Supplementary Information

A Formal Vinylogous Schmidt Reaction: Nitrogen Insertion of *para*-Quinone Methides Insertion

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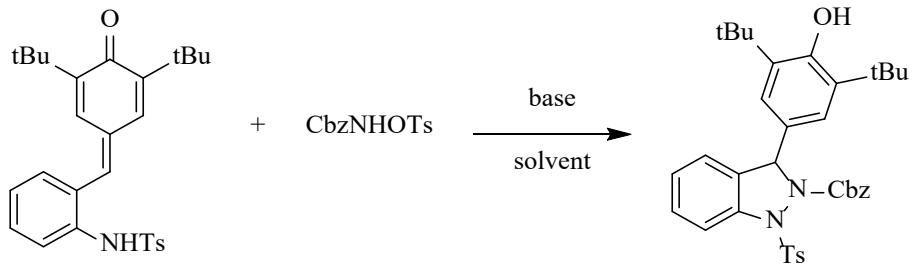
1. Supplementary Methods

General Information. The chemical reagents are commercially available and were used without further purification. Reactions were monitored by Thin Layer Chromatography (TLC) (Silica gel HF254 or GF254 from Qingdao Haiyang Chemical Co., Ltd., Qingdao, China), and the spots were visualized with ultraviolet irradiation (254 nm). Compounds were purified by solvent beating or silica gel column chromatography (200-300 mesh). ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker AVANCE-III HD 600 MHz/ 800 MHz spectrometer. Chemical shifts (ppm) were recorded with tetramethylsilane (TMS) as the internal reference standard. Data for ^{1}H NMR are reported as follows: chemical shift (ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublet, td = triplet of doublet, m = multiplet, br = broad), integration, and coupling constant (Hz). Data for ^{13}C NMR are reported in terms of chemical shift and multiplicity where appropriate. High resolution mass spectra (HRMS) were obtained from Thermo Scientific Q Exactive Plus. The melting points were determined by Büchi 510 apparatus without corrected.

2. Table S1. Optimization of Reaction Conditions of Procedure B.[a]

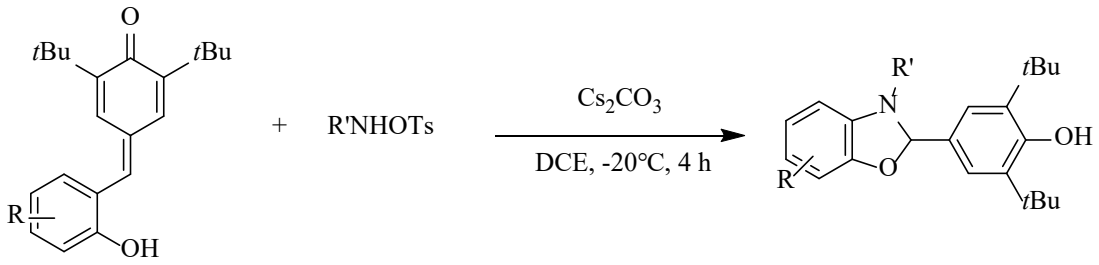


4a 2b 5a

Entry	Base	Solvent	Temperature	Yield (%)[b]
1	Cs_2CO_3	DCE	rt	60
2	Cs_2CO_3	CH_3CN	rt	< 10
3	Cs_2CO_3	Et_2O	rt	19
4	Cs_2CO_3	$CHCl_3$	rt	45
5	Cs_2CO_3	DCM	rt	71
6	Cs_2CO_3	DMF	rt	< 10
7	Cs_2CO_3	MTBE	rt	20
8	Cs_2CO_3	EA	rt	45
9	Cs_2CO_3	Toluene	rt	47
10	Cs_2CO_3	THF	rt	49
11	Cs_2CO_3	DCM	reflux	49
12	Cs_2CO_3	DCM	0 °C	53

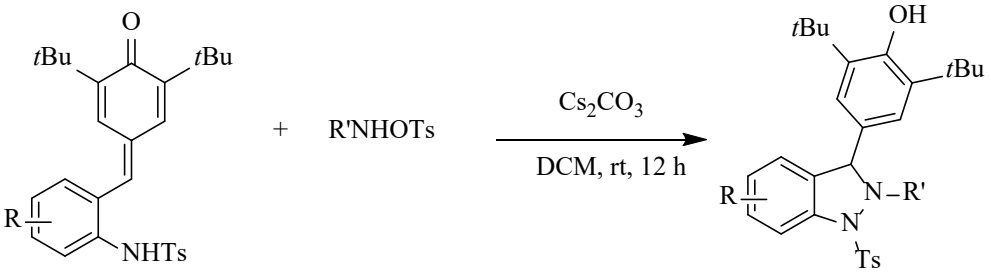
[a] Reaction was conducted as following unless otherwise noted: All reactions were conducted with 0.2 mmol of **4a** (1 equiv), 0.24 mmol of **2b** (1.2 equiv) and 0.24 mmol of base (1.2 equiv) in the indicated solvent (2.0 mL) for 12 h. [b] Yield of isolated **5a.**

3. General Procedure A for the synthesis of products 3a-3s and 6.



To a solution of 1 (0.1 mmol) and 2 (0.12 mmol) in DCE (2.0 mL) at -20 ºC was added Cs_2CO_3 (0.12 mmol). The reaction mixture was allowed to stir at -20 ºC for 4 h and then directly purified by silica gel chromatography to provide the desired products **3a-3s** and **6**.

4. General ProcedureB for the synthesis of products 5a-5k.

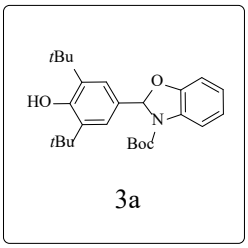


To a solution of 1 (0.1 mmol) and 2 (0.12 mmol) in DCM (2.0 mL) at rt was added Cs_2CO_3 (0.12 mmol). The reaction mixture was allowed to stir at rt for 12 h and then directly purified by silica gel chromatography to provide the desired products **5a-5k**.

5. Characterization data

Tert-butyl 2-(3,5-di-tert-butyl-4-hydroxyphenyl)benzo[d]oxazole-3(2H)-carboxylate (3a)

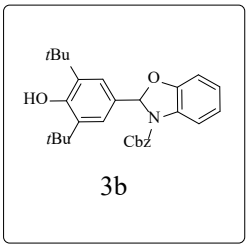
According to general procedure A, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **3a** as a white solid (31.9 mg, 75% yield). mp: 120-122 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.5 (s, 1H), 7.2 (s, 1H), 7.1 (s, 2H), 6.9 (pd, J = 7.6, 1.6 Hz, 3H), 6.8 (dd, J = 7.3, 1.7 Hz, 1H), 1.3 (s, 18H), 1.3 – 0.9 (m, 9H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 155.4, 150.1, 139.7, 130.0, 123.8, 122.8, 121.6, 113.3, 108.8, 94.9, 81.7, 34.9, 30.6, 28.0. HRMS (ESI): m/z [M+Na]$^+$ calcd for $C_{26}H_{35}NO_4Na^+$ 448.2464; found 448.2466.



3a

Benzyl 2-(3,5-di-tert-butyl-4-hydroxyphenyl)benzo[d]oxazole-3(2H)-carboxylate (3b)

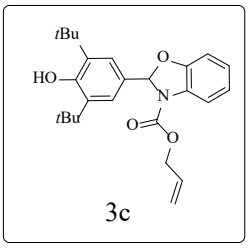
According to general procedure A, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **3b** as a white solid (27.5 mg, 60% yield). mp: 135-137 °C. ^{1}H NMR (800 MHz, DMSO-d_6) δ 7.55 (br, 1H), 7.31 – 7.16 (m, 5H), 7.14 (s, 2H), 7.07 (s, 1H), 6.98– 6.91 (m, 3H), 6.88 (d, J = 7.8 Hz, 1H), 5.25 (d, J = 12.8 Hz, 1H), 5.05 (br, 1H), 1.30 (s, 18H). ^{13}C NMR (200 MHz, DMSO-d_6) δ 160.5, 155.6, 150.2, 139.7, 139.1, 136.4, 129.4, 128.8, 128.3, 127.4, 124.3, 122.8, 121.7, 113.6, 109.0, 94.7, 67.2, 34.9, 30.5. HRMS (ESI): m/z [M+Na]$^+$ calcd for $C_{29}H_{33}NO_4Na^+$ 482.2307; found 482.2308.



3b

Allyl 2-(3,5-di-tert-butyl-4-hydroxyphenyl)benzo[d]oxazole-3(2H)-carboxylate (3c)

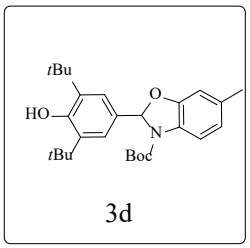
According to general procedure A, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **3c** as a white solid (21.2 mg, 52% yield). mp: 96-98 °C. ^{1}H NMR (800 MHz, DMSO-d_6) δ 7.52 (br, 1H), 7.22 (s, 1H), 7.16 (s, 2H), 7.06– 7.04 (m, 1H), 7.00 – 6.96 (m, 1H), 6.96 – 6.92 (m, 1H), 6.89 (d, J = 7.8 Hz, 1H), 5.95 – 5.76 (m, 1H), 5.20 – 4.90 (m, 2H), 4.70 (d, J = 10.4 Hz, 1H), 4.51 (br, 1H), 1.33 (s, 18H). ^{13}C NMR (200 MHz, DMSO-d_6) δ 155.5, 150.2, 140.0, 139.1, 132.8, 129.3, 127.4, 124.3, 122.8, 121.7, 117.4, 113.8, 109.0, 94.6, 66.1, 34.9, 30.6. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{25}H_{32}NO_4^+$ 410.2331; found 410.2326.



3c

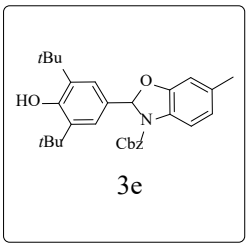
Tert-butyl 2-(3,5-di-tert-butyl-4-hydroxyphenyl)-6-methylbenzo[d]oxazole-3(2H)-carboxylate (3d)

According to general procedure A, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **3d** as a white solid (28.5 mg, 65% yield). mp: 123-125 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.36 (br, 1H), 7.22 (s, 1H), 7.12 (s, 2H), 6.85 (br, 1H), 6.71 – 6.66 (m, 2H), 2.23 (s, 3H), 1.33 (s, 18H), 1.17 (s, 9H). ^{13}C NMR (200 MHz, DMSO-d_6) δ 160.4, 155.3, 150.2, 139.6, 139.1, 133.1, 130.1, 127.7, 122.8, 122.0, 112.7, 109.5, 95.2, 81.3, 34.9, 30.6, 28.0, 21.3. HRMS (ESI): m/z [M+ Na]$^+$ calcd for $C_{27}H_{37}NO_4Na^+$ 462.2620; found 462.2625.



3d

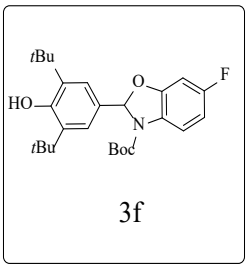
Benzyl 2-(3,5-di-tert-butyl-4-hydroxyphenyl)-6-methylbenzo[d]oxazole-3(2H)-carboxylate (3e)



3e

According to general procedure A, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **3e** as a white solid (19.9 mg, 42% yield). mp: 119-121 °C. ^{1}H NMR (800 MHz, DMSO-d_6) δ 7.41(s, 1H), 7.40 – 7.20 (m, 5H), 7.13 (s, 2H), 7.04 (br, 1H), 6.93 (br, 1H), 6.75 – 6.71 (m, 2H), 5.24 (d, J = 12.6 Hz, 1H), 5.03 (br, 1H), 2.25 (s, 3H), 1.30 (s, 18H). ^{13}C NMR (200 MHz, DMSO-d_6) δ δ 155.5, 155.3, 150.3, 139.7, 139.6, 136.5, 133.8, 129.4, 128.8, 128.2, 127.3, 122.8, 121.7, 113.1, 109.7, 94.8, 64.7, 34.9, 30.6, 21.3. HRMS (ESI): m/z [M+ Na]$^+$ calcd for $C_{30}H_{35}NO_4Na^+$ 496.2464; found 496.2463.

Tert-butyl 2-(3,5-di-tert-butyl-4-hydroxyphenyl)-6-fluorobenzo[d]oxazole-3(2H)-carboxylate (3f)

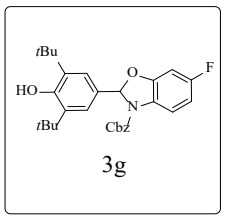


3f

According to general procedure A, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **3f** as a white solid (38.1 mg, 86% yield). mp: 140-142 °C. ^{1}H NMR (800 MHz, DMSO-d_6) δ 7.46 (s, brH), 7.25 (s, 1H), 7.14 (s, 2H), 6.95 (s, 1H), 6.84 (d, J_1 = 8.0 Hz, 1H), 6.73 – 6.70 (m, 1H), 1.34 (s, 18H), 1.19 (s, 9H). ^{13}C NMR (200 MHz, DMSO-d_6) δ 159.0 (d, J = 237.1 Hz), 155.5, 151.1 (d, J = 14.0 Hz), 150.1, 139.7, 129.5, 127.2, 122.9, 112.9, 106.9 (d, J = 23.6 Hz), 98.2, 96.2, 81.7, 34.9, 30.6, 28.0. HRMS (ESI): m/z [M+Na]$^+$ calcd for $C_{26}H_{34}FNO_4Na^+$ 466.2370; found 466.2376.

Benzyl 2-(3,5-di-tert-butyl-4-hydroxyphenyl)-6-fluorobenzo[d]oxazole-3(2H)-carboxylate

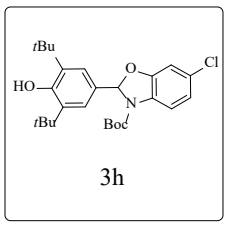
(3g)



3g

According to general procedure A, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **3g** as a white solid (34.8 mg, 73% yield). mp: 137-139 °C. ^{1}H NMR (800 MHz, DMSO-*d*6) δ 7.49 (s, brH), 7.39 – 7.21 (m, 5H), 7.14 (s, 3H), 6.95 (br, 1H), 6.90 (dd, *J* = 8.9, 2.7 Hz, 1H), 6.78 – 6.73 (m, 1H), 5.24 (d, *J* = 12.8 Hz, 1H), 5.04 (br, 1H), 1.30 (s, 18H). ^{13}C NMR (200 MHz, DMSO-*d*6) δ 159.3 (d, *J* = 240.0 Hz), 155.7, 151.2 (d, *J* = 13.7 Hz), 150.9, 139.8, 139.7, 136.3, 129.1, 128.8, 128.3, 127.3, 122.8, 113.4, 107.1 (d, *J* = 22.8 Hz), 98.3 (d, *J* = 31.1 Hz), 95.8, 67.3, 34.9, 30.5. HRMS (ESI): m/z [M+Na]$^+$ calcd for $C_{29}H_{32}FNO_4Na^+$ 500.2213; found 500.2210.

Tert-butyl 6-chloro-2-(3,5-di-tert-butyl-4-hydroxyphenyl)benzo[d]oxazole-3(2H)-carboxylate (3h)



3h

According to general procedure A, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **3h**as a white solid (38.6 mg, 84% yield). mp: 153-155 °C. ^{1}H NMR (800 MHz, DMSO-d_6) δ 7.48 (br, 1H), 7.26 (s, 1H), 7.13 (s, 2H), 7.00 – 6.92 (m, 3H), 1.34 (s, 18H), 1.18 (s, 9H). ^{13}C NMR (200 MHz, DMSO-d_6) δ 155.6, 151.1, 149.9, 139.7, 139.6, 130.0, 129.5, 127.2, 122.9, 121.3, 113.5, 109.4, 96.2, 81.9, 34.9, 30.6, 27.9. HRMS (ESI): m/z [M+ Na]$^+$ calcd for $C_{26}H_{34}ClNO_4Na^+$ 482.2074; found 482.2072

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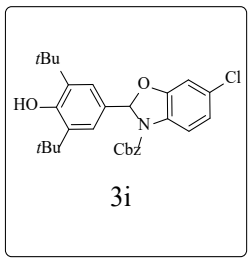
Benzyl 6-chloro-2-(3,5-di-tert-butyl-4-hydroxyphenyl)benzo[d]oxazole-3(2H)-carboxylate

(3i)

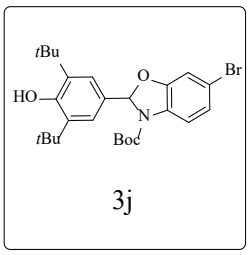


3i

According to general procedure A, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **3i** as a white solid (35.6 mg, 72% yield). mp: 117-118 °C. ^{1}H NMR (800 MHz, DMSO-d_6) δ 7.52 (br, 1H), 7.31 – 7.19 (m, 5H), 7.15 – 7.11 (m, 3H), 7.04 (s, 1H), 6.99 (d, *J* = 8.3 Hz, 1H), 6.93 (s, 1H), 5.25 (d, *J* = 12.6 Hz, 1H), 5.04 (br, 1H), 1.30 (s, 18H). ^{13}C NMR (200 MHz, DMSO-d_6) δ 155.7, 155.6, 151.1, 150.8, 139.8, 139.7, 136.2, 128.8, 128.3, 127.7, 127.3, 122.9, 121.4, 114.0, 109.6, 95.8, 67.4, 34.9, 30.5. HRMS (ESI): m/z [M+Na]$^+$ calcd for $C_{29}H_{32}ClNO_4Na^+$ 516.1918; found 516.1920.

Tert-butyl 6-bromo-2-(3,5-di-tert-butyl-4-hydroxyphenyl)benzo[d]oxazole-3(2H)-carboxylate

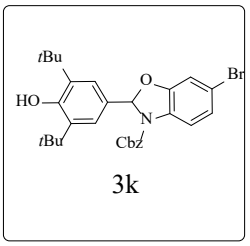
(3j)



3j

According to general procedure A, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **3j** as a white solid (36.3 mg, 72% yield). mp: 162-164 °C. ^{1}H NMR (800 MHz, DMSO-d_6) δ 7.43 (br, 1H), 7.26 (s, 1H), 7.13 (s, 2H), 7.10 – 7.08 (m, 2H) 6.94 (br, 1H), 1.34 (s, 18H), 1.18 (s, 9H). ^{13}C NMR (200 MHz, DMSO-d_6) δ 155.6, 151.2, 149.9, 139.7, 130.5, 129.4, 124.2, 122.9, 114.7, 114.2, 111.9, 96.1, 81.9, 34.9, 30.6, 27.9. HRMS (ESI): m/z [M+ Na]$^+$ calcd for $C_{26}H_{34}BrNO_4Na^+$ 526.1569; found 526.1583.

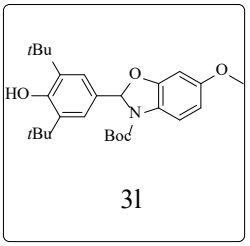
Benzyl 6-bromo-2-(3,5-di-tert-butyl-4-hydroxyphenyl)benzo[d]oxazole-3(2H)-carboxylate (3k)



3k

According to general procedure A, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **3k** as a white solid (25.8 mg, 48% yield). mp: 157-159 °C. ^{1}H NMR (800 MHz, DMSO-d_6) δ 7.63 (br, 1H), 7.47 – 7.20 (m, 5H), 7.17 – 7.09 (m, 4H), 6.93 (br, 1H), 6.87 (d, J = 8.4 Hz, 1H), 5.26 (d, J = 13.0 Hz, 1H), 5.06 (br, 1H), 1.30 (s, 18H). ^{13}C NMR (200 MHz, DMSO-d_6) δ 155.7, 150.9, 149.7, 139.8, 139.7, 136.1, 130.1, 128.8, 128.3, 127.4, 126.6, 122.9, 116.0, 112.4, 110.6, 95.9, 67.5, 34.9, 30.5. HRMS (ESI): m/z [M+Na]$^+$ calcd for $C_{29}H_{32}BrNO_4Na^+$ 560.1412; found 560.1420.

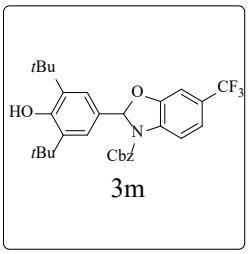
Tert-butyl 2-(3,5-di-tert-butyl-4-hydroxyphenyl)-6-methoxybenzo[d]oxazole-3(2H)-carboxylate (3l)



3l

According to general procedure A, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **3l** as a white solid (25.5 mg, 56% yield). mp: 130-132 °C. ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.74 – 7.64 (m, 1H), 7.20 (s, 1H), 7.12 (s, 2H), 6.87 (br, 1H), 6.51 (d, J = 2.5 Hz, 1H), 6.47 – 6.42 (m, 1H), 3.69 (s, 3H), 1.33 (s, 18H), 1.19 (s, 9H). ^{13}C NMR (200 MHz, DMSO-d_6) δ 159.3, 153.7, 144.9, 139.3, 139.0, 132.2, 130.5, 129.5, 129.2, 129.1, 126.6, 125.8, 123.6, 117.3, 67.0, 54.4, 35.0, 30.7, 30.5, 21.8. HRMS (ESI): m/z [M+ Na]$^+$ calcd for $C_{27}H_{37}NO_5Na^+$ 478.2569; found 478.2568.

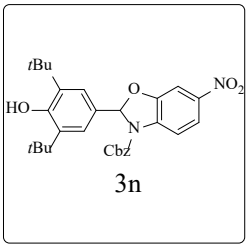
Benzyl 2-(3,5-di-tert-butyl-4-hydroxyphenyl)-6-(trifluoromethyl)benzo[d]oxazole-3(2H)-carboxylate (3m)



3m

According to general procedure A, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **3m** as a white solid (31.6 mg, 60% yield). mp: 155-157 °C. ^{1}H NMR (800 MHz, DMSO-d_6) δ 8.00 (d, J = 2.1 Hz, 1H), 7.95 – 7.91 (m, 1H), 7.50 (d, J = 9.1 Hz, 1H), 7.38 – 7.33 (m, 5H), 7.11 (s, 1H), 7.07 (s, 2H), 6.64 (s, 1H), 5.27 – 5.21 (m, 2H), 1.31 (s, 18H). ^{13}C NMR (200 MHz, DMSO-d_6) δ 161.1, 157.0, 154.7, 154.4, 140.0, 135.9, 132.3, 131.2, 130.3 (q, J = 32.0 Hz), 128.9, 128.9, 128.8, 128.5 (q, J = 30.0 Hz), 125.8, 124.3 (q, J = 254.0 Hz) 123.2, 120.3 (q, J = 4.0 Hz), 116.1 (q, J = 4.0 Hz), 114.5 (q, J = 4.0 Hz), 105.2, 68.5, 67.5, 35.0, 30.6. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{30}H_{32}F_3NO_4Na^+$ 550.2181; found 550.2172.

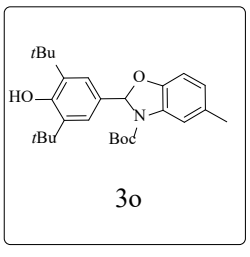
Benzyl 2-(3,5-di-tert-butyl-4-hydroxyphenyl)-6-nitrobenzo[d]oxazole-3(2H)-carboxylate (3n)



3n

According to general procedure A, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **3n** as a white solid (22.2 mg, 44% yield). mp: 123-125 °C. ^{1}H NMR (800 MHz, DMSO-d_6) δ 7.58 (s, 1H), 7.46 (d, J = 8.0 Hz, 1H), 7.42 (d, J = 8.0 Hz, 1H), 7.37 – 7.34 (m, 5H), 7.09 (s, 1H), 7.06 (s, 2H), 6.93 (s, 1H), 5.25 – 5.21 (m, 2H), 1.31 (s, 18H). ^{13}C NMR (200 MHz, DMSO-d_6) δ 161.3, 156.9, 154.8, 154.5, 148.9, 140.1, 135.9, 135.1, 130.9, 128.9, 128.8, 128.7, 128.5, 125.7, 123.4, 119.0, 114.2, 112.6, 103.5, 68.6, 67.6, 35.0, 30.6. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{29}H_{32}N_2O_6Na^+$ 527.2158; found 527.2162.

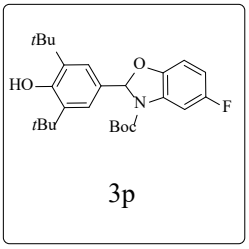
Tert-butyl 2-(3,5-di-tert-butyl-4-hydroxyphenyl)-5-methylbenzo[d]oxazole-3(2H)-carboxylate (3o)



3o

According to general procedure A, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **3o** as a white solid (20.2 mg, 46% yield). mp: 110-112 °C. ^{1}H NMR (800 MHz, DMSO-d_6) δ 7.38 (br, 1H), 7.20 (s, 1H), 7.13 (s, 2H), 6.85 (br, 1H), 6.74 – 6.67 (m, 2H), 2.26 (s, 3H), 1.34 (s, 18H), 1.20 (s, 9H). ^{13}C NMR (200 MHz, DMSO-d_6) δ 155.3, 150.1, 148.1, 139.6, 139.5, 130.4, 130.1, 123.6, 122.8, 114.0, 108.1, 95.2, 81.5, 34.9, 30.6, 28.0, 21.3. HRMS (ESI): m/z [M+ Na]$^+$ calcd for $C_{27}H_{37}NO_4Na^+$ 462.2620; found 462.2617

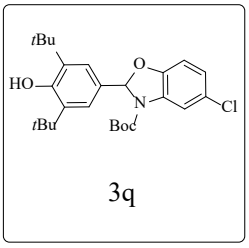
Tert-butyl 2-(3,5-di-tert-butyl-4-hydroxyphenyl)-5-fluorobenzo[d]oxazole-3(2H)-carboxylate (3p)



3p

According to general procedure A, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **3p** as a white solid (27.4 mg, 62% yield). mp: 132-134 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.25 (s, 2H), 7.13 (s, 2H), 6.94 (br, 1H), 6.84 – 6.79 (m, 1H), 6.77 – 6.70 (m, 1H), 1.53 – 1.23 (m, 27H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 157.3 (d, J = 232.5 Hz), 155.5, 149.9, 146.3, 139.7, 139.3, 129.5, 122.8, 108.8, 108.6, 101.8, 96.1, 82.1, 34.9, 30.6, 28.0. HRMS (ESI): m/z [M+ Na]$^+$ calcd for $C_{26}H_{34}FNO_4Na^+$ 466.2370; found 466.2365.

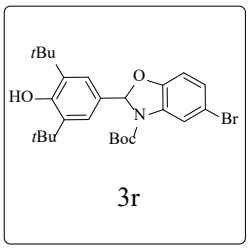
Tert-butyl 5-chloro-2-(3,5-di-tert-butyl-4-hydroxyphenyl)benzo[d]oxazole-3(2H)-carboxylate (3q)



3q

According to general procedure A, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **3q** as a white solid (18.4 mg, 40% yield). mp: 125-127 °C. ^{1}H NMR (800 MHz, DMSO-d_6) δ 7.48 (br, 1H), 7.26 (s, 1H), 7.13 (s, 2H), 6.98 (d, J = 8.0 Hz, 1H),6.94 (br, 1H), 6.85 (d, J = 8.0 Hz, 1H), 1.34 (s, 18H), 1.19 (s, 9H). ^{13}C NMR (200 MHz, DMSO-d_6) δ 155.6, 149.9, 149.2, 139.7, 139.6, 132.2, 129.5, 125.0, 122.9, 112.9, 109.6, 96.3, 82.2, 34.9, 30.6, 27.9. HRMS (ESI): m/z [M+ Na]$^+$ calcd for $C_{26}H_{34}ClNO_4Na^+$ 482.2074; found 482.2079.

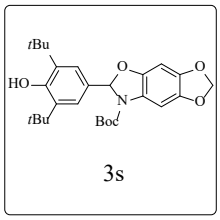
Tert-butyl 6-bromo-2-(3,5-di-tert-butyl-4-hydroxyphenyl)benzo[d]oxazole-3(2H)-carboxylate (3r)



3r

According to general procedure A, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **3r** as a white solid (21.2 mg, 42% yield). mp: 123-125 °C. ^{1}H NMR (800 MHz, DMSO-d_6) δ 7.61 (br, 1H), 7.26 (s, 1H), 7.13 (s, 2H), 7.10 (d, J = 8.4 Hz, 1H), 6.94 (br, 1H), 6.81 (d, J = 8.4 Hz, 1H), 1.34 (s, 18H), 1.18 (s, 9H). ^{13}C NMR (200 MHz, DMSO-d_6) δ 155.6, 149.9, 149.6, 139.7, 132.5, 129.4, 126.0, 122.9, 115.5, 112.4, 110.3, 96.2, 82.2, 34.9, 30.6, 27.9. HRMS (ESI): m/z [M+ Na]$^+$ calcd for $C_{26}H_{34}BrNO_4Na^+$ 526.1569; found 526,1570.

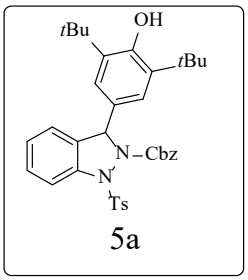
Tert-butyl 6-(3,5-di-tert-butyl-4-hydroxyphenyl)-[1,3]dioxolo[4',5':4,5]benzo[1,2-d]oxazole-7(6H)-carboxylate (3s)



3s

According to general procedure A, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **3s** as a white solid (23.5 mg, 50% yield). mp: 150-152 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.2 (s, 1H), 7.1 (s, 2H), 6.9 (s, 1H), 6.7 (s, 1H), 6.0 (d, J = 9.6 Hz, 2H), 1.3 (s, 18H), 1.3 – 1.0 (m, 9H).^{13}C NMR (125 MHz, DMSO-d_6) δ 155.3, 150.0, 144.3, 142.9, 141.0, 139.6, 129.9, 123.6, 122.7, 101.5, 96.6, 95.6, 93.5, 81.5, 34.9, 30.6, 28.0. HRMS (ESI): m/z [M+ Na]$^+$ calcd for $C_{27}H_{35}NO_6Na^+$ 492.2362; found 492.2361.

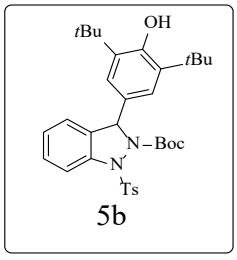
Benzyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-1-tosyl-1,3-dihydro-2H-indazole-2-carboxylate (5a)



5a

According to general procedure B, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **5a** as a white solid (43.5 mg, 71% yield). mp: 143-145 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.59 (d, J = 8.1 Hz, 1H), 7.45–7.43 (m, 2H), 7.38 –7.33 (m, 7H), 7.24 –7.23 (m, 1H), 7.01 (s, 2H), 6.81 (d, J = 8.7 Hz, 2H), 6.24 (s, 1H), 5.28 (s, 2H), 5.15 (s, 1H), 2.21 (s, 3H), 1.33 (s, 18H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.7, 153.3, 144.1, 139.8, 135.6, 135.3, 132.6, 131.7, 129.9, 129.4, 128.8, 128.6, 128.5, 128.2, 128.1, 126.0, 124.7, 124.2, 117.9, 68.9, 67.0, 34.3, 30.2, 21.8. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{36}H_{41}N_2O_5S^+$ 613.2736; found 613.2730.

Tert-butyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-1-tosyl-1,3-dihydro-2H-indazole-2-carboxylate (5b)

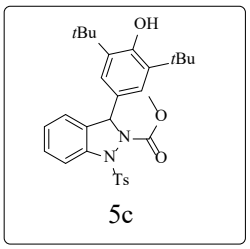


5b

According to general procedure B, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **5b** as a white solid (45.1 mg, 78% yield). mp: 152-154 °C. ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.73 (d, J = 8.0 Hz, 2H) , 7.58 (d, J = 8.0 Hz, 1H), 7.56 (d, J = 8.0 Hz, 1H), 7.48 – 7.44 (m, 1H), 7.36 – 7.32 (m, 3H), 7.10 – 7.02 (m, 3H), 5.71 (s, 1H), 2.37 (s, 3H), 1.32 (s, 18H), 1.17 (s, 9H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 153.9, 153.7, 152.5, 144.5, 138.9, 138.8, 136.7, 133.5, 129.6, 128.1, 127.8, 127.0, 125.9, 124.0, 121.4, 83.0, 65.7, 34.5, 30.1, 26.7, 21.1. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{33}H_{43}N_2O_5S^+$ 579.2893; found 579.2869.

Methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-1-tosyl-1,3-dihydro-2H-indazole-2-carboxylate

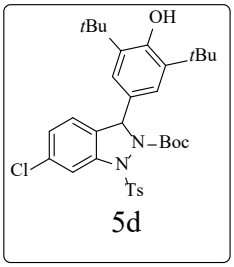
(5c)



5c

According to general procedure B, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **5c** as a white solid (34.3 mg, 64% yield). mp: 139-141 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.48 – 7.40 (m, 3H), 7.24 (d, J = 8.0 Hz, 2H), 6.97 (d, J = 7.1 Hz, 4H), 6.20 (s, 1H), 5.76 (s, 2H), 3.76 (s, 3H), 2.21 (s, 3H), 1.31 (s, 18H). ^{13}C NMR (200 MHz, DMSO-d_6) δ 159.3, 153.7, 144.9, 139.8, 139.3, 139.0, 132.2, 130.5, 130.2, 129.5, 129.2, 126.6, 125.8, 123.6, 117.3, 67.0, 54.4, 35.0, 30.7, 21.7. HRMS (ESI): m/z [M+Na]$^+$ calcd for $C_{30}H_{37}N_2O_5SNa^+$ 559.2237; found 559.2245.

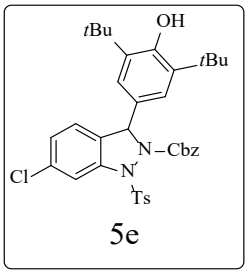
Tert-butyl 6-chloro-3-(3,5-di-tert-butyl-4-hydroxyphenyl)-1-tosyl-1,3-dihydro-2H-indazole-2-carboxylate (5d)



5d

According to general procedure B, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **5d** as a white solid (38.0 mg, 62% yield). mp: 159-161 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.75 (s, 1H), 7.64 (d, J = 8.0 Hz, 2H),7.29 – 7.25 (m, 1H), 7.21 (d, J = 8.0 Hz, 1H), 7.14 (d, J = 8.0 Hz, 2H), 7.11 (s, 2H), 5.45 (s, 1H), 5.29 (s, 1H), 2.35 (s, 3H), 1.37 (s, 18H), 1.25 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.0, 152.9, 144.4, 136.4, 135.9, 135.1, 133.8, 129.4, 128.5, 128.0, 127.3, 127.0, 125.8, 124.3, 122.6, 83.8, 66.4, 34.4, 30.1, 27.0, 21.7. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{33}H_{42}ClN_2O_5S^+$ 613.2503; found 613.2489

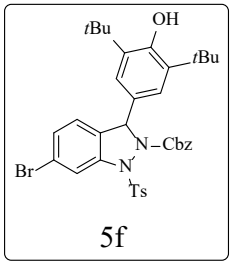
Benzyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-5-fluoro-1-tosyl-1,3-dihydro-2H-indazole- 2-carboxylate (5e)



5e

According to general procedure B, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **5e** as a white solid (37.5 mg, 58% yield). mp: 155-157 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.56 (d, J = 8.0 Hz, 1H), 7.45 – 7.44 (m, 2H), 7.38 – 7.32 (m, 4H), 7.31 (d, J = 8.0 Hz, 1H), 7.22 (d, J = 8.0 Hz, 1H), 6.89 – 6.81 (m, 4H), 6.32 (s, 1H), 5.35 – 5.23 (m, 2H), 5.14 (s, 1H), 2.23 (s, 3H), 1.32 (s, 18H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.4, 153.3, 144.3, 141.5, 135.4, 135.1, 132.6, 130.2, 130.2, 129.3, 128.9, 128.6, 128.3, 128.2, 128.1, 126.6, 124.6, 123.5, 116.2, 69.1, 66.8, 34.2, 30.2, 21.9. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{36}H_{40}ClN_2O_5S^+$ 647.2346; found 647.2342.

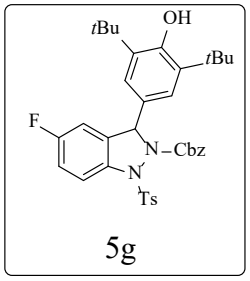
Benzyl 6-bromo-3-(3,5-di-tert-butyl-4-hydroxyphenyl)-1-tosyl-1,3-dihydro-2H-indazole-2-carboxylate (5f)



5f

According to general procedure B, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **5f** as a white solid (51.9 mg, 75% yield). mp: 167-169 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.75 (s, 1H), 7.44 – 7.32 (m, 8H), 7.11 (d, *J* = 6.0 Hz, 1H), 6.98 (s, 2H), 6.90 – 6.78 (m, 2H), 6.18 (s, 1H), 5.29 – 5.22 (m, 2H), 5.18 (s, 1H), 2.24 (s, 3H), 1.34 (s, 18H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.8, 153.6, 144.7, 141.3, 135.6, 135.5, 132.4, 131.0, 129.6, 129.2, 128.7, 128.5, 128.3, 125.9, 124.3, 122.2, 121.3, 69.2, 67.1, 34.5, 30.4, 22.0. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{36}H_{40}BrN_2O_5S^+$ 691.1841; found 691.1838

Benzyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-5-fluoro-1-tosyl-1,3-dihydro-2H-indazole-2-carboxylate (5g)

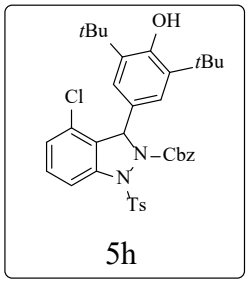


5g

According to general procedure B, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **5g** as a white solid (37.8 mg, 60% yield). mp: 140-142 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.50 –7.48 (m, 1H), 7.42 –7.32 (m, 7H), 7.09 – 7.01 (m, 3H), 6.95 (d, *J* = 7.8 Hz, 1H), 6.87 (d, *J* = 7.9 Hz, 2H), 6.21 (s, 1H), 5.27 – 5.22 (m, 2H), 5.19 (s, 1H), 2.24 (s, 3H), 1.35 (s, 18H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.1 (d, *J* = 243.0 Hz), 158.5, 153.5, 144.5, 135.8, 135.5, 135.4, 134.1 (d, *J* = 8.3 Hz), 132.4, 129.5, 129.2, 128.9, 128.5, 128.3, 128.2, 124.2, 119.2 (d, *J* = 8.3 Hz), 115.7 (d, *J* = 23.8 Hz), 111.7 (d, *J* = 24.9 Hz), 69.0, 67.1, 34.3, 30.2, 21.8. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{36}H_{40}FN_2O_5S^+$ 631.2642; found 631.2638.

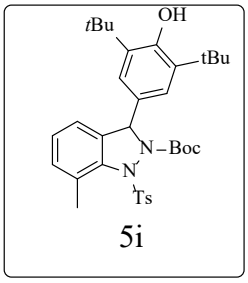
Benzyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-5-fluoro-1-tosyl-1,3-dihydro-2H-indazole-2-carboxylate (5h)

According to general procedure B, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **5h** as a white solid (49.2 mg, 76% yield). mp: 135-137 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.59 (s, 1H), 7.45 – 7.41 (m, 2H), 7.39 – 7.32 (m, 5H), 7.23 – 7.14 (m, 2H), 6.98 (s, 2H), 6.86 (d, *J* = 6.9 Hz, 2H), 6.20 (s, 1H), 5.30 – 5.22 (m, 2H), 5.18 (s, 1H), 2.24 (s, 3H), 1.34 (s, 18H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 153.6, 144.7, 140.9, 135.6, 135.5, 134.6, 132.1, 129.9, 129.6, 129.2, 128.7, 128.5, 128.3, 127.3, 126.4, 126.1, 125.5, 124.3, 118.4, 69.2, 67.0, 34.5, 30.4, 22.0. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{36}H_{40}ClN_2O_5S^+$ 647.2346; found 647.2344.



5h

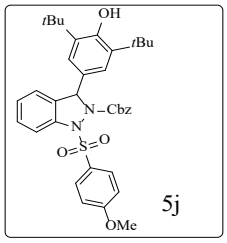
Tert-butyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-7-methyl-1-tosyl-1,3-dihydro-2H-indazole-2-carboxylate (5i)



5i

According to general procedure B, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **5i** as a white solid (23.6 mg, 40% yield). mp: 156-158 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.45 (d, *J* = 8.2 Hz, 2H), 7.35 – 7.32 (m, 1H), 7.29 – 7.26 (m, 1H), 7.22 (s, 2H), 7.10 (d, *J* = 8.0 Hz, 1H), 6.96 (d, *J* = 8.0 Hz, 2H), 5.54 (s, 1H), 5.28 (s, 1H), 2.60 (s, 3H), 2.28 (s, 3H), 1.35 (s, 18H), 1.25 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.8, 153.9, 143.7, 136.0, 135.6, 134.8, 133.8, 131.7, 131.3, 129.8, 129.6, 128.8, 126.3, 124.6, 124.5, 83.9, 67.1, 34.4, 30.1, 27.0, 21.6, 21.4. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{34}H_{45}N_2O_5S^+$ 593.3049; found 593.3041

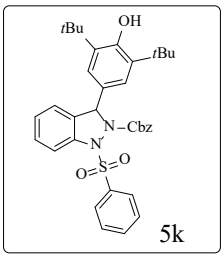
Benzyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-1-((4-methoxyphenyl)sulfonyl)-1,3-dihydro-2H-indazole-2-carboxylate (5j)



5j

According to general procedure B, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **5j** as a white solid (38.9 mg, 62% yield). mp: 174-176 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.1 Hz, 1H), 7.50 – 7.31 (m, 7H), 7.27 (s, 3H), 6.95 (s, 2H), 6.37 (d, *J* = 8.5 Hz, 2H), 6.23 (s, 1H), 5.37 – 5.29 (m, 2H), 5.15 (s, 1H), 3.65 (s, 3H), 1.33 (s, 18H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.1, 159.1, 153.0, 140.1, 135.6, 135.3, 131.4, 130.1, 128.6, 128.5, 128.2, 128.2, 126.2, 125.9, 124.8, 123.9, 118.2, 113.1, 69.0, 66.7, 55.1, 34.3, 30.2. HRMS (ESI): m/z $[M+ Na]^+$ calcd for $C_{36}H_{41}N_2O_6SNa^+$ 651.2499; found 651.2504.

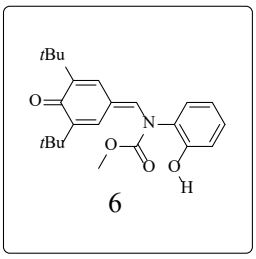
Benzyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-1-(phenylsulfonyl)-1,3-dihydro-2H-indazole-2-carboxylate (5k)



5k

According to general procedure B, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **5k** as a white solid (40.1 mg, 67% yield). mp: 168-170 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.72 (d, J = 8.1 Hz, 1H), 7.50 – 7.19 (m, 11H), 6.91 – 6.85 (m, 4H), 6.22 (s, 1H), 5.39 – 5.30 (m, 2H), 5.14 (s, 1H), 1.33 (s, 18H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 153.1, 139.9, 135.5, 135.3, 134.3, 133.6, 131.1, 130.0, 129.1, 128.7, 128.5, 128.2, 128.2, 127.7, 126.0, 125.0 123.8, 118.2, 69.1, 66.6, 34.3, 30.2. HRMS (ESI): m/z [M+ Na]$^+$ calcd for $C_{35}H_{39}N_2O_5SNa^+$ 621.2391; found 621.2400.

