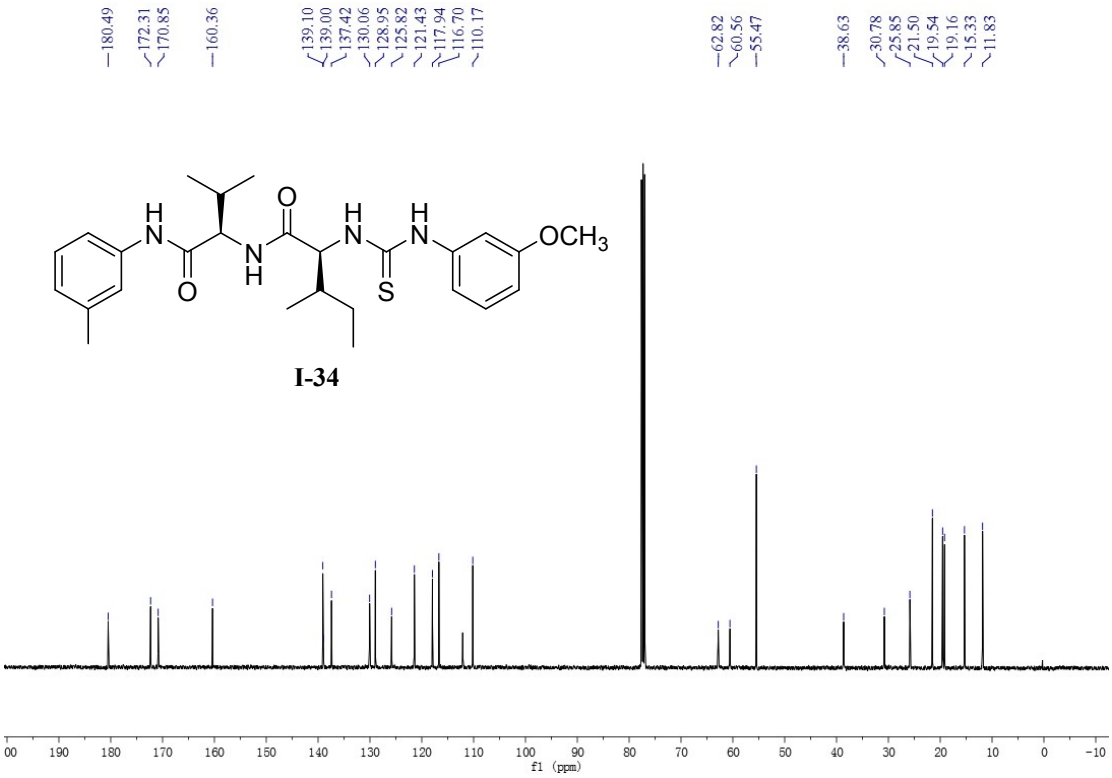


**I-33**

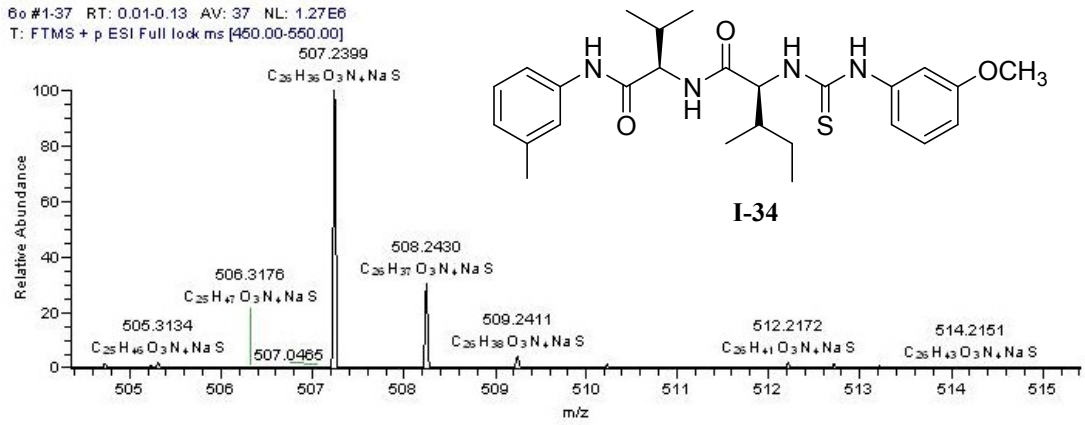

f1 (ppm)



