



Supporting Information

for

Eschenmoser coupling reactions starting from primary thioamides. When do they work and when not?

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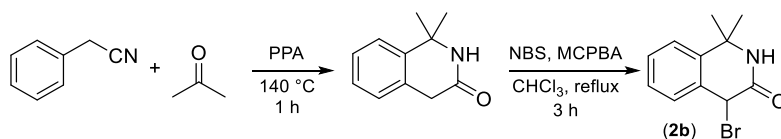
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Experimental part

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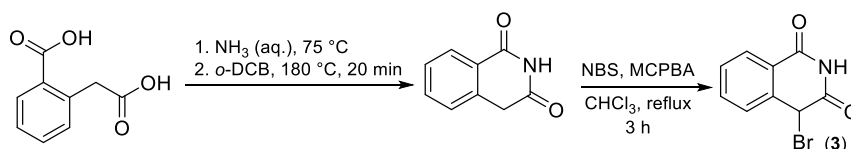
Synthesis of 4-bromo-1,1-dimethyl-1,4-dihydroisoquinoline-3(2H)-one (2b)



Polyphosphoric acid (450 g) was heated [1] to 135 °C in a 1-L-three-necked round-bottomed flask equipped with a reflux condenser and phenylacetonitrile (60 g, 0.51 mol) was added during 3 min under stirring. After 10 min, acetone (80 mL, 1.1 mol) was added dropwise during 1 hour and the reaction mixture was stirred at 140 °C for the next 1 hour. Then, another portion of acetone (15 mL) was added, the reaction mixture was stirred for 20 min, cooled, and poured into ice water (3 L). Extraction with dichloromethane (3 × 250 mL), washing of the combined organic layers with 5% aq. NaHCO₃ (2 × 250 mL), drying (anhydrous Na₂SO₄), and filtration of the organic phase through a plug of silica gel (60 g) gave a clear solution which was evaporated under reduced pressure. Yield 52 g (63%) of yellow solid 1,1-dimethyl-1,4-dihydroisoquinoline-3(2H)-one with m.p. 131-132 °C and ¹H NMR (500 MHz, CDCl₃) δ: 7.87 (bs, 1H, NH), 7.21 – 7.33 (m, 3H, Ar-H), 7.14 (d, *J* 7.2 Hz, 1H, Ar-H), 3.65 (s, 2H, CH₂), 1.60 (s, 6H, 2×CH₃) is in accord with ref. [2].

A solution of 1,1-dimethyl-1,4-dihydroisoquinoline-3(2H)-one (4.1 g, 23.4 mmol), *N*-bromosuccinimide (4.3 g, 24.3 mmol) and *m*-chlorobenzoic acid (0.6 g of 75% aq. solution) in CCl₄ (90 mL) was refluxed for 3.5 hours. The resulting yellow solution was washed with water (50 mL), 5% aq. NaHCO₃ (40 mL) and brine (50 mL) and dried with anhydrous Na₂SO₄. Evaporation of the solvent gave the crude product which was crystallized from hot acetonitrile/THF (2:1) with charcoal. Yield 3.9 g (66 %) of white crystalline **2b** with m.p. 206-207 °C. ¹H NMR (500 MHz, CDCl₃) δ: 8.01 (bs, 1H, NH), 7.36 – 7.43 (m, 2H, Ar-H), 7.29 – 7.36 (m, 2H, Ar-H), 5.52 (s, 1H, CH), 1.71 and 1.72 (2×s, 6H, 2×CH₃); ¹³C NMR (125 MHz, CDCl₃) δ: 167.3 (C=O), 141.2 (C), 131.5 (C), 129.8 (CH), 129.5 (CH), 128.1 (CH), 124.6 (CH), 57.0 (C), 41.7 (CH), 31.4 (CH₃), 30.4 (CH₃); HRMS: calcd. for C₁₁H₁₃BrNO [M+H⁺]: calcd. 254.0175, found 254.0178; Elemental analysis: calcd. C: 51.99, H: 4.76, N: 5.51, Br: 31.44; found C: 52.33, H: 4.77, N: 5.30, Br: 31.10.

Synthesis of 4-bromoisoquinoline-1,3(2H,4H)-dione (3)

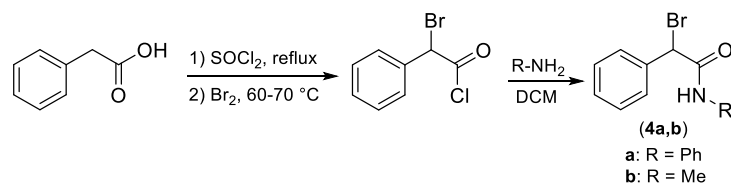


Homophthalic acid (10 g, 55.6 mmol) was mixed [3] with 25% aq. ammonia (15 mL, 0.2 mol), heated at 75 °C until complete dissolution, and then evaporated. The same operation was repeated once more with 25% aq. ammonia (10 mL, 0.13 mol). The resulting solid residue was suspended in *o*-chlorobenzene (25 mL) and heated at 175–180 °C for 20 min without a condenser. Then, the solvent was distilled off at 225 °C by bubbling of dry inert gas (nitrogen or argon) and the residue was dissolved in hot MeOH (30 mL). Cooling of the solution gave

6.8 g (71%) of isoquinoline-1,3(2*H*,4*H*)-dione as a white crystalline solid with mp. 237-238 °C and NMR spectra ¹H NMR (500 MHz, DMSO-*d*₆) δ (ppm): 11.30 (bs, 1H, NH), 8.01 (d, *J* 7.8 Hz, 1H, ArH), 7.64 (t, *J* 7.5 Hz, 1H, ArH), 7.45 (t, *J* 7.6 Hz, 1H, ArH), 7.37 (d, *J* 7.7 Hz, 1H, ArH), 4.03 (s, 2H, CH₂); ¹³C NMR (125 MHz, DMSO-*d*₆) δ (ppm): 171.1 (C=O), 165.5 (C=O), 136.8 (C), 133.6 (CH), 128.0 (CH), 127.6 (CH), 127.3 (CH), 125.1 (C), 36.1 (CH₂) both in accordance with ref. [4].

The above prepared isoquinoline-1,3(2*H*,4*H*)-dione (0.8 g, 5 mmol) was suspended in amylene-stabilized chloroform (60 mL) and *N*-bromosuccinimide (0.9 g, 5 mmol) together with *m*-chloroperoxybenzoic acid (0.12 g of 75% aq. solution) were added. The reaction mixture was refluxed for 3 h and then evaporated under vacuum. The solid residue was quickly crystallized from boiling acetonitrile and THF (10 + 1 mL) to give 0.8 g (65%) of pale brown crystals of compound **3** with mp. 174-176 °C. ¹H NMR (500 MHz, CDCl₃) δ: 8.52 (bs, 1H, NH), 8.22 (d, *J* 7.8 Hz, 1H, Ar-H), 7.72 (t, *J* 7.6 Hz, 1H, Ar-H), 7.55-7.62 (m, 2H, Ar-H), 5.66 (s, 1H, CH); ¹³C APT NMR (125 MHz, CDCl₃) δ (ppm): 167.6 (C=O), 163.1 (C=O), 136.5 (C), 134.8 (CH), 130.1 (CH), 129.5 (CH), 129.2 (CH), 123.8 (C), 38.1 (CH); HRMS: calcd. for C₉H₇BrNO₂ [M+H⁺]: calcd. 239.9655, found 239.9658; Elemental analysis: calcd. C: 45.03, H: 2.52, N: 5.83; found C: 45.09, H: 2.53, N: 5.50.

α-Bromo(phenyl)acetamides (**4a,b**)



A mixture [5] of phenylacetic acid (22 g, 160 mmol) and thionyl chloride (60 mL, 818 mmol) was refluxed for 1.5 h and then cooled to 35 °C. Bromine (9.8 mL, 192 mmol) and aq. hydrobromic acid (56%) (10 drops) were added and the resulting solution was heated at 60 °C for 1 h and then for 2 h at 70 °C. Excess of thionyl chloride was distilled off under reduced pressure (300–400 torr) to give an oily residue which was purified by distillation using a short column (bp 135-136 °C at 18 torr). Yield 31.2 g (91 %) of yellowish liquid. ¹H NMR (400 MHz, CDCl₃) δ: 7.44-7.53 (m, 2H, Ar-H), 7.36-7.44 (m, 3H, Ar-H), 5.66 (s, 1H, CH).

The corresponding amine (10 mmol) was dissolved in a mixture of dry DCM (25 mL) with pyridine (1 mL, 12 mmol). After cooling to –40 °C a solution of α-bromo(phenyl)acetyl chloride (2.2 g, 10 mmol) in DCM (10 mL) was added dropwise and the reaction mixture was stirred at –40 °C for 30 min and then for 2.5 h at room temperature. The reaction mixture was diluted with DCM (30 mL) and washed with aq. HCl (5%, 40 mL), water (30 mL), aq. NaHCO₃ (5%, 30 mL) and brine (30 mL). The organic layer was dried with anhydrous Na₂SO₄ and evaporated to obtain amides **4a,b**.

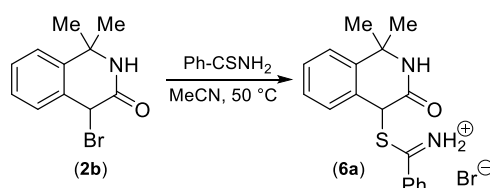
N-Phenyl-2-bromo(phenyl)acetamide (4a)

White crystalline solid (1.9 g, 65 %); mp. 142 – 143 °C (ref. [6] gives 144 – 145 °C); ¹H NMR (500 MHz, CDCl₃) δ: 8.34 (bs, 1H, NH), 7.48-7.56 (m, 4H, Ar-H), 7.30-7.41 (m, 5H, Ar-H), 7.16 (t, *J* 7.4, 1H, Ar-H), 5.56 (s, 1H, CH).

N-Methyl-2-bromo(phenyl)acetamide (4b)

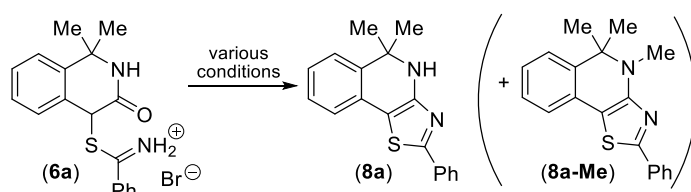
White crystalline solid crystallized from CHCl₃/n-hexane 1:2 (1.2 g, 52 %); mp. 94 – 96 °C (ref. [7] gives 99 – 100 °C); ¹H NMR (500 MHz, CDCl₃) δ: 7.41-7.46 (m, 2H, Ar-H), 7.30-7.40 (m, 3H, Ar-H), 6.70 (bs, 1H, NH), 2.90 (d, *J* 4.9, 3H, CH₃).

1,1-Dimethyl-3-oxo-1,2,3,4-tetrahydroisoquinolin-4-yl benzimidothioate hydrobromide (6a)



Compound **2b** (0.51 g, 2 mmol) was dissolved in acetonitrile (25 mL) at 50 °C and a hot solution (50 °C) of thiobenzamide (0.27 g, 2 mmol) in acetonitrile (5 mL) was added in one portion. The reaction mixture was stirred for 30 min at 50 °C and then cooled. The precipitated salt was filtered off, washed with cold acetonitrile (5 mL) and diethylether (10 mL). Yield 0.76 g (97%) of white solid with m.p. 176-177 °C. HRMS: calcd. for C₁₈H₁₉N₂OS [M+H⁺]: calcd. 311.1213, found 311.1216; Elemental analysis: calcd. C: 55.25, H: 4.89, N: 7.16, Br: 20.42; S: 8.19; found C: 55.15, H: 4.92, N: 7.12, S: 8.26, Br: 20.51. IR (cm⁻¹): 3025 (s), 2891 (s), 1635 (s), 1423 (m), 1329 (m), 767 (m).

Transformation of salt 6a to 5,5-dimethyl-2-phenyl-4,5-dihydrothiazolo[4,5-c]isoquinoline (8a) and 4,5,5-trimethyl-2-phenyl-4,5-dihydrothiazolo[4,5-c]isoquinoline (8a-Me)



In DMF:

Salt **6a** (100 mg, 0.25 mmol) was dissolved in DMF (0.5 mL) at room temperature and stirred for 12 h. The reaction mixture was then poured into cold water (50 mL) and extracted with EtOAc (2 × 10 mL). The organic layer was dried with anhydrous Na₂SO₄ and evaporated to give 90 mg (74%) of orange solid **8a** with mp 86-89 °C. ¹H NMR (500 MHz, CDCl₃) δ 7.86-7.94 (m, 2H, Ar-H), 7.35-7.42 (m, 3H, Ar-H), 7.19 (td, *J* 7.2 and 1.3 Hz, 2H, Ar-H), 7.13 (td, *J* 7.2 and 1.3 Hz, 2H, Ar-H), 4.62 (bs, 1H, NH), 1.56 (s, 6H, 2×CH₃); ¹³C NMR (125 MHz, CDCl₃) δ 164.4 (C), 155.4 (C), 136.5 (C), 133.7 (C), 129.8 (CH), 128.8 (CH), 128.4 (C), 127.5

(CH), 126.2 (CH), 125.8 (CH), 123.6 (CH), 122.3 (CH), 105.1 (C), 55.9 (C), 29.8 (CH₃); HRMS: calcd. for C₁₈H₁₇N₂S [M+H⁺]: calcd. 293.1113, found 293.1108; Elemental analysis: calcd. C: 73.94, H: 5.52, N: 9.58, S: 10.96; found C: 73.69, H: 5.56, N: 9.81, S: 11.02.

In MeCN:

Salt **6a** (400 mg, 1 mmol) was suspended in MeCN (30 mL) and stirred for 12 h at 70 °C in a tightly closed heavy-wall screw-capped vial. The resulting solution was neutralized with Et₃N (0.15 mL, 1.1 mmol) and evaporated with non-porous alumina. Column chromatography (silica gel, petrolether/EtOAc 4:1) gave 0.21 g (72%) of compound **8a** with the characteristics mentioned above.

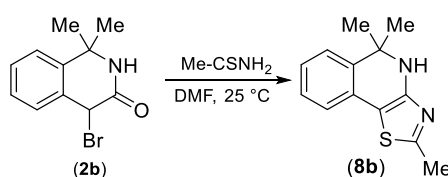
In (MeO)₃P:

Salt **6a** (186 mg, 0.5 mmol) was suspended in neat trimethyl phosphite (2 mL) and stirred without (entry 1 in the table below) or with an appropriate additive (TFA: entry 2; TEA: entry 3 in table below) for 12 h at 70 °C. The resulting solution was then diluted with CH₂Cl₂ (10 mL) and evaporated with non-porous alumina (5 g). The residue was submitted to column chromatography (silica gel) and eluted with hexane/EtOAc 95:5 to give **8a-Me** and then with hexane/EtOAc 60:40 to give product **8a** in the yields given below:

Entry	Additive (equiv)	Yield 8a mg (%)	Yield 8a-Me mg (%)	Overall yield 8a + 8a-Me (%)
1	None	53 (36)	26 (16)	52
2	CF ₃ COOH (0.8)	93 (61)	41(26)	87
3	Et ₃ N (0.7)	40 (27)	29 (18)	45

Compound **8a-Me**: mp 104-105 °C. ¹H NMR (500 MHz, CDCl₃) δ 7.94 (dd, *J* 8.2 and 1.2 Hz, 2H, Ar-H), 7.33-7.42 (m, 3H, Ar-H), 7.24 (d, *J* 7.8 Hz, 1H, Ar-H), 7.18 (dt, *J* 7.4 and 1.1 Hz, 1H, Ar-H), 7.08-7.13 (m, 2H, Ar-H), 3.27 (s, 3H, NCH₃), 1.56 (s, 6H, 2×CH₃); ¹³C NMR (125 MHz, CDCl₃) δ 162.8 (C), 157.6 (C), 136.2 (C), 134.0 (C), 129.5 (CH), 128.8 (CH), 128.7 (C), 127.5 (CH), 125.9 (CH), 125.8 (CH), 123.7 (CH), 122.0 (CH), 104.9 (C), 59.7 (C), 31.0 (NCH₃), 24.3 (CH₃); HRMS: calcd. for C₁₉H₁₉N₂S [M+H⁺]: calcd. 307.1264, found 307.1264; Elemental analysis: calcd. C: 74.47, H: 5.92, N: 9.14, S: 10.46; found C: 74.71, H: 5.90, N: 9.01, S: 10.42; IR (cm⁻¹): 3064 (m), 2975 (m), 1597 (m), 1550 (s), 1457 (m), 752 (m).

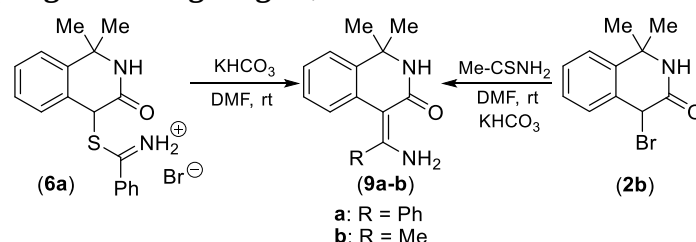
Synthesis of **8b**



Compound **2b** (254 mg, 1 mmol) was dissolved in DMF (1.5 mL) at 25 °C, then a solution of thioacetamide (75 mg, 1 mmol) in DMF (1 mL) was added in one portion and the mixtures

stirred for 16 h. All volatiles were evaporated in vacuo and the residue was dissolved in mixture of DCM and MeOH (3:1, 20 mL). The solution was co-evaporated with non-porous alumina (5 g) and the residue was submitted to column chromatography (silica gel) eluted with petrolether/EtOAc 4:1 – 2:1 to give **8b** with mp 104-107 °C. ¹H NMR (500 MHz, DMSO-*d*₆) δ 7.19 (d, *J* 7.5 Hz, 1H, Ar-H), 7.13 (t, *J* 7.5 Hz, 1H, Ar-H), 7.05 (t, *J* 7.5 Hz, 1H, Ar-H), 6.91 (d, *J* 7.5 Hz, 1H, Ar-H), 6.66 (bs, 1H, NH), 2.57 (s, 3H, CH₃), 1.44 (s, 6H, 2×CH₃); ¹³C NMR (125 MHz, DMSO-*d*₆) δ 163.2 (C), 155.4 (C), 136.1 (C), 128.7 (C), 127.3 (CH), 125.3 (CH), 123.6 (CH), 121.1 (CH), 100.2 (C), 55.2 (C), 29.8 (CH₃), 19.4 (CH₃); HRMS: calcd. for C₁₃H₁₅N₂S [M+H⁺]: calcd. 231.0951, found 231.0951; Elemental analysis: calcd. C: 67.79, H: 6.13, N: 12.16, S: 13.92; found C: 67.42, H: 6.16, N: 12.31, S: 14.02.

Eschenmoser coupling reaction giving **9a,b**



Salt **6a** (300 mg, 0.77 mmol) and finely powdered K₂CO₃ (230 mg, 2.3 mmol) were suspended in DMF (5 mL) and stirred in screw-capped vial for 48 h at room temperature. Then, DCM (10 mL) was added and the reaction mixture was filtered. The solid residue was washed with DCM (10 mL) and the combined filtrates were co-evaporated with non-porous alumina (5 g) and subjected to automated flash chromatography (25 g column with spherical SiO₂; hexane/EtOAc - gradient 10–100% EtOAc) to give product **9a**.

(Z)-4-(Amino(phenyl)methylidene)-1,1-dimethyl-1,4-dihydroisoquinolin-3(2H)-one (**9a**)

Yellow crystalline solid (132 mg, 62 %); mp 227 – 229 °C; ¹H NMR (500 MHz, CDCl₃) δ: 9.60 (bs, 1H, ½NH₂), 7.35-7.43 (m, 3H, Ar-H_{o+p}), 7.29-7.34 (m, 2H, Ar-H_m), 7.15 (dd, *J* 7.7 and 0.9 Hz, 1H, Ar-H₈), 6.91 (dt, *J* 7.6 and 1.1 Hz, 1H, Ar-H), 6.71 (dt, *J* 7.6 and 1.2 Hz, 1H, Ar-H), 6.41 (dd, *J* 8.0 and 0.8 Hz, 1H, Ar-H₅), 5.76 (bs, 1H, NH), 5.58 (bs, 1H, ½NH₂), 1.62 (s, 6H, 2×CH₃); ¹³C NMR (125 MHz, CDCl₃) δ (ppm): 171.1 (C=O), 156.1 (C), 139.3 (C), 138.7 (C), 133.2 (C), 129.6 (CH), 128.9 (CH), 128.7 (CH), 128.4 (CH), 125.6 (CH), 123.6 (CH), 121.9 (CH), 96.7 (C), 54.3 (C), 29.5 (CH₃); HRMS: calcd. for C₁₈H₁₉N₂O [M+H⁺]: calcd. 279.1492, found 279.1490; Elemental analysis: calcd. C: 77.67, H: 6.52, N: 10.06; found C: 77.66, H: 6.56, N: 10.32.

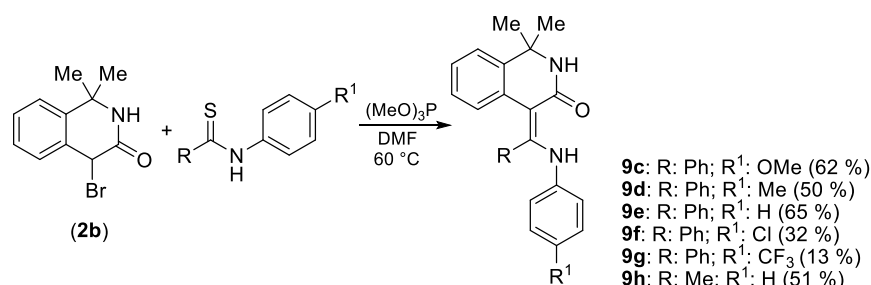
Compound **9b** was prepared from **2b** and thioacetamide without the isolation of intermediary salt **6b** as follows. Compound **2b** (0.51 g, 2 mmol) was dissolved in DMF (2 mL) at room temperature and a solution of thioacetamide (0.15 g, 2 mmol) in 1.5 mL of DMF was added in one portion. Then, finely powdered K₂CO₃ (0.6 g, 6 mmol) was added and the reaction mixture was stirred at 25 °C for 48 h. Then, the reaction mixture was diluted with MeCN (25 mL) and filtered through a plug of celite. All volatiles were evaporated, the residue was dissolved in

MeOH (20 mL), and co-evaporated again with non-porous alumina (5 g). Column chromatography (silica gel, petrolether/EtOAc 50:50–0:100 and then MeOH/EtOAc 5:95) gave compound **9b**.

(Z)-4-(1-Aminoethylidene)-1,1-dimethyl-1,4-dihydroisoquinolin-3(2H)-one (**9b**)

White crystalline solid (209 mg, 48 %); mp 186 – 188 °C; ^1H NMR (500 MHz, CDCl_3) δ : 9.24 (vbs, 1H, $\frac{1}{2}\text{NH}_2$), 7.16–7.24 (m, 2H, Ar-H), 7.12 (d, J 7.3 Hz, 1H, Ar-H), 7.07 (t, J 7.5 Hz, 1H, Ar-H), 5.82 (bs, 1H, NH), 4.55 (vbs, 1H, $\frac{1}{2}\text{NH}_2$), 2.25 (s, 3H, CH_3), 1.50 (s, 6H, $2\times\text{CH}_3$); ^{13}C NMR (125 MHz, CDCl_3) δ (ppm): 171.2 (C), 153.8 (C), 139.9 (C), 133.6 (C), 126.6 (CH), 126.1 (CH), 123.8 (CH), 122.1 (CH), 97.0 (C), 54.2 (C), 29.3 (CH_3), 21.8 (CH_3); HRMS: calcd. for $\text{C}_{13}\text{H}_{17}\text{N}_2\text{O}$ [$\text{M}+\text{H}^+$]: calcd. 217.1335, found 217.1338; Elemental analysis: calcd. C: 72.19, H: 7.46, N: 12.95; found C: 71.94, H: 7.46, N: 12.91.

Synthesis of **9c–h**



Compound **2b** (0.51 g, 2 mmol) was dissolved in DMF (5 mL) at room temperature and a solution of the corresponding secondary thioamide (2 mmol in 1.5 mL of DMF) was added in one portion. After 5 min, trimethyl phosphite (295 μL , 2.5 mmol, 1.25 equiv) was added and the reaction mixture was stirred at 60 °C for 16 h. Then, all volatiles were evaporated, the residue was dissolved in $\text{CHCl}_3/\text{EtOH}$ (1:1, 10 mL), and co-evaporated again with non-porous alumina (5 g). Column chromatography (silica gel, *n*-hexane/EtOAc 6:1–4:1) gave compounds **9c–h**.

(Z)-4-[[4-Methoxyphenyl]amino][phenyl]methylidene-1,1-dimethyl-1,4-dihydroisoquinolin-3(2H)-one (**9c**)

Yellow solid (477 mg, 62 %); mp 209 – 211 °C; ^1H NMR (500 MHz, CDCl_3) δ : 11.76 (bs, 1H, NH), 7.21–7.27 (m, 3H, Ar-H), 7.11–7.21 (m, 3H, Ar-H), 6.91 (t, J 7.5, 1H, Ar-H), 6.69 (t, J 7.6 Hz, 1H, Ar-H), 6.55–6.65 (m, 4H, Ar-H), 6.33 (d, J 8.0 Hz, 1H, Ar-H), 6.00 (s, 1H, Ar-H), 3.68 (s, 3H, OCH_3), 1.64 (s, 6H, $2\times\text{CH}_3$); ^{13}C NMR (125 MHz, CDCl_3) δ (ppm): 171.3 (C), 155.3 (C), 153.5 (C), 139.9 (C), 134.6 (C), 133.7 (C), 133.1 (C), 130.9 (CH), 129.0 (CH), 128.8 (CH), 128.5 (CH), 125.5 (CH), 113.6 (CH), 99.7 (C), 55.3 (OCH_3), 54.3 (C), 29.2 (CH_3); HRMS: calcd. for $\text{C}_{25}\text{H}_{25}\text{N}_2\text{O}_2$ [$\text{M}+\text{H}^+$]: calcd. 385.1911, found 385.1910; Elemental analysis: calcd. C: 78.10, H: 6.29, N: 7.29; found C: 78.30, H: 6.37, N: 7.36.

(Z)-4-[[4-(4-Methylphenyl)amino][phenyl]methylidene]-1,1-dimethyl-1,4-dihydroisoquinolin-3(2H)-one (9d)

Crude product obtained after chromatography was crystallized from MeOH/CHCl₃ (5:1). Yellow solid (368 mg, 50 %); mp 253 – 254 °C; ¹H NMR (500 MHz, CDCl₃) δ: 11.78 (bs, 1H, NH), 7.23-7.30 (m, 3H, Ar-H), 7.17-7.23 (m, 2H, Ar-H), 7.16 (d, *J* 7.6, 1H, Ar-H), 6.92 (t, *J* 7.4 Hz, 1H, Ar-H), 6.84 (d, *J* 7.9 Hz, 2H, Ar-H), 6.69 (t, *J* 7.5 Hz, 1H, Ar-H), 6.53 (d, *J* 8.0 Hz, 2H, Ar-H), 6.34 (d, *J* 7.9 Hz, 1H, Ar-H), 5.86 (s, 1H, Ar-H), 2.18 (s, 3H, CH₃), 1.65 (s, 6H, 2×CH₃); ¹³C NMR (125 MHz, CDCl₃) δ (ppm): 171.2 (C), 152.8 (C), 140.0 (C), 138.0 (C), 134.7 (C), 133.1 (C), 132.0 (C), 130.8 (CH), 129.1 (CH), 129.0 (CH), 128.9 (CH), 128.6 (CH), 125.6 (CH), 123.8 (CH), 122.7 (CH), 121.8 (CH), 100.3 (C), 54.4 (C), 29.2 (CH₃), 20.7 (CH₃); HRMS: calcd. for C₂₅H₂₅N₂O [M+H⁺]: calcd. 369.1961, found 369.1960; Elemental analysis: calcd. C: 81.49, H: 6.57, N: 7.60; found C: 81.48, H: 6.52, N: 7.77.

(Z)-1,1-Dimethyl-4-[phenyl(phenylamino)methylidene]-1,4-dihydroisoquinolin-3(2H)-one (9e)

Yellow solid (461 mg, 65 %); mp 231 – 232 °C; ¹H NMR (500 MHz, CDCl₃) δ: 11.81 (bs, 1H, NH), 7.24-7.30 (m, 3H, Ar-H), 7.18-7.23 (m, 2H, Ar-H), 7.16 (d, *J* 7.7, 1H, Ar-H), 7.03 (t, *J* 7.7 Hz, 1H, Ar-H), 6.93 (t, *J* 7.4 Hz, 2H, Ar-H), 6.84 (t, *J* 7.3 Hz, 1H, Ar-H), 6.70 (t, *J* 7.5 Hz, 2H, Ar-H), 6.62 (d, *J* 7.8 Hz, 1H, Ar-H), 6.36 (d, *J* 7.9 Hz, 1H, Ar-H), 6.26 (s, 1H, Ar-H), 1.65 (s, 6H, 2×CH₃); ¹³C NMR (125 MHz, CDCl₃) δ (ppm): 171.2 (C), 152.1 (C), 140.7 (C), 140.3 (C), 134.5 (C), 132.9 (C), 130.8 (CH), 129.2 (CH), 129.0 (CH), 128.6 (CH), 128.4 (CH), 125.6 (CH), 124.0 (CH), 122.4 (CH), 122.3 (CH), 121.8 (CH), 101.1 (C), 54.4 (C), 29.1 (CH₃); HRMS: calcd. for C₂₄H₂₂N₂O [M+H⁺]: calcd. 355.1805, found 355.1806; Elemental analysis: calcd. C: 81.33, H: 6.26, N: 7.90; found C: 81.16, H: 6.30, N: 7.93.

(Z)-4-[[4-(4-Chlorophenyl)amino][phenyl]methylidene]-1,1-dimethyl-1,4-dihydroisoquinolin-3(2H)-one (9f)

Yellow solid (251 mg, 32 %); mp 222 – 224 °C; ¹H NMR (500 MHz, CDCl₃) δ: 11.78 (bs, 1H, NH), 7.27-7.33 (m, 1H, Ar-H), 7.20-7.26 (m, 4H, Ar-H), 7.17 (d, *J* 7.7, 1H, Ar-H), 6.90-7.03 (m, 3H, Ar-H), 6.71 (t, *J* 7.4 Hz, 1H, Ar-H), 6.53 (d, *J* 8.6 Hz, 2H, Ar-H), 6.36 (d, *J* 7.9 Hz, 1H, Ar-H), 6.25 (s, 1H, Ar-H), 1.65 (s, 6H, 2×CH₃); ¹³C NMR (125 MHz, CDCl₃) δ (ppm): 171.1 (C), 151.5 (C), 140.3 (C), 139.4 (C), 134.2 (C), 132.6 (C), 130.7 (CH), 129.4 (CH), 129.0 (CH), 128.8 (CH), 128.4 (C), 127.4 (CH), 125.7 (CH), 124.3 (CH), 123.4 (CH), 121.9 (CH), 101.7 (C), 54.5 (C), 29.2 (CH₃); HRMS: calcd. for C₂₄H₂₂ClN₂O [M+H⁺]: calcd. 389.1415, found 389.1417; Elemental analysis: calcd. C: 74.12, H: 5.44, N: 7.20; found C: 74.34, H: 5.46, N: 7.09.

(Z)-4-[[4-(4-Trifluoromethylphenyl)amino][phenyl]methylidene]-1,1-dimethyl-1,4-dihydroisoquinolin-3(2H)-one (9g)

Crude product obtained after chromatography was crystallized from MeOH/EtOAc (2:1). Yellow solid (112 mg, 13 %); mp 234 – 236 °C; ¹H NMR (500 MHz, CDCl₃) δ: 11.86 (bs, 1H, NH), 7.32-7.37 (m, 1H, Ar-H), 7.23-7.30 (m, 6H, Ar-H), 7.19 (d, *J* 7.7, 1H, Ar-H), 6.98 (t, *J*

7.4 Hz, 1H, Ar-H), 6.74 (d, *J* 7.5 Hz, 2H, Ar-H), 6.60 (d, *J* 8.3 Hz, 2H, Ar-H), 6.40 (d, *J* 7.9 Hz, 1H, Ar-H), 6.06 (s, 1H, Ar-H), 1.67 (s, 6H, 2×CH₃); ¹³C NMR (125 MHz, CDCl₃) δ (ppm): 170.9 (C), 150.3 (C), 144.1 (C), 140.6 (C), 134.0 (C), 132.2 (C), 130.6 (CH), 129.7 (CH), 129.2 (CH), 129.0 (CH), 125.8 (CH), 125.7 (C, q, ³*J*_{C-F} = 3.7 Hz), 124.7 (CH), 124.3 (C, q, ¹*J*_{C-F} = 269.5 Hz), 123.4 (C, q, ²*J*_{C-F} = 32.7 Hz), 122.01 (CH), 121.0 (CH), 103.2 (C), 54.7 (C), 29.4 (CH₃); HRMS: calcd. for C₂₅H₂₂F₃N₂O [M+H⁺]: calcd. 423.1679, found 423.1682; Elemental analysis: not measured due to fluorine content damaging column.

(Z)-1,1-Dimethyl-4-[1-(phenylamino)ethylidene]-1,4-dihydroisoquinolin-3(2H)-one (9h)

Yellow solid (296 mg, 51 %); mp 191 – 193 °C; ¹H NMR (500 MHz, CDCl₃) δ: 12.05 (bs, 1H, NH), 7.34 (t, *J* 7.7 Hz, 1H, Ar-H), 7.20-7.27 (m, 3H, Ar-H), 7.14-7.19 (m, 3H, Ar-H), 7.07-7.12 (m, 1H, Ar-H), 5.74 (s, 1H, Ar-H), 2.34 (s, 3H, CH₃), 1.55 (s, 6H, 2×CH₃); ¹³C NMR (125 MHz, CDCl₃) δ (ppm): 171.3 (C), 153.5 (C), 140.1 (C), 139.7 (C), 133.6 (C), 128.9 (CH), 127.0 (CH), 126.2 (CH), 125.0 (CH), 124.7 (CH), 124.0 (CH), 122.2 (CH), 98.4 (CH), 54.3 (C), 29.4 (CH₃), 19.5 (CH₃); HRMS: calcd. for C₁₉H₂₁N₂O [M+H⁺]: calcd. 293.1648, found 293.1646; Elemental analysis: calcd. C: 78.05, H: 6.89, N: 9.57; found C: 78.32, H: 7.00, N: 9.35.

Synthesis of 11a–c

Compound **3** (0.24 g, 1 mmol) was dissolved in DMF (1.5 mL) at room temperature and a solution of the corresponding thioamide (1 mmol) in DMF (1.5 mL) was added in one portion and stirred for 12 h at room temperature. Then, all volatiles were evaporated with non-porous alumina (2 g), and the residue was submitted to flash column chromatography (silica gel cartridge, CH₂Cl₂/MeOH gradient 0–8% during 15 min) giving compounds **11a–c**.

(Z)-4-(Amino(phenyl)methylidene)isoquinoline-1,3(2H,4H)-dione (11a)

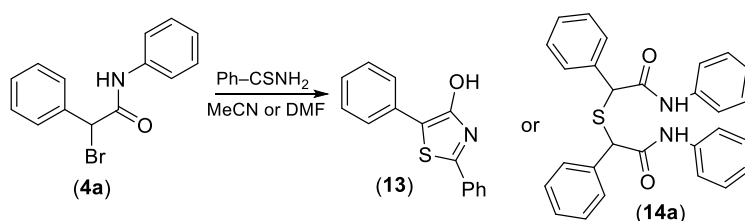
Yellow solid (0.2 g, 75 %); mp 282 – 283 °C; ¹H NMR (500 MHz, DMSO-*d*₆) δ: 11.08 (bs, 1H, NH), 10.80 (bd, *J* 2.8 Hz, 1H, ½NH₂), 8.60 (bd, *J* 2.4 Hz, 1H, ½NH₂), 7.93 (dd, *J* 7.6 and 1.6 Hz, 1H, Ar-H), 7.57 (t, *J* 7.4 Hz, 1H, Ar-H), 7.49 (t, *J* 7.6, 2H, Ar-H_m), 7.42 (d, *J* 7.2 Hz, 2H, Ar-H_o), 6.93-7.03 (m, 2H, Ar-H), 6.32 (d, *J* 8.0 Hz, 1H, Ar-H); ¹³C NMR APT (125 MHz, DMSO-*d*₆) δ (ppm): 166.9 (C=O), 166.1 (C=O), 163.9 (C), 137.7 (C), 137.4 (C), 131.0 (CH), 130.7 (CH), 129.3 (CH), 128.6 (CH), 127.2 (CH), 125.5 (CH), 122.7 (CH), 122.4 (C), 92.4 (C); HRMS: calcd. for C₁₆H₁₃N₂O₂ [M+H⁺]: calcd. 265.0972, found 265.0974; Elemental analysis: calcd. C: 72.72, H: 4.58, N: 10.60; found C: 72.55, H: 4.51, N: 10.40.

(Z)-4-(1-Aminoethylidene)isoquinoline-1,3(2H,4H)-dione (11b)

Light yellow solid (0.16 g, 78 %); mp 278 – 280.5 °C; ¹H NMR (500 MHz, DMSO-*d*₆) δ: 10.87 (bs, 1H, NH), 10.80 (bs, 1H, ½NH₂), 8.47 (bs, 1H, ½NH₂), 8.03 (d, *J* 7.8 Hz, 1H, Ar-H), 7.61 (d, *J* 8.3 Hz, 1H, Ar-H), 7.53 (t, *J* 7.7, 2H, Ar-H), 7.18 (t, *J* 7.3 Hz, 1H, Ar-H), 2.51 (s, 3H, CH₃); ¹³C NMR (125 MHz, DMSO-*d*₆) δ (ppm): 166.4, 165.9, 163.7, 138.0, 132.2, 127.5, 124.7, 122.1, 93.2, 23.8; HRMS: calcd. for C₁₁H₁₁N₂O₂ [M+H⁺]: calcd. 203.0815, found 203.0816; Elemental analysis: calcd. C: 65.34, H: 4.98, N: 13.85; found C: 65.40, H: 4.95, N: 13.99.

(Z)-4-(Phenyl(phenylamino)methylidene)isoquinoline-1,3(2H,4H)-dione (11c)

Yellow solid (0.3 g, 91 %); mp 268 – 270 °C; ¹H NMR (500 MHz, DMSO-*d*₆) δ: 13.12 (bs, 1H, NH), 11.41 (bs, 1H, NH), 7.97 (d, *J* 7.7 Hz, 1H, Ar-H), 7.44 (t, *J* 7.2 Hz, 1H, Ar-H), 7.24-7.39 (m, 4H, Ar-H), 7.15 (t, *J* 7.8, 2H, Ar-H), 7.01-7.08 (m, 2H, Ar-H), 6.96 (t, *J* 7.7 Hz, 1H, Ar-H), 6.86 (d, *J* 7.8 Hz, 2H, Ar-H) 6.25 (d, *J* 8.2 Hz, 1H, Ar-H); ¹³C NMR APT (125 MHz, DMSO-*d*₆) δ (ppm): 167.7 (C=O), 163.8 (C=O), 161.7 (C), 138.4 (C), 136.9 (C), 133.5 (C), 131.1 (CH), 130.5 (CH), 130.2 (CH), 129.4 (CH), 128.8 (CH), 127.3 (CH), 126.1 (CH), 125.4 (CH), 125.1 (CH), 123.5 (CH), 123.2 (C), 96.1 (C); HRMS: calcd. for C₂₂H₁₇N₂O₂ [M+H⁺]: calcd. 341.1285, found 341.1288; Elemental analysis: calcd. C: 77.63, H: 4.74, N: 8.23; found C: 77.90, H: 4.66, N: 8.19.

Experiments with 4a

N-Phenyl-2-bromo(phenyl)acetamide (**4a**, 145 mg, 0.5 mmol) was dissolved in MeCN or DMF (2.5 mL) and a solution of thiobenzamide (69 mg, 0.5 mmol) in the same solvent (2.5 ml) was added in one portion. The reaction mixture was stirred for 16 h at room temperature. In some experiments the base/thiophilic agent were also present. The crude reaction mixture was evaporated under vacuum and a sample was subjected to ¹H NMR analysis (see Table 3 in the main text). Pure constituents present in reaction mixture were obtained using column chromatography (silica gel, petrolether/DCM/EtOAc 250:100:40).

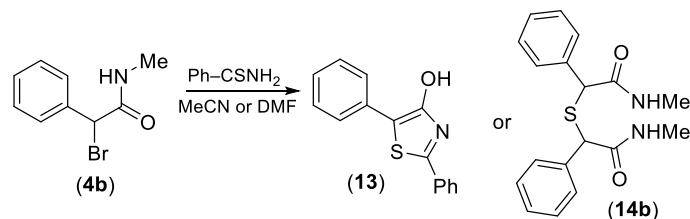
4-Hydroxy-2,5-diphenyl-1,3-thiazole (**13**) and thiobenzamide were identified by comparison of their ¹H and ¹³C NMR spectra in DMSO-*d*₆ with original samples prepared previously [8] in our laboratory.

2,2'-Thiobis(N-phenyl-2-phenylacetamide) (14a)

White solid (48 mg, 21 %); mp 212 – 215 °C; ¹H NMR (500 MHz, DMSO-*d*₆) δ: 10.22 and 10.26 (2×bs, 2H, 2×NH), 7.56 and 7.52 (2×d, *J* 7.9 and 7.5 Hz, 4H, Ar-H), 7.44-7.50 (m, 4H, Ar-H), 7.22-7.42 (m, 10H, Ar-H), 7.06 and 7.03 (2×t, *J* 7.4 Hz, 2H, Ar-H), 4.69 and 4.63 (2×s, 1H, 2×CH); ¹³C NMR (125 MHz, DMSO-*d*₆) δ (ppm): 167.7 and 167.6 (C=O), 138.8 and 138.7 (C), 137.4 and 137.2 (C), 128.9 and 128.8 (CH), 128.8 and 128.7 (CH), 128.4 and 128.3 (CH), 128.2 and 128.1 (CH), 123.9 and 123.8 (CH), 119.6, 119.5 (CH), 53.8 and 53.5 (CH); HRMS: calcd. for C₂₈H₂₅N₂O₂S [M+H⁺]: calcd. 453.1631, found 453.1639; Elemental analysis: calcd. C: 74.31, H: 5.35, N: 6.19, S: 7.09; found C: 74.64, H: 5.42, N: 5.82, S: 7.22.

Note: Both NMR spectra consist of two close sets of signals mutually approaching at heating. Unfortunately, the coalescence was not attained even at the highest temperature (75 °C) of measurement. Another explanation involves two sets of signals for diastereoisomers (set of two enantiomers and *meso*-form).

Experiments with 4b



N-Methyl-2-bromo(phenyl)acetamide (456 mg, 2 mmol) was dissolved in MeCN (10 mL) and a solution of thiobenzamide (274 mg, 2 mmol) in MeCN (5 mL) was added, followed by finely powdered KHCO₃ (600 mg, 6 mmol). The reaction mixture was stirred for 16 h at room temperature. Reaction contents were then filtered, and the filter cake washed with additional MeCN (5 mL). The filtrate was evaporated in vacuo with non-porous alumina (5 g) and subsequent column chromatography (silica gel, DCM/EtOAc/MeOH 30:10:1) gave yellow solid (124 mg) which was triturated with CHCl₃ (3 mL) and filtered.

4-Hydroxy-2,5-diphenyl-1,3-thiazole (**13**) and thiobenzamide were identified by comparison of their ¹H and ¹³C NMR spectra in DMSO-*d*₆ with original samples prepared previously [8] in our laboratory.

