

Electronic supplementary information

Construction of Fluorophoric Thiazolo-[2,3-b]quinazolinone Derivatives: A Multicomponent Domino synthetic approach

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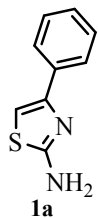
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1. General information

The reactions were performed in SINEO MAS-II Microwave Synthesizer, Power Voltage: AC 220 V \pm 10% 50Hz AC, Rated Input power: 1360W, Rated high frequency output power: 1000W, Operating frequency: 2450MHz. Melting points were taken in open capillaries using sulphuric acid-bath and are uncorrected. Reactions were monitored by thin-layer chromatography (TLC) using Merck silica gel 60 F254 precoated plates (0.25 mm) in appropriate mixture of ethyl acetate and hexane and visualized under UV-Lamp of 365 nm. Column chromatography was performed using silica gel (60-120 mesh) using hexanes and ethyl acetate mixture as eluent. Isolation of some of the compounds was carried in Prep. HPLC, Agilent technologies 1260. ^1H NMR and ^{13}C NMR spectra were recorded on Bruker (400 and 100 MHz, respectively) instrument internally referenced to tetramethylsilane (TMS) or DMSO signals. Chemical shifts were reported in parts per million and multiplicities are as indicated: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), and br (broad). Coupling constants, J , are reported in Hertz. Mass spectra were measured on Agilent 6110 LC-MS instrument (ESI). High-resolution mass spectrum of one of the compounds was recorded TOF mass spectrometer. All the reagents and solvents used were of the best grade available and were used without further purification.

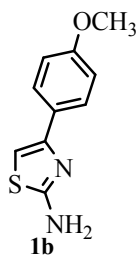
2. General procedure for the synthesis of 2-amino-4-aryl thiazole

A mixture of thiourea (15.2 gm, 0.2 mol), acetophenone (11.7 ml, 0.1 mol) and iodine (25.4 gm, 0.1 mol) was refluxed for 8 hours in dry benzene (5 ml) on a water bath. Further heating the mixture for 12 hours without refluxing yielded a hard mass which was kept in contact with ether (20 ml) overnight. After decanting off the ether, it was washed with cold water followed by very dilute solution of sodium thiosulfate. The residue was then extracted three times with boiling water, treated with conc. ammonia and kept overnight. The pale yellow solid was collected by filtration and recrystallized from ethanol.



4-phenylthiazol-2-amine

Pale Yellow, 85% yield; m.p: 149-151°C; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 5.21 (bs, 2H), 6.72 (s, 1H), 7.27-7.31 (t, 1H), 7.36 (t, 2H), 7.76 (d, $J = 7.6$ Hz, 2H).

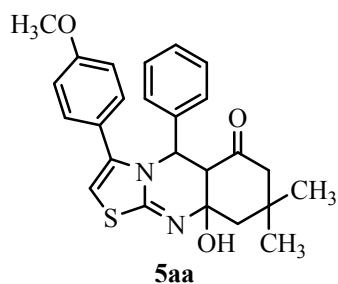


4-(4-methoxyphenyl)thiazol-2-amine

Yellow, 95% yield; m.p: 245-247°C; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 3.83 (s, 3H), 4.94 (bs, 2H), 6.54 (s, 1H), 6.90 (d, $J = 8.8$ Hz, 2H), 7.70 (d, $J = 8.8$ Hz, 2H).

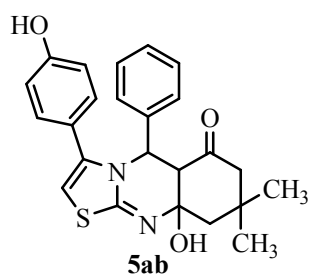
3. General procedure for the synthesis of 9a-hydroxy-8,8-dimethyl-3,5-diaryl-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

The reactions were performed in SINEO MAS-II Microwave Synthesizer. In a 25 ml microwave reaction vessel, a mixture of 2-amino-4-aryl thiazole (0.001 mol), aryl aldehyde (0.001 mol), and cyclic 1,3-dicarbonyl compound (0.001 mol) in 3ml glacial acetic acid was irradiated for a desired time varied from 10-15 minutes (monitored by TLC) at 300 W and 150°C. The reaction mixture was allowed to cool at room temperature and poured onto crushed ice. The solid products thus separated out were filtered, dried and washed with aqueous ethanol. Subsequently, it was recrystallized with water-ethanol (4:96) mixture.



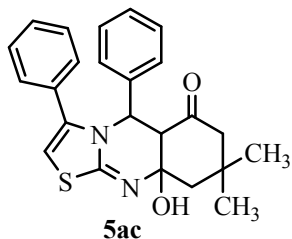
**9a-hydroxy-3-(4-methoxyphenyl)-8,8-dimethyl-5-phenyl-5,5a,7,8,9,9a-hexahydrothiazolo-
[2,3-b]quinazolin-6-one**

Light green, 73% yield; m.p: 160-163°C; ¹H NMR (400 MHz, DMSO-d₆) δ 0.98 (s, 3H), 0.99 (s, 3H), 1.91 (s, 2H), 2.04-2.17 (m, 2H), 2.68 (d, *J* = 8.4 Hz, 1H), 3.69 (s, 3H), 3.86 (d, *J* = 8.4 Hz, 1H), 6.69 (d, *J* = 8.8 Hz, 2H), 6.95 (s, 1H), 7.13 (t, 1H), 7.25 (d, *J* = 7.2 Hz, 2H), 7.33 (t, 2H), 7.49 (d, *J* = 8.8 Hz, 2H), 12.21 (bs, 1H); ¹³C NMR (100 MHz, DMSO-d₆) δ 28.41, 29.13, 31.59, 32.12, 36.86, 41.93, 55.39, 56.83, 87.52, 113.87, 115.0, 125.47, 127.17, 127.44, 128.16, 129.52, 129.75, 146.63, 158.86, 166.68, 196.71; **LC-MS (m/z):** [M+H]⁺ calcd for C₂₅H₂₆N₂O₃S: 434.5; found: 435.4.



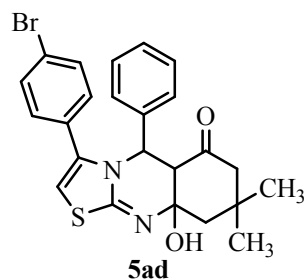
**9a-hydroxy-3-(4-hydroxyphenyl)-8,8-dimethyl-5-phenyl-5,5a,7,8,9,9a-hexahydrothiazolo-
[2,3-b]quinazolin-6-one**

Yellowish green, 71% yield; m.p: 189-191°C; ¹H NMR (400 MHz, DMSO-d₆) δ 0.99 (s, 3H), 1.01 (s, 3H), 1.91 (s, 2H), 2.15-2.24 (m, 2H), 2.96 (d, *J* = 8.4 Hz, 1H), 4.11 (d, *J* = 8.4 Hz, 1H), 6.54 (d, *J* = 8.8 Hz, 2H), 6.62 (d, *J* = 8.8 Hz, 2H), 6.87 (s, 1H), 7.05 (t, 1H), 7.20 (t, 2H), 7.34 (d, *J* = 7.6 Hz, 2H), 10.71 (bs, 1H), 11.98 (bs, 1H); ¹³C NMR (100 MHz, DMSO-d₆) δ 28.48, 29.00, 31.54, 32.02, 36.77, 42.34, 56.96, 87.83, 114.89, 115.16, 126.40, 127.11, 128.39, 128.95, 129.69, 134.27, 145.39, 156.65, 166.25, 195.79; **ESI-MS (m/z):** [M+H]⁺ calcd for C₂₄H₂₄N₂O₃S: 420.5; found: 421.2.



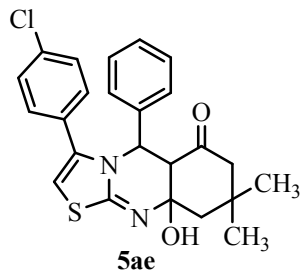
9a-hydroxy-8,8-dimethyl-3,5-diphenyl-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Greenish yellow, 62% yield; m.p: 158-160°C; ¹H NMR (400 MHz, DMSO-d₆) δ 0.99 (s, 3H), 1.04 (s, 3H), 1.91 (s, 2H), 2.28-2.33 (m, 2H), 2.35 (d, *J* = 8.4 Hz, 1H), 3.85 (d, *J* = 8.4 Hz, 1H), 6.99 (s, 1H), 7.12 (t, 1H), 7.17-7.23 (m, 3H), 7.27(d, *J* = 6.8 Hz, 2H), 7.34 (t, 2H), 7.41 (d, *J* = 7.6 Hz, 2H), 12.24 (bs, 1H); ¹³C NMR (100 MHz, DMSO-d₆) δ 28.31, 29.23, 31.32, 32.17, 37.06, 41.68, 56.21, 89.32, 116.07, 126.27, 126.67, 127.48, 127.88, 128.27, 128.41, 128.60, 129.33, 144.86, 146.73, 196.89; HRMS (*m/z*): [M+H]⁺ calcd for C₂₄H₂₄N₂O₂S: 405.1558; found: 405.1637.



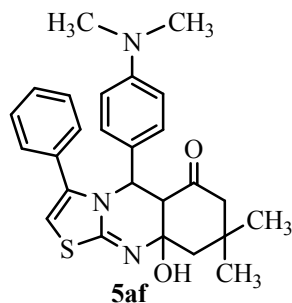
3-(4-bromophenyl)-9a-hydroxy-8,8-dimethyl-5-phenyl-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Pale yellow, 64% yield; m.p: 160-162°C; ¹H NMR (400 MHz, DMSO-d₆) δ 0.98 (s, 3H), 1.03 (s, 3H), 1.91 (s, 2H), 2.26-2.33 (m, 2H), 2.42 (d, *J* = 8.4 Hz, 1H), 3.87 (d, *J* = 8.4 Hz, 1H), 6.97 (d, *J* = 7.6 Hz, 2H), 7.06 (s, 1H), 7.20 (t, 1H), 7.26 (t, 2H), 7.34 (d, *J* = 8.4 Hz, 2H), 7.46 (d, *J* = 8.4 Hz, 2H), 11.99 (bs, 1H); ¹³C NMR (100 MHz, DMSO-d₆) δ 28.24, 29.01, 31.62, 32.21, 36.76, 41.69, 56.61, 89.53, 114.83, 124.06, 126.87, 127.69, 128.07, 129.11, 130.10, 131.39, 144.04, 145.63, 166.90, 196.40; ESI-MS (*m/z*): [M+H]²⁺ calcd for C₂₄H₂₃BrN₂O₂S: 485.4; found: 485.2.



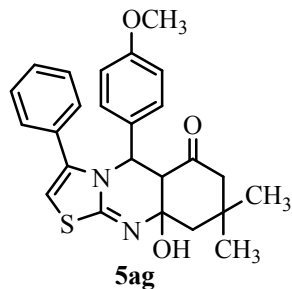
3-(4-chlorophenyl)-9a-hydroxy-8,8-dimethyl-5-phenyl-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Greenish yellow, 68% yield; m.p: 158-161°C; ¹H NMR (400 MHz, DMSO-d₆) δ 0.98 (s, 3H), 1.03 (s, 3H), 1.92 (s, 2H), 2.22-2.30 (m, 2H), 2.41 (d, *J* = 8.4 Hz, 1H), 3.86 (d, *J* = 8.4 Hz, 1H), 6.98 (d, *J* = 8.8 Hz, 2H), 7.06 (s, 1H), 7.15 (t, 1H), 7.23 (t, 2H), 7.33 (d, *J* = 7.2 Hz, 2H), 7.42 (d, *J* = 8.8 Hz, 2H), 12.28 (bs, 1H); ¹³C NMR (100 MHz, DMSO-d₆) δ 28.34, 29.01, 31.60, 32.20, 36.76, 41.71, 56.46, 89.47, 114.87, 126.96, 127.71, 128.45, 129.11, 129.80, 132.34, 134.13, 144.09, 145.55, 166.88, 196.40; **ESI-MS (m/z)**: [M+H]⁺ calcd for C₂₄H₂₃ClN₂O₂S: 438.9; found: 439.1.



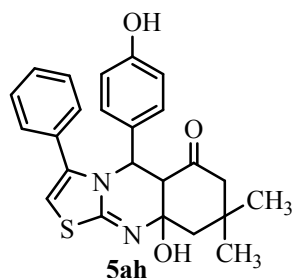
5-(4-(dimethylamino)phenyl)-9a-hydroxy-8,8-dimethyl-3-phenyl-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Brownish yellow, 59% yield; m.p: 160-163°C; ¹H NMR (400 MHz, DMSO-d₆) δ 0.97 (s, 3H), 1.01 (s, 3H), 1.91 (s, 2H), 2.10-2.20 (m, 2H), 2.79 (s, 6H), 2.86 (d, *J* = 8.4 Hz, 1H), 3.86 (d, *J* = 8.4 Hz, 1H), 6.68 (d, *J* = 8.8 Hz, 2H), 6.94 (s, 1H), 6.99 (d, *J* = 8.8 Hz, 2H), 7.11 (t, 1H), 7.18 (t, 2H), 7.24 (d, *J* = 6.8 Hz, 2H), 12.19 (bs, 1H); ¹³C NMR (100 MHz, DMSO-d₆) δ 28.52, 29.19, 31.63, 32.35, 36.21, 40.99, 43.70, 56.43, 89.77, 112.72, 112.78, 127.65, 128.48, 129.19, 130.76, 146.19, 149.60, 166.61, 196.71; **ESI-MS (m/z)**: [M+H]⁺ calcd for C₂₆H₂₉N₃O₂S: 447.6; found 448.3.



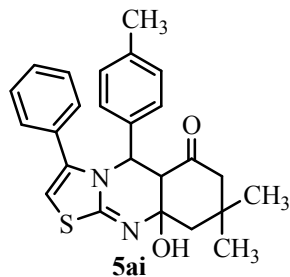
**9a-hydroxy-5-(4-methoxyphenyl)-8,8-dimethyl-3-phenyl-5,5a,7,8,9,9a-hexahydrothiazolo-
[2,3-b]quinazolin-6-one**

Yellowish green, 71% yield; m.p: 156-158°C; ¹H NMR (400 MHz, DMSO-d₆) δ 0.99 (s, 3H), 1.01 (s, 3H), 2.13 (s, 2H), 2.25-2.30 (m, 2H), 2.64 (d, *J* = 8.4 Hz, 1H), 3.64 (d, *J* = 8.4 Hz, 1H), 3.72 (s, 3H), 6.73 (d, *J* = 8.8 Hz, 2H), 6.88 (d, *J* = 8.4 Hz, 2H), 6.99 (s, 1H), 7.09 (t, 1H), 7.22 (t, 2H), 7.34 (d, *J* = 7.2 Hz, 2H), 12.21 (bs, 1H); ¹³C NMR (100 MHz, DMSO-d₆) δ 28.10, 29.07, 31.10, 32.10, 36.12, 41.28, 55.18, 55.44, 88.73, 113.37, 114.51, 127.82, 128.20, 128.71, 129.23, 135.31, 136.37, 146.74, 157.92, 166.31, 196.34; **ESI-MS (m/z):** [M+H]⁺ calcd for C₂₅H₂₆N₂O₃S: 434.5; found: 435.21.



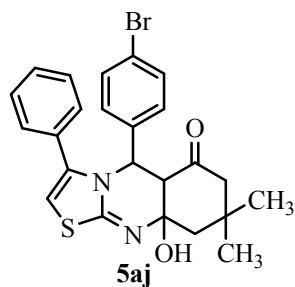
**9a-hydroxy-5-(4-hydroxyphenyl)-8,8-dimethyl-3-phenyl-5,5a,7,8,9,9a-hexahydrothiazolo-
[2,3-b]quinazolin-6-one**

Greenish yellow, 63% yield; m.p: 156-159°C; ¹H NMR (400 MHz, DMSO-d₆) δ 0.95 (s, 3H), 0.98 (s, 3H), 2.14 (s, 2H), 2.30-2.39 (m, 2H), 2.59 (d, *J* = 8.4 Hz, 1H), 3.82 (d, *J* = 8.4 Hz, 1H), 6.52 (d, *J* = 8.4 Hz, 2H), 6.86 (s, 1H), 6.95 (d, *J* = 7.6 Hz, 2H), 7.19 (t, 1H), 7.39 (t, 2H), 7.69 (d, *J* = 8.4 Hz, 2H), 10.88 (bs, 1H), 11.93 (bs, 1H); ¹³C NMR (100 MHz, DMSO-d₆) δ 28.29, 29.09, 31.75, 32.15, 36.43, 42.35, 56.35, 89.32, 106.34, 116.41, 127.88, 128.24, 128.59, 129.71, 129.86, 135.30, 143.70, 157.11, 166.90; **LC-MS (m/z):** [M+H]⁺ calcd for C₂₄H₂₄N₂O₃S: 420.5; found 421.3.



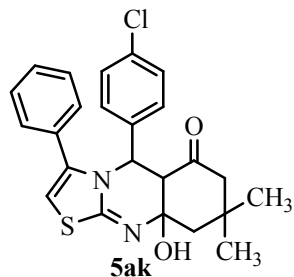
9a-hydroxy-8,8-dimethyl-3-phenyl-5-p-tolyl-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Light green, 58% yield; m.p: 158-161°C; $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 0.99 (s, 3H), 1.02 (s, 3H), 1.91 (s, 2H), 2.13-2.23 (m, 2H), 2.28 (s, 3H), 2.39 (d, $J = 8.4$ Hz, 1H), 3.81 (d, $J = 8.4$ Hz, 1H), 6.86 (d, $J = 8$ Hz, 2H), 6.97 (s, 1H), 6.99 (t, 1H), 7.12 (d, $J = 8$ Hz, 2H), 7.19 (t, 2H), 7.40 (d, $J = 6.8$ Hz, 2H), 11.96 (bs, 1H); $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 21.52, 28.39, 29.16, 31.60, 32.13, 36.53, 41.56, 56.61, 89.44, 115.02, 127.15, 127.71, 128.23, 128.80, 129.71, 134.29, 135.48, 136.54, 146.65, 166.75, 196.53; **LC-MS (m/z):** $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{25}\text{H}_{26}\text{N}_2\text{O}_2\text{S}$: 418.5; found 419.2.



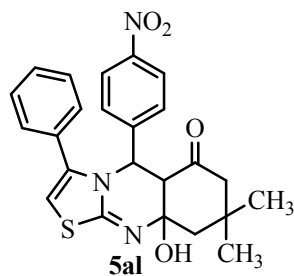
5-(4-bromophenyl)-9a-hydroxy-8,8-dimethyl-3-phenyl-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Light yellow, 63% yield; m.p: 180-182°C; $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 0.99 (s, 3H), 1.02 (s, 3H), 1.91 (s, 2H), 2.25-2.31 (m, 2H), 2.60 (d, $J = 8.4$ Hz, 1H), 3.82 (d, $J = 8.4$ Hz, 1H), 6.79 (d, $J = 7.6$ Hz, 2H), 7.02 (s, 1H), 7.13 (t, 1H), 7.30 (t, 2H), 7.38 (d, $J = 8.8$ Hz, 2H), 7.47 (d, $J = 8.8$ Hz, 2H), 12.28 (bs, 1H); $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 28.42, 28.95, 31.54, 32.61, 36.41, 41.32, 56.20, 89.81, 114.48, 122.89, 127.74, 128.12, 128.46, 129.40, 129.95, 131.94, 135.20, 144.02, 166.78, 196.45; **LC-MS (m/z):** $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{24}\text{H}_{23}\text{BrN}_2\text{O}_2\text{S}$: 483.4; found 484.1.



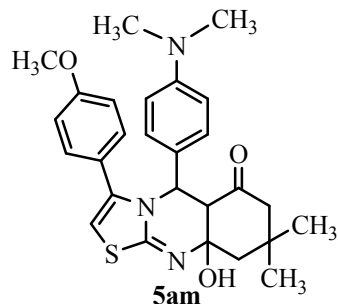
5-(4-chlorophenyl)-9a-hydroxy-8,8-dimethyl-3-phenyl-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

light green, 64% yield; m.p: 157-159°C; $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 0.95 (s, 3H), 0.99 (s, 3H), 1.91 (s, 2H), 2.26 (s, 2H), 2.42 (d, $J = 8.4$ Hz, 1H), 4.08 (d, $J = 8.4$ Hz, 1H), 6.92 (d, $J = 6.4$ Hz, 2H), 7.10 (s, 1H), 7.11 (t, 1H), 7.18 (t, 2H), 7.25 (d, $J = 7.6$ Hz, 2H), 7.38 (d, $J = 8.4$ Hz, 2H), 12.28 (bs, 1H); $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 28.59, 29.13, 31.12, 32.50, 36.69, 41.42, 56.26, 89.24, 115.70, 127.99, 128.31, 128.68, 129.22, 132.16, 135.37, 136.53, 143.98, 166.82, 196.62; **ESI-MS (m/z):** $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{24}\text{H}_{23}\text{ClN}_2\text{O}_2\text{S}$: 438.9; found 437.3.



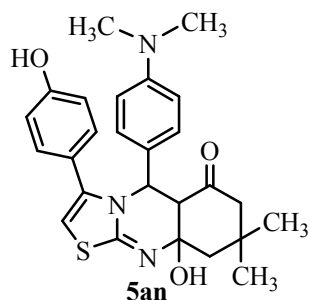
9a-hydroxy-8,8-dimethyl-5-(4-nitrophenyl)-3-phenyl-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Ocean blue, 62% yield; m.p: 188-191°C; $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 0.95 (s, 3H), 1.03 (s, 3H), 1.91 (s, 2H), 2.10-2.18 (m, 2H), 2.68 (d, $J = 8.4$ Hz, 1H), 4.04 (d, $J = 8.4$ Hz, 1H), 7.11 (s, 1H), 7.14 (t, 1H), 7.21 (t, 2H), 7.47 (d, $J = 8.8$ Hz, 2H), 8.08 (d, $J = 8.4$ Hz, 2H), 8.22 (d, $J = 8.8$ Hz, 2H), 11.95 (bs, 1H); $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 28.38, 29.22, 31.95, 32.81, 36.78, 42.16, 56.81, 89.36, 114.47, 123.60, 128.29, 128.69, 129.24, 129.89, 135.15, 144.82, 146.80, 146.92, 166.90, 196.73; **LC-MS (m/z):** $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{24}\text{H}_{23}\text{N}_3\text{O}_4\text{S}$: 449.5; found 450.1.



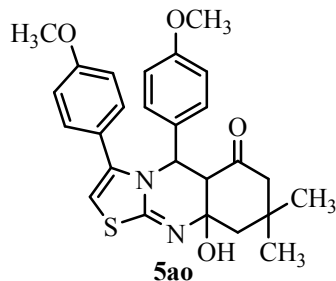
5-(4-(dimethylamino)phenyl)-9a-hydroxy-3-(4-methoxyphenyl)-8,8-dimethyl-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Brownish green, 58% yield; m.p: 160-163°C; $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 0.91 (s, 3H), 1.03 (s, 3H), 1.90 (s, 2H), 2.08-2.15 (m, 2H), 2.76 (s, 6H), 2.82 (d, $J = 8.4$ Hz, 1H), 3.51 (s, 3H), 4.08 (d, $J = 8.4$ Hz, 1H), 6.52 (d, $J = 8.4$ Hz, 2H), 6.66 (d, $J = 7.2$ Hz, 2H), 6.80 (s, 1H), 6.97 (d, $J = 8.8$ Hz, 2H), 7.08 (d, $J = 8.8$ Hz, 2H); $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 28.48, 29.19, 31.49, 32.14, 35.94, 40.87, 41.61, 55.54, 56.19, 89.67, 112.78, 114.84, 115.23, 127.34, 128.43, 129.19, 129.53, 144.28, 150.03, 156.98, 166.86, 196.87; **ESI-MS (m/z):** $[\text{M}-\text{H}]^+$ calcd for $\text{C}_{27}\text{H}_{31}\text{N}_3\text{O}_3\text{S}$: 477.6; found 476.3.



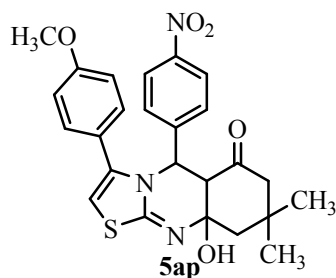
5-(4-(dimethylamino)phenyl)-9a-hydroxy-3-(4-hydroxyphenyl)-8,8-dimethyl-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Brown, 60% yield; m.p: 168-171°C; $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 0.98 (s, 3H), 1.03 (s, 3H), 1.93 (s, 2H), 2.11-2.18 (m, 2H), 2.87 (s, 6H), 2.95 (d, $J = 8.4$ Hz, 1H), 3.99 (d, $J = 8.4$ Hz, 1H), 6.57 (d, $J = 8.8$ Hz, 2H), 6.64 (d, $J = 8.8$ Hz, 2H), 6.78 (s, 1H), 6.89 (d, $J = 8.4$ Hz, 2H), 7.13 (d, $J = 8.4$ Hz, 2H), 10.46 (bs, 1H), 12.11 (bs, 1H); $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 28.32, 29.08, 31.54, 32.37, 37.02, 41.78, 43.73, 56.44, 89.46, 112.64, 115.26, 116.63, 126.69, 128.73, 129.24, 129.57, 143.67, 146.25, 157.14, 166.14, 196.67; **ESI-MS (m/z):** $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{26}\text{H}_{29}\text{N}_3\text{O}_3\text{S}$: 463.6; found 464.3.



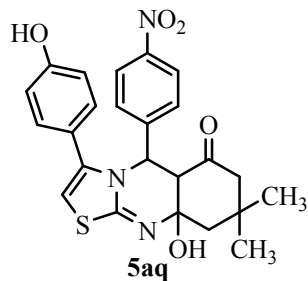
9a-hydroxy-3,5-bis(4-methoxyphenyl)-8,8-dimethyl-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Light green, 68% yield; m.p: 160-163°C; $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 0.98 (s, 3H), 0.99 (s, 3H), 1.91 (s, 2H), 2.06-2.15 (m, 2H), 2.21 (d, $J = 8.4$ Hz, 1H), 3.65 (d, $J = 8.4$ Hz, 1H), 3.69 (s, 3H), 3.74 (s, 3H), 6.69 (d, $J = 8.8$ Hz, 2H), 6.77 (d, $J = 8.4$ Hz, 2H), 6.94 (s, 1H), 7.09 (d, $J = 8.8$ Hz, 2H), 7.15 (d, $J = 8.8$ Hz, 2H), 12.20 (bs, 1H); $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 28.29, 29.02, 31.46, 32.19, 36.10, 41.09, 55.28, 55.39, 56.97, 87.89, 113.74, 115.15, 116.76, 127.97, 128.12, 128.80, 129.40, 146.26, 157.19, 158.72, 166.45, 196.45; **ESI-MS (m/z):** $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{26}\text{H}_{28}\text{N}_2\text{O}_4\text{S}$: 464.6; found 465.3.



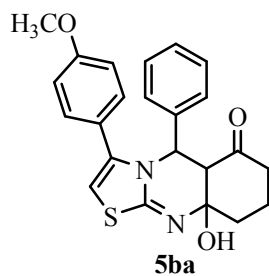
9a-hydroxy-3-(4-methoxyphenyl)-8,8-dimethyl-5-(4-nitrophenyl)-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Midnight blue, 68% yield; m.p: 196-199°C; $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 0.99 (s, 3H), 1.04 (s, 3H), 1.91 (s, 2H), 2.07-2.15 (m, 2H), 2.30 (d, $J = 8.4$ Hz, 1H), 3.70 (s, 3H), 3.77 (d, $J = 8.4$ Hz, 1H), 6.71 (d, $J = 8.8$ Hz, 2H), 7.06 (s, 1H), 7.13 (d, $J = 8.8$ Hz, 2H), 7.98 (d, $J = 8.8$ Hz, 2H), 8.22 (d, $J = 8.8$ Hz, 2H), 11.96 (bs, 1H); $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 28.41, 29.02, 31.58, 32.37, 37.29, 42.03, 55.42, 56.59, 89.94, 114.0, 114.26, 124.26, 127.70, 128.44, 129.57, 144.88, 147.48, 147.72, 159.03, 166.96, 196.59; **ESI-MS (m/z):** $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{25}\text{H}_{25}\text{N}_3\text{O}_5\text{S}$: 479.5; found 480.2.



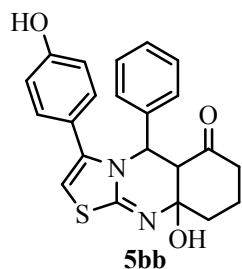
9a-hydroxy-3-(4-hydroxyphenyl)-8,8-dimethyl-5-(4-nitrophenyl)-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Midnight blue, 61% yield; m.p: 158-161°C; $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 0.98 (s, 3H), 1.03 (s, 3H), 1.90 (s, 2H), 2.03-2.14 (m, 2H), 2.54 (d, $J = 8.4$ Hz, 2H), 4.10 (d, $J = 8.4$ Hz, 1H), 6.63 (d, $J = 8.8$ Hz, 2H), 6.99 (s, 1H), 7.05 (d, $J = 8.8$ Hz, 2H), 7.96 (d, $J = 8.8$ Hz, 2H), 8.20 (d, $J = 8.8$ Hz, 2H), 9.53 (bs, 1H), 12.24 (bs, 1H); $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 28.35, 28.90, 31.42, 32.22, 37.19, 41.98, 56.32, 89.71, 114.51, 115.29, 122.68, 128.20, 129.10, 129.46, 144.64, 146.67, 147.44, 157.16, 166.56, 196.46; **LC-MS (m/z):** $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{24}\text{H}_{23}\text{N}_3\text{O}_5\text{S}$: 465.5; found 466.2.



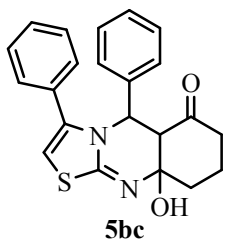
9a-hydroxy-3-(4-methoxyphenyl)-5-phenyl-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Yellowish green, 69% yield; m.p: 172-175°C; $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 1.92-1.98 (m, 2H), 2.25 (t, 2H), 2.63 (t, 2H), 2.68 (d, $J = 8.4$ Hz, 1H), 3.69 (s, 3H), 3.87 (d, $J = 8.4$ Hz, 1H), 6.69 (d, $J = 8.8$ Hz, 2H), 6.95 (s, 1H), 7.14 (t, 1H), 7.25 (d, $J = 7.2$ Hz, 2H), 7.33 (t, 2H), 7.51 (d, $J = 8.8$ Hz, 2H), 12.25 (bs, 1H); $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 20.21, 26.79, 36.75, 41.86, 55.29, 56.94, 87.40, 113.76, 115.89, 125.93, 127.22, 127.67, 128.31, 129.42, 130.11, 146.55, 158.76, 166.55, 196.67. **ESI-MS (m/z):** $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{23}\text{H}_{22}\text{N}_2\text{O}_3\text{S}$: 406.5; found: 407.3.



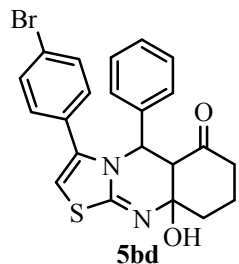
9a-hydroxy-3-(4-hydroxyphenyl)-5-phenyl-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Light yellow, 68% yield; m.p: 214-217°C; ¹H NMR (400 MHz, DMSO-d₆) δ 1.75-1.83 (m, 2H), 2.26 (t, 2H), 2.61 (t, 2H), 2.89 (d, *J* = 8.4 Hz, 1H), 4.16 (d, *J* = 8.4 Hz, 1H), 6.54 (d, *J* = 8.8 Hz, 2H), 6.62 (d, *J* = 8.8 Hz, 2H), 6.86 (s, 1H), 7.16 (t, 1H), 7.24 (t, 2H), 7.32 (d, *J* = 7.6 Hz, 2H), 10.74 (bs, 1H), 11.91 (bs, 1H); ¹³C NMR (100 MHz, DMSO-d₆) δ 20.18, 26.77, 36.73, 42.38, 56.76, 87.79, 114.83, 115.18, 126.33, 126.51, 128.33, 128.98, 129.43, 134.18, 145.02, 156.95, 165.30, 196.88; **ESI-MS (m/z)**: [M+H]⁺ calcd for C₂₂H₂₀N₂O₃S: 392.5; found: 393.2.



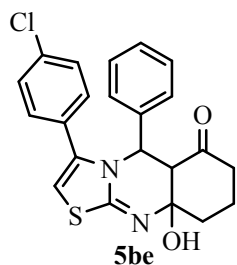
9a-hydroxy-3,5-diphenyl-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Yellow, 58% yield; m.p: 184-187°C; ¹H NMR (400 MHz, DMSO-d₆) δ 1.91-1.98 (m, 2H), 2.19 (t, 2H), 2.63 (t, 2H), 2.69 (d, *J* = 8.4 Hz, 1H), 3.91 (d, *J* = 8.4 Hz, 1H), 6.99 (s, 1H), 7.11 (t, 1H), 7.18-7.23 (m, 3H), 7.26 (d, *J* = 6.8 Hz, 2H), 7.34 (t, 2H), 7.41 (d, *J* = 7.6 Hz, 2H), 12.25 (s, 1H); ¹³C NMR (100 MHz, DMSO-d₆) δ 21.53, 26.90, 36.85, 41.89, 56.37, 89.73, 115.99, 126.23, 126.62, 127.75, 127.82, 128.24, 128.45, 128.55, 129.18, 144.73, 146.81, 196.95; **ESI-MS (m/z)**: [M+H]⁺ calcd for C₂₂H₂₀N₂O₂S: 376.5; found: 377.2.



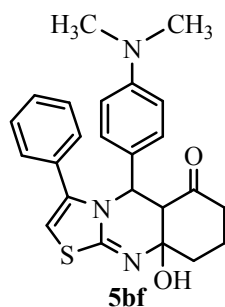
3-(4-bromophenyl)-9a-hydroxy-5-phenyl-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Greenish yellow, 59% yield; m.p: 206-208°C; ¹H NMR (400 MHz, DMSO-d₆) δ 1.93-1.99 (m, 2H), 2.25 (t, 2H), 2.55 (d, *J* = 8.4 Hz, 1H), 2.64 (t, 2H), 3.86 (d, *J* = 8.4 Hz, 1H), 6.96 (d, *J* = 7.6 Hz, 2H), 7.07 (s, 1H), 7.19 (t, 1H), 7.26 (t, 2H), 7.34 (d, *J* = 8.4 Hz, 2H), 7.60 (d, *J* = 8.4 Hz, 2H); ¹³C NMR (100 MHz, DMSO-d₆) δ 20.33, 26.91, 36.87, 41.80, 56.69, 89.60, 116.0, 124.16, 126.60, 127.80, 128.46, 129.24, 130.22, 131.51, 144.18, 145.75, 167.02, 196.81. **ESI-MS (m/z):** [M+H]⁺ calcd for C₂₂H₁₉BrN₂O₂S: 455.4; found: 456.9.



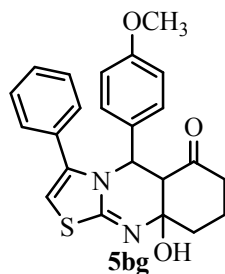
3-(4-chlorophenyl)-9a-hydroxy-5-phenyl-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Yellow, 64% yield; m.p: 202-205°C; ¹H NMR (400 MHz, DMSO-d₆) δ 1.93-1.99 (m, 2H), 2.25 (t, 2H), 2.43 (d, *J* = 8.4 Hz, 1H), 2.64 (t, 2H), 3.87 (d, *J* = 8.4 Hz, 1H), 6.94 (d, *J* = 8.8 Hz, 2H), 7.06 (s, 1H), 7.19 (t, 1H), 7.27 (t, 2H), 7.37 (d, *J* = 7.2 Hz, 2H), 7.42 (d, *J* = 8.8 Hz, 2H), 12.30 (bs, 1H); ¹³C NMR (100 MHz, DMSO-d₆) δ 20.32, 26.90, 36.85, 41.79, 56.39, 89.50, 115.9, 126.61, 127.82, 128.59, 129.25, 129.91, 132.45, 134.22, 144.20, 145.65, 167.0, 196.83. **ESI-MS (m/z):** [M+H]⁺ calcd for C₂₂H₁₉ClN₂O₂S: 410.9; found: 411.3.