Methyl 2-(3,5-di-tert-butyl-4-hydroxyphenyl)benzo[d]oxazole-3(2H)-carboxylate (6)



6

According to general procedure A, the crude product was purified by silica gel chromatography (hexane/ethyl ether = 150/1 to 100/1) to provide **6** as a white solid (27.6 mg,72% yield). mp: 130-132 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.77 – 7.59 (m, 1H), 7.57 – 7.49 (m, 2H), 7.48 (s, 1H), 7.45 – 7.37 (m, 2H), 7.32 – 7.26 (m, 2H), 3.83 (s, 3H), 1.27 (s, 9H), 1.21 (s, 9H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 186.4, 153.6, 149.7, 149.0, 147.5, 138.0, 135.4, 132.9, 132.1, 131.3, 128.4,128.2, 127.0, 123.2, 56.2, 35.5, 35.2, 29.8, 29.6. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{23}H_{30}NO_4^+$ 384.2175; found 384.2172.

6. Computational Details

All DFT-calculations were performed using Gaussian 16, Revision B.01.[1] The geometry optimization and frequency analysis were performed using meta-hybrid-GGA DFT functional ωB97xD.[2] The split-valence plus one polarization function Def2-SVP basis set was used for all atoms.[3] In all cases, the default integral grid (Ultrafine Grid) was employed. Frequency calculations were performed in order to obtain thermal corrections (298 K) and to confirm the nature of the stationary points (minima with no imaginary frequency or transition states with one imaginary frequency). All transition states were optimized using the default Berny algorithm implemented in the Gaussian 16 code.[1] For transition state structures, IRC calculations were undertaken to confirm that the transition states were connected to the correct minima. For further validation of energetics, single-point calculations were performed on the ωB97xD/Def2-SVP optimized geometries using meta-hybrid GGA functional M06-2X[4] employing a valence triple-ζ-type of basis set Def2-TZVPP[3] for all atoms. The solvent effects (chloroform (CH_3Cl): ε=4.7113) were evaluated implicitly by a self-consistent reaction field (SCRF) approach for all the intermediates and transition states, using the SMD continuum solvation model.[5] Unless specified otherwise, ΔG was used throughout the text. The ΔG value was obtained by augmenting the Eel energy terms at M06-2X(SMD-CH_3Cl)/Def2-TZVPP with the respective free energy corrections at the ωB97xD/Def2-SVP level in gas phase. The geometries were realized using CYLview20, Build 0001.[6]

7. Cartesian Coordinates and Energies of Calculated Structures (in Hartree)

A1:

Eel = -1296.543477

Zero-point correction = 0.288679

Thermal correction to Energy = 0.308530

Thermal correction to Enthalpy = 0.309474

Thermal correction to Gibbs Free Energy = 0.237815

C	-4.07068500	-0.99400000	-0.03418900
C	-4.96099100	-0.15295000	-0.94652600
H	-6.01707400	-0.37715200	-0.73620800
H	-4.78973900	0.91878400	-0.78782700
H	-4.76278300	-0.39385100	-2.00162400
C	-4.25851000	-0.63925900	1.43913800
H	-5.28702600	-0.87996300	1.74547800
H	-3.56748100	-1.22420800	2.06408800
H	-4.07930500	0.42841300	1.61621900
C	-4.30630900	-2.48194500	-0.26835700
H	-4.12539000	-2.74110900	-1.32160500
H	-3.63250500	-3.08313500	0.35898500
H	-5.34418800	-2.74370300	-0.01770200
O	-2.67344300	-0.81945700	-0.40959200
C	-2.06797100	0.36377200	-0.31092600
O	-2.54152400	1.41606100	0.00624700
N	-0.72145400	0.16037900	-0.61453700
H	-0.49903200	-0.61162000	-1.23634000
O	-0.01624300	1.29106700	-0.93391100
S	1.04188200	1.74613800	0.28551600
O	0.36134100	1.64102300	1.55300500
O	1.57944400	2.98007700	-0.22786400
C	2.25288900	0.45971400	0.17160900
C	2.15007800	-0.65497000	1.00036600
C	3.27782300	0.57670600	-0.76697300
C	3.09297900	-1.67164100	0.87731200
H	1.34377700	-0.71322600	1.73289300
C	4.20958200	-0.44888300	-0.87322300
H	3.34078100	1.46689600	-1.39530800
C	4.13351400	-1.58601500	-0.05576000
H	3.01990100	-2.54946800	1.52387300
H	5.01744400	-0.36446600	-1.60427000
C	5.17026500	-2.67188500	-0.15961600
H	6.06782400	-2.40198800	0.41976200
H	4.79603000	-3.62688200	0.23403600
H	5.48625100	-2.82623000	-1.20115000

Cs_2CO_3:

Eel = -304.178162
Zero-point correction = 0.016606
Thermal correction to Energy = 0.023711
Thermal correction to Enthalpy = 0.024655
Thermal correction to Gibbs Free Energy = -0.020120

C	-0.00147800	1.22547000	0.00000000
O	0.00000000	-0.10821200	0.00000000
O	-1.12220400	1.82757100	0.00000000
O	1.11793000	1.83011900	0.00000000
Cs	-2.73472400	-0.32827000	0.00000000
Cs	2.73550600	-0.32170600	0.00000000

$Cs_2CHO_3^+$:

Eel = -304.675349
Zero-point correction = 0.029181
Thermal correction to Energy = 0.036856
Thermal correction to Enthalpy = 0.037800
Thermal correction to Gibbs Free Energy = -0.008642

C	-1.25320500	0.02997800	0.00000000
O	-1.90536600	-1.18990900	0.00000000
O	0.00000000	-0.06395100	0.00000000
O	-1.95073200	1.04667600	0.00000000
Cs	0.53831300	-2.89897800	0.00000000
Cs	0.21115200	2.94405900	0.00000000
H	-2.85257800	-1.00187000	0.00000000

A2:

Eel = -1296.054284
Zero-point correction = 0.274455
Thermal correction to Energy = 0.293819
Thermal correction to Enthalpy = 0.294763
Thermal correction to Gibbs Free Energy = 0.225719

C	-3.00680600	0.70518500	0.14774300
C	-2.61078100	-0.75777900	-0.08607300
H	-3.50673300	-1.37679100	-0.25808700
H	-1.93884800	-0.83362600	-0.94997800

H	-2.07651800	-1.14459300	0.79573900
C	-3.68455500	1.29916400	-1.09361800
H	-4.60579100	0.74355100	-1.33608400
H	-3.95081300	2.35070100	-0.90340100
H	-2.99008600	1.26242600	-1.94144900
C	-3.94901900	0.79944900	1.35000600
H	-3.46160600	0.38572700	2.24533500
H	-4.19580600	1.85229200	1.55350100
H	-4.88250000	0.24519100	1.16230400
O	-1.88690900	1.48504000	0.54057000
C	-0.73523500	1.49955800	-0.23198400
O	-0.74801400	1.13575900	-1.40849600
N	0.25157900	1.95383600	0.54320700
O	1.42735800	2.05009800	-0.31338900
S	2.53251900	0.98263900	0.09531000
O	3.00497800	1.17214300	1.45682500
O	3.49933100	0.99799900	-0.99081200
C	1.63482100	-0.56114200	0.04949100
C	1.31320500	-1.20798200	1.23663200
C	1.25625600	-1.08848400	-1.18138800
C	0.60685900	-2.40691100	1.18815400
H	1.61105100	-0.75190800	2.18157500
C	0.55592700	-2.28979300	-1.21484300
H	1.49081400	-0.54345500	-2.09550000
C	0.21312200	-2.96049800	-0.03531400
H	0.34101600	-2.91387500	2.12021900
H	0.24447700	-2.70195500	-2.17862600
C	-0.62303500	-4.21263200	-0.08159500
H	-0.41081100	-4.80858400	-0.98177700
H	-0.45273400	-4.84763000	0.80045500
H	-1.69498600	-3.95366700	-0.10249600

B1:

Eel = -966.299519
Zero-point correction = 0.423702
Thermal correction to Energy = 0.446336
Thermal correction to Enthalpy = 0.447280
Thermal correction to Gibbs Free Energy = 0.372735

C	-2.03250400	-1.05424400	-0.08847900
C	-0.78065600	-1.56152500	-0.07496100
C	0.41709100	-0.73722900	-0.04253600
C	0.23427300	0.69715500	0.10244700

C	-0.98088700	1.28768300	0.10737200
C	-2.20036200	0.43316300	-0.06006700
H	-0.61843400	-2.63984100	-0.11490000
H	1.13224100	1.29499600	0.24857000
C	-3.28415800	-1.93825200	-0.14653600
C	-2.92050300	-3.42943400	-0.12624100
H	-2.37246300	-3.70876500	0.78723700
H	-3.84277300	-4.02895300	-0.15369500
H	-2.31500200	-3.72044800	-0.99875300
C	-4.17881900	-1.65523600	1.07665400
H	-4.52445500	-0.61476800	1.08687100
H	-5.06169200	-2.31365800	1.05400600
H	-3.63275400	-1.85467900	2.01229500
C	-4.06178700	-1.65879700	-1.44809200
H	-4.39797000	-0.61637900	-1.49498800
H	-3.43246000	-1.86607400	-2.32803000
H	-4.94598100	-2.31375500	-1.50302900
C	-1.15719500	2.80076900	0.28264600
C	0.19157400	3.50221700	0.49634700
H	0.86662900	3.37530900	-0.36448400
H	0.02347100	4.58214100	0.62367300
H	0.70867500	3.13982100	1.39844000
C	-2.03861500	3.08721300	1.51438300
H	-3.04267300	2.66317100	1.39468400
H	-1.58376400	2.66548100	2.42466800
H	-2.13662100	4.17485900	1.65869600
C	-1.80505000	3.39740300	-0.98301900
H	-1.90684900	4.48874900	-0.87170500
H	-1.17734000	3.20500100	-1.86757100
H	-2.79939200	2.97088300	-1.15932100
O	-3.30970700	0.93998100	-0.15055200
C	1.63446800	-1.33994500	-0.11897900
H	1.65013800	-2.43461500	-0.09157700
C	2.95069000	-0.70496200	-0.22215200
C	3.19808900	0.42691200	-1.01437500
C	4.04251700	-1.29144300	0.45417800
C	4.46878400	0.98663800	-1.11083900
H	2.37574500	0.85157300	-1.59314300
C	5.31763700	-0.73056200	0.36072200
C	5.52770400	0.40721000	-0.41450500
H	4.63367300	1.86373000	-1.73857000
H	6.14995700	-1.18981400	0.90203800
H	6.53042400	0.83460100	-0.48032000
O	3.79193500	-2.39453900	1.19098900

H	4.60809300	-2.72051000	1.58159400

A2-C1TS:

Eel = -2262.359906
Zero-point correction = 0.699813
Thermal correction to Energy = 0.741999
Thermal correction to Enthalpy = 0.742943
Thermal correction to Gibbs Free Energy = 0.625367

C	-2.11397300	0.84125100	1.72786200
C	-0.78807600	0.52183100	1.70136800
C	0.12778700	1.04313300	0.73404300
C	-0.40089300	1.88965000	-0.28943100
C	-1.72391700	2.21448700	-0.36691800
C	-2.66417600	1.68960200	0.65164400
H	-0.36267600	-0.13214000	2.46434700
H	0.30188200	2.26031800	-1.03404300
C	-3.03832900	0.37694000	2.86468700
C	-2.28194800	-0.45089000	3.91316300
H	-1.46818200	0.12316500	4.38363900
H	-2.97813100	-0.75501500	4.71118200
H	-1.85166700	-1.36759500	3.48085200
C	-3.62752200	1.61213000	3.57421200
H	-4.21244700	2.21804000	2.87095700
H	-4.28294100	1.29995400	4.40515900
H	-2.82199600	2.23751900	3.99168800
C	-4.17975000	-0.50000500	2.32109200
H	-4.75773300	0.04926100	1.56725600
H	-3.77498700	-1.41387400	1.85996800
H	-4.85493400	-0.79812900	3.14168700
C	-2.26184500	3.13372100	-1.47465500
C	-1.15049000	3.56174800	-2.44375200
H	-0.67834600	2.69801500	-2.93703600
H	-1.57746100	4.20652400	-3.22851800
H	-0.35977600	4.13599900	-1.93632600
C	-2.85970000	4.40434800	-0.83973300
H	-3.68238000	4.14623800	-0.16088000
H	-2.08912000	4.94767200	-0.26965100
H	-3.24377800	5.07964000	-1.62320600
C	-3.34591300	2.41085800	-2.29786000
H	-3.73366900	3.07988200	-3.08444500
H	-2.93062400	1.51980300	-2.79501500
H	-4.17939800	2.10745000	-1.65248100

O	-3.87765800	1.95460500	0.59943300
C	1.48208000	0.75862300	0.86364900
C	2.59369400	1.56955800	0.30974400
C	2.90193800	1.66399000	-1.06700000
C	3.35015400	2.31527700	1.22236700
C	3.91497600	2.54747000	-1.47593200
C	4.35731700	3.18365300	0.81099900
C	4.62733900	3.30288800	-0.55359000
H	4.13084600	2.60111800	-2.54466200
H	4.92033900	3.76236100	1.54603200
H	5.41267400	3.97913100	-0.90155700
H	1.75191700	0.19517700	1.76335400
N	1.76015500	-1.09544100	-0.35723700
C	2.72959300	-1.81900300	0.27361400
O	2.62053800	-2.80318300	0.97469600
O	3.89997900	-1.18373600	0.01143800
C	5.07731300	-1.39951400	0.79871400
C	5.61335900	-2.81560500	0.57831700
H	6.57523800	-2.94185100	1.10001600
H	4.89509600	-3.55703800	0.94933100
H	5.77439500	-2.99054900	-0.49612700
C	4.78719600	-1.13018000	2.27727200
H	4.05680900	-1.85106200	2.66668800
H	5.71537000	-1.20920500	2.86408200
H	4.38905700	-0.11110000	2.39714300
C	6.05418000	-0.35862800	0.25531900
H	6.22776300	-0.52716000	-0.81753600
H	5.63985500	0.65294700	0.37809600
H	7.01742900	-0.42012700	0.78498800
O	0.50705100	-1.70503800	-0.19480300
S	-0.06465700	-2.24774400	-1.62934000
O	0.13585500	-1.22021100	-2.63397100
O	0.41503700	-3.59498600	-1.87065600
C	-1.78032300	-2.30124600	-1.19988800
C	-2.51765900	-1.12122300	-1.26695900
C	-2.37552300	-3.51051800	-0.86122800
C	-3.87696800	-1.15815200	-0.99234000
H	-2.02134800	-0.18465600	-1.52518200
C	-3.74214800	-3.53033400	-0.58601500
H	-1.77049500	-4.41799000	-0.82642400
C	-4.50859900	-2.36173000	-0.64937700
H	-4.44638000	-0.22630100	-1.01580800
H	-4.22144400	-4.47541400	-0.31702000
C	-5.97550400	-2.36944400	-0.31438500

H	-6.14945300	-1.83351900	0.63242400
H	-6.56311600	-1.85641000	-1.09048100
H	-6.36373500	-3.39206000	-0.20519700
H	3.11679500	2.22398900	2.28736700
O	2.27518800	0.94889200	-1.99167200
H	1.93425100	0.11012300	-1.56428200

C1:

Eel = -2262.380820
Zero-point correction = 0.702577
Thermal correction to Energy = 0.744402
Thermal correction to Enthalpy = 0.745347
Thermal correction to Gibbs Free Energy = 0.630128

C	2.34225800	-0.88111500	1.56978300
C	1.02104500	-0.46762700	1.64575300
C	0.06573200	-0.77059400	0.66657700
C	0.47473700	-1.56463800	-0.41169400
C	1.78248600	-2.00362500	-0.56916300
C	2.79805400	-1.63481600	0.40880600
H	0.68563100	0.11722200	2.50584200
H	-0.26966000	-1.84267100	-1.15722700
C	3.33765400	-0.58714600	2.70461600
C	2.68691300	0.15368800	3.88106300
H	1.86371800	-0.42631300	4.32806800
H	3.43901700	0.32605100	4.66863800
H	2.29018500	1.13653100	3.58051200
C	3.90210000	-1.91787000	3.23913900
H	4.38821700	-2.46726800	2.42256300
H	4.63688700	-1.73413500	4.04290600
H	3.09095500	-2.53992600	3.65130600
C	4.49398300	0.28773500	2.18729800
H	4.96944000	-0.20832800	1.33023100
H	4.11455400	1.27248600	1.87067800
H	5.24636800	0.44757900	2.98000000
C	2.18369100	-2.87927600	-1.76772500
C	0.99556000	-3.18328100	-2.69153100
H	0.56403900	-2.26753400	-3.12626500
H	1.33188600	-3.82112000	-3.52548600
H	0.19008500	-3.71961100	-2.16539400
C	2.74302000	-4.21924100	-1.25240500
H	3.59811800	-4.03289800	-0.58929700
H	1.96875900	-4.76528100	-0.68953200

H	3.06875200	-4.85550500	-2.09427300
C	3.26267500	-2.16654100	-2.60643800
H	3.56864400	-2.79490900	-3.46117600
H	2.87727800	-1.21558000	-3.01055500
H	4.13853000	-1.96204100	-1.97692100
O	4.01589000	-1.95224900	0.25822600
C	-1.37313800	-0.36198100	0.87601500
C	-2.34355400	-1.41277100	0.35471700
C	-2.83438500	-1.47701500	-0.96379200
C	-2.72563000	-2.41788600	1.24746500
C	-3.70588500	-2.51629600	-1.32487700
C	-3.57594300	-3.45732500	0.88633700
C	-4.07385100	-3.49945300	-0.41579100
H	-4.06889700	-2.52830500	-2.35450900
H	-3.84729400	-4.22413500	1.61465900
H	-4.74731600	-4.30168300	-0.72756200
H	-1.54070500	-0.29407900	1.96372800
N	-1.69589400	0.99676200	0.32713300
C	-2.92182700	1.63477900	0.49899000
O	-3.12037000	2.78834600	0.21975300
O	-3.81303200	0.77143100	0.97790800
C	-5.23569600	0.94521700	0.76041000
C	-5.50633700	1.18147100	-0.72498400
H	-6.58920600	1.13094500	-0.91287300
H	-5.13762400	2.16449200	-1.04470500
H	-5.00619900	0.40923000	-1.32786900
C	-5.74998800	2.09112500	1.62947600
H	-5.28991000	3.04041000	1.32754500
H	-6.84330700	2.17167900	1.52975300
H	-5.51177700	1.90174000	2.68701600
C	-5.81814700	-0.39149300	1.20674100
H	-5.42500900	-1.20891400	0.58574900
H	-5.54715900	-0.59641200	2.25267000
H	-6.91511100	-0.37166300	1.12303900
O	-0.65369200	1.89097700	0.34394800
S	-0.17949600	2.41617400	-1.18173500
O	-0.58971700	1.37384000	-2.11030900
O	-0.63172300	3.77684400	-1.35476400
C	1.56824000	2.42547100	-0.97410200
C	2.28010500	1.24283400	-1.14565900
C	2.20464100	3.62588800	-0.66354000
C	3.66019300	1.26083600	-0.99792900
H	1.76208800	0.30916000	-1.36599500
C	3.58943300	3.62543100	-0.52530800

H	1.61973200	4.53867600	-0.54325800
C	4.33329100	2.44934700	-0.68906800
H	4.20580400	0.31712900	-1.07899500
H	4.10292200	4.55892500	-0.28061400
C	5.82603600	2.43572000	-0.50592000
H	6.09496200	1.77957500	0.33641700
H	6.32805600	2.03622300	-1.40014900
H	6.22321200	3.44081300	-0.30491200
H	-2.33267600	-2.37299400	2.26682900
O	-2.55718400	-0.59242900	-1.93637800
H	-1.87897500	0.06492200	-1.69939400

C2:

Eel = -2262.366116
Zero-point correction = 0.702986
Thermal correction to Energy = 0.745275
Thermal correction to Enthalpy = 0.746219
Thermal correction to Gibbs Free Energy = 0.630586

C	-2.48336900	-0.40198200	1.48020500
C	-1.09423000	-0.52185100	1.36554300
C	-0.31314800	0.41372300	0.68806500
C	-0.95469900	1.53364500	0.17432500
C	-2.32252200	1.75788500	0.30862700
C	-3.08536100	0.74937700	0.93034900
H	-0.60051800	-1.37857100	1.81461300
H	-0.33828200	2.26601600	-0.33209500
C	-3.30534900	-1.44997100	2.25852600
C	-2.42740200	-2.62034400	2.72800900
H	-1.64595000	-2.29709500	3.43161500
H	-3.05517600	-3.36028100	3.24929300
H	-1.93623200	-3.12933600	1.88450300
C	-3.91716000	-0.79032400	3.51018900
H	-4.59414100	0.02973100	3.23801700
H	-4.48757600	-1.53216100	4.09423100
H	-3.12355400	-0.38340600	4.15596800
C	-4.42199200	-2.05001800	1.38382100
H	-5.12228000	-1.28280400	1.03334600
H	-3.98734400	-2.55112900	0.50781100
H	-4.98924300	-2.80030000	1.95963100
C	-2.91431900	3.11613900	-0.12907400
C	-1.81708600	4.04764400	-0.67431800
H	-1.36395400	3.65310100	-1.59589800

H	-2.25705900	5.02909400	-0.91261100
H	-1.00744600	4.19446800	0.05637800
C	-3.51955800	3.83440900	1.09786900
H	-4.32672900	3.27518300	1.59559900
H	-2.73476600	3.99880000	1.85049500
H	-3.92858000	4.81511000	0.80515900
C	-3.96555100	2.95973300	-1.24798500
H	-4.34343300	3.94756200	-1.55715600
H	-3.51402900	2.48030100	-2.12901500
H	-4.84406000	2.35205400	-0.97714700
O	-4.44770900	0.86237200	1.04961000
C	1.21418400	0.39414800	0.65069500
C	1.83507400	1.39452800	-0.30864400
C	2.38572600	1.04085600	-1.53465000
C	1.89164800	2.76115800	0.18317000
C	3.01236000	1.98047800	-2.36222500
H	2.36819200	-0.00752600	-1.84505200
C	2.55495500	3.68842200	-0.69775300
C	3.09005000	3.30722500	-1.91862200
H	3.43986100	1.67669000	-3.32064500
H	2.62160600	4.72448300	-0.35166300
H	3.58379000	4.05925700	-2.54521900
O	1.37163100	3.09546400	1.28092300
H	1.50596300	0.75844100	1.65148700
N	1.80666600	-0.96063000	0.49374100
C	3.11518400	-1.26231600	0.82069000
O	3.60005500	-2.36413100	0.72855300
O	3.71870000	-0.15628200	1.24398500
C	5.14084100	0.05979600	1.09363900
C	5.58027000	-0.28017800	-0.32951400
H	6.64539100	-0.02978300	-0.44917200
H	5.44172700	-1.34777300	-0.54524500
H	4.99763100	0.31139800	-1.05115700
C	5.88560500	-0.77175100	2.13683300
H	5.72484000	-1.84283100	1.95604000
H	6.96411900	-0.55471600	2.09152000
H	5.52360300	-0.52458200	3.14630900
C	5.28616300	1.55587200	1.35141900
H	4.71130100	2.12558200	0.60583600
H	4.89542700	1.81285900	2.34664200
H	6.34574300	1.84916700	1.29633200
O	1.02169600	-2.06579700	0.33891600
S	0.94914900	-2.76660500	-1.18684600
O	1.99638200	-2.21625400	-2.01698800

O	0.83939500	-4.17998700	-0.90725100
C	-0.62717200	-2.17178800	-1.72293700
C	-0.75253700	-0.85403400	-2.15565300
C	-1.73512500	-3.00591400	-1.59923300
C	-2.02424900	-0.35758800	-2.41520000
H	0.12368700	-0.20849700	-2.24843600
C	-2.99510700	-2.49501600	-1.88754200
H	-1.59902600	-4.03629600	-1.26796800
C	-3.16261900	-1.15459900	-2.25548400
H	-2.13053200	0.68812600	-2.71023100
H	-3.87177100	-3.14034300	-1.79071500
C	-4.53864700	-0.56399600	-2.39098300
H	-4.84975100	-0.15541200	-1.41477400
H	-4.56037400	0.25835800	-3.12032900
H	-5.27979800	-1.31918800	-2.69020700
H	-4.72468000	1.70305700	0.68235200

C2-D1TS:

Eel = -2262.343789
Zero-point correction = 0.700041
Thermal correction to Energy = 0.742787
Thermal correction to Enthalpy = 0.743731
Thermal correction to Gibbs Free Energy = 0.625888

C	2.15621500	0.91705000	1.23409600
C	0.79815900	0.61463800	1.12784300
C	0.01601200	1.08969000	0.07825500
C	0.60506400	1.89292500	-0.88968800
C	1.96321300	2.22517100	-0.85538800
C	2.72659700	1.71531800	0.21878900
H	0.32838800	-0.05845200	1.84365900
H	-0.03109400	2.25348600	-1.69761300
C	2.99603100	0.37702000	2.40760600
C	2.13195400	-0.42539500	3.39222900
H	1.64967300	-1.29292000	2.91933000
H	2.76990400	-0.79234800	4.21216400
H	1.34210700	0.19697700	3.84107400
C	4.09029400	-0.57079600	1.88106000
H	4.75574800	-0.07106100	1.16549600
H	4.69948700	-0.94482400	2.72083100
H	3.63195900	-1.43719600	1.38346000
C	3.62438300	1.54680800	3.19089300
H	4.30690700	2.13899400	2.56938000

H	2.83796500	2.21472600	3.57690800
H	4.18976400	1.15744700	4.05378000
C	2.58544100	3.10904200	-1.95806100
C	1.53877300	3.55350300	-2.99216700
H	0.73451100	4.14545900	-2.53207200
H	2.02321500	4.18144600	-3.75640800
H	1.08081400	2.69648900	-3.50664500
C	3.66103800	2.32503100	-2.74381800
H	4.45826500	1.89401200	-2.11976400
H	3.19122400	1.48191900	-3.27247100
H	4.13966100	2.97274000	-3.49606700
C	3.16494400	4.40744300	-1.35145300
H	3.59699900	5.04131100	-2.14260600
H	2.36318800	4.97489900	-0.85619700
H	3.94641800	4.25142500	-0.59309000
O	4.06839000	1.96490900	0.31471200
C	-1.44458900	0.75443800	-0.05534400
C	-2.43202300	1.56789900	0.75503800
C	-2.26355800	1.76835800	2.14437600
C	-3.55315400	2.16942200	0.02834900
C	-3.16107000	2.51000000	2.87790100
H	-1.40194600	1.31072100	2.63539300
C	-4.47508400	2.91642200	0.86581800
C	-4.28151200	3.07320700	2.21368600
H	-3.02154500	2.65239300	3.95106200
H	-5.33593500	3.36111400	0.35943500
H	-5.01018700	3.64900500	2.79446200
O	-3.70427600	2.06899300	-1.20414700
H	-1.77908600	0.80992300	-1.10247800
N	-1.81539100	-0.44904300	0.60823500
C	-3.12198900	-0.99524600	0.31322900
O	-3.74165200	-1.58902700	1.15106800
O	-3.45898400	-0.79470000	-0.94273100
C	-4.73870600	-1.18987100	-1.48954200
C	-5.86835400	-0.48746600	-0.73846200
H	-6.83158400	-0.75193200	-1.20178700
H	-5.88986900	-0.78952400	0.31648500
H	-5.72564500	0.60050500	-0.80287400
C	-4.85737900	-2.71230400	-1.44044600
H	-4.94322000	-3.06611500	-0.40514200
H	-5.74634600	-3.03300000	-2.00521300
H	-3.96566000	-3.17392900	-1.88990000
C	-4.65787900	-0.67600100	-2.92305200
H	-4.46196200	0.40542000	-2.89707700

H	-3.83814800	-1.17443300	-3.46161500
H	-5.60231900	-0.87335000	-3.45274000
H	4.34793700	2.51283900	-0.41851200
O	-0.96130000	-1.77459100	-0.35074100
S	-0.15108400	-2.83757600	0.42668200
O	-0.02158700	-2.52159200	1.84569100
O	-0.60950300	-4.17715800	0.08307700
C	1.48589300	-2.67119300	-0.29337100
C	1.83744700	-1.60082800	-1.10871000
C	2.42782700	-3.65079300	0.02423900
C	3.14497200	-1.49699200	-1.57863000
H	1.09220200	-0.84636800	-1.35973500
C	3.72857600	-3.53729600	-0.45535100
H	2.13413900	-4.49903700	0.64582300
C	4.11195100	-2.45142300	-1.25335700
H	3.41810700	-0.64015200	-2.19946100
H	4.46547700	-4.30287800	-0.19638000
C	5.54035900	-2.28669700	-1.70131900
H	5.60444500	-1.73143700	-2.64864800
H	6.11545200	-1.72260500	-0.94825600
H	6.03789400	-3.25835500	-1.83745400

D1:

Eel = -1367.451519
Zero-point correction = 0.567863
Thermal correction to Energy = 0.599968
Thermal correction to Enthalpy = 0.600912
Thermal correction to Gibbs Free Energy = 0.504950

C	2.30630500	-1.18172600	0.69508800
C	0.96020800	-0.82491900	0.63051900
C	0.50749500	0.20598700	-0.18822100
C	1.42095700	0.89686200	-0.97685000
C	2.78486800	0.59637000	-0.96489400
C	3.20894000	-0.45170800	-0.11340200
H	0.21593400	-1.35442300	1.22338400
H	1.04415000	1.69512300	-1.61582700
C	2.78098900	-2.32739500	1.60940500
C	1.60855600	-2.95640900	2.37777700
H	0.85707100	-3.39408300	1.70345100
H	1.98932900	-3.76700300	3.01717200
H	1.10375200	-2.23059500	3.03345200
C	3.42918400	-3.44378800	0.76694100

H	4.31031800	-3.08485300	0.22233300
H	3.74248400	-4.27360100	1.42035800
H	2.70786600	-3.84257100	0.03671700
C	3.77948000	-1.79120700	2.65434100
H	4.67400600	-1.36622500	2.18423200
H	3.30807600	-1.01103600	3.27250600
H	4.09638200	-2.60656200	3.32400200
C	3.77539500	1.38401700	-1.85006800
C	3.06244200	2.46496300	-2.67803200
H	2.56233800	3.20852800	-2.04023300
H	3.80200000	3.00068200	-3.29185800
H	2.31632300	2.03415400	-3.36172500
C	4.46142600	0.44358400	-2.86663800
H	5.03328800	-0.38194900	-2.41759100
H	3.70643300	-0.02073800	-3.51813700
H	5.15770800	1.01294700	-3.50170400
C	4.81345400	2.12384600	-0.97621500
H	5.51082600	2.69110600	-1.61198200
H	4.30439300	2.83473200	-0.30864400
H	5.41983100	1.47151800	-0.33055800
O	4.51630600	-0.81277600	-0.03513300
C	-0.92803700	0.59011300	-0.22873900
C	-1.62436100	1.37175600	0.93362500
C	-0.86804500	1.72436000	2.14513900
C	-2.64925300	2.35195800	0.40281500
C	-1.00025700	2.93813000	2.70789900
H	-0.18354800	0.97447300	2.54537400
C	-2.70786400	3.64954200	1.08336600
C	-1.93379500	3.91126500	2.15938900
H	-0.41939500	3.20569800	3.59222500
H	-3.42386500	4.37297100	0.68969800
H	-2.01222600	4.88382800	2.65288500
O	-3.34672600	2.06865700	-0.55318900
H	-1.32484300	0.90278800	-1.20326400
N	-1.84315000	-0.02438200	0.65108500
C	-3.10365600	-0.54092400	0.32360100
O	-4.06546700	-0.40039000	1.02885600
O	-3.01254300	-1.24758700	-0.79571400
C	-4.17835500	-1.87748800	-1.39632600
C	-5.22399200	-0.81509700	-1.72889500
H	-6.03337300	-1.27037100	-2.31867000
H	-5.64950700	-0.37820500	-0.81763300
H	-4.76877400	-0.00613900	-2.31789200
C	-4.72486100	-2.95679500	-0.46430500

H	-5.11798800	-2.51616400	0.46004800
H	-5.53602300	-3.50173100	-0.96948900
H	-3.93358300	-3.67731300	-0.20845000
C	-3.61173700	-2.49694800	-2.66930900
H	-3.18934600	-1.71814600	-3.32042900
H	-2.81602100	-3.21621500	-2.42713500
H	-4.40494200	-3.02246600	-3.22023100
H	5.04750200	-0.27080900	-0.62058600

D1-E1TS:

Eel = -1367.433715
Zero-point correction = 0.567117
Thermal correction to Energy = 0.598373
Thermal correction to Enthalpy = 0.599317
Thermal correction to Gibbs Free Energy = 0.507087

C	-3.25679500	0.82271900	-0.44336500
C	-2.06687100	1.47225300	-0.70679300
C	-0.81478200	0.86418000	-0.46647800
C	-0.76624100	-0.40437800	0.14357300
C	-1.92140300	-1.07810900	0.49614900
C	-3.15915500	-0.46963200	0.15567900
H	-2.07519300	2.47354800	-1.13666100
H	0.21386500	-0.77295800	0.43821300
C	-4.61943400	1.46808700	-0.75782700
C	-4.44325500	2.85962700	-1.38446600
H	-3.89070300	2.81972900	-2.33578300
H	-5.43398900	3.28635100	-1.59942800
H	-3.92734900	3.55796900	-0.70759600
C	-5.39243800	0.60113600	-1.77138600
H	-5.60803000	-0.39887700	-1.37717300
H	-6.35058000	1.08350000	-2.02060300
H	-4.81730600	0.49022700	-2.70370500
C	-5.43664000	1.64736400	0.53705300
H	-5.66061200	0.68879500	1.01941800
H	-4.88999400	2.27798800	1.25525600
H	-6.39193200	2.14551900	0.30899600
C	-1.83807900	-2.41035400	1.27088900
C	-0.37317900	-2.79095400	1.54146500
H	0.16743500	-2.00986900	2.09599600
H	-0.34389200	-3.71733700	2.13430700
H	0.17373400	-2.97713900	0.60627300
C	-2.45340900	-3.56758700	0.45279100

H	-3.53453700	-3.48510900	0.25319000
H	-1.95779200	-3.64683300	-0.52595800
H	-2.30988800	-4.51906300	0.98690700
C	-2.52317600	-2.26830200	2.64773600
H	-2.44959000	-3.21525500	3.20389200
H	-2.02095400	-1.48761200	3.23740200
H	-3.58977100	-1.99976500	2.60239900
O	-4.31896300	-1.08625100	0.41820700
C	0.37075700	1.60596000	-0.67864000
H	0.29842400	2.69985700	-0.67255900
N	1.63150200	1.15003400	-0.80023700
C	2.44647000	1.77040400	0.20998900
C	3.25941400	2.87585300	-0.05163400
C	2.38104200	1.09945600	1.49288600
C	3.98311000	3.45059900	0.97781900
C	3.13122300	1.76743100	2.52849800
C	3.89456000	2.88393700	2.27081700
H	4.60982500	4.32521600	0.79698700
H	3.08007600	1.33473000	3.53042400
H	4.45507600	3.34474700	3.08945600
C	1.97787900	-0.09958200	-1.37522800
O	1.21025500	-0.76100200	-2.02256400
O	3.24289100	-0.33997200	-1.12309200
C	3.81845800	-1.67471800	-1.22450800
C	3.92622300	-2.08149800	-2.69069300
H	4.43059000	-3.05634800	-2.76500600
H	2.93228500	-2.16182600	-3.14899300
H	4.51907000	-1.34365000	-3.25132100
C	5.19250800	-1.49298400	-0.59166500
H	5.76826800	-0.73090000	-1.13600200
H	5.08848800	-1.16750200	0.45297500
H	5.74882300	-2.44097000	-0.61781500
C	2.96677500	-2.64118100	-0.40415800
H	3.50672600	-3.59043900	-0.27549600
H	2.76218800	-2.20047700	0.58379000
H	2.01173700	-2.84868200	-0.90492800
O	1.76870800	0.01289100	1.64962600
H	3.29774000	3.28151100	-1.06618100
H	-4.15726500	-1.95300500	0.80254200

E1:

Eel = -1367.459036
Zero-point correction = 0.568514

Thermal correction to Energy = 0.600328
Thermal correction to Enthalpy = 0.601272
Thermal correction to Gibbs Free Energy = 0.506916

C	-3.20443000	-1.36363900	-0.08696300
C	-1.86550700	-1.71901400	-0.14428100
C	-0.82556700	-0.77335000	-0.06693800
C	-1.16010300	0.57945000	0.11573200
C	-2.47598100	1.00130000	0.21551400
C	-3.49169700	0.01618900	0.08711800
H	-1.59363200	-2.76843500	-0.25500100
H	-0.35909900	1.30617900	0.19295700
C	-4.32290900	-2.41724900	-0.19806300
C	-3.74520200	-3.83102200	-0.36485900
H	-3.12767400	-4.13251800	0.49517800
H	-4.57281200	-4.55159900	-0.44017900
H	-3.14309400	-3.92917700	-1.28131100
C	-5.17903400	-2.41897700	1.08392100
H	-5.67552500	-1.45549700	1.24804000
H	-5.95631400	-3.19579300	1.01239100
H	-4.55699300	-2.64383700	1.96414500
C	-5.19842100	-2.12902000	-1.43375300
H	-5.69500800	-1.15396100	-1.36726100
H	-4.59030800	-2.14723700	-2.35154900
H	-5.97622700	-2.90283100	-1.52886000
C	-2.79575600	2.49654400	0.43239800
C	-1.50914800	3.32787400	0.56702900
H	-0.87939900	3.27314200	-0.33292100
H	-1.77600100	4.38371400	0.72201100
H	-0.90041300	3.01214300	1.42682600
C	-3.58892800	2.69897000	1.74289800
H	-4.56694600	2.19472900	1.78157400
H	-3.00790700	2.32366200	2.59807000
H	-3.77682800	3.77117400	1.90428200
C	-3.56098400	3.06220100	-0.78470600
H	-3.76846900	4.13256100	-0.63451800
H	-2.95033500	2.95816000	-1.69362600
H	-4.52517400	2.57320400	-0.99396000
O	-4.79148100	0.35481200	0.12702200
C	0.51527900	-1.28950900	-0.07006000
H	0.63369700	-2.36841100	0.07449800
N	1.65329500	-0.65195900	-0.17377200
C	1.80879700	0.72981100	-0.48028900
C	1.33166200	1.26641700	-1.67594200

C	2.46328400	1.48941000	0.55750200
C	1.44684600	2.62765600	-1.90538700
C	2.55527300	2.89993600	0.25743600
C	2.06257000	3.42964100	-0.91554200
H	1.09775700	3.06627300	-2.84128600
H	3.03705700	3.53416800	1.00538800
H	2.15867200	4.50508100	-1.09248900
C	2.85675000	-1.42347200	0.17201700
O	2.76917700	-2.44033800	0.79877000
O	3.88994700	-0.87458300	-0.38699600
C	5.26492200	-1.17738000	0.03085100
C	5.63798500	-2.56085900	-0.48968100
H	6.69020900	-2.77024500	-0.24733900
H	5.01304500	-3.33483400	-0.02470200
H	5.51932800	-2.61069600	-1.58236200
C	6.06192200	-0.07801100	-0.65824500
H	5.90760400	-0.11110600	-1.74630000
H	5.74074300	0.90632800	-0.28970800
H	7.13378300	-0.20537100	-0.44976500
C	5.37780000	-1.06489100	1.54770000
H	6.44209400	-1.07126600	1.82493700
H	4.90883700	-0.12909600	1.88483100
H	4.88124400	-1.90378700	2.05211700
O	2.87354500	0.93801500	1.60181400
H	0.86290700	0.61003400	-2.41481800
H	-4.88792300	1.30159700	0.25978300

F1:

Eel = -1366.994926
Zero-point correction = 0.554956
Thermal correction to Energy = 0.586360
Thermal correction to Enthalpy = 0.587304
Thermal correction to Gibbs Free Energy = 0.493411

C	-3.20460700	-1.37597900	-0.06045400
C	-1.88991700	-1.70828000	-0.15595300
C	-0.81982800	-0.74340300	-0.15692900
C	-1.18620600	0.64103200	-0.00832300
C	-2.47743400	1.05172900	0.10857400
C	-3.57453200	0.05569100	0.05651900
H	-1.59571600	-2.75652000	-0.24154000
H	-0.38097900	1.36797400	0.02580700
C	-4.32119900	-2.43031800	-0.06898800

C	-3.76231500	-3.85596700	-0.17682400
H	-3.10433000	-4.10628100	0.67022900
H	-4.59514800	-4.57707200	-0.17429000
H	-3.19615000	-4.00818100	-1.10933900
C	-5.13236500	-2.34273000	1.23867500
H	-5.58531600	-1.34977400	1.34682900
H	-5.93347500	-3.10126700	1.24244900
H	-4.48207200	-2.52941500	2.10825500
C	-5.25037600	-2.19706900	-1.27646400
H	-5.70247200	-1.19907200	-1.22744300
H	-4.68547900	-2.28178100	-2.21877100
H	-6.05427300	-2.95262400	-1.29164500
C	-2.82889000	2.53713600	0.28393300
C	-1.57069000	3.41508100	0.34443000
H	-0.96658600	3.34831600	-0.57309300
H	-1.86787700	4.46822100	0.47365600
H	-0.91561900	3.14851000	1.18790700
C	-3.60970500	2.73706800	1.59761000
H	-4.54339500	2.16129900	1.59181000
H	-3.00071500	2.41590300	2.45766400
H	-3.85212400	3.80445500	1.73448300
C	-3.68075500	3.01292200	-0.90932200
H	-3.93058200	4.08129400	-0.79447200
H	-3.11952700	2.89618200	-1.85024300
H	-4.61230600	2.43789600	-0.97998100
O	-4.76060400	0.40232300	0.11462500
C	0.45799400	-1.25786500	-0.25722300
H	0.55367700	-2.34742500	-0.25057300
N	1.66666800	-0.65680500	-0.36611200
C	1.85954700	0.76411700	-0.45639600
C	1.55043300	1.43860500	-1.62896800
C	2.38450200	1.40186900	0.73042300
C	1.67838800	2.82487800	-1.70194900
C	2.48310700	2.83558400	0.60067400
C	2.14323300	3.50448200	-0.56253400
H	1.42326200	3.36330500	-2.61668800
H	2.85055300	3.38094000	1.47473000
H	2.24074400	4.59513600	-0.59489600
C	2.79533400	-1.48237100	-0.16690100
O	2.72122300	-2.63831500	0.17680100
O	3.89716800	-0.82523400	-0.46786800
C	5.18411600	-1.18239300	0.09341000
C	5.72500100	-2.41077900	-0.63543800
H	6.73405300	-2.65085500	-0.26611500