2,2'-Thiobis(*N*-methyl-2-phenylacetamide) (**14b**)

White solid (104 mg, 16 %); mp 223 – 226 °C; ¹H NMR (500 MHz, DMSO-*d*₆) δ: 8.16 and 8.05 (2×bq, *J* 4.5 Hz, 1H, NH), 7.25–7.43 (m, 5H, Ar-H), 4.36 and 4.26 (2×s, 1H, CH-S), 2.59 and 2.48 (2×d, *J* 4.5 Hz, 3H, CH₃); ¹³C NMR (125 MHz, DMSO-*d*₆) δ (ppm): 169.2 and 169.2 (C=O), 137.9 and 137.7, 128.4 and 128.1 (CH), 128.3 and 127.7 (CH), 127.7 and 127.5 (CH), 53.2 and 53.0 (CH), 26.0 and 25.8 (CH₃); HRMS: calcd. for C₁₈H₂₁N₂O₂S [M+H⁺]: calcd. 329.1318, found 329.1323; Elemental analysis: calcd. C: 65.83, H: 6.14, N: 8.53, S: 9.76; found C: 65.72, H: 6.18, N: 8.89, S: 9.42.

Note: Both NMR spectra consist of two close sets of signals (ratio 1:4) mutually approaching at heating. Unfortunately, the coalescence was not attained even at the highest temperature (75 °C) of measurement. Another explanation involves two sets of signals for diastereoisomers (set of two enantiomers and *meso*-form).

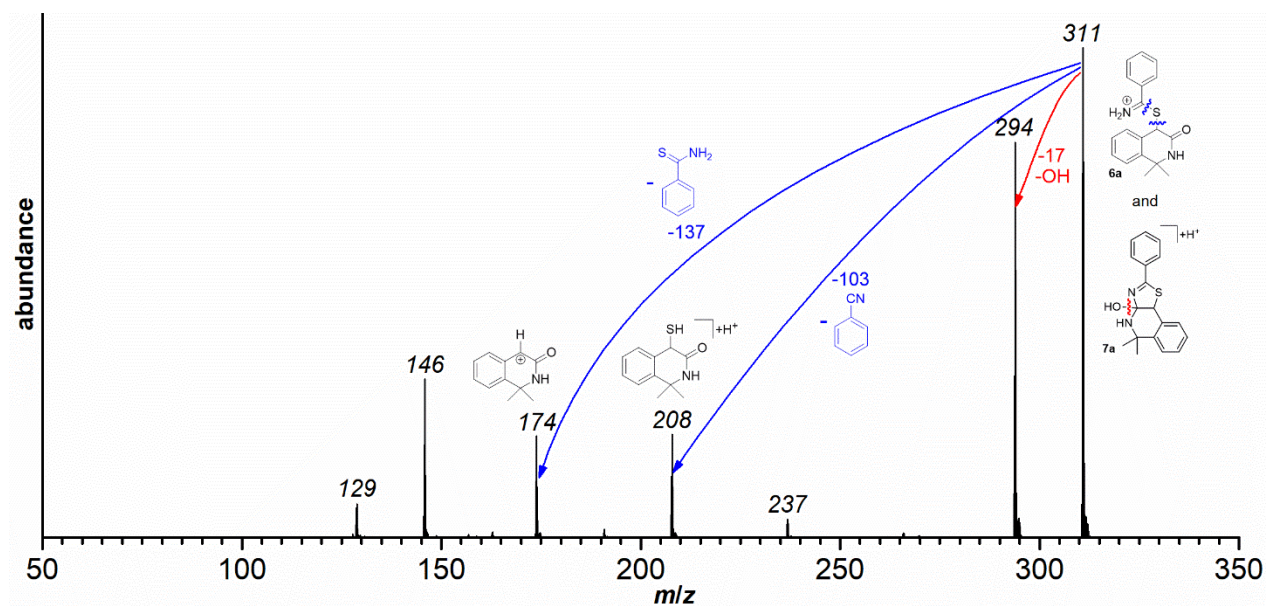
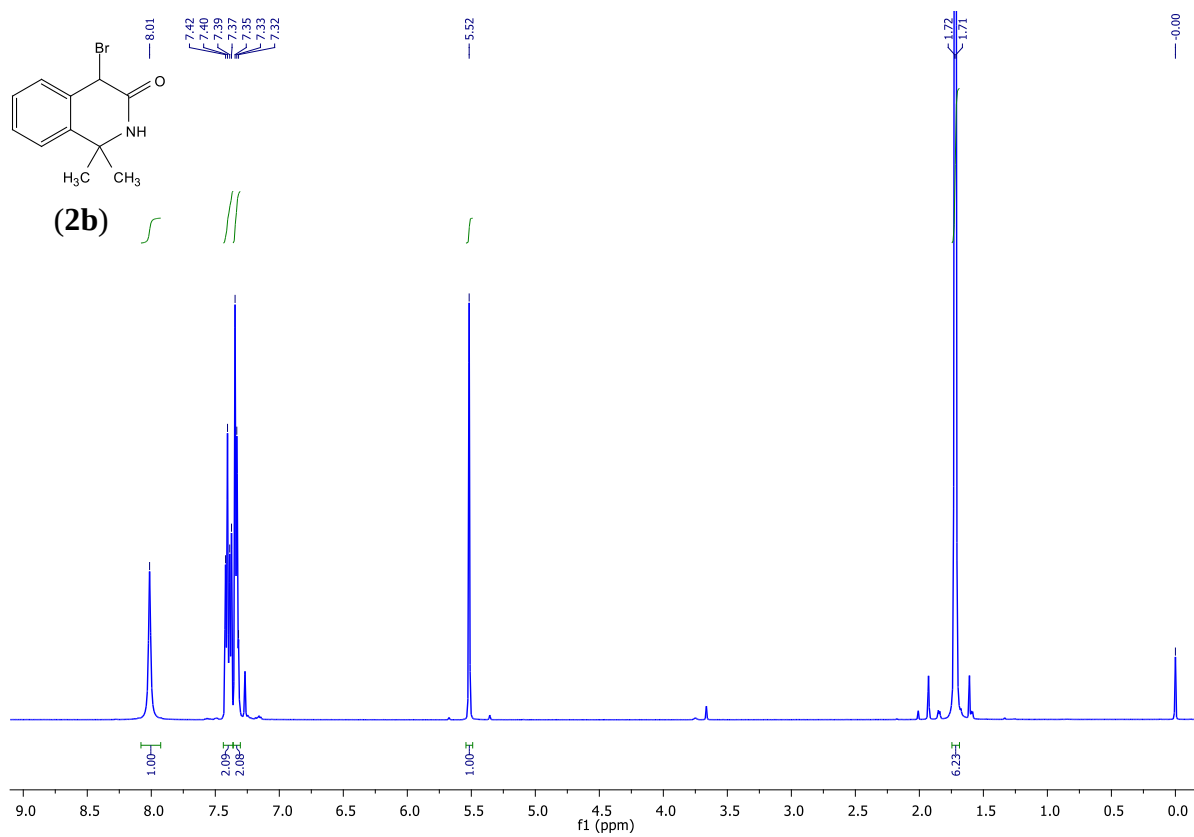
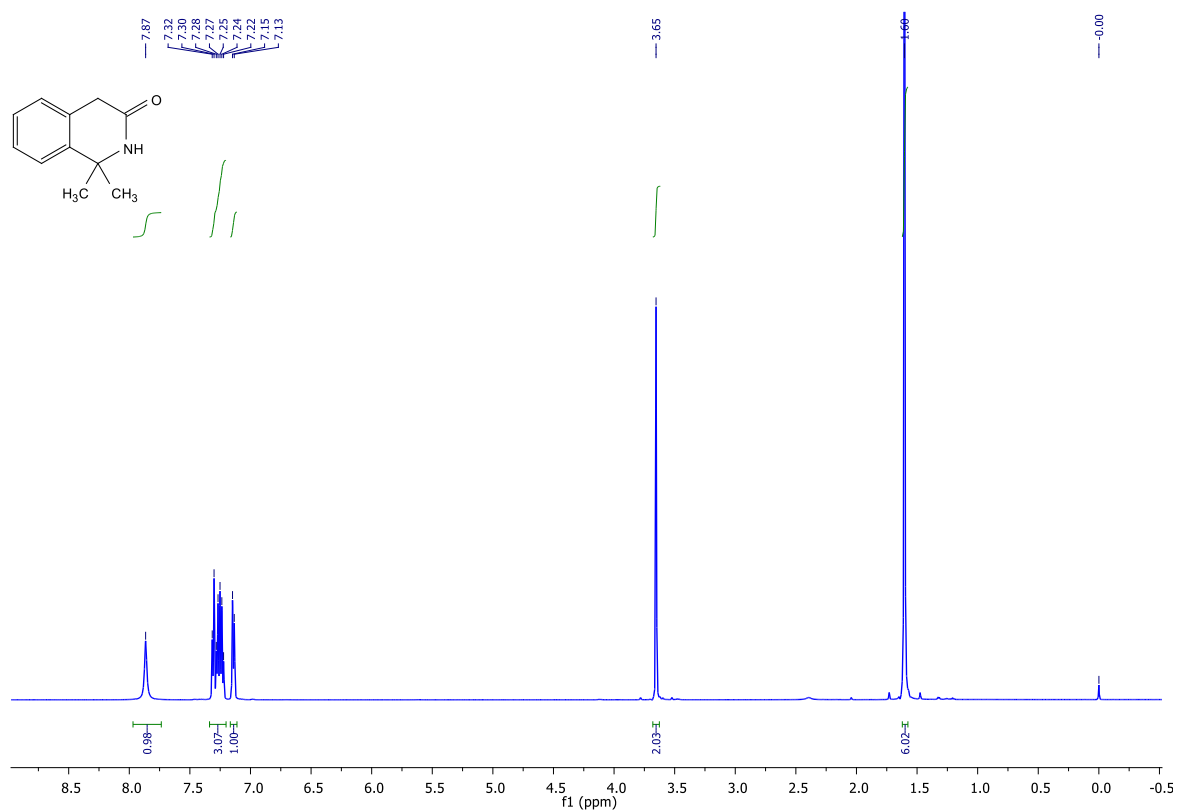
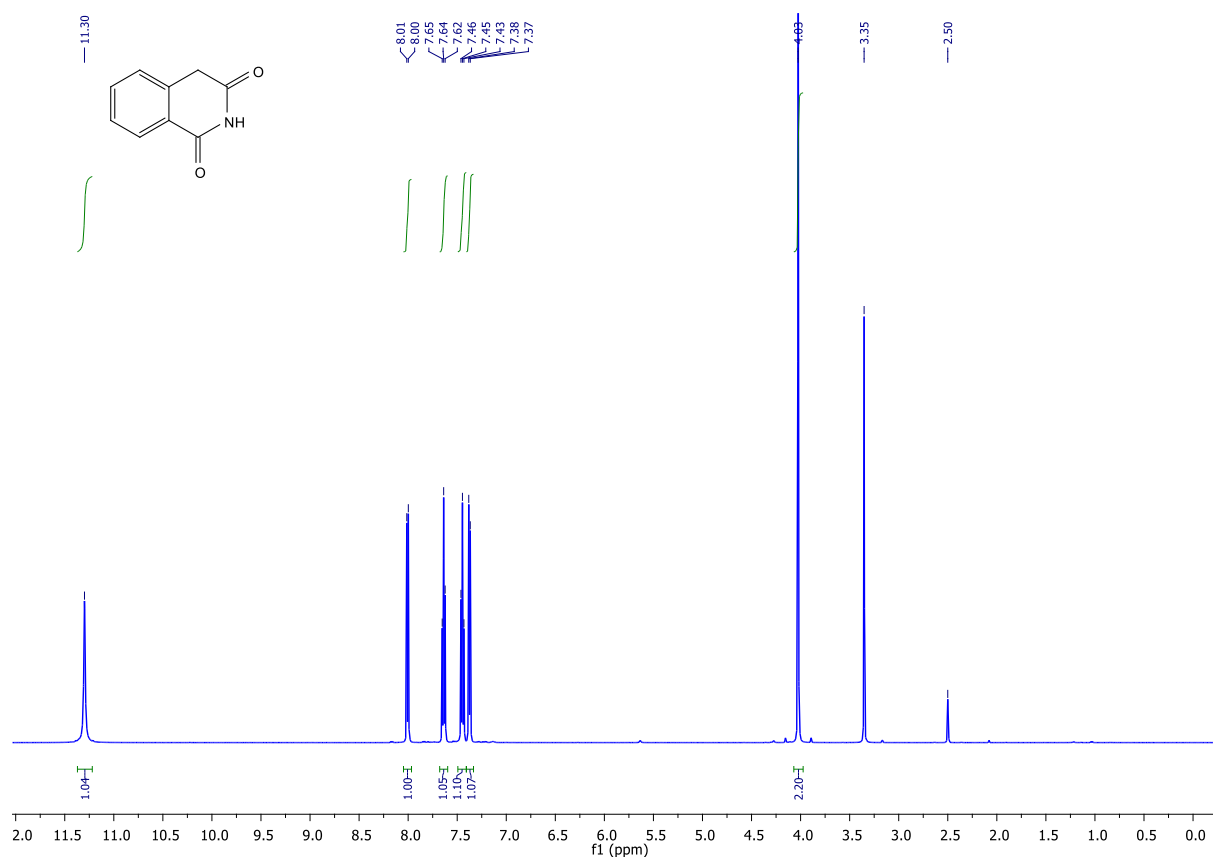
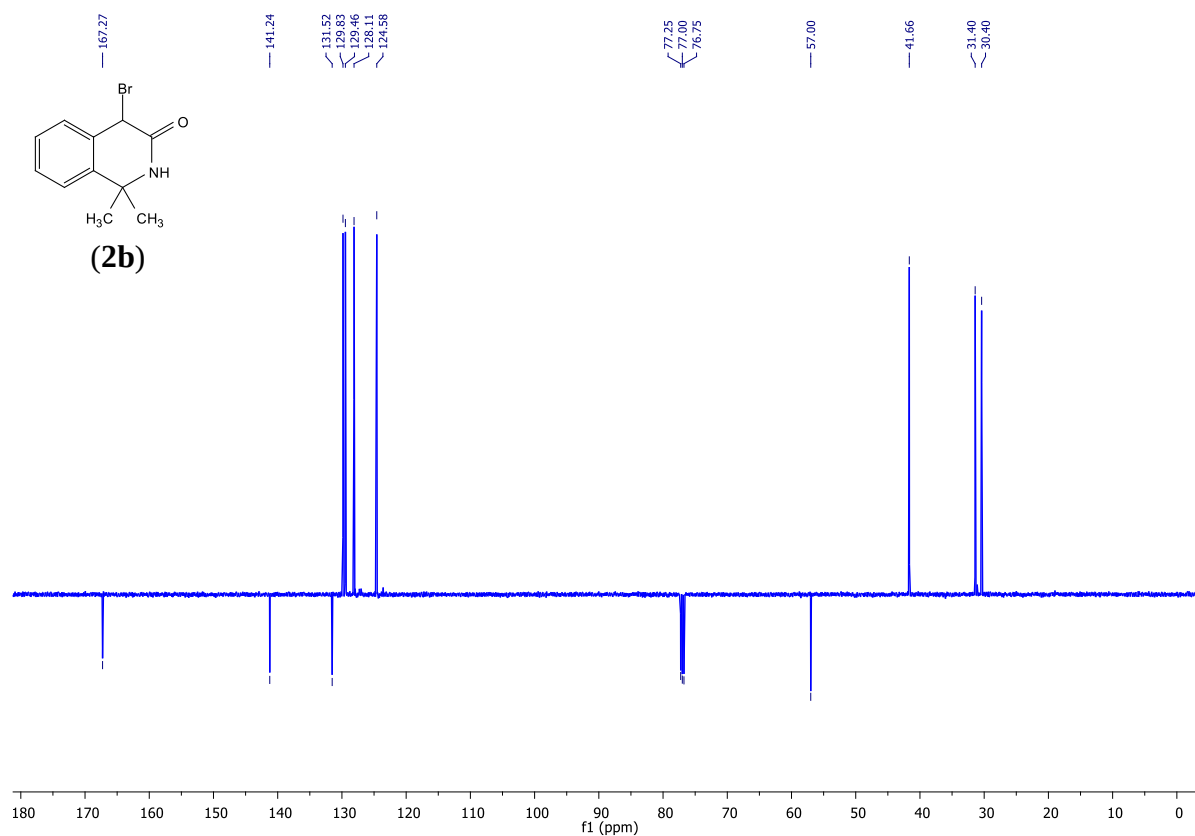
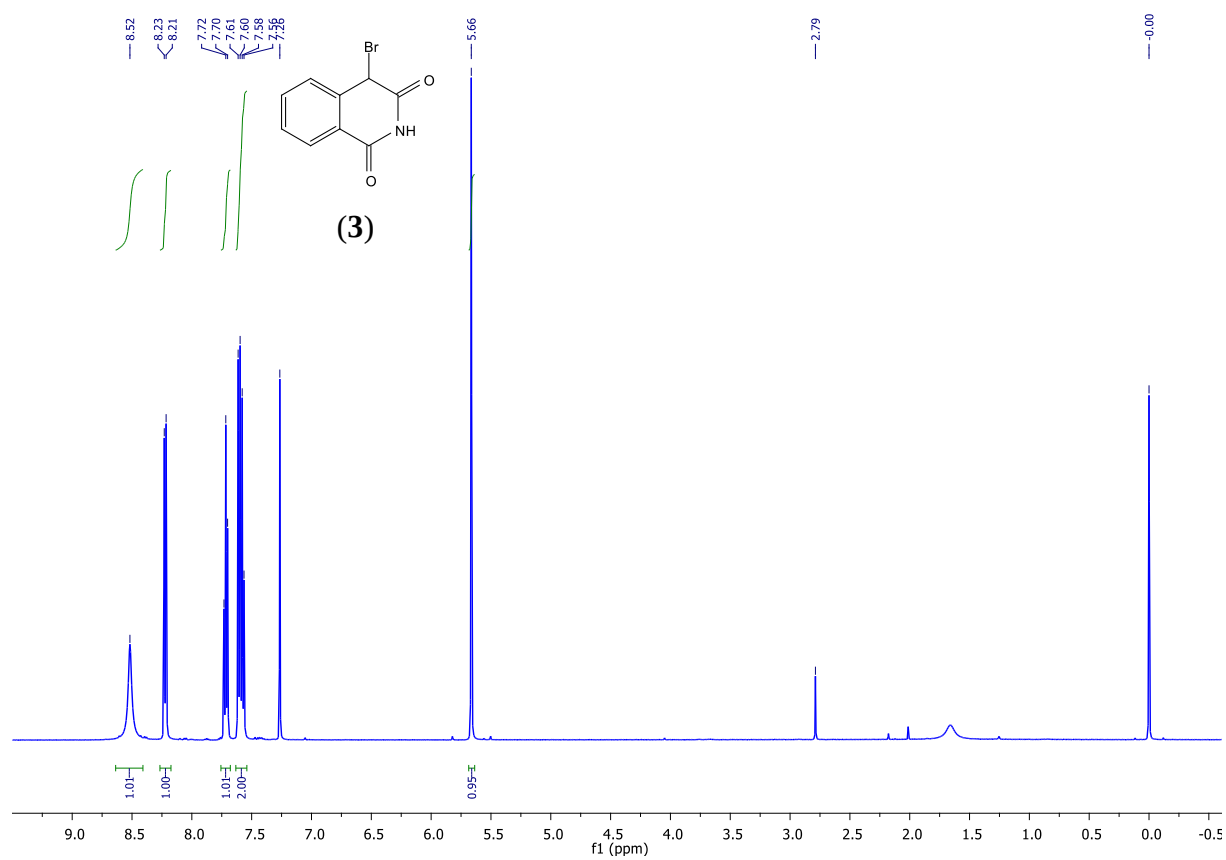
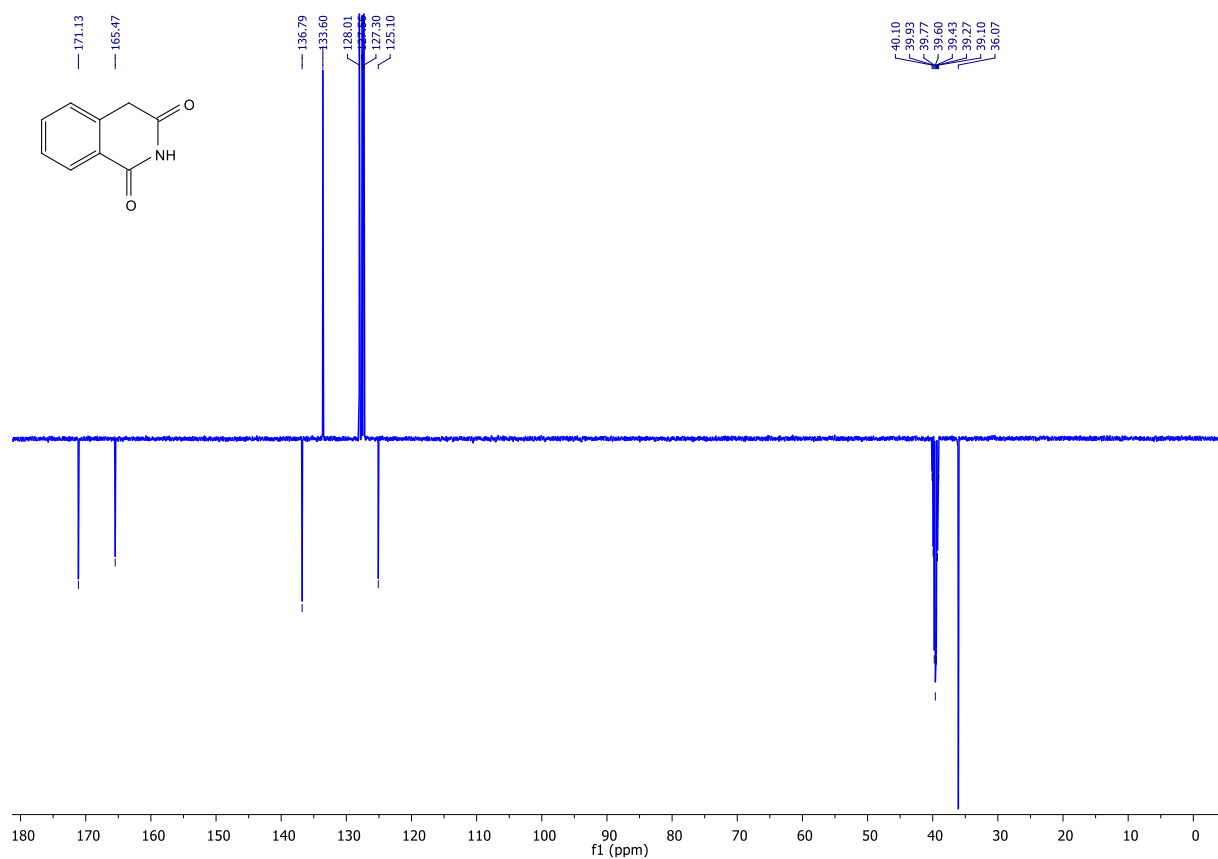
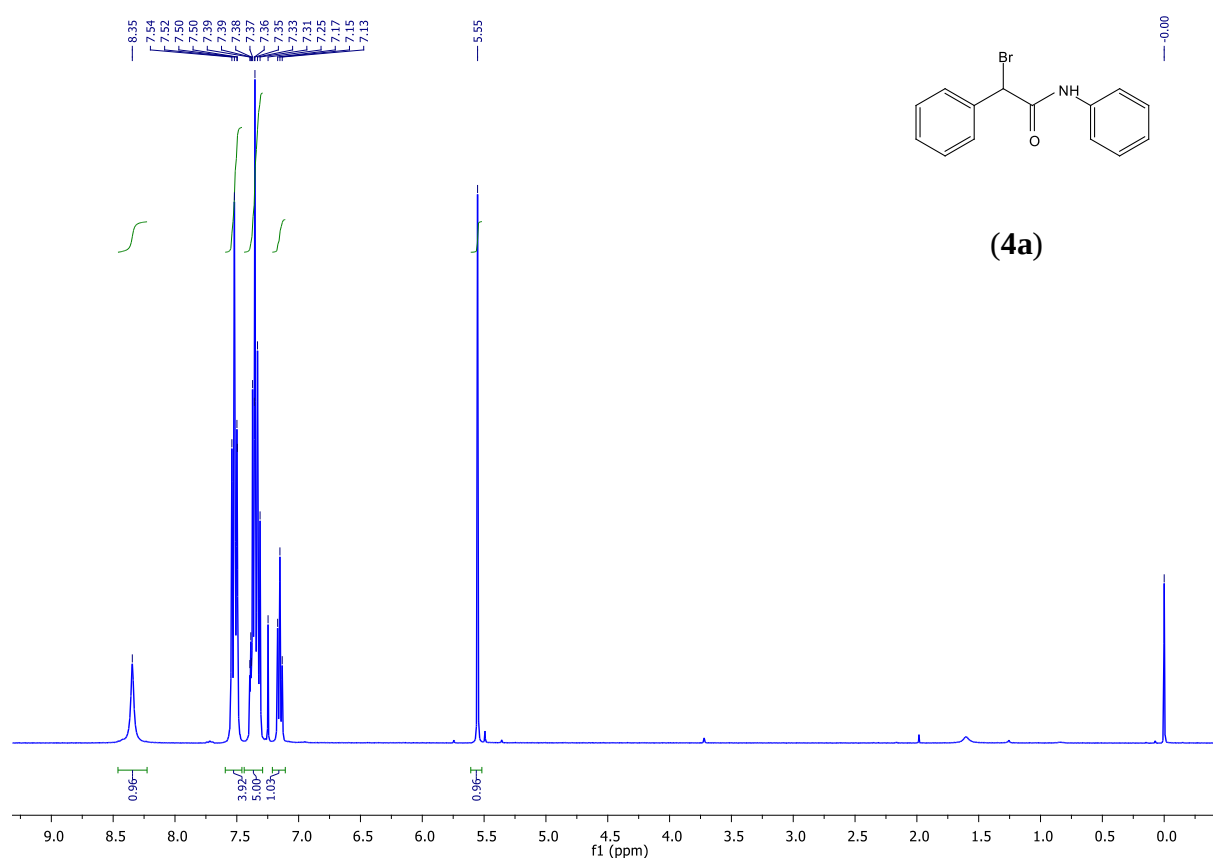
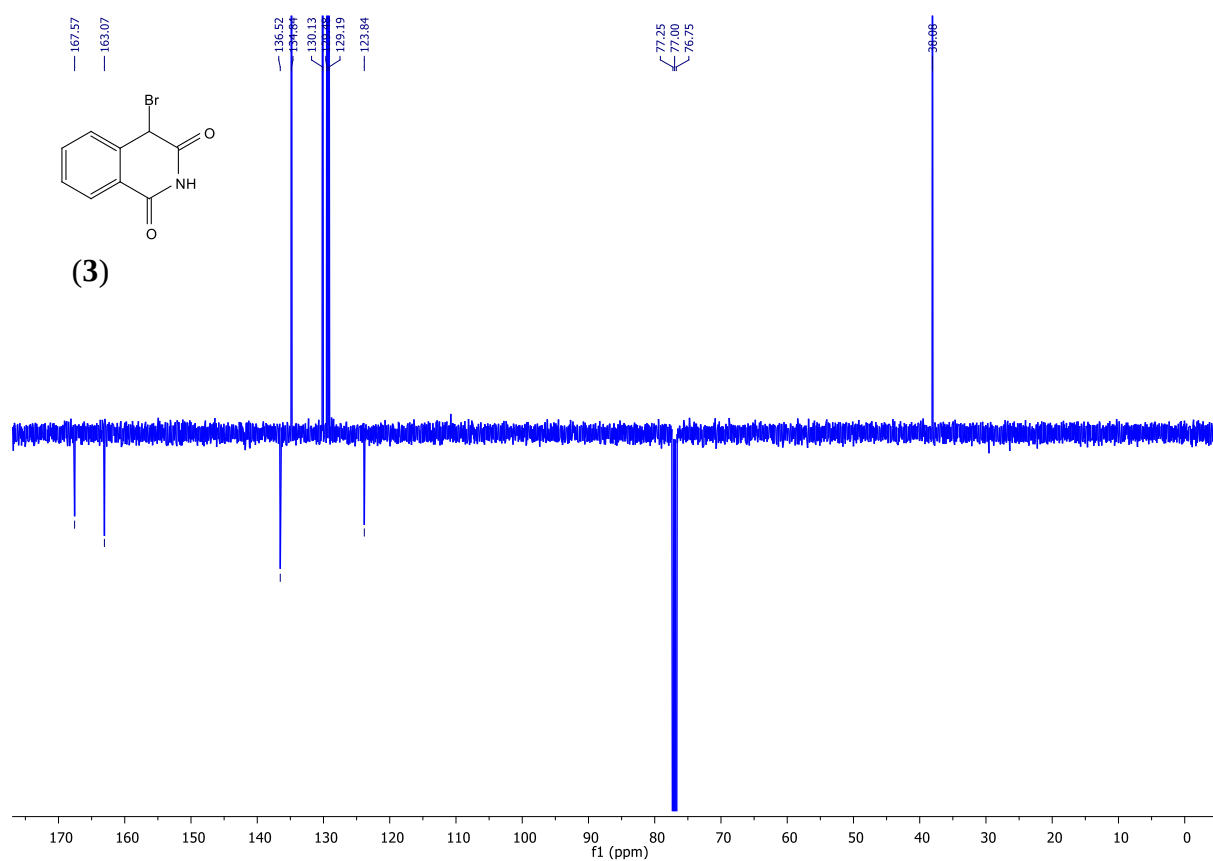


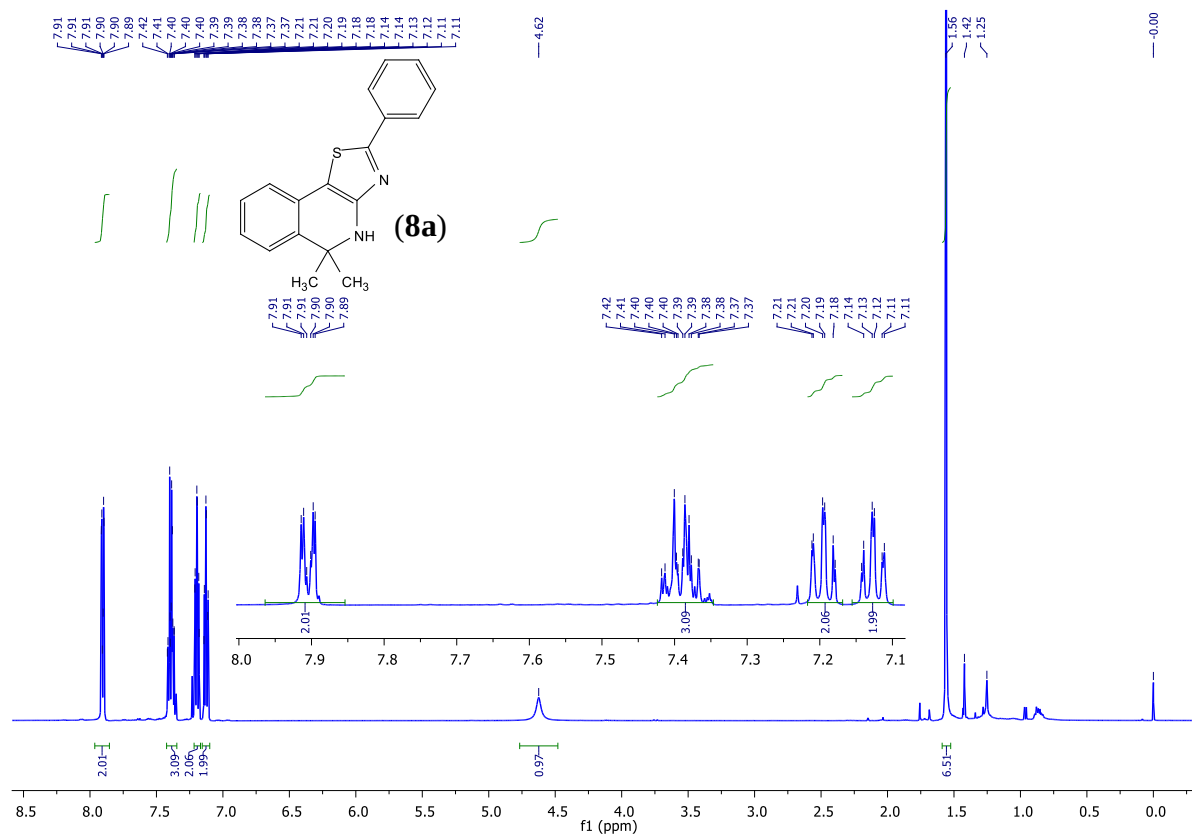
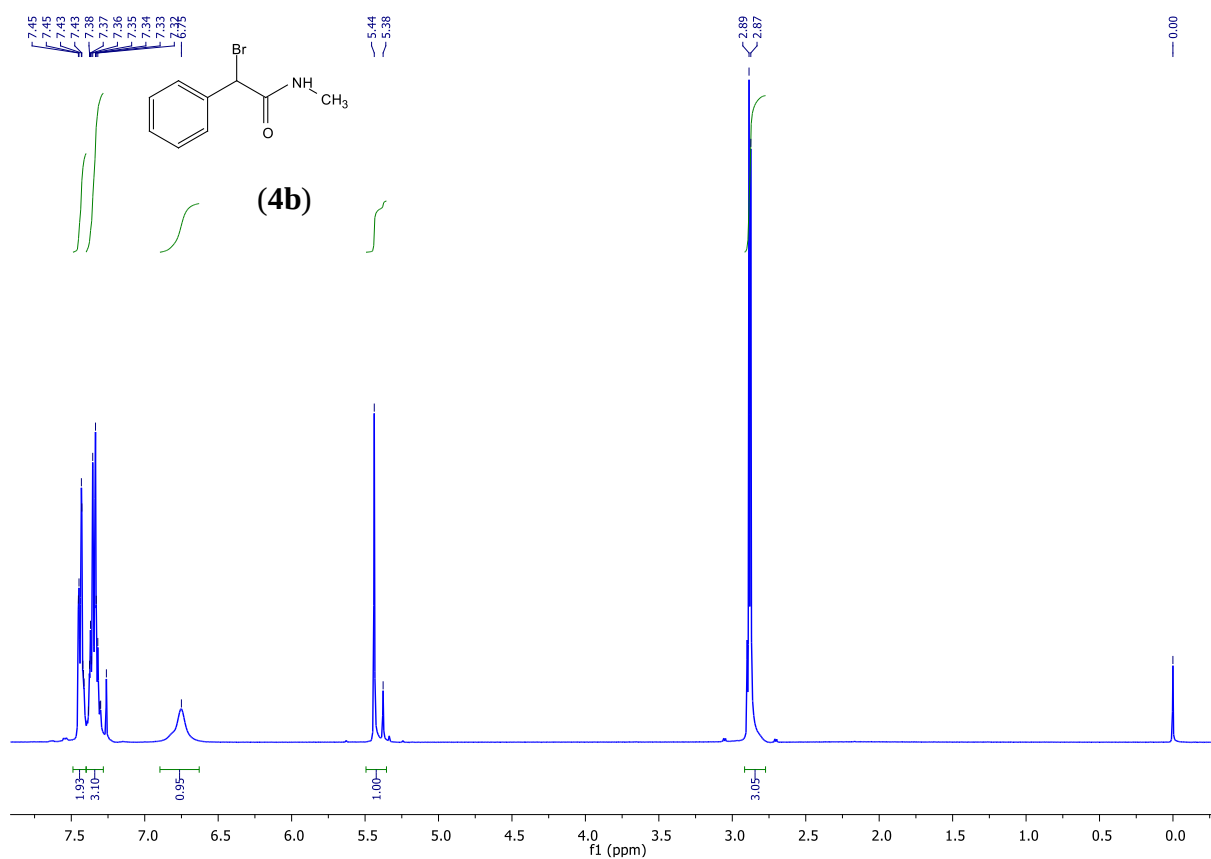
Figure S1. ESI-MS CID spectrum showing different fragmentation patterns of isobaric compounds **6a** and **7a**.

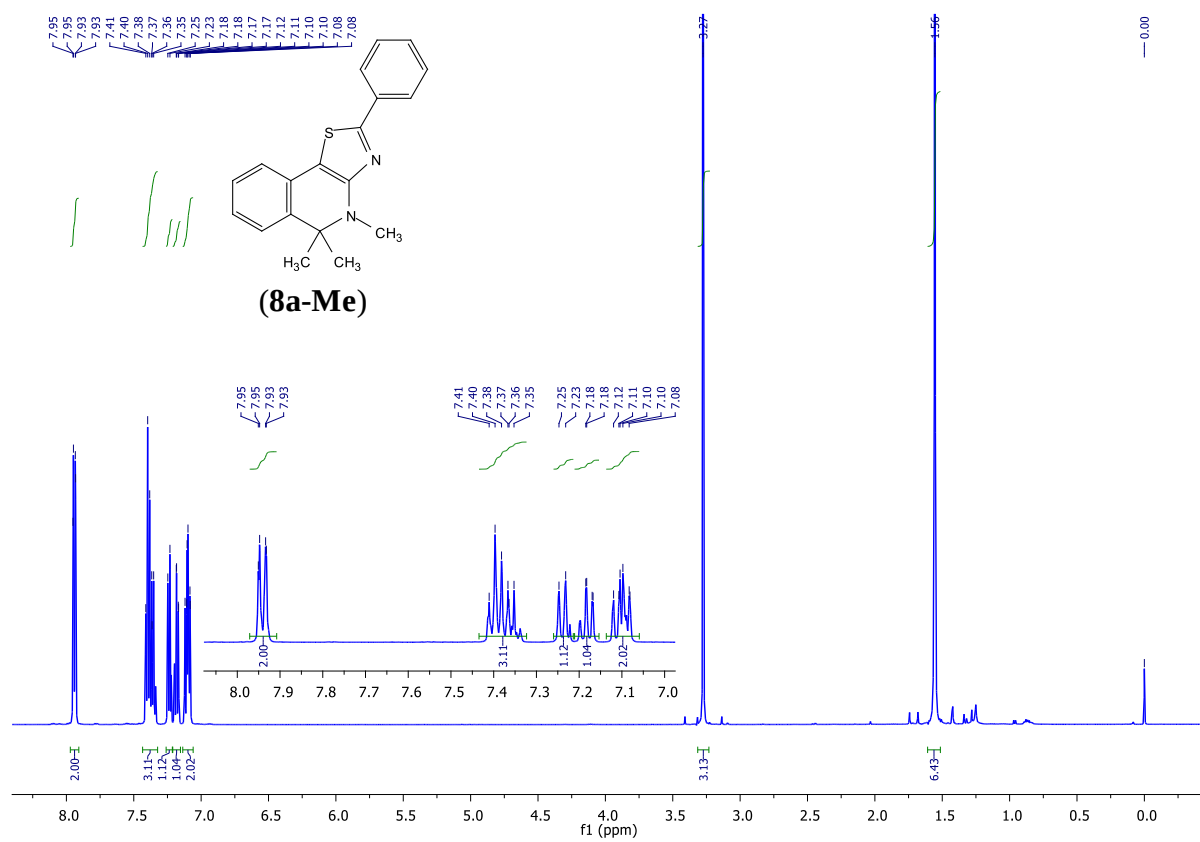
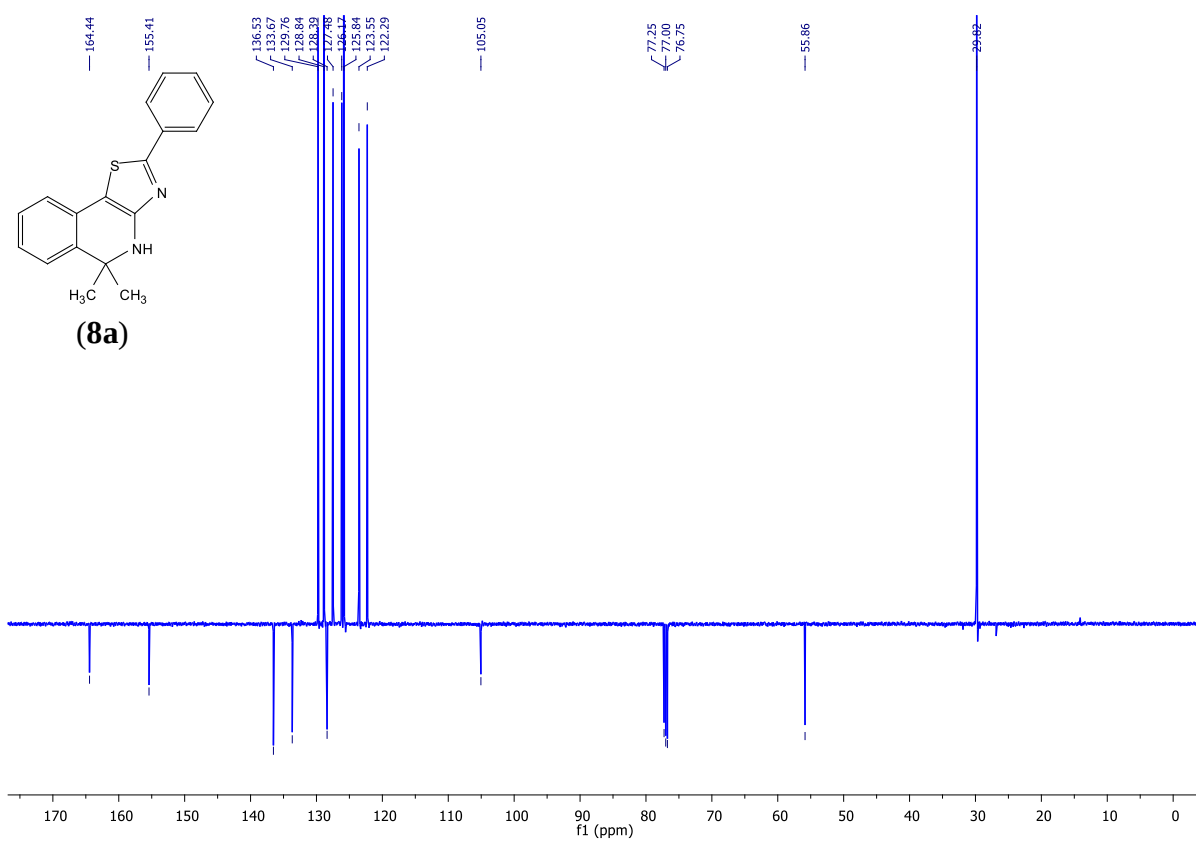


