Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Organic-base Catalyzed Asymmetric 1,4-Addition of Tritylthiol to *in Situ* Generated Aza-*o*-Quinone Methides at H_2O/DCM Interface

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Supporting Information

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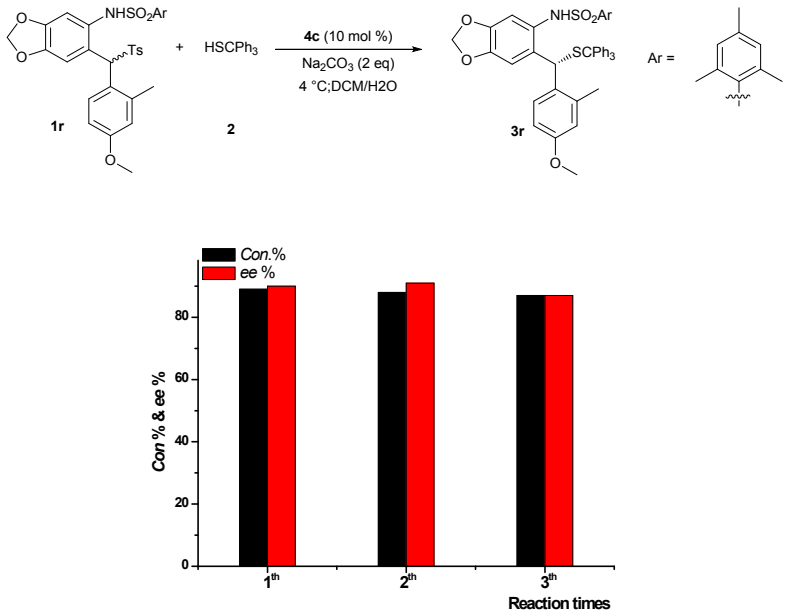
General Information

All reactions were carried out under an atmosphere of nitrogen using standard Schlenk techniques, unless otherwise noted. Commercially available reagents were used without further purification. Solvents were treated prior to use according to the standard methods. All reactions were monitored by TLC analysis. ^{1}H and ^{13}C spectra were recorded on a 400 MHz spectrometer (101 MHz for ^{13}C). Column chromatography was performed on silica gel (300-400 mesh). HPLC analysis was performed on Agilent HPLC 1100 or 1200 equipped with Daicel chiral AD-H column. High resolution mass spectra for all the new compounds were done by an LTQ-Orbitrap instrument (ESI) (Thermo Fisher Scientific, USA). Catalysts **4a**-**4g** were purchased from Daicel Chiral Technologies (China) Co., LTD. Tritylthiol **2** and Benzyl Thiols and Malononitrile were purchased from Energy Chemical Company.

Results and Experimental Procedures

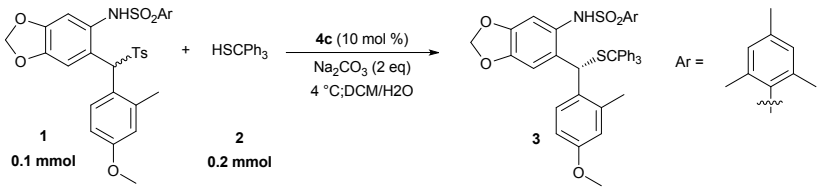
1. Catalyst recovery and recycle experiment



Reaction condition: A solution of substrate **1r** (0.32 mmol), tritylthiol **2** (2 equiv), Na_2CO_3 (2 equiv) and catalyst (10 mol%, 20 mg) in water (11.52 mL) and CH_2Cl_2 (1.28 mL) was stirred (1500r/min) at 4℃ for 12 hours. and purified by flash chromatography on silica gel (Hexanes/EtOAc = 10/1) to afford the corresponding product **3r**. The catalyst was also recovered by flash chromatography on silica gel (EtOAc/MeOH = 3/1).Catalyst recovery: 1^{th}: 90%, 18mg; 2^{th}: 83%, 15mg.

Figure S1. Catalyst recovery experiment.

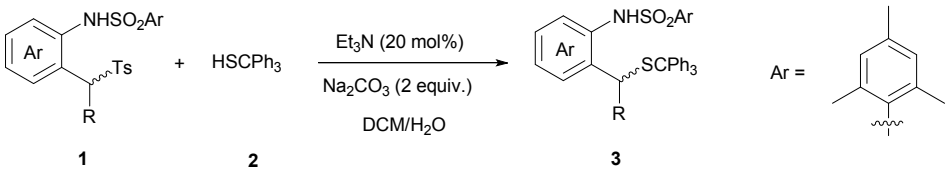
2. Exploration of catalyst loading, stirring rate and concentration of reagents.



Entry	Catalyst Loading	Stirring Rate	DCM/H_2O(mL)	*ee*.%
1	10 mol%	1500r/min	0.2/1.8	90
2	10 mol%	1500r/min	0.4/3.6	90
3	10 mol%	1500r/min	0.8/7.2	89
4	10mol%	750r/min	0.4/3.6	81
5	2mol%	1500r/min	0.4/3.6	79

Table S1. Catalyst loading, stirring rate and concentration of reagents investigation.

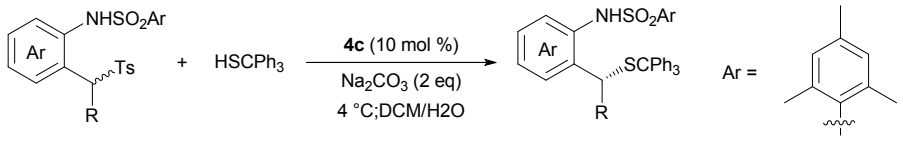
3. General experimental procedure for the racemic conjugate addition adducts 3



1 **2** **3**

At room temperature, a solution of Na_2CO_3 (0.20 mmol), tritylthiol **2** (0.20 mmol), Et_3N (20 mol%) and substrate **1** (0.10 mmol) in water (3.6 mL) and CH_2Cl_2 (400 μL) was stirred at for 12 hours. Then 5 mL saturated NH_4Cl aqueous solution was added, the organic phase was separated and the aqueous layer was extracted with CH_2Cl_2 (3 mL×3). The organic phases were collected and dried by Na_2SO_4. After the solvent was removed under reduced pressure, the residue was subjected to flash chromatography on silica gel (Hexanes/EtOAc = 10/1) to afforded the desired racemic products **3**.

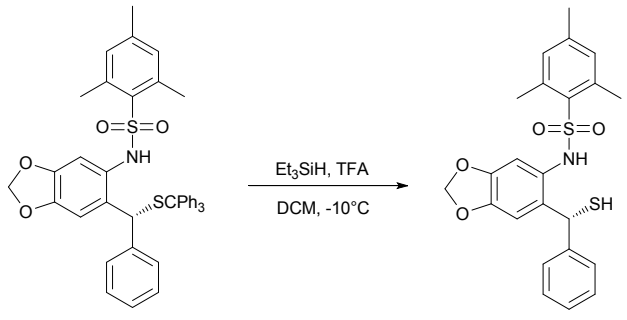
4. General experimental procedure for the asymmetric Michael addition adducts 3



1 **2** **3**

A solution of substrate **1** (0.10 mmol), tritylthiol **2** (0.20 mmol), Na_2CO_3 (0.20 mmol) and catalyst (10 mol%) in water (3.6 mL) and CH_2Cl_2 (400 μL) was stirred(1500r/min) at 4℃ for 8-12 hours. Then 5 mL saturated NH_4Cl aqueous solution was added, the organic phase was separated and the aqueous layer was extracted with CH_2Cl_2. The combined organic phases were dried over Na_2SO_4, then concentrated under the reduced pressure, and purified by flash chromatography on silica gel (Hexanes/EtOAc = 10/1) to afford the corresponding product **3**. Product **3w-3x** were prepared in water (3.6 mL) and $CHCl_3$ (400 μL) and stirred at 50℃ for 72 hours.

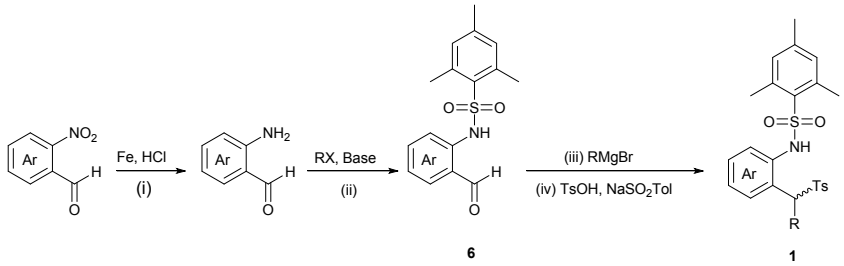
5. Gram-scale reaction



3l **5**

Under Ar atmosphere, to a solution of **3l** (2.10 g, 3.07 mmol) in CH_2Cl_2 (30 mL) was added Et_3SiH (900 uL) and TFA (1.50 mL). The resulting mixture was stirred for 0.5 hour at -10℃ temperature and quenched by saturated $NaHCO_3$. The organic phase was separated and dried over Na_2SO_4. The solvent was removed under reduced pressure, and the residue was purified by flash chromatography on silica gel (hexanes/ethyl acetate = 5/1) to give compound **5** as a white solid in 85% yield and 92% ee.

6. Preparation of substrates 2-(Tosylmethyl)anilines



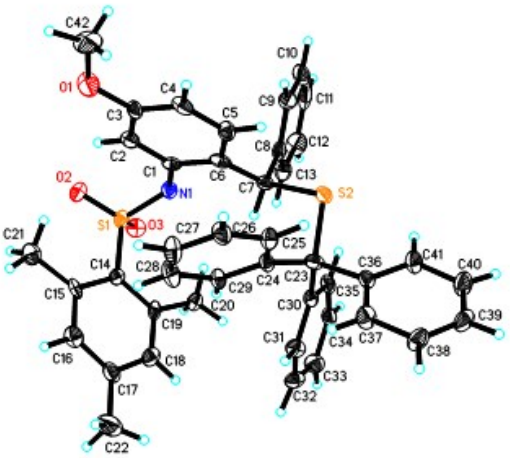
(iii) Under Ar, a solution of Grignard reagent (2.5 equiv.) was slowly added to aldehyde **6**[1] (9.0 mmol) in dry THF (10 mL). After being stirred at room temperature for 3 h, the reaction mixture was quenched by a saturated NH_4Cl (20 mL) and extracted with DCM. The combined extracts were washed with brine, then dried over Na_2SO_4, filtered and concentrated. The resulting crude solid was used without purification.

(iv) $TolSO_2Na$ (1.25 equiv.) and TsOH (1.75 equiv.) were placed in a dried Schlenk tube, and dry DCM (20 mL) was added. The resulting mixture was stirred at room temperature for 5 min. Then, the solution (15 mL) of the crude product diaryl methanols in DCM was added and stirred for 1.5 h. The reaction mixture was quenched and adjusted to pH = 8 by a saturated $NaHCO_3$. After extracted with DCM, the combined extracts were washed with 1 *N* HCl and brine, then dried over Na_2SO_4, filtered and concentrated. The resulting crude solid was purified on silica gel column chromatography (eluent: 3/1 (v/v) ethyl acetate/petroleum ether) to afford the desired product as white or brown solid (67%-84% yield).

References:

[1] (a) N. T. Patil, V. S. Raut, V. S. Shinde, G. Gayatri and G. N. Sastry, *Chem.-Eur. J.*, 2012, **18**, 5530-5535; (b) J. W. Jin, L. Zhang, G. R. Meng, J. H. Zhu and Q. Zhang, *Synthetic Commun*, 2014, **44**, 346-351; (c) V. Machtey, H. E. Gottlieb and G. Byk, *Arkivoc*, 2011, 308-U479; (d) C. Saá, A. Varela-Fernández and J. Varela, *Synthesis*, 2012, **44**, 3285-3295.

X-ray Crystal Structure of 3v



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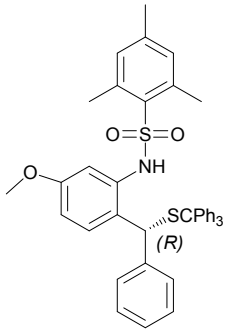


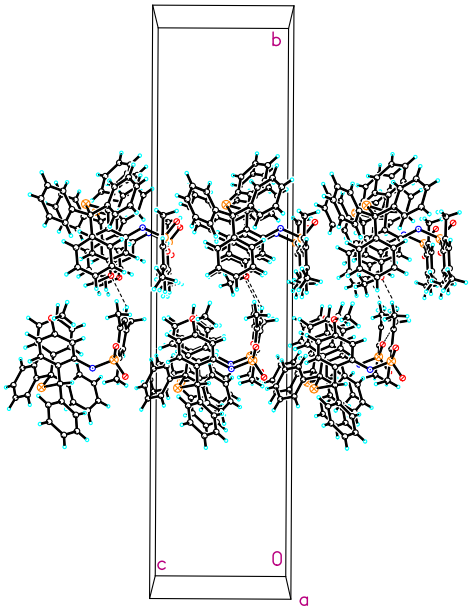


Table 1. Crystal data and structure refinement for mo_d8v18109_0m.

Identification code	mo_d8v18109_0m	
Empirical formula	C42 H38 N O3 S2	
Formula weight	668.85	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 9.4563(7) Å	α= 90°.
	b = 40.805(4) Å	β= 90.090(2)°.
	c = 9.7208(9) Å	γ = 90°.
Volume	3750.9(6) $Å^3$	
Z	4	
Density (calculated)	1.184 Mg/m^3	
Absorption coefficient	0.180 mm^{-1}	
F(000)	1412	
Crystal size	0.200 x 0.170 x 0.130 mm^3	
Theta range for data collection	2.095 to 24.998°.	
Index ranges	-9<=h<=11, -48<=k<=48, -11<=l<=11	
Reflections collected	26698	
Independent reflections	12519 [R(int) = 0.0538]	
Completeness to theta = 25.242°	96.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6584	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12519 / 1 / 874	
Goodness-of-fit on F^2	1.046	
Final R indices [I>2sigma(I)]	R1 = 0.0803, wR2 = 0.2166	
R indices (all data)	R1 = 0.0906, wR2 = 0.2316	
Absolute structure parameter	0.04(4)	
Largest diff. peak and hole	0.519 and -0.471 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mo_d8v18109_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	7230(3)	6112(1)	-795(3)	35(1)
S(2)	9271(3)	6653(1)	4720(3)	36(1)
S(3)	7743(3)	4002(1)	2752(3)	36(1)
S(4)	5584(3)	3495(1)	8201(3)	32(1)
N(1)	7100(11)	6280(2)	771(10)	35(2)
N(2)	7869(11)	3857(2)	4283(11)	37(2)
O(1)	4539(12)	5458(2)	3212(10)	59(3)
O(2)	6106(10)	5882(2)	-995(9)	42(2)
O(3)	7340(9)	6385(2)	-1705(8)	40(2)
O(4)	10145(12)	4717(3)	7038(13)	72(3)
O(5)	7738(10)	3714(2)	1929(9)	44(2)
O(6)	8849(10)	4238(2)	2546(10)	46(2)
C(1)	6741(11)	6117(3)	2019(11)	30(2)
C(2)	5842(14)	5851(3)	2049(13)	38(3)
C(3)	5468(14)	5719(3)	3295(13)	40(3)
C(4)	6006(15)	5842(3)	4494(13)	43(3)
C(5)	6895(13)	6115(3)	4483(12)	37(3)
C(6)	7292(13)	6257(3)	3231(12)	34(3)
C(7)	8165(12)	6566(3)	3207(11)	32(2)
C(8)	7242(13)	6865(3)	2976(13)	37(3)
C(9)	6049(14)	6915(3)	3845(16)	47(3)
C(10)	5239(16)	7197(4)	3634(18)	59(4)
C(11)	5540(20)	7426(4)	2590(20)	78(6)
C(12)	6719(18)	7374(4)	1710(20)	64(4)
C(13)	7527(15)	7091(3)	1923(14)	45(3)
C(14)	8886(12)	5895(3)	-828(10)	31(2)
C(15)	8914(14)	5549(3)	-908(12)	39(3)
C(16)	10237(15)	5404(3)	-945(13)	45(3)
C(17)	11503(15)	5580(3)	-916(13)	48(3)
C(18)	11400(14)	5922(3)	-861(12)	41(3)
C(19)	10132(13)	6084(3)	-794(10)	32(2)
C(20)	10181(14)	6456(3)	-824(15)	44(3)
C(21)	7656(17)	5321(3)	-941(18)	57(4)

C(22)	12902(19)	5406(5)	-888(19)	73(5)
C(23)	10939(13)	6448(3)	4265(12)	36(3)
C(24)	10609(13)	6083(3)	4147(11)	33(2)
C(25)	10265(14)	5906(3)	5311(13)	42(3)
C(26)	9820(15)	5578(3)	5229(14)	46(3)
C(27)	9663(18)	5437(4)	3983(15)	55(4)
C(28)	9984(18)	5600(4)	2796(14)	53(4)
C(29)	10453(13)	5927(3)	2897(12)	34(2)
C(30)	11677(12)	6600(3)	3003(10)	32(2)
C(31)	12820(14)	6440(3)	2397(12)	39(3)
C(32)	13544(13)	6574(4)	1314(12)	43(3)
C(33)	13233(15)	6898(4)	906(14)	50(3)
C(34)	12105(14)	7059(3)	1511(13)	41(3)
C(35)	11339(15)	6913(3)	2550(12)	40(3)
C(36)	12001(12)	6525(3)	5465(11)	33(3)
C(37)	13019(15)	6292(4)	5828(13)	47(3)
C(38)	14094(14)	6379(4)	6820(15)	48(3)
C(39)	14056(15)	6674(5)	7396(12)	57(4)
C(40)	13093(16)	6904(4)	7056(15)	53(4)
C(41)	12000(16)	6829(3)	6086(13)	44(3)
C(42)	3876(19)	5334(4)	4398(18)	69(5)
C(43)	8086(11)	4024(3)	5594(12)	29(2)
C(44)	9030(12)	4298(3)	5640(14)	36(3)
C(45)	9280(13)	4445(3)	6881(15)	45(3)
C(46)	8703(14)	4334(3)	8068(14)	44(3)
C(47)	7864(14)	4053(3)	8028(12)	37(3)
C(48)	7563(12)	3898(2)	6794(12)	30(2)
C(49)	6692(12)	3574(3)	6740(12)	31(2)
C(50)	7653(11)	3282(3)	6527(11)	29(2)
C(51)	7343(14)	3045(3)	5513(13)	40(3)
C(52)	8244(18)	2783(3)	5351(17)	56(4)
C(53)	9392(17)	2736(3)	6183(19)	60(4)
C(54)	9719(17)	2967(4)	7200(19)	63(4)
C(55)	8834(13)	3237(4)	7359(14)	45(3)
C(56)	6092(14)	4201(3)	2569(12)	34(3)
C(57)	5983(16)	4544(4)	2420(13)	48(3)
C(58)	4655(14)	4672(3)	2171(12)	43(3)
C(59)	3422(14)	4494(3)	2124(12)	41(3)

C(60)	3562(13)	4160(3)	2356(12)	38(3)
C(61)	4856(13)	4009(3)	2551(10)	36(3)
C(62)	4826(14)	3638(3)	2737(13)	39(3)
C(63)	7240(17)	4783(3)	2489(17)	56(4)
C(64)	1999(15)	4650(4)	1838(16)	57(4)
C(65)	3887(12)	3698(3)	7681(11)	28(2)
C(66)	4240(12)	4059(3)	7482(10)	30(2)
C(67)	4477(13)	4263(3)	8649(11)	35(3)
C(68)	4924(14)	4576(3)	8471(11)	35(3)
C(69)	5128(13)	4710(3)	7164(14)	40(3)
C(70)	4937(13)	4509(3)	6047(11)	34(3)
C(71)	4476(14)	4196(3)	6195(11)	36(3)
C(72)	3202(11)	3525(3)	6422(10)	28(2)
C(73)	2100(13)	3688(3)	5713(11)	35(3)
C(74)	1360(11)	3523(3)	4667(13)	39(3)
C(75)	1712(15)	3214(4)	4316(13)	46(3)
C(76)	2769(14)	3054(3)	5011(12)	36(3)
C(77)	3524(14)	3211(3)	6055(13)	39(3)
C(78)	2865(13)	3628(3)	8871(10)	30(2)
C(79)	1769(13)	3843(3)	9166(12)	36(3)
C(80)	797(14)	3786(3)	10161(12)	41(3)
C(81)	841(13)	3478(3)	10840(12)	37(3)
C(82)	1850(14)	3262(4)	10551(12)	46(3)
C(83)	2851(12)	3324(3)	9530(11)	33(3)
C(84)	11238(17)	4761(4)	6164(19)	62(4)

Table 3. Bond lengths [Å] and angles [°] for mo_d8v18109_0m.

S(1)-O(3)	1.428(8)
S(1)-O(2)	1.431(9)
S(1)-N(1)	1.674(10)
S(1)-C(14)	1.800(12)
S(2)-C(7)	1.838(11)
S(2)-C(23)	1.838(12)
S(3)-O(5)	1.423(9)
S(3)-O(6)	1.435(9)
S(3)-N(2)	1.607(11)
S(3)-C(56)	1.767(13)
S(4)-C(49)	1.796(12)
S(4)-C(65)	1.873(11)
N(1)-C(1)	1.425(14)
N(2)-C(43)	1.460(15)
O(1)-C(3)	1.382(15)
O(1)-C(42)	1.407(16)
O(4)-C(84)	1.351(19)
O(4)-C(45)	1.389(16)
C(1)-C(2)	1.378(18)
C(1)-C(6)	1.408(17)
C(2)-C(3)	1.373(18)
C(2)-H(2)	0.9500
C(3)-C(4)	1.367(19)
C(4)-C(5)	1.398(19)
C(4)-H(4)	0.9500
C(5)-C(6)	1.400(16)
C(5)-H(5)	0.9500
C(6)-C(7)	1.506(17)
C(7)-C(8)	1.517(16)
C(7)-H(7)	1.0000
C(8)-C(13)	1.405(18)
C(8)-C(9)	1.425(19)
C(9)-C(10)	1.40(2)
C(9)-H(9)	0.9500
C(10)-C(11)	1.41(3)
C(10)-H(10)	0.9500

C(11)-C(12)	1.42(3)
C(11)-H(11)	0.9500
C(12)-C(13)	1.398(19)
C(12)-H(12)	0.9500
C(13)-H(13)	0.9500
C(14)-C(19)	1.409(16)
C(14)-C(15)	1.412(17)
C(15)-C(16)	1.385(19)
C(15)-C(21)	1.510(19)
C(16)-C(17)	1.40(2)
C(16)-H(16)	0.9500
C(17)-C(18)	1.40(2)
C(17)-C(22)	1.50(2)
C(18)-C(19)	1.371(18)
C(18)-H(18)	0.9500
C(19)-C(20)	1.518(17)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-C(24)	1.528(18)
C(23)-C(30)	1.541(16)
C(23)-C(36)	1.569(16)
C(24)-C(29)	1.379(16)
C(24)-C(25)	1.381(18)
C(25)-C(26)	1.407(18)
C(25)-H(25)	0.9500
C(26)-C(27)	1.349(19)
C(26)-H(26)	0.9500
C(27)-C(28)	1.37(2)
C(27)-H(27)	0.9500
C(28)-C(29)	1.408(19)
C(28)-H(28)	0.9500

C(29)-H(29)	0.9500
C(30)-C(35)	1.390(18)
C(30)-C(31)	1.394(17)
C(31)-C(32)	1.371(18)
C(31)-H(31)	0.9500
C(32)-C(33)	1.41(2)
C(32)-H(32)	0.9500
C(33)-C(34)	1.384(19)
C(33)-H(33)	0.9500
C(34)-C(35)	1.379(18)
C(34)-H(34)	0.9500
C(35)-H(35)	0.9500
C(36)-C(41)	1.381(17)
C(36)-C(37)	1.397(17)
C(37)-C(38)	1.445(18)
C(37)-H(37)	0.9500
C(38)-C(39)	1.33(2)
C(38)-H(38)	0.9500
C(39)-C(40)	1.35(2)
C(39)-H(39)	0.9500
C(40)-C(41)	1.430(18)
C(40)-H(40)	0.9500
C(41)-H(41)	0.9500
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(43)-C(48)	1.368(16)
C(43)-C(44)	1.432(16)
C(44)-C(45)	1.366(18)
C(44)-H(44)	0.9500
C(45)-C(46)	1.35(2)
C(46)-C(47)	1.395(19)
C(46)-H(46)	0.9500
C(47)-C(48)	1.384(16)
C(47)-H(47)	0.9500
C(48)-C(49)	1.561(14)
C(49)-C(50)	1.511(15)
C(49)-H(49)	1.0000

C(50)-C(55)	1.390(17)
C(50)-C(51)	1.412(17)
C(51)-C(52)	1.378(19)
C(51)-H(51)	0.9500
C(52)-C(53)	1.37(2)
C(52)-H(52)	0.9500
C(53)-C(54)	1.40(2)
C(53)-H(53)	0.9500
C(54)-C(55)	1.39(2)
C(54)-H(54)	0.9500
C(55)-H(55)	0.9500
C(56)-C(61)	1.407(17)
C(56)-C(57)	1.413(19)
C(57)-C(58)	1.38(2)
C(57)-C(63)	1.538(19)
C(58)-C(59)	1.374(19)
C(58)-H(58)	0.9500
C(59)-C(60)	1.389(19)
C(59)-C(64)	1.513(19)
C(60)-C(61)	1.381(18)
C(60)-H(60)	0.9500
C(61)-C(62)	1.526(18)
C(62)-H(62A)	0.9800
C(62)-H(62B)	0.9800
C(62)-H(62C)	0.9800
C(63)-H(63A)	0.9800
C(63)-H(63B)	0.9800
C(63)-H(63C)	0.9800
C(64)-H(64A)	0.9800
C(64)-H(64B)	0.9800
C(64)-H(64C)	0.9800
C(65)-C(66)	1.522(16)
C(65)-C(78)	1.534(15)
C(65)-C(72)	1.553(14)
C(66)-C(71)	1.389(15)
C(66)-C(67)	1.426(15)
C(67)-C(68)	1.356(17)
C(67)-H(67)	0.9500

C(68)-C(69)	1.396(17)
C(68)-H(68)	0.9500
C(69)-C(70)	1.371(18)
C(69)-H(69)	0.9500
C(70)-C(71)	1.359(17)
C(70)-H(70)	0.9500
C(71)-H(71)	0.9500
C(72)-C(77)	1.366(17)
C(72)-C(73)	1.414(16)
C(73)-C(74)	1.405(17)
C(73)-H(73)	0.9500
C(74)-C(75)	1.35(2)
C(74)-H(74)	0.9500
C(75)-C(76)	1.369(19)
C(75)-H(75)	0.9500
C(76)-C(77)	1.396(18)
C(76)-H(76)	0.9500
C(77)-H(77)	0.9500
C(78)-C(79)	1.388(16)
C(78)-C(83)	1.398(17)
C(79)-C(80)	1.356(17)
C(79)-H(79)	0.9500
C(80)-C(81)	1.419(18)
C(80)-H(80)	0.9500
C(81)-C(82)	1.330(18)
C(81)-H(81)	0.9500
C(82)-C(83)	1.396(16)
C(82)-H(82)	0.9500
C(83)-H(83)	0.9500
C(84)-H(84A)	0.9800
C(84)-H(84B)	0.9800
C(84)-H(84C)	0.9800

O(3)-S(1)-O(2)	118.8(5)
O(3)-S(1)-N(1)	104.4(5)
O(2)-S(1)-N(1)	109.7(5)
O(3)-S(1)-C(14)	108.0(5)
O(2)-S(1)-C(14)	108.7(6)

N(1)-S(1)-C(14)	106.5(5)
C(7)-S(2)-C(23)	102.0(5)
O(5)-S(3)-O(6)	118.5(6)
O(5)-S(3)-N(2)	102.5(5)
O(6)-S(3)-N(2)	108.9(6)
O(5)-S(3)-C(56)	108.7(6)
O(6)-S(3)-C(56)	108.8(5)
N(2)-S(3)-C(56)	109.1(5)
C(49)-S(4)-C(65)	102.1(5)
C(1)-N(1)-S(1)	126.9(8)
C(43)-N(2)-S(3)	130.2(8)
C(3)-O(1)-C(42)	120.9(12)
C(84)-O(4)-C(45)	119.2(11)
C(2)-C(1)-C(6)	121.9(10)
C(2)-C(1)-N(1)	122.2(11)
C(6)-C(1)-N(1)	115.7(10)
C(3)-C(2)-C(1)	119.2(12)
C(3)-C(2)-H(2)	120.4
C(1)-C(2)-H(2)	120.4
C(4)-C(3)-C(2)	120.8(11)
C(4)-C(3)-O(1)	124.6(11)
C(2)-C(3)-O(1)	114.6(11)
C(3)-C(4)-C(5)	120.6(11)
C(3)-C(4)-H(4)	119.7
C(5)-C(4)-H(4)	119.7
C(4)-C(5)-C(6)	119.9(11)
C(4)-C(5)-H(5)	120.0
C(6)-C(5)-H(5)	120.0
C(5)-C(6)-C(1)	117.4(11)
C(5)-C(6)-C(7)	120.4(11)
C(1)-C(6)-C(7)	121.9(10)
C(6)-C(7)-C(8)	111.1(9)
C(6)-C(7)-S(2)	117.4(8)
C(8)-C(7)-S(2)	106.9(8)
C(6)-C(7)-H(7)	107.0
C(8)-C(7)-H(7)	107.0
S(2)-C(7)-H(7)	107.0
C(13)-C(8)-C(9)	119.4(12)

C(13)-C(8)-C(7)	121.7(12)
C(9)-C(8)-C(7)	118.9(11)
C(10)-C(9)-C(8)	117.7(15)
C(10)-C(9)-H(9)	121.1
C(8)-C(9)-H(9)	121.1
C(9)-C(10)-C(11)	122.8(16)
C(9)-C(10)-H(10)	118.6
C(11)-C(10)-H(10)	118.6
C(10)-C(11)-C(12)	119.4(15)
C(10)-C(11)-H(11)	120.3
C(12)-C(11)-H(11)	120.3
C(13)-C(12)-C(11)	117.7(17)
C(13)-C(12)-H(12)	121.2
C(11)-C(12)-H(12)	121.2
C(12)-C(13)-C(8)	123.0(15)
C(12)-C(13)-H(13)	118.5
C(8)-C(13)-H(13)	118.5
C(19)-C(14)-C(15)	122.3(11)
C(19)-C(14)-S(1)	117.1(9)
C(15)-C(14)-S(1)	120.6(9)
C(16)-C(15)-C(14)	116.5(11)
C(16)-C(15)-C(21)	116.6(11)
C(14)-C(15)-C(21)	127.0(11)
C(15)-C(16)-C(17)	123.6(12)
C(15)-C(16)-H(16)	118.2
C(17)-C(16)-H(16)	118.2
C(16)-C(17)-C(18)	117.0(12)
C(16)-C(17)-C(22)	120.9(13)
C(18)-C(17)-C(22)	122.0(14)
C(19)-C(18)-C(17)	122.9(12)
C(19)-C(18)-H(18)	118.6
C(17)-C(18)-H(18)	118.6
C(18)-C(19)-C(14)	117.7(11)
C(18)-C(19)-C(20)	117.0(11)
C(14)-C(19)-C(20)	125.0(11)
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5

C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(15)-C(21)-H(21A)	109.5
C(15)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(15)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(17)-C(22)-H(22A)	109.5
C(17)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(17)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(24)-C(23)-C(30)	115.1(10)
C(24)-C(23)-C(36)	112.3(10)
C(30)-C(23)-C(36)	102.8(9)
C(24)-C(23)-S(2)	106.6(8)
C(30)-C(23)-S(2)	113.5(8)
C(36)-C(23)-S(2)	106.2(8)
C(29)-C(24)-C(25)	117.1(11)
C(29)-C(24)-C(23)	122.5(11)
C(25)-C(24)-C(23)	119.8(10)
C(24)-C(25)-C(26)	121.5(11)
C(24)-C(25)-H(25)	119.3
C(26)-C(25)-H(25)	119.3
C(27)-C(26)-C(25)	119.3(13)
C(27)-C(26)-H(26)	120.4
C(25)-C(26)-H(26)	120.4
C(26)-C(27)-C(28)	121.7(13)
C(26)-C(27)-H(27)	119.2
C(28)-C(27)-H(27)	119.2
C(27)-C(28)-C(29)	118.3(12)
C(27)-C(28)-H(28)	120.8
C(29)-C(28)-H(28)	120.8
C(24)-C(29)-C(28)	122.1(11)
C(24)-C(29)-H(29)	119.0

C(28)-C(29)-H(29)	119.0
C(35)-C(30)-C(31)	118.4(11)
C(35)-C(30)-C(23)	121.1(10)
C(31)-C(30)-C(23)	120.0(11)
C(32)-C(31)-C(30)	121.8(12)
C(32)-C(31)-H(31)	119.1
C(30)-C(31)-H(31)	119.1
C(31)-C(32)-C(33)	119.0(12)
C(31)-C(32)-H(32)	120.5
C(33)-C(32)-H(32)	120.5
C(34)-C(33)-C(32)	119.1(13)
C(34)-C(33)-H(33)	120.5
C(32)-C(33)-H(33)	120.5
C(35)-C(34)-C(33)	120.9(13)
C(35)-C(34)-H(34)	119.6
C(33)-C(34)-H(34)	119.6
C(34)-C(35)-C(30)	120.5(12)
C(34)-C(35)-H(35)	119.7
C(30)-C(35)-H(35)	119.7
C(41)-C(36)-C(37)	120.1(11)
C(41)-C(36)-C(23)	120.2(11)
C(37)-C(36)-C(23)	119.5(10)
C(36)-C(37)-C(38)	119.0(12)
C(36)-C(37)-H(37)	120.5
C(38)-C(37)-H(37)	120.5
C(39)-C(38)-C(37)	119.1(13)
C(39)-C(38)-H(38)	120.5
C(37)-C(38)-H(38)	120.5
C(38)-C(39)-C(40)	123.1(13)
C(38)-C(39)-H(39)	118.5
C(40)-C(39)-H(39)	118.5
C(39)-C(40)-C(41)	120.1(14)
C(39)-C(40)-H(40)	120.0
C(41)-C(40)-H(40)	120.0
C(36)-C(41)-C(40)	118.6(12)
C(36)-C(41)-H(41)	120.7
C(40)-C(41)-H(41)	120.7
O(1)-C(42)-H(42A)	109.5

O(1)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
O(1)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(48)-C(43)-C(44)	119.5(11)
C(48)-C(43)-N(2)	121.2(9)
C(44)-C(43)-N(2)	118.6(10)
C(45)-C(44)-C(43)	118.4(11)
C(45)-C(44)-H(44)	120.8
C(43)-C(44)-H(44)	120.8
C(46)-C(45)-C(44)	122.5(12)
C(46)-C(45)-O(4)	114.3(12)
C(44)-C(45)-O(4)	123.2(13)
C(45)-C(46)-C(47)	118.7(12)
C(45)-C(46)-H(46)	120.7
C(47)-C(46)-H(46)	120.7
C(48)-C(47)-C(46)	121.0(11)
C(48)-C(47)-H(47)	119.5
C(46)-C(47)-H(47)	119.5
C(43)-C(48)-C(47)	119.6(10)
C(43)-C(48)-C(49)	118.7(10)
C(47)-C(48)-C(49)	121.6(10)
C(50)-C(49)-C(48)	110.8(9)
C(50)-C(49)-S(4)	108.7(7)
C(48)-C(49)-S(4)	115.6(8)
C(50)-C(49)-H(49)	107.1
C(48)-C(49)-H(49)	107.1
S(4)-C(49)-H(49)	107.1
C(55)-C(50)-C(51)	118.7(11)
C(55)-C(50)-C(49)	120.6(10)
C(51)-C(50)-C(49)	120.7(10)
C(52)-C(51)-C(50)	119.0(13)
C(52)-C(51)-H(51)	120.5
C(50)-C(51)-H(51)	120.5
C(53)-C(52)-C(51)	122.1(14)
C(53)-C(52)-H(52)	118.9
C(51)-C(52)-H(52)	118.9

C(52)-C(53)-C(54)	119.9(14)
C(52)-C(53)-H(53)	120.1
C(54)-C(53)-H(53)	120.1
C(55)-C(54)-C(53)	118.6(15)
C(55)-C(54)-H(54)	120.7
C(53)-C(54)-H(54)	120.7
C(50)-C(55)-C(54)	121.6(14)
C(50)-C(55)-H(55)	119.2
C(54)-C(55)-H(55)	119.2
C(61)-C(56)-C(57)	119.3(12)
C(61)-C(56)-S(3)	118.7(9)
C(57)-C(56)-S(3)	122.0(10)
C(58)-C(57)-C(56)	117.3(12)
C(58)-C(57)-C(63)	118.1(13)
C(56)-C(57)-C(63)	124.6(13)
C(59)-C(58)-C(57)	125.4(13)
C(59)-C(58)-H(58)	117.3
C(57)-C(58)-H(58)	117.3
C(58)-C(59)-C(60)	115.6(12)
C(58)-C(59)-C(64)	122.6(12)
C(60)-C(59)-C(64)	121.8(12)
C(61)-C(60)-C(59)	122.8(11)
C(61)-C(60)-H(60)	118.6
C(59)-C(60)-H(60)	118.6
C(60)-C(61)-C(56)	119.5(12)
C(60)-C(61)-C(62)	116.1(11)
C(56)-C(61)-C(62)	124.4(11)
C(61)-C(62)-H(62A)	109.5
C(61)-C(62)-H(62B)	109.5
H(62A)-C(62)-H(62B)	109.5
C(61)-C(62)-H(62C)	109.5
H(62A)-C(62)-H(62C)	109.5
H(62B)-C(62)-H(62C)	109.5
C(57)-C(63)-H(63A)	109.5
C(57)-C(63)-H(63B)	109.5
H(63A)-C(63)-H(63B)	109.5
C(57)-C(63)-H(63C)	109.5
H(63A)-C(63)-H(63C)	109.5

H(63B)-C(63)-H(63C)	109.5
C(59)-C(64)-H(64A)	109.5
C(59)-C(64)-H(64B)	109.5
H(64A)-C(64)-H(64B)	109.5
C(59)-C(64)-H(64C)	109.5
H(64A)-C(64)-H(64C)	109.5
H(64B)-C(64)-H(64C)	109.5
C(66)-C(65)-C(78)	114.4(9)
C(66)-C(65)-C(72)	115.5(9)
C(78)-C(65)-C(72)	104.3(8)
C(66)-C(65)-S(4)	105.9(7)
C(78)-C(65)-S(4)	104.8(7)
C(72)-C(65)-S(4)	111.6(7)
C(71)-C(66)-C(67)	117.1(11)
C(71)-C(66)-C(65)	122.7(10)
C(67)-C(66)-C(65)	119.9(9)
C(68)-C(67)-C(66)	119.9(10)
C(68)-C(67)-H(67)	120.1
C(66)-C(67)-H(67)	120.1
C(67)-C(68)-C(69)	121.8(11)
C(67)-C(68)-H(68)	119.1
C(69)-C(68)-H(68)	119.1
C(70)-C(69)-C(68)	118.0(11)
C(70)-C(69)-H(69)	121.0
C(68)-C(69)-H(69)	121.0
C(71)-C(70)-C(69)	121.3(10)
C(71)-C(70)-H(70)	119.4
C(69)-C(70)-H(70)	119.4
C(70)-C(71)-C(66)	121.8(11)
C(70)-C(71)-H(71)	119.1
C(66)-C(71)-H(71)	119.1
C(77)-C(72)-C(73)	118.5(11)
C(77)-C(72)-C(65)	122.6(10)
C(73)-C(72)-C(65)	118.5(10)
C(74)-C(73)-C(72)	119.6(11)
C(74)-C(73)-H(73)	120.2
C(72)-C(73)-H(73)	120.2
C(75)-C(74)-C(73)	120.5(12)

C(75)-C(74)-H(74)	119.7
C(73)-C(74)-H(74)	119.7
C(74)-C(75)-C(76)	120.0(12)
C(74)-C(75)-H(75)	120.0
C(76)-C(75)-H(75)	120.0
C(75)-C(76)-C(77)	120.9(12)
C(75)-C(76)-H(76)	119.6
C(77)-C(76)-H(76)	119.6
C(72)-C(77)-C(76)	120.4(12)
C(72)-C(77)-H(77)	119.8
C(76)-C(77)-H(77)	119.8
C(79)-C(78)-C(83)	117.3(10)
C(79)-C(78)-C(65)	120.7(10)
C(83)-C(78)-C(65)	121.1(10)
C(80)-C(79)-C(78)	123.0(12)
C(80)-C(79)-H(79)	118.5
C(78)-C(79)-H(79)	118.5
C(79)-C(80)-C(81)	117.8(12)
C(79)-C(80)-H(80)	121.1
C(81)-C(80)-H(80)	121.1
C(82)-C(81)-C(80)	120.6(11)
C(82)-C(81)-H(81)	119.7
C(80)-C(81)-H(81)	119.7
C(81)-C(82)-C(83)	121.1(11)
C(81)-C(82)-H(82)	119.5
C(83)-C(82)-H(82)	119.5
C(82)-C(83)-C(78)	119.7(11)
C(82)-C(83)-H(83)	120.1
C(78)-C(83)-H(83)	120.1
O(4)-C(84)-H(84A)	109.5
O(4)-C(84)-H(84B)	109.5
H(84A)-C(84)-H(84B)	109.5
O(4)-C(84)-H(84C)	109.5
H(84A)-C(84)-H(84C)	109.5
H(84B)-C(84)-H(84C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_d8v18109_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	37(2)	40(2)	29(1)	0(1)	-6(1)	-4(1)
S(2)	37(2)	39(2)	30(1)	-7(1)	-1(1)	5(1)
S(3)	34(2)	40(2)	34(1)	0(1)	12(1)	-2(1)
S(4)	32(1)	36(2)	28(1)	6(1)	2(1)	2(1)
N(1)	40(6)	37(6)	29(5)	-4(4)	-1(4)	-4(4)
N(2)	41(6)	28(5)	43(6)	1(4)	-1(5)	-1(4)
O(1)	83(8)	45(5)	47(5)	2(4)	15(5)	-14(5)
O(2)	40(5)	44(5)	43(5)	1(4)	-5(4)	-12(4)
O(3)	45(5)	45(5)	30(4)	13(4)	-6(4)	6(4)
O(4)	58(6)	59(6)	98(9)	-40(6)	22(6)	-34(5)
O(5)	50(5)	43(5)	40(5)	-9(4)	12(4)	8(4)
O(6)	34(5)	57(6)	49(5)	9(4)	15(4)	-6(4)
C(1)	25(5)	31(6)	34(6)	5(5)	6(4)	10(4)
C(2)	41(7)	35(6)	38(6)	-1(5)	10(5)	3(5)
C(3)	50(7)	24(6)	47(7)	-11(5)	16(6)	-9(5)
C(4)	54(8)	40(7)	36(6)	-1(5)	16(5)	7(6)
C(5)	46(7)	30(6)	36(6)	-1(5)	1(5)	-3(5)
C(6)	33(6)	34(6)	35(6)	8(5)	9(5)	17(5)
C(7)	29(6)	42(7)	24(5)	-1(5)	5(4)	1(5)
C(8)	41(6)	21(5)	49(7)	-6(5)	-17(6)	1(5)
C(9)	36(7)	34(7)	70(9)	-11(6)	-4(6)	11(5)
C(10)	49(9)	49(9)	79(10)	-31(8)	-15(7)	22(7)
C(11)	69(11)	45(9)	119(16)	-42(10)	-47(11)	8(8)
C(12)	61(10)	35(8)	97(12)	4(8)	-21(9)	12(7)
C(13)	55(8)	30(6)	51(7)	2(6)	-5(6)	-6(6)
C(14)	31(6)	43(7)	18(5)	-1(4)	-4(4)	-3(5)
C(15)	55(8)	29(6)	34(6)	-16(5)	2(5)	2(5)
C(16)	54(8)	37(7)	43(7)	1(5)	-9(6)	9(6)
C(17)	52(8)	49(8)	41(7)	-19(6)	-7(6)	10(6)
C(18)	39(7)	57(8)	28(6)	2(5)	-7(5)	-6(6)
C(19)	45(7)	35(6)	18(4)	-3(4)	-4(4)	-13(5)
C(20)	41(7)	39(7)	53(7)	-8(6)	2(6)	-13(5)

C(21)	57(9)	36(7)	78(10)	-6(7)	4(8)	1(7)
C(22)	66(11)	78(12)	75(10)	-11(9)	-1(9)	29(9)
C(23)	30(6)	51(7)	28(5)	-1(5)	2(5)	11(5)
C(24)	35(6)	32(6)	31(5)	-9(5)	-10(5)	7(5)
C(25)	44(7)	47(8)	36(6)	-7(5)	-7(5)	-4(6)
C(26)	58(8)	36(7)	43(7)	-3(6)	8(6)	-6(6)
C(27)	77(11)	35(7)	53(8)	-7(6)	-9(7)	-10(7)
C(28)	81(10)	43(8)	37(7)	-9(6)	-15(7)	8(7)
C(29)	45(7)	30(6)	27(5)	-2(4)	-3(5)	-2(5)
C(30)	35(6)	43(7)	19(5)	-5(5)	-4(4)	-2(5)
C(31)	39(7)	47(8)	31(6)	4(5)	-3(5)	8(6)
C(32)	31(6)	70(9)	29(6)	3(6)	-6(5)	5(6)
C(33)	48(8)	63(9)	38(7)	1(6)	4(6)	1(6)
C(34)	48(7)	33(7)	43(7)	-10(5)	1(6)	-6(5)
C(35)	50(7)	42(7)	29(6)	-11(5)	2(5)	-5(6)
C(36)	38(7)	37(6)	24(5)	-5(5)	2(5)	-2(5)
C(37)	53(8)	51(8)	37(6)	-1(6)	-20(6)	12(6)
C(38)	39(7)	49(8)	57(8)	4(7)	-16(6)	1(6)
C(39)	40(8)	106(13)	26(6)	-3(7)	-5(5)	-20(8)
C(40)	54(9)	50(8)	55(8)	-8(7)	-24(7)	5(7)
C(41)	55(8)	38(7)	38(6)	-4(5)	-12(6)	4(6)
C(42)	77(11)	59(9)	72(10)	20(8)	34(9)	-16(8)
C(43)	27(6)	18(5)	42(6)	-3(5)	2(5)	-4(4)
C(44)	32(7)	31(6)	47(7)	4(5)	19(5)	-5(5)
C(45)	28(6)	48(7)	60(8)	-25(6)	-3(6)	0(5)
C(46)	40(7)	49(8)	42(7)	-15(6)	-1(6)	-4(6)
C(47)	40(7)	46(7)	26(5)	-1(5)	-4(5)	4(5)
C(48)	36(6)	19(5)	36(6)	1(4)	3(5)	2(4)
C(49)	32(6)	25(6)	35(5)	2(4)	1(5)	-3(4)
C(50)	22(5)	33(6)	32(6)	-3(4)	10(4)	-1(4)
C(51)	34(6)	42(7)	44(7)	5(5)	7(5)	4(5)
C(52)	71(10)	20(6)	78(10)	-4(6)	22(8)	-3(6)
C(53)	50(9)	28(7)	104(12)	10(7)	8(9)	3(6)
C(54)	54(9)	51(9)	82(11)	24(8)	5(8)	7(7)
C(55)	34(7)	53(8)	47(7)	5(6)	-1(5)	10(6)
C(56)	46(7)	24(5)	31(6)	7(5)	4(5)	1(5)
C(57)	55(9)	54(8)	34(6)	2(6)	11(6)	-17(7)
C(58)	52(8)	47(8)	31(6)	8(5)	-4(5)	-2(6)

C(59)	48(7)	49(8)	27(6)	3(5)	-2(5)	3(6)
C(60)	27(6)	61(8)	27(5)	0(5)	3(4)	-14(5)
C(61)	35(6)	53(7)	19(5)	0(5)	3(4)	-4(6)
C(62)	50(7)	35(6)	34(6)	-7(5)	-3(5)	-14(6)
C(63)	59(9)	32(7)	76(10)	8(6)	-17(8)	-13(6)
C(64)	52(8)	67(10)	53(8)	12(7)	-1(7)	3(7)
C(65)	31(6)	25(6)	28(5)	-7(4)	2(4)	-2(4)
C(66)	25(5)	46(7)	18(5)	-2(4)	2(4)	2(5)
C(67)	44(7)	46(7)	16(5)	-4(5)	2(4)	8(5)
C(68)	49(7)	38(6)	19(5)	-2(4)	1(5)	0(5)
C(69)	38(6)	34(6)	48(7)	7(5)	6(5)	5(5)
C(70)	42(7)	38(7)	23(5)	8(5)	5(5)	-7(5)
C(71)	47(7)	43(7)	17(5)	7(5)	-3(5)	8(6)
C(72)	22(5)	42(6)	21(5)	-3(5)	-2(4)	1(4)
C(73)	32(6)	48(7)	24(5)	3(5)	4(5)	8(5)
C(74)	17(5)	56(8)	44(7)	-3(6)	0(5)	-1(5)
C(75)	54(8)	51(8)	33(6)	1(6)	2(6)	-8(6)
C(76)	47(7)	30(6)	31(6)	-1(5)	6(5)	-6(5)
C(77)	42(7)	32(6)	42(7)	-1(5)	6(5)	1(5)
C(78)	35(6)	39(6)	16(5)	4(4)	7(4)	-3(5)
C(79)	35(6)	41(7)	31(6)	2(5)	1(5)	5(5)
C(80)	44(7)	54(8)	26(6)	-13(5)	2(5)	-3(6)
C(81)	42(7)	35(6)	35(6)	13(5)	10(5)	7(5)
C(82)	51(8)	53(8)	33(6)	21(6)	17(6)	-11(6)
C(83)	33(6)	41(6)	27(5)	3(5)	9(5)	16(5)
C(84)	52(8)	39(8)	95(12)	-6(8)	6(8)	-12(7)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for mo_d8v18109_0m.

	x	y	z	U(eq)
H(2)	5485	5761	1217	46
H(4)	5772	5740	5344	52
H(5)	7231	6205	5324	45
H(7)	8814	6549	2399	38
H(9)	5812	6762	4544	56
H(10)	4455	7237	4221	71
H(11)	4954	7614	2465	93
H(12)	6952	7525	1004	77
H(13)	8304	7050	1329	54
H(16)	10286	5172	-992	53
H(18)	12246	6048	-871	50
H(20A)	11050	6532	-376	67
H(20B)	9359	6544	-335	67
H(20C)	10165	6532	-1781	67
H(21A)	7204	5332	-1848	86
H(21B)	6977	5387	-233	86
H(21C)	7972	5096	-763	86
H(22A)	13623	5552	-501	110
H(22B)	13170	5345	-1826	110
H(22C)	12828	5209	-318	110
H(25)	10330	6009	6186	51
H(26)	9633	5456	6043	55
H(27)	9321	5218	3928	66
H(28)	9891	5496	1926	64
H(29)	10670	6044	2078	41
H(31)	13103	6232	2745	47
H(32)	14245	6450	845	52
H(33)	13789	7004	226	60
H(34)	11857	7273	1207	49
H(35)	10573	7028	2958	48
H(37)	13004	6079	5429	57
H(38)	14818	6228	7057	58

H(39)	14740	6726	8079	69
H(40)	13140	7115	7460	64
H(41)	11289	6986	5875	53
H(42A)	4594	5282	5093	104
H(42B)	3351	5135	4162	104
H(42C)	3222	5498	4764	104
H(44)	9472	4377	4827	44
H(46)	8866	4446	8911	53
H(47)	7493	3966	8860	45
H(49)	6060	3588	5916	37
H(51)	6525	3066	4952	48
H(52)	8060	2629	4637	67
H(53)	9967	2547	6072	73
H(54)	10529	2940	7769	75
H(55)	9042	3393	8053	53
H(58)	4588	4901	2020	52
H(60)	2732	4029	2381	46
H(62A)	3845	3561	2712	59
H(62B)	5252	3581	3625	59
H(62C)	5362	3534	1994	59
H(63A)	7765	4775	1621	83
H(63B)	7866	4721	3249	83
H(63C)	6888	5006	2639	83
H(64A)	1895	4687	847	86
H(64B)	1936	4860	2325	86
H(64C)	1245	4504	2157	86
H(67)	4323	4180	9549	42
H(68)	5104	4708	9258	42
H(69)	5390	4933	7052	48
H(70)	5131	4591	5152	41
H(71)	4310	4067	5396	43
H(73)	1861	3907	5943	42
H(74)	606	3630	4203	47
H(75)	1227	3107	3587	55
H(76)	2990	2834	4778	43
H(77)	4267	3098	6514	46
H(79)	1696	4040	8647	43
H(80)	110	3946	10396	49

H(81)	144	3426	11508	45
H(82)	1889	3061	11047	55
H(83)	3520	3160	9285	40
H(84A)	11144	4610	5385	93
H(84B)	12130	4718	6647	93
H(84C)	11235	4988	5827	93

Table 6. Torsion angles [°] for mo_d8v18109_0m.

