Supporting Information

Ru(II)-catalyzed Allenylation and Sequential Annulation of *N*-Tosylbenzamides with Propargyl Alcohols

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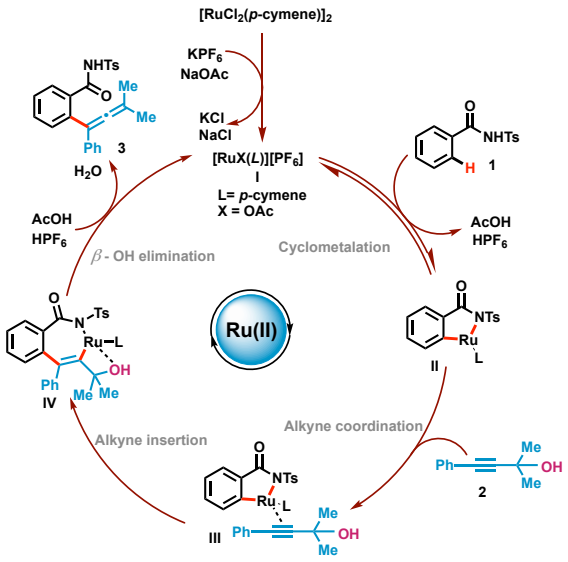
1. General Information

All reactions were carried out under nitrogen atmosphere in screw cap reaction tubes and the workups were performed under air. All the solvents used for the reactions were dried by following the reported procedures. Unless otherwise noted, all materials were purchased from commercial suppliers and used as received. Reactions were monitored using thin-layer chromatography. A gradient elution using petroleum ether and ethyl acetate was performed based on Merck aluminium TLC sheets (silica gel $60F_{254}$). TLC plates were visualized with UV light (254 nm) or $KMnO_4$ stain or Anisaldehyde stain. For column chromatography, silica gel (100–200 mesh) from SRL Co. was used. NMR studies were performed on Bruker Advance DPX at 400 MHz (^1H) or 500 MHz (^1H) and at 100 MHz (^{13}C) or 125 MHz (^{13}C), respectively. Chemical shifts (δ) are reported in ppm, using the residual solvent peak in $CDCl_3$ (δH = 7.26 and δC = 77.16) ppm as internal standards, and coupling constants (J) are given in Hz. HRMS were recorded with Bruker Maxis impact mass spectrometer using ESI-TOF techniques. FTIR measurements were performed on an Agilent Cary 630 FTIR Spectrometer.

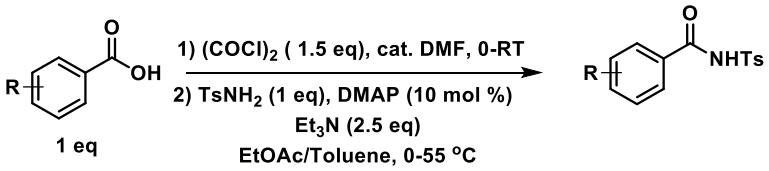
2. Proposed mechanism



3. Experimental Section

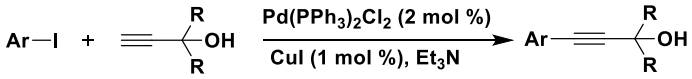
Preparation of Starting Materials

(a) Typical Procedure for the preparation of *N*-Tosyl Benzamides



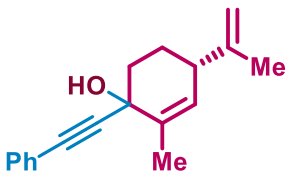
To a solution of substituted benzoic acid(3 mmol) and DMF (6μL) in DCM (20mL) under N_2 atmosphere was dropwise added oxalyl chloride (381μL, 4.5 mmol). The reaction was stirred until the solid suspension disappeared. Then solvent was removed under reduced pressure and the residue was dissolved in toluene (3mL). The above acyl chloride was then added dropwise to a solution of *p*-toluenesulfonamide (606mg, 3.0 mmol), DMAP (36 mg, 0.3 mmol) and Et_3N (1.04 mL, 7.5 mmol) in EtOAc (6 mL) at 0 °C over 15 minutes. The mixture was stirred at 55 °C until no further reaction was noticed (TLC analysis), cooled to room temperature and quenched with HCl (1N, 20 mL). The resulting mixture was extracted with EtOAc (20 mL ×3). The combined organic layers was dried over anhydrous Na_2SO_4, filtered and evaporated under reduced pressure. The residue was purified by flash silica gel chromatography with petroleum ether/EtOAc (2:1) to afford the benzamides 80-92% yields as white solids.

(b) Typical Procedure for the preparation of propargyl alcohols



To a solution of iodobenzene (3.18 mmol), CuI (21.83 mg, 1 mol%), and $PdCl_2(PPh_3)_2$ (80.47 mg, 2 mol%) in 15 mL NEt_3 under nitrogen atmosphere was added alkynol (3.82 mmol, 1.1 eq) at ambient temperature. Then the reaction mixture was heated to 50 °C for 6 h. The reaction was quenched with water (30 mL), extracted with dichloromethane (DCM) (3×30 mL). Drying collected organic layer over magnesium sulfate followed by concentration, the product was obtained as yellow oil by column chromatography (silica, hexane/ethyl acetate (5:1).

1ae



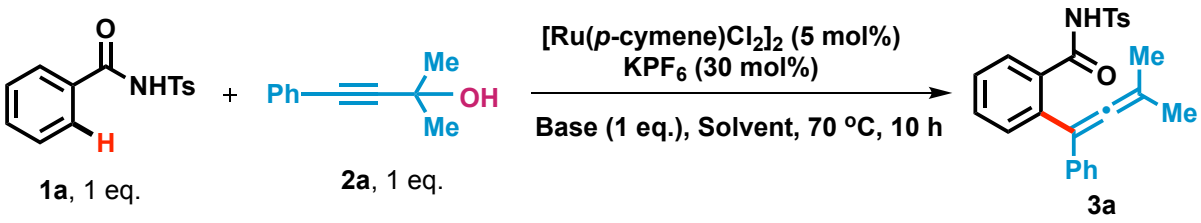
2-methyl-1-(phenylethynyl)-4-(prop-1-en-2-yl)cyclohex-2-en-1-ol

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.45 (dd, *J* = 6.6, 3.0 Hz, 2H), 7.33 (dd, *J* = 4.9, 1.7 Hz, 3H), 5.57 (dd, *J* = 3.4, 1.5 Hz, 1H), 4.80 (s, 2H), 2.66 – 2.60 (m, 1H), 2.39 (d, *J* = 12.0 Hz, 1H),

2.33 (s, 1H), 2.24 – 2.19 (m, 1H), 2.04 – 1.99 (m, 1H), 1.94 (s, 3H), 1.90 – 1.85 (m, 1H), 1.80 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 148.6, 135.9, 131.9, 128.5, 128.4, 124.7, 122.8, 109.4, 92.1, 84.3, 70.4, 43.7, 39.9, 31.2, 20.9, 17.4.

(c) General Optimization Table[a]

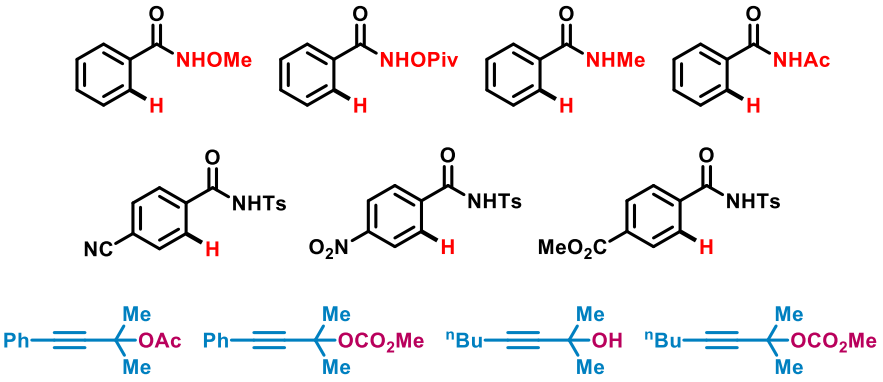


Entry	Base	Solvent	Yield
1	NaOPiv	DCE	45 (41)
2	Na_2CO_3	DCE	20
3	$NaHCO_3$	DCE	traces
4	**NaOAc**	**DCE**	**82 (81)**
5	KOAc	DCE	66
6	CsOAc	DCE	42
7	NaOAc	DCE	-[b]
8	NaOAc	DCE	-[c]
9	NaOAc	Toluene	61
10	NaOAc	MeCN	43
11	NaOAc	DCM	22
12	NaOAc	1,4-Dioxane	37
13	NaOAc	MeOH	traces
14	NaOAc	DMF	NR
15	NaOAc	DCE	63%[d]
16	NaOAc	DCE	70%[e]
17	NaOAc	DCE	39%[f]

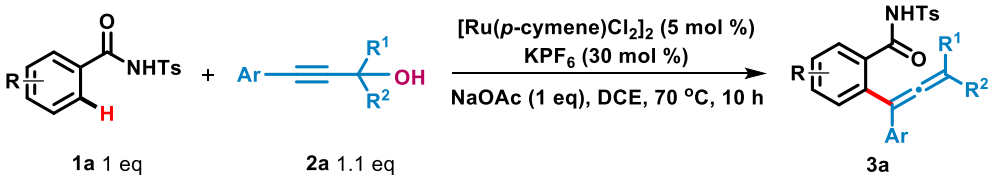
[a] [a]Unless specified in parenthesis, NMR yields were calculated using 1,2,3-trimethoxybenzene as external standard. Reaction conditions: **1a** (0.15 mmol). **2a** (0.15 mmol), $[RuCl_2(p\text{-cymene})]_2$ (5 mol%), KPF_6 (30 mol%), base (1 eq.), solvent (1.5 mL), 70 °C.[b]Reaction without Ru(II) catalyst. [c]Reaction without KPF_6. [d]Reaction at 60 °C. [e]Reaction at 90 °C. [f]30 mol% NaOAc.

(d) Failed substrates:

Following substrates failed to deliver the corresponding allenylation product under the established standard conditions.

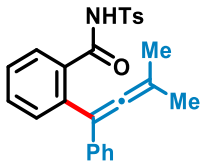


(e) Typical Procedure for the Synthesis of C-2 Allenyl *N*-Tosyl Benzamide



To an oven dried screw cap reaction tube equipped with a magnetic stir bar, was added *N*-Tosylbenzamide (0.2 mmol, 1 eq), [Ru(*p*-cymene)Cl_2]$_2$ (6 mg, 0.007 mmol), KPF_6 (7.3 mg, 0.045 mmol), NaOAc (16.4 mg, 0.2 mmol) and propargyl alcohol (0.2 mmol) followed by 1.0 ml DCE. After heating the reaction mixture at 70 °C for 8-10 h, it was cooled to room temperature and the solvent was evaporated under reduced pressure. The residue was purified by silica gel column chromatography (mesh 100-200; hexane: ethyl acetate 95:5 to 80:20) to give allenylated products. (Rf values from 0.4-0.5 in hexane : EA = 4:1)

3a.



2-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

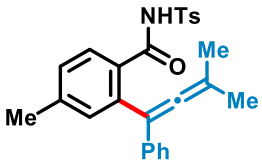
67 mg, 81%, colourless oil

^{1}H NMR (500 MHz, $CDCl_3$): δ 9.43 (s, 1H), 7.96 (d, *J* = 6.9 Hz, 1H), 7.55 (dd, *J* = 7.5, 1.2 Hz, 1H), 7.45 (t, *J* = 7.4 Hz, 3H), 7.32 (d, *J* = 7.6 Hz, 1H), 7.25 – 7.20 (m, 3H), 7.12 – 7.02 (m, 4H), 2.36 (s, 3H), 1.94 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 202.0, 164.5, 144.6, 136.4, 135.8, 133.1, 132.1, 130.8, 130.7, 129.6, 129.4, 129.1, 128.4, 127.5, 126.9, 126.6, 105.8, 101.7, 21.8, 20.2.

HRMS (ESI): $C_{25}H_{23}NNaO_3S$ $[M+Na]^+$ calculated = 440.1291; found = 440.1296.

3b.



4-methyl-2-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

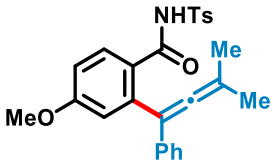
67 mg, 78%, colourless oil

^{1}H NMR (500 MHz, $CDCl_3$): δ 9.48 (s, 1H), 7.99 (d, *J* = 7.7 Hz, 1H), 7.62 – 7.43 (m, 4H), 7.34 (d, *J* = 7.4 Hz, 1H), 7.14 – 6.88 (m, 6H), 2.39 (s, 3H), 2.37 (s, 3H), 1.96 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 203.3, 163.5, 149.0, 145.1, 138.3, 138.0, 136.7, 134.4, 133.1, 129.7, 128.9, 128.5, 127.1, 126.7, 125.5, 121.4, 100.2, 91.5, 22.0, 20.2, 19.9.

HRMS (ESI): $C_{26}H_{26}NO_3S$ $[M+H]^+$ calculated = 432.1628; found = 432.1631.

3c.



4-methoxy-2-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

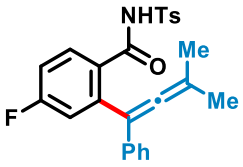
64 mg, 72%, colourless oil

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.54 (s, 1H), 7.99 (d, *J* = 8.8 Hz, 1H), 7.81 (d, *J* = 8.2 Hz, 2H), 7.38 – 7.30 (m, 4H), 7.25 – 7.23 (m, 2H), 7.09 – 7.03 (m, 3H), 3.85 (s, 3H), 2.34 (s, 3H), 1.96 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): *δ* 201.6, 165.7, 163.5, 140.6, 129.9, 129.4, 129.1, 128.8, 128.5, 128.4, 128.0, 126.6, 126.6, 125.3, 117.4, 114.5, 106.3, 101.9, 56.1, 21.7, 20.2.

HRMS (ESI): $C_{26}H_{26}NO_4S$ $[M+H]^+$ calculated = 448.1577; found = 448.1579.

3d.



4-fluoro-2-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

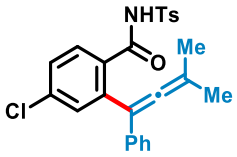
60 mg, 70%, pale yellow oil

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.41 (s, 1H), 7.97 (dd, *J* = 8.7, 5.8 Hz, 1H), 7.81 (d, *J* = 8.2 Hz, 2H), 7.44 (d, *J* = 8.2 Hz, 3H), 7.30 (d, *J* = 8.0 Hz, 1H), 7.26 – 7.21 (m, 4H), 7.16 – 6.95 (m, 1H), 2.36 (s, 3H), 1.94 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 201.8, 163.9, 163.4 (d, J_{C-F} = 231.9 Hz), 144.7, 143.6, 139.2, 135.7, 133.4 (d, J_{C-F} =3.6 Hz), 129.8, 129.4, 129.1, 128.3, 127.6, 126.5 (d, J_{C-F} = 8.6 Hz) , 119.0, 118.8, 115.7(d, J_{C-F} =28.0 Hz), 105.1, 102.3, 21.6, 20.1.

HRMS (ESI): $C_{25}H_{23}FNO_3S$ $[M+H]^+$ calculated = 436.1377; found = 436.1382.

3e.



4-chloro-2-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

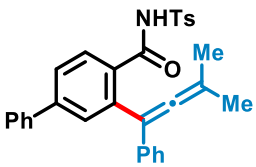
65 mg, 72%, yellow oil

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.40 (s, 1H), 7.87 (d, *J* = 8.5 Hz, 1H), 7.80 (d, *J* = 8.2 Hz, 4H), 7.45 (d, *J* = 8.3 Hz, 2H), 7.40 (dd, *J* = 8.5, 2.1 Hz, 1H), 7.31 – 7.23 (m, 5H), 7.09 (d, *J* = 8.1 Hz, 2H), 7.06 – 6.98 (m, 2H), 2.36 (s, 3H), 1.94 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 201.9, 163.5, 144.7, 143.6, 139.2, 135.7, 132.1, 131.8, 129.7, 129.4, 129.1, 128.7, 128.3, 127.6, 126.5, 126.4, 104.8, 102.3, 21.6, 20.1.

HRMS (ESI): $C_{25}H_{23}ClNO_3S$ $[M+H]^+$ calculated = 452.1082; found = 452.1086.

3f.



3-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosyl-[1,1'-biphenyl]-4-carboxamide

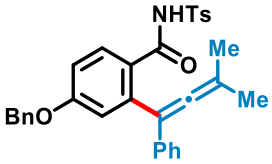
61 mg, 62%, colourless oil

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.53 (s, 1H), 8.06 (d, *J* = 8.2 Hz, 1H), 7.67 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.61 (d, *J* = 7.3 Hz, 2H), 7.54 (d, *J* = 1.6 Hz, 1H), 7.50 – 7.44 (m, 4H), 7.41 (d, *J* = 7.2 Hz, 1H), 7.25 (d, *J* = 2.3 Hz, 3H), 7.20 – 6.99 (m, 4H), 2.36 (s, 3H), 1.97 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 201.9, 164.2, 145.9, 144.6, 139.3, 136.3, 136.2, 135.2, 131.5, 130.5, 129.6, 129.4, 129.1, 129.1, 128.6, 128.4, 127.5, 127.4, 127.0, 126.6, 105.8, 101.8, 21.7, 20.2.

HRMS (ESI): $C_{31}H_{28}NO_3S$ $[M+H]^+$ calculated = 494.1784; found = 494.1792.

3g.



4-(benzyloxy)-2-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

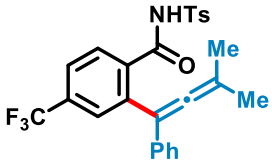
59 mg, 57%, yellow oil

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.57 (s, 1H), 8.03 (d, *J* = 8.8 Hz, 1H), 7.94 (m, 1H), 7.84 (d, *J* = 8.2 Hz, 1H), 7.41 (d, *J* = 8.2 Hz, 2H), 7.35 (d, *J* = 8.1 Hz, 1H), 7.27 (dd, *J* = 8.4, 5.0 Hz, 5H), 7.14 – 7.06 (m, 4H), 6.97 (dd, *J* = 8.8, 2.5 Hz, 1H), 6.83 (d, *J* = 2.5 Hz, 1H), 3.88 (s, 2H), 2.37 (s, 3H), 2.00 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 201.8, 170.7, 163.8, 135.7, 133.4, 131.7, 130.8, 129.1, 128.8, 128.5, 128.4, 128.3, 127.7, 126.8, 126.4, 118.2, 116.7, 114.3, 113.5, 109.7, 106.7, 99.4, 70.3, 30.0, 20.1.

HRMS (ESI): $C_{32}H_{30}NO_4S$ $[M+H]^+$ calculated = 524.1890; found = 524.1894.

3h.



2-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosyl-4-(trifluoromethyl)benzamide

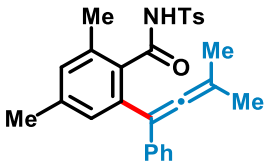
32 mg, 33%, colourless oil

^{1}H NMR (500 MHz, $CDCl_3$): δ 9.07 (s, 1H), 7.91 (d, *J* = 7.5 Hz, 1H), 7.84 (d, *J* = 8.2 Hz, 2H), 7.60 (t, *J* = 6.8 Hz, 2H), 7.49 (t, *J* = 7.6 Hz, 1H), 7.42 (d, *J* = 7.6 Hz, 1H), 7.34 (d, *J* = 8.1 Hz, 2H), 7.29 (m, 1H), 7.19 (d, *J* = 7.9 Hz, 1H), 7.13 (d, *J* = 8.1 Hz, 1H), 2.46 (s, 3H), 1.96 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 202.6, 164.4, 144.9, 143.7, 139.1, 136.4 (q, J_{C-F} = 255.3 Hz) 135.0, 133.1, 132.0, 130.3, 129.6 (q, J_{C-F} = 43.1 Hz), 129.3, 128.8, 128.3, 126.6, 123.8 (q, J_{C-F} = 3.8 Hz), 122.9 (q, J_{C-F} = 3.7 Hz), 104.9, 102.3, 21.6, 20.1.

HRMS (ESI): $C_{26}H_{23}F_3NO_3S$ $[M+H]^+$ calculated = 486.1345; found = 486.1332.

3i.



2,4-dimethyl-6-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

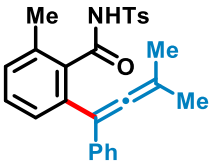
64 mg, 72%, colourless oil

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95 (d, J = 8.1 Hz, 2H), 7.29 – 7.18 (m, 6H), 7.08 (dd, J = 7.7, 1.6 Hz, 2H), 7.01 (s, 1H), 6.90 (s, 1H), 2.64 (s, 3H), 2.40 (s, 3H), 2.34 (s, 3H), 1.79 (s, 3H), 1.55 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 200.5, 167.9, 146.1, 144.4, 142.8, 141.1, 139.8, 139.4, 132.3, 129.1, 128.6, 128.0, 127.7, 125.3, 123.3, 119.8, 105.0, 102.6, 22.8, 22.1, 21.6, 20.2, 18.8.

HRMS (ESI): $C_{27}H_{28}NO_3S$ $[M+H]^+$ calculated = 446.1784; found = 446.1786.

3j.



2-methyl-6-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

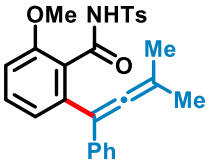
68 mg, 79%, colourless oil

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98 – 7.91 (m, 2H), 7.69 (d, J = 8.2 Hz, 2H), 7.33 (t, J = 7.7 Hz, 1H), 7.23 – 7.18 (m, 4H), 7.14 – 7.08 (m, 2H), 7.05 (d, J = 7.4 Hz, 2H), 2.43 (s, 3H), 2.27 (s, 3H), 1.65 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 202.2, 164.3, 144.5, 136.2, 135.7, 135.1, 134.2, 133.1, 132.0, 130.8, 129.3, 129.0, 128.5, 128.3, 127.3, 126.3, 106.0, 104.8, 22.6, 21.7, 18.4.

HRMS (ESI): $C_{26}H_{26}NO_3S$ $[M+H]^+$ calculated = 432.1628; found = 432.1626.

3k.



2-methoxy-6-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

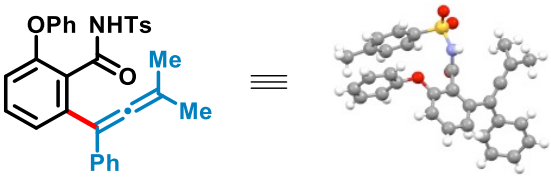
68 mg, 77%, colourless oil

^{1}H NMR (500 MHz, $CDCl_3$): δ 9.57 (s, 1H), 8.03 (d, *J* = 8.8 Hz, 1H), 7.84 (d, *J* = 8.2 Hz, 1H), 7.41 (d, *J* = 8.2 Hz, 1H), 7.35 (d, *J* = 8.1 Hz, 1H), 7.28 – 7.26 (m, 2H), 7.25 (s, 1H), 7.14 – 7.04 (m, 3H), 6.97 (dd, *J* = 8.8, 2.5 Hz, 1H), 6.83 (d, *J* = 2.5 Hz, 1H), 3.88 (s, 3H), 2.37 (s, 3H), 2.00 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$): *δ* 201.5, 165.6, 163.3, 140.4, 133.4, 129.8, 129.3, 128.6, 128.4, 128.3, 127.9, 126.5, 126.4, 125.2, 117.5, 113.4, 106.2, 101.8, 55.6, 21.6, 20.1.

HRMS (ESI): $C_{26}H_{26}NO_4S$ $[M+H]^+$ calculated = 448.1577; found = 448.1580.

3l.



2-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-6-phenoxy-*N*-tosylbenzamide

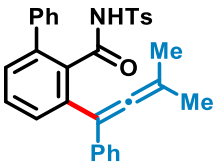
62 mg, 61%, yellow oil

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.32 (s, 1H), 7.73 (d, *J* = 8.2 Hz, 2H), 7.36 – 7.23 (m, 5H), 7.22 – 7.12 (m, 4H), 7.02 (dd, *J* = 15.1, 7.9 Hz, 3H), 6.87 (d, *J* = 8.1 Hz, 2H), 6.72 (d, *J* = 8.3 Hz, 1H), 2.30 (s, 3H), 1.84 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 202.8, 163.6, 155.8, 154.9, 144.6, 139.1, 137.7, 135.4, 131.4, 129.9, 129.3, 128.5, 128.4, 127.3, 126.8, 126.1, 125.6, 124.3, 119.6, 116.4, 103.9, 100.5, 21.7, 20.1.

HRMS (ESI): $C_{31}H_{28}NO_4S$ $[M+H]^+$ calculated = 510.1734; found = 510.1738.

3m.



3-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosyl-[1,1'-biphenyl]-2-carboxamide

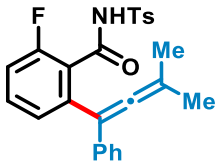
71 mg, 72%, yellow oil

^{1}H NMR (500 MHz, $CDCl_3$): δ 9.07 (s, 1H), 7.91 (d, *J* = 7.5 Hz, 1H), 7.84 (d, *J* = 8.2 Hz, 3H), 7.60 (t, *J* = 6.8 Hz, 3H), 7.49 (t, *J* = 7.6 Hz, 1H), 7.42 (d, *J* = 7.6 Hz, 1H), 7.32 (dd, *J* = 20.5, 10.2 Hz, 6H), 7.19 (d, *J* = 7.9 Hz, 1H), 7.14 (s, 1H), 2.39 (s, 3H), 1.96 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 202.0, 164.2, 157.8, 144.3, 135.9, 135.4, 135.1, 134.5, 132.9, 131.9, 131.0, 130.5, 129.5, 129.2, 128.8, 128.3, 128.2, 127.2, 126.3, 113.7, 106.5, 104.2, 21.6, 18.1.

HRMS (ESI): $C_{31}H_{28}NO_3S$ $[M+Na]^+$ calculated = 494.1784; found = 494.1788.

3n.



2-fluoro-6-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

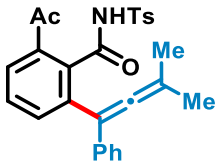
54 mg, 62%, colourless oil

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.24 (s, 1H), 7.82 (d, *J* = 8.3 Hz, 2H), 7.46 – 7.43 (m, 2H), 7.32 (dd, *J* = 5.0, 1.9 Hz, 2H), 7.26 (d, *J* = 3.2 Hz, 3H), 7.13 – 7.09 (m, 3H), 2.45 (s, 3H), 1.82 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 202.7, 161.3, 159.9 (d, $J_{C\text{-}F}$ = 252.2 Hz), 137.4 (d, $J_{C\text{-}F}$ = 7.8 Hz), 132.3 (d, $J_{C\text{-}F}$ = 3.1 Hz), 130.2, 129.6, 129.5, 129.2, 128.9, 128.6, 126.9, 125.3, 117.9 (d, $J_{C\text{-}F}$ = 4.4 Hz), 116.4 (d, $J_{C\text{-}F}$ = 18.8 Hz), 115.1 (d, $J_{C\text{-}F}$ = 21.7 Hz), 101.0, 96.5, 21.8, 20.0.

HRMS (ESI): $C_{25}H_{23}FNO_3S$ $[M+H]^+$ calculated = 436.1377; found = 436.1379.

3o.



2-acetyl-6-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

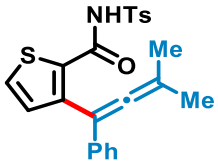
52 mg, 57%, yellow oil

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96 (d, *J* = 8.4 Hz, 2H), 7.62 (d, *J* = 7.6 Hz, 1H), 7.57 – 7.51 (m, 1H), 7.37 (dd, *J* = 7.5, 0.9 Hz, 1H), 7.25 (d, *J* = 8.1 Hz, 2H), 7.19 – 7.14 (m, 2H), 7.11 (s, 1H), 7.09 – 7.03 (m, 2H), 4.56 (s, 1H), 2.40 (s, 3H), 2.21 (s, 3H), 1.77 (s, 3H), 1.69 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 204.9, 203.0, 163.2, 148.7, 144.8, 138.1, 137.7, 136.4, 134.1, 132.8, 129.4, 128.6, 128.3, 126.8, 126.4, 125.2, 121.1, 102.3, 99.9, 91.2, 29.2, 21.7, 19.9, 19.6.

HRMS (ESI): $C_{27}H_{26}NO_4S$ $[M+H]^+$ calculated = 460.1577; found = 460.1568.

3p.



3-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylthiophene-2-carboxamide

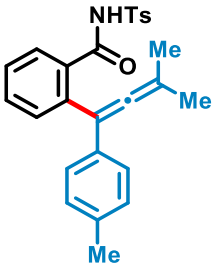
27 mg, 32%, yellow oil

^{1}H NMR (500 MHz, $CDCl_3$): δ 9.25 (s, 1H), 7.94 – 7.90 (m, 1H), 7.81 (d, *J* = 8.3 Hz, 1H), 7.57 (dd, *J* = 7.5, 1.4 Hz, 1H), 7.53 (d, *J* = 6.6 Hz, 1H), 7.45 (td, *J* = 7.6, 1.2 Hz, 1H), 7.31 – 7.28 (m, 1H), 7.14 (d, *J* = 8.1 Hz, 2H), 7.12 – 7.08 (m, 2H), 6.94 – 6.90 (m, 2H), 2.42 (s, 3H), 1.95 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 202.1, 164.5, 145.0, 133.3, 133.2, 132.0, 130.6, 129.8, 129.4, 129.0, 128.8, 128.3, 127.6, 126.6, 105.1, 102.0, 21.8, 20.2.

HRMS (ESI): $C_{23}H_{22}NO_3S_2$ $[M+H]^+$ calculated = 424.1036; found = 424.1037.

3r.



2-(3-methyl-1-(p-tolyl)buta-1,2-dien-1-yl)-*N*-tosylbenzamide

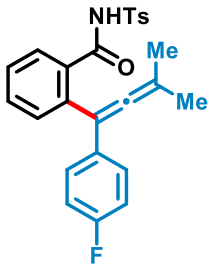
70 mg, 82%, colourless oil

^{1}H NMR (500 MHz, $CDCl_3$): δ 9.48 (s, 1H), 7.99 (d, *J* = 7.7 Hz, 1H), 7.63 – 7.39 (m, 4H), 7.34 (d, *J* = 7.4 Hz, 1H), 7.16 – 6.89 (m, 6H), 2.39 (s, 3H), 2.37 (s, 3H), 1.96 (s, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 201.6, 164.5, 144.5, 137.4, 136.0, 135.3, 133.4, 133.1, 132.1, 131.2, 130.8, 129.8, 129.3, 128.5, 128.5, 126.5, 105.7, 101.5, 21.8, 21.3, 20.3.

HRMS (ESI): $C_{26}H_{26}NO_3S$ $[M+H]^+$ calculated = 432.1628; found = 432.1627.

3s.



2-(1-(4-fluorophenyl)-3-methylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

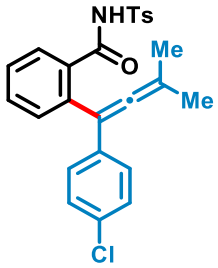
69 mg, 80%, yellow oil

^{1}H NMR (500 MHz, $CDCl_3$): δ 9.31 (s, 1H), 7.95 (d, *J* = 7.8 Hz, 1H), 7.59 (dd, *J* = 4.8, 3.5 Hz, 3H), 7.49 (d, *J* = 7.6 Hz, 1H), 7.33 (d, *J* = 7.5 Hz, 1H), 7.16 (d, *J* = 8.2 Hz, 2H), 7.00 (dd, *J* = 8.7, 5.3 Hz, 2H), 6.87 (t, *J* = 8.6 Hz, 2H), 2.41 (s, 3H), 1.97 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 201.9, 164.5, 162.3 (d, $J_{C\text{-}F}$ = 247.6 Hz), 144.9, 135.6, 133.2, 132.3 (d, $J_{C\text{-}F}$ = 3.1 Hz), 132.0, 131.4, 130.6, 129.4, 128.7, 128.4, 128.1 (d, $J_{C\text{-}F}$ = 8.1 Hz, 115.9 (d, $J_{C\text{-}F}$ = 21.8 Hz), 105.1, 101.8, 21.7, 20.3.

HRMS (ESI): $C_{25}H_{23}FNO_3S$ $[M+H]^+$ calculated = 436.1377; found = 436.1381.

3t.



2-(1-(4-chlorophenyl)-3-methylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

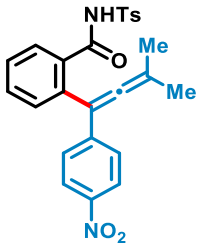
55 mg, 61%, yellow oil

^{1}H NMR (500 MHz, $CDCl_3$): *δ* ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.23 (s, 1H), 7.92 (d, *J* = 7.8 Hz, 1H), 7.57 – 7.52 (m, 2H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.30 (s, 2H), 7.12 (m, 3H), 6.92 (d, *J* = 8.4 Hz, 1H), 2.43 (s, 3H), 1.95 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 202.1, 164.5, 145.0, 143.8, 139.2, 135.3, 134.9, 133.2, 132.0, 130.6, 129.9, 129.4, 129.0, 128.4, 127.6, 126.6, 105.1, 102.1, 21.7, 20.2.

HRMS (ESI): $C_{25}H_{23}ClNO_3S$ $[M+H]^+$ calculated = 452.1082; found = 452.1087.

3u.



2-(1-(4-nitrophenyl)-3-methylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

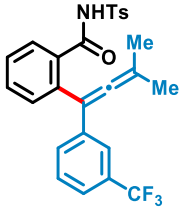
56 mg, 62%, yellow oil

^{1}H NMR (500 MHz, $CDCl_3$): δ 9.55 (s, 1H), 8.01 (d, J = 8.8 Hz, 1H), 7.82 (d, J = 8.2 Hz, 1H), 7.39 (d, J = 8.2 Hz, 2H), 7.33 (d, J = 8.1 Hz, 1H), 7.26 – 7.21 (m, 3H), 7.11 – 7.08 (m, 1H), 7.06 (d, J = 8.3 Hz, 1H), 6.95 (dd, J = 8.8, 2.5 Hz, 1H), 6.81 (d, J = 2.5 Hz, 1H), 2.35 (s, 3H), 1.98 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 201.9, 163.5, 144.7, 143.5, 139.1, 139.0, 137.5, 134.9, 132.1, 131.7, 129.7, 129.0, 128.3, 127.5, 126.4, 126.3, 104.8, 102.3, 21.5, 20.0.

HRMS (ESI): $C_{25}H_{23}N_2O_5S$ $[M+H]^+$ calculated = 463.1322; found = 463.1325.

3v.



2-(3-methyl-1-(3-(trifluoromethyl)phenyl)buta-1,2-dien-1-yl)-*N*-tosylbenzamide

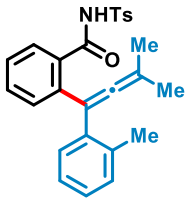
70 mg, 73%, yellow oil

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.05 (s, 1H), 7.88 (d, J = 7.5 Hz, 1H), 7.81 (d, J = 8.2 Hz, 2H), 7.57 (s, 2H), 7.47 (t, J = 7.6 Hz, 1H), 7.39 (d, J = 7.6 Hz, 1H), 7.30 (s, 3H), 7.16 (d, J = 7.9 Hz, 1H), 7.11 (s, 1H), 2.37 (s, 3H), 1.94 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 202.8, 164.7, 145.1, 144.0, 139.4, 136.6 (q, $J_{C\text{-}F}$ = 253.0 Hz), 135.2, 133.3, 132.2, 130.6, 129.9 (q, $J_{C\text{-}F}$ = 41.3 Hz), 129.5, 129.0, 128.5, 126.8, 124.1 (q, $J_{C\text{-}F}$ = 3.8 Hz), 123.1 (q, $J_{C\text{-}F}$ = 3.8 Hz), 105.1, 102.5, 21.9, 20.3.

HRMS (ESI): $C_{26}H_{23}F_3NO_3S$ $[M+H]^+$ calculated = 486.1345; found = 486.1347.

3w.



2-(3-methyl-1-(o-tolyl)buta-1,2-dien-1-yl)-*N*-tosylbenzamide

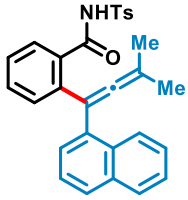
70 mg, 82%, colourless oil

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.77 (s, 1H), 7.67 (s, 2H), 7.41 (m, 2H), 7.28 – 6.93 (m, 7H), 6.68 (d, *J* = 6.7 Hz, 1H), 2.41 (s, 6H), 1.84 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$):) δ 198.7, 164.4, 144.5, 136.6, 136.0, 135.3, 134.3, 133.1, 132.6, 132.2, 130.7, 129.4, 129.1, 128.5, 128.4, 127.3, 126.4, 108.8, 108.5, 105.5, 27.6, 26.0, 21.7.

HRMS (ESI): $C_{26}H_{26}NO_3S$ $[M+H]^+$ calculated = 432.1628; found = 432.1635.

3x.



2-(3-methyl-1-(naphthalen-1-yl)buta-1,2-dien-1-yl)-*N*-tosylbenzamide

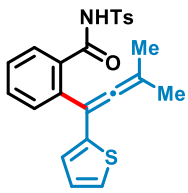
70 mg, 75%, colourless oil

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.26 (s, 1H), 7.95 (d, *J* = 7.8 Hz, 1H), 7.84 (d, *J* = 8.1 Hz, 3H), 7.60 – 7.54 (m, 2H), 7.49 (d, *J* = 7.6 Hz, 1H), 7.33 (t, *J* = 7.4 Hz, 4H), 7.15 (dd, *J* = 15.9, 8.3 Hz, 3H), 6.95 (d, *J* = 8.4 Hz, 1H), 2.43 (s, 3H), 1.98 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): *δ* 202.7, 163.5, 155.7, 154.8, 144.4, 139.0, 138.3, 137.6, 135.3, 132.8, 131.2, 129.8, 129.2, 128.4, 128.3, 127.1, 126.7, 126.4, 125.5, 124.2, 119.4, 116.3, 103.8, 100.3, 21.5, 20.0.

HRMS (ESI): $C_{29}H_{26}NO_3S$ $[M+H]^+$ calculated = 468.1628; found = 468.1632.

3y.



2-(3-methyl-1-(thiophen-2-yl)buta-1,2-dien-1-yl)-*N*-tosylbenzamide

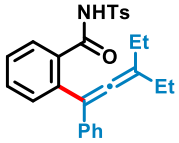
49 mg, 58%, yellow oil

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.25 (s, 1H), 7.98 – 7.87 (m, 1H), 7.81 (d, *J* = 8.3 Hz, 1H), 7.60 – 7.48 (m, 3H), 7.47 – 7.43 (m, 1H), 7.31 – 7.28 (m, 1H), 7.16 (s, 1H), 7.11 – 7.09 (m, 1H), 6.99 – 6.87 (m, 2H), 2.40 (s, 3H), 1.95 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 202.1, 164.5, 145.0, 135.2, 134.9, 133.3, 133.2, 131.9, 130.6, 129.8, 129.4, 129.0, 128.8, 128.3, 127.6, 126.6, 105.1, 102.0, 21.8, 20.2.

HRMS (ESI): $C_{23}H_{22}NO_3S_2$ $[M+H]^+$ calculated = 424.1036; found = 424.1035.

3z.



2-(3-ethyl-1-phenylpenta-1,2-dien-1-yl)-*N*-tosylbenzamide

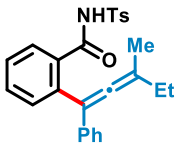
69 mg, 78%, colourless oil

^{1}H NMR (400 MHz, $CDCl_3$): *δ* 9.47 (s, 1H), 8.00 (d, *J* = 7.6 Hz, 1H), 7.56 (d, *J* = 7.1 Hz, 1H), 7.42 (m, 4H), 7.23 (s, 3H), 7.09 (d, *J* = 7.1 Hz, 4H), 2.37 (s, 3H), 2.25 (m, 4H), 1.20 (t, *J* = 7.2 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 201.5, 164.4, 144.5, 136.6, 135.9, 135.3, 133.2, 132.1, 140.0, 130.9, 129.4, 129.1, 128.5, 128.4, 127.4, 126.1, 114.5, 109.1, 26.2, 21.7, 13.0.

HRMS (ESI): $C_{27}H_{28}NO_3S$ $[M+H]^+$ calculated = 446.1784; found = 446.1788.

3aa.



2-(3-methyl-1-phenylpenta-1,2-dien-1-yl)-*N*-tosylbenzamide

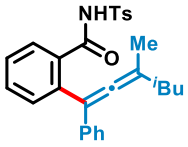
67 mg, 78%, colourless oil

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.49 (s, 1H), 7.98 (dd, *J* = 7.8, 1.1 Hz, 1H), 7.57 (td, *J* = 7.5, 1.3 Hz, 1H), 7.46 (dd, *J* = 7.7, 1.1 Hz, 1H), 7.43 (d, *J* = 8.3 Hz, 2H), 7.34 (d, *J* = 7.6 Hz, 1H), 7.25 – 7.19 (m, 3H), 7.07 (dd, *J* = 7.3, 3.4 Hz, 4H), 2.36 (s, 3H), 2.22 (qd, *J* = 15.7, 7.9 Hz, 2H), 1.96 (s, 3H), 1.19 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 201.6, 164.4, 144.6, 136.5, 135.9, 135.2, 133.2, 132.1, 131.0, 130.9, 129.4, 129.1, 128.6, 128.4, 127.5, 126.3, 108.1, 107.6, 27.64, 21.76, 18.62, 12.69.

HRMS (ESI): $C_{26}H_{26}NO_3S$ $[M+H]^+$ calculated = 432.1628; found = 432.1633.

3ab.



2-(3,4-dimethyl-1-phenylhexa-1,2-dien-1-yl)-N-tosylbenzamide

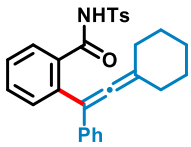
70 mg, 77%, colourless oil

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.49 (s, 1H), 7.98 (d, *J* = 6.9 Hz, 1H), 7.55 (dd, *J* = 7.5, 1.1 Hz, 1H), 7.50 – 7.39 (m, 3H), 7.33 (d, *J* = 7.5 Hz, 1H), 7.25 – 7.18 (m, 3H), 7.12 – 7.00 (m, 4H), 2.35 (s, 3H), 2.19 – 2.03 (m, 2H), 1.93 (s, 3H), 1.91 – 1.84 (m, 1H), 0.99 (d, *J* = 6.6 Hz, 3H), 0.91 (d, *J* = 6.6 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 202.3, 164.4, 144.6, 136.3, 135.8, 135.2, 134.7, 133.2, 132.1, 130.9, 129.4, 129.1, 128.6, 128.4, 127.4, 126.4, 106.1, 104.9, 43.8, 26.6, 22.9, 22.7, 21.8, 18.5.

HRMS (ESI): $C_{28}H_{30}NO_3S$ $[M+H]^+$ calculated = 460.1941; found = 460.1947.

3ac.



2-(2-cyclohexylidene-1-phenylvinyl)-*N*-tosylbenzamide

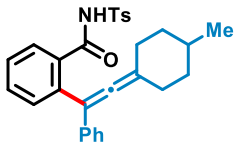
70 mg, 77%, colourless oil

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.45 (s, 1H), 7.96 (d, *J* = 7.7 Hz, 1H), 7.55 (d, *J* = 7.5 Hz, 1H), 7.45 (dd, *J* = 7.2, 5.4 Hz, 3H), 7.31 (d, *J* = 7.6 Hz, 1H), 7.26 – 7.20 (m, 3H), 7.13 – 7.00 (m, 4H), 2.47 – 2.38 (m, 2H), 2.36 (s, 3H), 2.32 – 2.23 (m, 2H), 1.75 – 1.73 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 198.7, 164.5, 144.6, 136.6, 136.1, 135.3, 133.1, 132.2, 130.8, 129.4, 129.1, 128.5, 128.4, 127.4, 126.4, 108.8, 108.5, 105.6, 31.1, 27.7, 26.1, 21.8.

HRMS (ESI): $C_{28}H_{28}NO_3S$ $[M+H]^+$ calculated = 458.1784; found = 458.1787.

3ad.



2-(2-cyclohexylidene-1-phenylvinyl)-*N*-tosylbenzamide

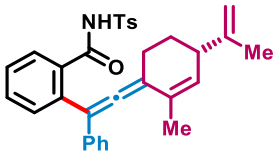
64 mg, 68%, colourless oil

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.44 (s, 1H), 7.94 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.54 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.48 – 7.41 (m, 3H), 7.33 – 7.29 (m, 1H), 7.23 (dd, *J* = 5.8, 4.2 Hz, 3H), 7.14 – 7.02 (m, 4H), 2.55 (m, 2H), 2.36 (s, 3H), 2.15 (m, 2H), 1.98 – 1.89 (m, 2H), 1.31 – 1.26 (m, 3H), 1.01 (d, *J* = 6.5 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 198.5, 164.5, 144.5, 136.5, 135.8, 135.2, 133.0, 132.2, 131.2, 130.6, 129.3, 129.1, 128.4, 128.4, 127.3, 126.3, 108.0, 105.5, 36.0, 32.2, 30.6, 22.2, 21.7.

HRMS (ESI): $C_{29}H_{30}NO_3S$ $[M+H]^+$ calculated = 472.1941; found = 472.1943.

3ae.



2-(2-methyl-4-(prop-1-en-2-yl)cyclohex-2-en-1-ylidene)-1-phenylvinyl)-N-tosylbenzamide

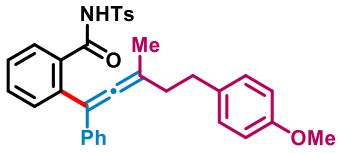
66 mg, 65%, colourless oil

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.38 (s, 1H), 7.97 (d, *J* = 7.7 Hz, 1H), 7.71 – 7.48 (m, 2H), 7.53 – 7.41 (m, 3H), 7.37 (d, *J* = 7.5 Hz, 1H), 7.32 – 7.18 (m, 3H), 7.14 – 7.04 (m, 3H), 5.79 (d, *J* = 4.5 Hz, 1H), 4.81 (s, 2H), 2.83 (d, *J* = 10.6 Hz, 1H), 2.48-2.31 (m, 5H), 2.10 (m, 1H), 1.91 (s, 3H), 1.81 (s, 3H), 1.62 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 203.8, 164.3, 148.2, 144.6, 136.1, 135.4, 135.3, 133.2, 132.1, 131.2, 130.9, 129.4, 129.2, 128.7, 128.5, 128.4, 128.2, 127.7, 126.5, 109.9, 109.5, 109.3, 41.2, 32.5, 31.2, 21.8, 21.1, 21.0.

HRMS (ESI): $C_{32}H_{32}NO_3S$ $[M+H]^+$ calculated = 510.2097; found = 510.2101.

3af.



(S)-2-(5-(4-methoxyphenyl)-3-methyl-1-phenylpenta-1,2-dien-1-yl)-N-tosylbenzamide

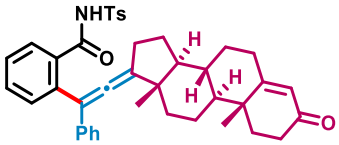
74 mg, 69%, colourless oil

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.12 (s, 1H), 7.91 (d, *J* = 7.3 Hz, 1H), 7.53 (t, *J* = 7.0 Hz, 1H), 7.43 (m, 3H), 7.18 (m, 4H), 7.07 (m, 4H), 6.87 (d, *J* = 6.5 Hz, 2H), 6.68 (d, *J* = 8.5 Hz, 2H), 3.75 (s, 3H), 2.84 (d, *J* = 7.1 Hz, 2H), 2.54 (t, *J* = 7.2 Hz, 2H), 2.35 (s, 3H), 1.98 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 202.1, 164.4, 157.9, 144.4, 136.0, 135.5, 135.2, 134.3, 133.0, 132.0, 131.1, 130.6, 129.6, 129.3, 128.9, 128.4, 128.3, 127.3, 126.4, 113.9, 106.6, 104.3, 55.2, 36.4, 32.6, 21.7, 18.2.

HRMS (ESI): $C_{33}H_{32}NO_4S$ $[M+H]^+$ calculated = 538.2047; found = 538.2055.

3ag.