H	5.06776900	-3.27351000	-0.46376200
H	5.78694400	-2.22025500	-1.71793700
C	6.02316000	0.05828700	-0.19542500
H	6.03918800	0.26849600	-1.27493400
H	5.58415600	0.92461300	0.31953600
H	7.05599900	-0.08866000	0.15485200
C	5.06382600	-1.40090200	1.60069000
H	6.07170900	-1.43759300	2.04213600
H	4.48630000	-0.56872100	2.03353800
H	4.54453900	-2.34153400	1.82585300
O	2.71775300	0.75076100	1.74908200
H	1.17533100	0.86679500	-2.48343300
C	-2.47598100	1.00130000	0.21551400

F1-G1TS:

Eel = -1366.980576
Zero-point correction = 0.553934
Thermal correction to Energy = 0.584730
Thermal correction to Enthalpy = 0.585674
Thermal correction to Gibbs Free Energy = 0.492543

C	-3.14537600	-1.19990300	0.09679400
C	-1.84630100	-1.57365700	0.29832800
C	-0.74014000	-0.71437200	0.03547400
C	-1.01785100	0.59293800	-0.46054000
C	-2.28684500	1.04498200	-0.68474400
C	-3.43429600	0.15749800	-0.40848100
H	-1.61159800	-2.56790000	0.68395400
H	-0.16513300	1.23820400	-0.66257500
C	-4.32089300	-2.14685700	0.38165200
C	-3.84672900	-3.51325000	0.89597000
H	-3.28804200	-3.42634400	1.84105500
H	-4.72052900	-4.15805600	1.08407900
H	-3.20508900	-4.02888100	0.16385800
C	-5.23639200	-1.53251700	1.45864900
H	-5.62372500	-0.56310400	1.12202700
H	-6.08620800	-2.20468700	1.66963800
H	-4.67777300	-1.38235800	2.39634500
C	-5.12583800	-2.38496200	-0.91096200
H	-5.50639000	-1.43374400	-1.30291900
H	-4.48938400	-2.85388800	-1.67889900
H	-5.97769900	-3.05904500	-0.71499200
C	-2.55255200	2.46362500	-1.21008000

C	-1.24888900	3.24199200	-1.44044900
H	-0.61002600	2.75850800	-2.19666200
H	-1.48688300	4.25429500	-1.80569700
H	-0.65911800	3.34887100	-0.51658400
C	-3.39019500	3.24634500	-0.17984700
H	-4.34665800	2.74007800	-0.00013600
H	-2.84608900	3.32429000	0.77482400
H	-3.58930000	4.26877300	-0.54497500
C	-3.30766900	2.39532800	-2.55158000
H	-3.50754000	3.41203000	-2.93200200
H	-2.70483100	1.86240200	-3.30486900
H	-4.26107900	1.86705800	-2.42673900
O	-4.60389700	0.53689000	-0.60271300
C	0.54763300	-1.16631600	0.31865600
H	0.71181300	-2.23303900	0.47612400
N	1.70252300	-0.43700400	-0.01214400
C	1.87022700	0.73979300	0.79224900
C	2.41469200	1.94293000	0.38460700
C	1.39573100	0.48946400	2.12033400
C	2.55257600	2.97890000	1.31502500
C	1.57219000	1.55707100	3.04103000
C	2.13189000	2.76425800	2.63269900
H	2.98127100	3.93712600	1.01437900
H	1.23856200	1.40850600	4.07060200
H	2.23690500	3.57133900	3.36489000
C	2.77129900	-1.17042100	-0.49183600
O	2.68725400	-2.32273000	-0.85608900
O	3.87833800	-0.42671700	-0.53664900
C	5.14770700	-0.96291300	-0.95819100
C	5.07834000	-1.41111100	-2.41840000
H	6.08042600	-1.70833200	-2.76360500
H	4.39220800	-2.25906800	-2.53272900
H	4.72616800	-0.58268400	-3.05137200
C	6.08699600	0.23077300	-0.80529400
H	5.75939900	1.05999500	-1.44901000
H	6.08302700	0.58618600	0.23494300
H	7.11316400	-0.05086200	-1.08496300
C	5.57385000	-2.10169100	-0.03114500
H	6.59661700	-2.42192600	-0.28195100
H	5.56246500	-1.75927300	1.01428800
H	4.89658700	-2.95891000	-0.12907000
O	0.84679300	-0.63748000	2.35604800
H	2.73992400	2.06621200	-0.65050600

G1:

Eel = -1367.508479
Zero-point correction = 0.570850
Thermal correction to Energy = 0.601890
Thermal correction to Enthalpy = 0.602834
Thermal correction to Gibbs Free Energy = 0.511138

C	-0.99841000	-1.65363800	0.54427100
C	0.12585100	-1.06942600	-0.03150500
C	0.02918200	-0.09848700	-1.02503700
C	-1.22244200	0.29487300	-1.46909200
C	-2.39925000	-0.24611700	-0.94049100
C	-2.26248300	-1.22716800	0.06824100
H	1.11776600	-1.35694300	0.31552900
H	-1.27354800	1.06862900	-2.23449200
C	-0.86174800	-2.69303700	1.67239500
C	0.61270600	-2.96518700	2.00940700
H	1.13269400	-2.06184500	2.36328300
H	0.66630800	-3.71179600	2.81583000
H	1.16818300	-3.36929000	1.14945100
C	-1.53470600	-2.16240900	2.95402800
H	-2.60713300	-1.98537000	2.80961400
H	-1.41301400	-2.89082300	3.77139900
H	-1.06514000	-1.21799700	3.27124400
C	-1.49191000	-4.03223400	1.24305500
H	-2.56259100	-3.93072800	1.03062400
H	-0.99367900	-4.41995900	0.34085200
H	-1.36876800	-4.77846400	2.04400700
C	-3.78156700	0.23526100	-1.43247200
C	-3.65339600	1.31623700	-2.51768700
H	-3.12156500	0.94604300	-3.40633400
H	-4.65752100	1.63009100	-2.83986100
H	-3.13222800	2.21160000	-2.14789500
C	-4.57516400	0.87807500	-0.27226300
H	-4.75778400	0.21070400	0.58251300
H	-4.02773300	1.74650900	0.12310000
H	-5.55612100	1.22763300	-0.62970000
C	-4.56675600	-0.93032600	-2.07526000
H	-5.54573200	-0.57713700	-2.43450700
H	-4.00993700	-1.32941400	-2.93586100
H	-4.75691300	-1.78386200	-1.40738700
O	-3.34798100	-1.80593300	0.64293700
C	1.28307600	0.55280900	-1.56162700

H	1.02235300	1.40837800	-2.20397700
C	3.21032900	-0.63844600	-1.65876700
C	3.33483900	0.15472500	-0.51446100
C	4.16788100	-1.56826600	-2.01062800
C	4.42692800	0.03439800	0.32868400
C	5.28315600	-1.69003900	-1.16630100
H	4.04931800	-2.17751200	-2.90706200
C	5.40784700	-0.90729400	-0.02191100
H	4.50129300	0.64786900	1.22463600
H	6.06076000	-2.41552800	-1.41343500
H	6.28165000	-1.02613900	0.62154400
H	-4.15318400	-1.47655200	0.24045900
O	2.06324100	-0.35935700	-2.32864700
N	2.19430100	0.96901100	-0.47925100
C	1.82215700	1.79447200	0.55053600
O	2.43905000	1.91065100	1.58293600
O	0.70051500	2.43856900	0.21441700
C	-0.18501800	3.01327500	1.21274700
C	0.49725300	4.17727600	1.92749200
H	-0.22755700	4.67881200	2.58600400
H	1.34618500	3.82869100	2.52701400
H	0.86166000	4.91175600	1.19398300
C	-0.62912100	1.91451900	2.17662100
H	0.22189400	1.52792000	2.75352200
H	-1.37085300	2.31666300	2.88213000
H	-1.08952700	1.08353900	1.62056100
C	-1.36526100	3.50465700	0.38178200
H	-1.03607300	4.25358000	-0.35315500
H	-1.82286200	2.66249800	-0.15600500
H	-2.12316400	3.96291400	1.03343400

OTs$^-$:

Eel = -894.969389
Zero-point correction = 0.131969
Thermal correction to Energy = 0.141988
Thermal correction to Enthalpy = 0.142932
Thermal correction to Gibbs Free Energy = 0.093927

O	-2.28386700	-0.01634400	1.45554400
S	-1.98815700	-0.00025700	0.01239600
O	-2.36431600	-1.23558600	-0.70037200
O	-2.36624200	1.24957400	-0.67355800
C	-0.16900100	0.00110900	-0.04491900

C	0.53497600	-1.20208000	-0.04343600
C	0.53429900	1.20372700	-0.04335700
C	1.92819900	-1.19936700	-0.02411800
H	-0.03479500	-2.13346600	-0.07680800
C	1.92838400	1.20124500	-0.02406800
H	-0.03588500	2.13486700	-0.07629500
C	2.64916700	0.00137500	-0.00820300
H	2.47099700	-2.15069600	-0.02880800
H	2.47088200	2.15267200	-0.02855300
C	4.15696700	-0.00133500	0.04761500
H	4.51904700	-0.08412300	1.08676000
H	4.58016700	-0.84953300	-0.51253100
H	4.57755500	0.92518600	-0.37209600

C2-D2TS:

Eel = -2262.336068
Zero-point correction = 0.699593
Thermal correction to Energy = 0.742076
Thermal correction to Enthalpy = 0.743020
Thermal correction to Gibbs Free Energy = 0.625629

C	-1.91367300	2.08456500	-0.80541200
C	-0.55243500	1.78059900	-0.77364300
C	0.01309600	1.04208400	0.26152800
C	-0.79327500	0.63044100	1.31024300
C	-2.16259000	0.91013500	1.35496800
C	-2.70863000	1.63043300	0.27373100
H	0.10833700	2.08563800	-1.58375200
H	-0.32989600	0.02879700	2.08781600
C	-2.52609300	2.86034300	-1.98723600
C	-1.45769500	3.24882800	-3.02053900
H	-0.96354200	2.36811800	-3.45673300
H	-1.93425700	3.80561800	-3.84286500
H	-0.68042300	3.89477000	-2.58592000
C	-3.56512000	1.98091100	-2.71106800
H	-4.38428500	1.69075800	-2.04122700
H	-3.99440300	2.52536600	-3.56844900
H	-3.08708500	1.06697800	-3.09846200
C	-3.17966900	4.16421200	-1.48933100
H	-3.98706500	3.96643500	-0.77407600
H	-2.42907400	4.80206100	-0.99696500
H	-3.59826200	4.72731300	-2.34013200
C	-3.01751400	0.41174800	2.53971500

C	-2.16081100	-0.33020000	3.57864100
H	-1.38973100	0.32306800	4.01275300
H	-2.80574000	-0.67952100	4.40045700
H	-1.66058500	-1.20709500	3.14270600
C	-4.07778500	-0.60660200	2.06636000
H	-4.74798700	-0.24379100	1.27096400
H	-3.58040100	-1.49777800	1.65811100
H	-4.71095800	-0.91962200	2.91248000
C	-3.66968200	1.60430400	3.27313100
H	-4.26786200	1.24861700	4.12779700
H	-2.88952800	2.27844000	3.65735600
H	-4.32792200	2.21678000	2.63929600
O	-4.04700500	1.91533300	0.21610000
C	1.48372400	0.67986500	0.26359300
C	2.35544200	1.89423100	0.57216800
C	3.45593800	2.12732100	-0.29119800
C	2.11256900	2.70725600	1.67205600
C	4.30216000	3.22516000	0.02629100
C	2.95312000	3.78451800	1.96640300
C	4.04625200	4.03020300	1.12993100
H	5.15426600	3.41511800	-0.63073500
H	2.75328000	4.42251800	2.83022900
H	4.71411400	4.87107800	1.34369500
H	1.65901700	-0.06314100	1.05305100
N	1.83151100	0.09507700	-1.04768500
C	3.03875600	-0.70127400	-1.16797500
O	3.39656600	-1.16266700	-2.21149100
O	3.50637300	-1.00569300	0.04493400
C	4.68299100	-1.81425300	0.23136600
C	5.88793100	-1.10241100	-0.38092600
H	6.80440900	-1.67806900	-0.17637800
H	5.76094500	-0.99925500	-1.46610100
H	5.99173200	-0.09536100	0.04854400
C	4.46463400	-3.20964500	-0.35539500
H	4.46279000	-3.17763000	-1.45131200
H	5.26420800	-3.88467400	-0.01151400
H	3.49106000	-3.60550700	-0.03050100
C	4.79890700	-1.88565800	1.75163500
H	4.89408500	-0.87354500	2.17159000
H	3.89520900	-2.35127700	2.17144900
H	5.67891700	-2.47869300	2.04350100
O	0.72092600	-1.24497200	-1.15409200
S	0.39846700	-2.41847500	-0.18532100
O	0.95767000	-3.67727200	-0.66055200

O	0.63511300	-2.10205800	1.22399300
C	-1.37640700	-2.52293800	-0.43274700
C	-2.08812900	-1.51410300	-1.07469700
C	-2.03339400	-3.65563000	0.04693800
C	-3.46645700	-1.63973100	-1.22796700
H	-1.55898300	-0.63666600	-1.44716600
C	-3.41247500	-3.76562700	-0.10883700
H	-1.46020700	-4.45088900	0.52787300
C	-4.15060900	-2.75969200	-0.74595700
H	-4.01732400	-0.83539400	-1.72268400
H	-3.92593600	-4.65439800	0.26884400
C	-5.64942900	-2.85385500	-0.86105600
H	-6.01443900	-2.35955100	-1.77309400
H	-5.99057100	-3.89934900	-0.87544500
H	-6.13508600	-2.35969800	-0.00265000
H	1.24564600	2.50139800	2.30764200
O	3.64182200	1.35939400	-1.30220700
H	-4.49613800	1.47232600	0.93718000

D2:

Eel = -1367.447700
Zero-point correction = 0.569808
Thermal correction to Energy = 0.601070
Thermal correction to Enthalpy = 0.602014
Thermal correction to Gibbs Free Energy = 0.509762

C	-0.75257200	-1.38855900	1.05204400
C	0.38334900	-0.79117900	0.51372300
C	0.38153800	-0.18467300	-0.74011500
C	-0.78664800	-0.18098400	-1.48555100
C	-1.96603700	-0.77263900	-1.01842300
C	-1.92401600	-1.38092600	0.25679000
H	1.30451700	-0.76752300	1.09528700
H	-0.77572200	0.32463200	-2.45061000
C	-0.73143000	-1.99802600	2.46600600
C	0.65027500	-1.84603500	3.12148500
H	0.94553200	-0.79106000	3.22861000
H	0.62063900	-2.28474600	4.13013200
H	1.43693900	-2.37071300	2.55800000
C	-1.74638100	-1.26342600	3.36461200
H	-2.77162900	-1.36054800	2.98836600
H	-1.71310600	-1.67810500	4.38461400
H	-1.49790000	-0.19259500	3.42756200

C	-1.05258800	-3.50371900	2.40282500
H	-2.05002900	-3.69159200	1.98836600
H	-0.31232300	-4.02898500	1.77928000
H	-1.01185800	-3.93872100	3.41413500
C	-3.26039500	-0.72338200	-1.85890400
C	-3.04671000	0.01250400	-3.19131000
H	-2.29142600	-0.48315000	-3.81869700
H	-3.99047100	0.02450700	-3.75676200
H	-2.74099900	1.05822400	-3.04000100
C	-4.36120500	0.05686100	-1.10493900
H	-4.63067900	-0.36511400	-0.12588300
H	-4.02906200	1.08876000	-0.91755900
H	-5.28101700	0.09861900	-1.70871800
C	-3.72860800	-2.14982200	-2.22536500
H	-4.64645300	-2.10523300	-2.83185000
H	-2.95311600	-2.66009400	-2.81558600
H	-3.94135400	-2.80278100	-1.36570000
O	-3.02016100	-1.97868700	0.79301000
C	1.63571600	0.50820300	-1.24107600
C	2.82163400	-0.41825900	-1.35212300
C	3.07533200	-1.49868700	-2.18370600
C	3.71643200	-0.08706700	-0.34202900
C	4.24997900	-2.23053500	-1.98889200
H	2.36644800	-1.77508800	-2.96723900
C	4.88679400	-0.80133600	-0.11925000
C	5.13745300	-1.88287600	-0.96618000
H	4.47395500	-3.08107100	-2.63500000
H	5.57039700	-0.52047400	0.68222000
H	6.04940100	-2.46674800	-0.82391700
O	3.31169400	0.97240300	0.39284800
H	1.42020800	1.02667500	-2.18746000
N	2.18464500	1.48984800	-0.27832200
C	1.39219400	2.27741100	0.53839000
O	1.64872200	2.57071100	1.67564300
O	0.33949700	2.66673100	-0.18464200
C	-0.83543000	3.25749400	0.43171700
C	-0.48671000	4.62378900	1.01732000
H	-1.40278100	5.11561400	1.37699300
H	0.21631000	4.52281200	1.85298300
H	-0.03140200	5.26324600	0.24656100
C	-1.40479700	2.30485900	1.48098800
H	-0.70505700	2.17215700	2.31638300
H	-2.34670300	2.71307800	1.87611000
H	-1.61152500	1.32218900	1.03226300

C	-1.80056600	3.39632800	-0.74072700
H	-1.37270400	4.04266200	-1.52068200
H	-2.00383100	2.40816500	-1.17783400
H	-2.74984300	3.83586600	-0.40187100
H	-3.75352700	-1.94298900	0.17703500

H1:

Eel = -1765.416201
Zero-point correction = 0.556807
Thermal correction to Energy = 0.588502
Thermal correction to Enthalpy = 0.589447
Thermal correction to Gibbs Free Energy = 0.495941

C	2.58142400	-0.72687500	1.07246000
C	1.27228300	-0.79632400	1.39713300
C	0.30670000	0.23492300	1.05678500
C	0.76746000	1.32597900	0.21661700
C	2.05565500	1.46835900	-0.16443700
C	3.06268500	0.46238200	0.30200000
H	0.88573900	-1.64132700	1.96846600
H	0.01307100	2.02577700	-0.13779000
C	3.59048200	-1.80941100	1.47468900
C	2.90921000	-2.95735200	2.23240700
H	2.13213000	-3.44895100	1.62593100
H	3.65902200	-3.72076200	2.48827500
H	2.45142900	-2.61823600	3.17455900
C	4.25251500	-2.40713900	0.21803000
H	4.77680800	-1.63911400	-0.36354100
H	4.98278700	-3.17793700	0.51061800
H	3.49924400	-2.88697500	-0.42617600
C	4.66351600	-1.20165800	2.39971600
H	5.23038700	-0.41460500	1.88884300
H	4.19950500	-0.77244600	3.30165300
H	5.36718800	-1.98556400	2.72196300
C	2.51933600	2.61863300	-1.06621300
C	1.34479600	3.51831000	-1.47568800
H	0.86287000	3.99314500	-0.60691700
H	1.71315100	4.32451800	-2.12742300
H	0.57552600	2.96564900	-2.03768300
C	3.15219000	2.05892600	-2.35488900
H	4.01908400	1.42439500	-2.13385000
H	2.41706100	1.46804300	-2.92341200
H	3.48547100	2.88778000	-2.99896300

C	3.54196800	3.48944500	-0.30928200
H	3.84946700	4.33885800	-0.93970300
H	3.09708500	3.89632700	0.61252500
H	4.43504700	2.91267100	-0.04198600
O	4.24853700	0.59435000	0.03005800
C	-0.96843600	0.11298600	1.51128500
H	-1.23086200	-0.82003900	2.01957200
C	-2.06861000	1.07759200	1.39970200
C	-1.87454100	2.45906700	1.56840800
C	-3.38577200	0.61139100	1.20340000
C	-2.94433100	3.34640700	1.51713900
H	-0.87287400	2.83302100	1.78668500
C	-4.45398200	1.50717500	1.14092300
C	-4.23741500	2.87243100	1.29923600
H	-2.76835600	4.41438700	1.66029300
H	-5.45554300	1.12002000	0.94642200
H	-5.07894900	3.56615800	1.25224700
N	-3.59891600	-0.79079600	1.05517600
H	-4.35859900	-1.17167100	1.61858800
S	-3.80320300	-1.41607600	-0.50993300
O	-4.56495200	-0.48121700	-1.32226800
O	-4.27659600	-2.76981800	-0.28392500
C	-2.14237300	-1.44404500	-1.12306100
C	-1.69815700	-0.40574500	-1.93700300
C	-1.30908300	-2.50700400	-0.78004300
C	-0.38727200	-0.43233400	-2.40176200
H	-2.37982800	0.40327700	-2.20391500
C	-0.00399600	-2.51633200	-1.25645400
H	-1.69067400	-3.31785800	-0.15704900
C	0.47810500	-1.48258100	-2.07216300
H	-0.02913500	0.37716400	-3.04245300
H	0.65651300	-3.34777500	-0.99855500
C	1.89595700	-1.49073900	-2.56687600
H	1.98395700	-0.99881300	-3.54547200
H	2.55105300	-0.94801500	-1.86716800
H	2.28709800	-2.51363300	-2.65516800

A2-I1TS:

Eel = -3061.466748
Zero-point correction = 0.832316
Thermal correction to Energy = 0.884090
Thermal correction to Enthalpy = 0.885035
Thermal correction to Gibbs Free Energy = 0.746796

C	-3.28772000	-1.75566400	-0.70483200
C	-2.02091600	-1.74412900	-1.20714400
C	-0.84872800	-1.75935600	-0.38332600
C	-1.03500100	-1.71863200	1.03517400
C	-2.26458500	-1.62738100	1.61427700
C	-3.47396900	-1.60588400	0.75461600
H	-1.85383600	-1.79135700	-2.28447000
H	-0.13892100	-1.73217600	1.65301500
C	-4.51692200	-1.96954600	-1.60306300
C	-4.11777700	-2.20105200	-3.06734400
H	-3.46741900	-3.08231200	-3.18301100
H	-5.02330200	-2.37368700	-3.67070100
H	-3.59729300	-1.32976100	-3.49453700
C	-5.27366800	-3.22218200	-1.11791900
H	-5.62082000	-3.08861100	-0.08554500
H	-6.14792200	-3.41430300	-1.76279200
H	-4.61968300	-4.10806600	-1.15657300
C	-5.45914700	-0.75506000	-1.56883700
H	-5.77678100	-0.54607700	-0.53979700
H	-4.95102600	0.13471300	-1.97008400
H	-6.35242600	-0.94978700	-2.18711800
C	-2.42396200	-1.54361600	3.13994600
C	-1.06862600	-1.63254600	3.85720400
H	-0.38234700	-0.82357200	3.56373800
H	-1.22557400	-1.55850400	4.94499400
H	-0.56187000	-2.59001700	3.65984200
C	-3.30147100	-2.70820300	3.63809400
H	-4.30207900	-2.66169600	3.19108800
H	-2.84237600	-3.67448700	3.37421000
H	-3.39971200	-2.66770600	4.73602000
C	-3.07169400	-0.20020200	3.52810800
H	-3.23161200	-0.15608500	4.61849200
H	-2.41237300	0.63928700	3.25528800
H	-4.04118100	-0.07789800	3.02844700
O	-4.60629300	-1.46565500	1.24360200
C	0.39034900	-1.90464200	-0.98609600
C	1.57686800	-2.55702600	-0.37819000
C	2.34100400	-2.07852300	0.70957800
C	1.88590700	-3.81725700	-0.90878800
C	3.28633500	-2.93257500	1.30275500
C	2.86058900	-4.63737600	-0.35239700
C	3.54297800	-4.19187200	0.77763800
H	3.84229800	-2.59113600	2.17464900

H	3.06972100	-5.61753400	-0.78527900
H	4.29590000	-4.82357300	1.25464300
H	0.36863100	-1.97701400	-2.07817300
N	1.10140800	0.25420000	-1.19521900
C	1.97040700	0.34790300	-2.23738700
O	1.81663900	0.81803800	-3.34561400
O	3.11750700	-0.23893600	-1.79652600
C	4.15275300	-0.68348000	-2.68497600
C	4.87402000	0.52707100	-3.28001500
H	5.70806600	0.19779500	-3.91930500
H	4.17564100	1.12918800	-3.87548500
H	5.28614300	1.15210400	-2.47289600
C	3.57211100	-1.58842200	-3.77345500
H	2.89944100	-1.02757200	-4.43471000
H	4.38805000	-2.02265700	-4.37155200
H	3.01269100	-2.41359000	-3.30602000
C	5.07945600	-1.48089600	-1.77043500
H	5.37457800	-0.87533400	-0.90182900
H	4.56050800	-2.37195900	-1.38657100
H	5.97782400	-1.80189800	-2.32028800
O	-0.12619900	0.86651700	-1.51263100
S	-0.39767900	2.15776900	-0.55702500
O	-0.05859200	1.81713200	0.81245100
O	0.17362700	3.34355800	-1.17571700
C	-2.15804400	2.25639000	-0.69306400
C	-2.93323100	1.63311000	0.28105300
C	-2.73554800	3.02920200	-1.69519300
C	-4.31106900	1.79658100	0.25446000
H	-2.45270500	1.02759900	1.04969100
C	-4.12096200	3.17403000	-1.71397600
H	-2.10094500	3.52063000	-2.43437800
C	-4.92428200	2.56908700	-0.74018400
H	-4.91679000	1.28408800	1.00527600
H	-4.58647000	3.77681000	-2.49823300
C	-6.42309000	2.69551700	-0.77545300
H	-6.87624200	1.73167700	-1.05816300
H	-6.82302800	2.96513200	0.21344500
H	-6.75202100	3.45319700	-1.50069500
H	1.31233600	-4.16888400	-1.77083000
N	2.14203000	-0.77423400	1.16456100
H	1.67748400	-0.16518400	0.44572800
S	3.35529000	-0.00012200	2.03382800
O	4.66421000	-0.26582600	1.44222000
O	3.17846700	-0.30580700	3.44834500

C	2.94157700	1.68842300	1.72747200
C	2.31409600	2.43262200	2.71609200
C	3.24364100	2.22903100	0.47822500
C	1.96232000	3.75053900	2.43618600
H	2.09329500	1.97075500	3.67937800
C	2.87270500	3.53767100	0.21483100
H	3.72586500	1.60931900	-0.28009600
C	2.21321800	4.31019400	1.18124900
H	1.44710700	4.34201500	3.19734800
H	3.05595300	3.95749100	-0.77619800
C	1.71534200	5.68253600	0.82314800
H	1.38505800	6.24387200	1.70881800
H	2.48690300	6.27077700	0.30375200
H	0.86089800	5.57537900	0.13599800

I1:

Eel = -3061.490432
Zero-point correction = 0.835146
Thermal correction to Energy = 0.886628
Thermal correction to Enthalpy = 0.887572
Thermal correction to Gibbs Free Energy = 0.751209

C	-3.45371600	-1.60890200	-0.62314400
C	-2.17967000	-1.60501200	-1.17121300
C	-1.01625000	-1.45806600	-0.40503400
C	-1.16635300	-1.35845200	0.98406500
C	-2.40565900	-1.32286300	1.60636700
C	-3.62432500	-1.39318300	0.80767700
H	-2.05439400	-1.73467800	-2.24917800
H	-0.26901600	-1.30977200	1.60041300
C	-4.69561600	-1.87230700	-1.49146200
C	-4.33803700	-2.16267400	-2.95582600
H	-3.68704000	-3.04618200	-3.05281200
H	-5.25951200	-2.36318900	-3.52700800
H	-3.83133200	-1.30915000	-3.43395600
C	-5.44523600	-3.09974500	-0.93749500
H	-5.73077800	-2.91883700	0.10687400
H	-6.35299400	-3.30262500	-1.53280500
H	-4.80087300	-3.99289000	-0.97860200
C	-5.63371600	-0.65209200	-1.47587800
H	-5.89503300	-0.40739900	-0.43737700
H	-5.13674900	0.21543100	-1.93870000
H	-6.55683400	-0.86327200	-2.04440900

C	-2.51665800	-1.20301900	3.13534400
C	-1.14293500	-1.17019000	3.82076500
H	-0.53436100	-0.30875600	3.50326100
H	-1.27773200	-1.09383600	4.91198500
H	-0.55904600	-2.08265900	3.62236600
C	-3.29485200	-2.41366600	3.68532900
H	-4.28742200	-2.46102900	3.21844700
H	-2.75321900	-3.34765000	3.46478900
H	-3.41217600	-2.33578100	4.78050200
C	-3.26229100	0.09352600	3.50801900
H	-3.37372300	0.17607300	4.60326700
H	-2.70247000	0.97857900	3.16213500
H	-4.25736700	0.09087500	3.04416700
O	-4.77259800	-1.27419400	1.32986900
C	0.33412000	-1.57260300	-1.07157100
C	1.29536700	-2.41118000	-0.23224400
C	2.16892500	-1.93225000	0.76648900
C	1.23618100	-3.78971400	-0.44780400
C	2.94931100	-2.84402800	1.49495800
C	2.01143300	-4.69330800	0.26903200
C	2.87675500	-4.20899300	1.24547000
H	3.61847300	-2.47825700	2.27224400
H	1.93537400	-5.76379000	0.06819900
H	3.49626000	-4.89222700	1.83071900
H	0.18763800	-2.13046900	-2.01114600
N	0.92055400	-0.25418900	-1.46661100
C	2.12814700	-0.12183000	-2.14977100
O	2.53766800	0.92064300	-2.59491000
O	2.73168400	-1.30148400	-2.20140000
C	4.12539000	-1.47049100	-2.56113200
C	5.01866100	-0.56251500	-1.72073800
H	6.07077100	-0.83433400	-1.89295900
H	4.88376000	0.48968600	-2.00220800
H	4.80910500	-0.68324100	-0.64724800
C	4.28423400	-1.20478800	-4.05665200
H	4.04197700	-0.15941900	-4.28908000
H	5.32152800	-1.40766600	-4.36328500
H	3.61669200	-1.86164700	-4.63439700
C	4.38455700	-2.93520300	-2.22355300
H	4.23148900	-3.11224400	-1.14902500
H	3.69261900	-3.58540700	-2.77829500
H	5.41719300	-3.20716500	-2.48786100
O	-0.00179300	0.67632100	-1.88191000
S	-0.12172600	2.02724800	-0.89557000

O	0.34817200	1.62271900	0.41918100
O	0.48717500	3.13852200	-1.59656700
C	-1.86290700	2.27149600	-0.88008200
C	-2.62155700	1.63431700	0.09571200
C	-2.43996500	3.13082900	-1.81385100
C	-3.99053800	1.86030700	0.13818900
H	-2.15302400	0.94808000	0.80152200
C	-3.81306800	3.34681700	-1.75392900
H	-1.81863500	3.62497800	-2.56192600
C	-4.60391700	2.71992800	-0.78099500
H	-4.58434700	1.31269900	0.87474100
H	-4.28142600	4.01634700	-2.48004900
C	-6.09233200	2.92943800	-0.72908400
H	-6.61256200	1.97138500	-0.88295300
H	-6.40082700	3.31068000	0.25628300
H	-6.43340000	3.63821400	-1.49690900
H	0.54681500	-4.15869700	-1.21162900
N	2.27633200	-0.55123600	1.01015700
H	1.49293900	0.06246200	0.76594200
S	3.34391300	0.13160500	2.09835800
O	4.69150500	-0.28558300	1.72168900
O	2.92538800	-0.08211600	3.47707700
C	3.08712900	1.82893200	1.67100900
C	2.38469900	2.64953700	2.54317400
C	3.48182200	2.27123700	0.40947100
C	2.05145000	3.93669200	2.12754600
H	2.07717300	2.26372700	3.51622300
C	3.12547000	3.54723700	0.00577800
H	4.01553600	1.60317800	-0.26562700
C	2.38916800	4.39073600	0.84992800
H	1.47767300	4.58352800	2.79601900
H	3.37537500	3.87547600	-1.00475400
C	1.91016200	5.72151700	0.34008900
H	1.49960600	6.34595900	1.14603100
H	2.71875200	6.27866000	-0.15648500
H	1.11844400	5.55110800	-0.40682500

I2:

Eel = -3061.495643
Zero-point correction = 0.836088
Thermal correction to Energy = 0.887825
Thermal correction to Enthalpy = 0.888769
Thermal correction to Gibbs Free Energy = 0.751464

C	2.00976900	-0.02477000	-1.02250300
C	0.72811000	-0.46623500	-0.68969600
C	0.33749200	-0.66394100	0.62859500
C	1.25847700	-0.41028200	1.64001000
C	2.54606700	0.06890500	1.38686100
C	2.89604200	0.27323800	0.03589700
H	-0.00875800	-0.62143700	-1.46885500
H	0.93117300	-0.55996800	2.66914300
C	2.38132300	0.20080500	-2.50444000
C	1.28817700	-0.34265200	-3.44019200
H	0.34212600	0.20394600	-3.31505400
H	1.61254100	-0.21245100	-4.48492500
H	1.11235300	-1.41638100	-3.27107600
C	2.48952800	1.71379500	-2.79415200
H	3.17989200	2.26268100	-2.13007500
H	2.82643200	1.88098000	-3.83007200
H	1.49926000	2.17700600	-2.67635500
C	3.68379900	-0.54210700	-2.87401000
H	4.57512200	-0.21254500	-2.32141600
H	3.56540100	-1.61798400	-2.68009000
H	3.89521100	-0.41093900	-3.94708100
C	3.50579000	0.42252000	2.54111000
C	2.92029200	0.02577300	3.90508800
H	2.71755200	-1.05519400	3.96544100
H	3.64256900	0.27407600	4.69859500
H	1.98644900	0.56280200	4.12766400
C	3.73937600	1.94514300	2.56402300
H	4.18614800	2.28944600	1.62229100
H	2.78597400	2.47428700	2.71498900
H	4.41691300	2.21874300	3.39003300
C	4.85602900	-0.30569200	2.39782000
H	5.52295600	-0.02978300	3.23127500
H	4.71791400	-1.39699600	2.43113800
H	5.35680000	-0.05099400	1.45662100
O	4.13719800	0.79952600	-0.21336000
C	-1.08311200	-1.03894500	1.05203000
C	-1.76416900	0.20544300	1.60028500
C	-2.05688600	0.25961700	2.95852500
C	-1.99411100	1.33822200	0.76877100
C	-2.56156200	1.41632400	3.55595800
H	-1.88496100	-0.63303300	3.56822600
C	-2.51476400	2.49935200	1.38879600
C	-2.78021700	2.53449900	2.75449100

H	-2.78223800	1.43763300	4.62540600
H	-2.73501200	3.36894200	0.76924900
H	-3.18154500	3.45279600	3.19304500
H	-0.98874300	-1.73984700	1.89990000
N	-1.82241000	-1.75232000	-0.00049000
C	-3.16832400	-1.76672000	-0.33217300
O	-3.59984800	-2.39825100	-1.26373800
O	-3.86897700	-1.04348600	0.52843600
C	-5.19555200	-0.55166200	0.20608700
C	-6.17352500	-1.72346700	0.11296500
H	-7.19733900	-1.33779000	-0.01087100
H	-5.92552000	-2.37204400	-0.73577800
H	-6.13814000	-2.32110300	1.03678500
C	-5.14716400	0.26496200	-1.08325100
H	-4.89720700	-0.37345200	-1.94087600
H	-6.13286400	0.72092600	-1.26196000
H	-4.39826600	1.06740200	-1.01803800
C	-5.53160200	0.33563700	1.39958100
H	-5.50181300	-0.24768800	2.33177800
H	-4.80546000	1.15518400	1.48366600
H	-6.53919500	0.76103600	1.27834100
N	-1.68465700	1.19689100	-0.55570600
S	-1.64563700	2.41202200	-1.56450800
O	-1.07113700	1.94157200	-2.83244500
O	-2.89954900	3.18169700	-1.67914400
C	-0.43678600	3.59764700	-0.92261300
C	-0.55170600	4.93587500	-1.29261800
C	0.64841800	3.17387100	-0.16073700
C	0.43230400	5.84525500	-0.91375500
H	-1.42150200	5.24789500	-1.87427800
C	1.62672300	4.09212900	0.21359500
H	0.72748100	2.12645700	0.13598100
C	1.53837000	5.43801500	-0.15761800
H	0.34016600	6.89417400	-1.21180200
H	2.47860700	3.74887800	0.80481400
C	2.58599600	6.43087500	0.27757700
H	2.28802000	6.93448500	1.21232100
H	3.55209800	5.93916200	0.46392400
H	2.74018700	7.21301000	-0.48102900
O	-1.08536700	-2.59583000	-0.77775100
S	-0.82779100	-4.14861100	-0.19946600
O	-1.37502600	-4.23049800	1.14047900
O	-1.21870200	-5.06195900	-1.24738700
C	0.93656000	-4.05083400	-0.15642400

C	1.57043000	-3.65473600	1.01595100
C	1.64138800	-4.19936800	-1.34811600
C	2.92792100	-3.36461400	0.97993600
H	0.99424800	-3.54338900	1.93557500
C	2.99951200	-3.90248400	-1.36412100
H	1.11955500	-4.51981500	-2.25116200
C	3.65383700	-3.44456300	-0.21355700
H	3.42297800	-3.02337500	1.89086800
H	3.55727200	-3.99970500	-2.29888700
C	5.08060000	-2.97354500	-0.26669700
H	5.09738400	-1.87214200	-0.31622200
H	5.64066200	-3.27032000	0.63213100
H	5.60523700	-3.36087900	-1.15152700
H	4.14038400	1.17085200	-1.09921000

I2-J2TS:

Eel = -3061.456964
Zero-point correction = 0.832872
Thermal correction to Energy = 0.884786
Thermal correction to Enthalpy = 0.885730
Thermal correction to Gibbs Free Energy = 0.747002

C	3.46558300	-1.08578400	1.15231700
C	2.43673500	-0.15359500	1.28563200
C	1.34952800	-0.11801000	0.41827000
C	1.32067600	-0.99020700	-0.66062900
C	2.33916600	-1.92021000	-0.87964300
C	3.37609400	-1.99131000	0.07278600
H	2.45644600	0.55532000	2.11249700
H	0.47867900	-0.92264700	-1.34361400
C	4.60876400	-1.16448900	2.18136100
C	4.54204000	-0.00170700	3.18342300
H	3.62262700	-0.02716700	3.78755500
H	5.39546100	-0.06628100	3.87696000
H	4.59110000	0.97412900	2.67506400
C	4.48870800	-2.47934500	2.97609900
H	4.56127900	-3.34958100	2.31130400
H	5.29184800	-2.54784200	3.72937100
H	3.52123500	-2.52407500	3.49972500
C	5.98375600	-1.09090300	1.49084800
H	6.13766500	-1.93158600	0.80530700
H	6.07087200	-0.15924200	0.91548400
H	6.78800600	-1.10238400	2.24550300

C	2.28643500	-2.83910300	-2.11893600
C	1.14812300	-2.43121400	-3.06915500
H	1.23714400	-1.38066100	-3.38298700
H	1.18787500	-3.06656000	-3.96894800
H	0.15925900	-2.55685000	-2.60763100
C	2.00353900	-4.29450200	-1.68670600
H	2.76198100	-4.73774500	-1.01793400
H	1.04367500	-4.33694600	-1.15100800
H	1.93468400	-4.94956600	-2.57018400
C	3.59374300	-2.73345700	-2.93555100
H	3.54359700	-3.39766500	-3.81322700
H	3.71783300	-1.70380900	-3.30385800
H	4.50605000	-2.98496100	-2.37611100
O	4.34439100	-2.95662200	-0.00744400
C	0.19126700	0.83403100	0.69916800
C	-0.50229100	0.41998500	1.98260200
C	-1.48570400	-0.56790600	1.79687700
C	-0.19282100	0.89699100	3.24488500
C	-2.12057900	-1.11251600	2.92277900
C	-0.83971500	0.36718500	4.36756300
C	-1.78748600	-0.63956800	4.19412600
H	-2.85336400	-1.90862300	2.79941100
H	-0.59916300	0.73599500	5.36710700
H	-2.28957800	-1.06800900	5.06588300
H	0.56649100	1.85822700	0.82421500
N	-0.70185400	0.82011200	-0.47902300
C	-1.99666600	1.46680900	-0.43121300
O	-2.76885900	1.39146700	-1.34182800
O	-2.16287300	2.14895200	0.69253000
C	-3.44844000	2.66808200	1.10507700
C	-4.47323900	1.53672000	1.16720100
H	-5.41063700	1.91612800	1.60177000
H	-4.68780100	1.13284000	0.17004700
H	-4.09849200	0.72104600	1.80293600
C	-3.87871700	3.78819900	0.16061900
H	-4.06712800	3.39331600	-0.84540900
H	-4.79654600	4.26273800	0.54065900
H	-3.08940200	4.55152700	0.09391700
C	-3.15988000	3.20047200	2.50560400
H	-2.79963300	2.38588900	3.15165500
H	-2.38344500	3.97872500	2.46632900
H	-4.07188000	3.63210700	2.94459100
O	-0.08190300	2.42032100	-1.23407600
S	0.92661200	2.31032800	-2.40394900

O	0.82008200	1.06590700	-3.15114200
O	0.87782800	3.56829900	-3.13751700
C	2.50127400	2.29470000	-1.54802400
C	3.45573700	1.33050400	-1.84190300
C	2.77173000	3.29702100	-0.61611100
C	4.69671500	1.37572900	-1.20726900
H	3.21069500	0.54218900	-2.55482100
C	4.01058100	3.33108200	0.01137400
H	2.00987500	4.04733100	-0.39539300
C	4.99811300	2.37991000	-0.28292000
H	5.44255500	0.61056300	-1.43824900
H	4.22536000	4.12165900	0.73644200
C	6.34468000	2.45848000	0.38965200
H	7.07355600	1.78803400	-0.08714100
H	6.74681800	3.48261300	0.35002200
H	6.27741600	2.17281000	1.45186100
H	0.55472500	1.68719700	3.35835300
H	4.06372100	-3.62443600	-0.63625300
N	-1.73269100	-0.78210700	0.46114500
S	-2.36416300	-2.11159900	-0.19430200
O	-2.34000900	-3.23094000	0.74981000
O	-1.79719200	-2.29974700	-1.52407600
C	-4.09006900	-1.70431600	-0.45507700
C	-5.03466100	-2.03125900	0.51288600
C	-4.46308100	-1.01727900	-1.60886700
C	-6.35982100	-1.63615200	0.33925600
H	-4.72781600	-2.60248800	1.39079400
C	-5.78980400	-0.63284200	-1.77035200
H	-3.70614500	-0.76802700	-2.35259800
C	-6.75546900	-0.92406300	-0.79773300
H	-7.10106900	-1.88939600	1.10251500
H	-6.07896900	-0.08215600	-2.66965900
C	-8.17704900	-0.45353800	-0.96691900
H	-8.52549800	-0.59215500	-2.00147300
H	-8.86399500	-0.99295900	-0.29883300
H	-8.26205900	0.62089100	-0.73521300