O(3)-S(1)-N(1)-C(1)	169.1(10)
O(2)-S(1)-N(1)-C(1)	40.8(11)
C(14)-S(1)-N(1)-C(1)	-76.7(11)
O(5)-S(3)-N(2)-C(43)	172.3(11)
O(6)-S(3)-N(2)-C(43)	46.0(12)
C(56)-S(3)-N(2)-C(43)	-72.6(12)
S(1)-N(1)-C(1)-C(2)	-31.4(16)
S(1)-N(1)-C(1)-C(6)	152.4(9)
C(6)-C(1)-C(2)-C(3)	0.1(18)
N(1)-C(1)-C(2)-C(3)	-175.8(11)
C(1)-C(2)-C(3)-C(4)	-1.7(19)
C(1)-C(2)-C(3)-O(1)	178.6(11)
C(42)-O(1)-C(3)-C(4)	11(2)
C(42)-O(1)-C(3)-C(2)	-169.1(14)
C(2)-C(3)-C(4)-C(5)	3(2)
O(1)-C(3)-C(4)-C(5)	-177.3(12)
C(3)-C(4)-C(5)-C(6)	-2.7(19)
C(4)-C(5)-C(6)-C(1)	1.1(17)
C(4)-C(5)-C(6)-C(7)	175.7(11)
C(2)-C(1)-C(6)-C(5)	0.2(16)
N(1)-C(1)-C(6)-C(5)	176.4(10)
C(2)-C(1)-C(6)-C(7)	-174.3(11)
N(1)-C(1)-C(6)-C(7)	1.9(15)
C(5)-C(6)-C(7)-C(8)	-98.9(12)
C(1)-C(6)-C(7)-C(8)	75.4(13)
C(5)-C(6)-C(7)-S(2)	24.5(14)
C(1)-C(6)-C(7)-S(2)	-161.2(9)
C(23)-S(2)-C(7)-C(6)	90.0(9)
C(23)-S(2)-C(7)-C(8)	-144.6(8)
C(6)-C(7)-C(8)-C(13)	-127.0(12)
S(2)-C(7)-C(8)-C(13)	103.8(11)
C(6)-C(7)-C(8)-C(9)	52.5(13)
S(2)-C(7)-C(8)-C(9)	-76.8(12)
C(13)-C(8)-C(9)-C(10)	-2.3(18)
C(7)-C(8)-C(9)-C(10)	178.3(11)
C(8)-C(9)-C(10)-C(11)	2(2)

C(9)-C(10)-C(11)-C(12)	-1(2)
C(10)-C(11)-C(12)-C(13)	1(2)
C(11)-C(12)-C(13)-C(8)	-2(2)
C(9)-C(8)-C(13)-C(12)	2(2)
C(7)-C(8)-C(13)-C(12)	-178.1(12)
O(3)-S(1)-C(14)-C(19)	43.2(9)
O(2)-S(1)-C(14)-C(19)	173.4(8)
N(1)-S(1)-C(14)-C(19)	-68.5(9)
O(3)-S(1)-C(14)-C(15)	-135.8(9)
O(2)-S(1)-C(14)-C(15)	-5.6(10)
N(1)-S(1)-C(14)-C(15)	112.5(9)
C(19)-C(14)-C(15)-C(16)	0.3(17)
S(1)-C(14)-C(15)-C(16)	179.3(9)
C(19)-C(14)-C(15)-C(21)	179.6(12)
S(1)-C(14)-C(15)-C(21)	-1.5(18)
C(14)-C(15)-C(16)-C(17)	-0.4(19)
C(21)-C(15)-C(16)-C(17)	-179.7(13)
C(15)-C(16)-C(17)-C(18)	-0.7(19)
C(15)-C(16)-C(17)-C(22)	176.9(14)
C(16)-C(17)-C(18)-C(19)	2.0(19)
C(22)-C(17)-C(18)-C(19)	-175.6(13)
C(17)-C(18)-C(19)-C(14)	-2.1(17)
C(17)-C(18)-C(19)-C(20)	-176.6(12)
C(15)-C(14)-C(19)-C(18)	0.9(16)
S(1)-C(14)-C(19)-C(18)	-178.1(8)
C(15)-C(14)-C(19)-C(20)	174.8(11)
S(1)-C(14)-C(19)-C(20)	-4.1(14)
C(7)-S(2)-C(23)-C(24)	-63.1(8)
C(7)-S(2)-C(23)-C(30)	64.7(10)
C(7)-S(2)-C(23)-C(36)	176.9(8)
C(30)-C(23)-C(24)-C(29)	-24.2(16)
C(36)-C(23)-C(24)-C(29)	-141.4(11)
S(2)-C(23)-C(24)-C(29)	102.7(12)
C(30)-C(23)-C(24)-C(25)	164.7(11)
C(36)-C(23)-C(24)-C(25)	47.5(15)
S(2)-C(23)-C(24)-C(25)	-68.5(12)
C(29)-C(24)-C(25)-C(26)	2.1(19)
C(23)-C(24)-C(25)-C(26)	173.7(12)

C(24)-C(25)-C(26)-C(27)	-3(2)
C(25)-C(26)-C(27)-C(28)	3(2)
C(26)-C(27)-C(28)-C(29)	-2(3)
C(25)-C(24)-C(29)-C(28)	-0.8(19)
C(23)-C(24)-C(29)-C(28)	-172.2(13)
C(27)-C(28)-C(29)-C(24)	1(2)
C(24)-C(23)-C(30)-C(35)	141.6(11)
C(36)-C(23)-C(30)-C(35)	-95.9(12)
S(2)-C(23)-C(30)-C(35)	18.4(14)
C(24)-C(23)-C(30)-C(31)	-46.1(14)
C(36)-C(23)-C(30)-C(31)	76.3(13)
S(2)-C(23)-C(30)-C(31)	-169.3(9)
C(35)-C(30)-C(31)-C(32)	-4.5(17)
C(23)-C(30)-C(31)-C(32)	-177.0(11)
C(30)-C(31)-C(32)-C(33)	7.5(19)
C(31)-C(32)-C(33)-C(34)	-6.9(19)
C(32)-C(33)-C(34)-C(35)	3(2)
C(33)-C(34)-C(35)-C(30)	-0.5(19)
C(31)-C(30)-C(35)-C(34)	0.9(17)
C(23)-C(30)-C(35)-C(34)	173.3(11)
C(24)-C(23)-C(36)-C(41)	-154.1(12)
C(30)-C(23)-C(36)-C(41)	81.6(13)
S(2)-C(23)-C(36)-C(41)	-37.9(14)
C(24)-C(23)-C(36)-C(37)	30.8(15)
C(30)-C(23)-C(36)-C(37)	-93.5(13)
S(2)-C(23)-C(36)-C(37)	147.0(10)
C(41)-C(36)-C(37)-C(38)	-2.3(19)
C(23)-C(36)-C(37)-C(38)	172.8(12)
C(36)-C(37)-C(38)-C(39)	2(2)
C(37)-C(38)-C(39)-C(40)	-3(2)
C(38)-C(39)-C(40)-C(41)	3(2)
C(37)-C(36)-C(41)-C(40)	2.7(19)
C(23)-C(36)-C(41)-C(40)	-172.4(12)
C(39)-C(40)-C(41)-C(36)	-3(2)
S(3)-N(2)-C(43)-C(48)	150.4(10)
S(3)-N(2)-C(43)-C(44)	-38.6(16)
C(48)-C(43)-C(44)-C(45)	-5.8(18)
N(2)-C(43)-C(44)-C(45)	-177.0(11)

C(43)-C(44)-C(45)-C(46)	2(2)
C(43)-C(44)-C(45)-O(4)	-178.2(12)
C(84)-O(4)-C(45)-C(46)	150.0(15)
C(84)-O(4)-C(45)-C(44)	-30(2)
C(44)-C(45)-C(46)-C(47)	2(2)
O(4)-C(45)-C(46)-C(47)	-177.4(12)
C(45)-C(46)-C(47)-C(48)	-3(2)
C(44)-C(43)-C(48)-C(47)	5.0(17)
N(2)-C(43)-C(48)-C(47)	176.0(11)
C(44)-C(43)-C(48)-C(49)	-172.3(10)
N(2)-C(43)-C(48)-C(49)	-1.4(16)
C(46)-C(47)-C(48)-C(43)	-0.5(18)
C(46)-C(47)-C(48)-C(49)	176.7(11)
C(43)-C(48)-C(49)-C(50)	75.1(13)
C(47)-C(48)-C(49)-C(50)	-102.2(13)
C(43)-C(48)-C(49)-S(4)	-160.7(9)
C(47)-C(48)-C(49)-S(4)	22.1(14)
C(65)-S(4)-C(49)-C(50)	-144.9(8)
C(65)-S(4)-C(49)-C(48)	89.7(9)
C(48)-C(49)-C(50)-C(55)	50.7(14)
S(4)-C(49)-C(50)-C(55)	-77.4(12)
C(48)-C(49)-C(50)-C(51)	-131.6(11)
S(4)-C(49)-C(50)-C(51)	100.3(11)
C(55)-C(50)-C(51)-C(52)	-2.2(17)
C(49)-C(50)-C(51)-C(52)	-179.9(11)
C(50)-C(51)-C(52)-C(53)	3(2)
C(51)-C(52)-C(53)-C(54)	-3(2)
C(52)-C(53)-C(54)-C(55)	2(2)
C(51)-C(50)-C(55)-C(54)	1.0(19)
C(49)-C(50)-C(55)-C(54)	178.8(12)
C(53)-C(54)-C(55)-C(50)	-1(2)
O(5)-S(3)-C(56)-C(61)	41.5(10)
O(6)-S(3)-C(56)-C(61)	171.8(9)
N(2)-S(3)-C(56)-C(61)	-69.5(10)
O(5)-S(3)-C(56)-C(57)	-137.5(10)
O(6)-S(3)-C(56)-C(57)	-7.2(12)
N(2)-S(3)-C(56)-C(57)	111.5(10)
C(61)-C(56)-C(57)-C(58)	-4.2(17)

S(3)-C(56)-C(57)-C(58)	174.8(9)
C(61)-C(56)-C(57)-C(63)	177.0(12)
S(3)-C(56)-C(57)-C(63)	-3.9(18)
C(56)-C(57)-C(58)-C(59)	3.4(19)
C(63)-C(57)-C(58)-C(59)	-177.8(13)
C(57)-C(58)-C(59)-C(60)	0.3(18)
C(57)-C(58)-C(59)-C(64)	-179.7(13)
C(58)-C(59)-C(60)-C(61)	-3.3(17)
C(64)-C(59)-C(60)-C(61)	176.7(12)
C(59)-C(60)-C(61)-C(56)	2.4(16)
C(59)-C(60)-C(61)-C(62)	-177.7(11)
C(57)-C(56)-C(61)-C(60)	1.5(16)
S(3)-C(56)-C(61)-C(60)	-177.5(8)
C(57)-C(56)-C(61)-C(62)	-178.4(11)
S(3)-C(56)-C(61)-C(62)	2.6(15)
C(49)-S(4)-C(65)-C(66)	-60.8(8)
C(49)-S(4)-C(65)-C(78)	177.9(7)
C(49)-S(4)-C(65)-C(72)	65.6(8)
C(78)-C(65)-C(66)-C(71)	-145.6(11)
C(72)-C(65)-C(66)-C(71)	-24.4(16)
S(4)-C(65)-C(66)-C(71)	99.6(12)
C(78)-C(65)-C(66)-C(67)	40.6(14)
C(72)-C(65)-C(66)-C(67)	161.8(10)
S(4)-C(65)-C(66)-C(67)	-74.2(11)
C(71)-C(66)-C(67)-C(68)	-0.5(18)
C(65)-C(66)-C(67)-C(68)	173.6(11)
C(66)-C(67)-C(68)-C(69)	1.7(19)
C(67)-C(68)-C(69)-C(70)	-3.6(19)
C(68)-C(69)-C(70)-C(71)	4.2(19)
C(69)-C(70)-C(71)-C(66)	-3(2)
C(67)-C(66)-C(71)-C(70)	1.1(18)
C(65)-C(66)-C(71)-C(70)	-172.8(11)
C(66)-C(65)-C(72)-C(77)	141.4(11)
C(78)-C(65)-C(72)-C(77)	-92.1(12)
S(4)-C(65)-C(72)-C(77)	20.5(14)
C(66)-C(65)-C(72)-C(73)	-45.1(14)
C(78)-C(65)-C(72)-C(73)	81.3(12)
S(4)-C(65)-C(72)-C(73)	-166.1(8)

C(77)-C(72)-C(73)-C(74)	0.6(17)
C(65)-C(72)-C(73)-C(74)	-173.2(10)
C(72)-C(73)-C(74)-C(75)	-1.3(18)
C(73)-C(74)-C(75)-C(76)	2.1(19)
C(74)-C(75)-C(76)-C(77)	-2.1(19)
C(73)-C(72)-C(77)-C(76)	-0.5(18)
C(65)-C(72)-C(77)-C(76)	172.9(10)
C(75)-C(76)-C(77)-C(72)	1.3(19)
C(66)-C(65)-C(78)-C(79)	36.3(15)
C(72)-C(65)-C(78)-C(79)	-90.9(12)
S(4)-C(65)-C(78)-C(79)	151.7(9)
C(66)-C(65)-C(78)-C(83)	-155.0(11)
C(72)-C(65)-C(78)-C(83)	77.9(13)
S(4)-C(65)-C(78)-C(83)	-39.5(12)
C(83)-C(78)-C(79)-C(80)	7.6(18)
C(65)-C(78)-C(79)-C(80)	176.7(11)
C(78)-C(79)-C(80)-C(81)	-5.7(19)
C(79)-C(80)-C(81)-C(82)	3.3(19)
C(80)-C(81)-C(82)-C(83)	-3(2)
C(81)-C(82)-C(83)-C(78)	5(2)
C(79)-C(78)-C(83)-C(82)	-6.9(17)
C(65)-C(78)-C(83)-C(82)	-176.0(11)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for mo_d8v18109_0m [Å and °].

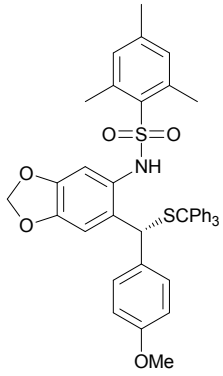
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(44)-H(44)...O(6)	0.95	2.36	3.022(16)	126.2
C(2)-H(2)...O(2)	0.95	2.28	2.973(15)	128.7
C(44)-H(44)...O(6)	0.95	2.36	3.022(16)	126.2
C(2)-H(2)...O(2)	0.95	2.28	2.973(15)	128.7
C(44)-H(44)...O(6)	0.95	2.36	3.022(16)	126.2
C(2)-H(2)...O(2)	0.95	2.28	2.973(15)	128.7
C(2)-H(2)...O(2)	0.95	2.28	2.973(15)	128.7
C(44)-H(44)...O(6)	0.95	2.36	3.022(16)	126.2

Symmetry transformations used to generate equivalent atoms:

CCDC 1816205 contains the structure and supplementary crystallographic data for the structure of **3v**. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif.

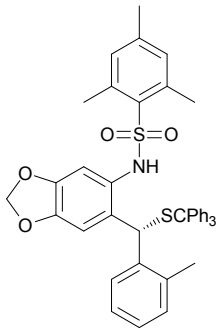
Compound Characterization Data of 3i-3z and 6a-6h

N-(6-((4-methoxyphenyl)(tritylthio)methyl)benzo[d][1,3]dioxol-5-yl)-2,4,6-trimethylbenzenesulfonamide (3i)



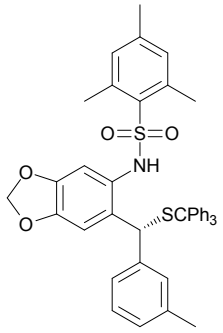
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.36 (m, 6H), 7.24 – 7.14 (m, 9H), 6.96 (d, *J* = 7.7 Hz, 2H), 6.88 (s, 1H), 6.84 (s, 2H), 6.70 (d, *J* = 7.7 Hz, 2H), 6.35 (s, 1H), 5.86 (d, *J* = 10.3 Hz, 2H), 5.72 (s, 1H), 4.97 (s, 1H), 3.77 (s, 3H), 2.37 (s, 6H), 2.28 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.43, 146.31, 145.70, 144.36, 142.32, 138.93, 134.81, 132.90, 132.01, 131.08, 129.72, 129.41, 127.92, 126.83, 126.66, 113.87, 109.79, 105.40, 101.41, 69.48, 55.26, 48.72, 22.99, 20.96.; $[\alpha]_D^{20}$ = -21.00 (c = 0.20, in $CHCl_3$); HRMS Calculated For $C_{43}H_{39}NNaO_5S_2$ $[M+Na]^+$: 736.2162, found: 736.2173.

2,4,6-trimethyl-N-(6-(o-tolyl(tritylthio)methyl)benzo[d][1,3]dioxol-5-yl)benzenesulfonamide (3j)



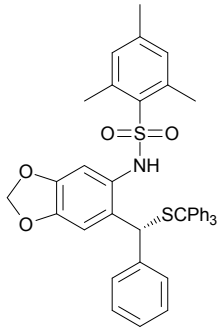
δ 7.48 – 7.39 (m, 6H), 7.38 – 7.27 (m, 2H), 7.27 – 7.15 (m, 8H), 7.08 – 7.02 (m, 1H), 6.99 (t, *J* = 6.8 Hz, 2H), 6.89 (s, 2H), 6.63 (s, 1H), 6.40 (s, 1H), 6.08 (s, 1H), 5.77 (s, 2H), 4.82 (s, 1H), 2.41 (s, 6H), 2.27 (s, 3H), 1.83 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.75, 144.50, 144.39, 142.40, 138.66, 137.42, 136.20, 135.50, 132.15, 130.78, 130.12, 129.68, 128.70, 127.92, 127.25, 126.75, 126.17, 125.77, 110.34, 102.87, 101.31, 68.98, 48.73, 22.70, 20.99, 19.36; $[\alpha]_D^{20}$ = 44.49 (c = 0.24, in $CHCl_3$); HRMS Calculated For $C_{43}H_{39}NNaO_4S_2$, $[M+Na]^+$: 720.2213, found: 720.2218.

2,4,6-trimethyl-N-(6-(m-tolyl(tritylthio)methyl)benzo[d][1,3]dioxol-5-yl)benzenesulfonamide (3k)



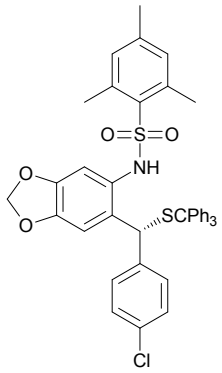
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.38 (m, 6H), 7.36 – 7.28 (m, 2H), 7.27– 7.10 (m, 8H), 7.06 (t, *J* = 7.3 Hz, 1H), 6.98 – 6.92 (m, 2H), 6.86 – 6.81 (m, 3H), 6.34 (s, 1H), 5.92 – 5.77 (m, 3H), 4.96 (s, 1H), 2.38 (s, 6H), 2.28 (s, 3H), 2.25 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.39, 145.56, 144.34, 142.31, 140.67, 138.92, 138.15, 134.87, 132.04, 130.38, 129.75, 128.99, 128.44, 127.93, 127.74, 126.97, 126.83, 125.35, 109.86, 105.12, 101.41, 69.57, 49.38, 22.94, 21.46, 20.99; $[\alpha]_D^{20}$ = -6.76 (c = 0.34, in $CHCl_3$); HRMS Calculated For $C_{43}H_{39}NNaO_4S_2$, $[M+Na]^+$: 720.2213, found: 720.2219.

2,4,6-trimethyl-N-(6-(phenyl(tritylthio)methyl)benzo[d][1,3]dioxol-5-yl)benzenesulfonamide (3l)



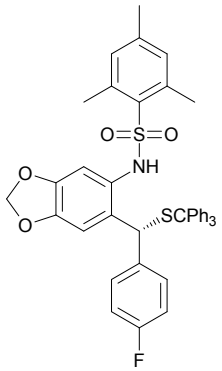
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.34 (m, 6H), 7.23 – 7.08 (m, 12H), 7.06 – 6.96 (m, 2H), 6.88 (s, 1H), 6.82 (s, 2H), 6.29 (s, 1H), 5.85 (d, *J* = 11.3 Hz, 2H), 5.68 (s, 1H), 4.98 (s, 1H), 2.34 (s, 6H), 2.26 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.37, 145.82, 144.31, 142.32, 140.87, 138.92, 134.83, 132.03, 131.13, 129.73, 128.45, 128.30, 127.94, 126.87, 126.81, 126.68, 109.82, 105.54, 101.44, 69.57, 49.23, 22.96, 20.98; $[\alpha]_D^{20}$ = 0.99 (c = 0.30, in $CHCl_3$); HRMS Calculated For $C_{42}H_{37}NNaO_4S_2$, $[M+Na]^+$: 706.2056, found: 706.2065.

N-(6-((4-chlorophenyl)(tritylthio)methyl)benzo[d][1,3]dioxol-5-yl)-2,4,6-trimethylbenzenesulfonamide (3m)



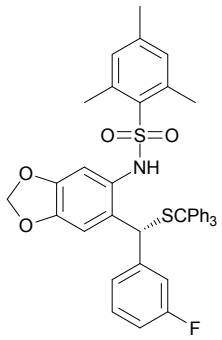
δ 7.46-7.33 (m, 6H), 7.24 – 7.14 (m, 9H), 7.02 (d, *J* = 8.5 Hz, 2H), 6.90 (d, *J* = 8.5 Hz, 2H), 6.83 (s, 2H), 6.78 (s, 1H), 6.25 (s, 1H), 5.88 (dd, *J* = 12.4, 1.3 Hz, 2H), 5.55 (s, 1H), 5.02 (s, 1H), 2.32 (s, 6H), 2.28 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.55, 146.54, 144.27, 142.48, 139.59, 138.93, 134.67, 132.57, 132.38, 131.99, 129.74, 129.69, 128.16, 128.00, 126.99, 126.18, 109.71, 106.78, 101.62, 69.65, 48.28, 23.04, 20.99; $[\alpha]_D^{20}$ = 10.74 (c = 0.46, in $CHCl_3$); HRMS Calculated For $C_{42}H_{36}ClNNaO_4S_2$, $[M+Na]^+$: 740.1666, found: 740.1673.

N-(6-((4-fluorophenyl)(tritylthio)methyl)benzo[d][1,3]dioxol-5-yl)-2,4,6-trimethylbenzenesulfonamide (3n)



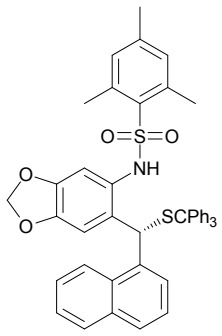
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.36 (m, 6H), 7.24 – 7.15 (m, 9H), 6.96 (dd, *J* = 8.6, 5.4 Hz, 2H), 6.84 (s, 2H), 6.76 (m, 3H), 6.25 (s, 1H), 5.87 (dd, *J* = 11.7, 1.1 Hz, 2H), 5.60 (s, 1H), 5.01 (s, 1H), 2.33 (s, 6H), 2.28 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.49 (d, J_{C-F} = 247.45 Hz), 146.43 (d, J_{C-F} = 8.08 Hz), 144.28, 142.41, 138.92, 136.73 (d, J_{C-F} = 3.03 Hz), 134.74, 132.47, 132.00, 129.98 (d, J_{C-F} = 8.08 Hz), 129.69, 127.97, 126.95, 126.21, 114.89 (d, J_{C-F} = 22.22 Hz), 109.71, 106.48, 101.57, 69.60, 48.25, 29.71, 23.01, 20.95; $[\alpha]_D^{20}$ = 15.50 (c = 0.20, in $CHCl_3$); HRMS Calculated For $C_{42}H_{36}FNNaO_4S_2$, $[M+Na]^+$: 724.1962, found: 724.1976.

N-(6-((3-fluorophenyl)(tritylthio)methyl)benzo[d][1,3]dioxol-5-yl)-2,4,6-trimethylbenzenesulfonamide (3o)



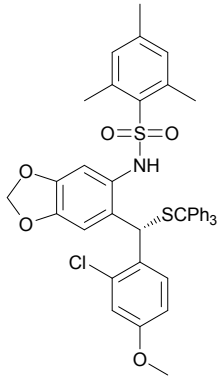
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.37 (m, 6H), 7.25 – 7.15 (m, 9H), 7.05 (dd, *J* = 14.3, 7.2 Hz, 1H), 6.85 (s, 2H), 6.84 – 6.73 (m, 3H), 6.64 (d, *J* = 10.2 Hz, 1H), 6.33 (s, 1H), 5.90 (d, *J* = 12.1 Hz, 2H), 5.62 (s, 1H), 5.05 (s, 1H), 2.35 (s, 6H), 2.29 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ162.46 (d, J_{C-F} = 246.44 Hz), 146.56 (d, J_{C-F} = 7.07 Hz), 144.25, 143.52 (d, J_{C-F} = 7.07 Hz), 142.46, 138.92, 134.61, 132.21, 132.03, 129.68, 129.45 (d, J_{C-F} = 8.08 Hz), 128.01, 127.01, 126.25, 124.10, 124.07, 115.43 (d, J_{C-F} = 22.22 Hz), 113.50 (d, J_{C-F} = 22.21 Hz), 109.72, 106.82, 101.63, 69.61, 48.39, 23.04, 20.96; $[\alpha]_D^{20}$ = 44.55 (c = 0.20, in $CHCl_3$); HRMS Calculated For $C_{42}H_{36}FNNaO_4S_2$, $[M+Na]^+$: 724.1962, found: 724.1968.

2,4,6-trimethyl-N-(6-(naphthalen-1-yl(tritylthio)methyl)benzo[d][1,3]dioxol-5-yl)benzenesulfonamide (3p)



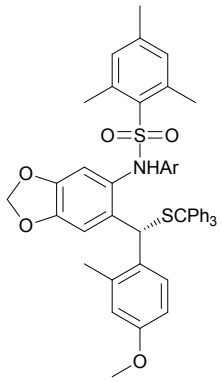
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 7.9 Hz, 1H), 7.67 – 7.57 (m, 2H), 7.53 (d, *J* = 7.1 Hz, 1H), 7.48 – 7.38 (m, 7H), 7.38 – 7.31 (m, 1H), 7.24 – 7.19(m, 1H), 7.19 – 7.06 (m, 9H), 6.81 (s, 2H), 6.76 (s, 1H), 6.41 (s, 1H), 6.14 (s, 1H), 5.75 (d, *J* = 11.7 Hz, 2H), 5.53 (s, 1H), 2.34 (s, 6H), 2.24 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.73, 144.76, 144.22, 142.35, 138.76, 135.19, 135.12, 133.89, 132.06, 130.38, 129.66, 128.53, 128.50, 128.35, 128.09, 127.94, 127.07, 126.74, 126.43, 125.83, 124.96, 124.02, 110.19, 103.62, 101.32, 69.19, 47.51, 22.70, 20.98; $[\alpha]_D^{20}$ = 0.5 (c = 0.20, in $CHCl_3$); HRMS Calculated For $C_{46}H_{39}NNaO_4S_2$, $[M+Na]^+$: 756.2213, found: 756.2222.

N-(6-((2-chloro-4-methoxyphenyl)(tritylthio)methyl)benzo[d][1,3]dioxol-5-yl)-2,4,6-trimethylbenzenesulfonamide (3q)



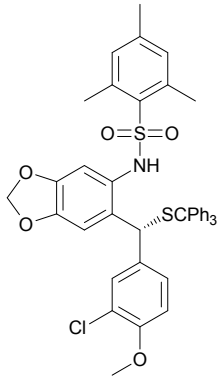
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.38 (m, 6H), 7.33 (d, *J* = 8.7 Hz, 1H), 7.22 – 7.10 (m, 9H), 6.88 (s, 2H), 6.74 (s, 2H), 6.62 (dd, *J* = 8.7, 2.5 Hz, 1H), 6.49 (s, 1H), 6.28 (s, 1H), 5.79 (d, *J* = 6.3 Hz, 2H), 5.13 (s, 1H), 3.74 (s, 3H), 2.44 (s, 6H), 2.27 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.01, 146.70, 144.25, 143.97, 142.39, 138.88, 135.38, 132.97, 132.11, 131.93, 129.71, 129.65, 128.47, 127.93, 126.78, 125.22, 114.83, 113.05, 109.91, 102.25, 101.32, 69.27, 55.55, 46.50, 22.83, 20.96; $[\alpha]_D^{20}$ = -8.50 (c = 0.20, in $CHCl_3$); HRMS Calculated For $C_{43}H_{38}ClNNaO_5S_2$, $[M+Na]^+$: 770.1772, found: 770.1781.

N-(6-((4-methoxy-2-methylphenyl)(tritylthio)methyl)benzo[d][1,3]dioxol-5-yl)-2,4,6-trimethylbenzenesulfonamide (3r)



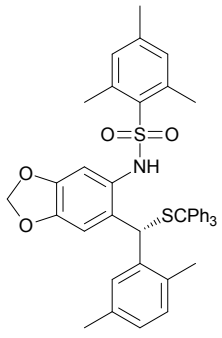
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.40 (m, 6H), 7.30 – 7.27 (m, 1H), 7.24 – 7.13 (m, 9H), 6.89 (s, 2H), 6.65 (s, 1H), 6.54 (m, 2H), 6.38 (s, 1H), 6.08 (s, 1H), 5.77 (q, *J* = 1.4 Hz, 2H), 4.76 (s, 1H), 3.73 (s, 3H), 2.41 (s, 6H), 2.27 (s, 3H), 1.82 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.55, 146.64, 144.45, 144.41, 142.39, 138.66, 137.65, 135.45, 132.13, 131.28, 129.68, 128.54, 127.95, 127.89, 126.72, 126.50, 116.28, 110.85, 110.31, 102.83, 101.27, 68.90, 55.17, 48.21, 22.70, 20.97, 19.61; $[\alpha]_D^{20}$ = -0.72 (c = 0.28, in $CHCl_3$); HRMS Calculated For $C_{44}H_{41}NNaO_5S_2$, $[M+Na]^+$: 750.2318, found: 750.2321.

N-(6-((3-chloro-4-methoxyphenyl)(tritylthio)methyl)benzo[d][1,3]dioxol-5-yl)-2,4,6-trimethylbenzenesulfonamide (3s)



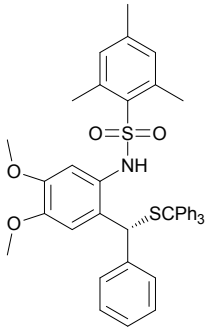
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.36 (m, 6H), 7.23 – 7.13 (m, 9H), 6.95 (d, *J* = 2.3 Hz, 1H), 6.88 – 6.81 (m, 3H), 6.79 (s, 1H), 6.63 (d, *J* = 8.6 Hz, 1H), 6.27 (s, 1H), 5.87 (dd, *J* = 9.8, 1.3 Hz, 2H), 5.61 (s, 1H), 4.97 (s, 1H), 3.82 (s, 3H), 2.34 (s, 6H), 2.26 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.65, 146.56, 146.43, 144.30, 142.41, 138.89, 134.61, 134.06, 132.18, 132.01, 130.17, 129.69, 127.99, 127.80, 126.96, 126.30, 121.99, 111.49, 109.79, 106.61, 101.61, 69.58, 56.14, 48.03, 23.04, 20.99; $[\alpha]_D^{20}$ = 8.38 (c = 0.36, in $CHCl_3$); HRMS Calculated For $C_{43}H_{38}ClNNaO_5S_2$, $[M+Na]^+$: 770.1772, found: 770.1775.

N-(6-((2,5-dimethylphenyl)(tritylthio)methyl)benzo[d][1,3]dioxol-5-yl)-2,4,6-trimethylbenzenesulfonamide (3t)



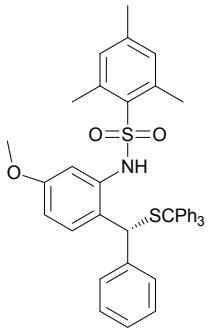
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 – 7.39 (m, 6H), 7.25 – 7.14 (m, 10H), 6.90 (s, 2H), 6.86 (s, 2H), 6.57 (d, *J* = 5.4 Hz, 2H), 6.10 (s, 1H), 5.77 (d, *J* = 1.2 Hz, 2H), 4.70 (s, 1H), 2.44 (s, 6H), 2.28 (s, 3H), 2.13 (s, 3H), 1.73 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.79, 144.43, 144.31, 142.39, 138.67, 136.88, 135.51, 135.20, 133.03, 132.15, 130.95, 130.66, 129.63, 128.95, 127.92, 126.70, 125.45, 110.31, 102.48, 101.27, 68.86, 49.11, 22.69, 20.98, 20.88, 18.81; $[\alpha]_D^{20}$ = 38.65 (c = 0.33, in $CHCl_3$); HRMS Calculated For $C_{44}H_{41}NNaO_4S_2$, $[M+Na]^+$: 734.2369, found: 734.2374.

N-(4,5-dimethoxy-2-(phenyl(tritylthio)methyl)phenyl)-2,4,6-trimethylbenzenesulfonamide (3u)



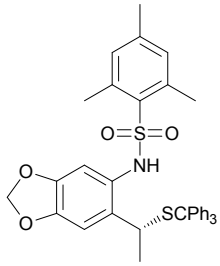
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.33 (m, 6H), 7.23 – 7.09 (m, 12H), 7.05 – 6.98 (m, 2H), 6.92 (s, 1H), 6.81 (s, 2H), 6.31 (s, 1H), 5.72 (s, 1H), 5.01 (s, 1H), 3.72 (s, 3H), 3.55 (s, 3H), 2.34 (s, 6H), 2.24 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.54, 146.87, 144.32, 142.30, 141.08, 139.14, 134.79, 131.92, 129.76, 129.01, 128.51, 128.26, 127.92, 126.90, 126.81, 125.81, 112.75, 108.17, 69.60, 55.82, 55.63, 49.24, 22.98, 20.92; $[\alpha]_D^{20}$ = 4.50 (c = 0.20, in $CHCl_3$); HRMS Calculated For $C_{43}H_{41}NNaO_4S_2$, $[M+Na]^+$: 722.2369, found: 722.2373.

N-(5-methoxy-2-(phenyl(tritylthio)methyl)phenyl)-2,4,6-trimethylbenzenesulfonamide (3v)



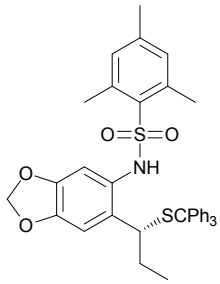
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (m, 6H), 7.21 – 7.10 (m, 13H), 7.05 – 6.98 (m, 2H), 6.83 (s, 2H), 6.47 – 6.40 (m, 2H), 6.36 (d, *J* = 2.5 Hz, 1H), 4.70 (s, 1H), 3.56 (s, 3H), 2.36 (s, 6H), 2.24 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.80, 144.24, 142.41, 140.57, 139.01, 135.03, 134.86, 132.04, 131.19, 129.75, 128.54, 128.51, 127.93, 126.98, 126.86, 125.04, 110.64, 106.57, 69.81, 55.13, 49.84, 22.76, 20.94; $[\alpha]_D^{20}$ = 2.08 (c = 0.24, in $CHCl_3$); HRMS Calculated For $C_{42}H_{39}NNaO_3S_2$, $[M+Na]^+$: 692.2264, found: 692.2269.

2,4,6-trimethyl-N-(6-(1-(tritylthio)ethyl)benzo[d][1,3]dioxol-5-yl)benzenesulfonamide (3w)



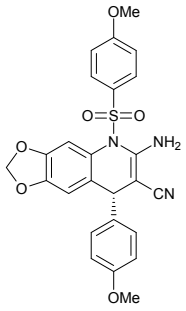
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.20 (m, 16H), 6.89 (s, 2H), 6.77 (s, 1H), 6.10 (s, 1H), 5.88 (dd, *J* = 5.8, 1.3 Hz, 2H), 3.81 (q, *J* = 7.1 Hz, 1H), 2.33 (s, 6H), 2.28 (s, 3H), 1.09 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, CDCl3) δ 147.10, 146.07, 144.74, 142.34, 139.08, 134.49, 134.46, 131.93, 130.17, 129.72, 128.07, 127.93, 126.92, 107.98, 107.39, 101.50, 68.35, 23.89, 23.11, 20.98; $[\alpha]_D^{20}$ = 31.50 (c = 0.20, in $CHCl_3$); HRMS Calculated For $C_{37}H_{35}NNaO_4S_2$, $[M+Na]^+$: 644.1900, found: 644.1904.

2,4,6-trimethyl-N-(6-(1-(tritylthio)propyl)benzo[d][1,3]dioxol-5-yl)benzenesulfonamide (3x)



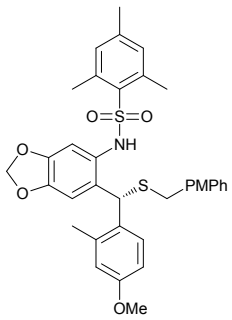
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 –7.35 (m, 6H), 7.26 – 7.16 (m, 10H), 6.89 (s, 2H), 6.06 (s, 1H), 5.90 – 5.84 (m, 2H), 3.57 (s, 1H), 2.49 (s, 1H), 2.39 (s, 6H), 2.28 (s, 3H), 1.65 – 1.40 (m, 2H), 0.56 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.19, 144.81, 143.79, 142.32, 138.97, 132.13, 132.02, 130.19, 129.70, 128.08, 127.95, 127.89, 127.28, 127.25, 126.82, 101.45, 68.37, 23.11, 23.04, 20.97, 11.80; $[\alpha]_D^{20}$ = 42.50 (c = 0.20, in $CHCl_3$); HRMS Calculated For $C_{38}H_{37}NNaO_4S_2$, $[M+Na]^+$: 658.2056, found: 658.2062.

6-amino-8-(4-methoxyphenyl)-5-((4-methoxyphenyl)sulfonyl)-5,8-dihydro-[1,3]dioxolo[4,5-g]quinoline-7-carbonitrile(6a)



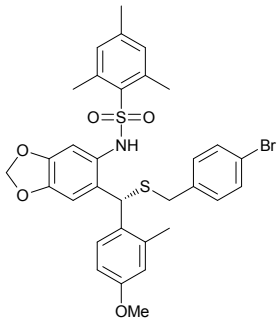
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, *J* = 8.7 Hz, 2H), 7.19 (s, 1H), 6.85 (d, *J* = 8.7 Hz, 2H), 6.81 – 6.68 (m, 4H), 6.05 – 5.93 (m, 3H), 5.31 (d, *J* = 19.2 Hz, 2H), 3.90 (s, 3H), 3.78 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.42, 158.86, 152.34, 146.95, 146.56, 132.62, 130.41, 130.08, 129.77, 128.05, 127.17, 118.74, 114.42, 114.10, 108.03, 107.15, 101.89, 55.81, 55.18, 41.24. $[\alpha]_D^{20}$ = -91.13 (c = 0.44, in $CHCl_3$). HRMS Calculated For $C_{25}H_{22}N_3O_6S_2$, $[M+H]^+$: 492.1224, found: 492.1239.

N-(6-((4-methoxy-2-methylphenyl)((4methoxybenzyl)thio)methyl)benzo[d][1,3]dioxol-5-yl)-2,4,6-trimethylbenzenesulfonamide (6b)



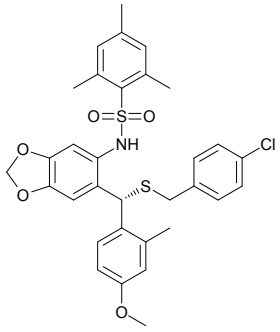
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.13 – 7.03 (m, 3H), 6.98-6.92 (m, 3H), 6.89-6.80 (m, 3H), 6.76 (d, *J* = 8.4 Hz, 1H), 6.56 (d, *J* = 2.1 Hz, 2H), 5.86 (s, 2H), 4.92 (s, 1H), 3.81 (s, 3H), 3.79 (s, 3H), 3.46 (dd, *J* = 31.0, 12.7 Hz, 2H), 2.51 (s, 6H), 2.30 (s, 3H), 2.18 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.86, 157.18, 146.78, 146.01, 142.48, 139.16, 134.93, 132.12, 131.23, 129.90, 129.76, 129.47, 129.15, 127.88, 127.34, 126.97, 114.18, 109.93, 109.01, 107.24, 101.54, 55.39, 55.33, 49.00, 36.63, 23.26, 21.01, 16.37; $[\alpha]_D^{20}$ = -29.95 (c =0.77, in $CHCl_3$); HRMS Calculated For $C_{33}H_{35}NNaO_6S_2$, $[M+Na]^+$: 628.1798, found:628.1790.

N-(6-(((4-bromobenzyl)thio)(4-methoxy-2-methylphenyl)methyl)benzo[d][1,3]dioxol-5-yl)-2,4,6-trimethylbenzenesulfonamide (6c)



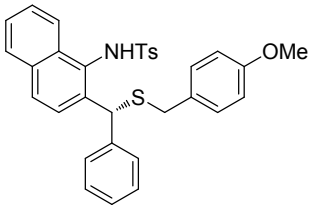
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 8.5 Hz, 1H), 7.41 (d, *J* = 8.1 Hz, 2H), 7.03 (d, *J* = 8.1 Hz, 2H), 6.95 (s, 2H), 6.83 (s, 1H), 6.76 (d, *J* = 8.6 Hz, 1H), 6.72 (s, 1H), 6.58 (s, 1H), 6.26 (s, 1H), 5.85 (s, 2H), 5.28 (s, 1H), 3.80 (s, 3H), 3.58 (s, 2H), 2.53 (s, 6H), 2.30 (s, 3H), 1.99 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.89, 146.97, 145.75, 142.62, 139.11, 138.61, 136.42, 132.15, 131.85, 130.52, 130.15, 128.71, 128.21, 127.97, 121.18, 116.55, 111.48, 109.14, 105.89, 101.55, 55.24, 46.08, 36.71, 23.00, 21.01, 19.29; $[\alpha]_D^{20}$ = -48.72 (c = 0.94, in $CHCl_3$); HRMS Calculated For $C_{32}H_{32}BrNNaO_5S_2$, $[M+Na]^+$: 676.0797, found: 676.0793.

N-(6-(((4-chlorobenzyl)thio)(4-methoxy-2-methylphenyl)methyl)benzo[d][1,3]dioxol-5-yl)-2,4,6-trimethylbenzenesulfonamide (6d)



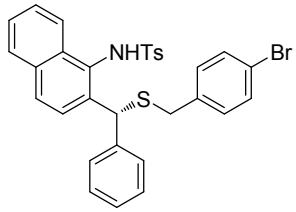
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, *J* = 8.5 Hz, 1H), 7.27 (s, 1H), 7.09 (d, *J* = 8.1 Hz, 2H), 6.95 (s, 2H), 6.84 (s, 1H), 6.77 (d, *J* = 8.5 Hz, 1H), 6.72 (s, 1H), 6.57 (s, 1H), 6.25 (s, 1H), 5.85 (s, 2H), 5.27 (s, 1H), 3.81 (s, 3H), 3.59 (s, 2H), 2.54 (s, 6H), 2.31 (s, 3H), 1.98 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.89, 146.96, 145.72, 142.61, 139.10, 138.63, 135.86, 134.89, 133.09, 132.14, 130.15, 128.92, 128.73, 128.16, 127.96, 116.54, 111.48, 109.12, 105.84, 101.53, 55.24, 46.00, 36.61, 22.98, 20.99, 19.28; $[\alpha]_D^{20}$ = -53.02 (c = 0.89, in $CHCl_3$); HRMS Calculated For $C_{32}H_{32}ClNNaO_5S_2$, $[M+Na]^+$: 632.1303, found: 632.1287.

N-(2-(((4-methoxybenzyl)thio)(phenyl)methyl)naphthalen-1-yl)-4-methylbenzenesulfonamide (6e)



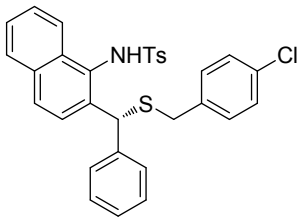
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, *J* = 8.1 Hz, 1H), 7.73 (d, *J* = 7.5 Hz, 1H), 7.65 (d, *J* = 8.7 Hz, 1H), 7.47 – 7.38 (m, 2H), 7.33 – 7.26 (m, 3H), 7.23–7.14 (m, 3H), 7.13 – 7.05 (m, 4H), 7.01 (d, *J* = 6.7 Hz, 2H), 6.93 (d, *J* = 8.5 Hz, 2H), 6.83 (s, 1H), 4.98 (s, 1H), 3.85 (s, 3H), 3.45 (dd, *J* = 34.6, 13.4 Hz, 2H), 2.39 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.06, 143.67, 138.20, 136.87, 135.78, 133.79, 132.08, 129.93, 129.54, 129.45, 129.39, 128.59, 128.44, 127.55, 127.52, 127.43, 126.50, 126.38, 125.88, 125.49, 114.40, 55.50, 48.80, 36.22, 21.53; $[\alpha]_D^{20}$ = 8.00 (c = 0.20, in $CHCl_3$); HRMS Calculated For $C_{32}H_{29}NNaO_2S_2$, $[M+Na]^+$: 562.1481, found: 562.1482.

(R)-N-(2-(((4-bromobenzyl)thio)(phenyl)methyl)naphthalen-1-yl)-4-methylbenzenesulfonamide (6f)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.4 Hz, 1H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.66 (d, *J* = 8.7 Hz, 1H), 7.51 – 7.19 (m, 10H), 7.16 – 6.97 (m, 6H), 6.82 (s, 1H), 5.12 (s, 1H), 3.47 (dd, *J* = 37.8, 13.4 Hz, 2H), 2.40 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.80, 138.03, 136.87, 136.62, 135.84, 133.80, 131.96, 131.93, 130.60, 129.60, 129.52, 129.36, 128.71, 128.58, 127.67, 127.63, 127.36, 126.55, 126.47, 125.80, 125.16, 121.25, 49.27, 36.32, 21.55; $[\alpha]_D^{20}$ = 15.55 (c = 0.81, in $CHCl_3$); HRMS Calculated For $C_{31}H_{30}BrN_2O_2S_2$, $[M+NH_4]^+$: 605.0927, found: 605.0898.

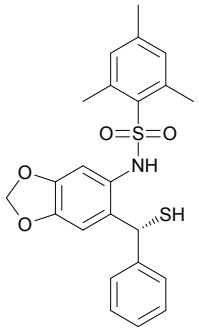
(R)-N-(2-(((4-chlorobenzyl)thio)(phenyl)methyl)naphthalen-1-yl)-4-methylbenzenesulfonamide (6g)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.4 Hz, 1H), 7.73 (d, *J* = 8.1 Hz, 1H), 7.66 (d, *J* = 8.7 Hz, 1H), 7.42 (t, *J* = 7.4 Hz, 1H), 7.39 – 7.19 (m, 11H), 7.15 – 7.03 (m, 6H), 6.82 (s, 1H), 5.13 (s, 1H), 3.49 (dd, *J* = 37.7, 13.4 Hz, 2H), 2.40 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.80, 138.09, 136.89, 136.10, 135.90, 133.80, 133.16, 131.96, 130.24, 129.59, 129.51, 129.36, 128.97, 128.71, 128.59, 127.66, 127.63, 127.36, 126.54, 126.46, 125.81, 125.14, 49.28, 36.27, 21.55.; $[\alpha]_D^{20}$ = 19.67 (c = 0.67, in $CHCl_3$); HRMS Calculated For $C_{31}H_{26}ClNNaO_2S_2$, $[M+Na]^+$: 566.0986, found: 566.0996.