2-((S)-2-((8R,9S,10R,13S,14S)-10,13-dimethyl-3-oxo-1,2,3,6,7,8,9,10,11,12,13,14,15,16-tetradecahydro-17H-cyclopenta[a]phenanthren-17-ylidene)-1-phenylvinyl)-N-tosylbenzamide

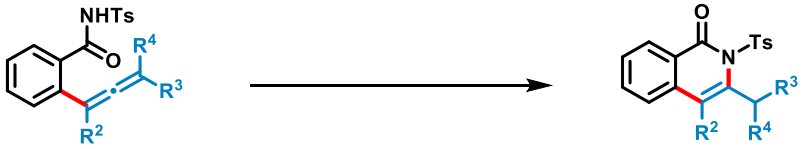
81 mg, 63%, colourless oil

^{1}H NMR (500 MHz, $CDCl_3$): δ 9.53 (s, 1H), 8.01 (d, *J* = 7.8 Hz, 1H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 1H), 7.42 (s, 1H), 7.33 (d, *J* = 7.7 Hz, 1H), 7.26 – 7.19 (m, 3H), 7.08 (d, *J* = 8.0 Hz, 4H), 5.79 (s, 1H), 2.79 (d, *J* = 7.5 Hz, 2H), 2.46 – 2.35 (m, 7H), 2.12 – 1.95 (m, 5H), 1.71 – 1.47 (m, 7H), 1.24 (s, 5H), 0.98 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 199.7, 196.2, 171.0, 164.4, 144.5, 136.2, 135.8, 135.1, 133.1, 132.1, 131.0, 130.8, 129.3, 129.0, 128.5, 128.3, 127.4, 126.0, 124.0, 118.5, 110.3, 55.3, 53.8, 47.0, 38.8, 36.2, 35.7, 34.0, 32.8, 31.9, 27.1, 25.0, 21.7, 21.1, 18.5, 17.4.

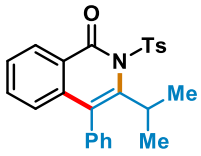
HRMS (ESI): $C_{41}H_{44}NO_4S$ $[M+H]^+$ calculated = 646.2986; found = 646.2990.

(f) Procedure for base assisted annulation of allenylated benzamides



To a mixture of allene **3** (0.15 mmol, 1 eq) in toluene, was added 0.5 eq K_2CO_3 and was heated in a preheated oil bath at 50 °C for 12 h. The crude reaction mixture was evaporated under reduced pressure and was directly purified by silica gel column chromatography (Hexane:EA = 10:1). (Rf values from 0.7-0.8 in hexane: EA = 9:1).

4a.



3-isopropyl-4-phenyl-2-tosylisoquinolin-1(2H)-one

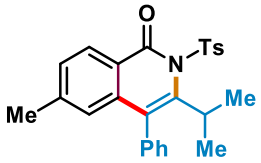
45 mg, 73%, colourless oil

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.42 (d, *J* = 8.0 Hz, 1H), 8.03 (d, *J* = 8.1 Hz, 2H), 7.59 (d, *J* = 7.3 Hz, 1H), 7.55 – 7.43 (m, 4H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.27 – 7.22 (m, 2H), 6.97 (d, *J* = 8.1 Hz, 1H), 2.75 (sep, *J* = 6.9 Hz, 1H), 2.46 (s, 3H), 1.23 (d, *J* = 6.9 Hz, 6H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 160.3, 158.6, 140.1, 137.2, 135.2, 133.6, 130.4, 129.5, 129.2, 128.9, 128.6, 128.2, 127.0, 125.1, 124.3, 120.4, 116.3, 30.4, 21.7, 20.3.

HRMS (ESI): $C_{25}H_{24}NO_3S$ $[M+H]^+$ calculated = 418.1471; found = 418.1467.

4b.



3-isopropyl-6-methyl-4-phenyl-2-tosylisoquinolin-1(2H)-one

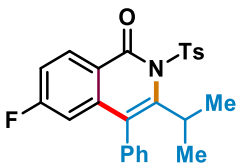
47 mg, 74%, yellow oil

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.29 (d, *J* = 8.2 Hz, 1H), 8.00 (d, *J* = 8.1 Hz, 2H), 7.73 – 7.65 (m, 1H), 7.48 (t, *J* = 6.7 Hz, 3H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.25 – 7.20 (m, 2H), 6.69 (s, 1H), 2.67 (sep, *J* = 6.9 Hz, 1H), 2.43 (s, 3H), 2.32 (s, 3H), 1.18 (d, *J* = 6.9 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 160.5, 158.7, 146.7, 142.8, 140.3, 137.3, 133.7, 130.4, 129.7, 129.5, 129.2, 129.0, 128.5, 126.9, 125.0, 118.0, 116.3, 30.4, 22.3, 21.7, 20.3.

HRMS (ESI): $C_{26}H_{26}NO_3S$ $[M+H]^+$ calculated = 432.1628; found = 432.1632.

4c.



6-fluoro-3-isopropyl-4-phenyl-2-tosylisoquinolin-1(2H)-one

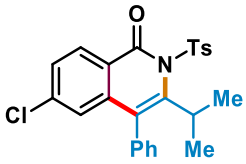
45 mg, 70%, colourless oil

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.41 (dd, *J* = 8.9, 5.7 Hz, 1H), 7.99 (d, *J* = 8.1 Hz, 2H), 7.50 (q, *J* = 5.6 Hz, 3H), 7.33 (d, *J* = 8.1 Hz, 2H), 7.25 – 7.16 (m, 2H), 7.12 (d, *J* = 2.3 Hz, 1H), 6.57 (dd, *J* = 9.8, 2.3 Hz, 1H), 2.72 (sep, *J* = 6.9 Hz, 1H), 2.44 (s, 3H), 1.21 (d, *J* = 6.9 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 167.1 (d, J_{C-F} = 257.5 Hz), 159.9, 143.1, 139.9, 133.0, 132.3 (d, J_{C-F} = 9.3 Hz), 130.2, 129.5 (d, J_{C-F} = 8.0 Hz), 128.9, 127.0, 116.6, 111.05 (d, J_{C-F} = 23.8 Hz), 30.5, 21.7, 20.3.

HRMS (ESI): $C_{25}H_{23}FNO_3S$ $[M+H]^+$ calculated = 436.1377; found = 436.1380.

4d.



6-chloro-3-isopropyl-4-phenyl-2-tosylisoquinolin-1(2H)-one

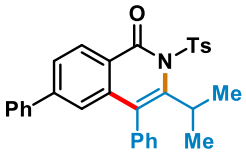
46 mg, 68%, pale yellow oil

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.32 (d, *J* = 8.6 Hz, 1H), 8.01 (d, *J* = 8.2 Hz, 2H), 7.69 (s, 1H), 7.53 (d, *J* = 7.3 Hz, 3H), 7.43 – 7.38 (m, 1H), 7.36 (d, *J* = 8.1 Hz, 1H), 7.23 (dd, *J* = 7.6, 1.6 Hz, 2H), 6.91 (d, *J* = 1.9 Hz, 1H), 2.72 (sep, *J* = 6.9 Hz, 1H), 2.46 (s, 3H), 1.23 (d, *J* = 6.9 Hz, 6H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 160.0, 159.4, 143.2, 142.2, 139.8, 138.6, 132.8, 130.5, 130.3, 129.5, 129.5, 128.9, 128.7, 127.0, 124.7, 118.8, 115.5, 30.5, 21.7, 20.3.

HRMS (ESI): $C_{25}H_{23}ClNO_3S$ $[M+H]^+$ calculated = 452.1082; found = 452.1080.

4e.



3-isopropyl-4,6-diphenyl-2-tosylisoquinolin-1(2H)-one

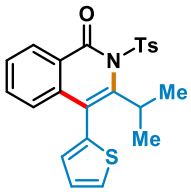
53 mg, 72%, brown oil

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.46 (d, *J* = 8.3 Hz, 1H), 8.02 (d, *J* = 7.9 Hz, 2H), 7.68 (dd, *J* = 19.6, 8.0 Hz, 2H), 7.51 – 7.39 (m, 8H), 7.27 (d, *J* = 3.7 Hz, 3H), 7.11 (s, 1H), 2.73 (sep. *J* = 6.8 Hz, 1H), 2.44 (s, 3H), 1.21 (d, *J* = 6.8 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 160.0, 158.9, 147.9, 142.7, 140.0, 139.4, 137.6, 133.4, 130.2, 129.4, 129.3, 129.1, 128.9, 128.7, 128.4, 127.3, 127.1, 126.8, 123.0, 119.1, 116.3, 30.3, 21.5, 20.1.

HRMS (ESI): $C_{31}H_{28}NO_3S$ $[M+H]^+$ calculated = 494.1784; found = 494.1787.

4f.



3-isopropyl-4-(thiophen-2-yl)-2-tosylisoquinolin-1(2H)-one

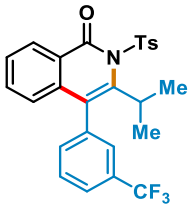
47 mg, 75%, colourless oil

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.41 (d, J = 8.0 Hz, 1H), 8.02 (d, J = 8.1 Hz, 2H), 7.71 (dd, J = 10.6, 7.6 Hz, 1H), 7.61 (d, J = 7.5 Hz, 1H), 7.50 (s, 1H), 7.47 (t, J = 7.7 Hz, 2H), 7.36 (d, J = 8.1 Hz, 1H), 7.20 (d, J = 8.2 Hz, 1H), 6.94 (d, J = 8.0 Hz, 1H), 2.72 (sep, J = 6.9 Hz, 1H), 2.46 (s, 3H), 1.24 (d, J = 6.9 Hz, 6H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 160.0, 158.7, 143.0, 139.9, 136.7, 135.2, 134.7, 132.0, 131.7, 129.5, 129.4, 129.0, 128.3, 126.9, 124.7, 120.3, 115.2, 30.4, 21.6, 20.3.

HRMS (ESI): $C_{23}H_{22}NO_3S_2$ $[M+H]^+$ calculated = 424.1036; found = 424.1038.

4g.



3-isopropyl-2-tosyl-4-(3-(trifluoromethyl)phenyl)isoquinolin-1(2H)-one

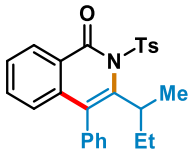
46 mg, 64%, yellow oil

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.40 (d, J = 7.9 Hz, 1H), 8.00 (d, J = 8.1 Hz, 2H), 7.68 (d, J = 8.5 Hz, 3H), 7.51 (s, 1H), 7.48-7.43 (m, 2H), 7.34 (d, J = 8.1 Hz, 2H), 6.85 (d, J = 8.0 Hz, 1H), 2.63 (sep, J= 6.7 Hz, 1H), 2.44 (s, 3H), 1.24 (d, J = 7.0 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 159.8, 159.0, 143.1, 135.4, 135.3, 135.2, 135.2 (q, J_{C-F} = 265.8), 134.6, 131.5, 131.4 (q, J_{C-F} = 3.0 Hz), 129.9, 129.5, 129.1, 128.6 (q, J_{C-F} = 39.5 Hz), 128.5 (overlapped), 127.0, 124.6, 120.4, 119.7, 115.1, 30.6, 21.7, 20.3.

HRMS (ESI): $C_{26}H_{23}F_3NO_3S$ $[M+H]^+$ calculated = 486.1345; found = 486.1348.

4h.



3-(sec-butyl)-4-phenyl-2-tosylisoquinolin-1(2H)-one

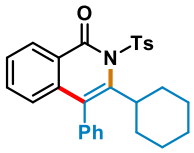
45 mg, 70 %, colourless oil

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.41 (d, *J* = 8.1 Hz, 1H), 7.99 (d, *J* = 8.0 Hz, 2H), 7.69 (s, 1H), 7.58 (t, *J* = 7.6 Hz, 1H), 7.47 (t, *J* = 6.7 Hz, 3H), 7.32 (d, *J* = 7.9 Hz, 2H), 7.21 (t, *J* = 6.9 Hz, 2H), 6.93 (d, *J* = 8.0 Hz, 1H), 2.43 (s, 3H), 1.74 (m, 1H), 1.50 – 1.38 (m, 2H), 1.18 (d, *J* = 6.9 Hz, 3H), 0.75 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 160.1, 157.6, 142.7, 137.0, 135.1, 133.5, 130.6, 130.3, 129.3, 129.1, 129.0, 128.8, 128.4, 128.0, 126.8, 124.9, 117.5, 37.2, 27.2, 21.5, 18.6, 12.2.

HRMS (ESI): $C_{26}H_{26}NO_3S$ $[M+H]^+$ calculated = 432.1628; found = 432.1625.

4i.



3-cyclohexyl-4-phenyl-2-tosylisoquinolin-1(2H)-one

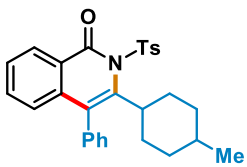
45 mg, 67%, yellow oil

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.42 (d, *J* = 8.0 Hz, 1H), 8.01 (d, *J* = 8.2 Hz, 2H), 7.72 – 7.66 (m, 1H), 7.57 (t, *J* = 7.7 Hz, 1H), 7.49 – 7.45 (m, 3H), 7.33 (d, *J* = 8.2 Hz, 2H), 7.20 (d, *J* = 5.5 Hz, 2H), 6.93 (d, *J* = 8.0 Hz, 1H), 2.58 (m, 1H), 2.43 (s, 3H), 1.67 (m, 6H), 1.05 (t, *J* = 7.2 Hz, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 160.3, 158.4, 142.9, 140.2, 137.3, 135.2, 133.6, 130.3, 129.5, 129.2, 129.0, 128.6, 128.2, 127.0, 125.1, 120.30, 116.7, 46.3, 40.2, 29.9, 25.9, 25.4, 21.7.

HRMS (ESI): $C_{28}H_{28}NO_3S$ $[M+H]^+$ calculated = 458.1784; found = 458.1791.

4j.



3-(4-methylcyclohexyl)-4-phenyl-2-tosylisoquinolin-1(2H)-one

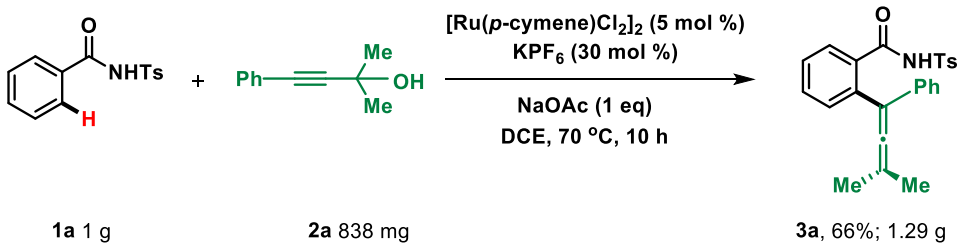
45 mg, 64%, yellow oil

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.34 (d, *J* = 8.0 Hz, 1H), 8.01 (d, *J* = 8.1 Hz, 2H), 7.56 (t, *J* = 7.5 Hz, 1H), 7.48 (t, *J* = 10.1 Hz, 3H), 7.40 (t, *J* = 7.7 Hz, 1H), 7.32 (d, *J* = 7.9 Hz, 2H), 7.23 (d, *J* = 7.5 Hz, 2H), 6.94 (d, *J* = 8.0 Hz, 1H), 2.44 (s, 3H), 2.34 (m, 1H), 2.20 – 2.04 (m, 2H), 1.59 (m, 4H), 1.43 (m, 3H), 1.15 (d, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 160.3, 158.5, 142.8, 140.2, 137.3, 135.0, 133.7, 130.4, 129.4, 129.2, 128.8, 128.5, 128.0, 126.9, 125.1, 120.3, 116.5, 40.5, 31.2, 26.7, 24.5, 21.7, 17.5.

HRMS (ESI): $C_{29}H_{30}NO_3S$ $[M+H]^+$ calculated = 472.1941; found = 472.1944.

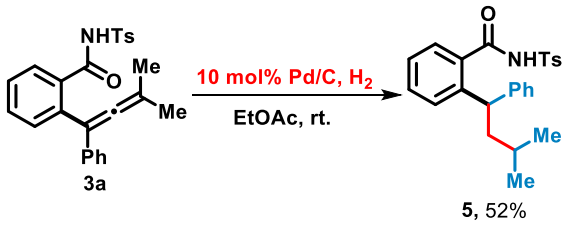
(g) Procedure for Gram Scale Reaction to synthesize 3a



1a 1 g **2a** 838 mg **3a**, 66%; 1.29 g

To an oven dried screw cap reaction tube equipped with a magnetic stir bar, was added *N*-Tosylbenzamide (1g, 4.7 mmol), [Ru(*p*-cymene)Cl_2]$_2$ (145 mg, 0.2 mmol), KPF_6 (262.86 mg, 1.4 mmol), NaOAc (390 mg, 4.7 mmol) and propargyl alcohol (838 mg, 5.2 mmol) followed by 6 ml DCE. After heating the reaction mixture at 70 °C for 8-10 h, it was cooled to room temperature and the solvent was evaporated under reduced pressure. The residue was purified by silica gel column chromatography (mesh 100-200; hexane: ethyl acetate 95:5 to 80:20) to give 1.29 g of the product **3a**.

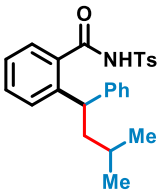
(h) Procedure for Pd/C Assisted Hydrogenation of 3a to obtain 5



5, 52%

A mixture of product **3a** (42 mg, 0.1 mmol) and Pd/C (35 mg, 0.01 mmol) was taken in a 25 ml round bottom flask. 10 ml ethyl acetate was added and H_2 gas was passed through the setup for 12 hours. The reaction was checked for complete conversion by TLC and product **5** was purified using silica gel column chromatography (EA: Hexane = 1:10).

5.



2-(3-methyl-1-phenylbutyl)-*N*-tosylbenzamide

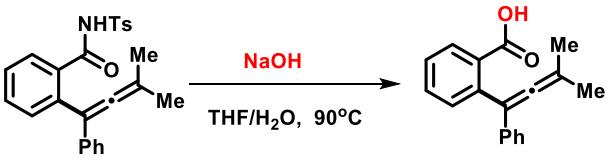
22 mg, 52%, white oil, Rf = 0.8 in hexane:EA = 4:1

^{1}H NMR (500 MHz, MeOD): δ 8.05 (d, *J* = 8.3 Hz, 2H), 7.50 (d, *J* = 8.2 Hz, 2H), 7.46 – 7.41 (m, 2H), 7.34 (d, *J* = 7.5 Hz, 1H), 7.25 (d, *J* = 7.8 Hz, 1H), 7.15 (t, *J* = 7.2 Hz, 2H), 7.11 (d, *J* = 7.0 Hz, 1H), 7.02 (d, *J* = 7.1 Hz, 2H), 4.34 (t, *J* = 7.9 Hz, 1H), 2.50 (s, 3H), 1.96 – 1.78 (m, 2H), 1.74 (dd, *J* = 13.8, 7.1 Hz, 1H), 0.80 (d, *J* = 6.6 Hz, 3H), 0.74 (d, *J* = 6.6 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 166.70, 145.36, 144.36, 144.23, 135.72, 133.36, 131.75, 129.74, 128.89, 128.65, 128.46, 128.08, 127.31, 126.40, 126.27, 45.25, 43.24, 25.72, 22.64, 22.48.

HRMS (ESI): $C_{25}H_{28}NO_3S$ $[M+H]^+$ calculated = 422.1784; found = 422.1786.

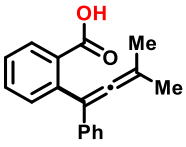
(i) Procedure for Base Catalyzed Hydrolysis of 3a



3a **6**, 65%

To a solution of **3a** (42 mg, 0.1 mmol) in THF (3 mL) was added a solution of NaOH (2M, 3 mL). The mixture was heated and stirred at 50 °C for 3 h, cooled to room temperature, acidified with a solution of HCl (3M) and extracted with ethyl acetate (2 x 15 mL). The combined organic layers were dried on NaSO4, filtrated and evaporated. The crude product was purified by silica gel chromatography using hexane/EtOAc (7:3) as the eluent. **5** was obtained as white solid.

6.



2-(3-methyl-1-phenylbuta-1,2-dien-1-yl)benzoic acid

17 mg, 65%, white oil, Rf = 0.3 in Hexane:EA = 9:1

IR ($CHCl_3$): *v* 3429, 2967, 2932, 1975, 1735, 1601, 1447, 1314, 1258, 1103, 798, 763, 706 cm^{-1}.

^1H NMR (500 MHz, $CDCl_3$): δ 8.17 – 8.12 (m, 2H), 7.91 (d, *J* = 7.6 Hz, 1H), 7.65 (dd, *J* = 10.8, 4.2 Hz, 2H), 7.51 (s, 1H), 7.45 (s, 1H), 7.35 (s, 1H), 7.31 (d, *J* = 7.0 Hz, 1H), 1.85 (s, 3H), 1.62 (s, 3H).

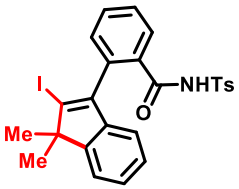
^{13}C NMR (125 MHz, $CDCl_3$): δ 202.8, 176.0, 138.5, 136.8, 134.8, 132.3, 130.8, 129.3, 129.1, 128.2, 127.7, 126.6, 125.5, 105.1, 99.4, 20.2.

HRMS (ESI): $C_{18}H_{16}NaO_2$ $[M+Na]^+$ calculated = 287.1043; found = 287.1041.

(j) Procedure for Iodonium Induced Cyclization of Allenylated Product

According to the method of preparation based on preceding literature[3], 1.2 equiv of *N*-iodosuccinimide was added to a solution of allenylated *N*-Tosylbenzamide **3a** (0.15 mmol, 1 equiv) in MeCN. The reaction mixture was stirred at room temperature for 30 minutes and checked for TLC. After completion of the reaction, the crude mixture was evaporated and directly subjected to column chromatography.

7.



2-(2-iodo-1,1-dimethyl-1H-inden-3-yl)-N-tosylbenzamide

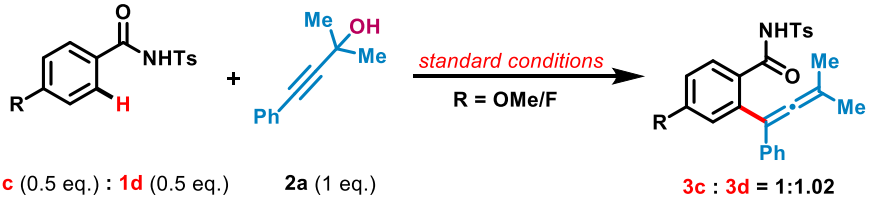
59 mg, 73%, yellow oil, Rf = 0.7 in Hexane:EA = 4:1

^1H NMR (500 MHz, $CDCl_3$): δ 7.97 (d, *J* = 8.2 Hz, 2H), 7.91 (d, *J* = 7.6 Hz, 1H), 7.64 – 7.52 (m, 1H), 7.48 (t, *J* = 7.4 Hz, 1H), 7.43 (d, *J* = 7.8 Hz, 1H), 7.25 (dd, *J* = 7.1, 4.8 Hz, 4H), 7.13 (dd, *J* = 8.0, 1.4 Hz, 2H), 2.43 (s, 3H), 2.11 (s, 3H), 1.71 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 153.7, 150.0, 143.4, 140.4, 138.8, 133.8, 129.9, 129.3, 129.1, 128.5, 127.9, 127.5, 126.0, 125.4, 125.1, 95.6, 35.4, 24.1, 21.7.

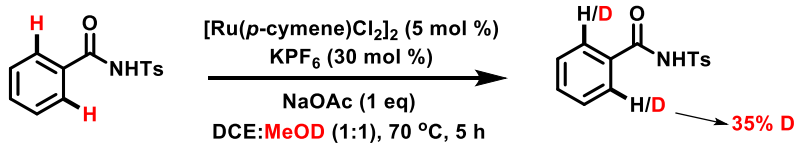
HRMS (ESI): $C_{25}H_{23}INO_3S$ $[M+H]^+$ calculated = 544.0438; found = 544.0441.

(k) Procedure for Intermolecular Competitive Experiment



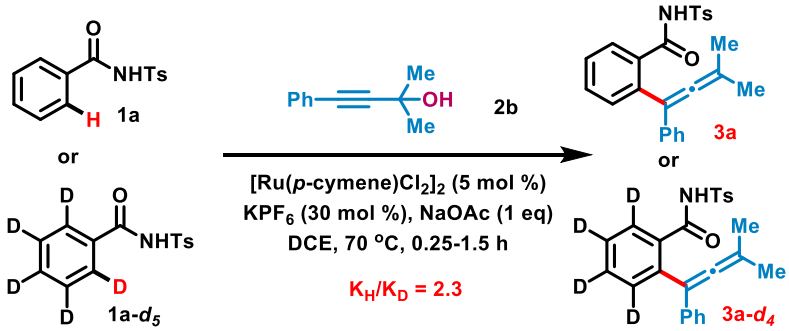
To an oven dried screw cap reaction tube equipped with a magnetic stir bar, was added **3c** 4-Methoxy-*N*-tosylbenzamide (18 mg,0.06 mmol), **3d** 4-Fluoro-*N*-tosylbenzamide (17.6 mg, 0.06 mmol), [Ru(*p*-cymene)Cl_2]$_2$ (3.7 mg,0.006 mmol), KPF_6 (6.6 mg, 0.036 mmol), NaOAc (9.8 mg, 0.06 mmol) and 2-methyl-4-phenylbut-3-yn-2-ol (21.12 mg, 0.132 mmol) followed by 1 ml DCE. After heating the reaction mixture at 70 °C for 5 h, it was cooled to room temperature and the solvent was evaporated under reduced pressure. The residue was taken up for NMR analysis.

(l) Procedure for H/D Exchange Experiment



To an oven dried screw cap reaction tube equipped with a magnetic stir bar, was added *N*-Tosylbenzamide (27.5 mg, 0.1 mmol), [Ru(*p*-cymene)Cl_2]$_2$ (3 mg, 0.005 mmol), KPF_6 (5.5 mg, 0.03 mmol) and NaOAc (8.2 mg, 0.1 mmol) followed by 1:1 DCE: MeOH-*d4*. After heating the reaction mixture at 70 °C for 5 h, it was cooled to room temperature and the solvent was evaporated under reduced pressure. The residue was taken up for NMR analysis.

(m) Procedure for Kinetic Isotopic Experiments



To an oven dried screw cap reaction tube equipped with a magnetic stir bar, 0.2 mmol of H_5-benzamide was subjected to standard reaction conditions. After an equal interval of 15 minutes, reaction mixture was concentrated and directly taken for NMR analysis upto 1.5 hours.

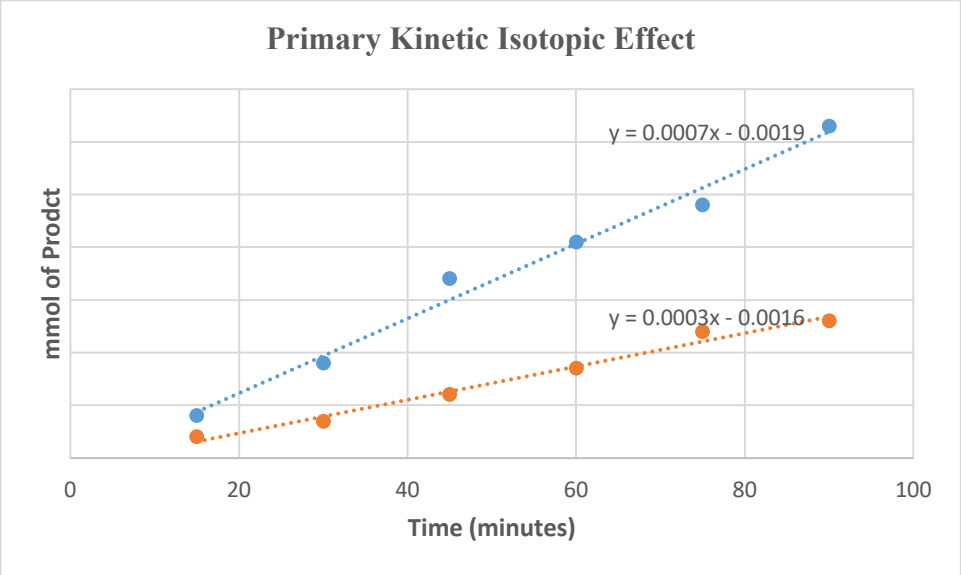
Identical set of experiments were performed using D_5-benzamide and NMR Analysis was carried out.

Studies for H5-Benzamide

S.No.	Time (minutes)	Rate Conversion	Mmol of Product
1	15	0.04	0.008
2	30	0.09	0.018
3	45	0.17	0.034
4	60	0.205	0.041
5	75	0.24	0.048
6	90	0.315	0.063

Studies for D5-Benzamide

S.No.	Time (minutes)	Rate Conversion	Mmol of Product
1	15	0.02	0.004
2	30	0.035	0.007
3	45	0.075	0.015
4	60	0.08	0.016
5	75	0.12	0.024
6	90	0.13	0.026



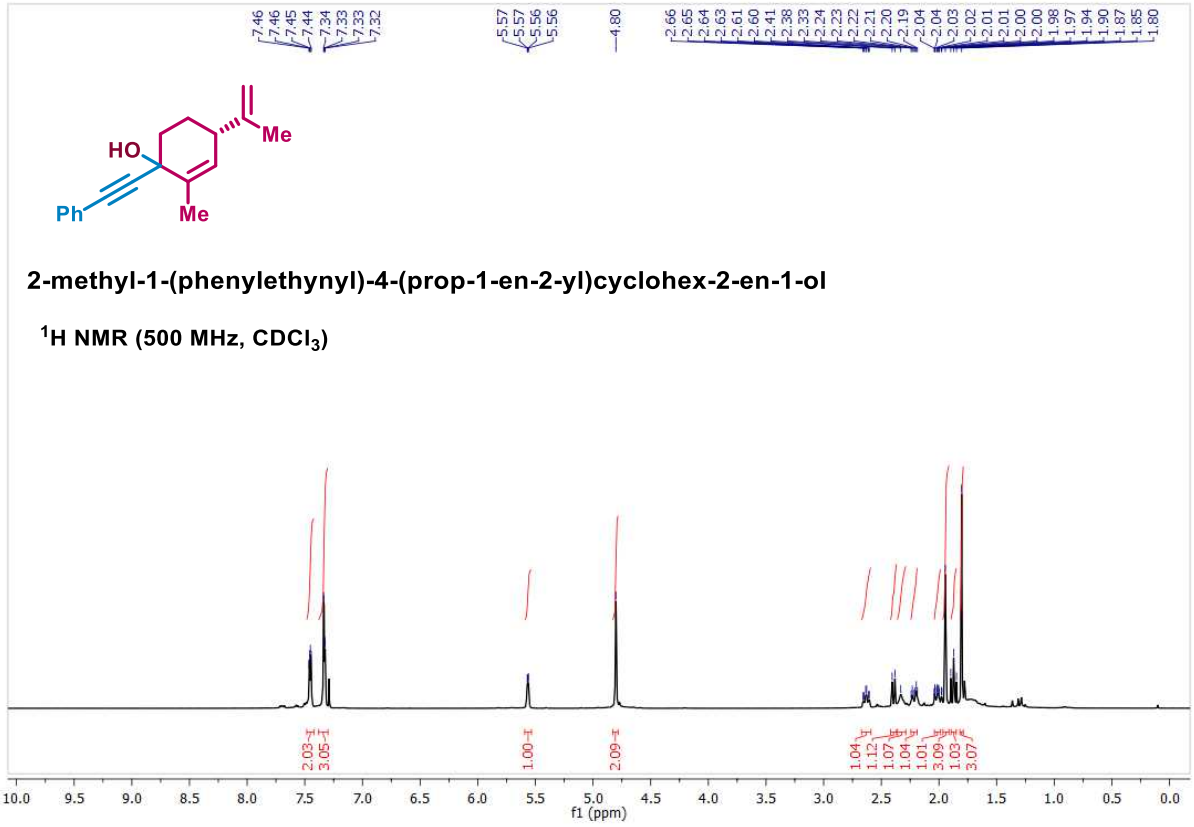
4. References

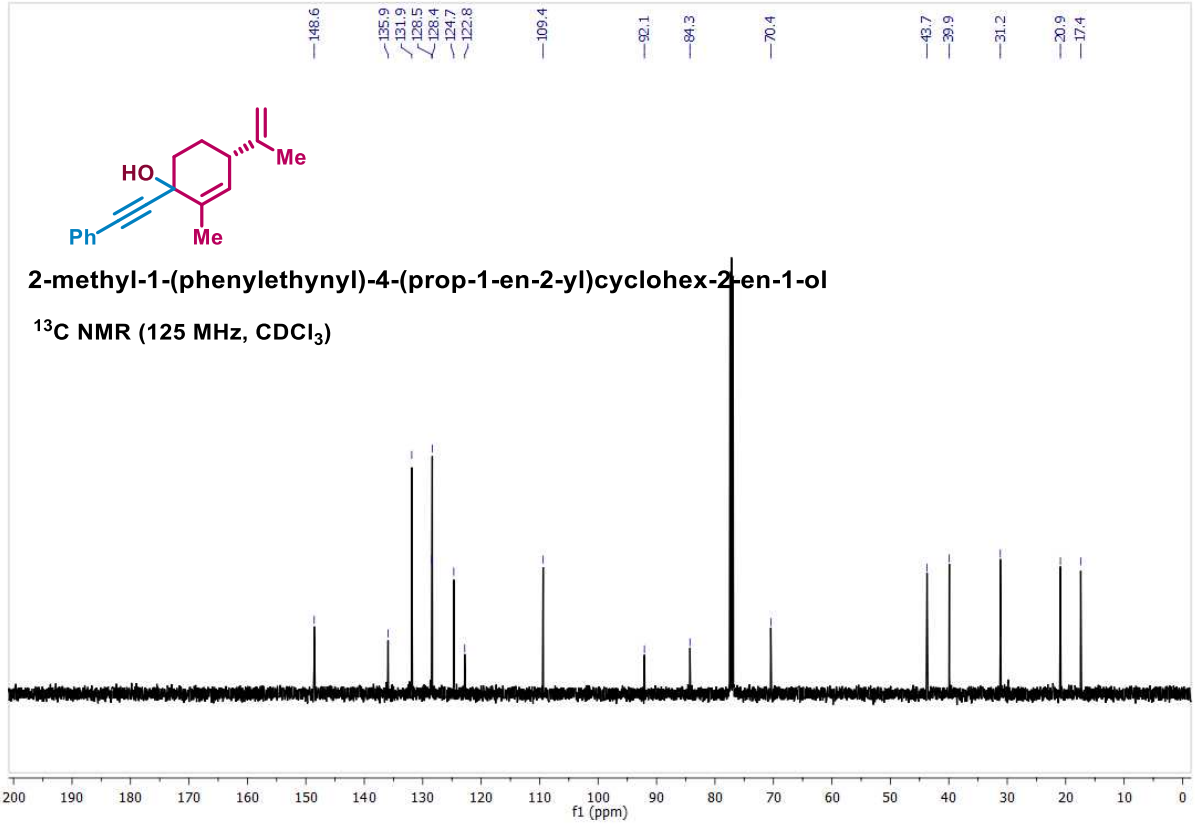
1. L. Yang, S. Li, L. Cai, Y. Ding, L. Fu, Z. Cai, H. Ji and G. Li, *Org. Lett.* 2017, **19**, 2746.

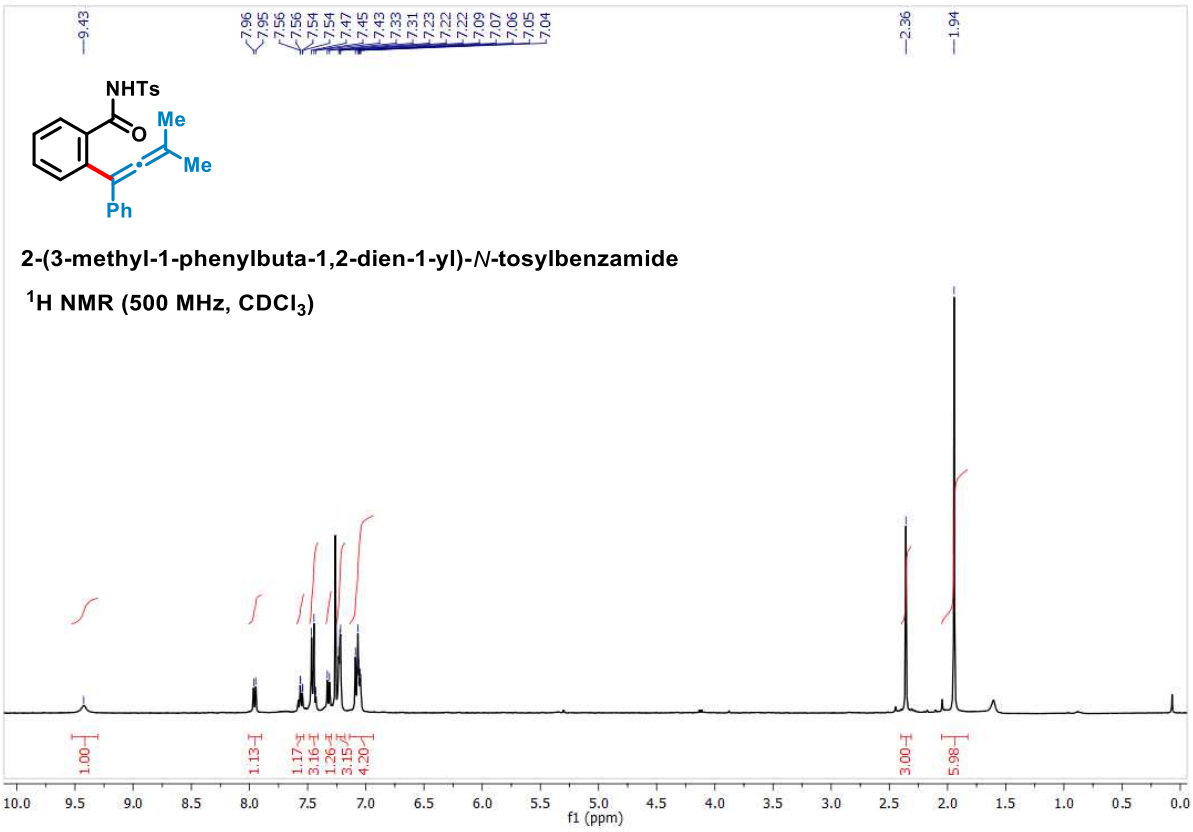
2. (a) B. S. L. Collins, M. G. Suero and M. J. Gaunt, *Angew. Chem., Int. Ed*. 2013, **52**, 5799; (b) C. Ma, Y. Zhang, H. Zhang, J. Li, Y. Nishiyama, H. Tanimoto, T. Morimoto and K. Kakiuchi, *Synlett*, 2017, **28**, 560.

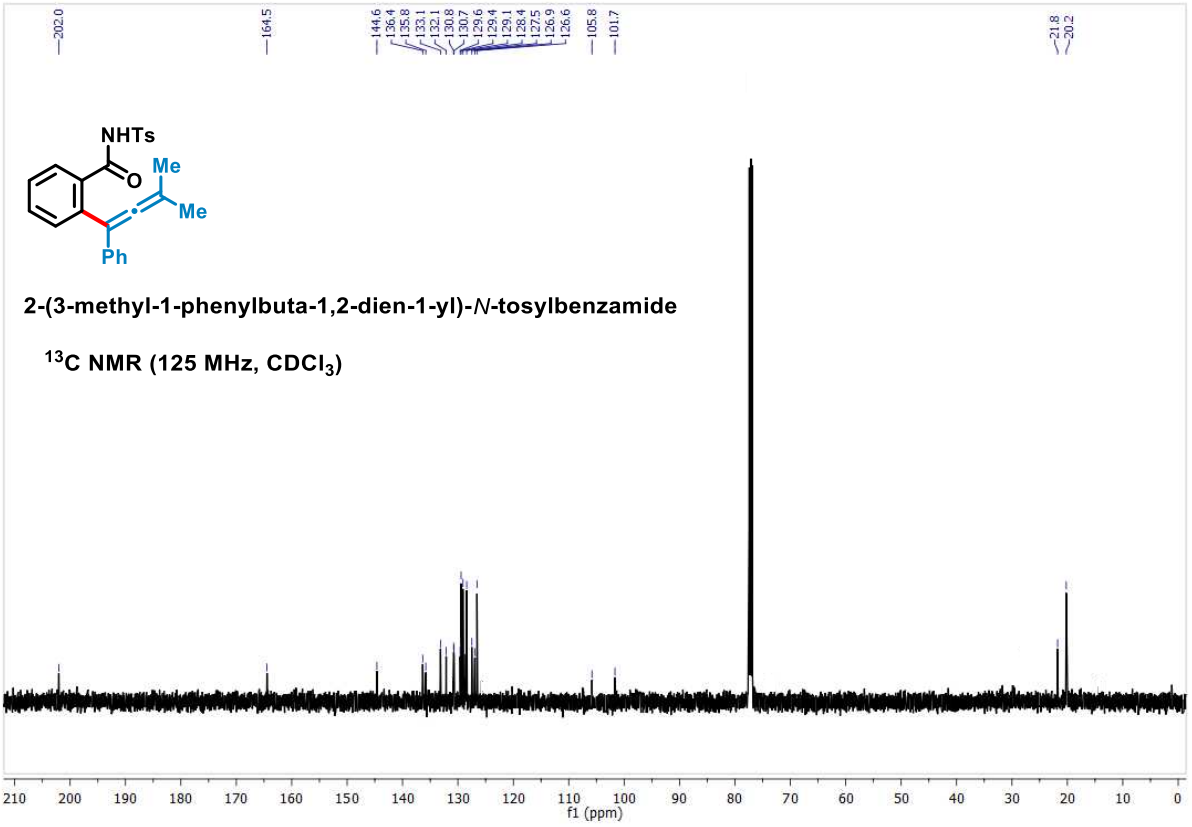
3. C. Grandclaudon, V. Michelet and P. Y. Toullec, *Org. Lett.*, 2016, **18**, 676.