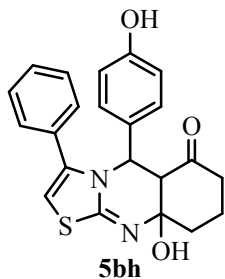
5-(4-(dimethylamino)phenyl)-9a-hydroxy-3-phenyl-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Brownish green, 57% yield; m.p: 178-181°C; ¹H NMR (400 MHz, DMSO-d₆) δ 1.91-1.98 (m, 2H), 2.23 (t, 2H), 2.61 (t, 2H), 2.81 (s, 6H), 2.86 (d, *J* = 8.4 Hz, 1H), 3.94 (d, *J* = 8.4 Hz, 1H), 6.68 (d, *J* = 8.8 Hz, 2H), 6.94 (s, 1H), 7.0 (d, *J* = 8.8 Hz, 2H), 7.11 (t, 1H), 7.18 (t, 2H), 7.24 (d, *J* = 6.8 Hz, 2H), 12.20 (bs, 1H); ¹³C NMR (100 MHz, DMSO-d₆) δ 20.41, 26.89, 36.96, 41.02, 43.13, 56.79, 89.64, 112.73, 112.79, 127.63, 128.23, 128.47, 129.1, 129.20, 132.24, 146.21, 149.61, 166.60, 196.84; **ESI-MS (m/z):** [M-H]⁺ calcd for C₂₄H₂₅N₃O₂S: 419.5; found 418.1.



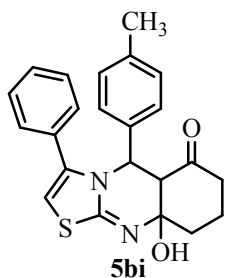
9a-hydroxy-5-(4-methoxyphenyl)-3-phenyl-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Yellow, 64% yield; m.p: 168-171°C; ¹H NMR (400 MHz, DMSO-d₆) δ 1.92 (m, 2H), 2.25 (t, 2H), 2.62 (t, 2H), 2.67 (d, *J* = 8.4 Hz, 1H), 3.67 (d, *J* = 8.4 Hz, 1H), 3.74 (s, 3H), 6.75 (d, *J* = 8.8 Hz, 2H), 6.90 (d, *J* = 8.4 Hz, 2H), 6.98 (s, 1H), 7.13 (t, 1H), 7.22 (t, 2H), 7.42 (d, *J* = 7.2 Hz, 2H), 12.23 (bs, 1H); ¹³C NMR (100 MHz, DMSO-d₆) δ 20.25, 26.78, 36.78, 41.04, 55.28, 55.39, 88.87, 113.69, 114.30, 127.59, 128.11, 128.81, 129.29, 135.39, 136.70, 146.42, 158.39, 166.59, 196.69; **ESI-MS (m/z):** [M+H]⁺ calcd for C₂₃H₂₂N₂O₃S: 406.5; found: 407.2.



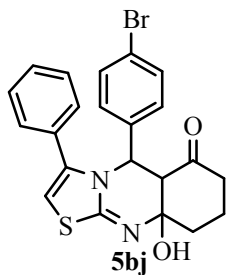
9a-hydroxy-5-(4-hydroxyphenyl)-3-phenyl-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Bright yellow, 57% yield; m.p: 228-231°C; $^1\text{H NMR}$ (400 MHz, DMSO-d_6) δ 1.91-1.98 (m, 2H), 2.23 (t, 2H), 2.54 (t, 2H), 2.96 (d, $J = 8.4$ Hz, 1H), 3.85 (d, $J = 8.4$ Hz, 1H), 6.60 (d, $J = 8.4$ Hz, 2H), 6.81 (s, 1H), 7.23 (d, $J = 7.6$ Hz, 2H), 7.32 (t, 1H), 7.43 (t, 2H), 7.88 (d, $J = 8.4$ Hz, 2H), 10.44 (bs, 1H), 12.23 (bs, 1H); $^{13}\text{C NMR}$ (100 MHz, DMSO-d_6) δ 21.81, 28.47, 36.80, 42.62, 56.94, 89.80, 106.79, 116.18, 127.66, 128.28, 129.12, 129.42, 130.19, 134.41, 144.57, 157.30, 161.2, 198.10; **ESI-MS (m/z):** $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{22}\text{H}_{20}\text{N}_2\text{O}_3\text{S}$: 392.5; found 393.3.



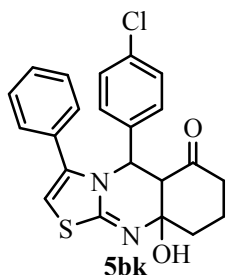
9a-hydroxy-3-phenyl-5-p-tolyl-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Yellowish green, 55% yield; m.p: 179-181°C; $^1\text{H NMR}$ (400 MHz, DMSO-d_6) δ 1.92-1.98 (m, 2H), 2.23 (t, 2H), 2.29 (s, 3H), 2.40 (d, $J = 8.4$ Hz, 1H), 2.64 (t, 2H), 3.81 (d, $J = 8.4$ Hz, 1H), 6.90 (d, $J = 8$ Hz, 2H), 6.97 (s, 1H), 7.07 (t, 1H), 7.13 (d, $J = 8$ Hz, 2H), 7.22 (t, 2H), 7.41 (d, $J = 6.8$ Hz, 2H), 11.99 (bs, 1H); $^{13}\text{C NMR}$ (100 MHz, DMSO-d_6) δ 20.24, 20.84, 26.78, 36.76, 41.43, 56.74, 89.63, 116.01, 127.03, 127.58, 128.22, 128.88, 129.59, 135.36, 135.50, 136.42, 146.52, 166.62, 196.65; **LC-MS (m/z):** 391.1 found for $\text{C}_{23}\text{H}_{22}\text{N}_2\text{O}_2\text{S}$.



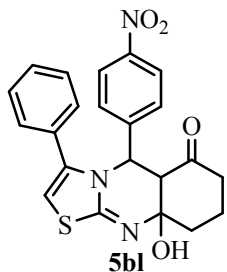
5-(4-bromophenyl)-9a-hydroxy-3-phenyl-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Yellow, 58% yield; m.p: 194-196°C; ¹H NMR (400 MHz, DMSO-d₆) δ 1.92-1.98 (m, 2H), 2.25-2.28 (t, 2H), 2.63-2.66 (t, 2H), 2.69-2.71 (d, *J* = 8.4 Hz, 1H), 3.86-3.88 (d, *J* = 8.4 Hz, 1H), 6.88 (d, *J* = 7.6 Hz, 2H), 7.05 (s, 1H), 7.19 (t, 1H), 7.27 (t, 2H), 7.39 (d, *J* = 8.8 Hz, 2H), 7.54 (d, *J* = 8.8 Hz, 2H), 12.27 (bs, 1H); ¹³C NMR (100 MHz, DMSO-d₆) δ 20.17, 26.79, 36.70, 41.32, 56.88, 89.28, 115.36, 122.90, 127.74, 128.12, 128.46, 129.95, 130.69, 131.16, 135.20, 144.02, 166.78; **ESI-MS (m/z):** [M+H]⁺ calcd for C₂₂H₁₉BrN₂O₂S: 455.3; found 456.1.



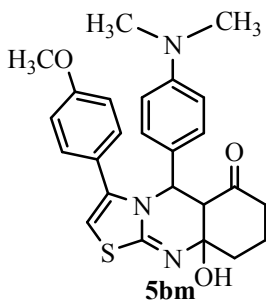
5-(4-chlorophenyl)-9a-hydroxy-3-phenyl-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Light yellow, 61% yield; m.p: 174-176°C; ¹H NMR (400 MHz, DMSO-d₆) δ 1.91-1.98 (m, 2H), 2.25 (t, 2H), 2.41 (d, *J* = 8.4 Hz, 1H), 2.63 (t, 2H), 3.87 (d, *J* = 8.4 Hz, 1H), 6.94 (d, *J* = 6.4 Hz, 1H), 7.06 (s, 1H), 7.13 (t, 1H), 7.20 (t, 2H), 7.26 (d, *J* = 7.6 Hz, 2H), 7.41 (d, *J* = 8.4 Hz, 2H), 12.29 (bs, 1H); ¹³C NMR (100 MHz, DMSO-d₆) δ 20.29, 26.90, 36.81, 41.36, 56.25, 89.39, 115.52, 127.88, 128.33, 128.59, 129.15, 129.72, 132.06, 135.31, 136.46, 143.70, 166.91; **ESI-MS (m/z):** [M+H]⁺ calcd for C₂₂H₁₉ClN₂O₂S: 410.9; found 411.4.



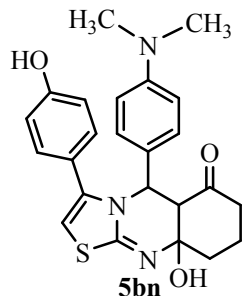
9a-hydroxy-5-(4-nitrophenyl)-3-phenyl-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Bluish green, 58% yield; m.p: 198-201°C; $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 1.93-1.99 (m, 2H), 2.25 (t, 2H), 2.62 (t, 2H), 2.72 (d, $J = 8.4$ Hz, 1H), 4.06 (d, $J = 8.4$ Hz, 1H), 6.80 (s, 1H), 7.11 (t, 1H), 7.25 (t, 2H), 7.47 (d, $J = 8.8$ Hz, 2H), 8.07 (d, $J = 8.4$ Hz, 2H), 8.21 (d, $J = 8.8$ Hz, 2H), 11.98 (bs, 1H); $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 20.12, 26.84, 36.63, 41.83, 56.95, 89.46, 114.78, 123.49, 128.16, 128.51, 129.09, 129.83, 135.08, 144.88, 146.80, 147.54, 166.96, 196.67; **LC-MS (m/z):** $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{22}\text{H}_{19}\text{N}_3\text{O}_4\text{S}$: 421.5; found 422.1.



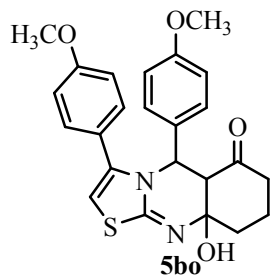
5-(4-(dimethylamino)phenyl)-9a-hydroxy-3-(4-methoxyphenyl)-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Brown, 56% yield; m.p: 184-187°C; $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 2.01-2.08 (m, 2H), 2.37 (t, 2H), 2.53 (t, 2H), 2.75 (s, 6H), 2.80 (d, $J = 8.4$ Hz, 1H), 3.54 (s, 3H), 4.07 (d, $J = 8.4$ Hz, 1H), 6.52 (d, $J = 8.4$ Hz, 2H), 6.66 (d, $J = 7.2$ Hz, 2H), 6.80 (s, 1H), 6.96 (d, $J = 8.8$ Hz, 2H), 7.07 (d, $J = 8.8$ Hz, 2H); $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 21.39, 26.77, 35.77, 40.51, 41.70, 55.63, 56.67, 89.77, 112.65, 114.85, 115.11, 127.52, 128.25, 129.06, 129.40, 144.19, 150.47, 156.78, 166.09, 196.54; **ESI-MS (m/z):** $[\text{M}-\text{H}]^+$ calcd for $\text{C}_{25}\text{H}_{27}\text{N}_3\text{O}_3\text{S}$: 449.6; found 450.3.



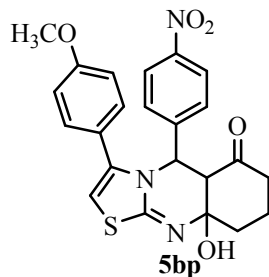
5-(4-(dimethylamino)phenyl)-9a-hydroxy-3-(4-hydroxyphenyl)-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Brownish green, 57% yield; m.p: 179-182°C; $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 1.91-1.97 (m, 2H), 2.24 (t, 2H), 2.62 (t, 2H), 2.81 (s, 6H), 2.85 (d, $J = 8.4$ Hz, 1H), 4.04 (d, $J = 8.4$ Hz, 1H), 6.53 (d, $J = 8.8$ Hz, 2H), 6.66 (d, $J = 8.8$ Hz, 2H), 6.81 (s, 1H), 6.97 (d, $J = 8.4$ Hz, 2H), 7.07 (d, $J = 8.4$ Hz, 2H), 10.56 (bs, 1H), 12.12 (bs, 1H); $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 20.41, 26.77, 36.94, 41.83, 43.84, 56.61, 89.52, 112.60, 115.32, 116.51, 126.60, 128.87, 129.20, 129.51, 143.75, 146.13, 157.03, 166.18, 196.87; **ESI-MS (m/z)**: $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{24}\text{H}_{25}\text{N}_3\text{O}_3\text{S}$: 435.5; found 436.4.



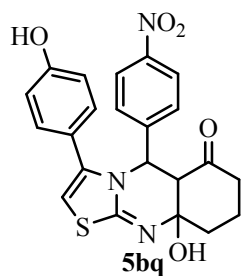
9a-hydroxy-3,5-bis(4-methoxyphenyl)-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Greenish yellow, 64% yield; m.p: 162-165°C; $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 1.92-1.98 (m, 2H), 2.25 (t, 2H), 2.32 (d, $J = 8.4$ Hz, 1H), 2.62 (t, 2H), 3.65 (d, $J = 8.4$ Hz, 1H), 3.70 (s, 3H), 3.74 (s, 3H), 6.69 (d, $J = 8.8$ Hz, 2H), 6.75 (d, $J = 8.4$ Hz, 2H), 6.92 (s, 1H), 7.07 (d, $J = 8.8$ Hz, 2H), 7.15 (d, $J = 8.8$ Hz, 2H), 12.19 (bs, 1H); $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 20.25, 26.78, 36.78, 41.10, 55.28, 55.39, 56.46, 87.15, 113.74, 114.25, 116.11, 127.98, 128.80, 129.29, 129.40, 146.27, 157.93, 158.72, 166.44, 196.69; **ESI-MS (m/z)**: $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{24}\text{H}_{24}\text{N}_2\text{O}_4\text{S}$: 436.5; found 437.3.



9a-hydroxy-3-(4-methoxyphenyl)-5-(4-nitrophenyl)-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Dark green, 63% yield; m.p: 208-211°C; $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 1.92-1.98 (m, 2H), 2.26 (t, 2H), 2.34 (d, $J = 8.4$ Hz, 1H), 2.64 (t, 2H), 3.69 (s, 3H), 3.71 (d, $J = 8.4$ Hz, 1H), 6.71 (d, $J = 8.8$ Hz, 2H), 7.07 (s, 1H), 7.14 (d, $J = 8.8$ Hz, 2H), 8.07 (d, $J = 8.8$ Hz, 2H), 8.22 (d, $J = 8.8$ Hz, 2H), 11.97 (bs, 1H); $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 28.41, 29.02, 31.58, 32.37, 37.29, 42.03, 55.42, 56.59, 89.94, 114.0, 114.26, 124.26, 127.70, 128.44, 129.57, 144.88, 147.48, 147.72, 159.03, 166.96, 196.59; **ESI-MS (m/z)**: $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{23}\text{H}_{21}\text{N}_3\text{O}_5\text{S}$: 451.5; found 452.4.



9a-hydroxy-3-(4-hydroxyphenyl)-5-(4-nitrophenyl)-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one

Teal green, 58% yield; m.p: 238-240°C; $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 1.92-1.98 (m, 2H), 2.24 (t, 2H), 2.57 (d, $J = 8.4$ Hz, 1H), 2.64 (t, 2H), 4.11 (d, $J = 8.4$ Hz, 1H), 6.55 (d, $J = 8.8$ Hz, 2H), 6.98 (s, 1H), 7.04 (d, $J = 8.8$ Hz, 2H), 7.94 (d, $J = 8.8$ Hz, 2H), 8.21 (d, $J = 8.8$ Hz, 2H), 9.67 (bs, 1H), 12.21 (bs, 1H); $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 21.46, 26.80, 36.60, 42.45, 56.26, 89.31, 114.72, 115.30, 123.50, 128.15, 129.06, 129.47, 144.45, 146.25, 147.41, 157.13, 165.85; **LC-MS (m/z)**: $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{22}\text{H}_{19}\text{N}_3\text{O}_5\text{S}$: 437.4; found 438.1.

4. ^1H NMR spectra of compounds **1a** and **1b**

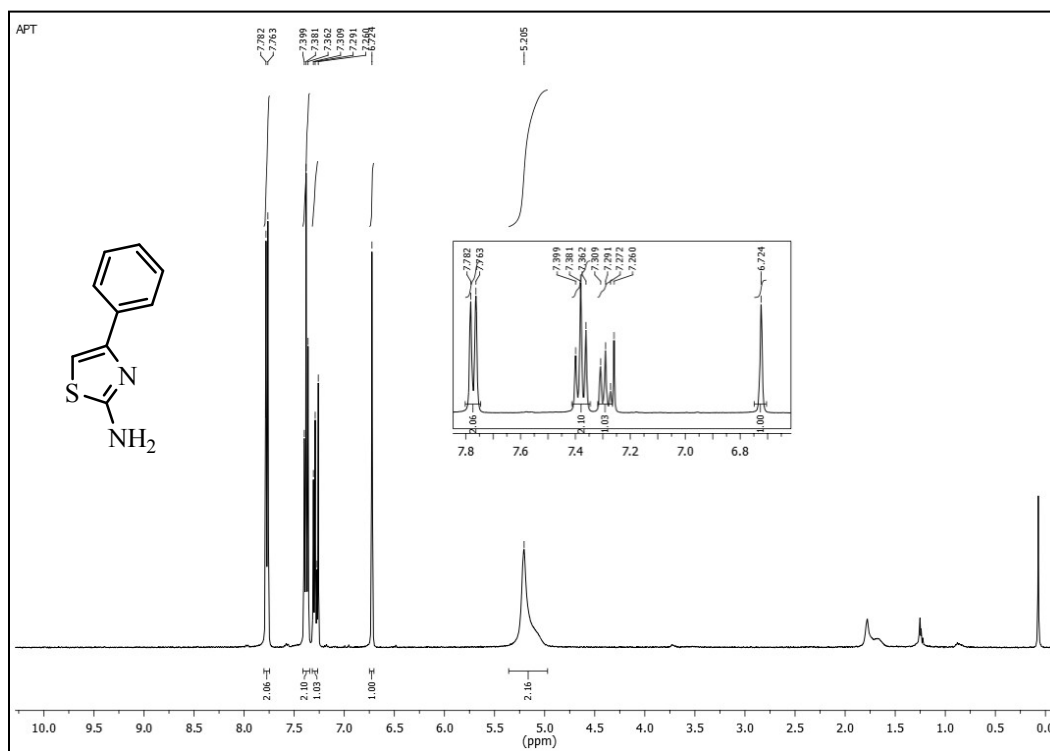


Figure S1. ^1H NMR spectrum of **1a** in CDCl_3

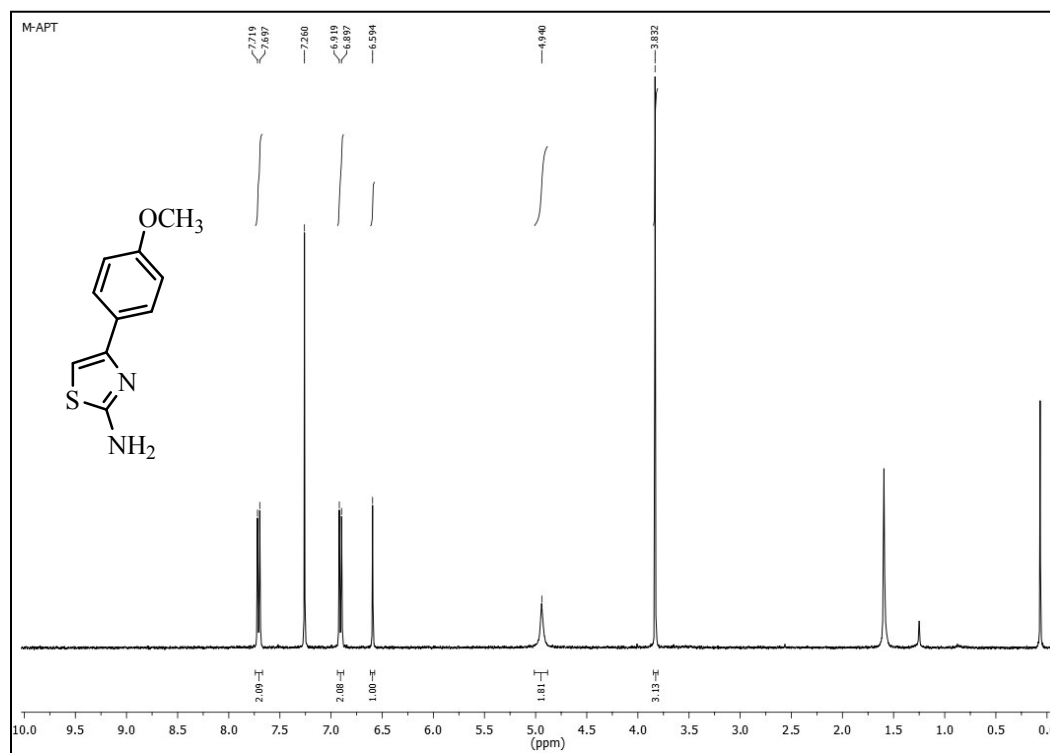
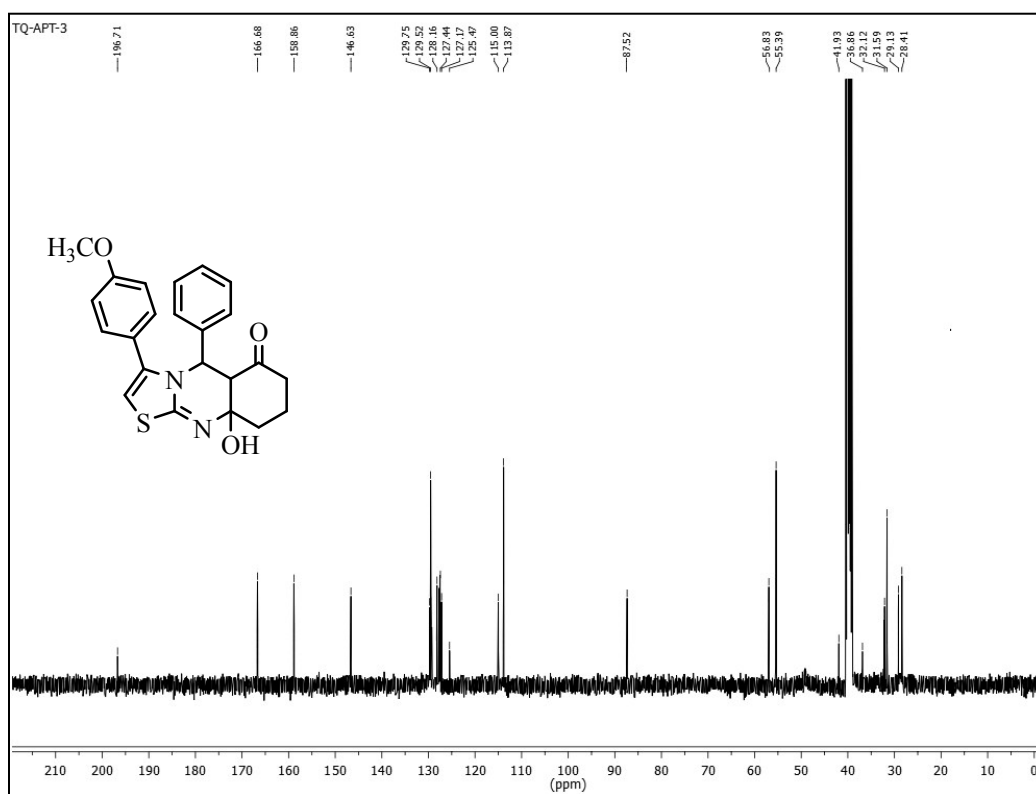
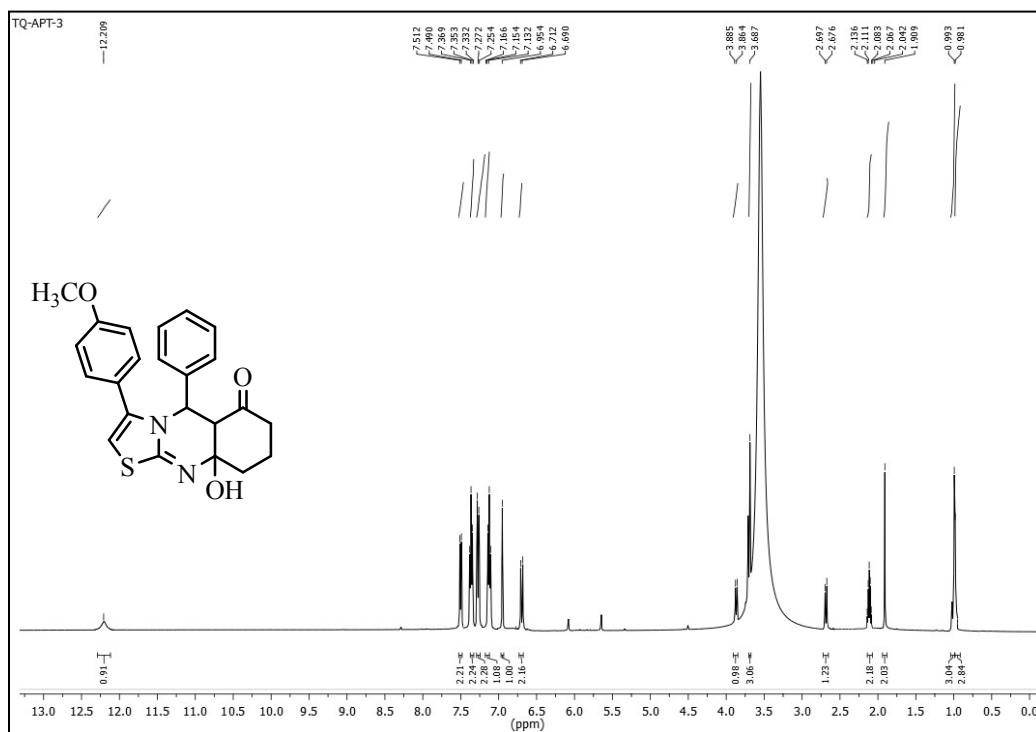