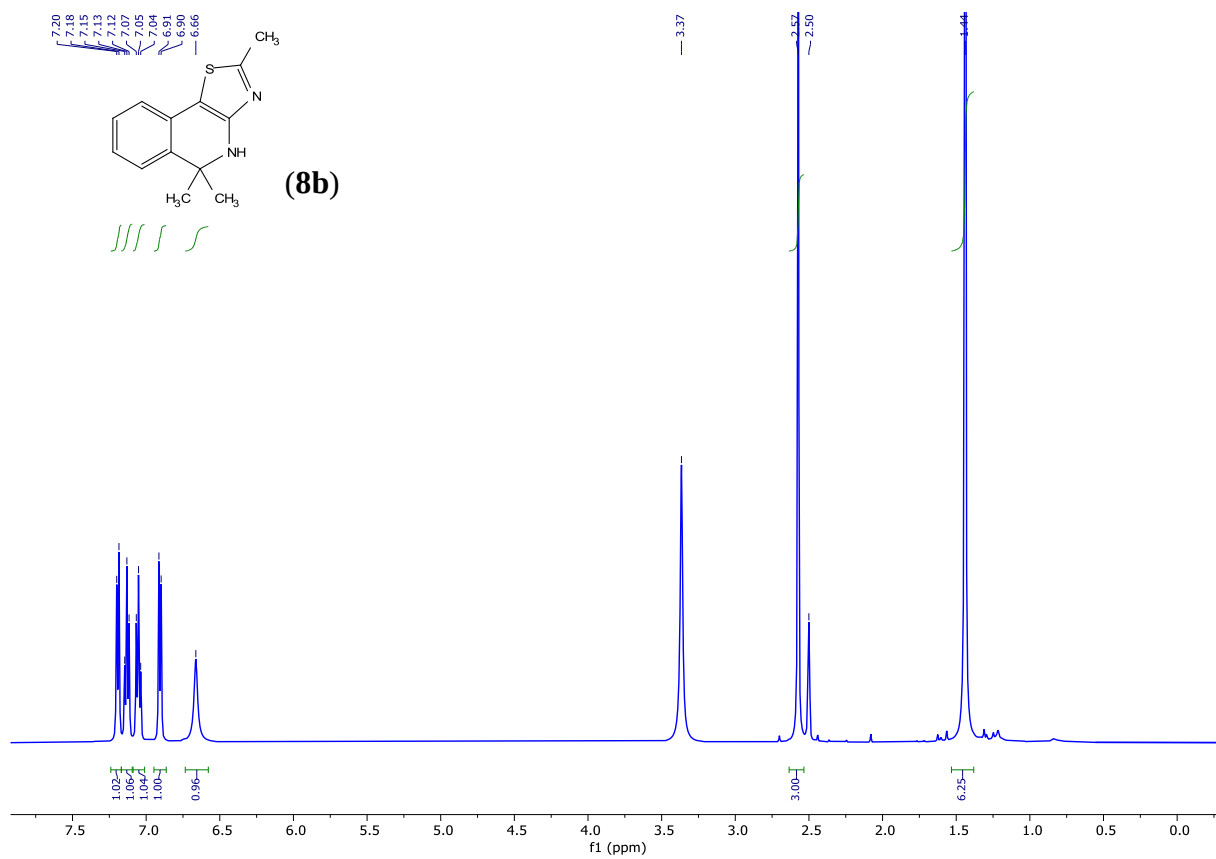
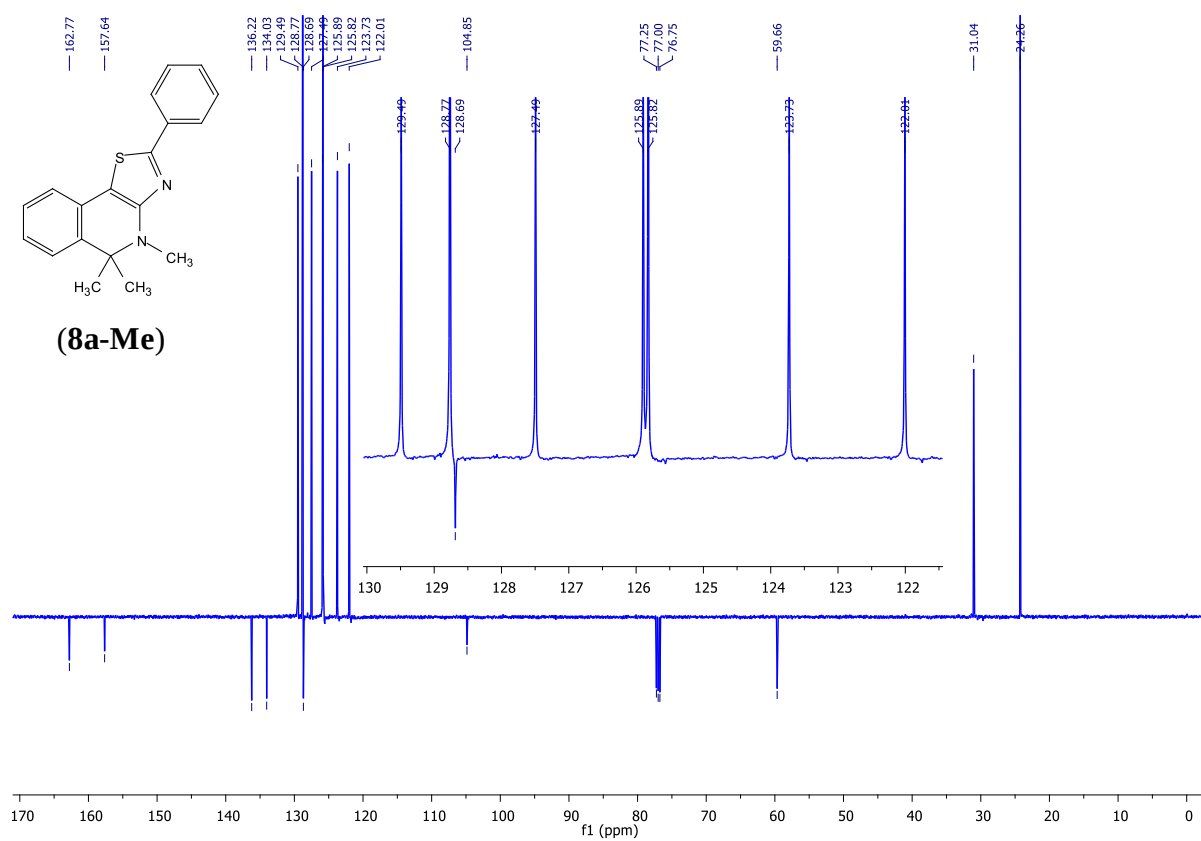


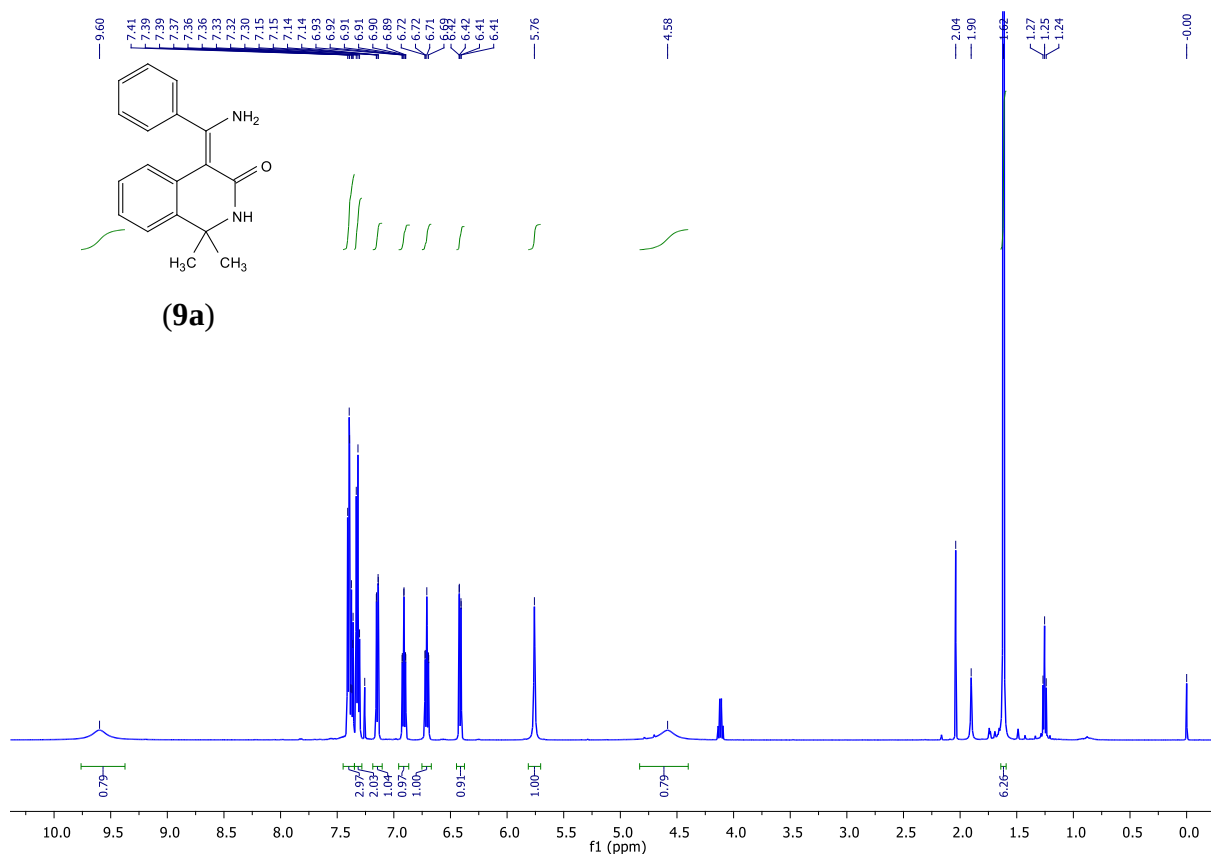
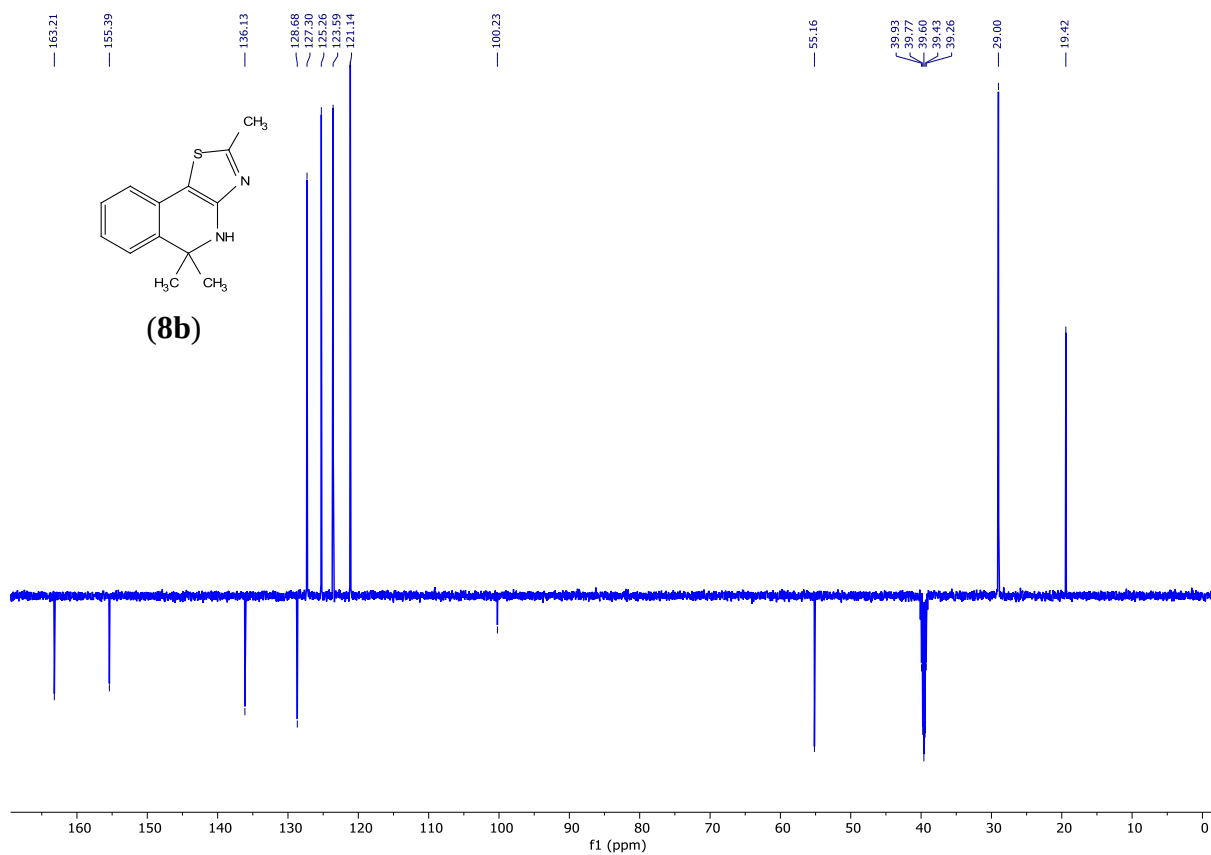


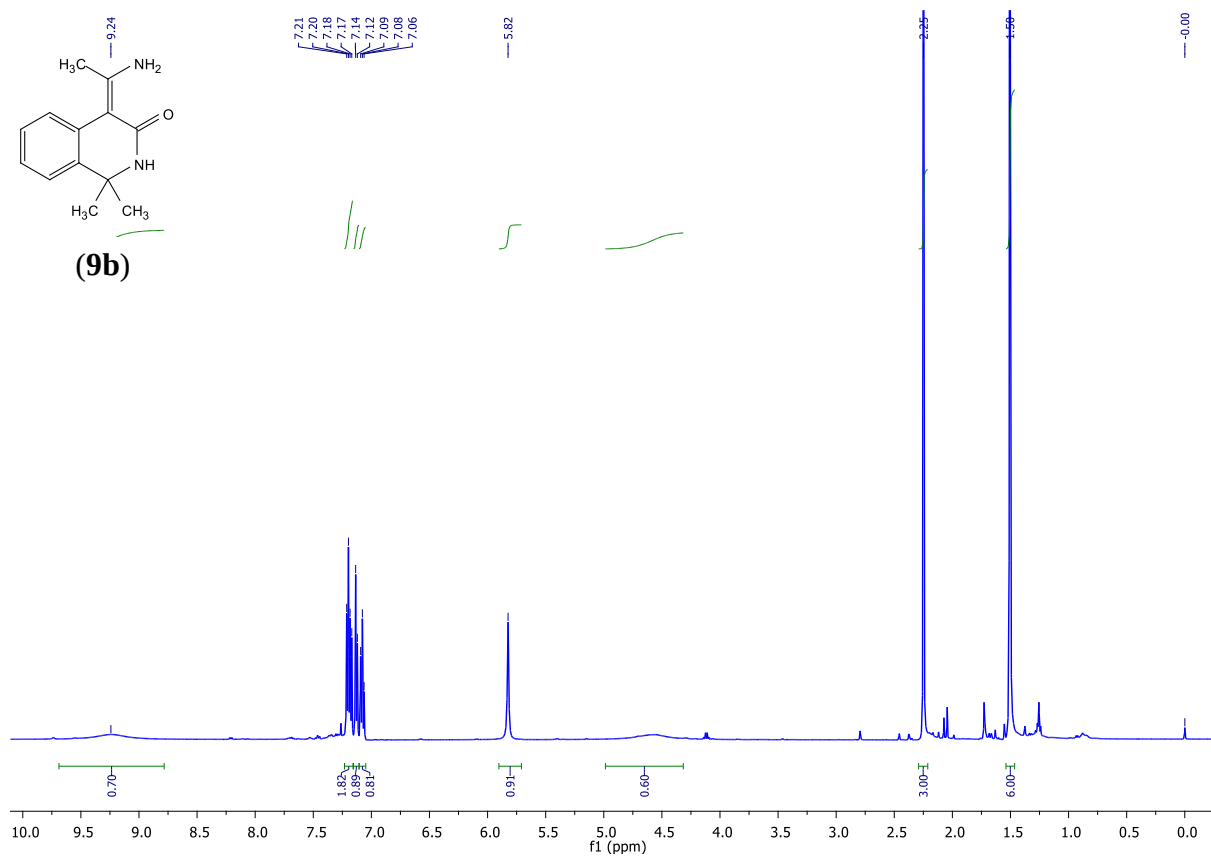
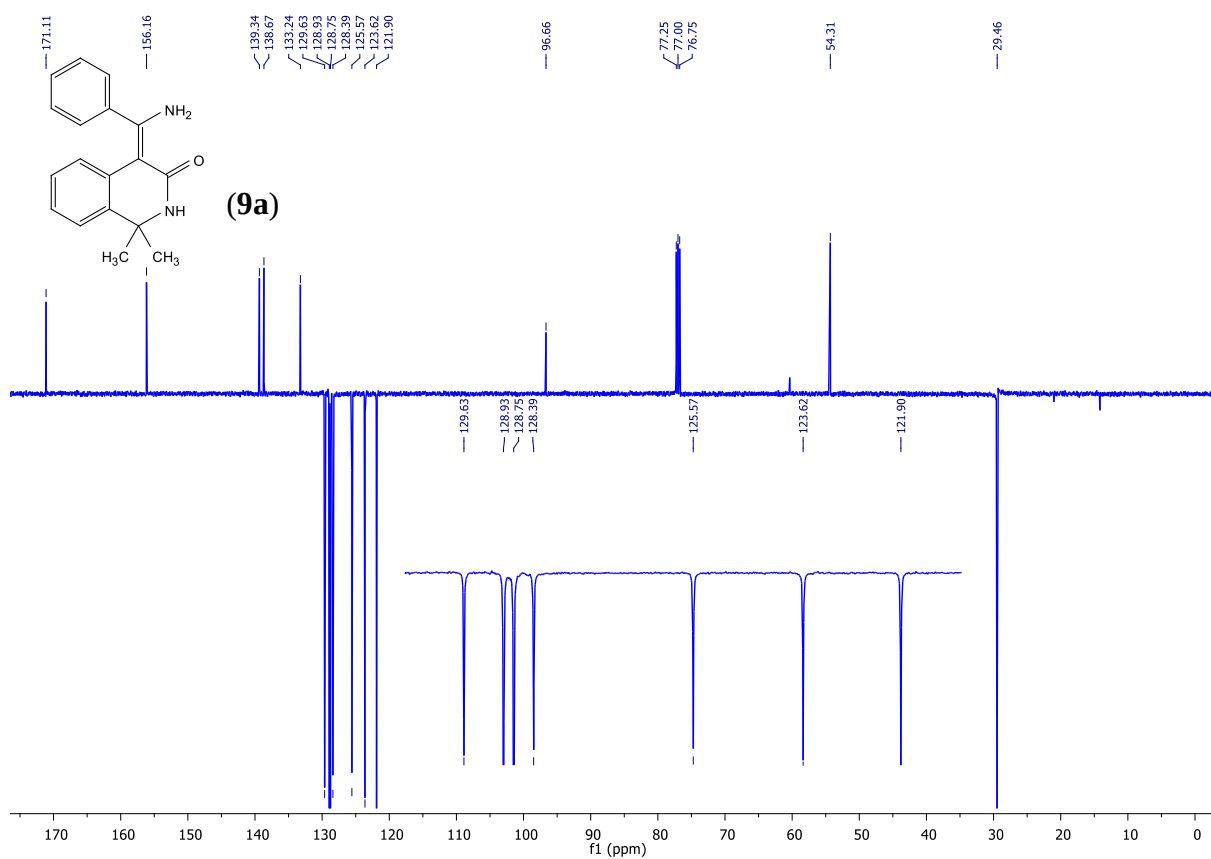


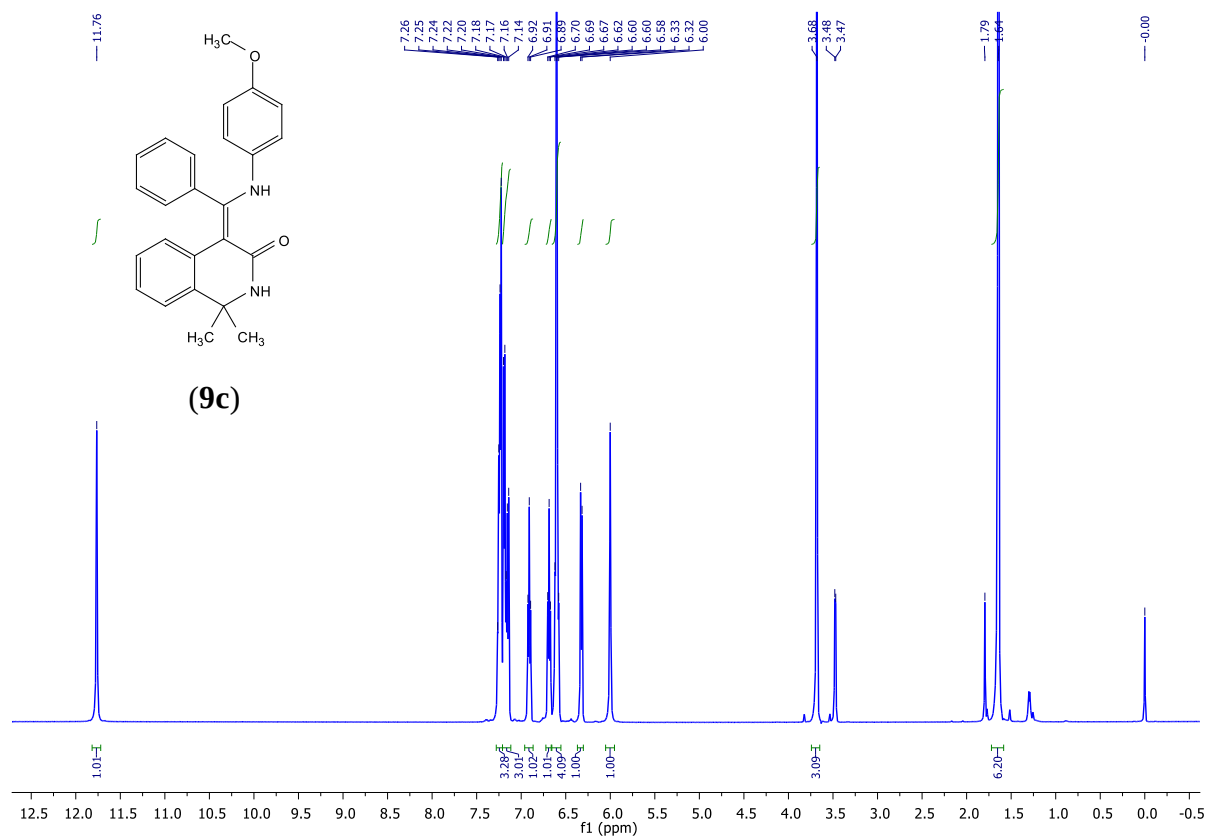
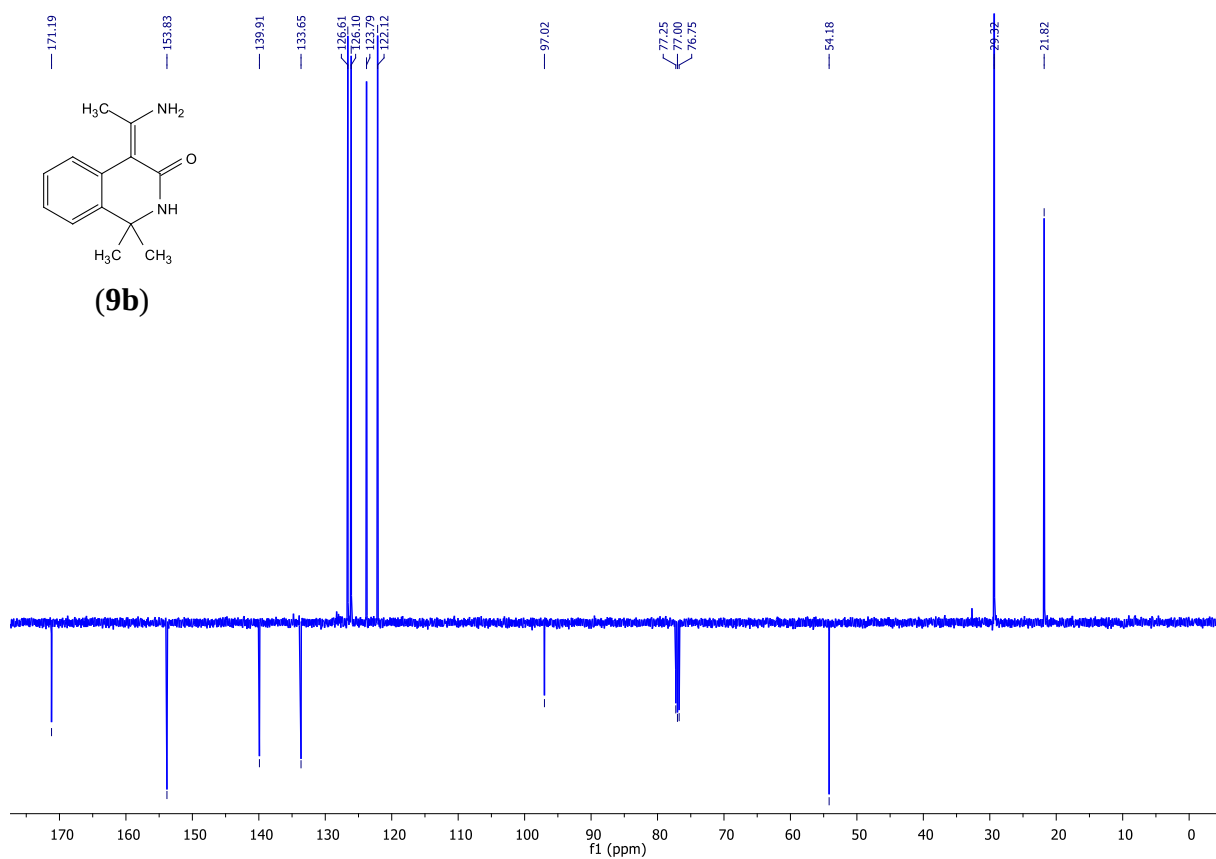


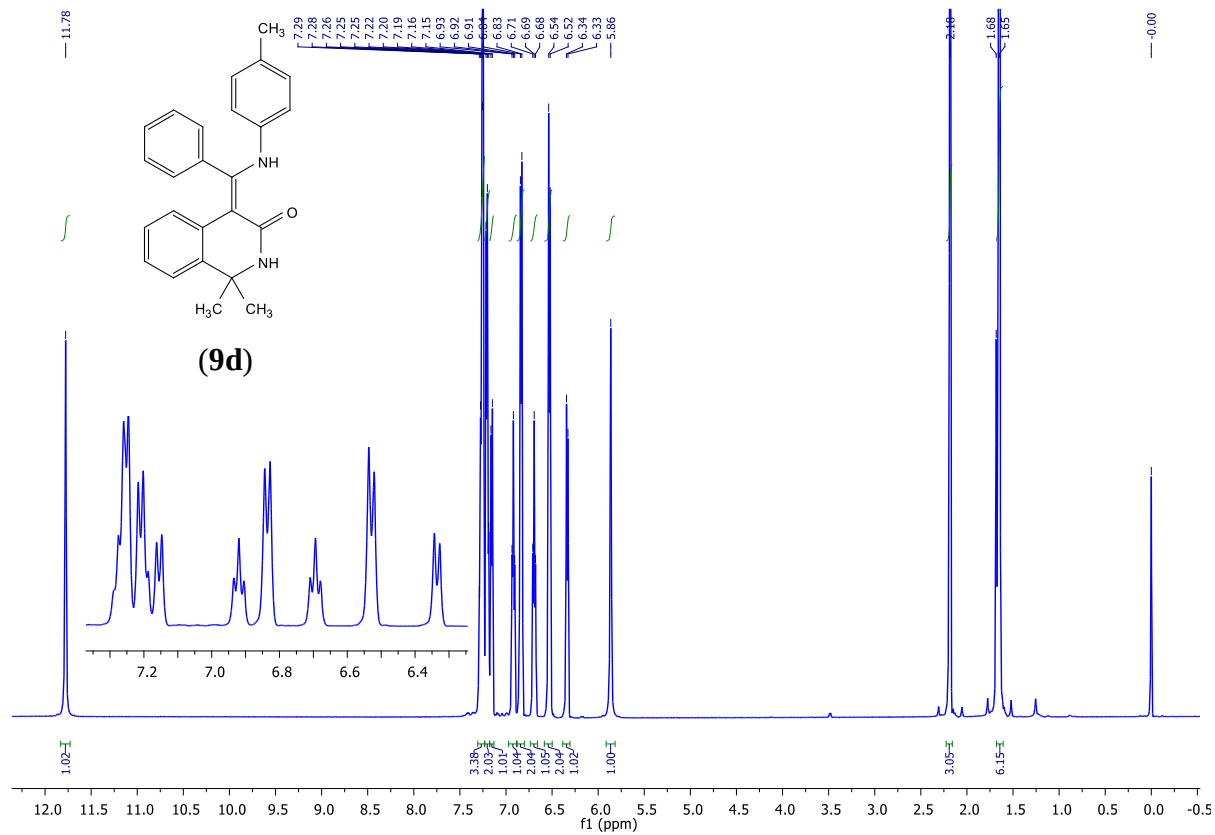
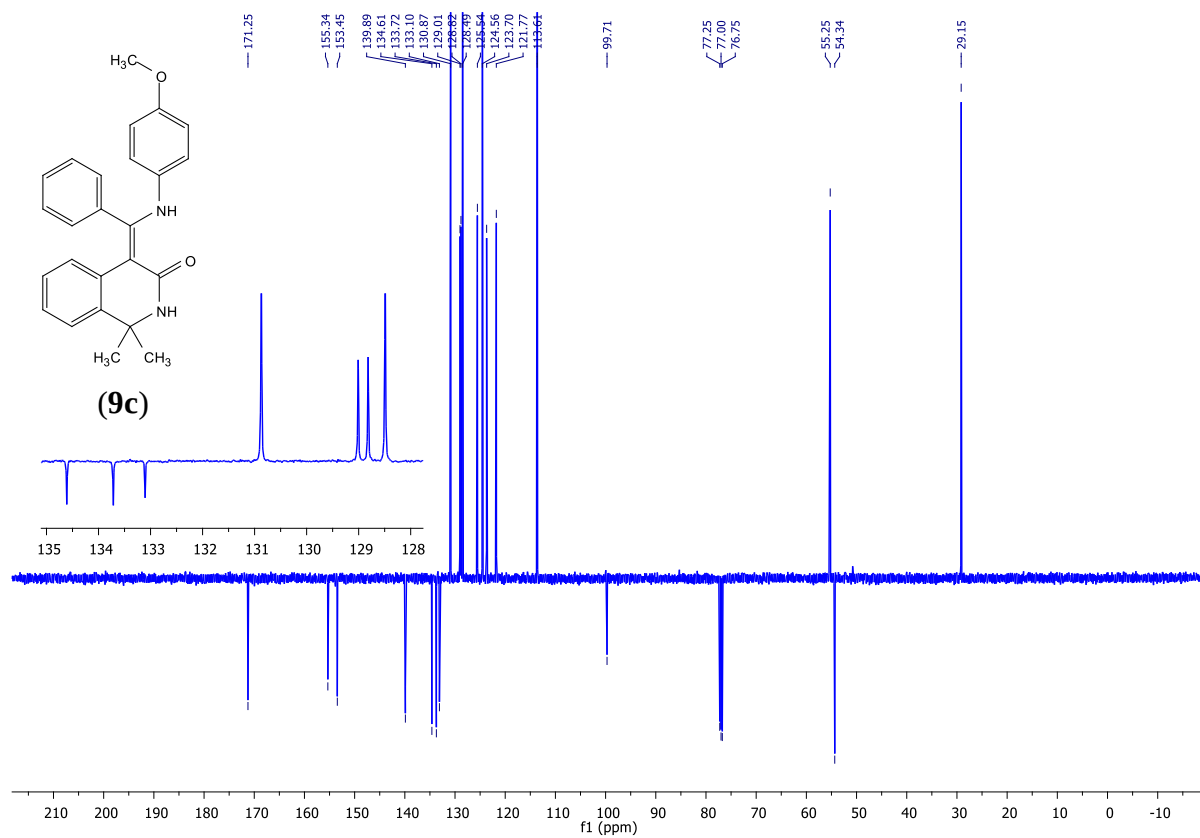


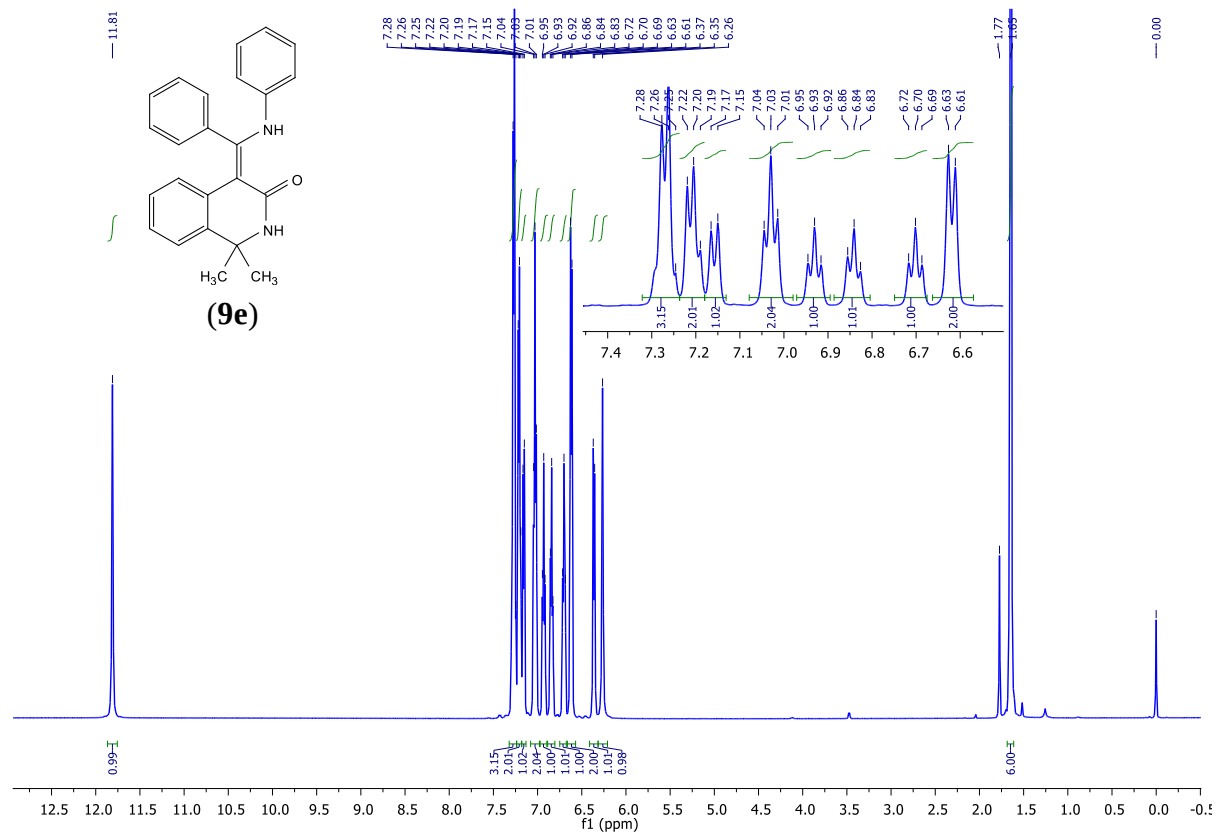
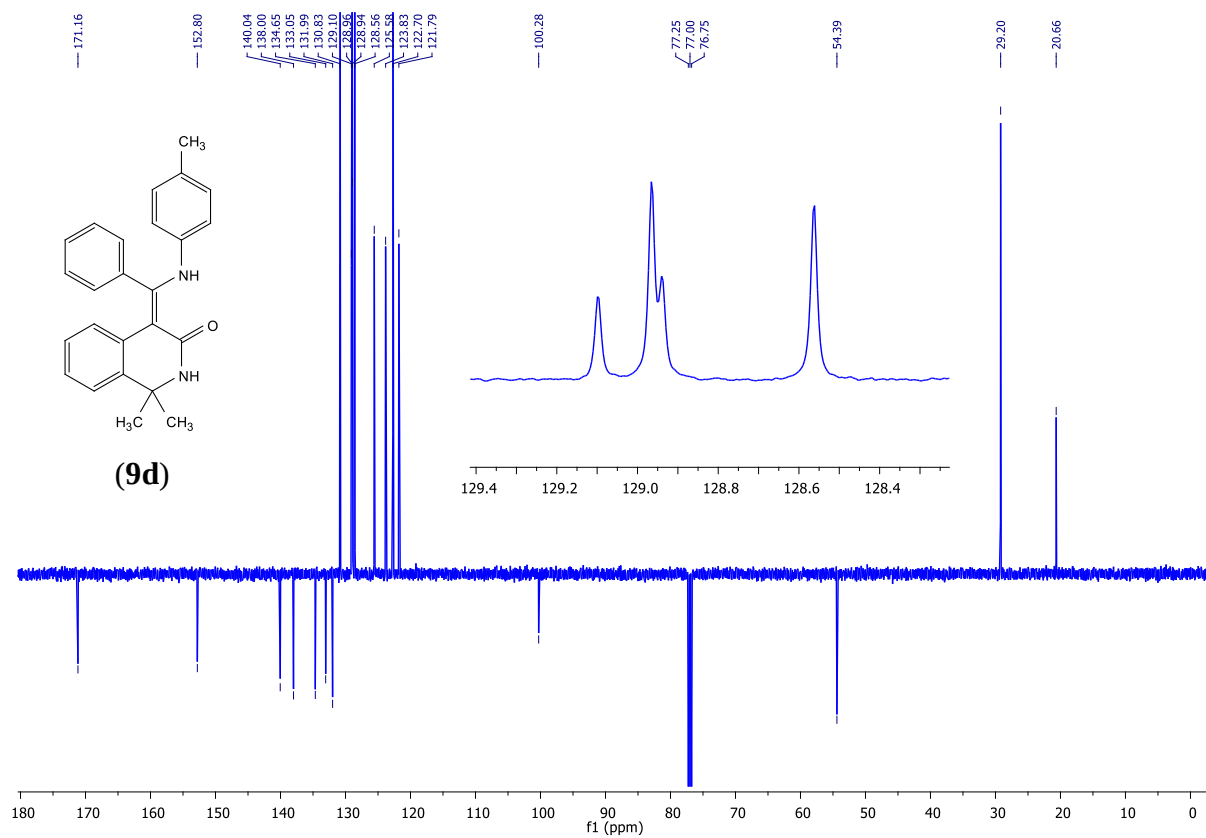


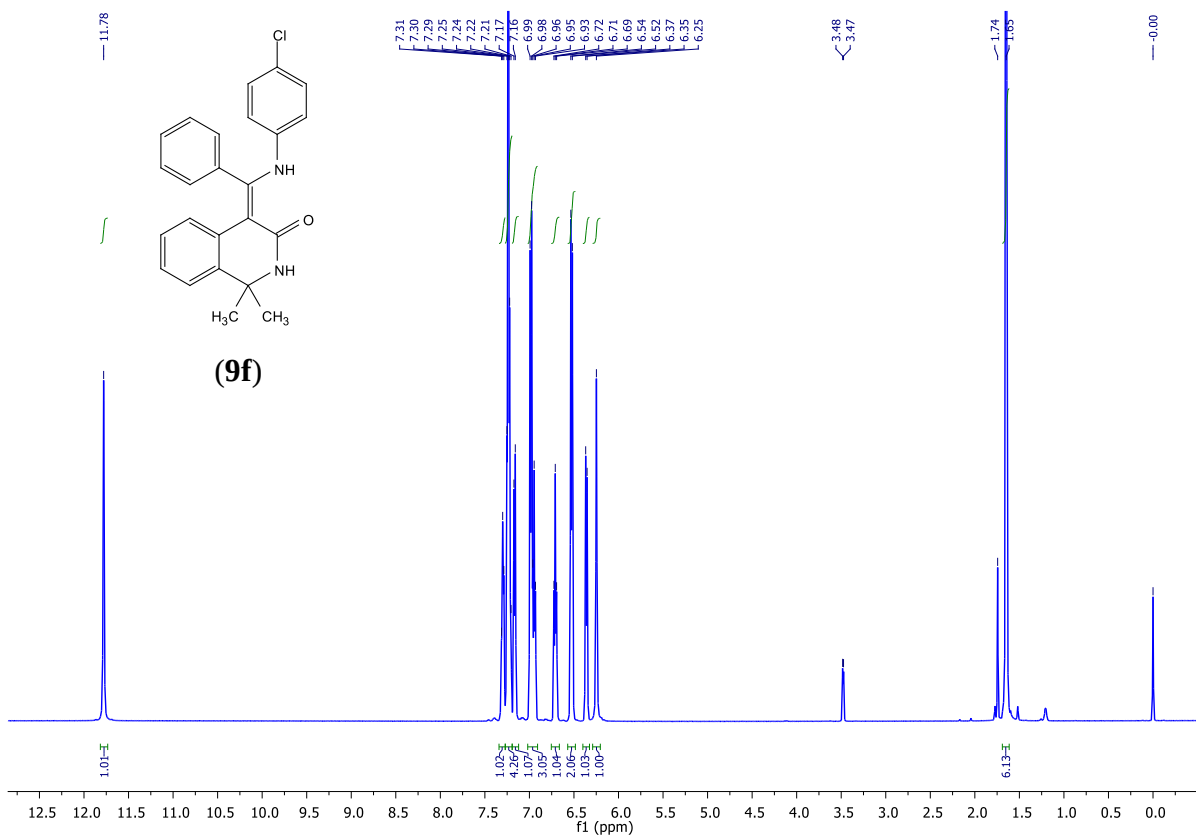
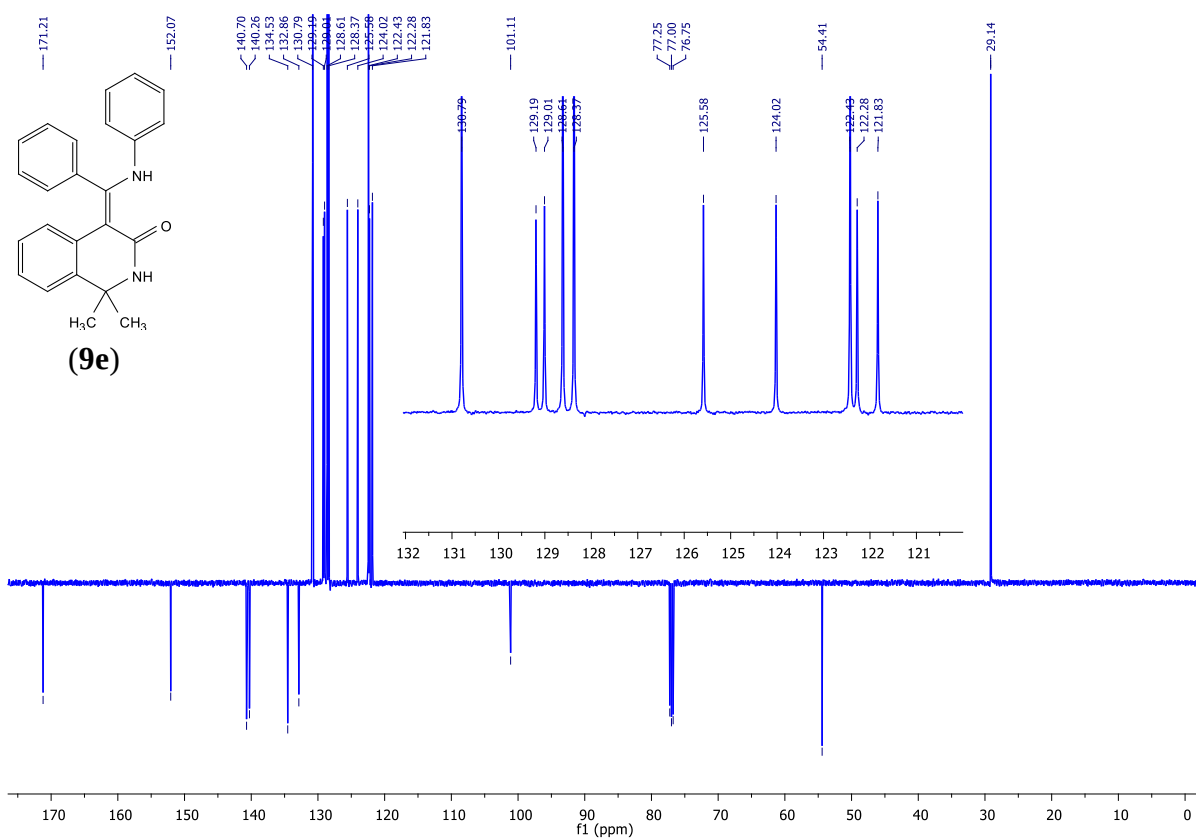