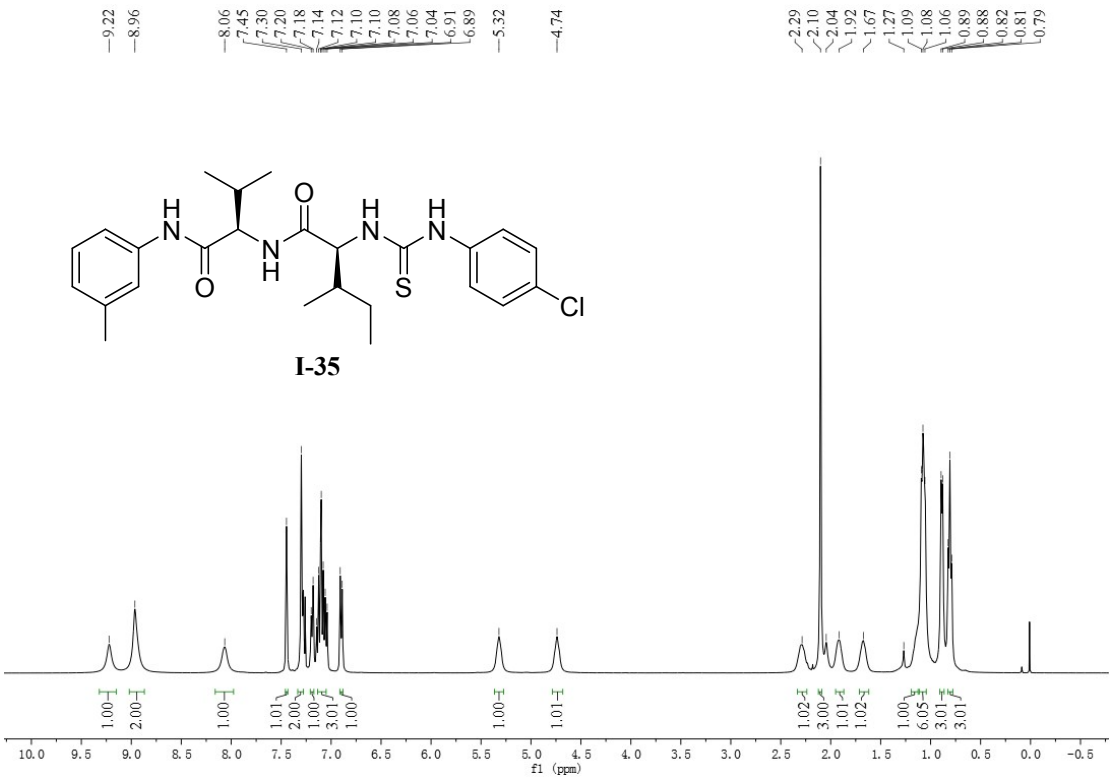
**I-34**


180.49
172.31
170.85
160.36
139.10
139.00
137.42
130.06
128.95
125.82
121.43
117.94
116.70
110.17
62.82
60.56
55.47
38.63
30.78
25.85
21.50
19.54
19.16
15.33
11.83
OCH3
f1 (ppm)