Figure S2. ^1H NMR spectrum of **1b** in CDCl_3

5. ^1H , ^{13}C NMR and mass spectra of compounds 5aa and 5aq



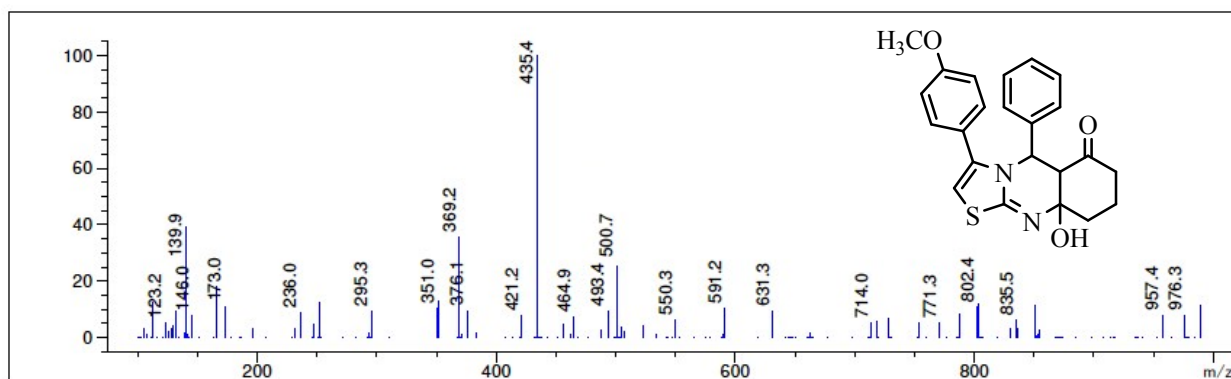


Figure S5. ESI-MS spectrum of 5aa

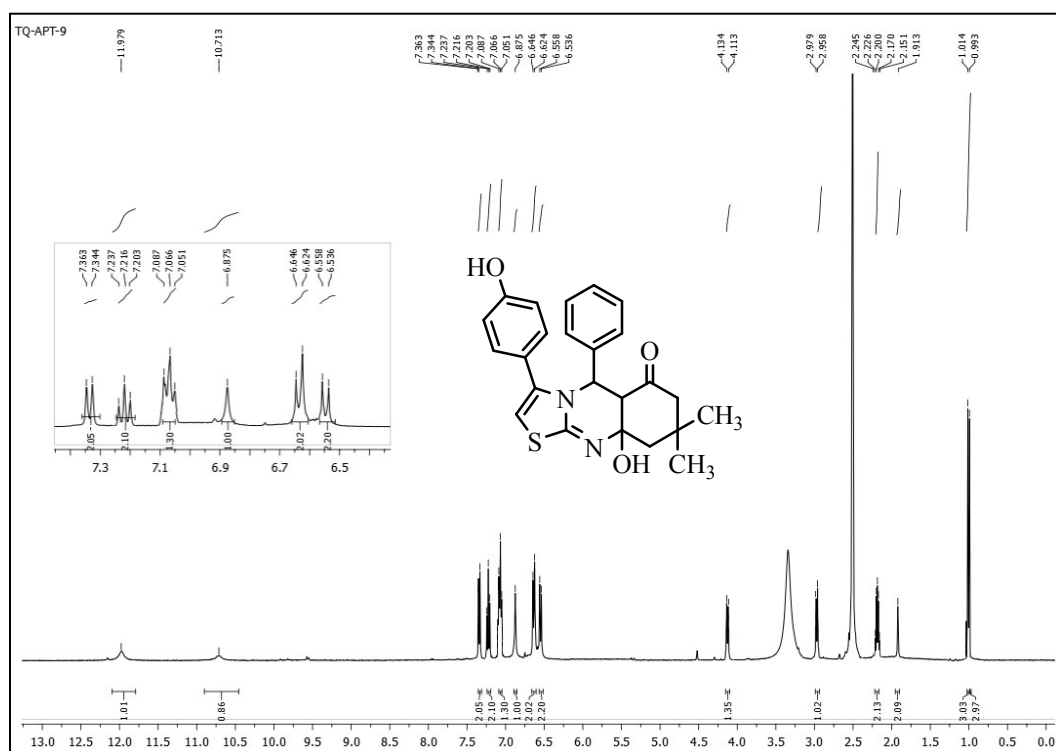


Figure S6. ¹H NMR spectrum of 5ab in DMSO-d₆

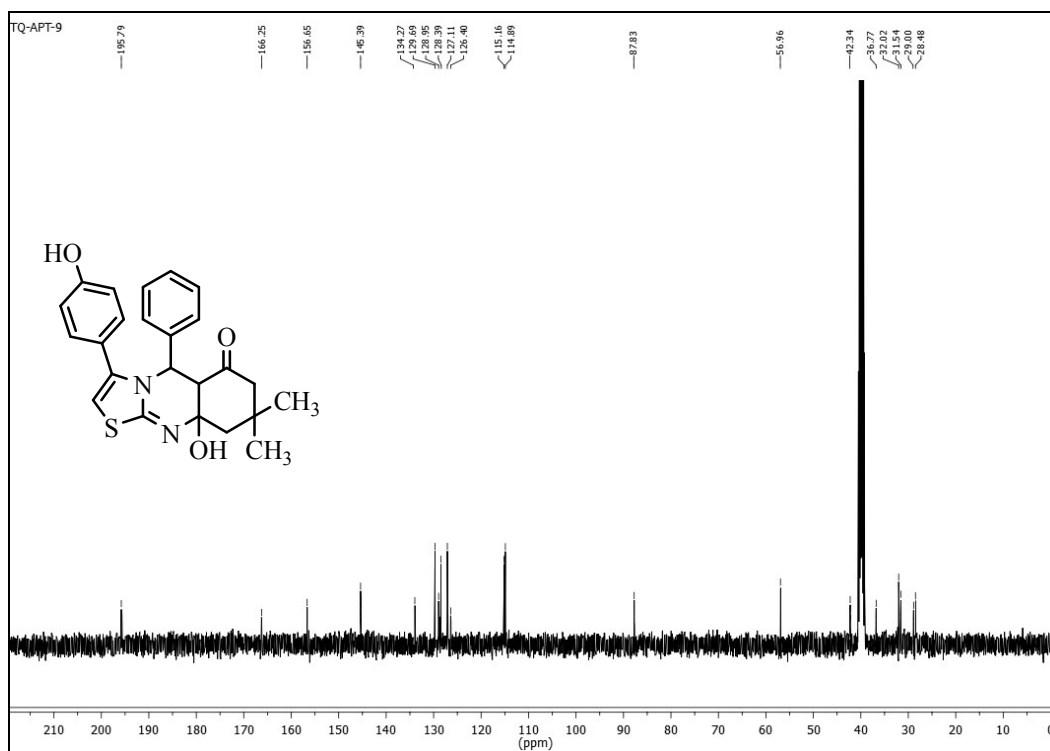


Figure S7. ¹³C NMR spectrum of **5ab** in DMSO-d₆

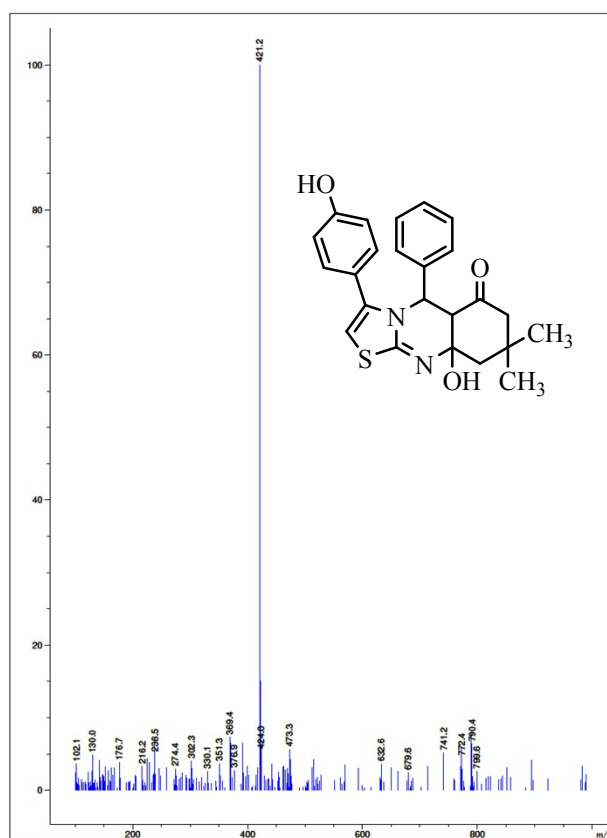


Figure S8. ESI-MS spectrum of **5ab**

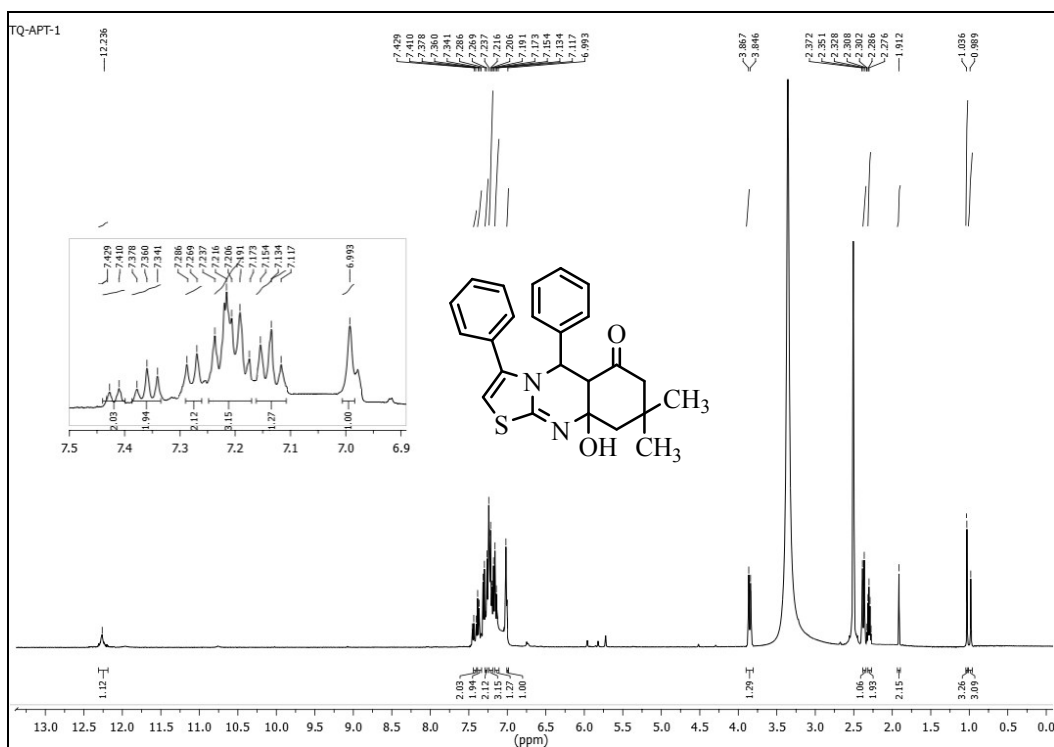


Figure S9. ^1H NMR spectrum of 5ac in DMSO-d_6

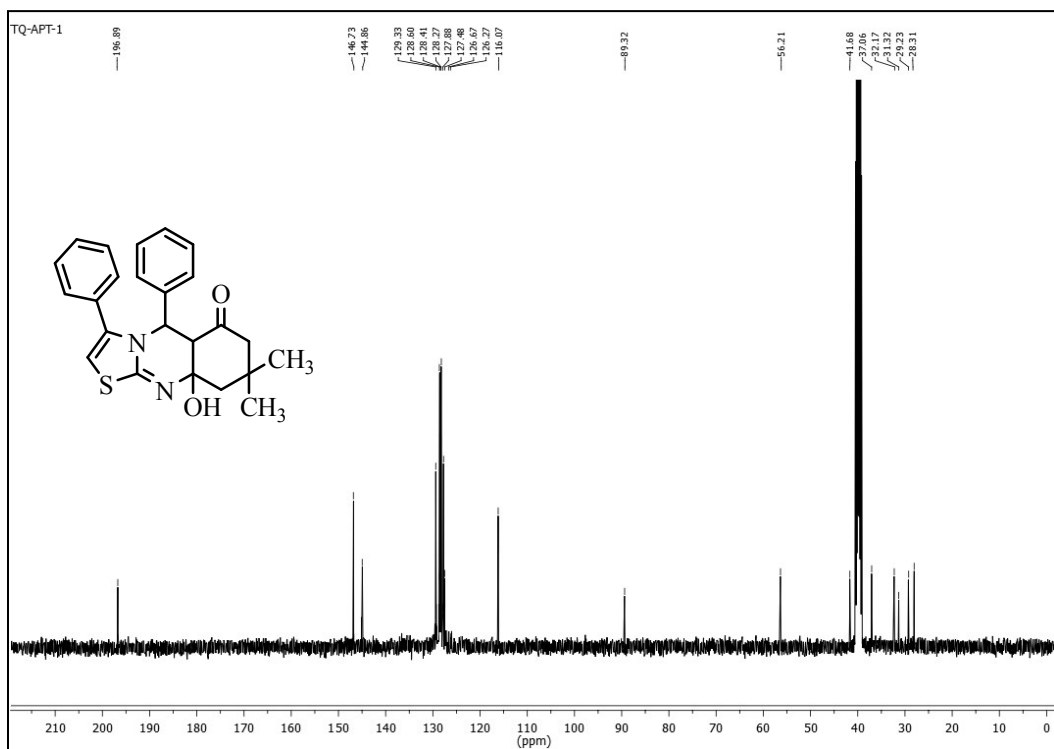


Figure S10. ^{13}C NMR spectrum of 5ac in DMSO-d_6

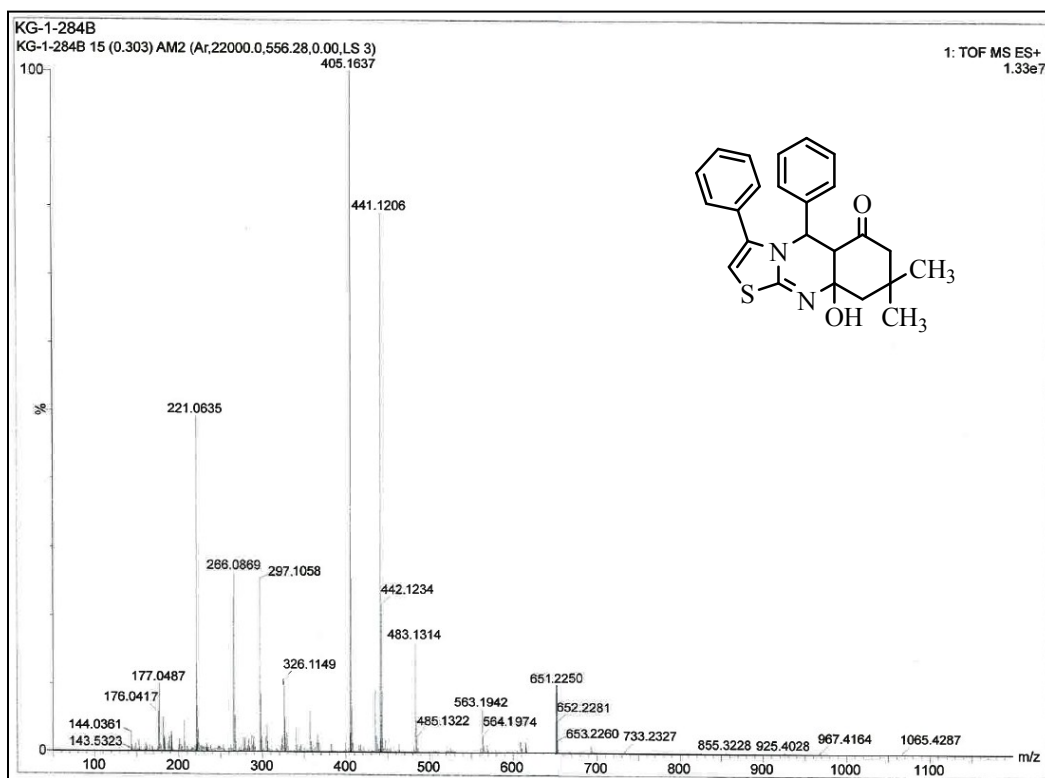


Figure S11. HRMS spectrum of 5ac

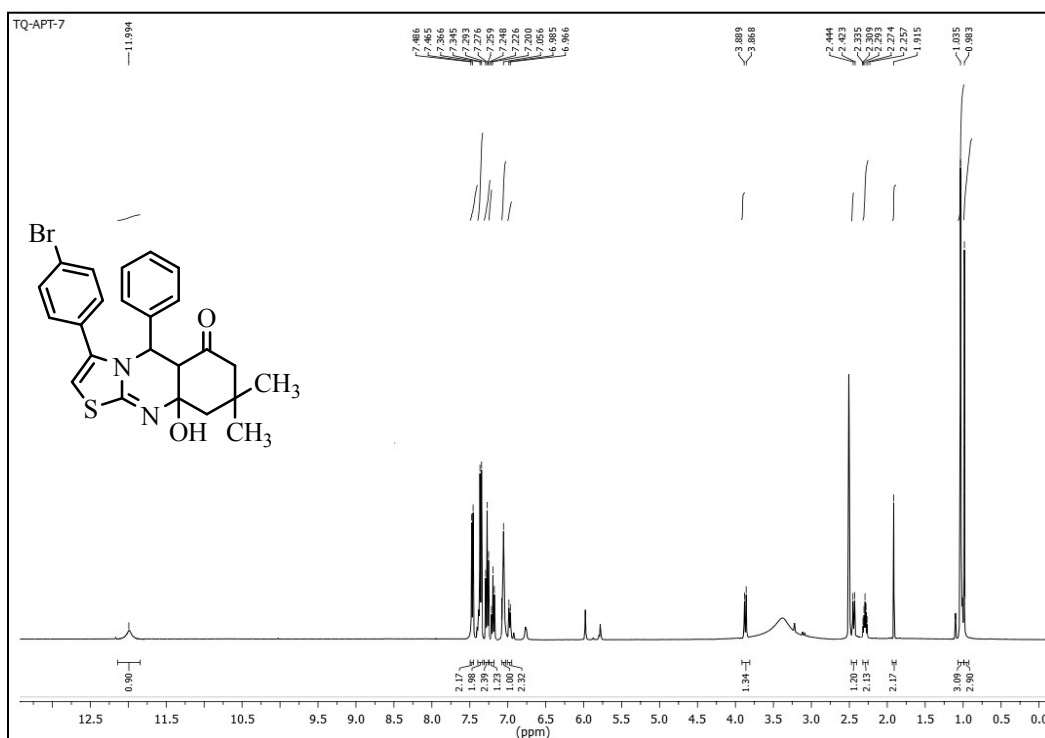


Figure S12. ¹H NMR spectrum of 5ad in DMSO-d₆

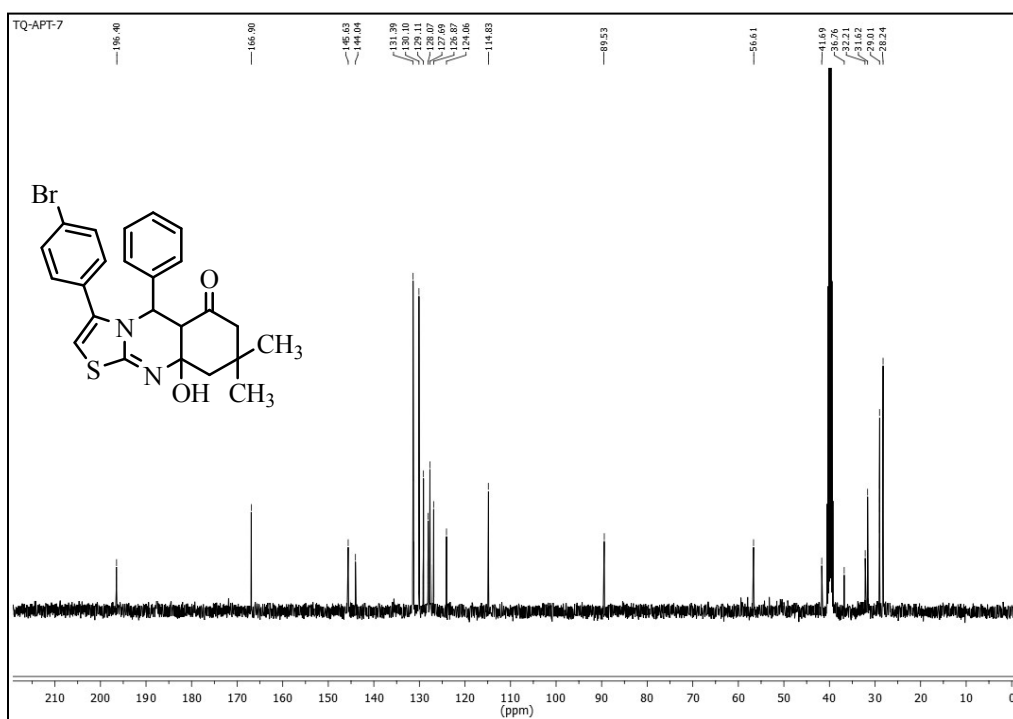


Figure S13. ¹³C NMR spectrum of 5ad in DMSO-d₆

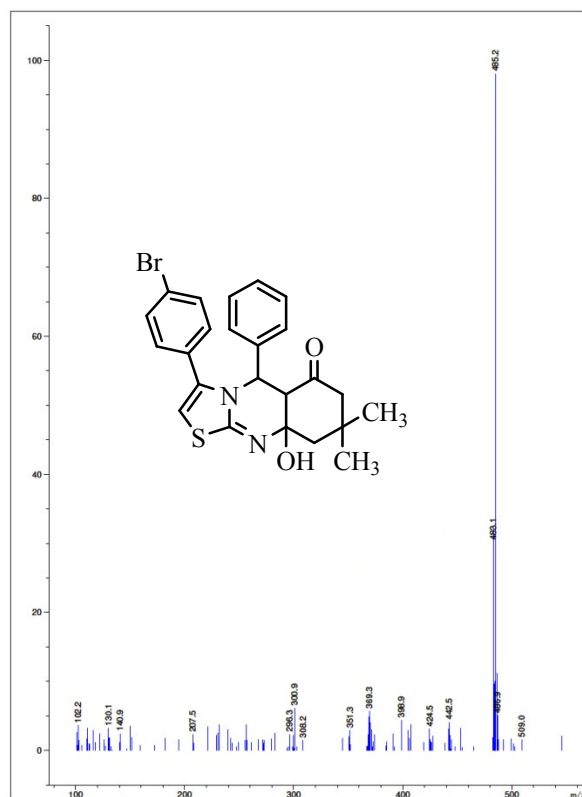


Figure S14. ESI-MS spectrum of 5ad

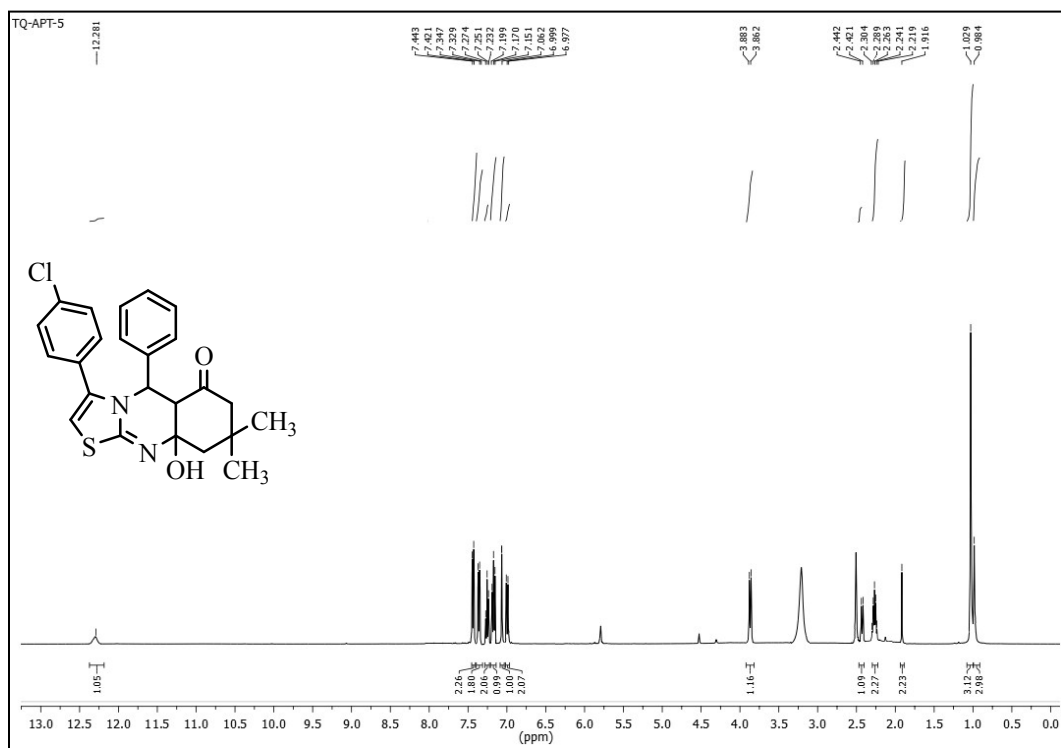


Figure S15. ^1H NMR spectrum of 5ae in DMSO-d_6

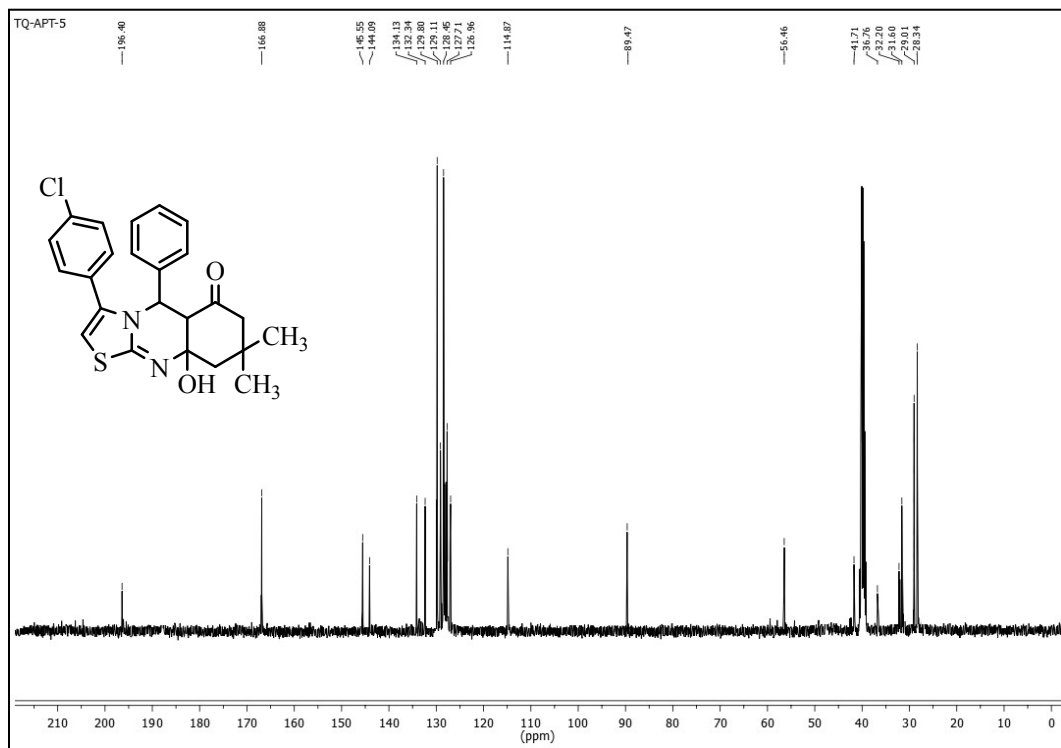


Figure S16. ^{13}C NMR spectrum of 5ae in DMSO-d_6

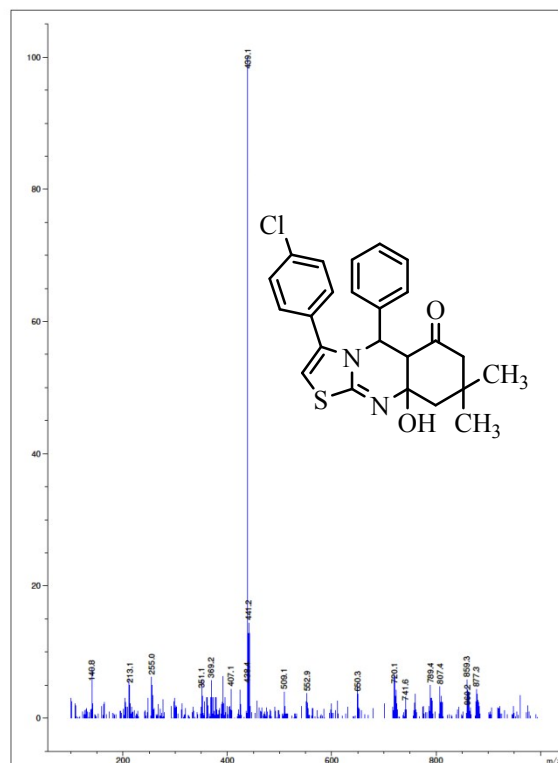


Figure S17. ESI-MS spectrum of 5ae

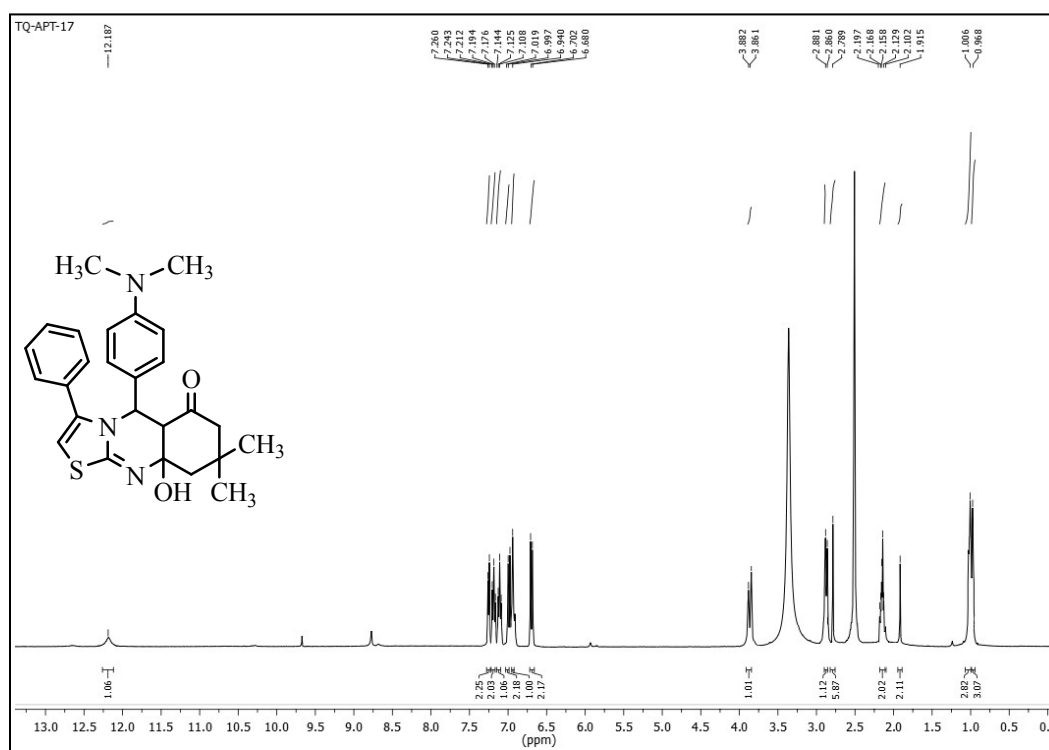


Figure S18. ^1H NMR spectrum of 5af in DMSO-d_6

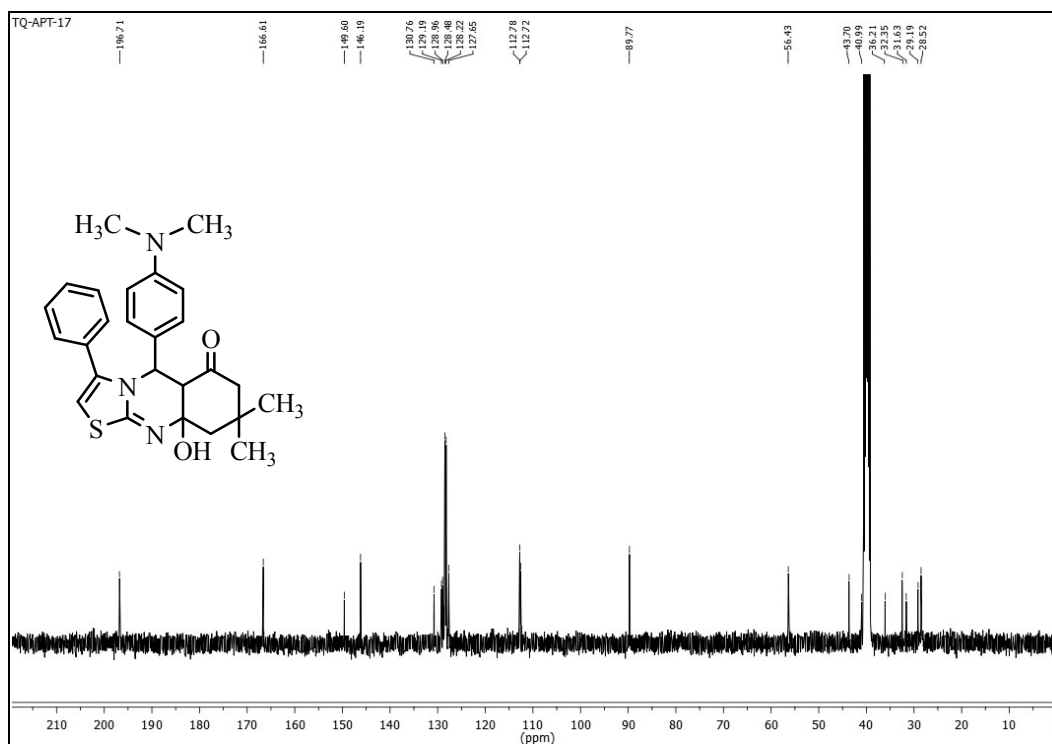


Figure S19. ^{13}C NMR spectrum of **5af** in DMSO-d_6

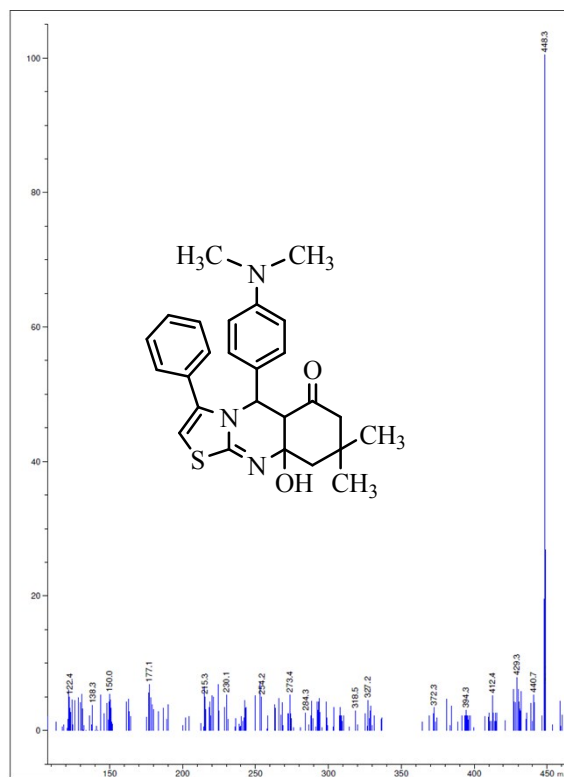


Figure S20. ESI-MS spectrum of **5af**

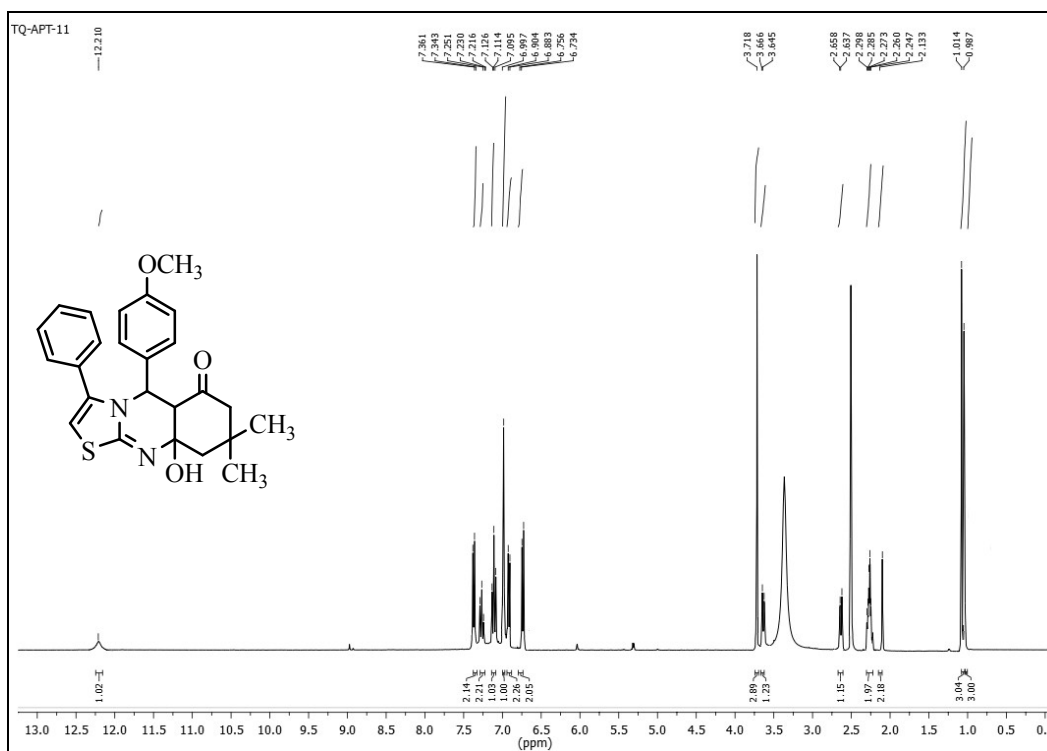


Figure S21. ^1H NMR spectrum of 5ag in DMSO-d_6