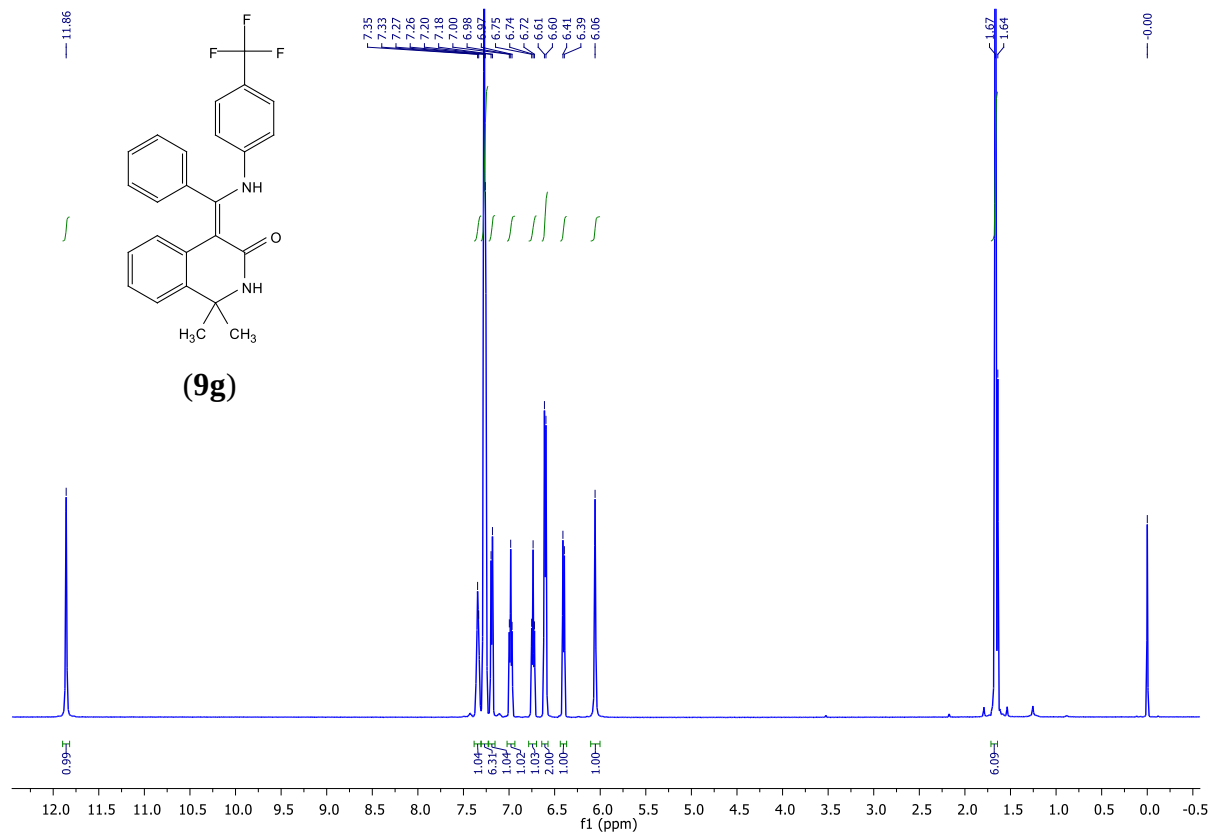
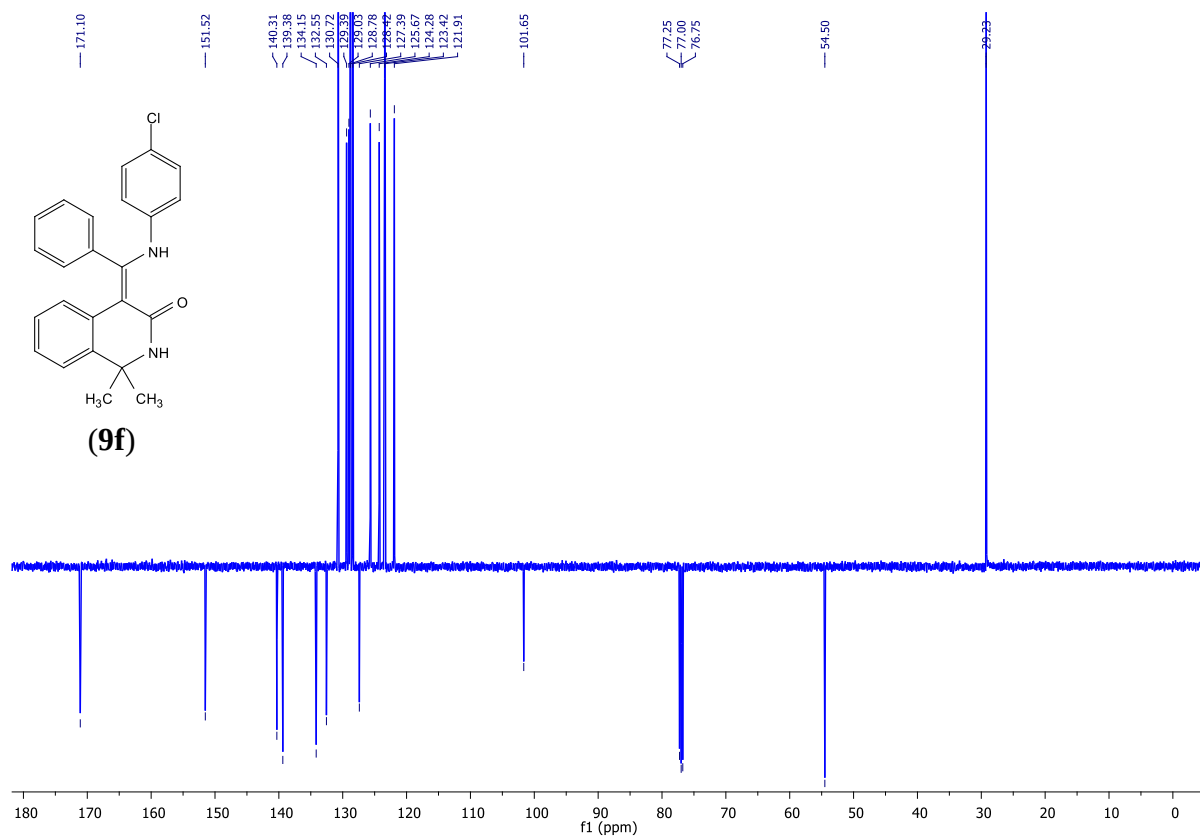


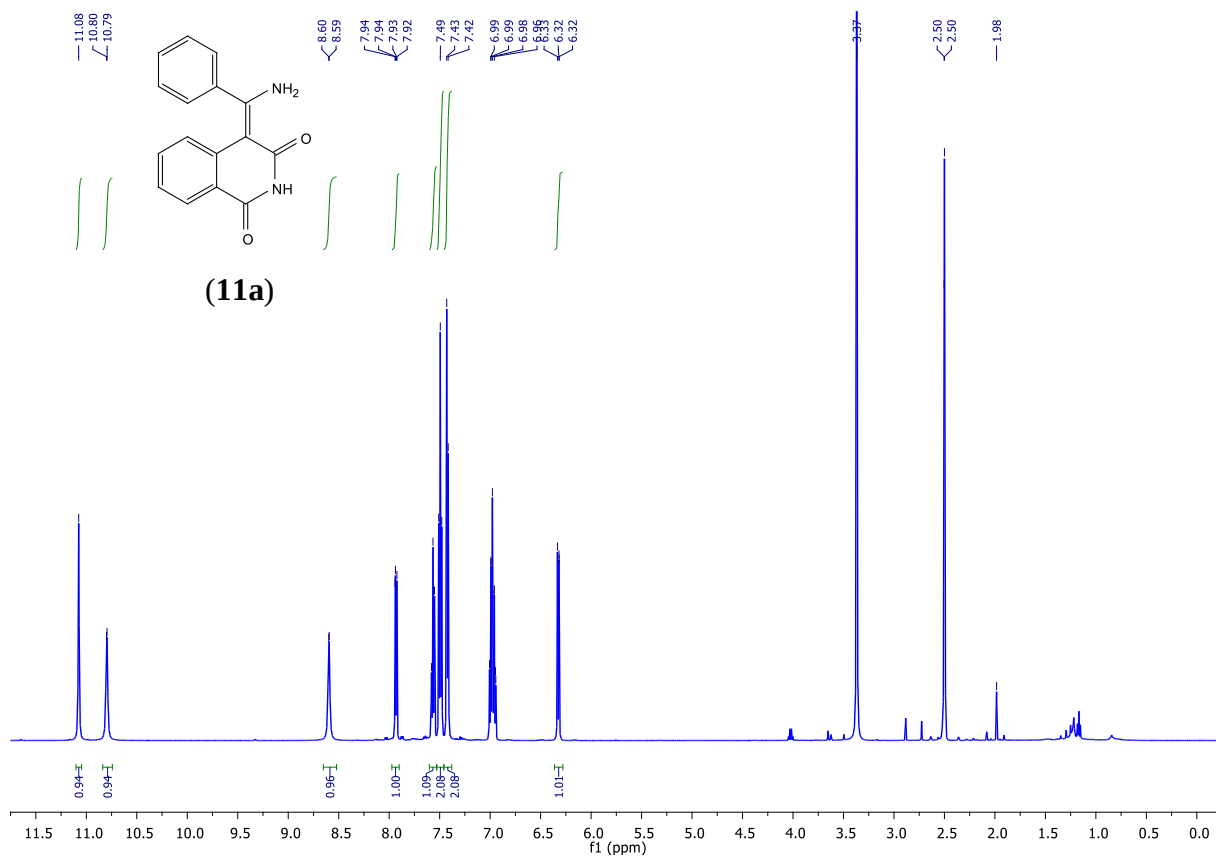
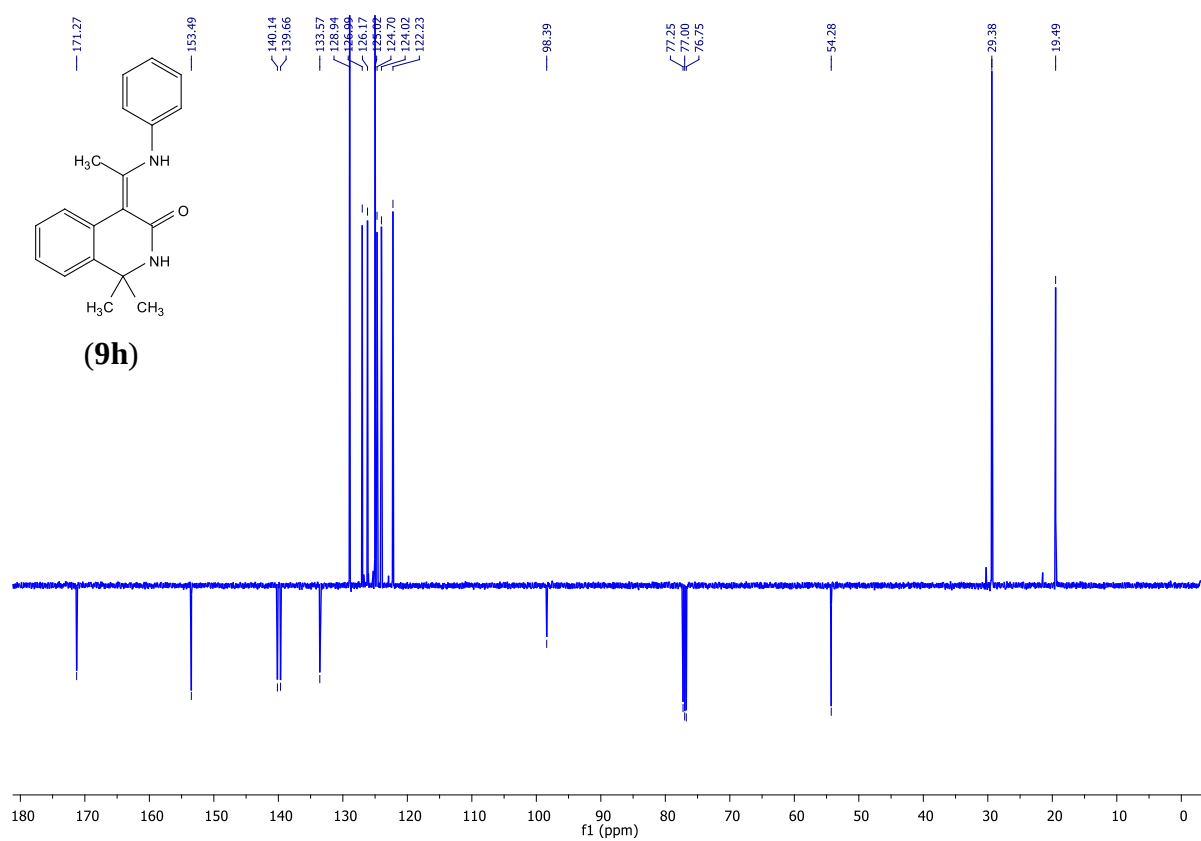


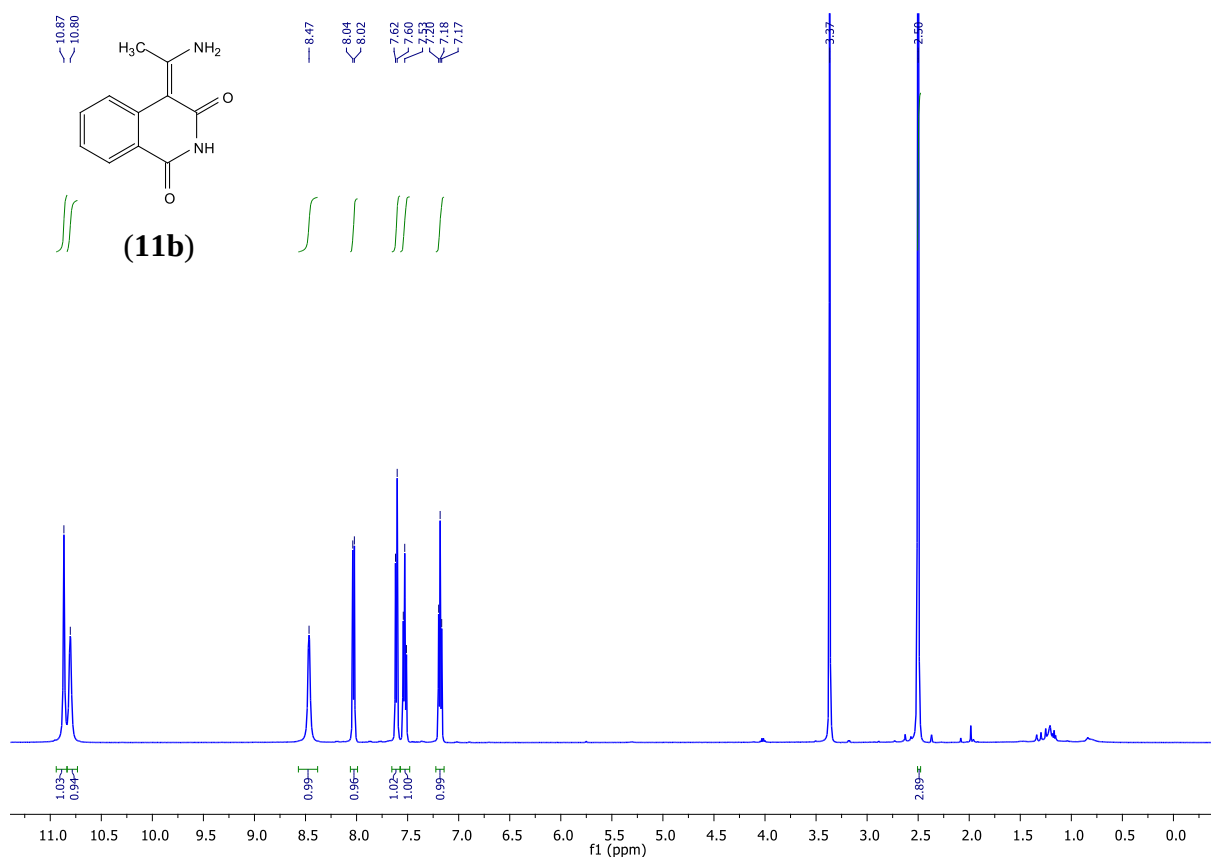
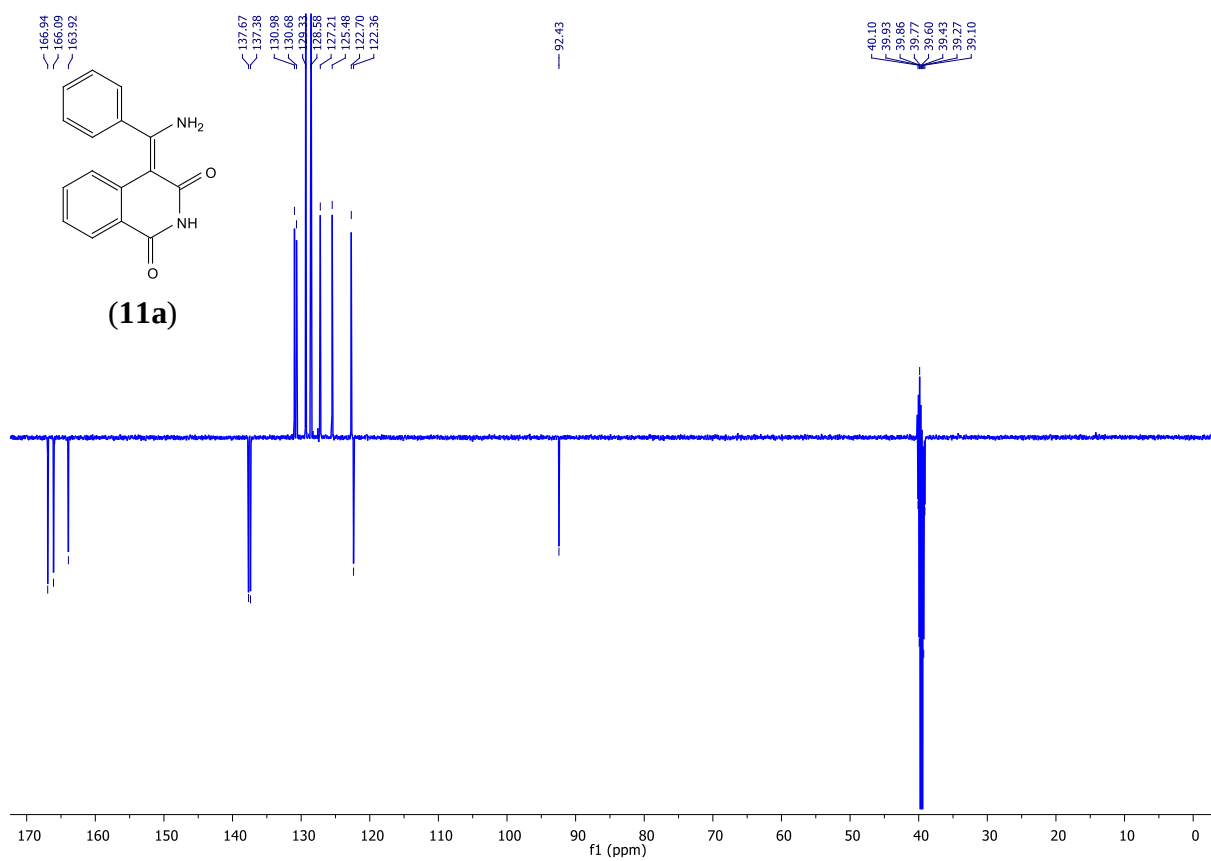


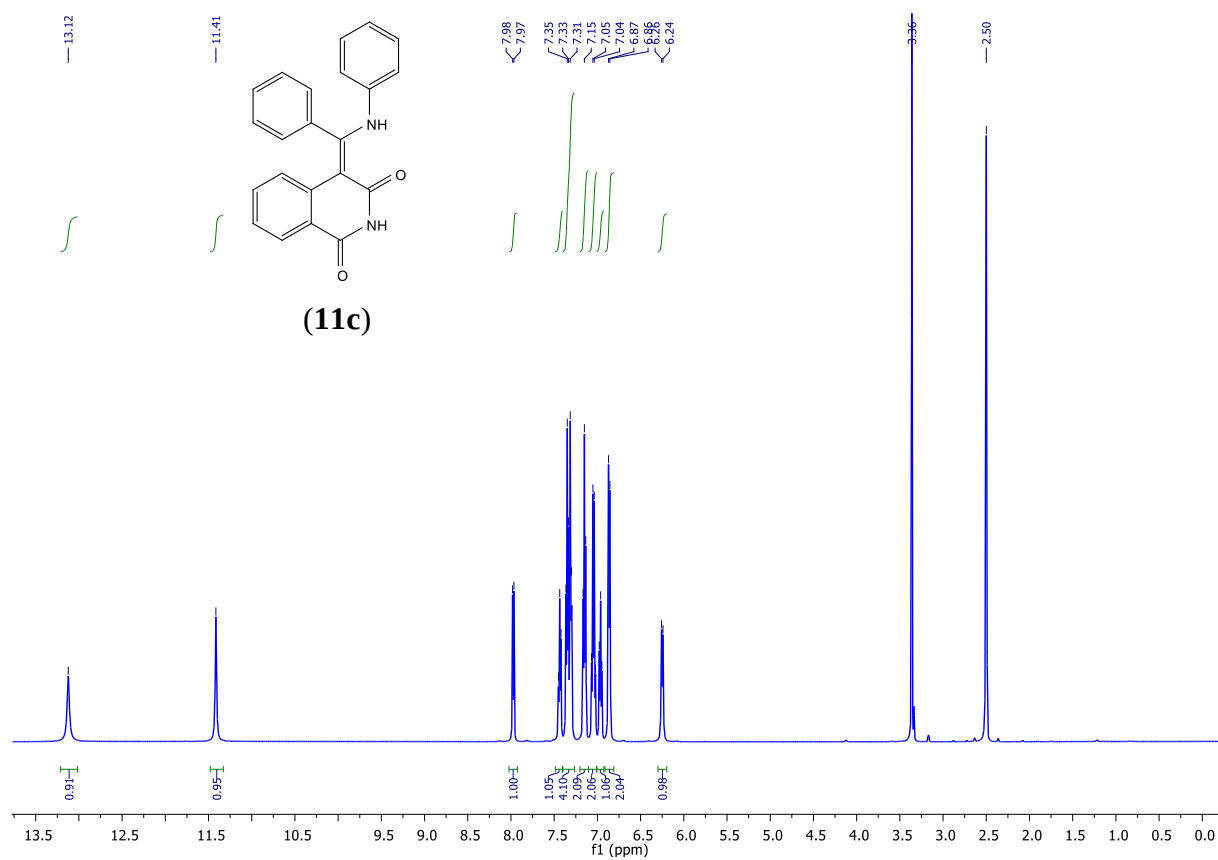
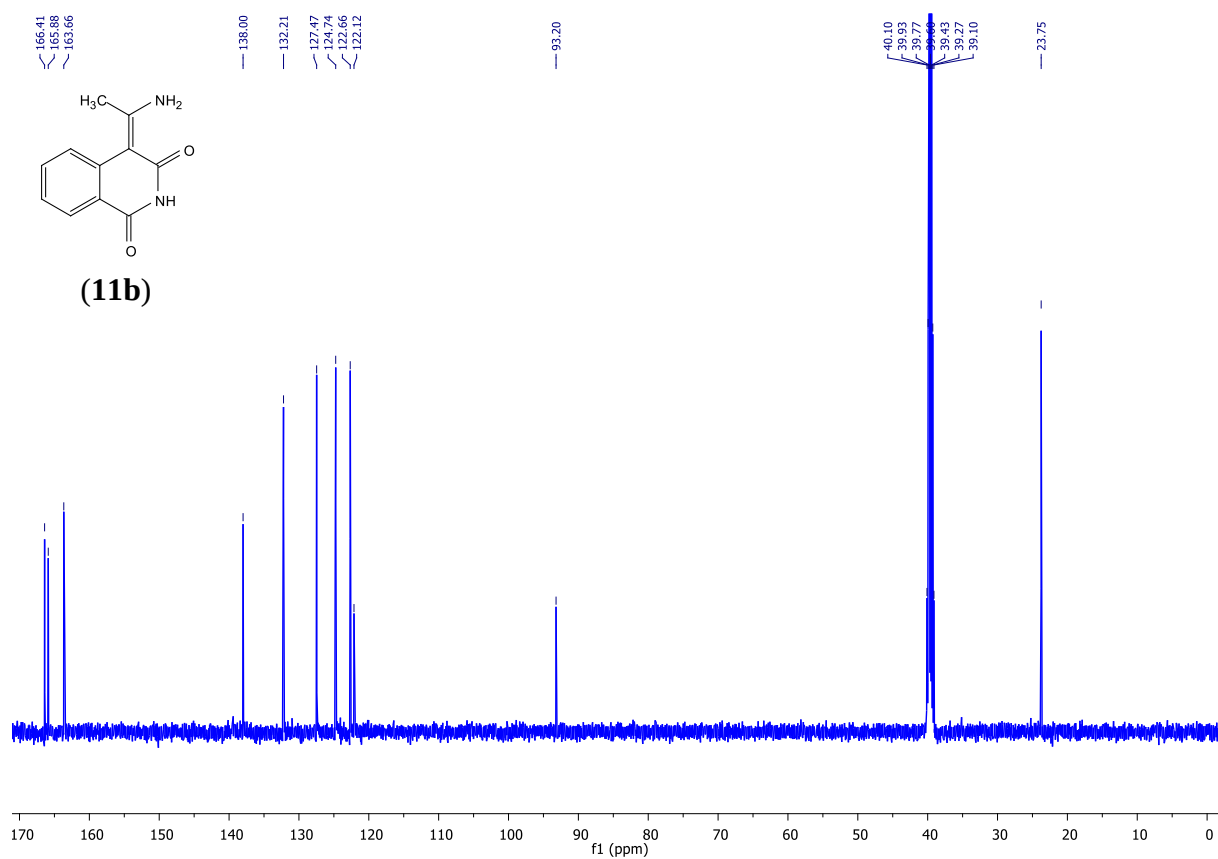


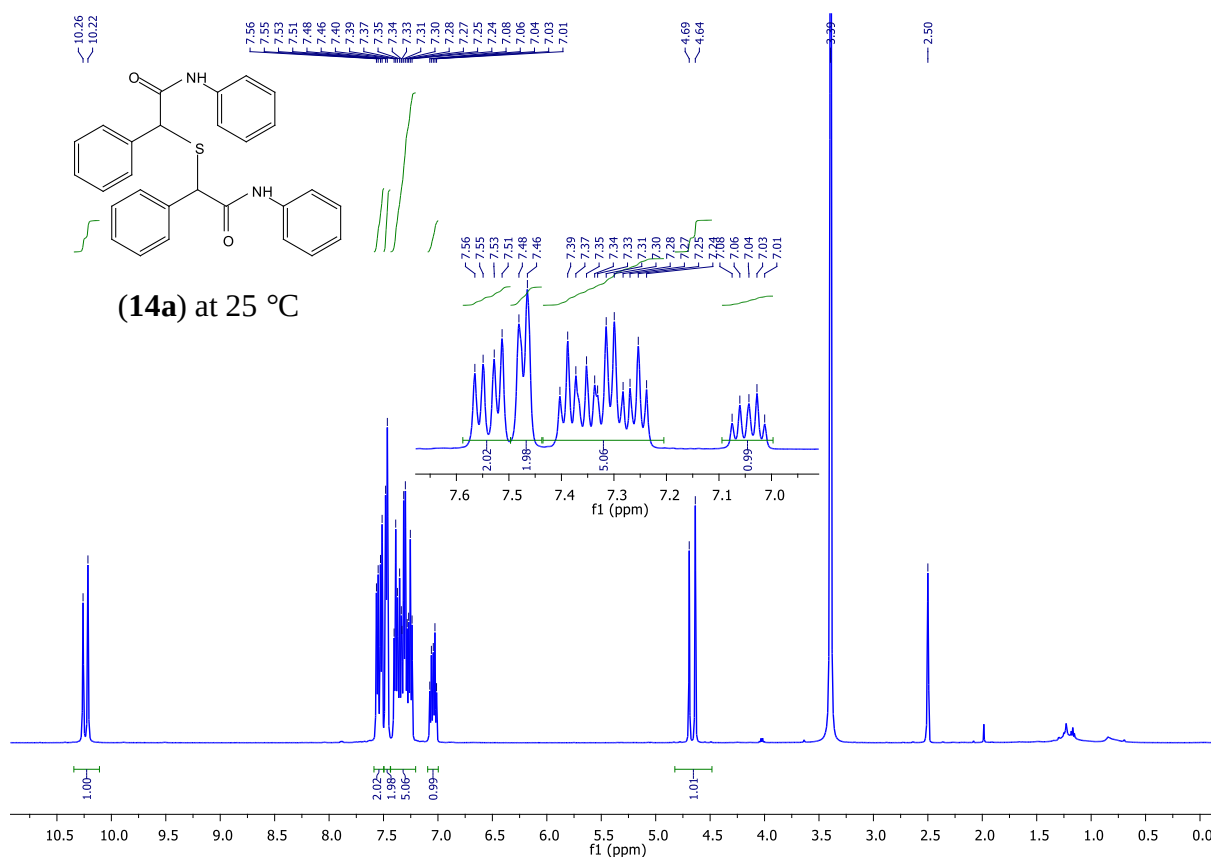
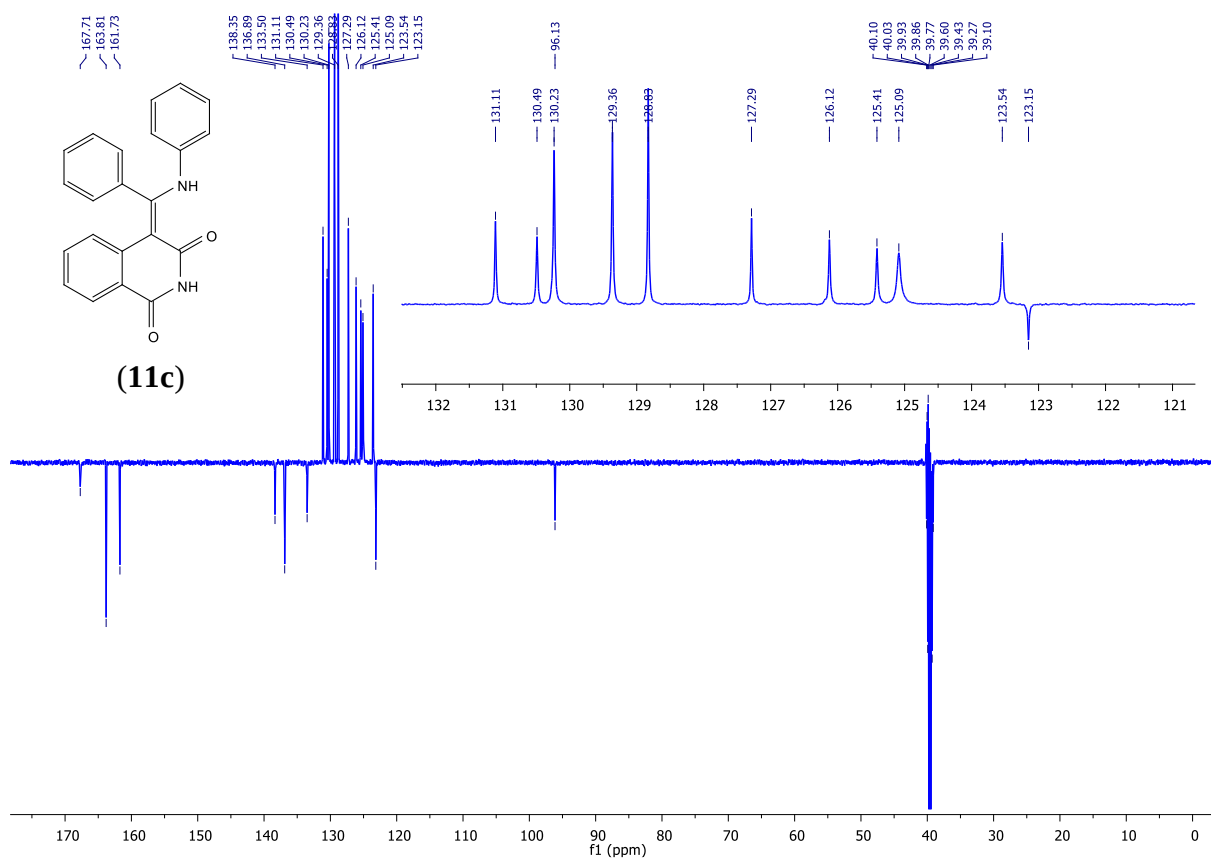


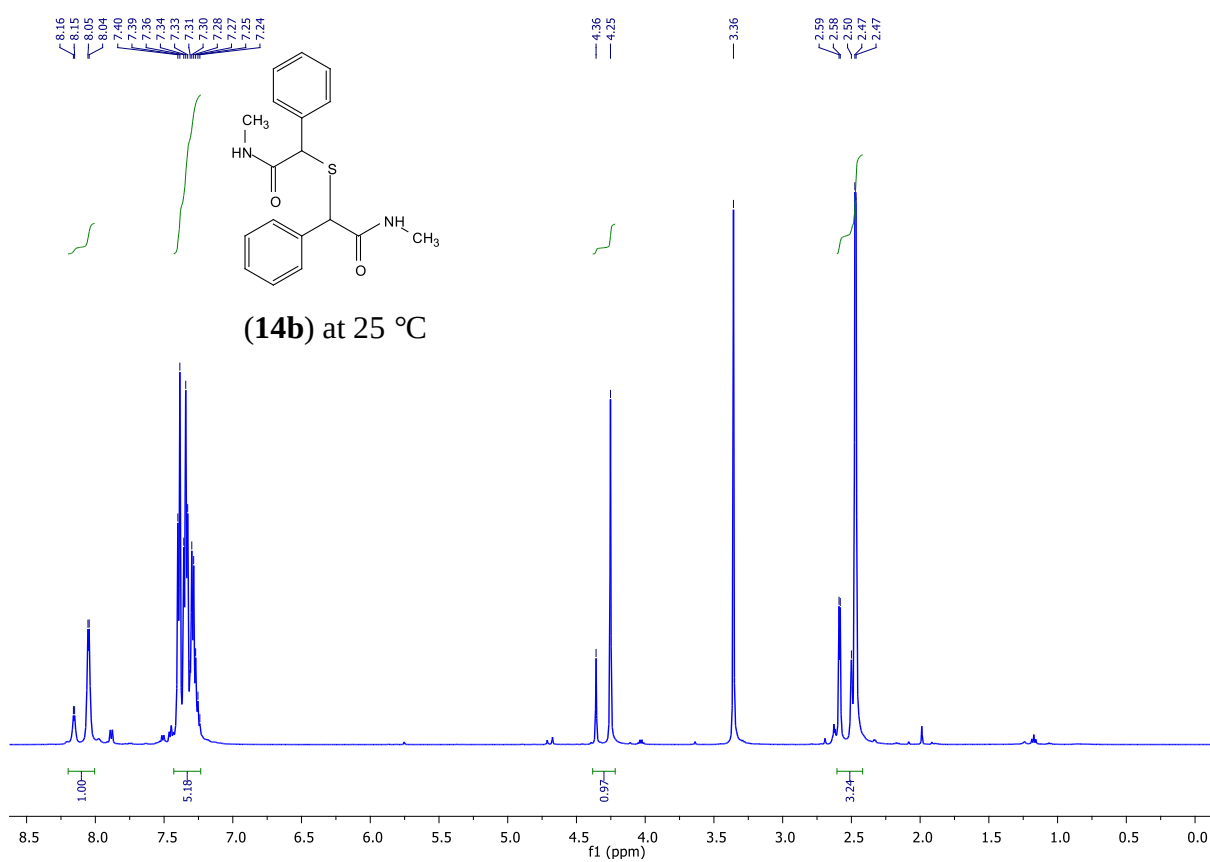
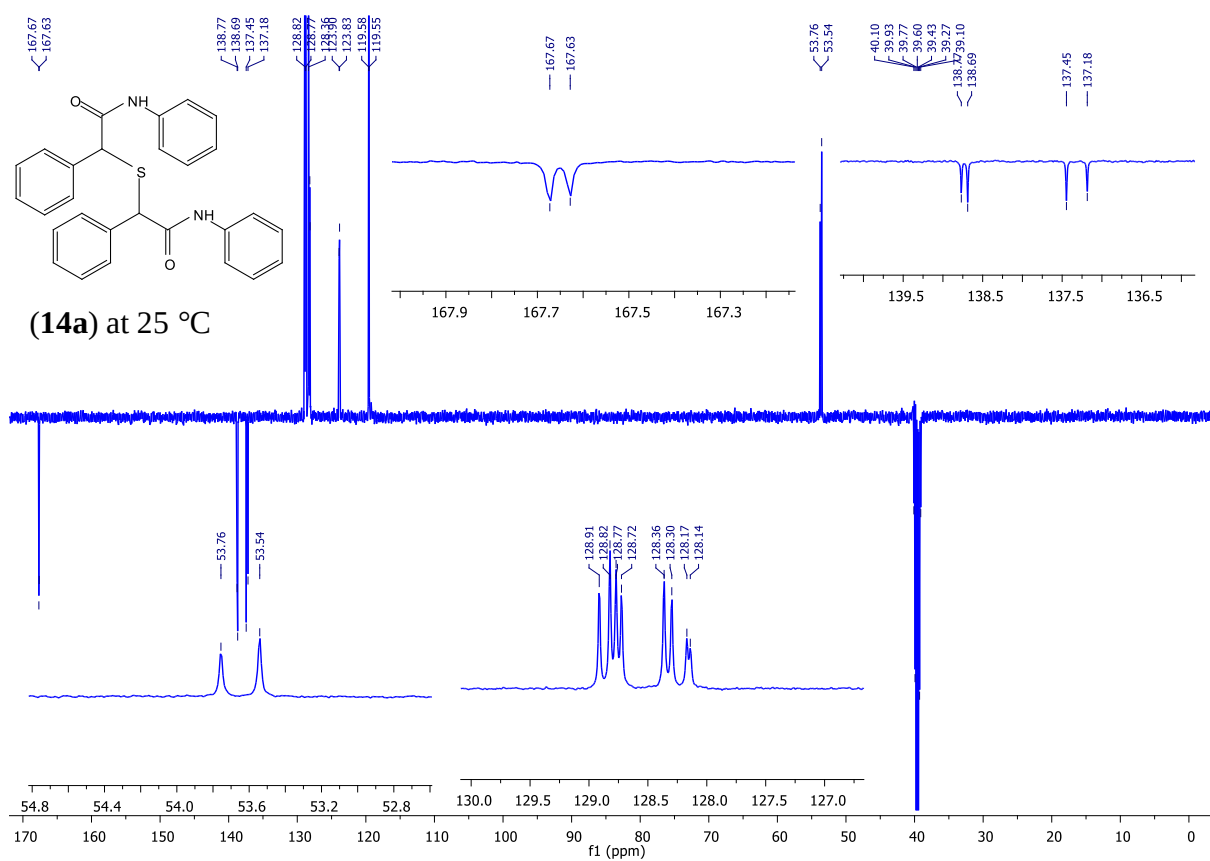


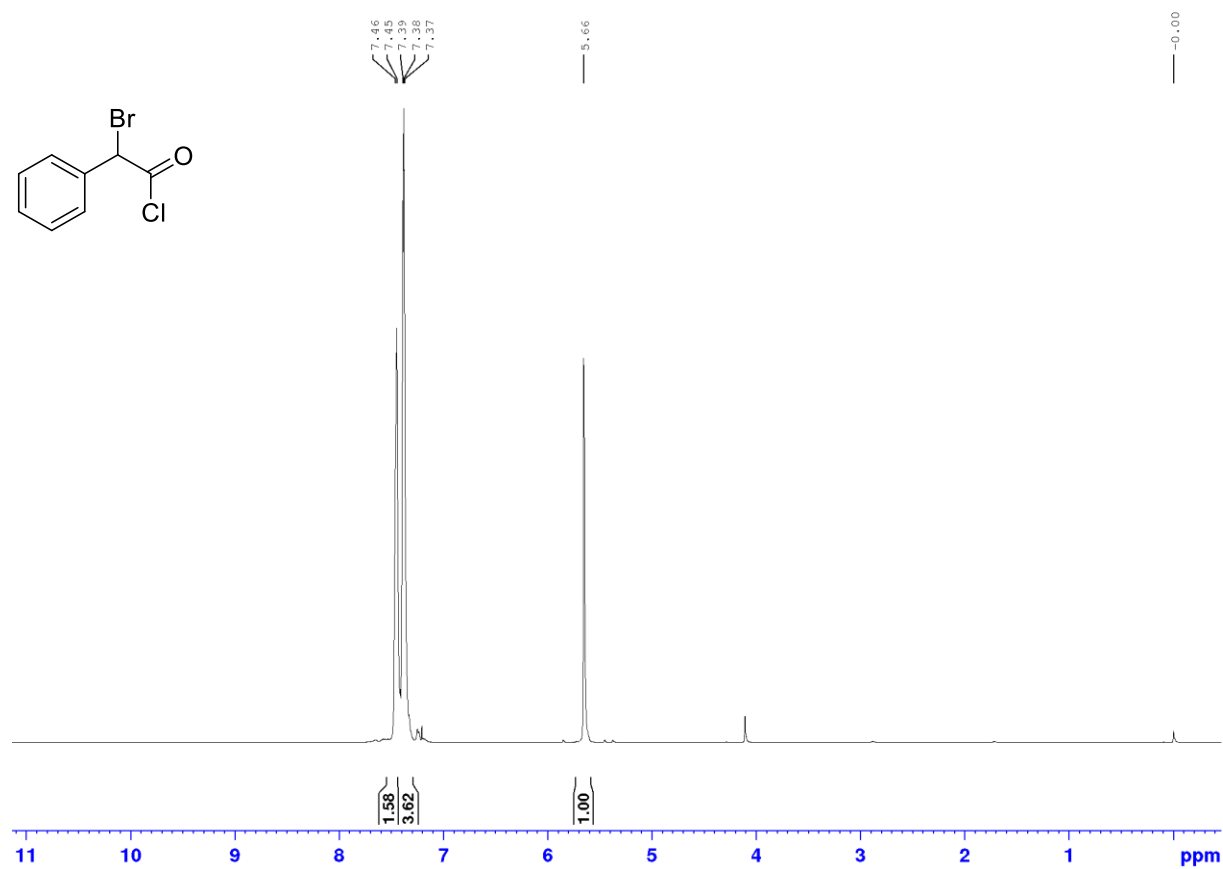
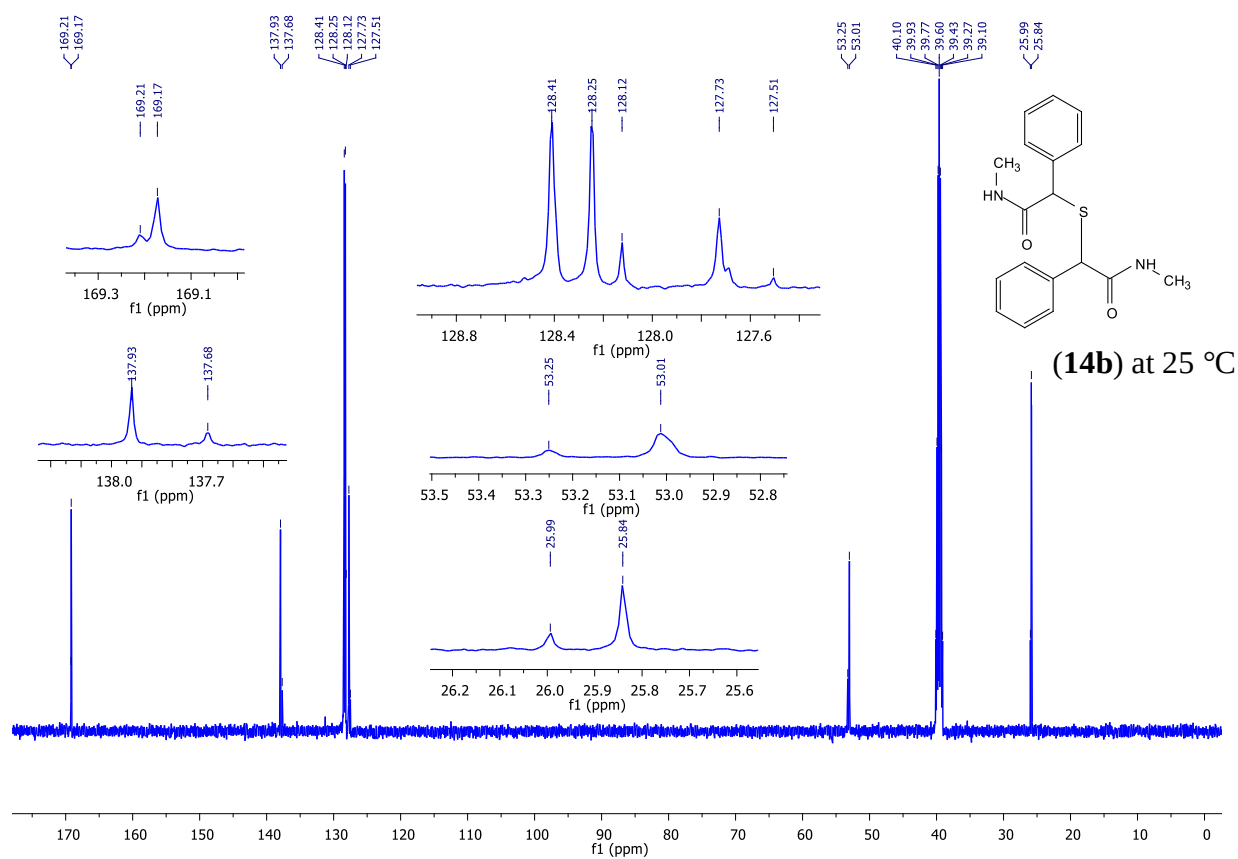