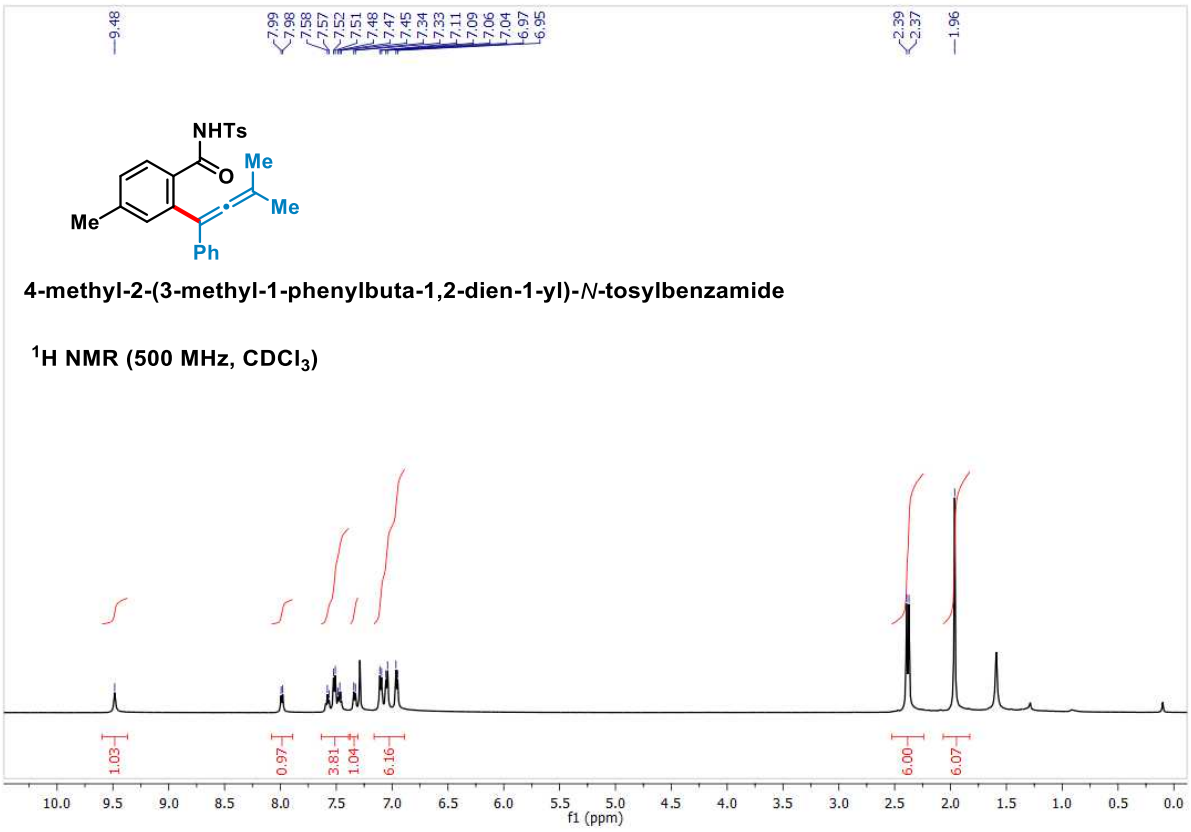
5. ^{1}H and ^{13}C NMR Spectra of Compounds





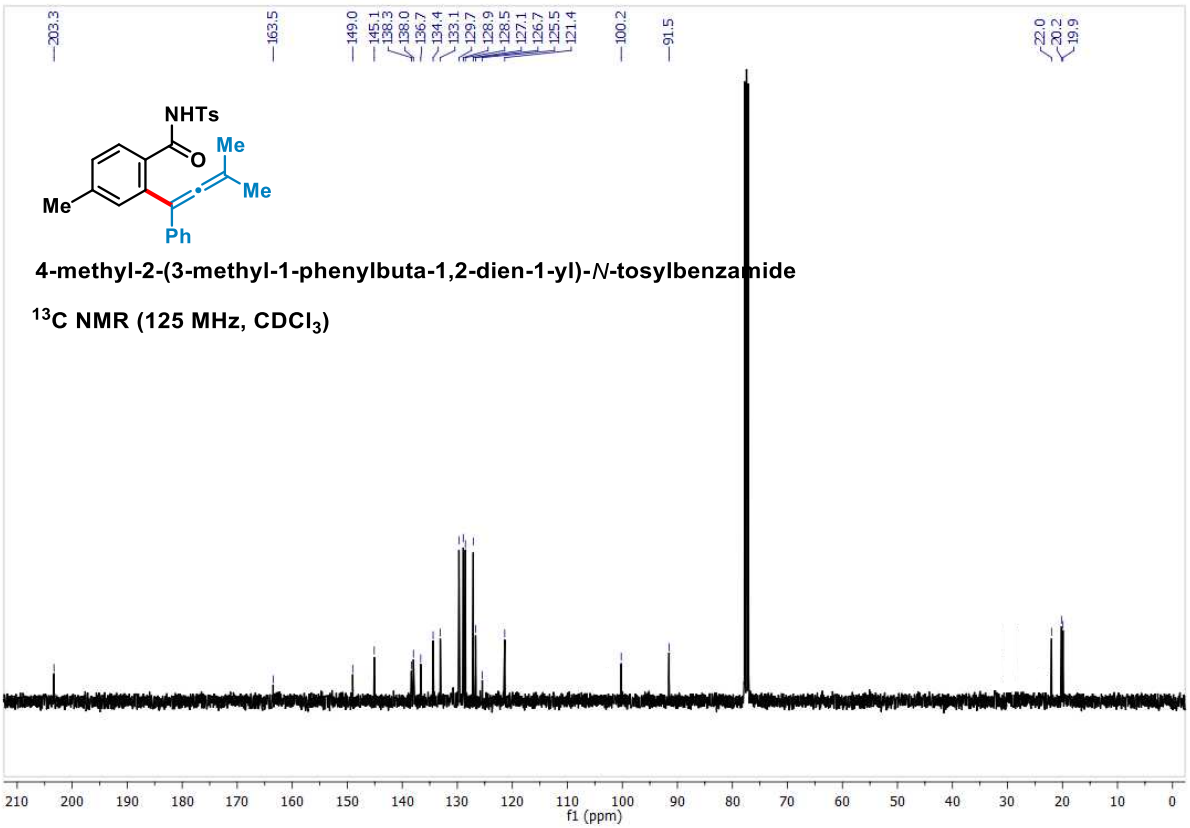

NHTs
O
Me
Me
Ph
2-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-N-tosylbenzamide
1H NMR (500 MHz, CDCl3)
f1 (ppm)


NHTs
O
Me
Me
Ph
2-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-N-tosylbenzamide
13C NMR (125 MHz, CDCl3)
f1 (ppm)



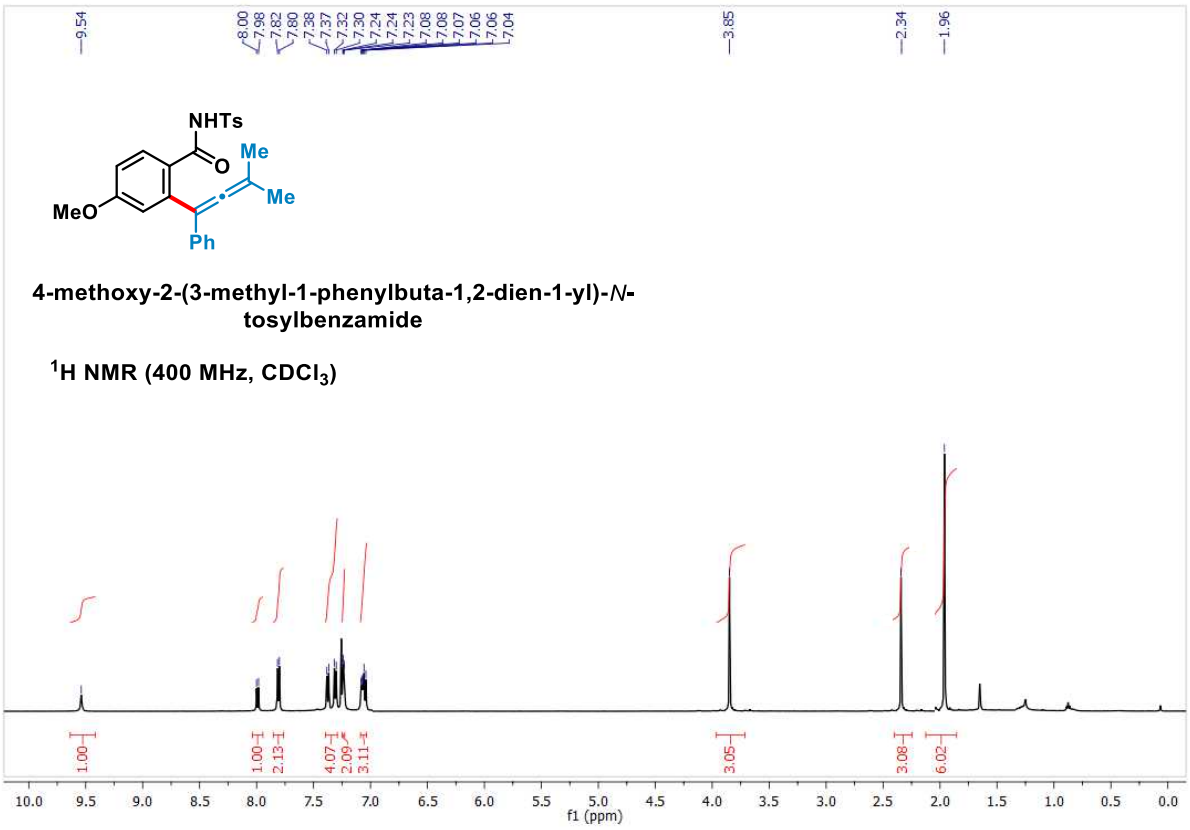
4-methyl-2-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{1}H NMR (500 MHz, $CDCl_3$)



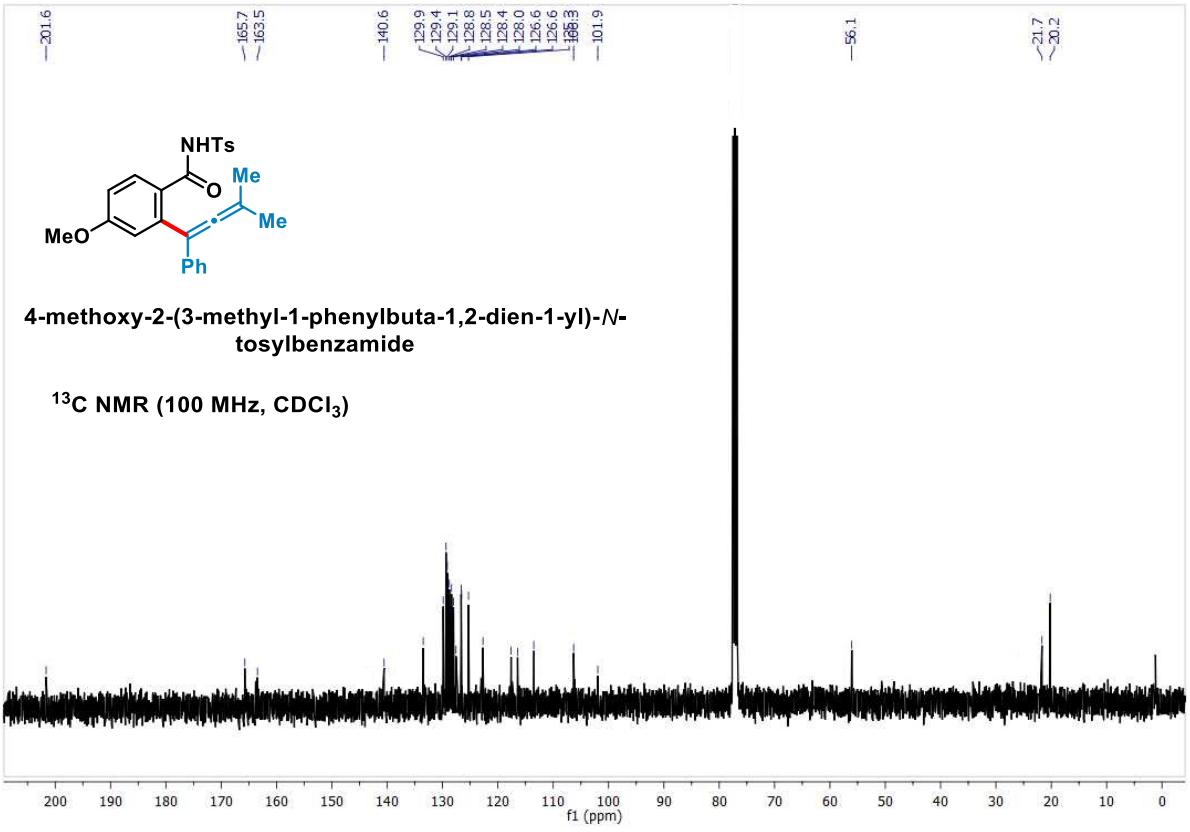
4-methyl-2-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{13}C NMR (125 MHz, $CDCl_3$)



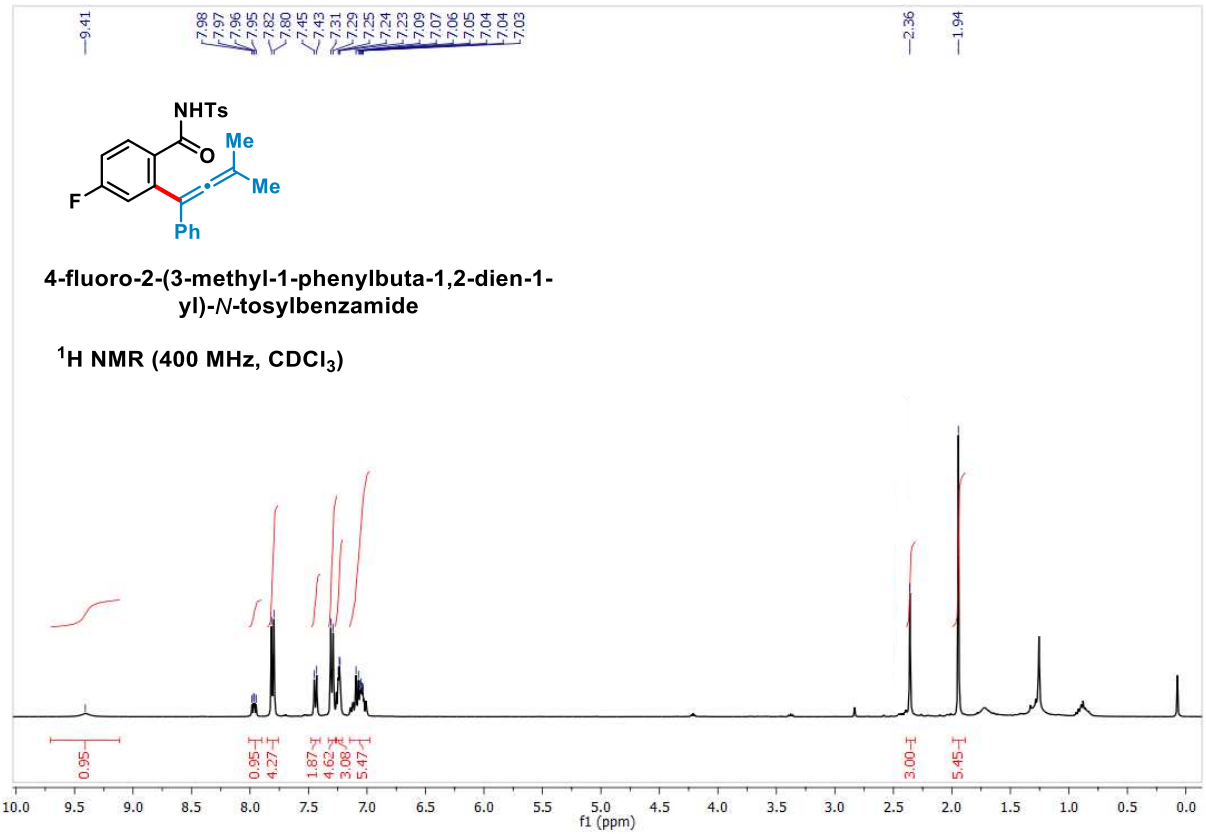
4-methoxy-2-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{1}H NMR (400 MHz, $CDCl_3$)



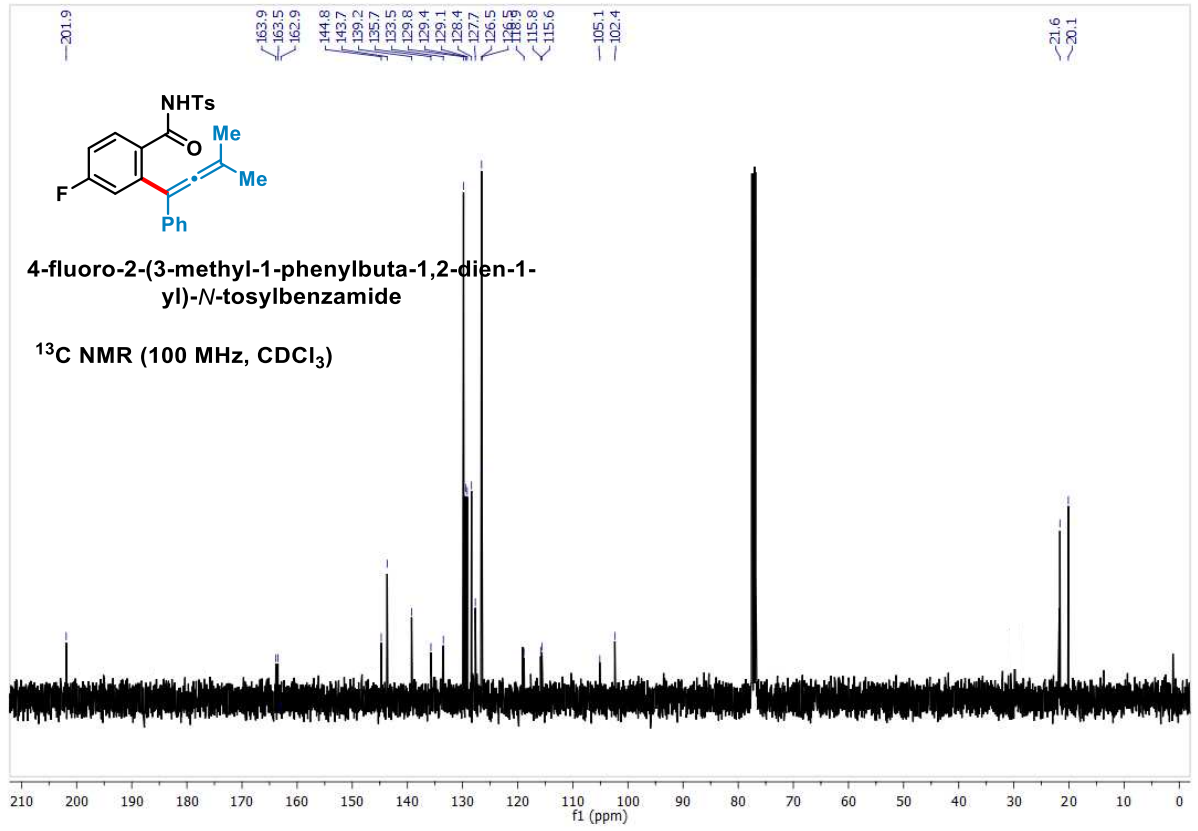
4-methoxy-2-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{13}C NMR (100 MHz, $CDCl_3$)



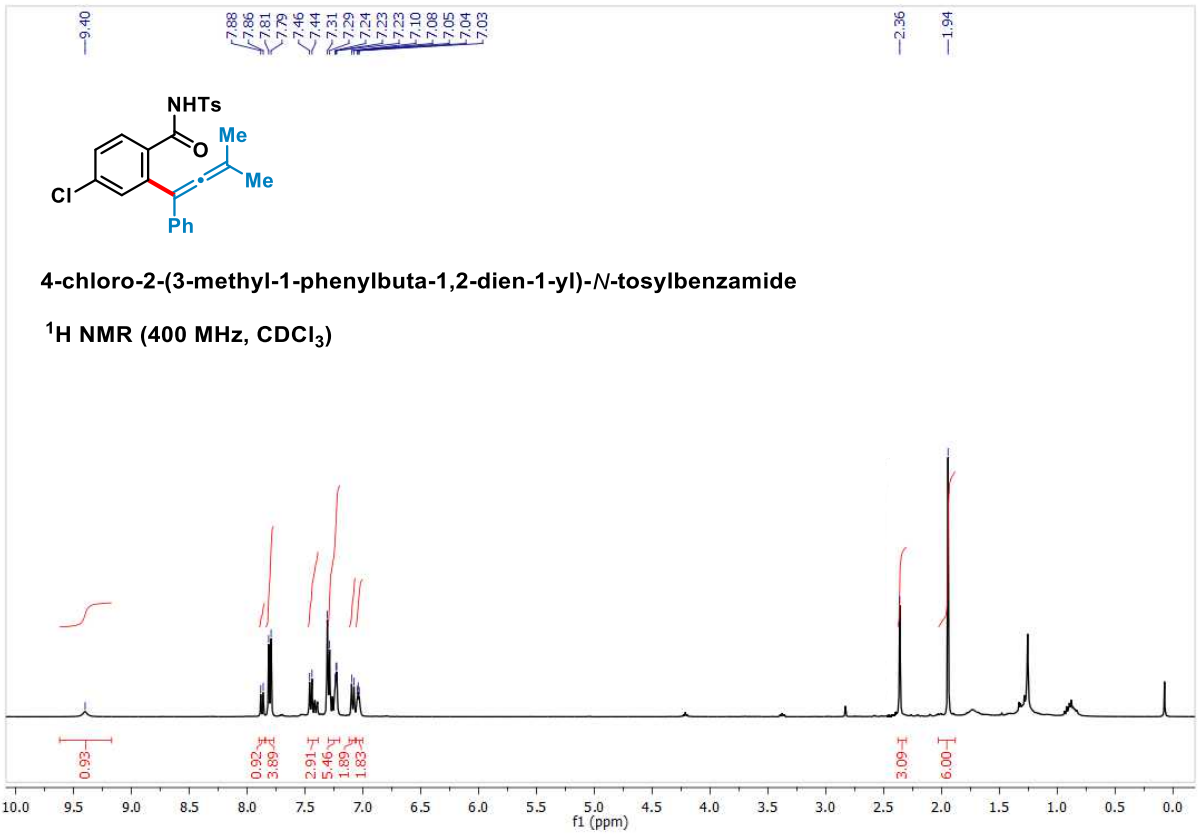
4-fluoro-2-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{1}H NMR (400 MHz, $CDCl_3$)



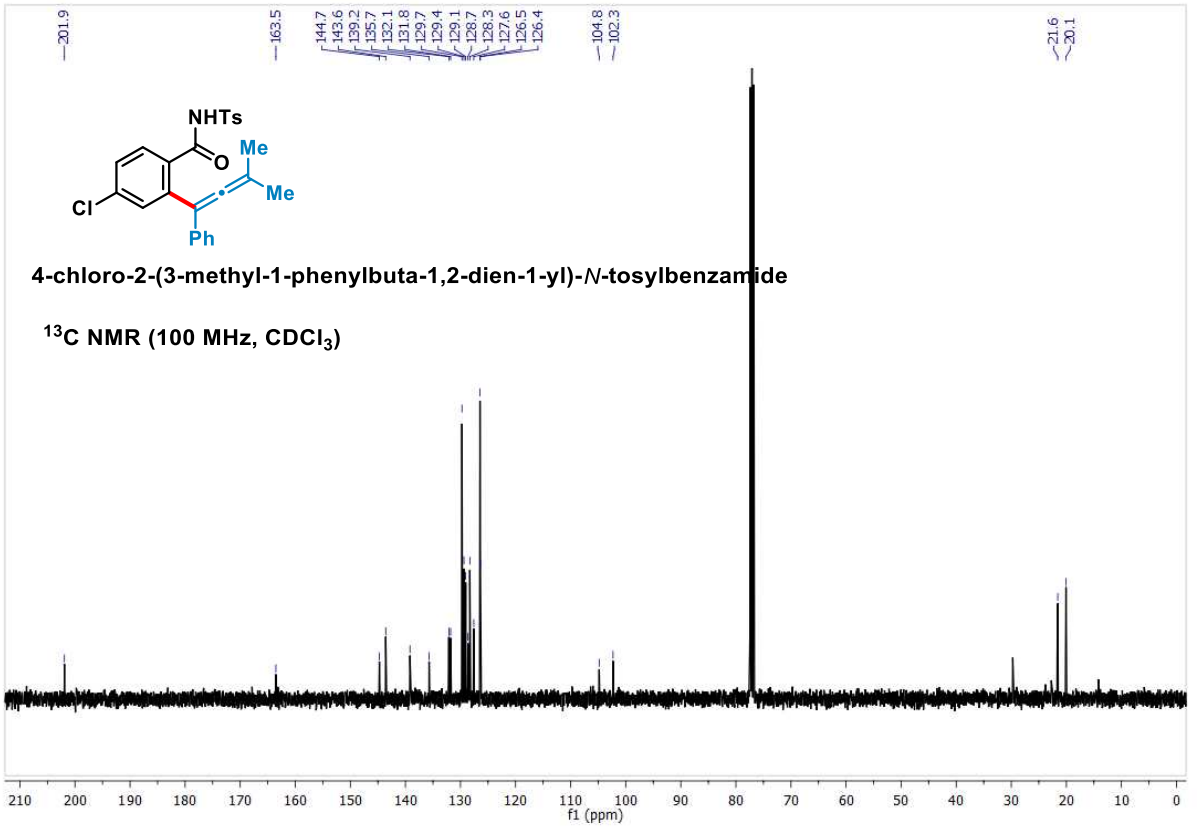
4-fluoro-2-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{13}C NMR (100 MHz, $CDCl_3$)



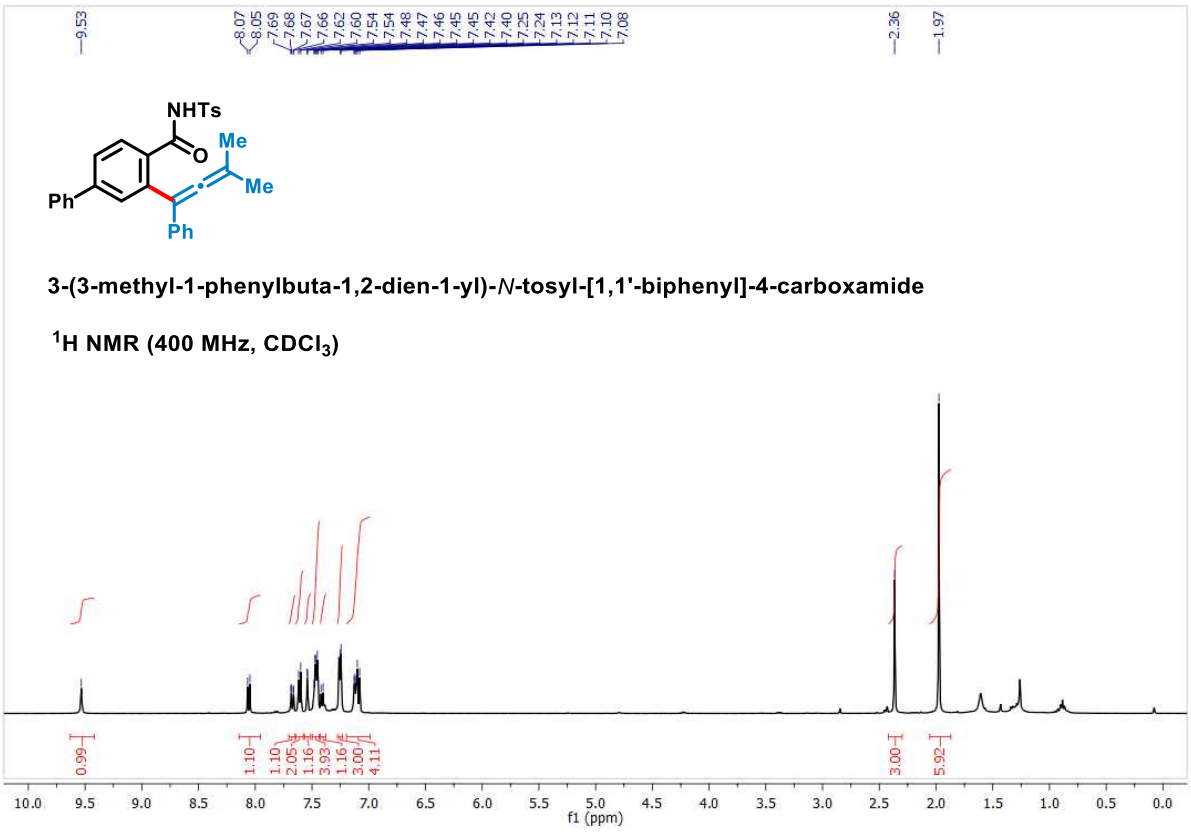
4-chloro-2-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{1}H NMR (400 MHz, $CDCl_3$)



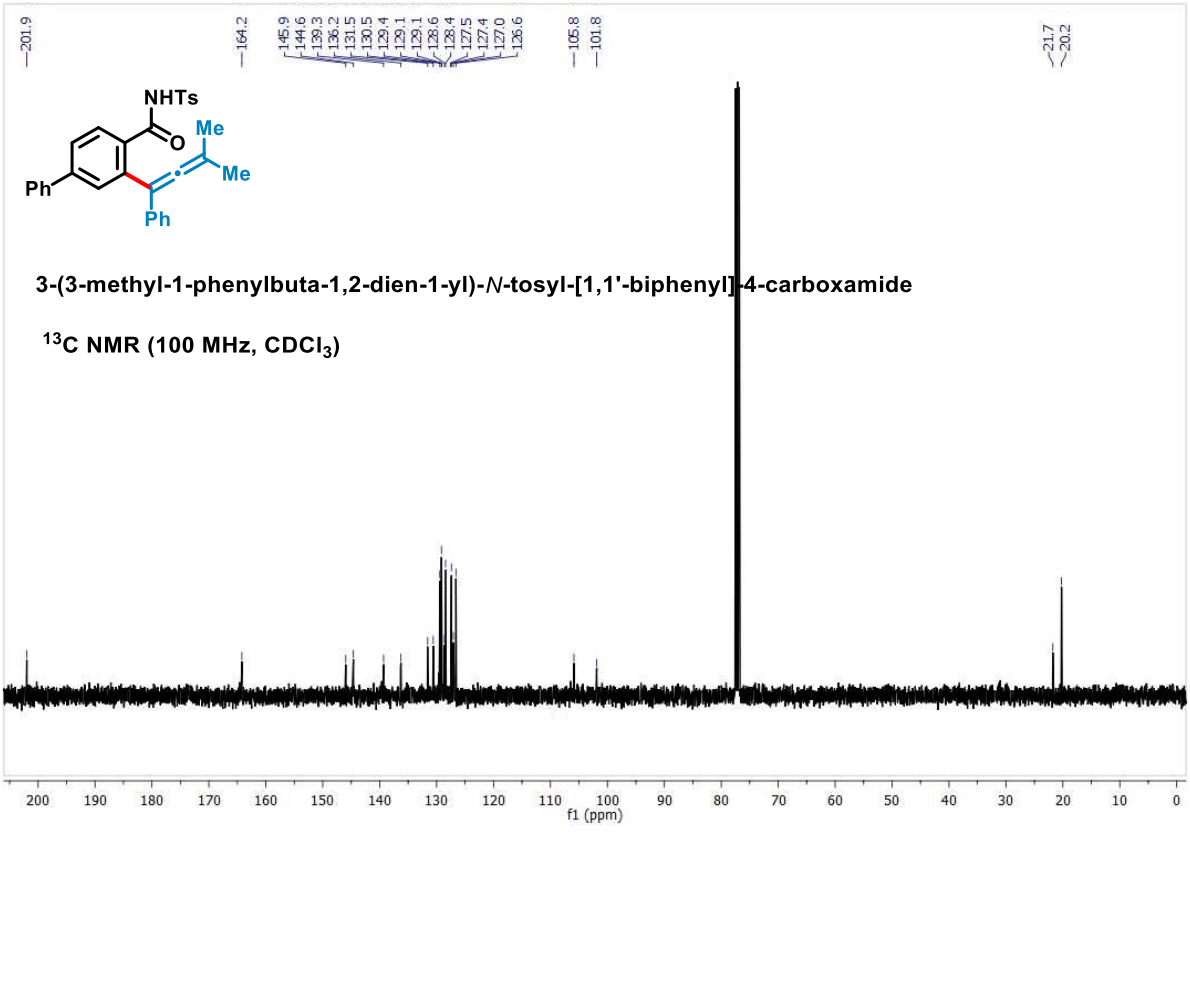
4-chloro-2-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{13}C NMR (100 MHz, $CDCl_3$)



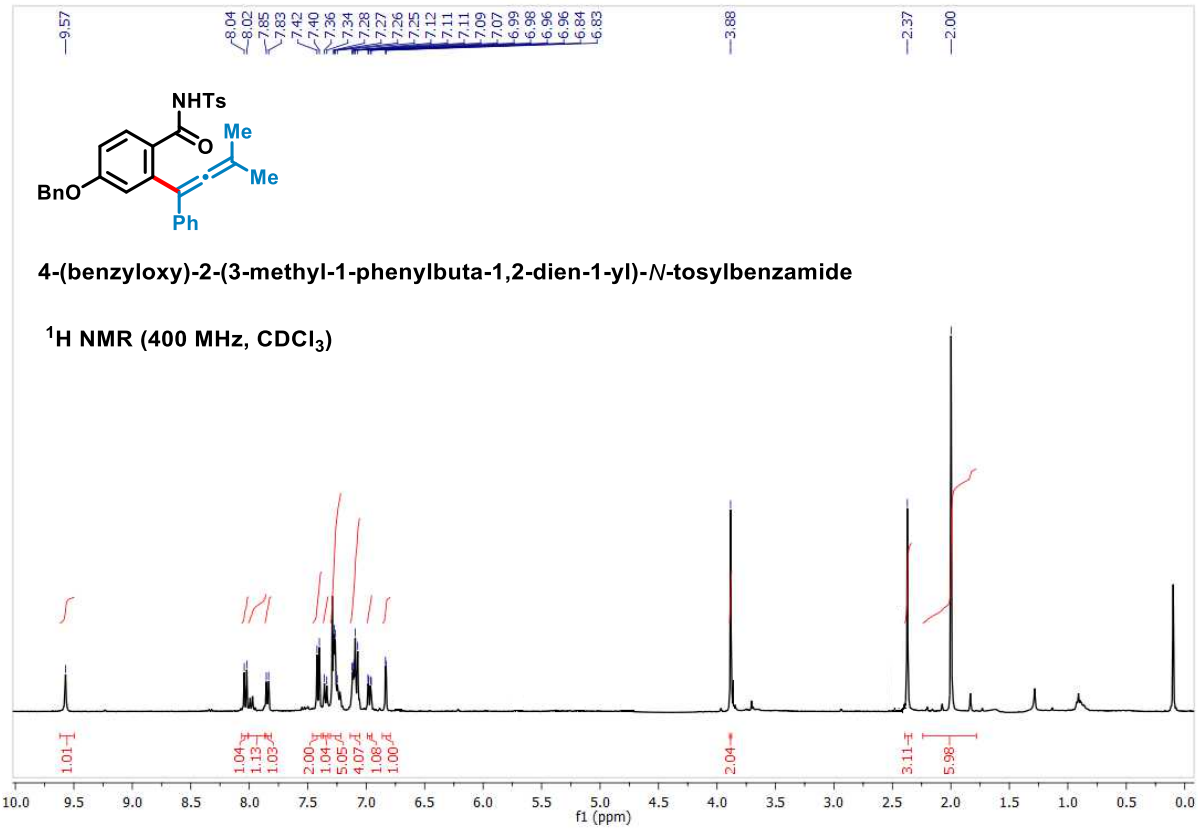
3-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosyl-[1,1'-biphenyl]-4-carboxamide

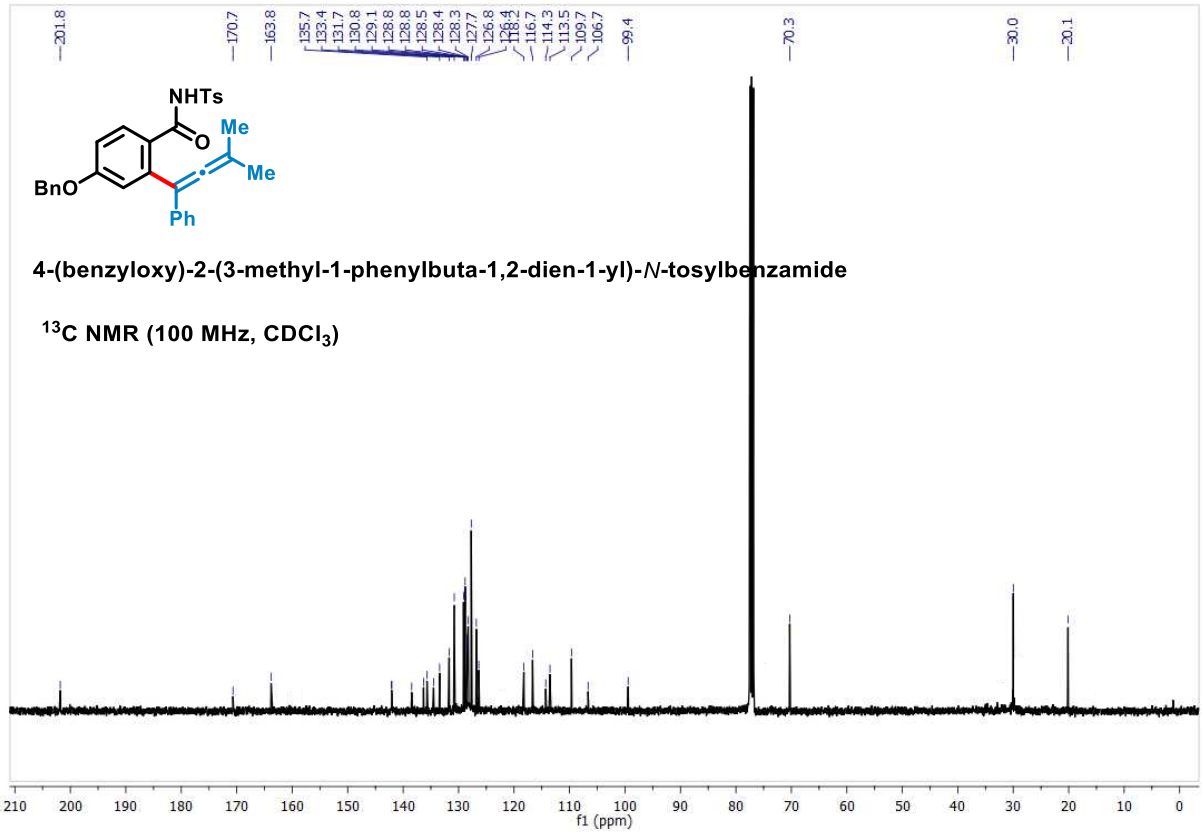
^{1}H NMR (400 MHz, $CDCl_3$)

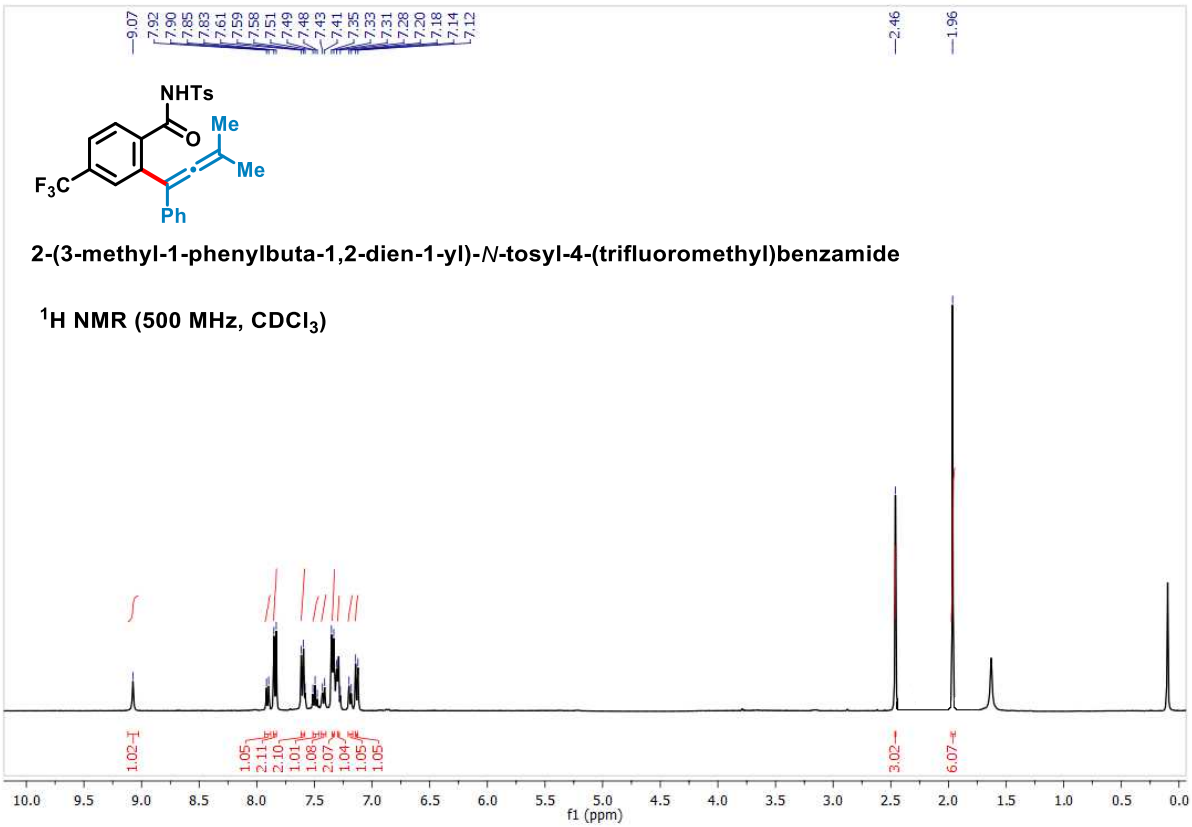


3-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosyl-[1,1'-biphenyl]-4-carboxamide

^{13}C NMR (100 MHz, $CDCl_3$)

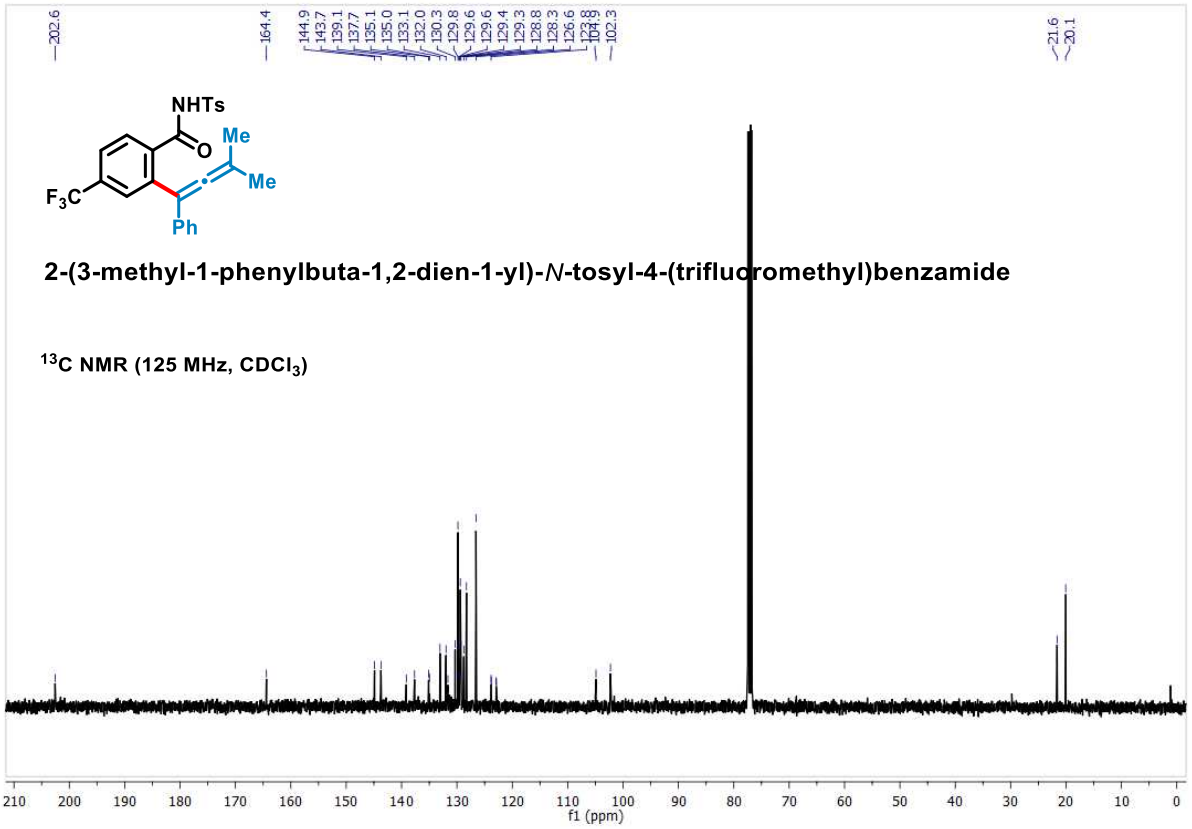

NHTs
Me
Me
BnO
Ph
4-(benzyloxy)-2-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-N-tosylbenzamide
1H NMR (400 MHz, CDCl3)
f1 (ppm)


NHTs
Me
Me
BnO
Ph
4-(benzyloxy)-2-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-N-tosylbenzamide
13C NMR (100 MHz, CDCl3)
f1 (ppm)



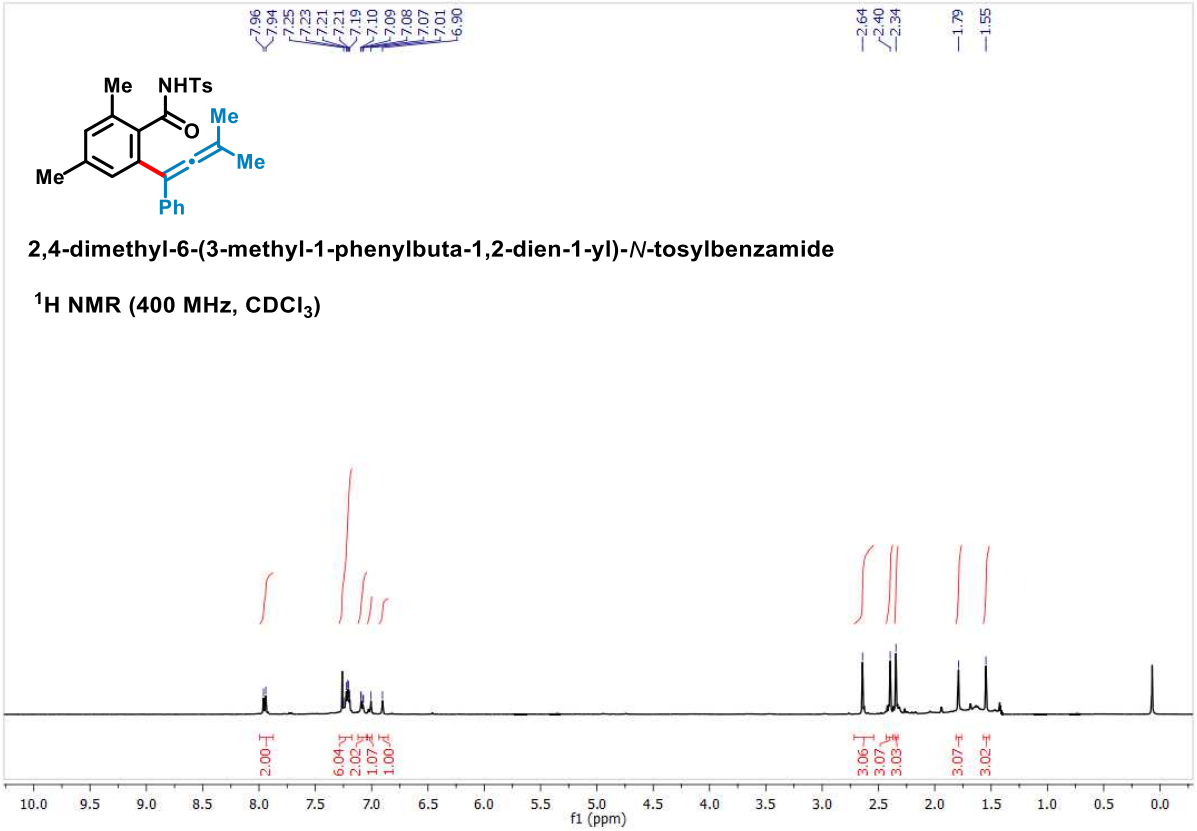
2-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosyl-4-(trifluoromethyl)benzamide

^{1}H NMR (500 MHz, $CDCl_3$)



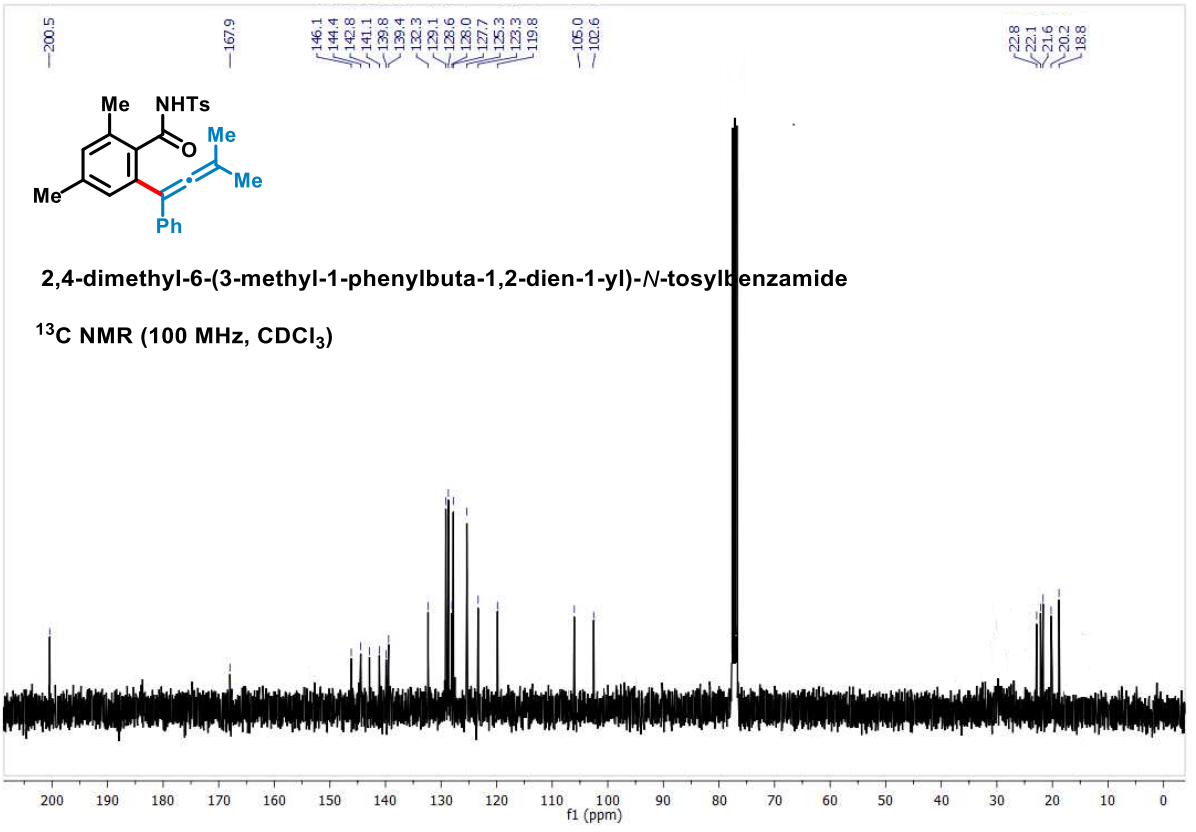
2-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosyl-4-(trifluoromethyl)benzamide

^{13}C NMR (125 MHz, $CDCl_3$)



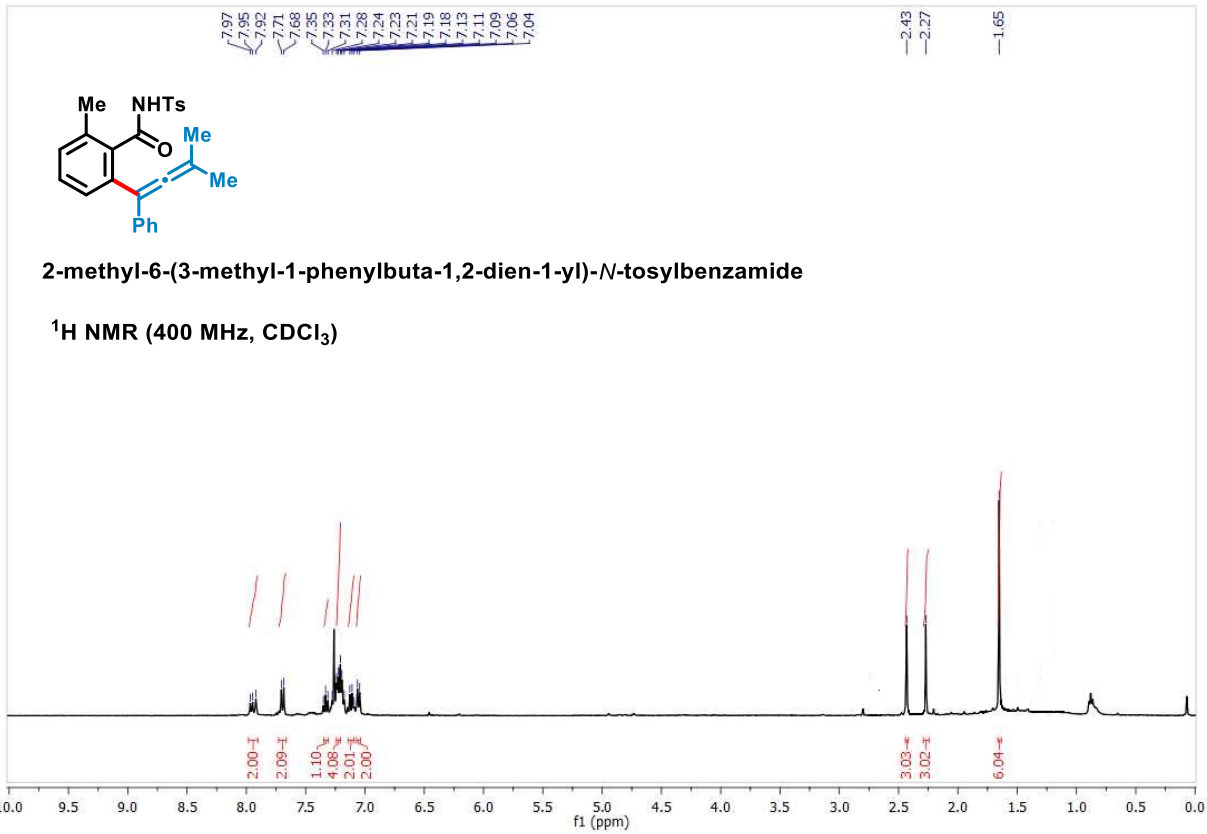
2,4-dimethyl-6-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{1}H NMR (400 MHz, $CDCl_3$)