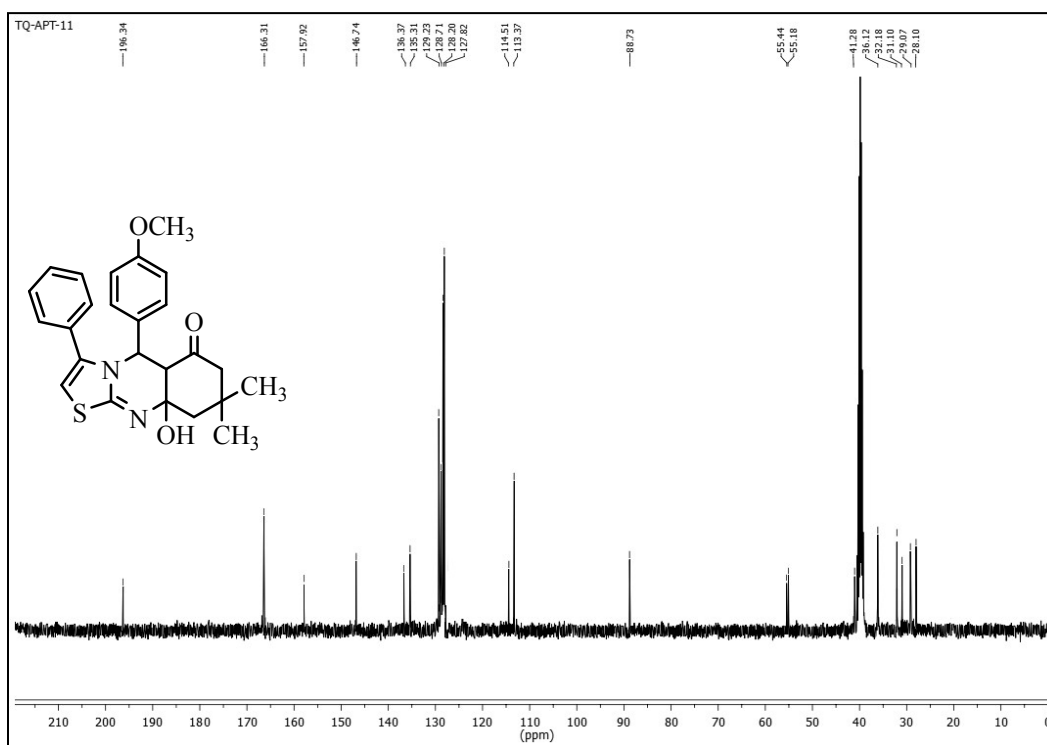


Figure S22. ^{13}C NMR spectrum of 5ag in DMSO-d_6

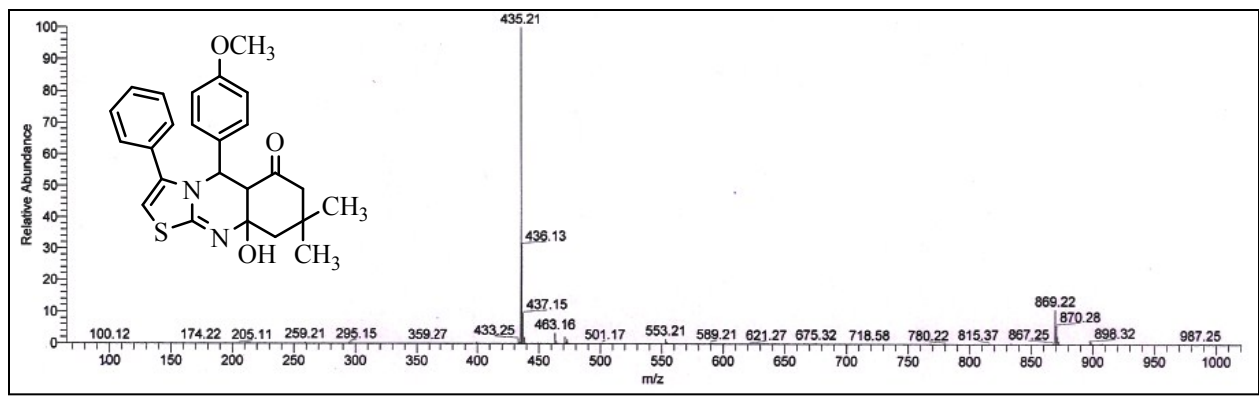


Figure S23. ESI-MS spectrum of 5ag

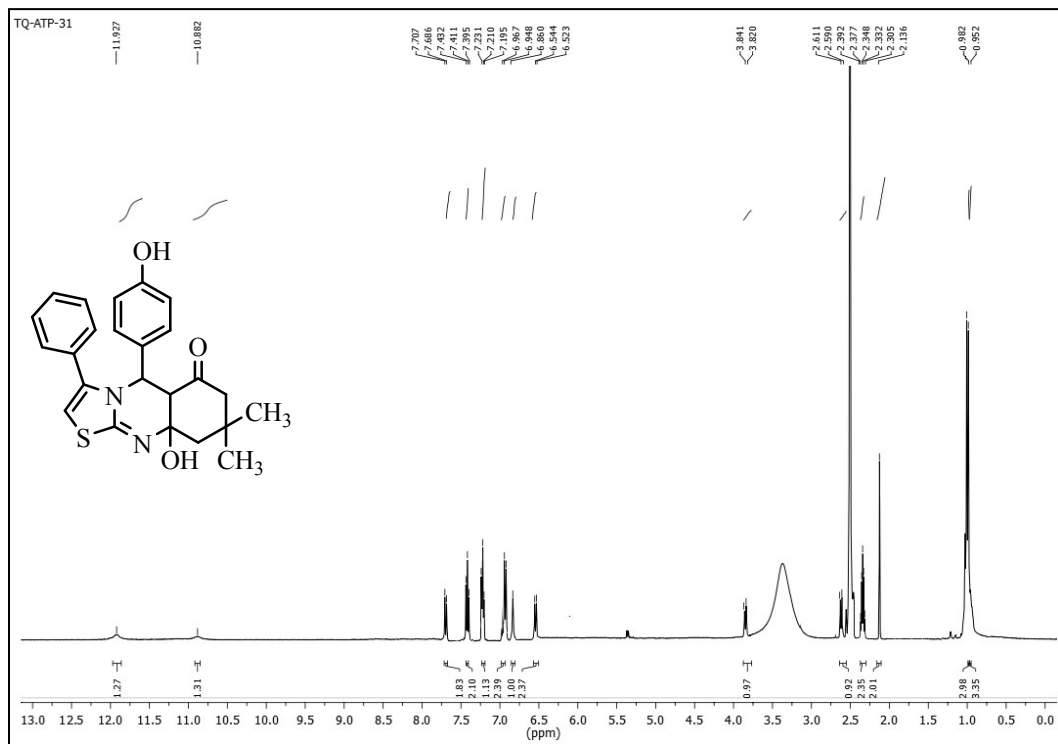


Figure S24. ¹H NMR spectrum of 5ah in DMSO-d₆

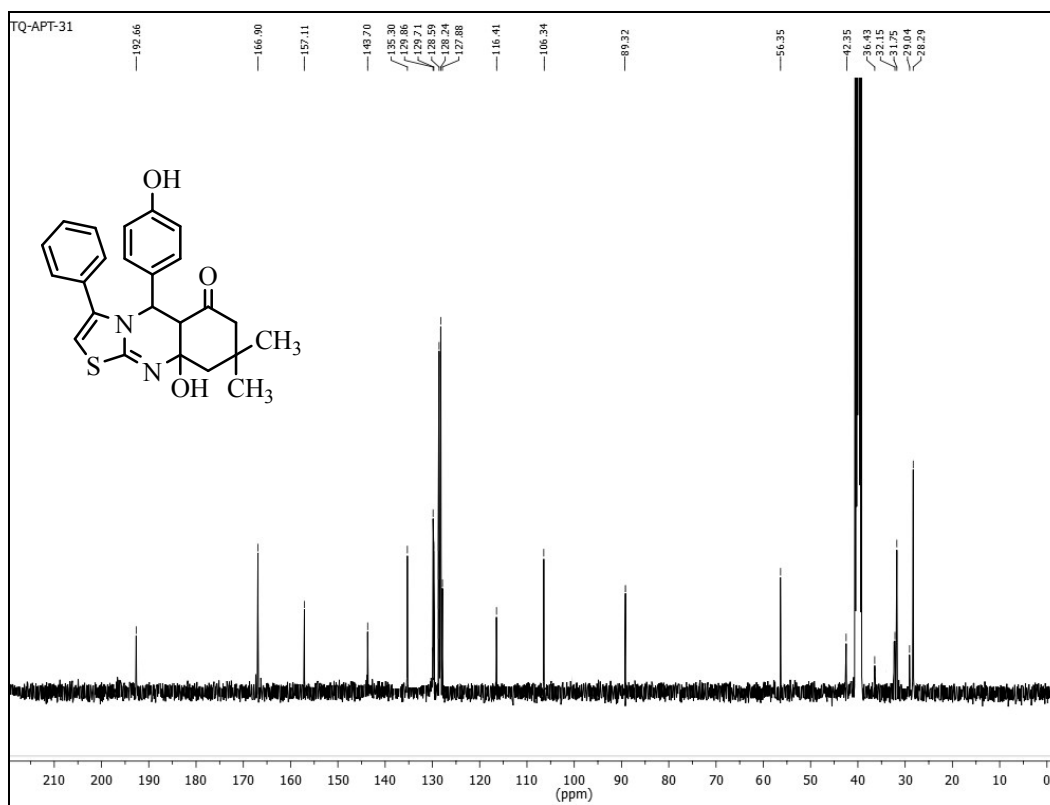


Figure S25. ^{13}C NMR spectrum of 5ah in DMSO-d_6

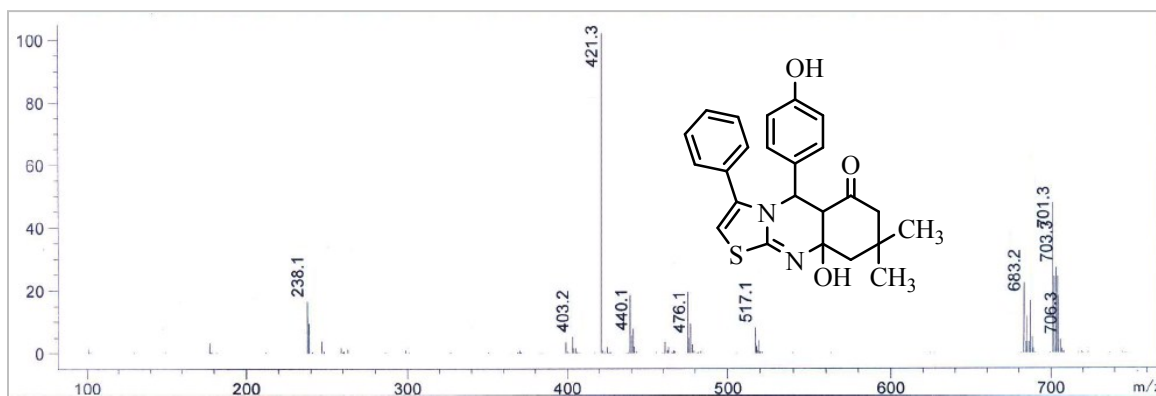


Figure S26. LC-MS spectrum of 5ah

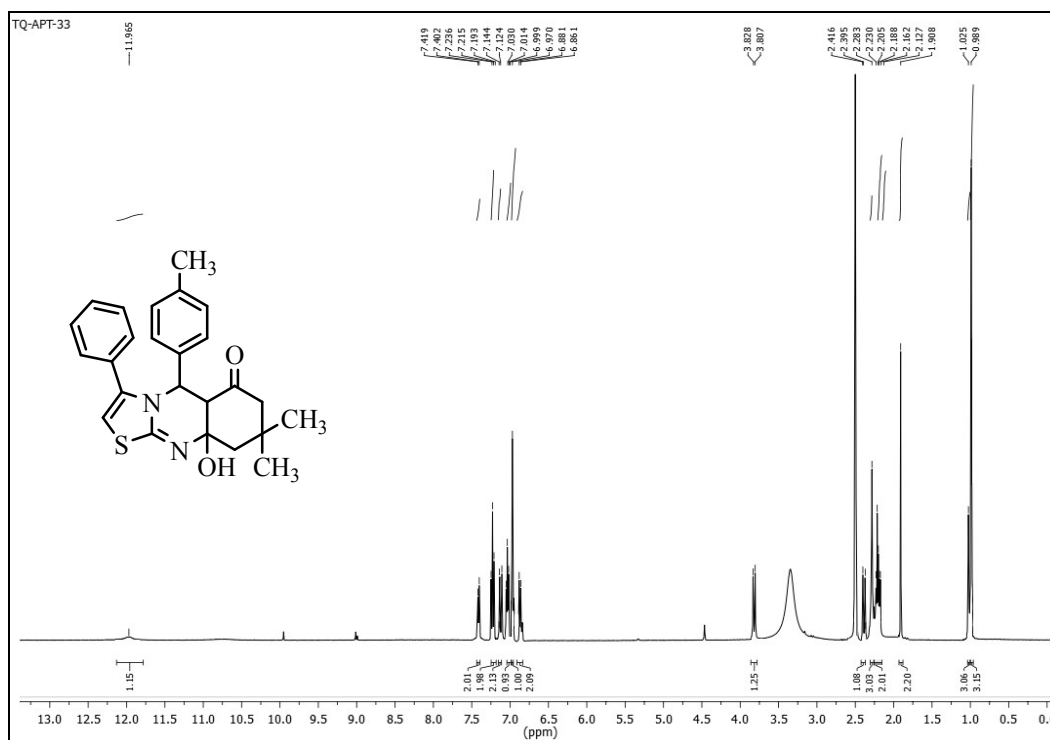


Figure S27. ^1H NMR spectrum of 5ai in DMSO-d_6

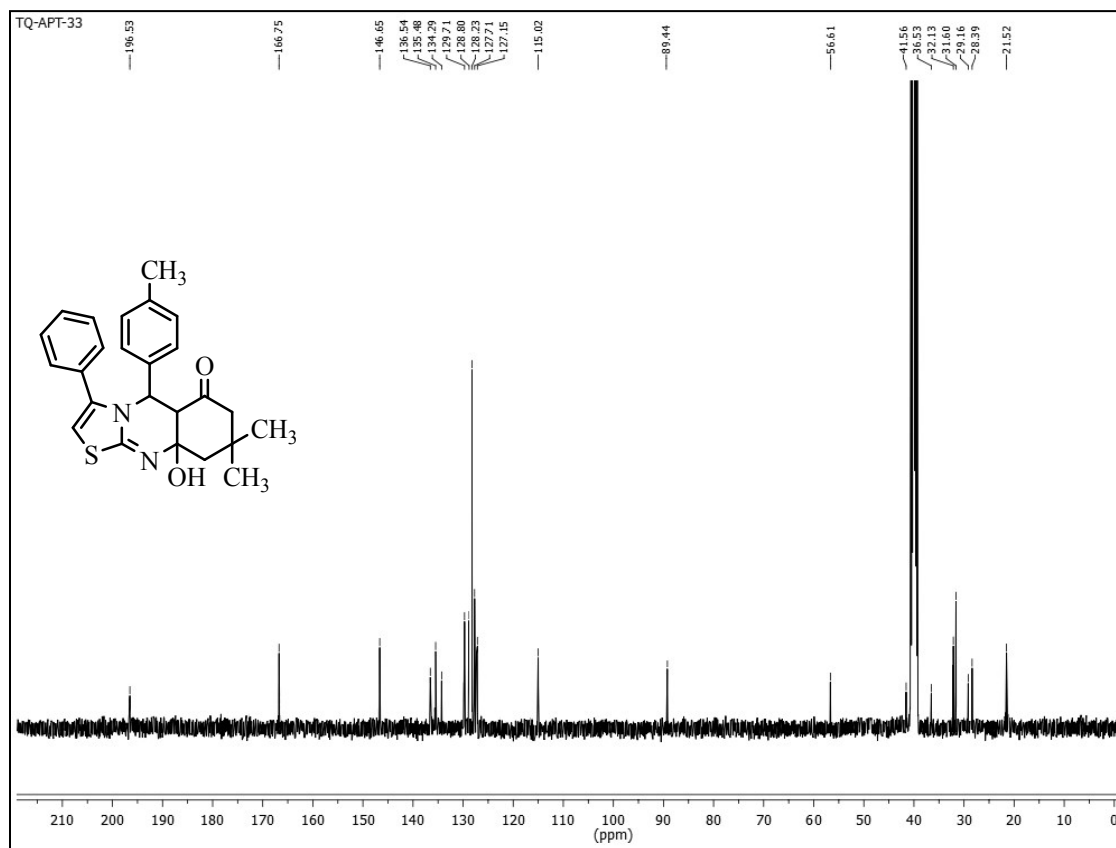


Figure S28. ^{13}C NMR spectrum of 5ai in DMSO-d_6

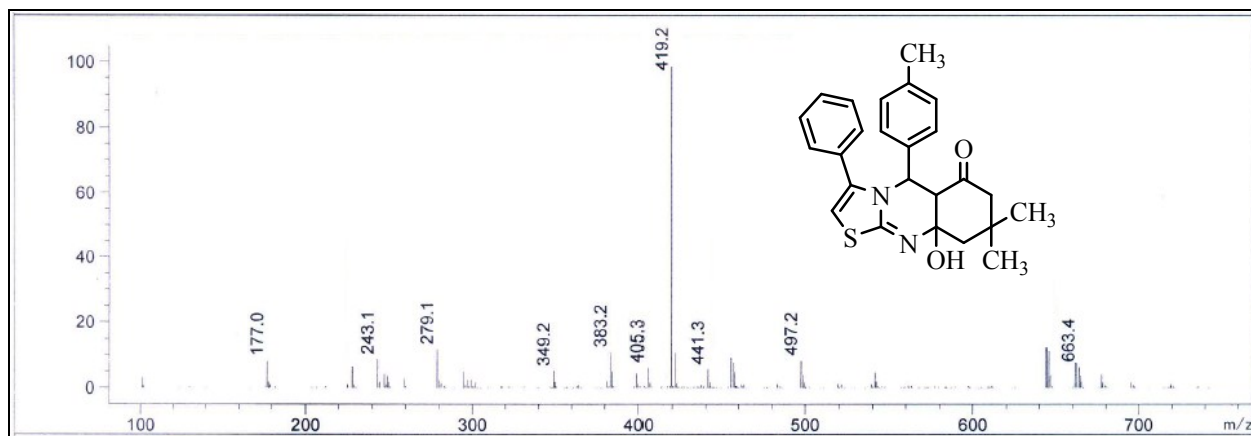


Figure S29. LC-MS spectrum of 5ai

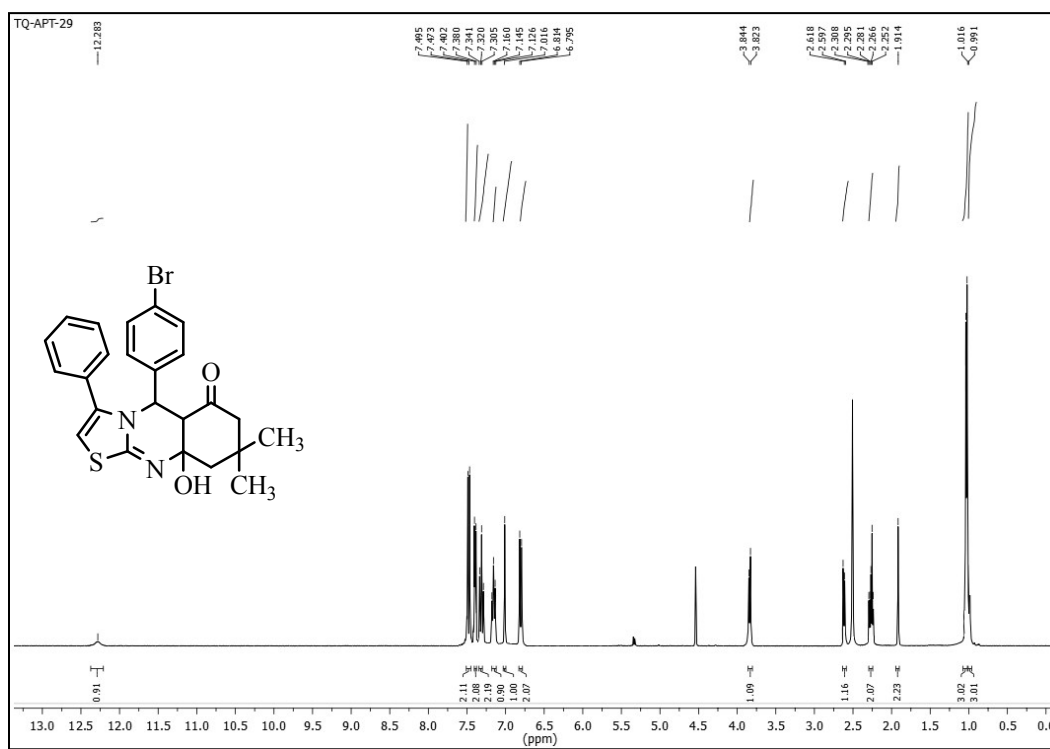


Figure S30. ¹H NMR spectrum of 5aj in DMSO-d₆

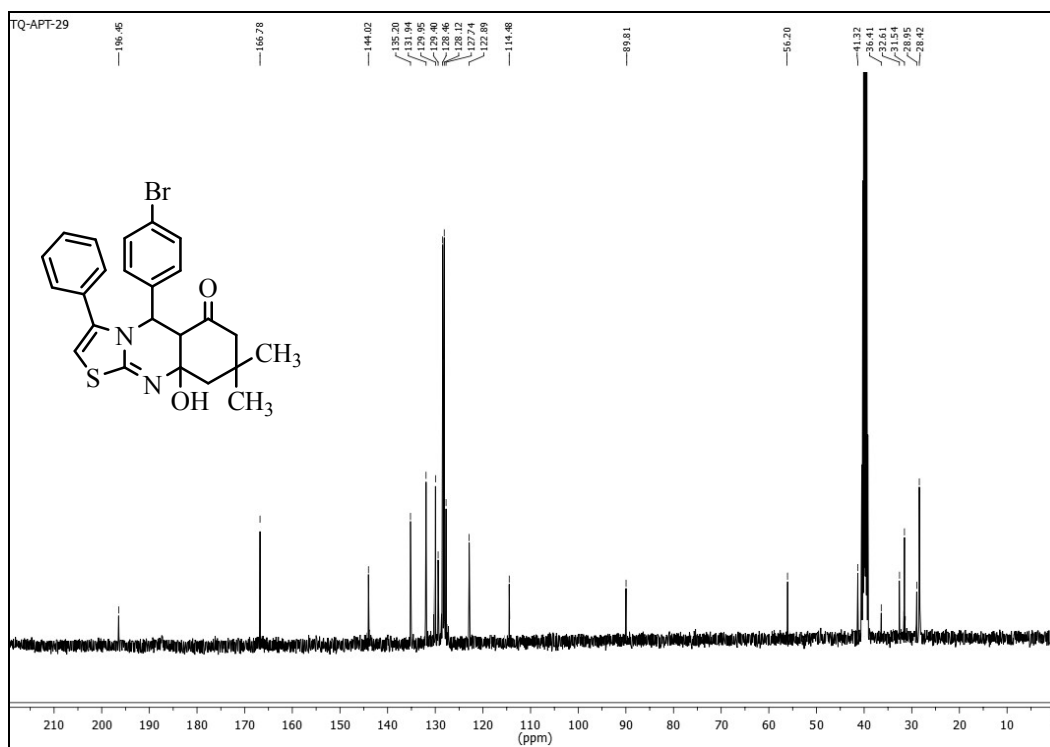


Figure S31. ^{13}C NMR spectrum of 5aj in DMSO-d_6

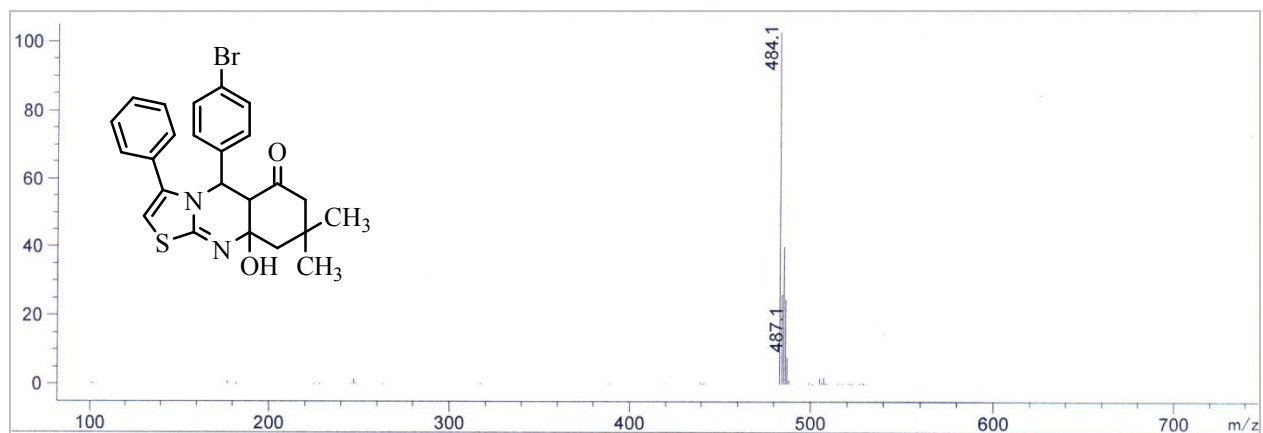


Figure S32. LC-MS spectrum of 5aj

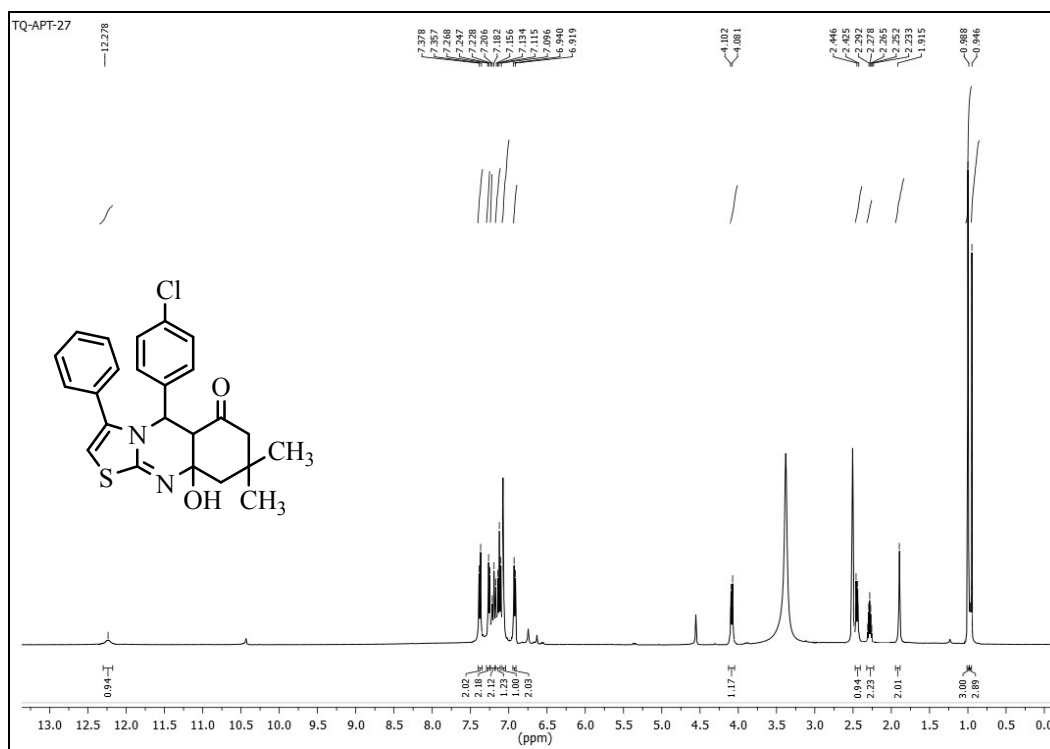


Figure S33. ^1H NMR spectrum of 5ak in DMSO-d_6

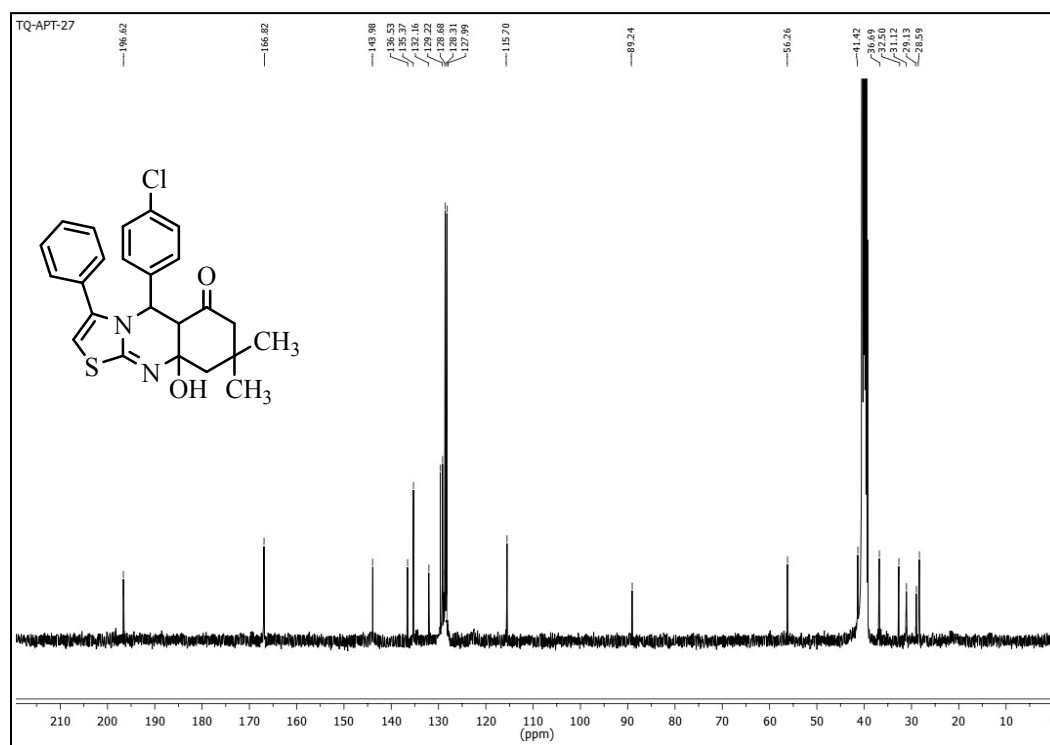


Figure S34. ^{13}C NMR spectrum of 5ak in DMSO-d_6

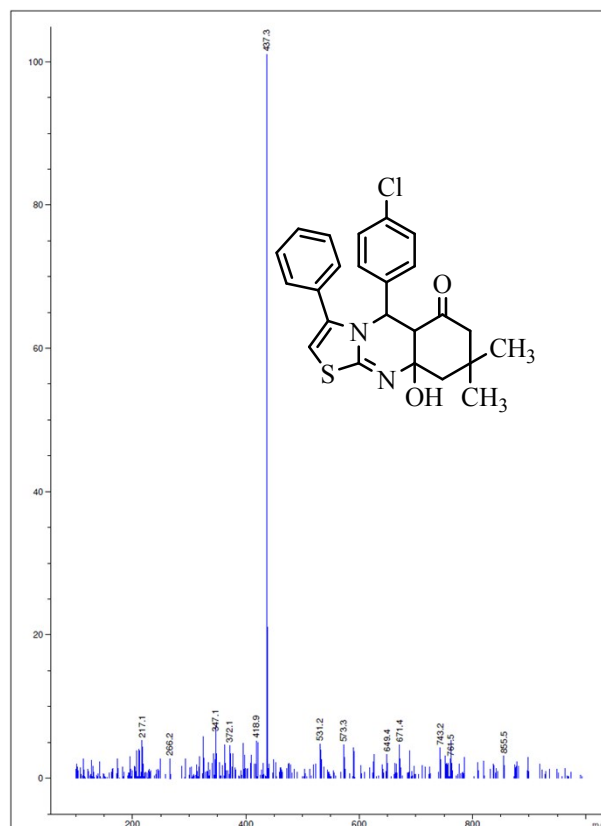


Figure S35. ESI-MS spectrum of 5ak

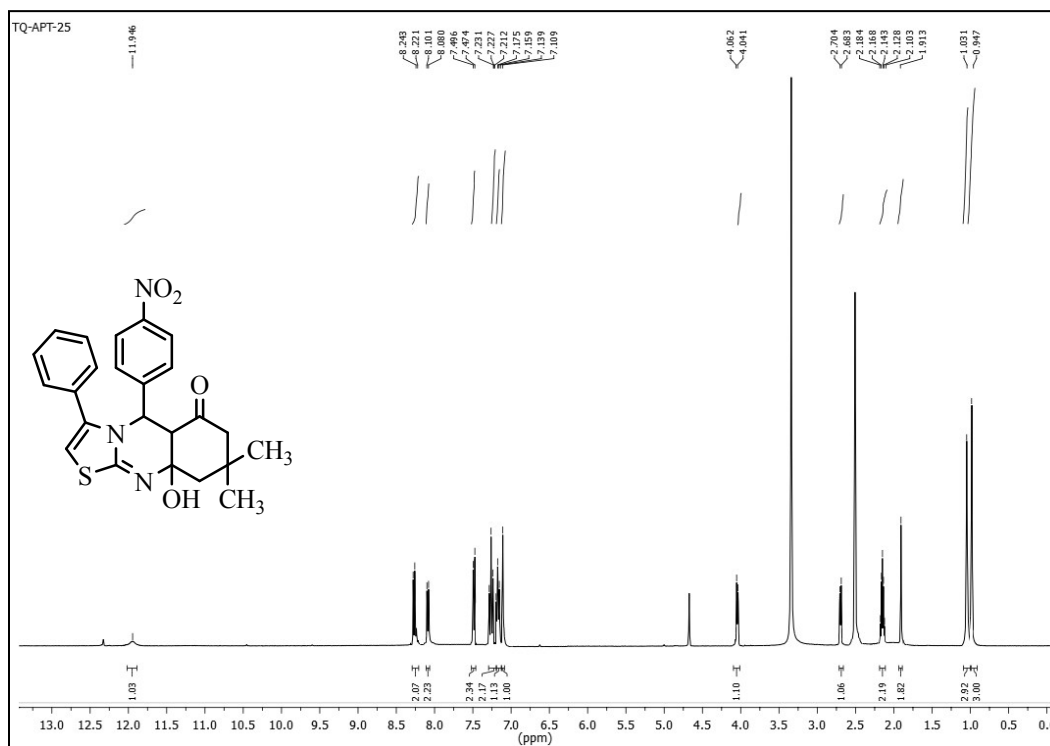


Figure S36. ¹H NMR spectrum of 5al in DMSO-d₆

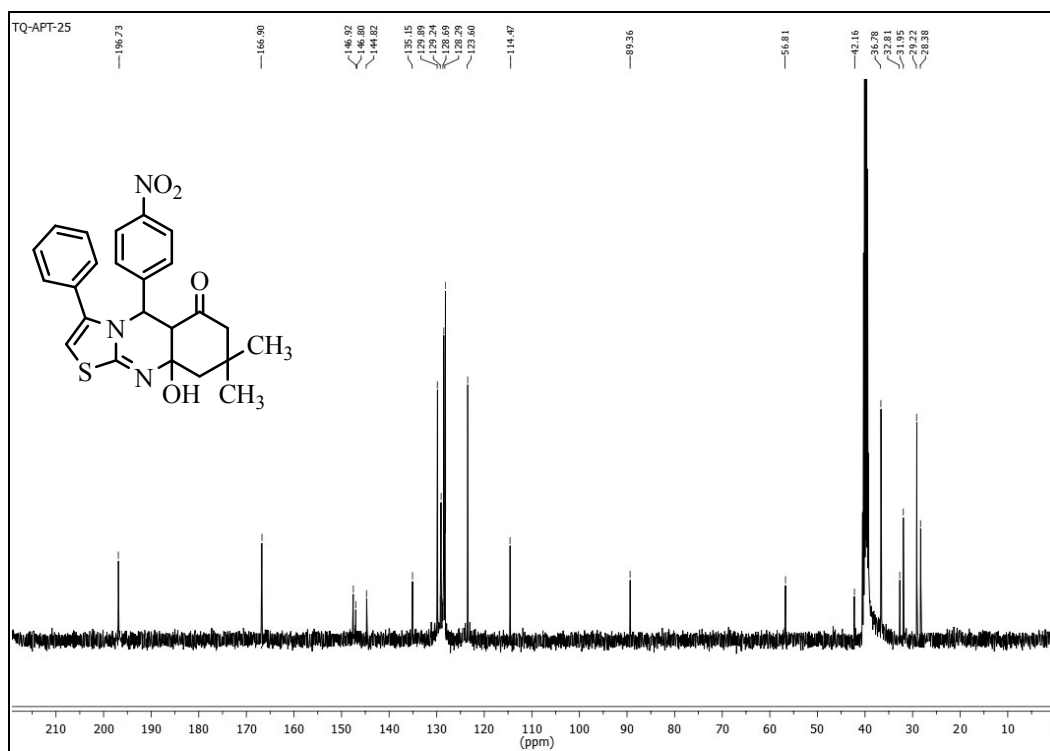


Figure S37. ^{13}C NMR spectrum of **5al** in DMSO-d_6

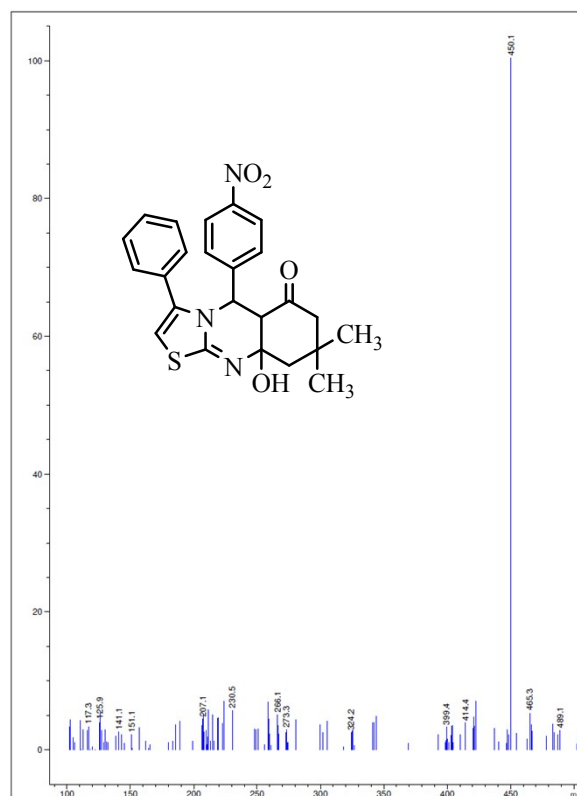


Figure S38. ESI-MS spectrum of **5al**

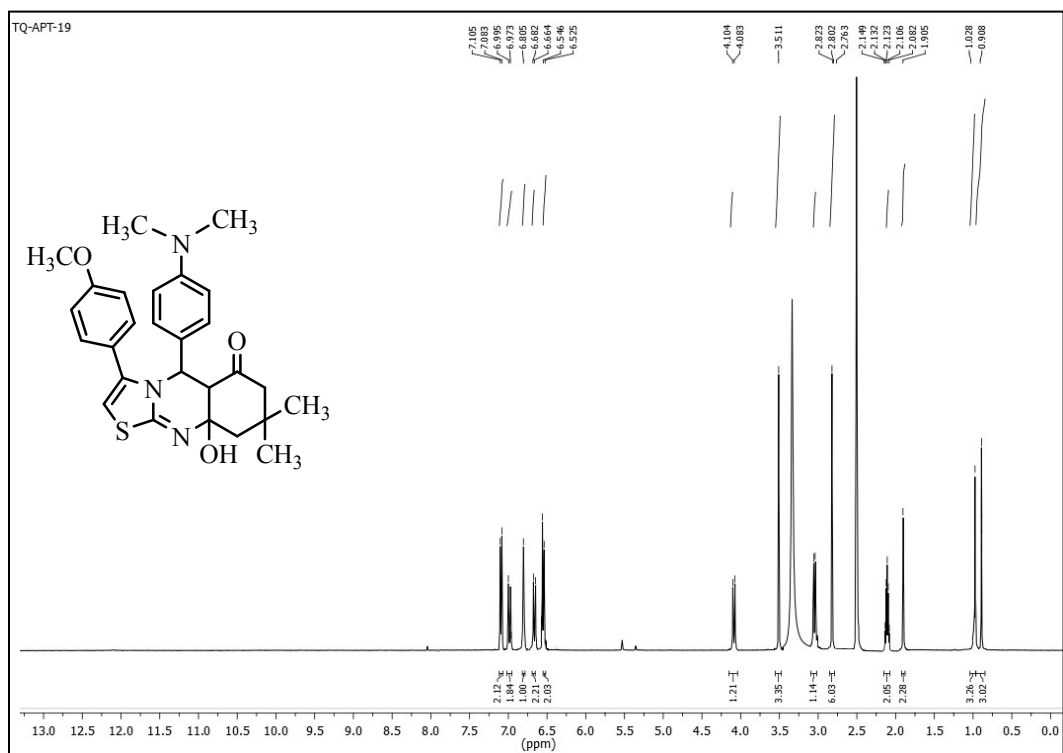


Figure S39. ^1H NMR spectrum of **5am** in DMSO-d_6

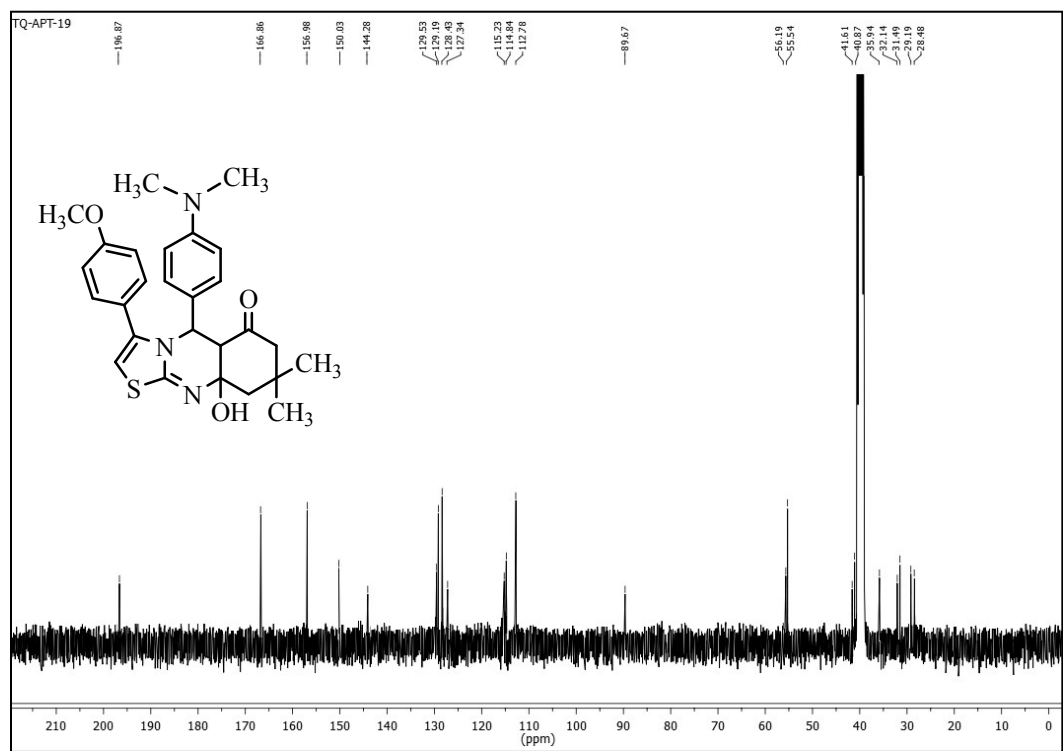