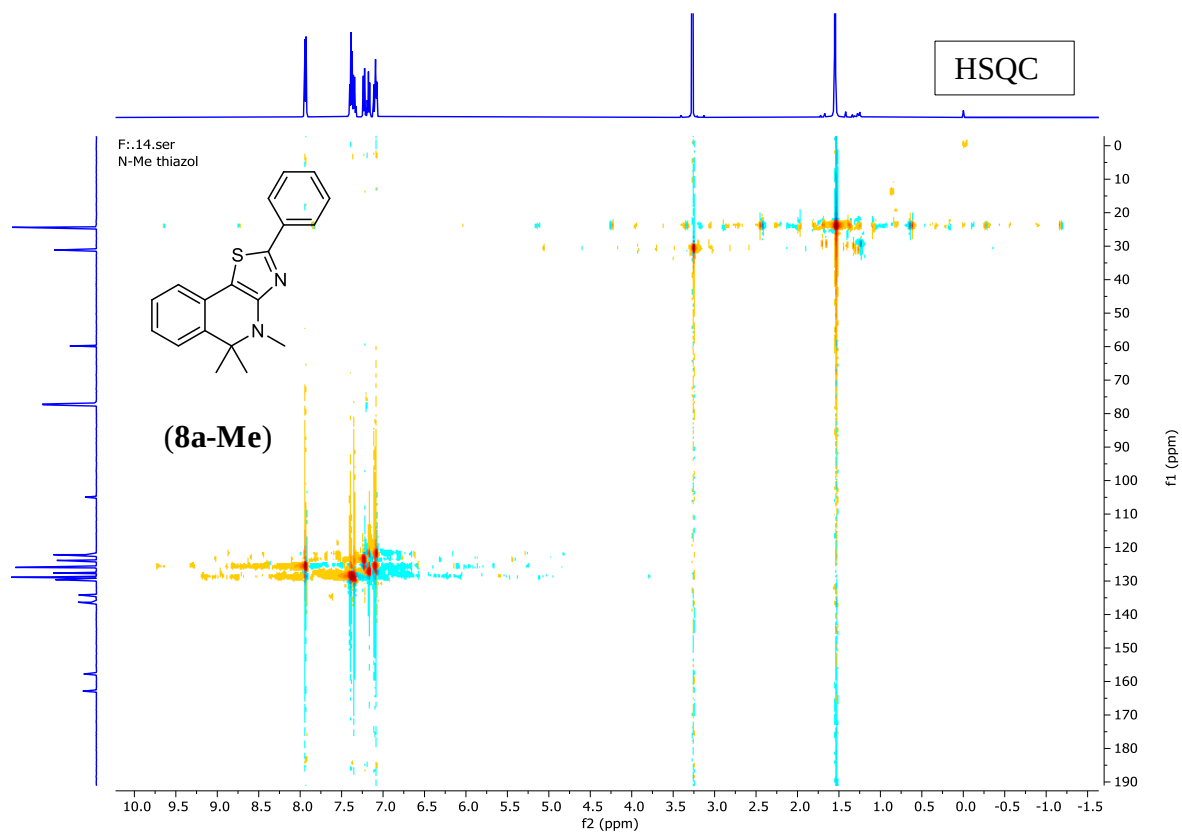
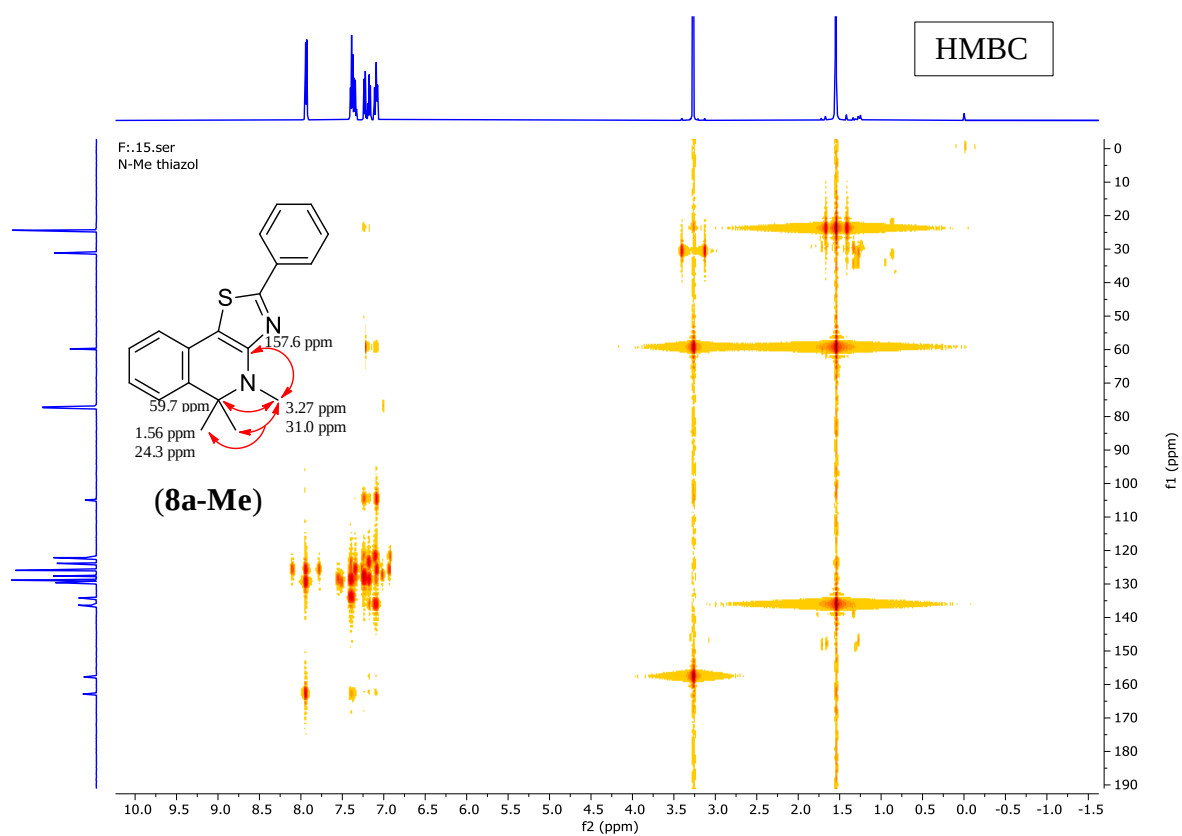


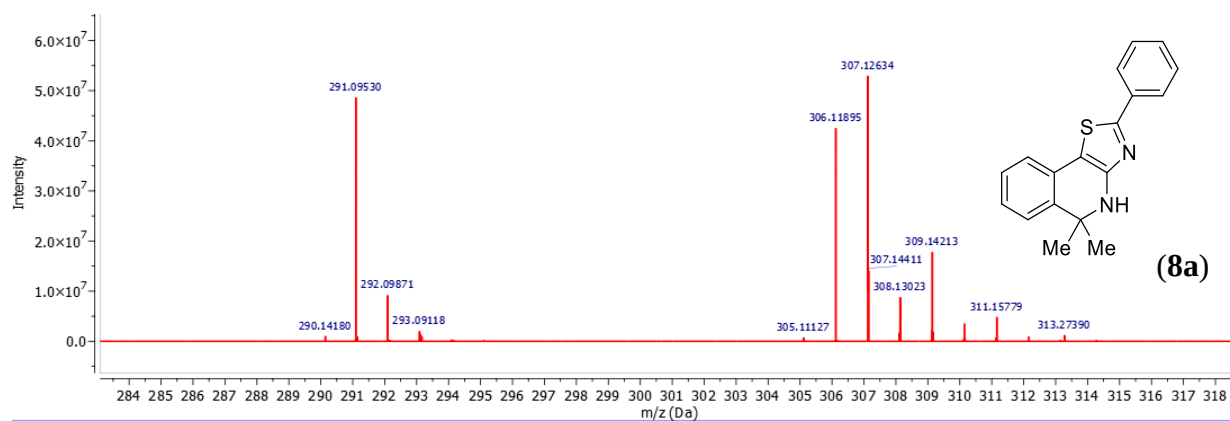
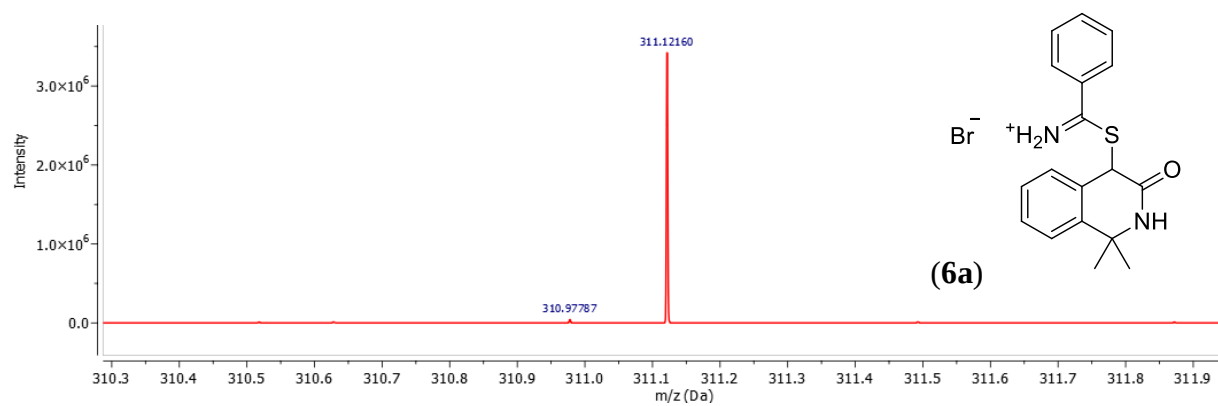
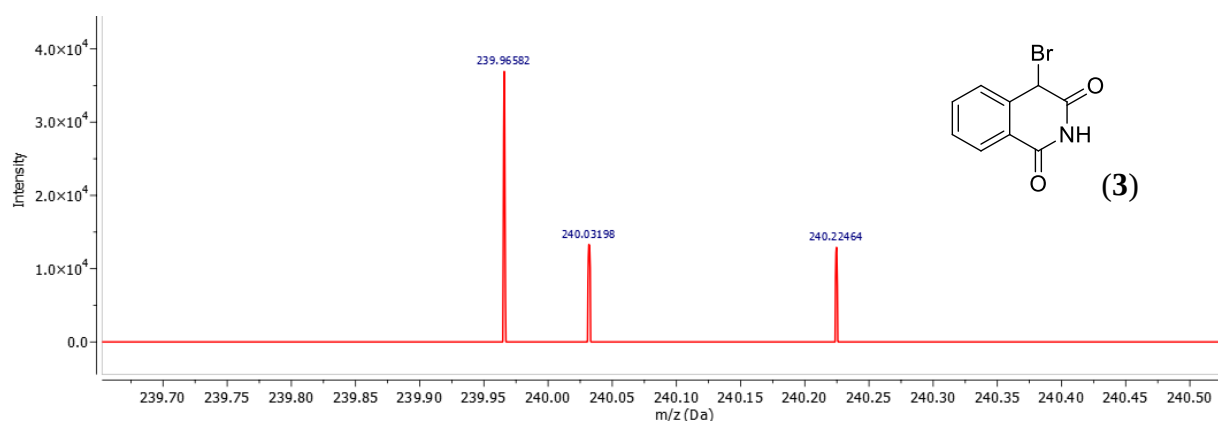
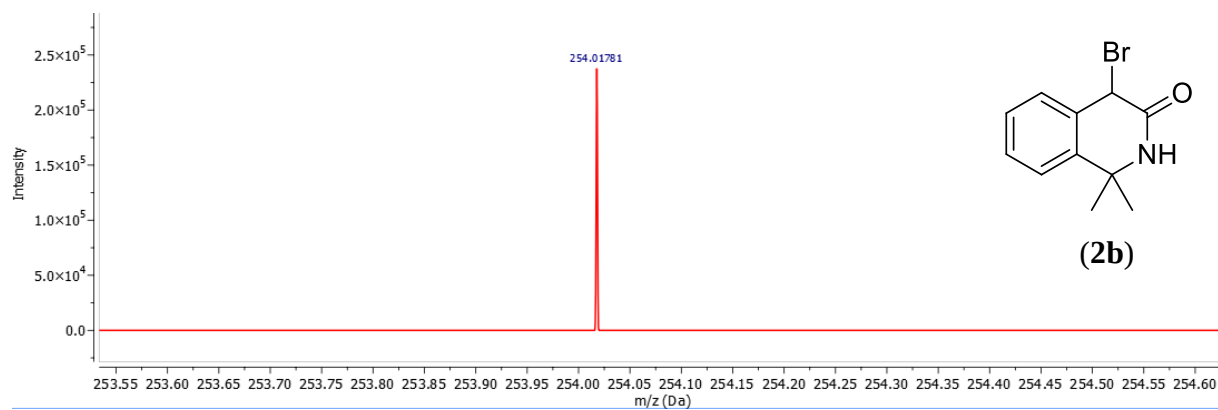


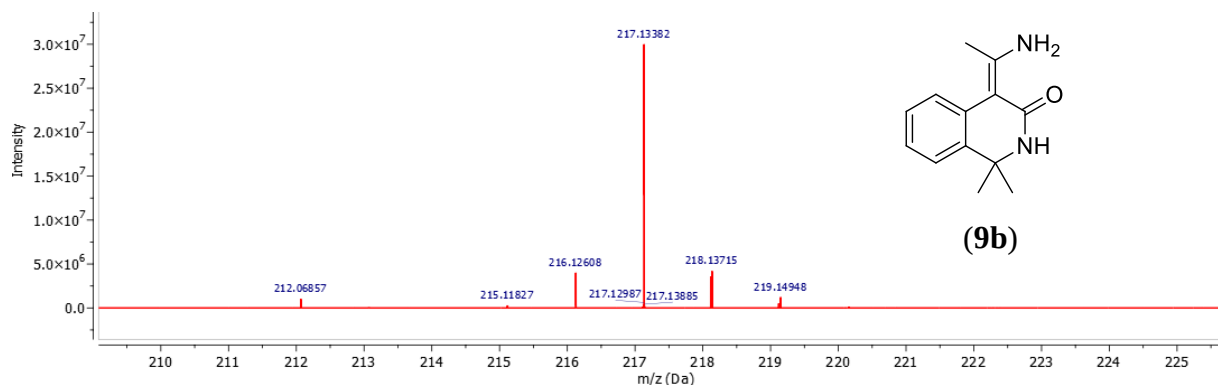
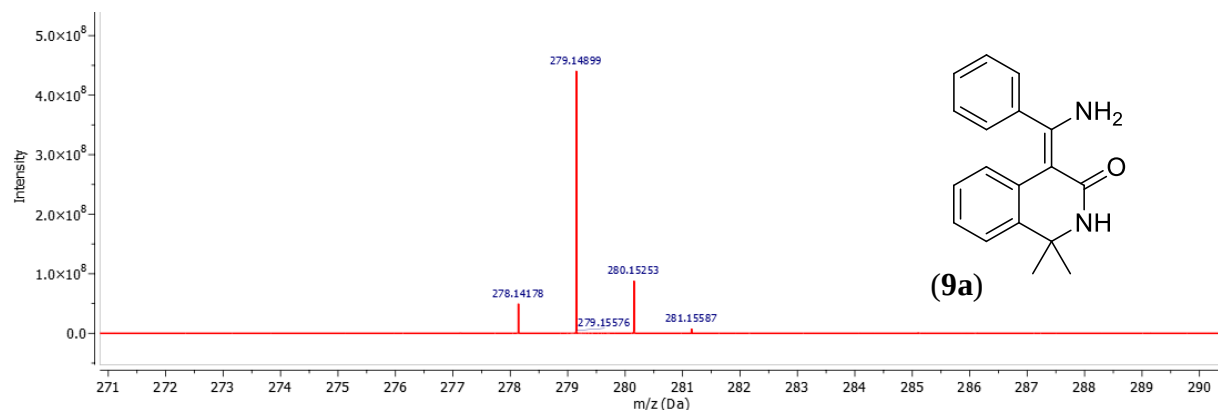
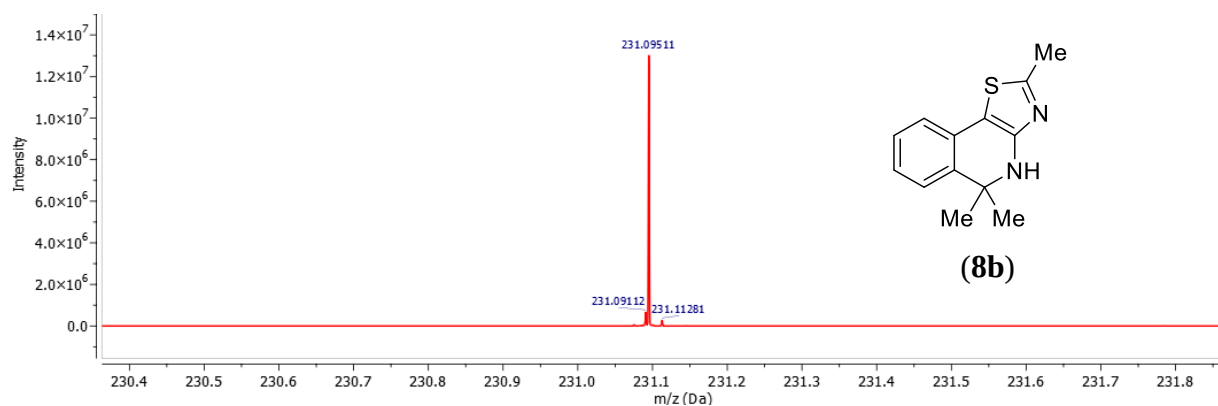
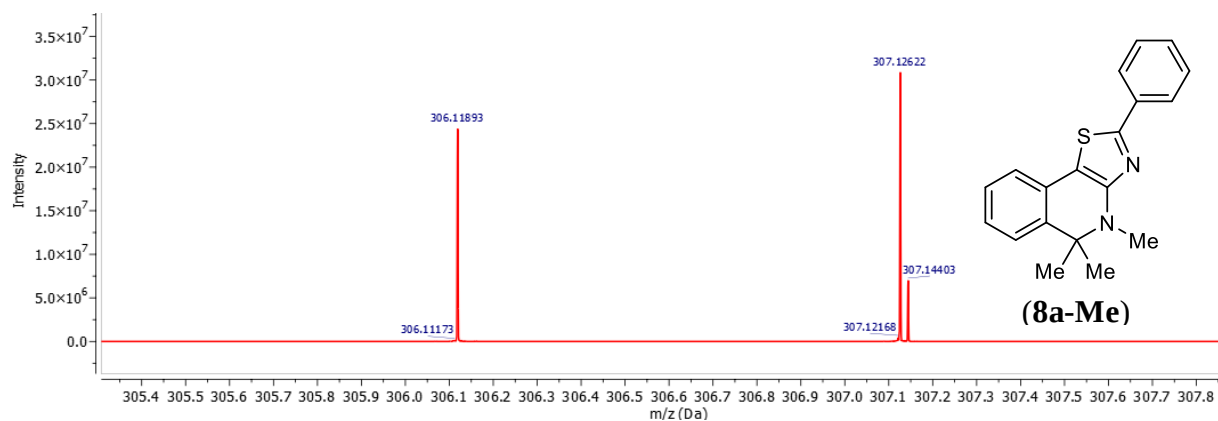


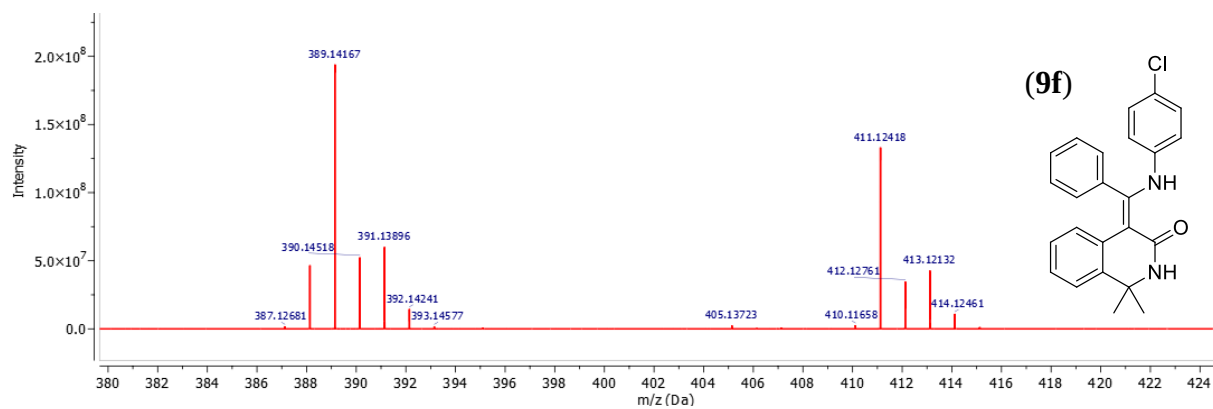
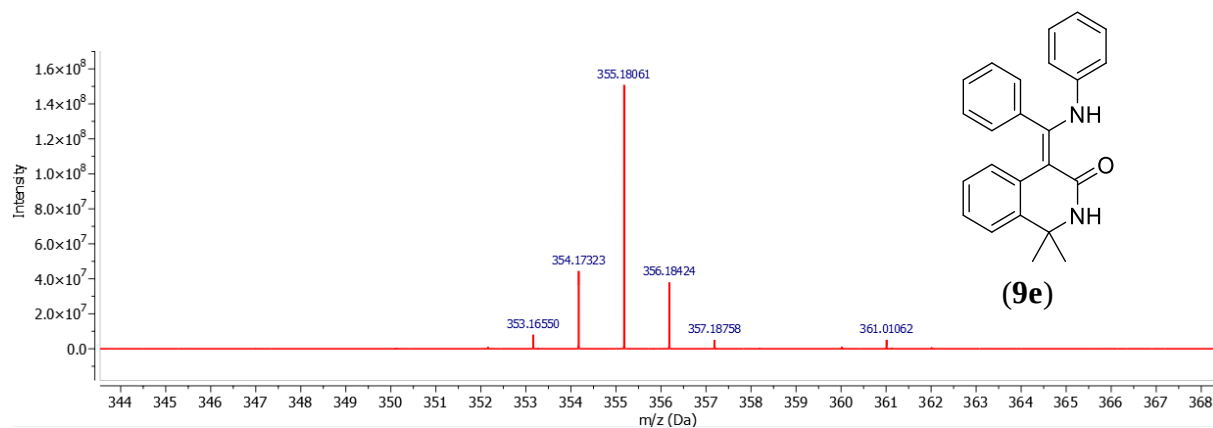
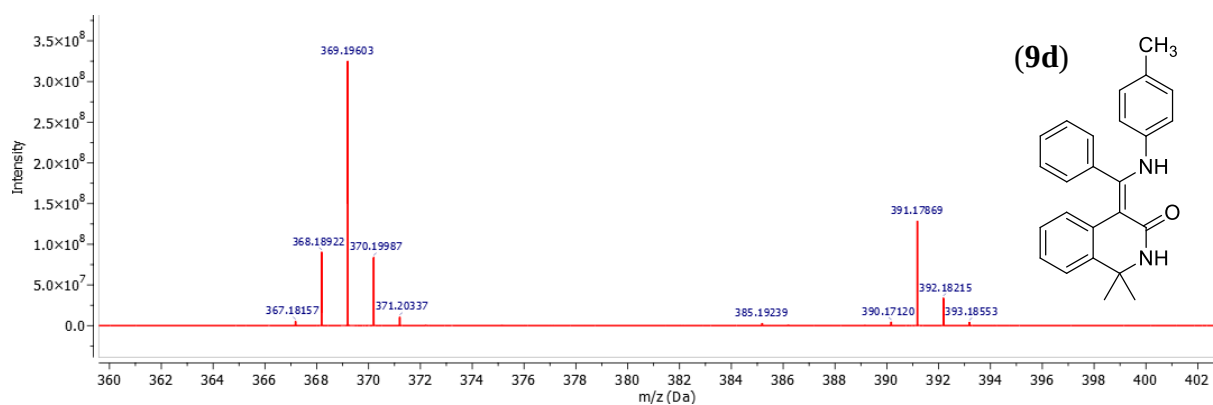
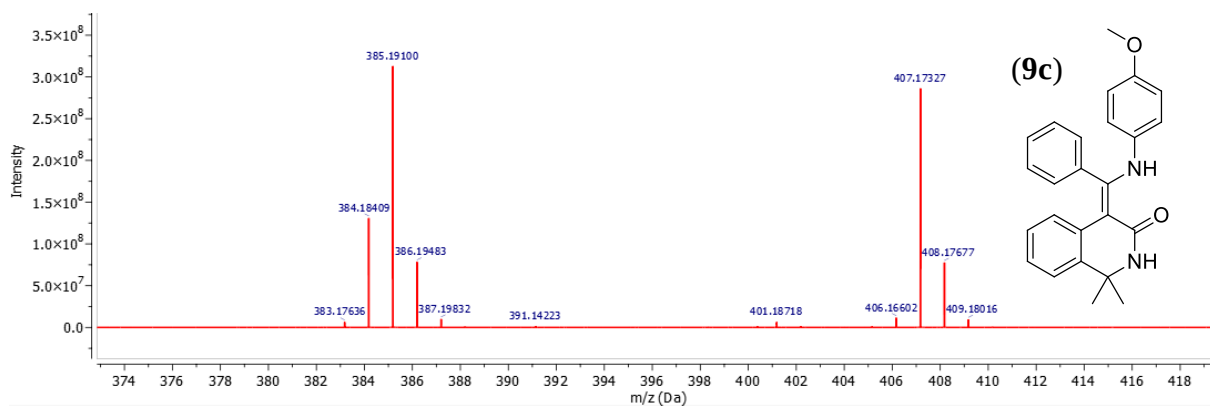


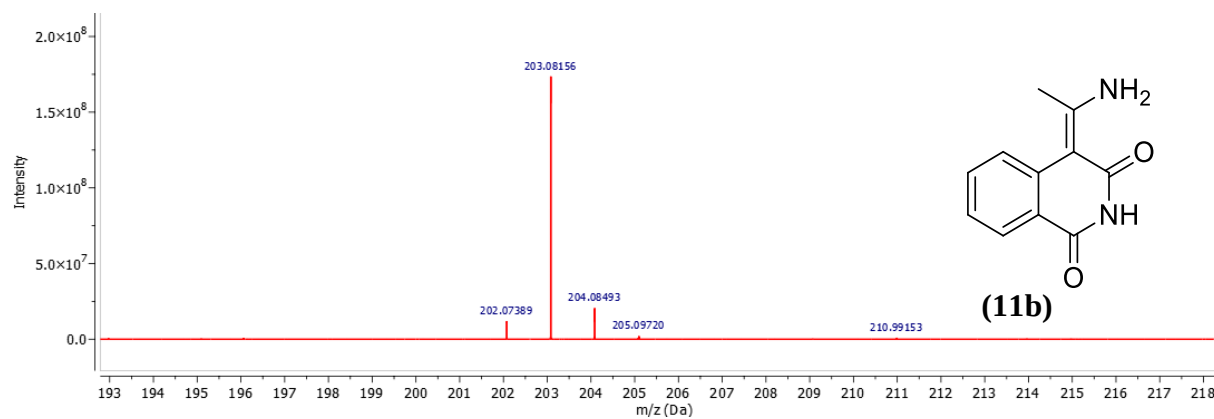
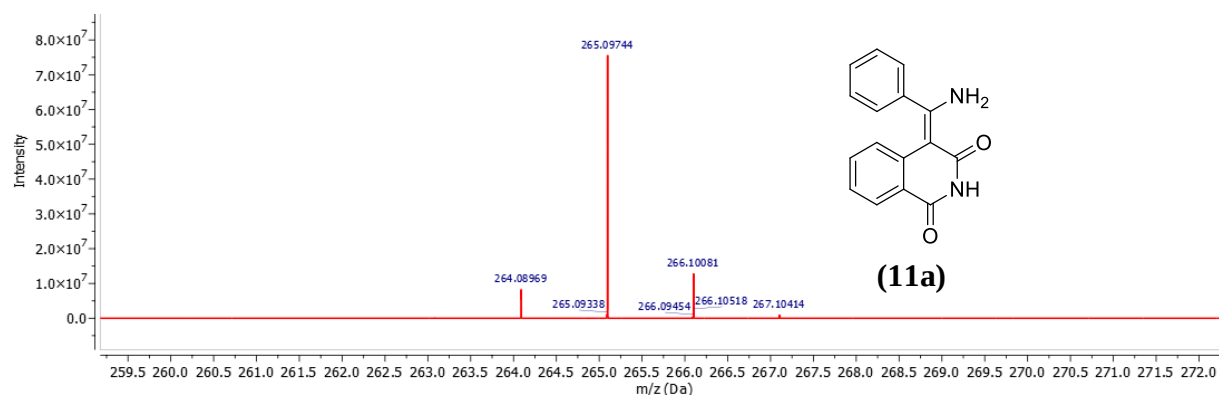
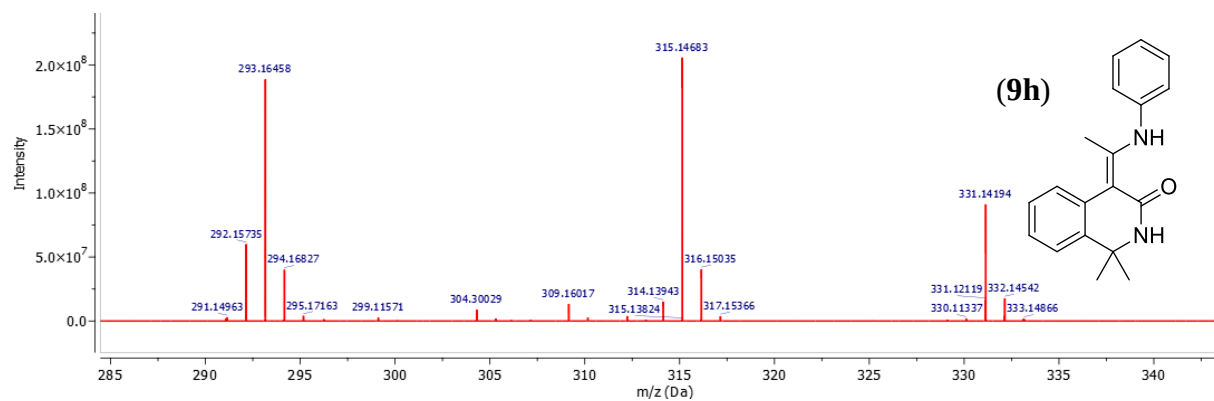
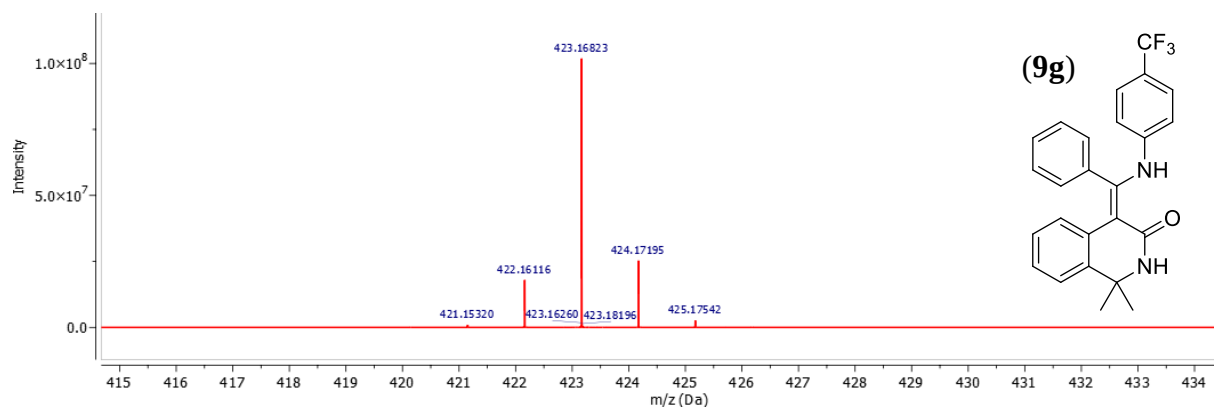


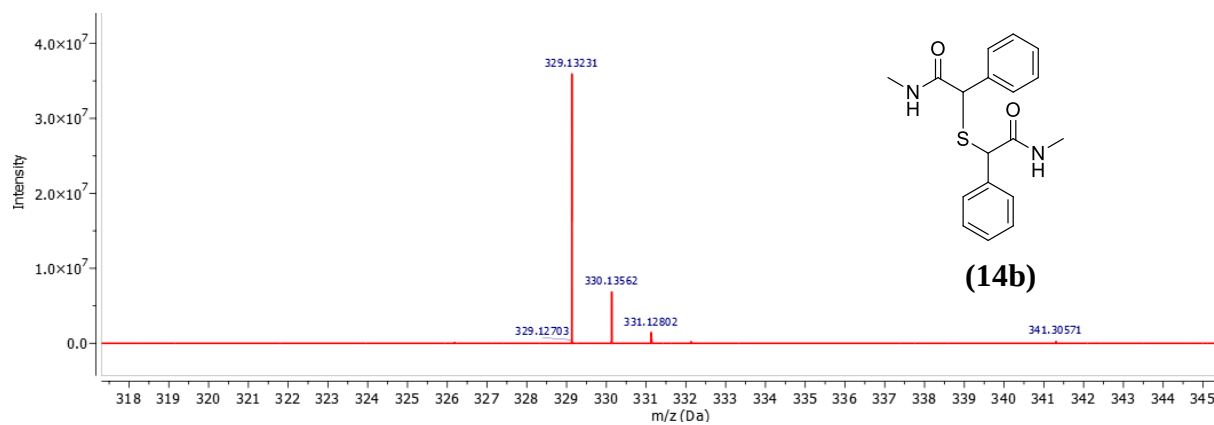
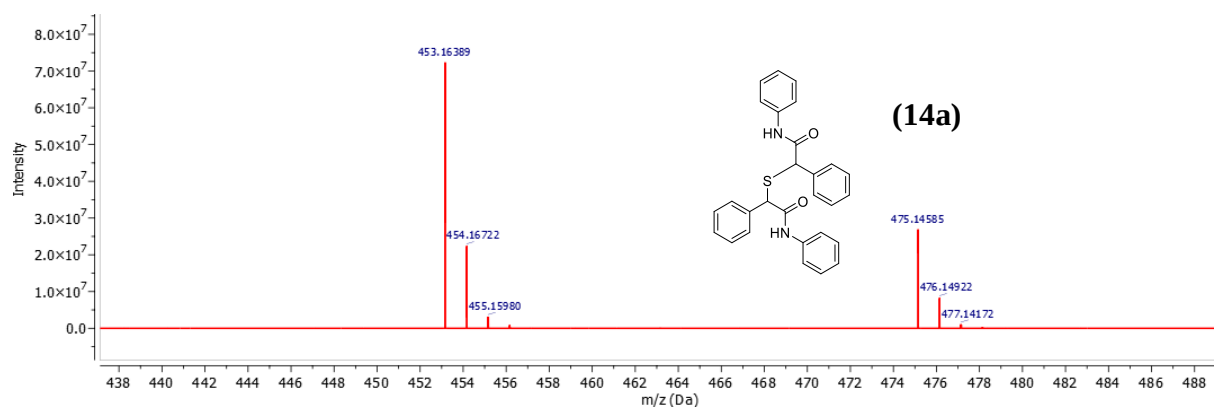
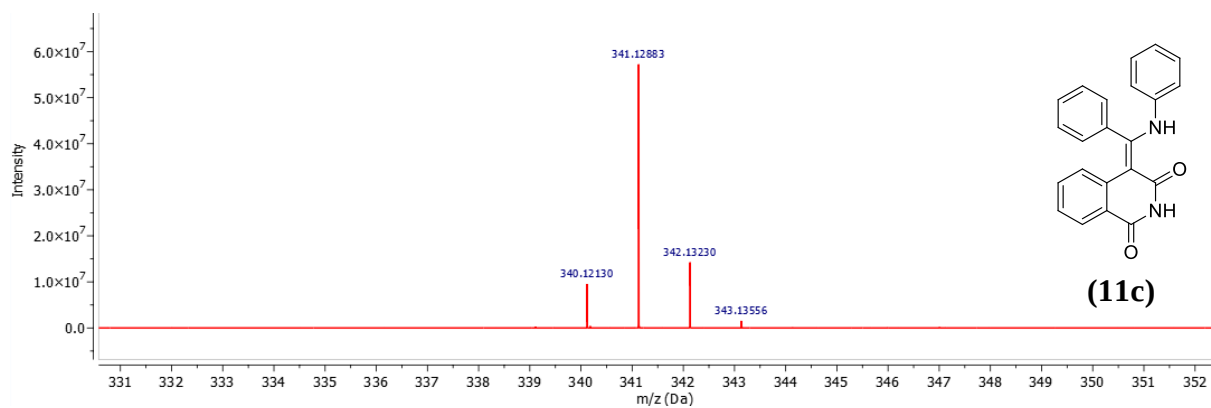


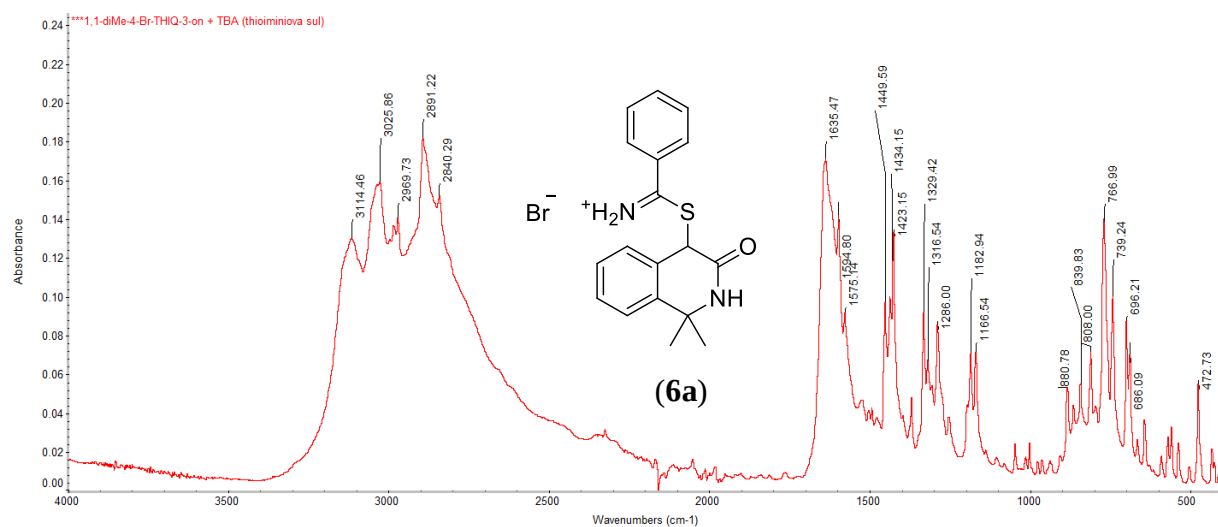




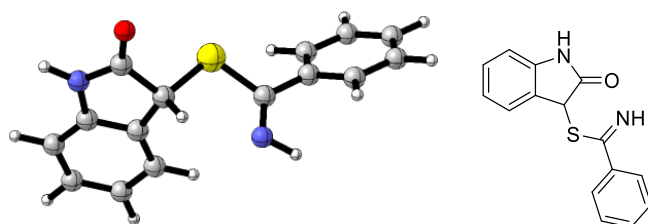






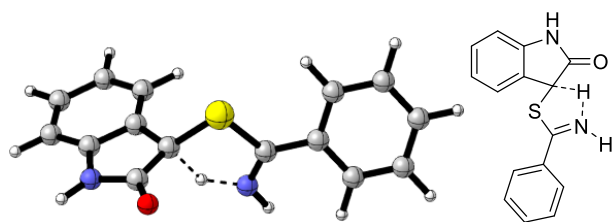


Coordinates



1-1 0 1 scf done: -1162.079869 Sum of electronic and thermal Free Energies -1161.887674
 imag. freq.: 0

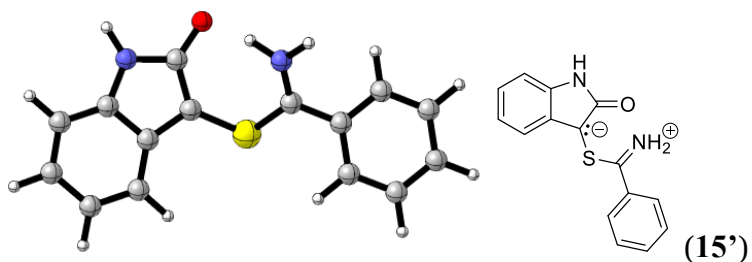
C	-2.8949580	-2.6569340	0.2264660
C	-1.8799140	-1.7277090	0.4884430
C	-2.1279900	-0.3864080	0.2493740
C	-3.3726010	0.0206730	-0.2512610
C	-4.3905220	-0.8833980	-0.5157300
C	-4.1307580	-2.2358810	-0.2675660
H	-2.7187510	-3.7104510	0.4088830
H	-0.9185980	-2.0506170	0.8693100
H	-5.3481780	-0.5542230	-0.9007750
H	-4.9066120	-2.9668250	-0.4648970
N	-3.3733740	1.4132450	-0.4149940
H	-4.1616090	1.9504110	-0.7535860
C	-2.1851000	1.9887150	-0.0504070
O	-1.9156710	3.1745070	-0.0868940
C	-1.2761490	0.8374260	0.4337080
H	-1.0051550	1.0087950	1.4783180
S	0.3049600	0.8505980	-0.4960730
C	1.3992250	0.1029650	0.7091180
C	2.7797270	-0.0955760	0.1887520
C	3.8694220	0.2040780	1.0174840
C	3.0104300	-0.5887340	-1.1014470
C	5.1691790	0.0118690	0.5606090
H	3.6966420	0.6032450	2.0103250
C	4.3137760	-0.7890890	-1.5501090
H	2.1762440	-0.8385380	-1.7455560
C	5.3942950	-0.4867230	-0.7231340
H	6.0063850	0.2564950	1.2040730
H	4.4830710	-1.1840760	-2.5450920
H	6.4078480	-0.6371760	-1.0767960
N	0.9882870	-0.1710370	1.8810850
H	1.7345910	-0.5888090	2.4394830