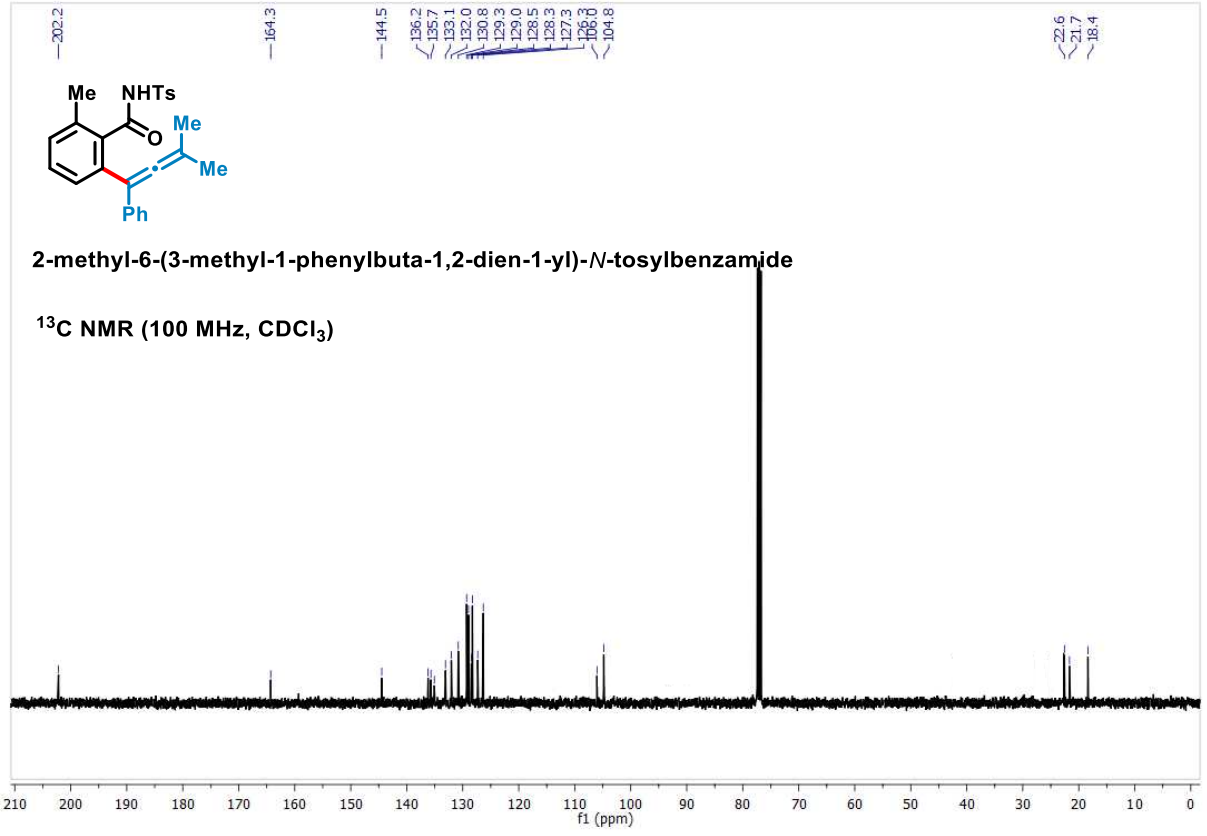
2,4-dimethyl-6-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{13}C NMR (100 MHz, $CDCl_3$)



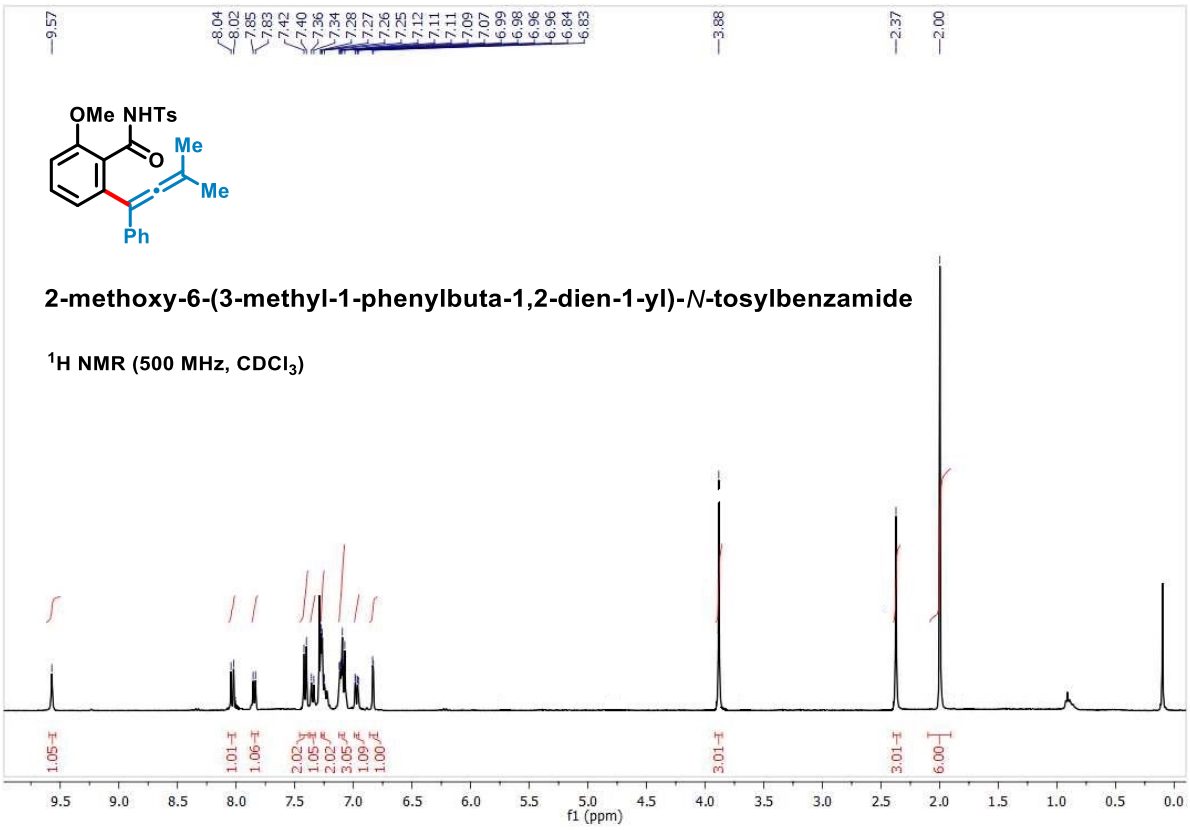
2-methyl-6-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

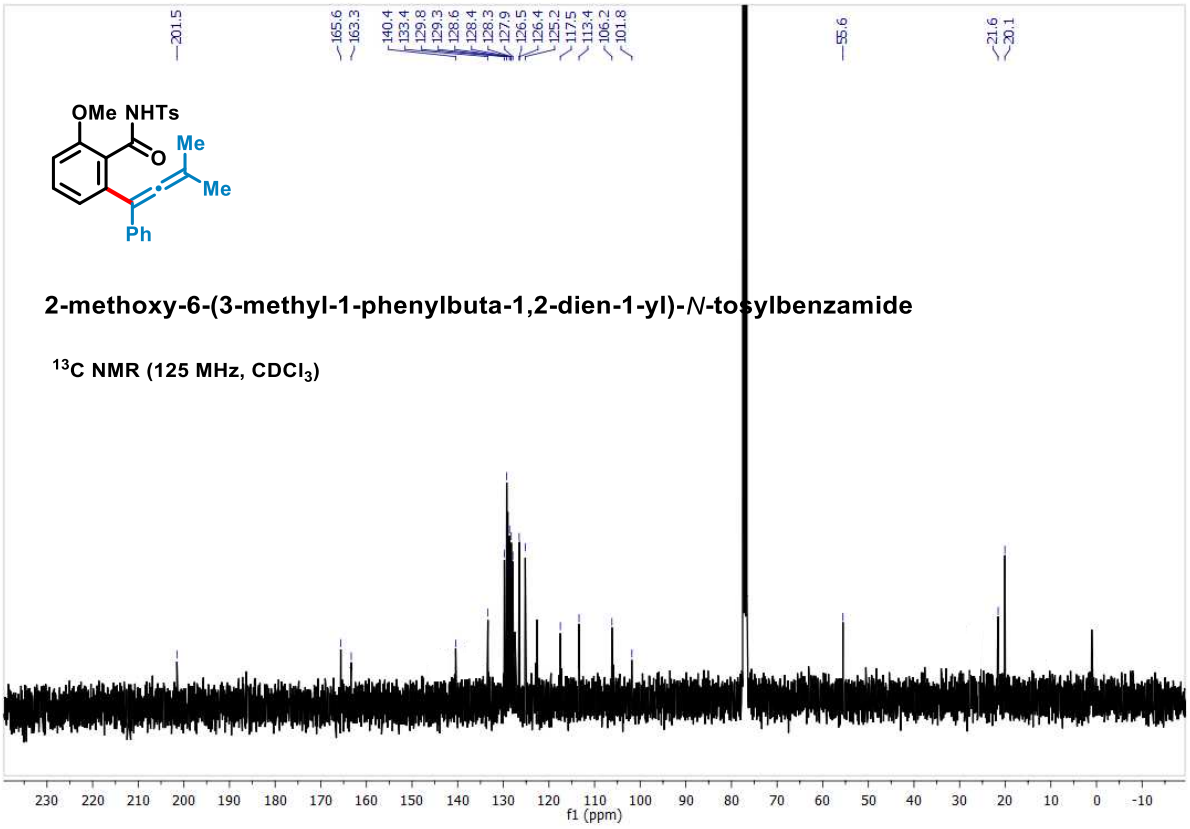
^{1}H NMR (400 MHz, $CDCl_3$)

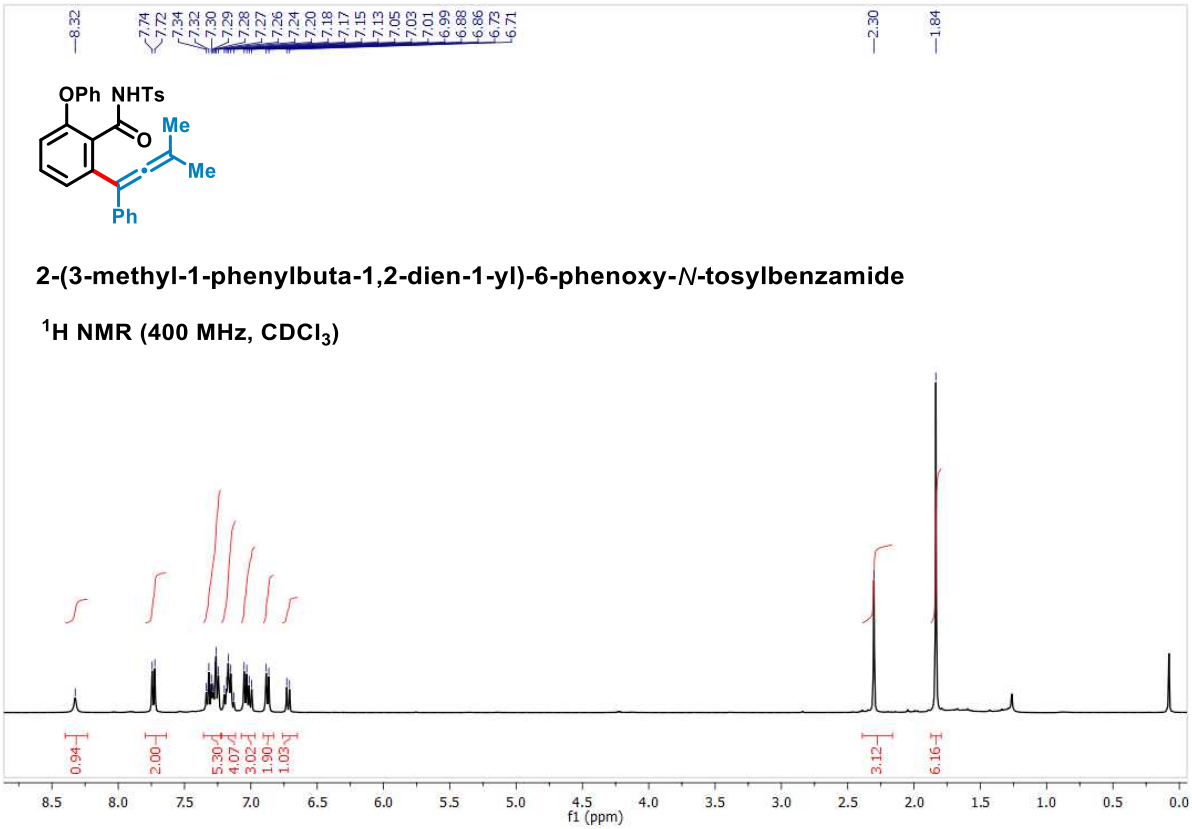


2-methyl-6-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{13}C NMR (100 MHz, $CDCl_3$)

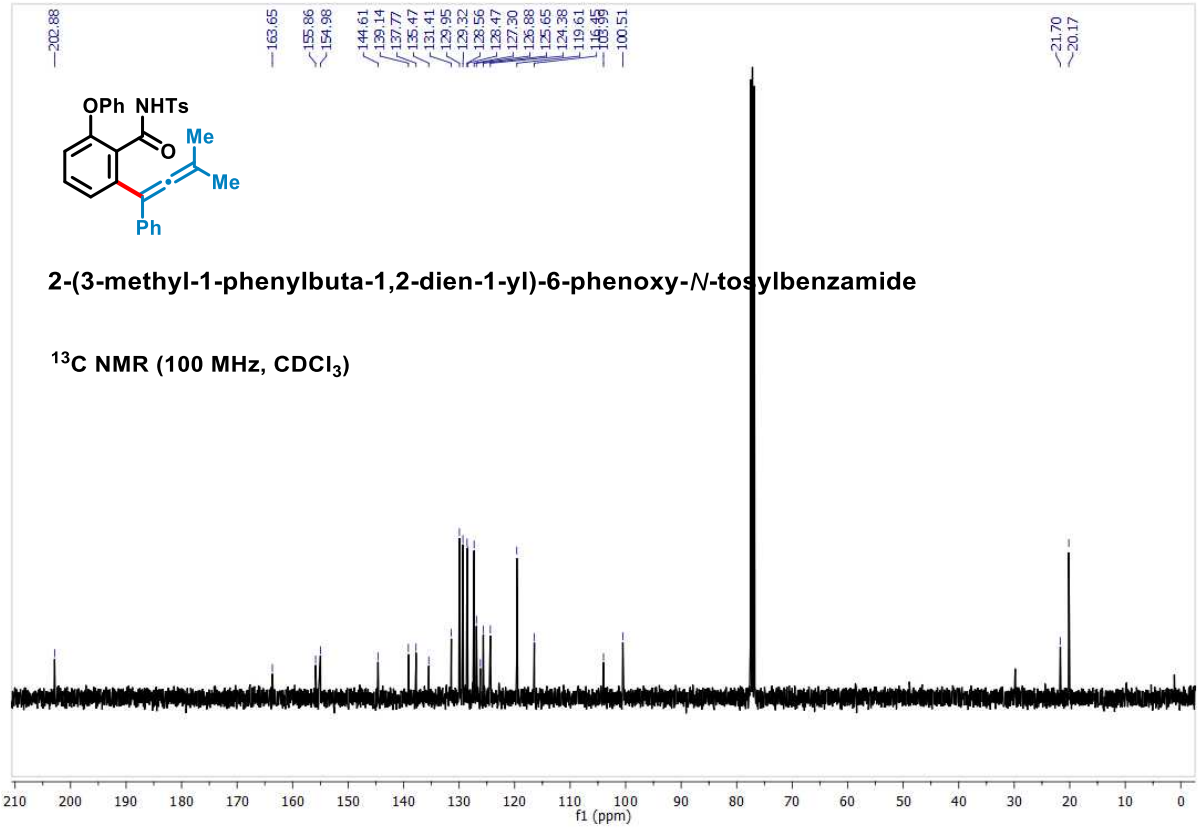

OMe NHTs
O
Me
Me
Ph
2-methoxy-6-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-N-tosylbenzamide
1H NMR (500 MHz, CDCl3)
f1 (ppm)


OMe NHTs
O
Me
Me
Ph
2-methoxy-6-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-N-tosylbenzamide
13C NMR (125 MHz, CDCl3)
f1 (ppm)



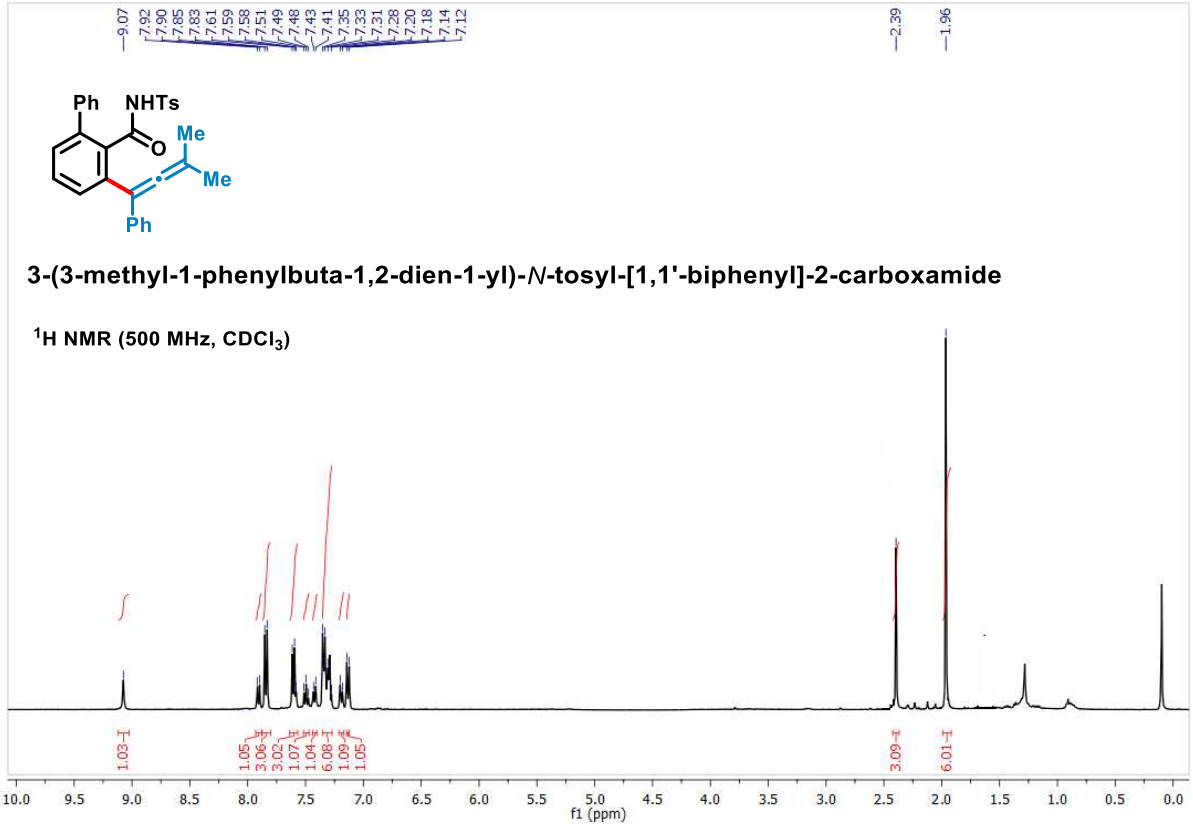
2-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-6-phenoxy-*N*-tosylbenzamide

^{1}H NMR (400 MHz, $CDCl_3$)



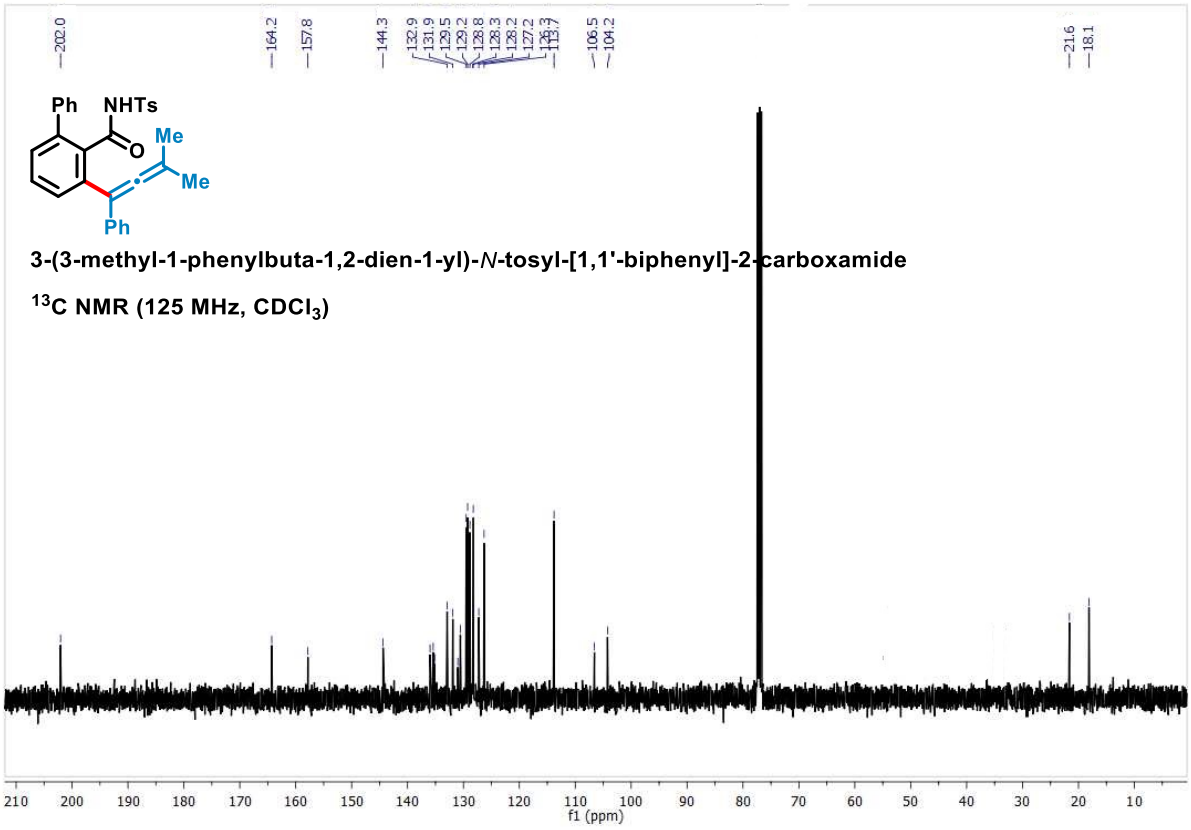
2-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-6-phenoxy-*N*-tosylbenzamide

^{13}C NMR (100 MHz, $CDCl_3$)



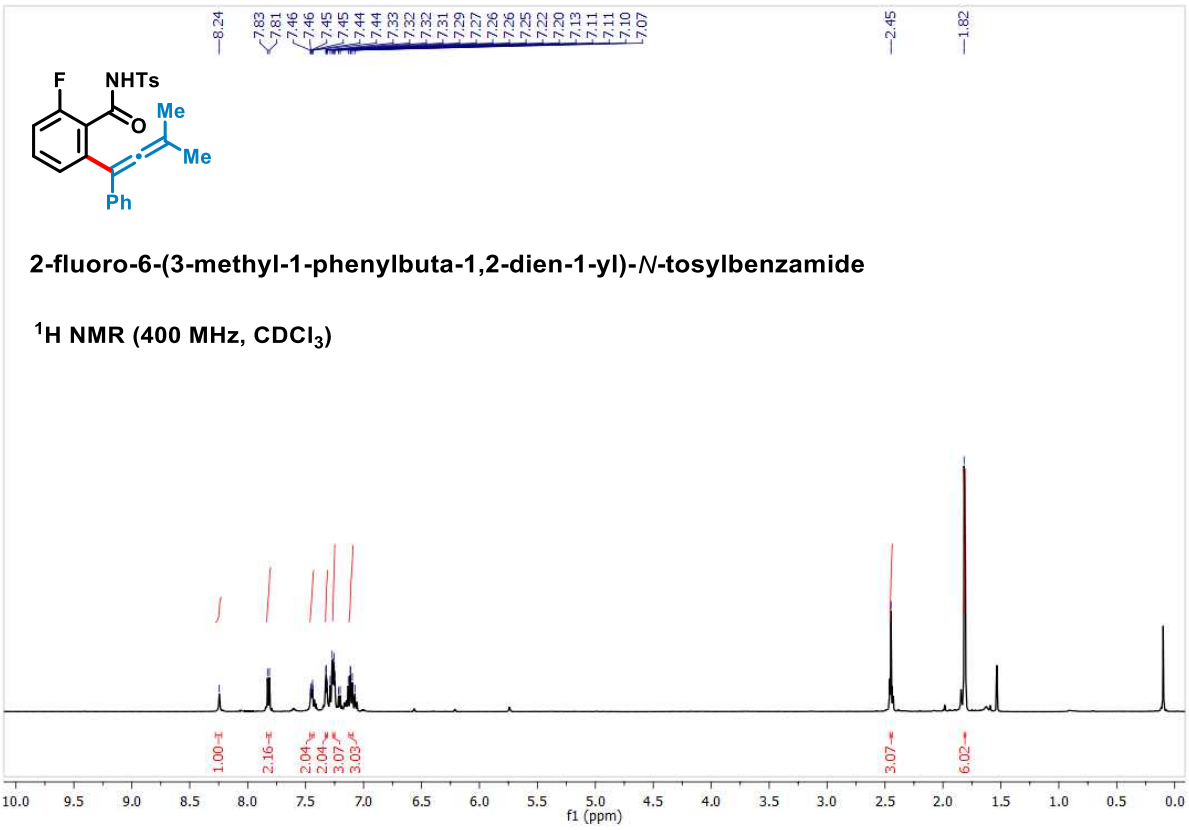
3-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosyl-[1,1'-biphenyl]-2-carboxamide

^{1}H NMR (500 MHz, $CDCl_3$)



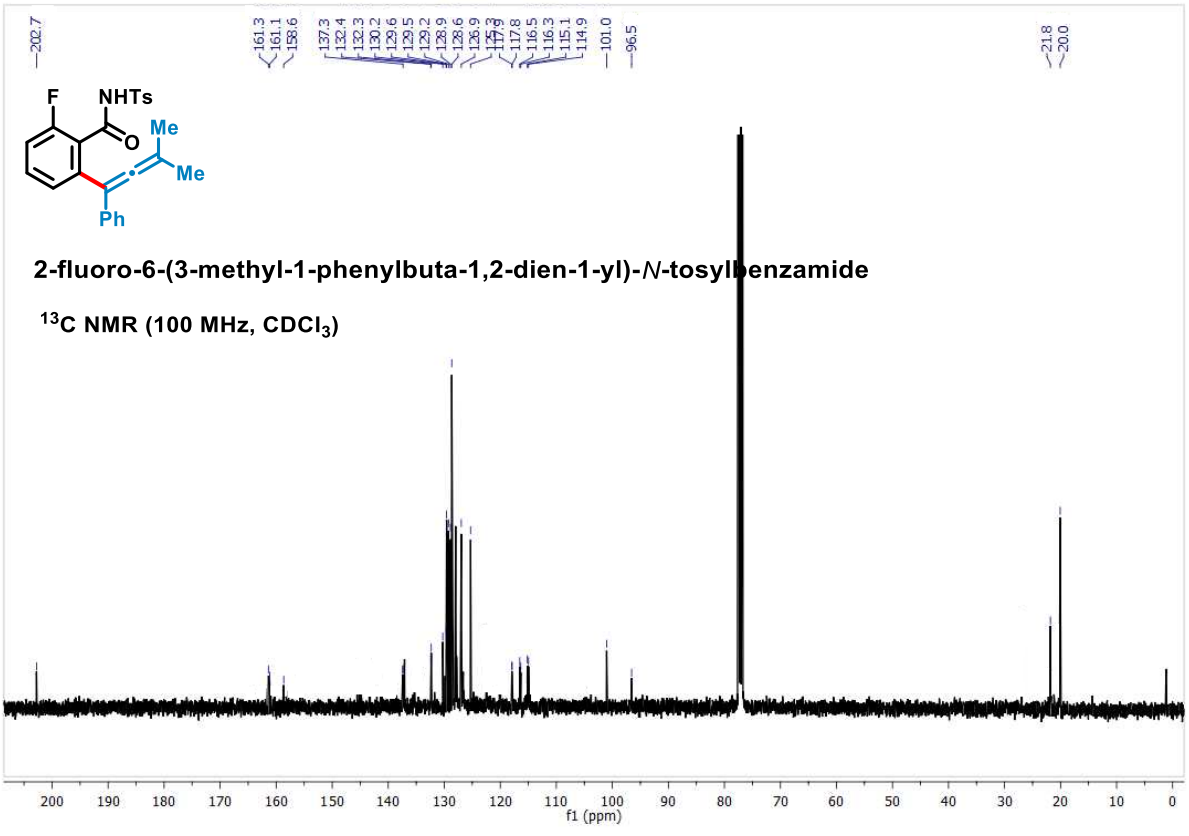
3-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosyl-[1,1'-biphenyl]-2-carboxamide

^{13}C NMR (125 MHz, $CDCl_3$)



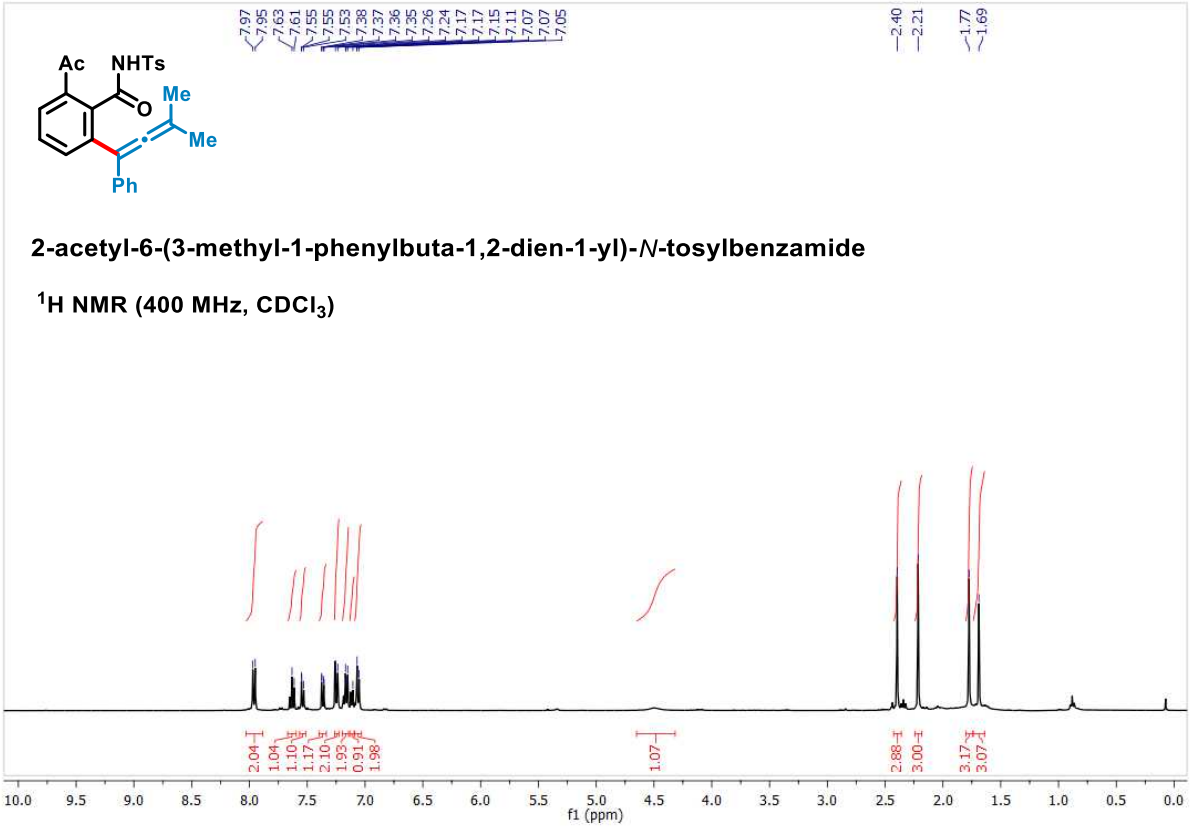
2-fluoro-6-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{1}H NMR (400 MHz, $CDCl_3$)



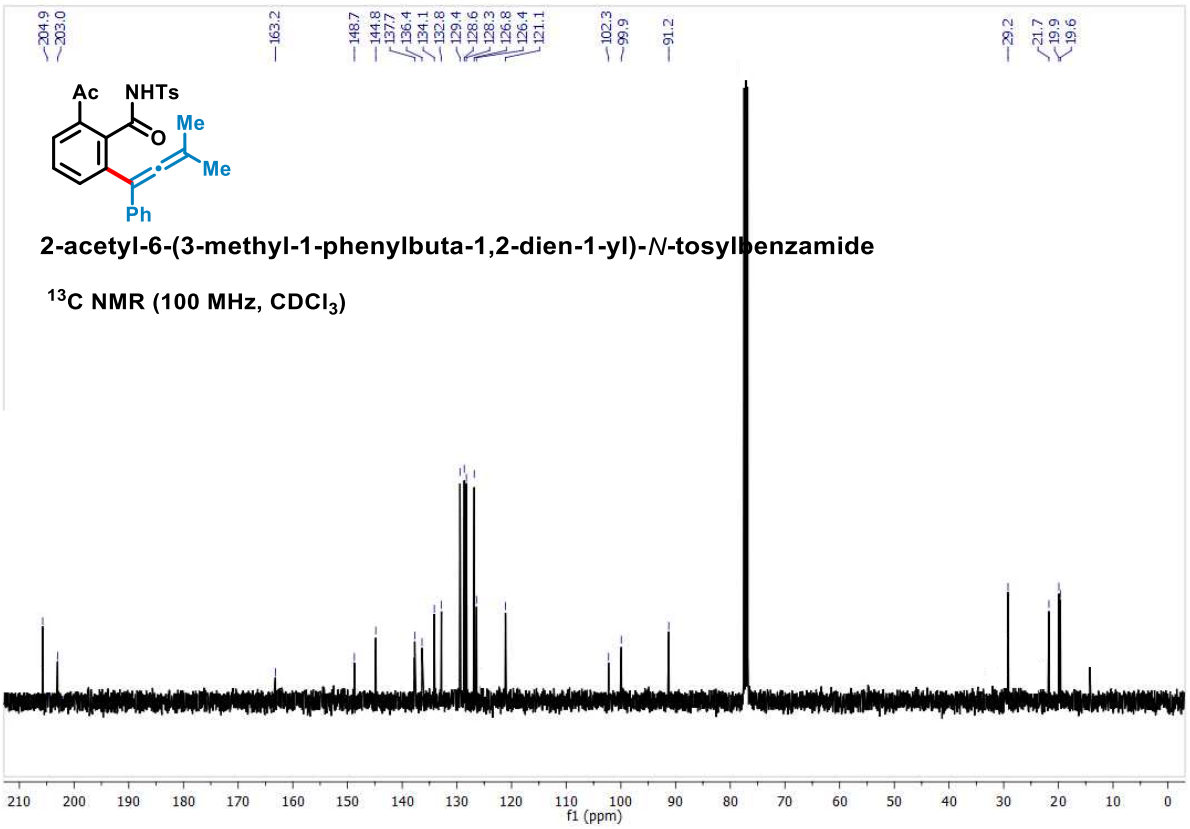
2-fluoro-6-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{13}C NMR (100 MHz, $CDCl_3$)



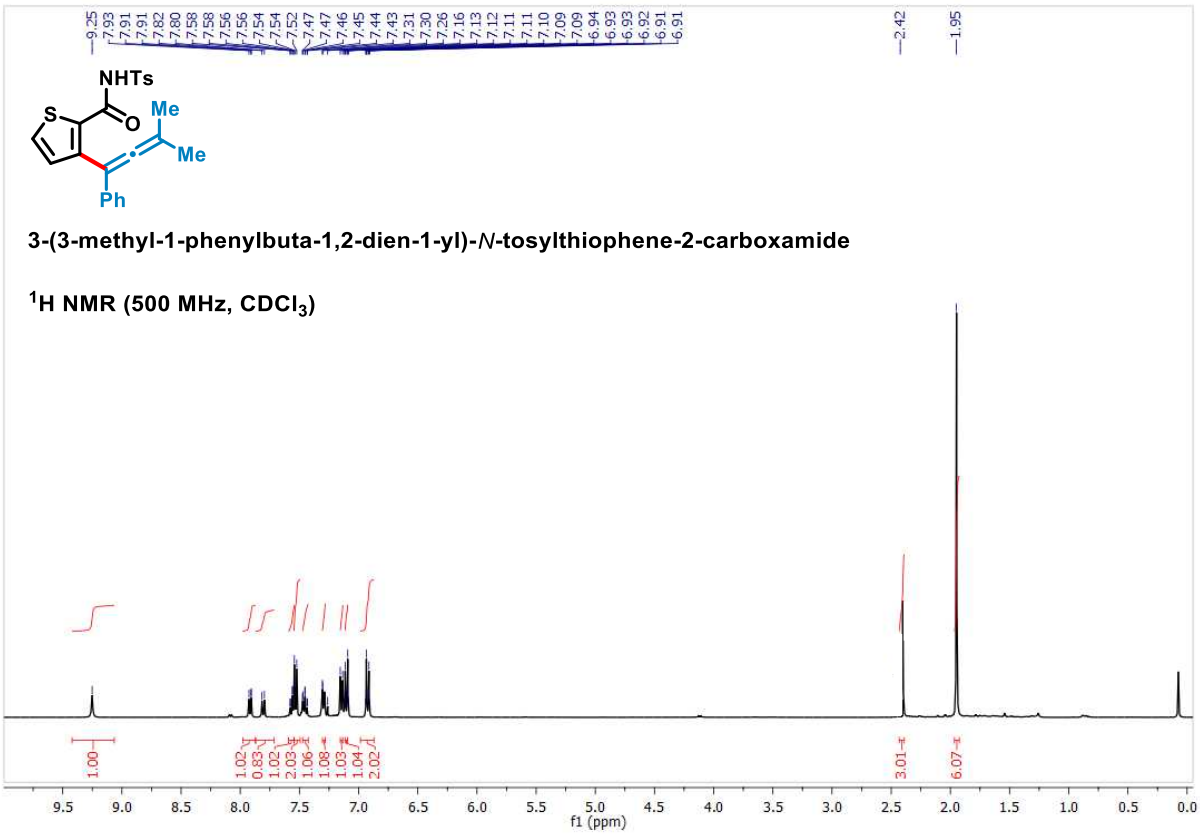
2-acetyl-6-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{1}H NMR (400 MHz, $CDCl_3$)



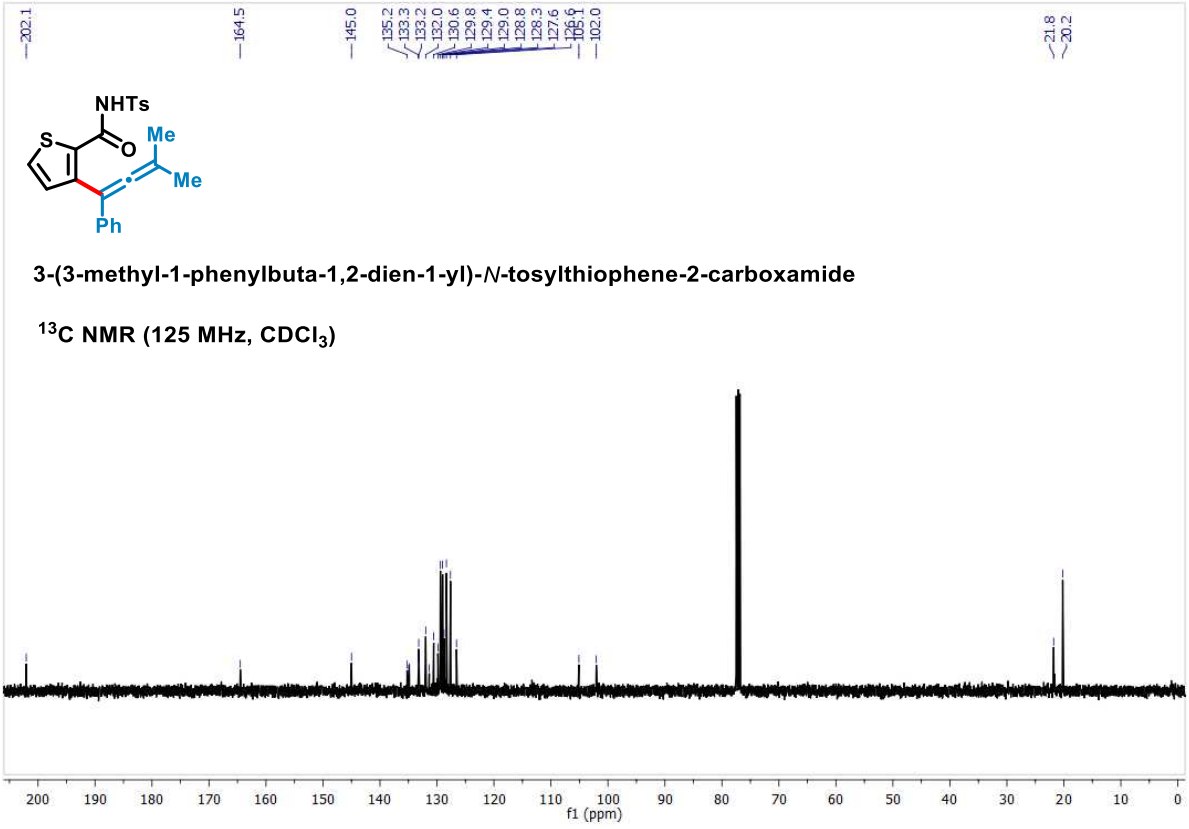
2-acetyl-6-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{13}C NMR (100 MHz, $CDCl_3$)



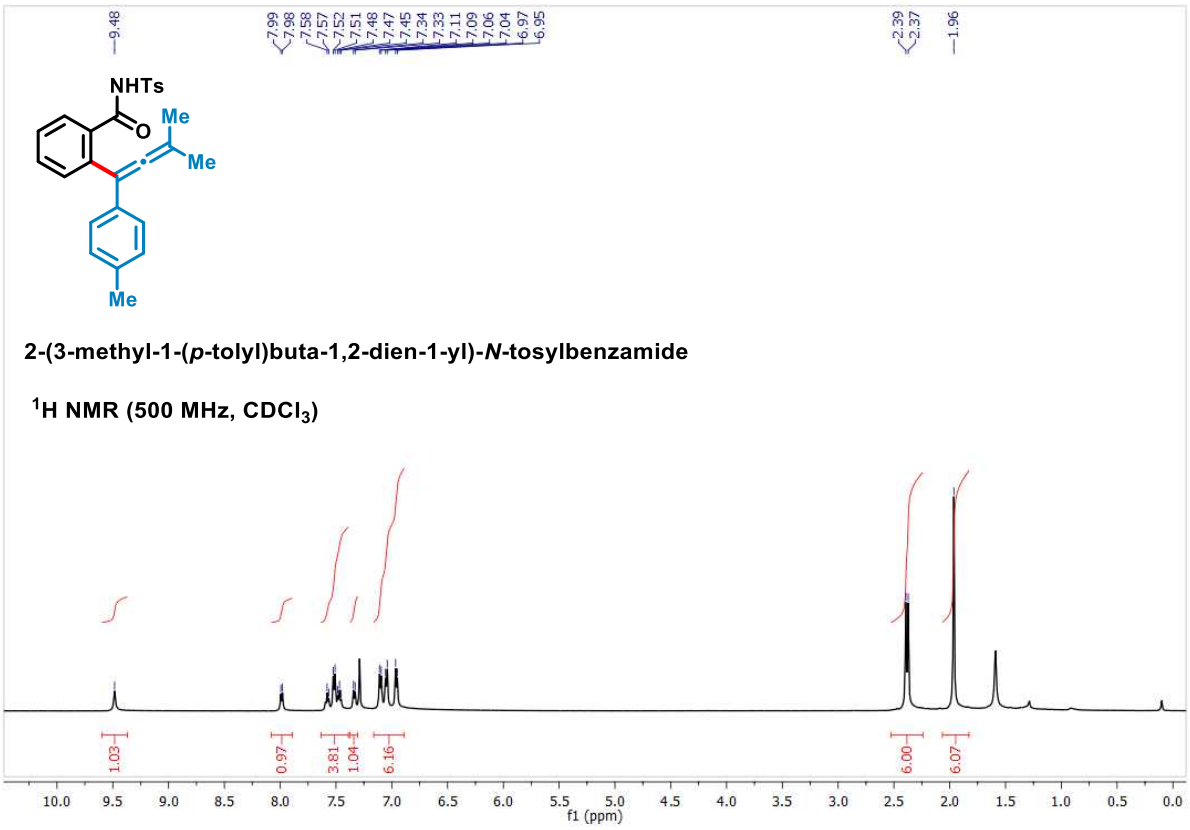
3-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylthiophene-2-carboxamide

^{1}H NMR (500 MHz, $CDCl_3$)



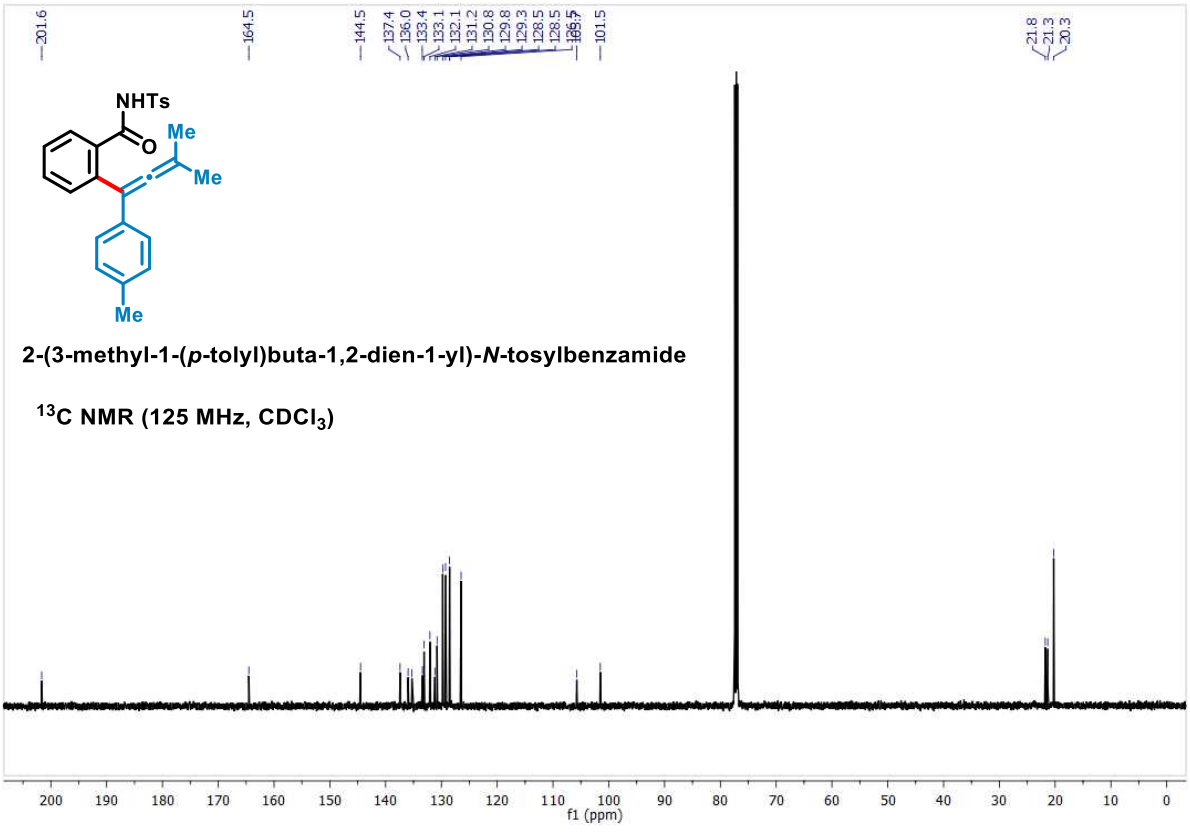
3-(3-methyl-1-phenylbuta-1,2-dien-1-yl)-*N*-tosylthiophene-2-carboxamide