Compound Characterization Data of 5

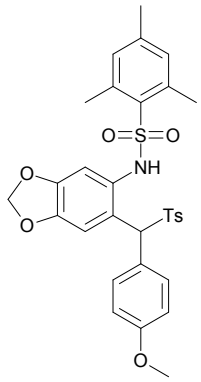
(R)-N-(6-(mercapto(phenyl)methyl)benzo[d][1,3]dioxol-5-yl)-2,4,6-trimethylbenzenesulfonamide (5)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.21 (m, 3H), 7.18 – 7.11 (m, 2H), 6.97 (s, 2H), 6.76 (s, 1H), 6.57 (s, 1H), 6.53 (s, 1H), 5.89 (dd, *J* = 3.2, 1.2 Hz, 2H), 5.30 (d, *J* = 6.0 Hz, 1H), 2.53 (s, 6H), 2.32 (s, 3H), 2.15 (d, *J* = 6.0 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.87, 146.79, 142.79, 141.21, 139.36, 134.33, 134.00, 132.21, 128.58, 128.19, 127.52, 126.57, 108.93, 108.33, 101.72, 42.70, 23.32, 20.96; $[\alpha]_D^{20}$ = 44.59 (c = 0.44, in $CHCl_3$); HRMS Calculated For $C_{23}H_{23}NNaO_4S_2$, $[M+Na]^+$: 464.0961, found: 464.0958.

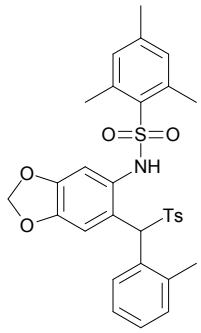
Compound Characterization Data of 1i-1z

N-(6-((4-methoxyphenyl)(tosyl)methyl)benzo[d][1,3]dioxol-5-yl)-2,4,6-trimethylbenzenesulfonamide (1i)



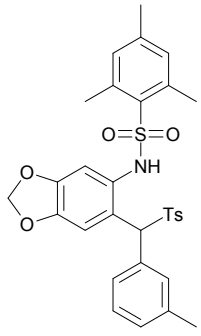
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.2 Hz, 2H), 7.38 – 7.31 (m, 3H), 7.20 (d, *J* = 8.2 Hz, 2H), 7.05 (s, 1H), 6.97 (s, 2H), 6.77 (d, *J* = 8.7 Hz, 2H), 6.30 (s, 1H), 5.95 (s, 1H), 5.92 (d, *J* = 6.2 Hz, 2H), 3.76 (s, 3H), 2.54 (s, 6H), 2.37 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.67, 147.97, 147.21, 144.71, 142.65, 139.31, 135.05, 134.57, 132.11, 131.25, 129.55, 129.50, 128.89, 124.59, 124.20, 114.08, 110.37, 109.29, 101.95, 69.25, 55.22, 23.09, 21.62, 20.99; HRMS Calculated For $C_{31}H_{35}N_2O_7S_2$, $[M+NH_4]^+$: 611.1880, found: 611.1889.

2,4,6-trimethyl-N-(6-(o-tolyl(tosyl)methyl)benzo[d][1,3]dioxol-5-yl)benzenesulfonamide (1j)



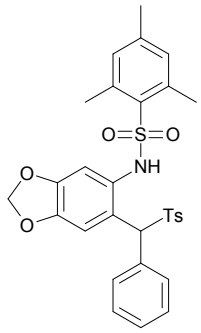
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 7.8 Hz, 1H), 7.99 (s, 1H), 7.69 (d, *J* = 8.2 Hz, 2H), 7.28 – 7.11 (m, 5H), 7.01 (m, 3H), 6.39 (s, 1H), 6.15 (s, 1H), 5.88 (d, *J* = 5.1 Hz, 2H), 2.64 (s, 6H), 2.35 (s, 3H), 2.34 (s, 3H), 2.11 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.21, 146.55, 144.84, 142.58, 138.66, 138.04, 135.76, 135.26, 132.24, 131.08, 131.05, 130.72, 129.59, 129.50, 128.73, 128.65, 125.93, 121.41, 110.77, 106.65, 101.92, 65.92, 22.89, 21.65, 21.03, 19.82; HRMS Calculated For $C_{31}H_{35}N_2O_6S_2$, $[M+NH_4]^+$: 595.1931, found: 595.1934.

2,4,6-trimethyl-N-(6-(m-tolyl(tosyl)methyl)benzo[d][1,3]dioxol-5-yl)benzenesulfonamide (1k)



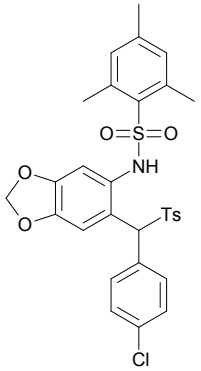
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.1 Hz, 2H), 7.38 (s, 1H), 7.25 – 7.17 (m, 3H), 7.13 (t, *J* = m, 2H), 7.05 (m, 2H), 6.98 (s, 2H), 6.37 (s, 1H), 5.92 (m, 3H), 2.55 (s, 6H), 2.37 (s, 3H), 2.33 (s, 3H), 2.26 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.05, 147.15, 144.78, 142.61, 139.27, 138.46, 135.03, 134.75, 132.57, 132.13, 130.56, 129.50, 128.98, 128.51, 126.92 , 123.75 , 110.50, 109.28 (s), 101.96 (s), 69.91 (s), 23.12, 21.62, 21.41, 21.03; HRMS Calculated For $C_{31}H_{35}N_2O_6S_2$, $[M+NH_4]^+$: 595.1931, found: 595.1952.

2,4,6-trimethyl-N-(6-(phenyl(tosyl)methyl)benzo[d][1,3]dioxol-5-yl)benzenesulfonamide (1l)



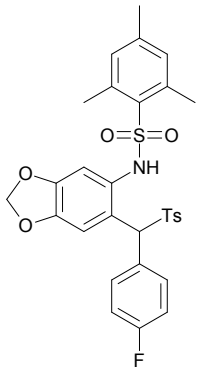
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.2 Hz, 2H), 7.46 (dd, *J* = 8.5, 5.3 Hz, 2H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.16 (s, 1H), 6.97 (m, 5H), 6.24 (s, 1H), 6.07 (s, 1H), 5.93 (d, *J* = 5.4 Hz, 2H), 2.53 (s, 6H), 2.38 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.06, 147.24, 144.83, 142.69, 139.31, 134.97, 134.57, 132.74, 132.13, 129.97, 129.60, 129.54, 128.94, 128.70, 128.58, 123.84, 110.42, 109.36, 101.99, 69.85, 23.11, 21.61, 20.99; HRMS Calculated For $C_{30}H_{33}N_2O_6S_2$, $[M+NH_4]^+$: 581.1775, found: 581.1781.

N-(6-((4-chlorophenyl)(tosyl)methyl)benzo[d][1,3]dioxol-5-yl)-2,4,6-trimethylbenzenesulfonamide (1m)



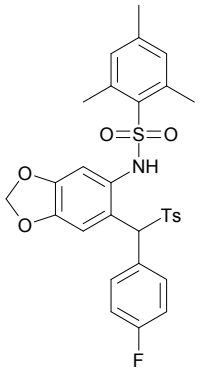
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.2 Hz, 2H), 7.42 (d, *J* = 8.5 Hz, 2H), 7.23 (m, 4H), 7.10 (s, 1H), 6.98 (m, 3H), 6.24 (s, 1H), 6.06 (s, 1H), 5.92 (d, *J* = 5.8 Hz, 2H), 2.52 (s, 6H), 2.39 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.16, 147.43, 145.11, 142.84, 139.34, 134.75, 134.74, 134.19, 132.14, 131.37, 131.24, 129.74, 129.44, 128.95, 128.89, 123.91, 110.18, 109.52, 102.10, 68.90, 23.08, 21.67, 21.03; HRMS Calculated For $C_{30}H_{32}ClN_2O_6S_2$, $[M+NH_4]^+$: 615.1385, found: 615.1386.

N-(6-((4-fluorophenyl)(tosyl)methyl)benzo[d][1,3]dioxol-5-yl)-2,4,6-trimethylbenzenesulfonamide (1n)



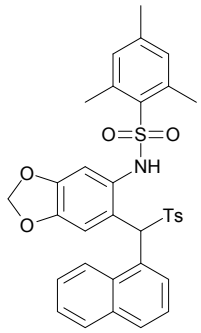
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.2 Hz, 2H), 7.46 (dd, *J* = 8.5, 5.3 Hz, 2H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.16 (s, 1H), 7.01 (s, 1H), 6.99 – 6.91 (m, 4H), 6.24 (s, 1H), 6.07 (s, 1H), 5.93 (d, *J* = 5.4 Hz, 2H), 2.53 (s, 6H), 2.38 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.70 (d, $J_{C\text{-}F}$ = 249.47 Hz), 148.12, 147.39, 145.01, 142.80, 139.34, 134.79, 134.27, 132.13, 131.80 (d, $J_{C\text{-}F}$ = 8.08 Hz), 129.68, 129.46, 128.88, 128.65 (d, $J_{C\text{-}F}$ = 4.04 Hz), 124.04, 115.75 (d, $J_{C\text{-}F}$ = 21.21 Hz), 110.21, 109.45, 102.07, 68.89, 23.08, 21.65, 21.02; HRMS Calculated For $C_{30}H_{32}FN_2O_6S_2$, $[M+NH_4]^+$: 599.1680, found: 599.1699.

N-(6-((3-fluorophenyl)(tosyl)methyl)benzo[d][1,3]dioxol-5-yl)-2,4,6-trimethylbenzenesulfonamide (1o)



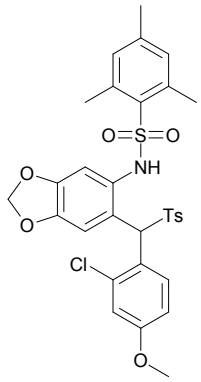
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.2 Hz, 2H), 7.33 – 7.19 (m, 4H), 7.16 (s, 1H), 7.07 – 6.91 (m, 5H), 6.36 (s, 1H), 5.97 (s, 1H), 5.93 (d, *J* = 5.5 Hz, 2H), 2.53 (s, 6H), 2.38 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.58 (d, $J_{C\text{-}F}$ =248.46 Hz), 148.23, 147.40, 145.12, 142.89, 139.30, 135.03 (d, $J_{C\text{-}F}$ =8.08 Hz), 134.75, 134.35, 132.16, 130.20 (d, $J_{C\text{-}F}$ =8.08 Hz), 129.68, 129.54, 128.94, 125.62 (d, $J_{C\text{-}F}$ =3.03 Hz), 123.55, 117.00 (d, $J_{C\text{-}F}$ =23.23 Hz), 115.64 (d, $J_{C\text{-}F}$ =21.21 Hz), 110.17, 109.70, 102.09, 69.13, 23.12, 21.64, 20.95; HRMS Calculated For $C_{30}H_{32}FN_2O_6S_2$, $[M+NH_4]^+$: 599.1680, found: 599.1692.

2,4,6-trimethyl-N-(6-(naphthalen-1-yl(tosyl)methyl)benzo[d][1,3]dioxol-5-yl)benzenesulfonamide (1p)



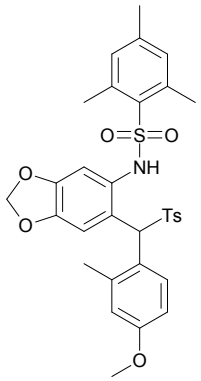
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (d, *J* = 7.2 Hz, 1H), 8.15 (s, 1H), 8.04 (d, *J* = 8.5 Hz, 1H), 7.75 (m, 4H), 7.52 – 7.44 (m, 2H), 7.39 (t, *J* = 7.1 Hz, 1H), 7.13 (d, *J* = 8.1 Hz, 2H), 7.05 (s, 2H), 6.97 (s, 2H), 6.21 (s, 1H), 5.84 (dd, *J* = 17.9, 1.3 Hz, 2H), 2.71 (s, 6H), 2.37 (s, 3H), 2.26 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.49, 146.44, 144.82, 142.65, 138.83, 135.80, 135.23, 133.84, 132.29, 131.37, 130.98, 129.64, 129.48, 128.70, 128.65, 128.45, 127.49, 127.41, 126.04, 124.56, 123.05, 121.62, 110.75, 106.47, 101.86, 65.56, 22.90, 21.52, 21.04; HRMS Calculated For $C_{34}H_{35}N_2O_6S_2$, $[M+NH_4]^+$: 631.1931, found: 631.1937.

N-(6-((2-chloro-4-methoxyphenyl)(tosyl)methyl)benzo[d][1,3]dioxol-5-yl)-2,4,6-trimethylbenzenesulfonamide (1q)



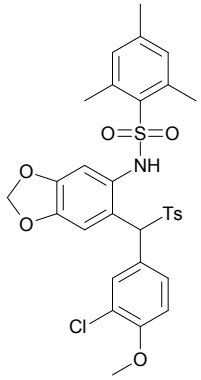
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.8 Hz, 1H), 7.85 (s, 1H), 7.66 (d, *J* = 8.3 Hz, 2H), 7.22 (d, *J* = 8.2 Hz, 2H), 7.08 (s, 1H), 7.00 (s, 2H), 6.85 (dd, *J* = 8.9, 2.7 Hz, 1H), 6.74 (d, *J* = 2.7 Hz, 1H), 6.64 (s, 1H), 6.33 (s, 1H), 5.95 – 5.89 (m, 2H), 3.75 (s, 3H), 2.65 (s, 6H), 2.38 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.09, 148.29, 146.36, 144.94, 142.41, 138.73, 136.15, 136.03, 135.01, 132.20, 131.64, 131.28, 129.66, 128.67, 122.17, 120.58, 115.06, 113.02, 110.13, 106.67, 101.92, 65.04, 55.52, 22.99, 21.68, 21.00; HRMS Calculated For $C_{31}H_{34}ClN_2O_7S_2$, $[M+NH_4]^+$: 645.1490, found: 645.1503.

N-(6-((4-methoxy-2-methylphenyl)(tosyl)methyl)benzo[d][1,3]dioxol-5-yl)-2,4,6-trimethylbenzenesulfonamide (1r)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.7 Hz, 1H), 7.97 (s, 1H), 7.69 (d, *J* = 8.2 Hz, 2H), 7.21 (d, *J* = 8.1 Hz, 2H), 7.12 (s, 1H), 7.02 (s, 2H), 6.79 (dd, *J* = 8.7, 2.7 Hz, 1H), 6.55 (d, *J* = 2.6 Hz, 1H), 6.31 (s, 1H), 6.14 (s, 1H), 5.89 (d, *J* = 3.6 Hz, 2H), 3.75 (s, 3H), 2.64 (s, 6H), 2.37 (s, 3H), 2.35 (s, 3H), 2.07 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.44, 148.10, 146.55, 144.70, 142.54, 139.80, 138.69, 135.75, 135.40, 132.21, 130.91, 130.83, 129.58, 128.68, 122.74, 122.01, 116.33, 111.23, 110.72, 106.73, 101.87, 65.49, 55.14, 22.86, 21.64, 21.01, 20.09; HRMS Calculated For $C_{32}H_{37}N_2O_7S_2$, $[M+NH_4]^+$: 625.2037, found: 625.2041.

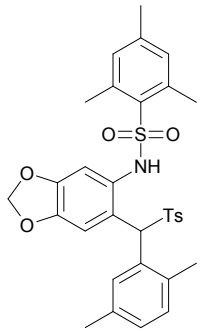
N-(6-((3-chloro-4-methoxyphenyl)(tosyl)methyl)benzo[d][1,3]dioxol-5-yl)-2,4,6-trimethylbenzenesulfonamide (1s)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.2 Hz, 2H), 7.42 (dd, *J* = 8.6, 2.1 Hz, 1H), 7.29 (d, *J* = 2.1 Hz, 1H), 7.24 (s, 1H), 7.22 (d, *J* = 3.4 Hz, 2H), 6.98 (m, 3H), 6.81 (d, *J* = 8.6 Hz, 1H), 6.35 (s, 1H), 5.93 (d, *J* = 4.4 Hz, 2H), 5.90 (s, 1H), 3.86 (s, 3H), 2.53 (s, 6H), 2.39 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.14, 148.14, 147.34, 145.02, 142.82, 139.25, 134.80, 134.40, 132.16, 131.47, 129.69, 129.48, 129.41, 128.89, 125.65, 123.82, 122.68, 111.86, 110.17, 109.62, 102.06, 68.62, 56.12, 23.12, 21.65, 21.06; HRMS Calculated For $C_{31}H_{34}ClN_2O_7S_2$, $[M+NH_4]^+$: 645.1490, found: 645.1503.

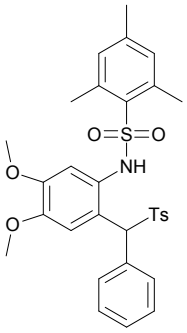
N-(6-((2,5-dimethylphenyl)(tosyl)methyl)benzo[d][1,3]dioxol-5-yl)-2,4,6-

trimethylbenzenesulfonamide (1t)



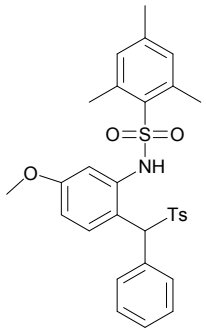
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (s, 1H), 7.88 (s, 1H), 7.69 (d, *J* = 8.2 Hz, 2H), 7.20 (d, *J* = 8.1 Hz, 2H), 7.14 (s, 1H), 7.02 (s, 2H), 6.92 (dd, *J* = 28.0, 7.7 Hz, 2H), 6.34 (s, 1H), 6.15 (s, 1H), 5.89 (d, *J* = 3.0 Hz, 2H), 2.64 (s, 6H), 2.42 – 2.31 (m, 9H), 2.05 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.16, 146.45, 144.75, 142.54, 138.65, 135.81, 135.38, 135.34, 134.82, 132.22, 131.07, 130.85, 130.46, 130.00, 129.53, 129.32, 128.73, 121.45, 110.81, 106.55, 101.86, 66.01, 22.85, 21.63, 21.26, 21.01, 19.28; HRMS Calculated For $C_{32}H_{37}N_2O_6S_2$, $[M+NH_4]^+$: 609.2088, found: 609.2100.

N-(4,5-dimethoxy-2-(phenyl(tosyl)methyl)phenyl)-2,4,6-trimethylbenzenesulfonamide (1u)



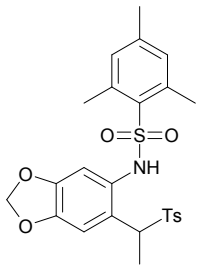
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.2 Hz, 2H), 7.43 (dd, *J* = 6.5, 2.9 Hz, 2H), 7.26 (m, 3H), 7.20 (s, 1H), 7.18 (d, *J* = 3.0 Hz, 2H), 7.10 (s, 1H), 6.96 (s, 2H), 6.23 (s, 1H), 6.00 (s, 1H), 3.77 (s, 3H), 3.49 (s, 3H), 2.49 (s, 6H), 2.37 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.12, 148.30, 144.74, 142.67, 139.70, 135.07, 134.39, 132.81, 131.96, 130.00, 129.49, 128.97, 128.65, 128.56, 128.21, 122.46, 113.02, 111.97, 69.73, 55.91, 55.55, 23.12, 21.61, 20.91; HRMS Calculated For $C_{31}H_{37}N_2O_6S_2$, $[M+NH_4]^+$: 597.2088, found: 597.2077.

N-(5-methoxy-2-(phenyl(tosyl)methyl)phenyl)-2,4,6-trimethylbenzenesulfonamide (1v)



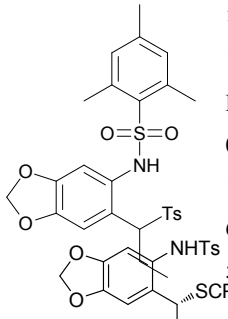
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (s, 1H), 7.62 (d, *J* = 8.3 Hz, 2H), 7.45 (d, *J* = 8.9 Hz, 1H), 7.41 (dd, *J* = 6.6, 2.9 Hz, 2H), 7.25 (m, 3H), 7.18 (d, *J* = 8.1 Hz, 2H), 6.99 (s, 2H), 6.75 (dd, *J* = 8.8, 2.7 Hz, 1H), 6.39 (d, *J* = 2.7 Hz, 1H), 5.92 (s, 1H), 3.57 (s, 3H), 2.56 (s, 6H), 2.36 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.07, 144.77, 142.65, 139.38, 136.94, 134.94, 134.88, 132.74, 132.10, 132.08, 130.10, 129.50, 128.95, 128.62, 128.52, 120.67, 113.73, 112.94, 69.92, 55.19, 23.05, 21.61, 20.96; HRMS Calculated For $C_{30}H_{35}N_2O_5S_2$, $[M+NH_4]^+$: 567.1982, found: 567.1987.

2,4,6-trimethyl-N-(6-(1-tosylethyl)benzo[d][1,3]dioxol-5-yl)benzenesulfonamide (1w)



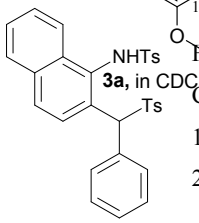
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 8.1 Hz, 2H), 7.15 (s, 1H), 6.95 (s, 2H), 6.61 (s, 1H), 6.43 (s, 1H), 5.95 (dd, *J* = 5.4, 1.2 Hz, 2H), 4.54 (q, *J* = 7.04 Hz, 1H); 2.52 (s, 6H), 2.46 (s, 3H), 2.30 (s, 3H), 1.31 (d, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.08, 147.12, 145.22, 142.66, 139.01, 134.56, 133.37, 132.11, 129.86, 129.74, 129.18, 109.19, 108.11, 101.98, 59.72, 29.70, 23.11, 21.71, 20.95, 14.36; HRMS Calculated For $C_{25}H_{31}N_2O_6S_2$, $[M+NH_4]^+$: 519.1618, found: 519.1616.

2,4,6-trimethyl-N-(6-(1-tosylpropyl)benzo[d][1,3]dioxol-5-yl)benzenesulfonamide (1x)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.2 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 7.12 (s, 1H), 6.95 (s, 2H), 6.49 (d, *J* = 7.4 Hz, 2H), 5.96 (d, *J* = 8.2 Hz, 2H), 4.45 (dd, *J* = 11.5, 4.1 Hz, 1H), 2.53 (s, 6H), 2.45 (s, 3H), 2.30 (s, 3H), 2.04 – 1.90 (m, 1H), 1.88 – 1.71 (m, 1H), 0.54 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.00, 147.14, 145.17, 142.56, 139.07, 134.85, 133.50, 132.08, 131.11, 129.69, 129.31, 122.36, 109.65, 107.93, 101.95, 66.14, 23.09, 21.68, 21.14, 20.93, 10.26; HRMS Calculated For $C_{26}H_{33}N_2O_6S_2$, $[M+NH_4]^+$: 533.1775, found: 533.1781.

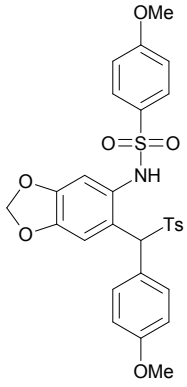
4-methyl-N-(2-(phenyl(tosyl)methyl)naphthalen-1-yl)benzenesulfonamide (1y)



3a, in $CDCl_3$

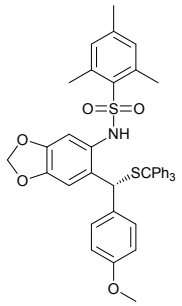
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.60 (m, 9H), 7.50 (d, *J* = 8.6 Hz, 1H), 7.40 (t, *J* = 7.5 Hz, 1H), 7.33 – 7.13 (m, 9H), 6.61 (s, 1H), 2.43 (s, 3H), 2.36 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ144.72, 144.03, 137.60, 135.17, 134.26, 132.61, 132.27, 132.16, 130.44, 129.77, 129.53, 128.97, 128.94, 128.63, 128.60, 127.89, 127.49, 126.87, 126.85, 126.56, 124.34, 70.45, 21.65, 21.60. HRMS Calculated For $C_{231}H_{27}N_{Na}O_4S_2$, $[M+Na]^+$: 564.1274, found: 564.1268.

4-methoxy-N-(6-((4-methoxyphenyl)(tosyl)methyl)benzo[d][1,3]dioxol-5-yl)benzenesulfonamide (1z)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.9 Hz, 2H), 7.58 (d, *J* = 8.3 Hz, 2H), 7.25-7.15 (m, 5H), 7.10 (s, 1H), 6.97 (d, *J* = 8.9 Hz, 2H), 6.75 (d, *J* = 8.8 Hz, 2H), 6.53 (s, 1H), 5.95 (dd, *J* = 8.1, 1.4 Hz, 2H), 5.74 (s, 1H), 3.88 (s, 3H), 3.77 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.21, 159.69, 148.03, 147.31, 144.74, 135.01, 131.87, 131.27, 129.56, 129.46, 129.39, 128.80, 124.38, 123.90, 114.44, 114.01, 110.18, 109.48, 102.04, 69.25, 55.69, 55.24, 21.65; HRMS Calculated For $C_{29}H_{31}N_2O_8S_2$, $[M+NH_4]^+$: 599.1516, found: 599.1526.

Copy of NMR Spectra and HPLC Chromatograms of 3i-3x



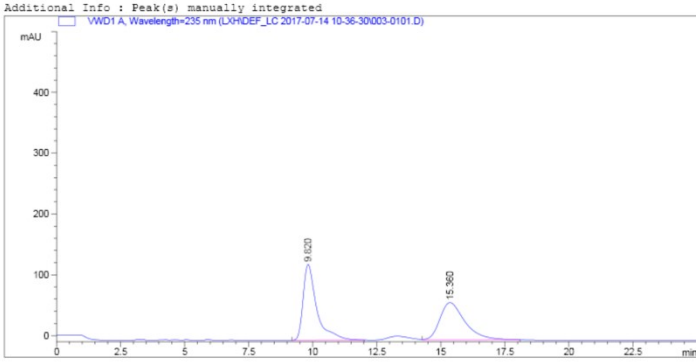
3i

yield: 93%

93%*ee*

```
Sample Info     : ADH0CE-KE039, 1.0ml/min, 25C,90/10, 235nm, 37bar
```

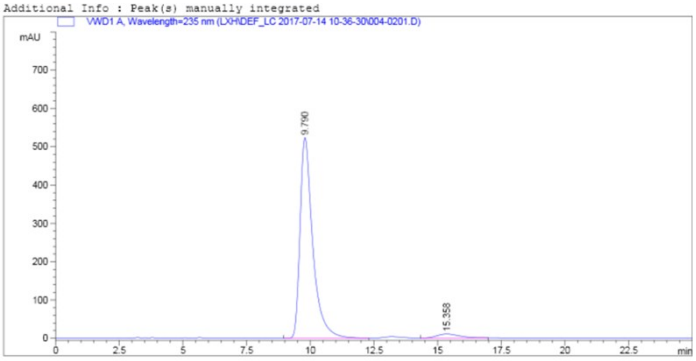
```
Additional Info : Peak(s) manually integrated
```



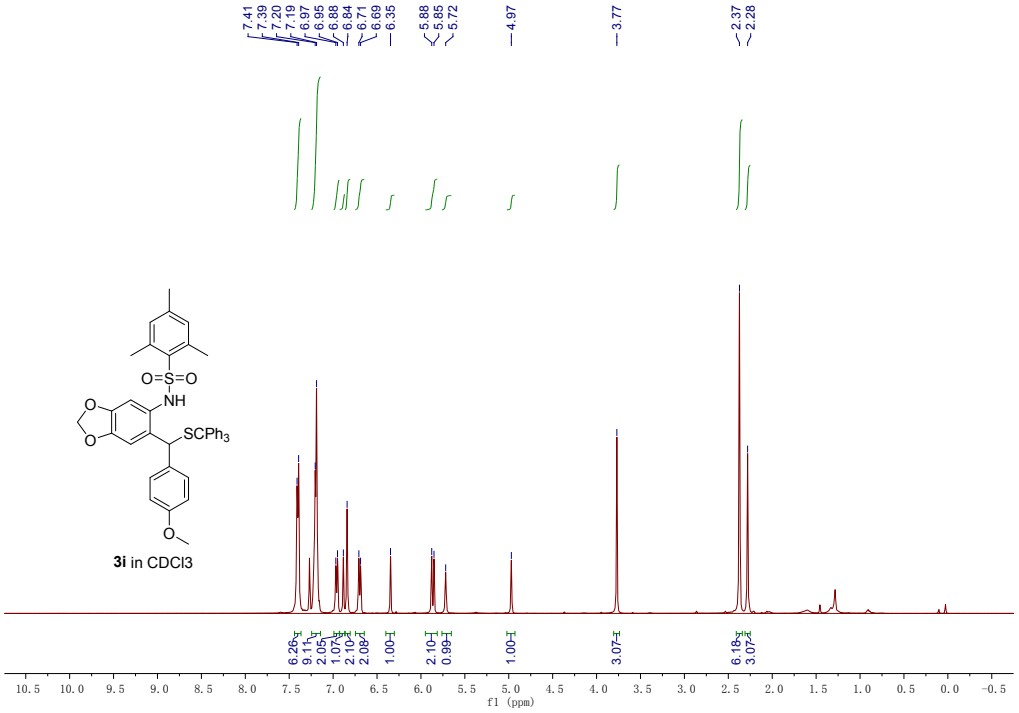

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s    [mAU   ]     %
----|-------|----|-------|----------|----------|--------|
   1   9.820 BB    0.5447 4597.55859  124.42519  52.1345
   2  15.360 VB    1.0336 4221.09814   61.51069  47.8655
```

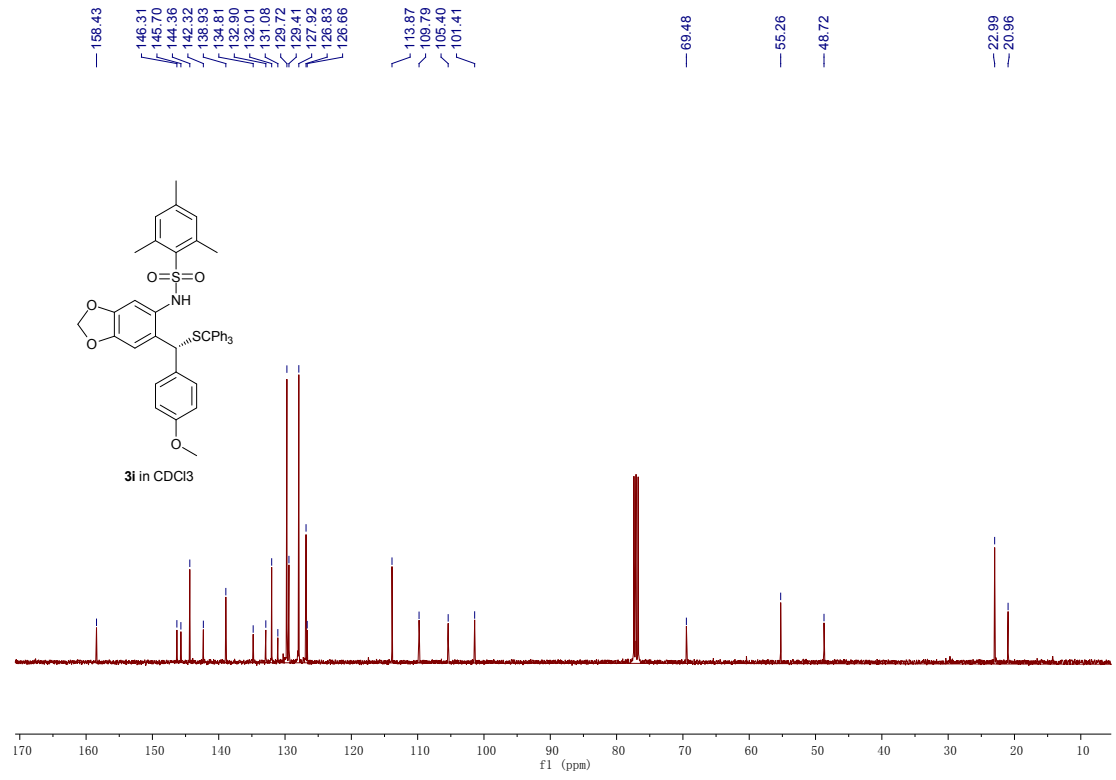
```
Sample Info     : ADH0CE-KE039, 1.0ml/min, 25C,90/10, 235nm, 37bar
```

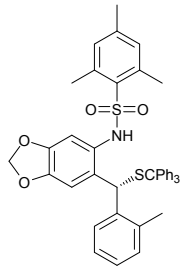
```
Additional Info : Peak(s) manually integrated
```




```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s    [mAU   ]     %
----|-------|----|-------|----------|----------|--------|
   1   9.790 BB    0.5147 1.81306e4   523.52203  96.6537
   2  15.358 VB    0.8990  627.71405   10.38212   3.3463
```


7.41
7.39
7.20
7.19
6.97
6.95
6.88
6.84
6.71
6.69
6.35
5.88
5.85
5.72
4.97
3.77
2.37
2.28
O=S=O
NH
O
O
SCPh3
O
3i in CDCl3
6.26
9.11
2.05
1.07
2.10
2.08
1.00
2.10
0.99
1.00
3.07
6.18
3.07
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


158.43
146.31
145.70
144.36
142.32
138.93
134.81
132.90
132.01
131.08
129.72
129.41
127.92
126.83
126.66
113.87
109.79
105.40
101.41
69.48
55.26
48.72
22.99
20.96
O=S=O
NH
O
O
SCPh3
O
3i in CDCl3
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

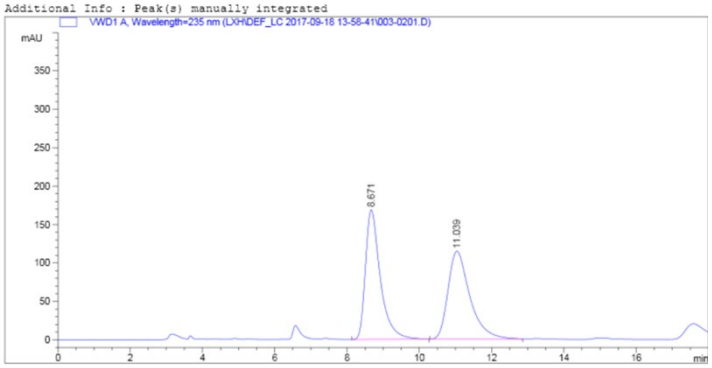


3j

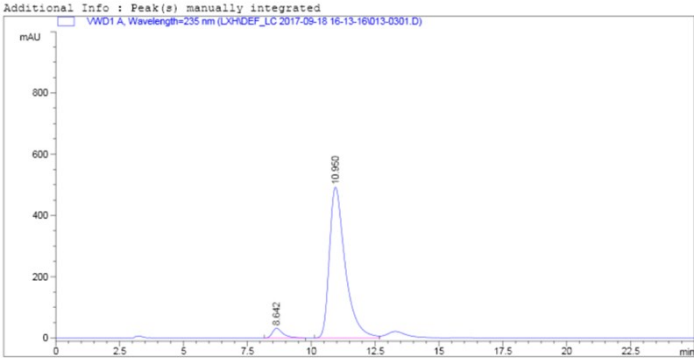
yield: 96%

92%*ee*

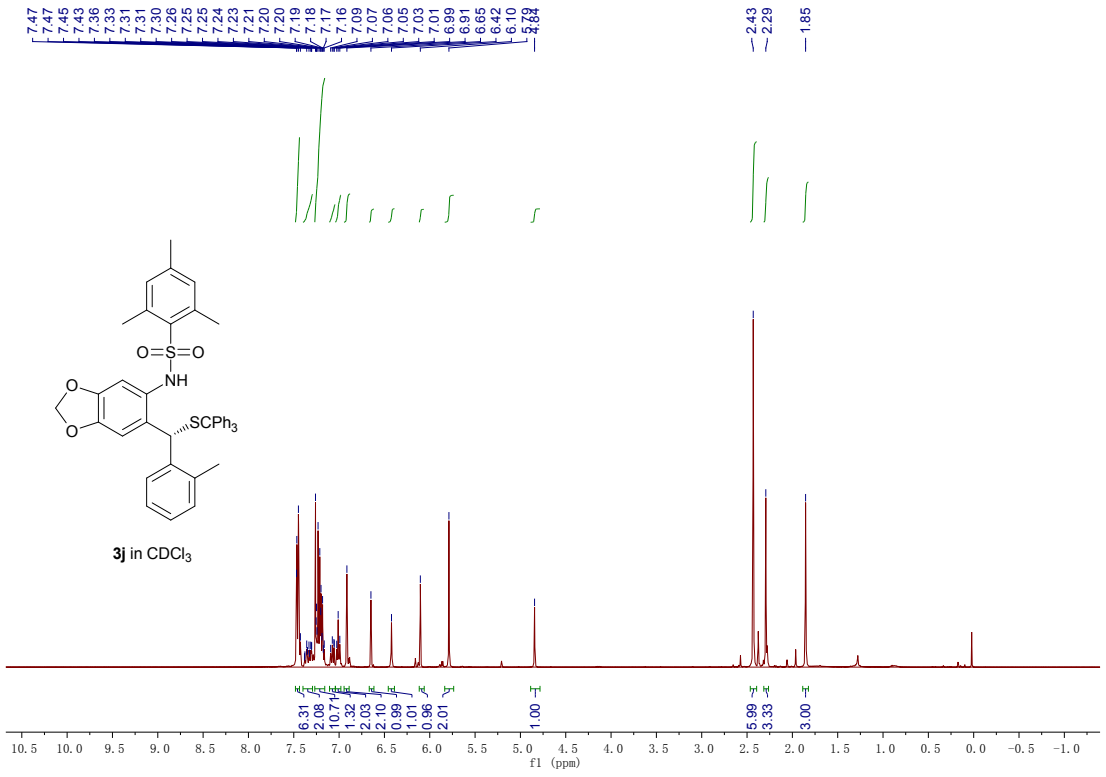
```
Sample Info     : ADH0CE-KE039; 95/5; 1.0mL/min; 235nm; 35bar; 25C

Additional Info : Peak(s) manually integrated
```



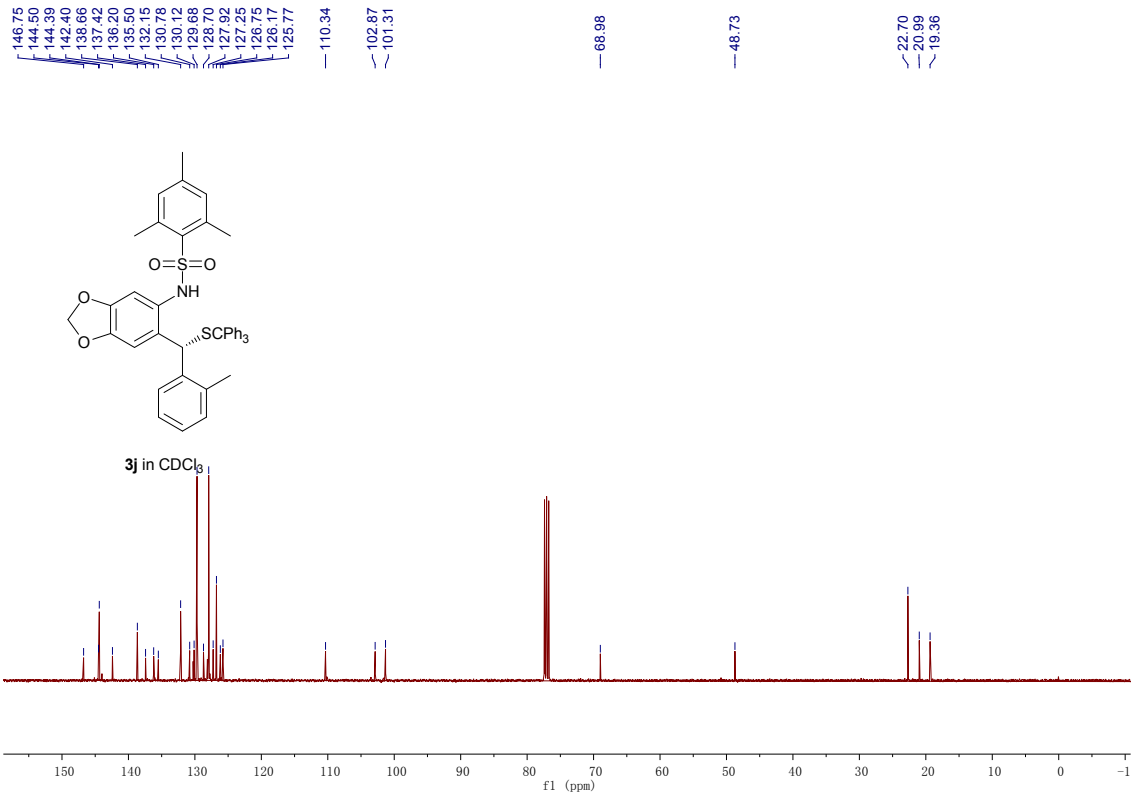

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s    [mAU   ]     %
----|-------|----|-------|---------|----------|--------|
   1   8.671 BB    0.4262 4814.49951  168.64966  50.0790
   2  11.039 BB    0.6275 4799.31543  114.46513  49.9210

 Sample Info     : ADH0CE-KE039; 95/5; 1.0mL/min; 235nm; 35bar; 25C

Additional Info : Peak(s) manually integrated
```



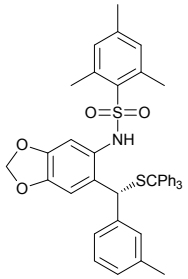

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s    [mAU   ]     %
----|-------|----|-------|---------|----------|--------|
   1   8.642 BB    0.4207  884.26459   31.36345   4.0076
   2  10.950 BV    0.6439 2.11805e4   491.60004  95.9924
```



3j in $CDCl_3$



3j in $CDCl_3$



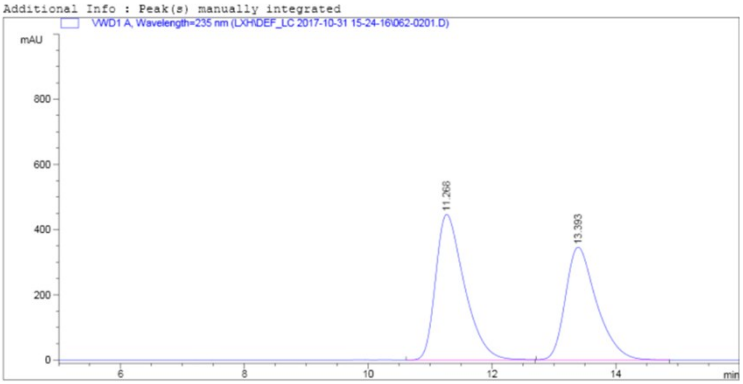
3k

yield: 89%

85%*ee*

```
Sample Info     : ADH0CE-EA056, 90/10, 1.0, 25C, 40bar
```

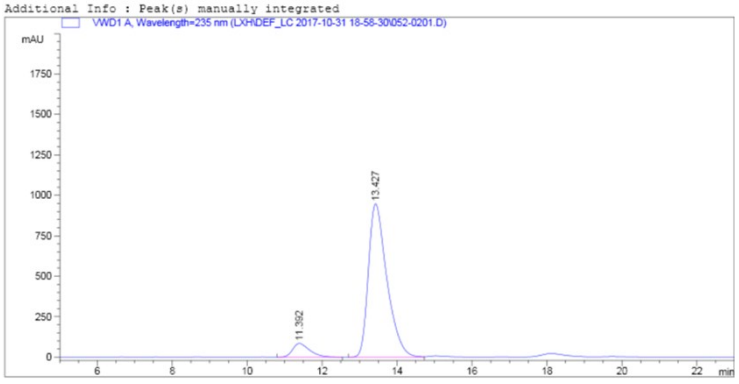
```
Additional Info : Peak(s) manually integrated
```



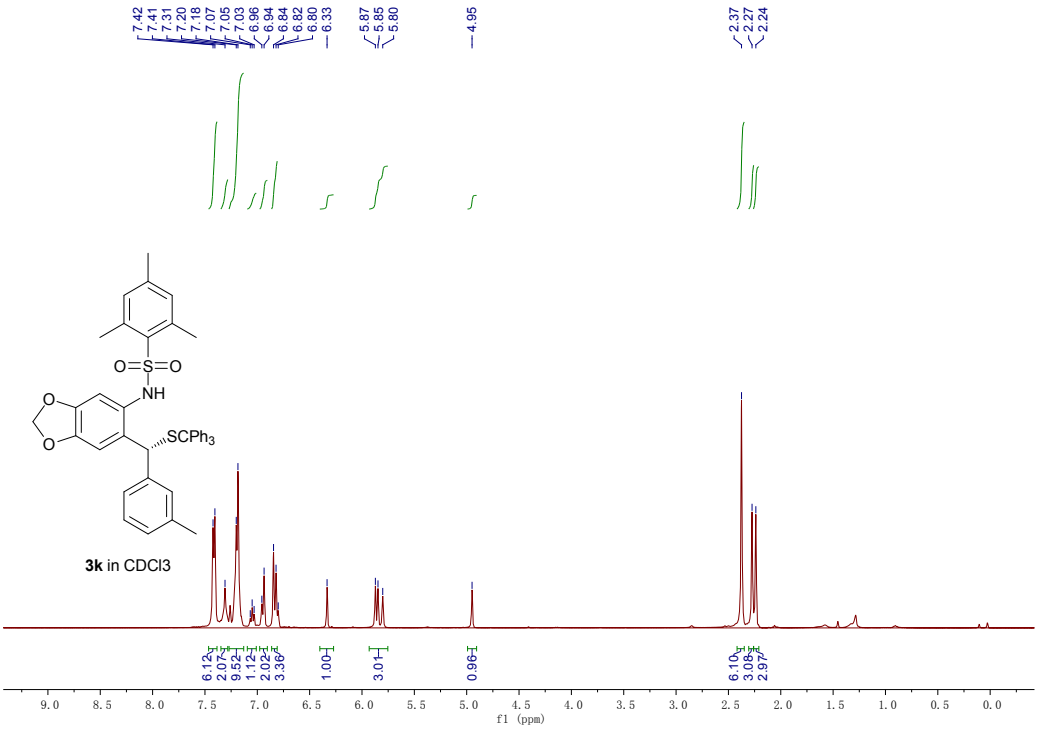

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s    [mAU   ]      %
----|-------|----|-------|----------|----------|-------|
   1  11.268 VB    0.4884 1.44627e4   446.73260  54.5413
   2  13.393 BB    0.5247 1.20543e4   345.70782  45.4587
```

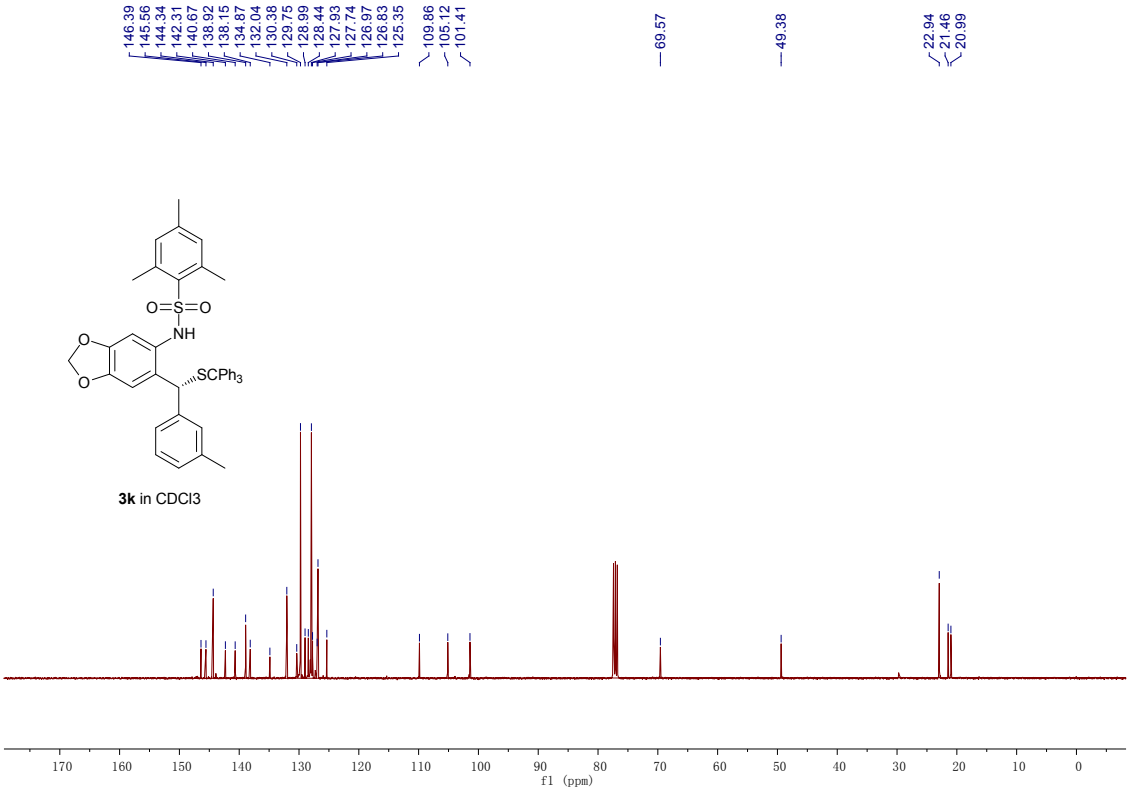
```
Sample Info     : ADH0CE-EA056, 90/10, 1.0, 25C, 40bar
```