31

1-TS1 0 1 scf done: -1162.054171 Sum of electronic and thermal Free Energies -1161.865353
imag. freq.: 1 (-1593.5)

C	3.5154870	2.3991040	0.3947370
C	2.2824270	1.7785390	0.1553840
C	2.2445440	0.4016370	-0.0267140
C	3.4448490	-0.3423560	0.0318270
C	4.6709050	0.2593660	0.2781150
C	4.6919120	1.6481950	0.4587680
H	3.5561820	3.4737030	0.5327310
H	1.3709460	2.3645550	0.1073980
H	5.5820520	-0.3263510	0.3224710
H	5.6374130	2.1440070	0.6476360
N	3.1425320	-1.6841680	-0.1936750
H	3.8224380	-2.4309690	-0.2371760
C	1.7884800	-1.8818570	-0.4432600
O	1.2834360	-2.9632820	-0.7342360
C	1.1489770	-0.5618980	-0.2198410
H	0.4081040	-0.6893790	0.9960600
S	-0.3342950	-0.1491900	-1.1009040
C	-1.4052230	-0.2031950	0.3445750
C	-2.8321500	0.0935720	0.1953220
C	-3.7600160	-0.4708530	1.0842360
C	-3.2811130	0.9353580	-0.8321200
C	-5.1141780	-0.1931110	0.9448370
H	-3.4247150	-1.1409430	1.8668560
C	-4.6369440	1.2170910	-0.9596430
H	-2.5733370	1.3888770	-1.5152520
C	-5.5544550	0.6528280	-0.0743050
H	-5.8270300	-0.6391690	1.6281590
H	-4.9759960	1.8778890	-1.7484800
H	-6.6112730	0.8700620	-0.1784390
N	-0.7878120	-0.5383050	1.4127930
H	-1.2616810	-0.5777580	2.3100380

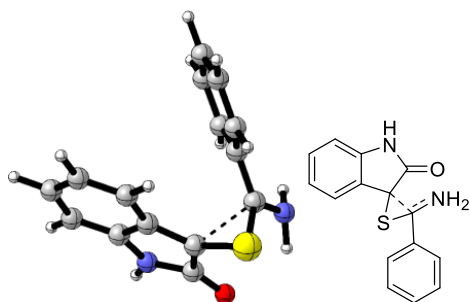


31

1-2 0 1 scf done: -1162.070177 Sum of electronic and thermal Free Energies -1161.876540

imag. freq.: 0

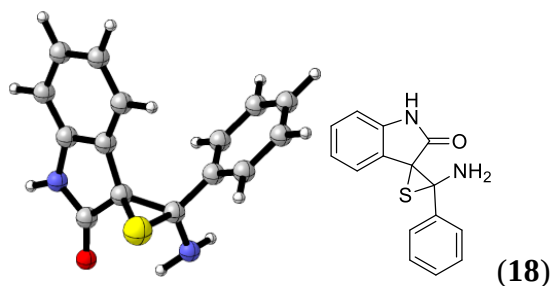
C	-3.9541310	-2.2703880	0.1861750
C	-2.6497770	-1.8283420	-0.0471420
C	-2.3989110	-0.4531950	-0.1243530
C	-3.4880760	0.4542240	0.0372670
C	-4.7843740	0.0161950	0.2708260
C	-5.0100540	-1.3630660	0.3449530
H	-4.1514170	-3.3350510	0.2484020
H	-1.8436460	-2.5447070	-0.1631760
H	-5.5960420	0.7250460	0.3927820
H	-6.0136200	-1.7300700	0.5275700
N	-2.9851410	1.7400980	-0.0803360
H	-3.5138530	2.5917480	0.0436900
C	-1.6112840	1.7255530	-0.3193850
O	-0.9139230	2.7742850	-0.4352860
C	-1.2290790	0.3565820	-0.3392780
H	0.4107760	2.2321290	0.3883020
S	0.3189980	-0.3112820	-0.8075120
C	1.5289170	0.5440540	0.0831490
C	2.8921510	-0.0048360	0.0700680
C	3.9914500	0.8682610	0.0317550
C	3.1079890	-1.3909370	0.1076600
C	5.2839080	0.3586140	0.0337310
H	3.8350460	1.9387800	-0.0286350
C	4.4043430	-1.8921470	0.1124870
H	2.2668860	-2.0705320	0.1624280
C	5.4925840	-1.0204720	0.0748860
H	6.1283710	1.0363000	-0.0061960
H	4.5652920	-2.9627250	0.1535130
H	6.5021460	-1.4147470	0.0771990
N	1.2543280	1.6782180	0.6801780
H	1.9863410	2.1403070	1.2087770



31

1-TS2 0 1 scf done:-1162.055802 Sum of electronic and thermal Free Energies -1161.861967
imag. freq.: 1 (-336.7)

C	-0.9981720	2.9218090	0.9530800
C	-0.6407100	1.6103180	1.2805300
C	-1.1898350	0.5606210	0.5480940
C	-2.0967540	0.8395470	-0.5069870
C	-2.4586410	2.1377540	-0.8344820
C	-1.8932000	3.1806300	-0.0901240
H	-0.5766000	3.7476850	1.5146610
H	0.0516770	1.4111280	2.0893400
H	-3.1532800	2.3370480	-1.6424510
H	-2.1577210	4.2045680	-0.3287660
N	-2.4938660	-0.3671200	-1.0769590
H	-3.1497490	-0.4631660	-1.8397700
C	-1.9063060	-1.4535700	-0.4369640
O	-2.0732070	-2.6376840	-0.7481260
C	-1.0266240	-0.8743740	0.5771240
H	-0.0346120	-3.3631070	-0.6265020
S	-0.0684660	-1.8458310	1.7100880
C	0.7800640	-1.6925280	0.1683620
C	1.6887450	-0.5596370	-0.1064850
C	1.8124600	-0.0724040	-1.4168730
C	2.4098850	0.0556420	0.9217700
C	2.6497520	1.0034400	-1.6883510
H	1.2317100	-0.5127410	-2.2195400
C	3.2545240	1.1276240	0.6437210
H	2.3137590	-0.3077320	1.9368710
C	3.3765630	1.6048280	-0.6593210
H	2.7273930	1.3796710	-2.7018560
H	3.8135940	1.5908840	1.4484340
H	4.0279460	2.4444740	-0.8728190
N	0.7796060	-2.7557870	-0.6721840
H	1.1195790	-2.5959280	-1.6137960

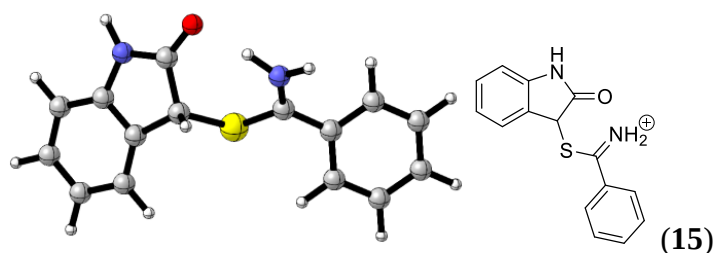


31

1-3 0 1 scf done: -1162.073785 Sum of electronic and thermal Free Energies -1161.879172

imag. freq.: 0

C	-1.1178380	2.8925580	0.8488430
C	-0.4981490	1.6407880	0.9292570
C	-1.1262440	0.5475930	0.3523810
C	-2.3700620	0.7054630	-0.2774510
C	-2.9997260	1.9376220	-0.3659860
C	-2.3493240	3.0359890	0.2061630
H	-0.6376260	3.7571820	1.2913590
H	0.4524230	1.5293400	1.4350880
H	-3.9596050	2.0426840	-0.8572040
H	-2.8158650	4.0129530	0.1522740
N	-2.8120060	-0.5379500	-0.7515420
H	-3.6914250	-0.6917170	-1.2283660
C	-1.9349280	-1.5466150	-0.4656030
O	-2.0668230	-2.7242130	-0.7601880
C	-0.7543580	-0.8885750	0.2478860
H	-0.0086910	-3.0763580	-1.0094020
S	0.0110550	-1.7680630	1.6823520
C	0.6425190	-1.4094130	-0.0364310
C	1.7395560	-0.3916530	-0.1838000
C	1.7136640	0.4493710	-1.3007580
C	2.7860250	-0.2888330	0.7304830
C	2.7205080	1.3916910	-1.4928370
H	0.8964980	0.3759980	-2.0097760
C	3.7952810	0.6536540	0.5375650
H	2.8052640	-0.9357800	1.5992100
C	3.7628500	1.4973960	-0.5716750
H	2.6869130	2.0469230	-2.3558190
H	4.6036850	0.7297330	1.2558650
H	4.5442280	2.2346840	-0.7172470
N	0.8488220	-2.5497680	-0.8624280
H	1.2537840	-2.2839050	-1.7547140

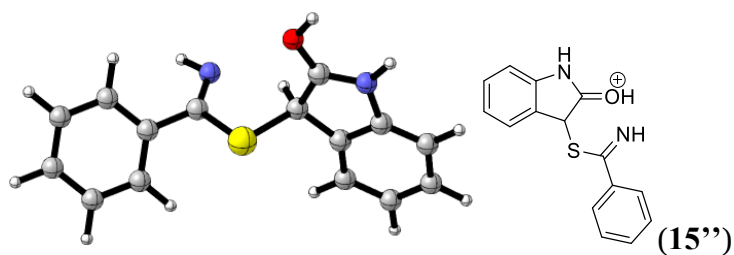


32

1-4 1 1 scf done: -1162.540262 Sum of electronic and thermal Free Energies -1162.333094

imag. freq.: 0

C	-2.2483930	-2.7206070	-0.1247690
C	-1.5790650	-1.4920670	-0.0762660
C	-2.3302960	-0.3389890	0.0791920
C	-3.7257090	-0.4093740	0.1824840
C	-4.4050160	-1.6148620	0.1399480
C	-3.6388800	-2.7752940	-0.0187440
H	-1.6812200	-3.6355170	-0.2452250
H	-0.4993890	-1.4458550	-0.1585830
H	-5.4836870	-1.6565980	0.2265880
H	-4.1404860	-3.7352140	-0.0578440
N	-4.2468560	0.8880980	0.3397020
H	-5.2314590	1.1019460	0.4494780
C	-3.2792700	1.8338840	0.3537330
O	-3.4275430	3.0429550	0.4947220
C	-1.9322900	1.1079450	0.1696290
H	-1.2558110	1.3388580	0.9948890
S	-1.0693780	1.5908780	-1.3986390
C	-0.4044360	3.1658250	-1.0655990
C	0.6931130	3.5986860	-1.9304090
C	0.7607360	4.9461200	-2.3261500
C	1.6607720	2.6857550	-2.3808590
C	1.7869840	5.3691490	-3.1586460
H	-0.0044660	5.6450950	-2.0102070
C	2.6885540	3.1229180	-3.2064980
H	1.6290150	1.6528420	-2.0591850
C	2.7515350	4.4602290	-3.5974120
H	1.8305070	6.4045310	-3.4738710
H	3.4433650	2.4214370	-3.5400820
H	3.5521040	4.7953160	-4.2465230
N	-0.8834690	3.9404280	-0.1336460
H	-0.4135690	4.8136920	0.0893410
H	-1.7905420	3.7421680	0.3173180

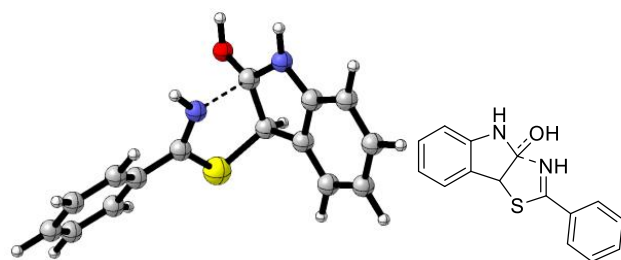


32

1-5 1 1 scf done: -1162.496961 Sum of electronic and thermal Free Energies -1162.292359

imag. freq.: 0

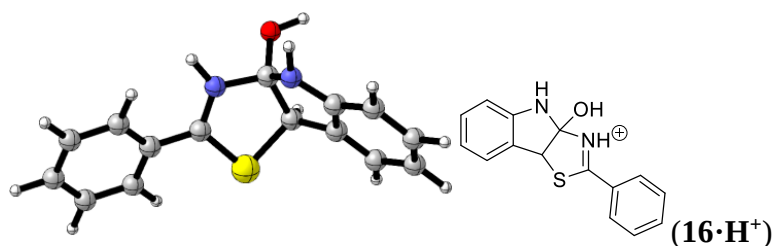
C	3.8231940	-2.1553680	-0.6831850
C	2.5465680	-1.5854010	-0.7411700
C	2.3790370	-0.3114300	-0.2261790
C	3.4687260	0.3600080	0.3315380
C	4.7400930	-0.1754910	0.3996810
C	4.8993740	-1.4627690	-0.1232620
H	3.9785950	-3.1519750	-1.0783360
H	1.7134000	-2.1265380	-1.1729150
H	5.5662410	0.3719590	0.8352060
H	5.8768800	-1.9283470	-0.0901370
N	3.0215300	1.6371540	0.7841340
H	3.6268370	2.3245350	1.2314280
C	1.7447400	1.7972740	0.5438860
O	1.0175670	2.8338630	0.8270670
C	1.1803470	0.5950430	-0.1540080
H	0.8114090	0.9190290	-1.1418030
S	-0.3041660	-0.0929250	0.6655490
C	-1.5643850	0.4225770	-0.5230600
C	-2.9135800	-0.0975740	-0.1899780
C	-4.0264800	0.7327240	-0.3816620
C	-3.0967860	-1.3995740	0.2929210
C	-5.3038720	0.2633690	-0.0965400
H	-3.8871900	1.7471170	-0.7366710
C	-4.3793530	-1.8667880	0.5676400
H	-2.2465970	-2.0569500	0.4282590
C	-5.4830360	-1.0372810	0.3763280
H	-6.1590280	0.9137170	-0.2388280
H	-4.5150460	-2.8800490	0.9270660
H	-6.4800510	-1.4015530	0.5957340
N	-1.2453110	1.1733130	-1.4927870
H	-2.0379520	1.3592650	-2.1089550
H	1.5214280	3.5431630	1.2723530



32

1-TS4 1 1 scf done: -1162.496053 Sum of electronic and thermal Free Energies -1162.289356
 imag. freq.: 1 (-264.1)

C	3.3989110	-2.0628810	0.8898970
C	2.5898390	-1.7533530	-0.2093110
C	2.3616360	-0.4200910	-0.5011690
C	2.9334720	0.5816930	0.2899180
C	3.7374620	0.2990660	1.3807770
C	3.9629720	-1.0506590	1.6691630
H	3.5886770	-3.1000620	1.1385730
H	2.1488290	-2.5386860	-0.8117450
H	4.1699430	1.0887070	1.9826900
H	4.5852140	-1.3116420	2.5170690
N	2.5559370	1.8428310	-0.2234410
H	2.7552720	2.7216960	0.2432570
C	1.5939840	1.6946980	-1.1498370
O	1.2216800	2.6560240	-1.9704820
C	1.5933580	0.2437650	-1.6209020
S	-0.0767340	-0.4078440	-1.9727570
C	-0.8782490	0.5272490	-0.6877540
C	-2.2947970	0.2375380	-0.4040470
C	-2.8119940	0.5082610	0.8712110
C	-3.1307350	-0.3020700	-1.3909010
C	-4.1477150	0.2447360	1.1492850
H	-2.1684200	0.9022960	1.6489120
C	-4.4688380	-0.5544760	-1.1086060
H	-2.7521370	-0.5030370	-2.3863780
C	-4.9785050	-0.2837620	0.1605510
H	-4.5393320	0.4462510	2.1392300
H	-5.1120920	-0.9610870	-1.8796570
H	-6.0201850	-0.4869190	0.3802820
N	-0.1335980	1.3811450	-0.1051650
H	-0.5485610	1.9892290	0.5993670
H	2.1412220	0.1903810	-2.5668950
H	1.4398140	3.5367210	-1.6175320

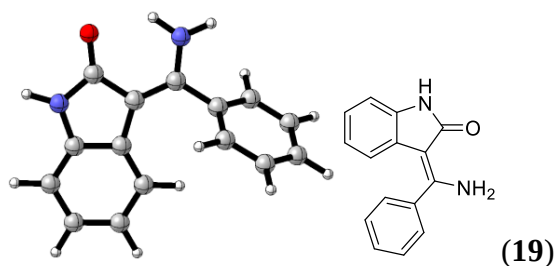


32

1-6 1 1 scf done: -1162.516500 Sum of electronic and thermal Free Energies -1162.308157

imag. freq.: 0

C	4.5941480	-1.2428760	-0.3802730
C	3.5497190	-0.8358810	-1.2160970
C	2.4604490	-0.1922920	-0.6499720
C	2.4032260	0.0532810	0.7287340
C	3.4374800	-0.3411460	1.5699170
C	4.5300450	-0.9948520	0.9935520
H	5.4560280	-1.7477300	-0.7992530
H	3.5892970	-1.0174760	-2.2842000
H	3.3976510	-0.1451660	2.6345550
H	5.3479160	-1.3111230	1.6311540
N	1.2109600	0.7035530	1.0648090
H	1.1491640	1.2648710	1.9059530
C	0.5562630	1.1837220	-0.1247410
O	0.6148580	2.5701080	-0.2949630
C	1.2205210	0.3562990	-1.2772670
S	-0.0346760	-0.9530560	-1.7274990
C	-1.2822310	-0.1721220	-0.8195530
C	-2.6492810	-0.6639600	-0.7992940
C	-3.4709310	-0.4230100	0.3160930
C	-3.1458090	-1.3962170	-1.8905840
C	-4.7707550	-0.9081220	0.3297890
H	-3.0888790	0.1087450	1.1789780
C	-4.4501990	-1.8690780	-1.8692380
H	-2.5269290	-1.5700710	-2.7623640
C	-5.2622800	-1.6273070	-0.7608940
H	-5.3992260	-0.7324850	1.1941680
H	-4.8341210	-2.4232610	-2.7168130
H	-6.2788570	-2.0024470	-0.7452010
N	-0.8752680	0.8663530	-0.1349040
H	-1.5129670	1.4325670	0.4192150
H	1.3765190	0.9607530	-2.1680360
H	1.5115440	2.8690100	-0.0795840

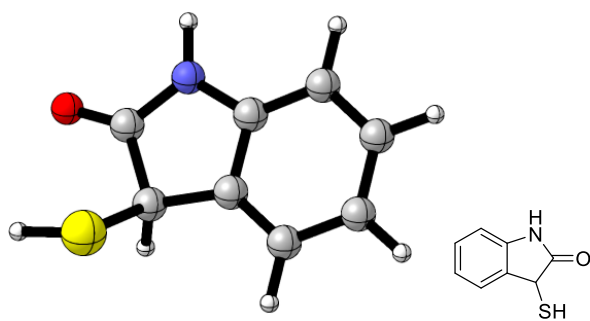


30

1-7 0 1 scf done: -763.880154 Sum of electronic and thermal Free Energies -763.685142

imag. freq.: 0

C	-1.3112920	3.1095820	0.4666960
C	-0.5364870	1.9724380	0.2177980
C	-1.1650310	0.7718470	-0.1215860
C	-2.5833740	0.7485180	-0.1759740
C	-3.3612420	1.8714730	0.0657820
C	-2.7058450	3.0644400	0.3862130
H	-0.8188370	4.0398020	0.7270070
H	0.5402700	2.0332470	0.2936870
H	-4.4427610	1.8192890	0.0136650
H	-3.2882910	3.9581670	0.5792160
N	-2.9954310	-0.5468550	-0.4786220
H	-3.9570640	-0.8511120	-0.5449390
C	-1.9176910	-1.4040040	-0.6025710
O	-2.0081690	-2.6204210	-0.8322740
C	-0.7142900	-0.5863000	-0.4145600
H	-0.0762640	-3.0502390	-0.7396860
C	0.5557020	-1.1307140	-0.5009340
C	1.7908830	-0.3088850	-0.4413940
C	2.0094840	0.6988240	-1.3861890
C	2.7573190	-0.5625240	0.5376640
C	3.1811190	1.4490020	-1.3476540
H	1.2631240	0.8898190	-2.1478980
C	3.9220180	0.2010640	0.5825600
H	2.5889450	-1.3429800	1.2707820
C	4.1360080	1.2062700	-0.3596420
H	3.3475100	2.2241290	-2.0868590
H	4.6605230	0.0100470	1.3527420
H	5.0444180	1.7969770	-0.3260400
N	0.7409000	-2.4541700	-0.6394570
H	1.6622440	-2.8219760	-0.8235920

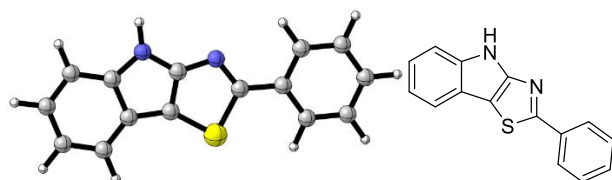


18

1-8 0 1 scf done: -837.455305 Sum of electronic and thermal Free Energies -837.357356

imag. freq.: 0

C	2.6750950	-1.6417410	-0.2290630
C	1.3465860	-2.0683900	-0.3537260
C	0.3438070	-1.1149140	-0.4091530
C	0.6627890	0.2492300	-0.3433660
C	1.9717630	0.6909910	-0.2219860
C	2.9770600	-0.2807650	-0.1634900
H	3.4727980	-2.3736230	-0.1847010
H	1.1091740	-3.1249410	-0.4051750
H	2.2060200	1.7476800	-0.1757110
H	4.0097750	0.0345980	-0.0675330
N	-0.5135270	1.0055390	-0.4358460
H	-0.5470370	2.0172160	-0.4205880
C	-1.6287750	0.2229320	-0.5788940
O	-2.7752930	0.6111530	-0.7081020
C	-1.1475460	-1.2410910	-0.5449480
H	-1.4575920	-1.7542270	-1.4558050
S	-1.8713540	-2.1303250	0.9062430
H	-3.1612690	-1.9567310	0.5418320

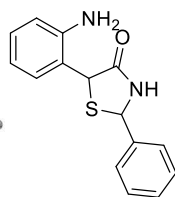
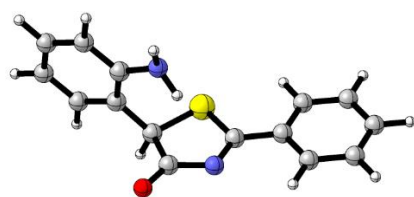


28

1-9 0 1 scf done: -1085.609928 Sum of electronic and thermal Free Energies -1085.440856

imag. freq.: 0

C	-4.0718390	-2.3093150	0.0761240
C	-2.6936620	-2.4598160	0.0008370
C	-1.8812580	-1.3218730	0.1084360
C	-2.4921230	-0.0366000	0.2930610
C	-3.8774260	0.1060730	0.3677340
C	-4.6560980	-1.0409530	0.2574180
H	-4.7108880	-3.1810500	-0.0057290
H	-2.2481340	-3.4380500	-0.1387490
H	-4.3279110	1.0819350	0.5073700
H	-5.7353060	-0.9555150	0.3123480
N	-1.5016960	0.9299530	0.3724990
H	-1.6520660	1.9209120	0.4976690
C	-0.2850850	0.3032220	0.2438150
C	-0.4766540	-1.0648490	0.0823050
S	1.0758380	-1.8187670	-0.0766970
C	1.8337670	-0.2082590	0.0906090
C	3.2861530	-0.0415090	0.0501380
C	3.8385460	1.2428220	0.1937340
C	4.1493890	-1.1334840	-0.1292330
C	5.2160230	1.4234510	0.1581240
H	3.1797480	2.0902510	0.3325680
C	5.5268790	-0.9467810	-0.1639400
H	3.7525410	-2.1359540	-0.2431640
C	6.0667990	0.3313800	-0.0206230
H	5.6279690	2.4198760	0.2703090
H	6.1790060	-1.8011080	-0.3033320
H	7.1407500	0.4752410	-0.0479590
N	0.9816320	0.7789300	0.2492280



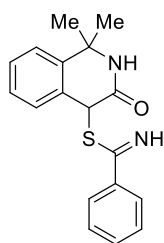
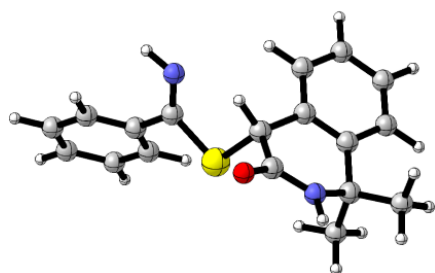
(17)

31

1-10 0 1 scf done:-1162.081041 Sum of electronic and thermal Free Energies -1161.889224

imag. freq.: 0

C	-4.3397410	-1.4747780	-0.6120430
C	-3.0652460	-1.9431320	-0.3136700
C	-2.0141260	-1.0759440	0.0051300
C	-2.2526630	0.3179760	0.0255660
C	-3.5451960	0.7812980	-0.2787720
C	-4.5711090	-0.0980850	-0.5941610
H	-5.1360380	-2.1687280	-0.8524810
H	-2.8669310	-3.0095370	-0.3243890
H	-3.7287260	1.8506050	-0.2621780
H	-5.5563260	0.2936010	-0.8219610
N	-1.2477060	1.2461970	0.2675150
H	-1.5800890	2.1745150	0.4955200
C	-0.0272020	-1.2844970	1.6554660
O	-0.6279760	-1.3963060	2.7027410
C	-0.6674630	-1.6747020	0.3015580
S	0.6281050	-1.3019050	-0.9563850
C	1.7239630	-0.7785880	0.3303610
C	3.0716120	-0.3109700	0.0033470
C	3.9443330	0.0527200	1.0426870
C	3.5080050	-0.2175950	-1.3268390
C	5.2256890	0.5008520	0.7512460
H	3.6068560	-0.0221430	2.0678520
C	4.7909390	0.2320090	-1.6127720
H	2.8501660	-0.4911570	-2.1434360
C	5.6515570	0.5916260	-0.5752390
H	5.8947620	0.7788880	1.5569580
H	5.1191840	0.3021900	-2.6427850
H	6.6525920	0.9414740	-0.7998990
N	1.2798060	-0.8213800	1.5536910
H	-0.4797420	0.9796930	0.8663760
H	-0.7633440	-2.7617330	0.3231490

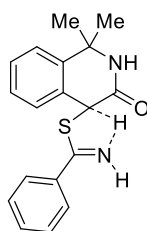
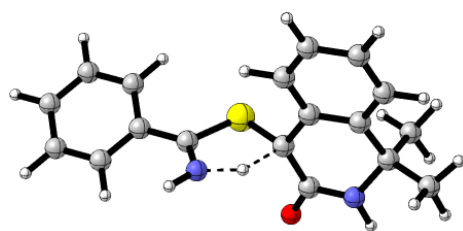


(6a''')

2b-1 0 1 scf done: -1280.076091 Sum of electronic and thermal Free Energies -1279.803591

imag. freq.: 0

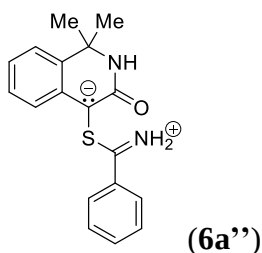
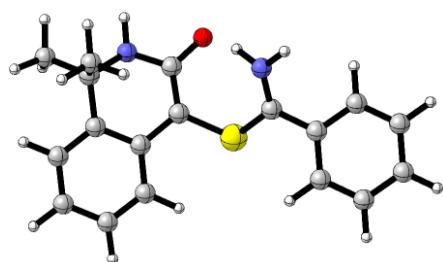
C	2.4378870	2.7956400	0.7848470
C	1.7254670	1.6225960	1.0018120
C	1.9755190	0.4848980	0.2256320
C	2.9662250	0.5124090	-0.7627760
C	3.6710910	1.7014060	-0.9790100
C	3.4093340	2.8355900	-0.2161200
H	2.2389280	3.6724220	1.3905000
H	0.9612650	1.5776940	1.7690290
H	4.4329700	1.7475740	-1.7465410
H	3.9692950	3.7459870	-0.3976130
N	2.8106070	-1.9314860	-0.8803310
H	3.2459420	-2.8001970	-1.1690670
C	1.8481350	-2.0466980	0.0540700
O	1.5437910	-3.1183820	0.5766000
C	1.1548010	-0.7522200	0.4441420
H	0.8403620	-0.8401420	1.4829410
S	-0.4540880	-0.6760120	-0.4928610
C	-1.5939300	-0.1712240	0.7941480
C	-2.9643440	0.0872640	0.2721260
C	-4.0672860	-0.3754770	1.0024890
C	-3.1739620	0.7959650	-0.9173370
C	-5.3593480	-0.1310480	0.5486710
H	-3.9096840	-0.9391300	1.9146860
C	-4.4699480	1.0465940	-1.3620560
H	-2.3293140	1.1707310	-1.4821160
C	-5.5636530	0.5820810	-0.6332850
H	-6.2064050	-0.5012620	1.1145880
H	-4.6236030	1.6076430	-2.2765330
H	-6.5711360	0.7736710	-0.9843970
N	-1.2285670	-0.0923560	2.0097760
H	-2.0010880	0.2176170	2.6016850
C	3.2330740	-0.7216560	-1.6162210
C	4.7268280	-0.9054750	-1.9160770
H	4.8780720	-1.8495080	-2.4468500
H	5.0999890	-0.1046940	-2.5544380
H	5.3095120	-0.9245440	-0.9925030
C	2.4457200	-0.6228120	-2.9383330
H	2.6058790	-1.5243730	-3.5357350
H	1.3752840	-0.5153240	-2.7510800
H	2.7818660	0.2434480	-3.5126280



40

2b-TS1 0 1 scf done:-1280.042945 Sum of electronic and thermal Free Energies -
1279.773908 imag. freq.: 1 (-1568.6)

C	2.5776420	2.8475330	0.3404490
C	1.6646540	1.8079600	0.2089760
C	2.0886270	0.4797820	0.0293020
C	3.4712900	0.2126860	-0.0035200
C	4.3794120	1.2659430	0.1331180
C	3.9457620	2.5786930	0.3036830
H	2.2222530	3.8633010	0.4754920
H	0.6028500	2.0236230	0.2429720
H	5.4430050	1.0655540	0.0923470
H	4.6683580	3.3804500	0.4050640
N	2.9331910	-2.1637730	0.1713940
H	3.2317230	-3.1324310	0.1416430
C	1.5884240	-2.0143310	-0.0616990
O	0.8476520	-3.0026460	-0.1438440
C	1.1039260	-0.6256620	-0.0516590
H	0.2985340	-0.5777860	1.1598540
S	-0.3753900	-0.3452500	-1.0161340
C	-1.4818950	-0.1935090	0.3871450
C	-2.9049720	0.0784700	0.1650970
C	-3.8569260	-0.3626670	1.0970970
C	-3.3261130	0.7741250	-0.9769380
C	-5.2068870	-0.1095180	0.8860630
H	-3.5430040	-0.9190850	1.9720930
C	-4.6778330	1.0332100	-1.1769510
H	-2.5990480	1.1321780	-1.6953230
C	-5.6193840	0.5906480	-0.2486550
H	-5.9379200	-0.4614320	1.6042990
H	-4.9950880	1.5816200	-2.0559020
H	-6.6728560	0.7891420	-0.4090540
N	-0.8946790	-0.3706610	1.5106680
H	-1.3895060	-0.2766790	2.3916760
C	3.9566140	-1.2036450	-0.2889280
C	5.2485670	-1.5545100	0.4567560
H	5.4840990	-2.6109090	0.2978940
H	6.0929940	-0.9707100	0.0889680
H	5.1386020	-1.3807590	1.5297170
C	4.1680520	-1.3637940	-1.8092530
H	4.9375400	-0.6742070	-2.1654400
H	4.4814470	-2.3865120	-2.0403780
H	3.2396050	-1.1546040	-2.3471890

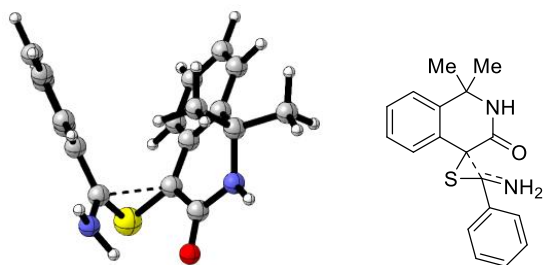


40

2b-2 0 1 scf done: -1280.055151 Sum of electronic and thermal Free Energies -1279.781381

imag. freq.: 0

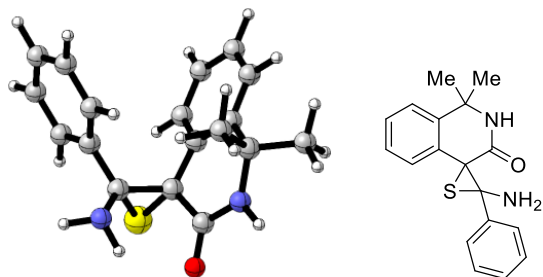
C	-3.1232660	-2.7796130	-0.0936630
C	-2.0594680	-1.8972450	-0.2482360
C	-2.2177340	-0.5063950	-0.0641970
C	-3.5064930	-0.0351210	0.3067860
C	-4.5589260	-0.9345610	0.4545260
C	-4.3865110	-2.3055070	0.2530530
H	-2.9598690	-3.8411460	-0.2468190
H	-1.0897030	-2.2969880	-0.5178780
H	-5.5352710	-0.5671550	0.7463330
H	-5.2217530	-2.9854460	0.3746100
N	-2.7466670	2.2194560	-0.1780340
H	-2.8393170	3.2221980	-0.0624560
C	-1.4296150	1.8396520	-0.3524860
O	-0.5727500	2.7402930	-0.6127430
C	-1.1439900	0.4594610	-0.2439750
S	0.4221390	-0.1697710	-0.7786180
C	1.6599970	0.5924810	0.1520110
C	2.9989320	-0.0134700	0.1274990
C	4.1360740	0.8105820	0.1283910
C	3.1543470	-1.4081600	0.1131800
C	5.4051850	0.2451690	0.1165060
H	4.0264430	1.8885260	0.1098800
C	4.4273940	-1.9659930	0.1032900
H	2.2829040	-2.0499990	0.1369410
C	5.5531370	-1.1423520	0.1040330
H	6.2788240	0.8860640	0.1069600
H	4.5410230	-3.0434790	0.1028550
H	6.5444270	-1.5805230	0.0948160
N	1.4234970	1.7167720	0.7848510
H	2.1623010	2.1470920	1.3302240
C	-3.6745700	1.4386360	0.6606750
H	0.6213120	2.2946640	0.4444670
C	-5.0809050	1.9763290	0.3814640
H	-5.3765920	1.7811470	-0.6519460
H	-5.8193440	1.5320560	1.0502310
H	-5.0946350	3.0575610	0.5477650
C	-3.3313030	1.6377450	2.1534860
H	-3.4064560	2.6971560	2.4186130
H	-4.0219350	1.0709260	2.7830900
H	-2.3137730	1.2987840	2.3639910



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2b-TS2 0 1 scf done: -1280.047399 Sum of electronic and thermal Free Energies -
1279.772556 imag. freq.: 1 (-227.2)

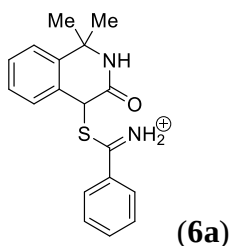
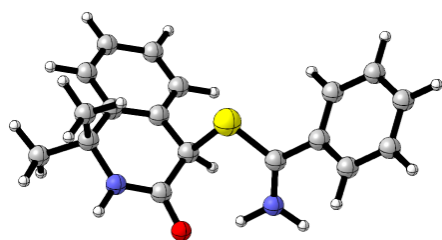
C	-0.6565730	2.9104850	-1.4164800
C	-0.1273580	1.6269130	-1.4896760
C	0.6787320	1.1098470	-0.4600650
C	0.9594130	1.9342310	0.6566020
C	0.4192140	3.2165970	0.7156500
C	-0.3901870	3.7105400	-0.3084270
H	-1.2754180	3.2825620	-2.2254850
H	-0.3309380	1.0134200	-2.3566100
H	0.6236580	3.8465910	1.5722460
H	-0.8011360	4.7112010	-0.2389170
N	2.7265320	0.3759880	1.2617420
H	3.4359210	0.0603260	1.9130280
C	2.3858620	-0.5694430	0.3306910
O	3.0380260	-1.6247120	0.2326400
C	1.2374660	-0.2363820	-0.5022500
S	0.8106310	-1.3880970	-1.8062900
C	0.0080310	-1.8930800	-0.3151190
C	-1.3363860	-1.4079190	0.0495350
C	-2.1753420	-0.8150640	-0.9048000
C	-1.8019370	-1.5255000	1.3717850
C	-3.4364450	-0.3453760	-0.5487730
H	-1.8437860	-0.7378620	-1.9304440
C	-3.0609310	-1.0539950	1.7227990
H	-1.1810410	-1.9653630	2.1424810
C	-3.8838430	-0.4586760	0.7651330
H	-4.0691910	0.1073830	-1.3034340
H	-3.3977180	-1.1451740	2.7490600
H	-4.8646060	-0.0899750	1.0427840
N	0.5433770	-2.9566210	0.3426890
H	0.2264290	-3.1230170	1.2904700
C	1.7859020	1.3721950	1.8062440
H	1.5484930	-3.0661530	0.2245610
C	2.6338700	2.4350930	2.5121090
H	3.2534260	2.9809510	1.7970940
H	2.0091360	3.1453040	3.0546290
H	3.2890300	1.9492820	3.2408140
C	0.8440440	0.6940900	2.8236590
H	0.1449040	1.4224380	3.2419630
H	0.2699420	-0.0974370	2.3404970
H	1.4268850	0.2571250	3.6401650



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2b-3 0 1 scf done:-1280.069908 Sum of electronic and thermal Free Energies -1279.794157
 imag. freq.: 0

C	0.6960690	2.6389950	1.3881670
C	0.2484900	1.3251580	1.3483770
C	-0.6478490	0.8938240	0.3626200
C	-1.1338730	1.8216130	-0.5707610
C	-0.6674650	3.1403560	-0.5286960
C	0.2460520	3.5506480	0.4349980
H	1.3931120	2.9475520	2.1588690
H	0.5949940	0.6155370	2.0861600
H	-1.0244480	3.8582860	-1.2557120
H	0.5921080	4.5779000	0.4491070
N	-2.8468400	0.2049890	-1.1935830
H	-3.6971120	-0.0106390	-1.7024330
C	-2.3790740	-0.8080750	-0.4421760
O	-2.9945860	-1.8681000	-0.3275220
C	-1.0406510	-0.5560130	0.2451950
S	-0.7067550	-1.6647190	1.6898890
C	0.0341790	-1.5733670	-0.0749500
C	1.4701880	-1.1222730	-0.1595450
C	2.3869950	-1.3317330	0.8689630
C	1.8934220	-0.4867460	-1.3322070
C	3.7054960	-0.8962970	0.7392210
H	2.0655120	-1.8239450	1.7779530
C	3.2059580	-0.0411540	-1.4581870
H	1.1917630	-0.3314100	-2.1411000
C	4.1167140	-0.2427780	-0.4203820
H	4.4075040	-1.0649850	1.5479840
H	3.5167160	0.4642650	-2.3656240
H	5.1390030	0.1049800	-0.5171920
N	-0.2611020	-2.5847950	-1.0096390
H	0.4050350	-3.3482440	-0.9625010
C	-2.1297570	1.4087620	-1.6428770
H	-1.2101060	-2.9357930	-0.9219980
C	-1.3983860	1.0959070	-2.9624520
H	-0.8401550	1.9697190	-3.3056510
H	-0.7041320	0.2661400	-2.8244990
H	-2.1233860	0.8176720	-3.7324800
C	-3.2024340	2.4804810	-1.8828620
H	-3.6855400	2.7656070	-0.9458350
H	-2.7752380	3.3691900	-2.3469380
H	-3.9619530	2.0855760	-2.5633840

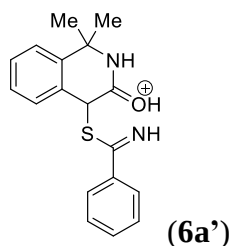
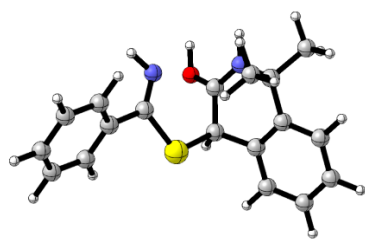


41

2b-4 1 1 scf done: -1280.541116 Sum of electronic and thermal Free Energies -1280.253915

imag. freq.: 0

C	2.3761160	2.7609300	1.4648070
C	1.6317290	1.6349250	1.7847760
C	1.8006610	0.4446280	1.0660380
C	2.7349470	0.3699190	0.0282310
C	3.4710020	1.5167860	-0.2926200
C	3.2931600	2.7004540	0.4138370
H	2.2440090	3.6782510	2.0261570
H	0.9099280	1.6681260	2.5933790
H	4.1906060	1.4862910	-1.1003590
H	3.8764090	3.5749540	0.1497080
N	2.3947490	-2.0655830	-0.0178330
H	2.7031130	-2.9783510	-0.3378980
C	1.4836480	-2.0778290	0.9494050
O	1.0653370	-3.1254610	1.4729080
C	0.9469550	-0.7388830	1.4124690
S	-0.7439810	-0.4388760	0.6426950
C	-1.8377180	-1.4315760	1.5633270
C	-3.2598040	-1.0961250	1.4598420
C	-4.2063710	-2.1345950	1.4357170
C	-3.6822160	0.2396190	1.3693760
C	-5.5570040	-1.8339750	1.3260730
H	-3.8829210	-3.1680610	1.4683950
C	-5.0372950	0.5289050	1.2690950
H	-2.9599360	1.0445860	1.4113620
C	-5.9737510	-0.5042200	1.2450890
H	-6.2842460	-2.6361500	1.2941050
H	-5.3623670	1.5607190	1.2151070
H	-7.0294070	-0.2740070	1.1609010
N	-1.4277420	-2.4418550	2.2748100
H	-2.0871820	-2.9446970	2.8614830
H	0.7646370	-0.7882410	2.4860730
C	2.9429020	-0.9122860	-0.7633570
H	-0.4570510	-2.8039530	2.1829270
C	2.2229820	-0.8199120	-2.1222000
H	2.6410170	-0.0008830	-2.7106330
H	2.3541980	-1.7524740	-2.6770070
H	1.1539560	-0.6408890	-1.9874070
C	4.4333330	-1.2163530	-0.9731860
H	4.8981740	-0.4675740	-1.6139150
H	4.9602800	-1.2434650	-0.0172000
H	4.5406950	-2.1879080	-1.4628410

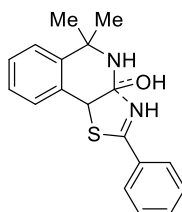
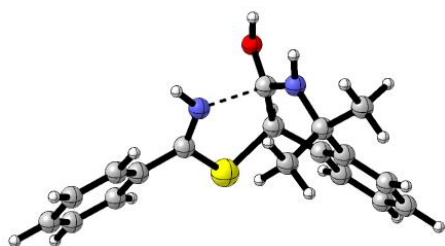