^{13}C NMR (125 MHz, $CDCl_3$)



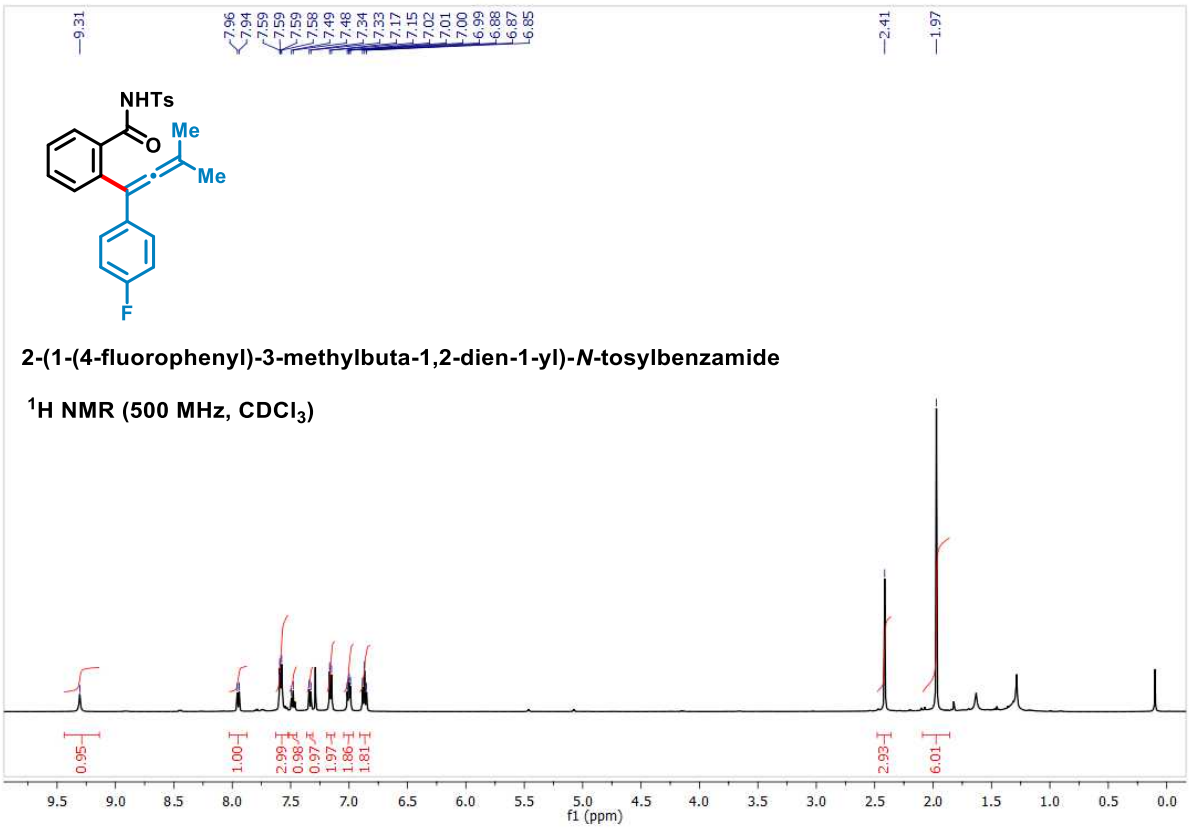
2-(3-methyl-1-(*p*-tolyl)buta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{1}H NMR (500 MHz, $CDCl_3$)



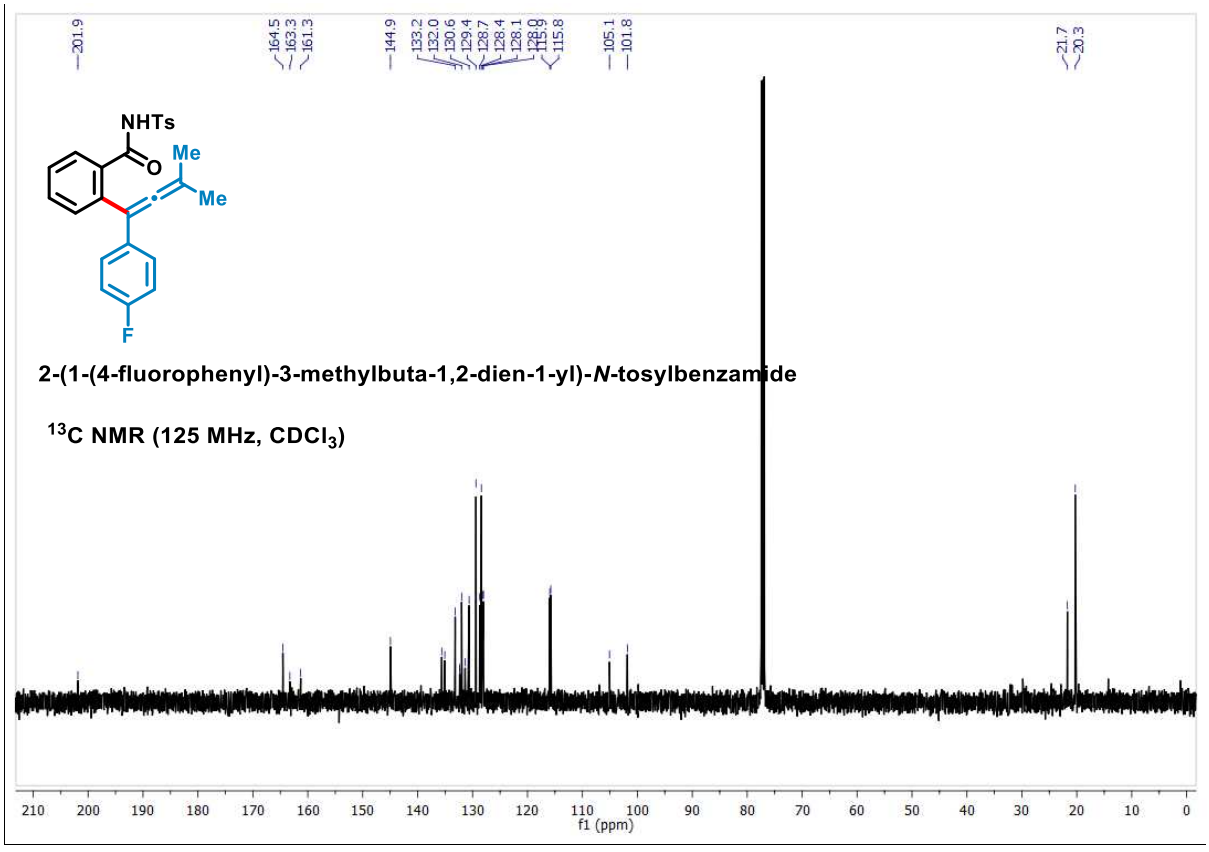
2-(3-methyl-1-(*p*-tolyl)buta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{13}C NMR (125 MHz, $CDCl_3$)



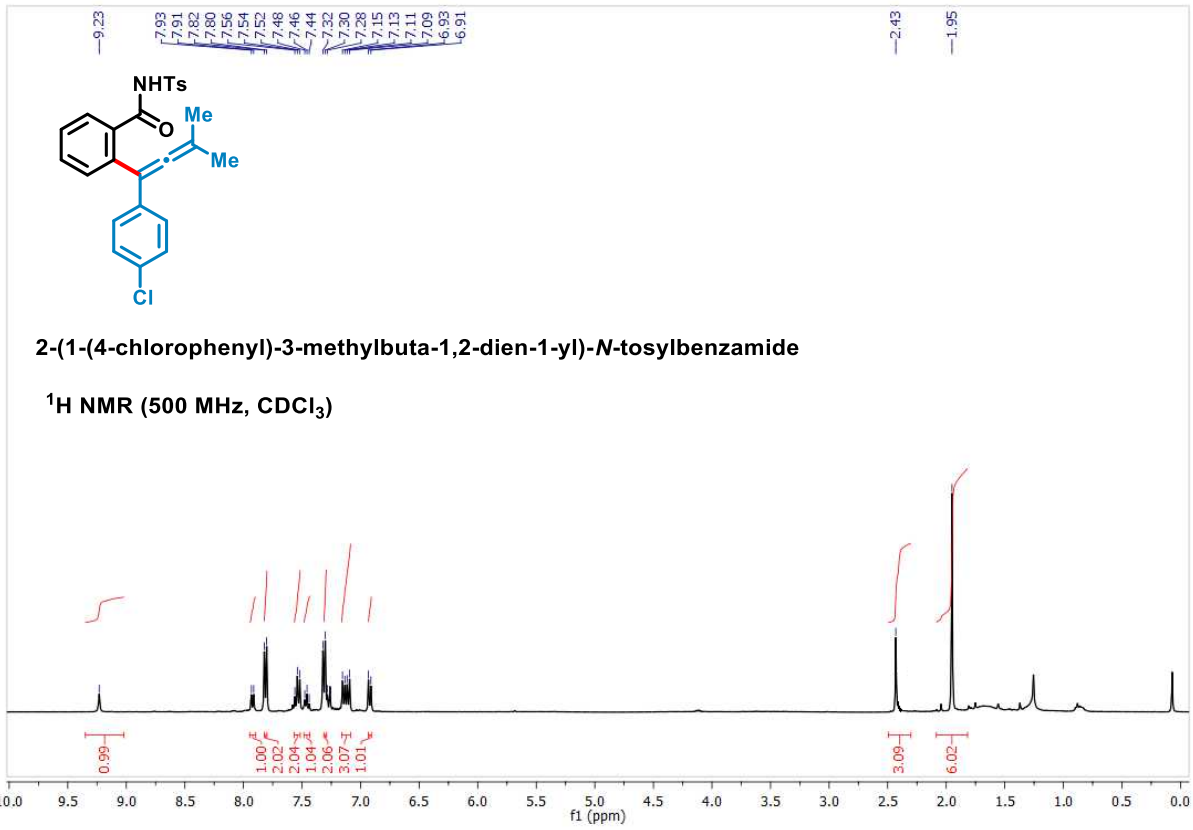
2-(1-(4-fluorophenyl)-3-methylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{1}H NMR (500 MHz, $CDCl_3$)



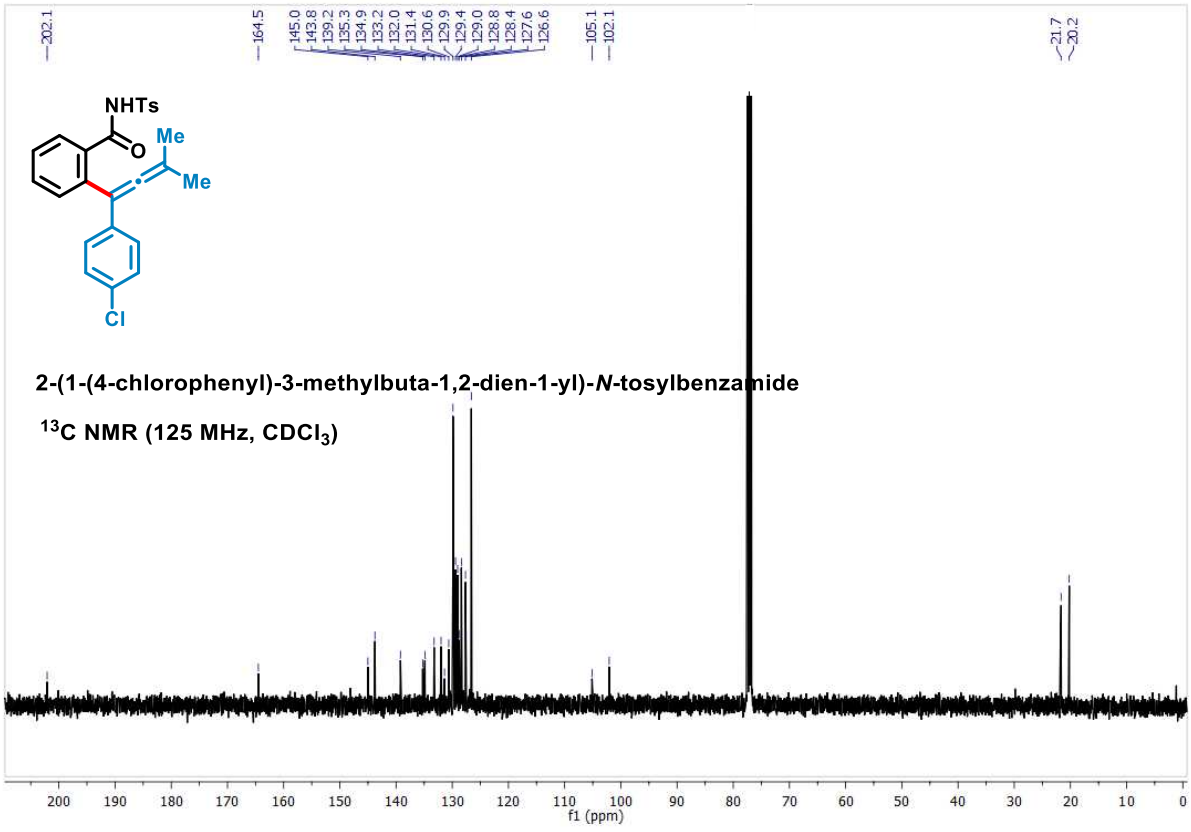
2-(1-(4-fluorophenyl)-3-methylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{13}C NMR (125 MHz, $CDCl_3$)



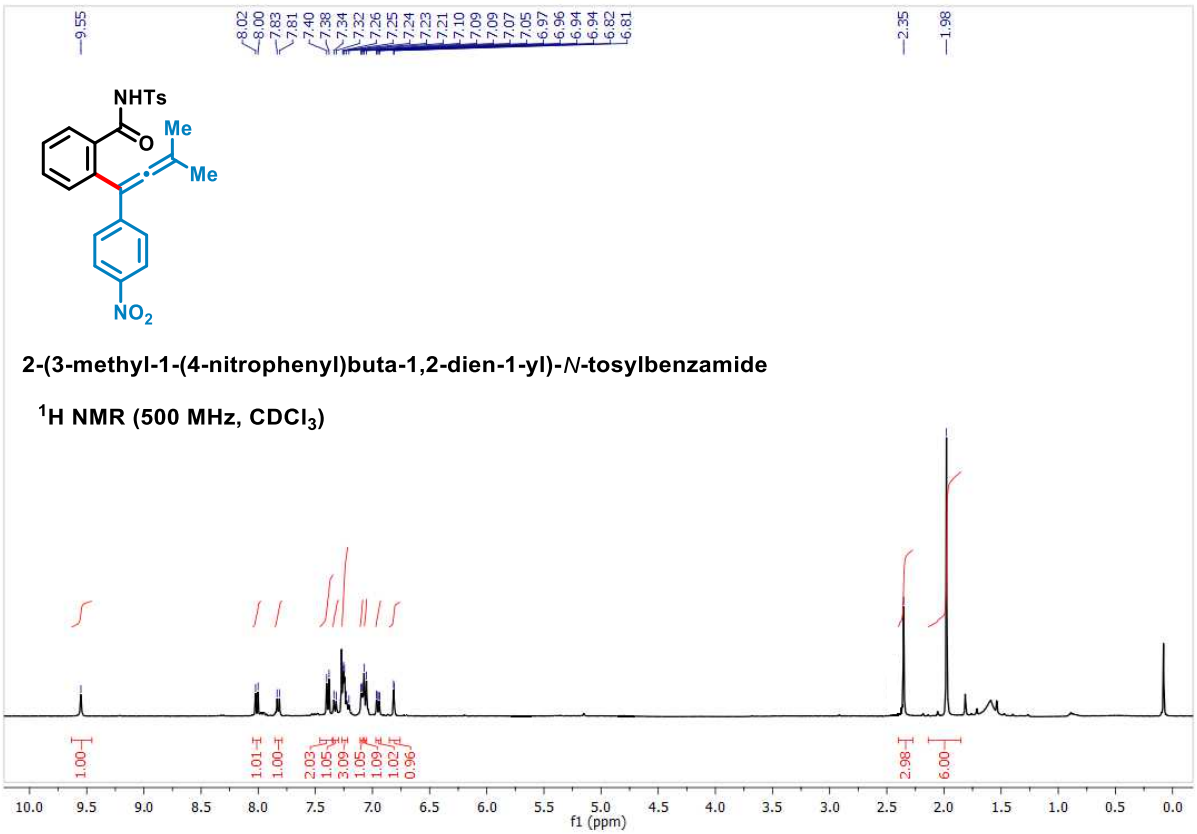
2-(1-(4-chlorophenyl)-3-methylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{1}H NMR (500 MHz, $CDCl_3$)



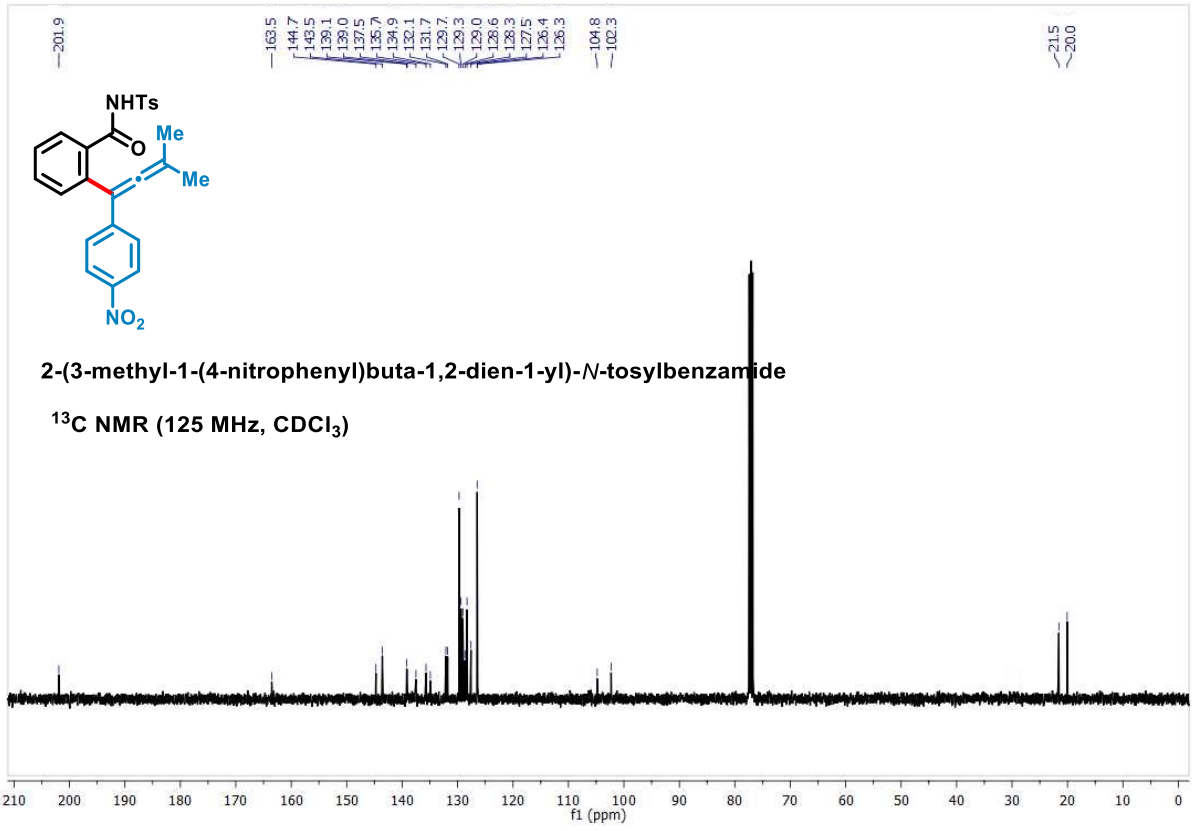
2-(1-(4-chlorophenyl)-3-methylbuta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{13}C NMR (125 MHz, $CDCl_3$)



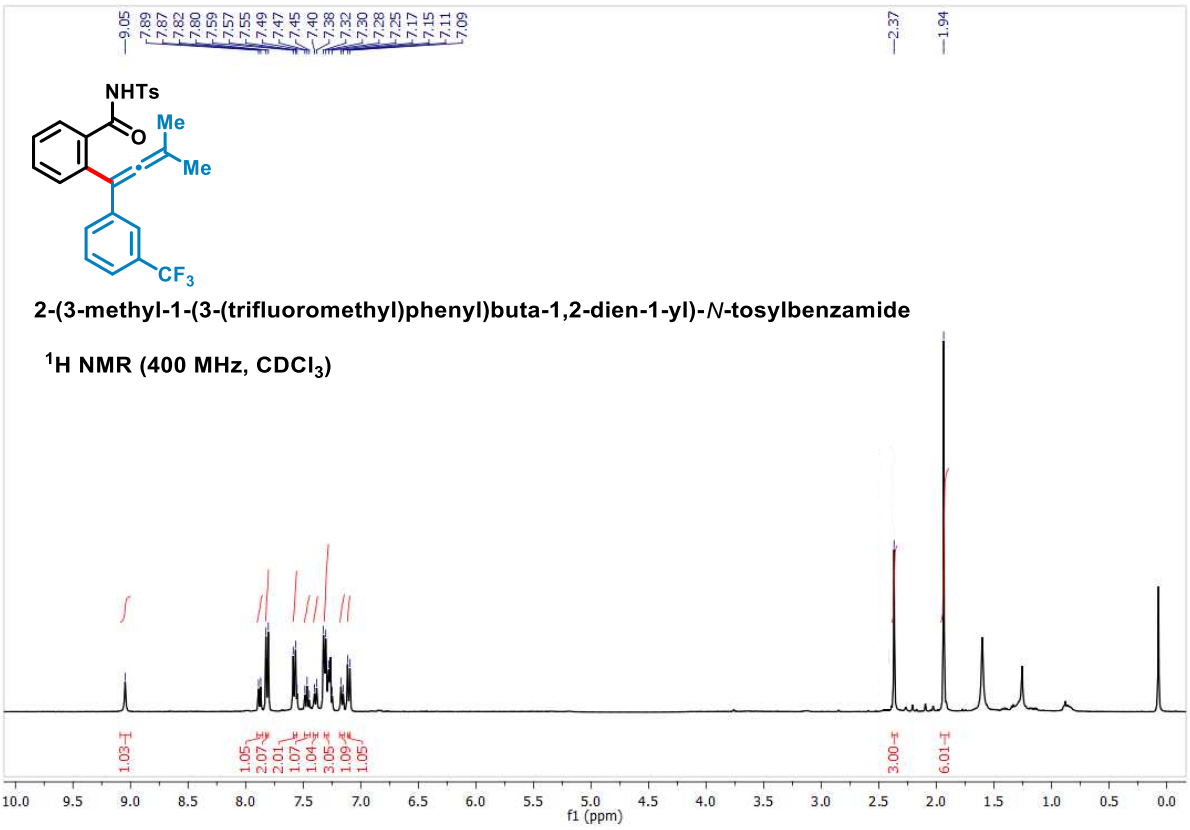
2-(3-methyl-1-(4-nitrophenyl)buta-1,2-dien-1-yl)-*N*-tosylbenzamide

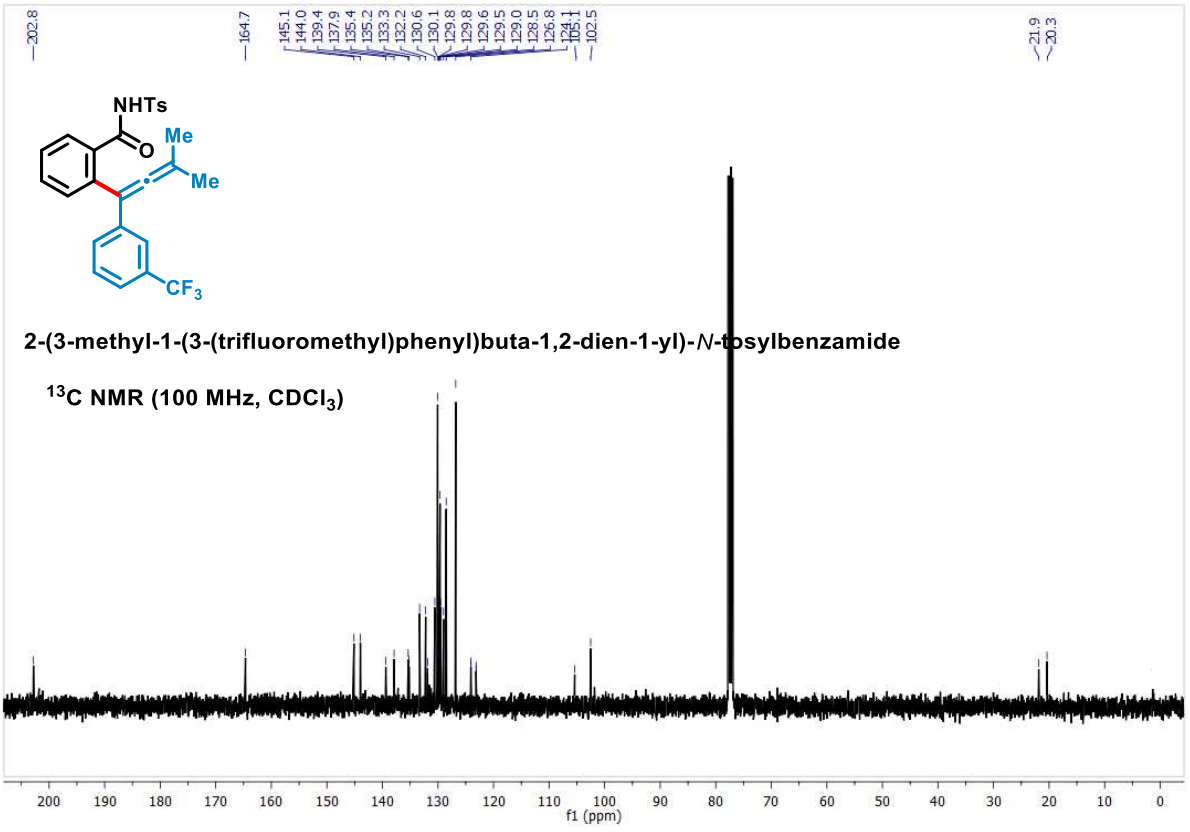
^{1}H NMR (500 MHz, $CDCl_3$)

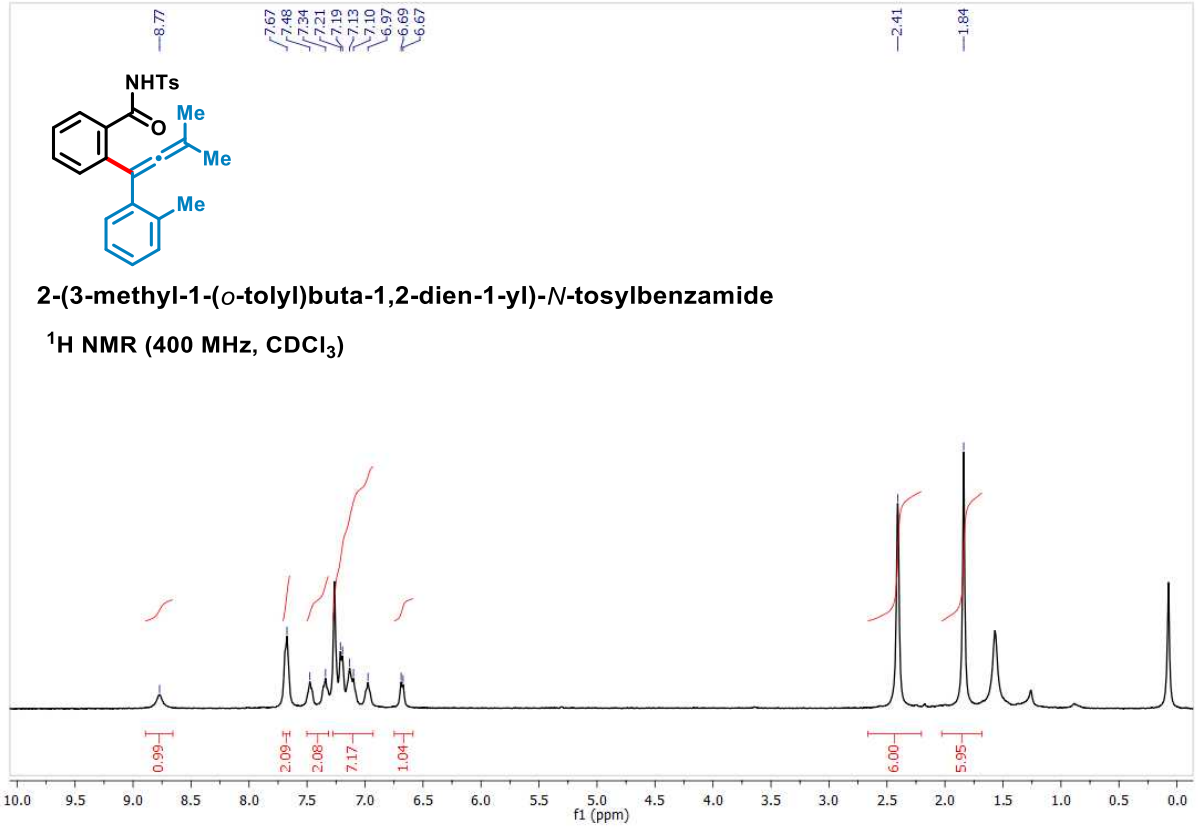


2-(3-methyl-1-(4-nitrophenyl)buta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{13}C NMR (125 MHz, $CDCl_3$)

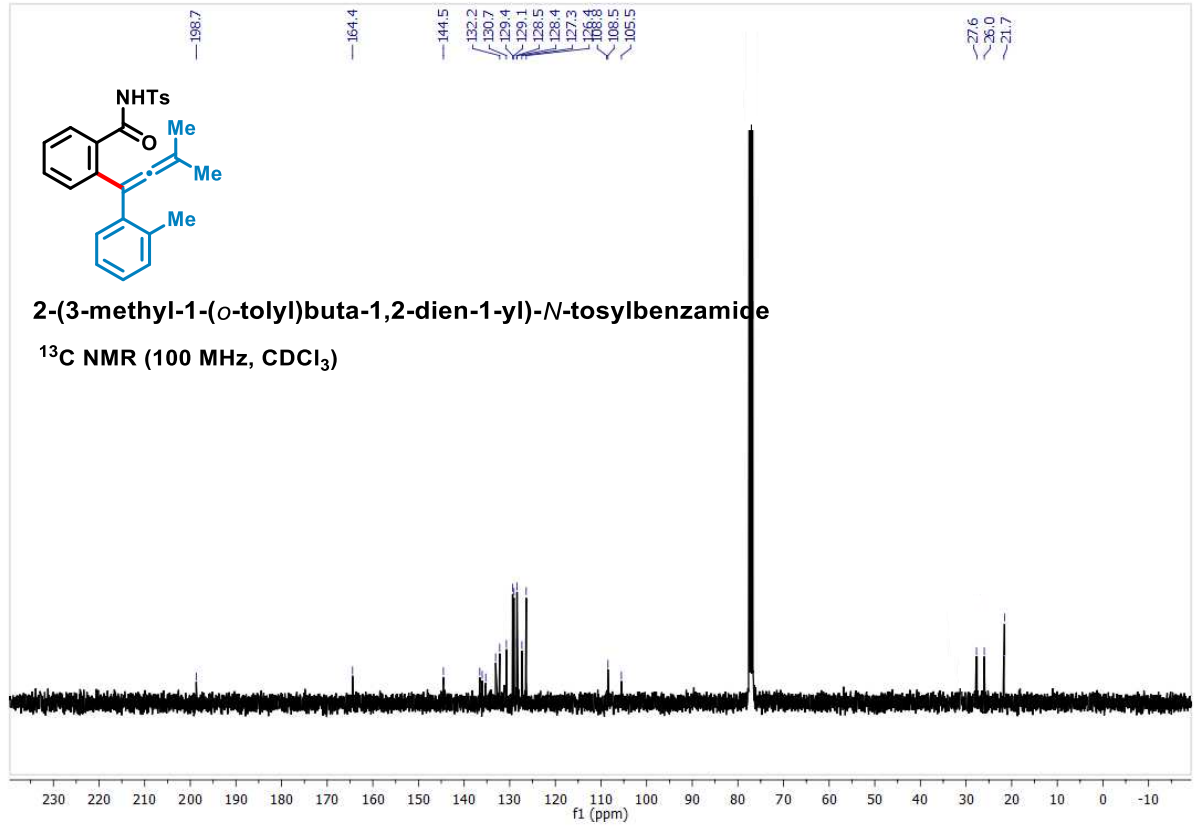

NHTs
Me
Me
CF3
2-(3-methyl-1-(3-(trifluoromethyl)phenyl)buta-1,2-dien-1-yl)-N-tosylbenzamide
1H NMR (400 MHz, CDCl3)
f1 (ppm)


NHTs
Me
Me
CF3
2-(3-methyl-1-(3-(trifluoromethyl)phenyl)buta-1,2-dien-1-yl)-N-tosylbenzamide
13C NMR (100 MHz, CDCl3)
f1 (ppm)



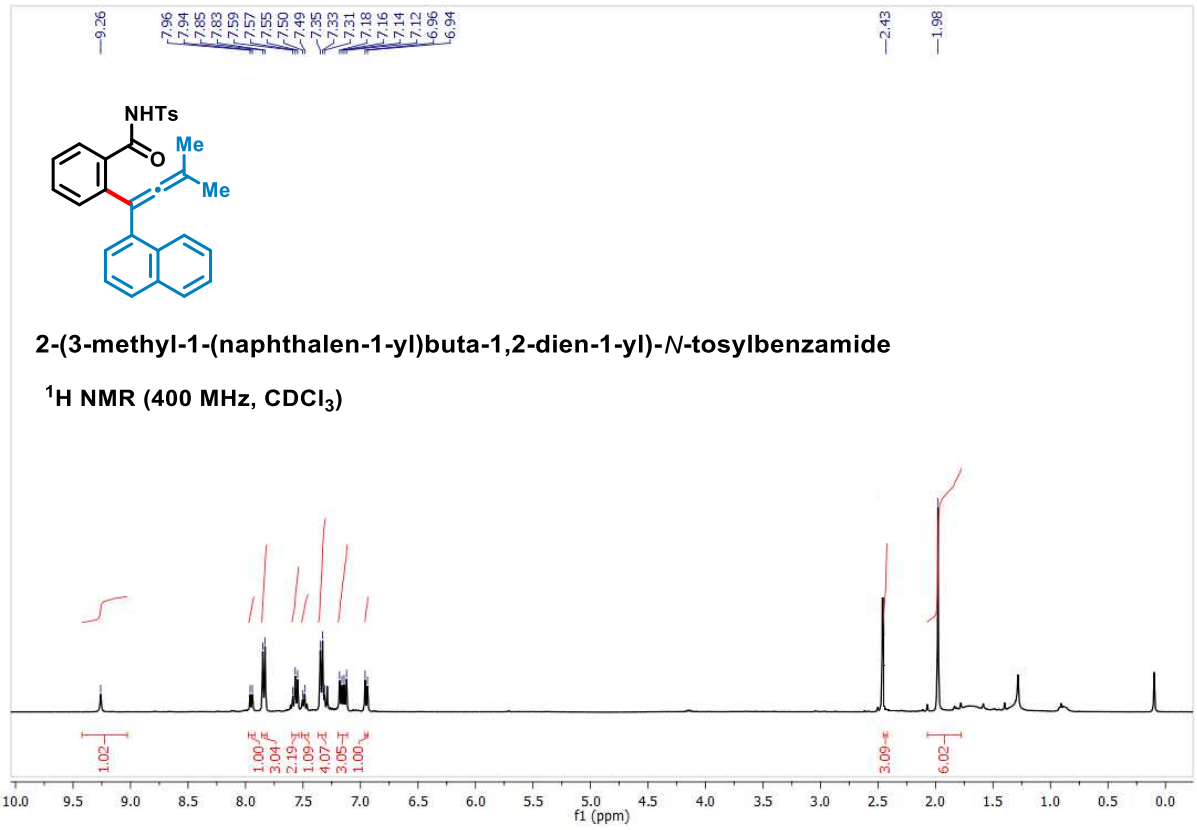
2-(3-methyl-1-(*o*-tolyl)buta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{1}H NMR (400 MHz, $CDCl_3$)



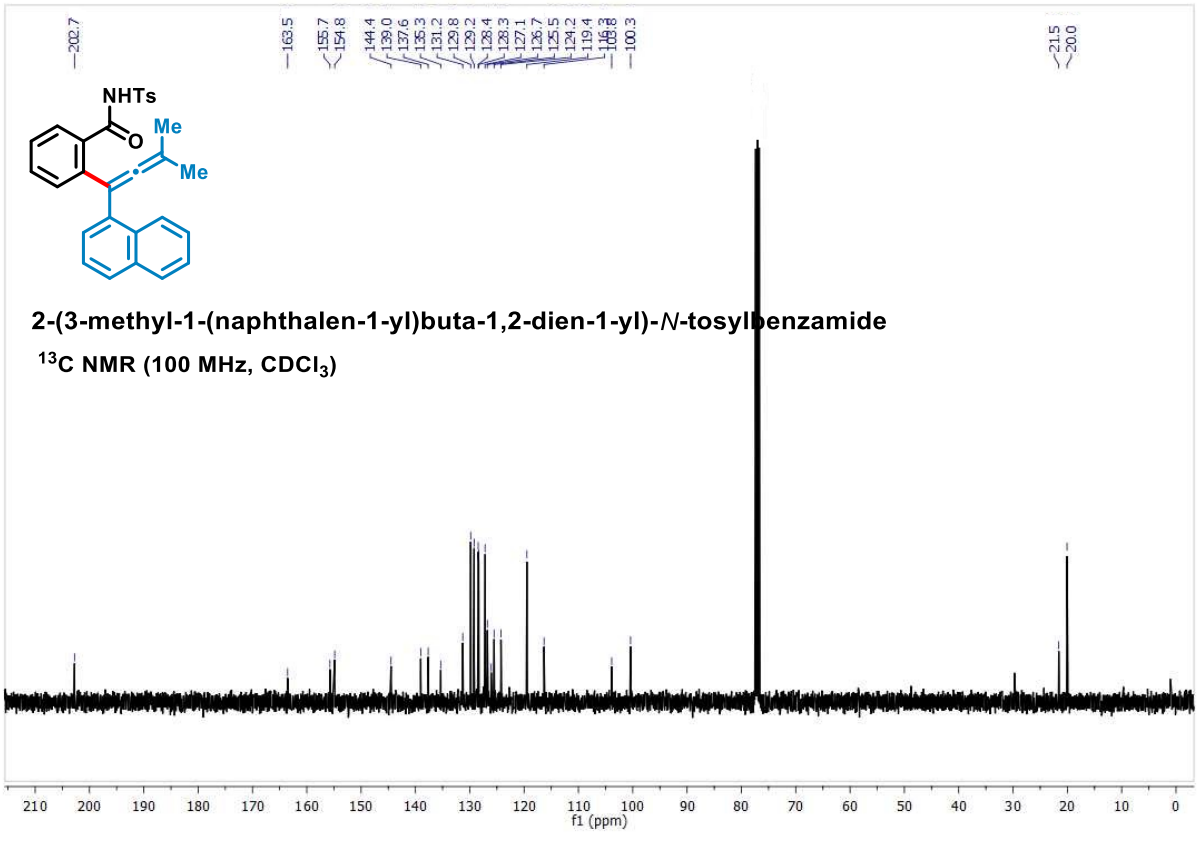
2-(3-methyl-1-(*o*-tolyl)buta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{13}C NMR (100 MHz, $CDCl_3$)



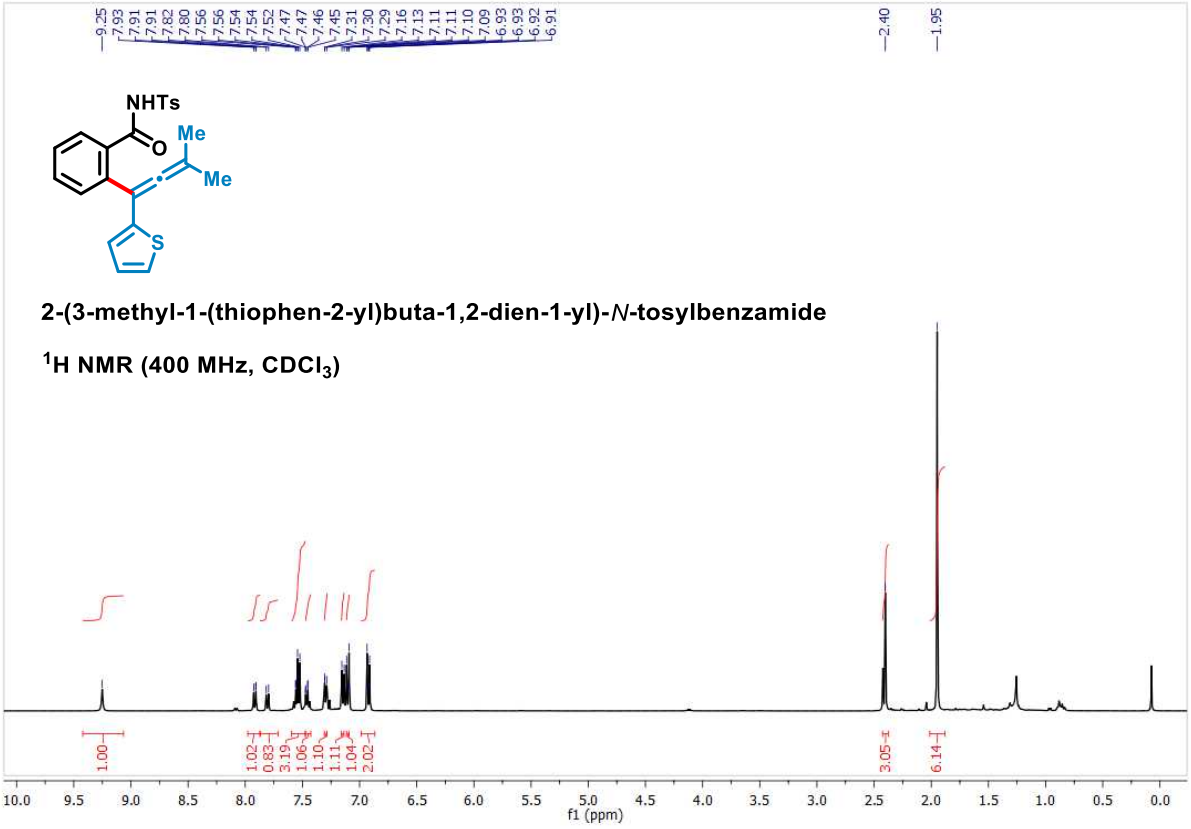
2-(3-methyl-1-(naphthalen-1-yl)buta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{1}H NMR (400 MHz, $CDCl_3$)



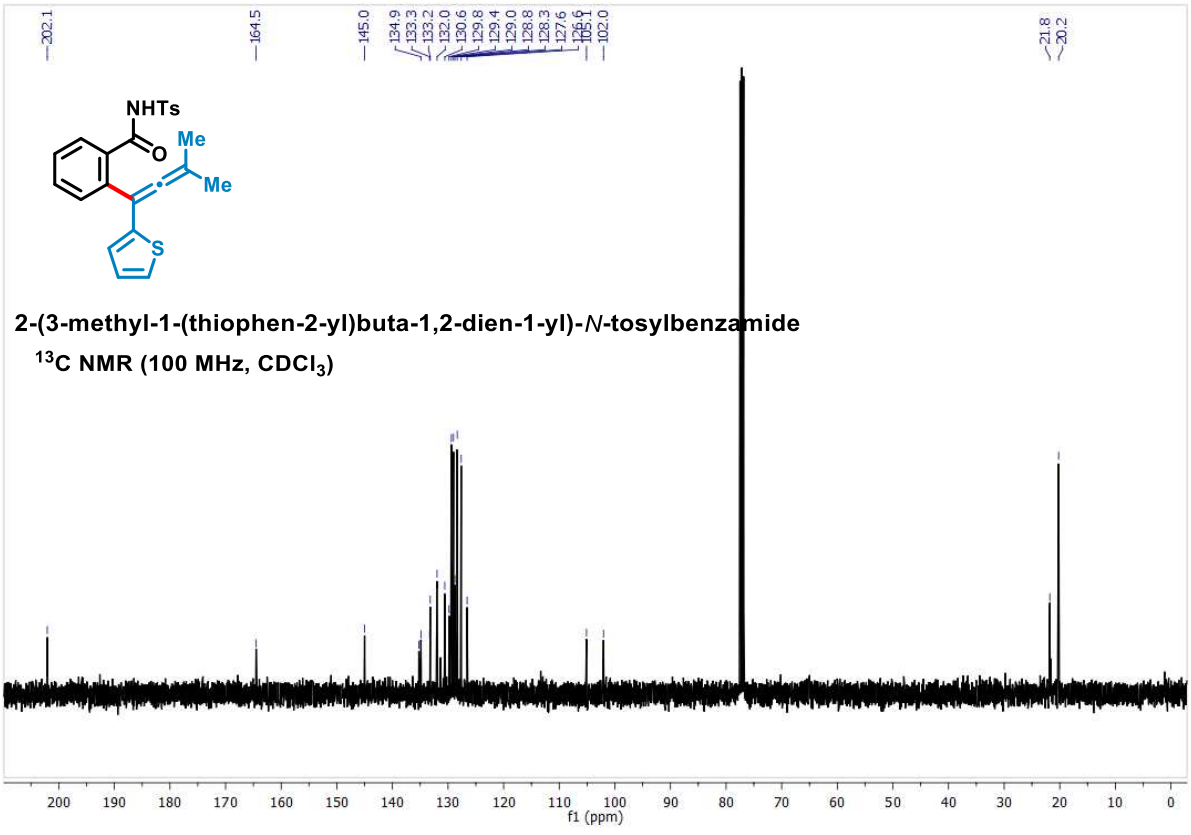
2-(3-methyl-1-(naphthalen-1-yl)buta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{13}C NMR (100 MHz, $CDCl_3$)