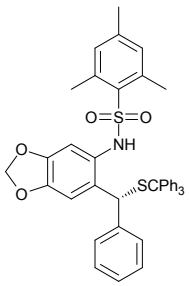
```
Additional Info : Peak(s) manually integrated
```




```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s    [mAU   ]      %
----|-------|----|-------|----------|----------|-------|
   1  11.392 VB    0.4719 2638.58545   84.19658   7.5192
   2  13.427 BV    0.5133 3.24525e4   947.21875  92.4808
```


7.42
7.41
7.31
7.20
7.18
7.07
7.05
7.03
6.96
6.94
6.84
6.82
6.80
6.33
5.87
5.85
5.80
4.95
2.37
2.27
2.24
O=S=O
NH
O
O
SCPh3
3k in CDCl3
6.12
2.07
9.52
1.12
2.02
3.36
1.00
3.01
0.96
6.10
3.08
2.97
f1 (ppm)


146.39
145.56
144.34
142.31
140.67
138.92
138.15
134.87
132.04
130.38
129.75
128.99
128.44
127.93
127.74
126.97
126.83
125.35
109.86
105.12
101.41
69.57
49.38
22.94
21.46
20.99
O=S=O
NH
O
O
SCPh3
3k in CDCl3
f1 (ppm)



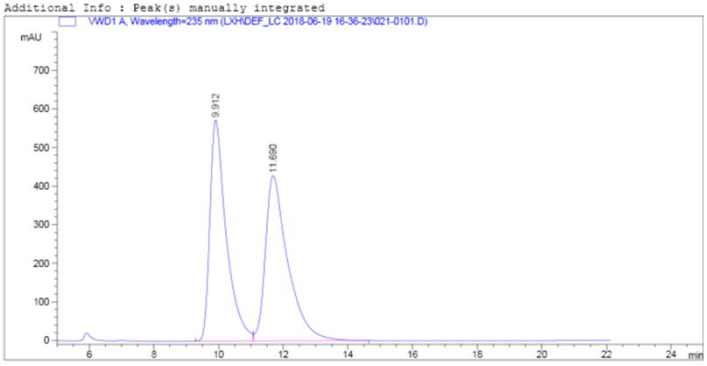
3l

yield: 96%

96%*ee*

```
Sample Info     : ADH0CE-EA039; 90/10; 1.0mL/min; 38bar; 235nm; 25C
```

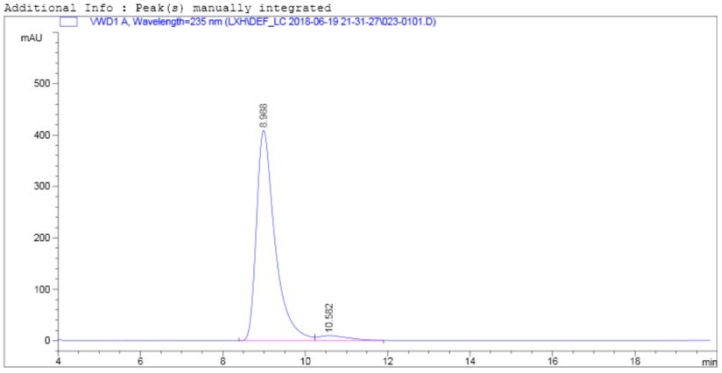
```
Additional Info : Peak(s) manually integrated
```



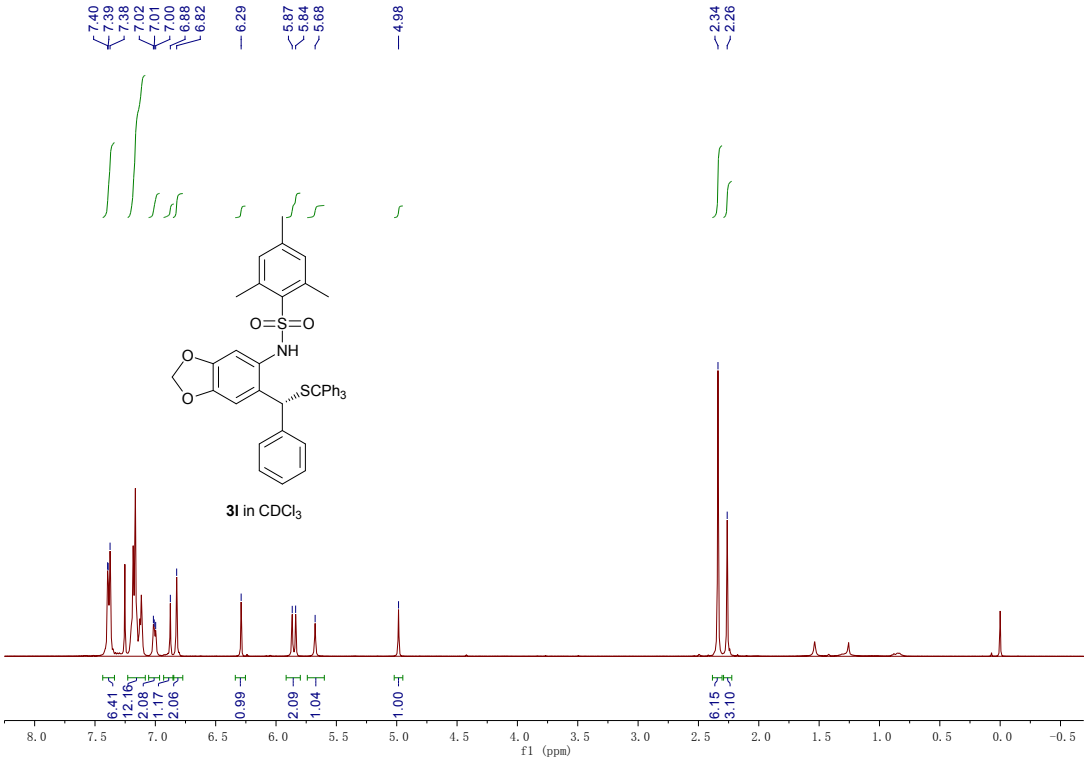

```
================================================================================
                          Area Percent Report
================================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1   9.912 BV     0.5113 2.00963e4   572.76062  49.2922
   2  11.690 VB     0.6975 2.06734e4   427.99033  50.7078
```

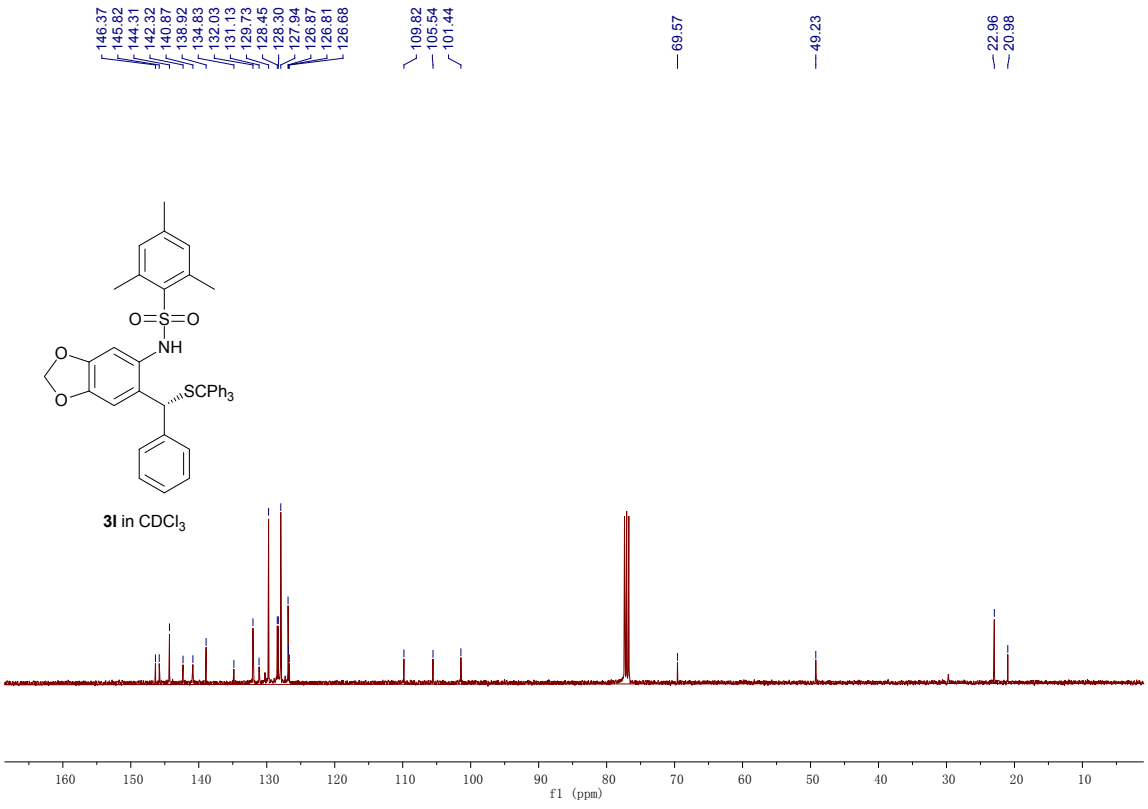
```
Sample Info     : ADH0CE-EA039; 90/10; 1.0mL/min; 38bar; 235nm; 25C
```

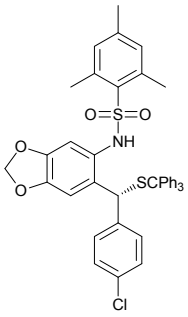
```
Additional Info : Peak(s) manually integrated
```




```
================================================================================
                          Area Percent Report
================================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1   8.988 BV     0.4653 1.27963e4   409.20364  96.4881
   2  10.582 VB     0.6861  465.74411    9.53847   3.5119
```


7.40
7.39
7.38
7.02
7.01
7.00
6.88
6.82
6.29
5.87
5.84
5.68
4.98
2.34
2.26
O=S=O
NH
O
O
SCPh3
3l in CDCl3
6.41
12.16
2.08
1.17
2.06
0.99
2.09
1.04
1.00
6.15
3.10
f1 (ppm)


146.37
145.82
144.31
142.32
140.87
138.92
134.83
132.03
131.13
129.73
128.45
128.30
127.94
126.87
126.81
126.68
109.82
105.54
101.44
69.57
49.23
22.96
20.98
O=S=O
NH
O
O
SCPh3
3l in CDCl3
f1 (ppm)



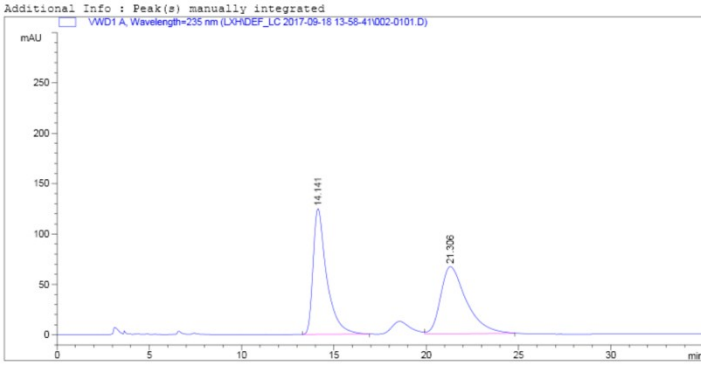
3m

yield: 89%

89%*ee*

```
Sample Info     : ADH0CE-KE039; 95/5; 1.0mL/min; 235nm; 35bar; 25C
```

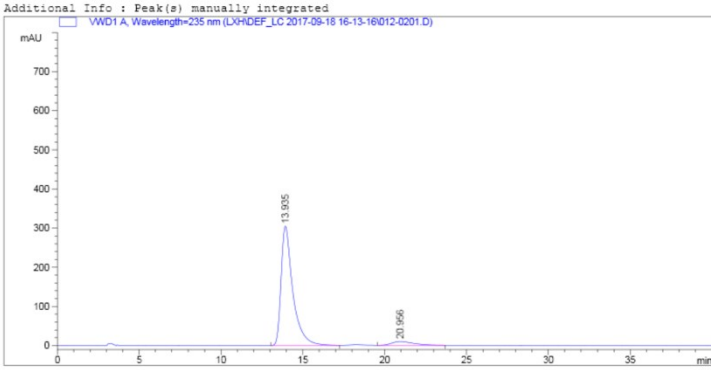
```
Additional Info : Peak(s) manually integrated
```



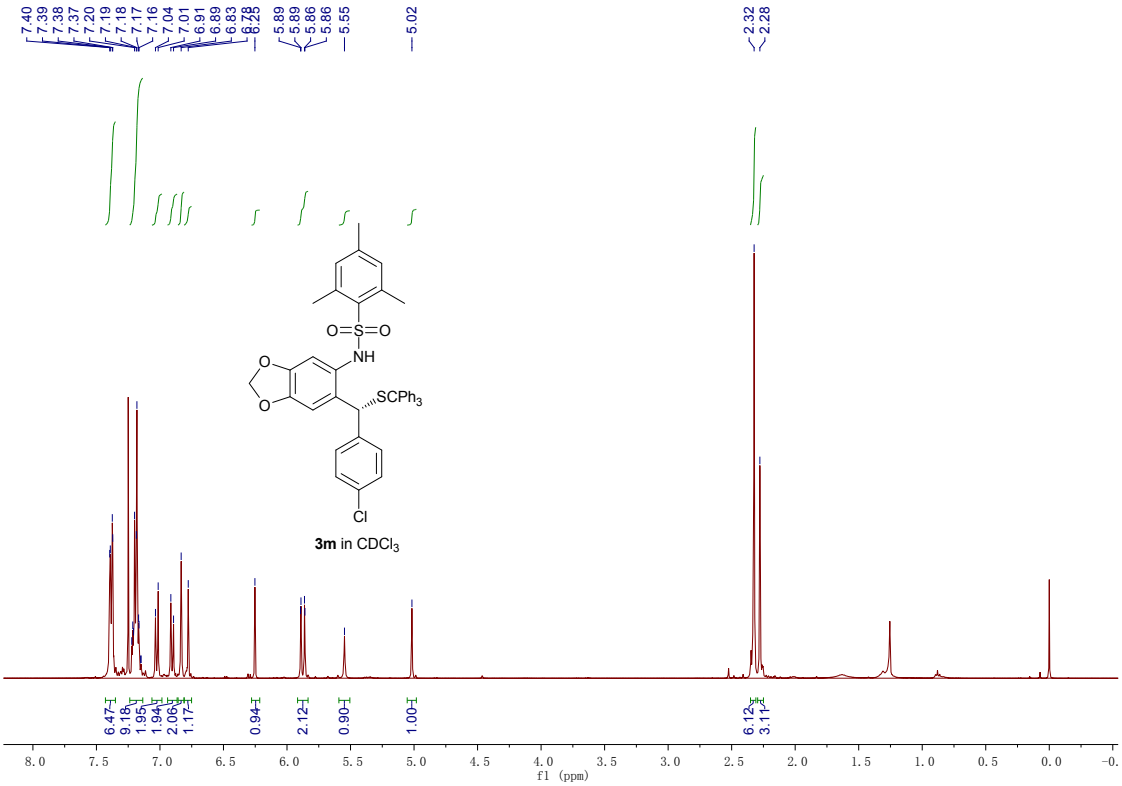

```
================================================================================
                            Area Percent Report
================================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  14.141 BB     0.7511 6393.85449  124.70413  49.7851
   2  21.306 VB     1.4403 6449.05078   66.65602  50.2149
```

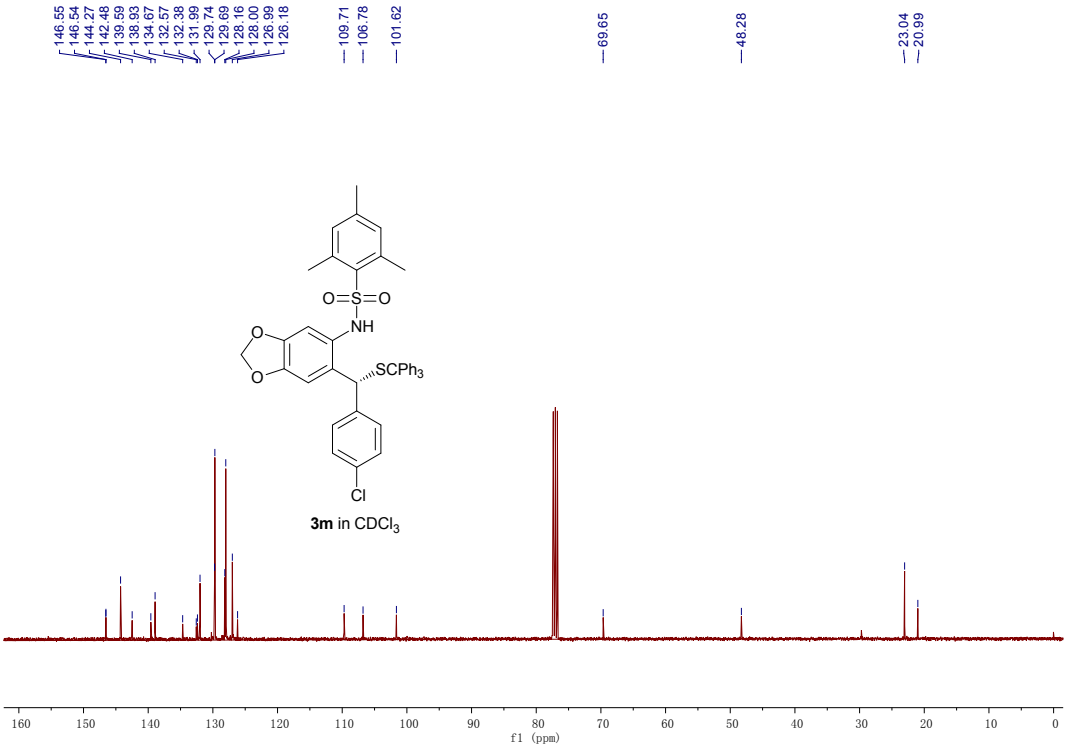
```
Sample Info     : ADH0CE-KE039; 95/5; 1.0mL/min; 235nm; 35bar; 25C
```

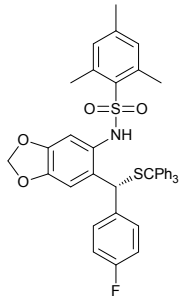
```
Additional Info : Peak(s) manually integrated
```




```
================================================================================
                            Area Percent Report
================================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  13.935 BB     0.7317 1.51569e4   304.74921  94.2706
   2  20.956 VB     1.3021  921.17480    9.69536   5.7294
```


7.40
7.39
7.38
7.37
7.20
7.19
7.18
7.17
7.16
7.04
7.01
6.91
6.89
6.83
6.78
6.25
5.89
5.89
5.86
5.86
5.55
5.02
2.32
2.28
O=S=O
NH
O
O
SCPh3
Cl
3m in CDCl3
6.47
9.18
1.95
1.94
2.06
1.17
0.94
2.12
0.90
1.00
6.12
3.11
f1 (ppm)

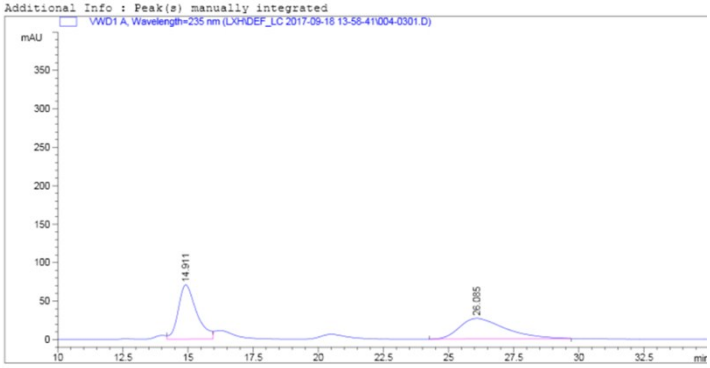

146.55
146.54
144.27
142.48
139.59
138.93
134.67
132.57
132.38
131.99
129.74
129.69
128.16
128.00
126.99
126.18
109.71
106.78
101.62
69.65
48.28
23.04
20.99
O=S=O
NH
O
O
SCPh3
Cl
3m in CDCl3
f1 (ppm)



3n
yield: 96%
93%*ee*

```
Sample Info     : ADH0CE-KE039; 95/5; 1.0mL/min; 235nm; 35bar; 25C
```

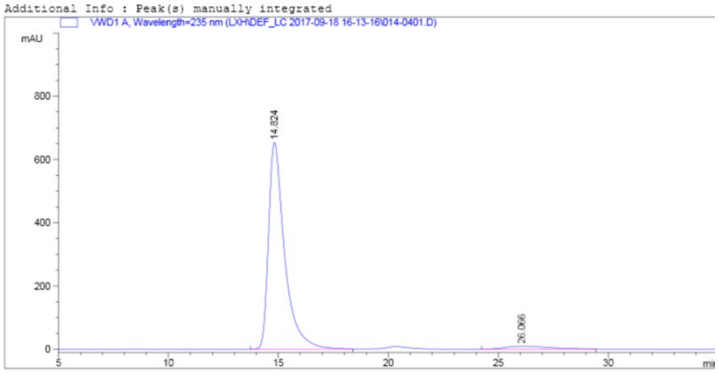
```
Additional Info : Peak(s) manually integrated
```



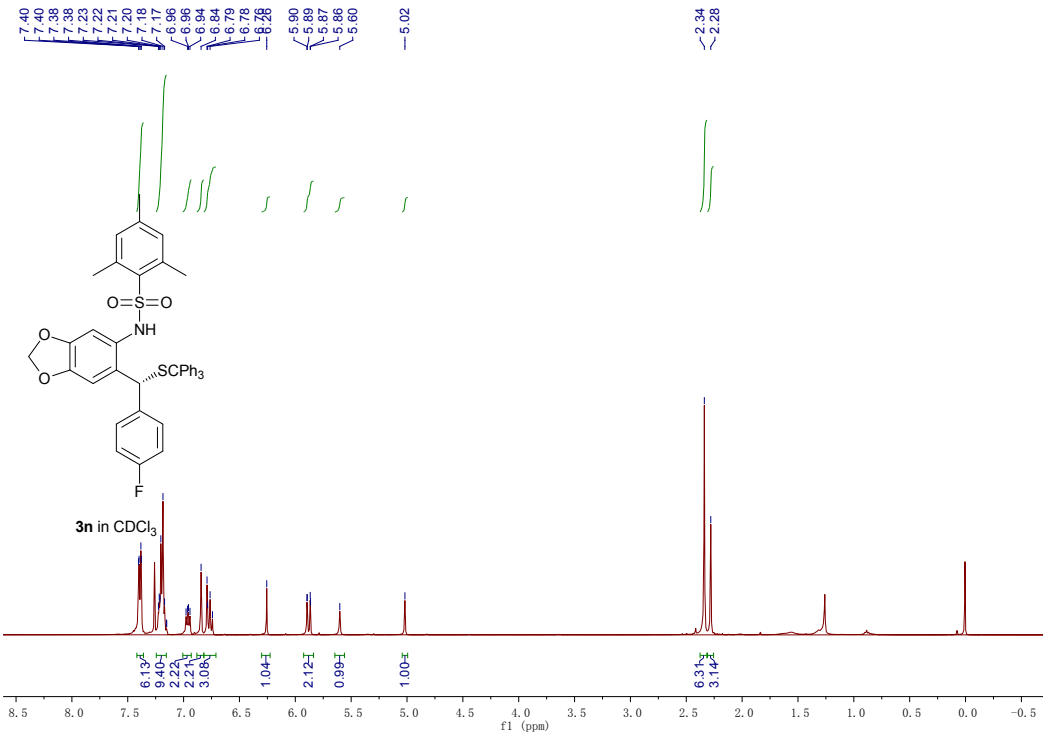

```
=====================================================================
                    Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]      [min]  mAU   *s    [mAU   ]      %
----|-------|----|-------|---------|----------|--------|
   1  14.911 VV    0.7321 3451.81152   70.59170  51.4262
   2  26.085 BB    1.6803 3260.35132   26.71100  48.5738
```

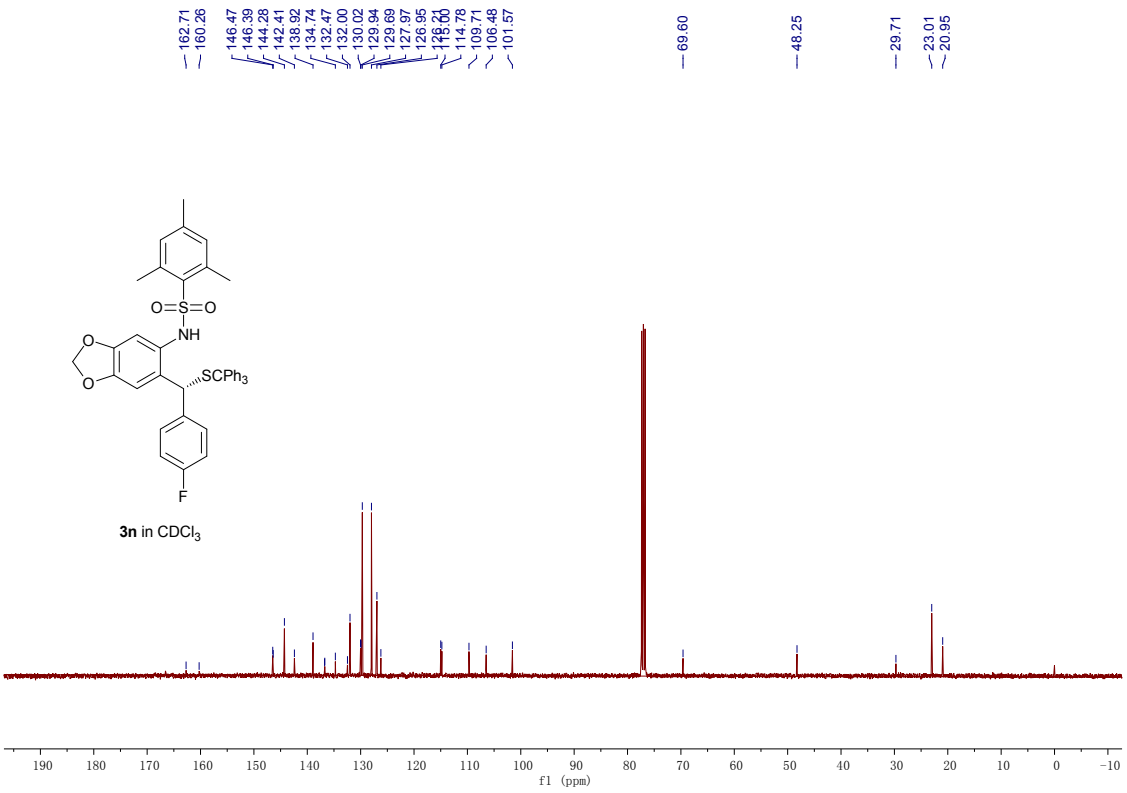
```
Sample Info     : ADH0CE-KE039; 95/5; 1.0mL/min; 235nm; 35bar; 25C
```

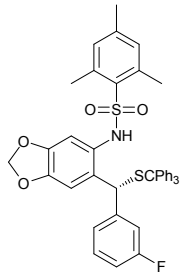
```
Additional Info : Peak(s) manually integrated
```




```
=====================================================================
                    Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]      [min]  mAU   *s    [mAU   ]      %
----|-------|----|-------|---------|----------|--------|
   1  14.824 BB    0.7474 3.31711e4   654.08942  96.4159
   2  26.066 BB    1.5595 1233.09436    9.36441   3.5841
```


7.40
7.40
7.38
7.38
7.23
7.22
7.21
7.20
7.18
7.17
6.96
6.94
6.84
6.79
6.78
6.28
6.26
5.90
5.89
5.87
5.86
5.60
5.02
2.34
2.28
O=S=O
NH
O
O
SCPh3
F
3n in CDCl3
6.13
9.40
2.22
2.21
3.08
1.04
2.12
0.99
1.00
6.31
3.14
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


162.71
160.26
146.47
146.39
144.28
142.41
138.92
134.74
132.47
132.00
130.02
129.94
129.69
127.97
126.95
126.21
115.00
114.78
109.71
106.48
101.57
69.60
48.25
29.71
23.01
20.95
O=S=O
NH
O
O
SCPh3
F
3n in CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



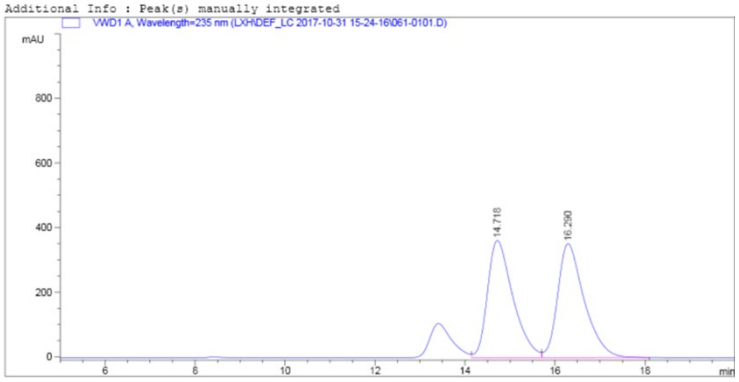
3o

yield: 93%

91%*ee*

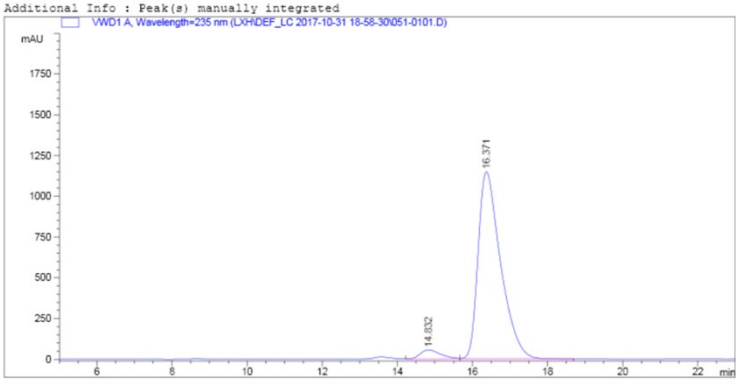
```
Sample Info     : ADH0CE-EA056, 90/10, 1.0, 25C, 40bar
```

```
Additional Info : Peak(s) manually integrated
```

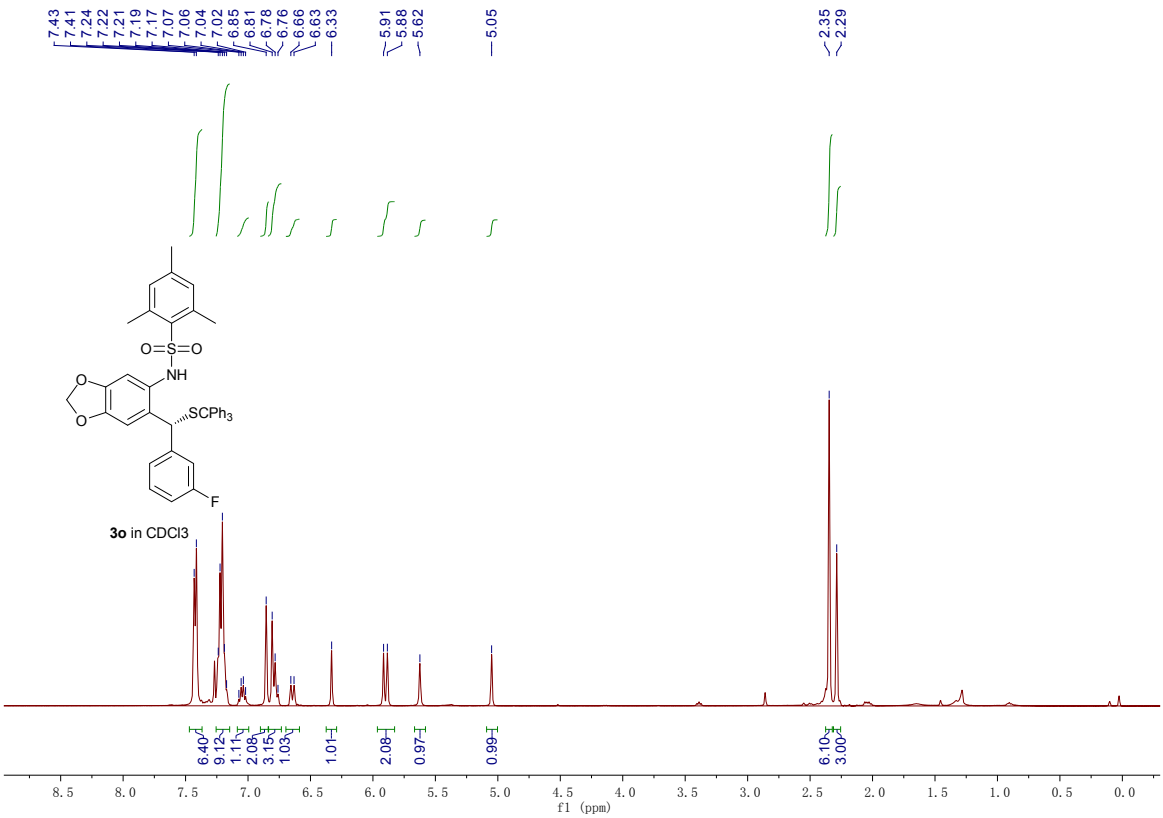


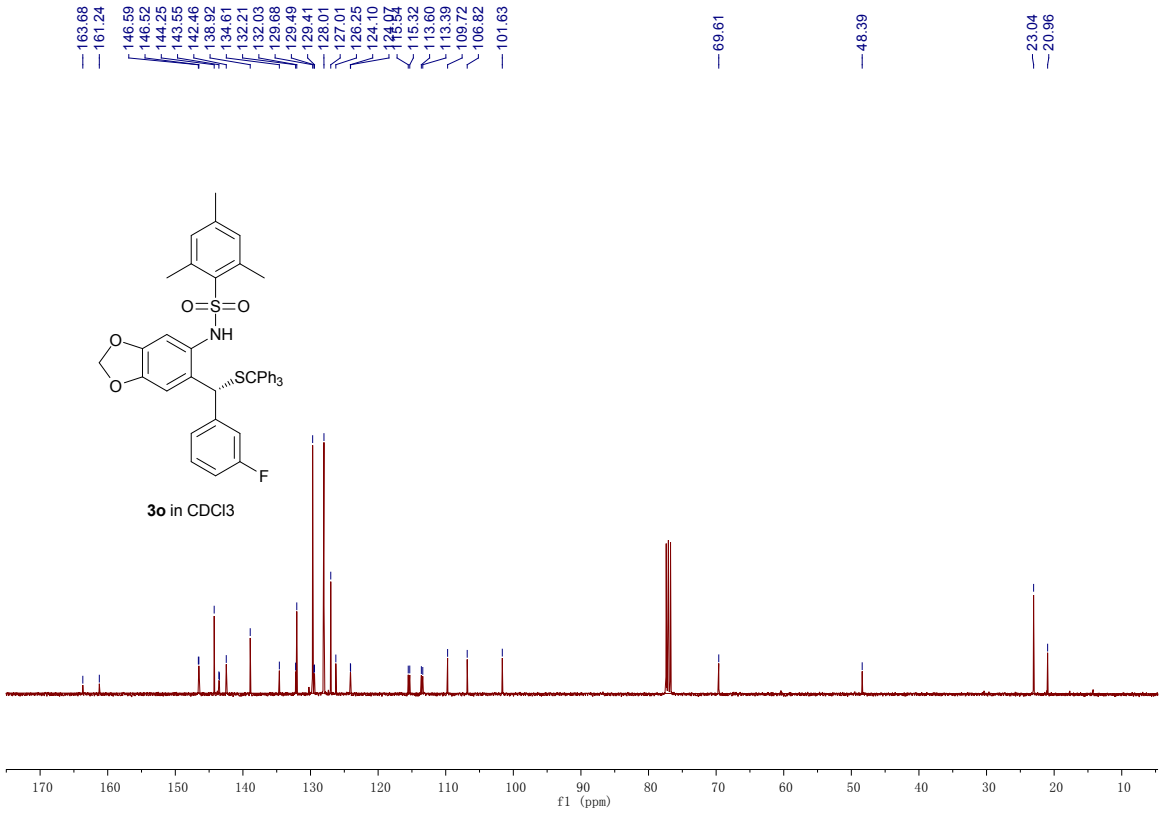

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  14.718 VV     0.5900 1.42005e4   362.12323  49.6627
   2  16.290 VB     0.6106 1.43934e4   352.31696  50.3373

Sample Info     : ADH0CE-EA056, 90/10, 1.0, 25C, 40bar
```

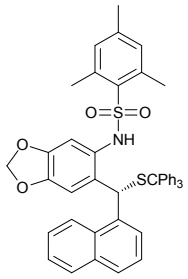
```
Additional Info : Peak(s) manually integrated
```




```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  14.832 VV     0.5785 2178.34741   56.60683   4.3539
   2  16.371 VB     0.6227 4.78536e4  1149.14465  95.6461
```


7.43
7.41
7.24
7.22
7.21
7.19
7.17
7.07
7.06
7.04
7.02
6.85
6.81
6.78
6.76
6.66
6.63
6.33
5.91
5.88
5.62
5.05
2.35
2.29
O=S=O
NH
O
O
SCPh3
F
3o in CDCl3
6.40
9.12
1.11
2.08
3.15
1.03
1.01
2.08
0.97
0.99
6.10
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


163.68
161.24
146.59
146.52
144.25
143.55
142.46
138.92
134.61
132.21
132.03
129.68
129.49
129.41
128.01
127.01
126.25
124.10
124.07
115.54
115.32
113.60
113.39
109.72
106.82
101.63
69.61
48.39
23.04
20.96
O=S=O
NH
O
O
SCPh3
F
3o in CDCl3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)



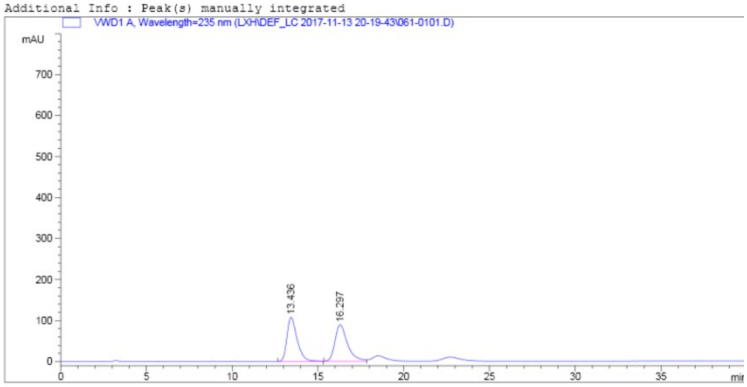
3p

yield: 95%

91%*ee*

```
Sample Info     : ADH-EA056. 95/5, 1.0, 40, 25c
```

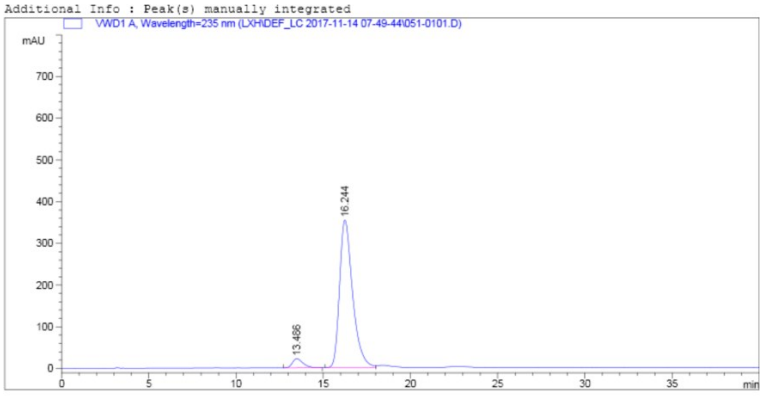
```
Additional Info : Peak(s) manually integrated
```



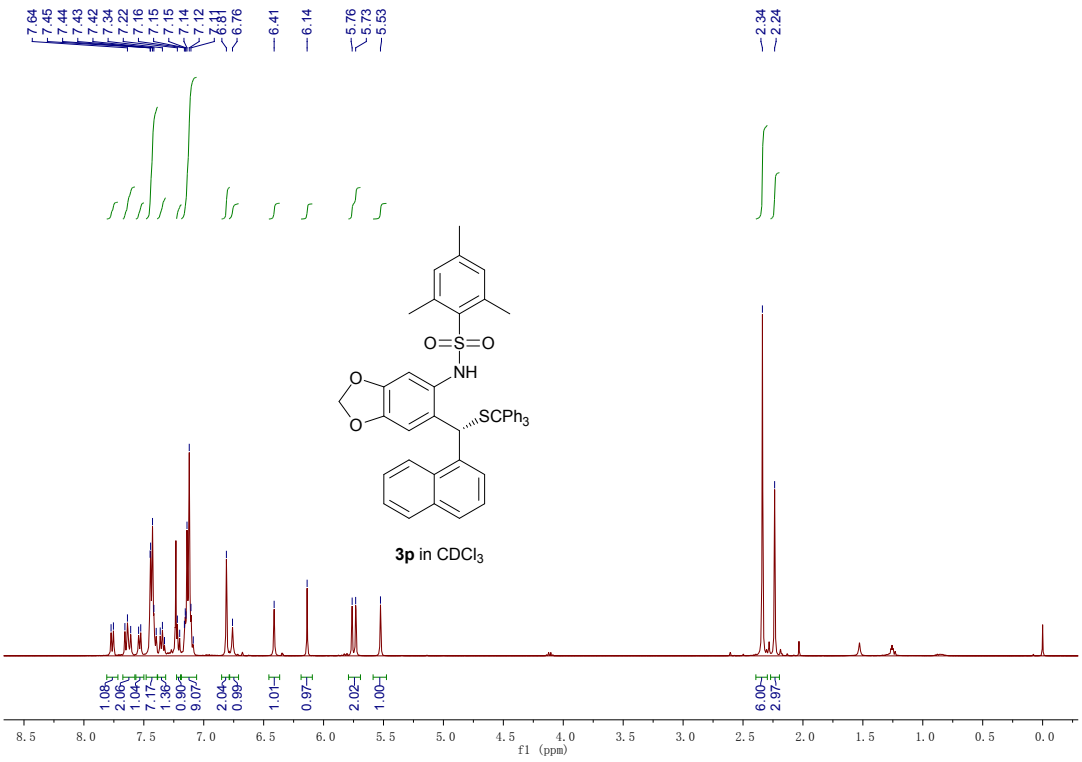

```
================================================================
                    Area Percent Report
================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  13.436 BB    0.6130 4369.15479  107.37801  49.2773
   2  16.297 BV    0.7612 4497.31006   88.80531  50.7227
```

```
Sample Info     : ADH0CE-EA056, 95/5, 1.0, 40bar, 25C, 235nm
```

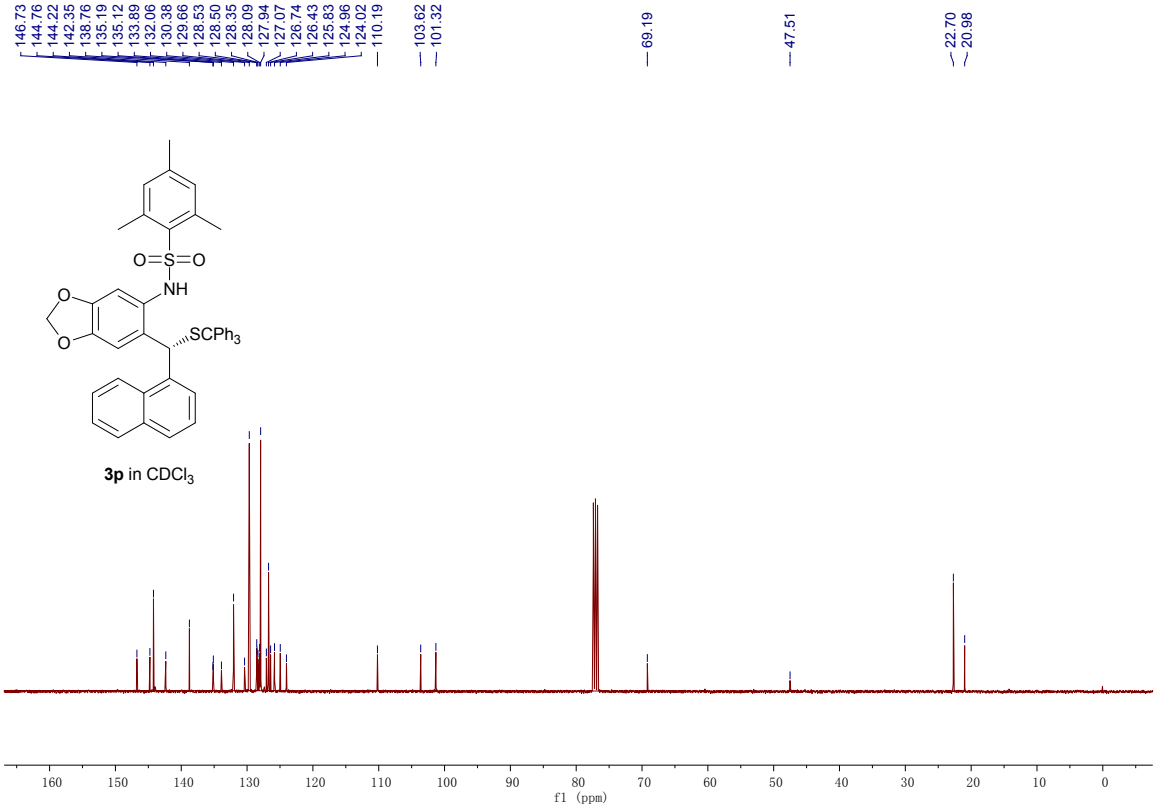
```
Additional Info : Peak(s) manually integrated
```



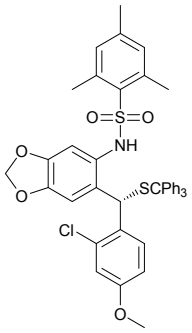

```
================================================================
                    Area Percent Report
================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  13.486 BB    0.6340  923.04181   21.98178   4.7783
   2  16.244 BV    0.7867 1.83944e4   354.02988  95.2217
```



3p in $CDCl_3$



3p in $CDCl_3$

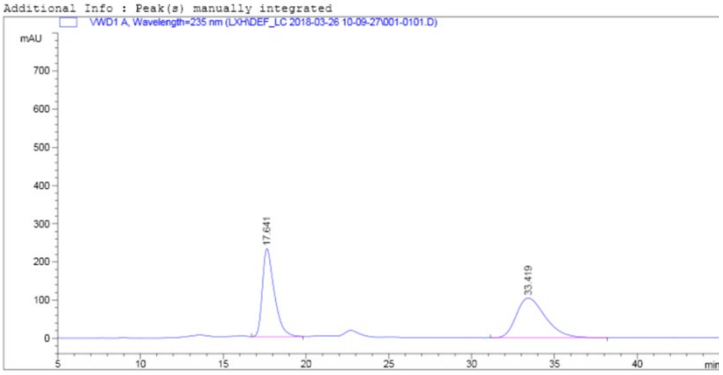


3q

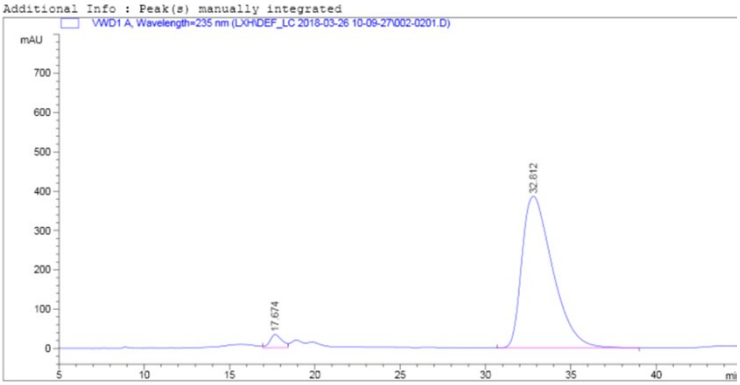
yield:80%

94%*ee*

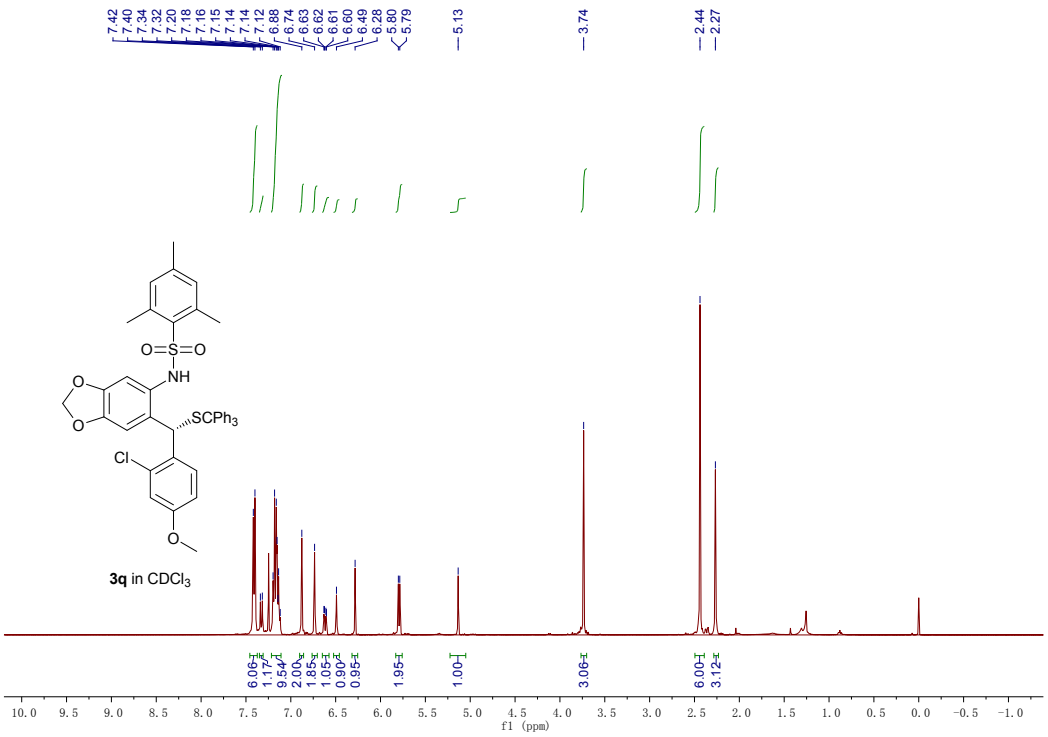
```
Sample Info     : ADH-056, 95/5, 1ml/min, 25C, 40bar, 235nm