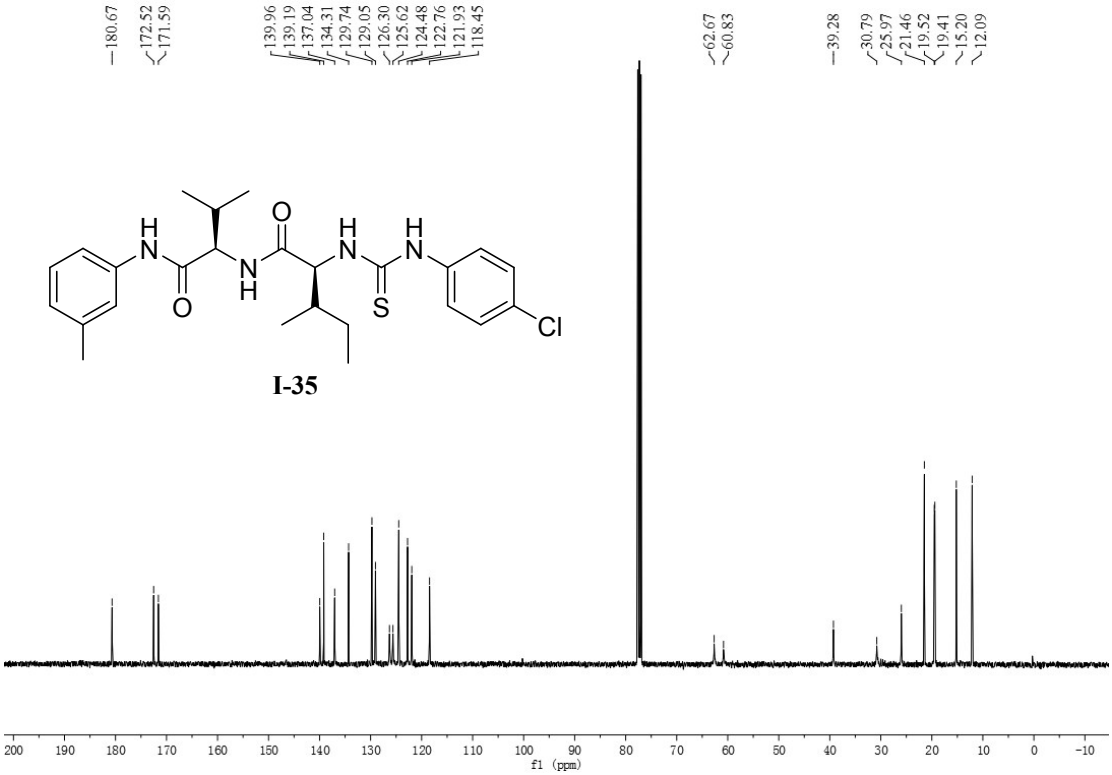
**I-34**


6o #1-37 RT: 0.01-0.13 AV: 37 NL: 1.27E6
T: FTMS + p ESI Full lock ms [450.00-550.00]
507.2399
C26H36O3N4NaS
508.2430
C26H37O3N4NaS
506.3176
C25H47O3N4NaS
505.3134
C25H46O3N4NaS
507.0465
509.2411
C26H38O3N4NaS
512.2172
C26H41O3N4NaS
514.2151
C26H43O3N4NaS
Relative Abundance
m/z
OCH3