J2:

Eel = -2166.591354
Zero-point correction = 0.703537
Thermal correction to Energy = 0.743971
Thermal correction to Enthalpy = 0.744915
Thermal correction to Gibbs Free Energy = 0.633129

C	-2.24834900	-1.78068300	-0.71051500
C	-0.96656000	-1.29688100	-0.97621100
C	-0.69515400	0.06540800	-1.07311200
C	-1.73654600	0.96608000	-0.88486100
C	-3.05312500	0.55698700	-0.66107600
C	-3.28924900	-0.83016000	-0.58060100
H	-0.13531000	-1.98321600	-1.13297100
H	-1.51745900	2.02893100	-0.93906500
C	-2.50660100	-3.30145900	-0.62606300
C	-1.19553400	-4.09826200	-0.72363400
H	-0.49529300	-3.82814200	0.08073900
H	-1.41309800	-5.17318800	-0.63290500
H	-0.68436000	-3.94328200	-1.68417400
C	-3.14776700	-3.69346700	0.72372300
H	-4.11911300	-3.22168200	0.92965400
H	-3.30129000	-4.78275800	0.76539900
H	-2.48332600	-3.41489800	1.55335100
C	-3.39165700	-3.75616000	-1.80781700
H	-4.38290300	-3.27736900	-1.84702200
H	-2.89552300	-3.52386100	-2.76152800
H	-3.56056500	-4.84344400	-1.76420200
C	-4.19684600	1.59026700	-0.59809500
C	-3.66200100	3.02848500	-0.68720600
H	-3.13892800	3.22290000	-1.63563900
H	-4.50516700	3.73302700	-0.62779200
H	-2.97364500	3.26481300	0.13903600
C	-4.99012000	1.48726600	0.71728200
H	-5.44485700	0.49872200	0.84762600
H	-4.33757600	1.68765500	1.57956000
H	-5.79551000	2.23867800	0.72671400
C	-5.13935600	1.36835000	-1.79798200
H	-5.94618600	2.11874900	-1.79108800
H	-4.58796600	1.47076500	-2.74553900
H	-5.59738000	0.37183300	-1.77029900
O	-4.57979000	-1.21675700	-0.37107300
C	0.69628800	0.51012900	-1.50799100
C	0.92732600	2.00095500	-1.55454700
C	0.36157800	2.97902600	-2.36390600
C	1.88733300	2.34842300	-0.60567400
C	0.74392100	4.30880200	-2.17840600
H	-0.37743100	2.71158500	-3.12224400
C	2.28635500	3.66730500	-0.40921300
C	1.68782000	4.64457500	-1.20416900

H	0.30608100	5.09059400	-2.80194600
H	3.03437500	3.91228400	0.34252500
H	1.97895000	5.68864000	-1.07185000
H	0.88653800	0.04977200	-2.49016100
N	1.82006300	0.08462800	-0.63809900
C	2.64363000	-0.95157100	-1.07181700
O	2.19543100	-1.85649800	-1.74169500
O	3.87776900	-0.80601900	-0.64807200
C	4.80841900	-1.91970800	-0.53949400
C	5.19559300	-2.41266300	-1.93079300
H	5.98249300	-3.17669000	-1.84416000
H	4.33146300	-2.84680100	-2.44885500
H	5.58944000	-1.58064200	-2.53314700
C	4.17732600	-3.01771200	0.31352000
H	3.31268900	-3.46722400	-0.19280900
H	4.91819000	-3.80815800	0.50230000
H	3.85817400	-2.59733800	1.27834400
C	5.99489100	-1.29123100	0.18153700
H	6.42541400	-0.48073300	-0.42416200
H	5.66414800	-0.86993500	1.14081600
H	6.77332700	-2.04654400	0.36215900
H	-4.65668900	-2.16823100	-0.46075400
N	2.38704700	1.18340400	0.02592700
S	2.36933200	1.04634300	1.74351000
O	3.22374600	-0.07821100	2.06733400
O	2.65638800	2.38275200	2.22892700
C	0.71055100	0.59075200	2.15073800
C	-0.26205200	1.57406500	2.31627700
C	0.40727500	-0.76152600	2.28992500
C	-1.56290200	1.18390200	2.61802900
H	0.00369600	2.62856800	2.22263900
C	-0.89501100	-1.12761700	2.59607400
H	1.19171800	-1.50924200	2.17071400
C	-1.90189700	-0.16833600	2.75729700
H	-2.33039500	1.94882200	2.75725200
H	-1.13473500	-2.18566800	2.72134200
C	-3.31129500	-0.59882800	3.05324300
H	-3.83735000	-0.84031900	2.11628800
H	-3.32792800	-1.49694200	3.68723000
H	-3.88187000	0.19304600	3.55751800

I2-J1TS:

Eel = -3061.440277

Zero-point correction = 0.832936
Thermal correction to Energy = 0.884641
Thermal correction to Enthalpy = 0.885585
Thermal correction to Gibbs Free Energy = 0.750214

C	-2.05935400	2.03805400	-1.30065300
C	-0.71017200	1.68286200	-1.23010300
C	-0.26567400	0.40509500	-1.56907900
C	-1.20077000	-0.51435600	-2.03986800
C	-2.56828100	-0.24213500	-2.09352600
C	-2.98404600	1.03975700	-1.67591900
H	0.04334200	2.38943500	-0.88594000
H	-0.84385900	-1.50243000	-2.31573200
C	-2.50857700	3.47015900	-0.95066200
C	-1.30581700	4.40546600	-0.76221700
H	-0.68007100	4.44755000	-1.66637700
H	-1.66827400	5.42535500	-0.55823800
H	-0.64273300	4.12803900	0.06661500
C	-3.36064900	4.06527100	-2.09041200
H	-4.28247200	3.49809300	-2.26319400
H	-3.63223100	5.10549200	-1.84671500
H	-2.78187100	4.08130400	-3.02751200
C	-3.31300000	3.45252700	0.36281000
H	-4.21470500	2.83066900	0.27343200
H	-2.69040200	3.05853900	1.18192900
H	-3.62283300	4.47420000	0.63757600
C	-3.56303300	-1.32043100	-2.57525800
C	-2.83406700	-2.60075300	-3.01426900
H	-2.24920200	-3.03897700	-2.19266000
H	-3.57478200	-3.34524800	-3.34684200
H	-2.15312200	-2.40940500	-3.85716100
C	-4.35499800	-0.81236200	-3.79970400
H	-4.93394300	0.10277100	-3.60769000
H	-3.66289300	-0.58121200	-4.62340000
H	-5.05774600	-1.58621500	-4.14925100
C	-4.51320500	-1.75022100	-1.43531900
H	-5.22651800	-2.50640500	-1.80095700
H	-3.93448000	-2.19240900	-0.61272400
H	-5.10711400	-0.93855400	-0.98521300
O	-4.30919100	1.36517900	-1.61476000
C	1.15805600	-0.10137800	-1.46517600
C	2.42264800	0.68502400	-1.80248400
C	2.84786500	1.88715500	-1.11610500
C	3.31926300	0.03442800	-2.69261200

C	4.21446500	2.28450700	-1.32223000
C	4.59785100	0.48713500	-2.90847900
C	5.04488400	1.61672000	-2.18474000
H	4.56582700	3.15188400	-0.76564600
H	5.25732700	-0.02090900	-3.61505100
H	6.07023300	1.97315700	-2.31886800
H	1.19460800	-1.02852900	-2.05466800
N	1.68771000	-0.31607700	-0.13894200
C	2.78561100	-1.25413100	-0.00547700
O	3.70154300	-1.03522800	0.73373700
O	2.60000300	-2.33156000	-0.74485200
C	3.44255700	-3.51101800	-0.64847900
C	3.47534800	-4.01328300	0.79388300
H	3.95862600	-5.00172000	0.82005200
H	4.03802400	-3.32822300	1.44007600
H	2.45153300	-4.10631200	1.18520700
C	4.83368600	-3.17890800	-1.18165800
H	5.32104800	-2.42258500	-0.55268900
H	5.45226000	-4.08932500	-1.18963600
H	4.76989200	-2.78946400	-2.20855100
C	2.71316700	-4.50482600	-1.54595600
H	1.67943200	-4.62537400	-1.19255000
H	2.67986800	-4.13383600	-2.58132200
H	3.22714500	-5.47736700	-1.53565800
O	0.60038100	-1.24760400	0.94174900
S	-0.22816200	-2.54299000	0.78443900
O	-0.31992900	-3.01600900	-0.59778000
O	0.18930700	-3.54331200	1.76946500
C	-1.83649400	-1.96551500	1.31115300
C	-2.18194000	-0.62203800	1.20322000
C	-2.73673000	-2.89377000	1.83223800
C	-3.45226200	-0.21366600	1.59934200
H	-1.45679500	0.10075000	0.82734100
C	-4.00347700	-2.46980800	2.22334400
H	-2.43314600	-3.93631400	1.94366000
C	-4.38273200	-1.12603200	2.10634000
H	-3.71856700	0.84123200	1.50141100
H	-4.71018100	-3.19672500	2.63322900
C	-5.77112500	-0.67804400	2.48061500
H	-5.77403900	0.36119500	2.83946300
H	-6.44213000	-0.72478600	1.60658700
H	-6.20584000	-1.31603800	3.26391800
H	2.96920800	-0.86390900	-3.20774600
H	-4.83451800	0.57623800	-1.75677300

N	1.98370600	2.58852300	-0.37709300
S	2.30342000	3.37282400	0.99099400
O	1.49035000	4.58905800	1.03080300
O	3.73066000	3.49782000	1.31623300
C	1.59153200	2.23477500	2.17517400
C	0.24205200	2.33278600	2.49924500
C	2.35705300	1.17019700	2.64480800
C	-0.35332500	1.33019600	3.26197600
H	-0.33432000	3.18668300	2.13807300
C	1.74938500	0.17771500	3.40261800
H	3.40825700	1.09582200	2.36488000
C	0.38190600	0.22411600	3.69939300
H	-1.42053000	1.39160700	3.49414200
H	2.33879700	-0.68614800	3.72040800
C	-0.27838300	-0.92904700	4.40693300
H	0.17925100	-1.11776500	5.39139500
H	-1.35391400	-0.75123400	4.55380100
H	-0.16579400	-1.84714400	3.80787200

J1:

Eel = -2166.550831
Zero-point correction = 0.701165
Thermal correction to Energy = 0.742552
Thermal correction to Enthalpy = 0.743496
Thermal correction to Gibbs Free Energy = 0.627927

C	1.46896800	-1.81741800	-1.27210700
C	0.20297000	-1.47100100	-0.79757500
C	-0.07653500	-1.41874000	0.56420800
C	0.92040200	-1.75349500	1.48102100
C	2.20249400	-2.12152200	1.08069300
C	2.46489400	-2.11781300	-0.31188100
H	-0.59785500	-1.21503700	-1.48533100
H	0.67034000	-1.73454900	2.54180300
C	1.75293700	-1.84730800	-2.78958400
C	0.48869400	-1.52273700	-3.60163100
H	0.11363200	-0.51406100	-3.37867400
H	0.73312700	-1.55533400	-4.67417900
H	-0.31078700	-2.25711500	-3.42123300
C	2.79548100	-0.76935200	-3.16534600
H	3.74020800	-0.82424600	-2.60114800
H	3.04762100	-0.84713300	-4.23433900
H	2.37179100	0.23051300	-2.99288600

C	2.20778300	-3.25848300	-3.22524800
H	3.13722200	-3.61484500	-2.75561100
H	1.43017700	-3.99771700	-2.98110300
H	2.36846400	-3.28008500	-4.31404200
C	3.26620800	-2.56080800	2.10663200
C	2.71148200	-2.54026300	3.53928800
H	1.85992900	-3.22652600	3.66350600
H	3.49885300	-2.86413900	4.23650100
H	2.39537700	-1.53188800	3.84785200
C	4.48302100	-1.61664200	2.07788900
H	4.92956800	-1.55639600	1.07780300
H	4.18833500	-0.60510300	2.39799200
H	5.25479600	-1.97569900	2.77716700
C	3.70531900	-4.00835500	1.80698800
H	4.43025400	-4.34620300	2.56461500
H	2.83931500	-4.68752300	1.84000500
H	4.17479300	-4.09562200	0.82019900
O	3.73269000	-2.42142600	-0.68609600
C	-1.42322300	-1.07140700	1.06888800
C	-2.05136300	0.39738900	1.04504800
C	-2.83932400	0.68398100	2.25514400
C	-1.28383900	1.52135900	0.42227000
C	-2.71538600	1.85173600	2.91067600
H	-3.49562600	-0.10667900	2.62801100
C	-1.15417500	2.73063200	1.22767100
C	-1.83550200	2.87533200	2.38832600
H	-3.27334700	2.03968400	3.82909800
H	-0.56316800	3.55612300	0.83712700
H	-1.74177600	3.81318800	2.94135500
H	-1.72302800	-1.61562300	1.97507200
N	-2.45896700	-0.68883800	0.19849800
C	-3.73426600	-1.24970500	0.18639200
O	-3.93404200	-2.42766600	0.33702100
O	-4.62858800	-0.29868900	-0.04086100
C	-6.05448700	-0.57795800	-0.12996500
C	-6.55133100	-1.14675900	1.19765200
H	-7.64542000	-1.25338400	1.16551600
H	-6.10921700	-2.13068100	1.39830300
H	-6.30047200	-0.46292100	2.02296400
C	-6.32674000	-1.52037200	-1.29971300
H	-5.89242500	-2.51168000	-1.12071700
H	-7.41254500	-1.62982300	-1.43663300
H	-5.90308500	-1.10719300	-2.22684800
C	-6.65428700	0.79940800	-0.38859100

H	-6.40881000	1.48650100	0.43399200
H	-6.25667500	1.22274100	-1.32177600
H	-7.74803200	0.72637200	-0.47233800
N	-0.80048600	1.31232200	-0.75645500
S	0.11021200	2.44492100	-1.58564900
O	0.46892600	1.79569700	-2.83586500
O	-0.56984400	3.73527300	-1.62018300
C	1.60295100	2.63097600	-0.62410000
C	2.05175900	3.91047500	-0.31278900
C	2.33886000	1.50403800	-0.26378700
C	3.25550000	4.05787700	0.37403600
H	1.45718500	4.77695600	-0.60910600
C	3.53855500	1.66875900	0.41559600
H	1.97592400	0.50524300	-0.50800400
C	4.01798700	2.94466200	0.74416600
H	3.60952900	5.06144600	0.62322700
H	4.11299400	0.78331600	0.69394100
C	5.33512000	3.10293000	1.45566600
H	5.47315300	2.32287200	2.21841100
H	6.17151400	3.01574000	0.74362900
H	5.41607800	4.08351100	1.94494600
H	3.81616800	-2.36211800	-1.64070100

J1-K1TS:

Eel = -2166.547480
Zero-point correction = 0.700839
Thermal correction to Energy = 0.741400
Thermal correction to Enthalpy = 0.742345
Thermal correction to Gibbs Free Energy = 0.630305

C	1.35298600	-1.85965900	-0.91112200
C	0.23216800	-1.69482100	-0.10983000
C	0.34545100	-1.49166800	1.27980400
C	1.63317500	-1.45830800	1.86190200
C	2.78944700	-1.56647100	1.11534700
C	2.62345000	-1.73449900	-0.29092500
H	-0.75488900	-1.75454700	-0.54942800
H	1.69654500	-1.32199600	2.94105500
C	1.20645600	-2.15476500	-2.41881400
C	-0.26954400	-2.35525200	-2.79778600
H	-0.85124000	-1.43863000	-2.63382400
H	-0.33416400	-2.60212000	-3.86795000
H	-0.72598200	-3.18284800	-2.23380900

C	1.72101200	-0.96171600	-3.25508000
H	2.77298200	-0.68220900	-3.07539000
H	1.63075700	-1.19189800	-4.32767000
H	1.10725000	-0.07411500	-3.04529700
C	1.93607400	-3.46840100	-2.78163300
H	3.02273100	-3.46534000	-2.60809100
H	1.52322200	-4.30445900	-2.19742300
H	1.78229900	-3.69237000	-3.84793100
C	4.18357600	-1.51576800	1.76817900
C	4.08002600	-1.39445300	3.29610700
H	3.55306000	-2.25066300	3.74462600
H	5.09244000	-1.37110900	3.72565800
H	3.57280700	-0.46822000	3.60691300
C	4.96670900	-0.28878500	1.26264200
H	5.08757000	-0.29888800	0.17244400
H	4.45009300	0.63950100	1.55244200
H	5.96940000	-0.26977000	1.71766000
C	4.95633900	-2.81444900	1.46274800
H	5.93270800	-2.79613500	1.97172700
H	4.40008500	-3.69046100	1.83086600
H	5.13497600	-2.94486400	0.38917400
O	3.74891200	-1.77295100	-1.01794300
C	-0.75525800	-1.32016900	2.16419800
C	-1.97882800	0.22510000	2.22983300
C	-2.32844700	0.63756900	3.54494700
C	-1.60970900	1.18221200	1.21290600
C	-2.22921700	1.95147900	3.91009700
H	-2.66138300	-0.12951900	4.24754000
C	-1.52188700	2.54984900	1.65034300
C	-1.81421000	2.90432700	2.94030400
H	-2.48230400	2.27076300	4.92204700
H	-1.25762400	3.31901400	0.92708400
H	-1.74430300	3.95686200	3.22553800
H	-0.52346800	-1.37337500	3.23328800
N	-2.09361400	-1.15589500	1.88560800
C	-2.85746300	-1.68923600	0.84287900
O	-2.63053900	-2.77158300	0.36337800
O	-3.83866000	-0.86026400	0.56681000
C	-4.68782800	-0.99691700	-0.61392000
C	-5.69867700	-2.10739300	-0.34828000
H	-6.39754200	-2.18541400	-1.19408800
H	-5.18751900	-3.07254600	-0.22770500
H	-6.27842500	-1.89315600	0.56180300
C	-3.85450400	-1.26382900	-1.86481100

H	-3.41519700	-2.26846100	-1.85407100
H	-4.50776800	-1.17638900	-2.74529800
H	-3.04967400	-0.52232300	-1.96243800
C	-5.34672500	0.37474300	-0.70253800
H	-5.88407100	0.60616700	0.22856700
H	-4.58269300	1.14800900	-0.87157700
H	-6.06242700	0.39628900	-1.53691000
N	-1.41030800	0.71286400	-0.01549900
S	-1.18083600	1.68653900	-1.29712100
O	-1.02960800	0.80446400	-2.45429900
O	-2.19176200	2.74241900	-1.37392700
C	0.40179700	2.49489100	-1.06863700
C	0.53033200	3.83797600	-1.41381400
C	1.50188000	1.76834700	-0.62170700
C	1.77619200	4.45112400	-1.31271000
H	-0.34937400	4.38961100	-1.75096700
C	2.74159300	2.39295800	-0.52964200
H	1.38655400	0.72132500	-0.34094600
C	2.90111000	3.74021000	-0.87609800
H	1.87651100	5.50653600	-1.57973300
H	3.60213400	1.81833100	-0.18030800
C	4.24915900	4.40704600	-0.80066300
H	4.95100600	3.82939300	-0.18312700
H	4.69127600	4.50513700	-1.80517300
H	4.17186900	5.41939600	-0.37768800
H	3.53604700	-1.81223700	-1.95594000

K1:

Eel = -2166.565824
Zero-point correction = 0.701187
Thermal correction to Energy = 0.742406
Thermal correction to Enthalpy = 0.743350
Thermal correction to Gibbs Free Energy = 0.629271

C	3.36446200	0.16017800	1.15846700
C	2.10117700	0.68031700	1.37996400
C	0.92636200	-0.00942800	1.01655800
C	1.04119200	-1.22903700	0.32905700
C	2.27180100	-1.77479400	0.01932700
C	3.42764700	-1.08449100	0.47412000
H	1.99624400	1.65356500	1.85830100
H	0.13826400	-1.69641800	-0.03952500
C	4.63624400	0.89915500	1.61379500

C	4.29012800	2.22707500	2.30376600
H	3.68023700	2.07912000	3.20821500
H	5.21938800	2.72680900	2.61415400
H	3.75609000	2.91668900	1.63213700
C	5.40676700	0.03644500	2.63263300
H	5.73388900	-0.91597900	2.19872600
H	6.30060100	0.57758700	2.98046300
H	4.77898600	-0.17944100	3.51101500
C	5.52878600	1.22832000	0.40123600
H	5.88484400	0.32429900	-0.10590400
H	4.97736500	1.84045800	-0.32720700
H	6.40822200	1.80397100	0.72964700
C	2.35188500	-3.06234500	-0.82767000
C	0.94520200	-3.56283200	-1.19735300
H	0.36627700	-2.81596800	-1.76039900
H	1.03484600	-4.46309200	-1.82301900
H	0.36311200	-3.83236500	-0.30375500
C	3.03208900	-4.20433900	-0.03976700
H	4.08799000	-4.03449000	0.22696500
H	2.49507200	-4.38845800	0.90227100
H	3.00895700	-5.13108200	-0.63261200
C	3.09057300	-2.77793900	-2.15376600
H	3.13913700	-3.69280400	-2.76344900
H	2.54787900	-2.01649500	-2.73301200
H	4.12147800	-2.41177300	-2.03153700
O	4.65325500	-1.57843000	0.24926600
C	-0.30136600	0.69258000	1.19688200
H	-0.20624100	1.77313600	1.34787700
N	-1.55825000	0.30937800	1.15693300
C	-2.58315300	1.33549800	1.12080300
C	-2.91827900	1.93363500	2.33878900
C	-3.23336100	1.65168000	-0.10135500
C	-3.91109700	2.89685200	2.40866200
C	-4.25646600	2.63438400	0.02599100
C	-4.58395700	3.23481600	1.22682900
H	-4.16464200	3.36684200	3.35978800
H	-4.77918300	2.89770300	-0.89491300
H	-5.37894400	3.98423400	1.24817500
C	-2.01761100	-1.08046800	1.22928800
O	-1.32508100	-1.95404700	1.66437200
O	-3.26237000	-1.10731300	0.87779000
C	-4.03069200	-2.33654600	0.65260700
C	-4.36293500	-2.94208700	2.01108000
H	-5.00921800	-3.82103200	1.87204600

H	-3.44891400	-3.26163300	2.53056200
H	-4.89813400	-2.21487000	2.63911000
C	-5.26496400	-1.80266800	-0.06244300
H	-5.79918700	-1.08365900	0.57505900
H	-4.96279400	-1.28526000	-0.98425200
H	-5.94447800	-2.62944700	-0.31346400
C	-3.25146600	-3.29511100	-0.24146000
H	-3.92250600	-4.11034300	-0.54865300
H	-2.88492300	-2.76500800	-1.13072800
H	-2.39307700	-3.72973300	0.28674300
H	-2.38373200	1.61751100	3.23878900
H	4.59529900	-2.42793000	-0.19768000
N	-3.03806100	1.16835800	-1.35721700
S	-1.86403900	0.35429300	-2.01350000
O	-2.12767300	0.18475900	-3.43321500
O	-1.46972200	-0.90590300	-1.31887000
C	-0.38170600	1.37845800	-1.87105800
C	-0.44754100	2.71212000	-1.47601100
C	0.85187700	0.80584300	-2.18102600
C	0.72600900	3.45713900	-1.36130600
H	-1.41676100	3.16772700	-1.26562000
C	2.01580400	1.55821000	-2.07133600
H	0.89082900	-0.23782100	-2.49839100
C	1.97327300	2.89690900	-1.65722800
H	0.66550600	4.50507900	-1.05464600
H	2.97850000	1.09958900	-2.31427100
C	3.22888400	3.71992200	-1.53694500
H	3.07548400	4.73859700	-1.92193000
H	3.54436500	3.81398300	-0.48523400
H	4.06198800	3.26812900	-2.09338900

L1:

Eel = -2166.107068
Zero-point correction = 0.687195
Thermal correction to Energy = 0.728177
Thermal correction to Enthalpy = 0.729121
Thermal correction to Gibbs Free Energy = 0.615090

C	3.42965000	-0.20433400	-1.15102400
C	2.19264600	-0.71015600	-1.38500700
C	0.97549400	-0.03234700	-1.00565800
C	1.10159800	1.20064700	-0.27293800
C	2.30279500	1.74639100	0.03805100

C	3.54893600	1.09030300	-0.42628000
H	2.07670400	-1.66779000	-1.89671900
H	0.18560200	1.64315900	0.10122600
C	4.71176800	-0.91465600	-1.60739900
C	4.40658800	-2.24307200	-2.31310100
H	3.79693000	-2.09870900	-3.21882700
H	5.34998500	-2.72084100	-2.62092500
H	3.87762900	-2.94911200	-1.65380600
C	5.47010500	-0.01723600	-2.60533900
H	5.74462600	0.93596700	-2.13747600
H	6.38933700	-0.52120000	-2.94868300
H	4.84525500	0.19138100	-3.48846200
C	5.61305100	-1.22061300	-0.39538300
H	5.90542700	-0.29453000	0.11332000
H	5.08603200	-1.86459900	0.32464400
H	6.52384000	-1.74997600	-0.72238300
C	2.39829800	3.01476400	0.89687500
C	1.00560100	3.53426100	1.28421800
H	0.41889900	2.79778200	1.85428400
H	1.11395100	4.43664700	1.90687900
H	0.41383800	3.80567000	0.39650800
C	3.11963900	4.12964000	0.11490100
H	4.13900800	3.82586700	-0.15305800
H	2.56750900	4.36682600	-0.80849400
H	3.16981400	5.04731400	0.72495900
C	3.17009100	2.69936300	2.19290500
H	3.23848900	3.60063500	2.82461300
H	2.64702200	1.92281400	2.77395800
H	4.18643200	2.34961000	1.97065800
O	4.65685300	1.58483400	-0.19841000
C	-0.20510200	-0.67405900	-1.27612400
H	-0.13211300	-1.70681000	-1.63187300
N	-1.51069300	-0.27897700	-1.13451300
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C	-2.78796700	-1.95322000	-2.32328100
C	-3.23976200	-1.62616900	0.07618300
C	-3.75855300	-2.93829200	-2.43558000
C	-4.24340200	-2.62545500	-0.08888800
C	-4.49521900	-3.26199100	-1.29016600
H	-3.94722900	-3.42998500	-3.39185500
H	-4.81361700	-2.87389400	0.80824700
H	-5.27724700	-4.02519500	-1.33802800
C	-1.94875800	1.05891300	-1.25171700
O	-1.25813200	1.96840400	-1.63238100

O	-3.23603500	1.11036300	-0.97584600
C	-3.96859200	2.34739800	-0.80737700
C	-4.20298400	2.96893700	-2.18249200
H	-4.83062800	3.86798400	-2.08485800
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H	-4.71610500	2.25509700	-2.84466600
C	-5.26806400	1.85719200	-0.17533100
H	-5.77536400	1.14637500	-0.84419400
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H	-5.94180000	2.70299400	0.02755900
C	-3.24124100	3.30130500	0.13838100
H	-3.92338000	4.12165600	0.40958200
H	-2.92869000	2.75983400	1.04182400
H	-2.34554800	3.72450500	-0.33281700
H	-2.21063000	-1.64483700	-3.19979000
N	-3.13746600	-1.12252000	1.33552300
S	-1.98967700	-0.32081300	2.06144700
O	-2.31448600	-0.24062000	3.48222900
O	-1.59711700	0.97773600	1.45811600
C	-0.49682200	-1.32874200	1.92972800
C	-0.55693700	-2.67694400	1.58918400
C	0.73542800	-0.73107800	2.18734100
C	0.62198400	-3.41161100	1.47206000
H	-1.52531100	-3.14605200	1.40782900
C	1.90611900	-1.47202600	2.07185400
H	0.77247600	0.32758200	2.44791400
C	1.86907400	-2.82275000	1.70430700
H	0.56874300	-4.46841100	1.19391900
H	2.86902400	-0.98416400	2.24838500
C	3.13737500	-3.61549100	1.52906200
H	2.99335800	-4.67265200	1.79767200
H	3.47436900	-3.58373100	0.48009100
H	3.95396300	-3.21145200	2.14475400

L1-M1TS:

Eel = -2166.104568
Zero-point correction = 0.687631
Thermal correction to Energy = 0.727808
Thermal correction to Enthalpy = 0.728752
Thermal correction to Gibbs Free Energy = 0.615752

C	2.33146200	-2.16601300	-0.69493300
C	1.05058400	-1.89162800	-1.08870000

C	0.08151000	-1.31063900	-0.22059500
C	0.46872700	-1.03483100	1.12256300
C	1.73243400	-1.25970900	1.58736000
C	2.75172800	-1.81997400	0.67711200
H	0.73269600	-2.08857400	-2.11383600
H	-0.28366500	-0.60618100	1.78159500
C	3.36402000	-2.77171700	-1.65680200
C	2.75740700	-3.06004300	-3.03707300
H	2.39062100	-2.14392400	-3.52588000
H	3.52722600	-3.50043400	-3.69093400
H	1.92241200	-3.77609100	-2.97781600
C	4.53199600	-1.78544000	-1.85761800
H	5.02395900	-1.57502300	-0.89984700
H	5.27509000	-2.20929300	-2.55441600
H	4.16856200	-0.83804100	-2.28704200
C	3.89575700	-4.09862700	-1.08260300
H	4.35984100	-3.93312500	-0.10224900
H	3.07423600	-4.82394600	-0.96639700
H	4.64545500	-4.53822700	-1.76263200
C	2.12931500	-0.90949300	3.02886000
C	0.93924700	-0.36617900	3.83326300
H	0.12287400	-1.10225000	3.90712900
H	1.26781000	-0.13027600	4.85825500
H	0.52708700	0.55610400	3.39490400
C	3.21724600	0.18215400	3.01205600
H	4.09931700	-0.16453900	2.45810000
H	2.83146600	1.09452500	2.53013200
H	3.52014200	0.43725300	4.04213200
C	2.65620300	-2.16450300	3.75042000
H	2.94418700	-1.91771600	4.78669300
H	1.87522000	-2.94115200	3.79020700
H	3.52925200	-2.57127200	3.22540000
O	3.92642500	-1.98736600	1.05367700
C	-1.16440700	-0.96072400	-0.74490400
H	-1.41919200	-1.31289900	-1.74484200
N	-2.28712300	-0.67209000	0.06569200
C	-2.24380200	0.58758800	0.74137000
C	-2.73479400	0.83193300	2.01130700
C	-1.63486100	1.59434200	-0.04865100
C	-2.66302800	2.12667700	2.53304100
C	-1.60227800	2.89730100	0.48064800
C	-2.10636400	3.14353000	1.75756600
H	-3.04539100	2.33609500	3.53404300
H	-1.20257500	3.70916600	-0.12488700

H	-2.06067900	4.16161800	2.15367600
C	-3.47970300	-1.25273600	-0.33334800
O	-3.54933200	-2.13822600	-1.15430500
O	-4.51025900	-0.73120200	0.33249900
C	-5.87449300	-1.12101500	0.06423100
C	-6.07825800	-2.59951100	0.39453200
H	-7.14411000	-2.85664900	0.29878600
H	-5.49404000	-3.23438500	-0.28256400
H	-5.76550900	-2.80299600	1.42981700
C	-6.67190600	-0.23938900	1.02150500
H	-6.38380900	-0.44552900	2.06265200
H	-6.47340700	0.82211800	0.81597500
H	-7.74939700	-0.43019300	0.90852400
C	-6.23635200	-0.80296700	-1.38634300
H	-7.30954900	-0.98478700	-1.54860600
H	-6.02555500	0.25443200	-1.60451400
H	-5.65987900	-1.42740300	-2.07971000
H	-3.17843400	0.01478100	2.58166100
N	-1.14638500	1.10890800	-1.22772400
S	-0.20706600	1.93911300	-2.24177700
O	-0.79670200	3.23413100	-2.59644100
O	0.16173000	1.01350800	-3.30775400
C	1.29603500	2.32309400	-1.33250100
C	1.54980100	3.61405000	-0.88272100
C	2.19692200	1.29531000	-1.06337300
C	2.69979500	3.86401300	-0.13208700
H	0.85140700	4.41419900	-1.13334400
C	3.33707100	1.55225200	-0.31431200
H	1.99832500	0.29183200	-1.43597900
C	3.60304200	2.84076700	0.17047100
H	2.89549600	4.87841700	0.22737000
H	4.02214300	0.72991100	-0.09033500
C	4.83395600	3.09388400	1.00059400
H	5.74818600	2.84879000	0.43747700
H	4.90037500	4.14428400	1.31896200
H	4.83047000	2.46054200	1.90159600

M1:

Eel = -2166.622266
Zero-point correction = 0.703627
Thermal correction to Energy = 0.744436
Thermal correction to Enthalpy = 0.745380
Thermal correction to Gibbs Free Energy = 0.630941

C	-0.30831000	1.69414800	1.83891200
C	0.52933400	0.89738700	1.06690200
C	0.05691700	0.15881300	-0.01245800
C	-1.28892500	0.20826100	-0.33576200
C	-2.19321200	0.99195500	0.38693100
C	-1.67643600	1.73431800	1.47428900
H	1.58928500	0.83434300	1.30907700
H	-1.63297400	-0.38433100	-1.18340900
C	0.24007200	2.48309700	3.04133100
C	1.74780700	2.24733000	3.22211800
H	2.32926900	2.58397400	2.35011900
H	2.10030700	2.82062600	4.09259400
H	1.97981400	1.18761700	3.40715300
C	0.02906000	3.99411800	2.82462400
H	-1.03325500	4.25040900	2.73454400
H	0.44826900	4.55745100	3.67343900
H	0.54622100	4.32702000	1.91080400
C	-0.45470700	2.01301900	4.33451000
H	-1.53501200	2.19876500	4.30981900
H	-0.28843800	0.93519100	4.48574400
H	-0.03394600	2.54693300	5.20136500
C	-3.68776700	1.03724200	0.00067300
C	-3.99111900	0.13908200	-1.20953300
H	-3.73592200	-0.91082700	-1.01002900
H	-5.06646000	0.18750500	-1.43849200
H	-3.44888500	0.46014200	-2.11040800
C	-4.10348300	2.46911400	-0.40582000
H	-3.95939900	3.22969600	0.37570700
H	-3.51331100	2.80107800	-1.27261500
H	-5.16729300	2.49141300	-0.68893100
C	-4.56020100	0.50488400	1.15975600
H	-5.62453300	0.52575000	0.87835400
H	-4.28539900	-0.53589700	1.38492000
H	-4.46173200	1.06151100	2.10317800
O	-2.47624000	2.52760000	2.23171000
C	1.02151600	-0.65485100	-0.84851000
H	0.48152100	-1.07588600	-1.71151300
C	3.09514900	-1.44343000	0.01088300
C	3.36187900	-0.27947200	-0.71901400
C	4.10023000	-2.10019100	0.70490800
C	4.63835000	0.26005000	-0.77551700
C	5.39050900	-1.55652700	0.65233900
H	3.88790500	-3.00829900	1.26568100

C	5.65536000	-0.40079600	-0.07428100
H	4.82202200	1.17077400	-1.34067000
H	6.19597700	-2.05651400	1.19363200
H	6.66823300	0.00559600	-0.10082900
H	-3.37868100	2.49634000	1.91082200
N	2.16251300	0.15053300	-1.31195500
C	2.01351700	1.30267500	-2.04458800
O	2.88972000	2.11896300	-2.20418500
O	0.77998200	1.36126800	-2.55357000
C	0.18960600	2.62691100	-2.95999300
C	0.94002500	3.21894700	-4.15113400
H	0.39508500	4.09919400	-4.52368100
H	1.95670500	3.51670700	-3.87145700
H	1.00019900	2.48186500	-4.96570700
C	0.16435500	3.56654100	-1.75553600
H	1.18236900	3.83967500	-1.44694800
H	-0.37730500	4.48834800	-2.01359800
H	-0.34686600	3.08393200	-0.90801700
C	-1.22658900	2.23409300	-3.36294900
H	-1.20727100	1.50082700	-4.18237200
H	-1.75066100	1.79053000	-2.50644300
H	-1.78443600	3.12012400	-3.69869100
N	1.71848000	-1.74909800	-0.12747300
S	0.95582300	-2.71644400	1.02672600
O	1.73730800	-3.93936000	1.08100600
O	0.69766500	-1.98612600	2.25600000
C	-0.59335600	-3.04928800	0.23015000
C	-1.77013900	-2.77679600	0.92096600
C	-0.61024900	-3.64680800	-1.02780400
C	-2.98482400	-3.10783200	0.33099300
H	-1.71949700	-2.30015000	1.90121100
C	-1.83639700	-3.94168800	-1.61559200
H	0.32739600	-3.87281700	-1.54008300
C	-3.03966600	-3.68063000	-0.94654400
H	-3.91460600	-2.90995000	0.87039600
H	-1.85934700	-4.39848400	-2.60780500
C	-4.36724800	-3.97802700	-1.58931200
H	-4.26081900	-4.65784300	-2.44536400
H	-5.06457200	-4.43309600	-0.87120600
H	-4.83390100	-3.04882200	-1.95523400