Additional Info : Peak(s) manually integrated
```

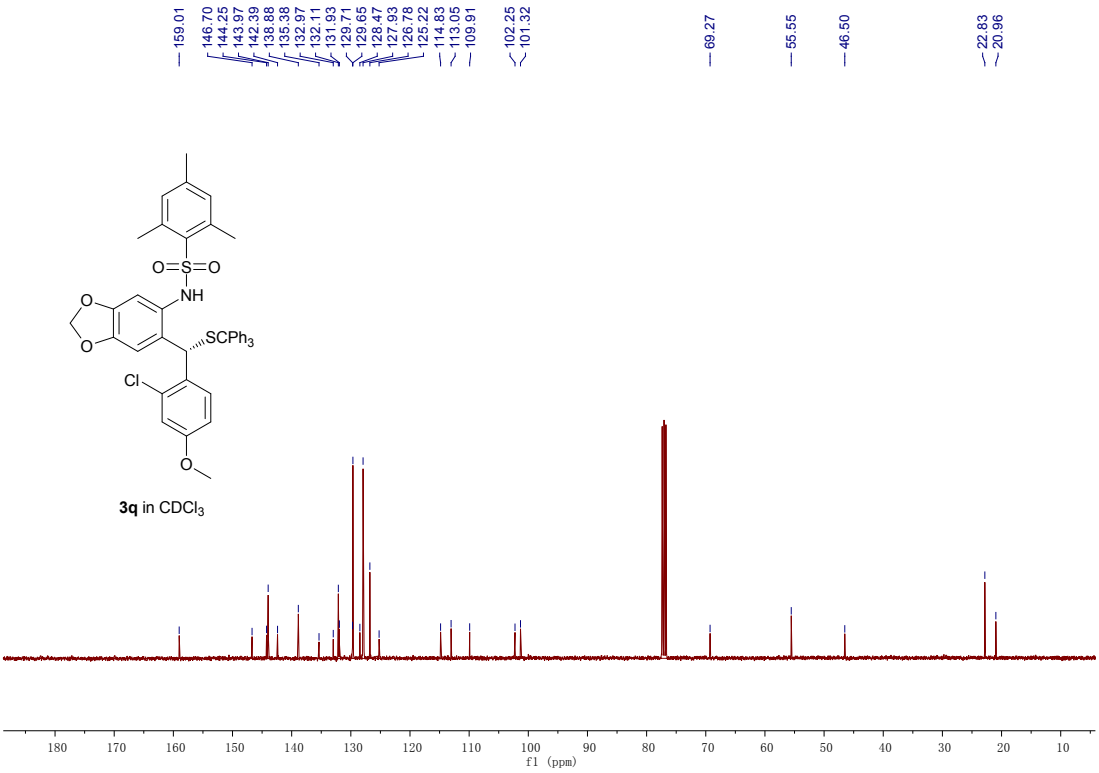


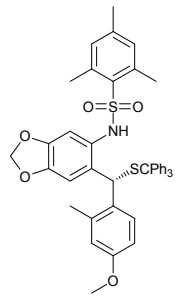

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  17.641 VB    0.7478 1.15757e4   230.96606  47.4655
   2  33.419 BB    1.8628 1.28119e4   104.17798  52.5345

Sample Info     : ADH-056, 95/5, 1ml/min, 25C, 40bar, 235nm

Additional Info : Peak(s) manually integrated
```




```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  17.674 VV    0.7217 1606.39233   32.94791   3.2223
   2  32.812 BB    1.9034 4.82460e4   385.70547  96.7777
```


7.42
7.40
7.34
7.32
7.20
7.18
7.16
7.15
7.14
7.14
7.12
6.88
6.74
6.63
6.62
6.61
6.60
6.49
6.28
5.80
5.79
5.13
3.74
2.44
2.27
O=S=O
NH
O
O
SCPh3
Cl
O
3q in CDCl3
6.06
1.17
9.54
2.05
1.85
1.05
0.90
0.95
1.95
1.00
3.06
6.00
3.12
f1 (ppm)

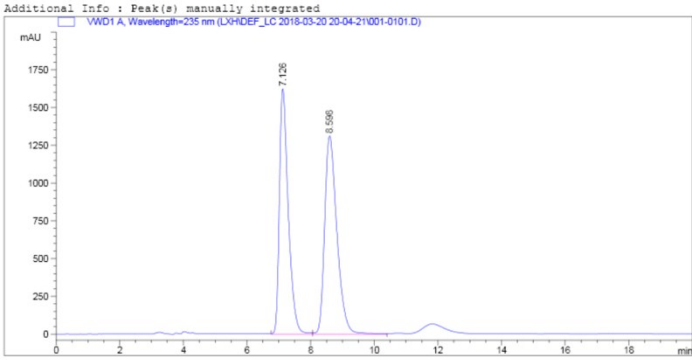

159.01
146.70
144.25
143.97
142.39
138.88
135.38
132.97
132.11
131.93
129.71
129.65
128.47
127.93
126.78
125.22
114.83
113.05
109.91
102.25
101.32
69.27
55.55
46.50
22.83
20.96
O=S=O
NH
O
O
SCPh3
Cl
O
3q in CDCl3
f1 (ppm)



3r
yield:88%
90%*ee*

```
Sample Info     : ADH0CE-EA056; 95/5; 1.0; 25; 235; 40bar
```

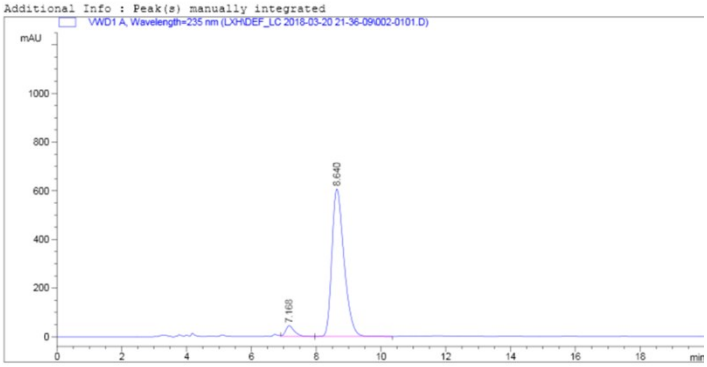
```
Additional Info : Peak(s) manually integrated
```



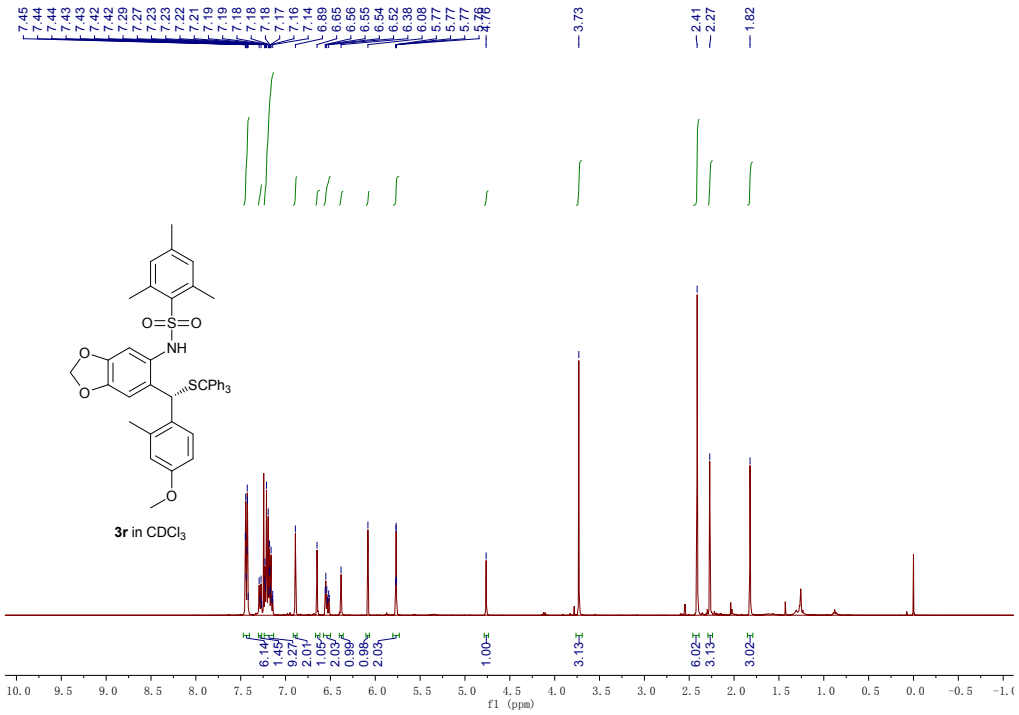

```
================================================================================
                            Area Percent Report
================================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1   7.126 VV     0.2899 3.14481e4  1624.41370  47.2098
   2   8.598 VV     0.4073 3.51653e4  1311.96777  52.7902
```

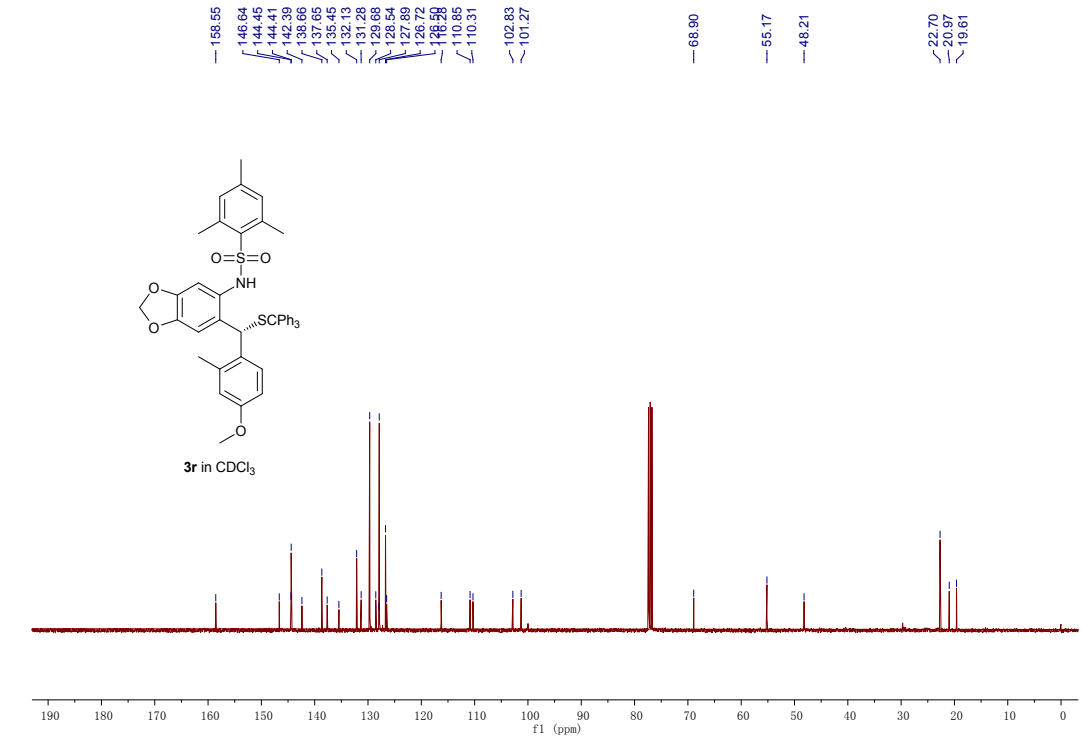
```
Sample Info     : ADH0CE-EA056; 95/5; 1.0; 25; 235; 40bar
```

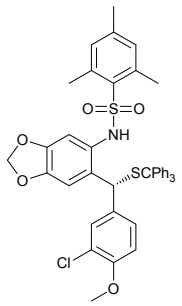
```
Additional Info : Peak(s) manually integrated
```




```
================================================================================
                            Area Percent Report
================================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1   7.168 VV     0.2828  856.72272   44.79903   5.1350
   2   8.640 VB     0.3960 1.58274e4   606.89929  94.8650
```


7.45
7.44
7.44
7.43
7.43
7.42
7.42
7.29
7.27
7.23
7.23
7.22
7.21
7.19
7.19
7.18
7.18
7.18
7.17
7.16
7.14
6.89
6.65
6.56
6.55
6.54
6.52
6.38
6.08
5.77
5.77
5.76
4.76
3.73
2.41
2.27
1.82
O=S=O
NH
O
O
SCPh3
O
3r in CDCl3
6.14
1.45
9.27
2.01
1.05
2.03
0.99
0.98
2.03
1.00
3.13
6.02
3.13
3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5
f1 (ppm)


158.55
146.64
144.45
144.41
142.39
138.66
137.65
135.45
132.13
131.28
129.68
128.54
127.89
126.72
110.85
110.31
102.83
101.27
68.90
55.17
48.21
22.70
20.97
19.61
O=S=O
NH
O
O
SCPh3
O
3r in CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



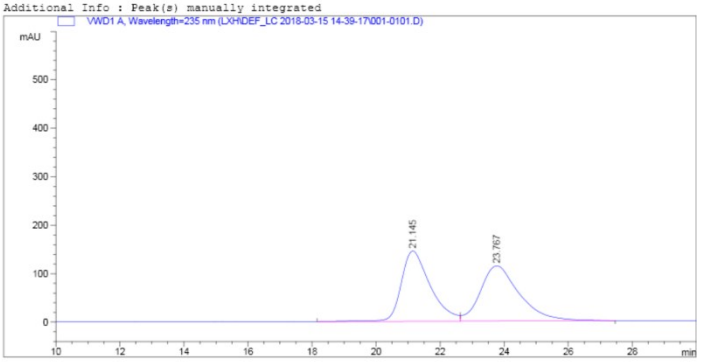
3s

yield:94%

90%*ee*

Sample Info : ADH-056; 97/3; 1.0mL/min; 40bar; 25C; 235nm

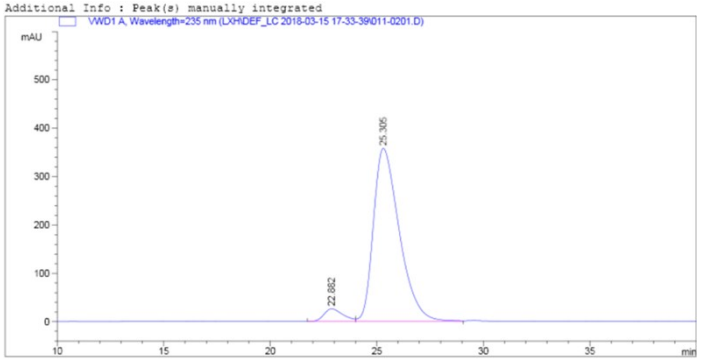
Additional Info : Peak(s) manually integrated



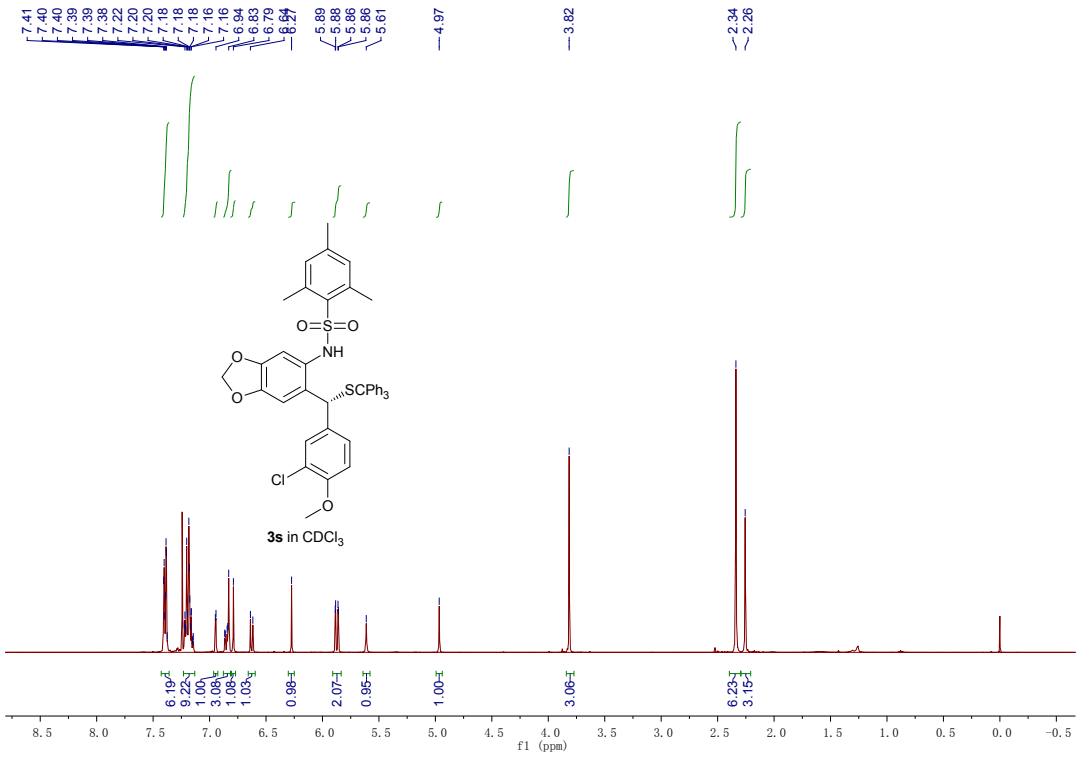

```
================================================================================
                          Area Percent Report
================================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  21.145 BV    0.9597 9102.51270  144.96864  48.5743
   2  23.767 VB    1.2304 9636.86230  113.71144  51.4257
```

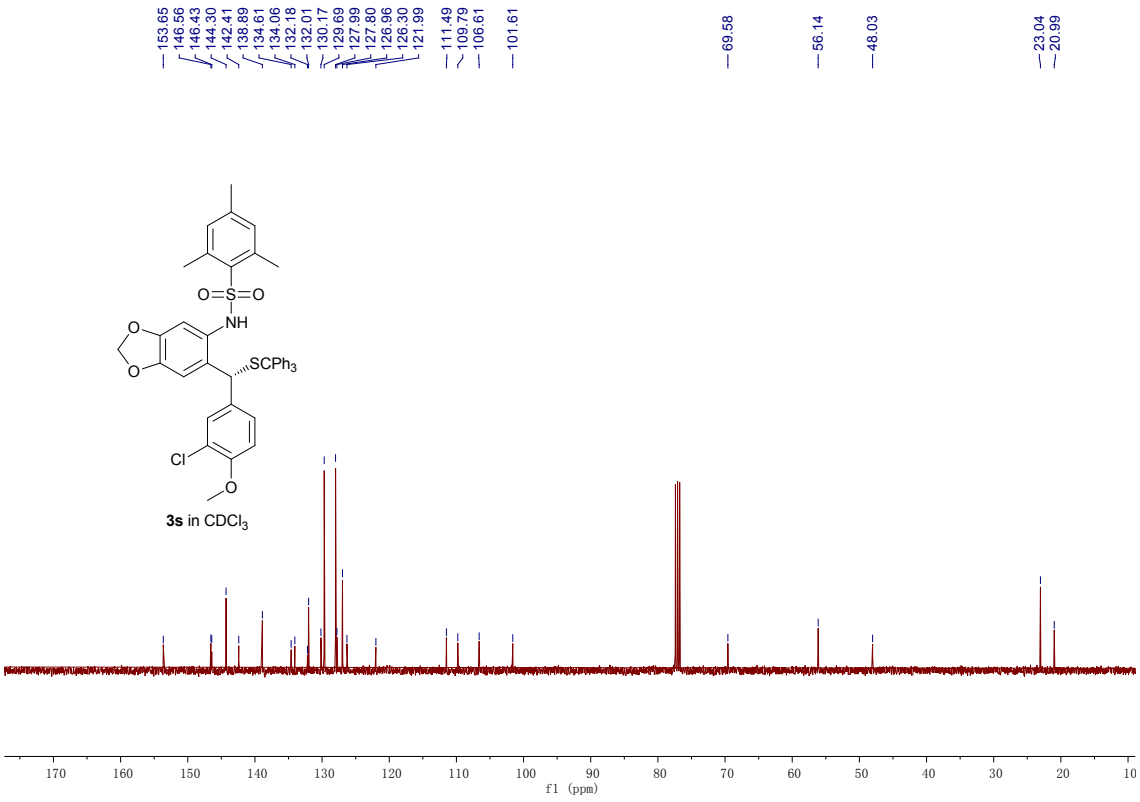
Sample Info : ADH-056; 97/3; 0.9mL/min; 37bar; 25C; 235nm

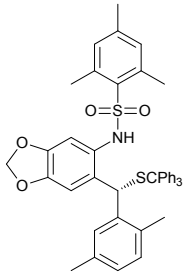
Additional Info : Peak(s) manually integrated




```
================================================================================
                          Area Percent Report
================================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  22.882 BV    0.9337 1605.44360   26.13131   5.0418
   2  25.305 VB    1.3019 3.02370e4   357.79697  94.9582

Totals :                  3.18424e4   383.92827
```


7.41
7.40
7.40
7.39
7.39
7.38
7.22
7.20
7.20
7.18
7.18
7.16
7.16
6.94
6.83
6.79
6.64
6.27
5.89
5.88
5.86
5.86
5.61
4.97
3.82
2.34
2.26
O=S=O
NH
O
O
SCPh3
Cl
O
3s in CDCl3
6.19
9.22
1.00
3.08
1.08
1.03
0.98
2.07
0.95
1.00
3.06
6.23
3.15
f1 (ppm)


153.65
146.56
146.43
144.30
142.41
138.89
134.61
134.06
132.18
132.01
130.17
129.69
127.99
127.80
126.96
126.30
121.99
111.49
109.79
106.61
101.61
69.58
56.14
48.03
23.04
20.99
O=S=O
NH
O
O
SCPh3
Cl
O
3s in CDCl3
f1 (ppm)



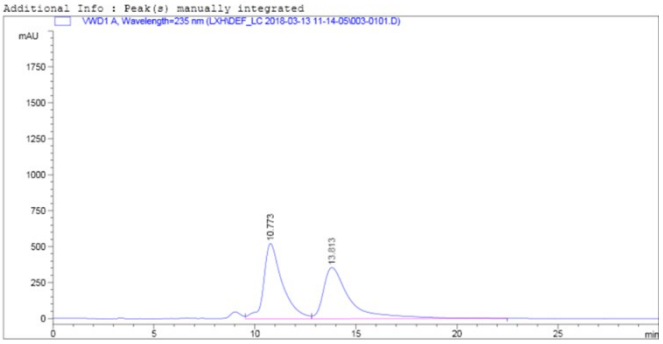
3t

yield:98%

91%*ee*

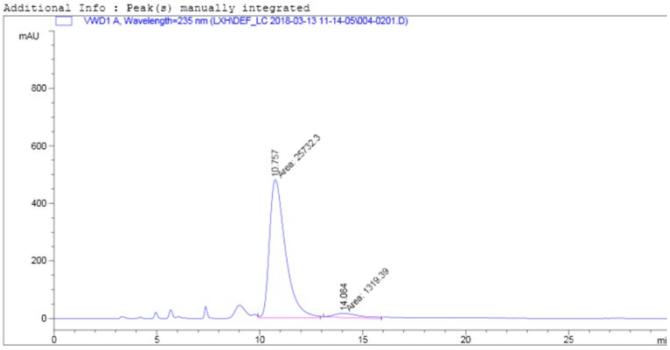
```
Sample Info     : ODH-NE054; 97/3; 1.0mL/min; 40bar; 25C; 235nm
```

```
Additional Info : Peak(s) manually integrated
```

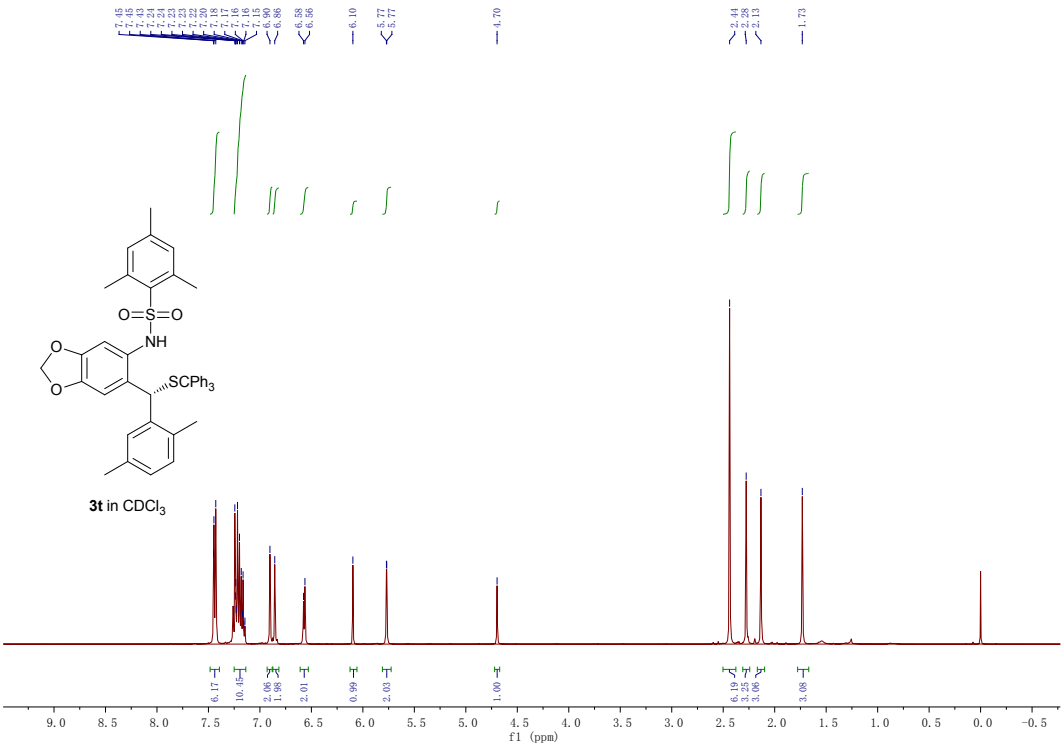



```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  10.773 VV     0.9185 3.33563e4   522.19012  50.9460
   2  13.813 VB     1.3221 3.21175e4   355.42850  49.0540

Sample Info     : ODH-NE054; 97/3; 1.0mL/min; 40bar; 25C; 235nm
```

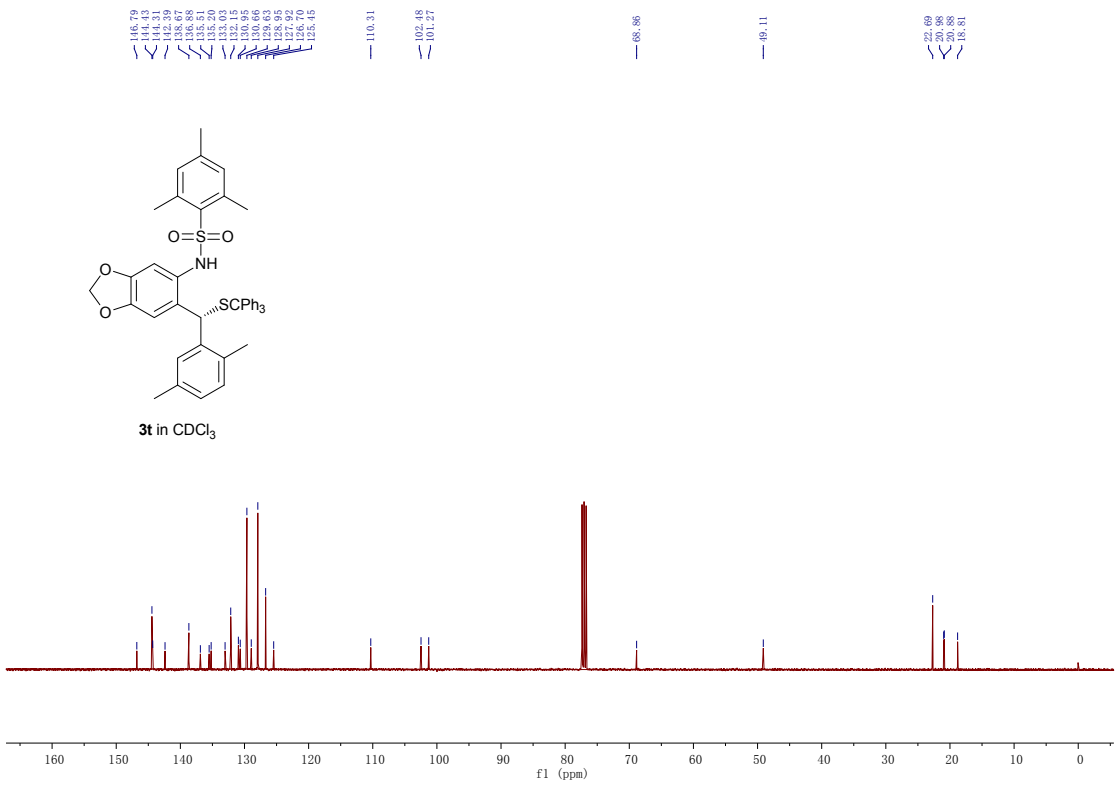
```
Additional Info : Peak(s) manually integrated
```



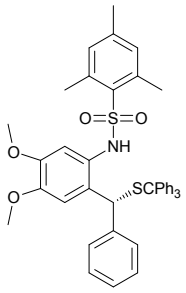

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  10.757 MM     0.8952 2.57323e4   479.07101  95.1227
   2  14.084 MM     1.5647 1319.39441   14.05414   4.8773
```



3t in $CDCl_3$



3t in $CDCl_3$



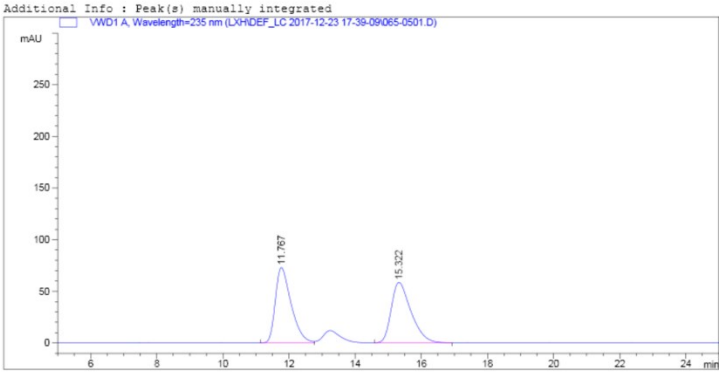
3u

yield: 79%

90%*ee*

```
Sample Info     : ADH0CE-EA056, 1ml/min, 95/5, 25C, 235nm, 59bar
```

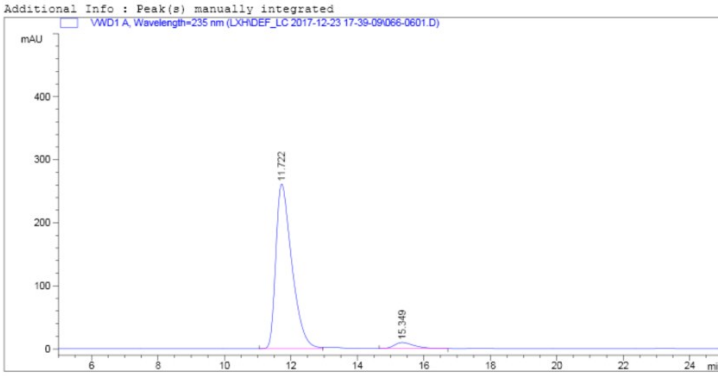
```
Additional Info : Peak(s) manually integrated
```



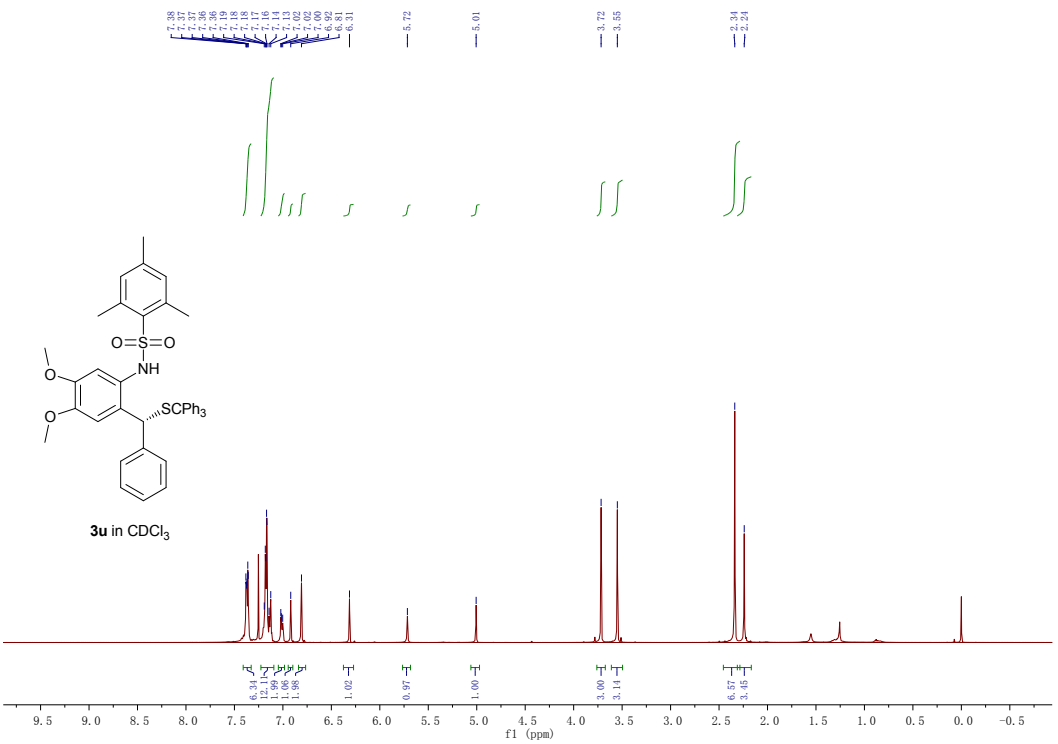

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  11.767 BV    0.4981 2423.21436   72.96810  49.9186
   2  15.322 BB    0.6225 2431.11475   58.58047  50.0814
```

```
Sample Info     : ADH0CE-EA056, 1ml/min, 95/5, 25C, 235nm, 59bar
```

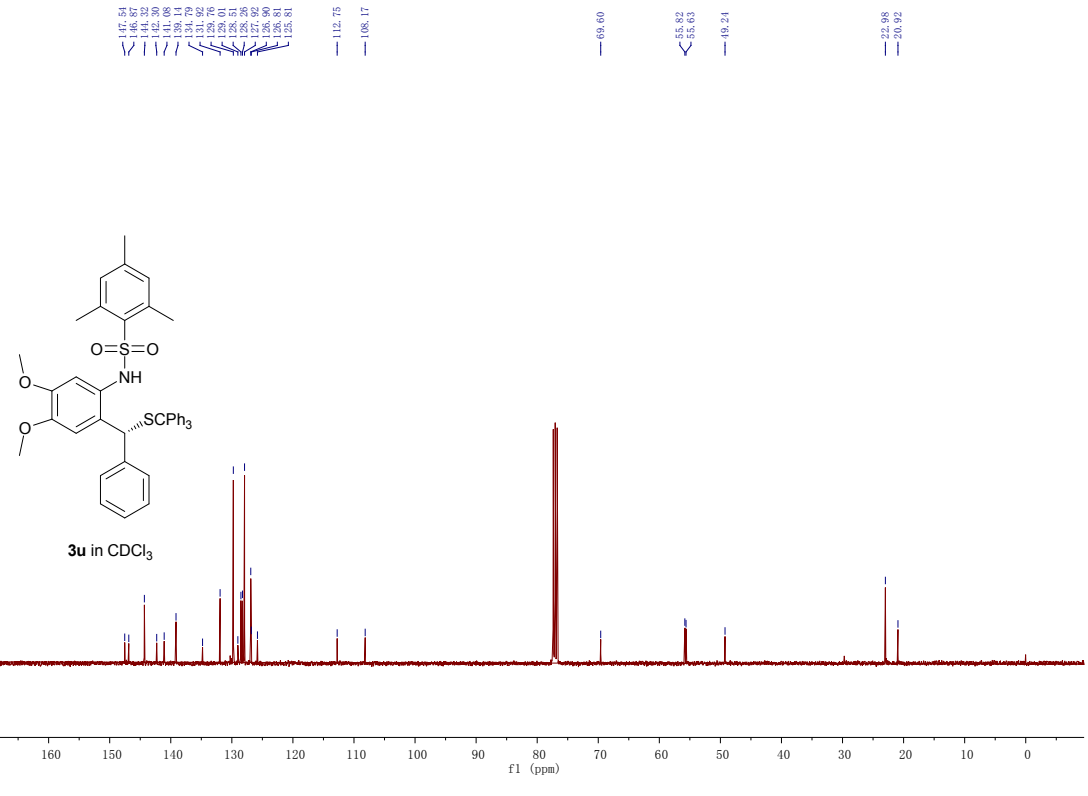
```
Additional Info : Peak(s) manually integrated
```



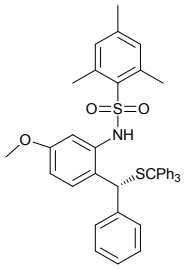

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  11.722 BV    0.5028 8745.36719  261.15497  95.5486
   2  15.349 BB    0.6174  407.43201    9.80364   4.4514
```



3u in $CDCl_3$



3u in $CDCl_3$

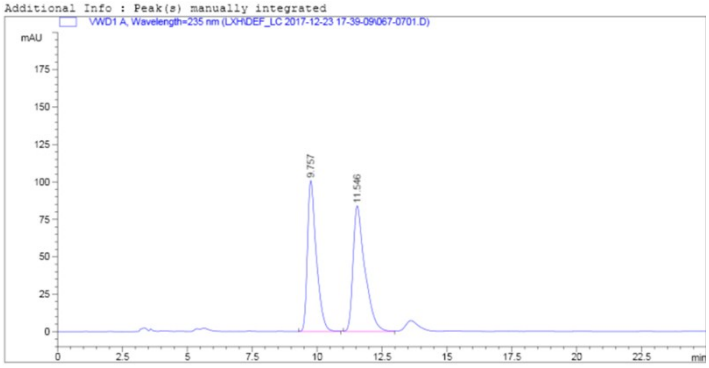


3v

yield: 88%

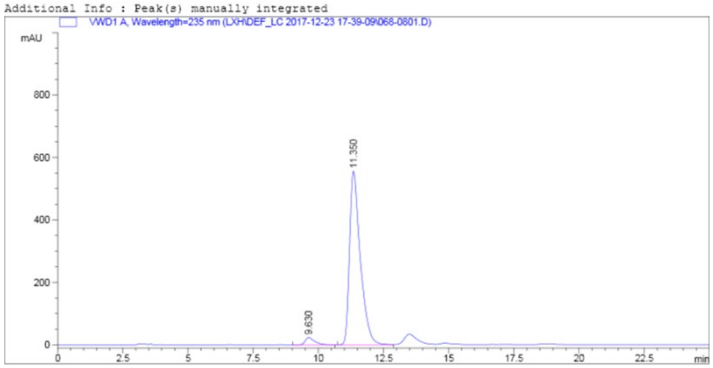
93%*ee*

```
Sample Info     : ADH0CE-EA056, 1ml/min, 95/5, 25C, 235nm, 59bar

Additional Info : Peak(s) manually integrated
```

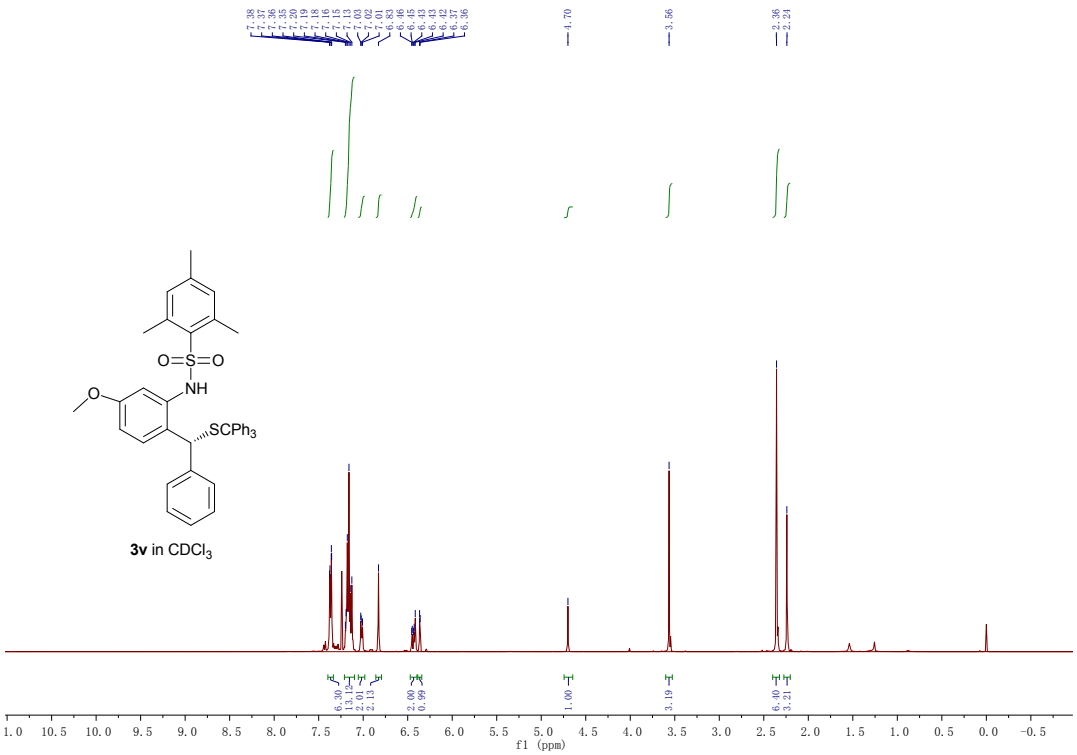


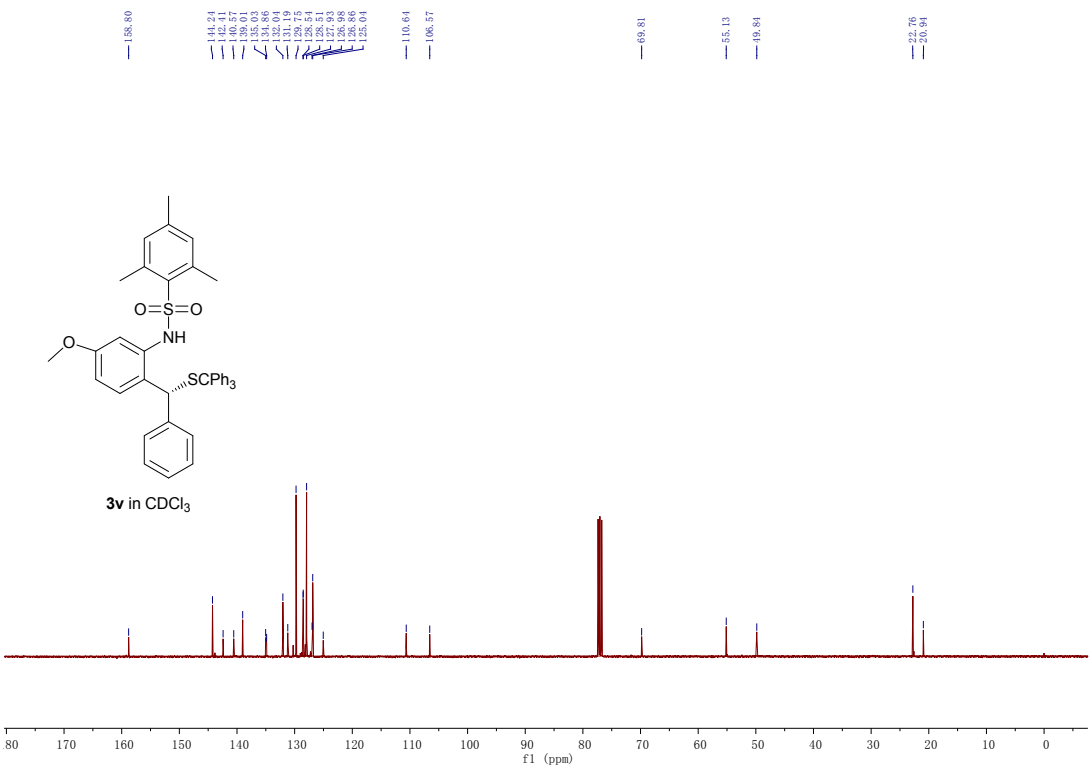

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1   9.757 BB    0.3470 2394.78247  100.82117  47.3765
   2  11.546 BB    0.4559 2660.00708   83.87397  52.6235
```

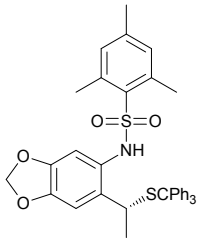
```
Sample Info     : ADH0CE-EA056, 1ml/min, 95/5, 25C, 235nm, 59bar

Additional Info : Peak(s) manually integrated
```




```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1   9.630 VB    0.3464  553.77612   23.24668   3.3767
   2  11.350 BV    0.4172 1.58463e4   555.55170  96.6233
```


7.38
7.37
7.36
7.35
7.20
7.19
7.18
7.16
7.15
7.13
7.04
7.03
7.02
7.01
6.48
6.46
6.45
6.43
6.42
6.37
6.36
4.70
3.56
2.36
2.24
O=S=O
NH
O
SCPh3
3v in CDCl3
6.30
13.12
10.14
2.13
2.00
0.99
1.00
3.19
6.40
3.21
f1 (ppm)


158.80
144.24
142.41
140.57
139.01
135.03
134.86
132.04
131.19
129.75
128.54
128.51
127.93
126.98
126.86
125.04
110.64
106.57
69.81
55.13
49.84
22.76
20.94
O=S=O
NH
O
SCPh3
3v in CDCl3
f1 (ppm)

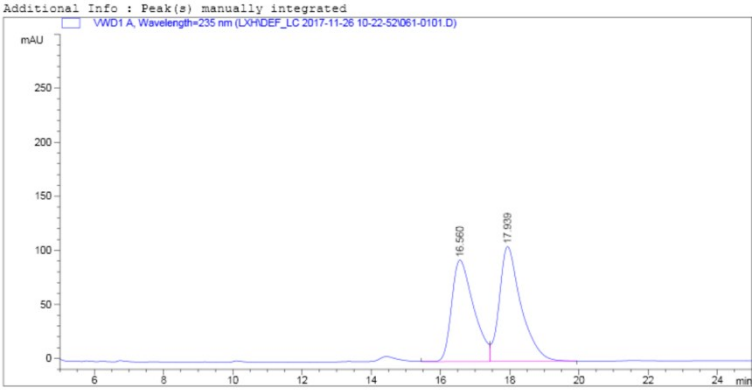


3w

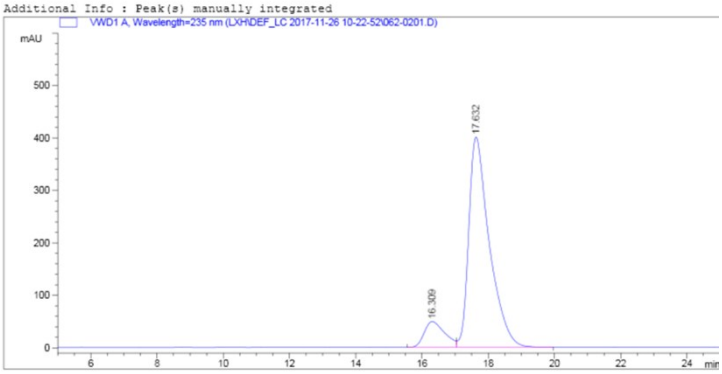
yield: 87%

78%*ee*

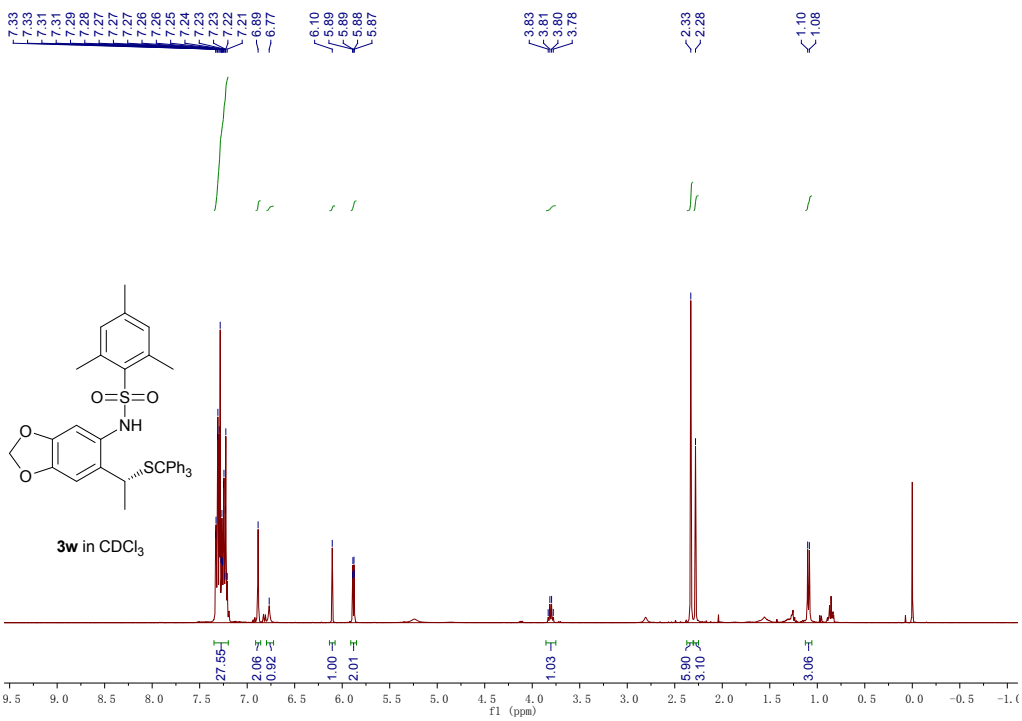
```
Sample Info     : ADH0CE-KE056, 95/5, 1.0, 235, 39, 25

Additional Info : Peak(s) manually integrated
```