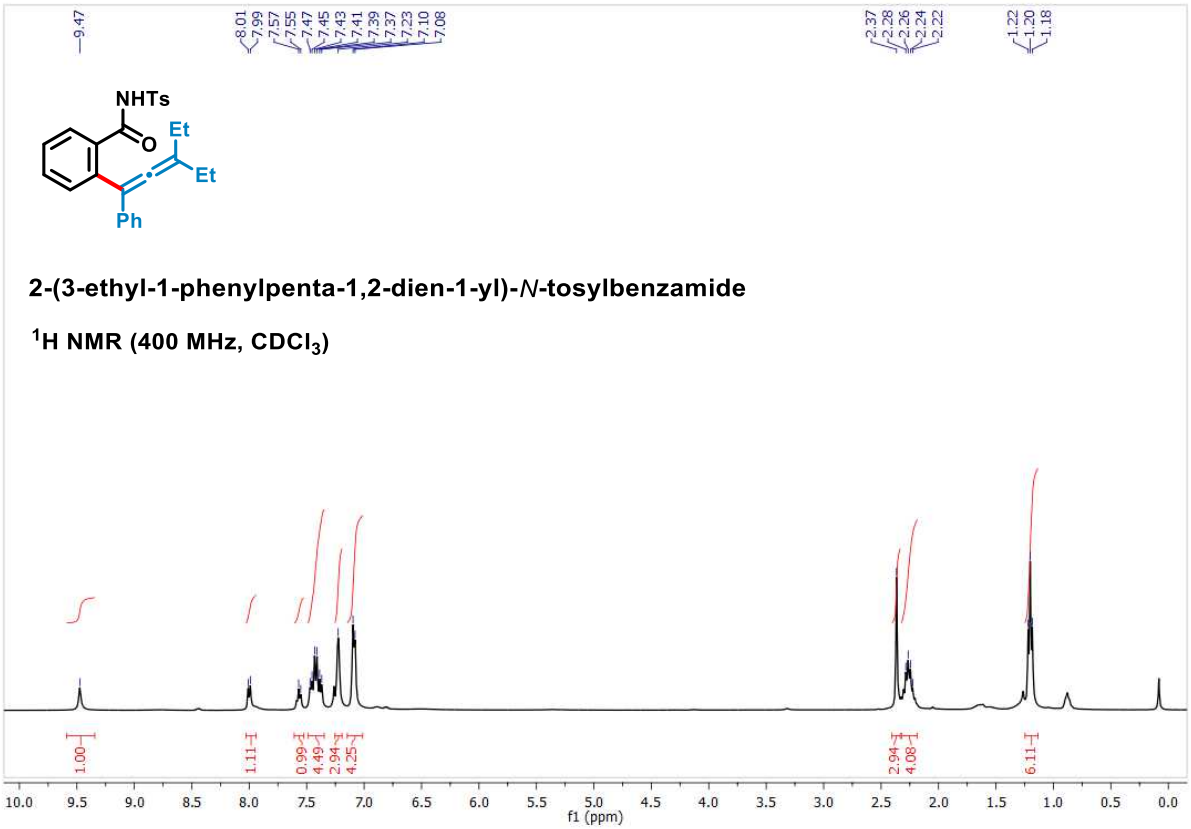
2-(3-methyl-1-(thiophen-2-yl)buta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{1}H NMR (400 MHz, $CDCl_3$)



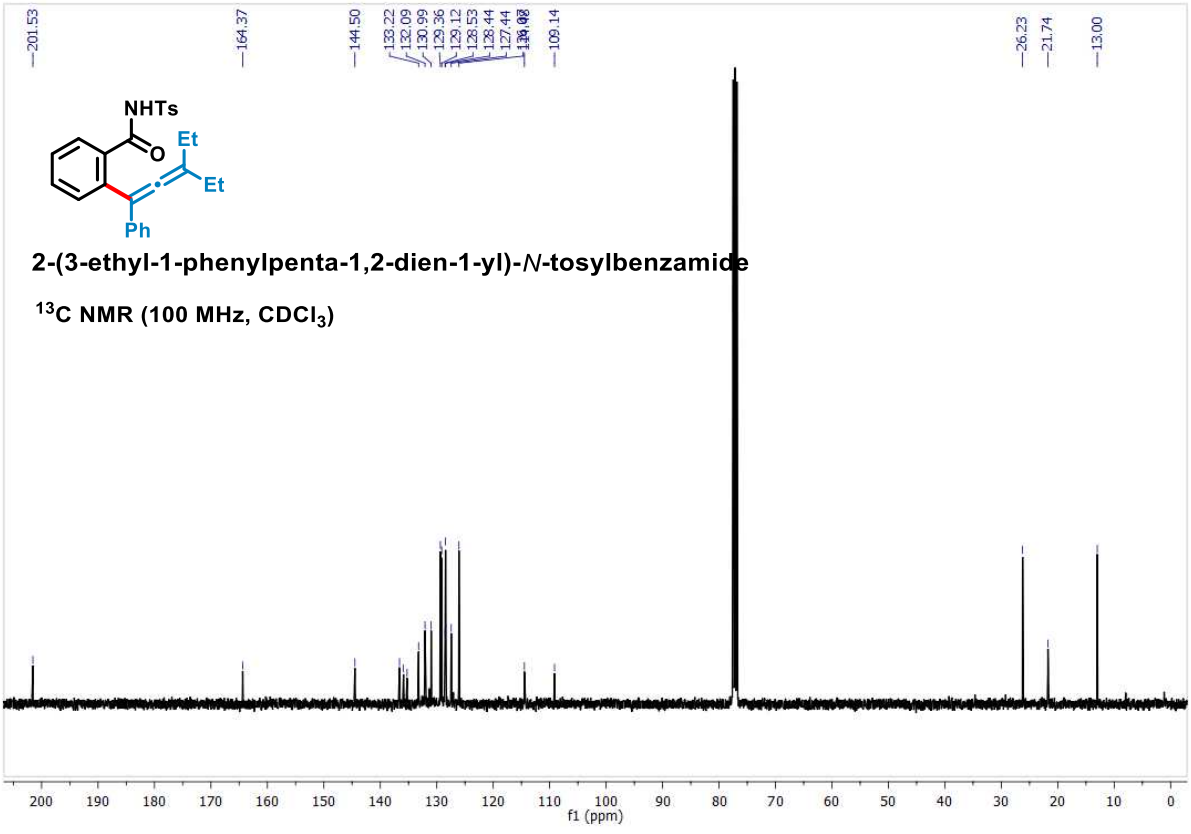
2-(3-methyl-1-(thiophen-2-yl)buta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{13}C NMR (100 MHz, $CDCl_3$)



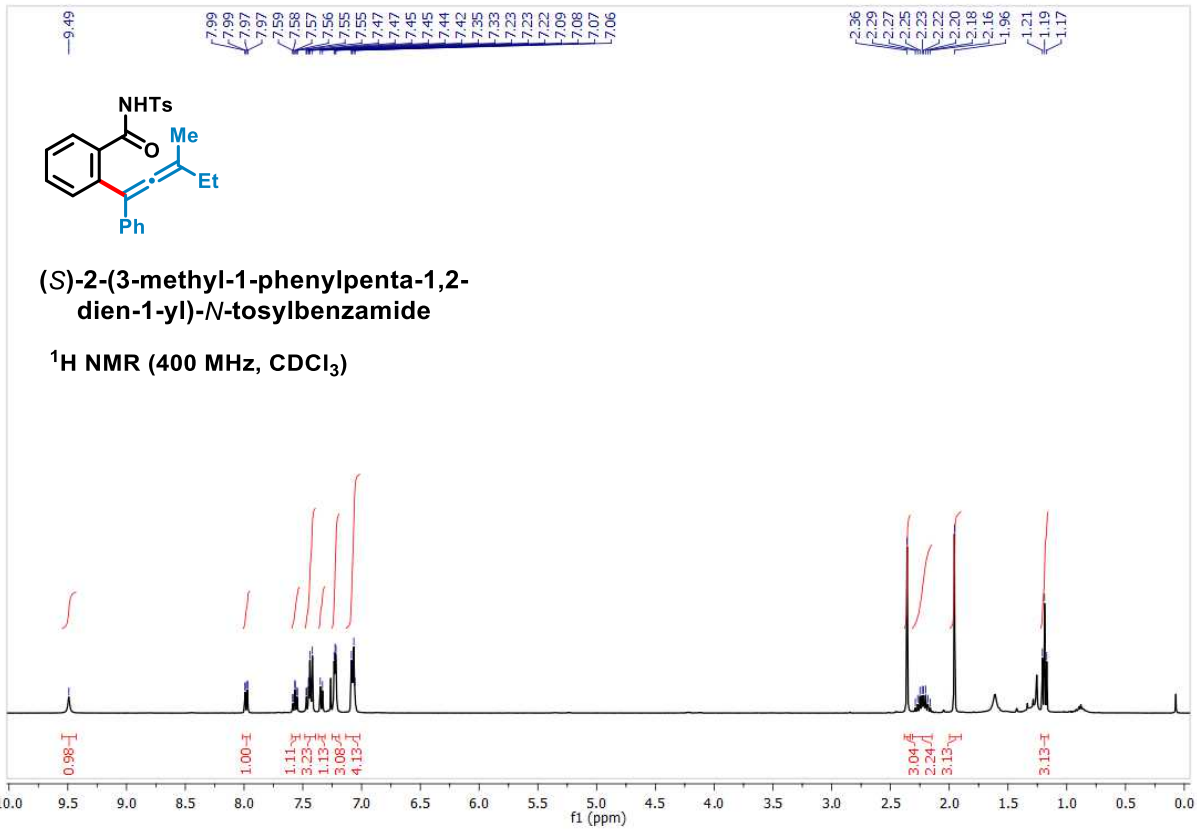
2-(3-ethyl-1-phenylpenta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{1}H NMR (400 MHz, $CDCl_3$)



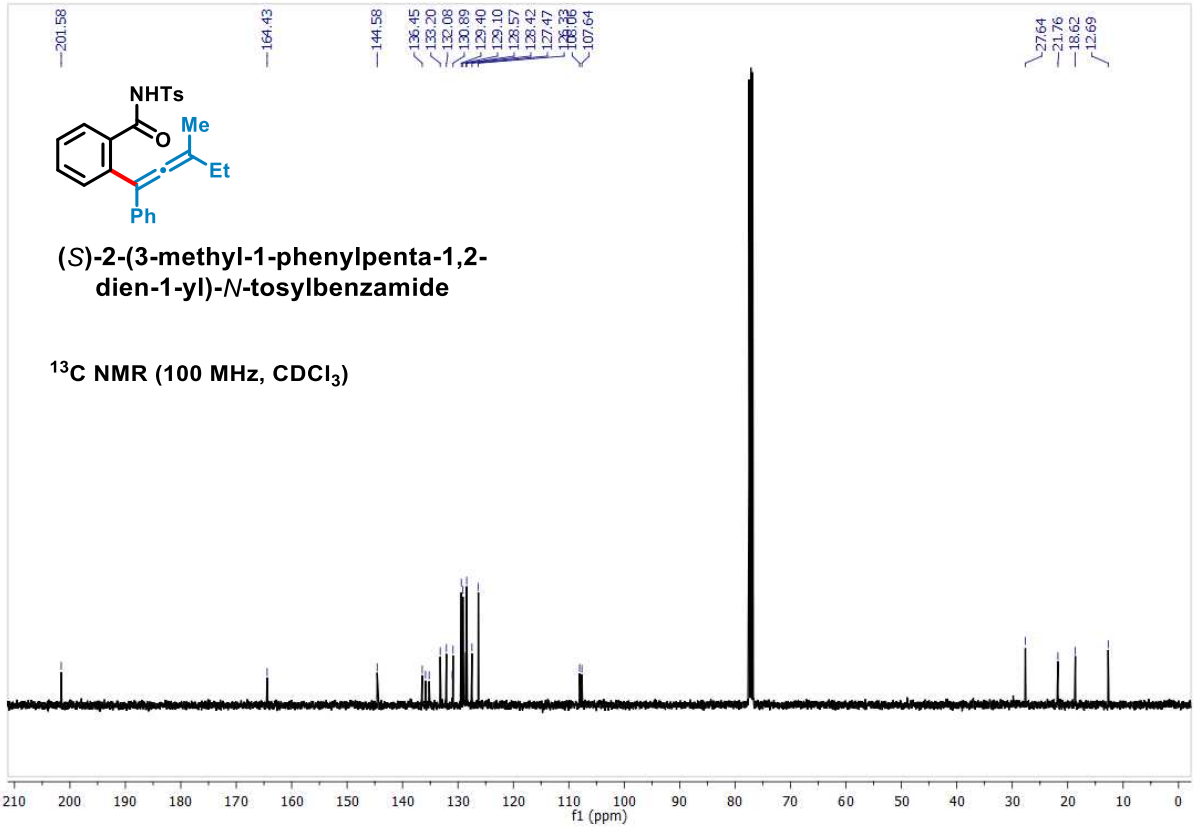
2-(3-ethyl-1-phenylpenta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{13}C NMR (100 MHz, $CDCl_3$)



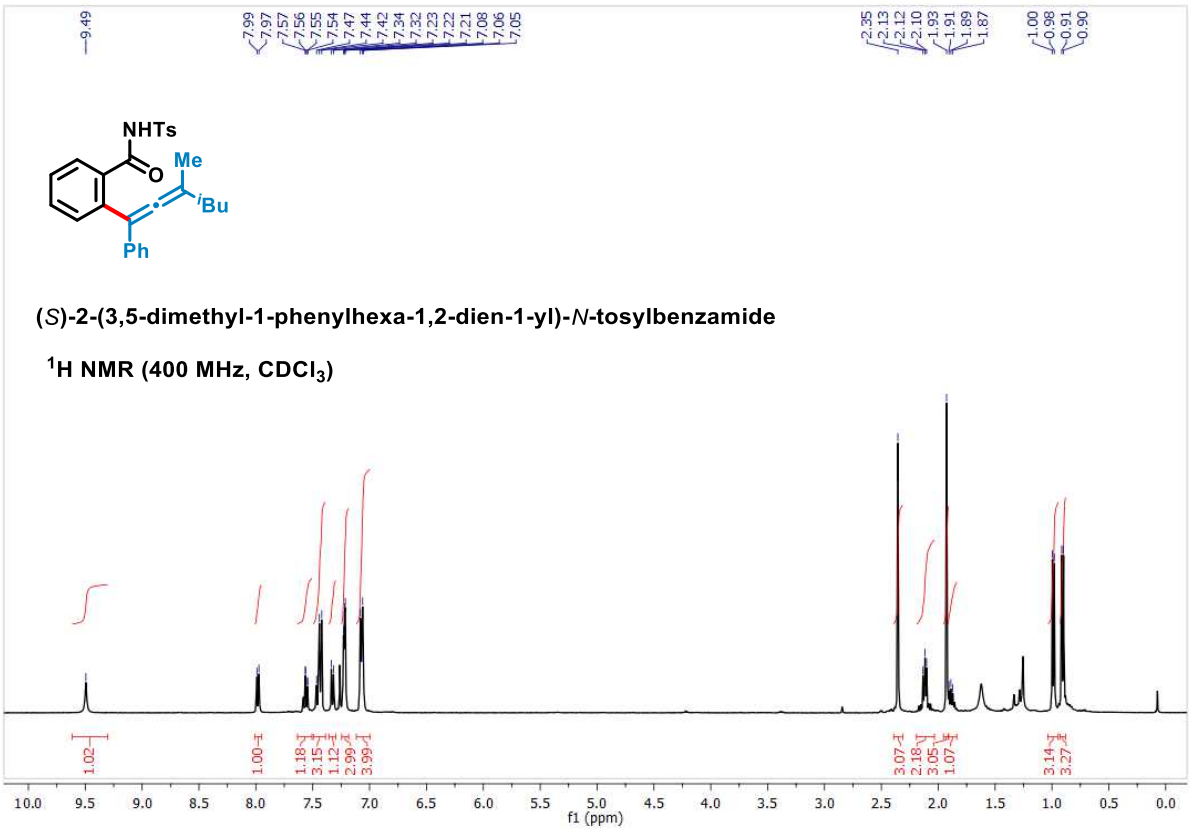
(*S*)-2-(3-methyl-1-phenylpenta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{1}H NMR (400 MHz, $CDCl_3$)



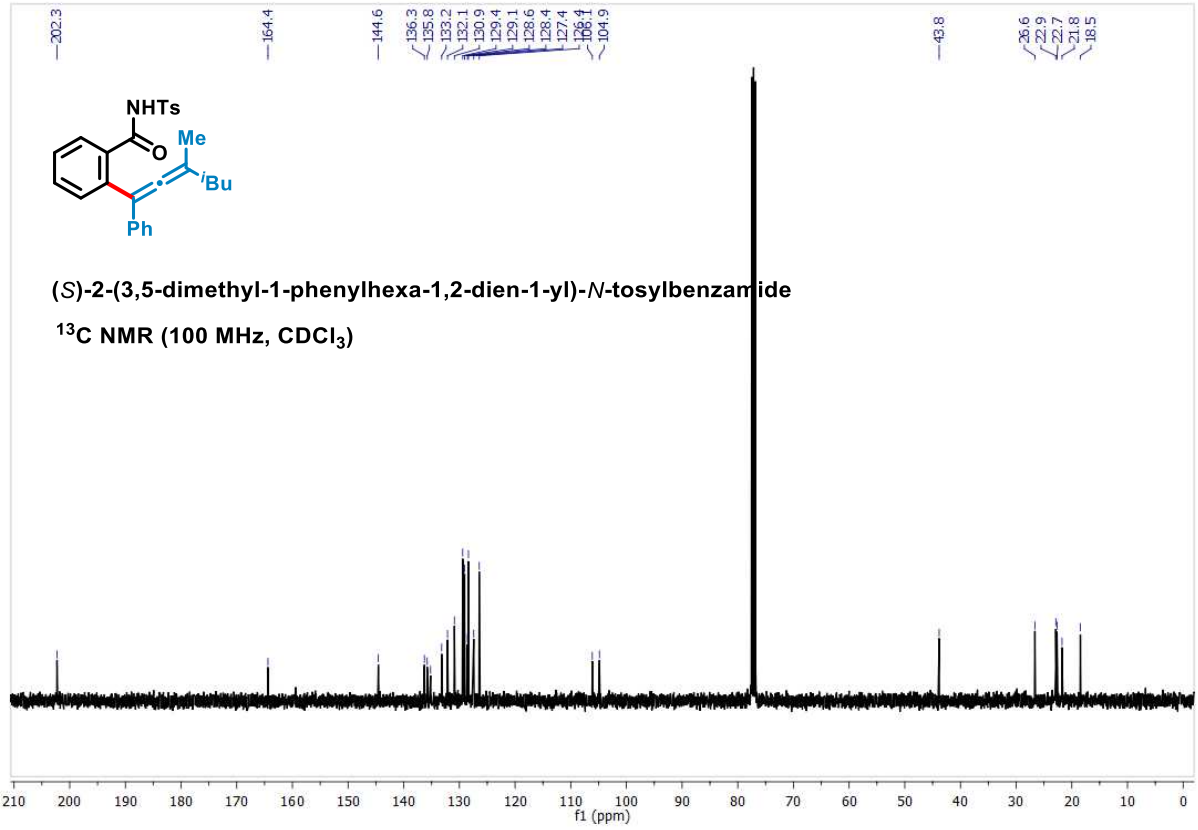
(*S*)-2-(3-methyl-1-phenylpenta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{13}C NMR (100 MHz, $CDCl_3$)



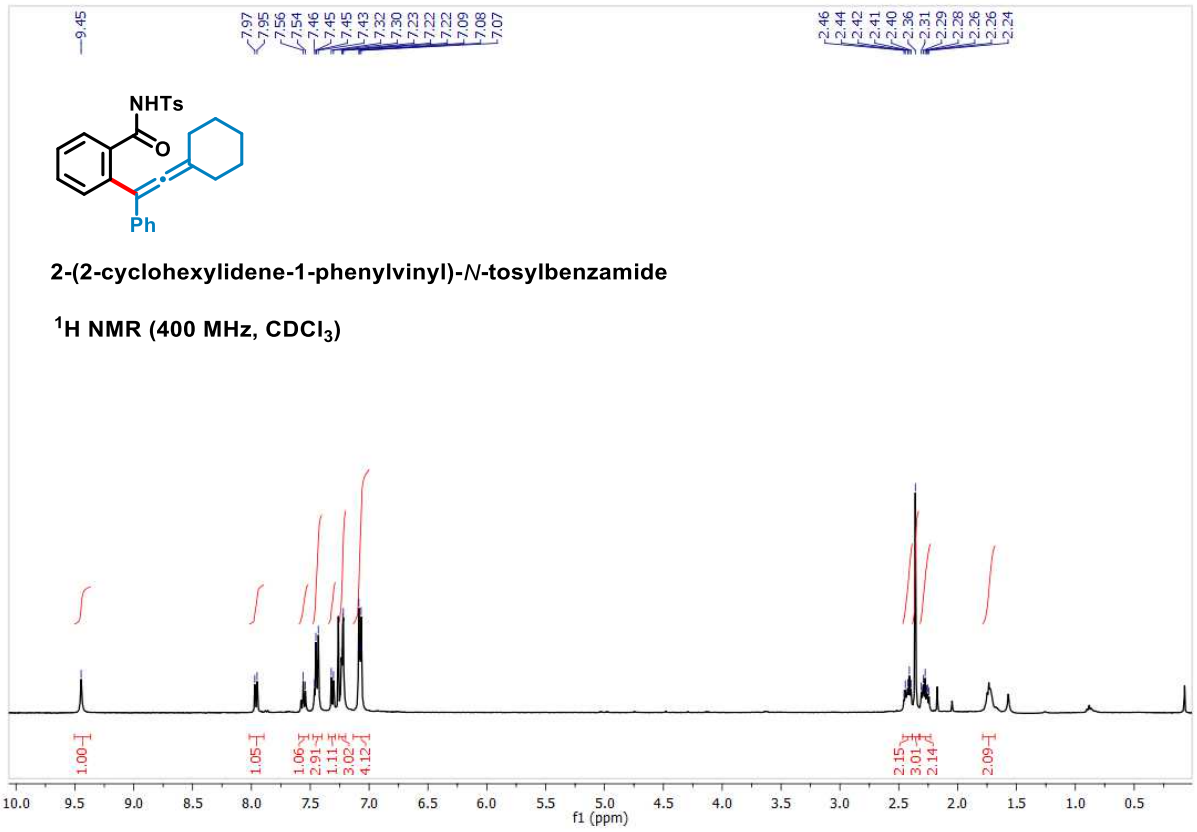
(*S*)-2-(3,5-dimethyl-1-phenylhexa-1,2-dien-1-yl)-*N*-tosylbenzamide

^{1}H NMR (400 MHz, $CDCl_3$)



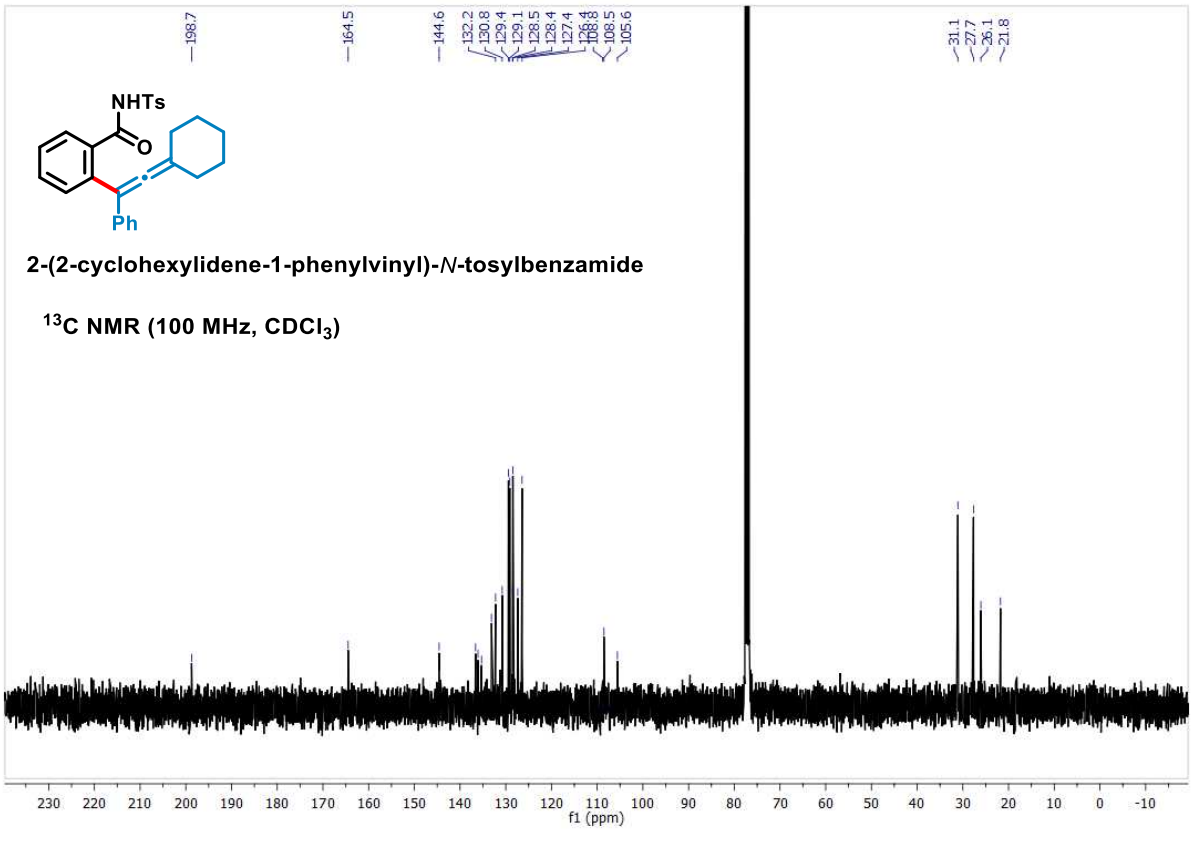
(*S*)-2-(3,5-dimethyl-1-phenylhexa-1,2-dien-1-yl)-*N*-tosylbenzamide

^{13}C NMR (100 MHz, $CDCl_3$)



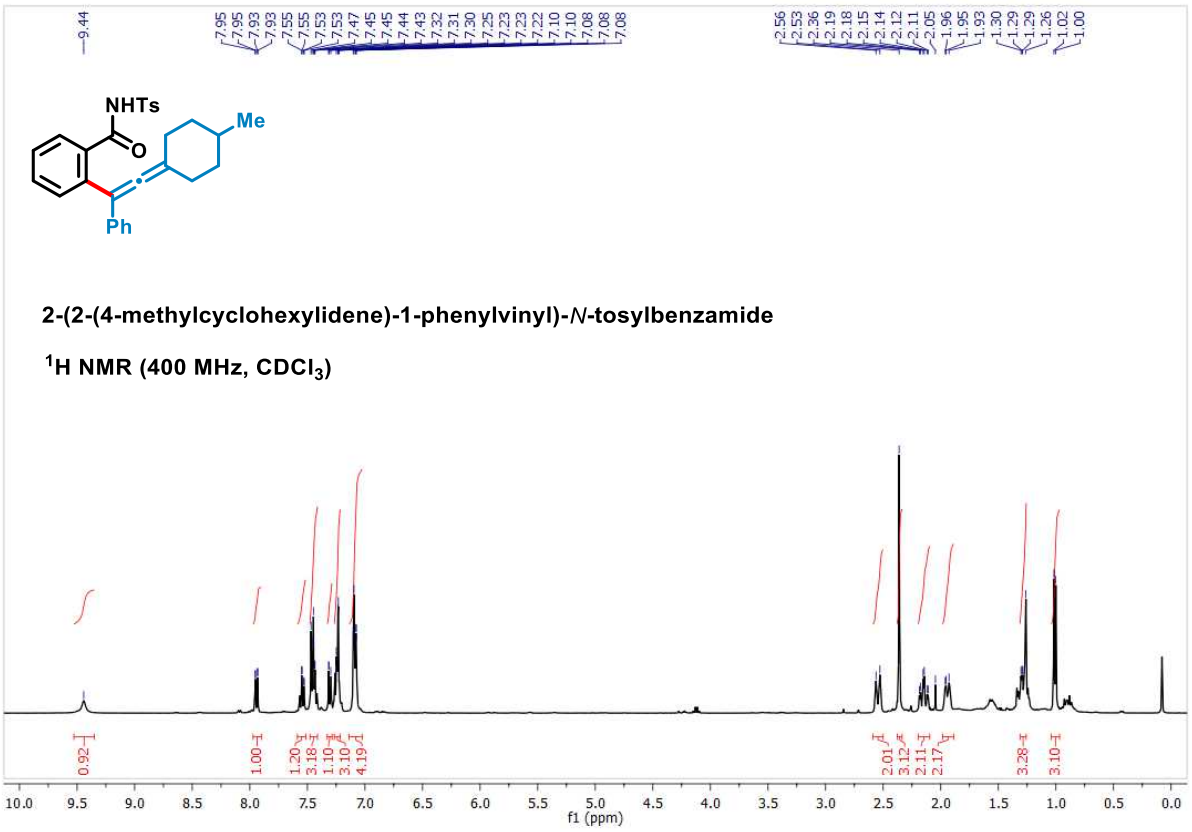
2-(2-cyclohexylidene-1-phenylvinyl)-*N*-tosylbenzamide

^{1}H NMR (400 MHz, $CDCl_3$)



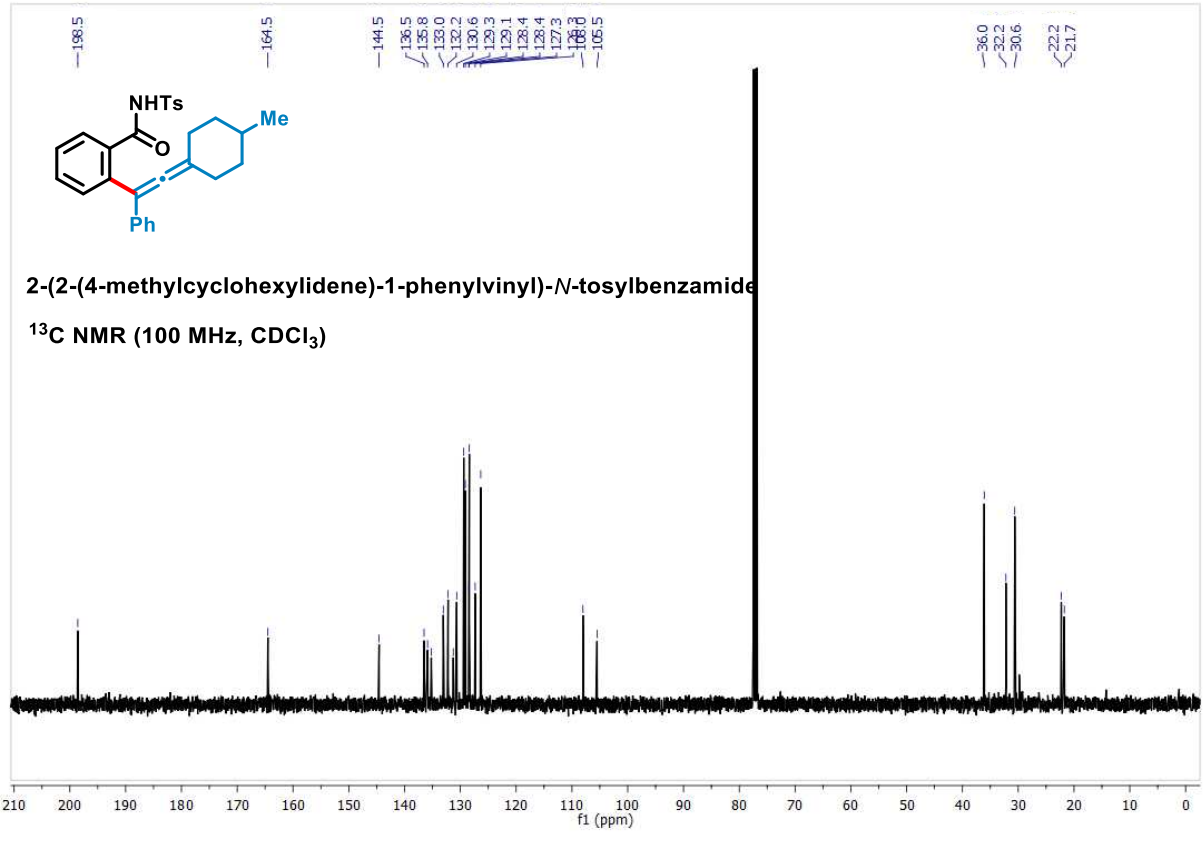
2-(2-cyclohexylidene-1-phenylvinyl)-*N*-tosylbenzamide

^{13}C NMR (100 MHz, $CDCl_3$)



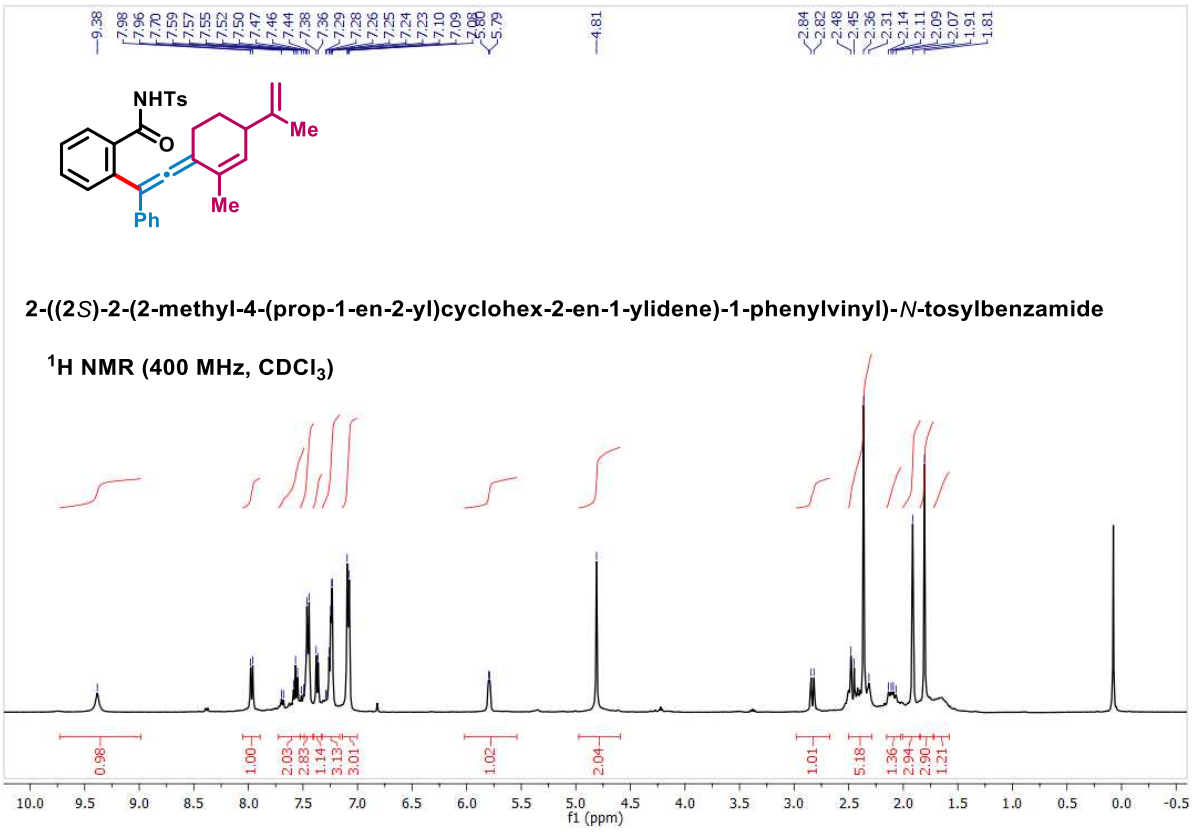
2-(2-(4-methylcyclohexylidene)-1-phenylvinyl)-*N*-tosylbenzamide

^{1}H NMR (400 MHz, $CDCl_3$)



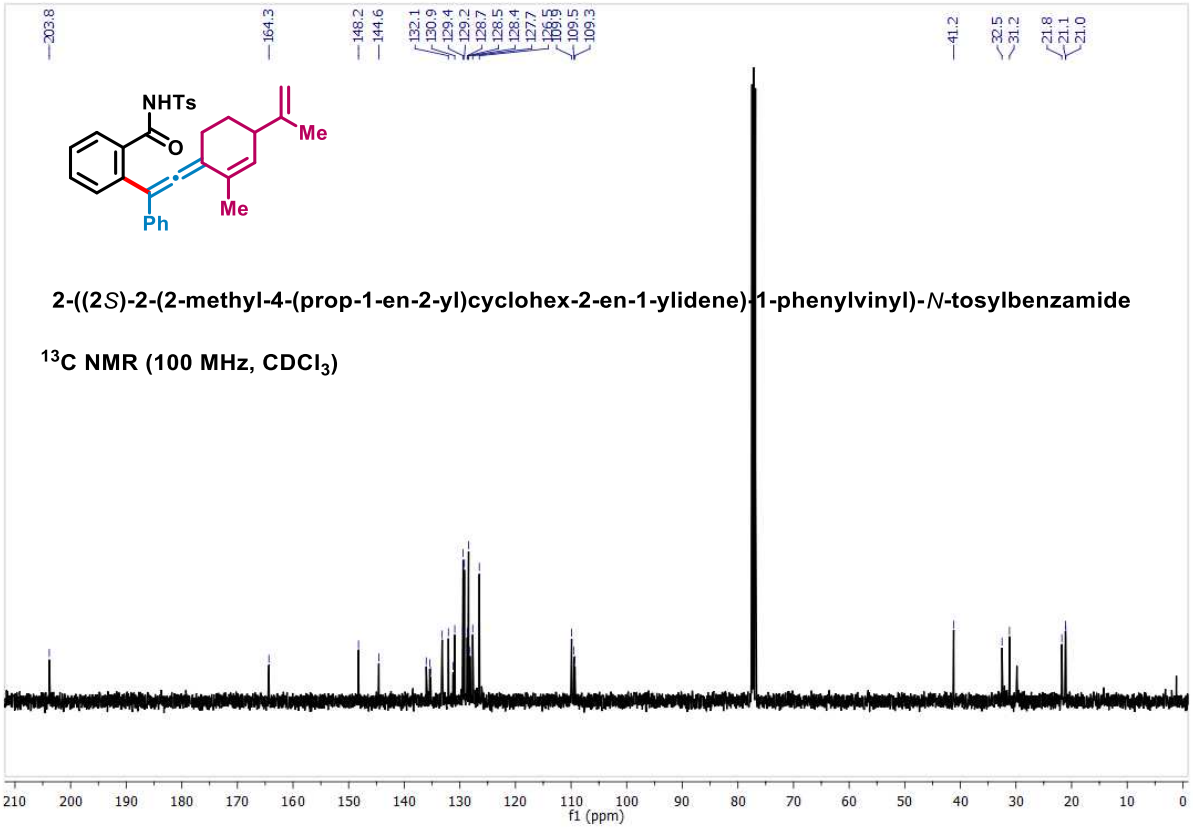
2-(2-(4-methylcyclohexylidene)-1-phenylvinyl)-*N*-tosylbenzamide

^{13}C NMR (100 MHz, $CDCl_3$)



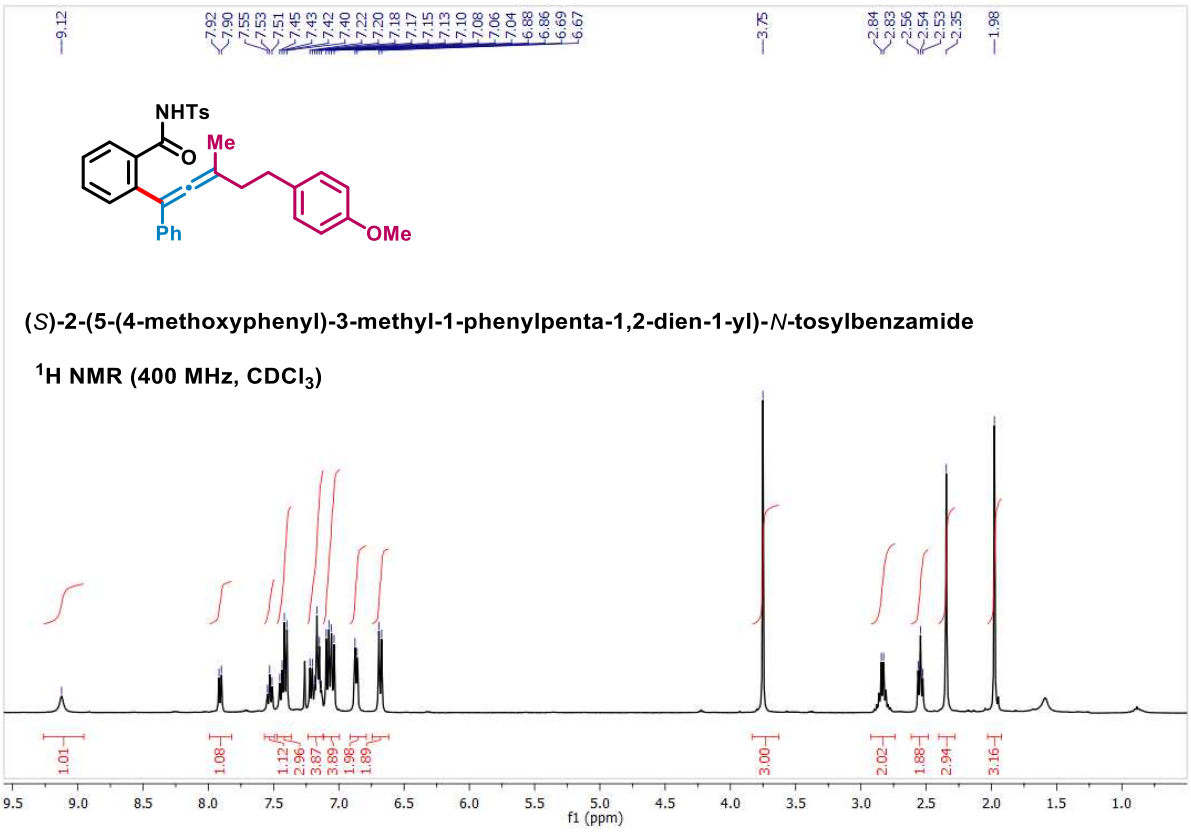
2-((2*S*)-2-(2-methyl-4-(prop-1-en-2-yl)cyclohex-2-en-1-ylidene)-1-phenylvinyl)-*N*-tosylbenzamide

^{1}H NMR (400 MHz, $CDCl_3$)



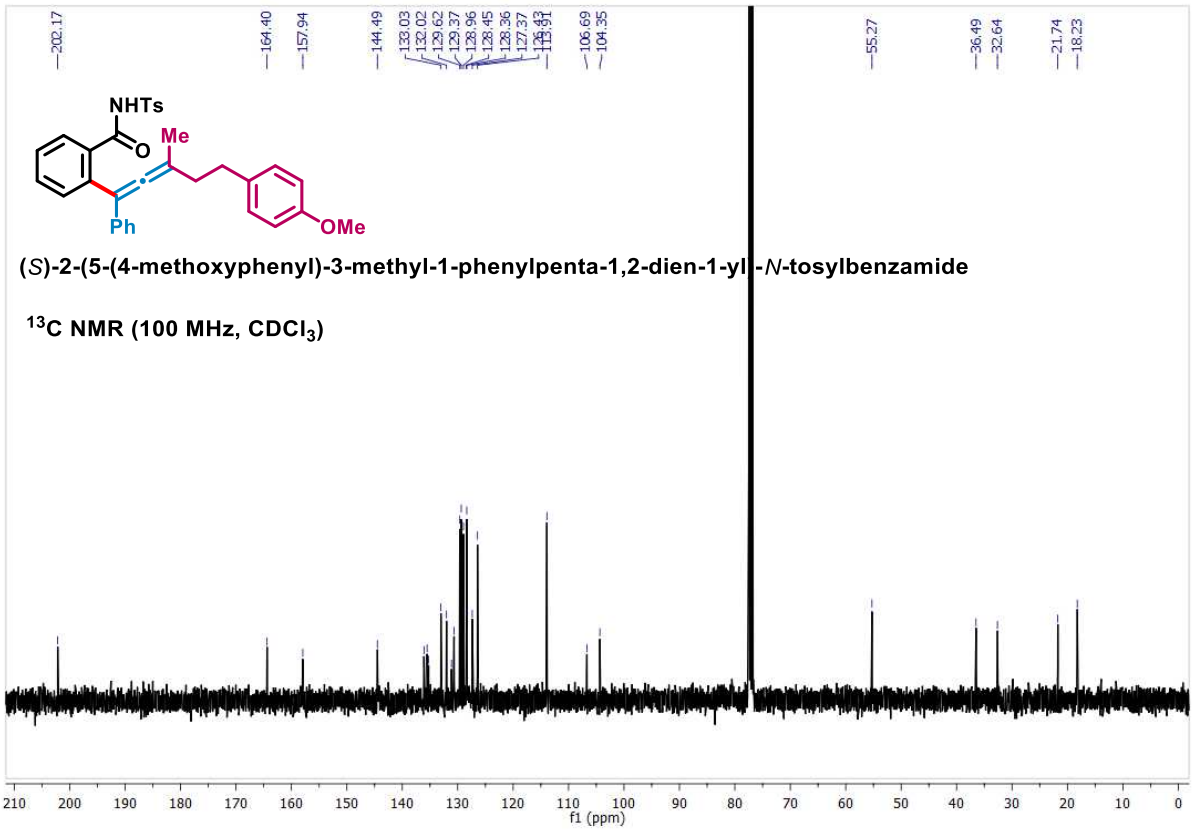
2-((2*S*)-2-(2-methyl-4-(prop-1-en-2-yl)cyclohex-2-en-1-ylidene)-1-phenylvinyl)-*N*-tosylbenzamide

^{13}C NMR (100 MHz, $CDCl_3$)



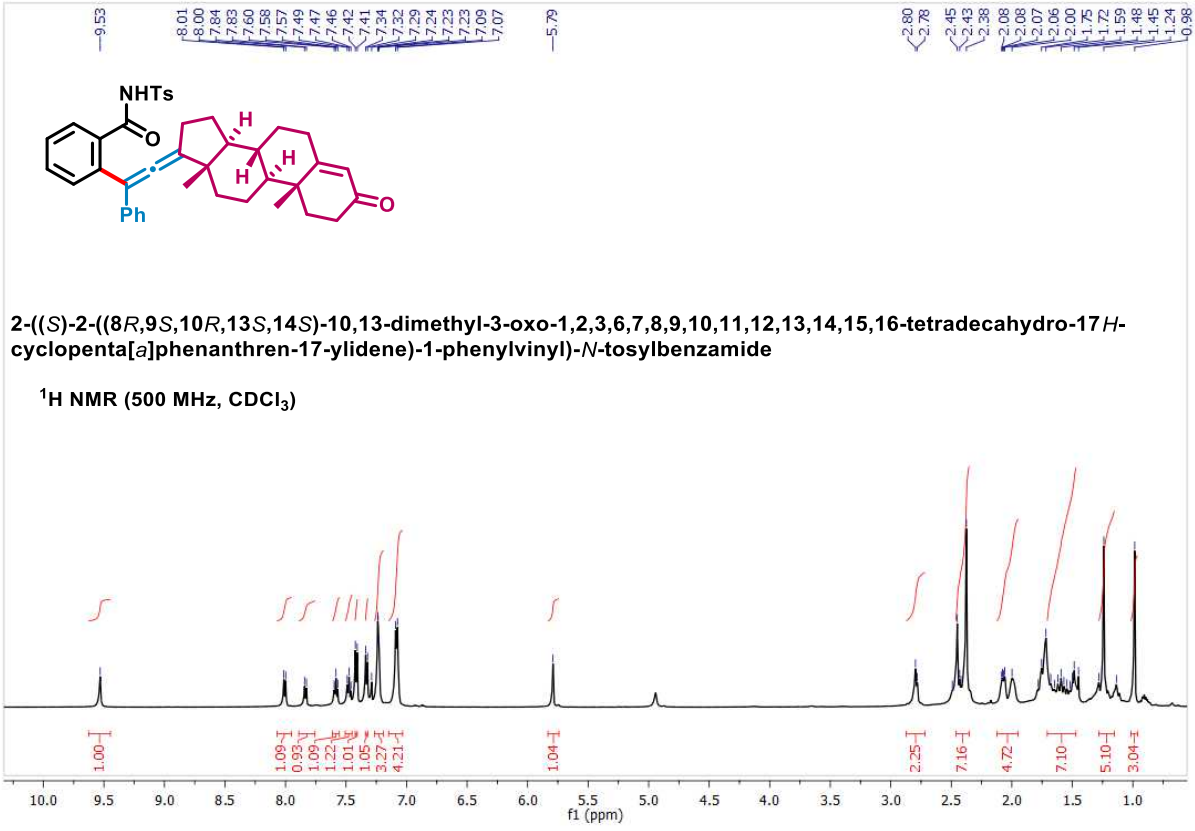
(*S*)-2-(5-(4-methoxyphenyl)-3-methyl-1-phenylpenta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{1}H NMR (400 MHz, $CDCl_3$)