41

2b-5 1 1 scf done: -1280.499128 Sum of electronic and thermal Free Energies -1280.212620

imag. freq.: 0

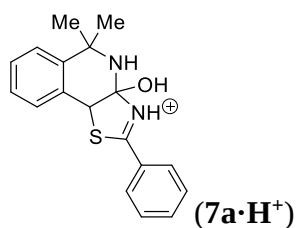
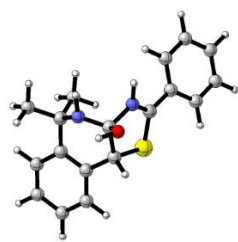
C	3.8692850	-2.3501780	-0.2839330
C	2.9111700	-1.5869560	-0.9408080
C	2.3654690	-0.4604190	-0.3207220
C	2.7986110	-0.0678130	0.9499260
C	3.7591320	-0.8442160	1.6023320
C	4.2852750	-1.9806440	0.9944440
H	4.2891930	-3.2250660	-0.7658570
H	2.5775670	-1.8623880	-1.9351260
H	4.1039890	-0.5646830	2.5889110
H	5.0296760	-2.5702040	1.5167320
N	1.7068400	2.0882230	0.5517590
H	1.6772460	3.0729200	0.8126170
C	1.2517820	1.7306050	-0.6032450
O	0.8676510	2.5759890	-1.5271870
C	1.2751790	0.3028760	-1.0208960
S	-0.3479780	-0.6257840	-0.7495860
C	-1.5957050	0.5306840	-0.1853780
C	-2.9318240	-0.1203590	-0.1059650
C	-3.7121950	0.0894100	1.0391640
C	-3.4265600	-0.9175200	-1.1454910
C	-4.9725250	-0.4900260	1.1392030
H	-3.3231520	0.6914760	1.8519710
C	-4.6932990	-1.4873600	-1.0429490
H	-2.8373160	-1.0724570	-2.0408540
C	-5.4656120	-1.2782190	0.0983910
H	-5.5675610	-0.3317270	2.0310890
H	-5.0764390	-2.0918740	-1.8566660
H	-6.4485090	-1.7282290	0.1780980
N	-1.3067500	1.7148700	0.1648530
H	-2.1406110	2.2252430	0.4613510
H	1.4117550	0.2807560	-2.1005090
C	2.2133890	1.1682630	1.6178640
H	0.7886900	3.4871450	-1.1882650
C	1.0412690	0.7941040	2.5399680
H	0.5794060	1.6951370	2.9494420
H	0.2844920	0.2168980	2.0094630
H	1.4258630	0.1894720	3.3631180
C	3.2625450	1.9809200	2.3823250
H	3.6232790	1.4174010	3.2415320
H	4.1084690	2.2319330	1.7395430
H	2.8112560	2.9034560	2.7567500



41

2b-TS4 1 1 scf done: -1280.494112 Sum of electronic and thermal Free Energies -
1280.207648 imag. freq.: 1 (-244.7)

C	-4.0602250	-2.0699280	0.2786080
C	-3.0433570	-1.3949620	0.9444040
C	-2.3476710	-0.3627430	0.3092180
C	-2.6911810	0.0268070	-0.9902540
C	-3.7094530	-0.6629340	-1.6525920
C	-4.3848340	-1.7080800	-1.0279300
H	-4.5949620	-2.8706000	0.7757940
H	-2.7804990	-1.6708600	1.9600240
H	-3.9856670	-0.3828830	-2.6607610
H	-5.1734520	-2.2294480	-1.5580010
N	-1.4883130	2.0906690	-0.5749710
H	-1.4167110	3.0709400	-0.8287110
C	-0.9125640	1.6979120	0.5515190
O	-0.7872270	2.5667000	1.5630850
C	-1.1856960	0.2751770	1.0296520
S	0.2776530	-0.8817830	0.9103560
C	1.4902040	0.2810990	0.3674300
C	2.8611950	-0.2215350	0.1523810
C	3.6381650	0.3319630	-0.8747970
C	3.3915780	-1.2402930	0.9543750
C	4.9316650	-0.1281570	-1.0912130
H	3.2232000	1.1024020	-1.5136190
C	4.6904630	-1.6894390	0.7377050
H	2.8056840	-1.6648450	1.7608200
C	5.4606320	-1.1364670	-0.2844020
H	5.5254730	0.2959940	-1.8921800
H	5.1003180	-2.4690290	1.3686700
H	6.4705460	-1.4914260	-0.4540920
N	1.0627560	1.4580950	0.1470840
H	1.7219570	2.1699380	-0.1649580
H	-1.3973150	0.3484980	2.0950090
C	-1.9516850	1.1814730	-1.6546450
H	-0.7813060	3.4843350	1.2414270
C	-2.8689620	2.0361040	-2.5348900
H	-3.2034660	1.4693200	-3.4026160
H	-3.7415590	2.3784540	-1.9748330
H	-2.3172910	2.9068600	-2.8997810
C	-0.7625870	0.6627880	-2.4830030
H	-0.1788380	1.5011050	-2.8704290
H	-0.1081930	0.0180110	-1.8969790
H	-1.1438910	0.0808110	-3.3243800

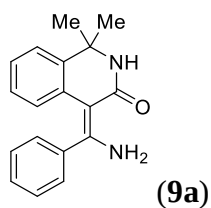
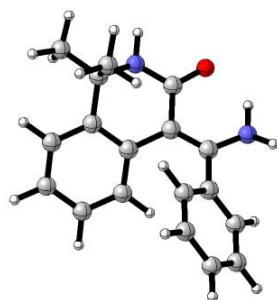


41

2b-6 1 1 scf done: -1280.512077 Sum of electronic and thermal Free Energies -1280.221708

imag. freq.: 0

C	-3.8533770	-2.4462310	-0.1681520
C	-2.7549860	-2.1172200	0.6176230
C	-2.0870670	-0.9031820	0.4287380
C	-2.5384060	0.0127740	-0.5308470
C	-3.6391600	-0.3327970	-1.3184820
C	-4.2878070	-1.5531640	-1.1466470
H	-4.3661420	-3.3889590	-0.0179180
H	-2.4047190	-2.8053150	1.3798100
H	-4.0026490	0.3561180	-2.0697380
H	-5.1409700	-1.7991100	-1.7684510
N	-1.3023690	1.7221240	0.6534020
H	-0.9533610	2.6769850	0.6586360
C	-0.4423740	0.8614690	1.3783830
O	-0.4145240	1.2610160	2.7279960
C	-0.8478960	-0.6355360	1.2318090
S	0.6131590	-1.5259640	0.4669610
C	1.5957760	-0.1070840	0.4987340
C	2.9564450	-0.0949240	-0.0177980
C	3.4948990	1.0867310	-0.5543000
C	3.7251610	-1.2694810	0.0057460
C	4.7899090	1.0869150	-1.0537820
H	2.8977720	1.9883320	-0.6118260
C	5.0230040	-1.2547660	-0.4869130
H	3.3239100	-2.1808940	0.4327740
C	5.5555670	-0.0794420	-1.0171710
H	5.2006030	1.9949030	-1.4781530
H	5.6190690	-2.1584500	-0.4555510
H	6.5672740	-0.0727250	-1.4054230
N	0.9861800	0.9467150	0.9644440
H	1.4585730	1.8425320	1.0606380
H	-0.9388990	-1.0497480	2.2332510
C	-1.8270280	1.3501970	-0.6831200
H	-1.2944340	1.6155990	2.9272870
C	-2.7933080	2.4813980	-1.0543940
H	-3.1929400	2.3430110	-2.0588580
H	-3.6211430	2.5359570	-0.3445730
H	-2.2569100	3.4344030	-1.0402930
C	-0.7287030	1.2535850	-1.7625480
H	-0.1441560	2.1771100	-1.7869770
H	-0.0524800	0.4144710	-1.5969640
H	-1.1909460	1.1085090	-2.7414840

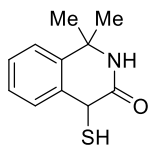
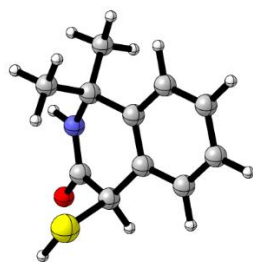


39

2b-7 0 1 scf done:-881.867664 Sum of electronic and thermal Free Energies -881.591334

imag. freq.: 0

C	0.1372490	2.6597410	1.6071870
C	0.3601060	1.3430140	1.2230210
C	-0.5771070	0.6407680	0.4444830
C	-1.7941530	1.2796100	0.1299310
C	-2.0096870	2.6014090	0.5211930
C	-1.0461570	3.3020660	1.2440750
H	0.8817920	3.1787100	2.2008880
H	1.2707460	0.8494280	1.5350740
H	-2.9384010	3.0949850	0.2635010
H	-1.2285420	4.3293010	1.5386980
N	-2.7382820	-0.9113690	-0.2313530
H	-3.5365420	-1.4950860	-0.4514470
C	-1.5607730	-1.5904670	-0.1201450
O	-1.5542200	-2.8396320	-0.1390010
C	-0.3630520	-0.7559590	0.0219390
C	0.8808590	-1.2957730	-0.2672860
C	2.0870620	-0.4606780	-0.5131650
C	3.3050230	-0.7759280	0.0998220
C	2.0263110	0.6194380	-1.4018170
C	4.4381960	-0.0045610	-0.1506300
H	3.3582140	-1.6091500	0.7908250
C	3.1615410	1.3801690	-1.6602710
H	1.0885770	0.8586290	-1.8878280
C	4.3690100	1.0753160	-1.0295090
H	5.3729570	-0.2462130	0.3423880
H	3.1054060	2.2113720	-2.3539390
H	5.2512250	1.6740540	-1.2258420
N	1.0907590	-2.6288810	-0.3877180
H	1.9012990	-2.9501430	-0.8971030
C	-2.8283300	0.4961400	-0.6678690
H	0.2672140	-3.2241630	-0.3322570
C	-2.5183880	0.6072350	-2.1749860
H	-2.5928640	1.6479580	-2.5000530
H	-1.5090930	0.2492910	-2.3909560
H	-3.2311600	0.0090110	-2.7501690
C	-4.2657890	0.9477930	-0.4006360
H	-4.4899270	0.9354750	0.6684600
H	-4.4413000	1.9523170	-0.7869010
H	-4.9592290	0.2724830	-0.9099810

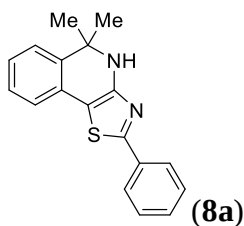
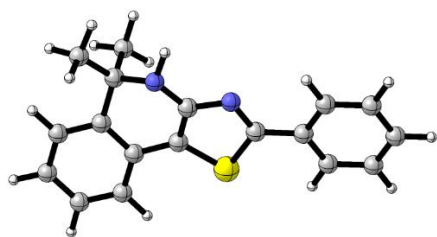


27

2b-8 0 1 scf done: -955.451843Sum of electronic and thermal Free Energies -955.273226

imag. freq.:0

C	-1.9253800	3.1124090	-0.8737930
C	-1.2231770	1.9495930	-1.1635100
C	-1.6301540	0.7189650	-0.6349370
C	-2.7672430	0.6451280	0.1772840
C	-3.4610110	1.8247730	0.4721120
C	-3.0453380	3.0477440	-0.0437270
H	-1.6039110	4.0606500	-1.2888230
H	-0.3461740	1.9853750	-1.8008600
H	-4.3352340	1.7922090	1.1096410
H	-3.5996950	3.9480090	0.1959650
N	-2.6762190	-1.7967600	-0.0396790
H	-3.1366930	-2.6918870	0.0800990
C	-1.5694870	-1.8166880	-0.8038220
O	-1.1721430	-2.8289990	-1.3837720
C	-0.8150610	-0.5078730	-0.9281210
H	-0.3953690	-0.4599870	-1.9309180
S	0.6396510	-0.5493110	0.2494010
C	-3.2242440	-0.6851200	0.7619460
C	-4.7513680	-0.8391820	0.7117720
H	-5.0264630	-1.8415180	1.0516370
H	-5.2421600	-0.1212200	1.3687390
H	-5.1219640	-0.6999540	-0.3062050
C	-2.7336990	-0.8143910	2.2180300
H	-3.0432650	-1.7789560	2.6298620
H	-1.6455320	-0.7461440	2.2665080
H	-3.1623300	-0.0192420	2.8321740
H	1.2000360	-1.6674860	-0.2618540

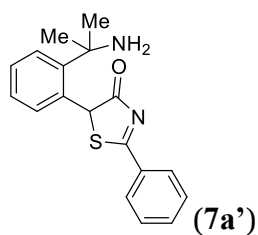
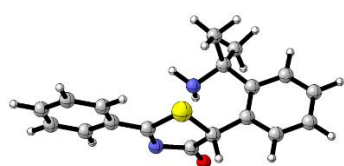


37

2b-9 0 1 scf done:-1203.605921 Sum of electronic and thermal Free Energies -1203.355998

imag. freq.: 0

C	-3.8617720	-2.1858190	-0.3180040
C	-2.4874670	-1.9746730	-0.3266770
C	-1.9638000	-0.6732010	-0.3016730
C	-2.8456610	0.4379290	-0.2678920
C	-4.2179860	0.2015190	-0.2469350
C	-4.7308580	-1.0972940	-0.2713670
H	-4.2516540	-3.1971710	-0.3394720
H	-1.8128460	-2.8239140	-0.3426890
H	-4.9073700	1.0360700	-0.2243240
H	-5.8034380	-1.2530830	-0.2588230
N	-0.9699160	1.9090770	0.3110840
H	-0.5448870	2.8292780	0.3120010
C	-0.0926450	0.8802930	0.0689830
C	-0.5506840	-0.3801800	-0.2580200
S	0.8120400	-1.4591840	-0.3997670
C	1.8855400	-0.1133200	-0.0174010
C	3.3393510	-0.2679970	0.0363930
C	4.1349520	0.8203880	0.4326030
C	3.9658090	-1.4787830	-0.2974600
C	5.5179220	0.6952110	0.4924290
H	3.6588310	1.7569040	0.6927750
C	5.3495680	-1.5987320	-0.2348660
H	3.3773780	-2.3332310	-0.6125550
C	6.1320850	-0.5132270	0.1599420
H	6.1190280	1.5430000	0.8009870
H	5.8172870	-2.5407120	-0.4968440
H	7.2107640	-0.6082180	0.2076200
N	1.2589000	1.0204290	0.1979340
C	-2.2795150	1.8613250	-0.3850070
C	-3.1658720	2.9156040	0.2800540
H	-4.1131120	3.0288260	-0.2483130
H	-3.3685410	2.6575350	1.3217910
H	-2.6562830	3.8829870	0.2543780
C	-2.1035400	2.1964570	-1.8809080
H	-1.6807850	3.1996140	-1.9921060
H	-1.4361730	1.4805880	-2.3667640
H	-3.0693830	2.1658560	-2.3912820

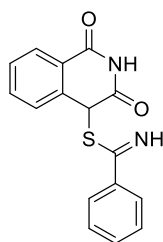
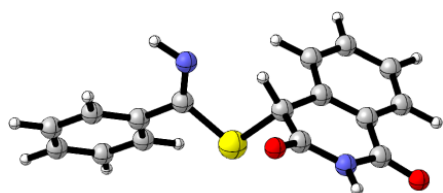


40

2b-10 0 1 scf done:-1280.057740 Sum of electronic and thermal Free Energies -1279.783924

imag. freq.: 0

C	4.3057810	1.9984210	0.2969440
C	2.9807770	1.9026760	0.7007210
C	2.1473820	0.8381820	0.3174140
C	2.6776200	-0.1826310	-0.5091470
C	4.0154890	-0.0551280	-0.9131730
C	4.8255070	1.0068510	-0.5263830
H	4.9150020	2.8352550	0.6183720
H	2.5683680	2.6774120	1.3375990
H	4.4439300	-0.8085370	-1.5591700
H	5.8534730	1.0525510	-0.8681970
N	0.7447660	-1.6811310	-0.1882210
H	0.0287160	-2.1820230	-0.7065970
C	0.2272680	-0.1714920	1.7946260
O	0.9125600	-0.6734920	2.6618040
C	0.7415280	0.9386510	0.8679930
S	-0.6151200	1.2110780	-0.3401320
C	-1.6800480	0.2077030	0.6562260
C	-3.0942480	0.0566010	0.2897280
C	-3.8760320	-0.9053180	0.9491020
C	-3.6782480	0.8456320	-0.7113300
C	-5.2134880	-1.0699100	0.6115390
H	-3.4232780	-1.5182010	1.7173470
C	-5.0175040	0.6780450	-1.0454170
H	-3.0955970	1.6010530	-1.2255650
C	-5.7877590	-0.2791620	-0.3853530
H	-5.8093540	-1.8162110	1.1239110
H	-5.4598710	1.2958040	-1.8178510
H	-6.8318440	-0.4086280	-0.6463890
N	-1.1526250	-0.3968680	1.6713090
C	1.8844590	-1.3808510	-1.0685090
C	2.7630690	-2.6429520	-1.2043410
H	3.5491480	-2.5440800	-1.9546640
H	3.2262830	-2.8962620	-0.2462780
H	2.1220460	-3.4752570	-1.5066310
C	1.3466860	-1.0032050	-2.4599020
H	0.7848010	-1.8437130	-2.8803090
H	0.6857760	-0.1376930	-2.4063060
H	2.1727180	-0.7694900	-3.1344100
H	1.0431950	-2.2920740	0.5670070
H	0.7117400	1.8336950	1.4974520

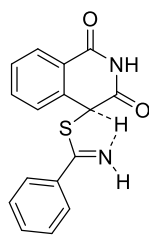
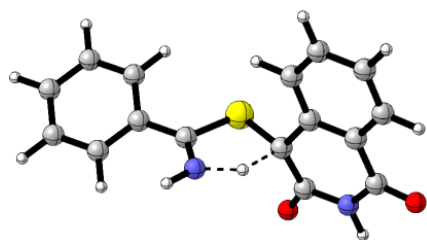


33

3-1 0 1 scf done: -1275.472293 Sum of electronic and thermal Free Energies -1275.272260

imag. freq.: 0

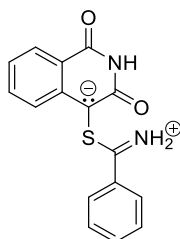
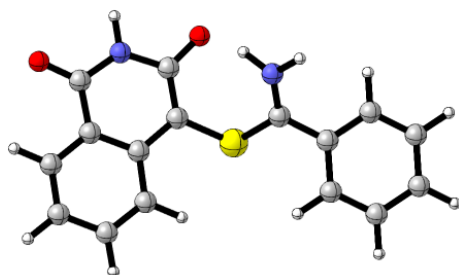
C	2.5333080	2.9038870	0.5322890
C	1.7282450	1.7922590	0.7495400
C	2.0711390	0.5552280	0.1981140
C	3.2355050	0.4490710	-0.5717110
C	4.0405470	1.5734510	-0.7952070
C	3.6903160	2.7977910	-0.2462770
H	2.2611470	3.8572120	0.9703930
H	0.8274610	1.8791140	1.3460410
H	4.9374820	1.4670470	-1.3919030
H	4.3141930	3.6672970	-0.4152130
N	2.8972380	-1.9597900	-0.7437470
H	3.2561800	-2.8642870	-1.0371360
C	1.7849850	-1.9808700	0.0728190
O	1.3098180	-3.0305960	0.4606740
C	1.1804060	-0.6330240	0.4110730
H	0.8217150	-0.6789330	1.4426510
S	-0.3897640	-0.4629460	-0.5677310
C	-1.5920730	-0.2525290	0.7522040
C	-2.9592050	0.0220240	0.2342500
C	-4.0545040	-0.6085160	0.8401470
C	-3.1741770	0.9073580	-0.8295340
C	-5.3450140	-0.3545380	0.3878040
H	-3.8917100	-1.3083020	1.6516470
C	-4.4695400	1.1655050	-1.2713800
H	-2.3373000	1.4126900	-1.2957860
C	-5.5554910	0.5342370	-0.6671870
H	-6.1857830	-0.8537690	0.8553240
H	-4.6288240	1.8627040	-2.0857000
H	-6.5621360	0.7323590	-1.0170480
N	-1.2521830	-0.3667520	1.9700280
H	-2.0438730	-0.2013230	2.5932260
C	3.6570670	-0.8556040	-1.1269580
O	4.6230720	-1.0117760	-1.8542930



33

3-TS1 0 1 scf done: -1275.451948 Sum of electronic and thermal Free Energies -1275.254321
imag. freq.: 1 (-1617.6)

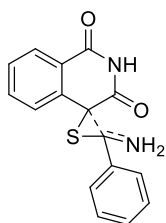
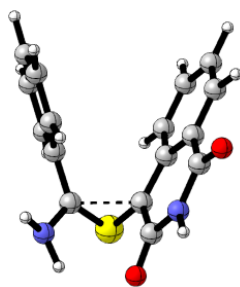
C	2.5935590	2.8622340	0.0740070
C	1.6630960	1.8507130	-0.1159980
C	2.0539160	0.5006960	-0.1231190
C	3.4183190	0.2089010	0.0822260
C	4.3504010	1.2377420	0.2750750
C	3.9468810	2.5626240	0.2696330
H	2.2634750	3.8951230	0.0719750
H	0.6214520	2.1044600	-0.2663670
H	5.3892530	0.9722780	0.4263600
H	4.6688670	3.3568610	0.4169070
N	2.9238950	-2.1513710	-0.1199800
H	3.2515640	-3.1118170	-0.1473510
C	1.5680210	-1.9713680	-0.3962900
O	0.8806610	-2.9501160	-0.6660060
C	1.0756320	-0.5970260	-0.2475570
H	0.3800020	-0.6398320	0.9532550
S	-0.4489170	-0.2677290	-1.1367240
C	-1.4774090	-0.2150730	0.3328520
C	-2.9092860	0.0676600	0.1894540
C	-3.8179830	-0.4409770	1.1299170
C	-3.3799840	0.8417660	-0.8803980
C	-5.1754510	-0.1750260	0.9993600
H	-3.4650520	-1.0588340	1.9468180
C	-4.7389680	1.1124900	-0.9993170
H	-2.6867720	1.2529200	-1.6041470
C	-5.6377020	0.6038540	-0.0625510
H	-5.8737530	-0.5782690	1.7231200
H	-5.0949180	1.7216700	-1.8215380
H	-6.6969180	0.8123520	-0.1597640
N	-0.8367090	-0.4622090	1.4109230
H	-1.3023640	-0.4282170	2.3131940
C	3.8920890	-1.1868830	0.0979720
O	5.0574300	-1.5191510	0.2855270



33

3-2 0 1 scf done: -1275.471947 Sum of electronic and thermal Free Energies -1275.269299
imag. freq.: 0

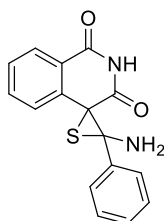
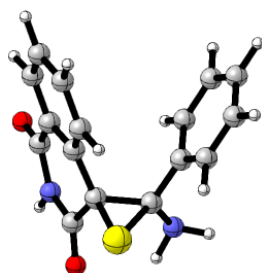
C	-2.9719270	-2.7226180	0.1545880
C	-1.9442480	-1.8254180	-0.0683550
C	-2.1753930	-0.4264970	-0.0708750
C	-3.5076870	0.0081510	0.1801500
C	-4.5351900	-0.9198060	0.4082610
C	-4.2828050	-2.2791170	0.3938200
H	-2.7555430	-3.7854710	0.1497670
H	-0.9438580	-2.2019740	-0.2371700
H	-5.5319580	-0.5401020	0.5970330
H	-5.0802310	-2.9911660	0.5691610
N	-2.7522840	2.2792680	0.0151690
H	-2.9401080	3.2748720	0.0668260
C	-1.4268400	1.9303280	-0.2529640
O	-0.5936940	2.8669710	-0.3891760
C	-1.1470560	0.5515730	-0.3041600
S	0.4247770	-0.0124820	-0.9003250
C	1.6476380	0.6101040	0.1609710
C	2.9721470	-0.0179690	0.1055410
C	4.1227290	0.7805780	0.2152800
C	3.0998410	-1.4061340	-0.0566020
C	5.3803470	0.1933870	0.1658460
H	4.0319800	1.8563300	0.3076620
C	4.3624250	-1.9852720	-0.0993990
H	2.2164970	-2.0288500	-0.1176630
C	5.5018280	-1.1883020	0.0099360
H	6.2659060	0.8132460	0.2387010
H	4.4571390	-3.0585860	-0.2117820
H	6.4849830	-1.6429200	-0.0276130
N	1.4131540	1.6516070	0.9153000
H	2.1319300	1.9864960	1.5483940
C	-3.8278810	1.4376160	0.2188340
H	0.6199020	2.2724480	0.6618360
O	-4.9507160	1.9034230	0.4257390



33

3-TS2 0 1 scf done: -1275.454283 Sum of electronic and thermal Free Energies -1275.251284
imag. freq.: 1 (-389.7)

C	-0.8380510	2.7943720	-1.1101950
C	-0.2524870	1.5518590	-1.3001030
C	0.7010780	1.0552460	-0.3938690
C	1.0602760	1.8754610	0.7010220
C	0.4616350	3.1277780	0.8820890
C	-0.4905460	3.5893800	-0.0125790
H	-1.5728510	3.1491410	-1.8241390
H	-0.5335610	0.9521480	-2.1539200
H	0.7631090	3.7259360	1.7328340
H	-0.9542150	4.5578570	0.1316440
N	2.6863540	0.2244060	1.3765510
H	3.4244110	-0.0706400	2.0078940
C	2.4083180	-0.6491480	0.3272250
O	3.0548290	-1.6941290	0.2342730
C	1.2891050	-0.2719140	-0.5156140
S	0.8980160	-1.3424580	-1.9087520
C	0.0798330	-1.7978200	-0.4073810
C	-1.2632620	-1.2680920	-0.0581200
C	-2.2454570	-1.0898240	-1.0340840
C	-1.5383350	-0.9247100	1.2717770
C	-3.4954730	-0.5839770	-0.6833210
H	-2.0333020	-1.3442340	-2.0652160
C	-2.7828990	-0.4092480	1.6164270
H	-0.7684420	-1.0347410	2.0273280
C	-3.7652040	-0.2391490	0.6392610
H	-4.2538190	-0.4525410	-1.4464240
H	-2.9829530	-0.1302710	2.6444930
H	-4.7337710	0.1661770	0.9086520
N	0.5064450	-2.9097960	0.2465160
H	0.1380280	-3.0619130	1.1790500
C	2.0898940	1.4394850	1.6593240
H	1.4860680	-3.1525740	0.1339440
O	2.4384630	2.0819190	2.6446010

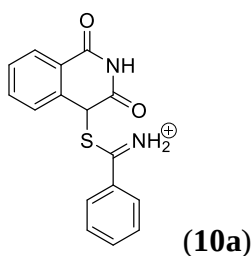
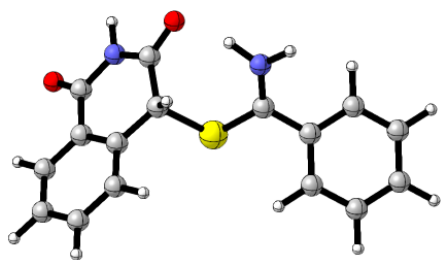


33

3-3 0 1 scf done: -1275.466100 Sum of electronic and thermal Free Energies -1275.262935

imag. freq.: 0

C	0.6621680	2.6381010	1.4686010
C	0.2262870	1.3177610	1.4450780
C	-0.7271700	0.8988210	0.5154530
C	-1.2566400	1.8472380	-0.3744890
C	-0.8109090	3.1733500	-0.3518380
C	0.1529860	3.5700230	0.5630010
H	1.4040150	2.9399110	2.1989070
H	0.6290060	0.6037530	2.1491260
H	-1.2396560	3.8795940	-1.0512200
H	0.4972130	4.5970820	0.5816730
N	-2.8756200	0.2163160	-1.1578190
H	-3.6987130	0.0106250	-1.7177300
C	-2.4697650	-0.7774650	-0.2937750
O	-3.1193420	-1.7994250	-0.1810080
C	-1.1332990	-0.5408770	0.3820370
S	-0.7037670	-1.6991060	1.7443570
C	-0.0663880	-1.5410650	-0.0477250
C	1.3404900	-1.0385410	-0.2279230
C	2.3602790	-1.3263610	0.6756280
C	1.6189460	-0.2708430	-1.3640690
C	3.6494310	-0.8418720	0.4546960
H	2.1445610	-1.9165030	1.5577140
C	2.9030080	0.2197600	-1.5793890
H	0.8252830	-0.0473550	-2.0671180
C	3.9218700	-0.0636470	-0.6683660
H	4.4368250	-1.0687620	1.1643780
H	3.1074780	0.8259220	-2.4545890
H	4.9218940	0.3205660	-0.8346030
N	-0.4027990	-2.5237270	-0.9963520
H	0.3137560	-3.2381040	-1.0663080
C	-2.3286220	1.4845570	-1.3229340
H	-1.3097170	-2.9507710	-0.8405410
O	-2.7746110	2.2288810	-2.1797070

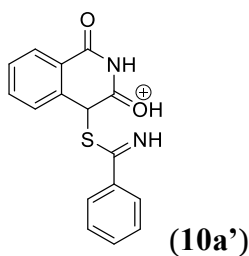
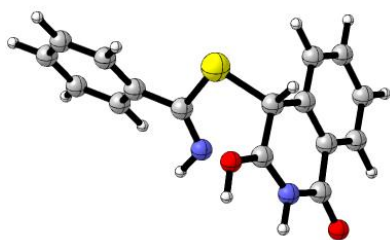


34

3-4 1 1 scf done: -1275.930411 Sum of electronic and thermal Free Energies -1275.714494

imag. freq.: 0

C	-2.1546900	1.2765130	-4.0507350
C	-1.4798690	0.5525690	-3.0732940
C	-1.9645900	0.5252480	-1.7656990
C	-3.1329100	1.2280930	-1.4445030
C	-3.8052400	1.9576640	-2.4303390
C	-3.3148560	1.9840420	-3.7287840
H	-1.7764540	1.2874730	-5.0659910
H	-0.5774840	0.0071100	-3.3238200
H	-4.7118940	2.4875320	-2.1683320
H	-3.8372770	2.5467910	-4.4927740
N	-3.0867830	0.2768450	0.8072540
H	-3.5457220	0.1568430	1.7072910
C	-1.9889380	-0.4942180	0.5752660
O	-1.6105210	-1.3362600	1.3806200
C	-1.2188780	-0.2290740	-0.7037840
S	0.2988700	0.7991840	-0.2871050
C	1.4584170	-0.3411530	0.3383260
C	2.8554420	0.0908910	0.3232890
C	3.6962890	-0.2775440	1.3887290
C	3.3580930	0.8733490	-0.7295770
C	5.0214670	0.1326990	1.3935870
H	3.3031810	-0.8508550	2.2193280
C	4.6888730	1.2706240	-0.7172560
H	2.7247660	1.1367400	-1.5667230
C	5.5190260	0.9044160	0.3418220
H	5.6645870	-0.1402400	2.2212670
H	5.0793940	1.8608580	-1.5370910
H	6.5552440	1.2216730	0.3494750
N	1.1097150	-1.4949780	0.8305480
H	1.8210850	-2.1695170	1.0973510
H	-0.8414610	-1.1760280	-1.0894260
C	-3.7086180	1.1638890	-0.0840540
H	0.1257910	-1.7269060	1.0202600
O	-4.6815030	1.7908620	0.2844820

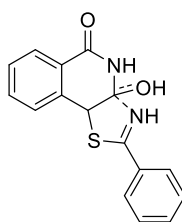
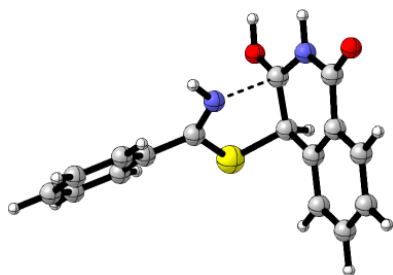


34

3-5 1 1 scf done: -1275.884410 Sum of electronic and thermal Free Energies -1275.670400

imag. freq.: 0

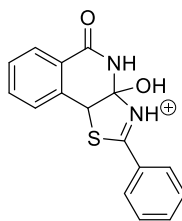
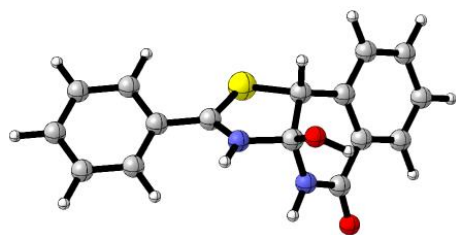
C	2.5369150	2.6107440	-0.9540900
C	1.7607410	2.1430060	0.1007830
C	1.7893920	0.7948370	0.4522740
C	2.6304150	-0.0738400	-0.2592140
C	3.4069380	0.4009540	-1.3255800
C	3.3571120	1.7398380	-1.6752730
H	2.5004210	3.6617030	-1.2153140
H	1.1259490	2.8299690	0.6451770
H	4.0415630	-0.2915520	-1.8630640
H	3.9550740	2.1095020	-2.4990850
N	1.9062770	-1.9241930	1.1789310
H	1.9620070	-2.9252990	1.3740550
C	0.9935100	-1.1867230	1.7781340
O	0.2211780	-1.6800440	2.6991540
C	0.9711840	0.3000270	1.6226500
S	-0.7473770	0.9589020	1.6646930
C	-1.4292560	-0.1011740	0.3879090
C	-2.8151840	0.2195010	-0.0217500
C	-3.1972630	0.0175630	-1.3550200
C	-3.7491530	0.7103390	0.8994280
C	-4.4976480	0.3013100	-1.7570430
H	-2.4735360	-0.3417060	-2.0772930
C	-5.0518600	0.9838550	0.4927740
H	-3.4743980	0.8549530	1.9379290
C	-5.4274990	0.7821600	-0.8344270
H	-4.7840870	0.1520030	-2.7914690
H	-5.7725310	1.3510120	1.2137430
H	-6.4410950	1.0007180	-1.1500880
N	-0.6737850	-1.0183240	-0.0586580
H	-1.1180850	-1.6116840	-0.7601360
H	1.4109860	0.6888820	2.5520410
C	2.7362030	-1.4894340	0.0946510
H	0.3129310	-2.6481230	2.7991900
O	3.4457280	-2.3154960	-0.4285750



34

3-TS4 1 1 scf done: -1275.884150 Sum of electronic and thermal Free Energies -1275.668418
imag. freq.: 1 (-94.8))

C	2.4315170	-2.8665770	-1.0060540
C	1.7174370	-1.7336800	-1.3808480
C	1.9272390	-0.5195410	-0.7287100
C	2.8870650	-0.4557370	0.2930070
C	3.5988900	-1.6019690	0.6721660
C	3.3687830	-2.8060990	0.0276630
H	2.2540120	-3.8021220	-1.5230620
H	0.9896780	-1.8002730	-2.1792150
H	4.3285240	-1.5270360	1.4679790
H	3.9175050	-3.6929920	0.3197850
N	2.4419660	1.9348720	0.5534350
H	2.6439580	2.7933480	1.0645100
C	1.3702200	1.8792500	-0.2345490
O	0.7268640	2.9734860	-0.5469250
C	1.1710890	0.7167590	-1.1625830
S	-0.6236880	0.4124470	-1.4421510
C	-1.0805710	0.5091650	0.2840970
C	-2.4557630	0.0976800	0.6295250
C	-2.7083820	-0.4702890	1.8861270
C	-3.5083840	0.2678740	-0.2791330
C	-3.9992240	-0.8581660	2.2262500
H	-1.8948040	-0.6281150	2.5845340
C	-4.7996440	-0.1126770	0.0718720
H	-3.3327340	0.7187870	-1.2491170
C	-5.0467220	-0.6774520	1.3223990
H	-4.1868960	-1.3064180	3.1947570
H	-5.6112500	0.0334460	-0.6308580
H	-6.0524370	-0.9790380	1.5912460
N	-0.1663890	0.9186240	1.0663310
H	-0.4187860	1.0209950	2.0491370
H	1.5441650	1.0470310	-2.1403410
C	3.1980390	0.8072990	0.9720670
H	0.9539660	3.7238410	0.0343390
O	4.0353660	0.9700550	1.8311430

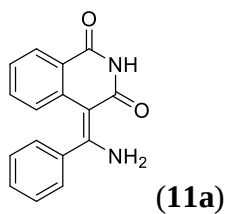
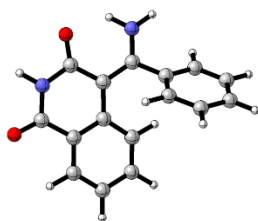


34

3-6 1 1 scf done: -1275.912198 Sum of electronic and thermal Free Energies -1275.694568

imag. freq.: 0

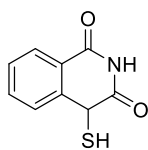
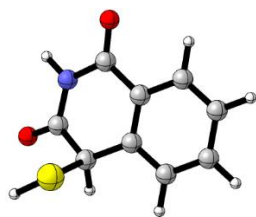
C	4.1292240	2.2539550	-0.2383550
C	2.8779640	2.1089130	0.3550280
C	2.1879790	0.9032580	0.2384070
C	2.7587100	-0.1616420	-0.4708460
C	4.0151440	-0.0115390	-1.0608680
C	4.6970480	1.1947060	-0.9476020
H	4.6627230	3.1922970	-0.1437200
H	2.4334490	2.9289630	0.9074090
H	4.4474380	-0.8460770	-1.5976900
H	5.6721380	1.3087430	-1.4058340
N	0.9373920	-1.6219600	0.2083950
H	0.5068760	-2.5413650	0.1898640
C	0.4245790	-0.6902250	1.1742560
O	0.7392890	-1.0371800	2.4920570
C	0.8269810	0.7554810	0.8348470
S	-0.5184630	1.3392070	-0.3336550
C	-1.6225010	0.1735170	0.3130510
C	-3.0302690	0.1579520	-0.0307670
C	-3.7527440	-1.0493080	-0.0087050
C	-3.6693360	1.3521090	-0.4071920
C	-5.0960820	-1.0511970	-0.3535790
H	-3.2625800	-1.9825480	0.2404080
C	-5.0152520	1.3383190	-0.7428380
H	-3.1250200	2.2884900	-0.4068850
C	-5.7285410	0.1393720	-0.7166480
H	-5.6494600	-1.9821470	-0.3482490
H	-5.5090440	2.2611500	-1.0208170
H	-6.7789160	0.1314340	-0.9831920
N	-1.0463850	-0.7010730	1.1029840
H	-1.5637620	-1.4375170	1.5784400
H	0.7167670	1.3606760	1.7329280
C	2.0593330	-1.4682000	-0.5764560
H	1.6149590	-1.4519140	2.4994740
O	2.4399000	-2.3783480	-1.2972380



32

3-7 0 1 scf done:-877.272124 Sum of electronic and thermal Free Energies -877.067220 imag.
freq.: 0

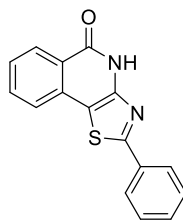
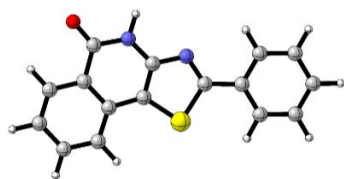
C	0.1441310	2.7701430	1.3180030
C	0.2690300	1.4395500	0.9546720
C	-0.7700900	0.7583160	0.2838020
C	-1.9752260	1.4741210	0.0854930
C	-2.0883380	2.8237360	0.4489430
C	-1.0299320	3.4840540	1.0464560
H	0.9660780	3.2562250	1.8318670
H	1.1785740	0.9174310	1.2096230
H	-3.0293900	3.3276190	0.2670860
H	-1.1188680	4.5260760	1.3294480
N	-3.0510960	-0.5741370	-0.5694460
H	-3.8895010	-1.0780450	-0.8404560
C	-1.9077320	-1.3519390	-0.4174320
O	-2.0230430	-2.5780340	-0.5783090
C	-0.6743260	-0.6402670	-0.1380770
C	0.5378020	-1.3133530	-0.3649780
C	1.8373730	-0.6151900	-0.5485290
C	2.9648470	-1.0203530	0.1731690
C	1.9487640	0.4157470	-1.4882790
C	4.1864400	-0.3800720	-0.0239770
H	2.8790890	-1.8150410	0.9051030
C	3.1735680	1.0410490	-1.6936140
H	1.0774670	0.7220480	-2.0539910
C	4.2926150	0.6510790	-0.9558740
H	5.0527080	-0.6860830	0.5511710
H	3.2555520	1.8340770	-2.4279280
H	5.2441020	1.1468620	-1.1108270
N	0.6030980	-2.6409110	-0.5059740
H	1.4501160	-3.0670670	-0.8545430
C	-3.1717020	0.7954850	-0.4347510
H	-0.2660970	-3.1695160	-0.4874870
O	-4.2357190	1.3509620	-0.6921290



20

3-8 0 1 scf done: -950.848211 Sum of electronic and thermal Free Energies -950.741470
imag. freq.: 0

C	2.6914130	-1.7614030	-0.3458330
C	1.3231910	-1.9333080	-0.5295650
C	0.4527250	-0.8536770	-0.3740420
C	0.9700990	0.4029180	-0.0348900
C	2.3463400	0.5706790	0.1542450
C	3.2046480	-0.5093500	0.0019610
H	3.3601470	-2.6044040	-0.4750070
H	0.9255450	-2.9064330	-0.7939410
H	2.7264200	1.5514900	0.4099100
H	4.2705990	-0.3790620	0.1454440
N	-1.2422220	1.3885740	-0.3122070
H	-1.8193590	2.2241870	-0.3516900
C	-1.8249430	0.2174350	-0.7501450
O	-2.9400070	0.2067800	-1.2370310
C	-1.0278020	-1.0492190	-0.5237950
H	-1.2521470	-1.7461840	-1.3286460
S	-1.6628290	-1.8138570	1.0620770
C	0.0818030	1.5825410	0.0750270
H	-2.9335030	-1.9822610	0.6330330
O	0.4513750	2.6854450	0.4392420

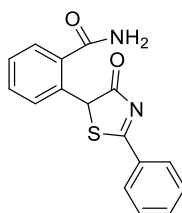
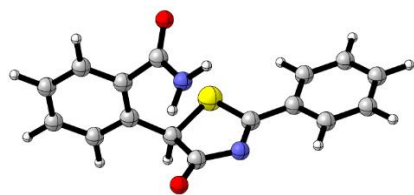


30

3-9 0 1 scf done:-1199.019284 Sum of electronic and thermal Free Energies -1198.840643

imag. freq.: 0

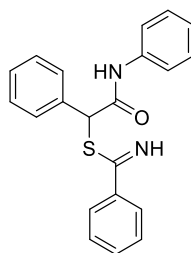
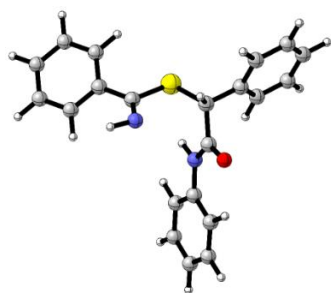
C	-3.7757800	-2.5661330	0.0347520
C	-2.4261440	-2.2622300	0.0288860
C	-1.9988000	-0.9218840	0.0841360
C	-2.9726410	0.1111780	0.1454990
C	-4.3342900	-0.2221740	0.1501250
C	-4.7370990	-1.5457370	0.0954130
H	-4.0910310	-3.6023020	-0.0080300
H	-1.6924020	-3.0588890	-0.0183770
H	-5.0616400	0.5783760	0.1972530
H	-5.7916370	-1.7941780	0.0993550
N	-1.2327030	1.7921190	0.1966590
H	-0.9368680	2.7618710	0.2364150
C	-0.2725240	0.8120330	0.1379970
C	-0.6257710	-0.5196640	0.0824600
S	0.8293410	-1.4778680	0.0176770
C	1.7791750	0.0126730	0.0685930
C	3.2414160	-0.0013220	0.0448180
C	3.9423750	1.2129170	0.1324740
C	3.9641670	-1.1989390	-0.0647510
C	5.3317540	1.2226780	0.1112870
H	3.3897640	2.1395700	0.2175510
C	5.3541300	-1.1828740	-0.0848020
H	3.4490790	-2.1503940	-0.1367930
C	6.0432630	0.0268190	0.0029010
H	5.8616620	2.1657170	0.1798320
H	5.8990750	-2.1156180	-0.1701110
H	7.1269530	0.0374270	-0.0132410
N	1.0553670	1.1048900	0.1303390
C	-2.5924450	1.5392380	0.2054010
O	-3.3992890	2.4661760	0.2598930