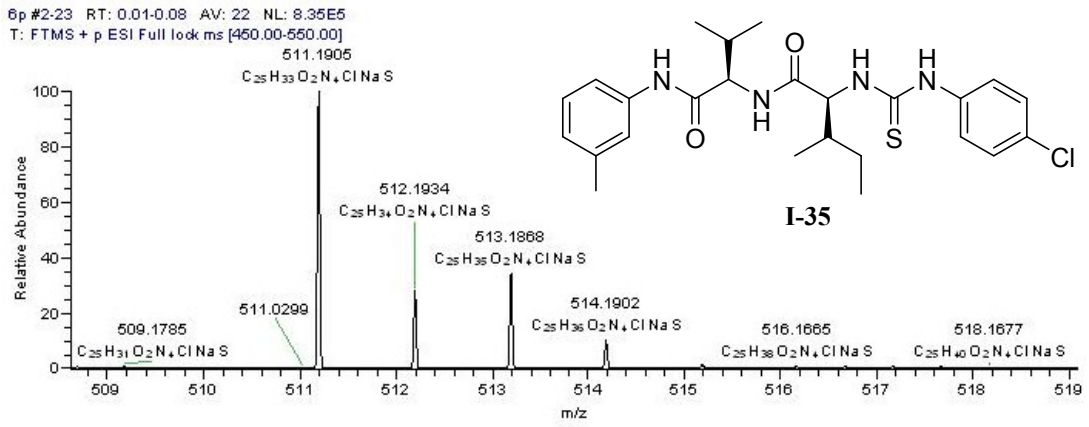
**I-34**


9.22
8.96
8.06
7.45
7.30
7.20
7.18
7.14
7.12
7.10
7.10
7.08
7.06
7.04
6.91
6.89
5.32
4.74
2.29
2.10
2.04
1.92
1.67
1.27
1.09
1.08
1.06
0.89
0.88
0.82
0.81
0.79
1.00
2.00
1.00
1.01
2.00
1.00
3.01
1.00
1.00
1.01
1.02
3.00
1.01
1.02
1.00
6.05
3.01
3.01
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)

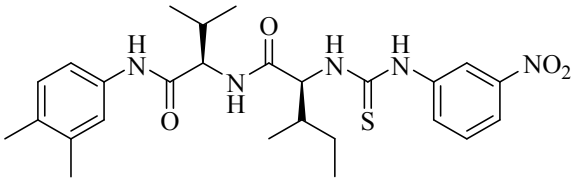
**I-35**


180.67
172.52
171.59
139.96
139.19
137.04
134.31
129.74
129.05
126.30
125.62
124.48
122.76
121.93
118.45
62.67
60.83
39.28
30.79
25.97
21.46
19.52
19.41
15.20
12.09
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