8. Copies of NMR Spectra

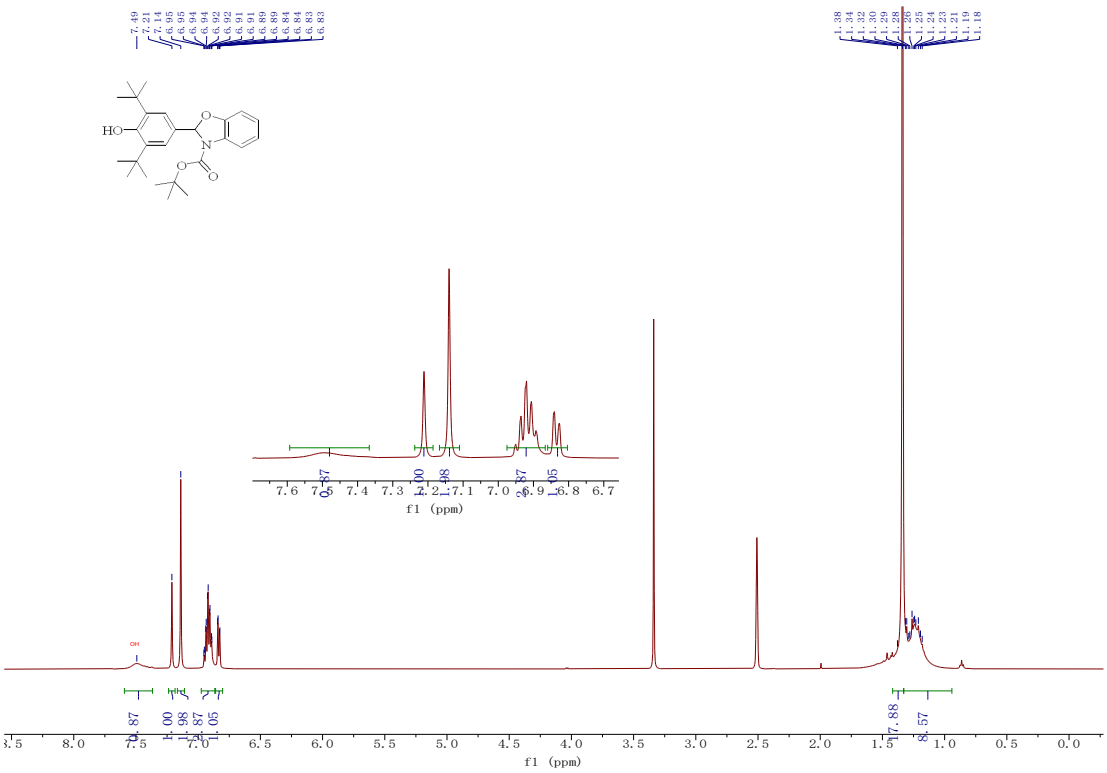


Figure S1. ^{1}H NMR (500 MHz, DMSO-d_6) of **3a**

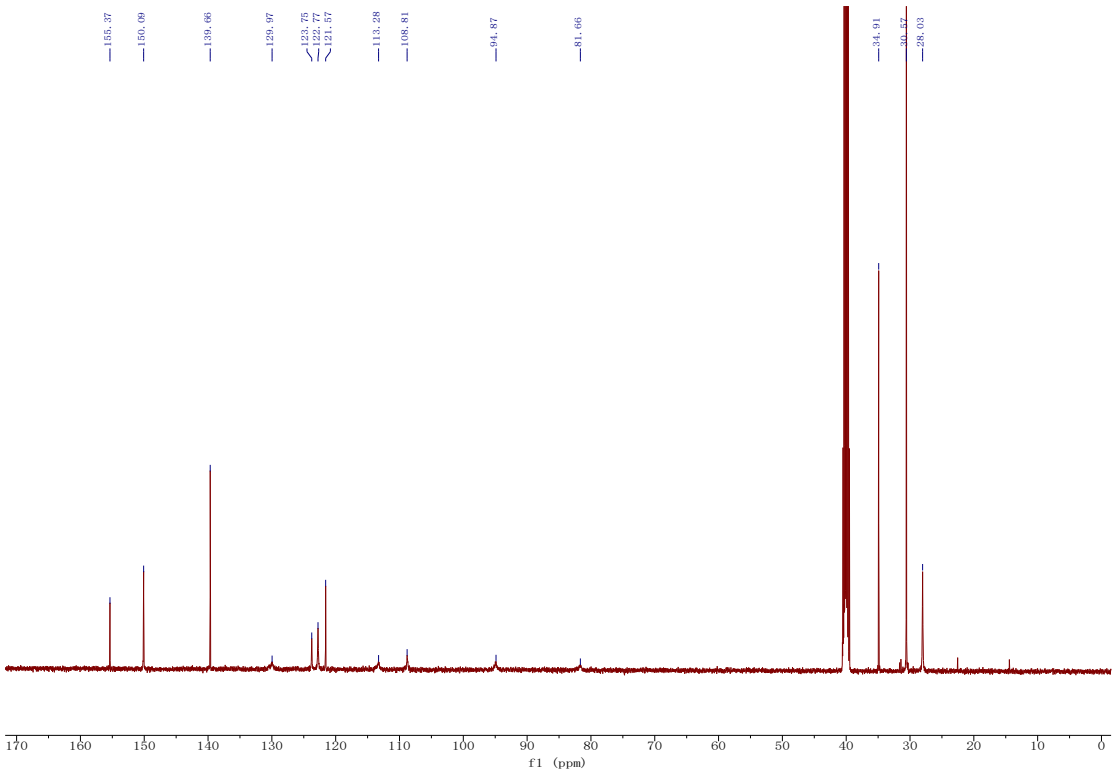


Figure S2. ^{13}C NMR (125 MHz, DMSO-d_6) of **3a**

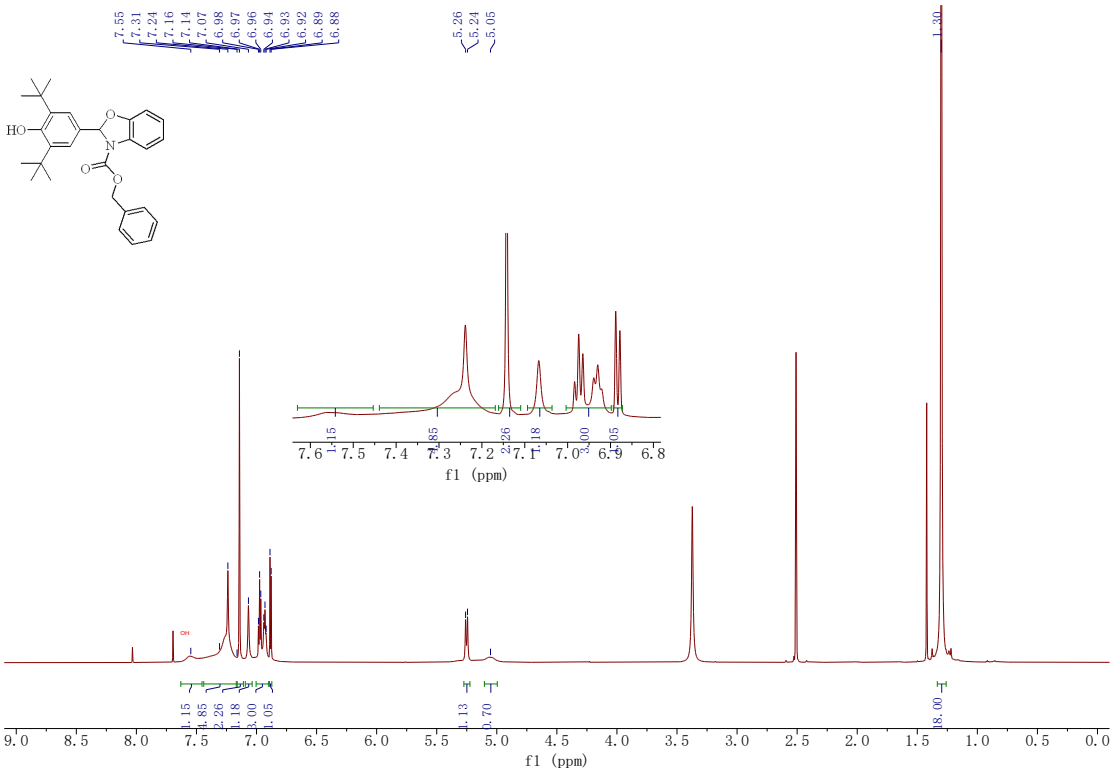


Figure S3. ^{1}H NMR (800 MHz, DMSO-d_6) of **3b**

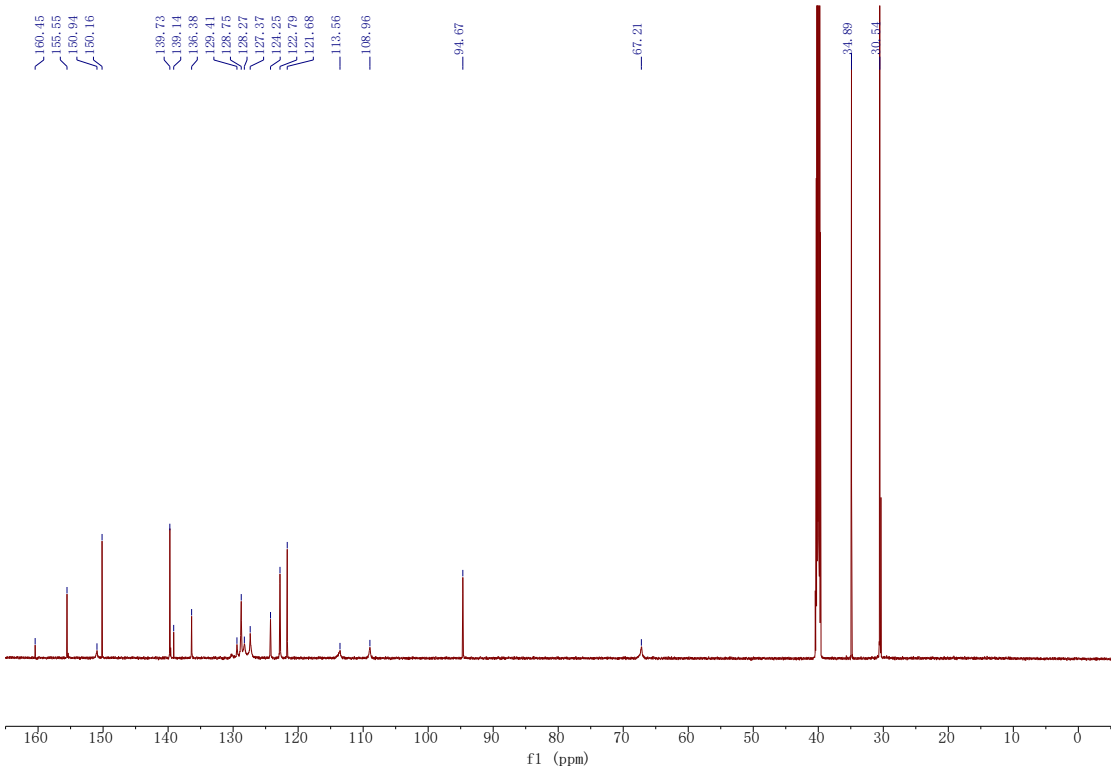


Figure S4. ^{13}C NMR (200 MHz, DMSO-d_6) of **3b**

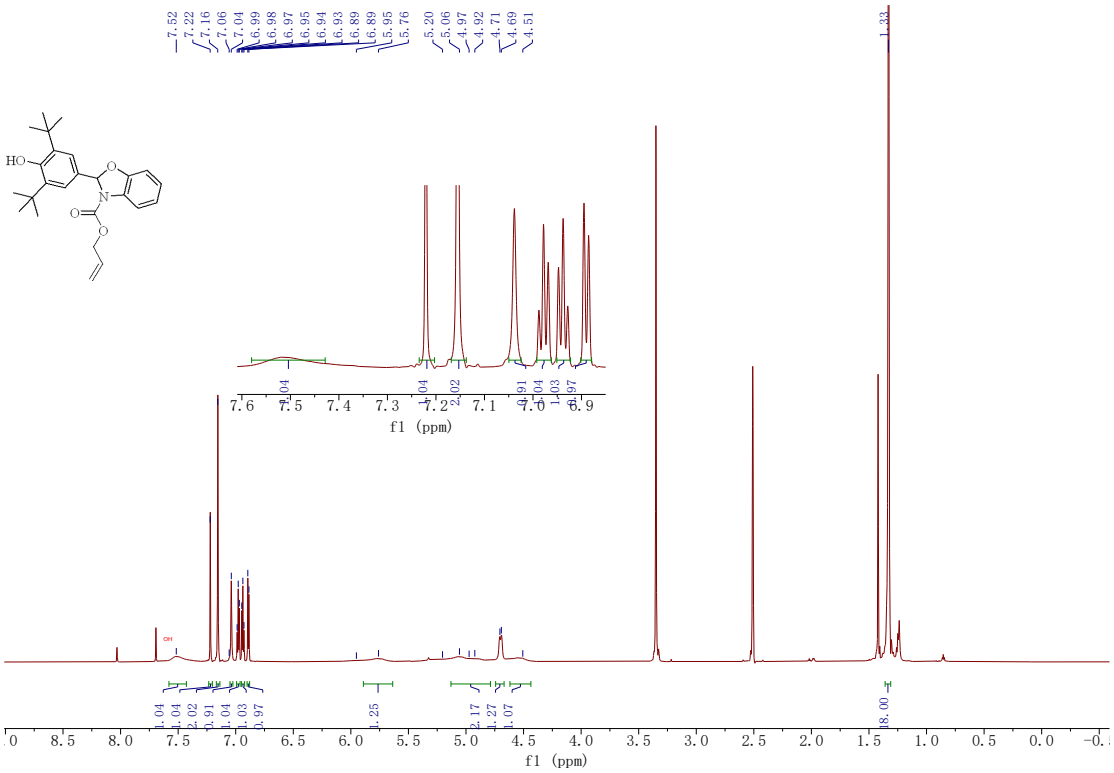


Figure S5. ^{1}H NMR (800 MHz, DMSO-d_6) of **3c**

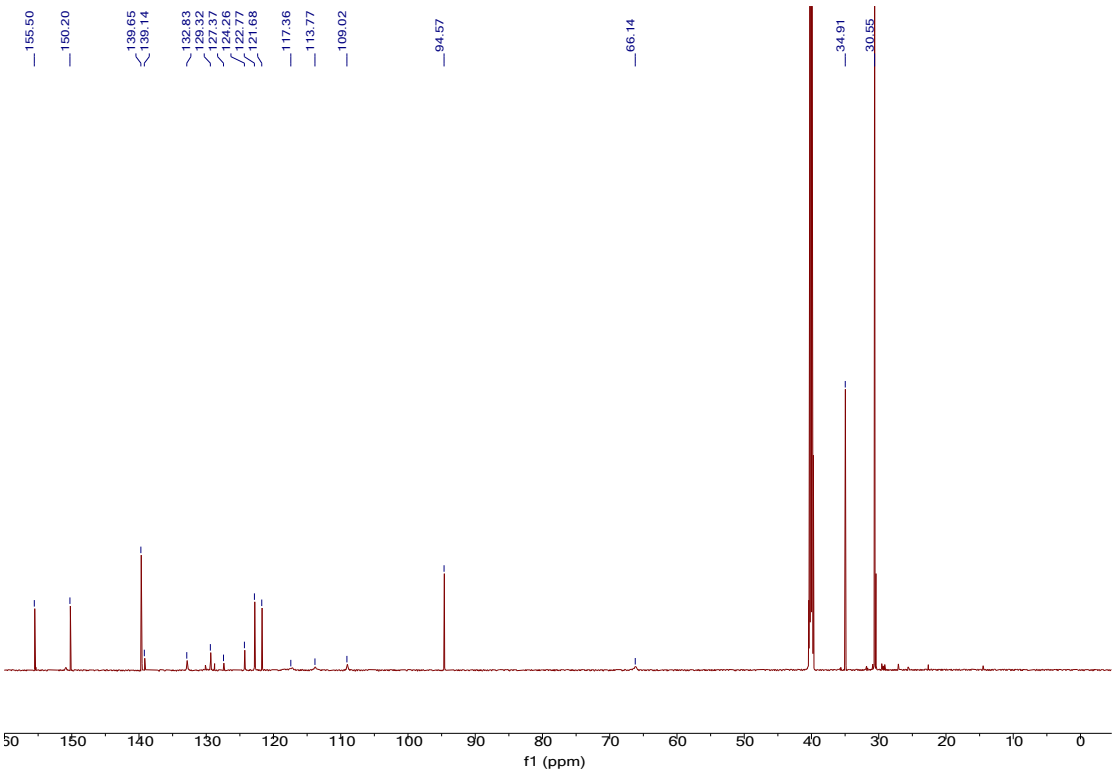


Figure S6. ^{13}C NMR (200 MHz, DMSO-d_6) of **3c**

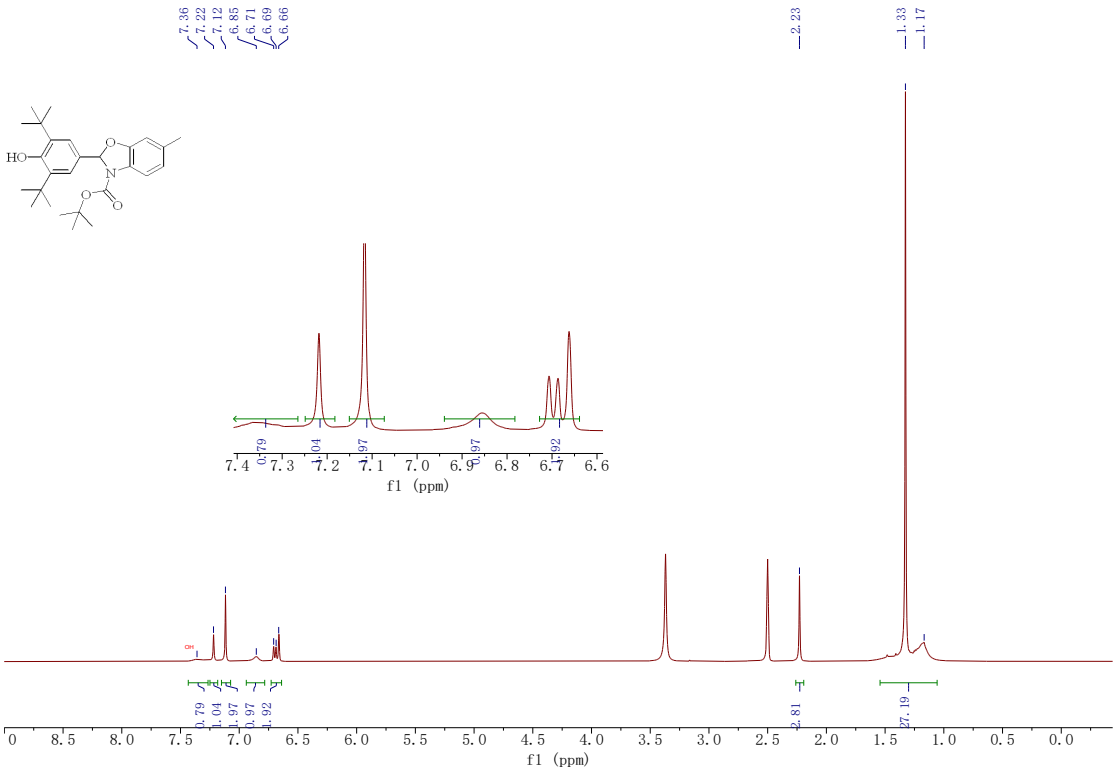


Figure S7. ^{1}H NMR (800 MHz, DMSO-d_6) of **3d**

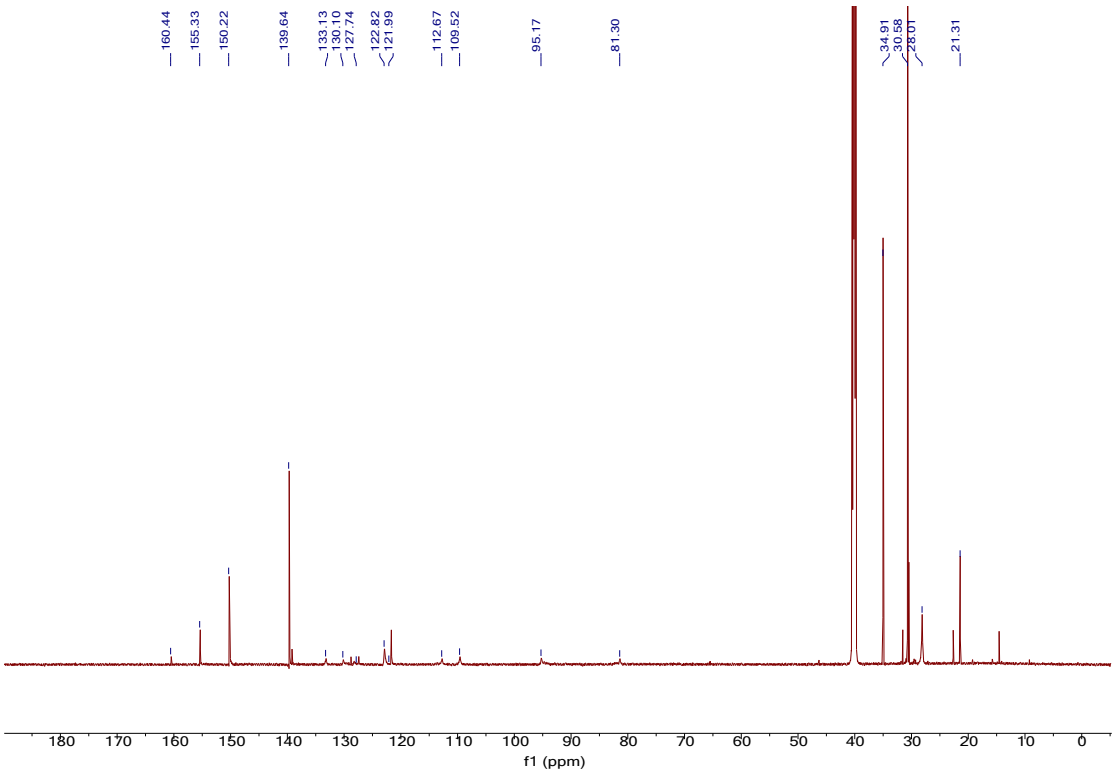


Figure S8. ^{13}C NMR (200 MHz, DMSO-d_6) of **3d**

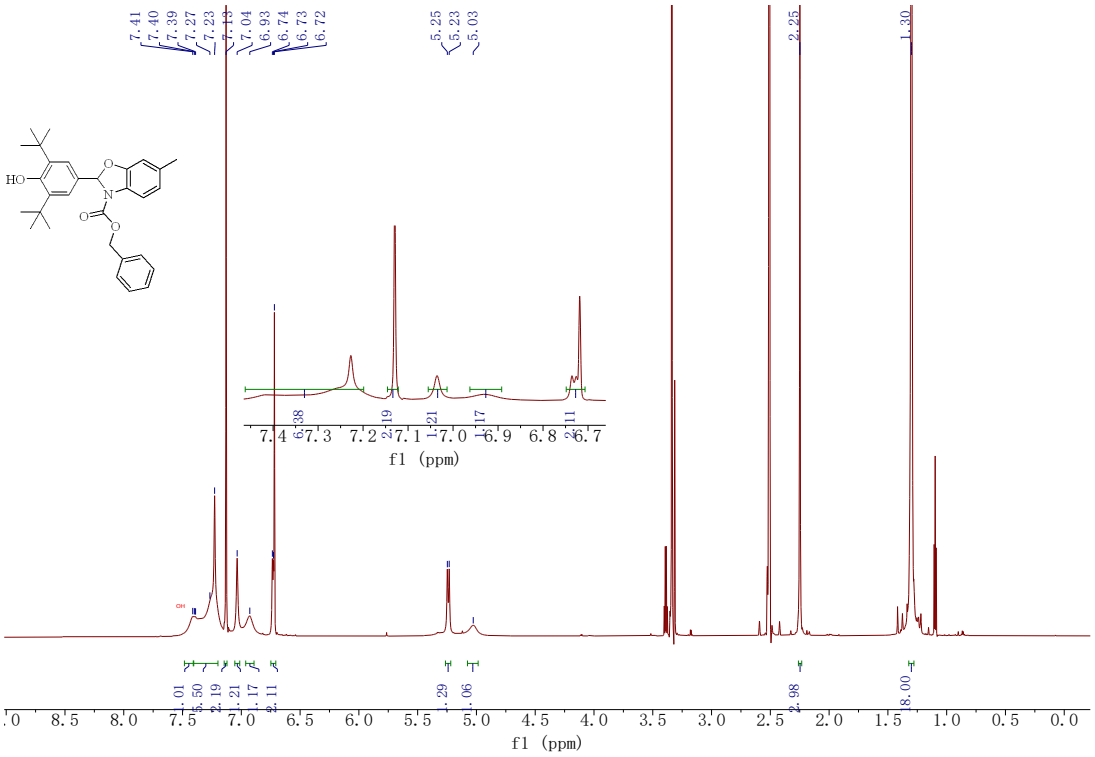


Figure S9. ^{1}H NMR (800 MHz, DMSO-d_6) of **3e**

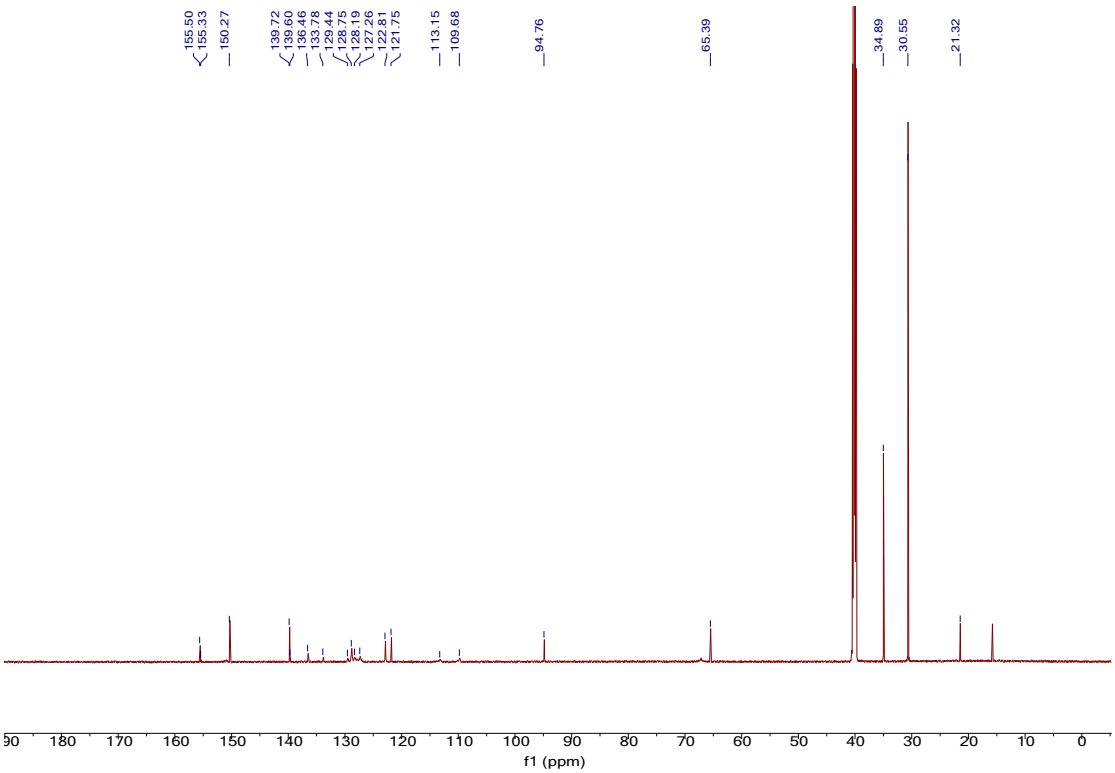


Figure S10. ^{13}C NMR (200 MHz, DMSO-d_6) of **3e**

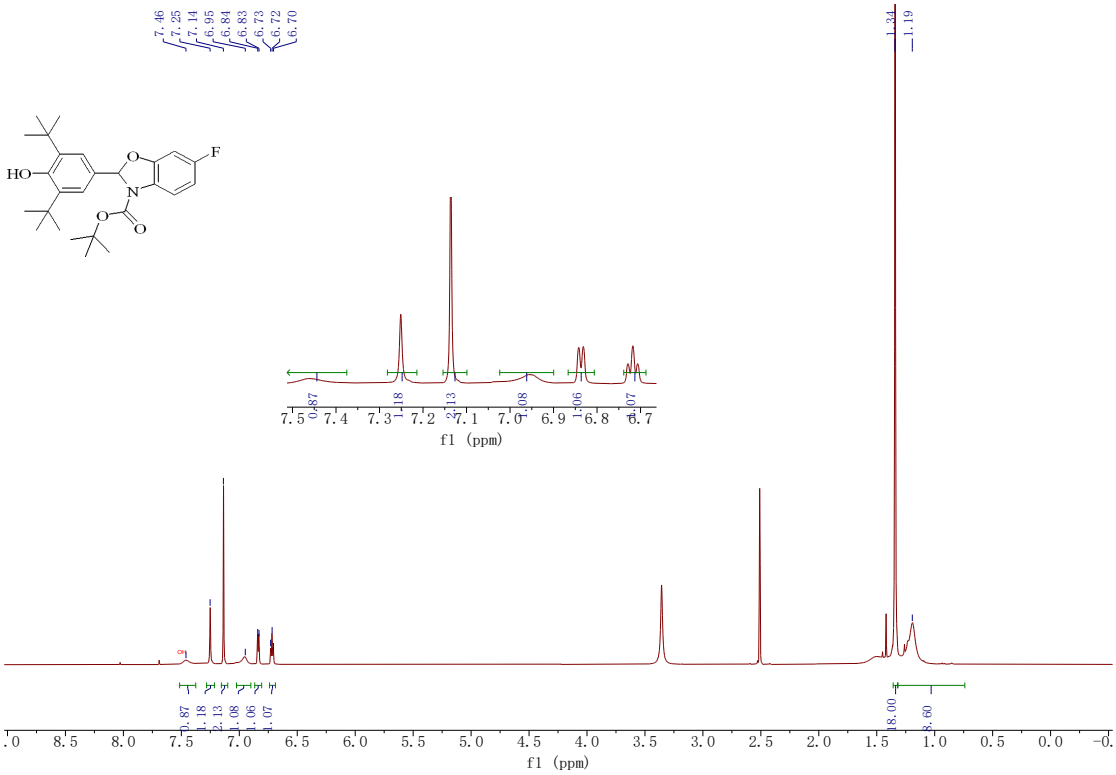


Figure S11. ^{1}H NMR (800 MHz, DMSO-d_6) of **3f**

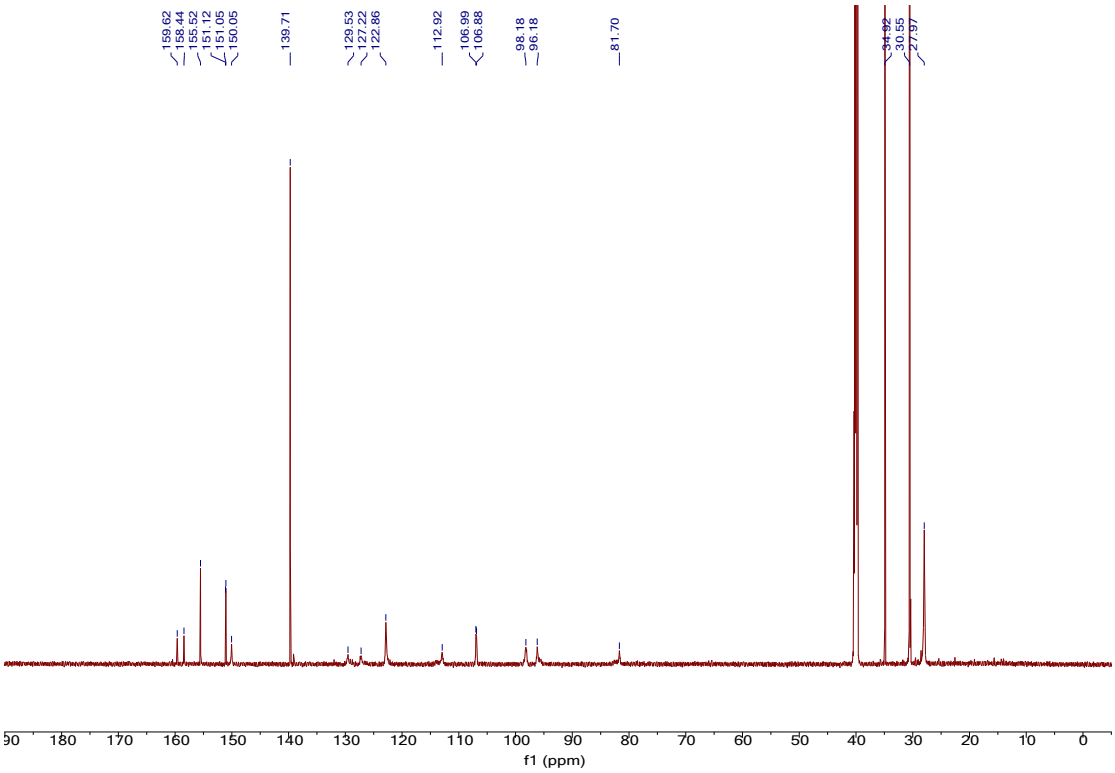


Figure S12. ^{13}C NMR (200 MHz, DMSO-d_6) of **3f**

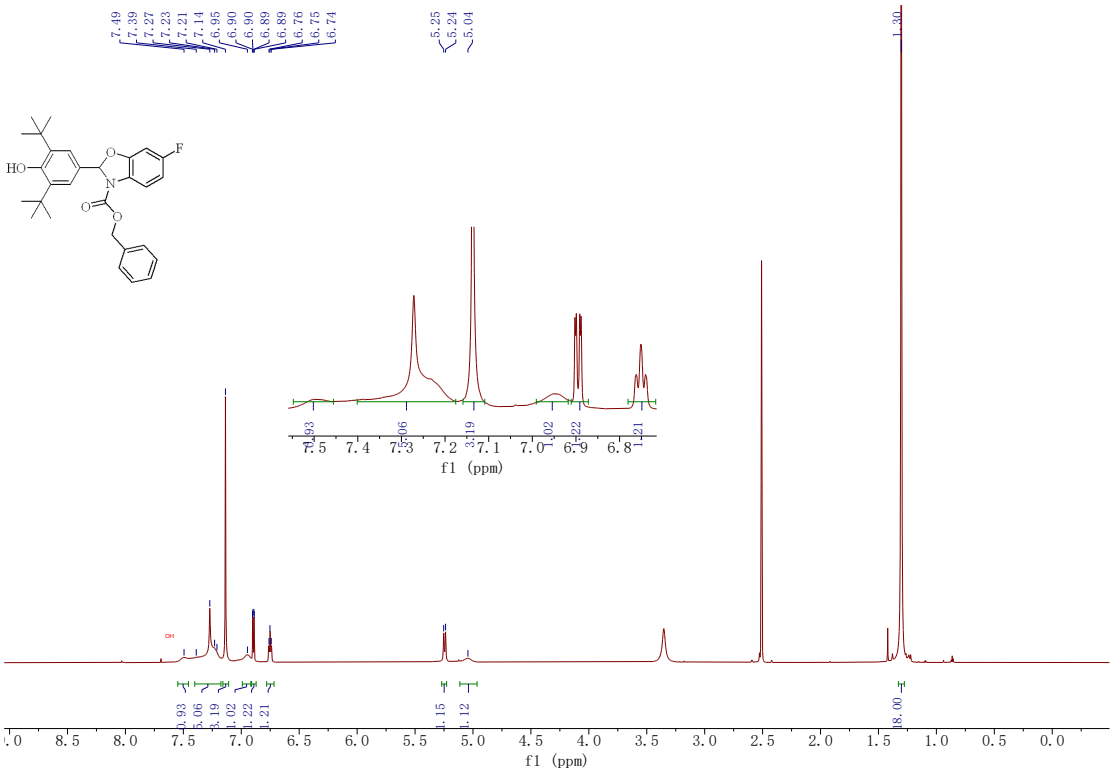


Figure S13. [1]H NMR (800 MHz, DMSO-d_6) of **3g**

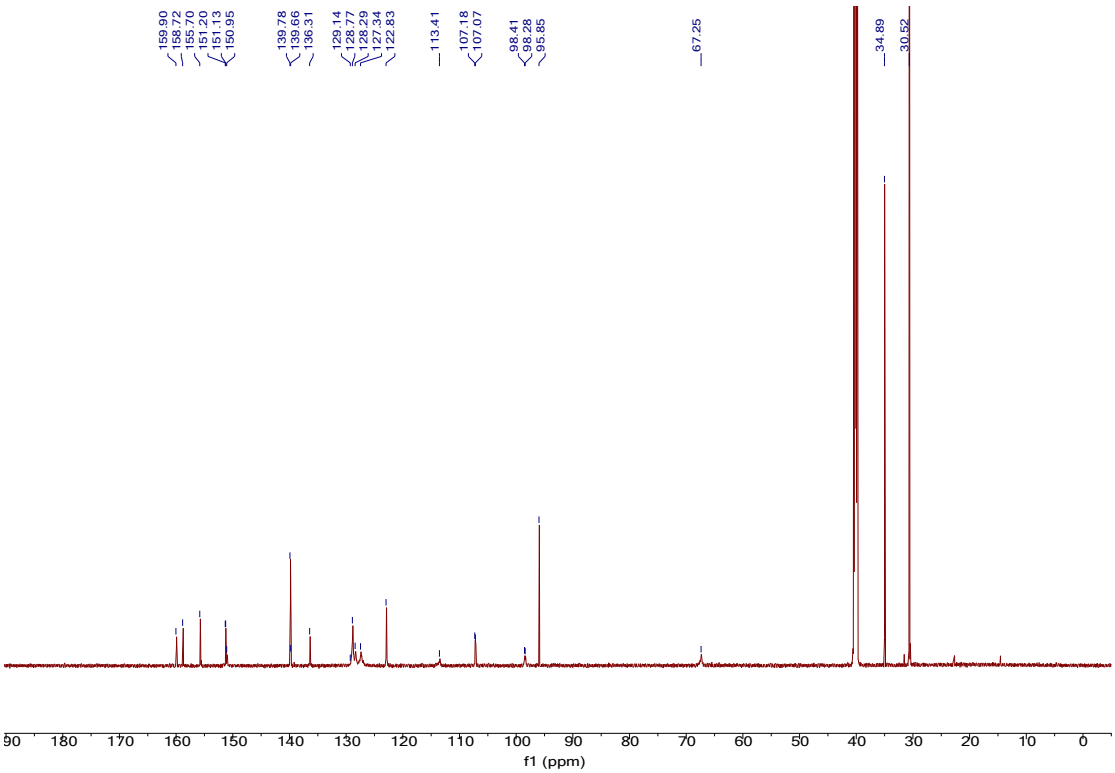


Figure S14. [13]C NMR (200 MHz, DMSO-d_6) of **3g**

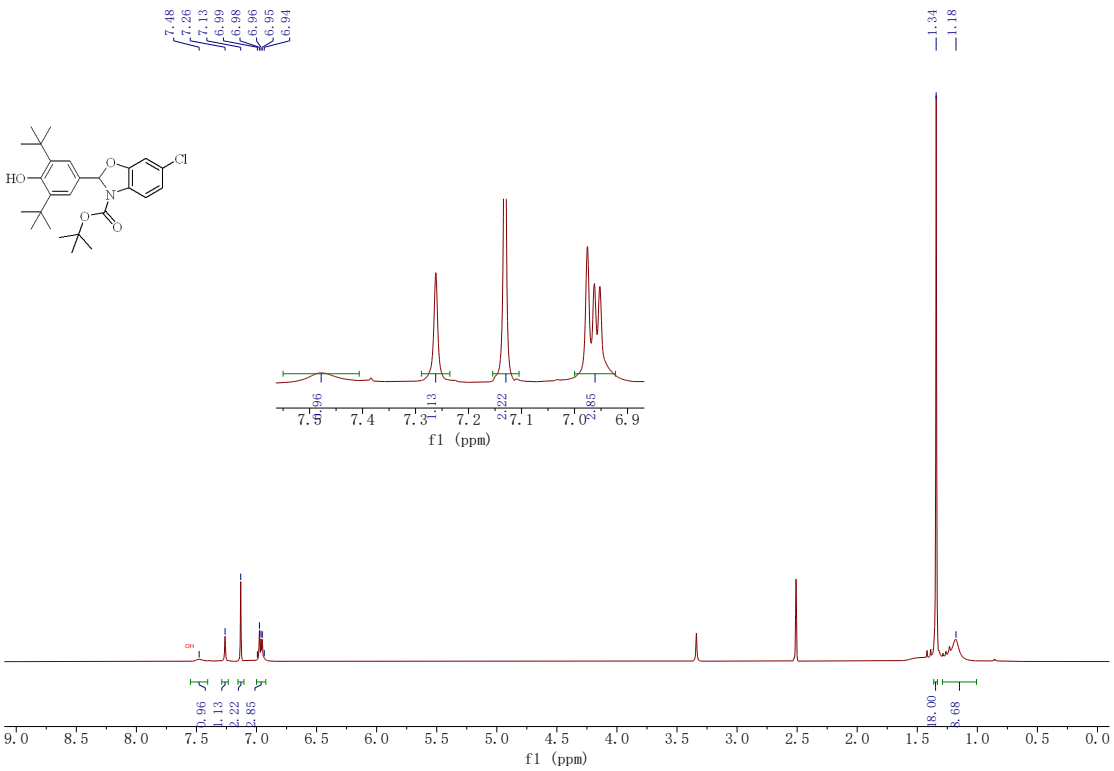


Figure S15. ^{1}H NMR (800 MHz, DMSO-d_6) of **3h**

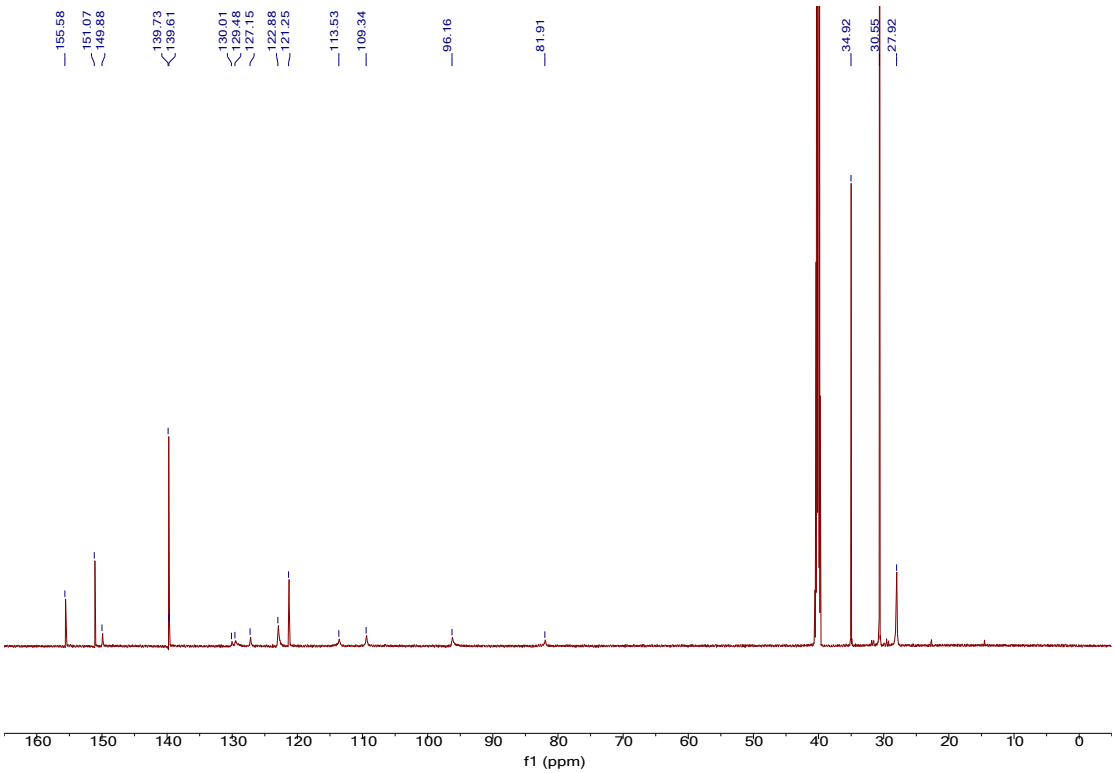


Figure S16. ^{13}C NMR (200 MHz, DMSO-d_6) of **3h**

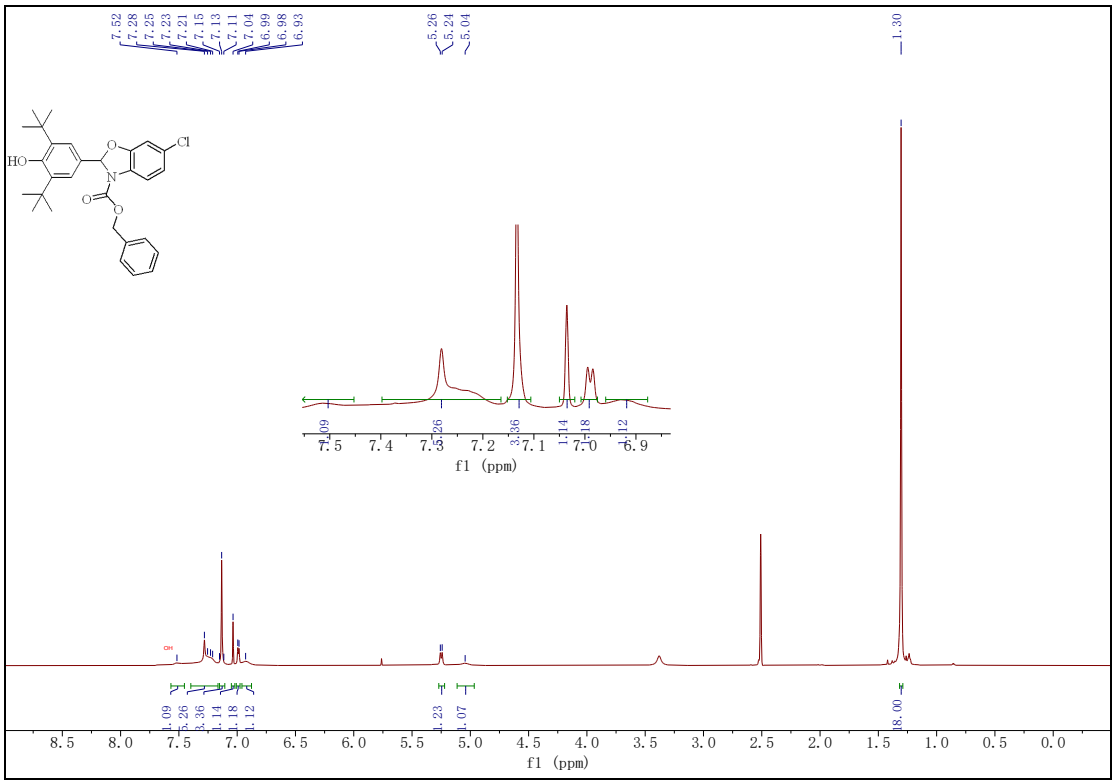


Figure S17. ^{1}H NMR (800 MHz, DMSO-d_6) of **3i**

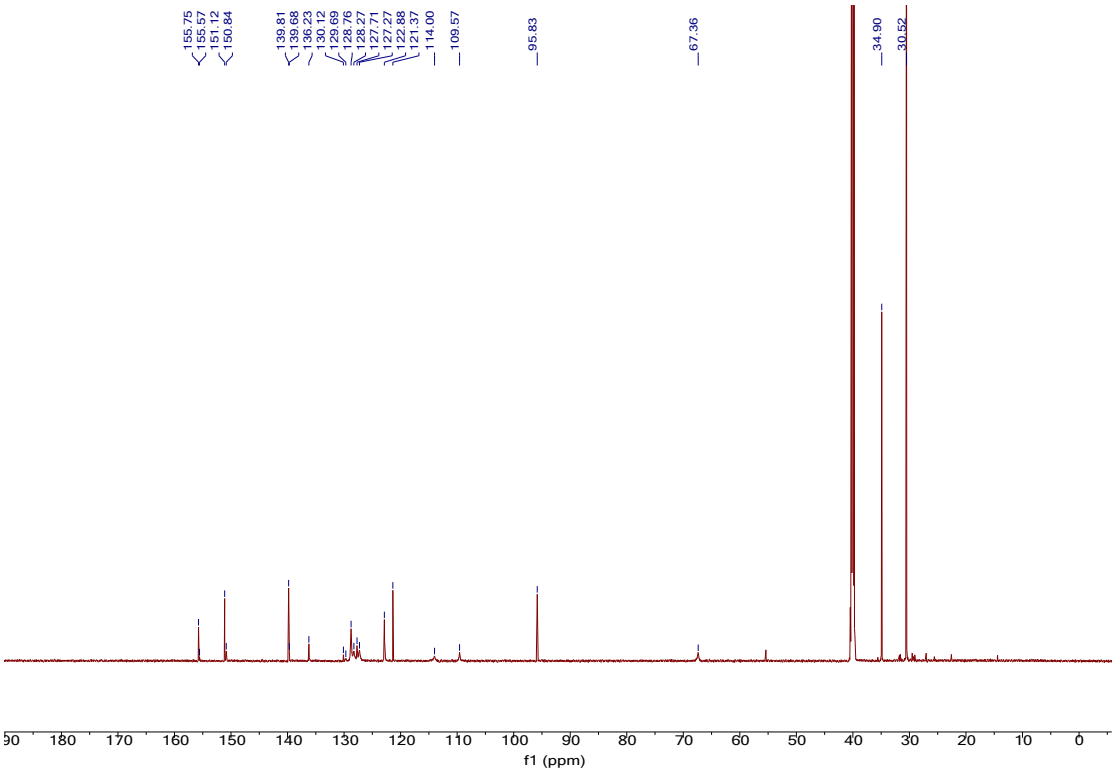


Figure S18. ^{13}C NMR (200 MHz, DMSO-d_6) of **3i**

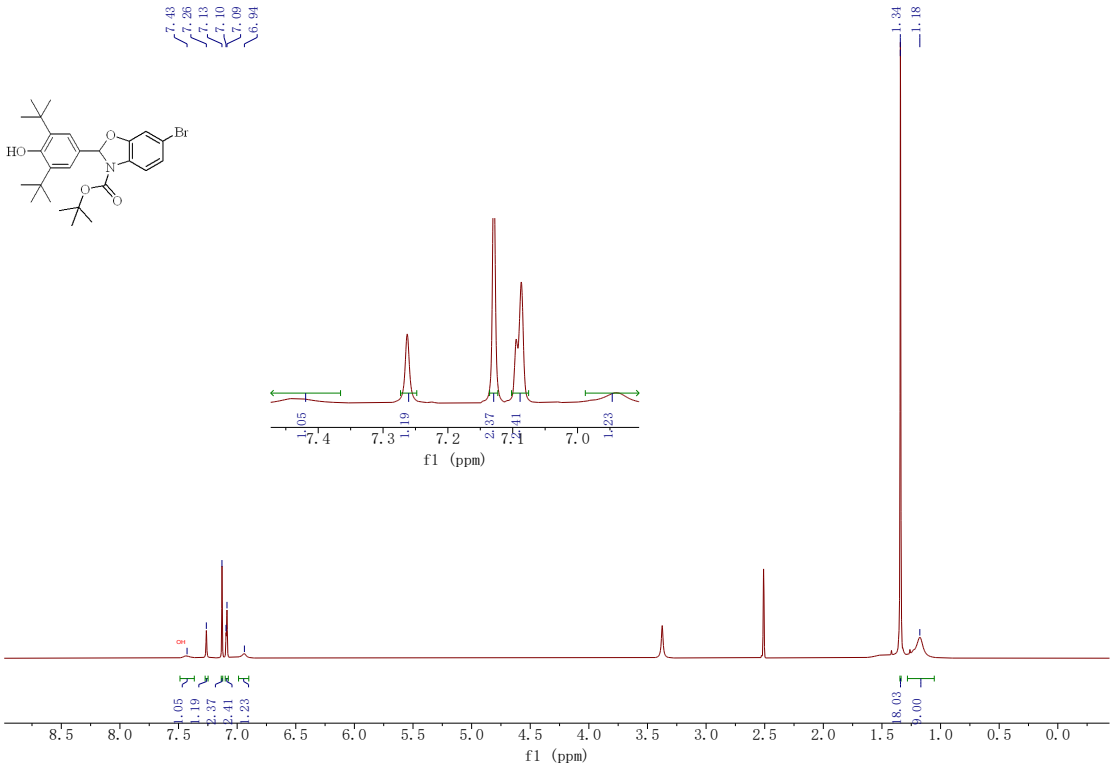


Figure S19. ^{1}H NMR (800 MHz, DMSO-d_6) of **3j**

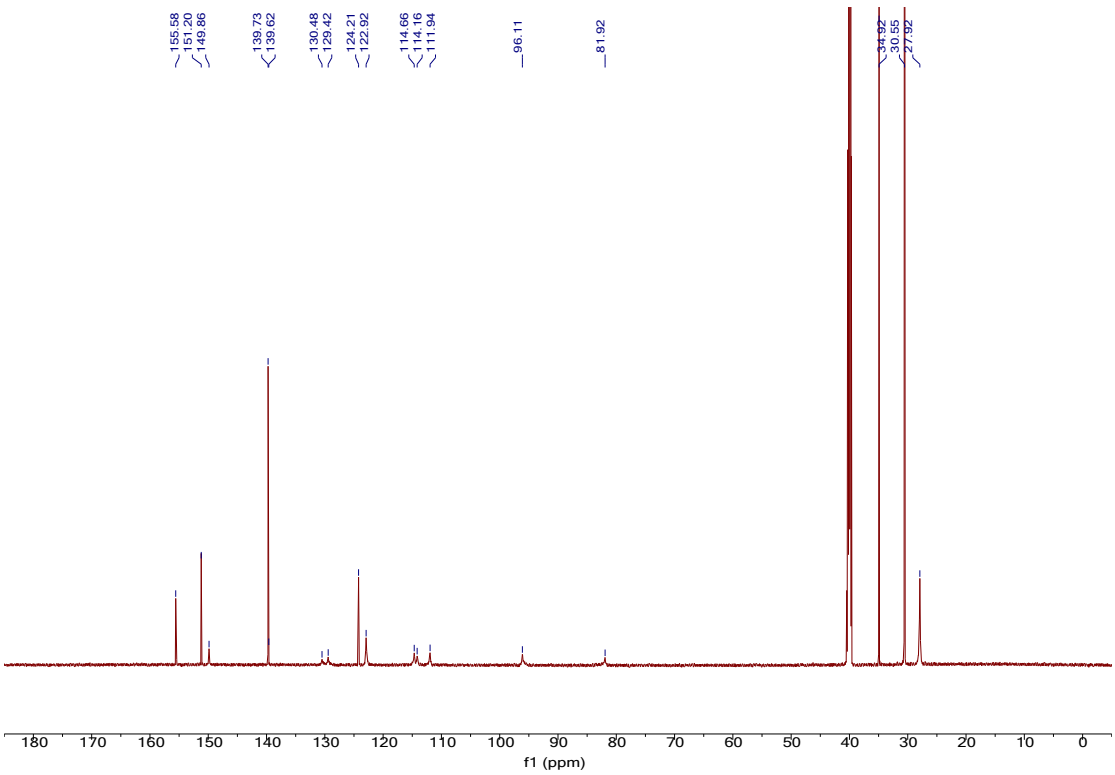


Figure S120. ^{13}C NMR (200 MHz, DMSO-d_6) of **3j**

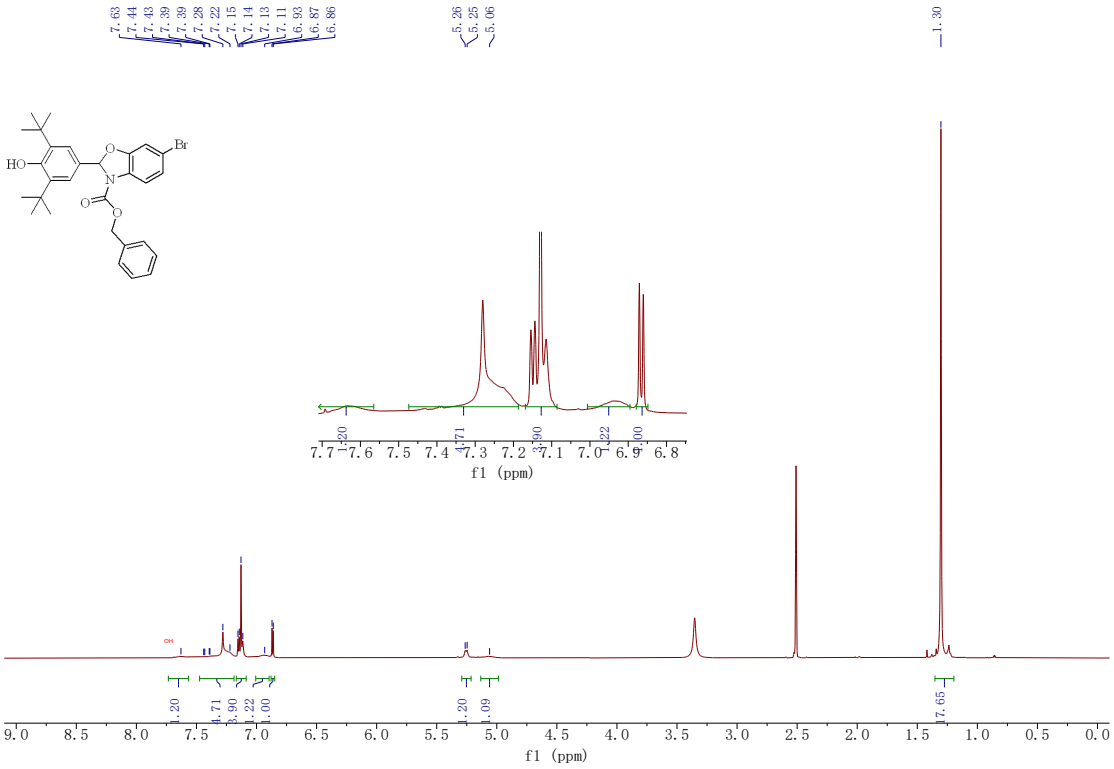


Figure S21. ^{1}H NMR (800 MHz, DMSO-d_6) of **3k**

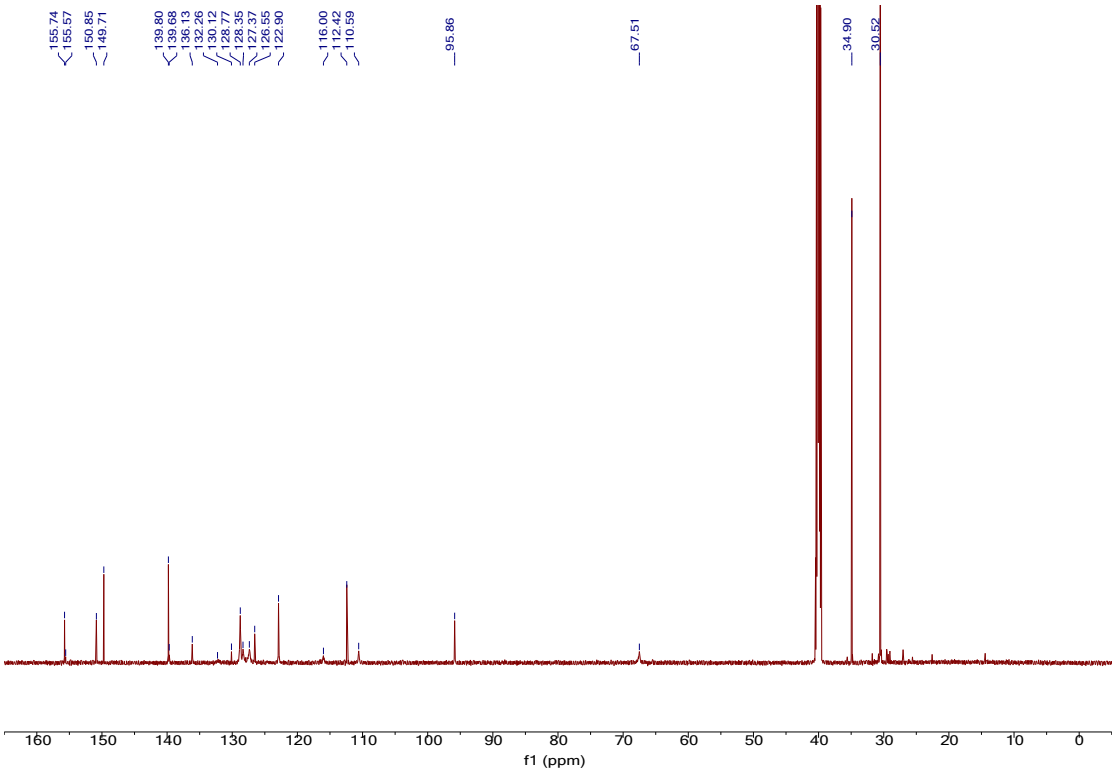