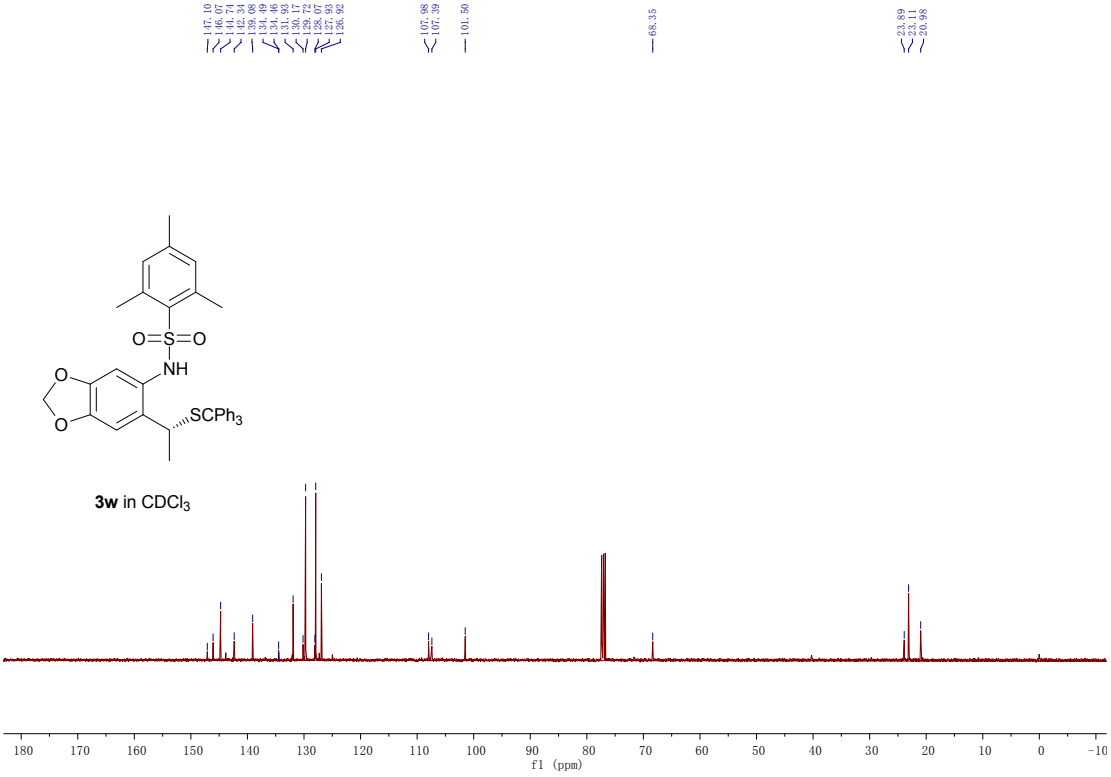


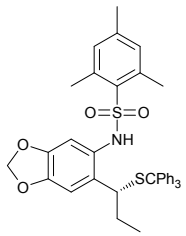

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]  mAU   *s    [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  16.560 VV    0.6617 4153.37500   93.88424  47.2587
   2  17.939 VB    0.6374 4635.22070  106.17902  52.7413


  Sample Info     : ADH0CE-KE056, 95/5, 1.0, 235, 39, 25

  Additional Info : Peak(s) manually integrated
```




```
  =====================================================================
                          Area Percent Report
  =====================================================================

  Sorted By             :      Signal
  Multiplier:                   :      1.0000
  Dilution:                     :      1.0000
  Use Multiplier & Dilution Factor with ISTDs


  Signal 1: VWD1 A, Wavelength=235 nm

  Peak RetTime Type  Width     Area      Height     Area
    #   [min]       [min]  mAU   *s    [mAU   ]      %
  ----|-------|----|-------|----------|----------|--------|
     1  16.309 BV    0.6504 2119.95215   49.13711  10.9265
     2  17.632 VB    0.6340 1.72821e4   400.85913  89.0735
```


7.33
7.33
7.31
7.31
7.29
7.28
7.27
7.27
7.26
7.26
7.25
7.24
7.23
7.23
7.22
7.21
6.89
6.77
6.10
5.89
5.89
5.88
5.87
3.83
3.81
3.80
3.78
2.33
2.28
1.10
1.08
O=S=O
NH
O
O
SCPh3
3w in CDCl3
27.55
2.06
0.92
1.00
2.01
1.03
5.90
3.10
3.06
f1 (ppm)


147.10
146.07
144.71
142.34
139.68
134.49
134.46
131.93
130.17
128.72
128.07
127.93
126.92
107.98
107.39
101.50
68.35
23.89
23.11
20.98
O=S=O
NH
O
O
SCPh3
3w in CDCl3
f1 (ppm)



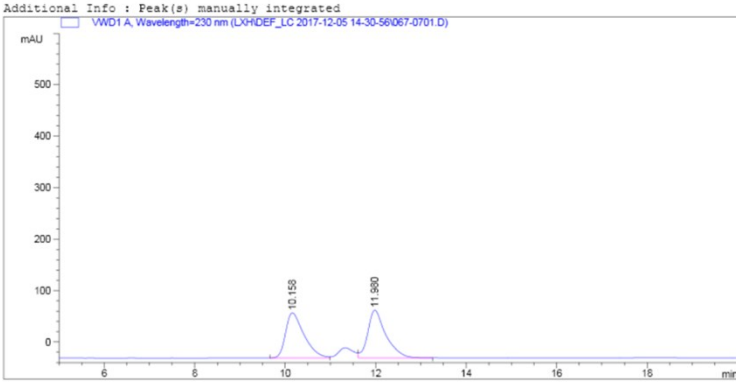
3x

yield: 89%

84%*ee*

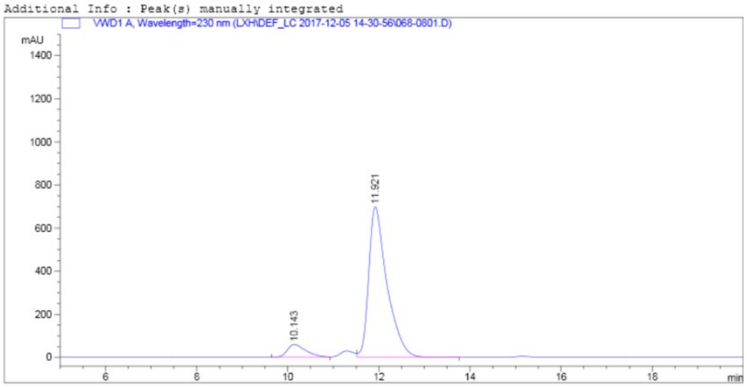
```
Sample Info     : ADH0CE-EA056, 95/5; 1.0; 235nm, 40bar,25C
```

```
Additional Info : Peak(s) manually integrated
```

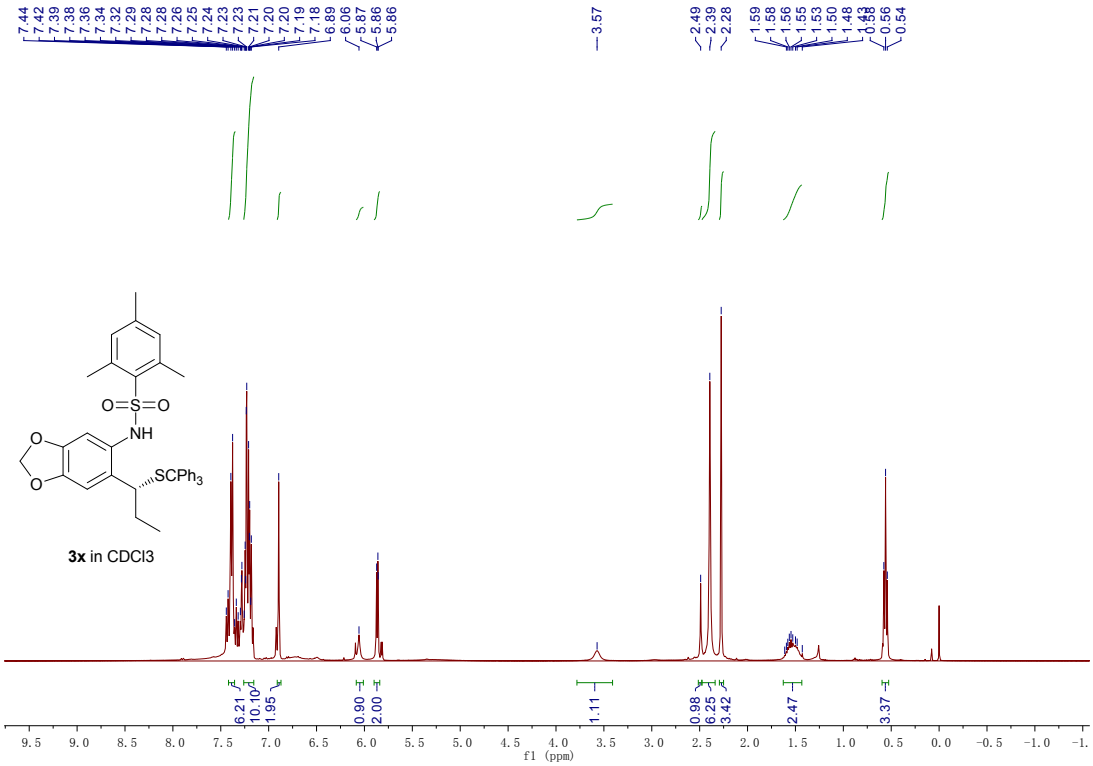


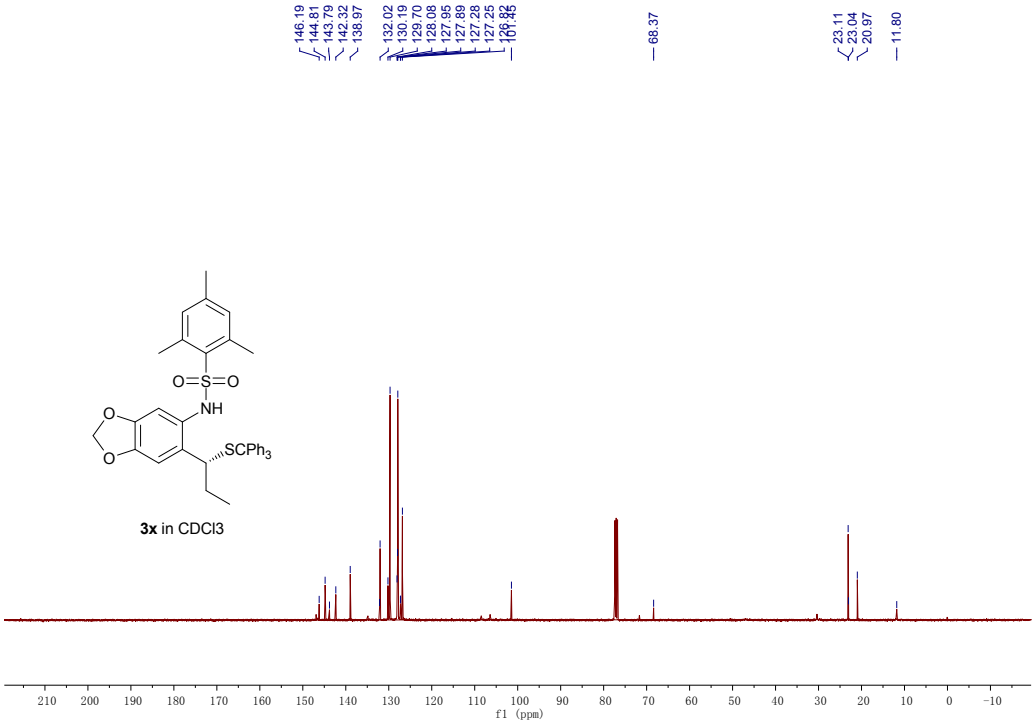

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=230 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s    [mAU   ]      %
----|-------|----|-------|----------|----------|-------|
   1  10.158 BV     0.4194 2485.95068   87.73550  49.0659
   2  11.980 VB     0.4025 2580.60645   92.95734  50.9341
Sample Info     : ADH0CE-EA056, 95/5; 1.0; 235nm, 40bar,25C
```

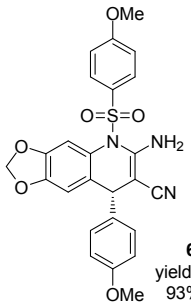
```
Additional Info : Peak(s) manually integrated
```




```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=230 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s    [mAU   ]      %
----|-------|----|-------|----------|----------|-------|
   1  10.143 BV     0.4253 1726.20593   60.11020   8.1672
   2  11.921 VB     0.4059 1.94097e4   698.09943  91.8328
```


7.44
7.42
7.39
7.38
7.36
7.34
7.32
7.29
7.28
7.28
7.26
7.25
7.24
7.23
7.23
7.21
7.20
7.20
7.19
7.18
6.89
6.06
5.87
5.86
5.86
3.57
2.49
2.39
2.28
1.59
1.58
1.56
1.55
1.53
1.50
1.48
0.56
0.54
O=S=O
NH
SCPh3
3x in CDCl3
6.21
10.10
1.95
0.90
2.00
1.11
0.98
6.25
3.42
2.47
3.37
f1 (ppm)

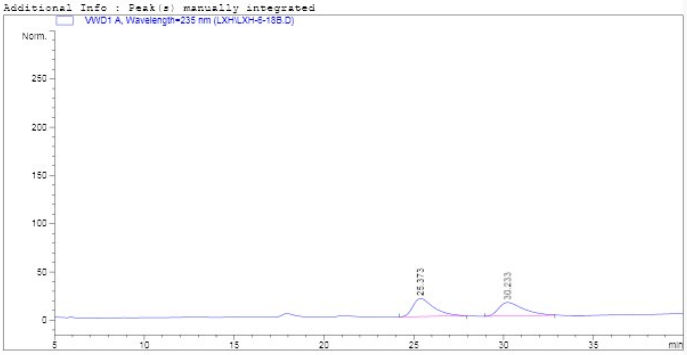

146.19
144.81
143.79
142.32
138.97
132.02
130.19
129.70
128.08
127.95
127.89
127.28
127.25
68.37
23.11
23.04
20.97
11.80
O=S=O
NH
SCPh3
3x in CDCl3
f1 (ppm)



6a
yield: 61%
93% ee

Sample Info : ADH-039, 1.0ml/min, 25C,80/20, 235nm, 40bar

Additional Info : Peak(s) manually integrated



Area Percent Report

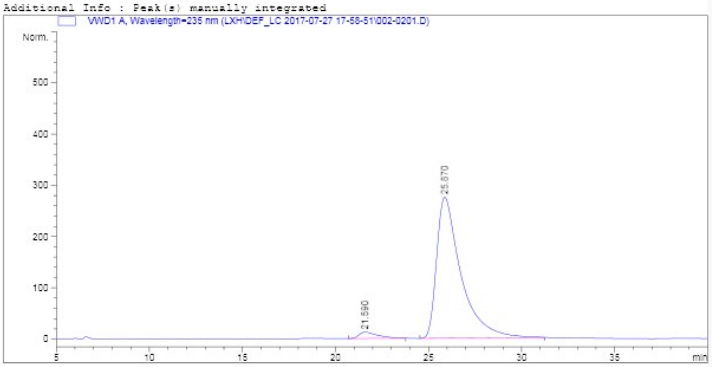
Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=235 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	25.373	BB	1.1676	1522.29089		18.65261	53.4183
2	30.233	BB	1.3228	1327.46472		13.89503	46.5817

Sample Info : ADH-039, 1.0ml/min, 25C,80/20, 235nm, 40bar

Additional Info : Peak(s) manually integrated

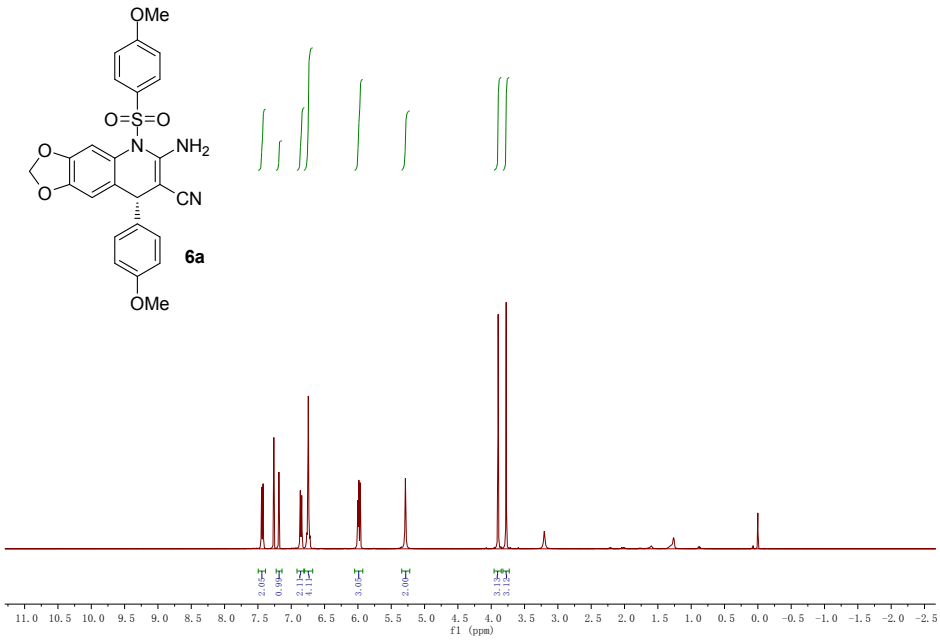


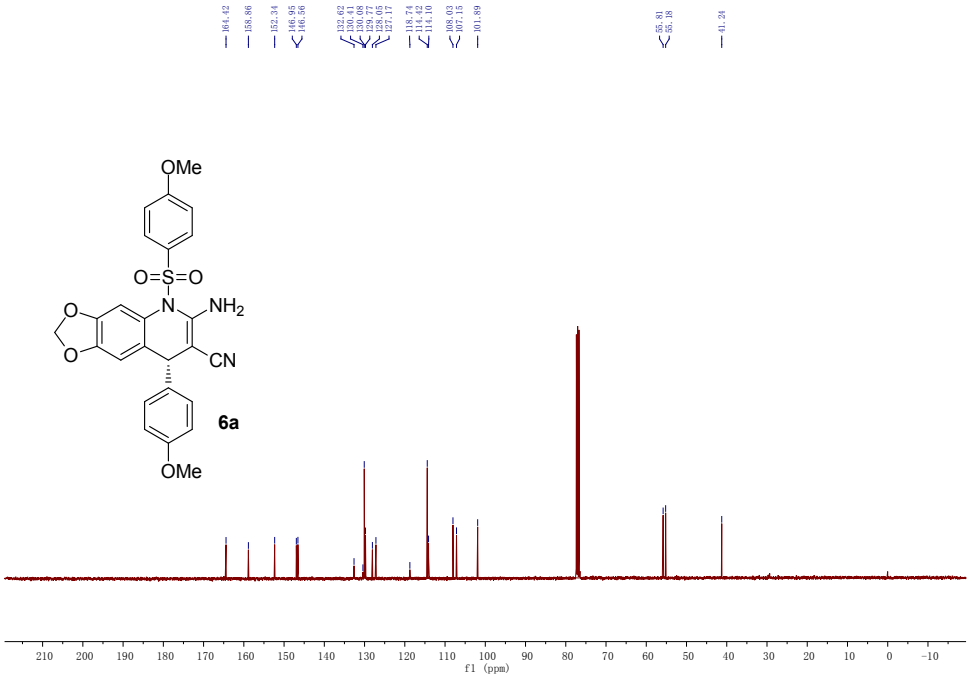
Area Percent Report

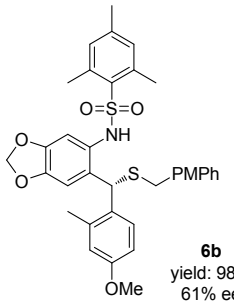
Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=235 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	*s	Height [mAU]	Area %
1	21.590	BB	0.9795	859.41003		12.84066	0.3253
2	25.870	BB	1.3141	2.49851e4		275.16528	96.6747

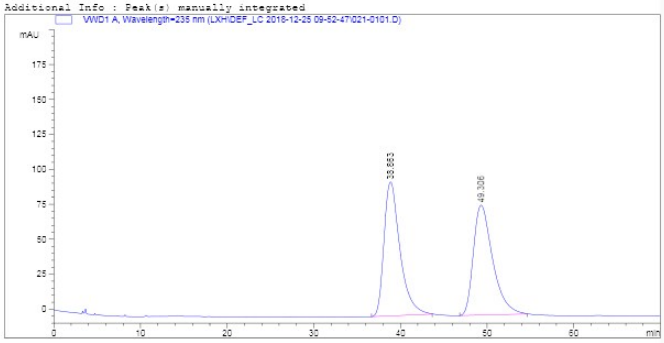

OMe
O=S=O
N
NH2
O
O
CN
6a
OMe
2.05
0.99
2.11
4.13
3.05
2.00
3.13
3.15
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0 -2.5
f1 (ppm)


164.42
158.86
152.34
146.95
146.56
132.62
130.41
130.08
129.77
128.05
127.17
118.74
114.42
114.10
108.03
107.15
101.89
65.81
65.18
41.24
OMe
O=S=O
N
NH2
O
O
CN
6a
OMe
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



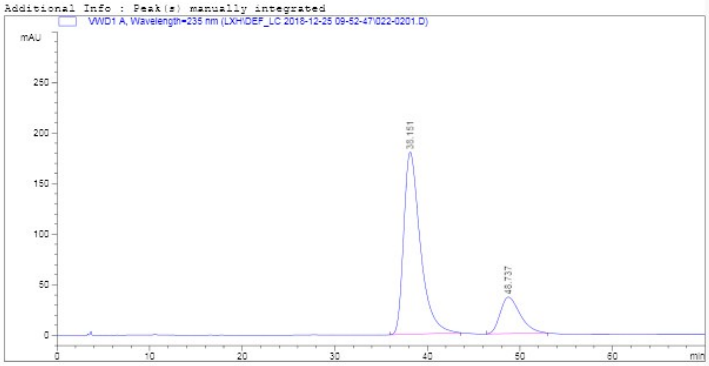
6b
yield: 98%
61% ee

```
Sample Info     : IC00CE-WJ021, 90/10, 1.0ml/min, 25C, 230nm,  36bar

Additional Info : Peak(s) manually integrated
```

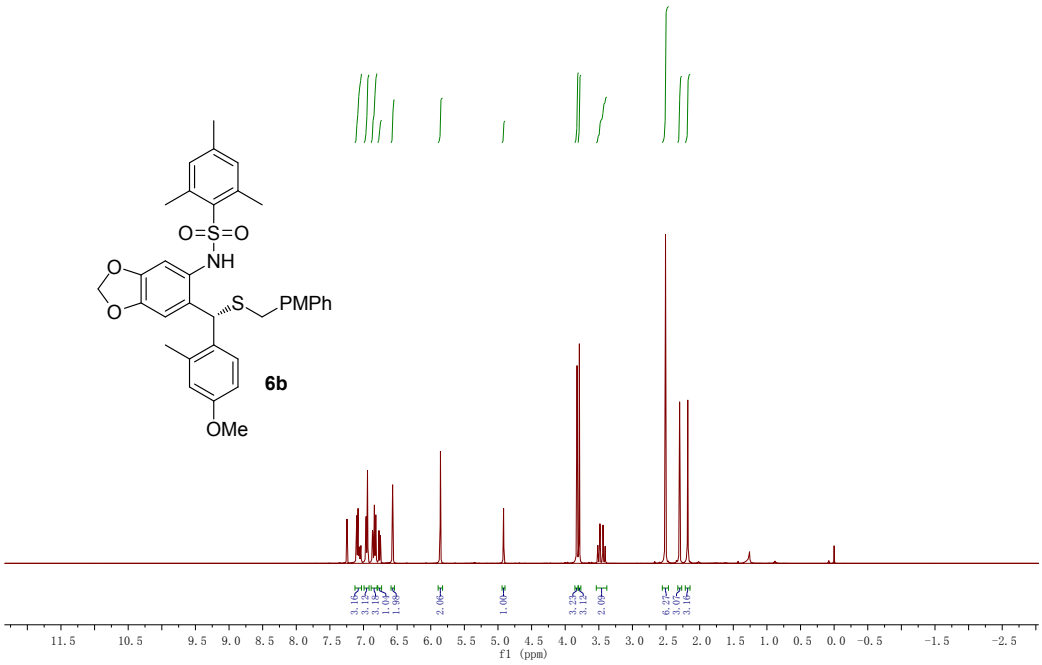


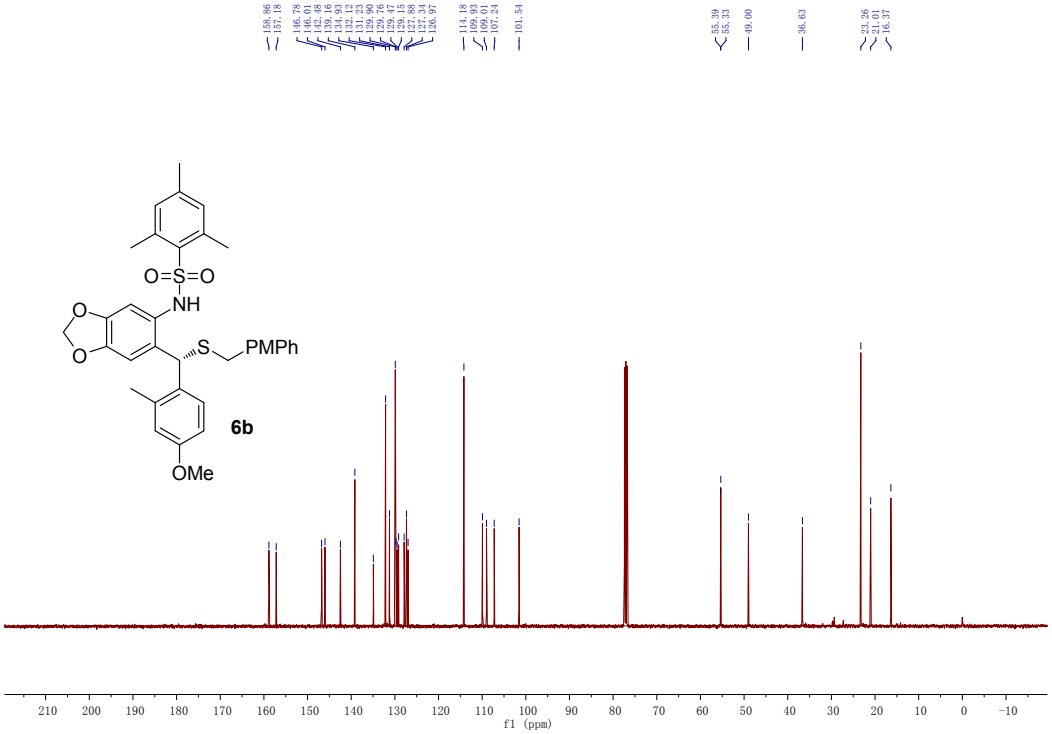

```
================================================================================
                            Area Percent Report
================================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s    [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  38.863 BB    1.8577 1.23012e4    95.79994  50.2578
   2  49.306 BB    2.1979 1.21749e4    78.63862  49.7422
```

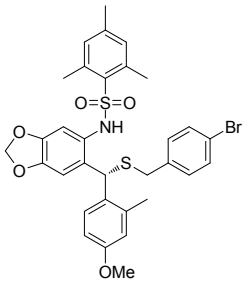
```
Sample Info     : IC00CE-WJ021, 90/10, 1.0ml/min, 25C, 230nm,  36bar

Additional Info : Peak(s) manually integrated
```




```
================================================================================
                            Area Percent Report
================================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s    [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  38.151 BB    1.8880 2.24340e4   179.99419  80.5309
   2  48.737 BB    2.0289 5423.69281   36.02211  19.4691
```


O=S=O
NH
O
O
S
PMPh
6b
OMe
f1 (ppm)

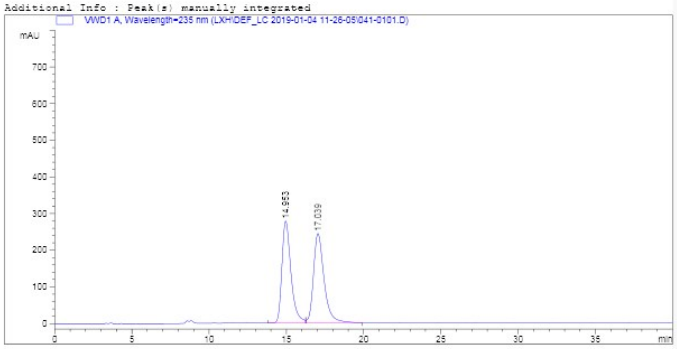

O=S=O
NH
O
O
S
PMPh
6b
OMe
f1 (ppm)



6c
yield: 91%
65% ee

```
Sample Info     : IC00CE-WJ021; 90/10; 1.0; 98bar; 235nm
```

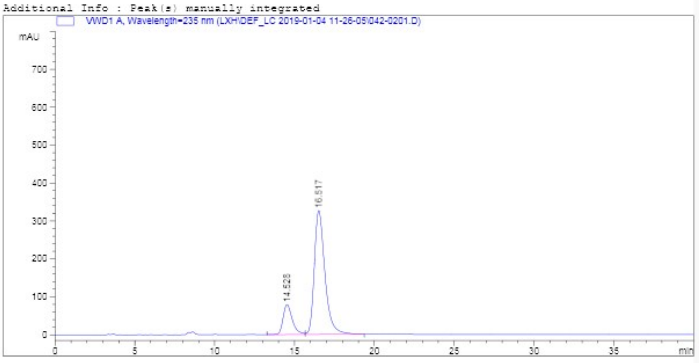
Additional Info : Peak(s) manually integrated



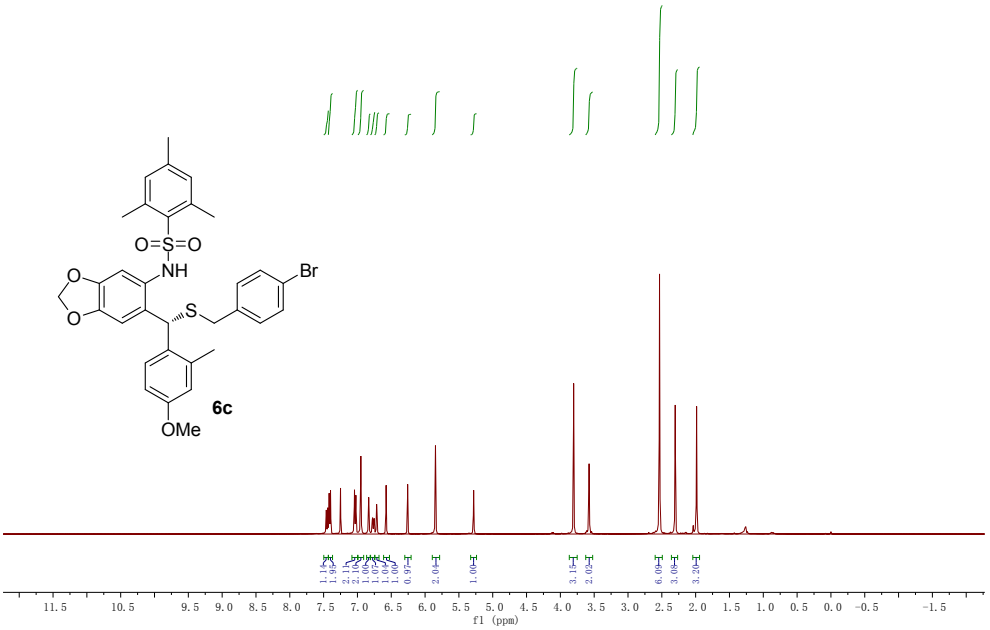

```
=====================================================================
                    Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]      [min]  mAU   *s    [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  14.953 BV    0.6175 1.13189e4   275.14008  49.2691
   2  17.039 VB    0.7236 1.16547e4   243.82382  50.7309
```

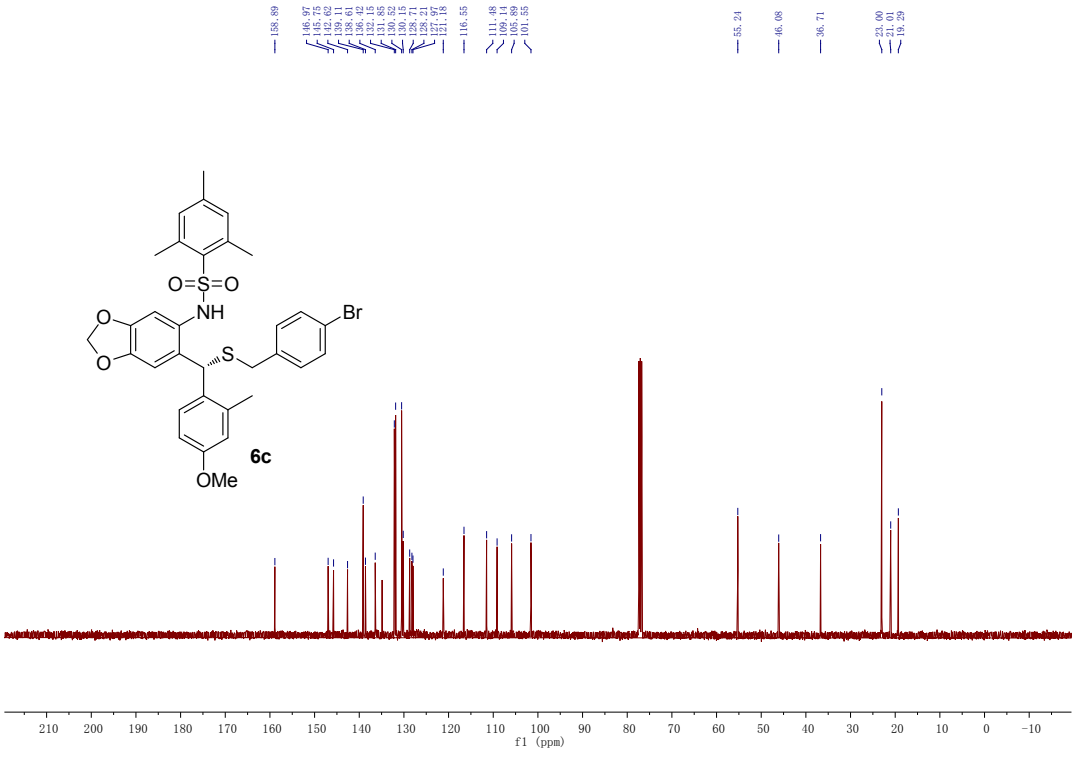
```
Sample Info     : IC00CE-WJ021; 90/10; 1.0; 98bar; 235nm
```

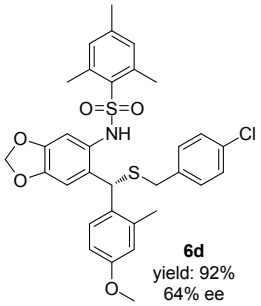
Additional Info : Peak(s) manually integrated




```
=====================================================================
                    Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]      [min]  mAU   *s    [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  14.528 BV    0.6091 3161.49268   78.82658  17.3446
   2  16.517 VB    0.6999 1.50660e4   326.51437  82.6554
```

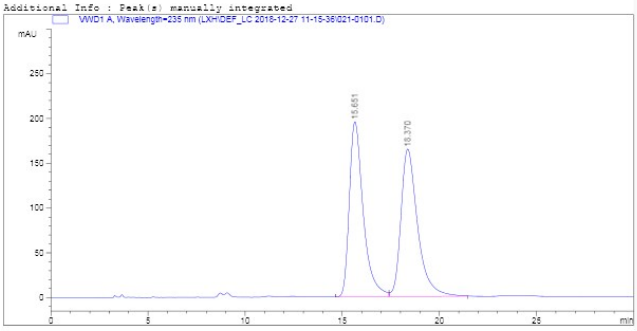

O=S=O
NH
Br
O
O
S
6c
OMe
1.14
1.93
2.15
2.10
1.07
1.04
1.00
0.97
2.04
1.06
3.15
2.02
6.09
3.08
3.20
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.5
f1 (ppm)


158.89
146.97
145.75
142.62
139.11
138.61
136.42
132.15
131.85
130.22
130.15
128.71
128.21
127.67
121.18
116.55
111.48
109.14
108.11
105.89
101.55
55.24
46.08
36.71
23.00
21.01
19.29
O=S=O
NH
Br
O
O
S
6c
OMe
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

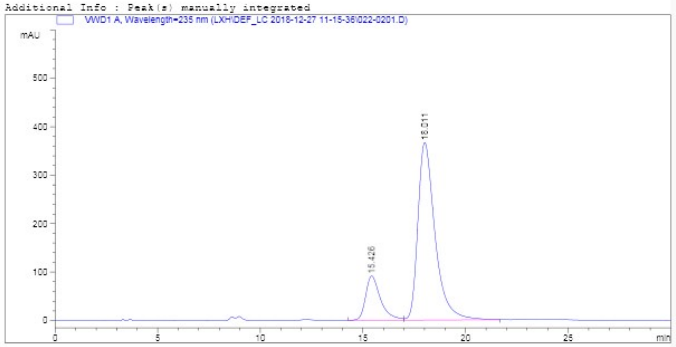


6d
yield: 92%
64% ee

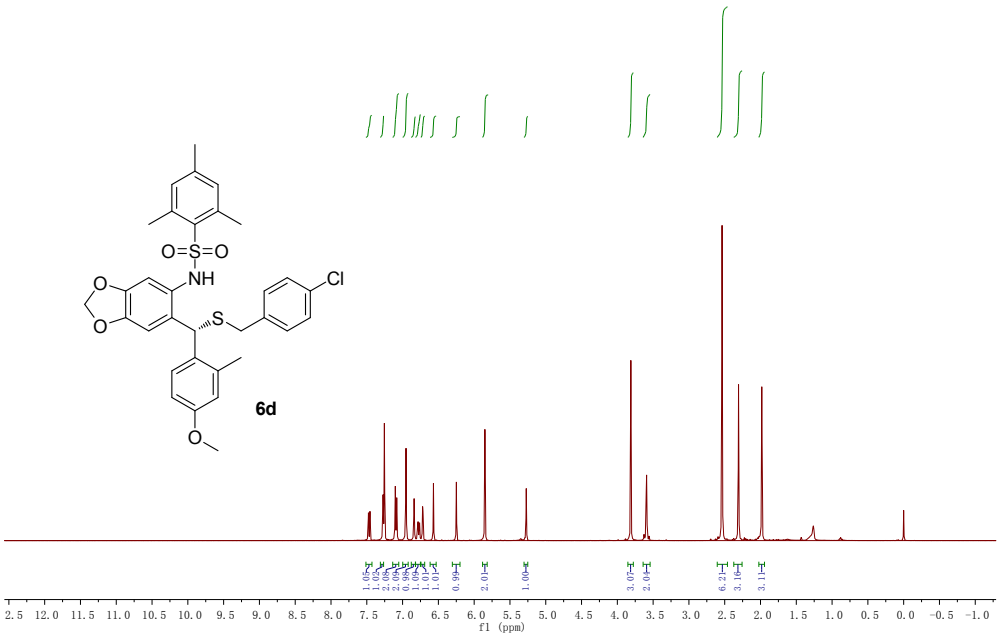
```
Sample Info      : IC00CE-WJ021; 90/10; 1.0; 235nm; 35bar

Additional Info : Peak(s) manually integrated
```

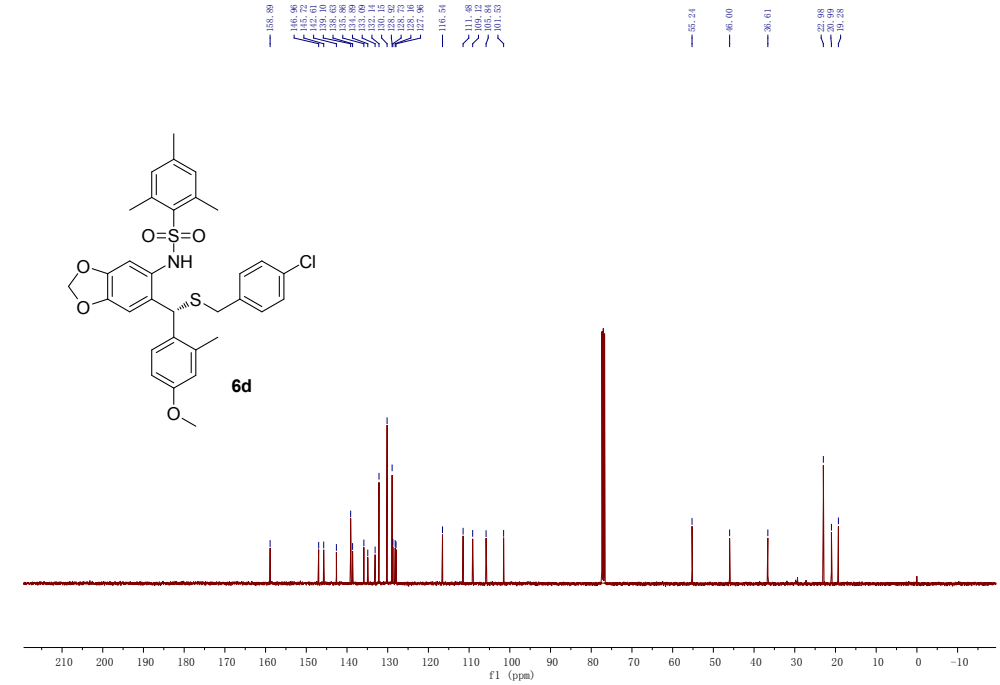


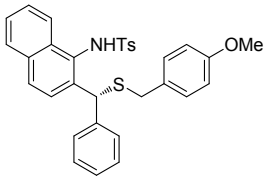

```
=====================================================================
                    Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]  mAU   *s    [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  15.651 BV     0.7482 9729.58301  195.65778  49.7817
   2  18.370 VB     0.9000 9825.00293  164.64156  50.2183

Sample Info      : IC00CE-WJ021; 90/10; 1.0; 235nm; 35bar

Additional Info : Peak(s) manually integrated
```




```
=====================================================================
                    Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]  mAU   *s    [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  15.426 BV     0.7517 4603.60645   91.47147  17.8006
   2  18.011 VB     0.8751 2.12584e4   366.27634  82.1994
```

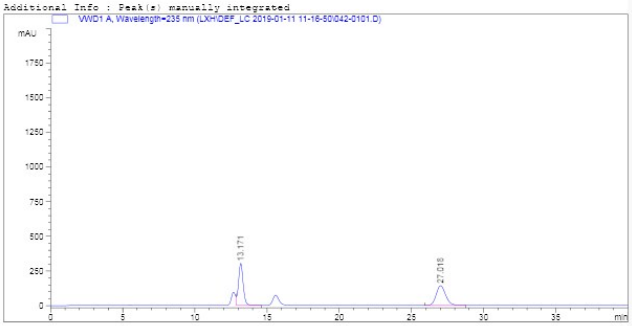

O=S=O
NH
Cl
O
O
S
O
6d
1.05
1.02
2.08
2.08
1.09
1.01
1.04
0.99
2.01
1.00
3.07
2.04
6.21
3.16
3.11
2.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


158.89
146.96
145.72
142.61
139.10
138.63
135.86
133.89
133.09
132.14
130.15
129.52
128.73
125.16
123.86
116.54
111.48
109.72
105.84
101.53
55.24
46.00
36.61
22.98
20.99
19.28
O=S=O
NH
Cl
O
O
S
O
6d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



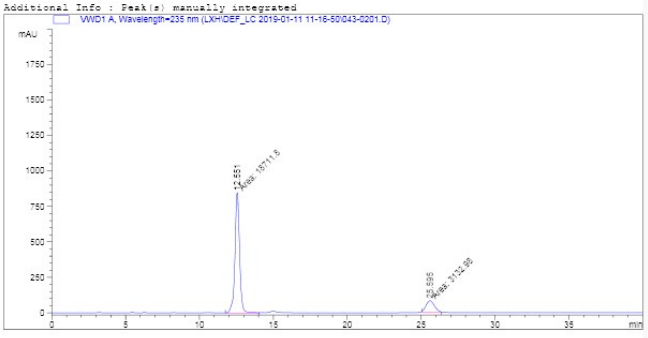
6e
yield: 87%
71% ee

```
Sample Info     : IA00CE-WE015; 90/10; 1.0; 86bar; 235nm

Additional Info : Peak(s) manually integrated
```

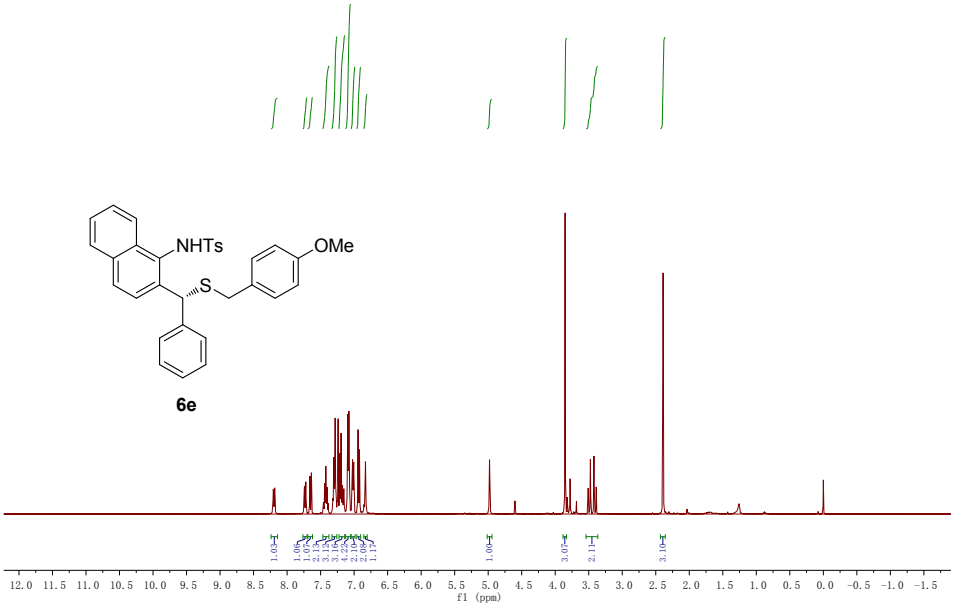


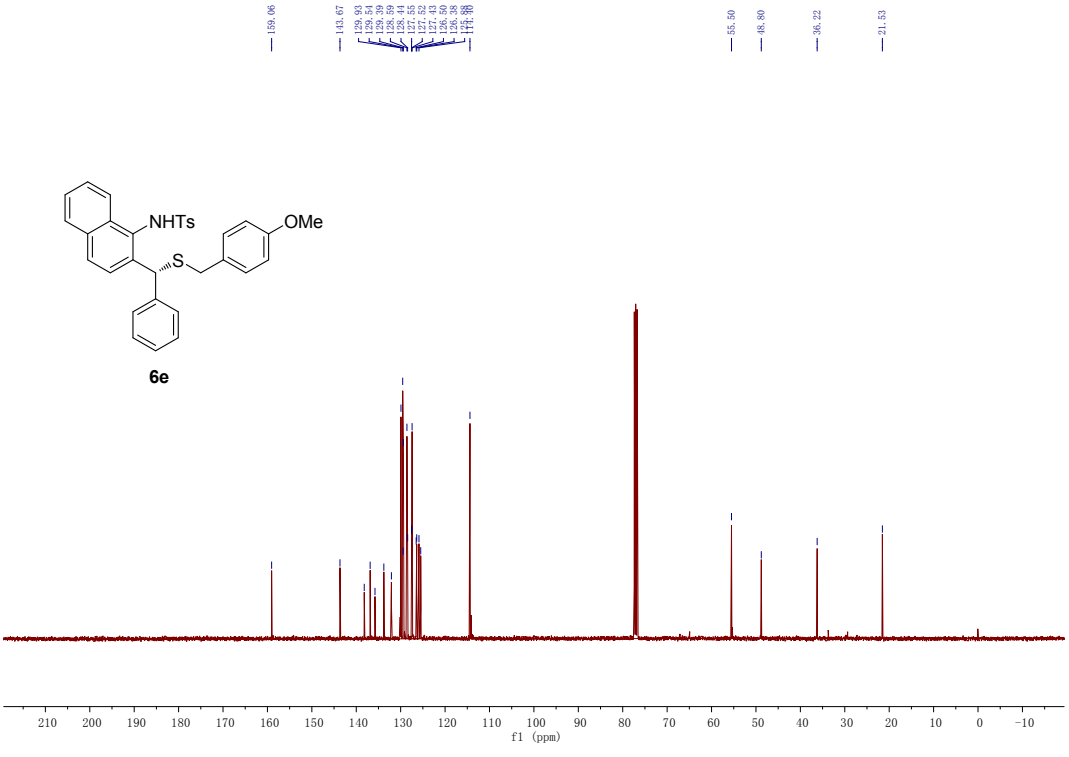

```
=====================================================================
                    Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]        [min]  mAU   *s    [mAU   ]      %
---|------|----|-------|----------|----------|--------|
   1  13.171 VB    0.9423 6852.00695  303.19250  51.4448
   2  27.018 BB    0.7063 6467.13672  141.92349  48.5552
```

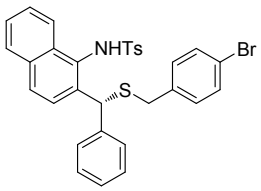
```
Sample Info     : IA00CE-WE015; 90/10; 1.0; 86bar; 235nm

Additional Info : Peak(s) manually integrated
```




```
=====================================================================
                    Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]        [min]  mAU   *s    [mAU   ]      %
---|------|----|-------|----------|----------|--------|
   1  12.551 MM    0.3674 1.87118e4  848.78491  85.6580
   2  25.595 MM    0.6580 3132.98389   79.35986  14.3420
```