**I-35**

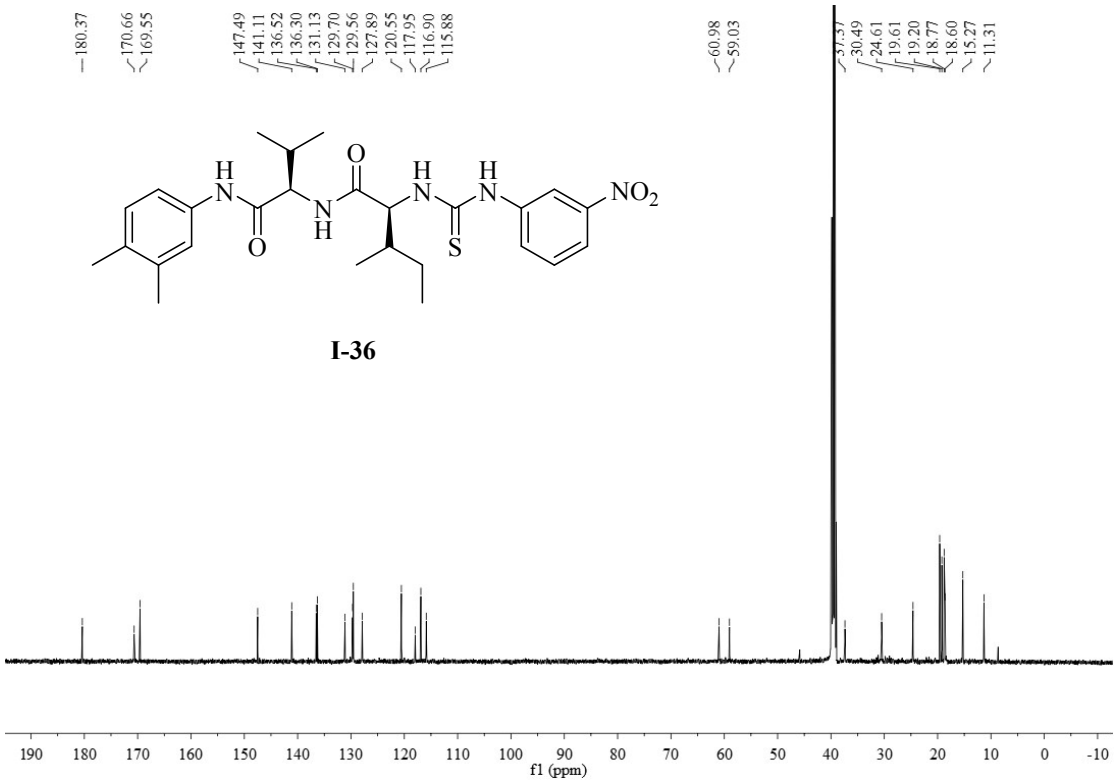

6p #2-23 RT: 0.01-0.08 AV: 22 NL: 8.35E5
T: FTMS + p ESI Full lock ms [450.00-550.00]
511.1905
C25H33O2N4ClNaS
512.1934
C25H34O2N4ClNaS
513.1868
C25H35O2N4ClNaS
514.1902
C25H36O2N4ClNaS
509.1785
C25H31O2N4ClNaS
511.0299
516.1665
C25H38O2N4ClNaS
518.1677
C25H40O2N4ClNaS
Relative Abundance
m/z

I-35

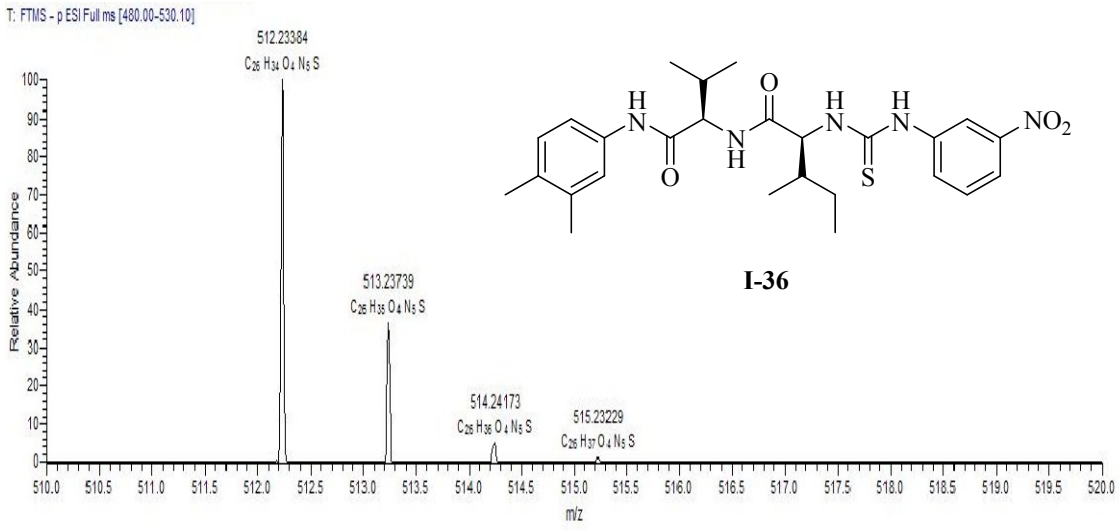


I-36


f1 (ppm)


180.37
170.66
169.55
147.49
141.11
136.52
136.30
131.13
129.70
129.56
127.89
120.55
117.95
116.90
115.88
60.98
59.03
31.37
30.49
24.61
19.61
19.20
18.77
18.60
15.27
11.31
NO2
f1 (ppm)

**I-36**


T: FTMS - p ESI Full ms [480.00-530.10]
512.23384
C26 H34 O4 N5 S
513.23739
C26 H35 O4 N5 S
514.24173
C26 H36 O4 N5 S
515.23229
C26 H37 O4 N5 S
Relative Abundance
m/z
NO2

**I-36**