Figure S22. ^{13}C NMR (200 MHz, DMSO-d_6) of **3k**

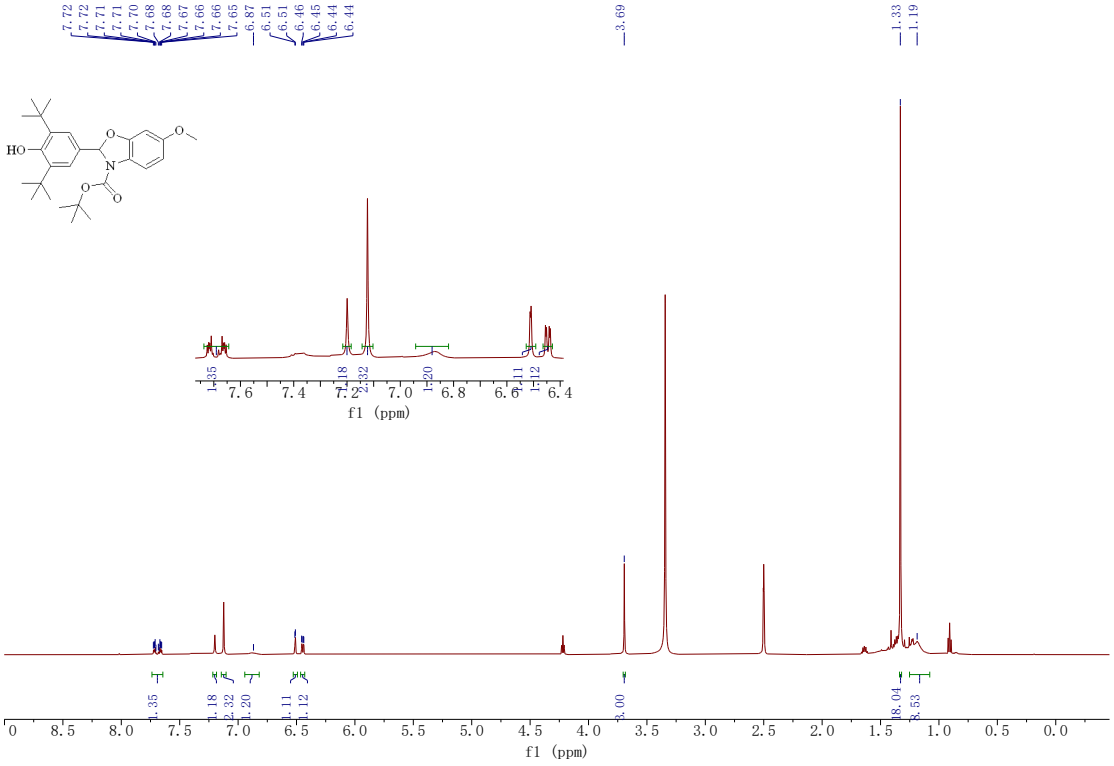


Figure S23. ^{1}H NMR (800 MHz, DMSO-d_6) of **3l**

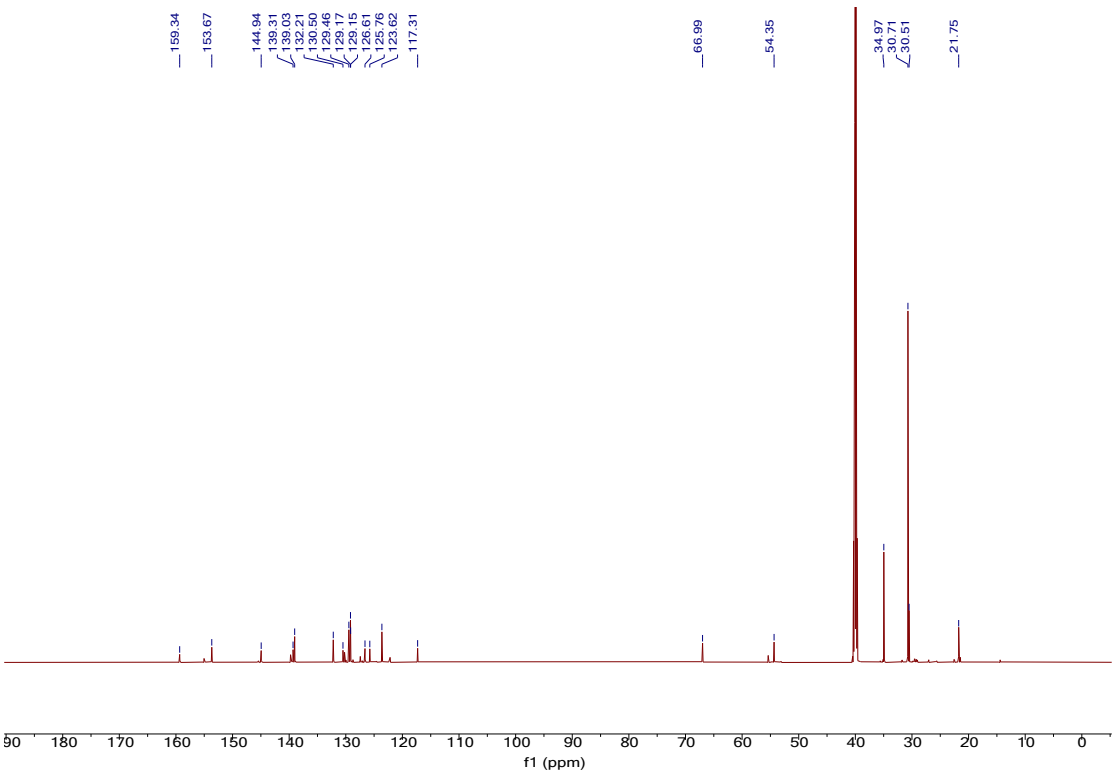


Figure S24. ^{13}C NMR (200 MHz, DMSO-d_6) of **3l**

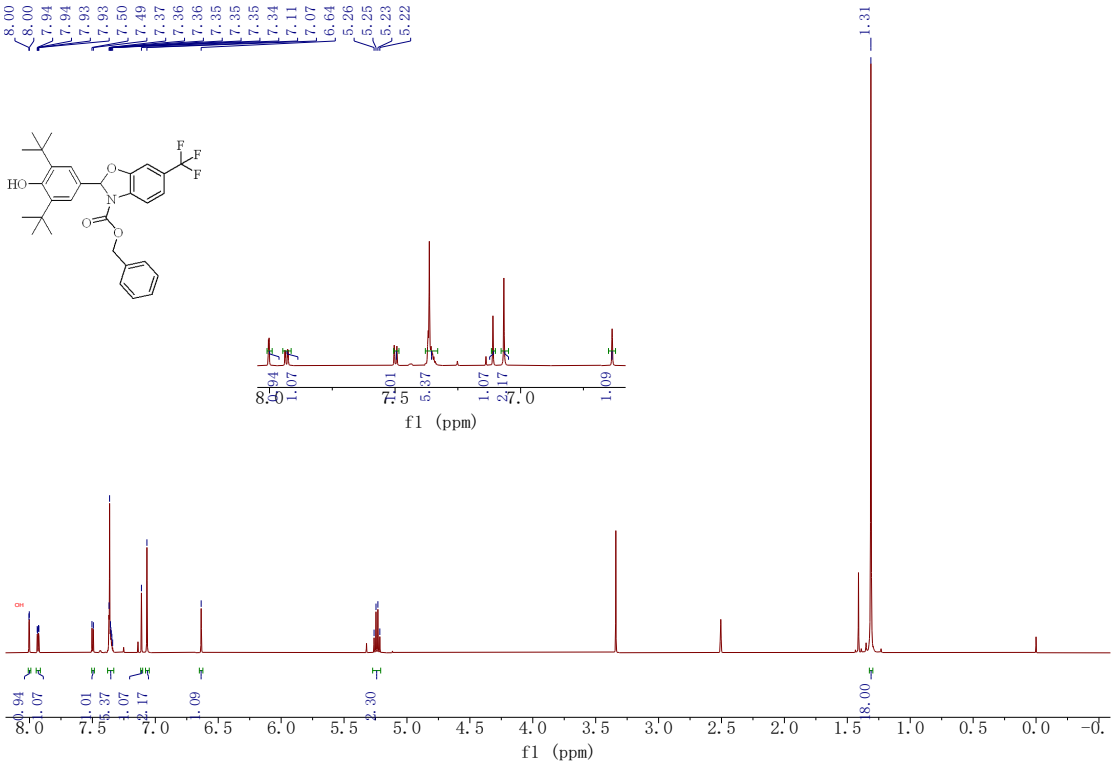


Figure S25. ^{1}H NMR (800 MHz, DMSO-d_6) of **3m**

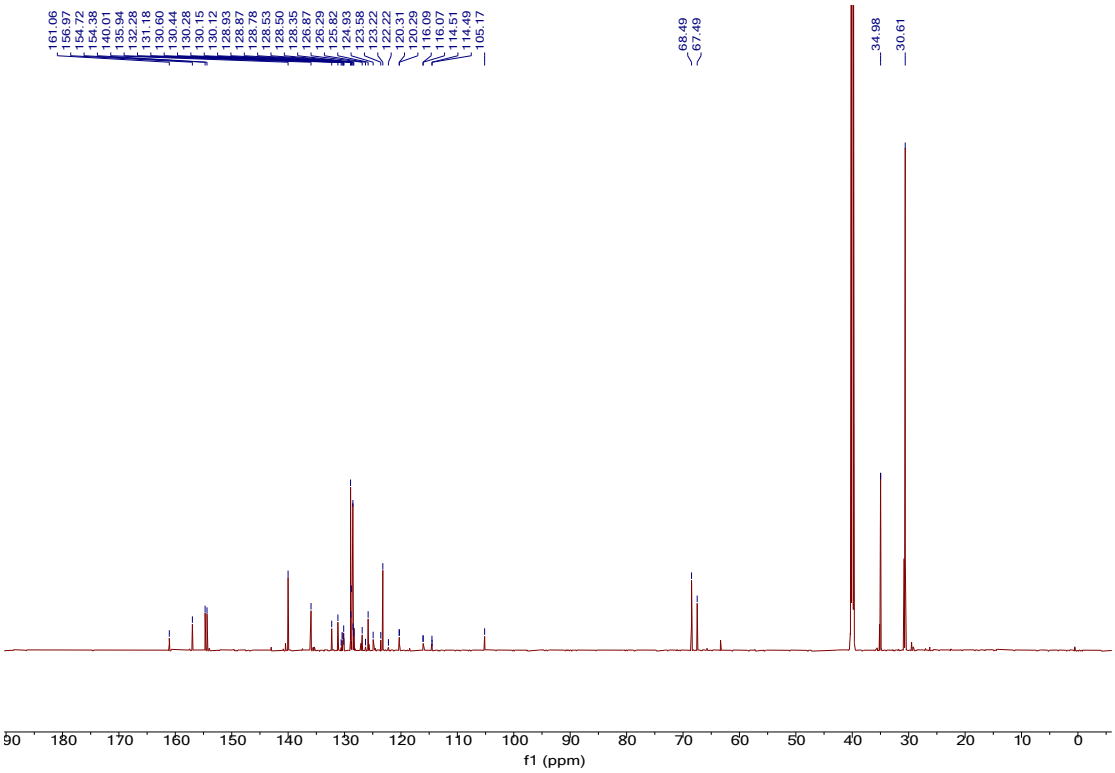


Figure S26. ^{13}C NMR (200 MHz, DMSO-d_6) of **3m**

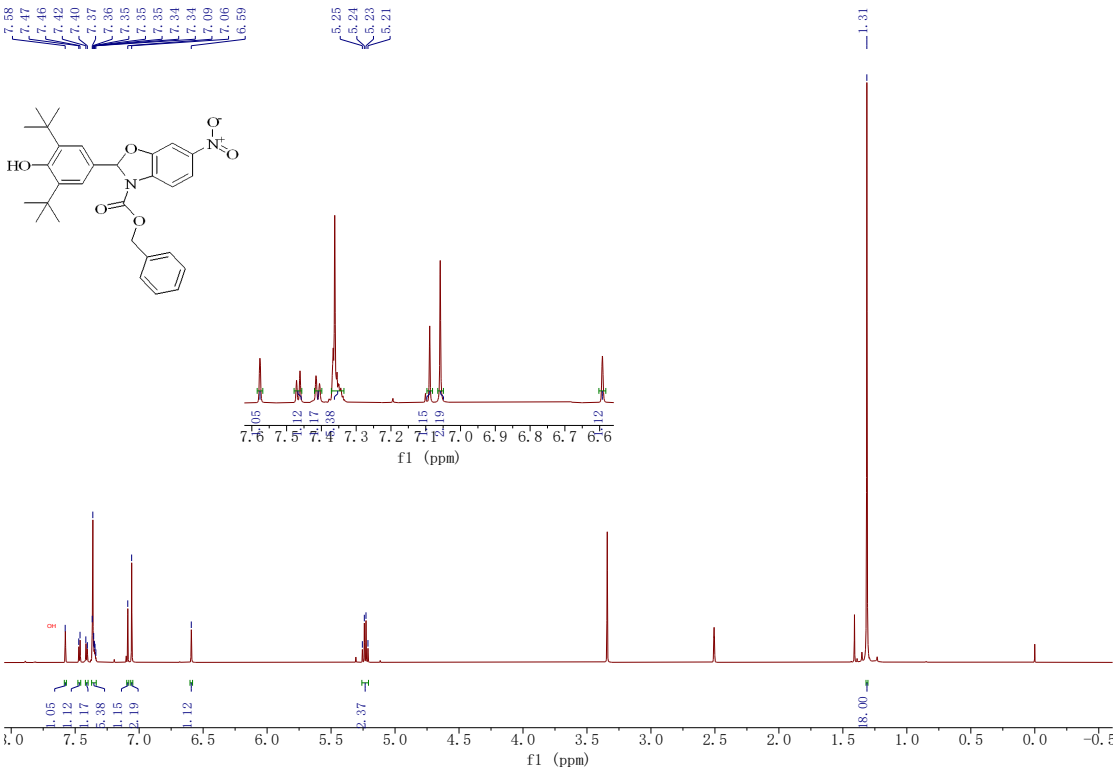


Figure S27. [1]H NMR (800 MHz, DMSO-d_6) of **3n**

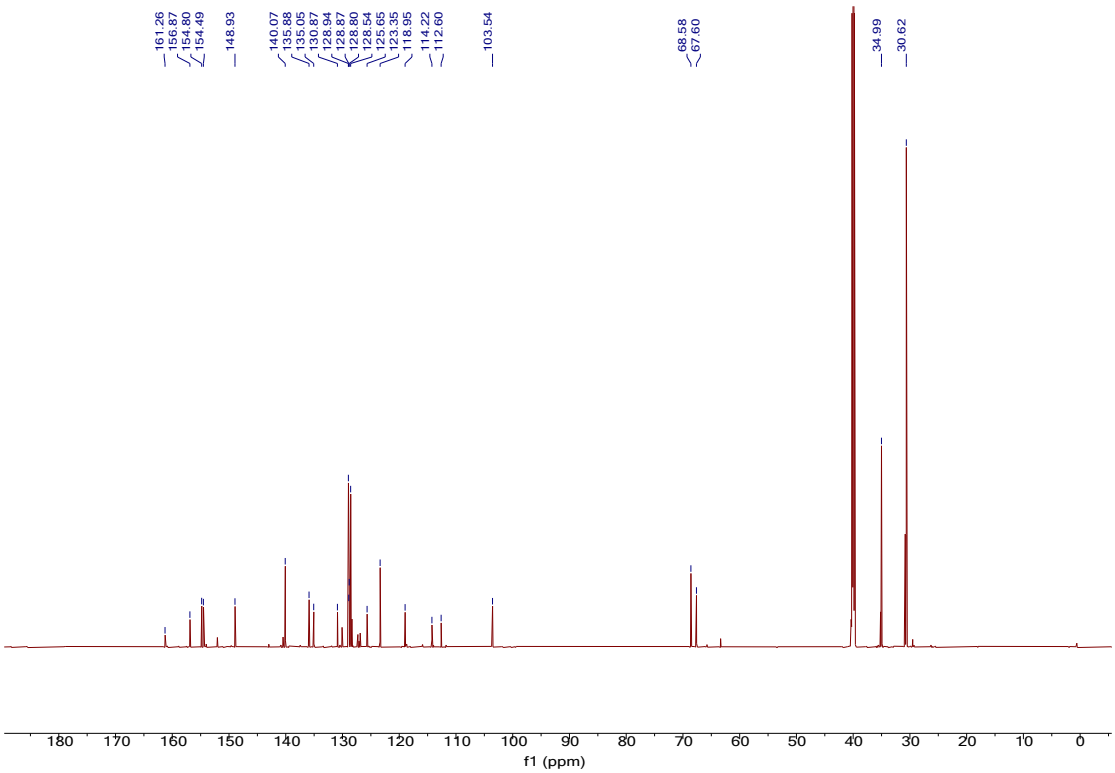


Figure S28. [13]C NMR (200 MHz, DMSO-d_6) of **3n**

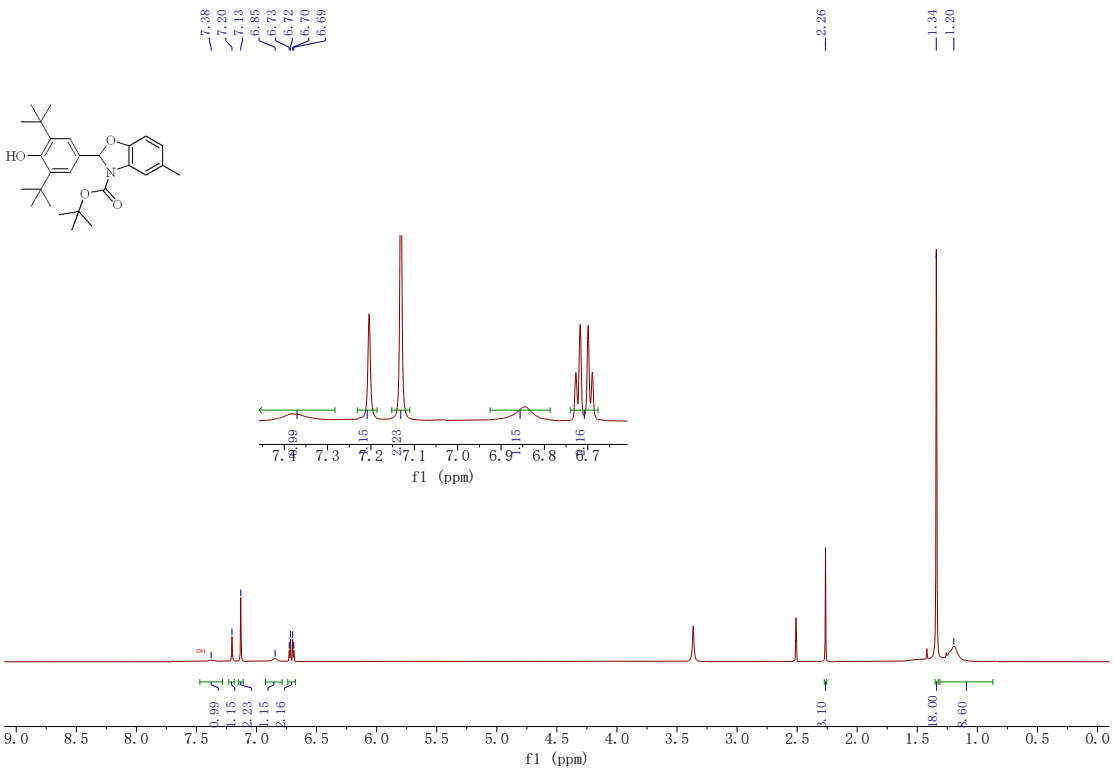


Figure S29. ^{1}H NMR (800 MHz, DMSO-d_6) of **3o**

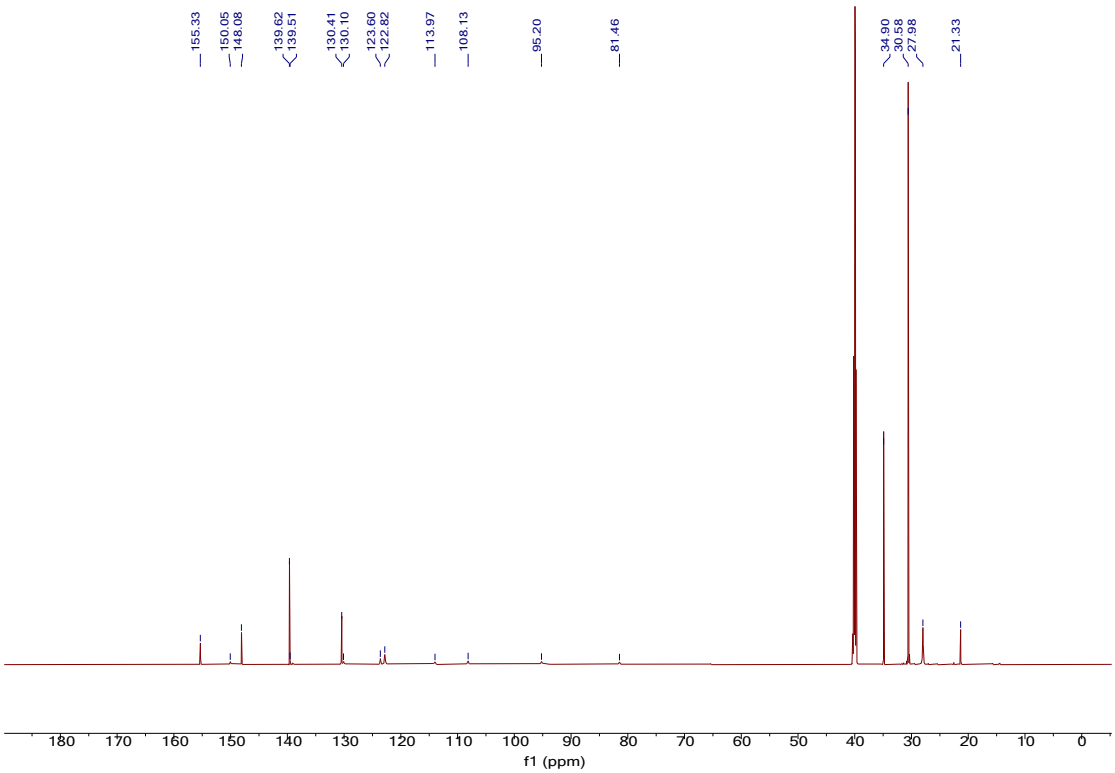


Figure S30. ^{13}C NMR (200 MHz, DMSO-d_6) of **3o**

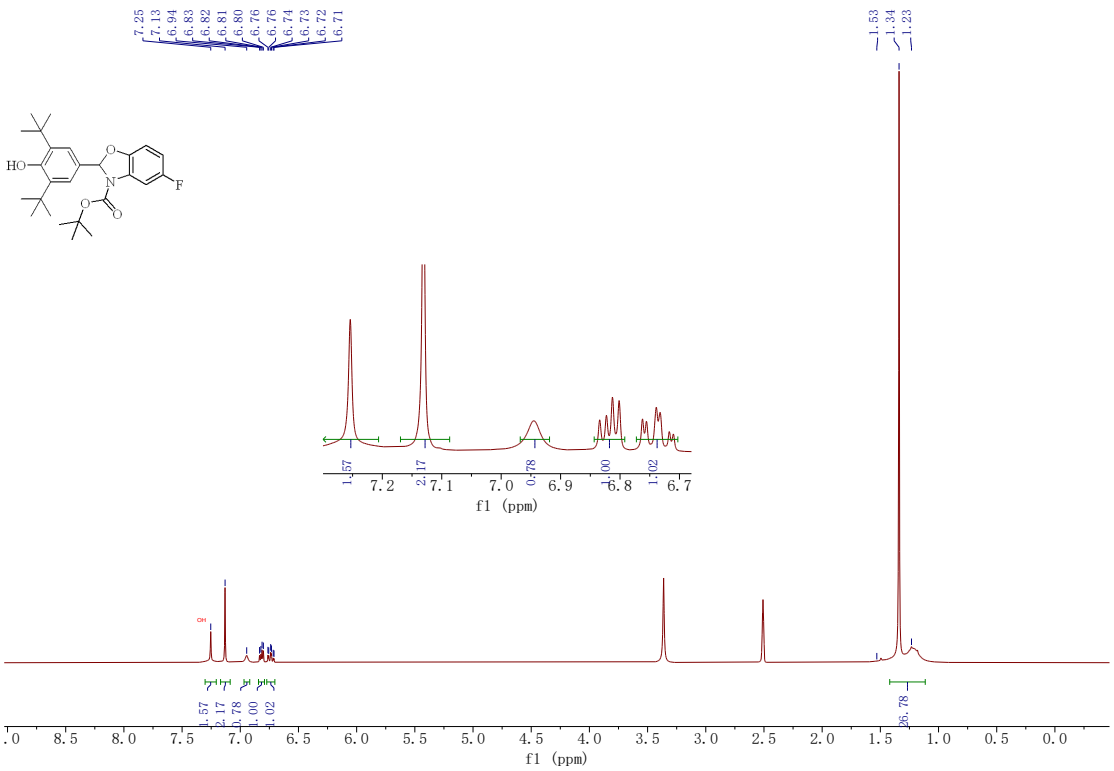


Figure S31. [1]H NMR (400 MHz, DMSO-d_6) of **3p**

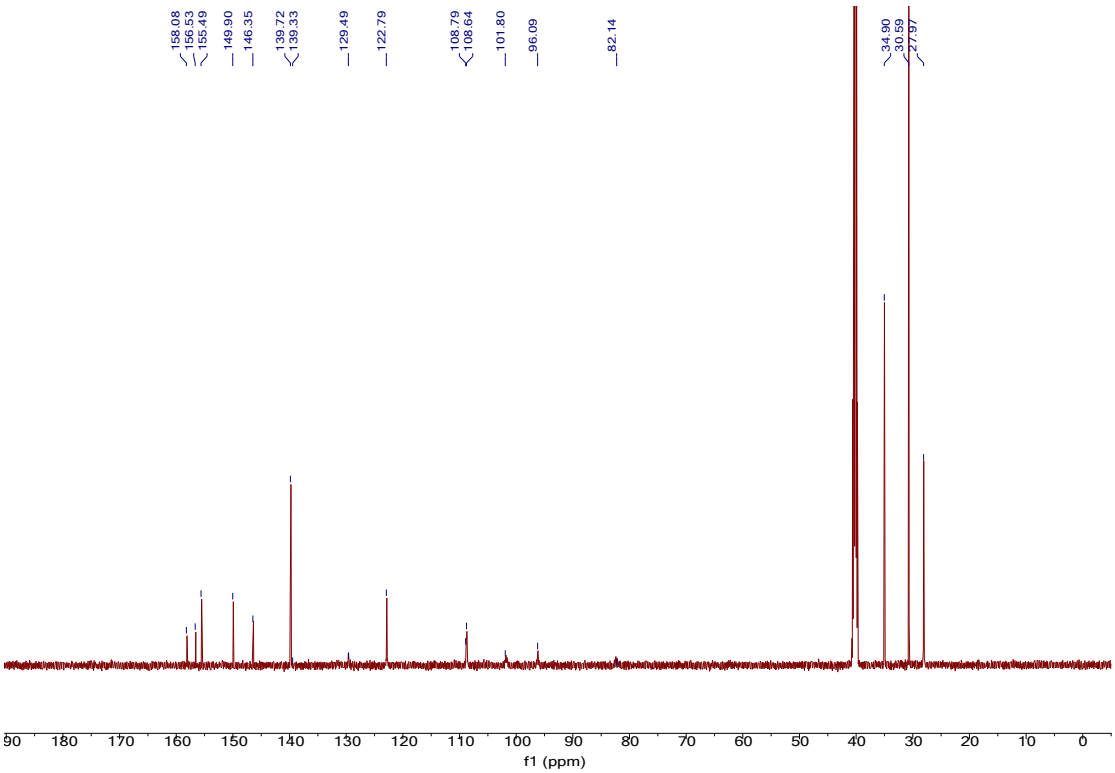


Figure S32. [13]C NMR (150 MHz, DMSO-d_6) of **3p**

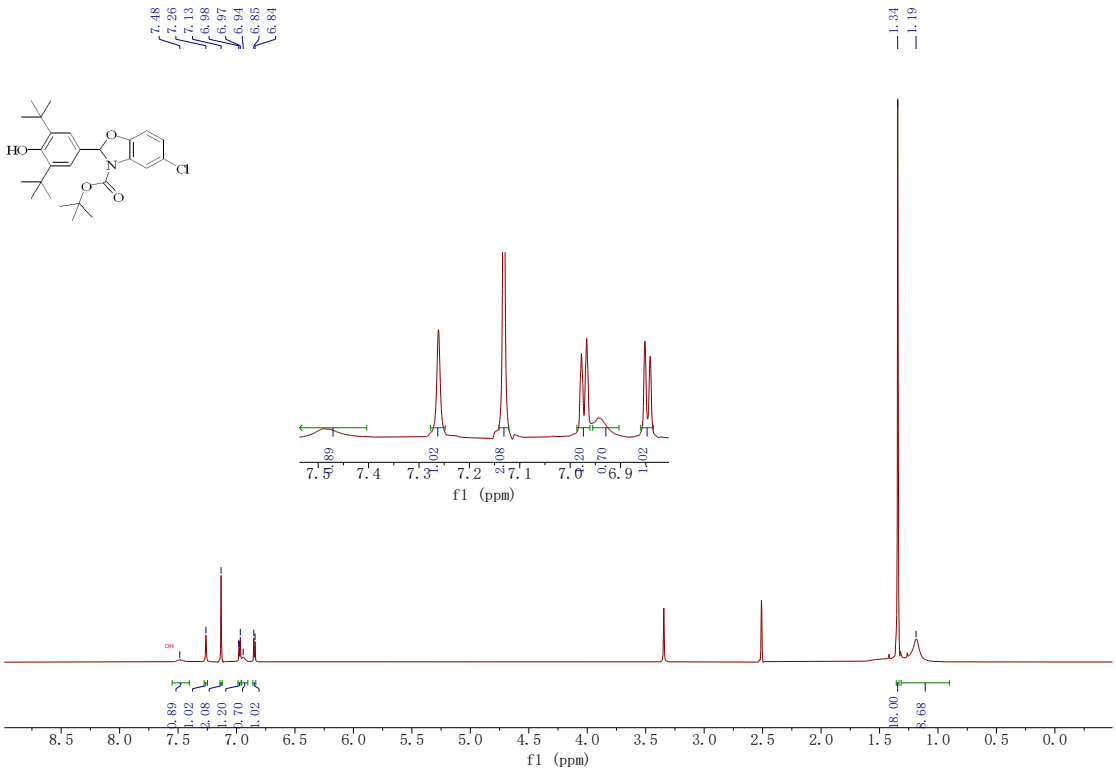


Figure S33. ^{1}H NMR (800 MHz, DMSO-d_6) of **3q**

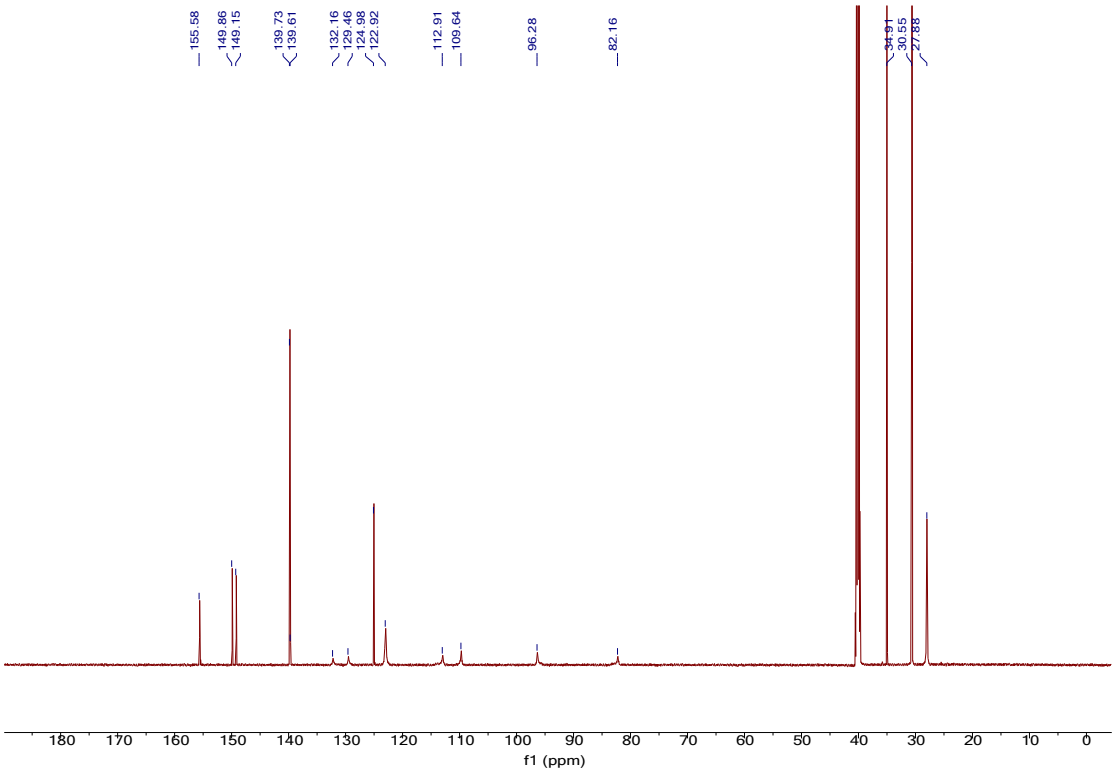


Figure S34. ^{13}C NMR (200 MHz, DMSO-d_6) of **3q**

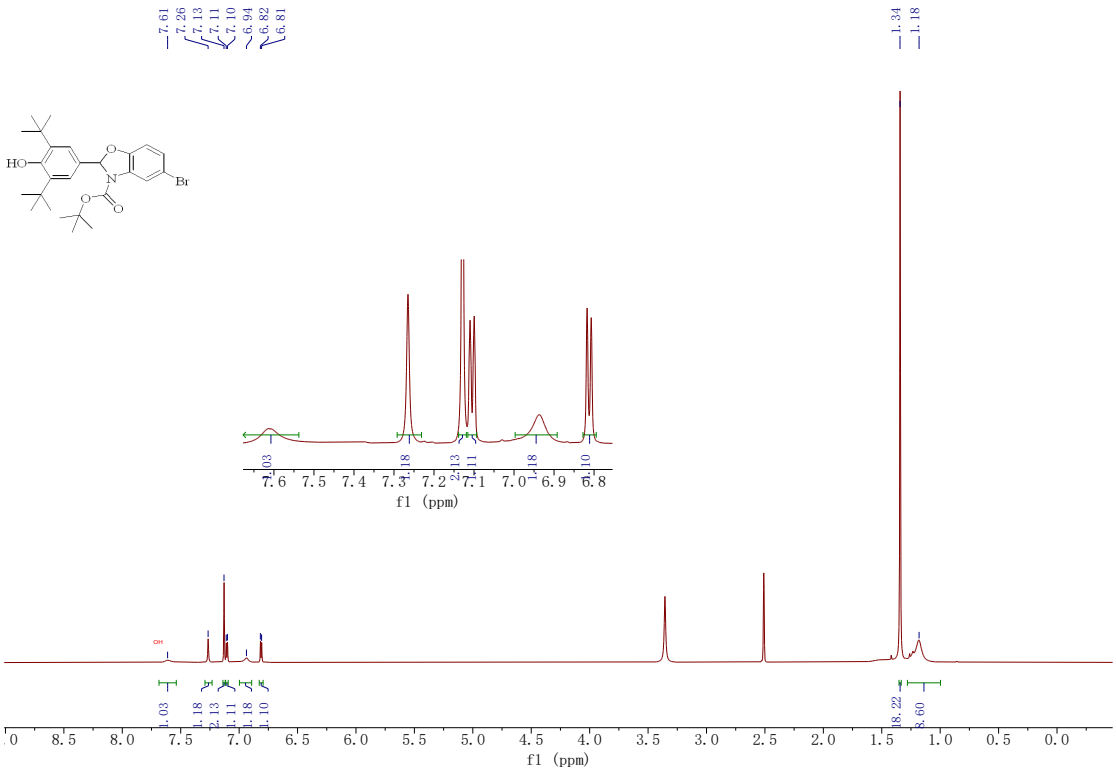


Figure S35. ^{1}H NMR (800 MHz, DMSO-d_6) of **3r**

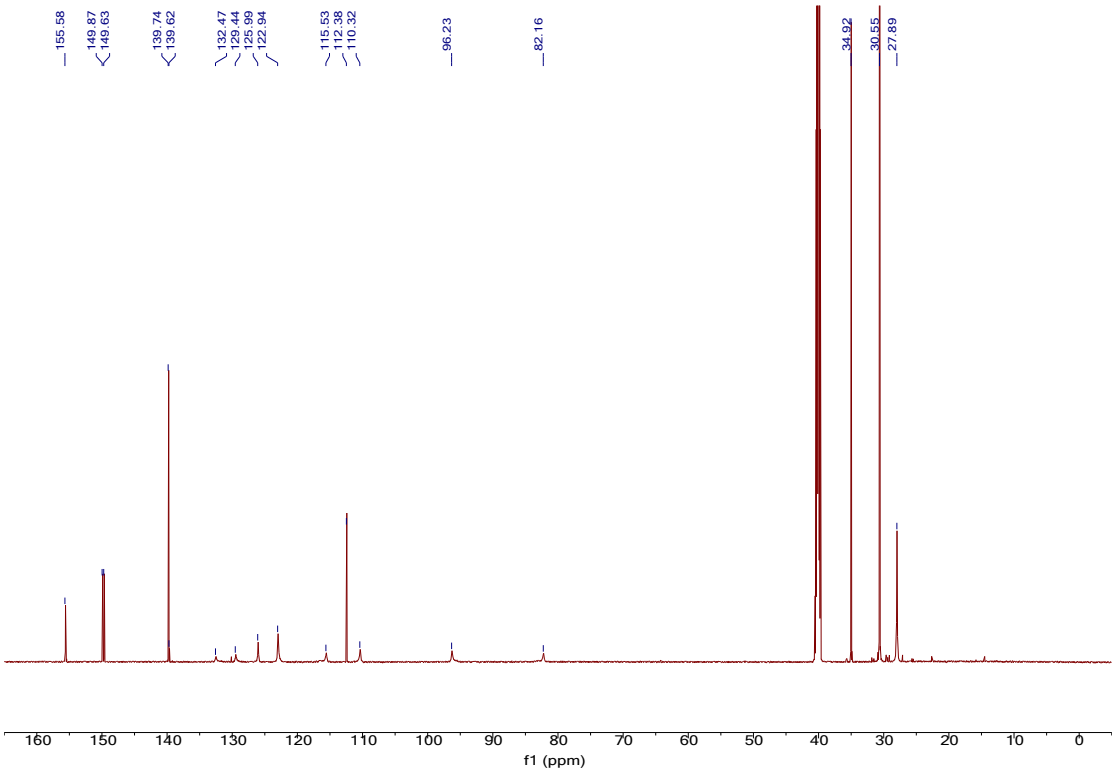


Figure S36. ^{13}C NMR (200 MHz, DMSO-d_6) of **3r**

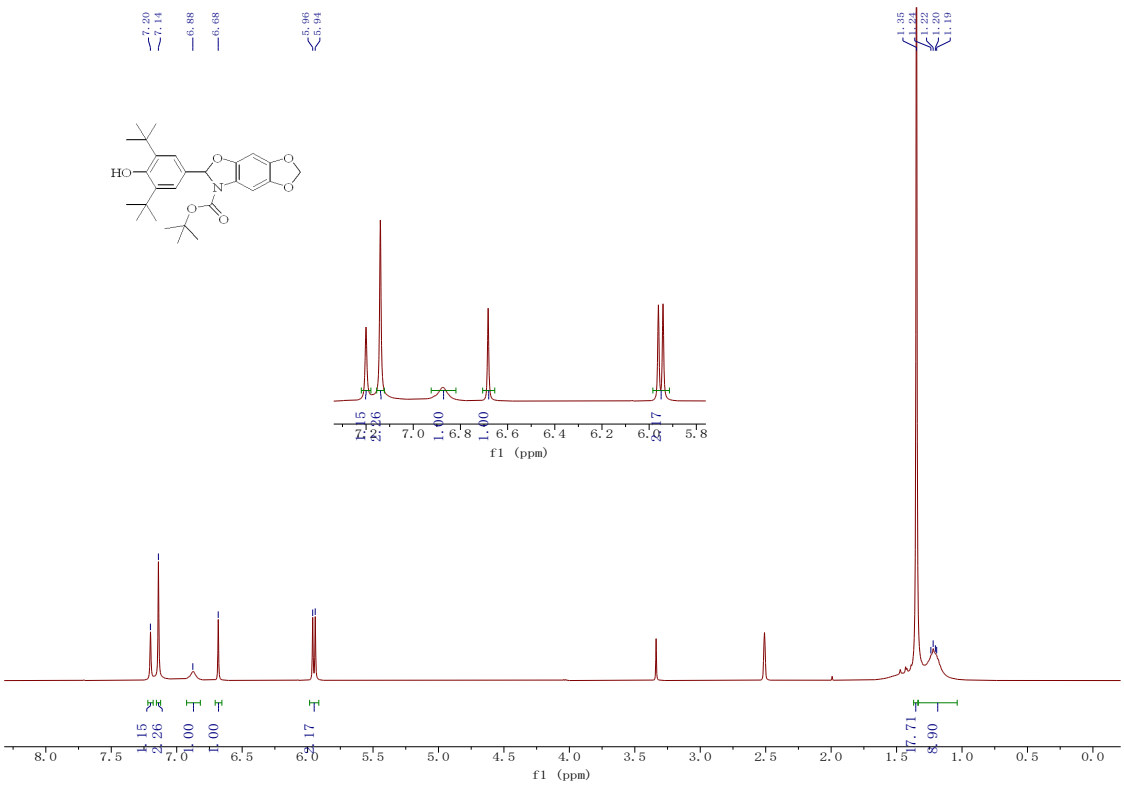


Figure S37. ^{1}H NMR (500 MHz, DMSO-d_6) of **3s**

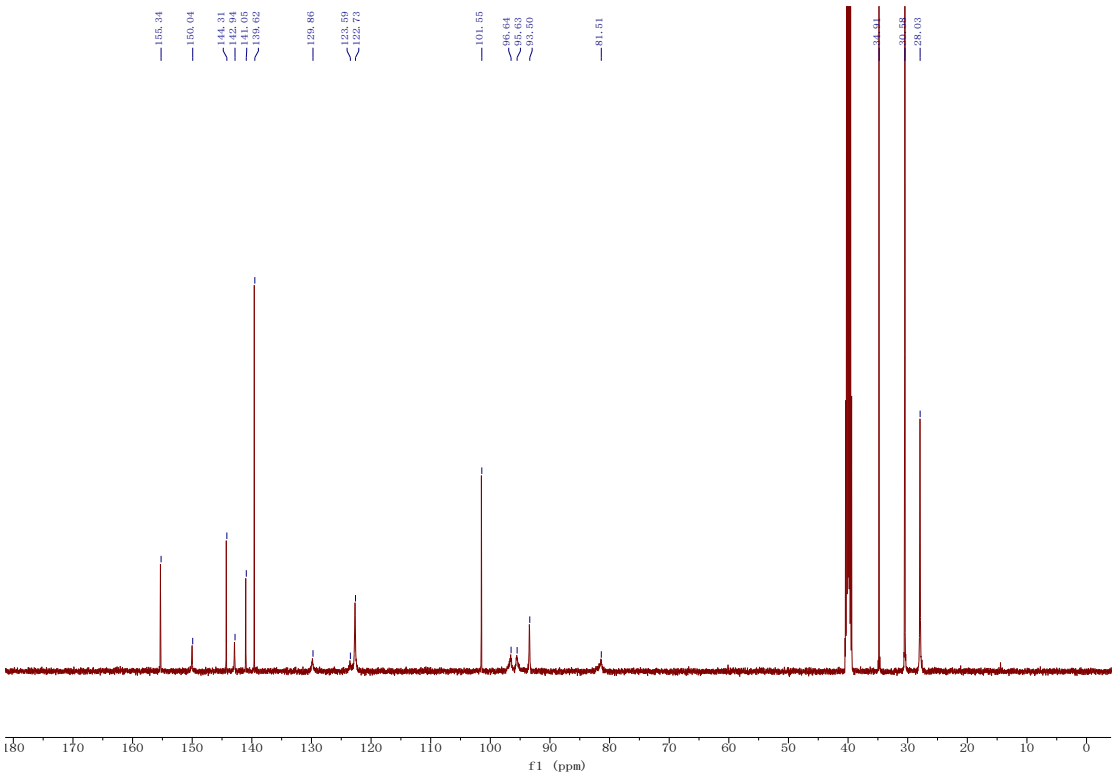


Figure S38. ^{13}C NMR (125 MHz, DMSO-d_6) of **3s**

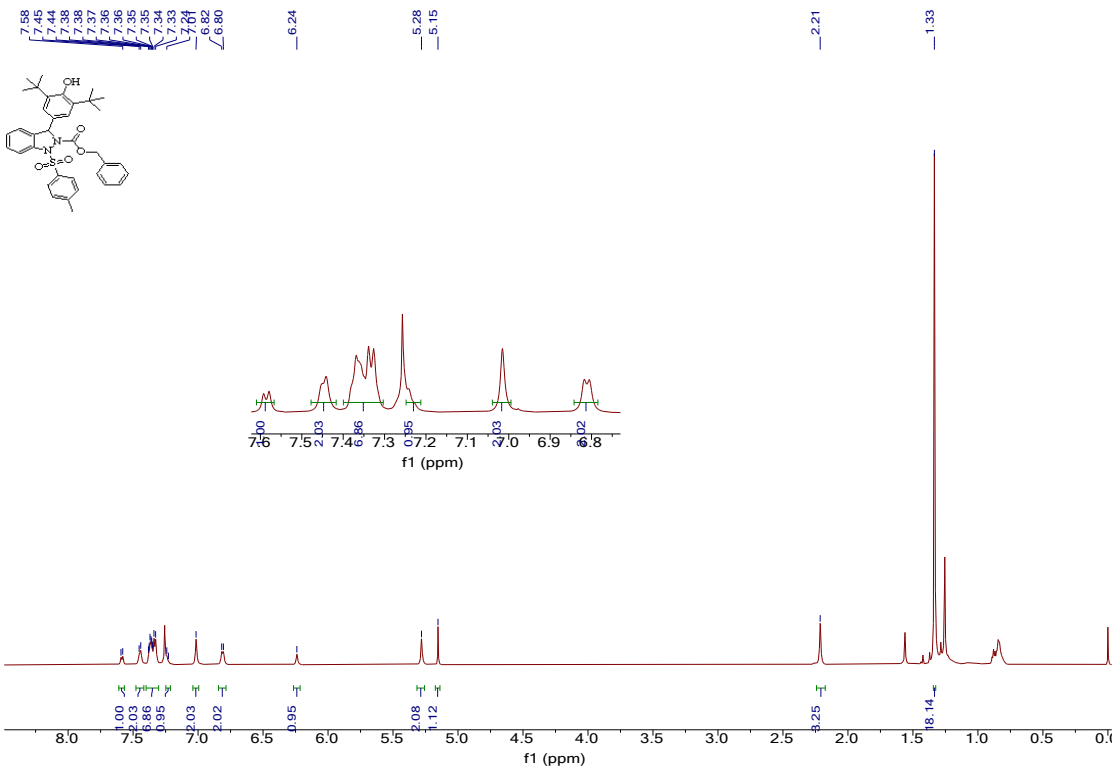


Figure S39. ^{1}H NMR (600 MHz, $CDCl_3$) of **5a**

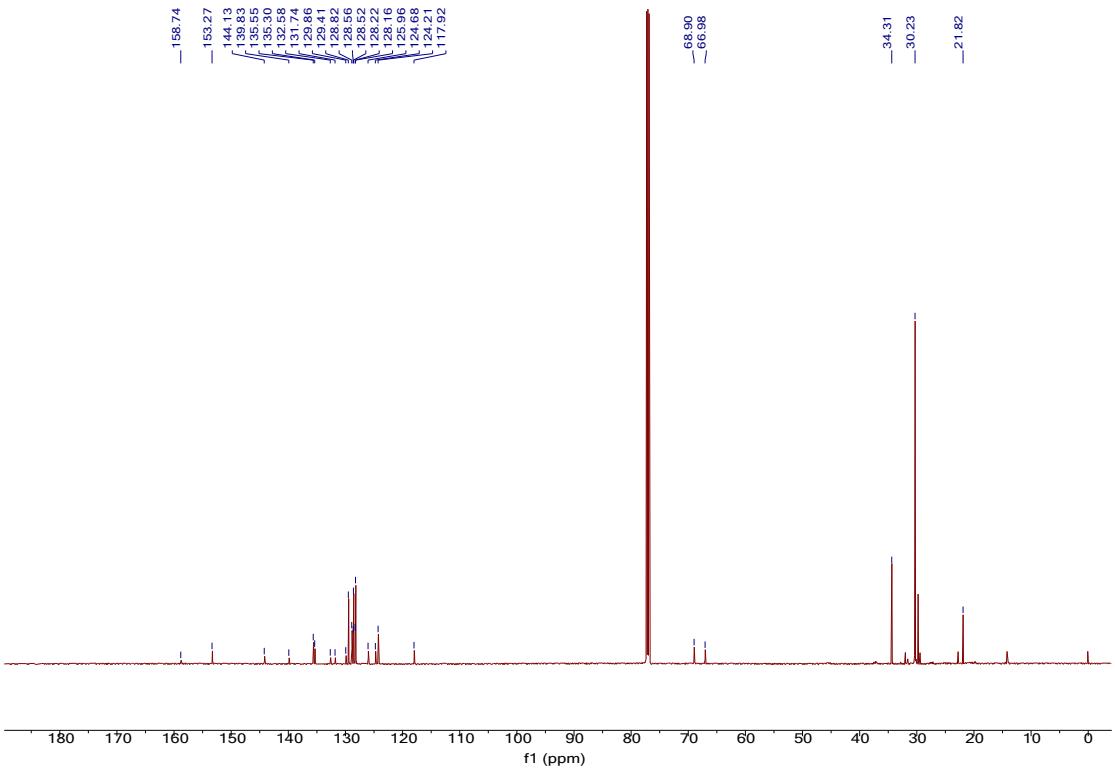


Figure S40. ^{13}C NMR (150 MHz, $CDCl_3$) of **5a**

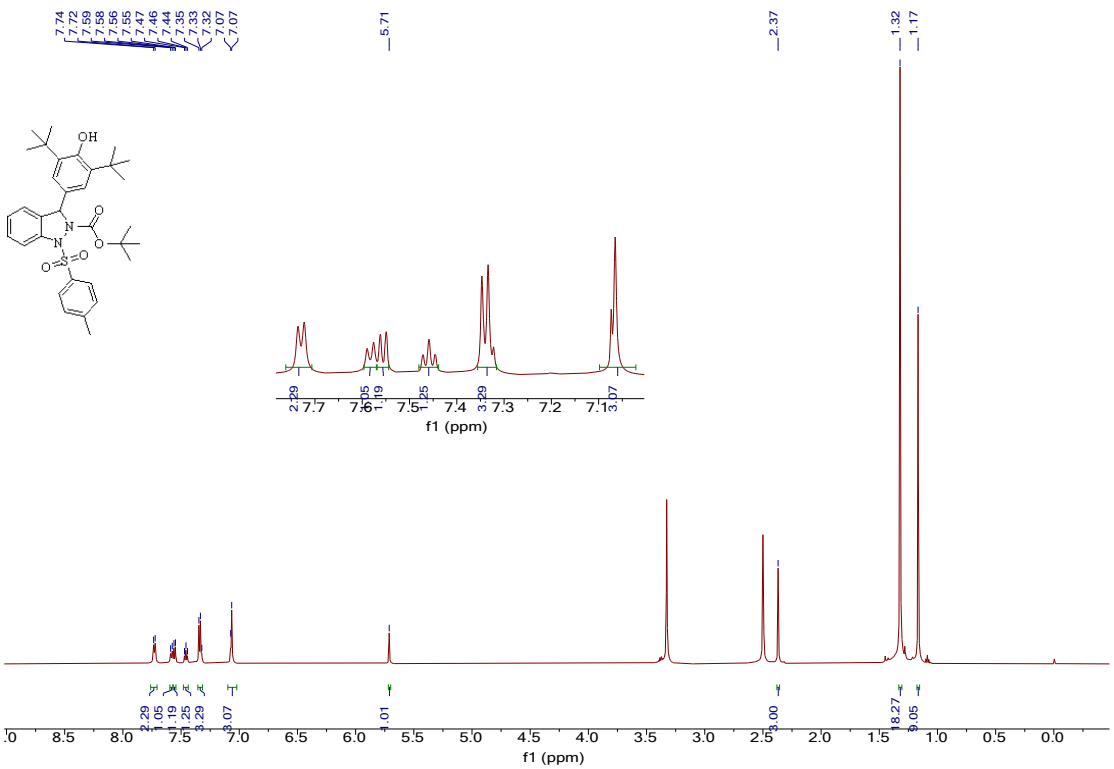


Figure S41. [1]H NMR (600 MHz, DMSO-d_6) of **5b**

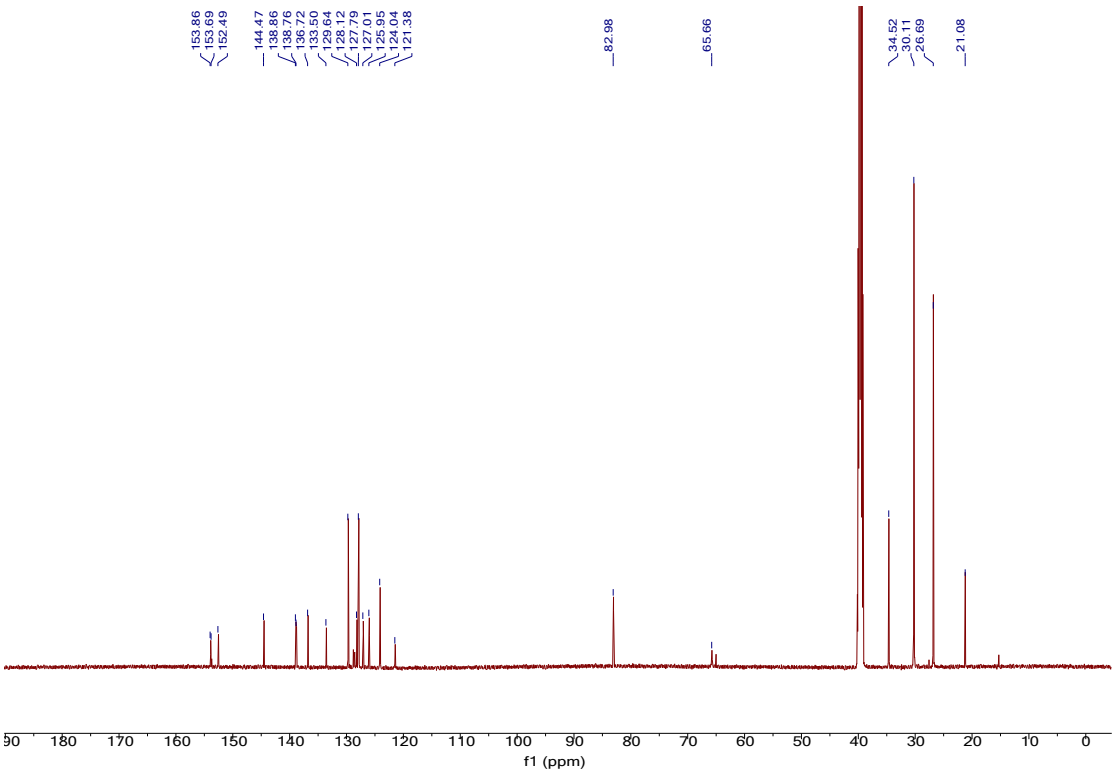


Figure S42. [13]C NMR (150 MHz, DMSO-d_6) of **5b**

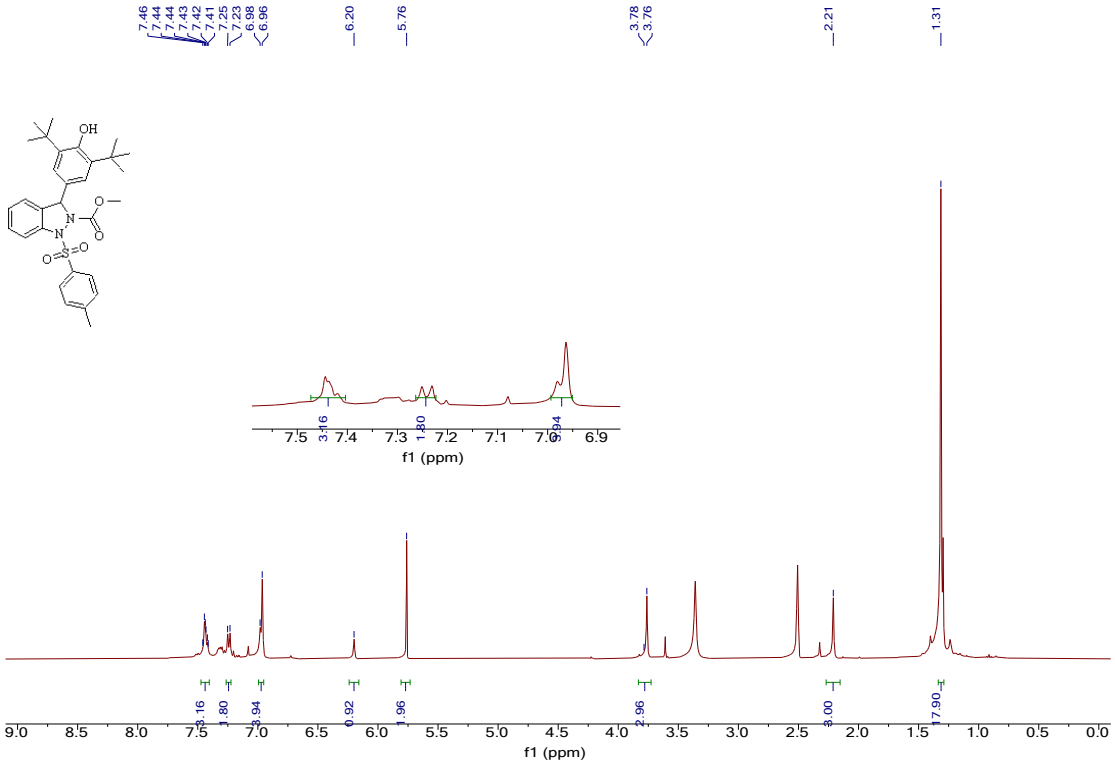


Figure S43. ^{1}H NMR (400 MHz, DMSO-d_6) of **5c**