Figure S40. ^{13}C NMR spectrum of **5am** in DMSO-d_6

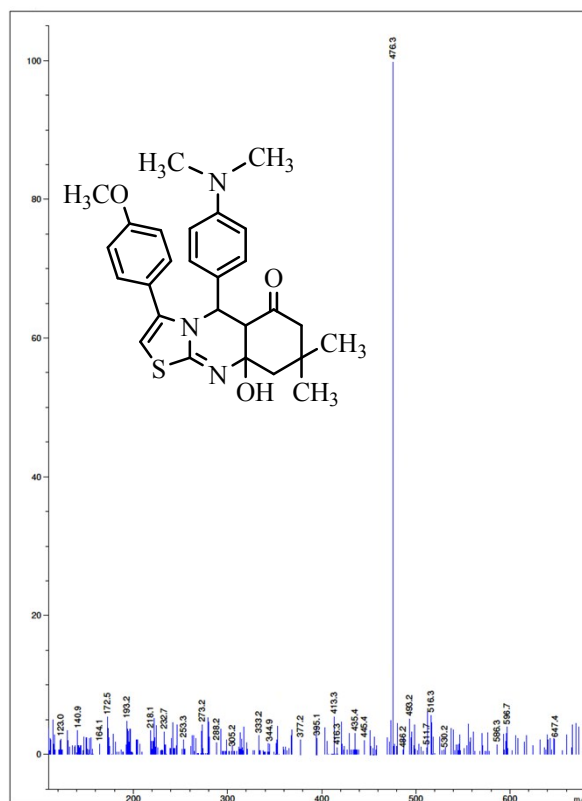


Figure S41. ESI-MS spectrum of 5am

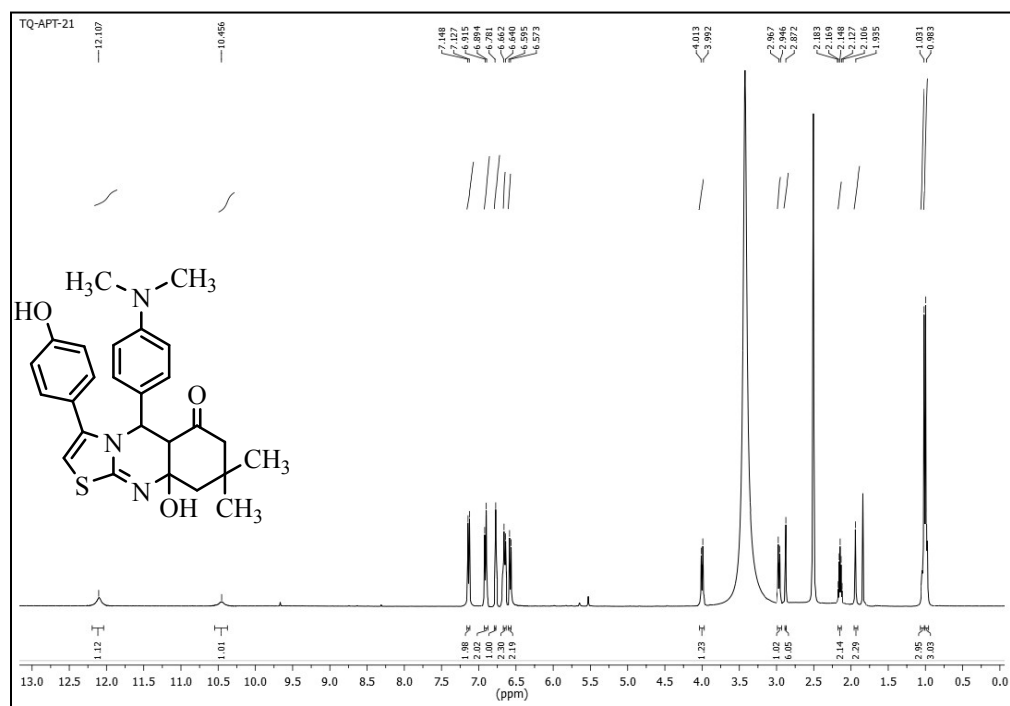


Figure S42. ¹H NMR spectrum of 5am in DMSO-d₆

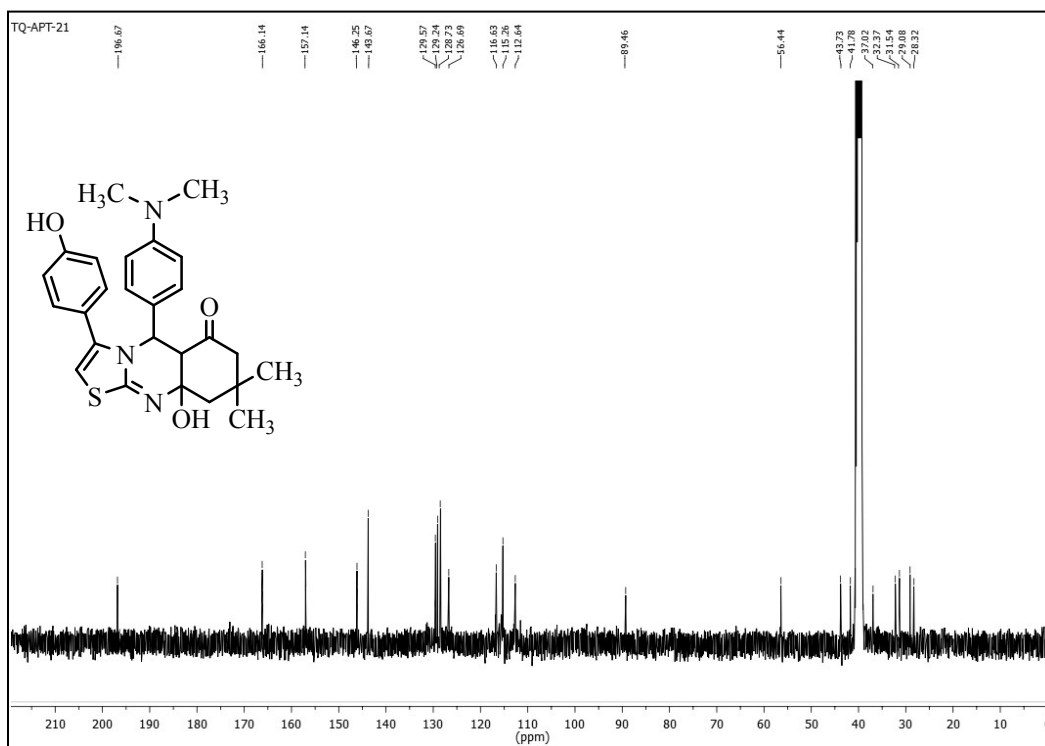


Figure S43. ^{13}C NMR spectrum of 5an in DMSO-d_6

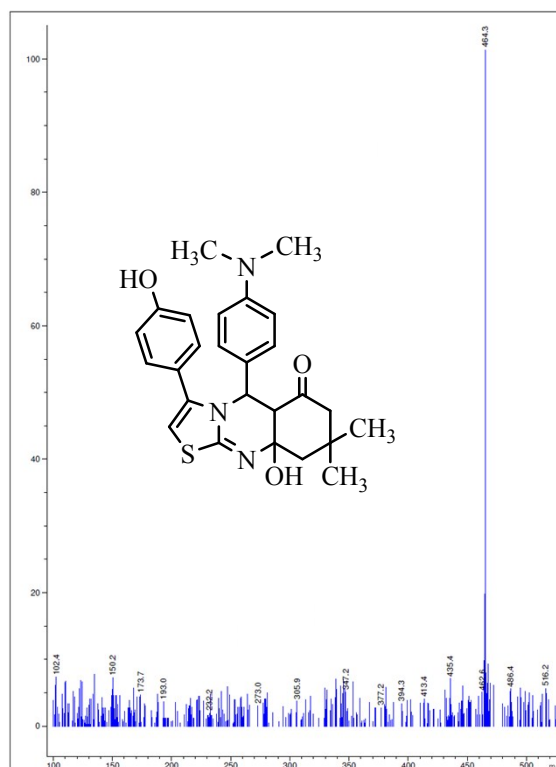


Figure S44. ESI-MS spectrum of 5an

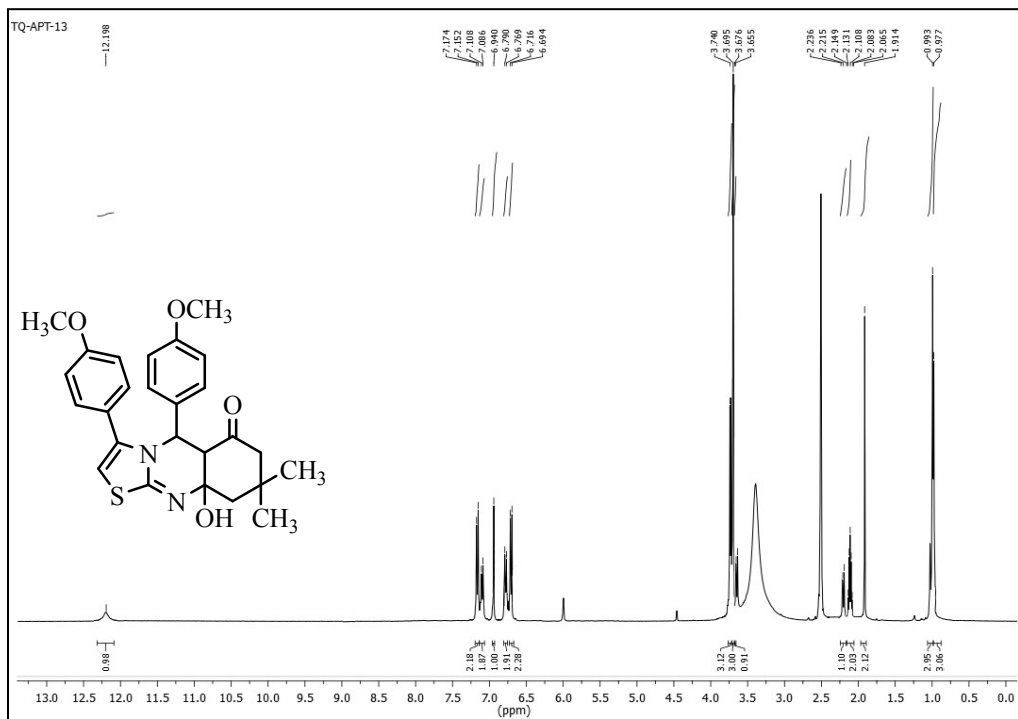


Figure S45. ^1H NMR spectrum of **5ao** in DMSO-d_6

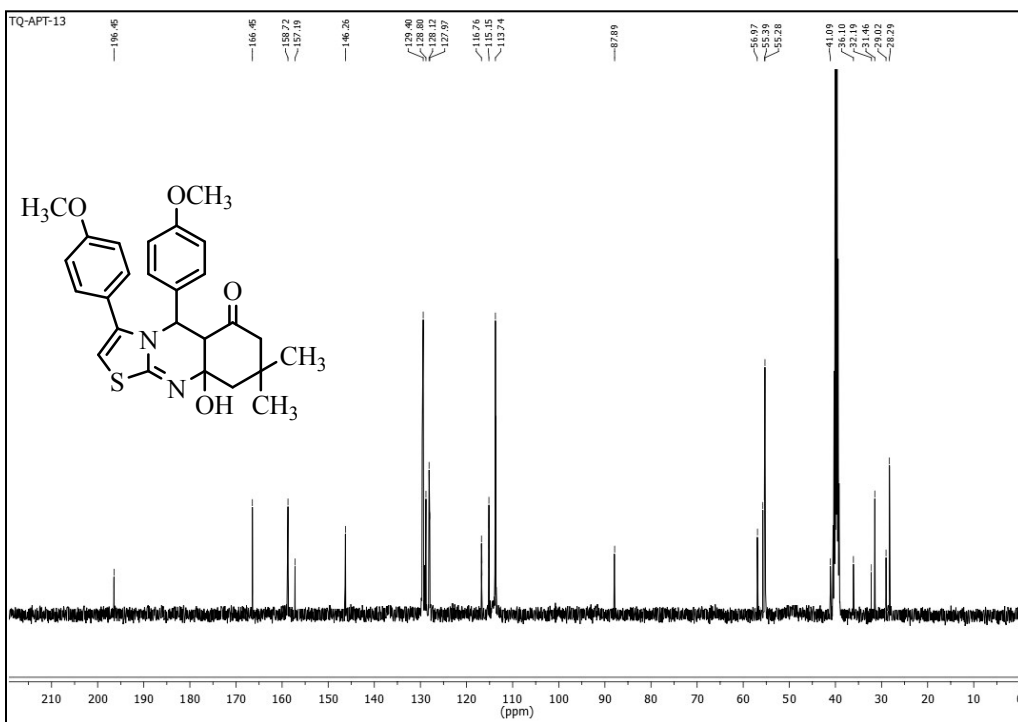


Figure S46. ^{13}C NMR spectrum of **5ao** in DMSO-d_6

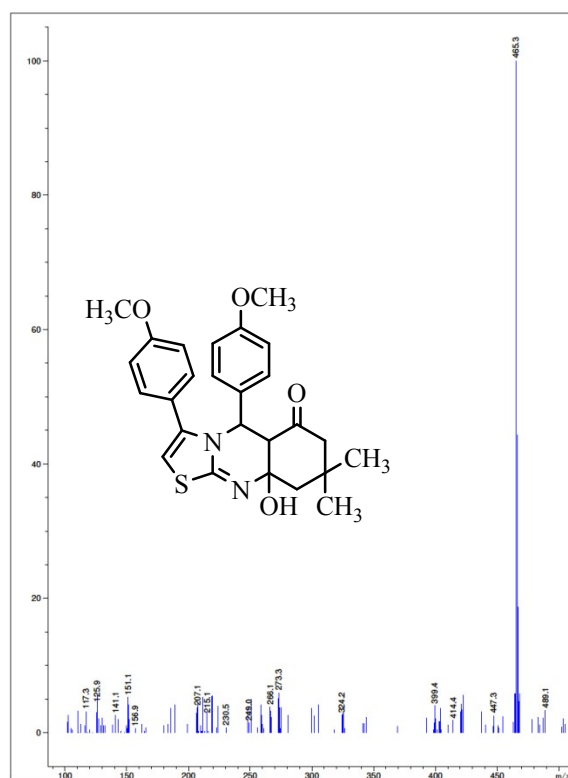


Figure S47. ESI-MS spectrum of 5ao

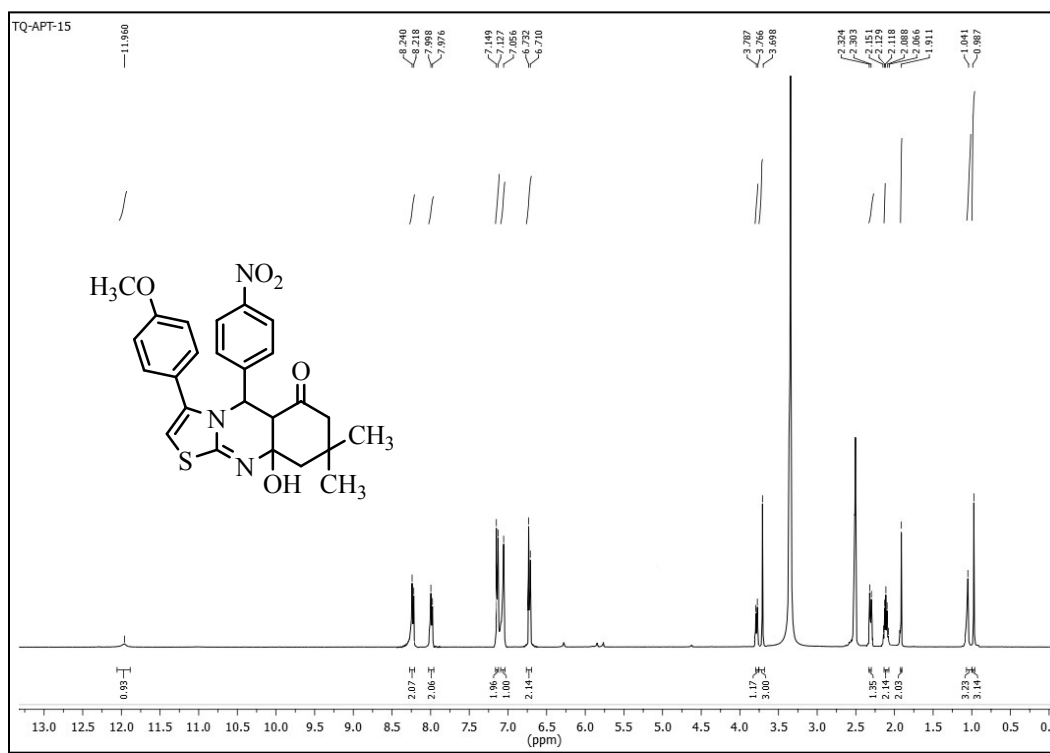


Figure S48. ¹H NMR spectrum of 5ap in DMSO-d₆

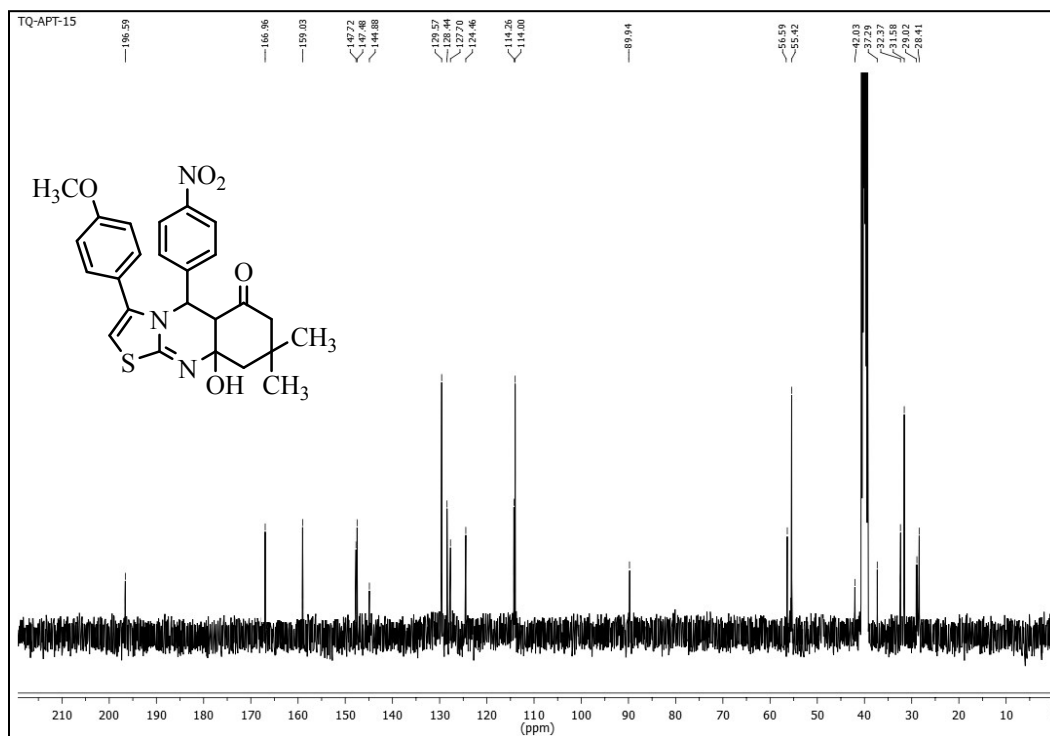


Figure S49. ^{13}C NMR spectrum of **5ap** in DMSO-d_6

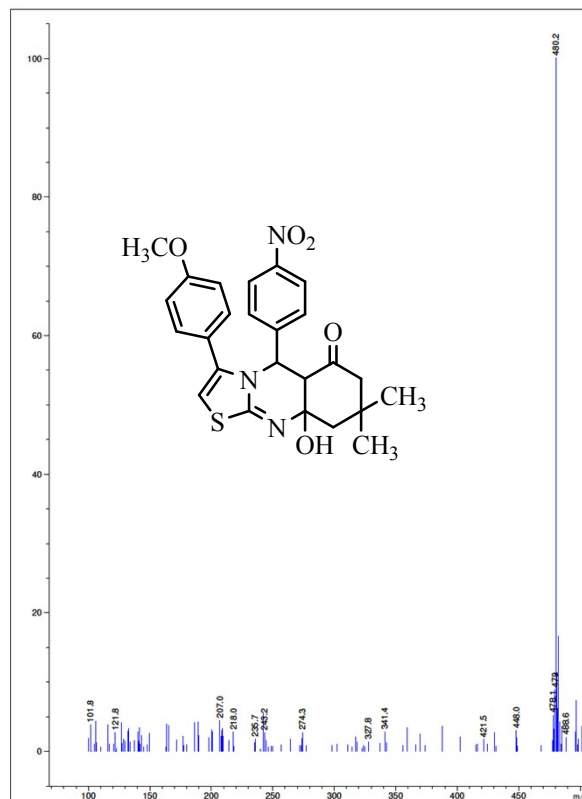


Figure S50. ESI-MS spectrum of **5ap**

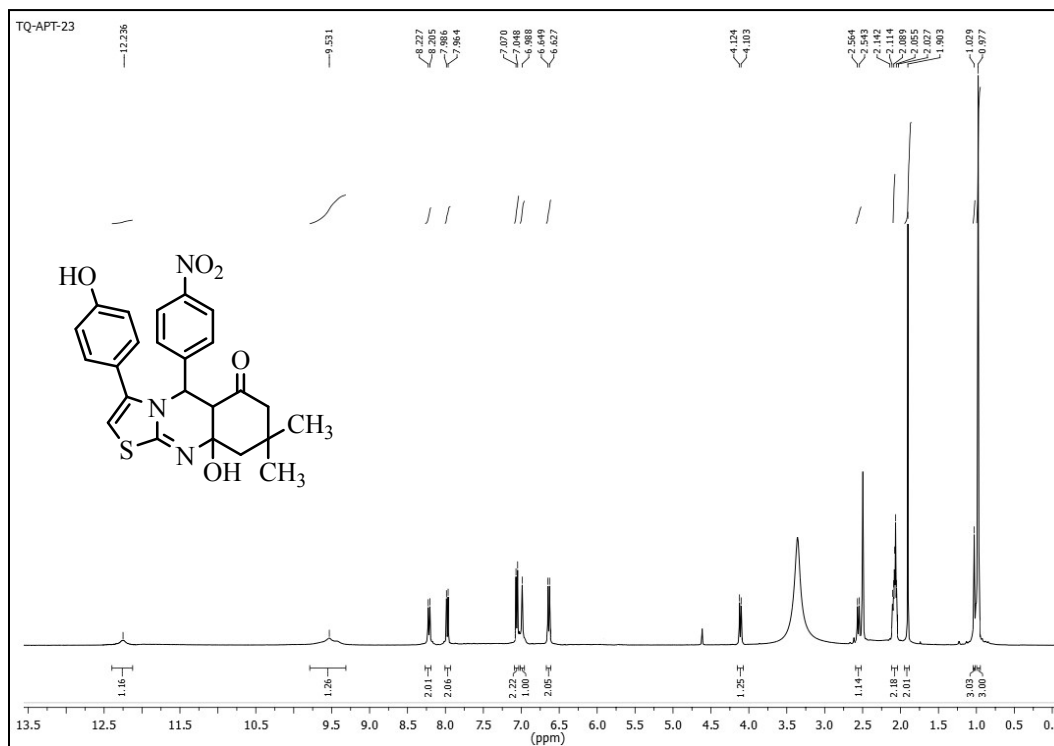


Figure S51. ^1H NMR spectrum of **5aq** in DMSO-d_6

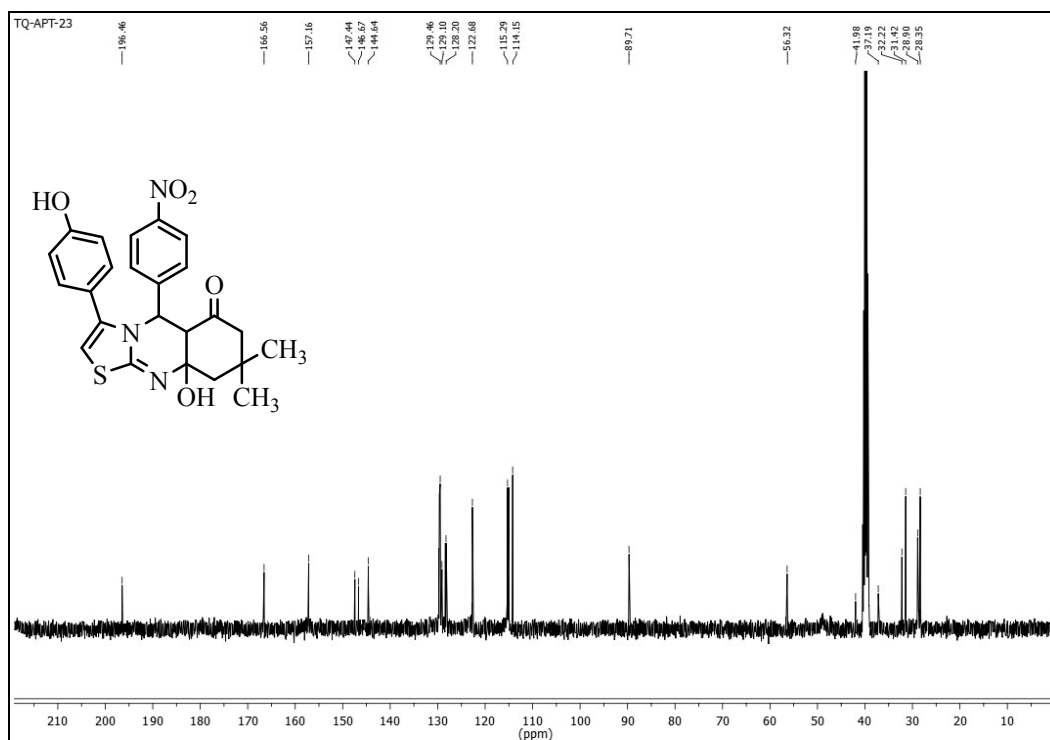


Figure S52. ^{13}C NMR spectrum of 5aq in DMSO-d_6

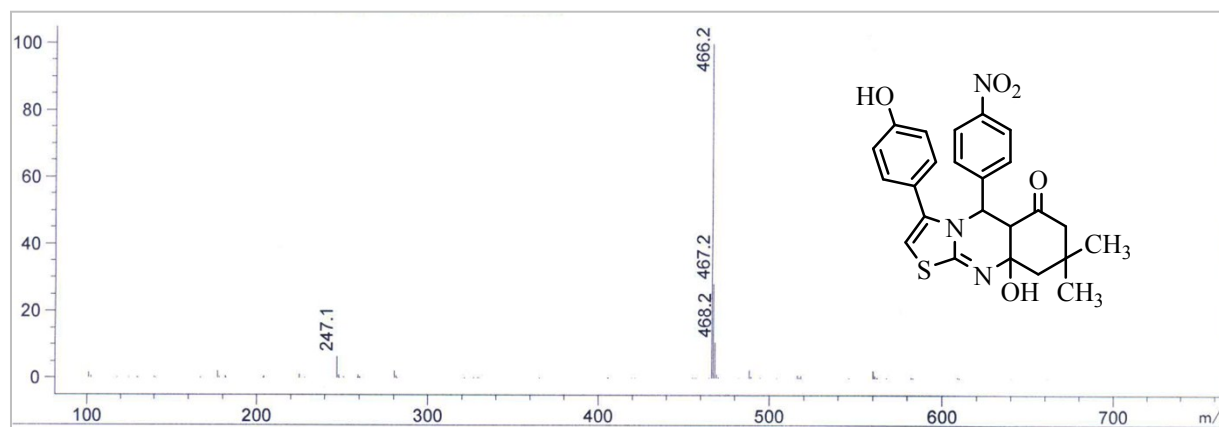


Figure S53. LC-MS spectrum of 5aq

6. ^1H , ^{13}C NMR and mass spectra of compounds 5aa and 5aq

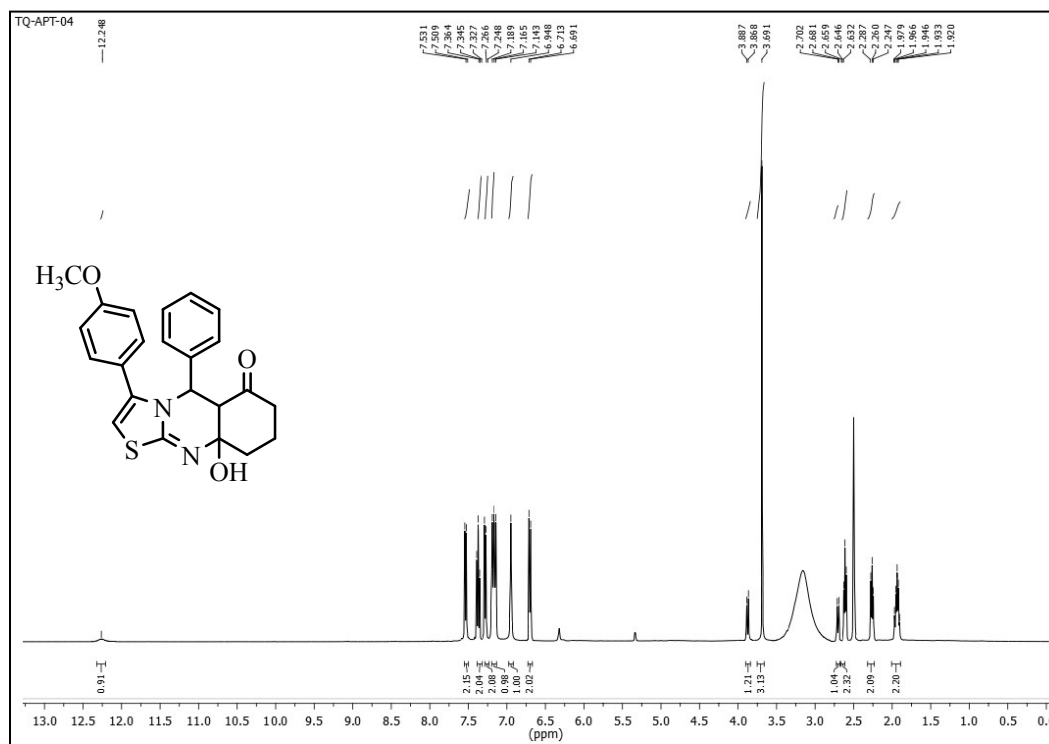


Figure S54. ^1H NMR spectrum of 5ba in DMSO- d_6

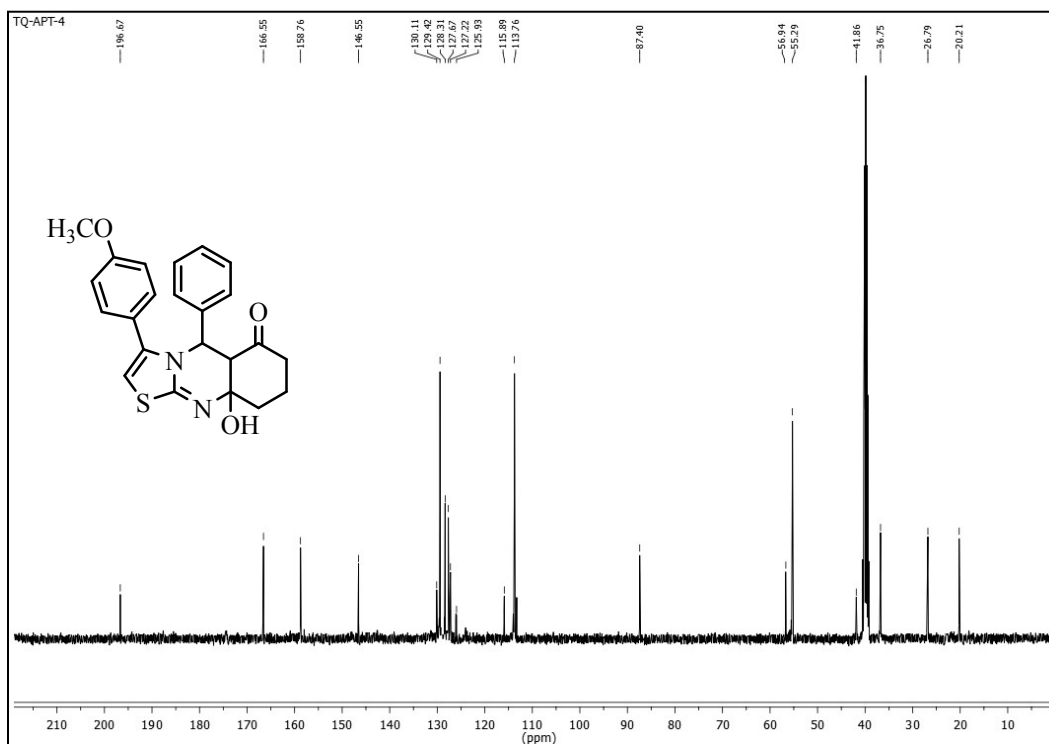


Figure S55. ^{13}C NMR spectrum of 5ba in DMSO- d_6

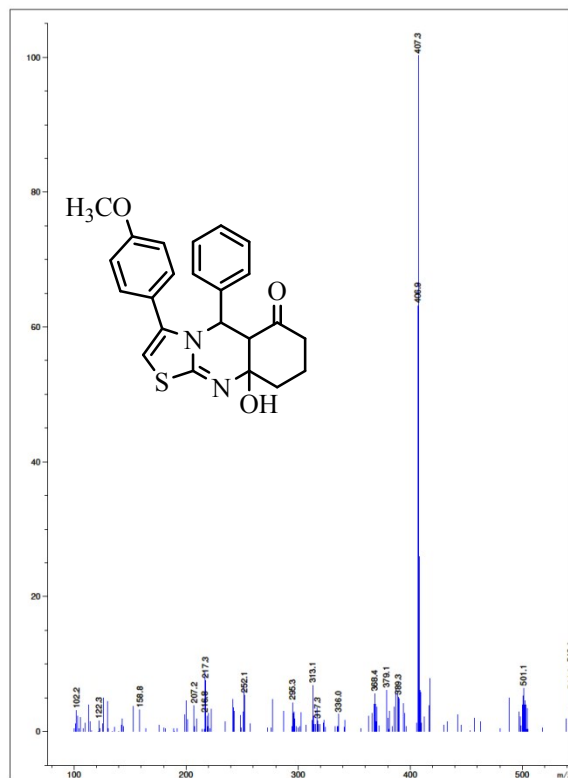


Figure S56. ESI-MS spectrum of 5ba

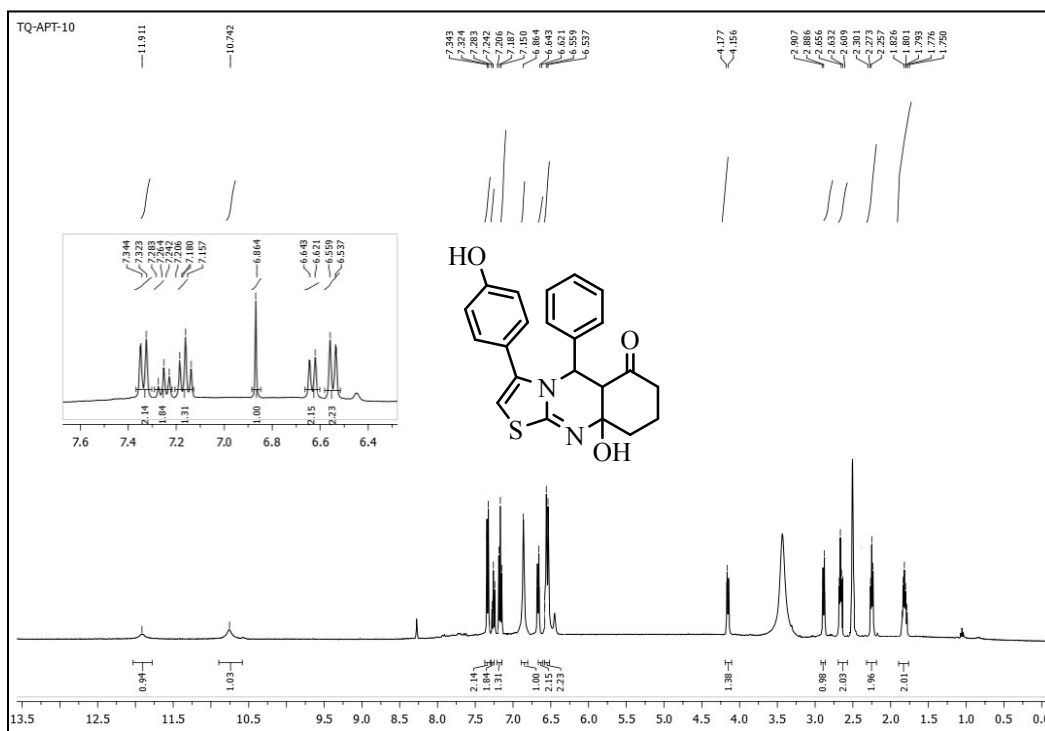