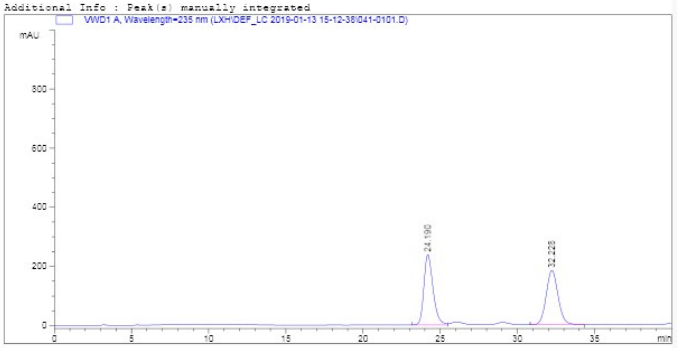

NHTs
OMe
S
6e
1.03
1.00
1.00
3.07
2.11
3.10
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.0 −1.5
f1 (ppm)


159.06
143.67
129.93
129.54
129.39
128.59
128.44
127.55
127.32
127.03
126.50
126.38
55.50
48.80
36.22
21.53
NHTs
OMe
S
6e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)



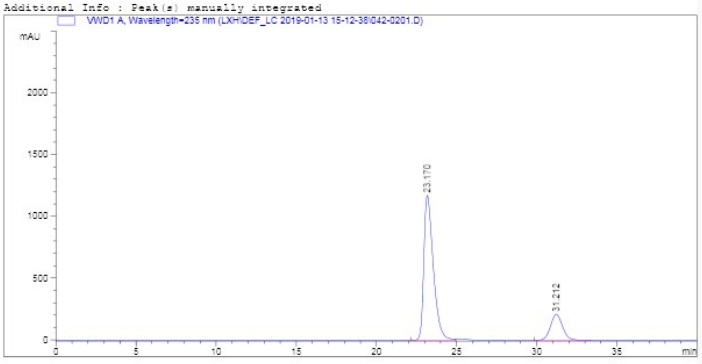
6f
yield: 82%
63% ee

```
Sample Info     : IA00CE-WE015; 90/10; 1.0; 98bar; 235nm

Additional Info : Peak(s) manually integrated
```

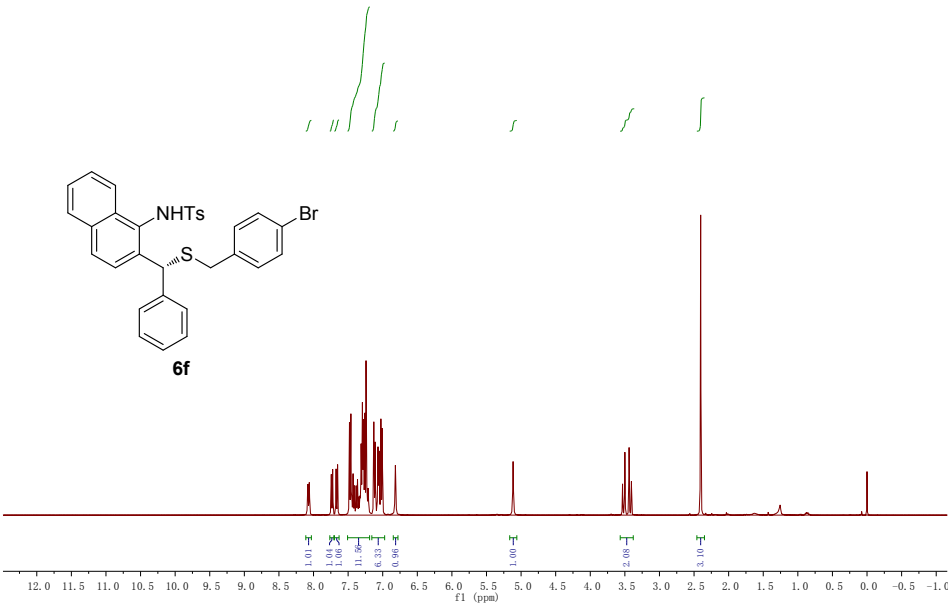



```
=====================================================================
                    Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  24.190 BV    0.6029 9835.87305  235.81427  49.9146
   2  32.228 BB    0.8233 9869.51270  154.56949  50.0854
```

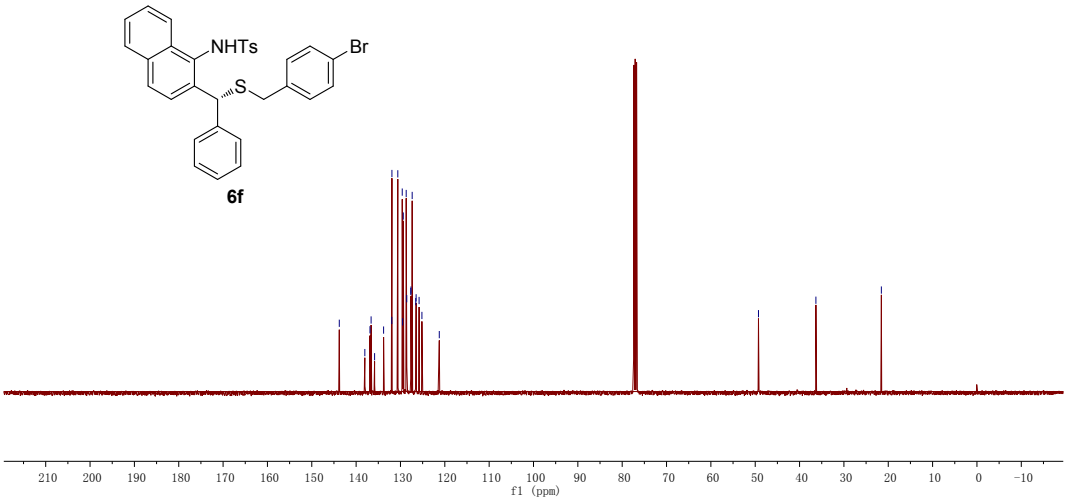
```
Sample Info     : IA00CE-WE015; 90/10; 1.0; 98bar; 235nm

Additional Info : Peak(s) manually integrated
```

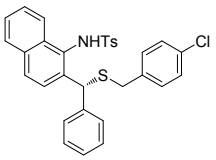



```
=====================================================================
                    Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  23.170 VB    0.6208 4.80684e4  1172.87146  81.4257
   2  31.212 BB    0.8060 1.09650e4   209.92316  18.5743
```


NHTs
Br
S
6f
1.01
1.04
1.06
11.56
6.33
0.96
1.00
2.08
3.10
f1 (ppm)

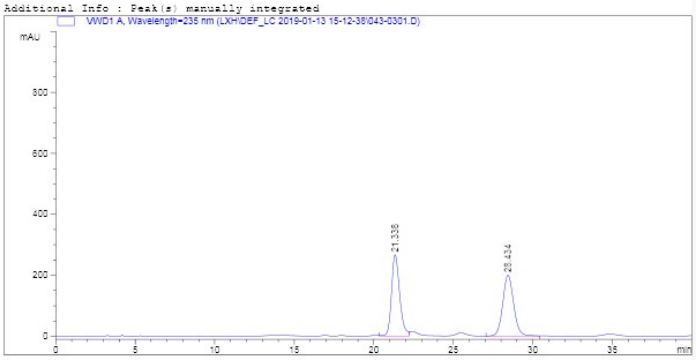

143.80
138.03
136.87
136.62
135.84
133.80
131.96
131.65
130.69
129.60
129.52
129.36
128.71
128.58
127.67
127.63
127.36
126.55
126.47
125.80
125.16
121.25
49.27
36.32
21.55


NHTs
Br
S
6f
f1 (ppm)



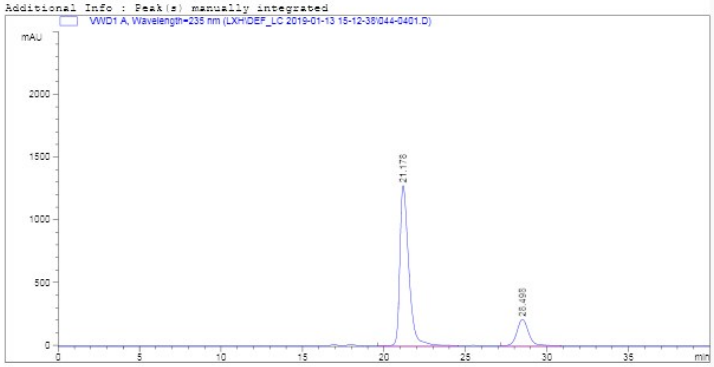
6g
yield: 85%
65% ee

```
Sample Info     : IA00CE-WE015; 90/10; 1.0; 98bar; 235nm

Additional Info : Peak(s) manually integrated
```

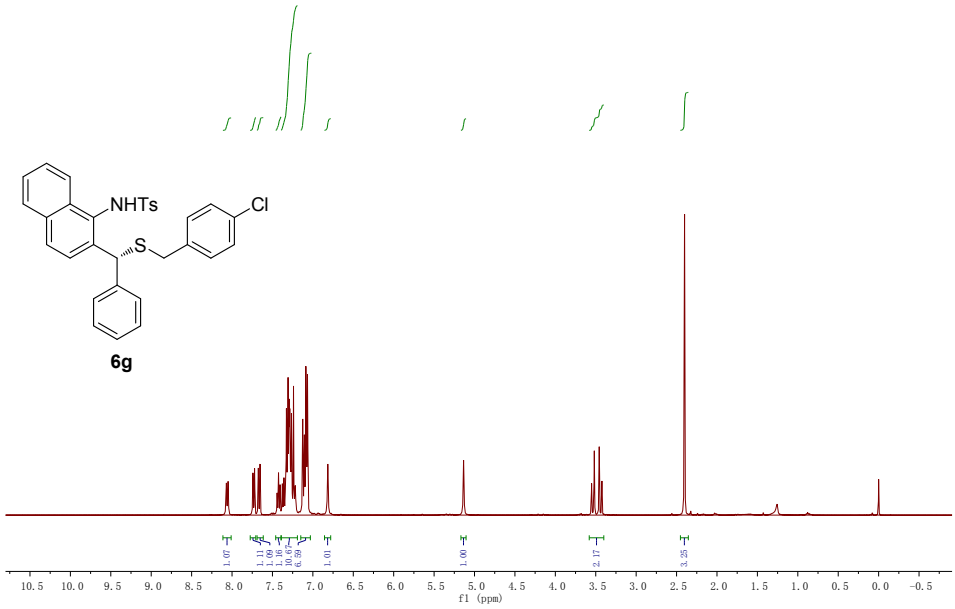


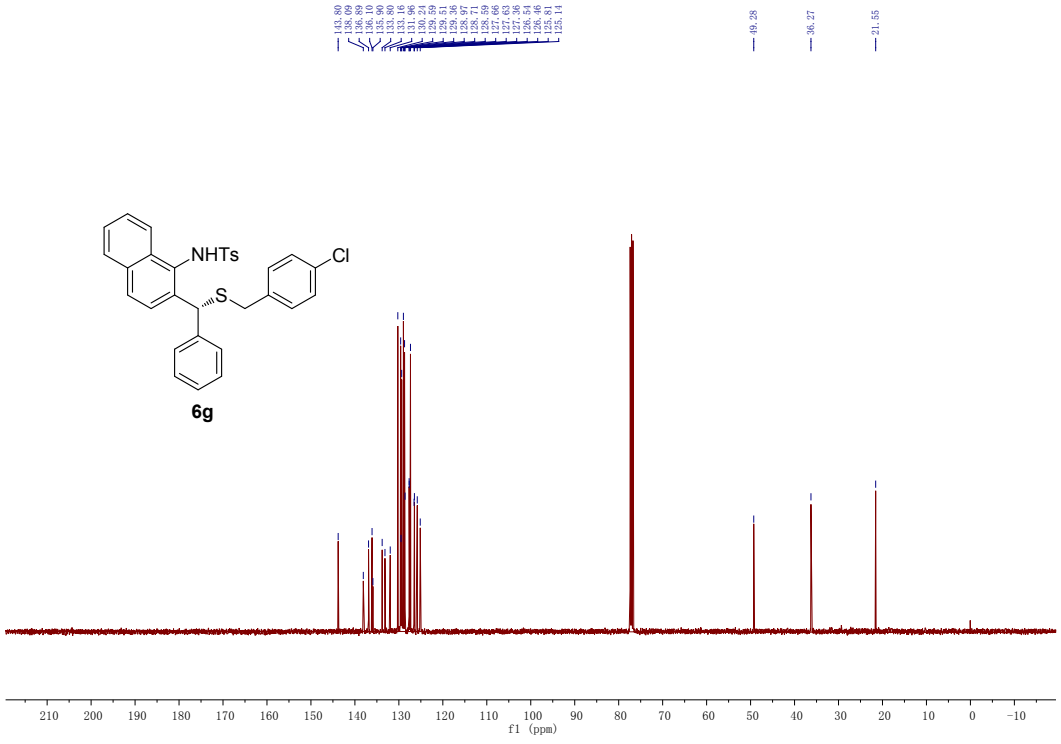

```
=====================================================================
                      Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  21.338 VV    0.5423 9457.71875  266.88919  50.0482
   2  28.434 BB    0.7323 9439.50000  199.57759  49.9518
```

```
Sample Info     : IA00CE-WE015; 90/10; 1.0; 98bar; 235nm

Additional Info : Peak(s) manually integrated
```

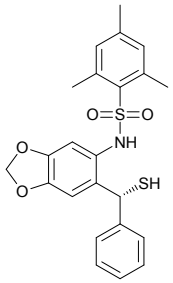



```
=====================================================================
                      Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  21.178 BB    0.5691 4.75704e4  1274.56316  82.5990
   2  28.498 BB    0.7415 1.00848e4   208.65015  17.4010
```


NHTs
Cl
S
6g
1.07
1.11
1.00
1.16
0.97
0.99
1.01
1.00
2.17
3.25
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


143.80
138.09
136.69
136.10
135.90
133.90
133.46
131.14
130.24
129.59
129.31
128.98
128.97
128.71
128.69
127.66
127.63
127.36
126.54
126.46
125.81
125.14
49.28
36.27
21.55
NHTs
Cl
S
6g
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

Copy of NMR Spectra and HPLC Chromatograms of 5

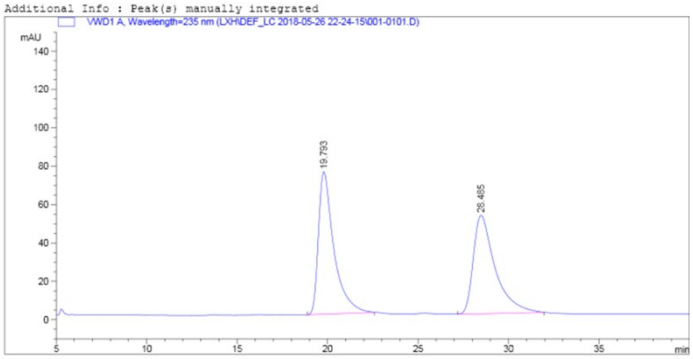


5

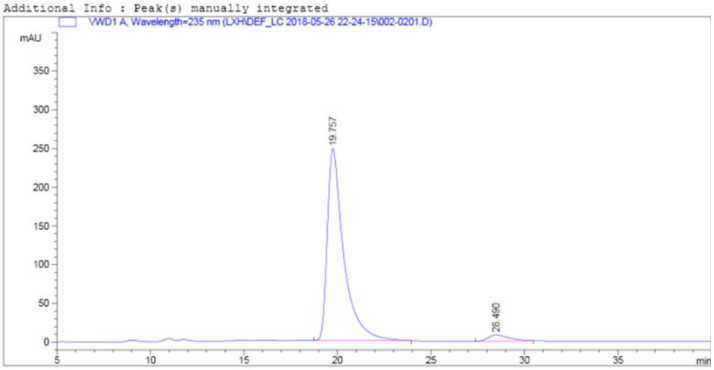
yield:85%

92%*ee*

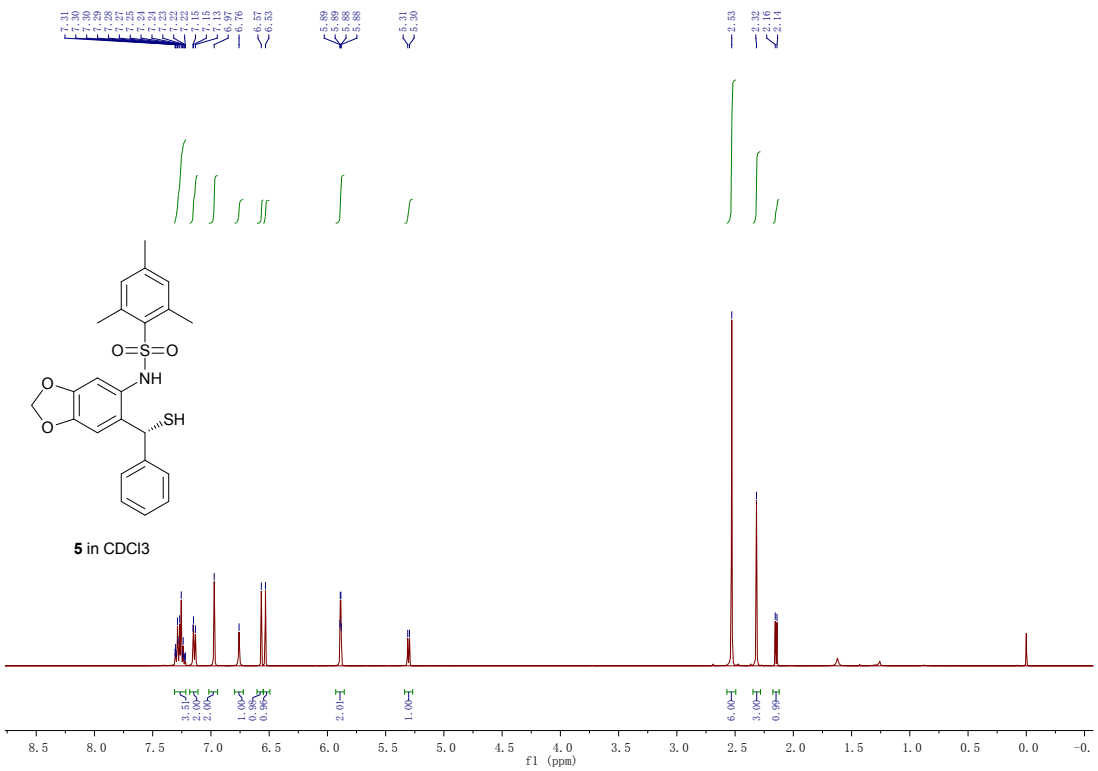
```
Sample Info     : ADH0CE-KE039; 90/10; 1.0; 38bar; 235nm; 25C

Additional Info : Peak(s) manually integrated
```

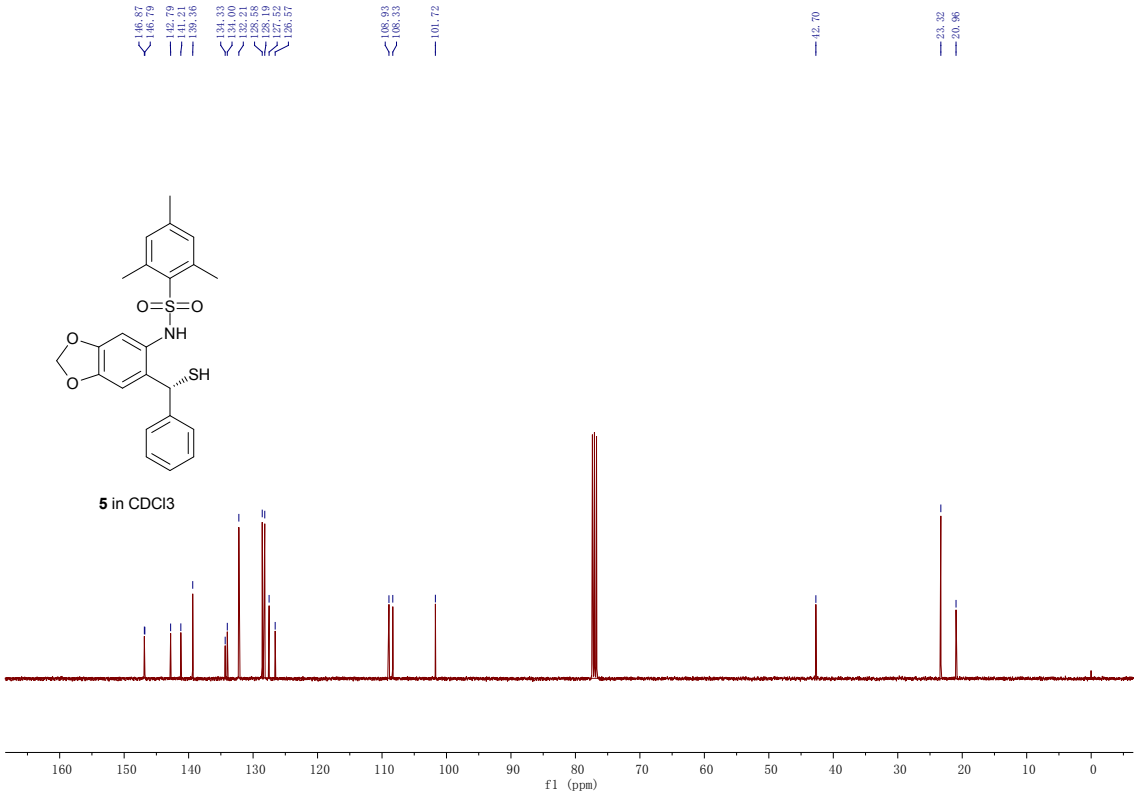



```
=====================================================================
                      Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  19.793 BB     0.8653 4394.97363   74.24725  50.5131
   2  28.485 BB     1.2298 4305.68848   51.29343  49.4869

Sample Info     : ADH0CE-KE039; 90/10; 1.0; 38bar; 235nm; 25C

Additional Info : Peak(s) manually integrated
```

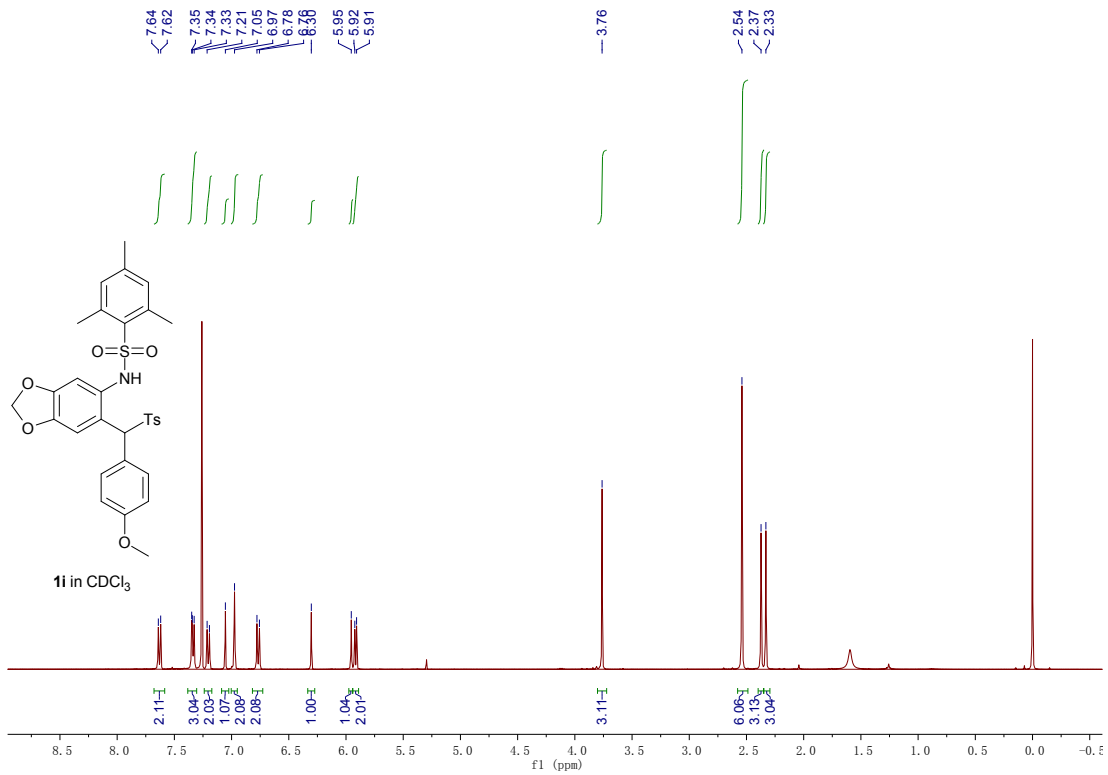


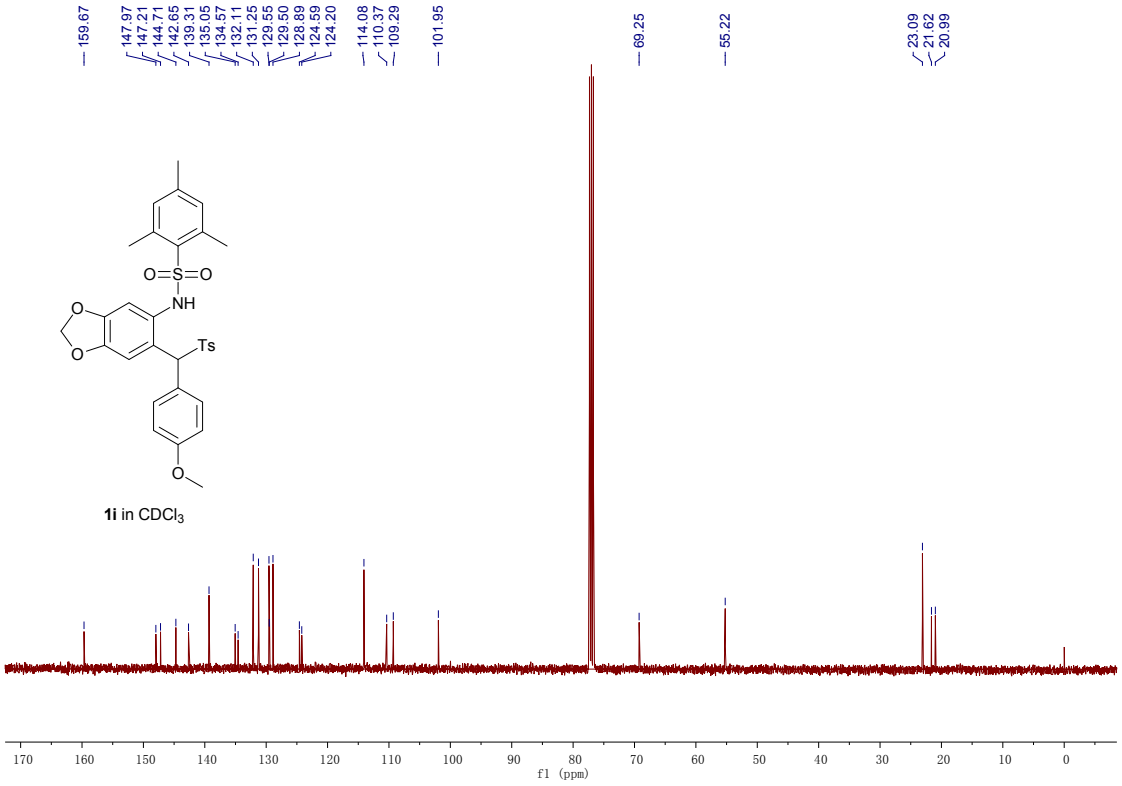

```
=====================================================================
                      Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=235 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  19.757 BB     0.8880 1.51243e4   247.89548  96.1223
   2  28.490 BB     1.0884  610.14111    7.95560   3.8777
```

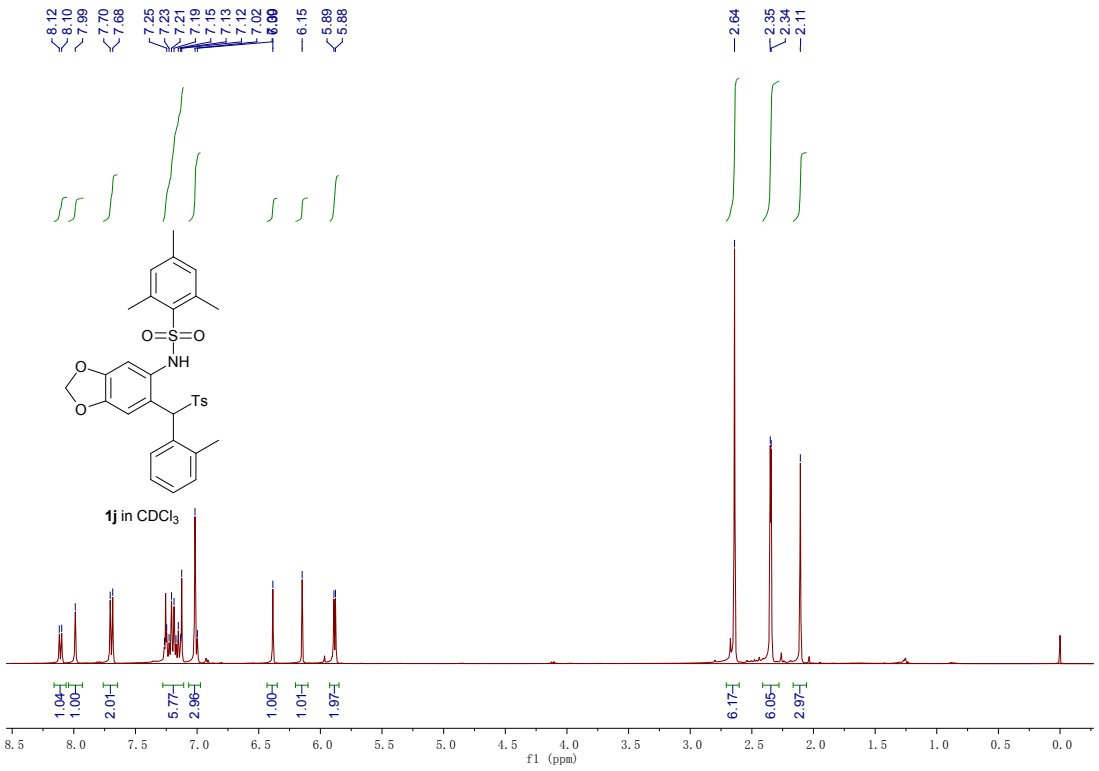


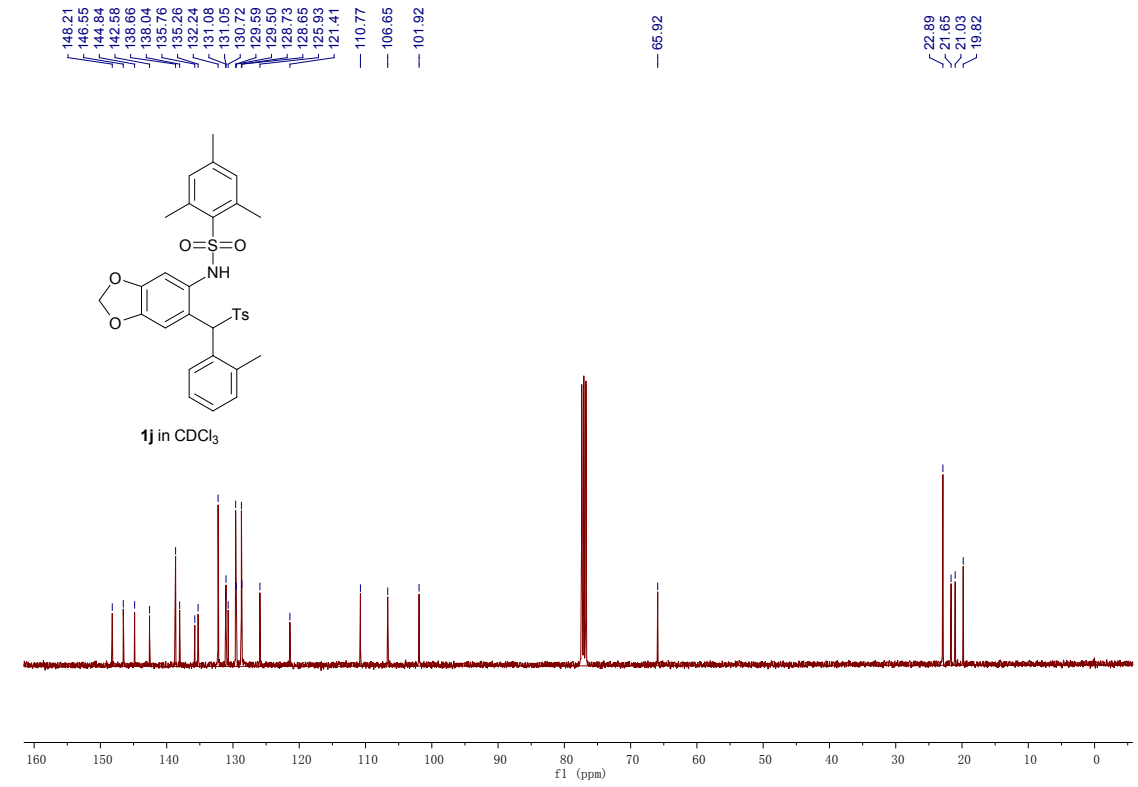


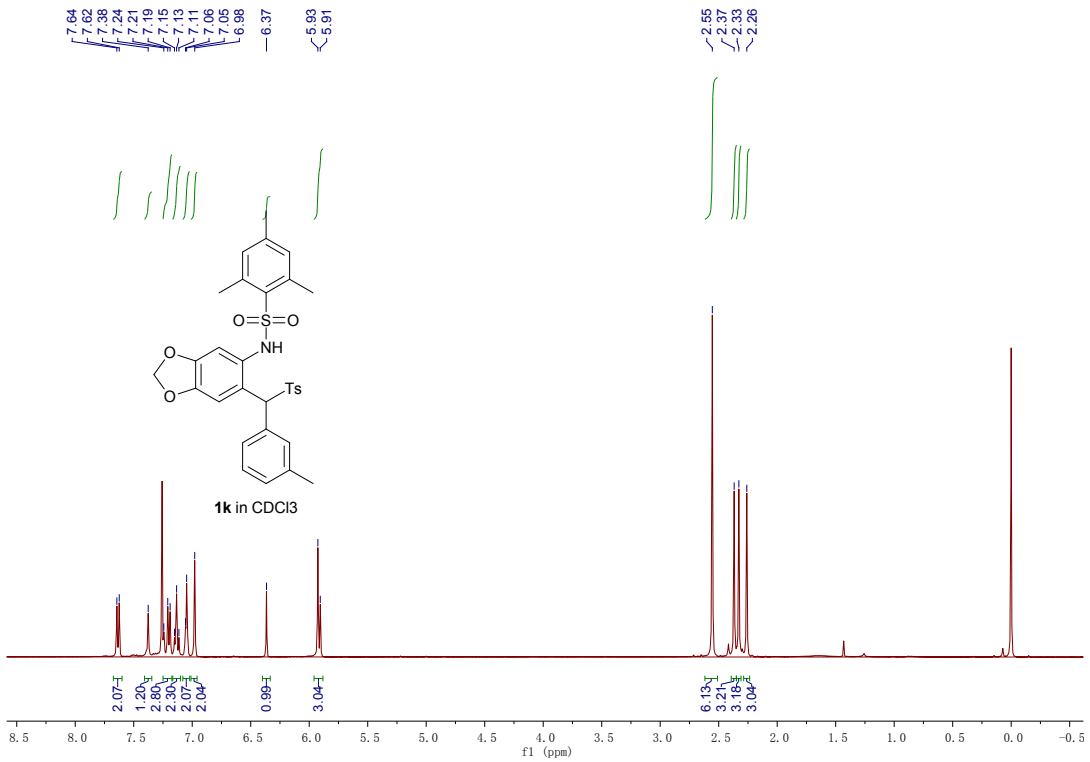
Copy of NMR Spectra of 1i-1z

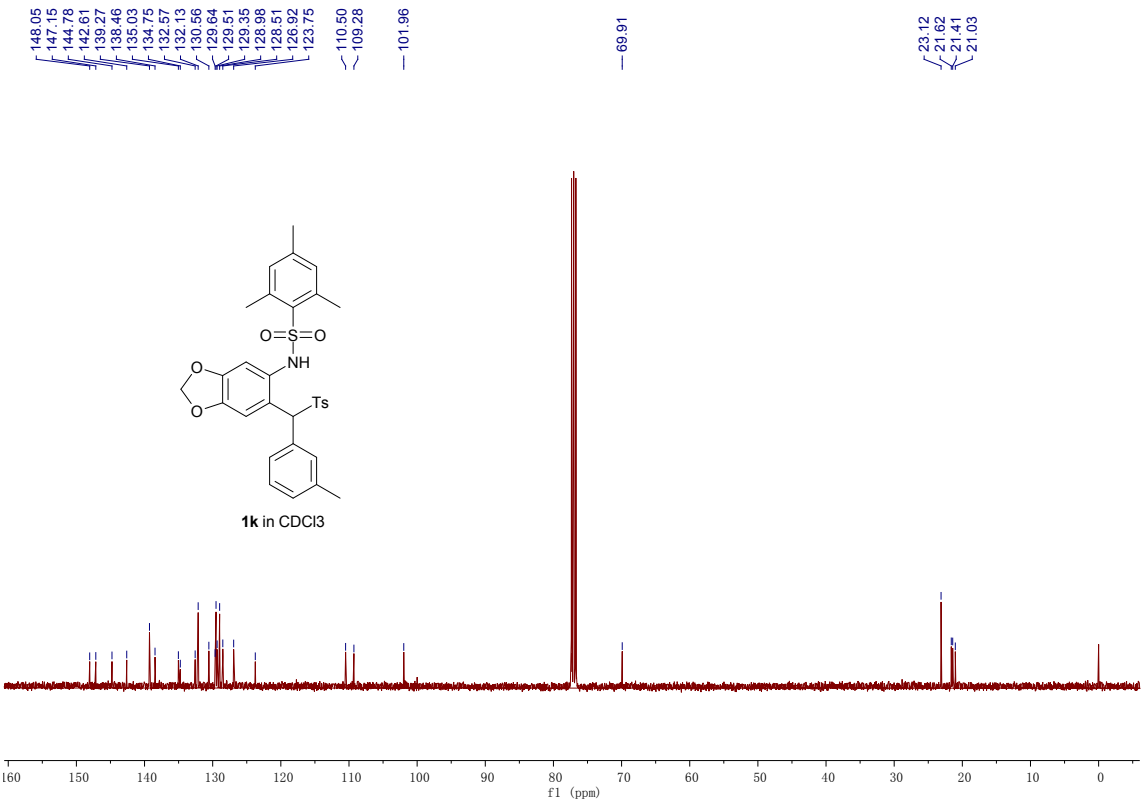

7.64
7.62
7.35
7.34
7.33
7.21
7.05
6.97
6.78
6.76
6.30
5.95
5.92
5.91
3.76
2.54
2.37
2.33
O=S=O
NH
Ts
O
O
O
1i in CDCl3
2.11
3.04
2.02
1.07
2.08
2.08
1.00
1.04
2.01
3.11
6.06
3.13
3.04
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

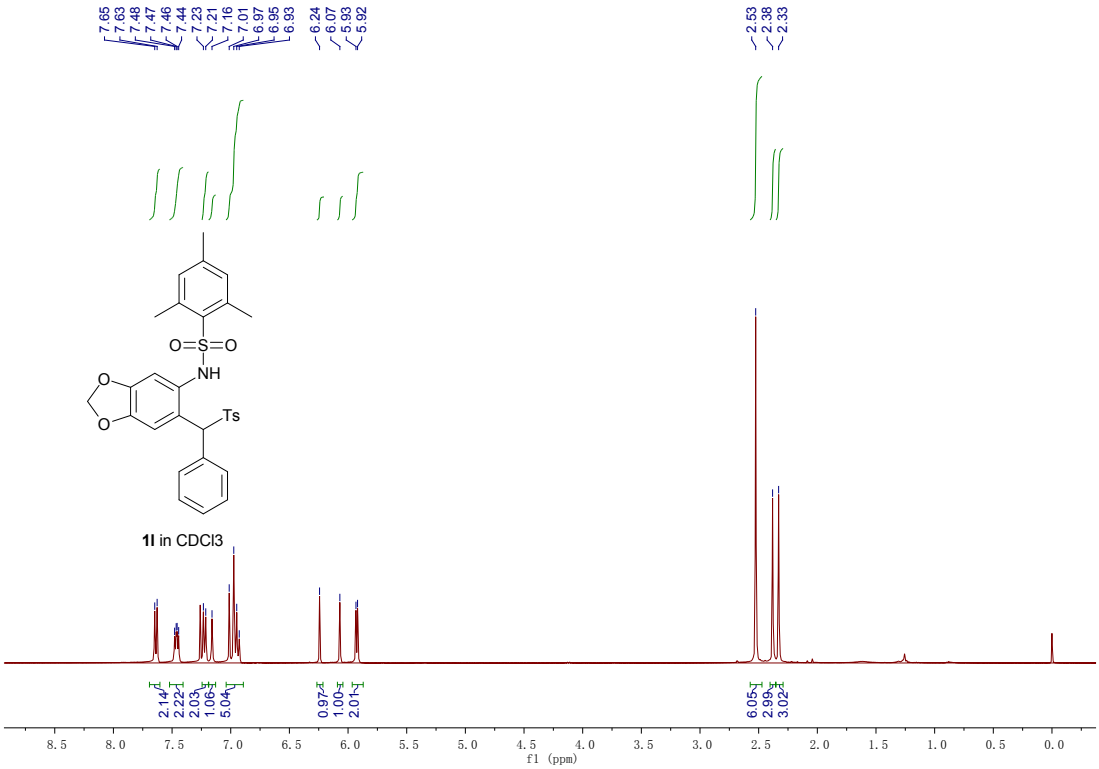

159.67
147.97
147.21
144.71
142.65
139.31
135.05
134.57
132.11
131.25
129.55
129.50
128.89
124.59
124.20
114.08
110.37
109.29
101.95
69.25
55.22
23.09
21.62
20.99
O=S=O
NH
Ts
O
O
O
1i in CDCl3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

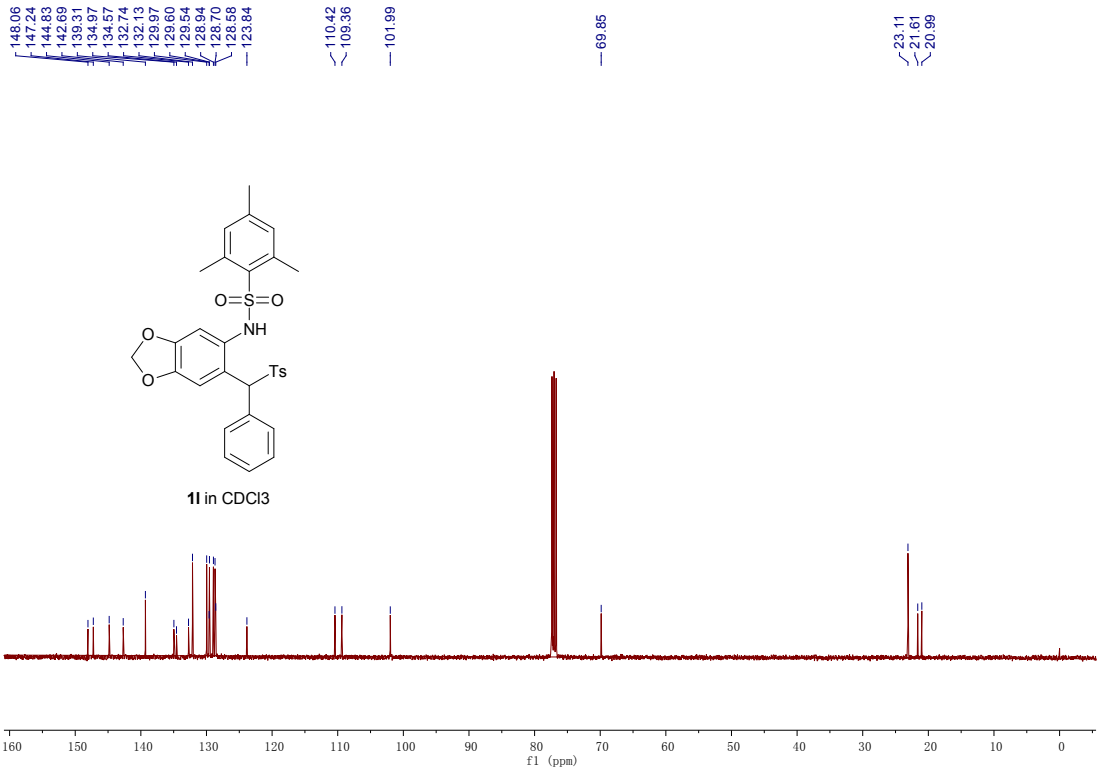

8.12
8.10
7.99
7.70
7.68
7.25
7.23
7.21
7.19
7.15
7.13
7.12
7.02
6.15
5.89
5.88
2.64
2.35
2.34
2.11
O=S=O
NH
O
O
Ts
1j in CDCl3
1.04
1.00
2.01
5.77
2.96
1.00
1.01
1.97
6.17
6.05
2.97
f1 (ppm)

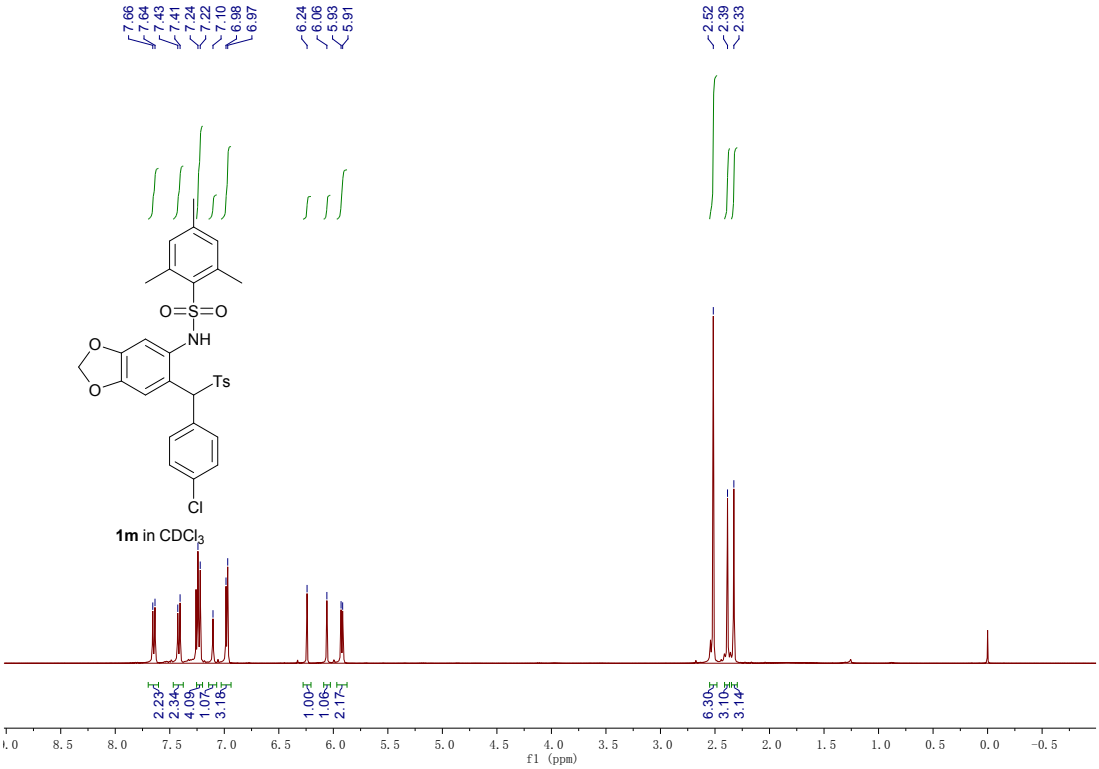

148.21
146.55
144.84
142.58
138.66
138.04
135.76
135.26
132.24
131.08
131.05
130.72
129.59
129.50
128.73
128.65
125.93
121.41
110.77
106.65
101.92
65.92
22.89
21.65
21.03
19.82
O=S=O
NH
O
O
Ts
1j in CDCl3
f1 (ppm)

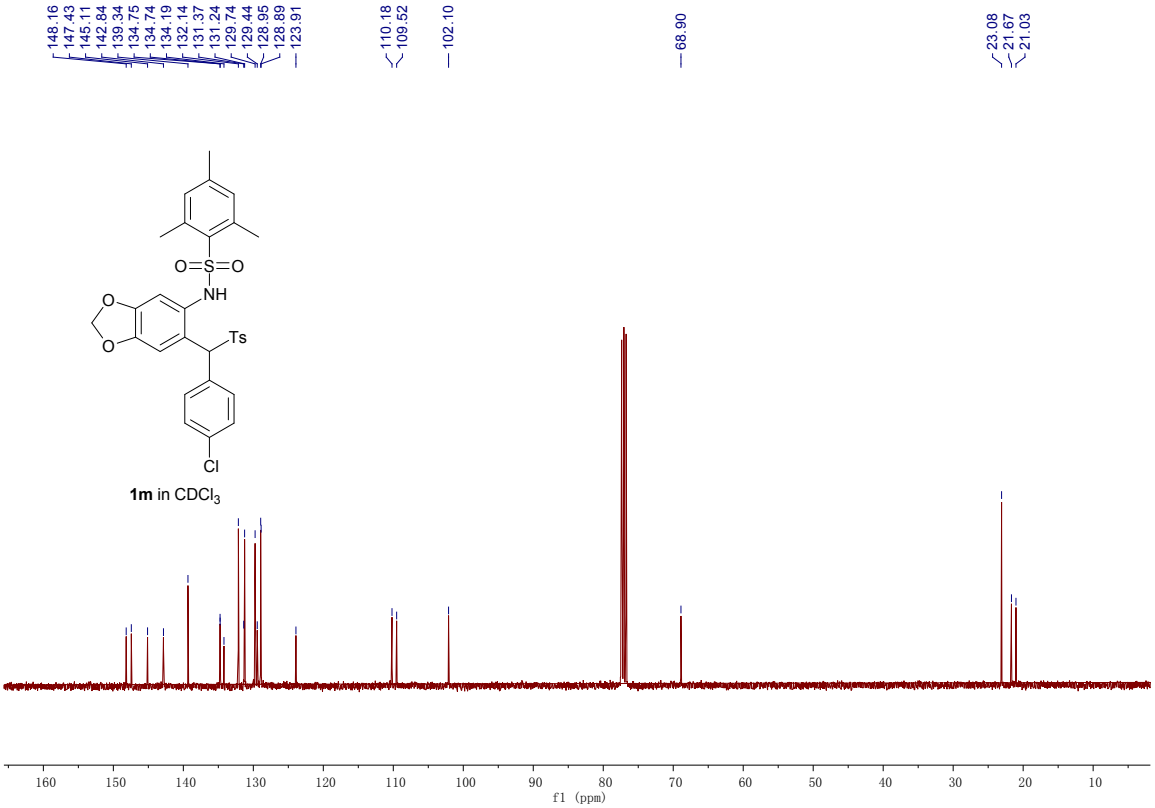

7.64
7.62
7.38
7.24
7.21
7.19
7.15
7.13
7.11
7.06
7.05
6.98
6.37
5.93
5.91
2.55
2.37
2.33
2.26
O=S=O
NH
O
O
Ts
1k in CDCl3
2.07
1.20
2.80
2.30
2.07
2.04
0.99
3.04
6.13
3.21
3.18
3.04
f1 (ppm)