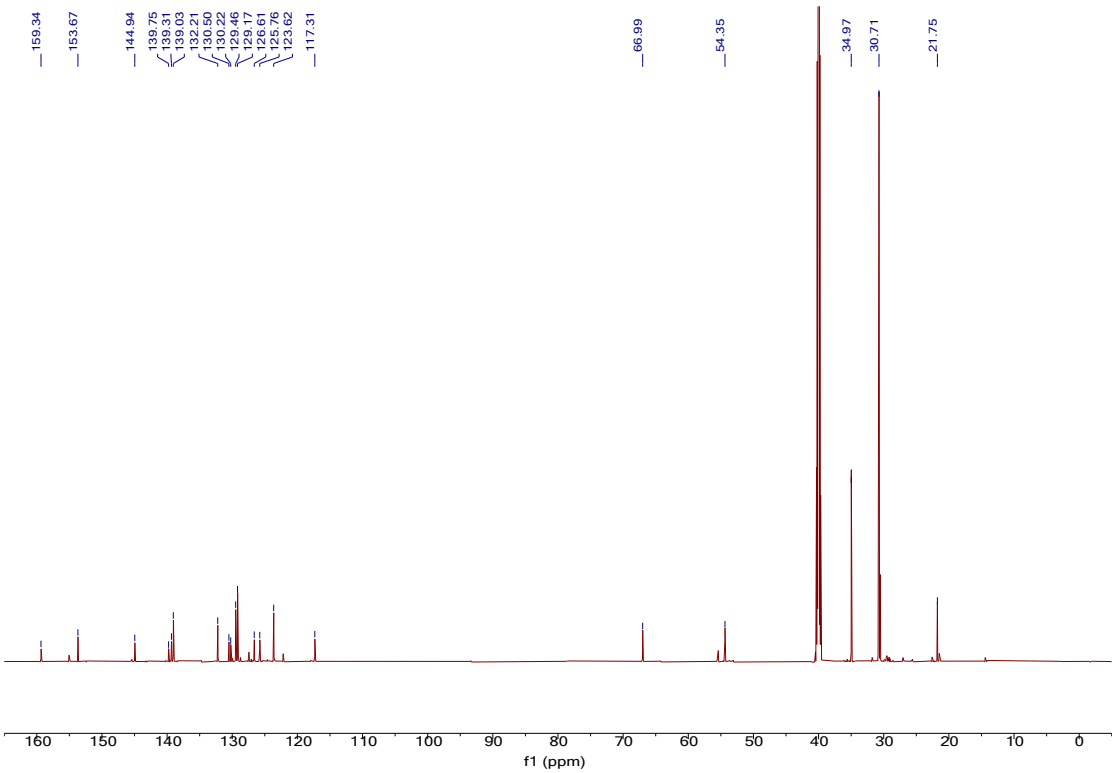


Figure S44. ^{13}C NMR (200 MHz, DMSO-d_6) of **5c**

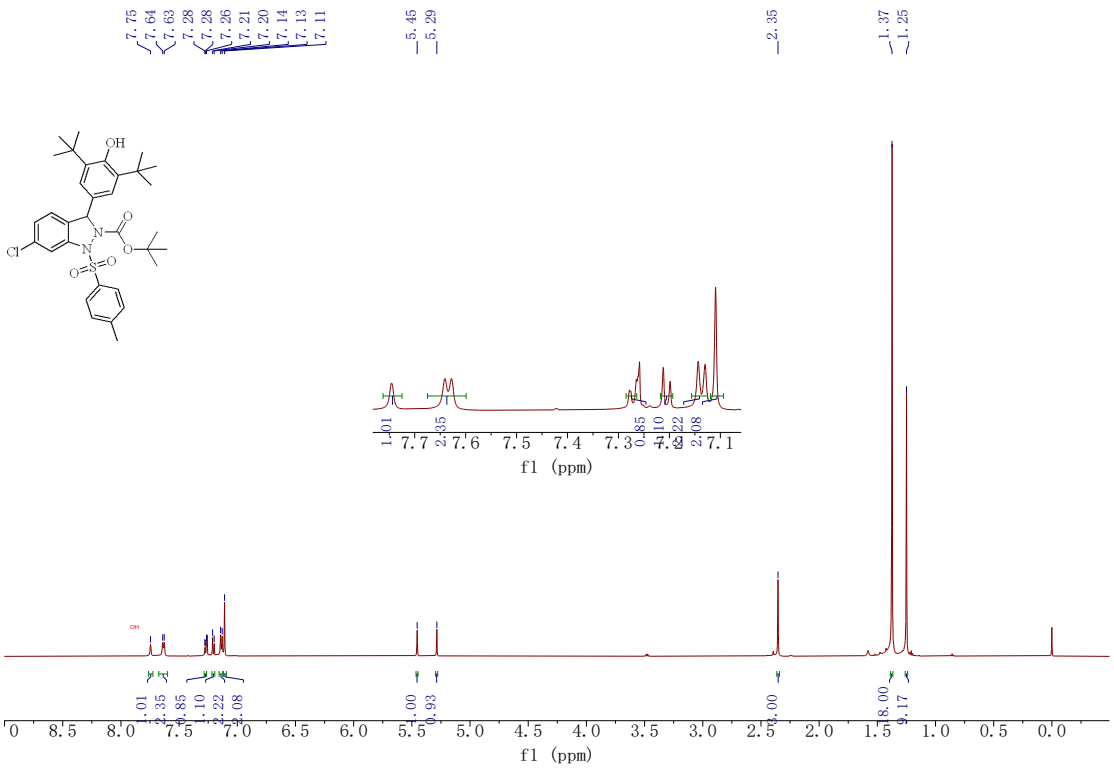


Figure S45. ^{1}H NMR (600 MHz, $CDCl_3$) of **5d**

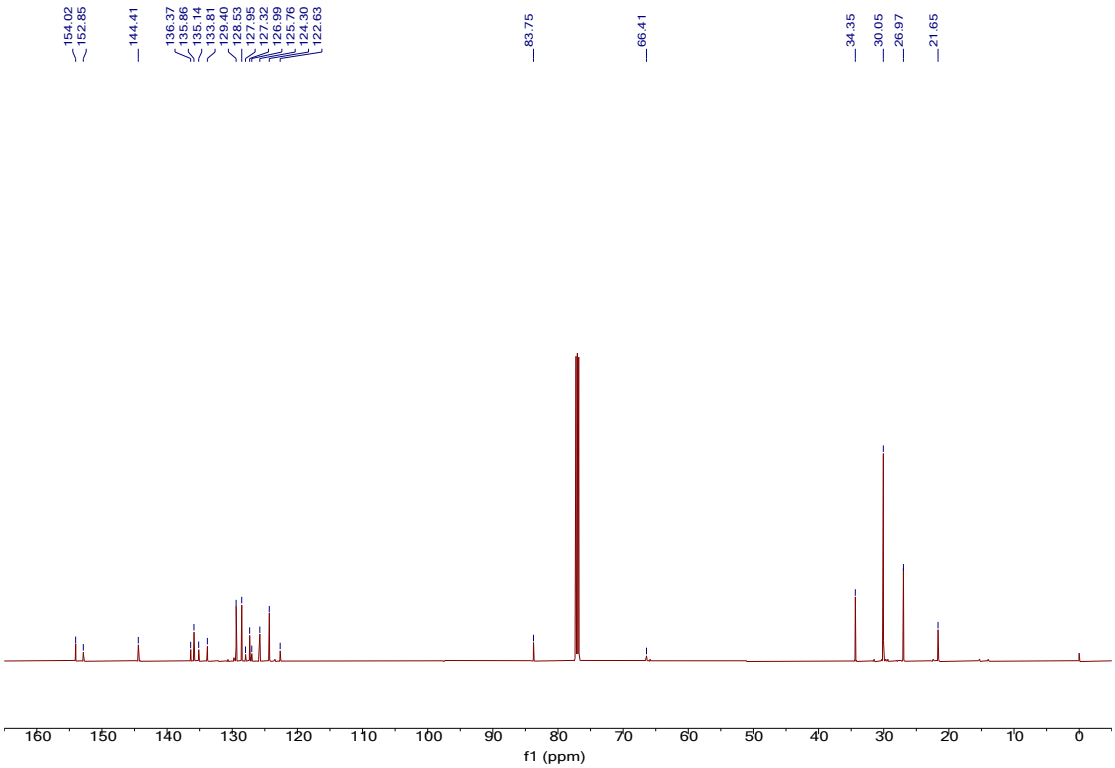


Figure S46. ^{13}C NMR (150 MHz, $CDCl_3$) of **5d**

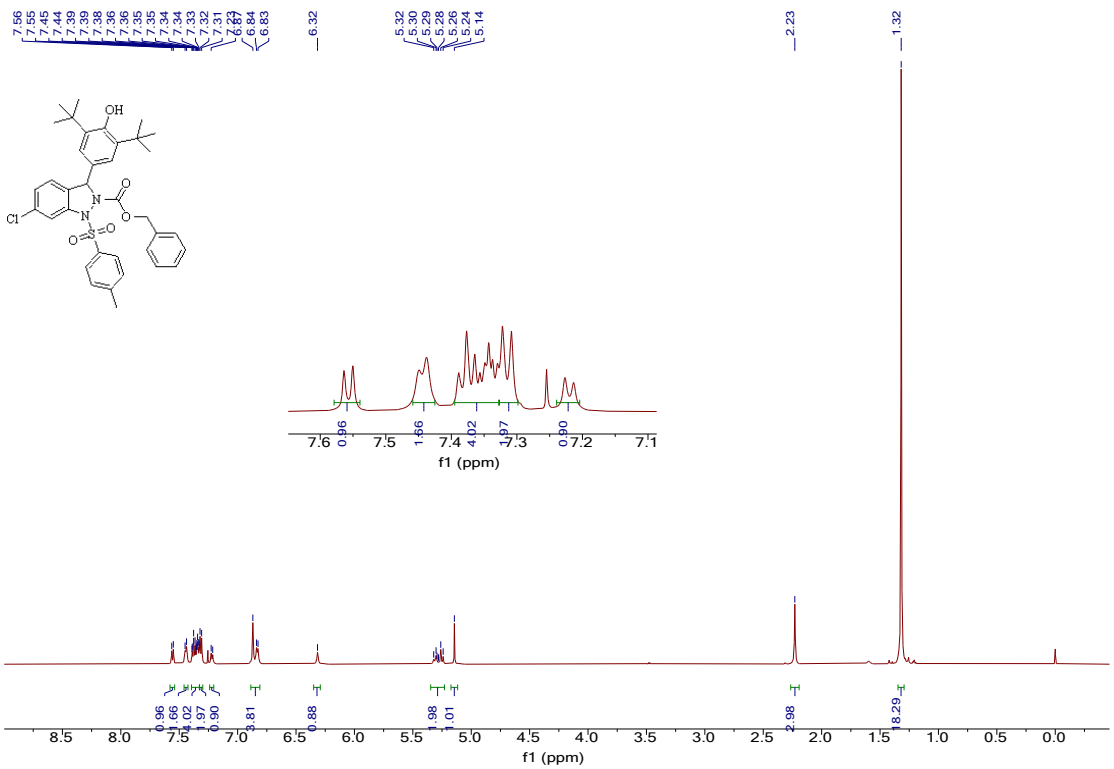


Figure S47. ^{1}H NMR (600 MHz, $CDCl_3$) of **5e**

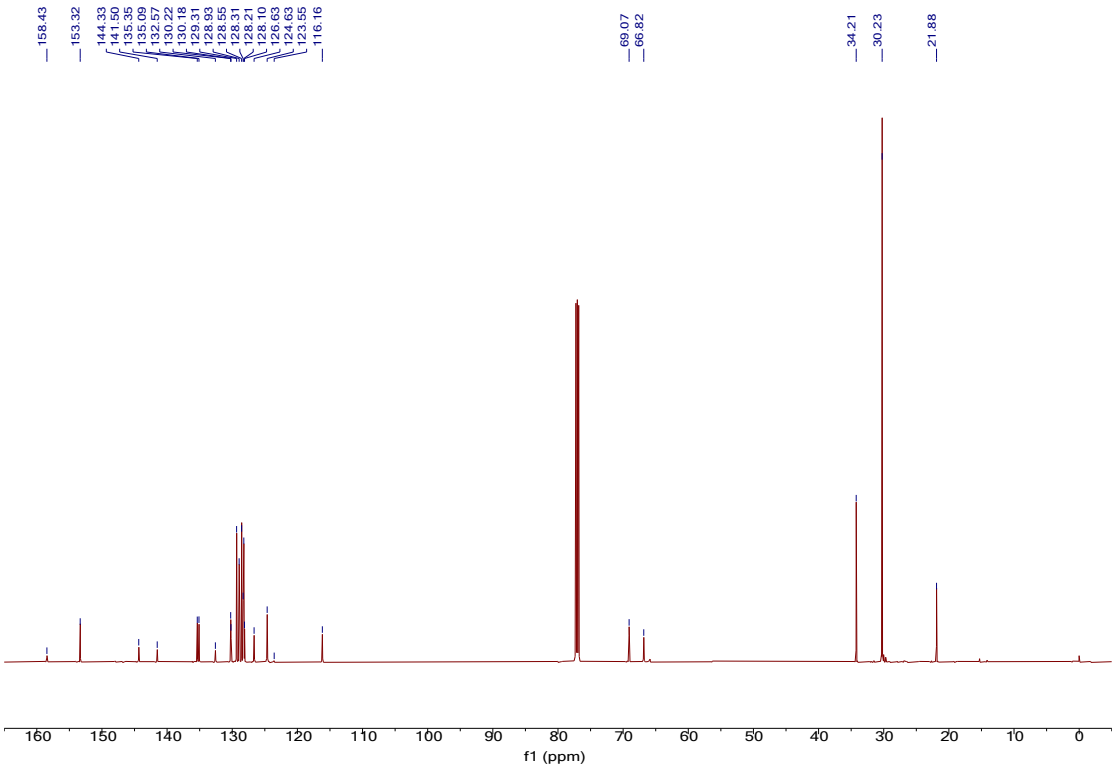


Figure S48. ^{13}C NMR (150 MHz, $CDCl_3$) of **5e**

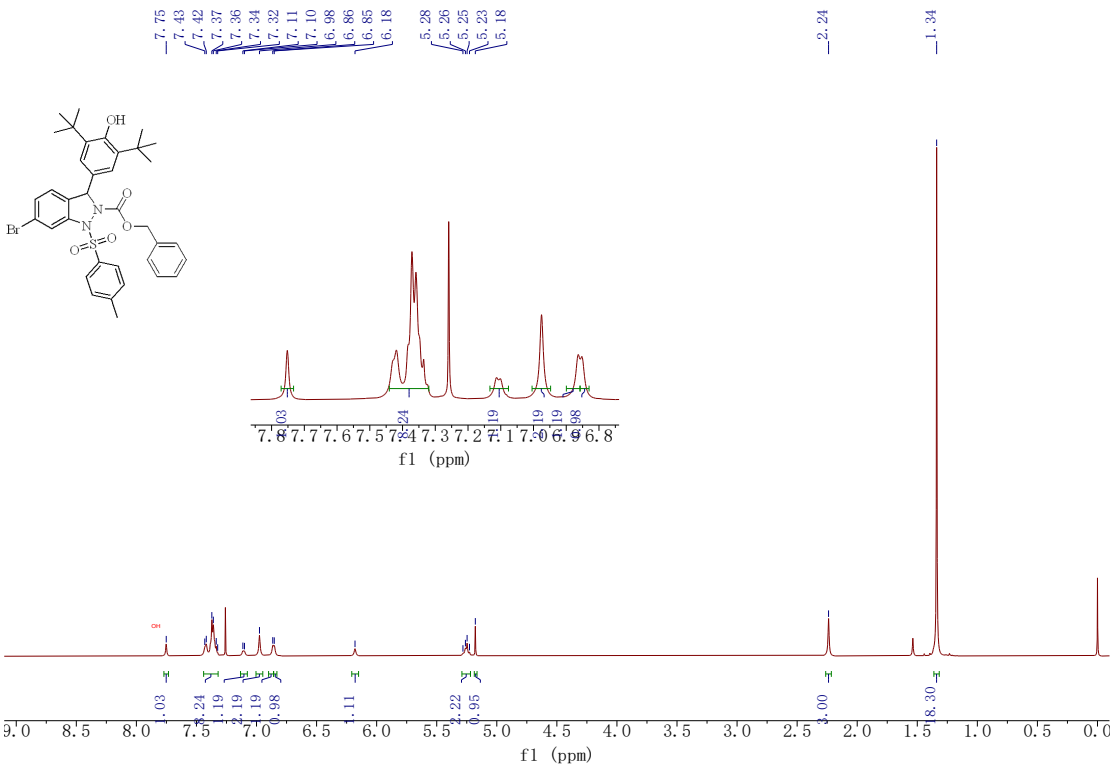


Figure S49. ^{1}H NMR (600 MHz, $CDCl_3$) of **5f**

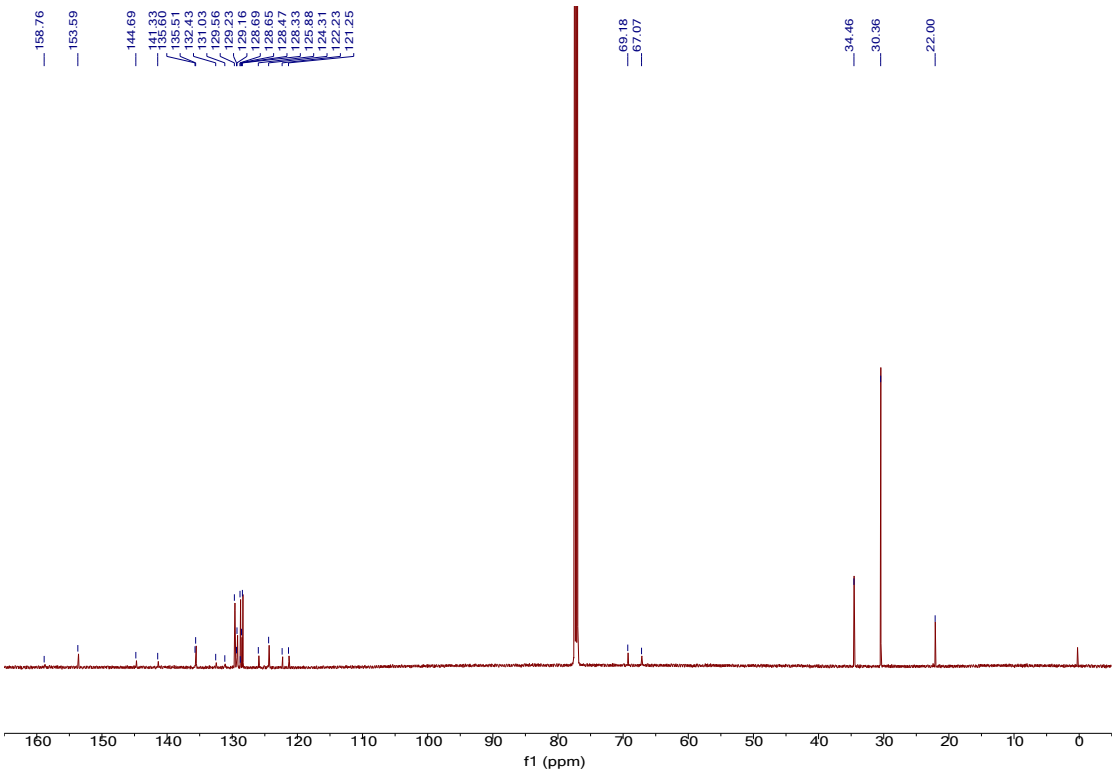


Figure S50. ^{13}C NMR (150 MHz, $CDCl_3$) of **5f**

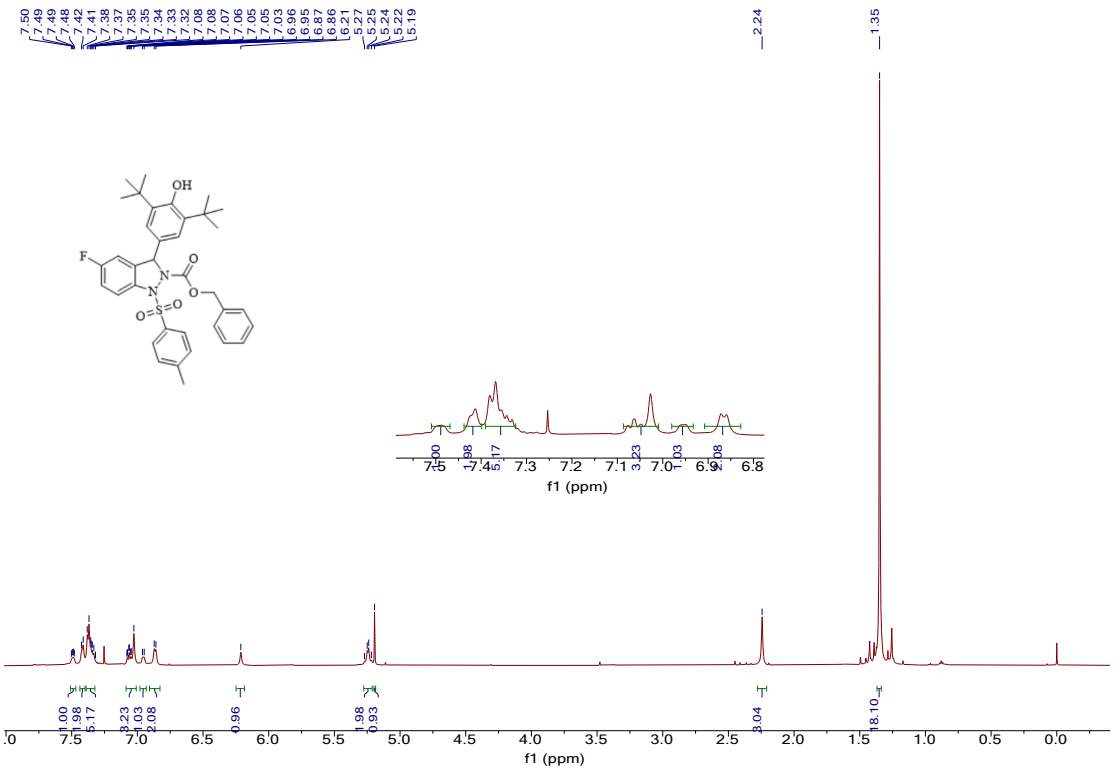


Figure S51. ^{1}H NMR (600 MHz, $CDCl_3$) of **5g**

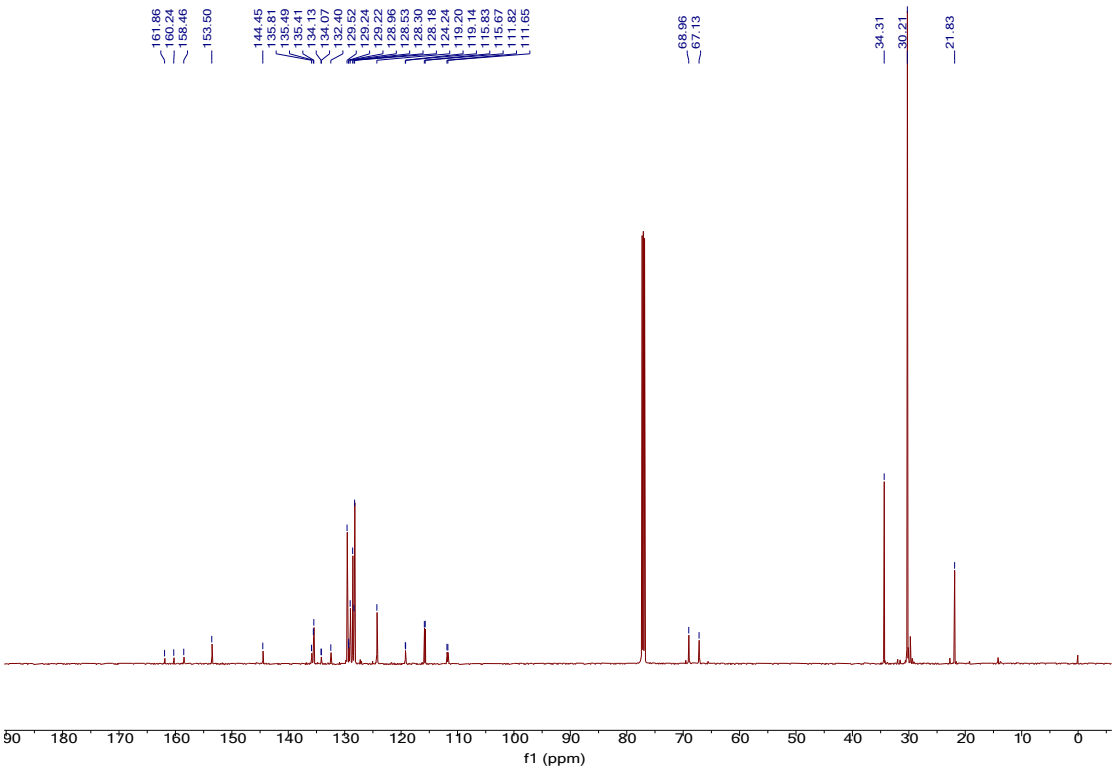


Figure S52. ^{13}C NMR (150 MHz, $CDCl_3$) of **5g**

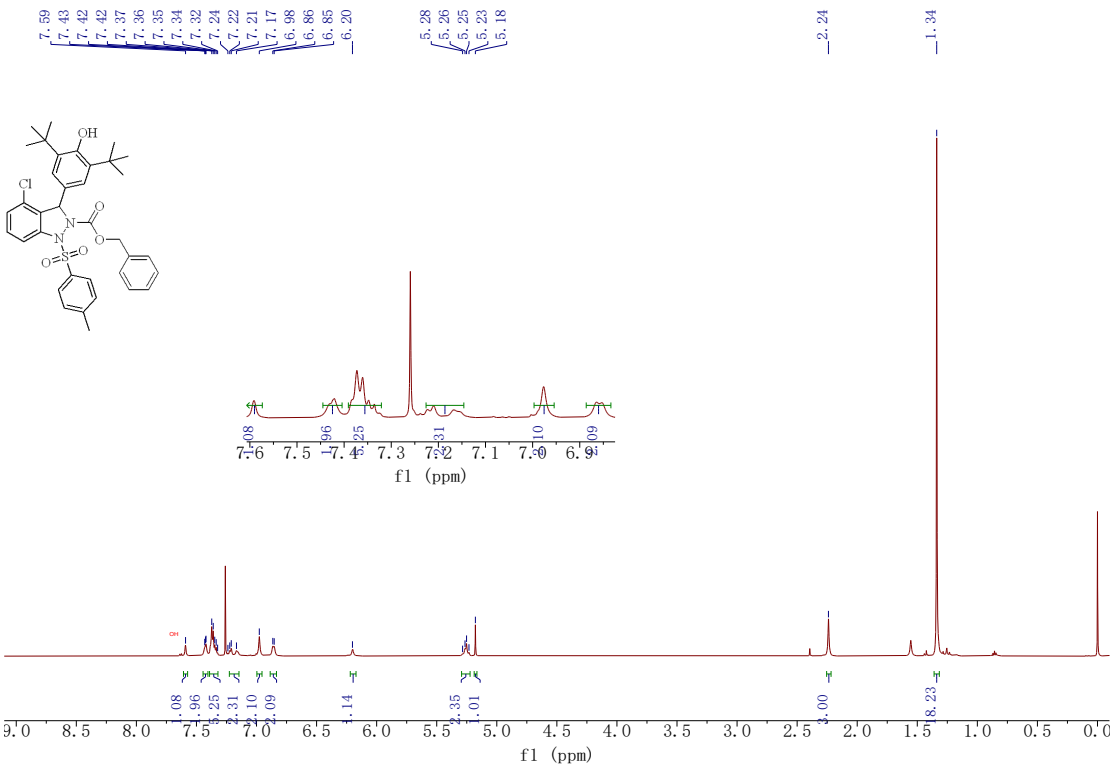


Figure S53. ^{1}H NMR (600 MHz, $CDCl_3$) of **5h**

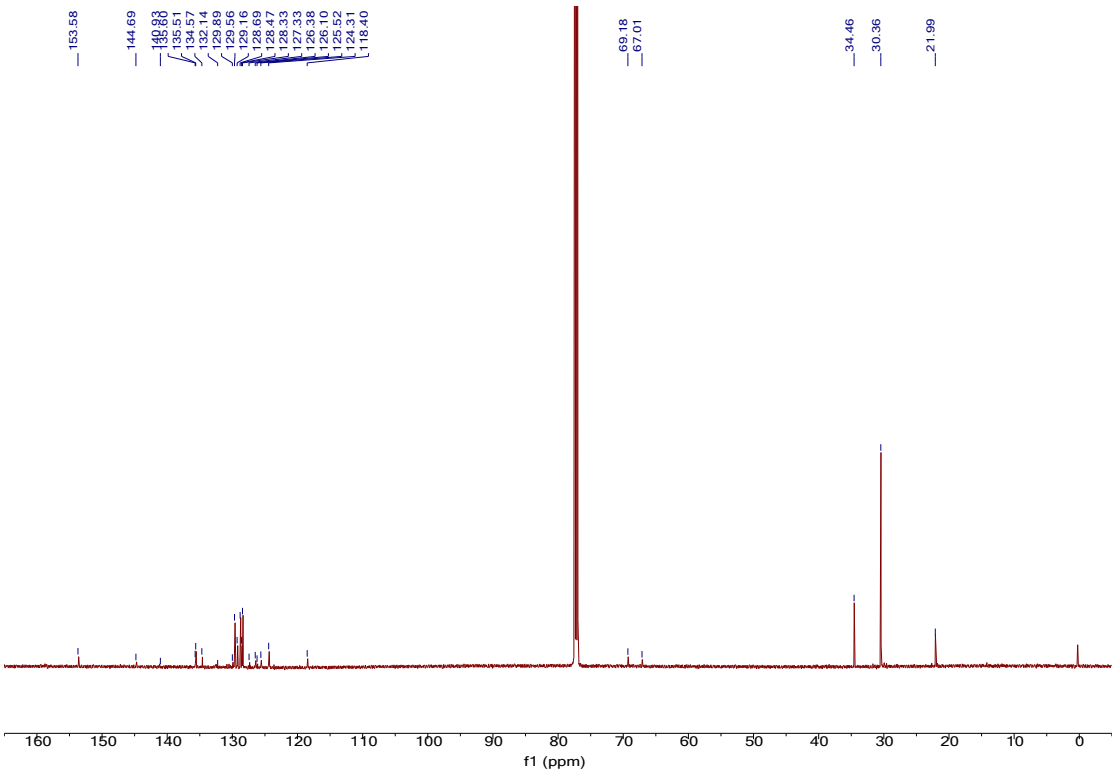


Figure S54. ^{13}C NMR (150 MHz, $CDCl_3$) of **5h**

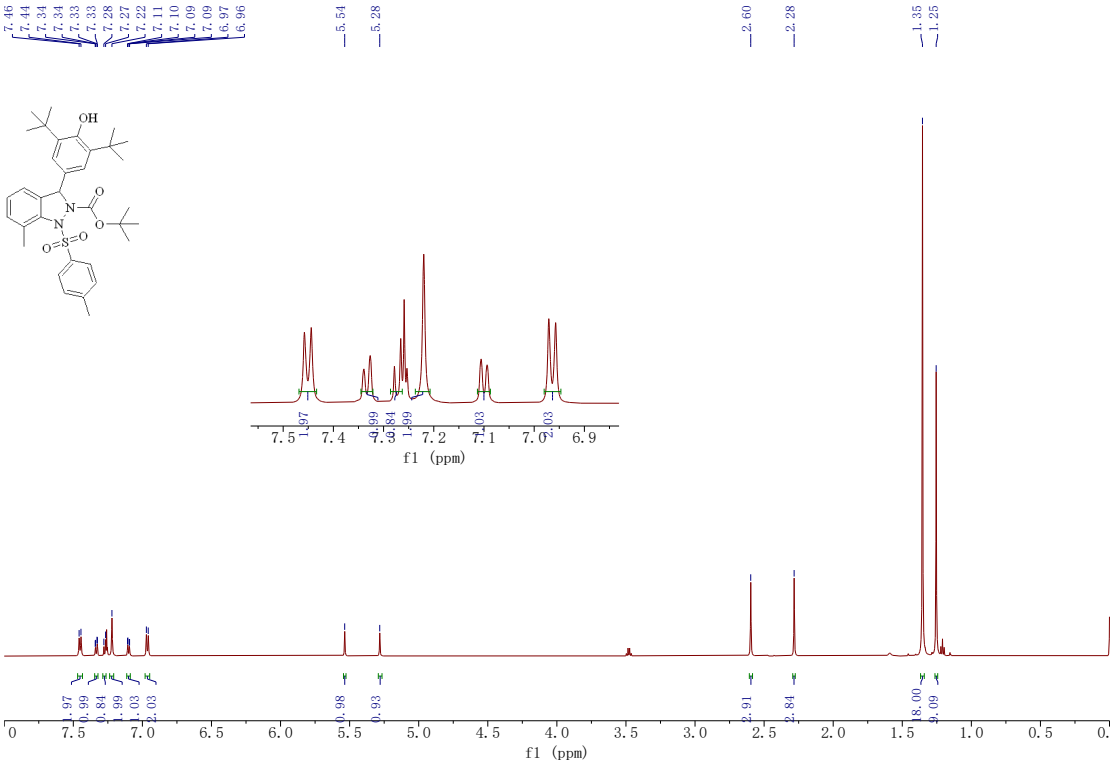


Figure S55. ^{1}H NMR (600 MHz, $CDCl_3$) of **5i**

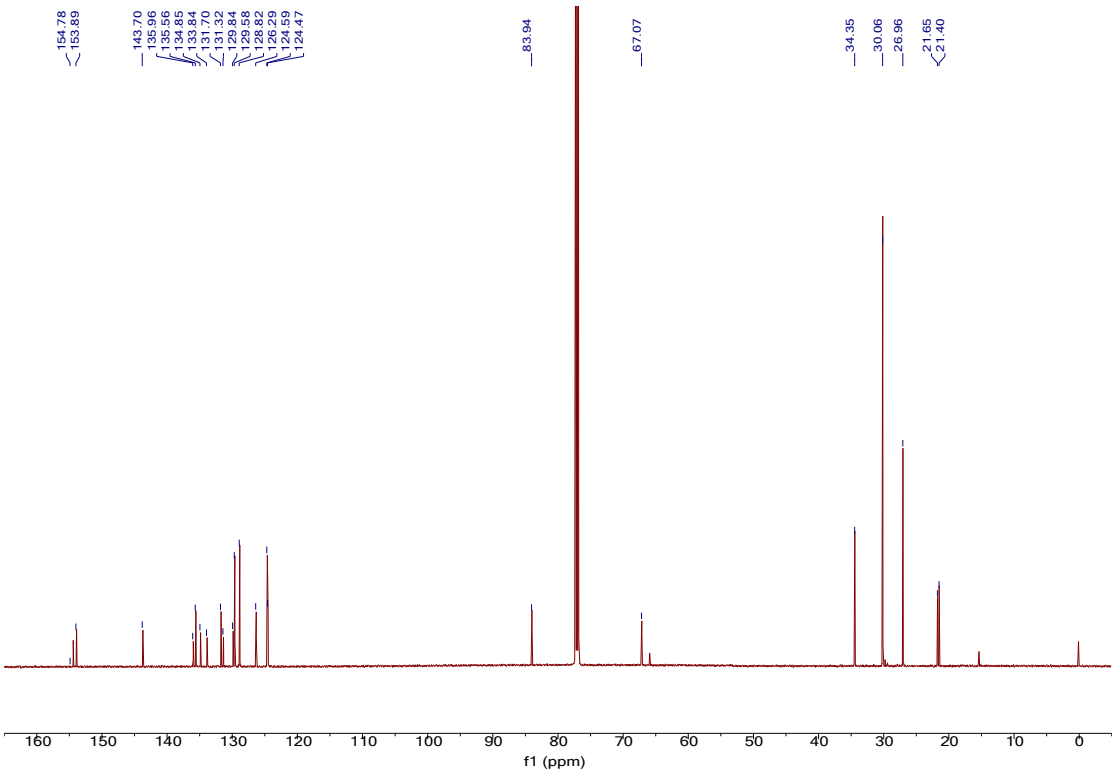


Figure S56. ^{13}C NMR (150 MHz, $CDCl_3$) of **5i**

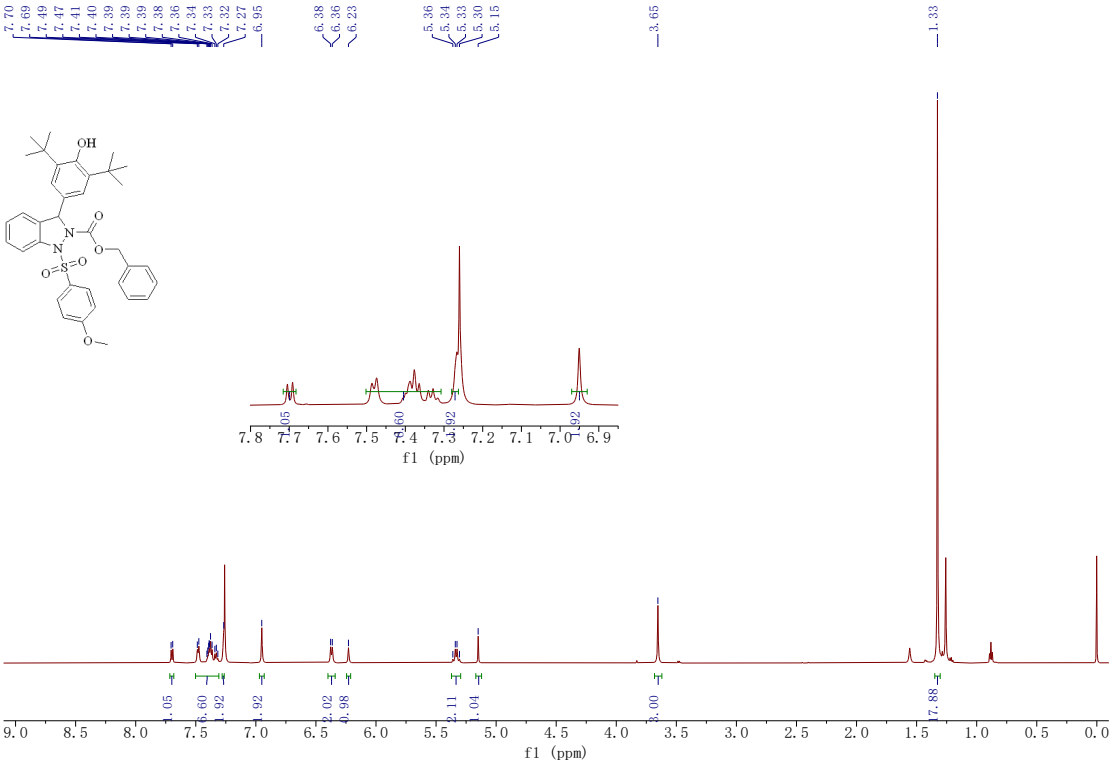


Figure S57. ^{1}H NMR (600 MHz, $CDCl_3$) of **5j**

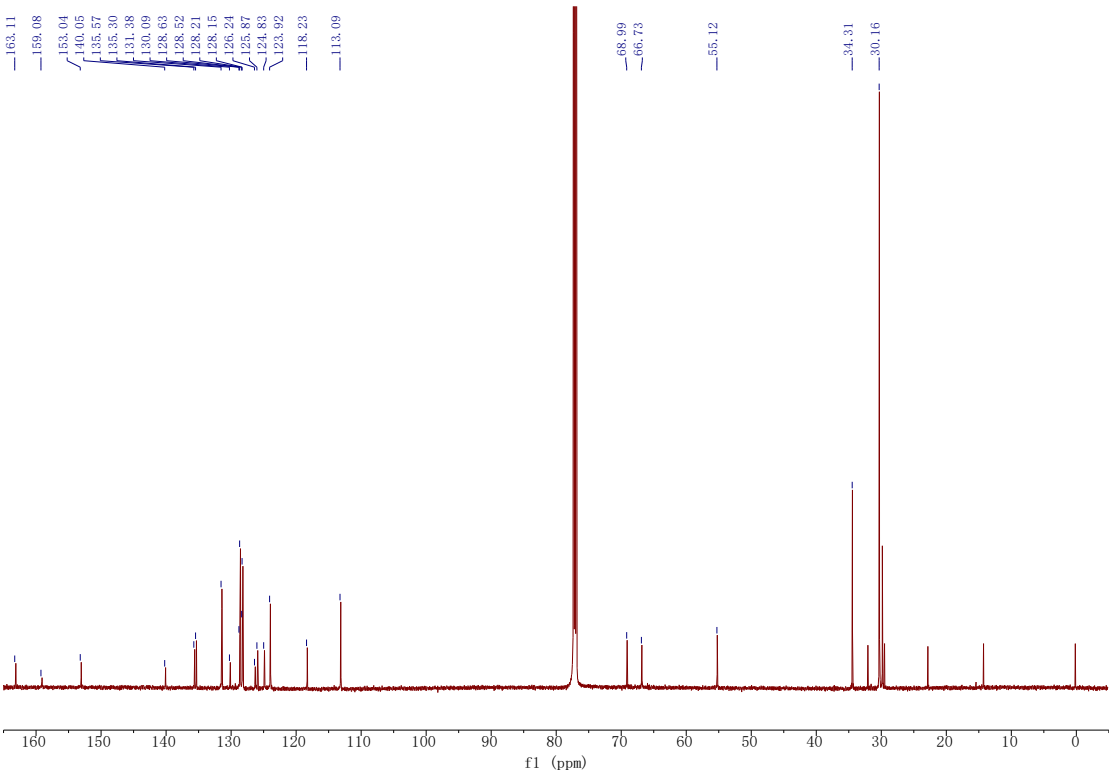


Figure S58. ^{13}C NMR (150 MHz, $CDCl_3$) of **5j**

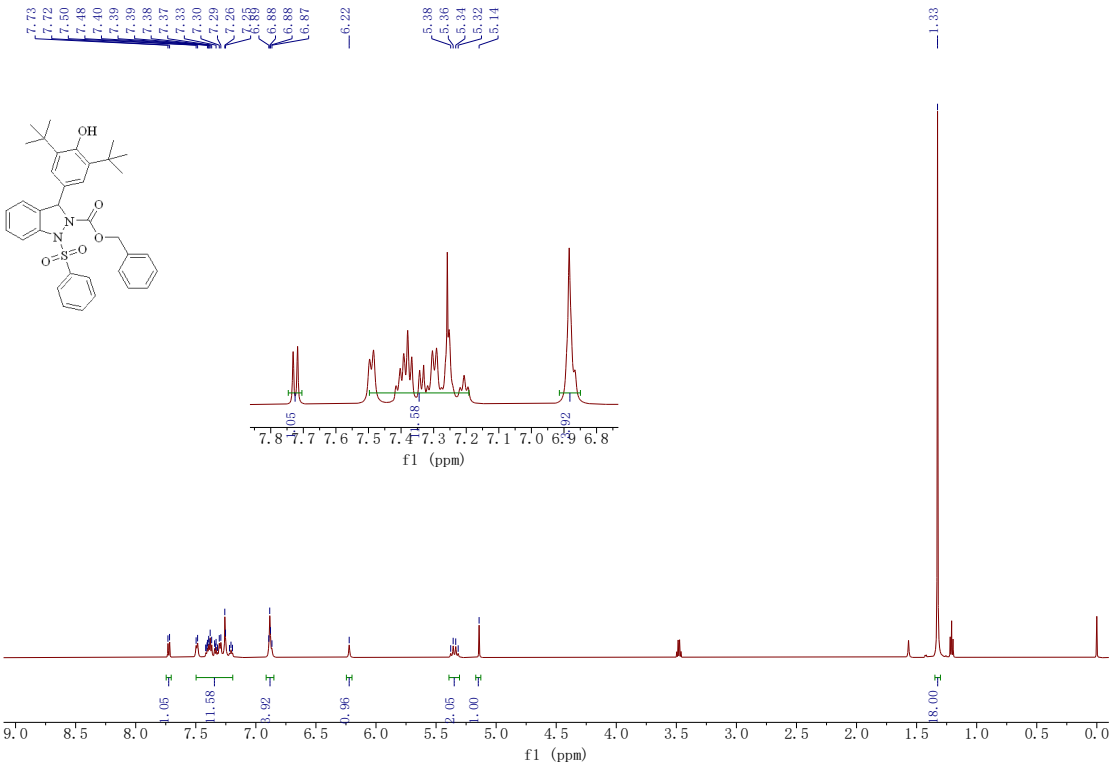


Figure S59. ^{1}H NMR (600 MHz, $CDCl_3$) of **5k**

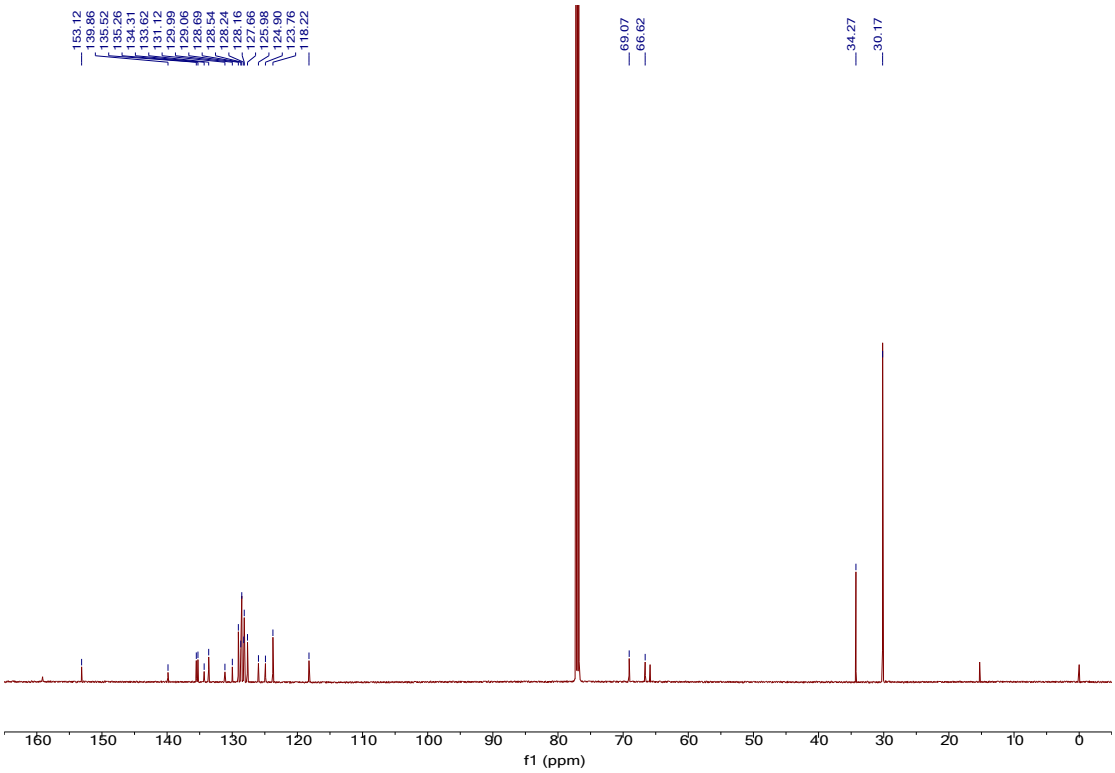


Figure S60. ^{13}C NMR (150 MHz, $CDCl_3$) of **5k**

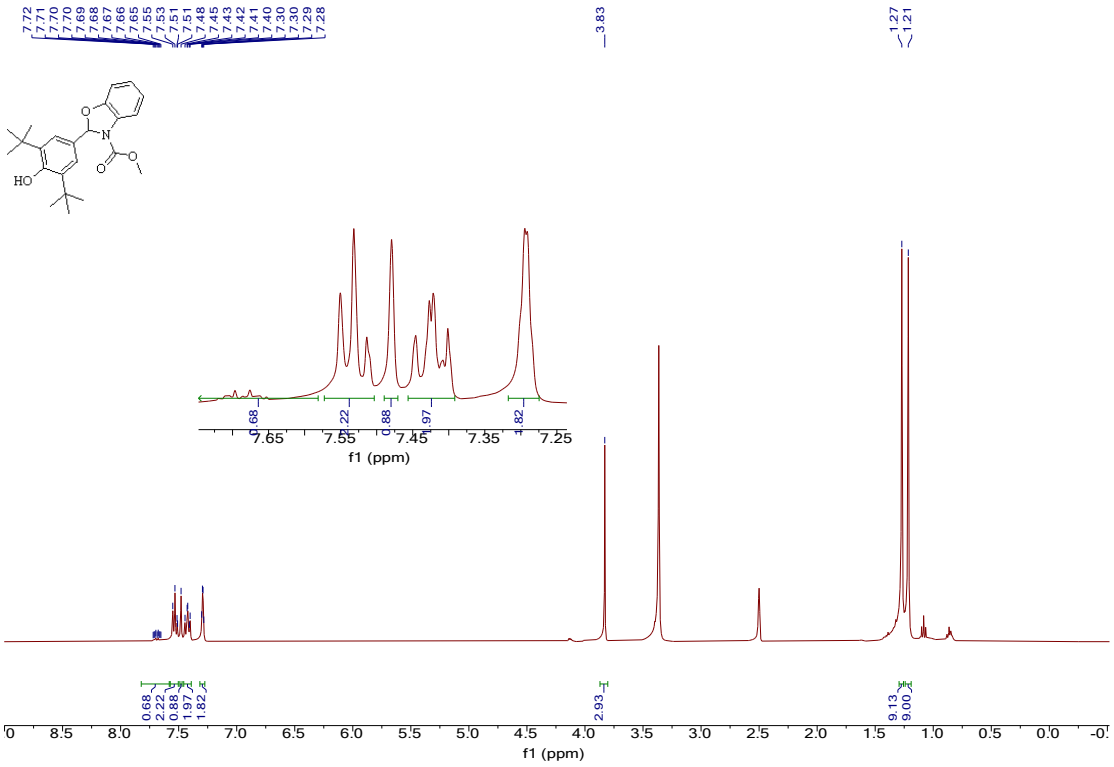


Figure S61. ^{1}H NMR (400 MHz, DMSO-d_6) of **6**

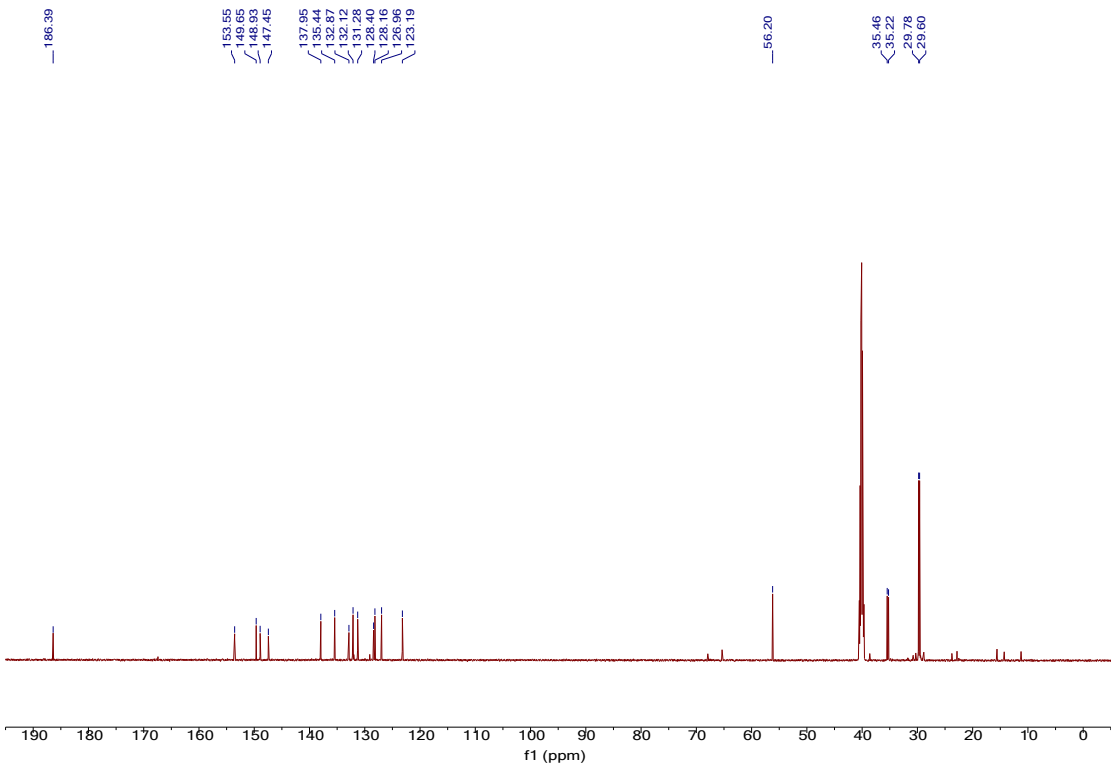
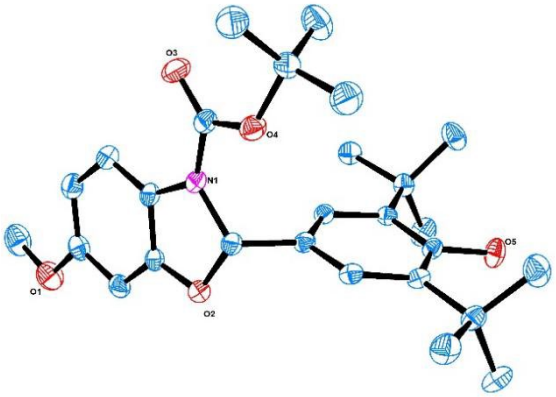


Figure S62. ^{13}C NMR (150 MHz, DMSO-d_6) of **6**

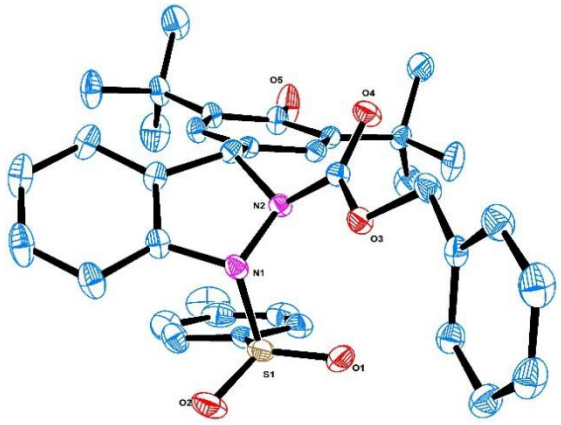
9. X-Ray Data