Figure S57. ¹H NMR spectrum of 5bb in DMSO-d₆

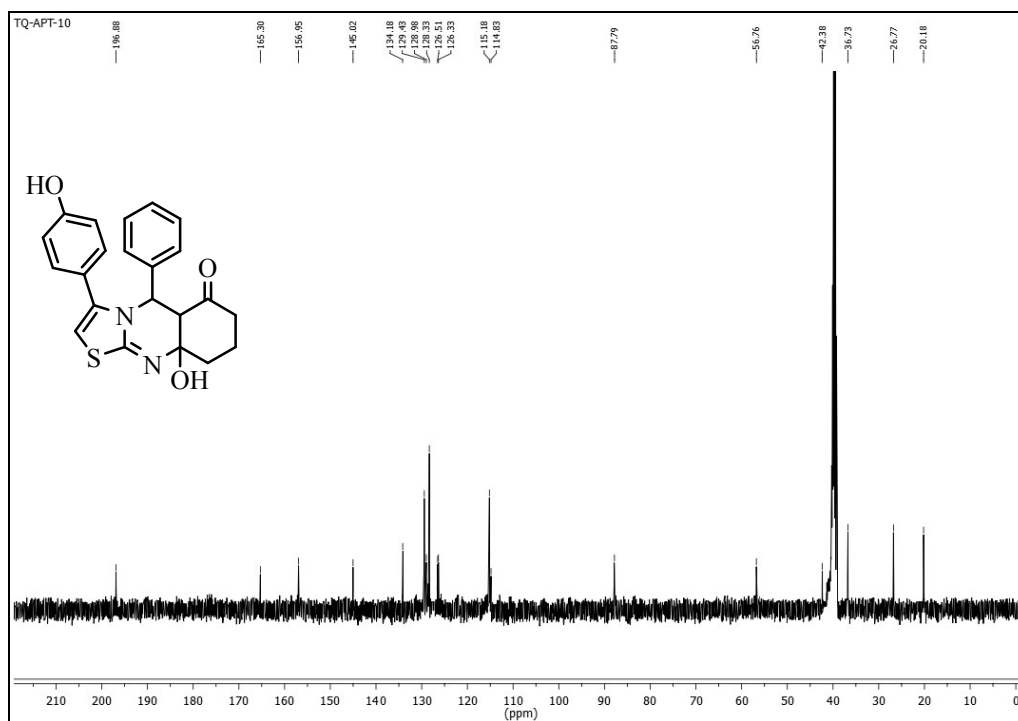


Figure S58. ¹³C NMR spectrum of **5bb** in DMSO-d₆

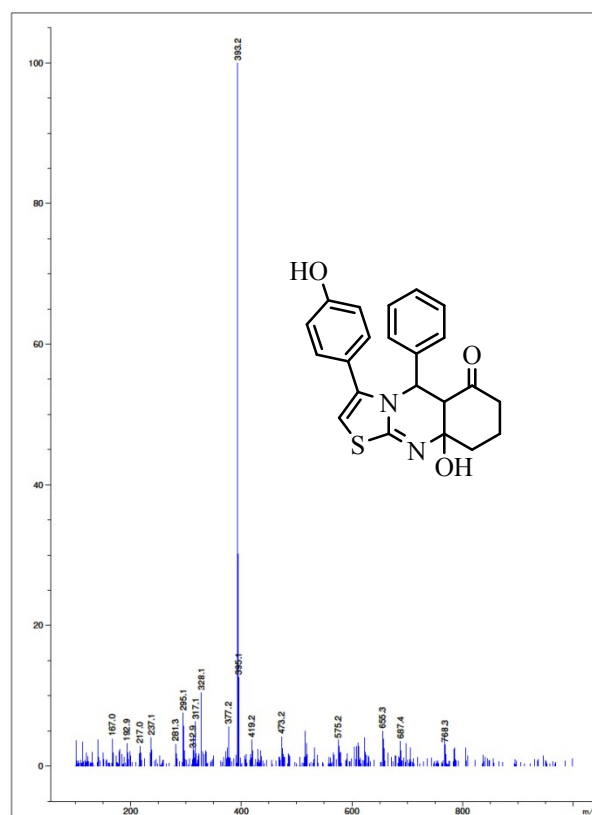


Figure S59. ESI-MS spectrum of **5bb**

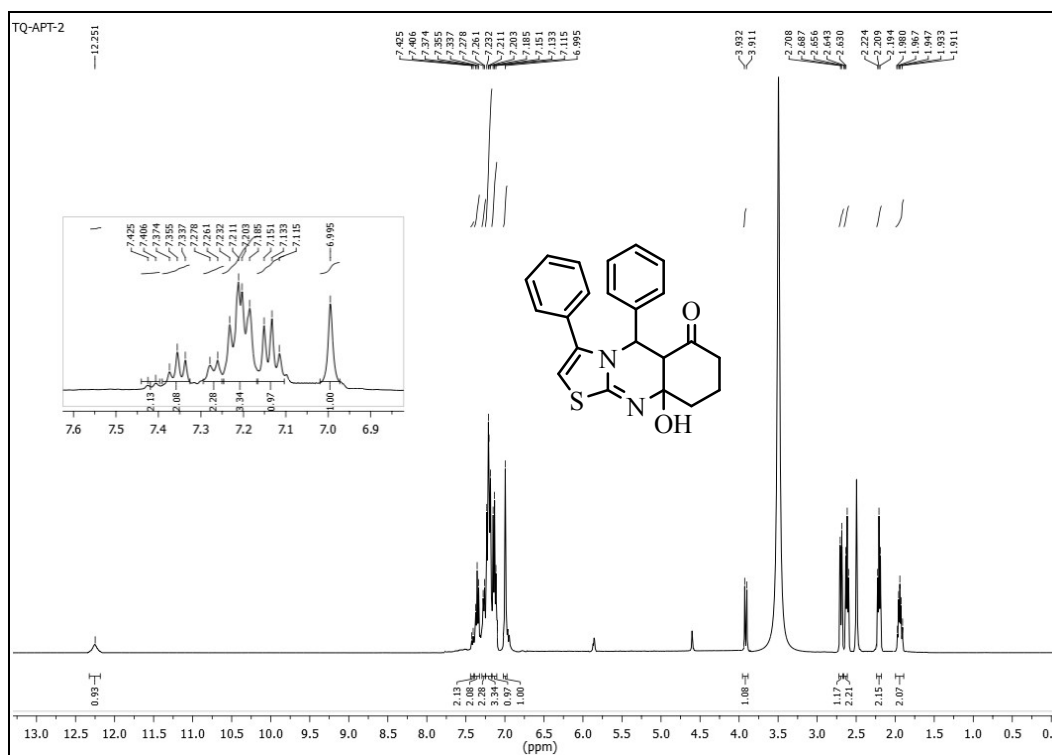


Figure S60. ^1H NMR spectrum of **5bc** in DMSO-d_6

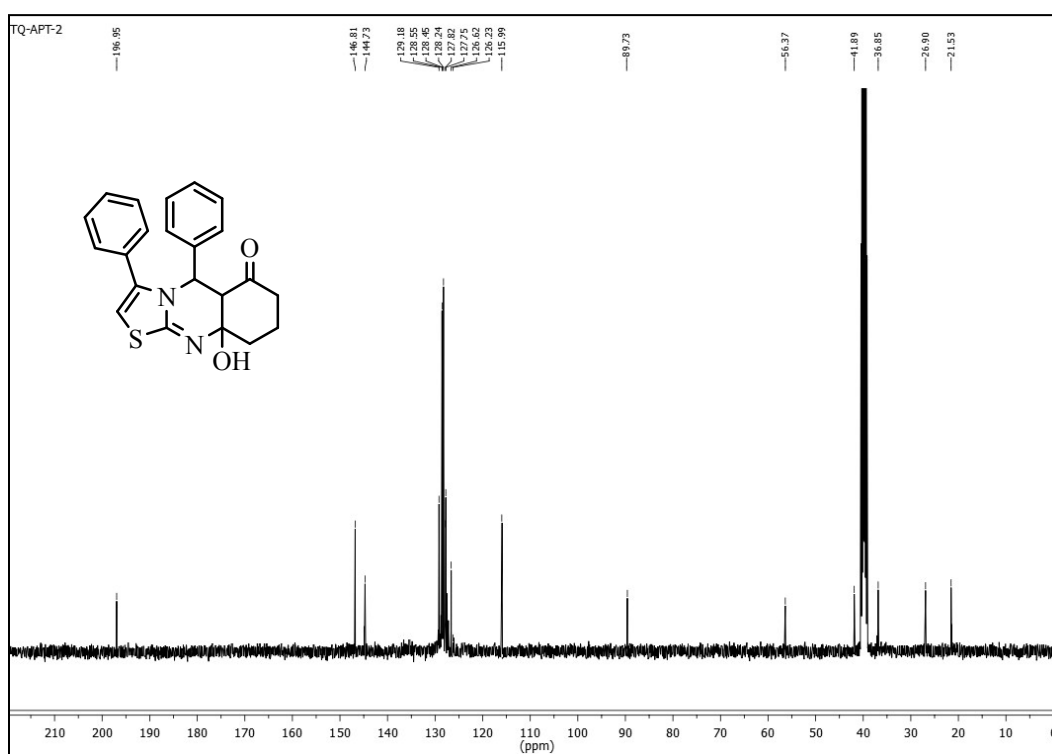


Figure S61. ^{13}C NMR spectrum of **5bc** in DMSO-d_6

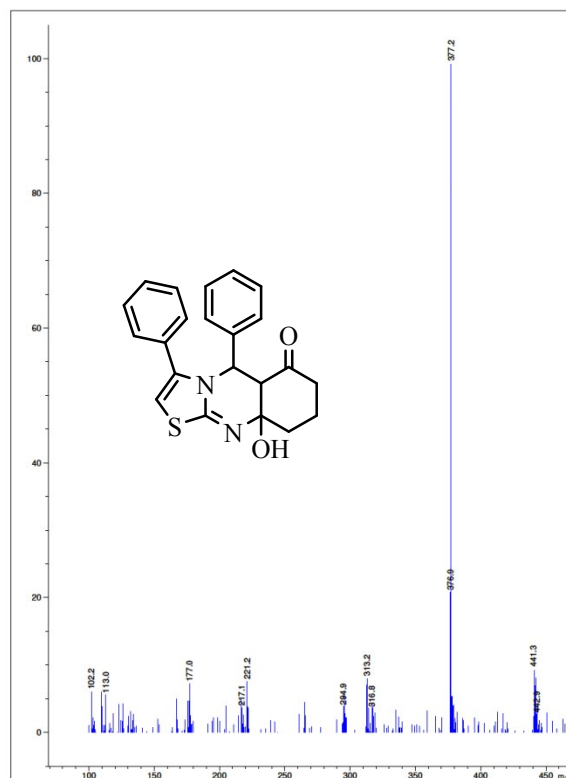


Figure S62. ESI-MS spectrum of 5bc

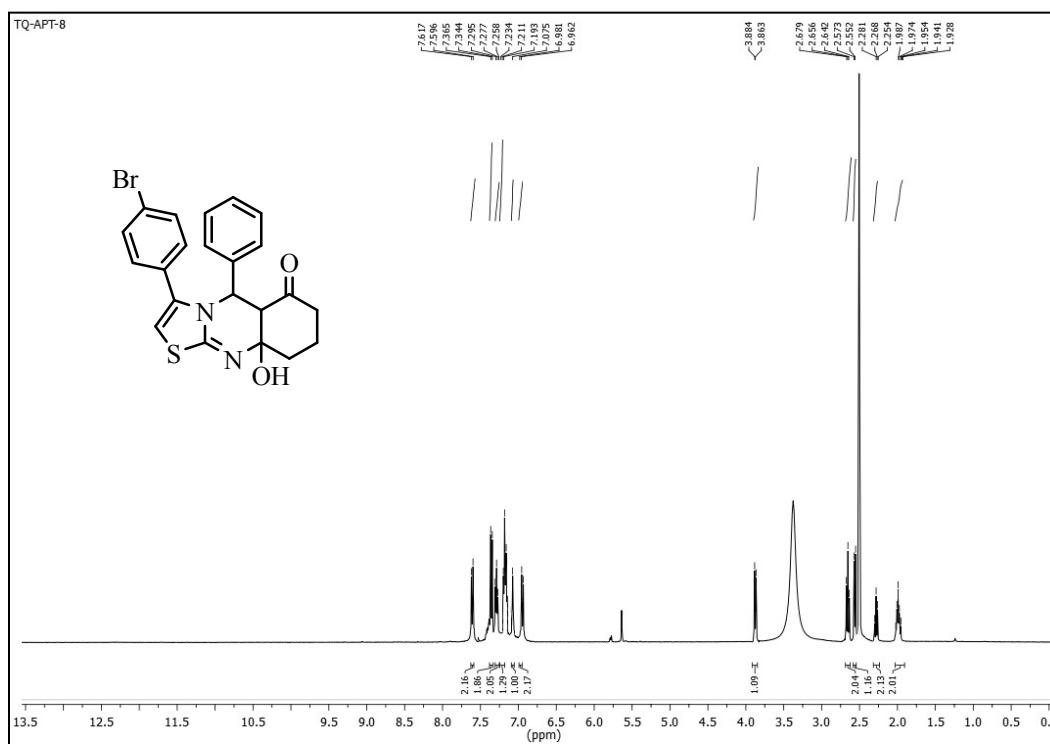


Figure S63. ¹H NMR spectrum of 5bd in DMSO-d₆

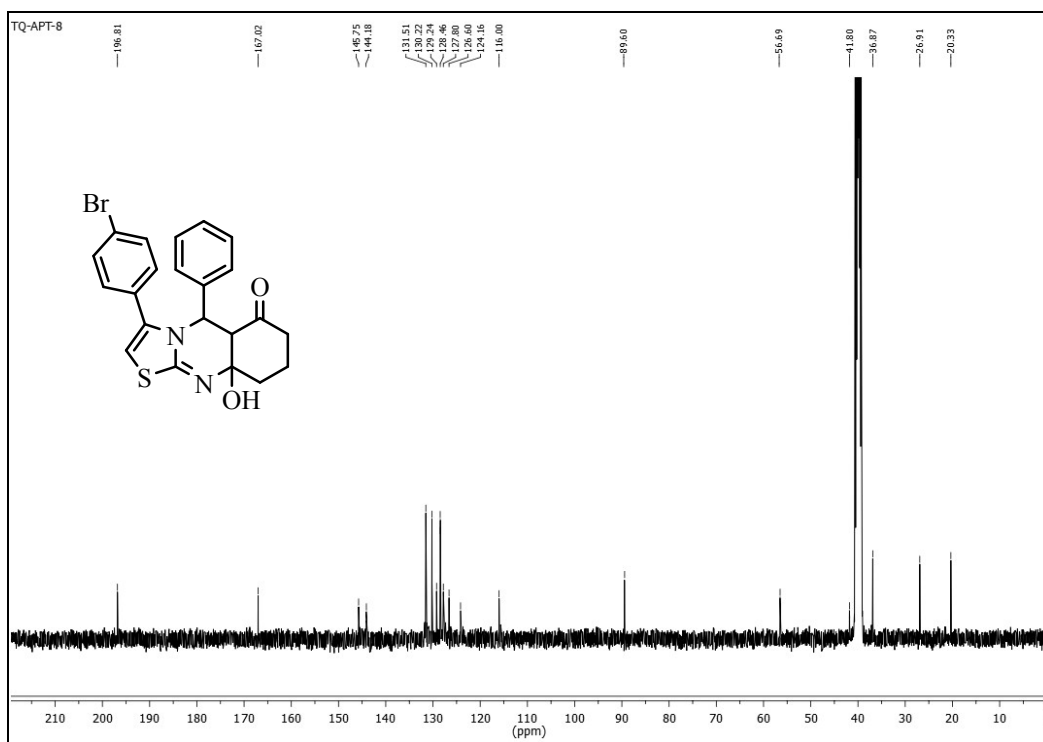


Figure S64. ^{13}C NMR spectrum of **5bd** in DMSO-d_6

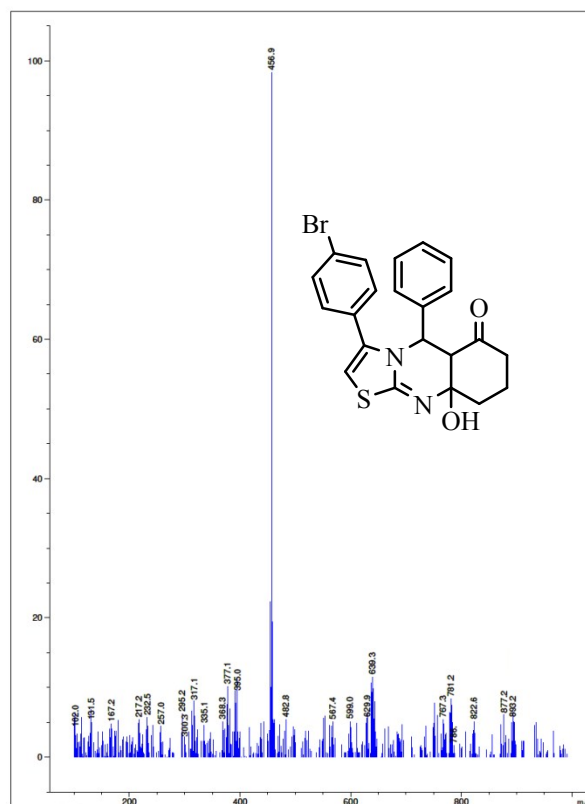


Figure S65. ESI-MS spectrum of **5bd**

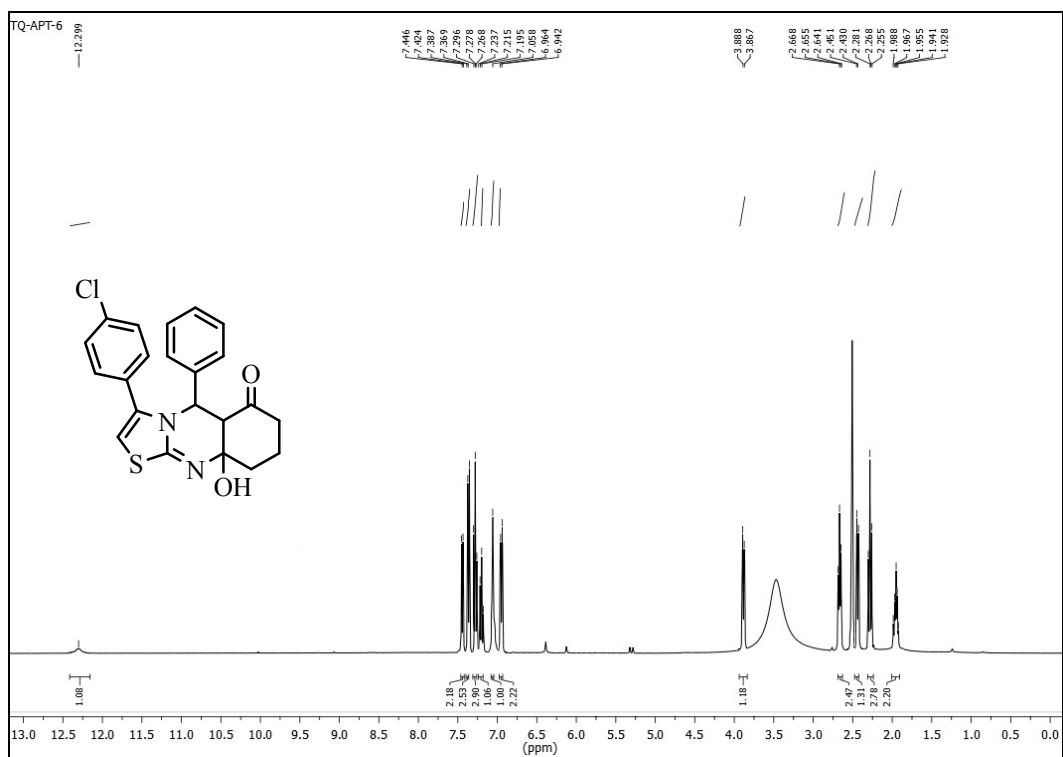


Figure S66. ¹H NMR spectrum of **5be** in DMSO-d₆

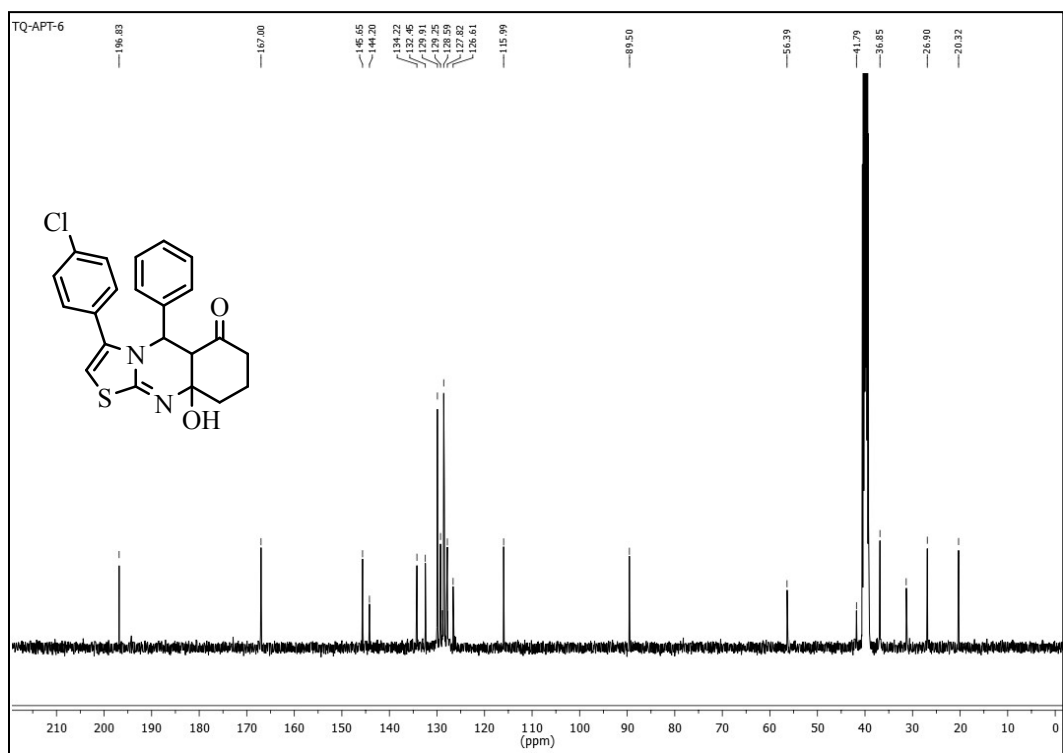


Figure S67. ¹³C NMR spectrum of **5be** in DMSO-d₆

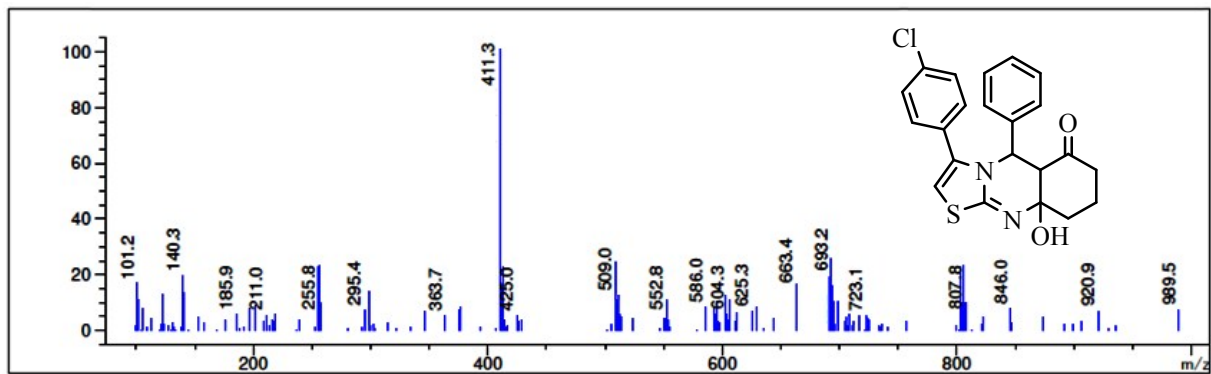


Figure S68. ESI-MS spectrum of 5be

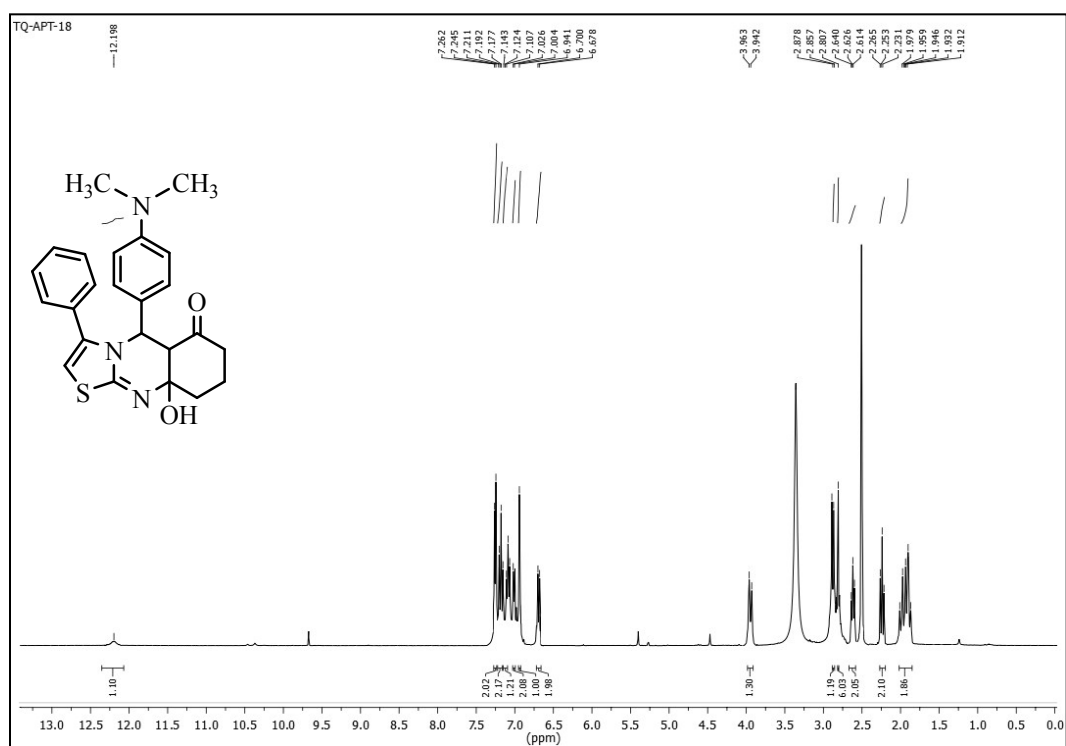


Figure S69. ¹H NMR spectrum of 5bf in DMSO-d₆

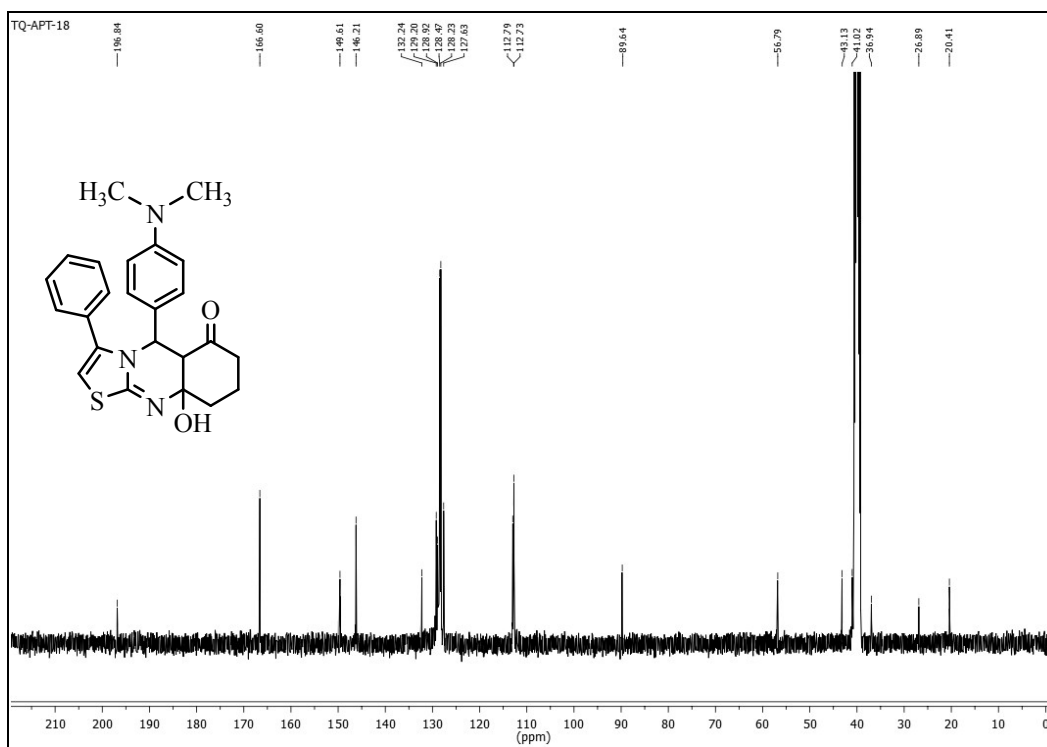


Figure S70. ^{13}C NMR spectrum of **5bf** in DMSO-d_6

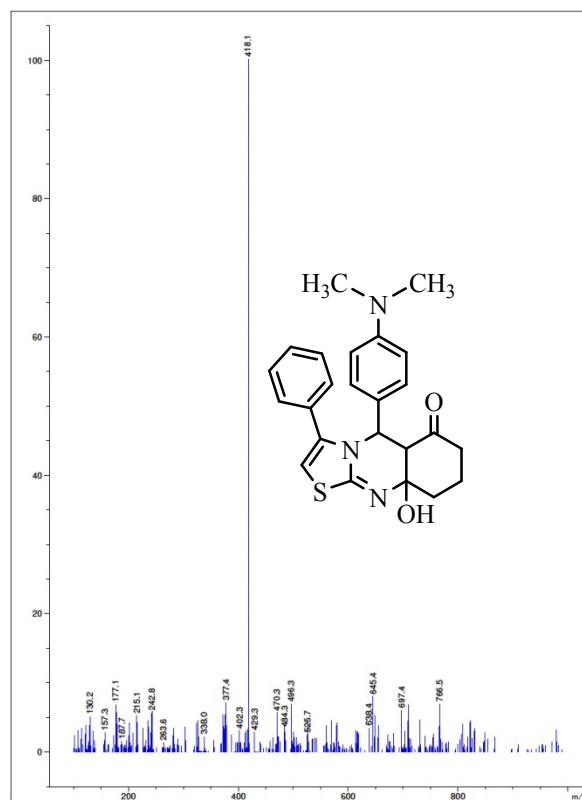


Figure S71. ESI-MS spectrum of **5bf**

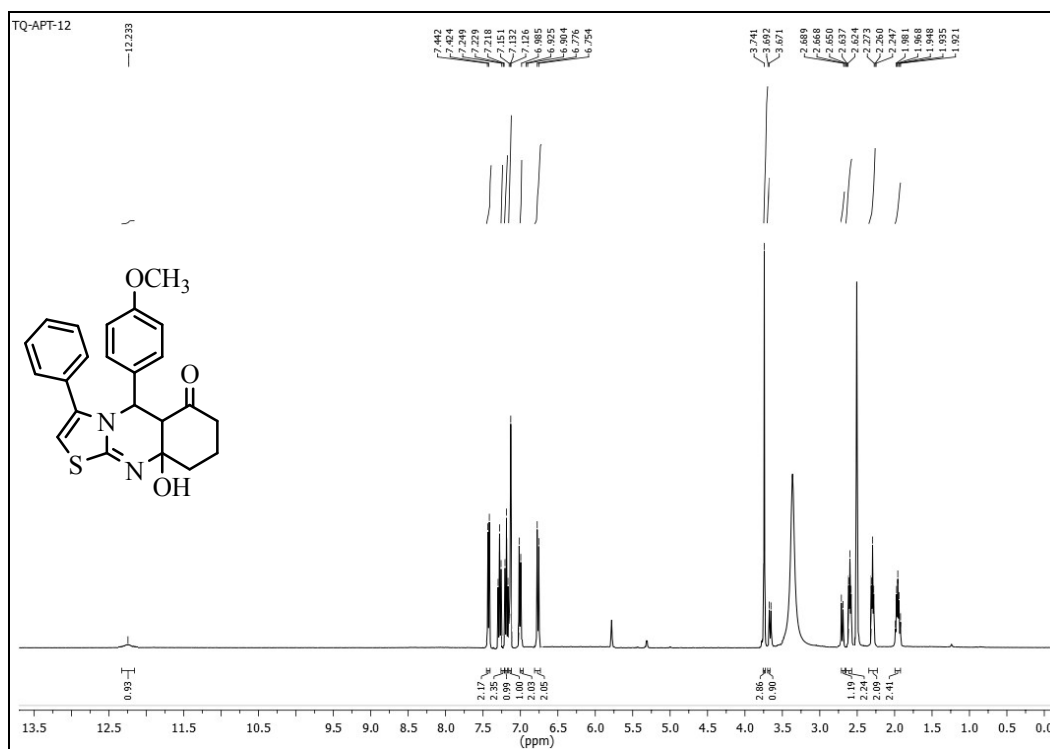


Figure S72. ^1H NMR spectrum of **5bg** in DMSO-d_6

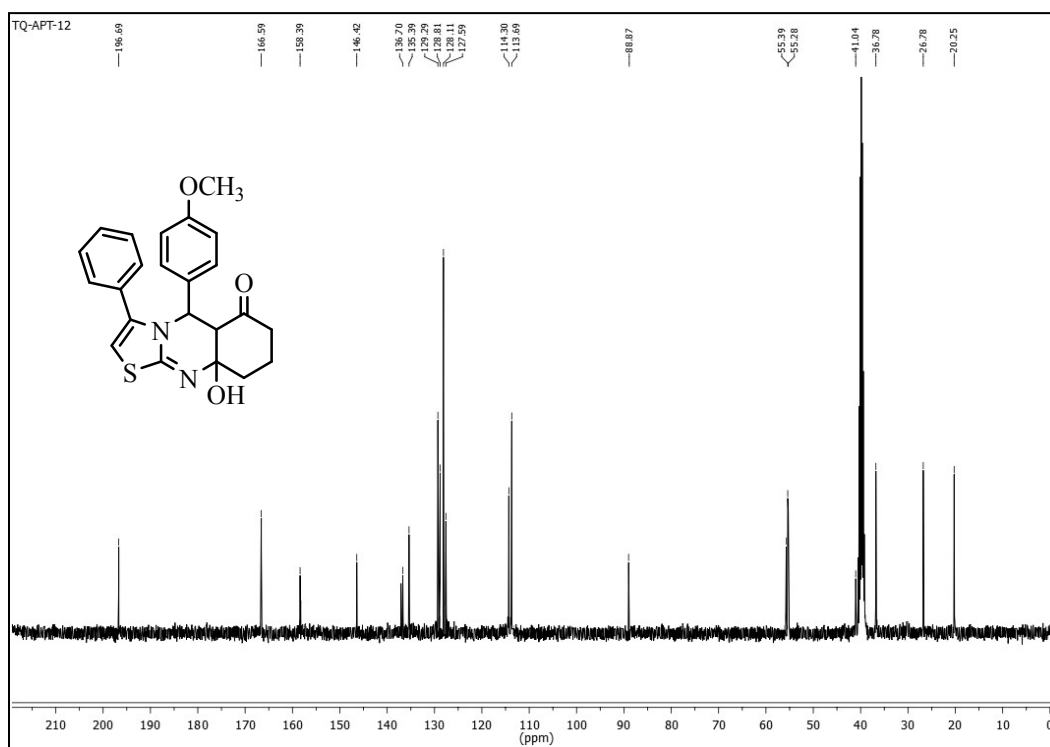


Figure S73. ^{13}C NMR spectrum of **5bg** in DMSO-d_6

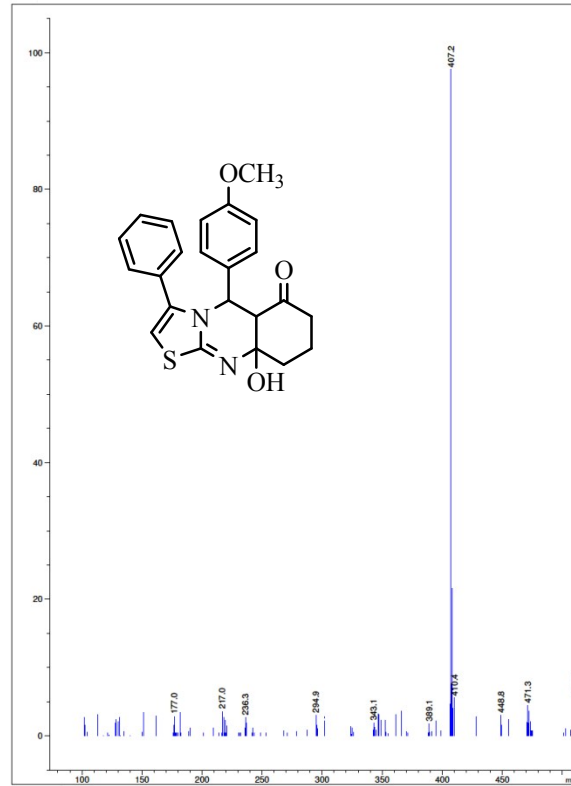


Figure S74. ESI-MS spectrum of **5bg**

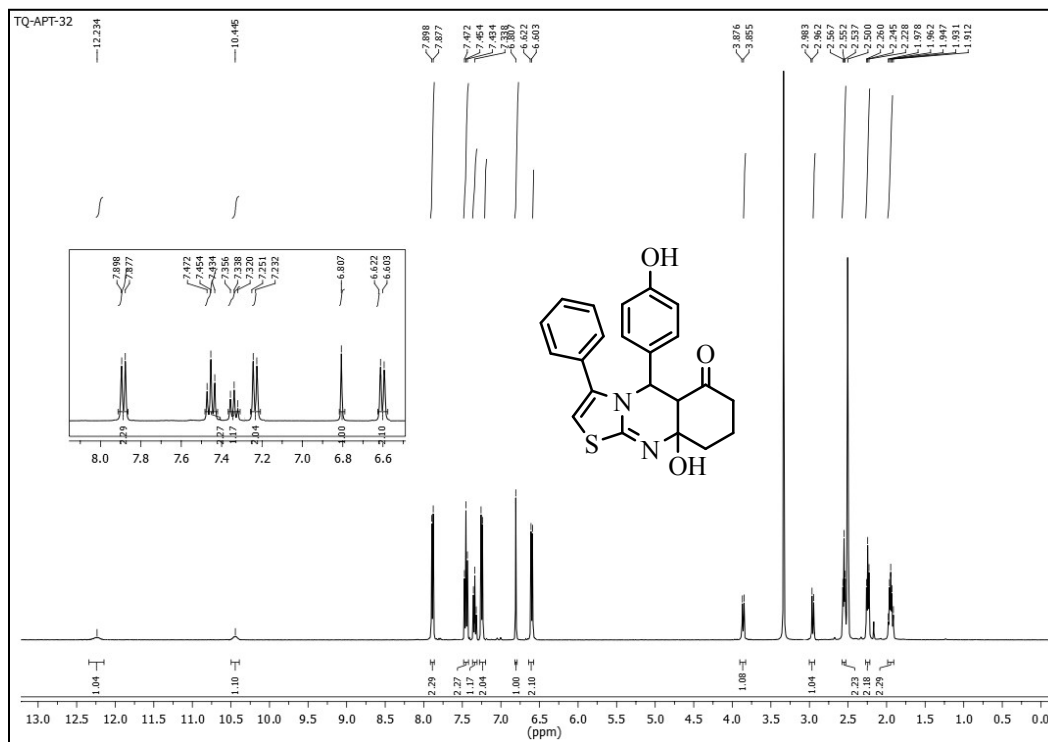