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3-10 0 1 scf done:-1275.470761 Sum of electronic and thermal Free Energies -1275.270406
imag. freq.: 0

C	-4.4616070	-1.6339420	-0.4595490
C	-3.1402240	-1.9915500	-0.2081320
C	-2.1312620	-1.0279140	-0.1032360
C	-2.4731070	0.3257140	-0.2808360
C	-3.7967220	0.6752710	-0.5593160
C	-4.7925120	-0.2935910	-0.6374660
H	-5.2238010	-2.4014270	-0.5266520
H	-2.8797490	-3.0375980	-0.0931530
H	-4.0439930	1.7200590	-0.7063540
H	-5.8162060	-0.0021670	-0.8413160
N	-0.8325180	1.6068820	0.9513220
H	-0.1951200	2.3841600	1.0641770
C	-0.1154600	-1.1872040	1.5414460
O	-0.7485710	-1.2844100	2.5711800
C	-0.7301840	-1.5265850	0.1635920
S	0.5368520	-1.0139800	-1.0585980
C	1.6639390	-0.6739900	0.2667780
C	3.0275050	-0.2330880	-0.0296610
C	3.8803540	0.1181390	1.0301620
C	3.4973120	-0.1483490	-1.3489500
C	5.1757070	0.5446060	0.7698780
H	3.5151930	0.0545150	2.0465930
C	4.7948210	0.2783750	-1.6035190
H	2.8589170	-0.4193990	-2.1818690
C	5.6356530	0.6255290	-0.5458440
H	5.8284710	0.8149680	1.5914440
H	5.1501270	0.3392820	-2.6251140
H	6.6474610	0.9584400	-0.7464810
N	1.2222320	-0.8151860	1.4798870
C	-1.4773450	1.4573970	-0.2295760
H	-1.1803560	1.1646870	1.7897790
H	-0.7490910	-2.6189590	0.1323860
O	-1.2880620	2.1881470	-1.1968020

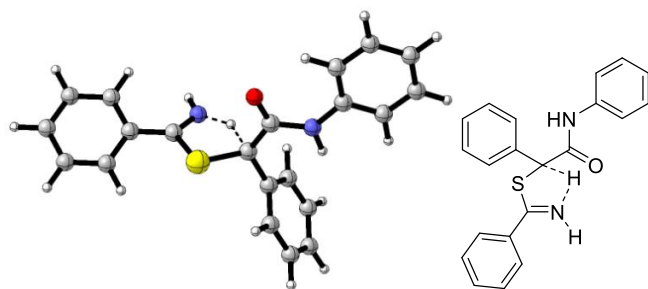


43

4a-1 0 1 scf done: -1394.426737 Sum of electronic and thermal Free Energies -1394.141577

imag. freq.: 0

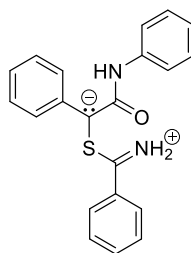
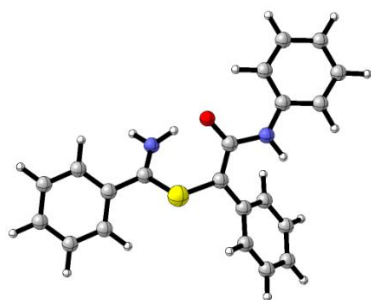
C	0.3120110	1.2033870	-5.3010780
C	0.6620130	0.1417600	-4.4692300
C	-0.0927840	-0.1415060	-3.3277500
C	-1.2034570	0.6542380	-3.0268210
C	-1.5526390	1.7160090	-3.8587130
C	-0.7962000	1.9934020	-4.9972220
H	0.9029560	1.4109400	-6.1859840
H	1.5240120	-0.4731190	-4.7037580
H	-2.4167340	2.3248610	-3.6181260
H	-1.0700820	2.8187850	-5.6444840
N	-1.4849950	-2.0350420	-0.9329880
C	-0.8735990	-2.2186140	-2.1302940
O	-1.2301960	-3.0125410	-2.9907090
C	0.3175780	-1.2913480	-2.4314170
H	1.0528430	-1.9109900	-2.9404710
S	1.1708620	-0.5703520	-0.9612590
C	1.8837430	-2.0457030	-0.2277140
C	2.6902300	-1.7760410	0.9924620
C	2.6018320	-2.6612150	2.0756420
C	3.5409280	-0.6668460	1.0777260
C	3.3561050	-2.4401070	3.2233550
H	1.9305720	-3.5107530	2.0246130
C	4.3016790	-0.4556410	2.2249590
H	3.6282720	0.0179550	0.2428160
C	4.2091300	-1.3385470	3.2998160
H	3.2739620	-3.1243010	4.0599450
H	4.9680940	0.3974460	2.2767420
H	4.7976560	-1.1688670	4.1941500
N	1.6428620	-3.1832790	-0.7432160
H	2.1258620	-3.9226470	-0.2287390
H	-1.0429120	-1.3643340	-0.3144060
H	-1.8014730	0.4453950	-2.1468510
C	-2.6047440	-2.6944160	-0.3930940
C	-2.9573520	-2.3628240	0.9234880
C	-3.3674330	-3.6342860	-1.0974530
C	-4.0564440	-2.9606620	1.5273990
H	-2.3628510	-1.6337170	1.4644260
C	-4.4672160	-4.2264970	-0.4768870
H	-3.1002400	-3.8932090	-2.1097930
C	-4.8200500	-3.8986610	0.8302710
H	-4.3158190	-2.6927330	2.5453650
H	-5.0522970	-4.9531250	-1.0296900
H	-5.6772990	-4.3656420	1.3009280



43

4a-TS1 0 1 scf done:-1394.388776 Sum of electronic and thermal Free Energies -1394.108051 imag.
freq.: 1 (-1324.8)

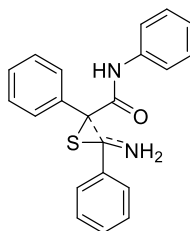
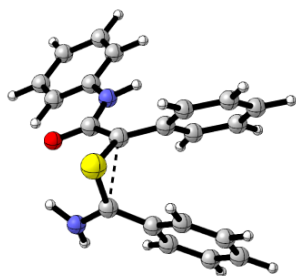
C	-3.7877850	-1.2553440	1.4361410
C	-2.7376430	-0.3494350	1.2891870
C	-2.1514730	-0.1152030	0.0355220
C	-2.6477200	-0.8286760	-1.0670410
C	-3.6863660	-1.7447580	-0.9211650
C	-4.2636680	-1.9595160	0.3314860
H	-4.2256390	-1.4171250	2.4150720
H	-2.3650840	0.1901900	2.1533610
H	-4.0522820	-2.2850810	-1.7874890
H	-5.0754100	-2.6694290	0.4438760
N	-2.6860640	2.6528450	-0.0482670
C	-1.3561500	2.3241010	-0.2571580
O	-0.5026720	3.1811140	-0.5051920
C	-1.0483150	0.8916730	-0.0863720
H	-0.2307920	0.8570700	1.1668220
S	0.3911400	0.3516280	-1.0029630
C	1.4597880	0.1760940	0.4229540
C	2.8341250	-0.3009810	0.2477580
C	3.8368090	0.1050560	1.1420090
C	3.1591520	-1.1583850	-0.8129620
C	5.1415530	-0.3428410	0.9744240
H	3.6007670	0.7851440	1.9517080
C	4.4649050	-1.6113050	-0.9684650
H	2.3900940	-1.4887800	-1.5002110
C	5.4573410	-1.2034810	-0.0779480
H	5.9131220	-0.0182360	1.6624930
H	4.7063570	-2.2834790	-1.7832230
H	6.4753330	-1.5538850	-0.2037180
N	0.9021620	0.5285920	1.5219170
H	1.3786920	0.4506570	2.4141050
H	-3.3168640	1.8758380	0.0952680
H	-2.2178210	-0.6599710	-2.0483510
C	-3.2877160	3.9130330	0.0494630
C	-4.6703910	3.9369250	0.3048900
C	-2.6016900	5.1296640	-0.0887420
C	-5.3493950	5.1432400	0.4200520
H	-5.2033780	2.9977580	0.4130440
C	-3.2977930	6.3323430	0.0313880
H	-1.5421800	5.1204740	-0.2891640
C	-4.6677500	6.3546140	0.2848780
H	-6.4156520	5.1359920	0.6178190
H	-2.7532170	7.2641350	-0.0779170
H	-5.1966330	7.2962720	0.3746860



43

4a-2 0 1 scf done:-1394.398170 Sum of electronic and thermal Free Energies -1394.112684 imag.
freq.: 0

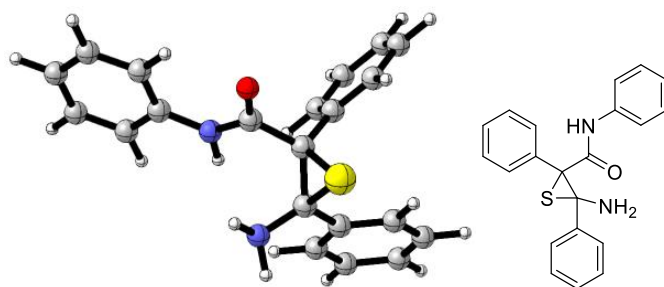
C	-3.3047010	-2.2261160	-0.7126570
C	-2.2577600	-1.3745490	-1.0544710
C	-2.1318220	-0.0930480	-0.4800620
C	-3.1172260	0.2861040	0.4577350
C	-4.1764000	-0.5571490	0.7799900
C	-4.2787700	-1.8231280	0.2012240
H	-3.3668260	-3.2049950	-1.1762620
H	-1.5310910	-1.7074630	-1.7869110
H	-4.9144080	-0.2296770	1.5046740
H	-5.0985780	-2.4833350	0.4601450
N	-2.4054730	2.7138350	-1.2106900
C	-1.1236160	2.2085070	-0.9947700
O	-0.1363400	3.0033750	-0.9917520
C	-1.0179260	0.8112580	-0.8094920
S	0.5434420	0.0255100	-1.1167740
C	1.6588890	0.5774990	0.1008790
C	2.8713960	-0.2140510	0.3432800
C	4.0826380	0.4349570	0.6342060
C	2.8304380	-1.6156290	0.2888260
C	5.2307380	-0.3102640	0.8707500
H	4.1303190	1.5174310	0.6464670
C	3.9827910	-2.3540580	0.5319220
H	1.8956650	-2.1217090	0.0846450
C	5.1823320	-1.7042520	0.8214960
H	6.1650220	0.1949200	1.0847970
H	3.9432240	-3.4362700	0.5010440
H	6.0797960	-2.2828930	1.0073870
N	1.4412540	1.7127500	0.7098960
H	2.0775110	2.0349980	1.4310530
H	0.7784640	2.3790710	0.2483020
H	-3.1210700	2.0198850	-1.3763710
H	-3.0392110	1.2488340	0.9488260
C	-2.9001940	3.9971730	-0.9712570
C	-2.1098870	5.0931560	-0.5858350
C	-4.2871320	4.1845140	-1.1213570
C	-2.7071160	6.3313100	-0.3546810
H	-1.0439980	4.9655690	-0.4808680
C	-4.8661350	5.4264490	-0.8921320
H	-4.9034450	3.3412660	-1.4161730
C	-4.0811820	6.5143130	-0.5043720
H	-2.0806760	7.1652910	-0.0561060
H	-5.9375430	5.5425630	-1.0143550
H	-4.5319530	7.4835240	-0.3257300



43

4a-TS2 0 1 scf done:-1394.390863 Sum of electronic and thermal Free Energies -1394.102754 imag.
freq.: 1 (-57.7)

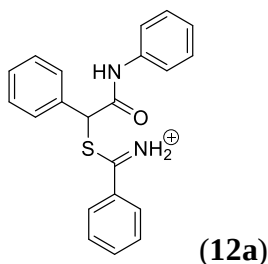
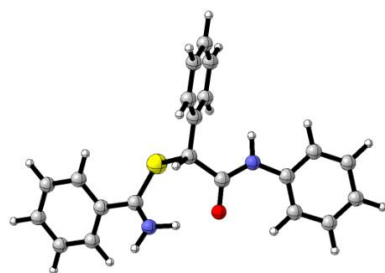
C	2.0168640	2.5516200	0.7093190
C	0.7840390	2.0258080	1.0813940
C	-0.0402780	1.3732810	0.1482880
C	0.4339070	1.2529160	-1.1729730
C	1.6668290	1.7794810	-1.5444850
C	2.4665170	2.4323790	-0.6063420
H	2.6312500	3.0517040	1.4500290
H	0.4563760	2.1090840	2.1111970
H	2.0127040	1.6604600	-2.5653840
H	3.4316360	2.8337900	-0.8938010
N	-2.5701120	1.7750060	-1.2091640
C	-2.5680650	0.8658840	-0.1604720
O	-3.5876890	0.2124430	0.1279600
C	-1.3103300	0.7542190	0.5529120
S	-1.3600400	-0.1480470	2.1016220
C	-1.1098610	-1.3940560	0.8801700
C	0.2277180	-1.6888220	0.3444680
C	1.3816470	-1.3505700	1.0662450
C	0.3729060	-2.2550610	-0.9338980
C	2.6440390	-1.5752060	0.5281240
H	1.2845690	-0.9055700	2.0469100
C	1.6364510	-2.4804160	-1.4663090
H	-0.4960710	-2.4901300	-1.5365300
C	2.7775650	-2.1396030	-0.7390700
H	3.5241310	-1.3041560	1.0995480
H	1.7299560	-2.9067640	-2.4584150
H	3.7619250	-2.3074590	-1.1606600
N	-2.1732890	-2.1365670	0.5241590
H	-2.1083290	-2.7123790	-0.3069510
H	-3.0792150	-1.6971790	0.6709030
H	-0.1567250	0.7139400	-1.9036610
H	-1.7436610	2.3490900	-1.2984810
C	-3.5701040	2.0533110	-2.1447840
C	-4.7675870	1.3296560	-2.2642880
C	-3.3306390	3.1213300	-3.0293090
C	-5.6907050	1.6792590	-3.2491140
H	-4.9640020	0.5127410	-1.5885140
C	-4.2605030	3.4558420	-4.0052910
H	-2.4065100	3.6837250	-2.9402880
C	-5.4518360	2.7368840	-4.1246920
H	-6.6107890	1.1099780	-3.3277720
H	-4.0528520	4.2831010	-4.6750740
H	-6.1784360	2.9983680	-4.8850280



43

4a-3 0 1 scf done:-1394.417909 Sum of electronic and thermal Free Energies -1394.129325 imag.
freq.: 0

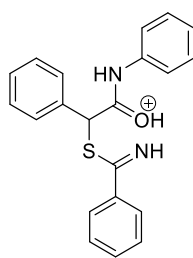
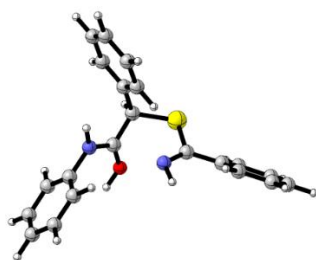
C	-0.8232820	3.2746560	0.8774150
C	-1.0895370	1.9276800	1.1194390
C	-0.8697170	0.9768470	0.1240460
C	-0.3873210	1.3879230	-1.1234510
C	-0.1144980	2.7319000	-1.3630240
C	-0.3321570	3.6798650	-0.3625820
H	-0.9947830	4.0049030	1.6602660
H	-1.4533680	1.6105840	2.0891290
H	0.2712600	3.0375880	-2.3289970
H	-0.1172290	4.7261610	-0.5481220
N	-2.4823790	-1.1741540	-1.5824420
C	-2.5666980	-0.7856160	-0.2799160
O	-3.6055980	-0.6041480	0.3345870
C	-1.1940900	-0.4835280	0.3452040
S	-0.9169280	-1.1842860	2.0164620
C	-0.0884340	-1.4920360	0.2752100
C	1.3278800	-1.0115930	0.1023180
C	1.9835060	-0.2275180	1.0553150
C	1.9877790	-1.3071710	-1.0980280
C	3.2666250	0.2557120	0.8137300
H	1.4863720	0.0007920	1.9882840
C	3.2723950	-0.8237650	-1.3377250
H	1.4888720	-1.9020880	-1.8515340
C	3.9169160	-0.0386550	-0.3840020
H	3.7595950	0.8603240	1.5666020
H	3.7656700	-1.0595490	-2.2740500
H	4.9166060	0.3372360	-0.5700640
N	-0.3352330	-2.7255710	-0.3526460
H	0.3509370	-3.4286480	-0.0993500
H	-1.2680050	-3.0900640	-0.1971220
H	-1.5494090	-1.3470800	-1.9369360
H	-0.2116220	0.6567510	-1.9031820
C	-3.5160860	-1.4123190	-2.5088920
C	-3.1288230	-1.8421630	-3.7866090
C	-4.8751260	-1.2353500	-2.2207560
C	-4.0855230	-2.0927360	-4.7623680
H	-2.0745730	-1.9740490	-4.0057820
C	-5.8231430	-1.4904200	-3.2113620
H	-5.1792680	-0.9061860	-1.2398590
C	-5.4416590	-1.9185670	-4.4809000
H	-3.7695440	-2.4243550	-5.7449210
H	-6.8731780	-1.3504380	-2.9797330
H	-6.1883710	-2.1138020	-5.2416280



44

4a-4 1 1 scf done: -1394.885825 Sum of electronic and thermal Free Energies -1394.584281 imag.
freq.: 0

C	-0.1317340	3.6524540	-0.3336650
C	-0.1876480	2.3977490	-0.9351190
C	-0.3340480	1.2481730	-0.1533370
C	-0.4133380	1.3689000	1.2405420
C	-0.3526090	2.6247160	1.8391820
C	-0.2133380	3.7679650	1.0534480
H	-0.0209290	4.5382120	-0.9483120
H	-0.1207340	2.3062150	-2.0132960
H	-0.4133700	2.7076950	2.9179060
H	-0.1667450	4.7448870	1.5205950
N	-2.7481220	-0.2468130	-0.1039800
C	-1.7664090	-0.8295580	-0.8088890
O	-1.8919510	-1.8793290	-1.4504120
C	-0.4172650	-0.0935120	-0.8365640
H	-0.1554720	0.0201050	-1.8895280
S	0.9435800	-1.1527100	-0.1006080
C	1.3877910	-2.2841190	-1.3472110
C	2.7237580	-2.8737070	-1.2370660
C	2.9064190	-4.2234300	-1.5847710
C	3.8134150	-2.1150850	-0.7798250
C	4.1643270	-4.7996300	-1.4788470
H	2.0607730	-4.8210120	-1.9032360
C	5.0700890	-2.6999040	-0.6864090
H	3.6850470	-1.0690420	-0.5340340
C	5.2466220	-4.0392930	-1.0324010
H	4.3002010	-5.8432530	-1.7351110
H	5.9125670	-2.1086440	-0.3489390
H	6.2277610	-4.4926290	-0.9529460
N	0.5669670	-2.6235620	-2.2985440
H	0.8825500	-3.2224830	-3.0561560
H	-2.5114040	0.6250790	0.3553050
H	-0.5281780	0.4874150	1.8627740
C	-4.0873540	-0.6606440	0.0839510
C	-4.8810240	0.1640700	0.8924550
C	-4.6324240	-1.8178410	-0.4823910
C	-6.2088000	-0.1652910	1.1335760
H	-4.4495170	1.0585130	1.3292040
C	-5.9670360	-2.1340780	-0.2305700
H	-4.0264770	-2.4554380	-1.1057460
C	-6.7601850	-1.3181180	0.5725650
H	-6.8122420	0.4800860	1.7613180
H	-6.3850640	-3.0318240	-0.6716240
H	-7.7958420	-1.5755480	0.7607520
H	-0.4349160	-2.3685410	-2.2290950

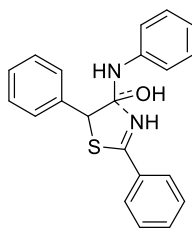
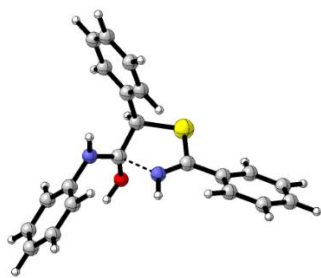


(12a')

44

4a-5 1 1 scf done:-1394.848244 Sum of electronic and thermal Free Energies -1394.549276 imag.
freq.: 0

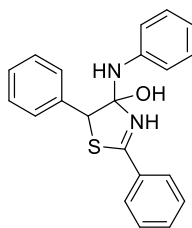
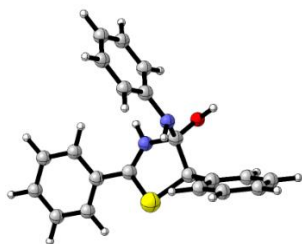
C	-1.9126830	4.3656160	0.2166270
C	-1.4818910	3.3509230	-0.6357710
C	-0.6387820	2.3411430	-0.1632300
C	-0.2282510	2.3569680	1.1742630
C	-0.6602280	3.3718970	2.0235430
C	-1.5025290	4.3773340	1.5480870
H	-2.5633270	5.1454890	-0.1617000
H	-1.7999570	3.3414560	-1.6724940
H	-0.3364030	3.3779070	3.0578880
H	-1.8344170	5.1670620	2.2123400
N	-2.0352640	-0.0986750	-0.1800370
C	-1.0053700	-0.0290740	-0.9746630
O	-0.6864960	-0.9993280	-1.7854420
C	-0.2233070	1.2486850	-1.1246430
S	1.5991550	0.9554580	-1.2312210
C	1.8716000	-0.2906790	0.0238000
C	3.2867110	-0.7287420	0.1264970
C	3.8177820	-0.9991920	1.3949010
C	4.0907950	-0.8922350	-1.0085520
C	5.1339860	-1.4289880	1.5236690
H	3.2047510	-0.8551740	2.2769060
C	5.4051990	-1.3318570	-0.8740210
H	3.6879330	-0.7042120	-1.9964150
C	5.9294750	-1.5983690	0.3897380
H	5.5405170	-1.6267750	2.5086380
H	6.0169530	-1.4697930	-1.7578100
H	6.9546010	-1.9353910	0.4917840
N	0.8933220	-0.6917370	0.7280180
H	1.1697440	-1.4239040	1.3839370
H	-0.4539350	1.5855080	-2.1418050
H	-1.2484120	-1.7879460	-1.6459450
H	-2.1890500	0.6902800	0.4449930
H	0.4197610	1.5763290	1.5501040
C	-2.8392660	-1.2780940	-0.0018540
C	-3.6814270	-1.7012400	-1.0279300
C	-2.7461370	-1.9679470	1.2051390
C	-4.4399980	-2.8556650	-0.8392410
H	-3.7556150	-1.1298700	-1.9457710
C	-3.5181160	-3.1117170	1.3828970
H	-2.0791150	-1.6117420	1.9805870
C	-4.3596810	-3.5566280	0.3621020
H	-5.0996180	-3.1960070	-1.6281630
H	-3.4580380	-3.6579940	2.3164500
H	-4.9553680	-4.4502960	0.5061610



44

4a-TS4 1 1 scf done:-1394.843252 Sum of electronic and thermal Free Energies -1394.543639 imag.
freq.: 1 (-294.2)

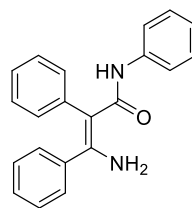
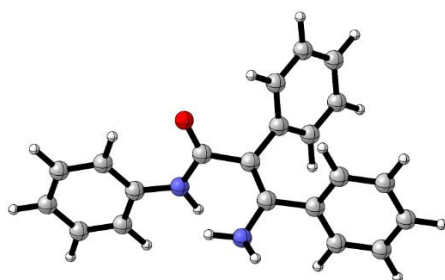
C	-1.8760280	4.4187140	0.1016840
C	-1.4893010	3.3884290	-0.7534980
C	-0.5953350	2.4062360	-0.3189310
C	-0.0887090	2.4670250	0.9840390
C	-0.4787740	3.4950730	1.8377730
C	-1.3724870	4.4727820	1.3995180
H	-2.5662500	5.1773920	-0.2485800
H	-1.8820710	3.3437360	-1.7633240
H	-0.0811860	3.5339640	2.8452990
H	-1.6708270	5.2738680	2.0659930
N	-2.0332810	-0.0112110	-0.1927620
C	-0.9300710	-0.0373060	-0.9591090
O	-0.8503070	-0.9213230	-1.9491800
C	-0.2429140	1.2889210	-1.2754530
S	1.5769530	1.0328230	-1.4600280
C	1.6982450	-0.2893150	-0.2844840
C	3.0419750	-0.7792430	0.0702640
C	3.2531960	-1.3630800	1.3276430
C	4.1082580	-0.6721120	-0.8327180
C	4.5141820	-1.8353900	1.6711830
H	2.4406250	-1.4274200	2.0416610
C	5.3650560	-1.1562360	-0.4862820
H	3.9588660	-0.2364680	-1.8136820
C	5.5704890	-1.7362120	0.7648580
H	4.6741920	-2.2768510	2.6476680
H	6.1819680	-1.0813340	-1.1939600
H	6.5522440	-2.1077100	1.0347060
N	0.5831130	-0.7056870	0.1732270
H	0.5716500	-1.5038170	0.8056990
H	-0.5872680	1.5581580	-2.2758490
H	-1.4052950	-1.7011850	-1.7649340
H	-2.0360350	0.7010900	0.5301720
H	0.6086400	1.7187630	1.3385970
C	-2.7967580	-1.1941220	0.0846060
C	-3.6719150	-1.6981270	-0.8776480
C	-2.6501570	-1.8238850	1.3214540
C	-4.3918970	-2.8607260	-0.6020260
H	-3.8055740	-1.1756660	-1.8178830
C	-3.3877900	-2.9721280	1.5929550
H	-1.9667330	-1.4128240	2.0552770
C	-4.2522350	-3.4954850	0.6299850
H	-5.0717700	-3.2571950	-1.3466650
H	-3.2821470	-3.4621690	2.5536640
H	-4.8197250	-4.3936220	0.8439360



44

4a-6 1 1 scf done:-1394.860797 Sum of electronic and thermal Free Energies -1394.558431 imag.
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C	2.7174490	-0.8969460	1.0896660
C	4.0071360	-1.1725300	1.5373330
C	5.1052540	-0.8947880	0.7252200
H	5.7570110	-0.1417790	-1.1844430
H	3.4688990	0.3334860	-1.9862570
H	4.1510030	-1.6087160	2.5188980
H	6.1080690	-1.1120830	1.0743930
N	1.0233490	1.8337950	1.0202120
C	0.6476120	1.4720620	-0.3078430
O	1.0498770	2.4275480	-1.2463680
C	1.1555440	0.0478470	-0.6918360
S	-0.2113950	-1.0984970	-0.1753920
C	-1.3697680	0.1845890	-0.2949740
C	-2.7970950	-0.0404990	-0.1604340
C	-3.6210140	0.9743940	0.3580580
C	-3.3522470	-1.2776000	-0.5278500
C	-4.9830460	0.7498690	0.4954380
H	-3.1946210	1.9142360	0.6862400
C	-4.7174750	-1.4875100	-0.3930210
H	-2.7270050	-2.0577950	-0.9448640
C	-5.5325300	-0.4765300	0.1172210
H	-5.6158910	1.5270450	0.9061230
H	-5.1463940	-2.4368770	-0.6889970
H	-6.5975720	-0.6455660	0.2247720
N	-0.8277990	1.3618840	-0.4732370
H	-1.3913530	2.2010520	-0.5784450
H	1.1558140	0.0247800	-1.7810180
H	1.9041340	2.7769710	-0.9503490
H	1.2751110	1.0431810	1.5998550
H	1.8746430	-1.1289220	1.7315710
C	0.3651800	2.8489130	1.7521350
C	0.2534960	2.6912250	3.1397910
C	-0.1453880	4.0062650	1.1515960
C	-0.3567620	3.6735930	3.9120660
H	0.6467630	1.7935860	3.6052280
C	-0.7709430	4.9756730	1.9338850
H	-0.0530070	4.1616570	0.0849740
C	-0.8794340	4.8210470	3.3142530
H	-0.4319010	3.5350730	4.9847400
H	-1.1665470	5.8633910	1.4532770
H	-1.3610200	5.5827160	3.9159220

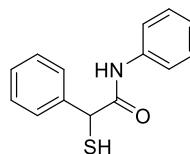
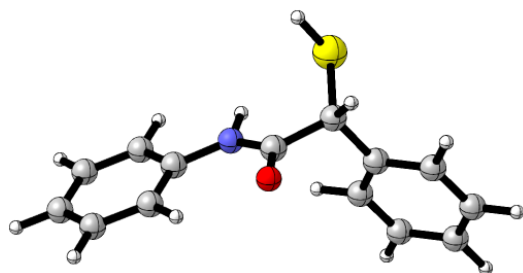


42

4a-7 0 1 scf done: -996.202979 Sum of electronic and thermal Free Energies -995.916555 imag. freq.:

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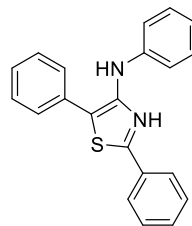
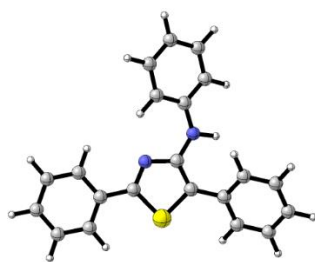
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C	0.9612060	1.2852320	-0.7516120
C	1.5982950	1.0837700	-1.9860120
C	2.3664640	2.0872450	-2.5705390
C	2.5018070	3.3240920	-1.9396680
H	1.9564240	4.5020540	-0.2221290
H	0.6084050	2.7117970	0.8161280
H	2.8529550	1.9052720	-3.5226650
H	3.0979840	4.1078690	-2.3934840
N	-2.1802420	-0.3766150	-0.3121720
C	-1.2626640	0.5211800	0.1823320
O	-1.5830030	1.5200200	0.8214880
C	0.1575880	0.1893770	-0.1452910
C	0.6862650	-1.0461790	0.0999650
C	2.1385870	-1.3306000	-0.0827160
C	3.1072580	-0.5361090	0.5408640
C	2.5473460	-2.4208730	-0.8596570
C	4.4605530	-0.8162130	0.3754050
H	2.7981380	0.3006990	1.1544120
C	3.9028010	-2.6939420	-1.0325180
H	1.8036290	-3.0422970	-1.3446580
C	4.8630040	-1.8916830	-0.4172370
H	5.2012520	-0.1950760	0.8663050
H	4.2078660	-3.5317110	-1.6494180
H	5.9175570	-2.1050250	-0.5506550
N	-0.0291610	-2.1526090	0.5210430
H	0.4987490	-2.8420760	1.0388590
H	-0.9653600	-2.0134520	0.8766750
H	-1.8172080	-1.0601990	-0.9641650
H	1.4913890	0.1290700	-2.4872250
C	-3.5770180	-0.4108990	-0.1442550
C	-4.2844480	-1.3538340	-0.9061000
C	-4.2753820	0.4170520	0.7451460
C	-5.6635900	-1.4686890	-0.7807770
H	-3.7443450	-1.9947010	-1.5952680
C	-5.6591820	0.2888910	0.8602880
H	-3.7401580	1.1481910	1.3297650
C	-6.3626810	-0.6467610	0.1046810
H	-6.1924570	-2.2028000	-1.3781940
H	-6.1888270	0.9343580	1.5523540
H	-7.4384350	-0.7349390	0.2018650



30

4a-8 0 1 scf done:-1069.799504 Sum of electronic and thermal Free Energies -1069.611334
imag. freq.: 0

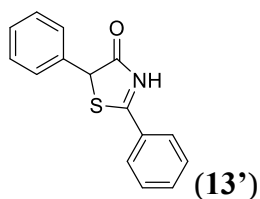
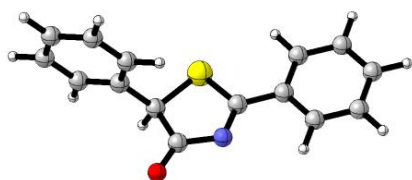
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C	3.4998480	-0.0817730	0.7907180
C	2.2508540	0.0328910	0.1746030
C	1.9181860	-0.8431930	-0.8645340
C	2.8234660	-1.8180370	-1.2781890
C	4.0682790	-1.9282720	-0.6587150
H	5.3690150	-1.1387350	0.8656250
H	3.7609360	0.5961310	1.5958340
H	2.5546680	-2.4929550	-2.0828090
H	4.7705140	-2.6888260	-0.9805820
N	-1.0256670	0.5867560	-0.0073440
C	-0.0863370	0.5081130	0.9680510
O	-0.2387220	-0.0332520	2.0563730
C	1.2895250	1.1104640	0.6332460
H	1.6585080	1.5416940	1.5613070
S	1.3021710	2.4624530	-0.6421250
H	0.5699710	3.3543180	0.0636720
H	0.9524760	-0.7722570	-1.3518860
H	-0.7501090	1.1062920	-0.8346720
C	-2.3334080	0.0645010	-0.0316600
C	-3.0842800	0.2955060	-1.1936540
C	-2.8993100	-0.6598290	1.0249420
C	-4.3820000	-0.1898500	-1.2980040
H	-2.6422170	0.8552950	-2.0111320
C	-4.2028240	-1.1409340	0.9044030
H	-2.3267930	-0.8396780	1.9210720
C	-4.9510620	-0.9128010	-0.2481890
H	-4.9487950	-0.0027910	-2.2030170
H	-4.6328940	-1.7007280	1.7274970
H	-5.9631630	-1.2915750	-0.3294470



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4a-9 0 1 scf done:-1317.954243 Sum of electronic and thermal Free Energies -1317.692920
 imag. freq.: 0

C	4.3730570	-1.3456350	-1.0236100
C	3.0076520	-1.0826530	-0.9657610
C	2.5048870	-0.0734000	-0.1270260
C	3.4146510	0.6613880	0.6545940
C	4.7795840	0.4009350	0.5856590
C	5.2664250	-0.6026200	-0.2525320
H	4.7393980	-2.1278670	-1.6788190
H	2.3277660	-1.6547210	-1.5870760
H	5.4637800	0.9762830	1.1991200
H	6.3300560	-0.8053670	-0.3012830
C	0.3943050	1.3957900	0.0835930
C	1.0673210	0.1930680	-0.0498080
S	-0.1125150	-1.0985390	-0.1242110
C	-1.3998810	0.0776620	0.0739810
C	-2.8125690	-0.3036960	0.1407660
C	-3.7736700	0.6693390	0.4599050
C	-3.2330480	-1.6190960	-0.1047330
C	-5.1195130	0.3292790	0.5327350
H	-3.4547320	1.6855410	0.6524410
C	-4.5807630	-1.9541970	-0.0299300
H	-2.5125830	-2.3876290	-0.3616750
C	-5.5294660	-0.9823840	0.2887420
H	-5.8509540	1.0895080	0.7820970
H	-4.8900690	-2.9746520	-0.2238200
H	-6.5794860	-1.2449790	0.3463060
N	-0.9714780	1.3104120	0.1547880
H	3.0498910	1.4232500	1.3321920
N	1.0102160	2.6363760	0.0559390
H	1.9293800	2.6517200	-0.3640820
C	0.6718680	3.7815390	0.7792920
C	1.4491790	4.9347880	0.5702610
C	-0.3818930	3.8338940	1.7048890
C	1.1765720	6.1066420	1.2648140
H	2.2683400	4.8974950	-0.1405220
C	-0.6454310	5.0182390	2.3906880
H	-0.9903120	2.9597630	1.8839110
C	0.1229200	6.1621700	2.1800210
H	1.7911900	6.9824550	1.0875370
H	-1.4638930	5.0391580	3.1022340
H	-0.0917710	7.0778710	2.7181520

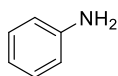
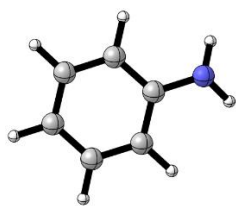


29

4a-10 0 1 scf done:-1106.696467 Sum of electronic and thermal Free Energies -1106.520003

imag. freq.: 0

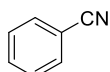
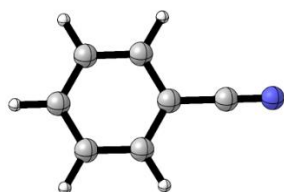
C	-4.6414410	-0.2730100	-1.0532390
C	-3.4598270	-0.9958260	-1.2206570
C	-2.3005440	-0.6177870	-0.5417790
C	-2.3325540	0.4941650	0.3073040
C	-3.5109140	1.2141010	0.4748990
C	-4.6690270	0.8325520	-0.2062770
H	-5.5367200	-0.5754430	-1.5844580
H	-3.4370070	-1.8575670	-1.8785020
H	-3.5275850	2.0721500	1.1371920
H	-5.5864270	1.3949530	-0.0748510
C	-0.4039200	-1.8805300	0.6115340
O	-1.0180310	-2.5673180	1.3987710
C	-1.0319540	-1.4117480	-0.7232500
S	0.3028640	-0.4691740	-1.5660330
C	1.3719760	-0.7466510	-0.1772840
C	2.7278310	-0.1956450	-0.1768420
C	3.5989150	-0.5152930	0.8782300
C	3.1738570	0.6452870	-1.2074880
C	4.8882130	-0.0005650	0.8970290
H	3.2542120	-1.1666700	1.6703310
C	4.4646090	1.1587130	-1.1829110
H	2.5165260	0.9088750	-2.0276750
C	5.3234920	0.8369650	-0.1317420
H	5.5561550	-0.2520210	1.7123550
H	4.7998090	1.8095560	-1.9814490
H	6.3305010	1.2376780	-0.1143900
N	0.9021690	-1.4479240	0.8101450
H	-1.2303080	-2.3024290	-1.3206160
H	-1.4365970	0.7967390	0.8391930



14

Aniline 0 1 scf done:-287.723325 Sum of electronic and thermal Free Energies -287.635892
imag. freq.: 0

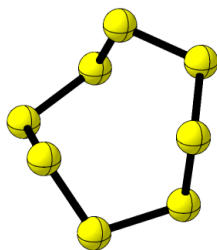
C	-2.5121820	-0.1027190	0.0030460
C	-3.4025270	0.8683500	0.4910560
C	-3.0018700	-1.3934270	-0.2585640
C	-4.7404920	0.5526930	0.7094030
H	-3.0356550	1.8691040	0.6952900
C	-4.3417220	-1.6980190	-0.0366590
H	-2.3234420	-2.1512690	-0.6369830
C	-5.2237960	-0.7311170	0.4496900
H	-5.4108280	1.3187710	1.0843270
H	-4.6989020	-2.7002770	-0.2480860
H	-6.2664140	-0.9723470	0.6201830
N	-1.1594580	0.1914530	-0.1616600
H	-0.6675750	-0.3992040	-0.8198650
H	-0.9457280	1.1709640	-0.2993830



13

Benzonitrile 0 1 scf done:-324.613608 Sum of electronic and thermal Free Energies -
324.544930 imag. freq.: 0

C	-2.1661780	0.1829640	0.6849520
C	-3.2569020	-0.2108120	-0.1478530
C	-4.5054630	-0.4889300	0.4281340
C	-3.0696420	-0.3158440	-1.5341850
C	-5.5623270	-0.8716680	-0.3892490
H	-4.6354320	-0.4036860	1.4996580
C	-4.1362930	-0.6997620	-2.3381930
H	-2.1004220	-0.0980980	-1.9649070
C	-5.3794980	-0.9771270	-1.7685410
H	-6.5288020	-1.0876980	0.0499860
H	-3.9975540	-0.7825620	-3.4094380
H	-6.2075280	-1.2760680	-2.4007750
N	-1.2828930	0.5018680	1.3593710

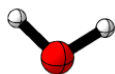


8

S₈ 0 1 scf done:-3185.802156 Sum of electronic and thermal Free Energies -3185.830556

imag. freq.: 0

S	-0.1189120	1.3415240	-1.7606760
S	0.9091380	-0.4353310	-2.1578950
S	-0.5003860	-2.0236470	-1.7278510
S	-1.4877350	-1.4748750	0.0205220
S	-0.4633130	-2.0110380	1.7489100
S	0.9505660	-0.4142700	2.1420300
S	-0.0872460	1.3559210	1.7444010
S	0.7978890	2.1058900	-0.0194530



3

H₂O 0 1 scf done:-76.467526 Sum of electronic and thermal Free Energies -76.464204

imag. freq.: 0

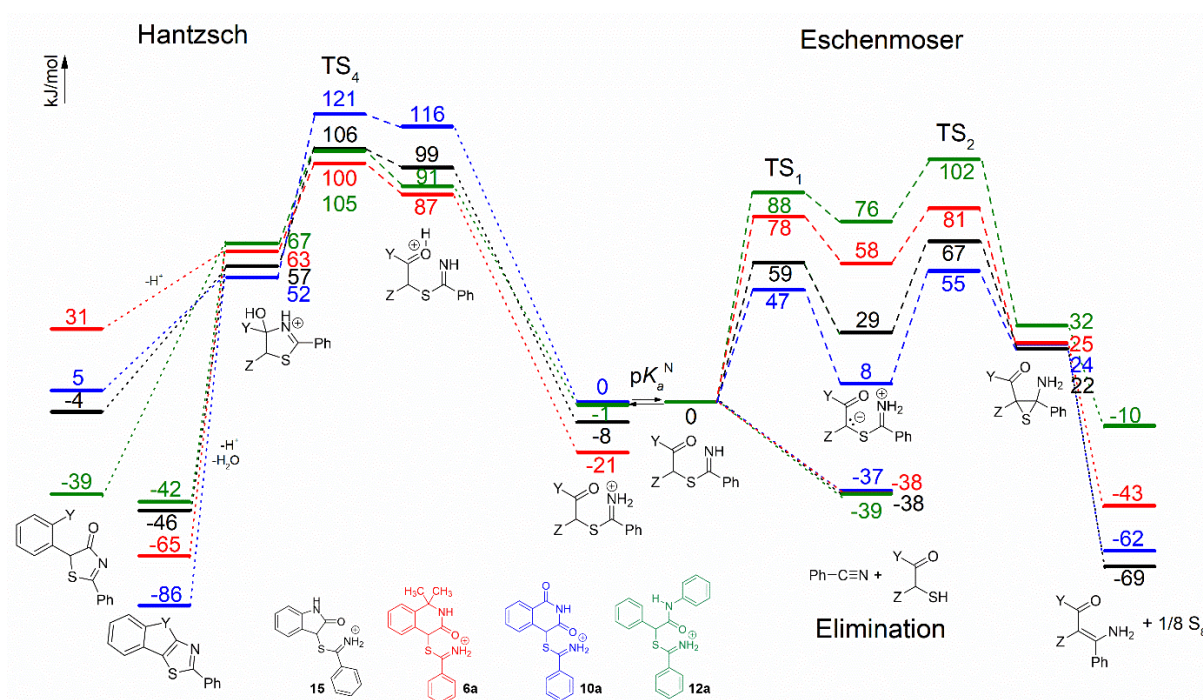
O	-0.0143780	-0.0203440	0.0000000
H	0.9499460	0.0223580	-0.0000000
H	-0.2960230	0.9029220	0.0000000



1

H⁺ 1 1 scf done:-0.213677 Sum of electronic and thermal Free Energies -0.223677 imag. freq.: 0

H	-1.8870440	0.1986360	0.0000000
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Extended version of Figure 2 in the main text - Comparison of energy profiles (relative Gibbs energies at 298 K in $\text{kJ}\cdot\text{mol}^{-1}$ for the ECR (right) and Hantzsch (left) pathways for salts **6a**, **10a**, **12a**, and **15** calculated at the B3LYP-D3/6-311++G(d,p) level of theory in *N,N*-dimethylformamide (SMD).

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