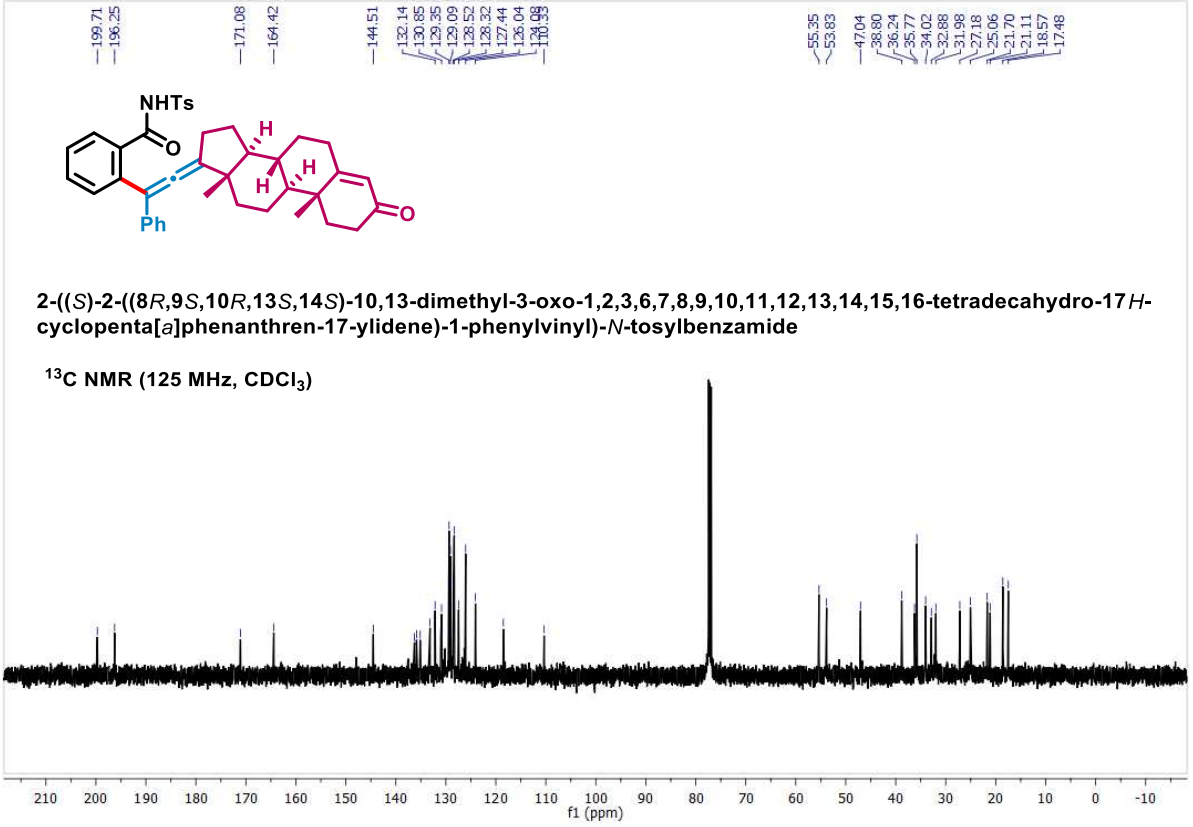
(*S*)-2-(5-(4-methoxyphenyl)-3-methyl-1-phenylpenta-1,2-dien-1-yl)-*N*-tosylbenzamide

^{13}C NMR (100 MHz, $CDCl_3$)



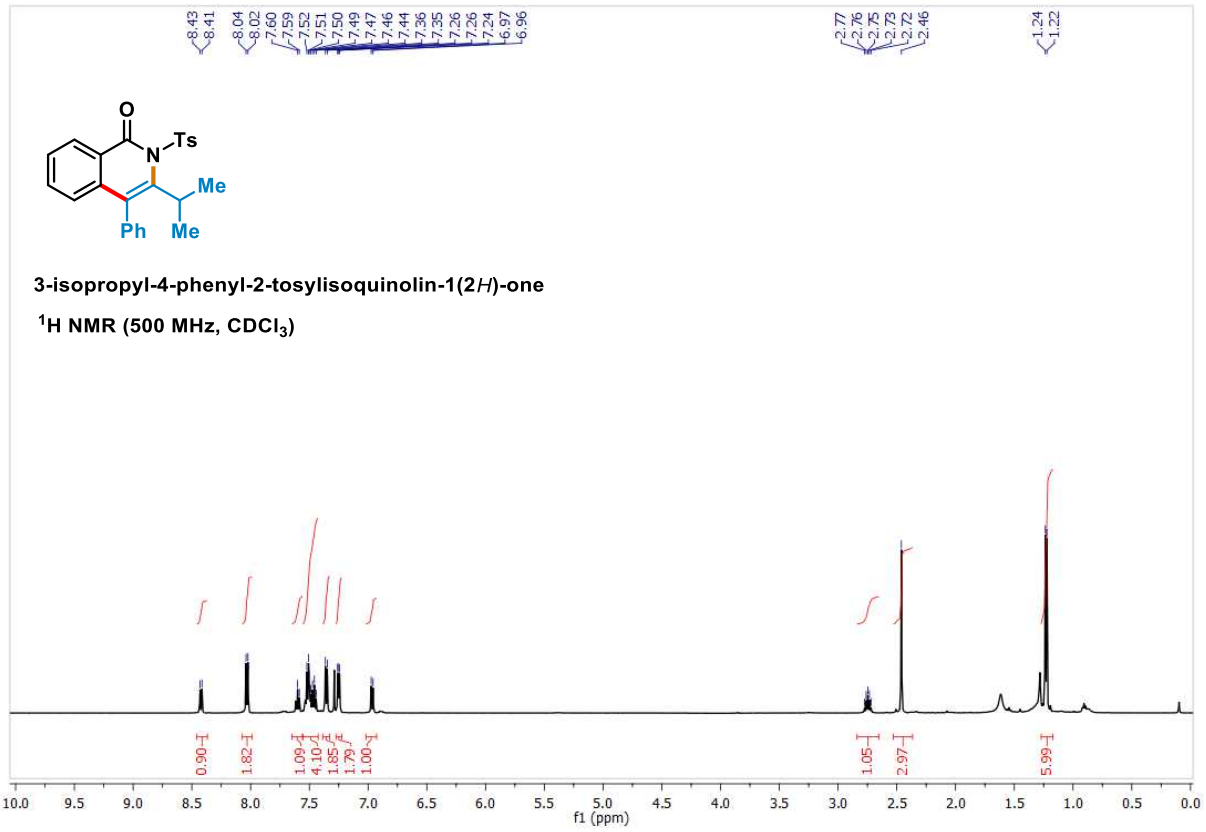
**2-((*S*)-2-((8*R*,9*S*,10*R*,13*S*,14*S*)-10,13-dimethyl-3-oxo-1,2,3,6,7,8,9,10,11,12,13,14,15,16-tetradecahydro-17*H*-cyclopenta[*a*]phenanthren-17-ylidene)-1-phenylvinyl)-*N*-tosylbenzamide

^{1}H NMR (500 MHz, $CDCl_3$)



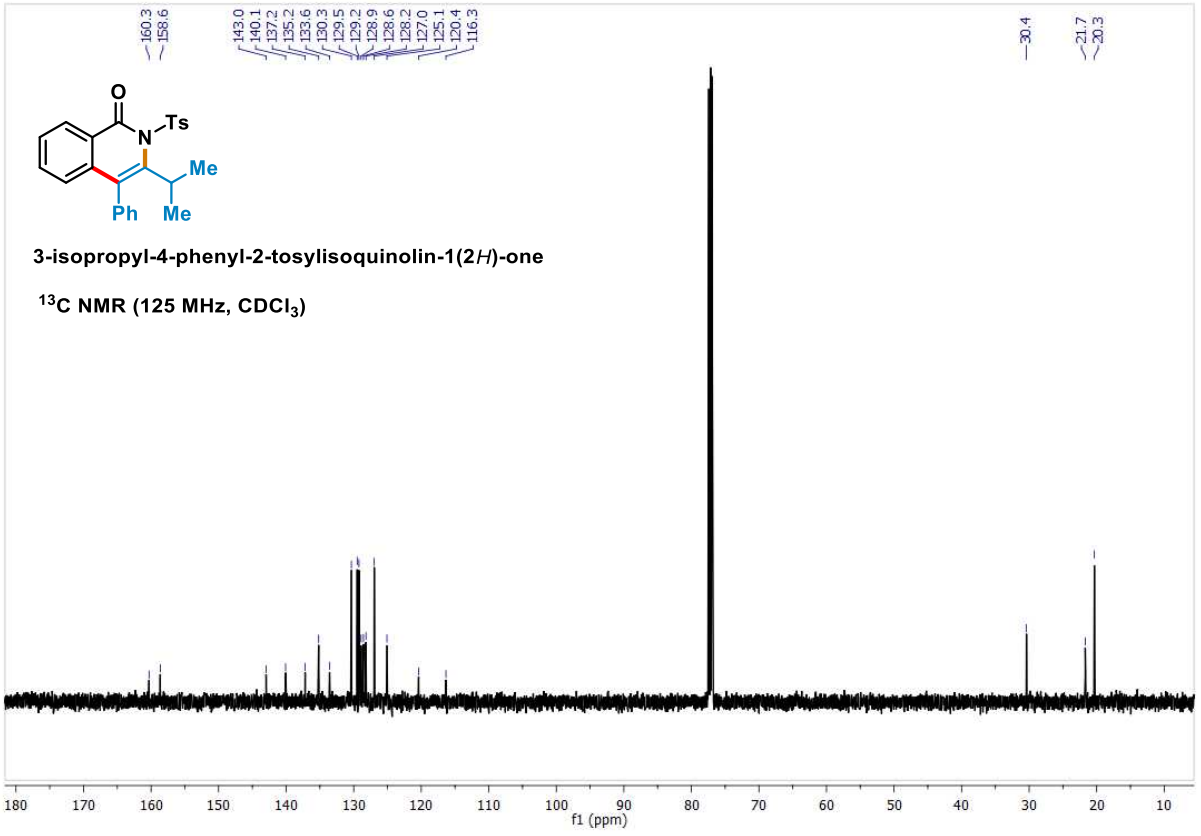
**2-((*S*)-2-((8*R*,9*S*,10*R*,13*S*,14*S*)-10,13-dimethyl-3-oxo-1,2,3,6,7,8,9,10,11,12,13,14,15,16-tetradecahydro-17*H*-cyclopenta[*a*]phenanthren-17-ylidene)-1-phenylvinyl)-*N*-tosylbenzamide

^{13}C NMR (125 MHz, $CDCl_3$)



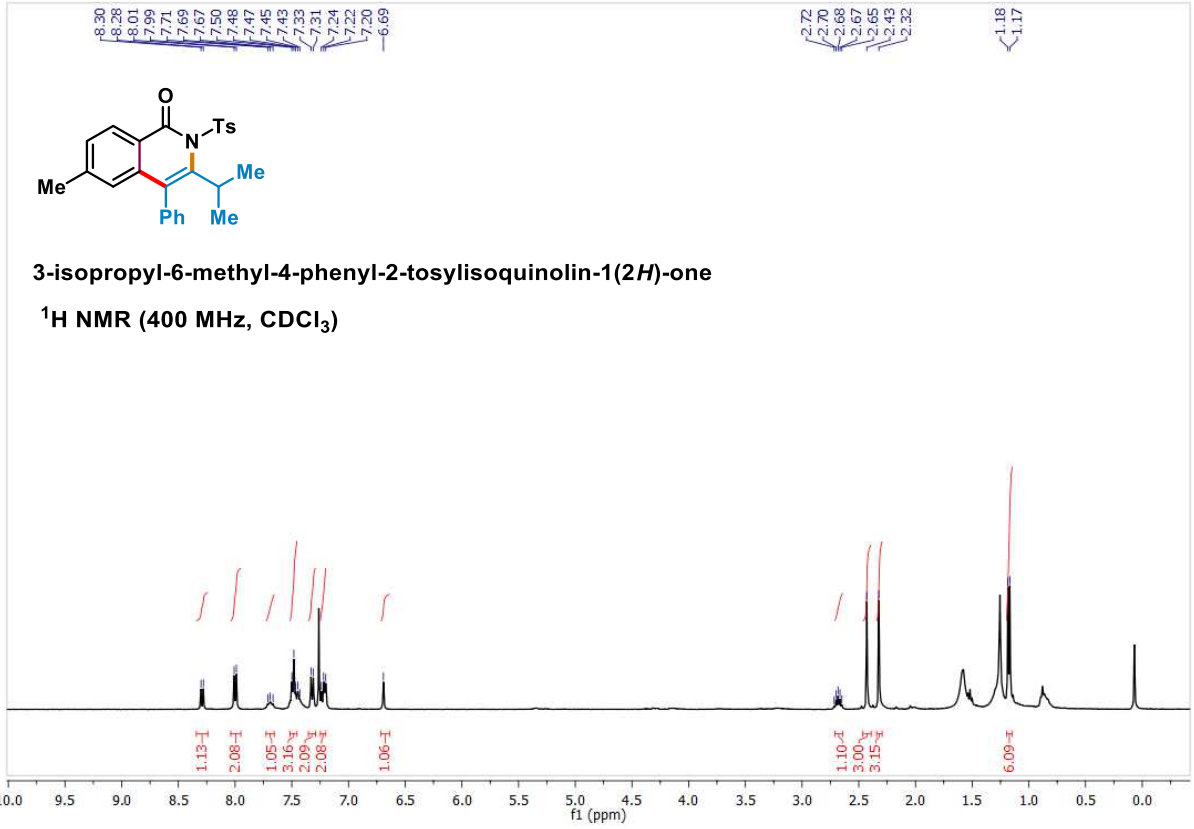
3-isopropyl-4-phenyl-2-tosylisoquinolin-1(2*H*)-one

^{1}H NMR (500 MHz, $CDCl_3$)



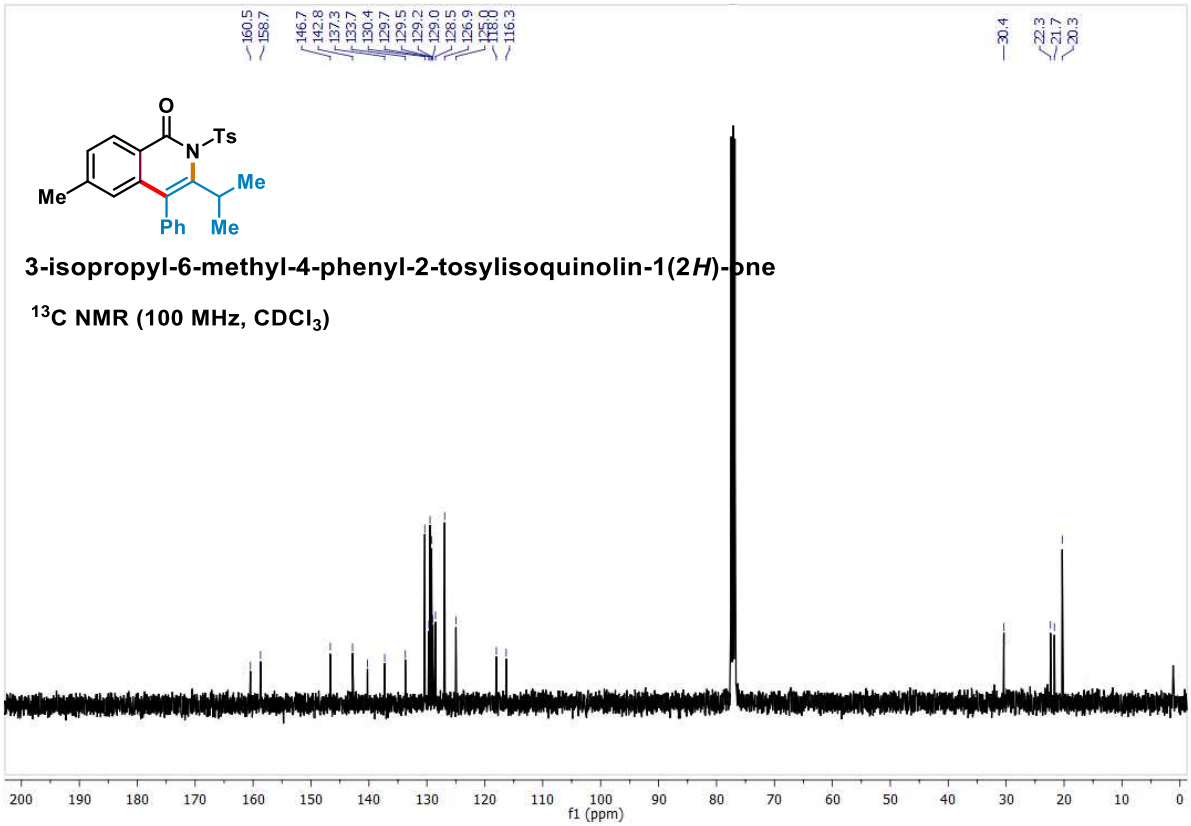
3-isopropyl-4-phenyl-2-tosylisoquinolin-1(2*H*)-one

^{13}C NMR (125 MHz, $CDCl_3$)



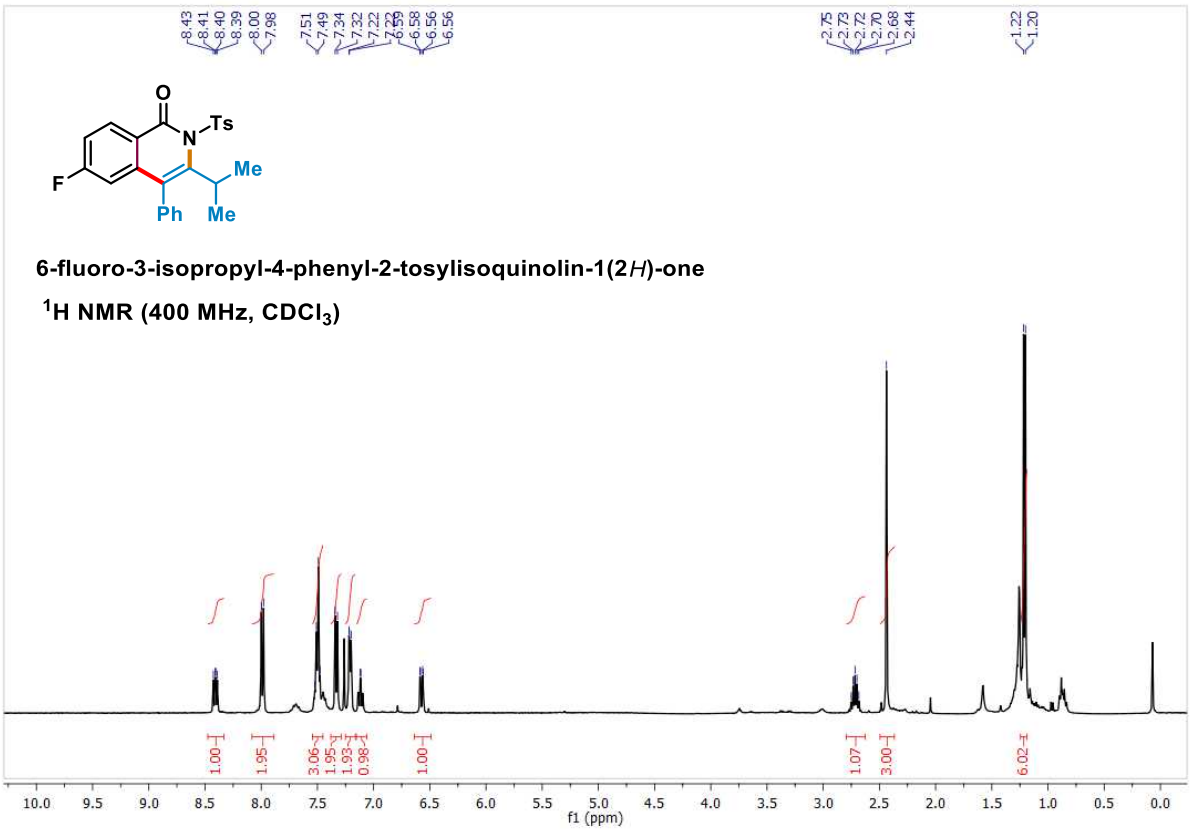
3-isopropyl-6-methyl-4-phenyl-2-tosylisoquinolin-1(2*H*)-one

^{1}H NMR (400 MHz, $CDCl_3$)



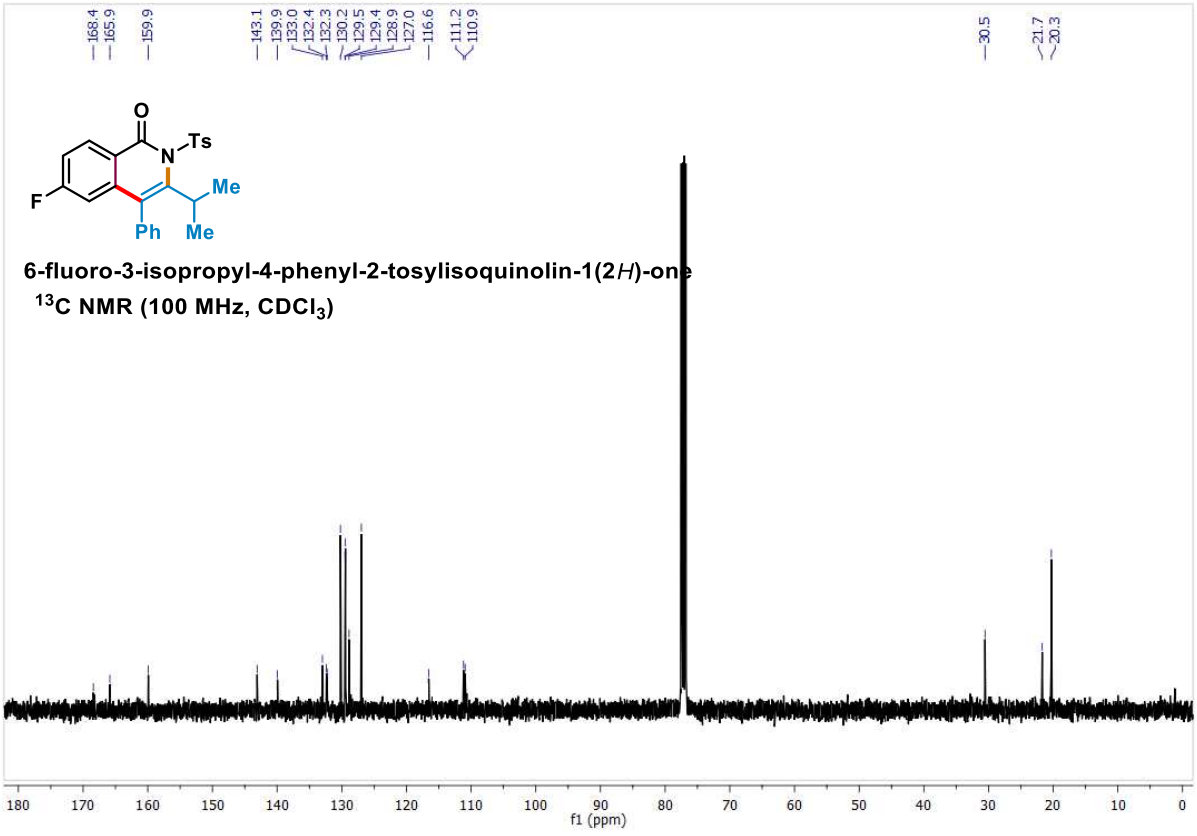
3-isopropyl-6-methyl-4-phenyl-2-tosylisoquinolin-1(2*H*)-one

^{13}C NMR (100 MHz, $CDCl_3$)



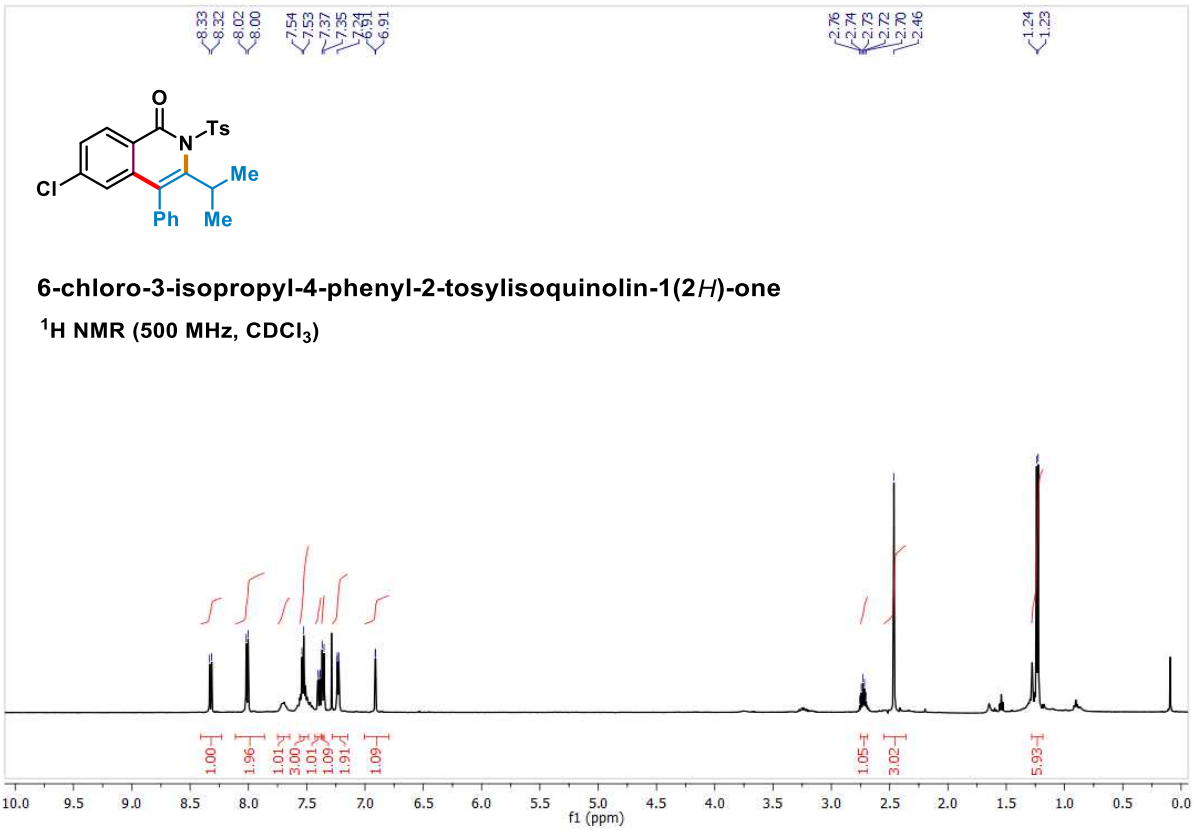
6-fluoro-3-isopropyl-4-phenyl-2-tosylisoquinolin-1(2*H*)-one

^{1}H NMR (400 MHz, $CDCl_3$)



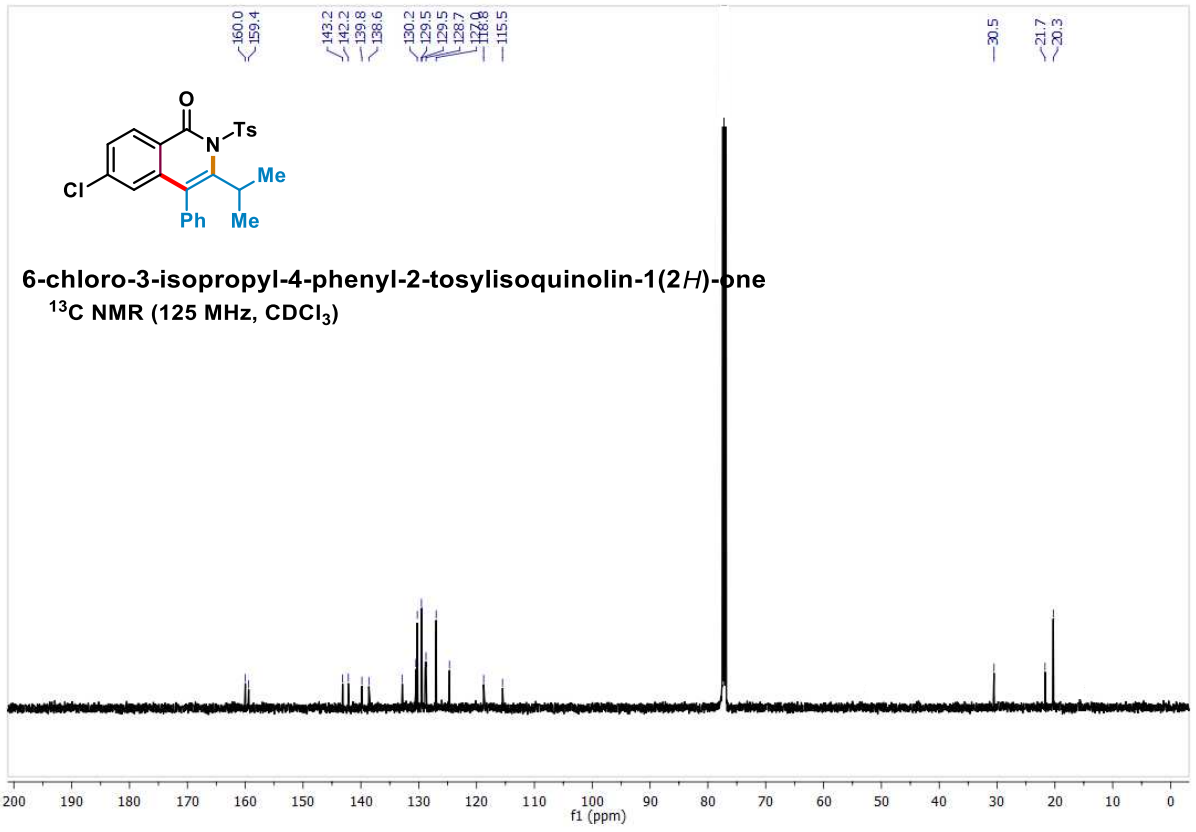
6-fluoro-3-isopropyl-4-phenyl-2-tosylisoquinolin-1(2*H*)-one

^{13}C NMR (100 MHz, $CDCl_3$)



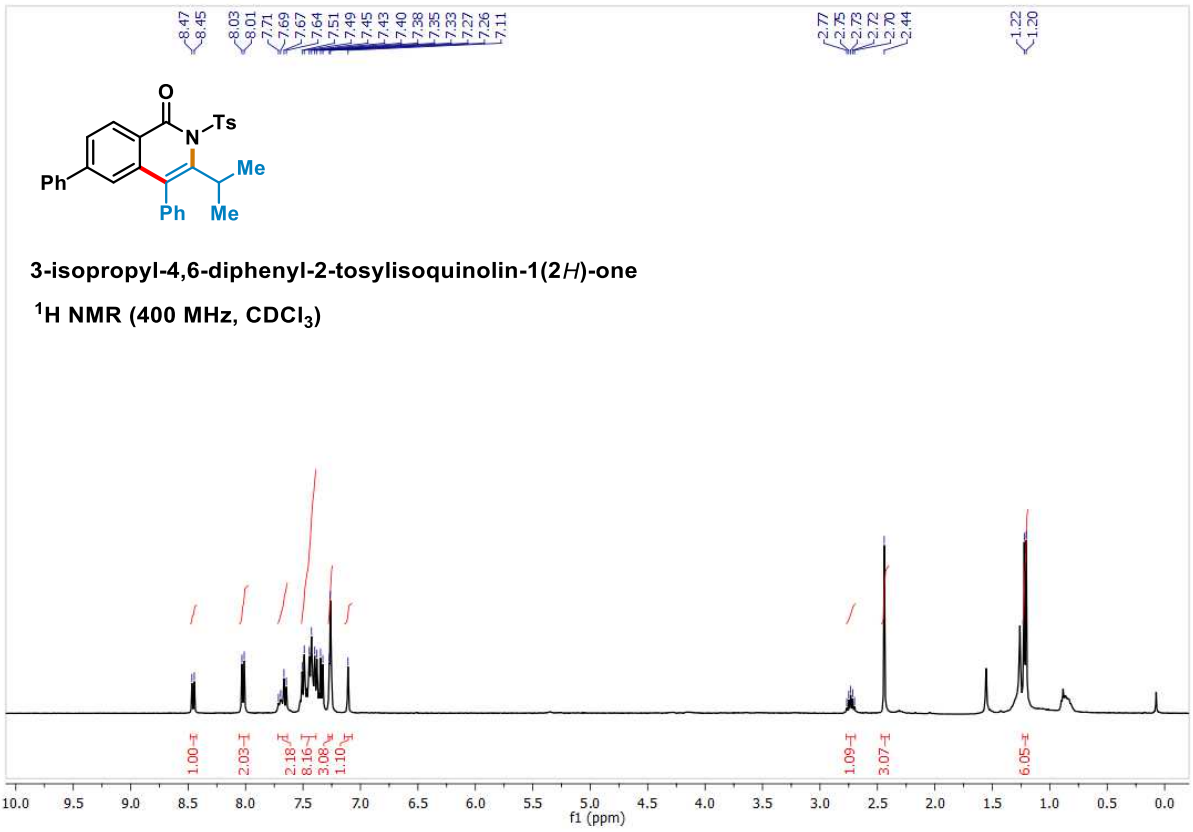
6-chloro-3-isopropyl-4-phenyl-2-tosylisoquinolin-1(2*H*)-one

^{1}H NMR (500 MHz, $CDCl_3$)



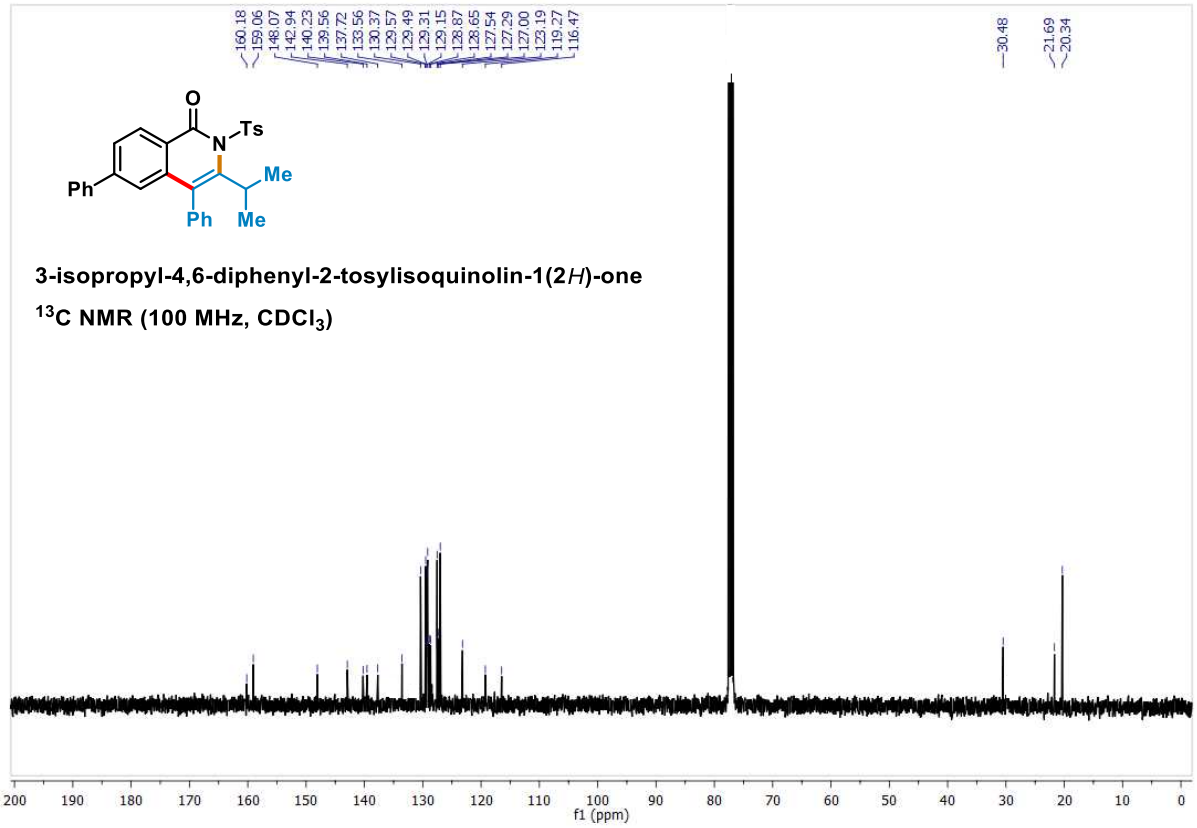
6-chloro-3-isopropyl-4-phenyl-2-tosylisoquinolin-1(2*H*)-one

^{13}C NMR (125 MHz, $CDCl_3$)



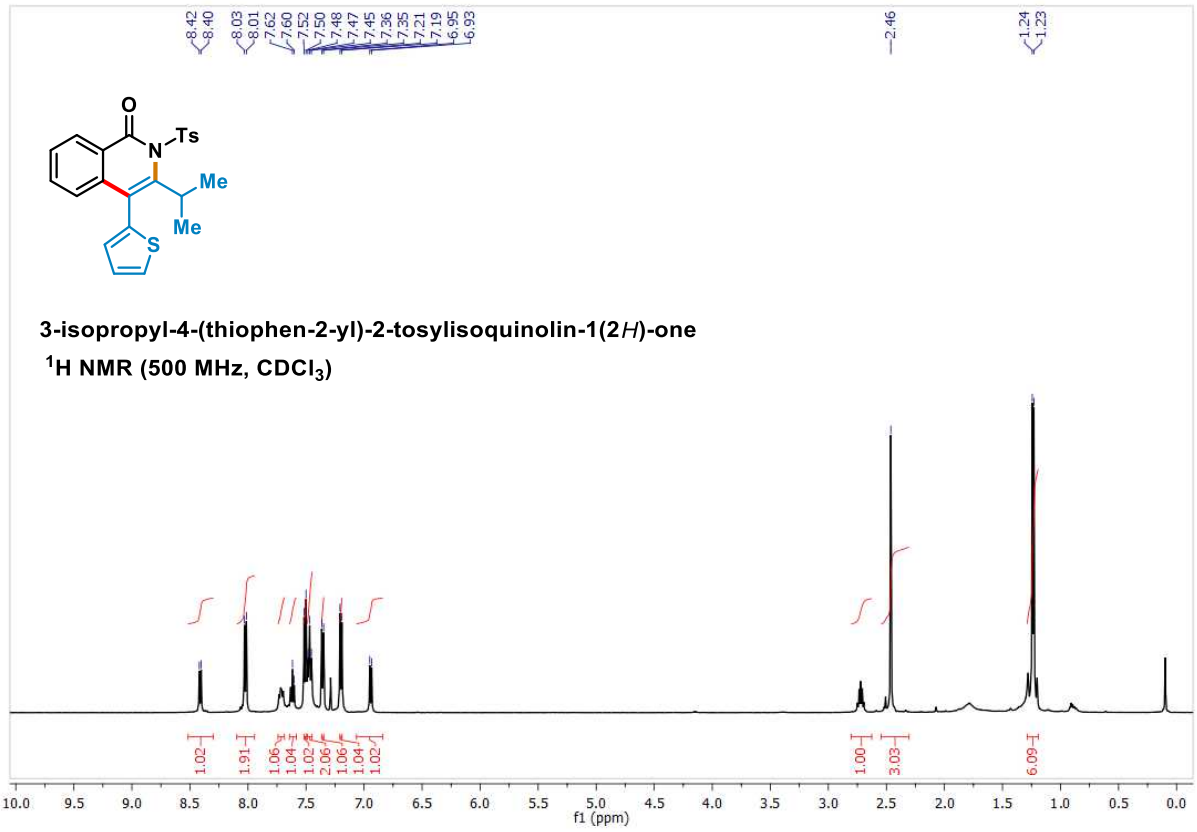
3-isopropyl-4,6-diphenyl-2-tosylisoquinolin-1(2*H*)-one

^{1}H NMR (400 MHz, $CDCl_3$)



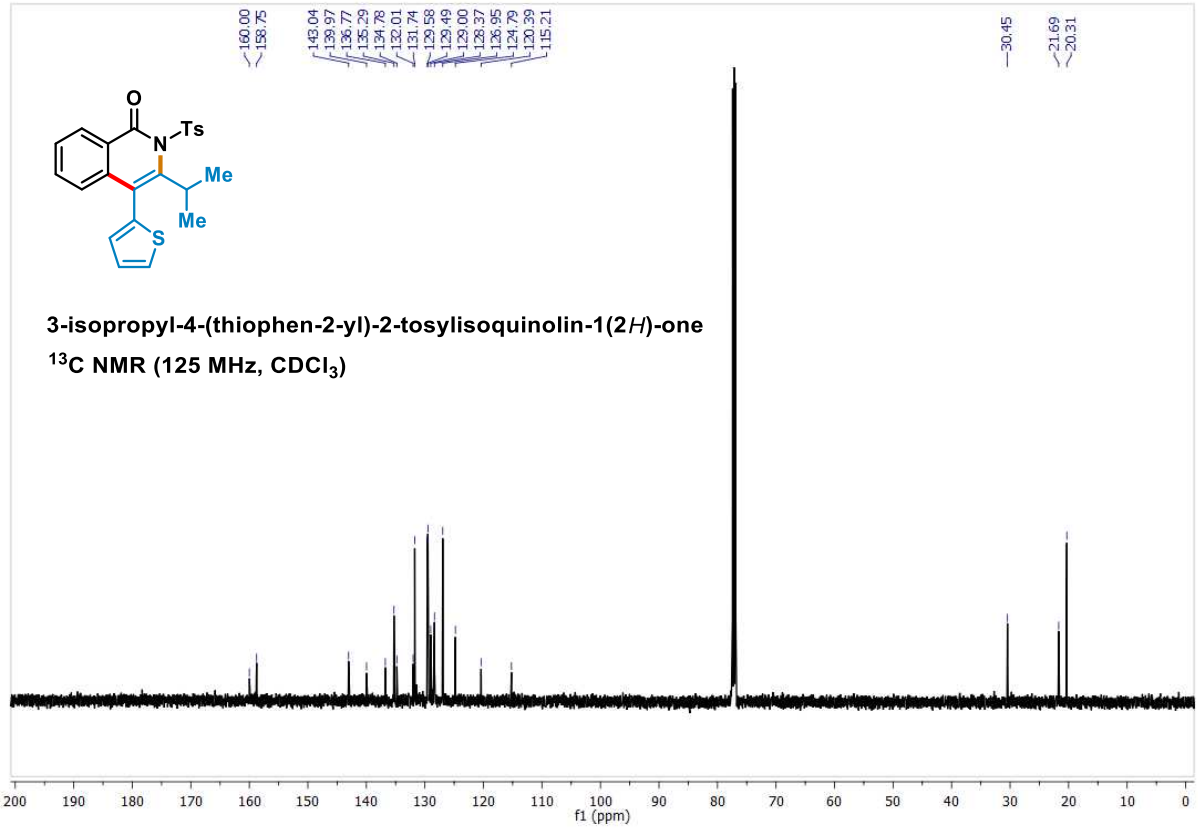
3-isopropyl-4,6-diphenyl-2-tosylisoquinolin-1(2*H*)-one

^{13}C NMR (100 MHz, $CDCl_3$)



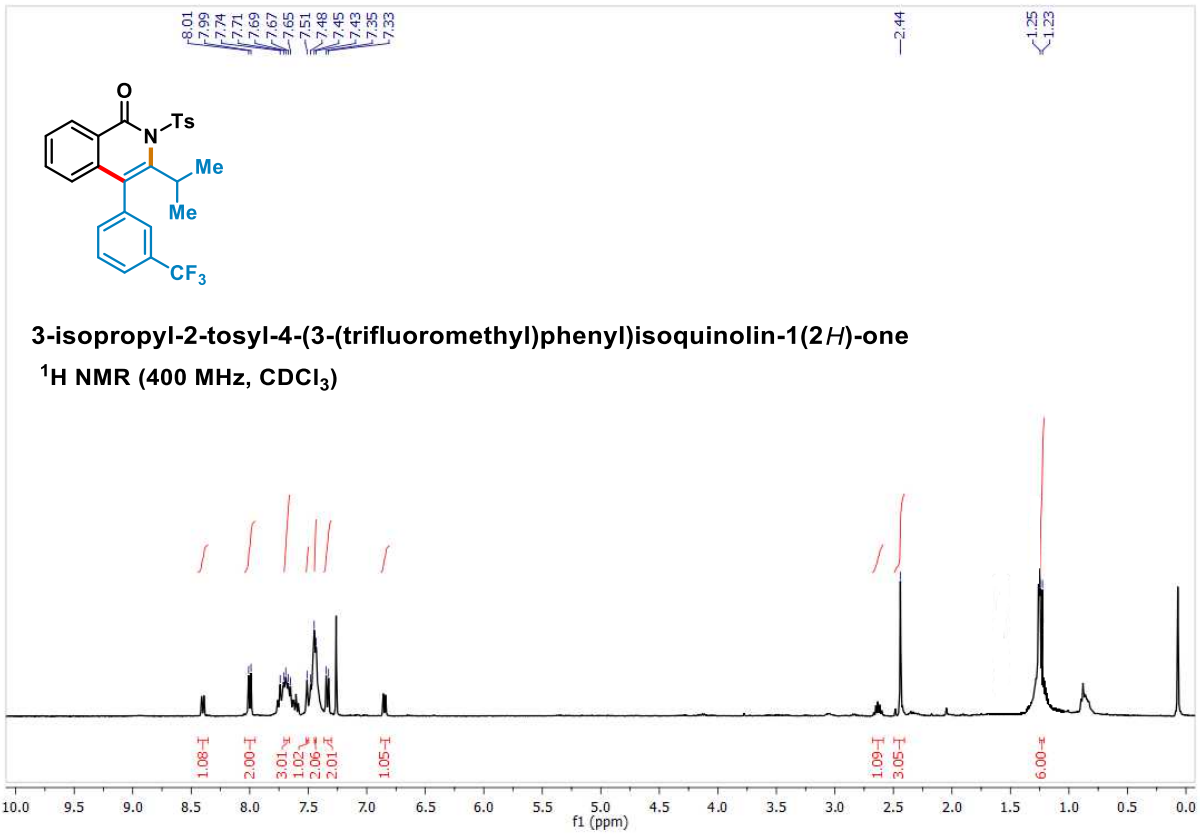
3-isopropyl-4-(thiophen-2-yl)-2-tosylisoquinolin-1(2*H*)-one

^{1}H NMR (500 MHz, $CDCl_3$)



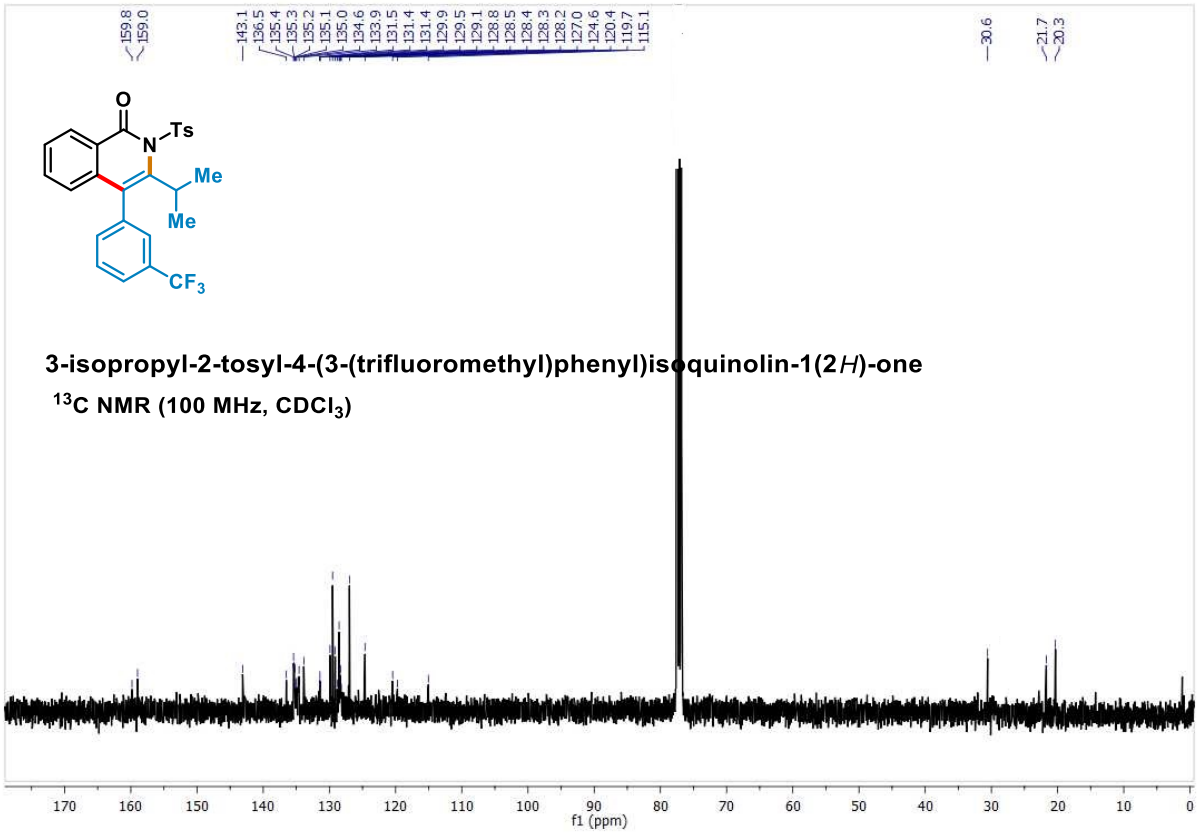
3-isopropyl-4-(thiophen-2-yl)-2-tosylisoquinolin-1(2*H*)-one