Figure S75. ¹H NMR spectrum of **5bh** in DMSO-d₆

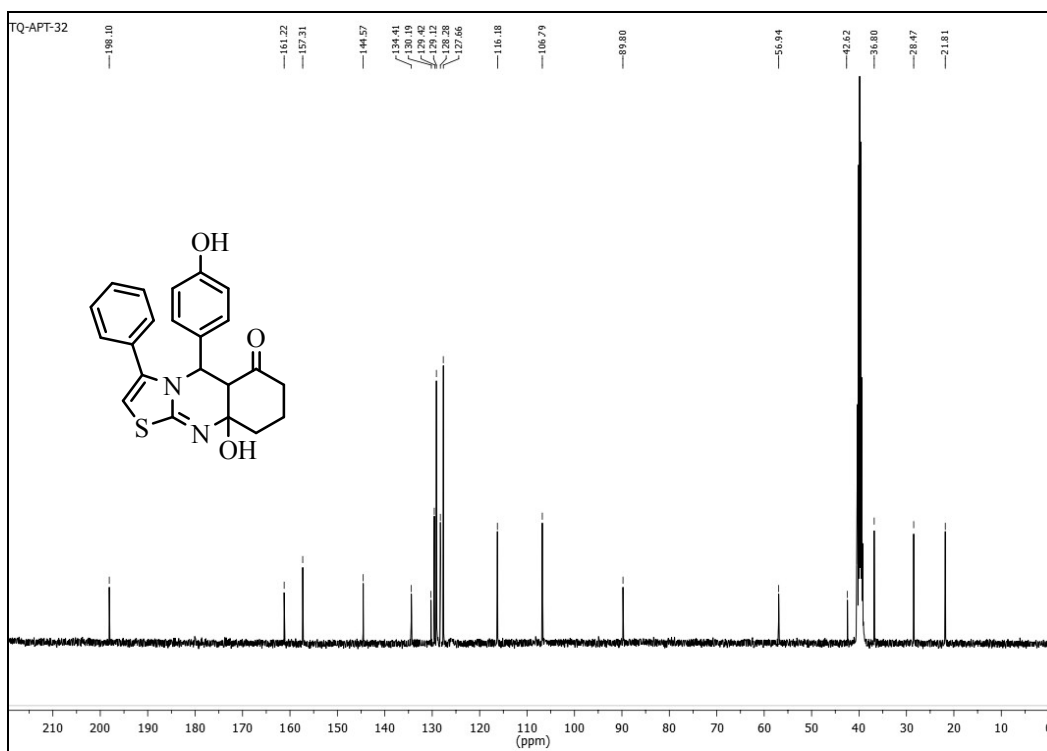


Figure S76. ^{13}C NMR spectrum of **5bh** in DMSO-d_6

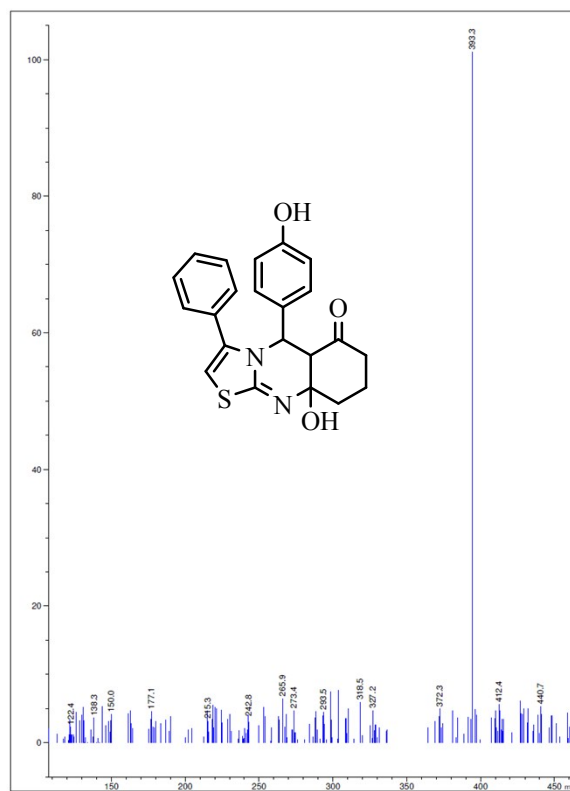


Figure S77. ESI-MS spectrum of **5bh**

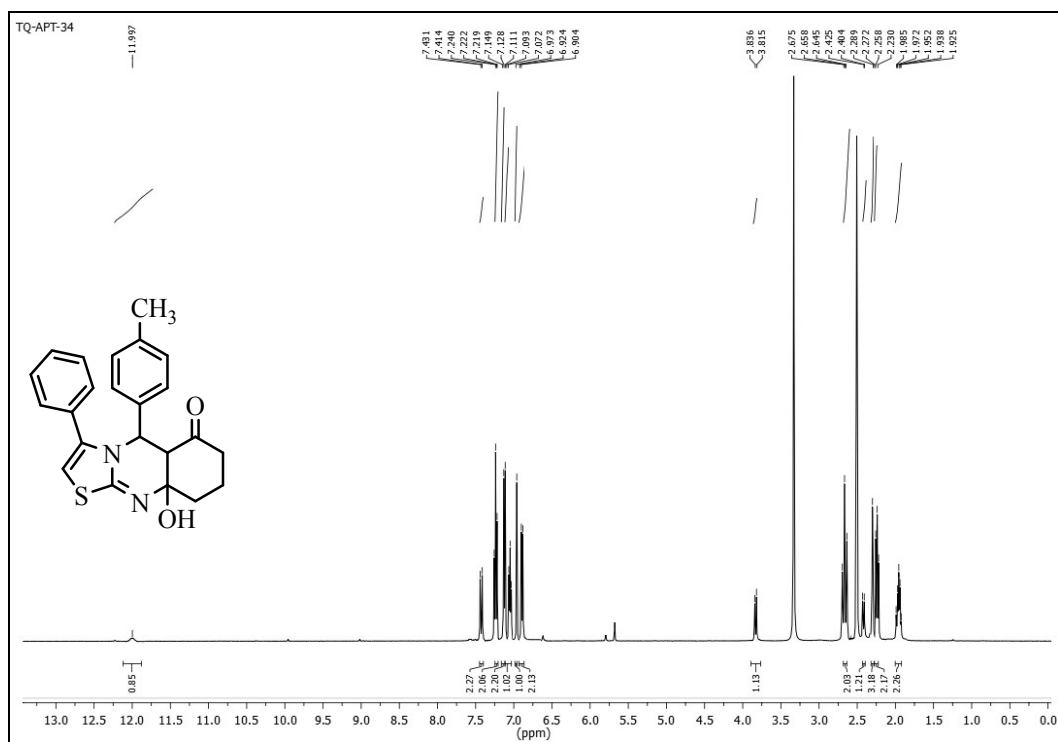


Figure S78. ^1H NMR spectrum of **5bi** in DMSO-d_6

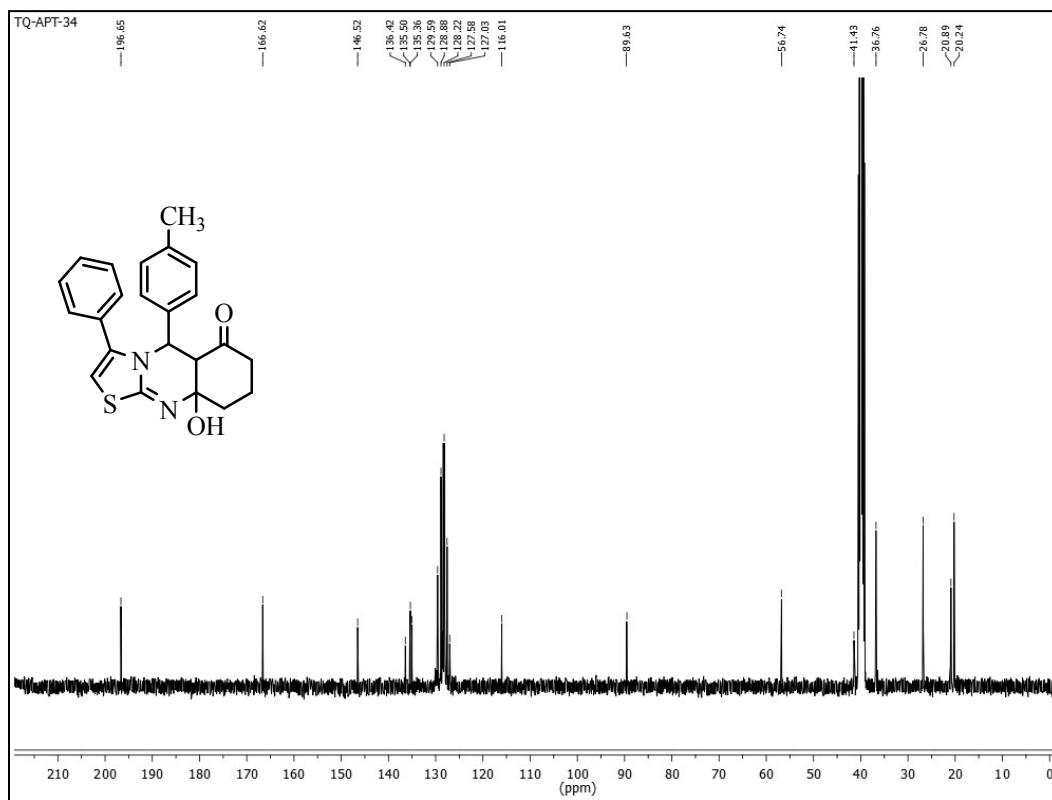


Figure S79. ^{13}C NMR spectrum of **5bi** in DMSO-d_6

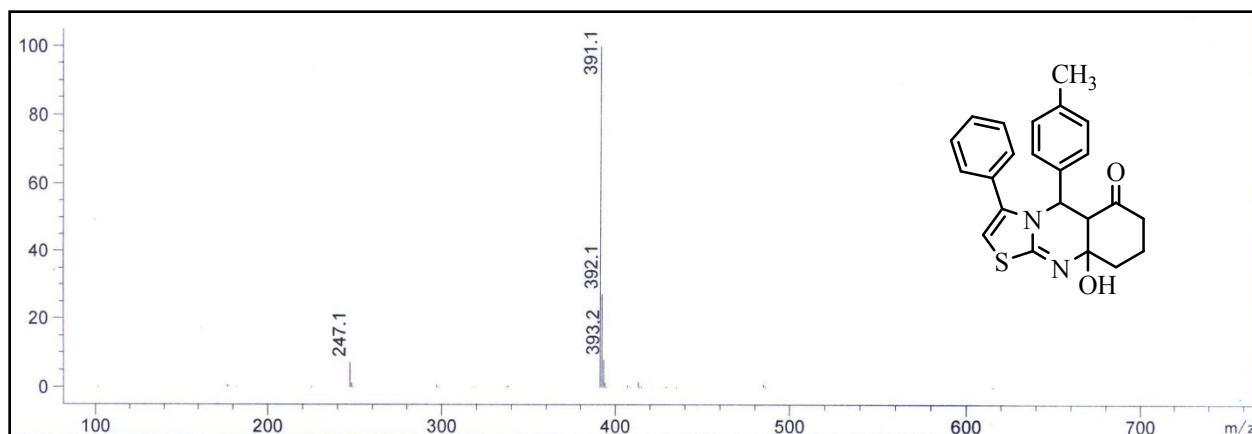


Figure S80. LC-MS spectrum of **5bi**

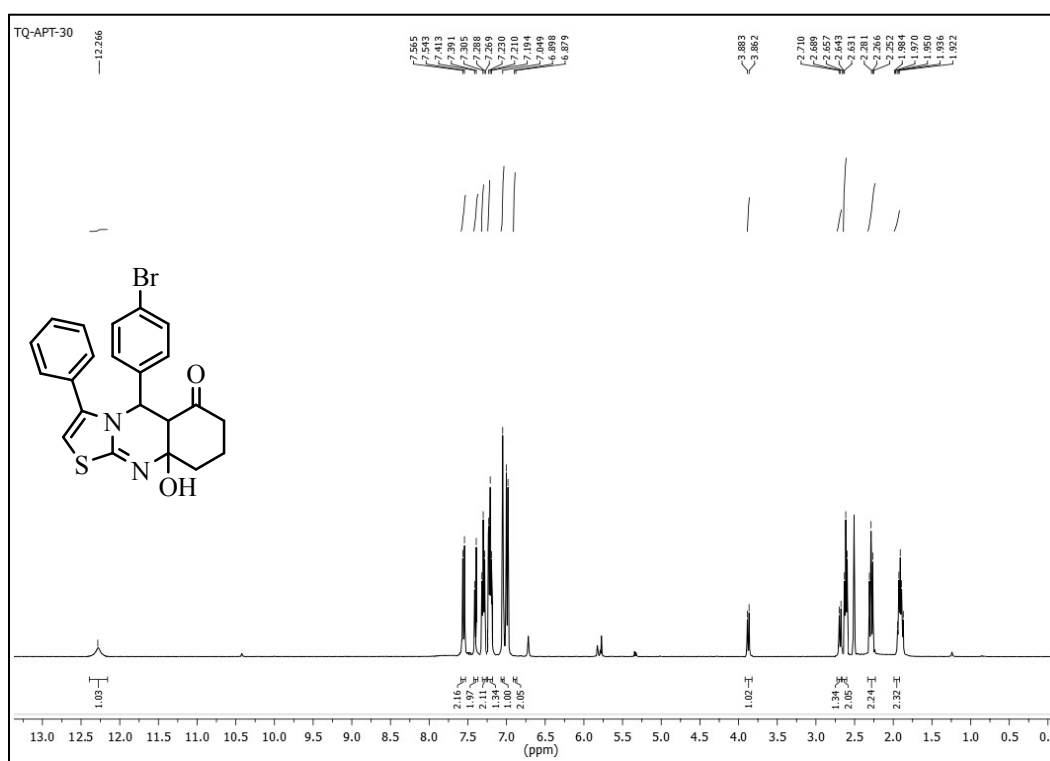


Figure S81. ^1H NMR spectrum of **5bj** in DMSO-d_6

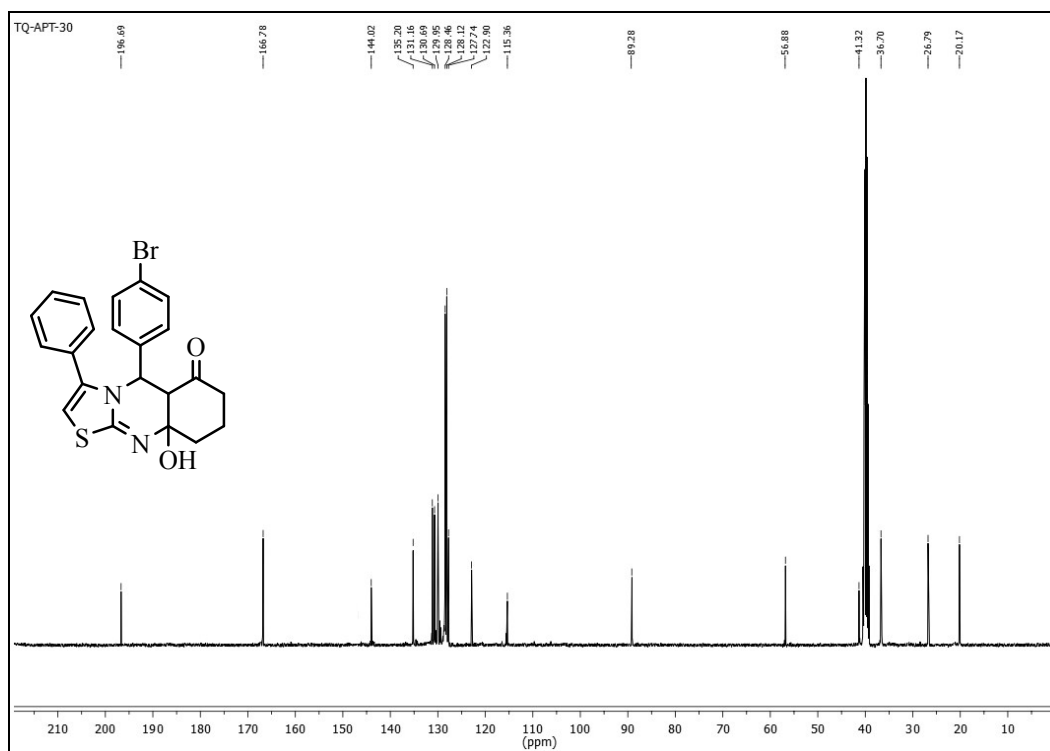


Figure S82. ¹³C NMR spectrum of 5bj in DMSO-d₆

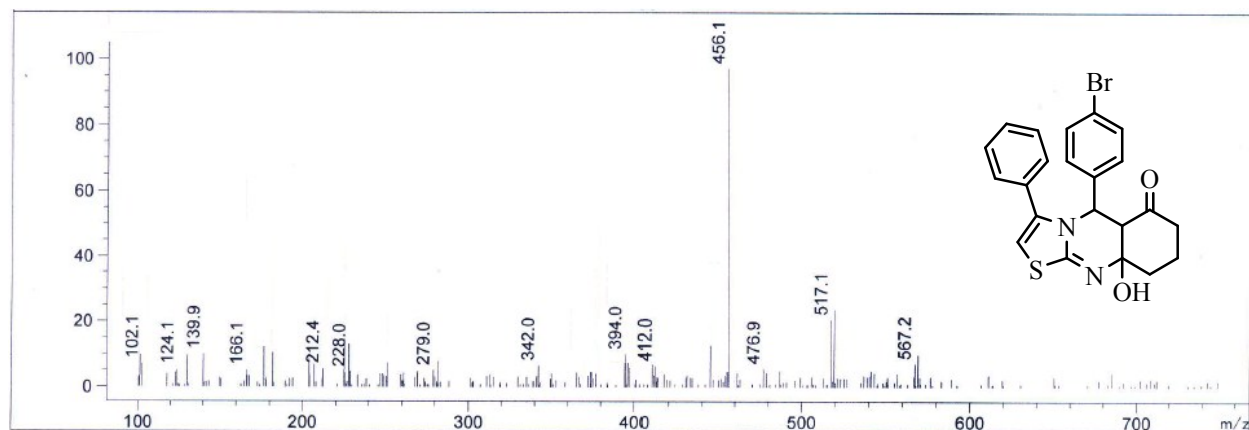


Figure S83. LC-MS spectrum of 5bj

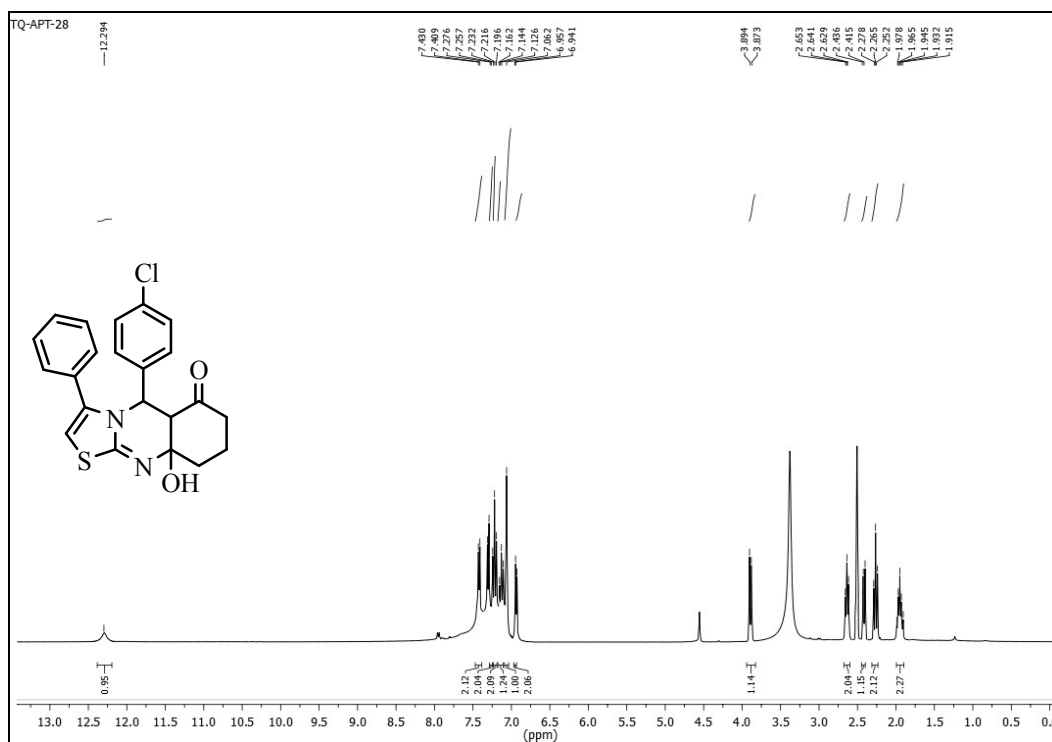


Figure S84. ^1H NMR spectrum of **5bk** in DMSO-d_6

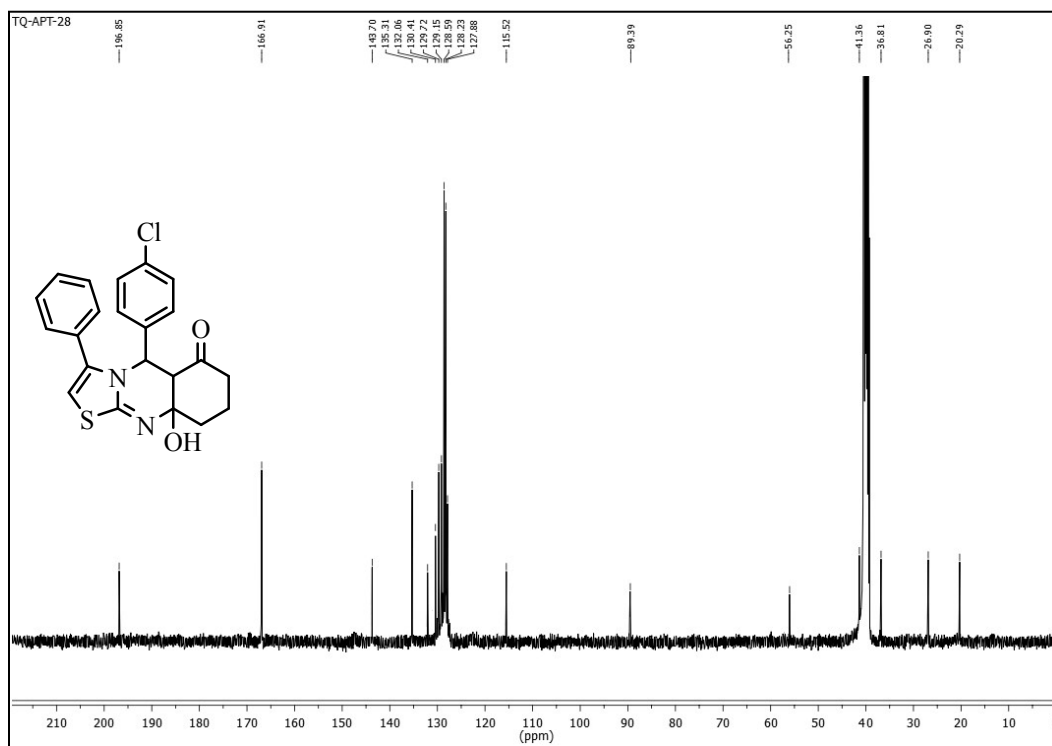


Figure S85. ^{13}C NMR spectrum of **5bk** in DMSO-d_6

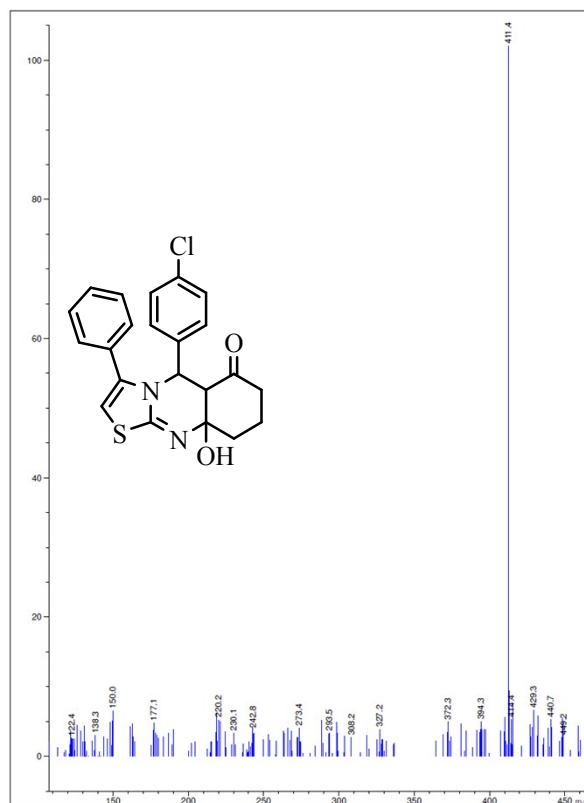


Figure S86. ESI-MS spectrum of 5bk

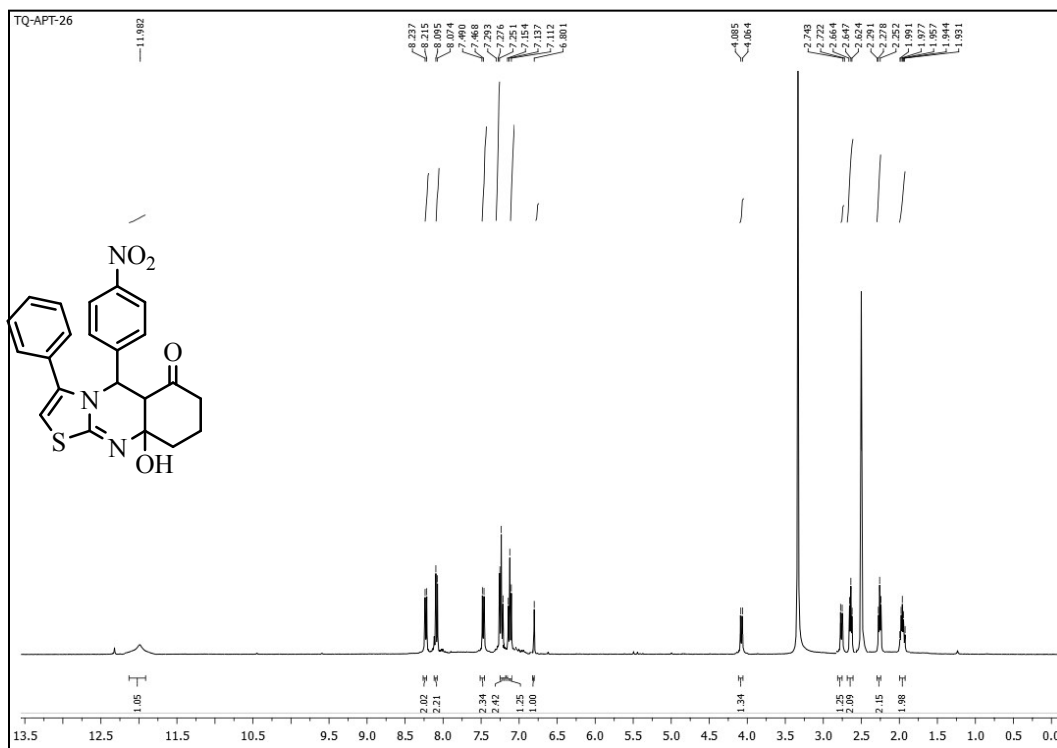


Figure S87. ¹H NMR spectrum of 5bl in DMSO-d₆

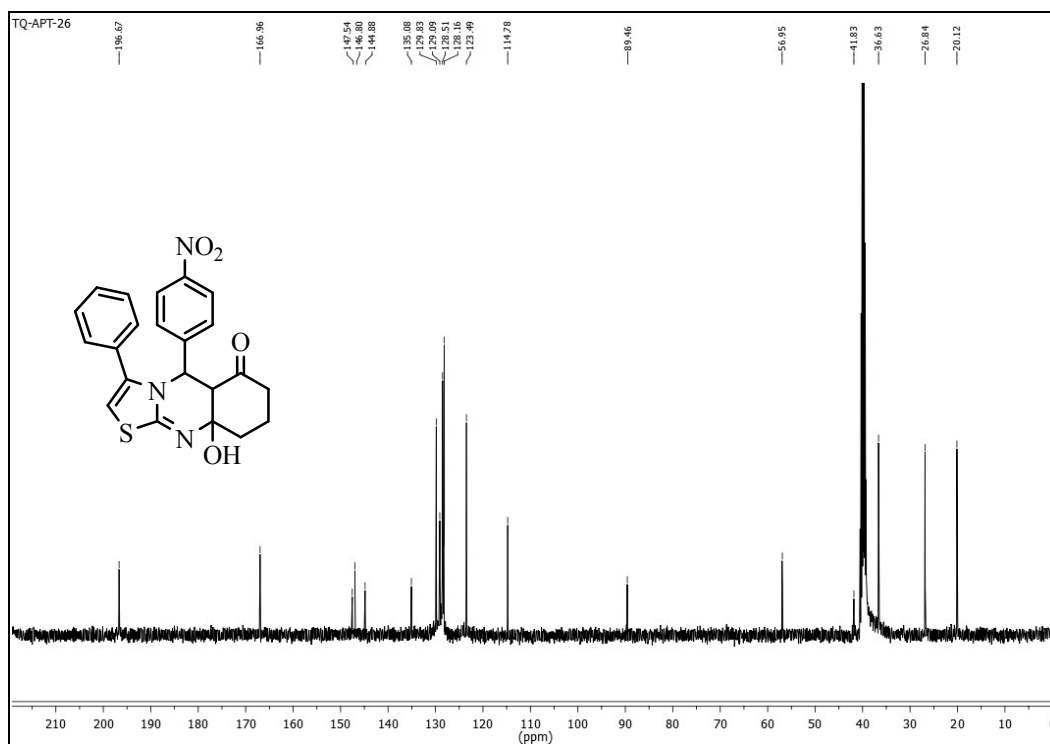


Figure S88. ^{13}C NMR spectrum of **5bl** in DMSO-d_6

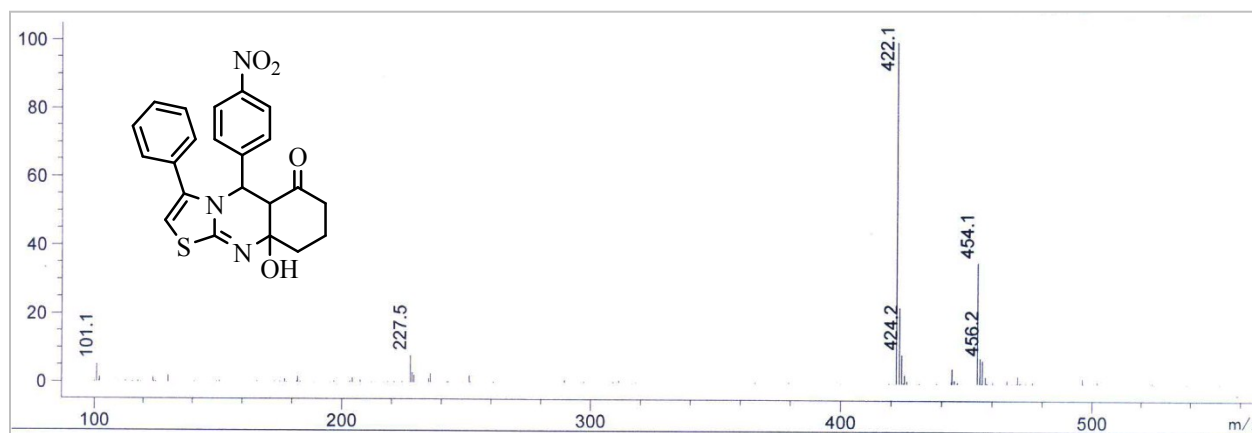


Figure S89. ESI-MS spectrum of **5bl**

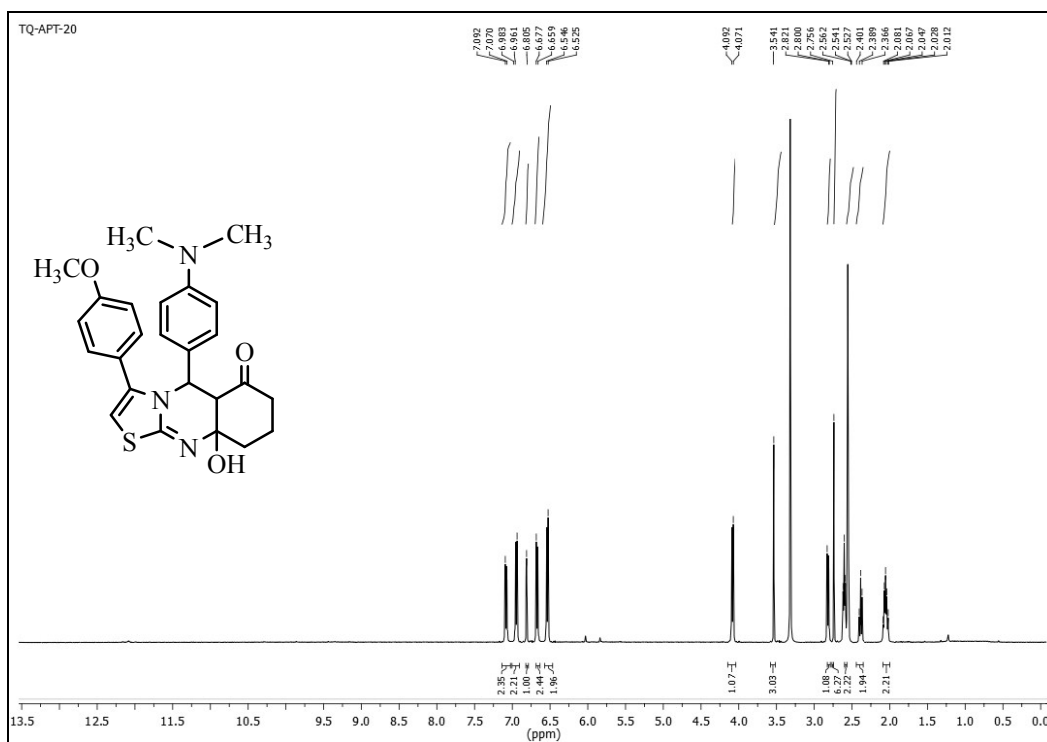


Figure S90. ¹H NMR spectrum of **5bm** in DMSO-d₆

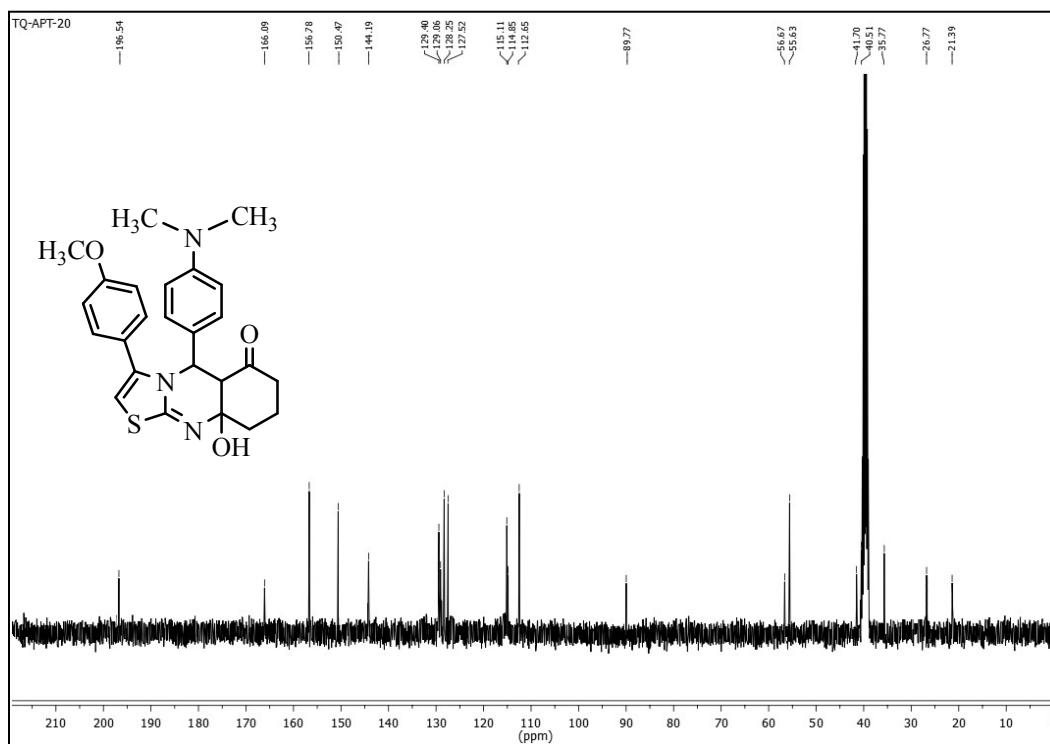


Figure S91. ¹³C NMR spectrum of **5bm** in DMSO-d₆

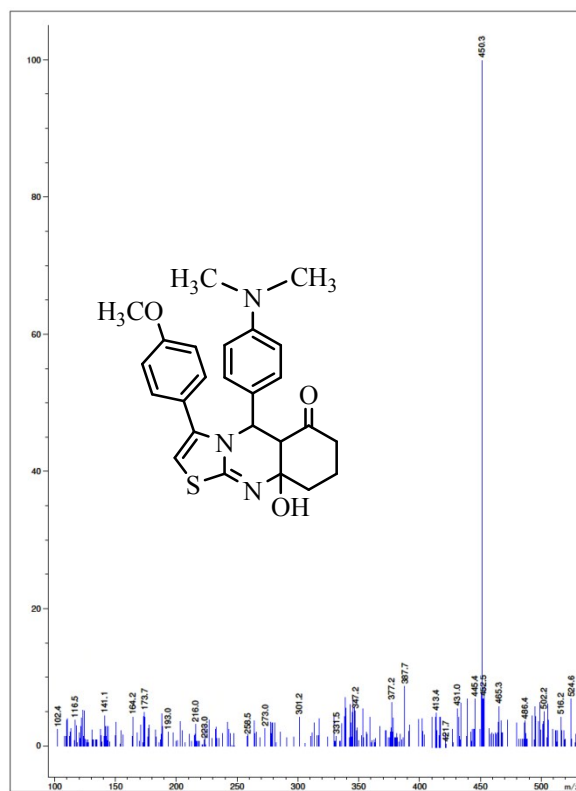


Figure S92. ESI-MS spectrum of 5bm

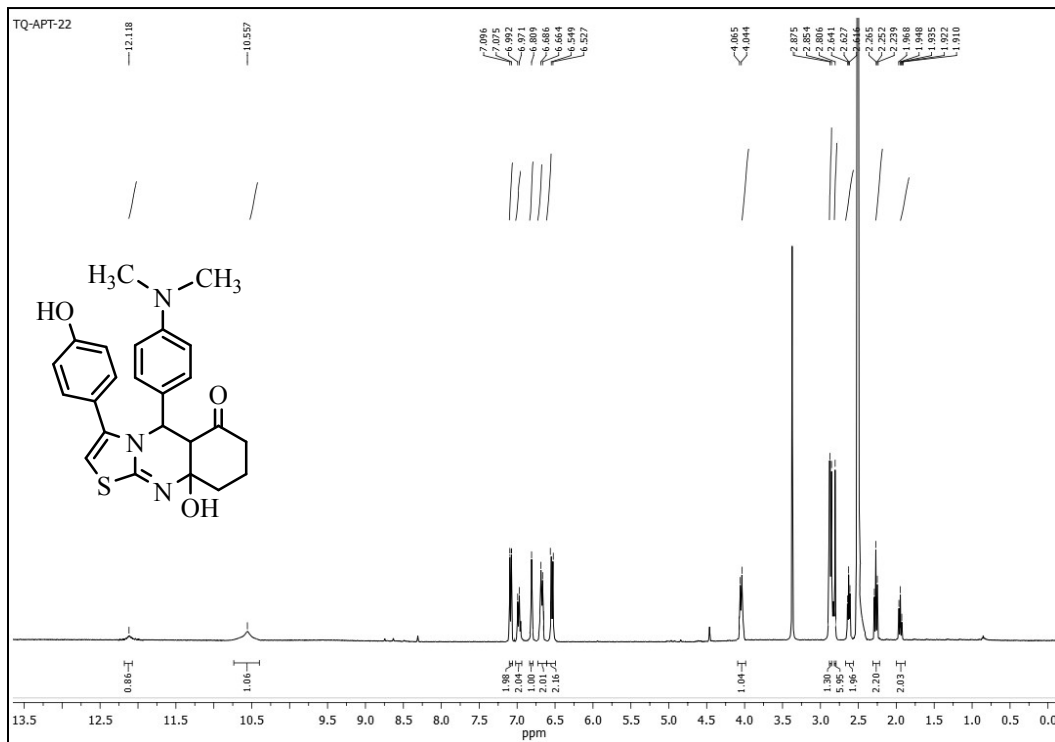