Crystal structure of the compound **3l**. The sample was dissolved at room temperature in ethyl ether and then hexane was slowly added to reach the following ratio: ethyl ether/hexane : 1/5. The solution was left at room temperature to wait for crystallisation. (CCDC：2323527)



Identification code	Datablock: a		
Bond precision	C-C = 0.0029 A	Wavelength= 0.71073	
Cell:	a= 25.190(2)	b= 9.8501(9)	c= 21.7157(19)
	alpha= 90	beta= 105.144(3)	gamma= 90
Temperature:	193 K		
	Calculated	Reported	
Volume	5201.1(8)	5201.1(8)	
Space group	C 2/c	C 1 2/c 1	
Hall group	-C 2yc	-C 2yc	
Moiety formula	C27 H37 N O5	C27 H37 N O5	
Sum formula	C27 H37 N O5	C27 H37 N O5	
Mr	455.58	455.57	
Dx,g cm-3	1.164	1.164	
Z	8	8	
Mu (mm-1)	0.079	0.079	
F000	1968.0	1968.0	
F000’	1968.93		
h,k,lmax	32, 12, 28	32, 12, 28	
Nref	5976	5958	
Tmin,Tmax	0.991, 0.992	0.678, 0.746	
Tmin’	0.991		
Correction method= # Reported T Limits: Tmin= 0.678 Tmax= 0.746 AbsCorr= MULTI-SCAN			
Data completeness= 0.997	Theta(max)= 27.494		
R(reflections)= 0.0595(47)		wR2(reflections)= 0.1713(5958)	
S= 1.057	Npar= 308		

Crystal structure of the compound **5a**. The sample was dissolved at room temperature in ethyl ether and then hexane was slowly added to reach the following ratio: ethyl ether/hexane : 1/5. The solution was left at room temperature to wait for crystallisation. (CCDC：2323528)



Identification code	2105068646_0m		
Bond precision	C-C = 0.0038 A	Wavelength= 1.34139	
Cell:	a= 10.1195(5)	b= 11.8196(6)	c= 27.3168(14)
	alpha= 90	beta= 90	gamma= 90
Temperature:	296 K		
	Calculated	Reported	
Volume	3267.3(3)	3267.3(3)	
Space group	P 21 21 21	P 21 21 21	
Hall group	P 2ac 2ab	P 2ac 2ab	
Moiety formula	C36 H40 N2 O5 S	C36 H40 N2 O5 S	
Sum formula	C36 H40 N2 O5 S	C36 H40 N2 O5 S	
Mr	612.76	612.76	
Dx,g cm-3	1.246	1.246	
Z	4	4	
Mu (mm-1)	0.803	0.800	
F000	1304.0	1304.0	
F000’	1307.94		
h,k,lmax	12, 14, 33	12, 14, 33	
Nref	6248[3533]	6228	
Tmin,Tmax	0.953, 0.961	0.619, 0.751	
Tmin’	0.953		
Correction method= # Reported T Limits: Tmin= 0.619 Tmax= 0.751 AbsCorr = MULTI-SCAN			
Data completeness= 1.76/1.00	Theta(max)= 55.022		
R(reflections)= 0.0353(5551)		wR2(reflections)= 0.0933(6228)	
S= 1.041	Npar= 405		