^{13}C NMR (125 MHz, $CDCl_3$)



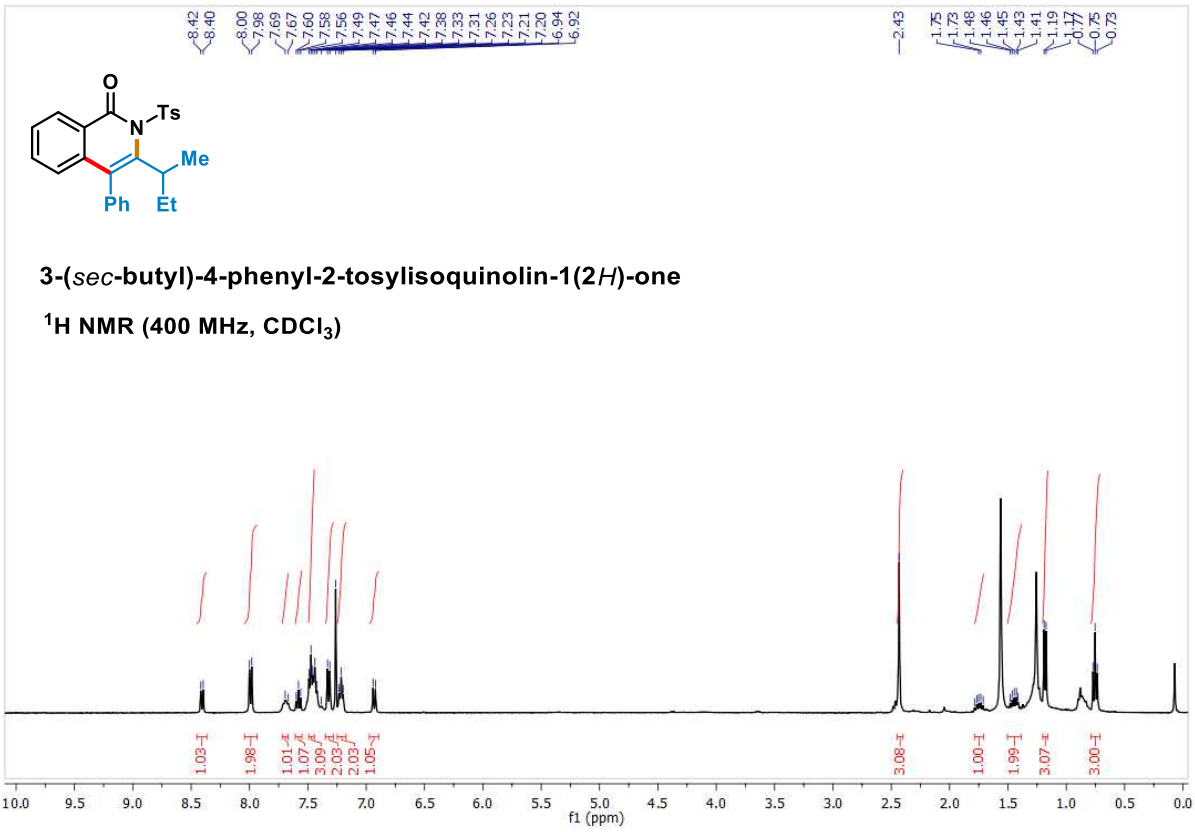
3-isopropyl-2-tosyl-4-(3-(trifluoromethyl)phenyl)isoquinolin-1(2*H*)-one

^{1}H NMR (400 MHz, $CDCl_3$)



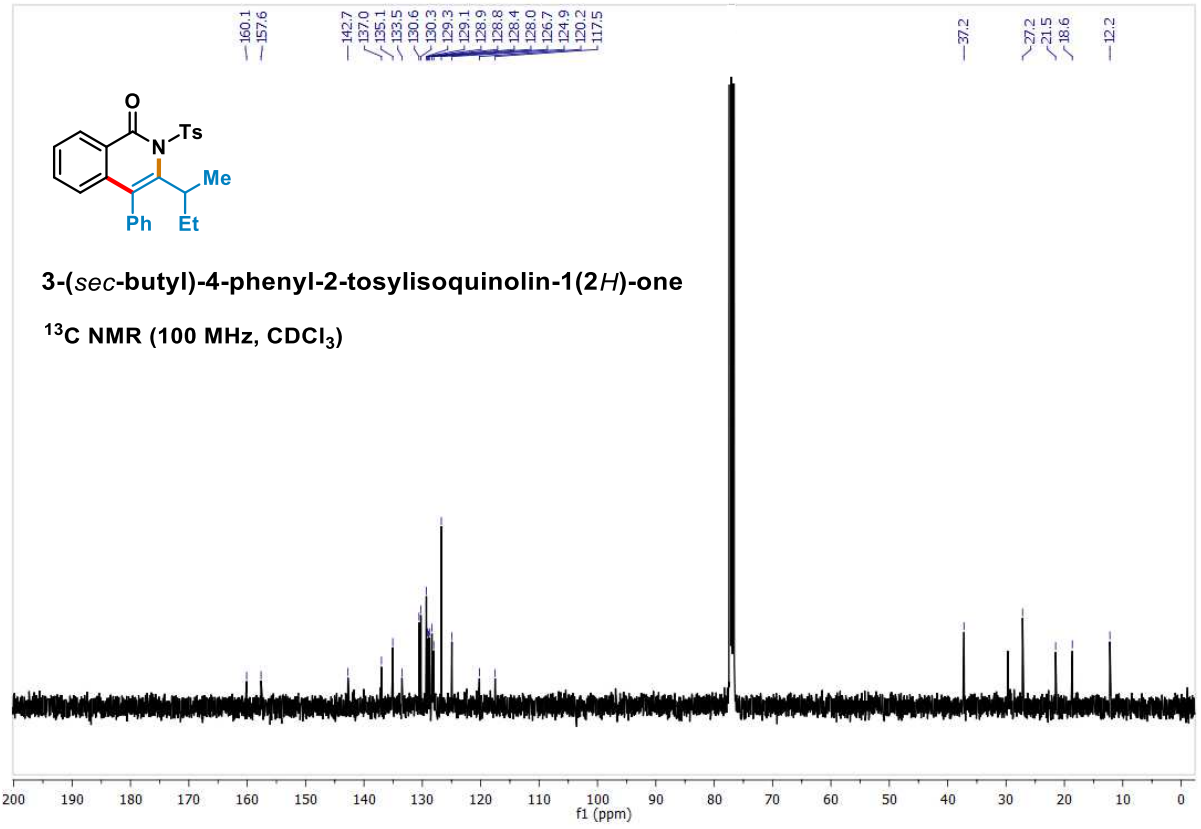
3-isopropyl-2-tosyl-4-(3-(trifluoromethyl)phenyl)isoquinolin-1(2*H*)-one

^{13}C NMR (100 MHz, $CDCl_3$)



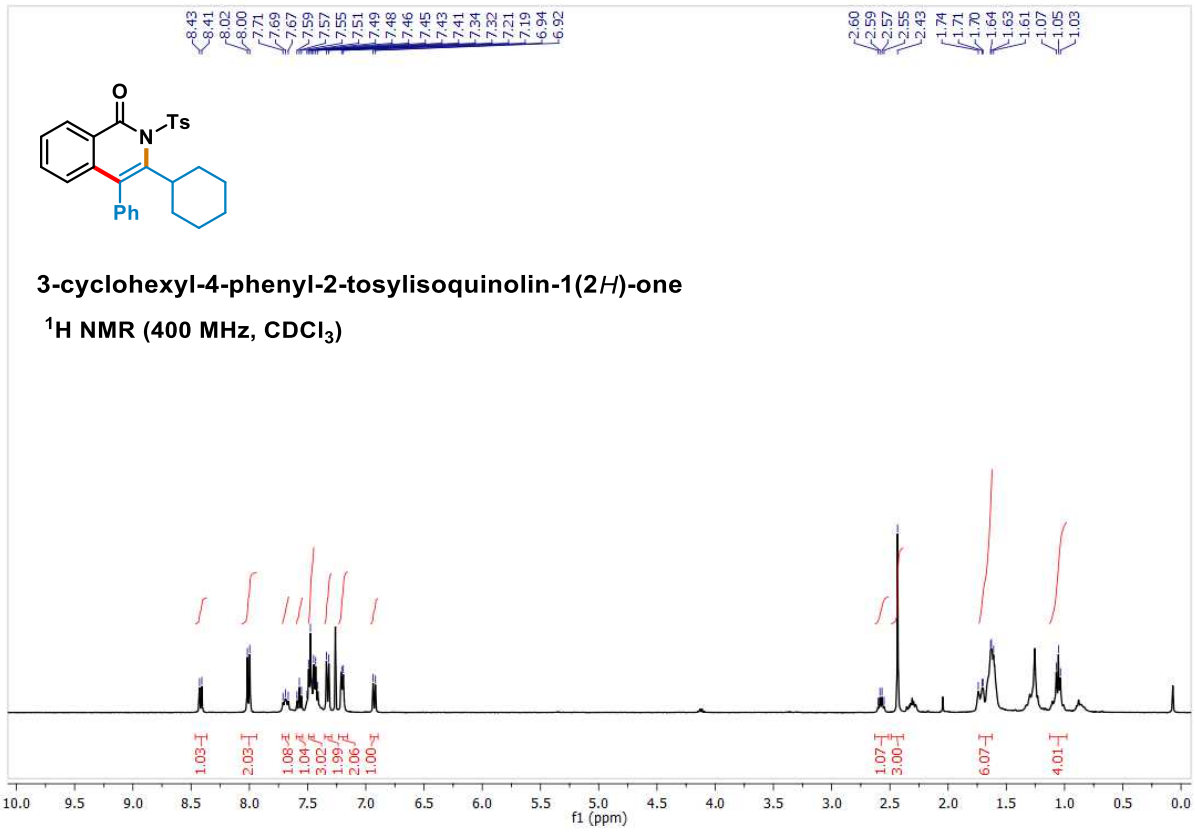
3-(*sec*-butyl)-4-phenyl-2-tosylisoquinolin-1(2*H*)-one

^{1}H NMR (400 MHz, $CDCl_3$)



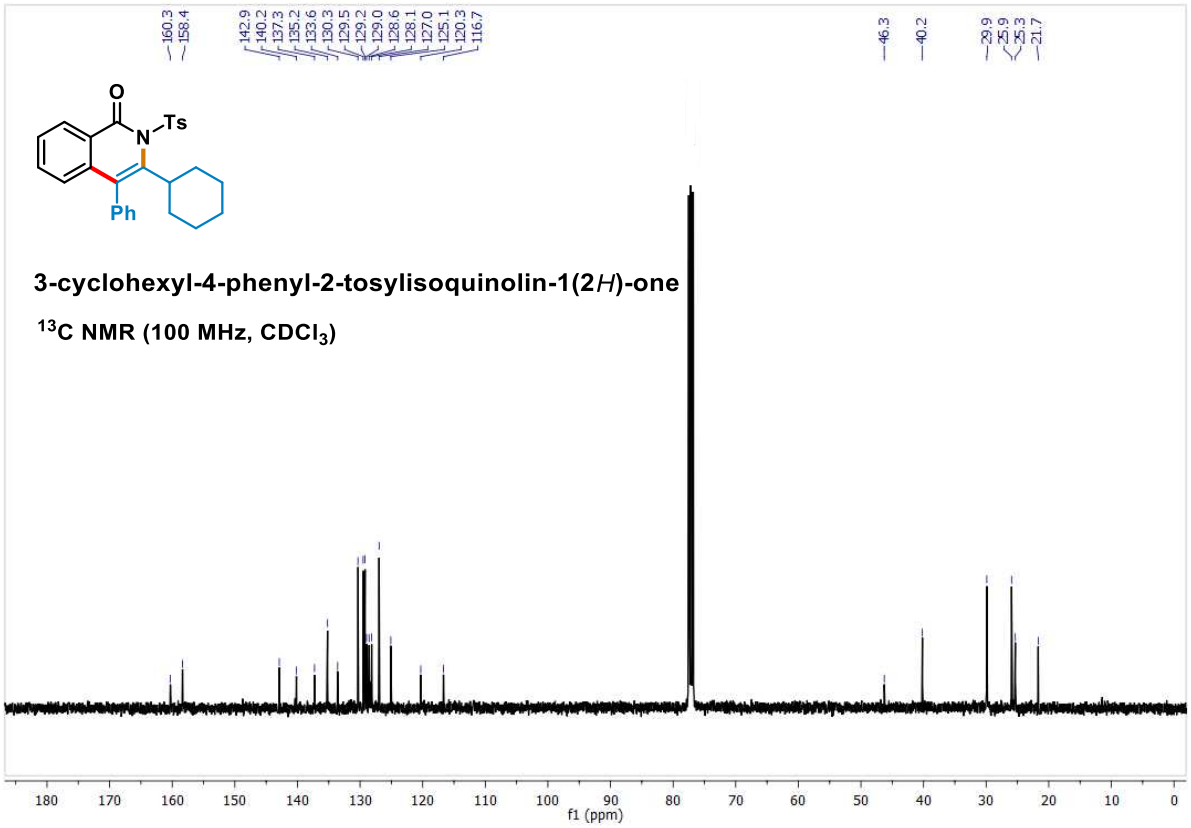
3-(*sec*-butyl)-4-phenyl-2-tosylisoquinolin-1(2*H*)-one

^{13}C NMR (100 MHz, $CDCl_3$)



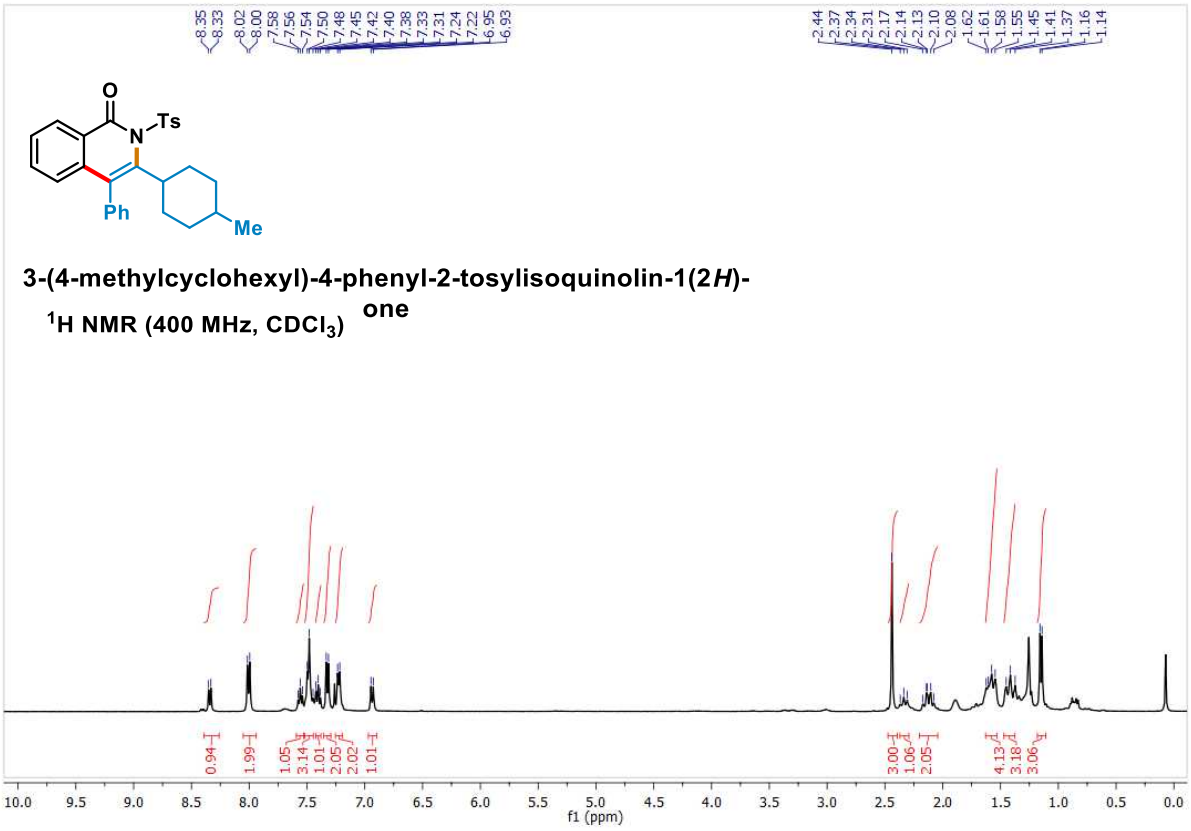
3-cyclohexyl-4-phenyl-2-tosylisoquinolin-1(2*H*)-one

^{1}H NMR (400 MHz, $CDCl_3$)



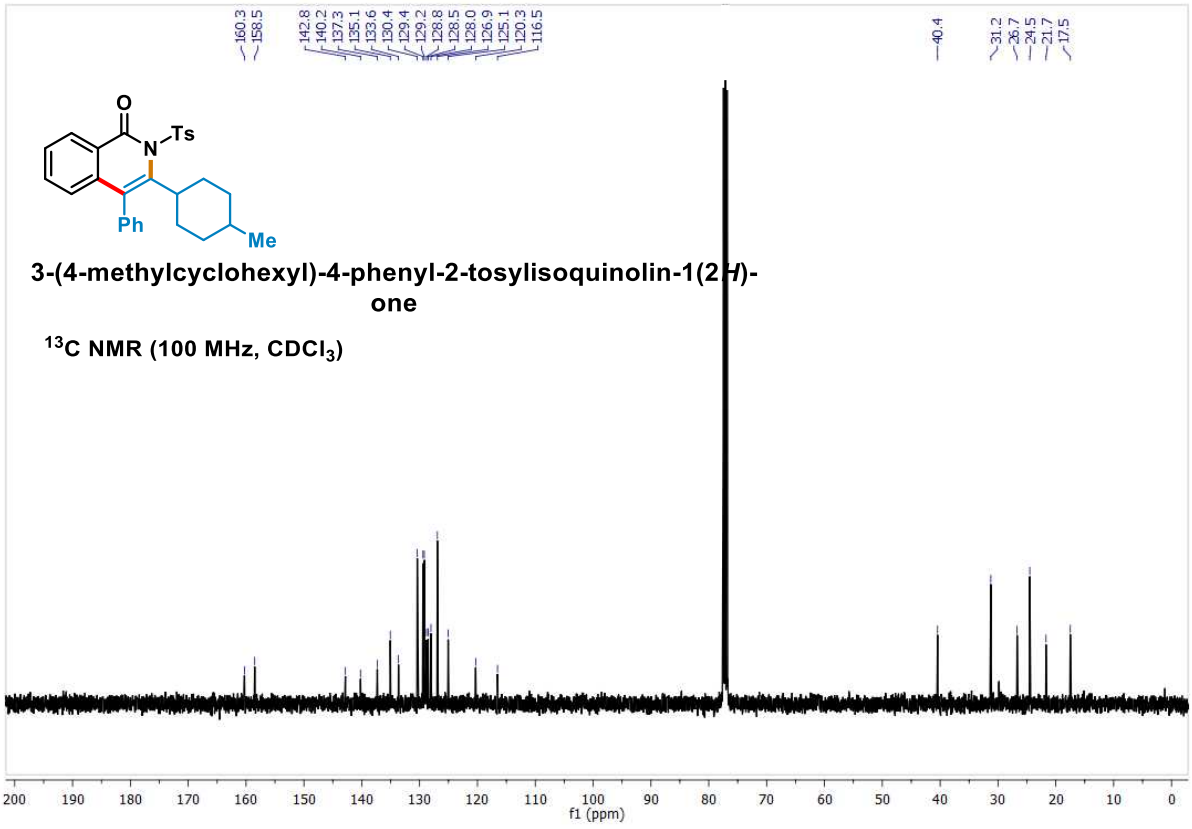
3-cyclohexyl-4-phenyl-2-tosylisoquinolin-1(2*H*)-one

^{13}C NMR (100 MHz, $CDCl_3$)



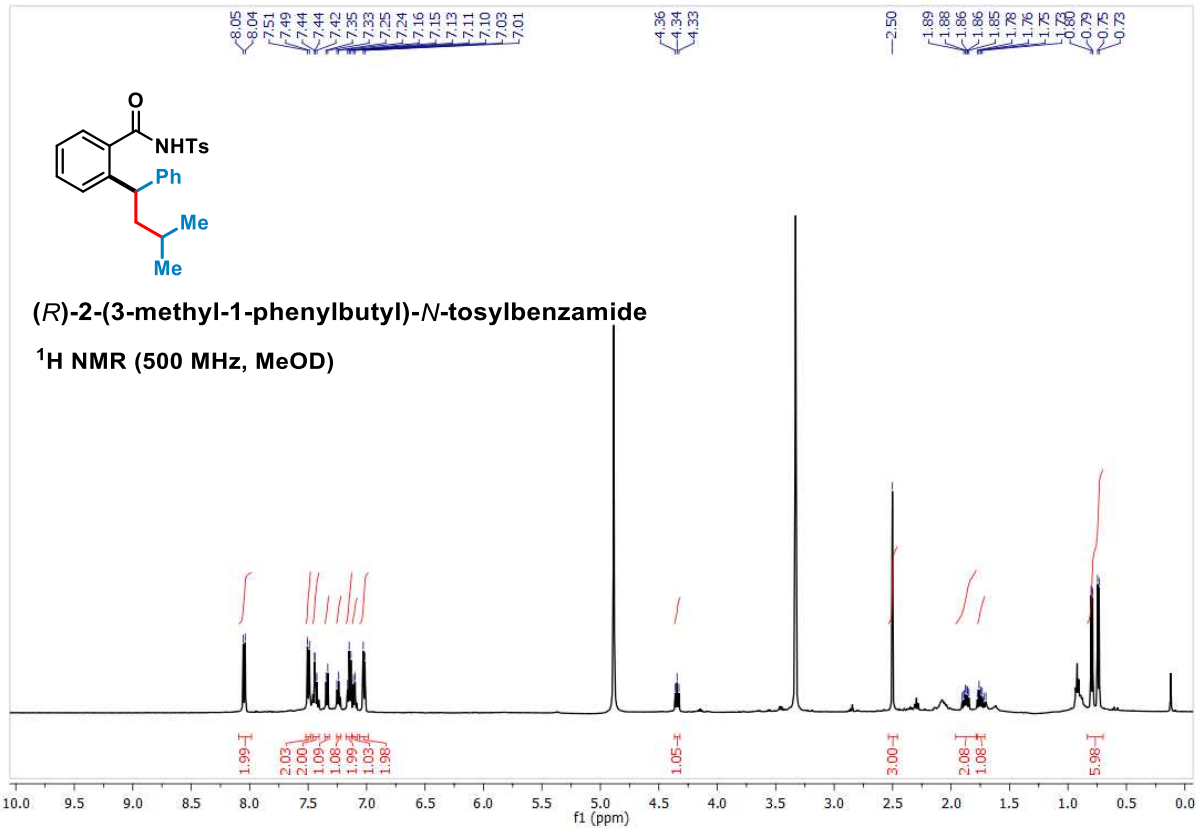
3-(4-methylcyclohexyl)-4-phenyl-2-tosylisoquinolin-1(2*H*)-one

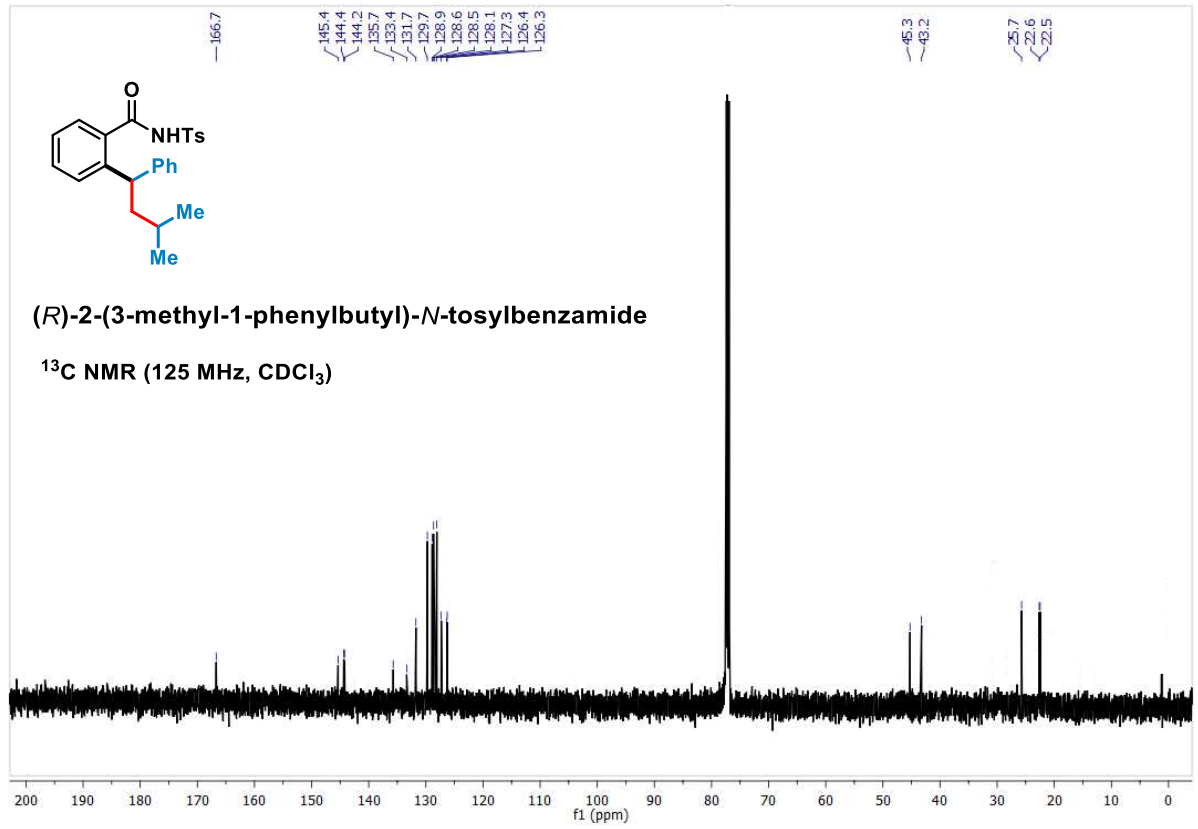
^{1}H NMR (400 MHz, $CDCl_3$)

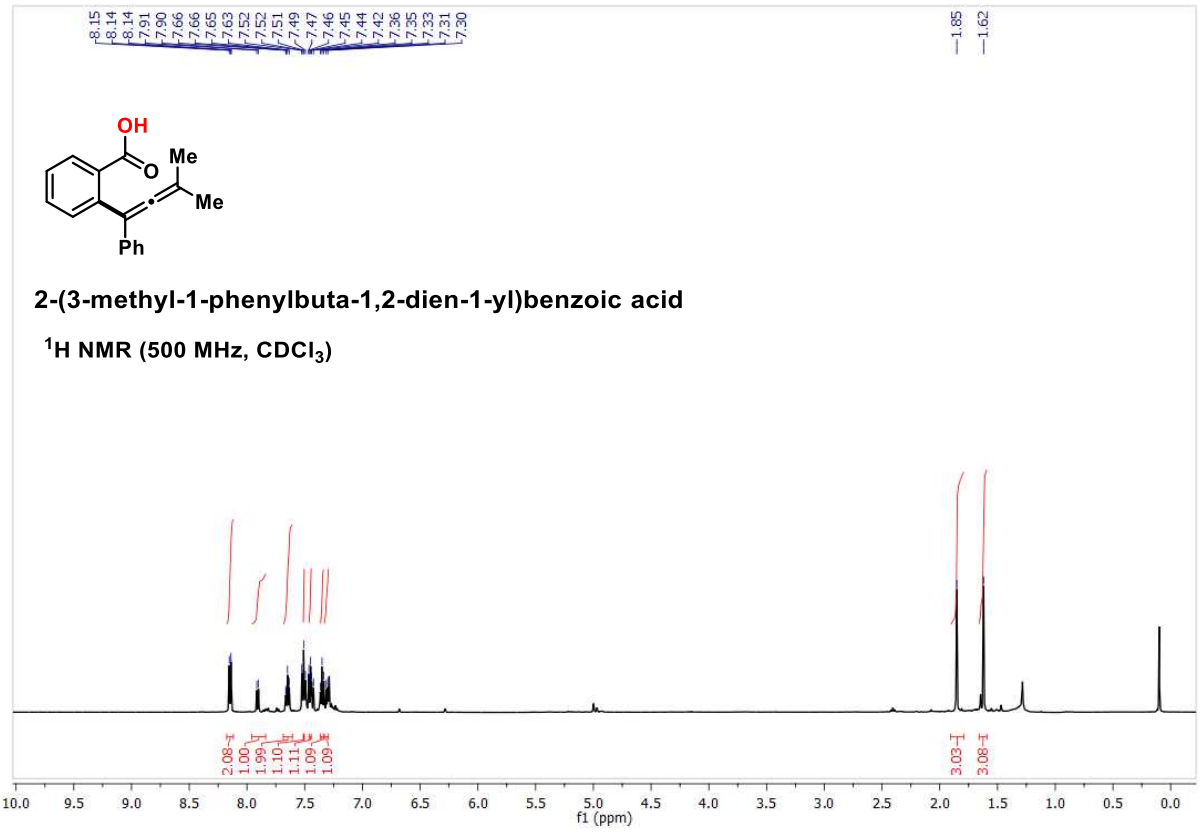


3-(4-methylcyclohexyl)-4-phenyl-2-tosylisoquinolin-1(2*H*)-one

^{13}C NMR (100 MHz, $CDCl_3$)

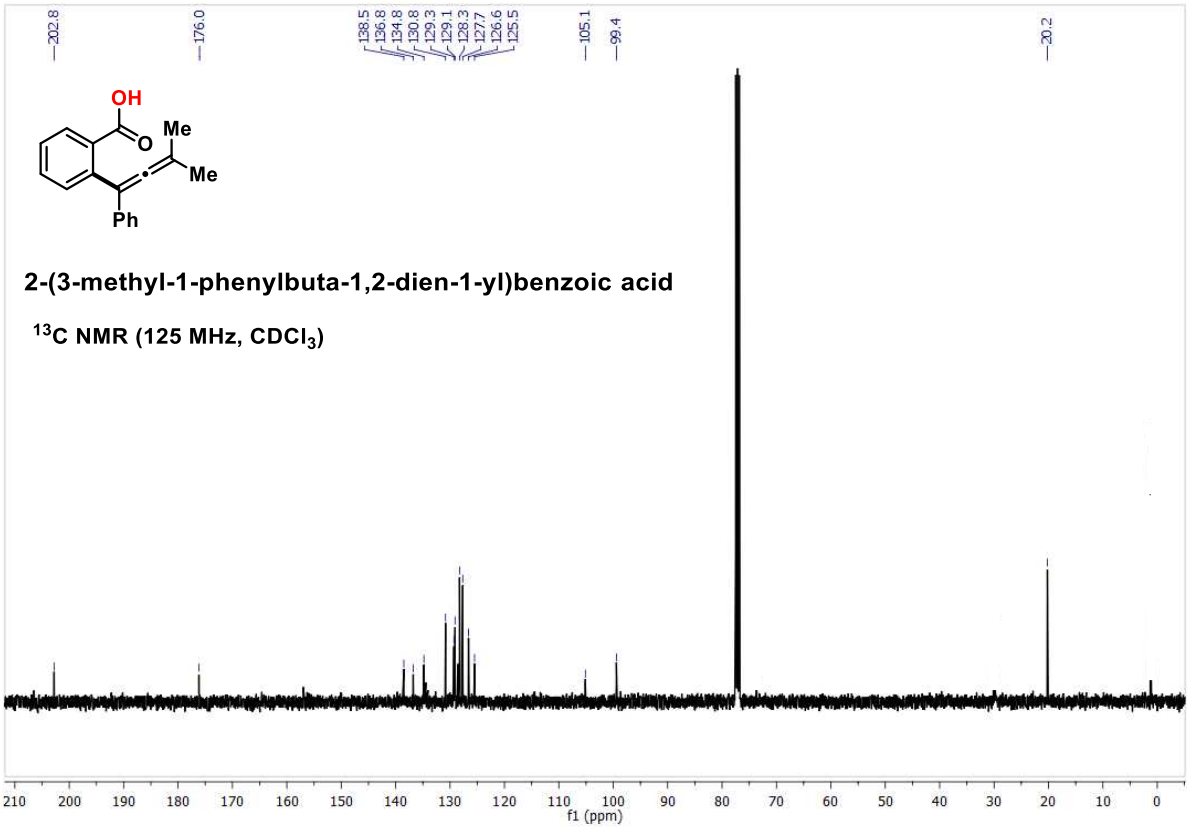

NHTs
Ph
Me
Me
(R)-2-(3-methyl-1-phenylbutyl)-N-tosylbenzamide
1H NMR (500 MHz, MeOD)
f1 (ppm)


NHTs
Ph
Me
Me
(R)-2-(3-methyl-1-phenylbutyl)-N-tosylbenzamide
13C NMR (125 MHz, CDCl3)
f1 (ppm)



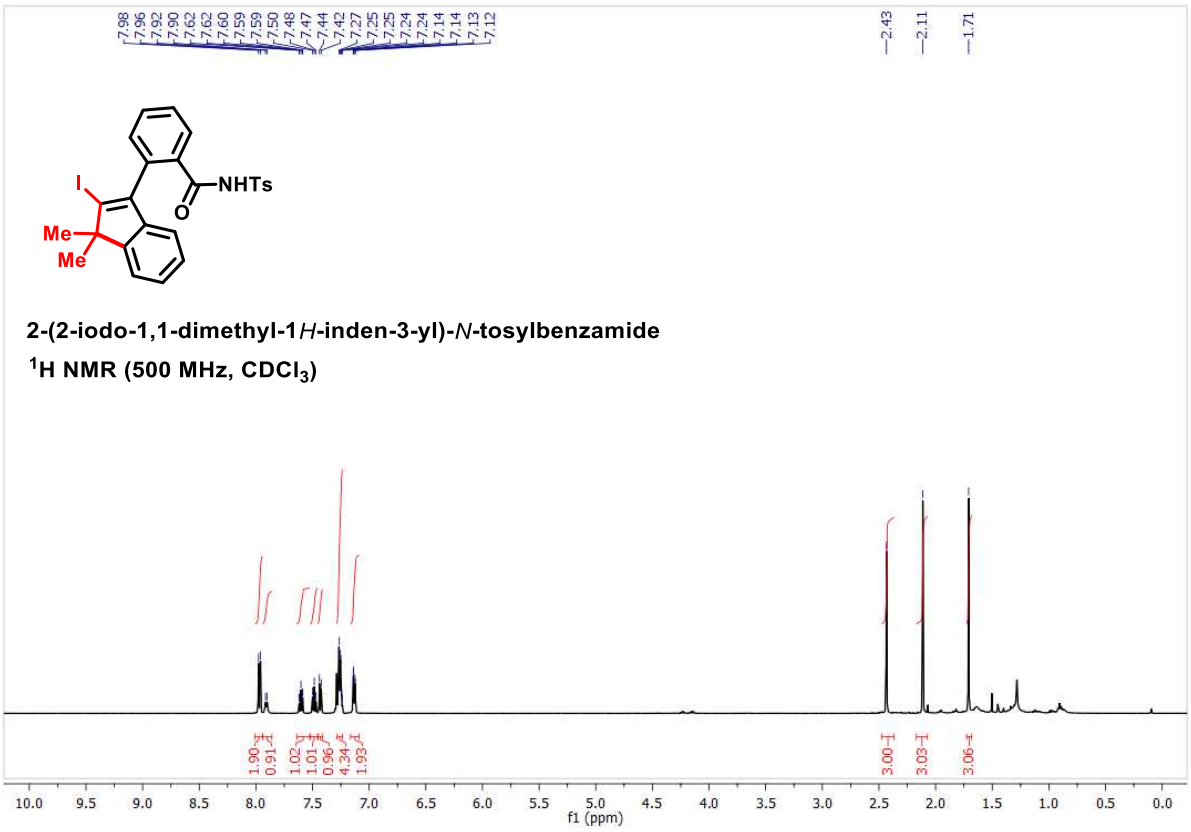
2-(3-methyl-1-phenylbuta-1,2-dien-1-yl)benzoic acid

^{1}H NMR (500 MHz, $CDCl_3$)



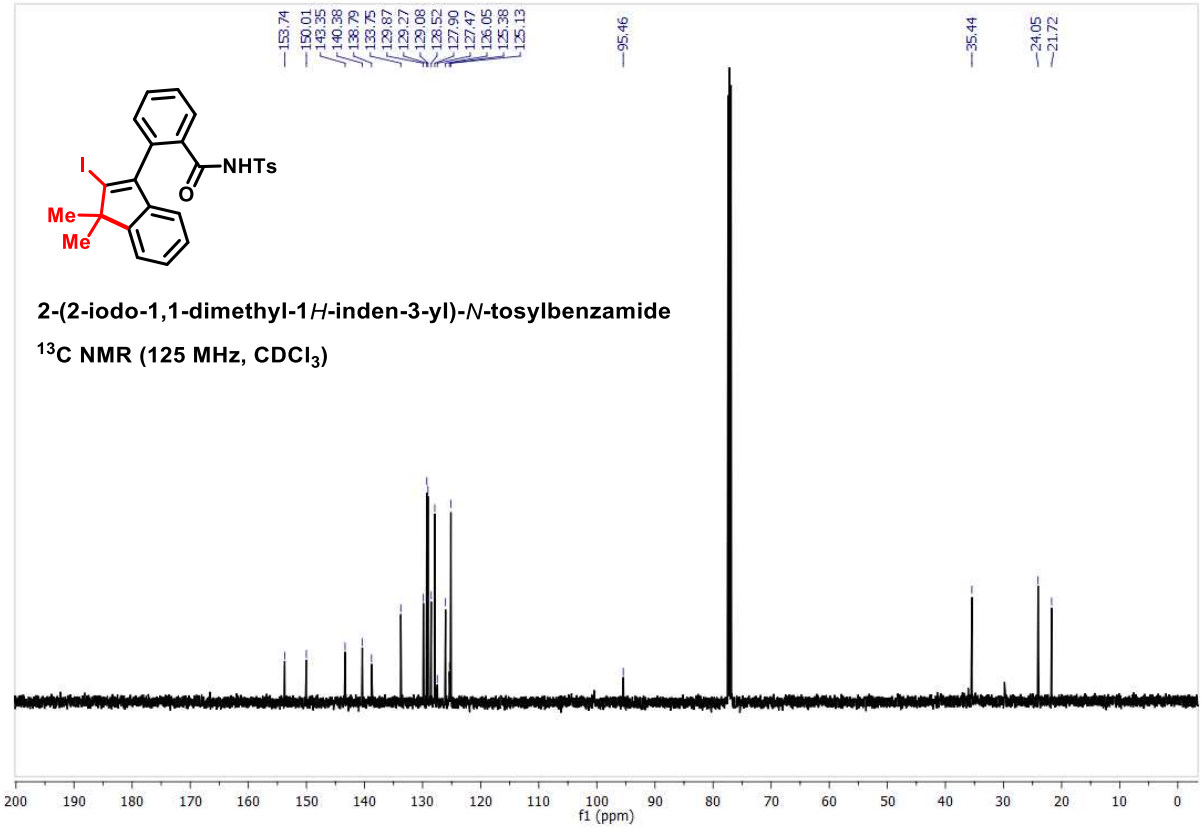
2-(3-methyl-1-phenylbuta-1,2-dien-1-yl)benzoic acid

^{13}C NMR (125 MHz, $CDCl_3$)



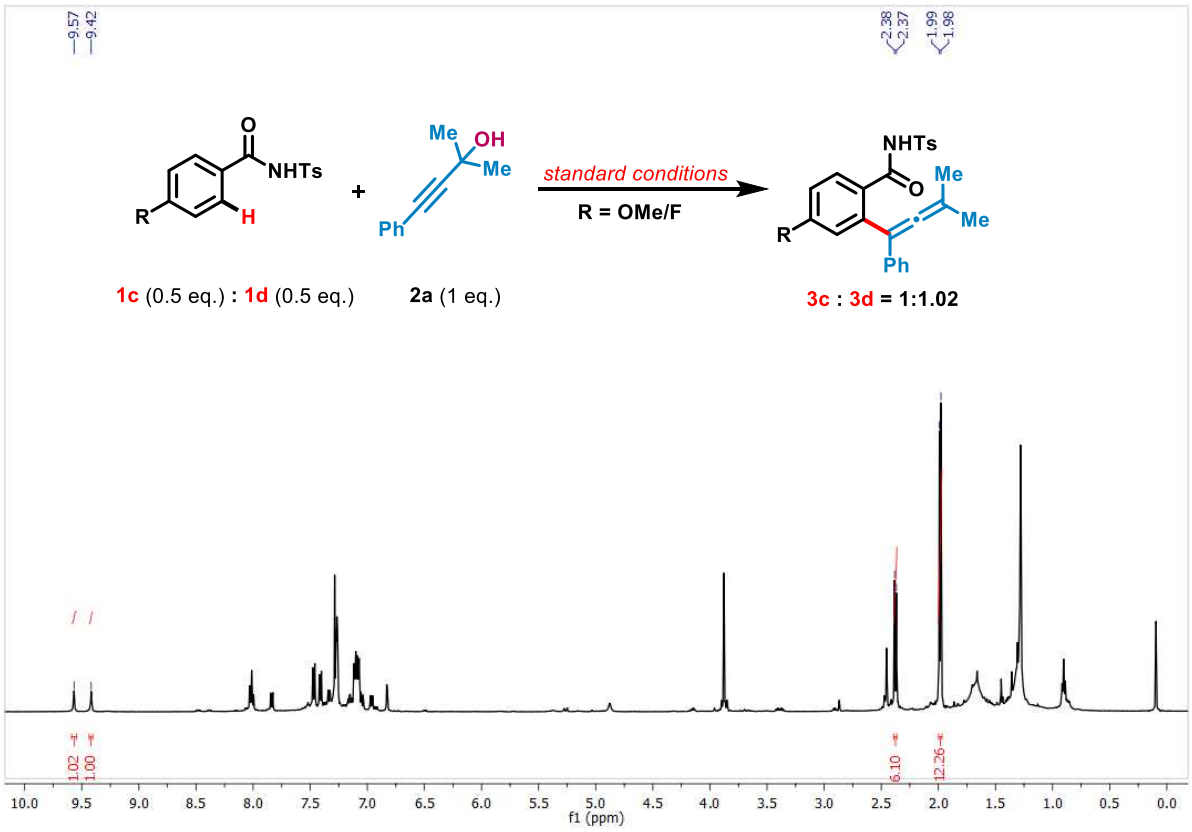
2-(2-iodo-1,1-dimethyl-1*H*-inden-3-yl)-*N*-tosylbenzamide

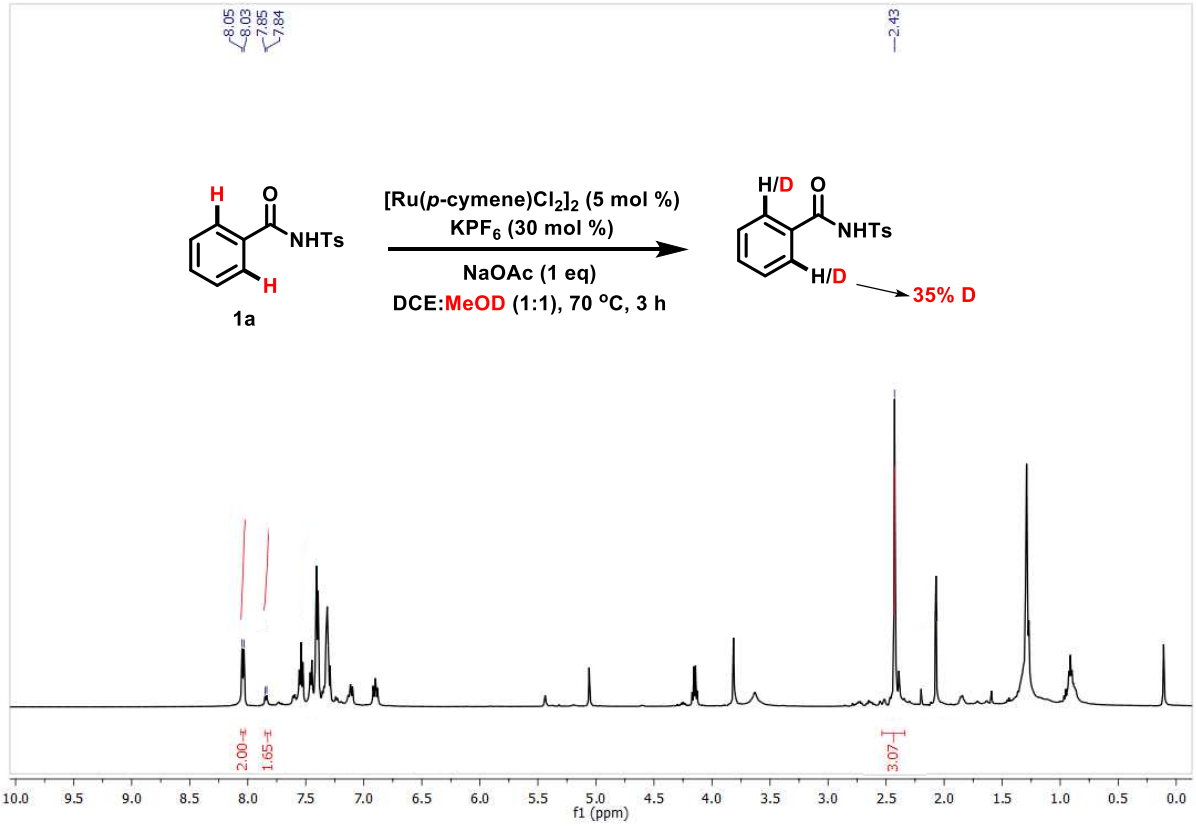
^{1}H NMR (500 MHz, $CDCl_3$)



2-(2-iodo-1,1-dimethyl-1*H*-inden-3-yl)-*N*-tosylbenzamide

^{13}C NMR (125 MHz, $CDCl_3$)


9.57
9.42
2.38
2.37
1.99
1.98
NHTs
R
H
Me
OH
Me
Ph
standard conditions
R = OMe/F
NHTs
O
Me
Me
R
Ph
1c (0.5 eq.) : 1d (0.5 eq.)
2a (1 eq.)
3c : 3d = 1:1.02
1.02
1.00
6.10
12.26
f1 (ppm)


8.05
8.03
7.85
7.84
2.43
H
O
NHTs
H
1a
[Ru(p-cymene)Cl2]2 (5 mol %)
KPF6 (30 mol %)
NaOAc (1 eq)
DCE:MeOD (1:1), 70 °C, 3 h
H/D
O
NHTs
H/D
35% D
2.00
1.65
3.07
f1 (ppm)