Figure S93. ¹H NMR spectrum of 5bn in DMSO-d₆

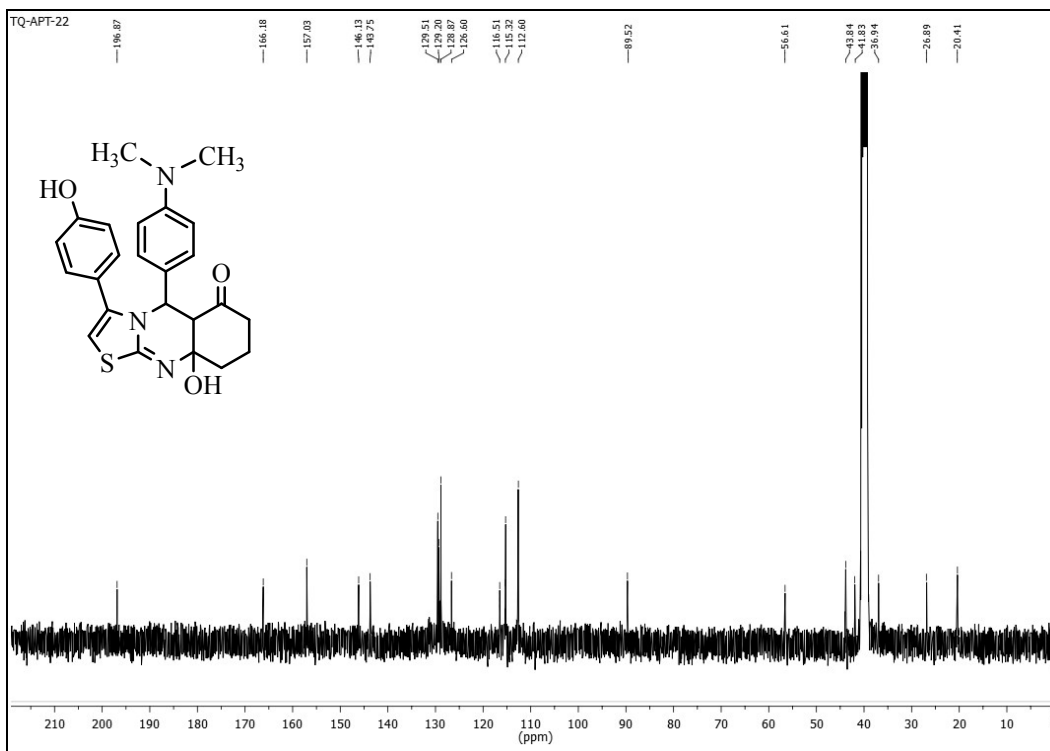


Figure S94. ^{13}C NMR spectrum of 5bn in DMSO-d_6

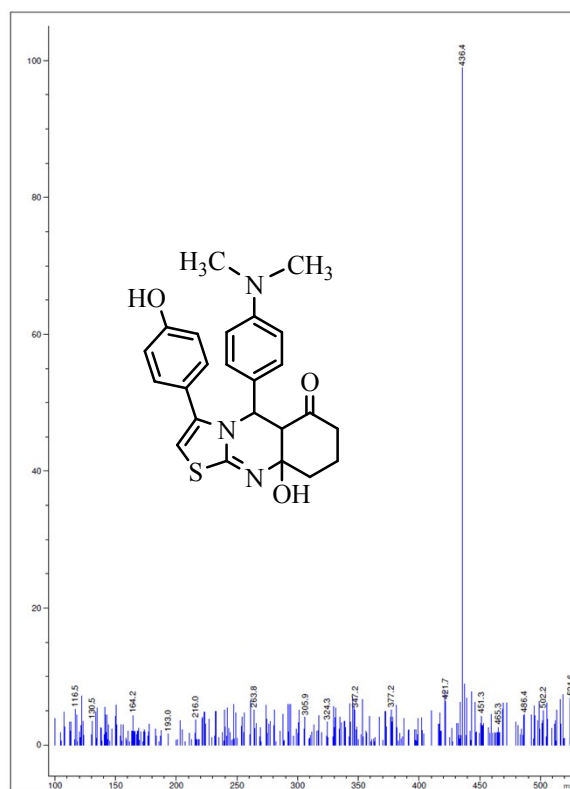


Figure S95. ESI-MS spectrum of 5bn

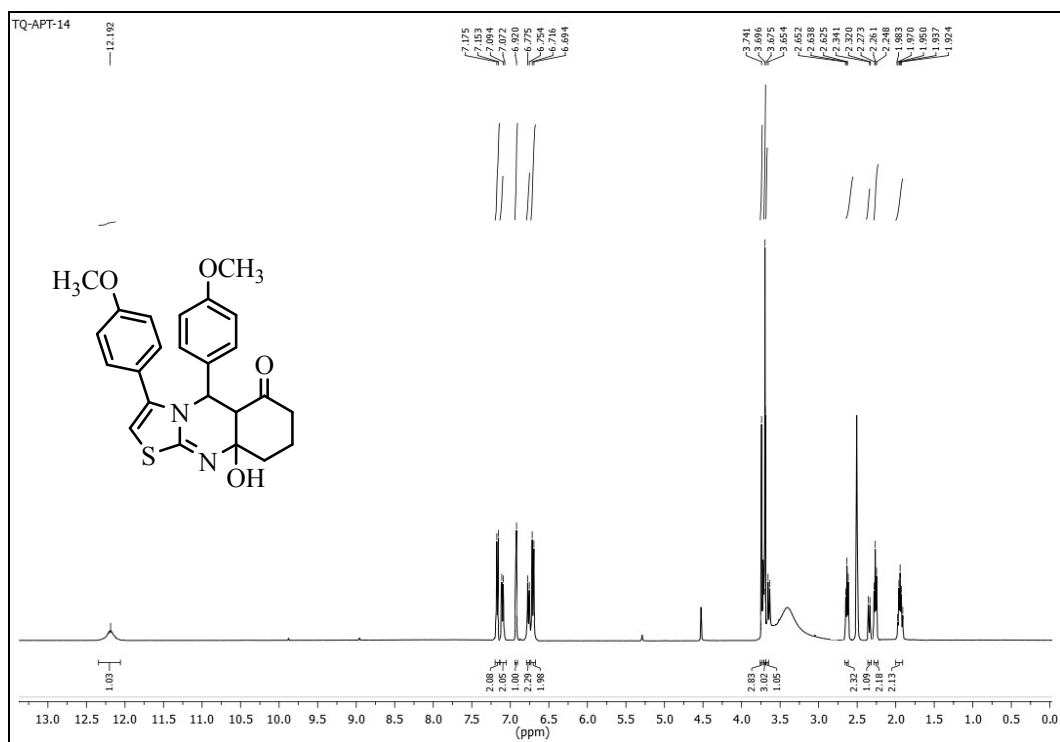


Figure S96. ^1H NMR spectrum of **5bo** in DMSO-d_6

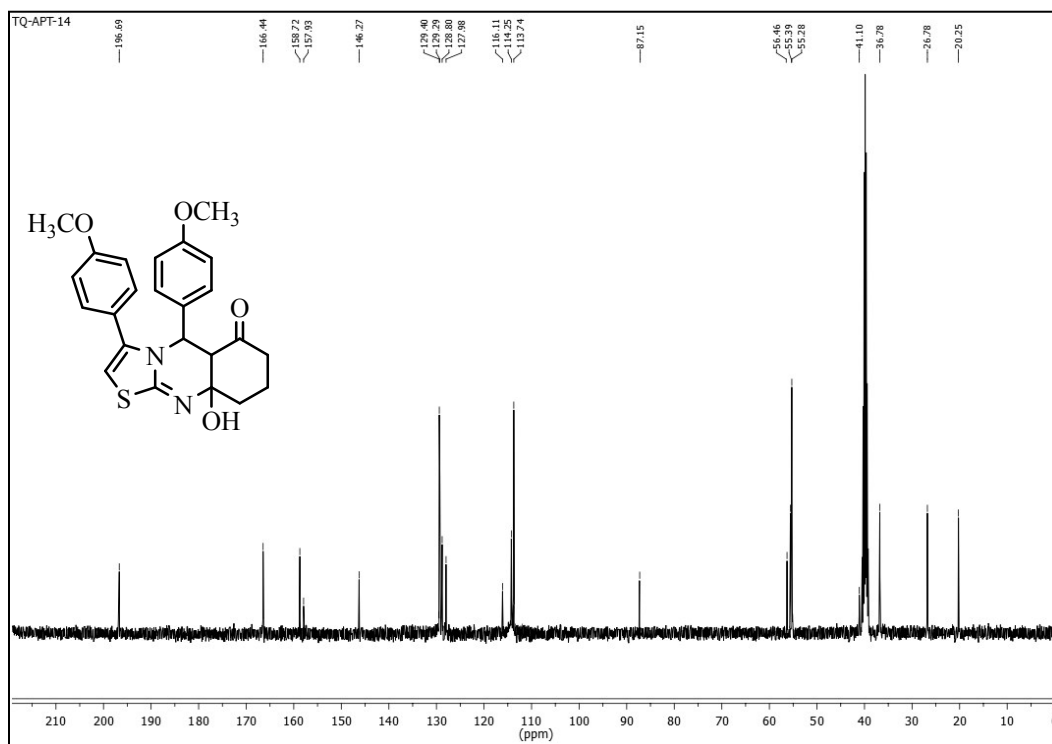


Figure S97. ^{13}C NMR spectrum of **5bo** in DMSO-d_6

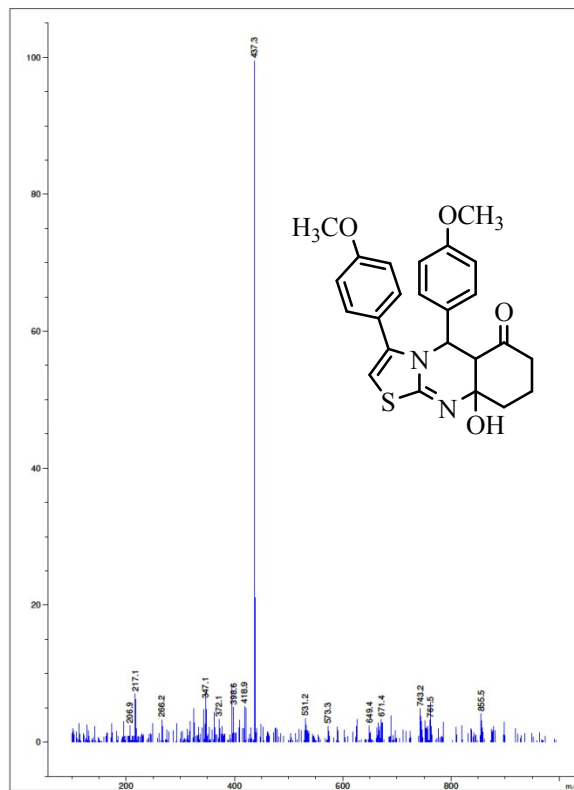


Figure S98. ESI-MS spectrum of **5bo**

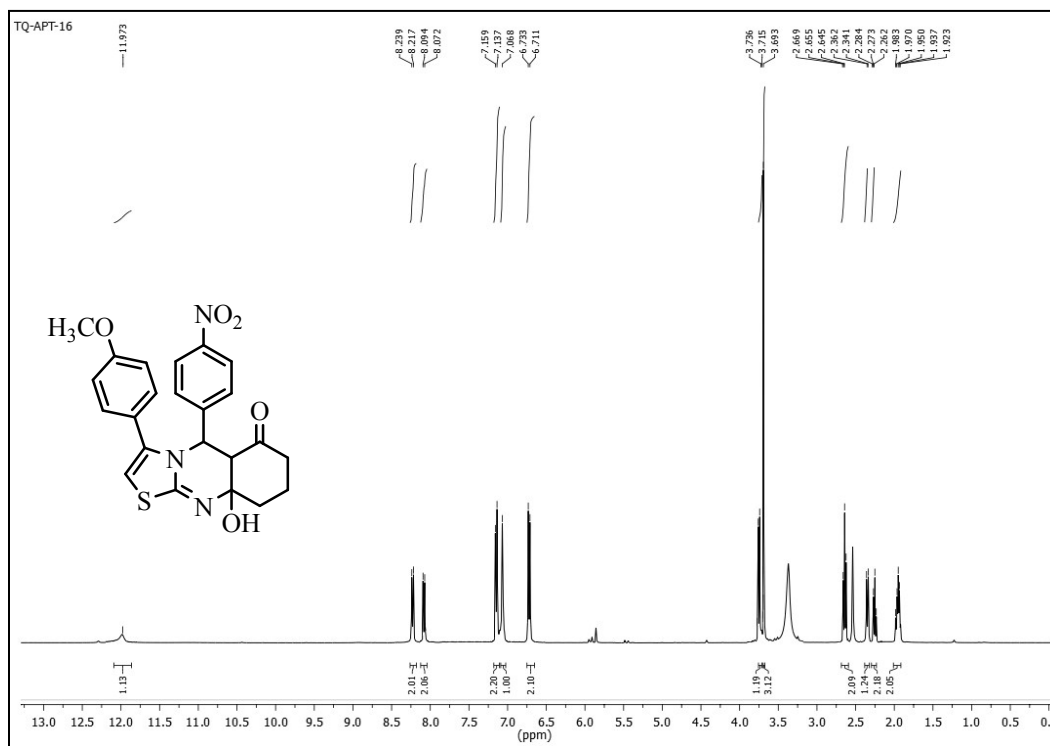


Figure S99. ^1H NMR spectrum of **5bp** in DMSO-d_6

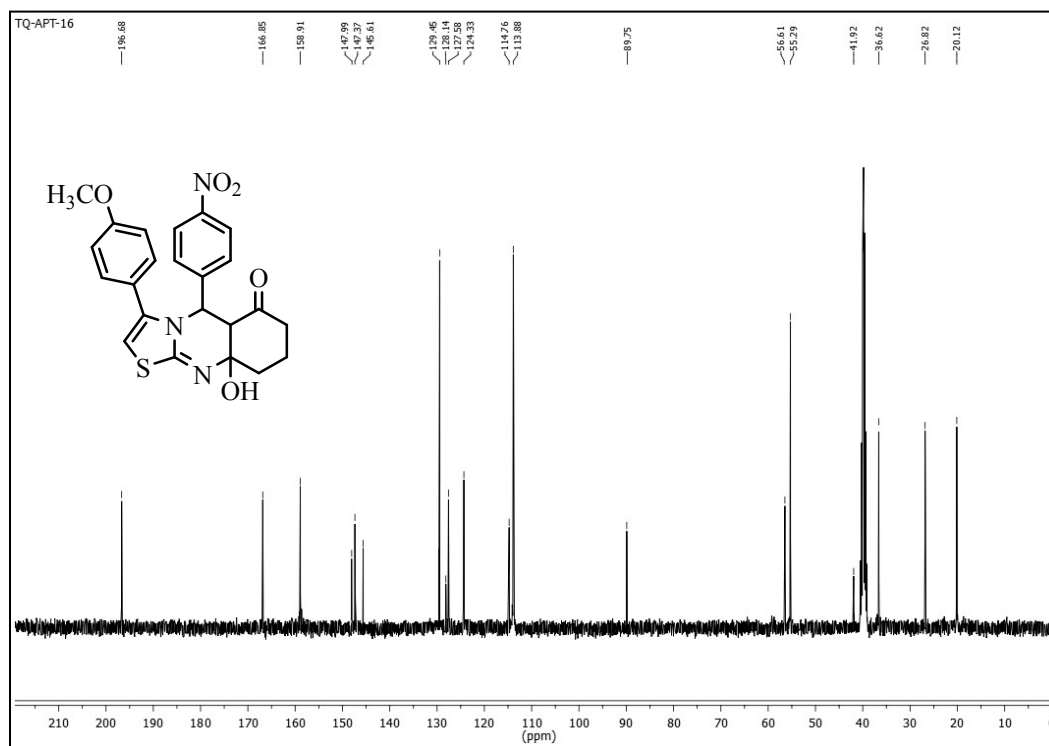


Figure S100. ^{13}C NMR spectrum of **5bp** in DMSO-d_6

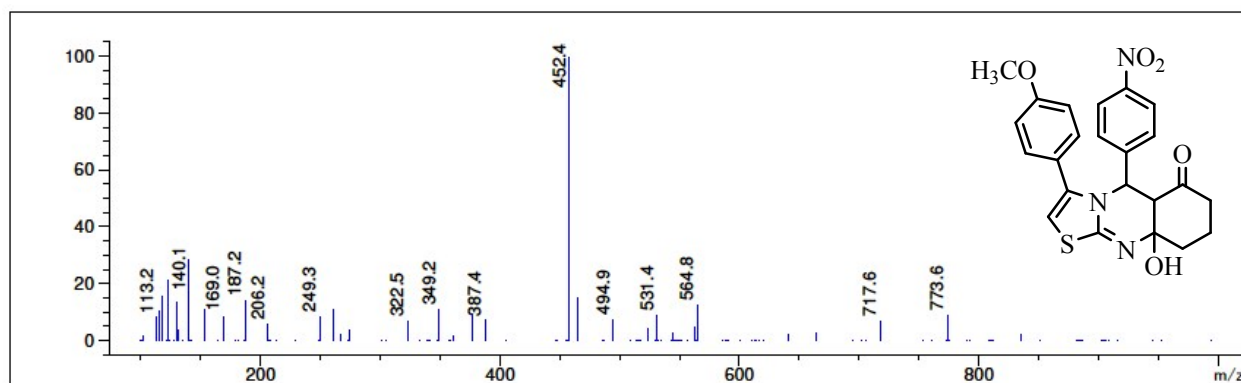


Figure S101. LC-MS spectrum of **5bp**

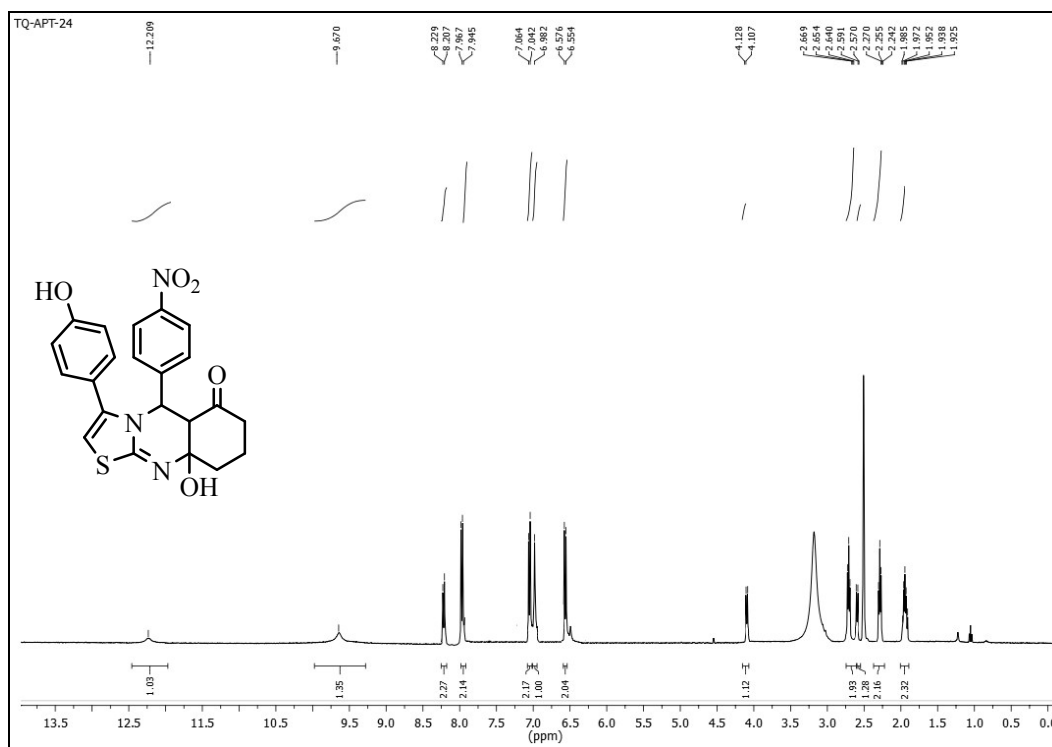


Figure S102. ^1H NMR spectrum of **5bq** in DMSO-d_6

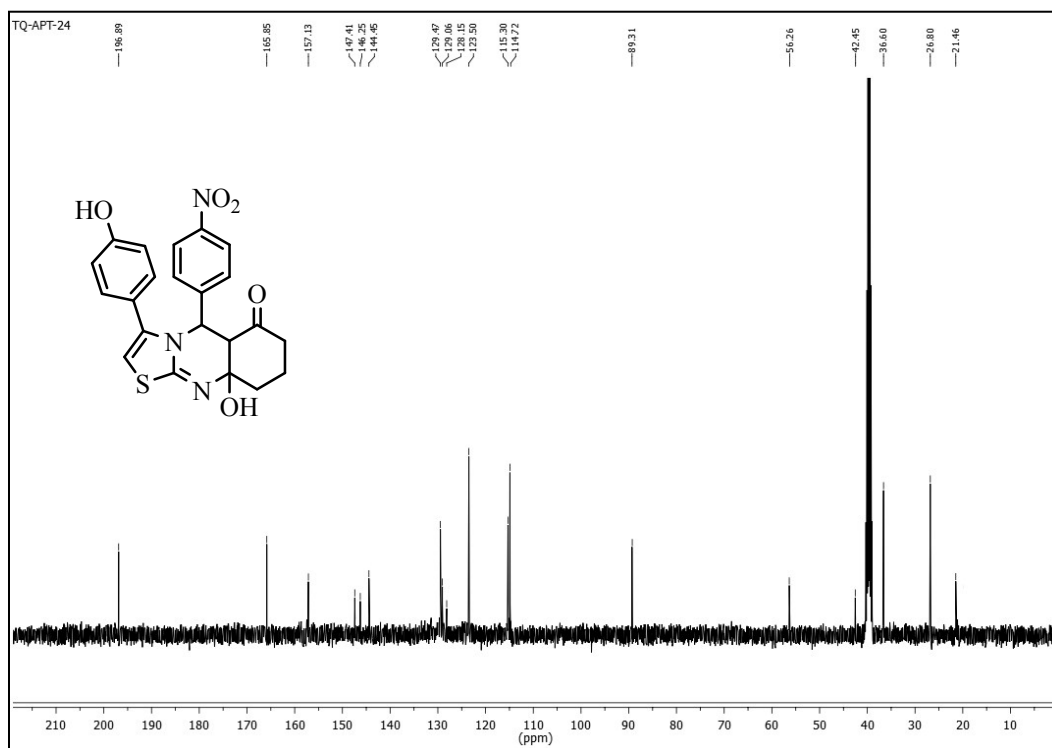


Figure S103. ^{13}C NMR spectrum of **5bq** in DMSO-d_6

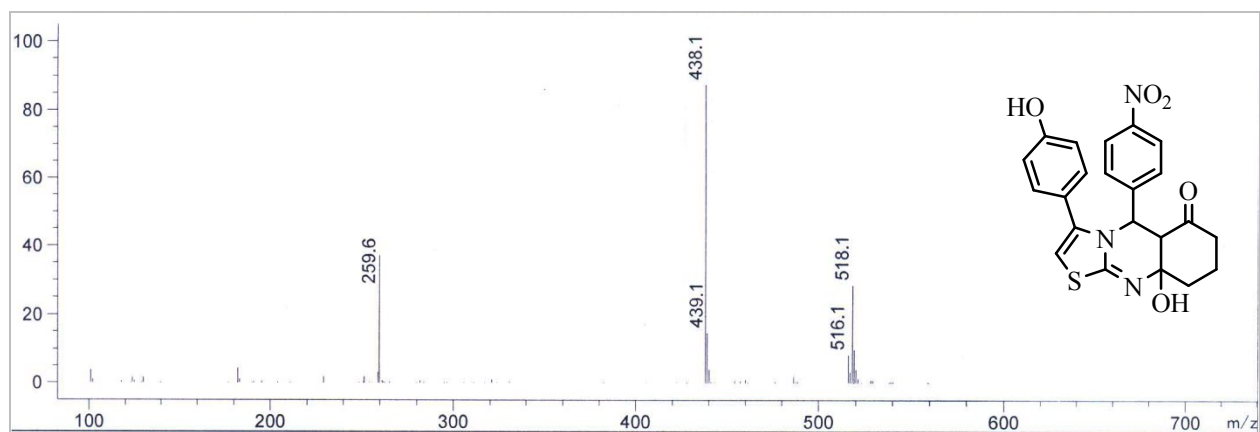


Figure S104. LC-MS spectrum of **5bq**

5. Table S1. Absorption and Emission maxima at 10 μ M conc. in MeOH.

entry	absorption λ_{\max} (nm)	emission λ_{\max} (nm)	entry	λ_{\max} (nm)	λ_{em} (nm)
5aa	406	466	5ba	406	466
5ab	378	464	5bb	406	464
5ac	406	466	5bc	408	468
5ad	370	466	5bd	402	466
5ae	406	466	5be	404	462
5af	276	462	5bf	348	390
5ag	406	464	5bg	406	464
5ah	400	464	5bh	400	466
5ai	276	358	5bi	280	354
5aj	404	462	5bj	400	454
5ak	404	462	5bk	404	462
5al	332	-	5bl	400	-
5am	406	464	5bm	404	464
5an	404	464	5bn	402	462
5ao	406	464	5bo	466	524
5ap	382	-	5bp	572	-
5aq	398	-	5bq	400	-