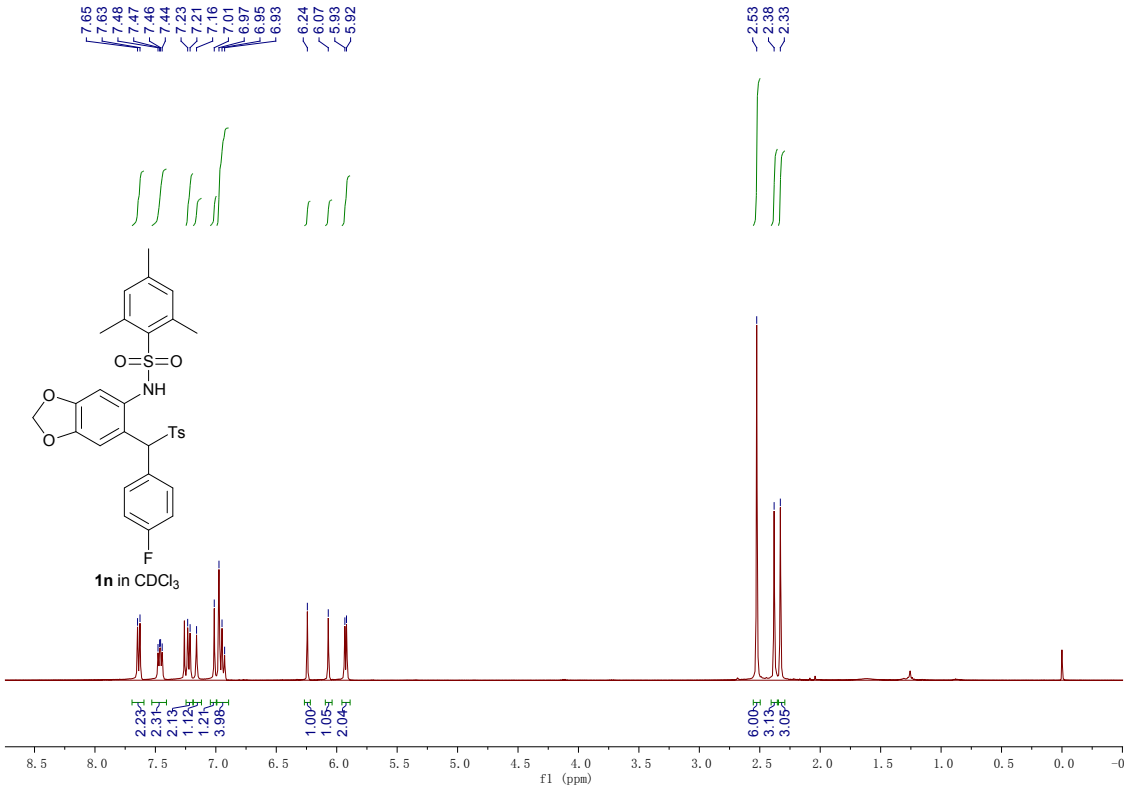

148.05
147.15
144.78
142.61
139.27
138.46
135.03
134.75
132.57
132.13
130.56
129.64
129.51
129.35
128.98
128.51
126.92
123.75
110.50
109.28
101.96
69.91
23.12
21.62
21.41
21.03
O=S=O
NH
O
O
Ts
1k in CDCl3
f1 (ppm)

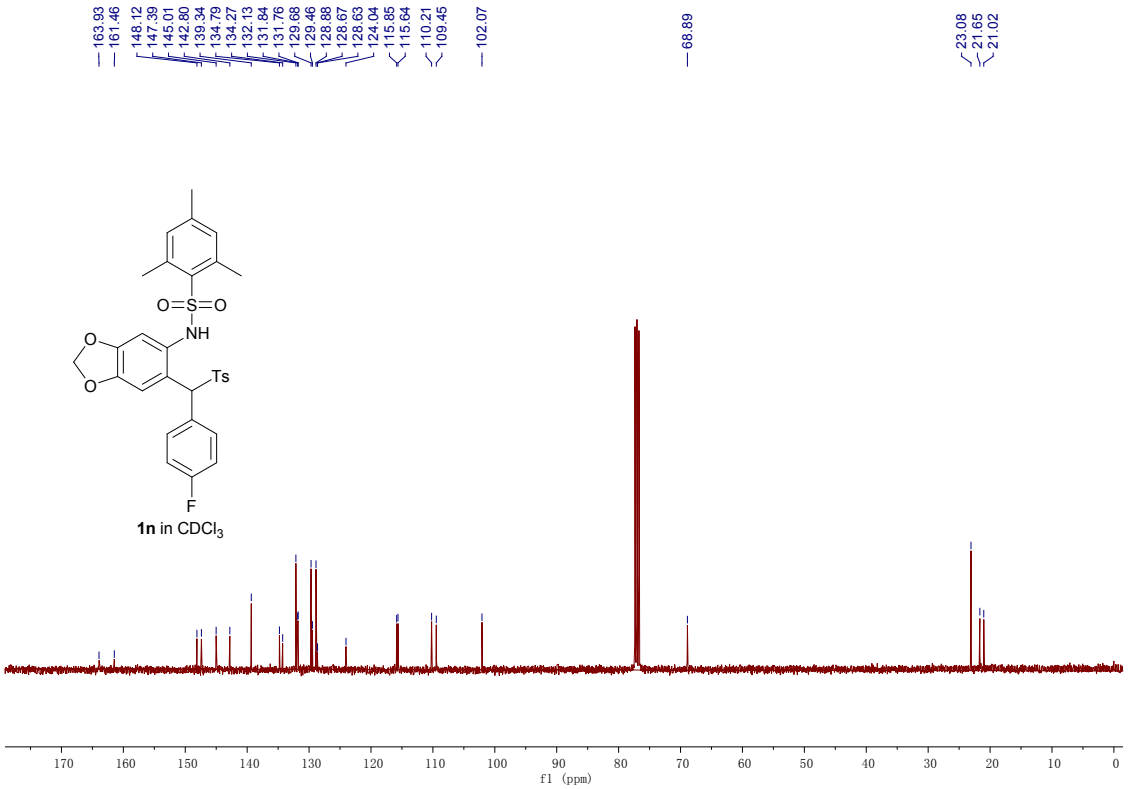

7.65
7.63
7.48
7.47
7.46
7.44
7.23
7.21
7.16
7.01
6.97
6.95
6.93
6.24
6.07
5.93
5.92
2.53
2.38
2.33
O=S=O
NH
O
O
Ts
1l in CDCl3
2.14
2.22
2.03
1.06
5.04
0.97
1.00
2.01
6.05
2.99
3.02
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

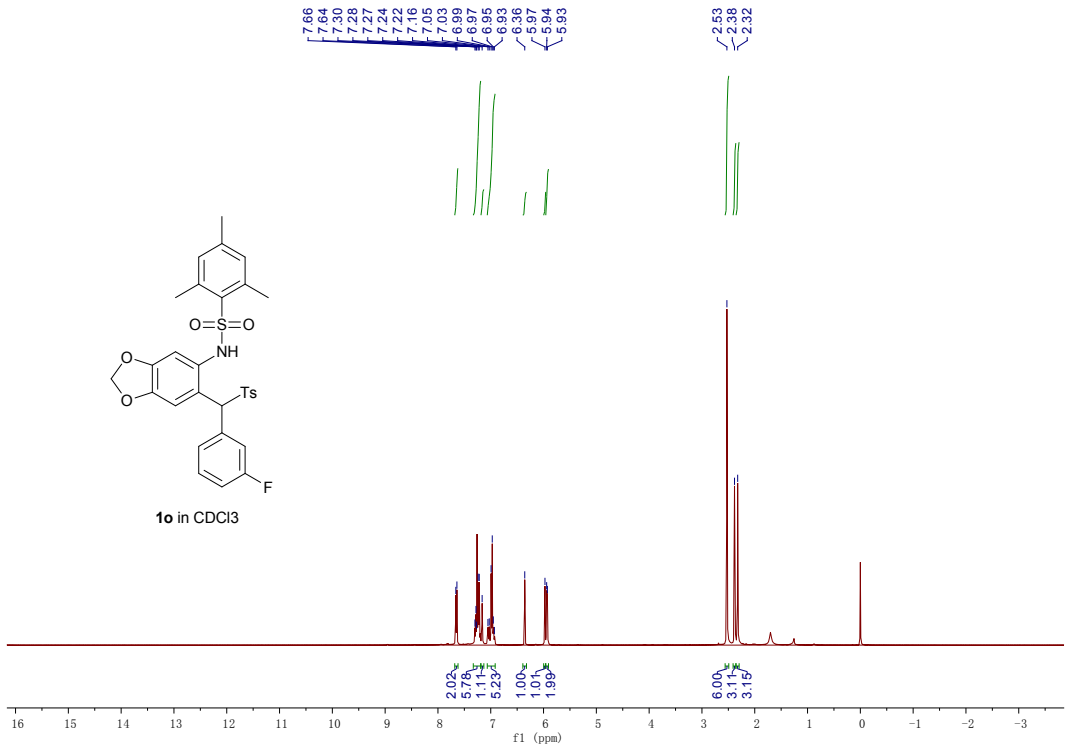

148.06
147.24
144.83
142.69
139.31
134.97
134.57
132.74
132.13
129.97
129.60
129.54
128.94
128.70
128.58
123.84
110.42
109.36
101.99
69.85
23.11
21.61
20.99
O=S=O
NH
O
O
Ts
1l in CDCl3
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

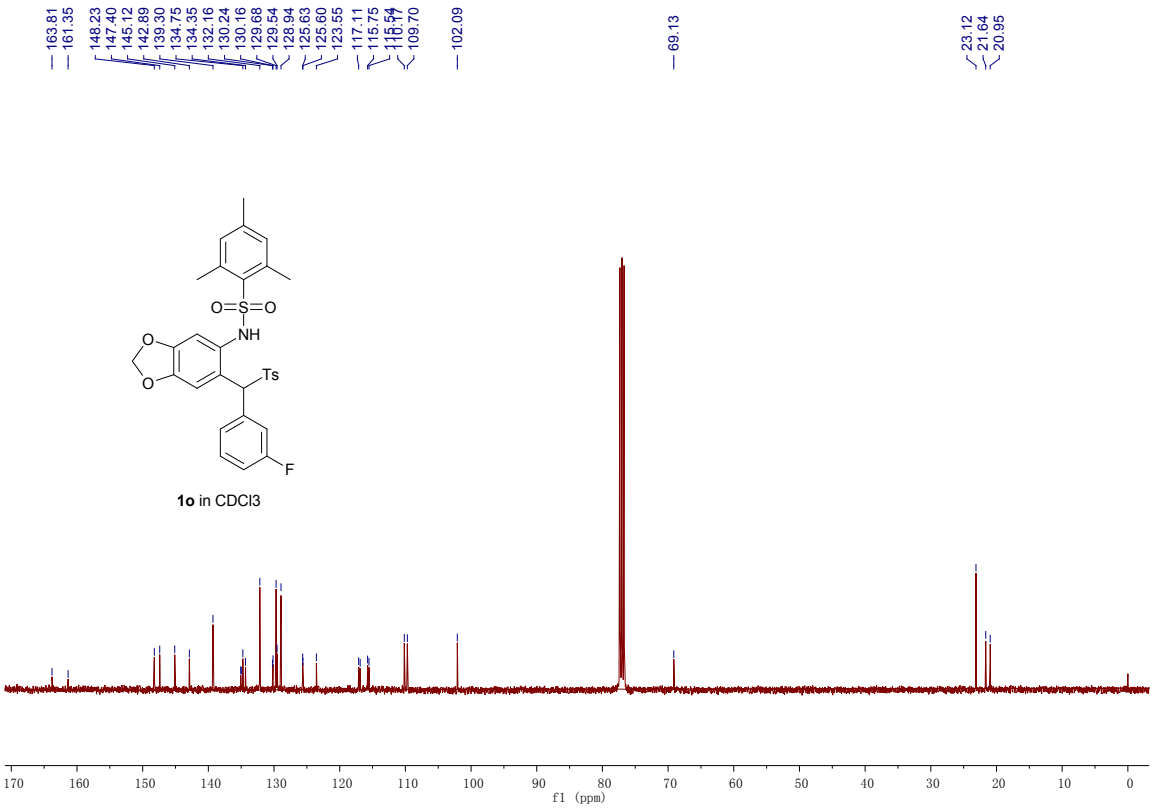

7.66
7.64
7.43
7.41
7.24
7.22
7.10
6.98
6.97
6.24
6.06
5.93
5.91
2.52
2.39
2.33
O=S=O
NH
Ts
Cl
1m in CDCl3
2.23
2.34
4.09
1.07
3.16
1.00
1.06
2.17
6.30
3.10
3.14
f1 (ppm)

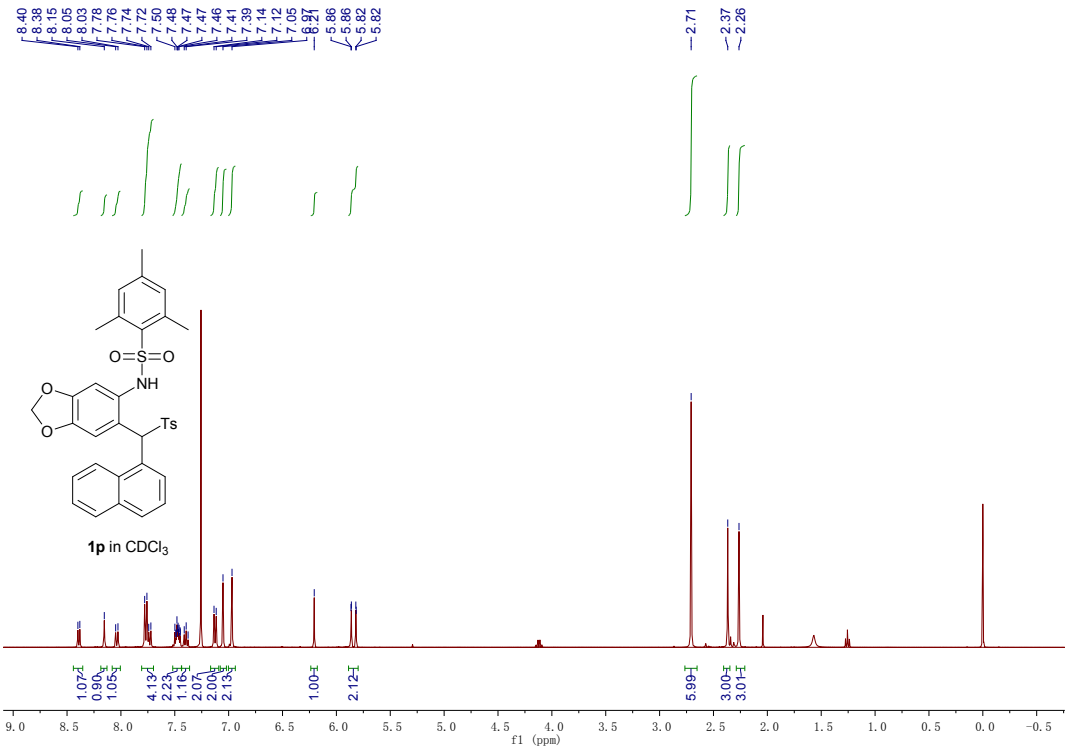

148.16
147.43
145.11
142.84
139.34
134.75
134.74
134.19
132.14
131.37
131.24
129.74
129.44
128.95
128.89
123.91
110.18
109.52
102.10
68.90
23.08
21.67
21.03
O=S=O
NH
Ts
Cl
1m in CDCl3
f1 (ppm)

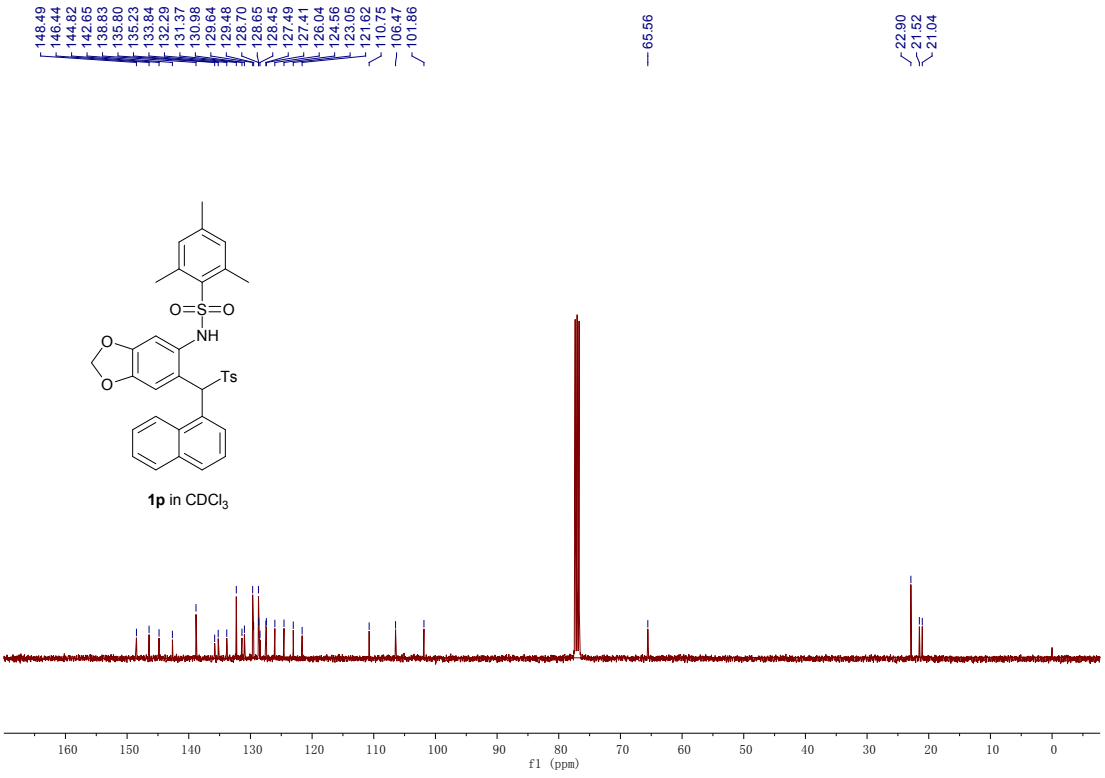

7.65
7.63
7.48
7.47
7.46
7.44
7.23
7.21
7.16
7.01
6.97
6.95
6.93
6.24
6.07
5.93
5.92
2.53
2.38
2.33
O=S=O
NH
Ts
O
O
F
1n in CDCl3
2.23
2.31
2.13
1.12
1.21
3.98
1.00
1.05
2.04
6.00
3.13
3.05
f1 (ppm)

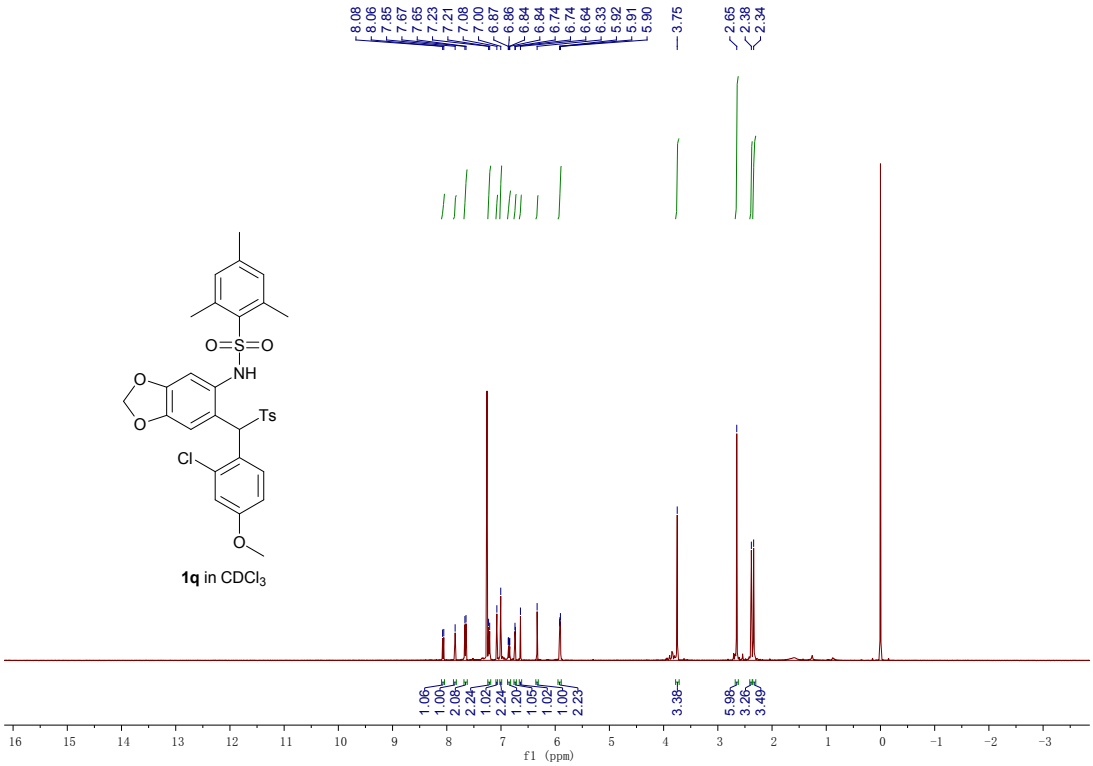

163.93
161.46
148.12
147.39
145.01
142.80
139.34
134.79
134.27
132.13
131.84
131.76
129.68
129.46
128.88
128.67
128.63
124.04
115.85
115.64
110.21
109.45
102.07
68.89
23.08
21.65
21.02
O=S=O
NH
Ts
O
O
F
1n in CDCl3
f1 (ppm)

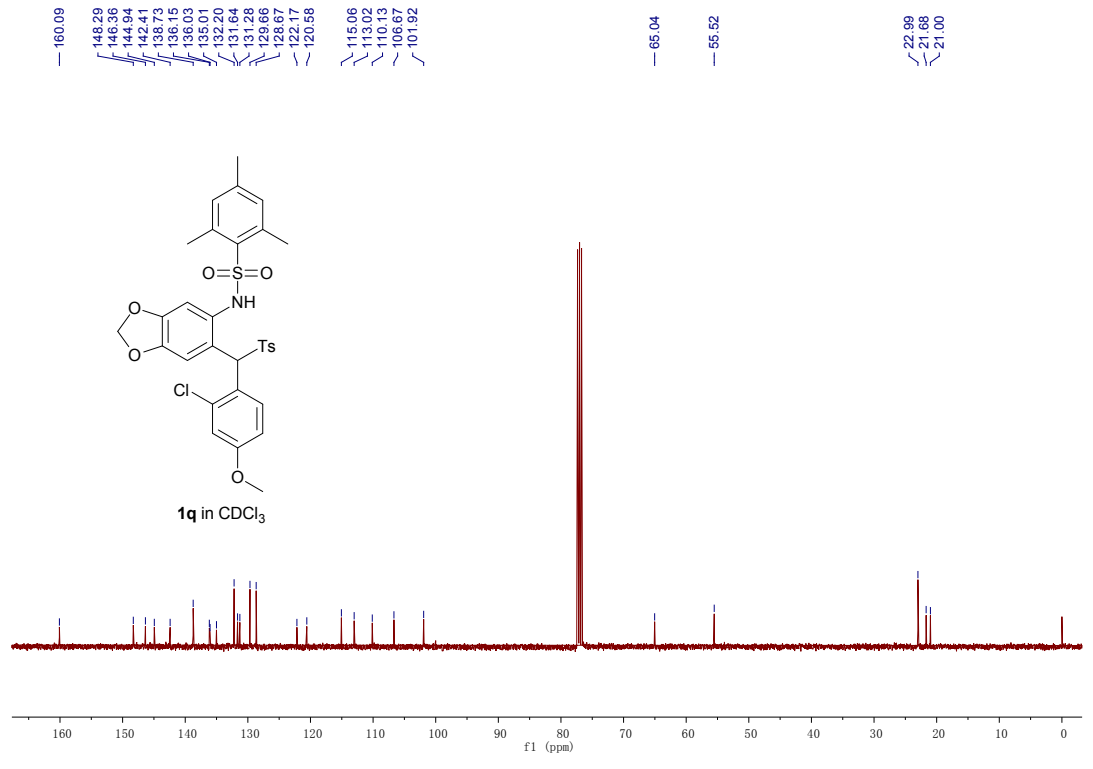

7.66
7.64
7.30
7.28
7.27
7.24
7.22
7.16
7.05
7.03
6.99
6.97
6.95
6.93
6.36
5.97
5.94
5.93
2.53
2.38
2.32
O=S=O
NH
O
O
Ts
F
1o in CDCl3
2.02
5.78
1.11
5.23
1.00
1.01
1.99
6.00
3.11
3.15
f1 (ppm)

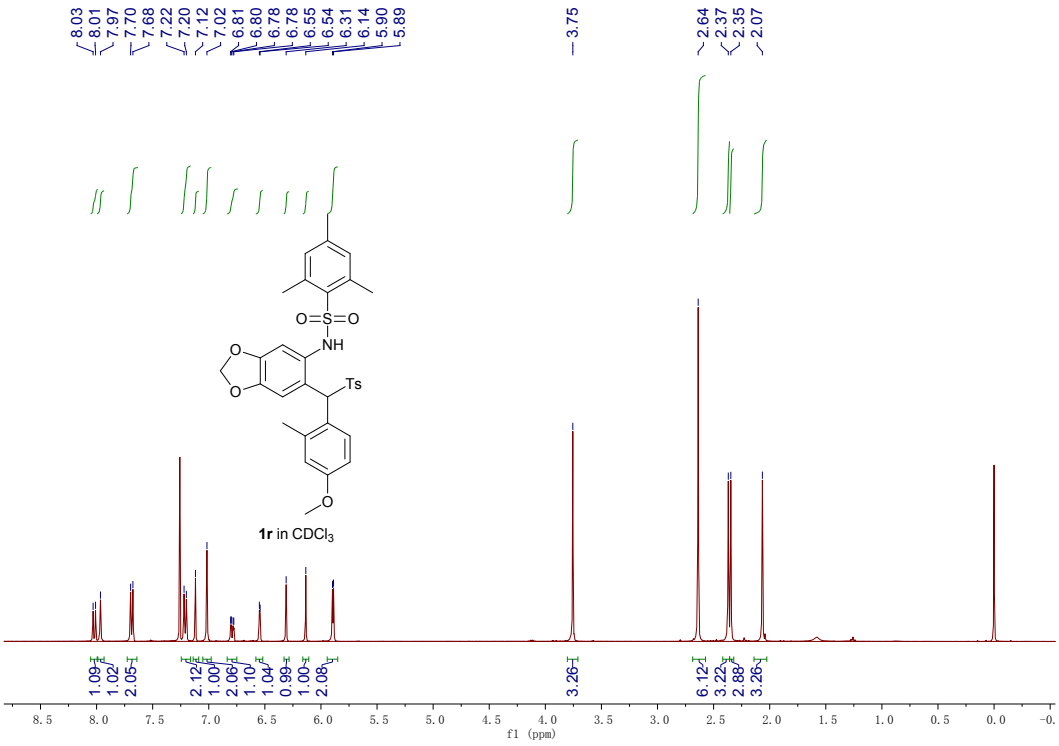

163.81
161.35
148.23
147.40
145.12
142.89
139.30
134.75
134.35
132.16
130.24
130.16
129.68
129.54
128.94
125.63
125.60
123.55
117.11
115.75
109.70
102.09
69.13
23.12
21.64
20.95
O=S=O
NH
O
O
Ts
F
1o in CDCl3
f1 (ppm)

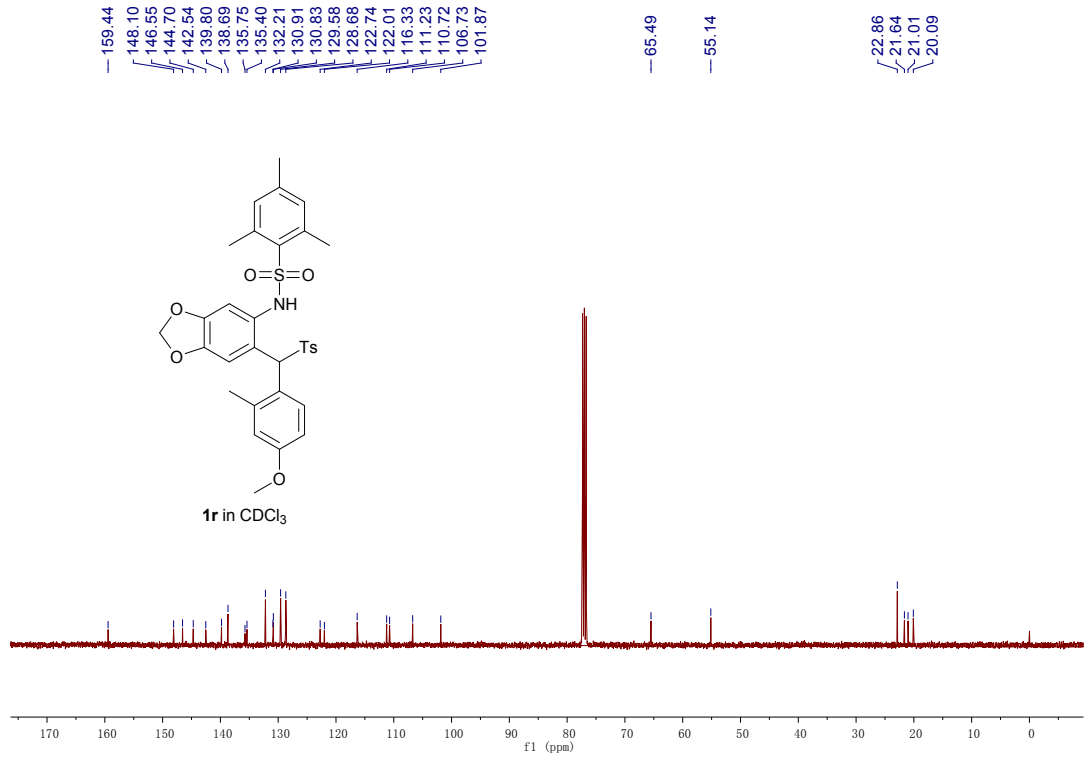

8.40
8.38
8.15
8.05
8.03
7.78
7.76
7.74
7.72
7.50
7.48
7.47
7.47
7.46
7.41
7.39
7.14
7.12
7.05
6.97
6.21
5.86
5.86
5.82
5.82
2.71
2.37
2.26
O=S=O
NH
O
O
Ts
1p in CDCl3
1.07
0.90
1.05
4.13
2.23
1.16
2.07
2.00
2.13
1.00
2.12
5.99
3.00
3.01
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

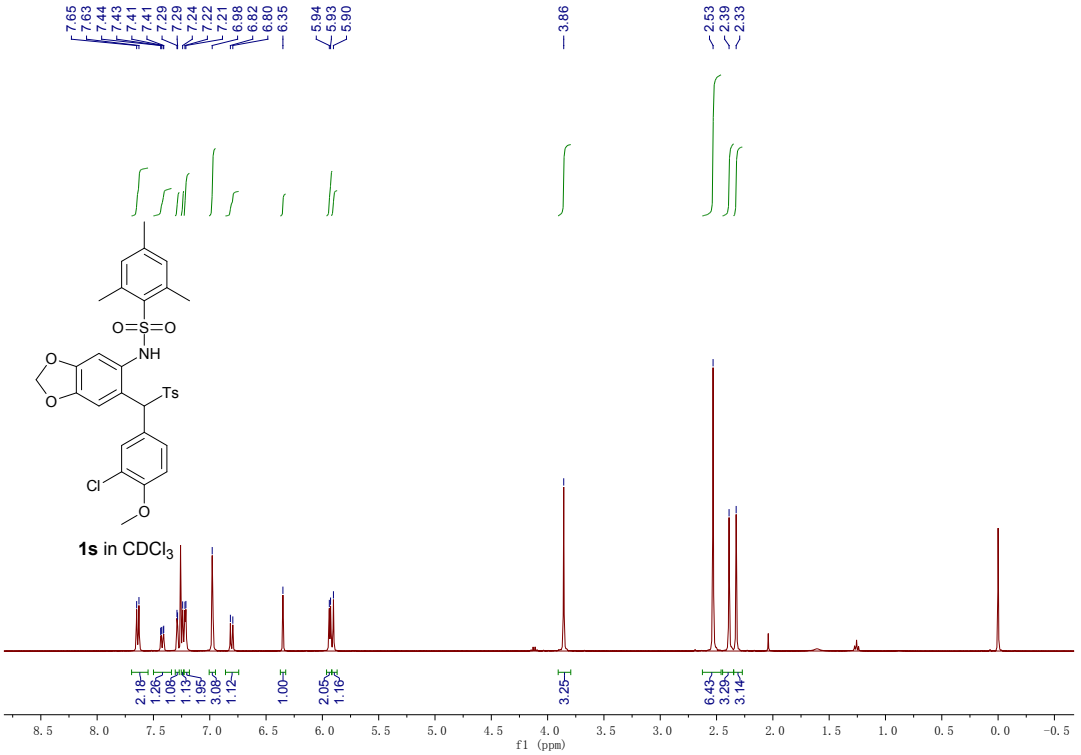

148.49
146.44
144.82
142.65
138.83
135.80
135.23
133.84
132.29
131.37
130.98
129.64
129.48
128.70
128.65
128.45
127.49
127.41
126.04
124.56
123.05
121.62
110.75
106.47
101.86
65.56
22.90
21.52
21.04
O=S=O
NH
O
O
Ts
1p in CDCl3
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

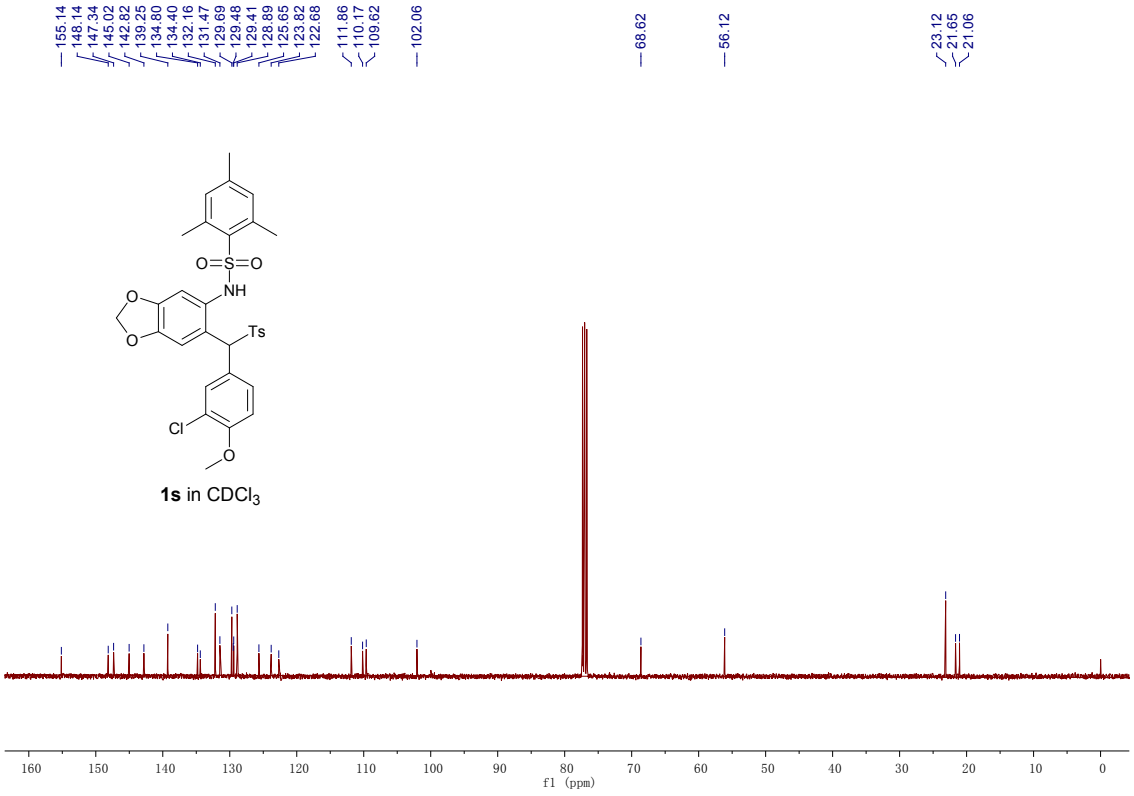

8.08
8.06
7.85
7.67
7.65
7.23
7.21
7.08
7.00
6.87
6.86
6.84
6.84
6.74
6.74
6.64
6.33
5.92
5.91
5.90
3.75
2.65
2.38
2.34
O=S=O
NH
O
O
Ts
Cl
O
1q in CDCl3
1.06
1.00
2.08
2.24
1.02
2.24
1.20
1.05
1.02
1.00
2.23
3.38
5.98
3.26
3.49
f1 (ppm)

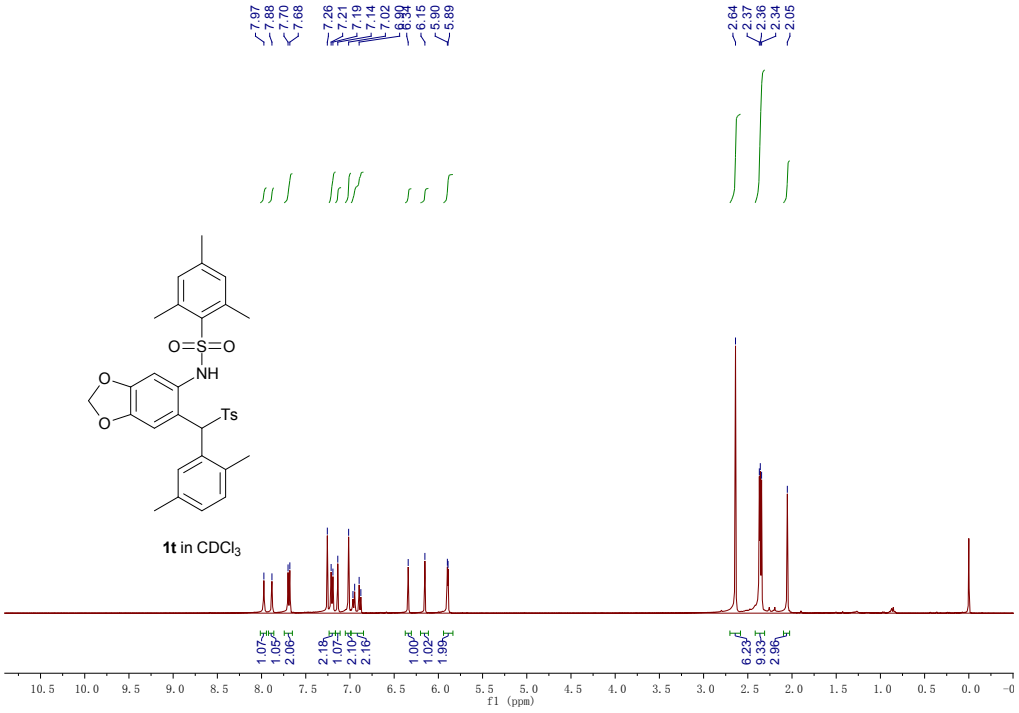

160.09
148.29
146.36
144.94
142.41
138.73
136.15
136.03
135.01
132.20
131.64
131.28
129.66
128.67
122.17
120.58
115.06
113.02
110.13
106.67
101.92
65.04
55.52
22.99
21.68
21.00
O=S=O
NH
O
O
Ts
Cl
O
1q in CDCl3
f1 (ppm)

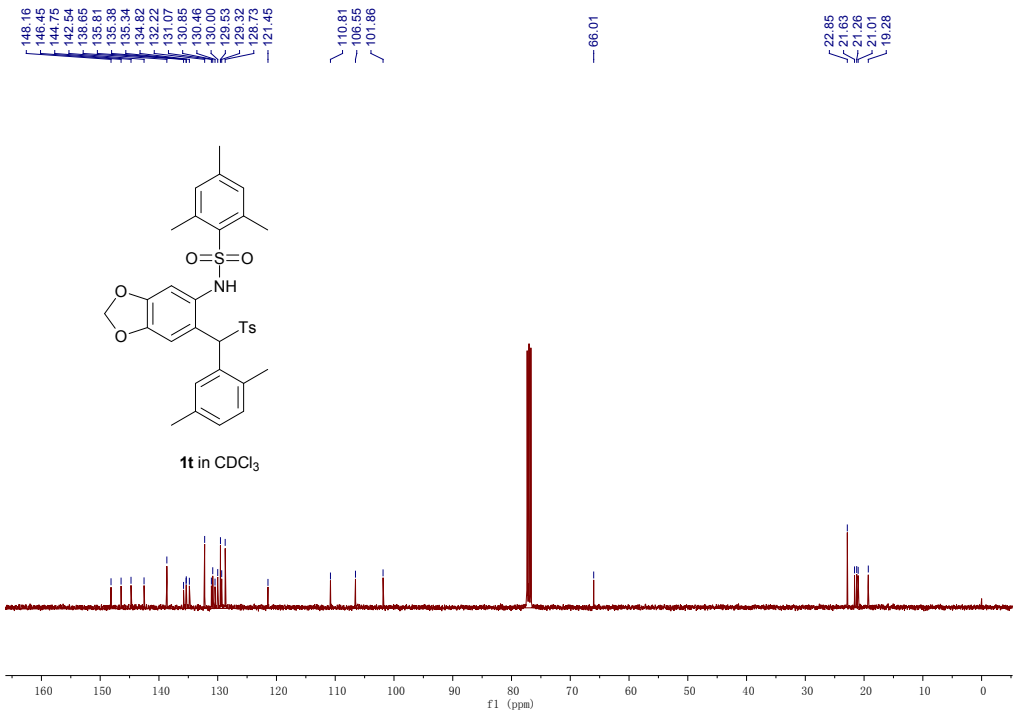

8.03
8.01
7.97
7.70
7.68
7.22
7.20
7.12
7.02
6.81
6.80
6.78
6.78
6.55
6.54
6.31
6.14
5.90
5.89
3.75
2.64
2.37
2.35
2.07
O=S=O
NH
O
O
Ts
O
1r in CDCl3
1.09
1.02
2.05
2.12
1.00
2.06
1.10
1.04
0.99
1.00
2.08
3.26
6.12
3.22
2.88
3.26
f1 (ppm)

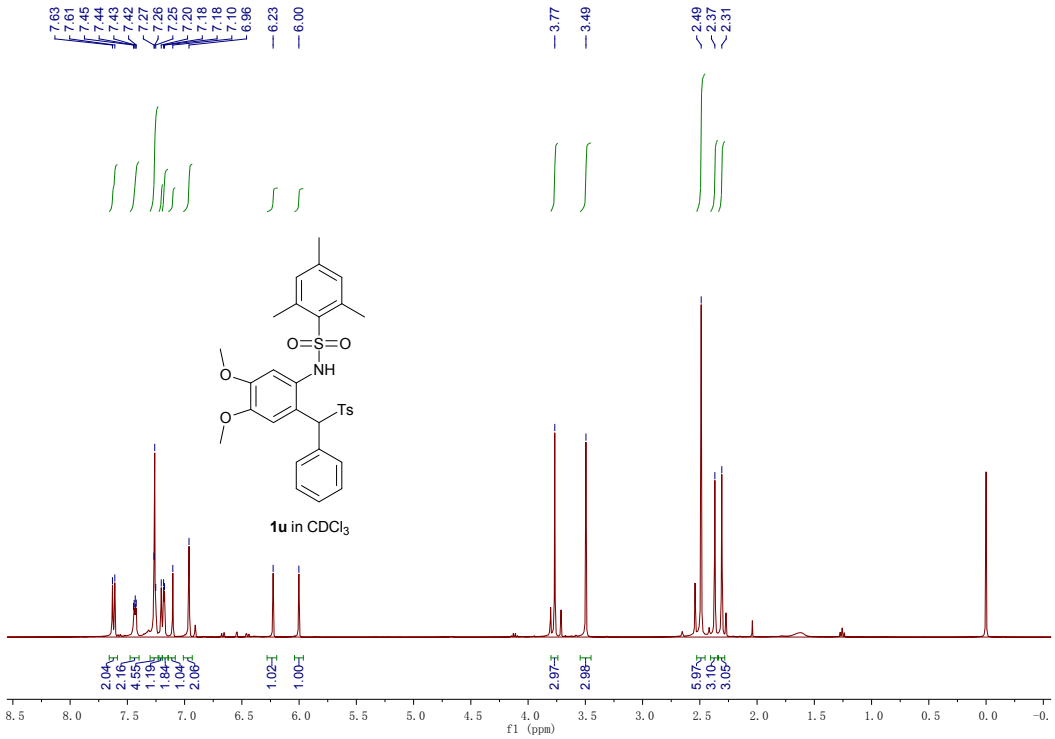

159.44
148.10
146.55
144.70
142.54
139.80
138.69
135.75
135.40
132.21
130.91
130.83
129.58
128.68
122.74
122.01
116.33
111.23
110.72
106.73
101.87
65.49
55.14
22.86
21.64
21.01
20.09
O=S=O
NH
O
O
Ts
O
1r in CDCl3
f1 (ppm)

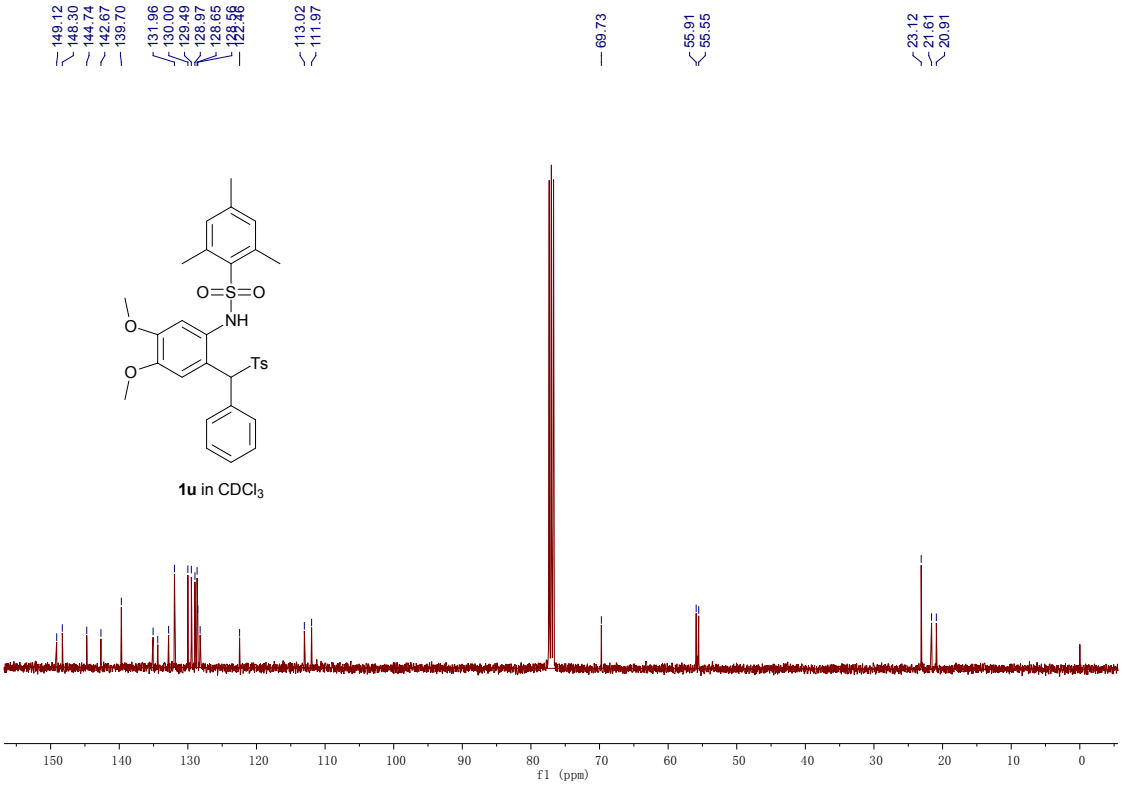

7.65
7.63
7.44
7.43
7.41
7.41
7.29
7.29
7.24
7.22
7.21
6.98
6.82
6.80
6.35
5.94
5.93
5.90
3.86
2.53
2.39
2.33
O=S=O
NH
O
O
Ts
Cl
O
1s in CDCl3
2.18
1.26
1.08
1.13
1.95
3.08
1.12
1.00
2.05
1.16
3.25
6.43
3.29
3.14
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

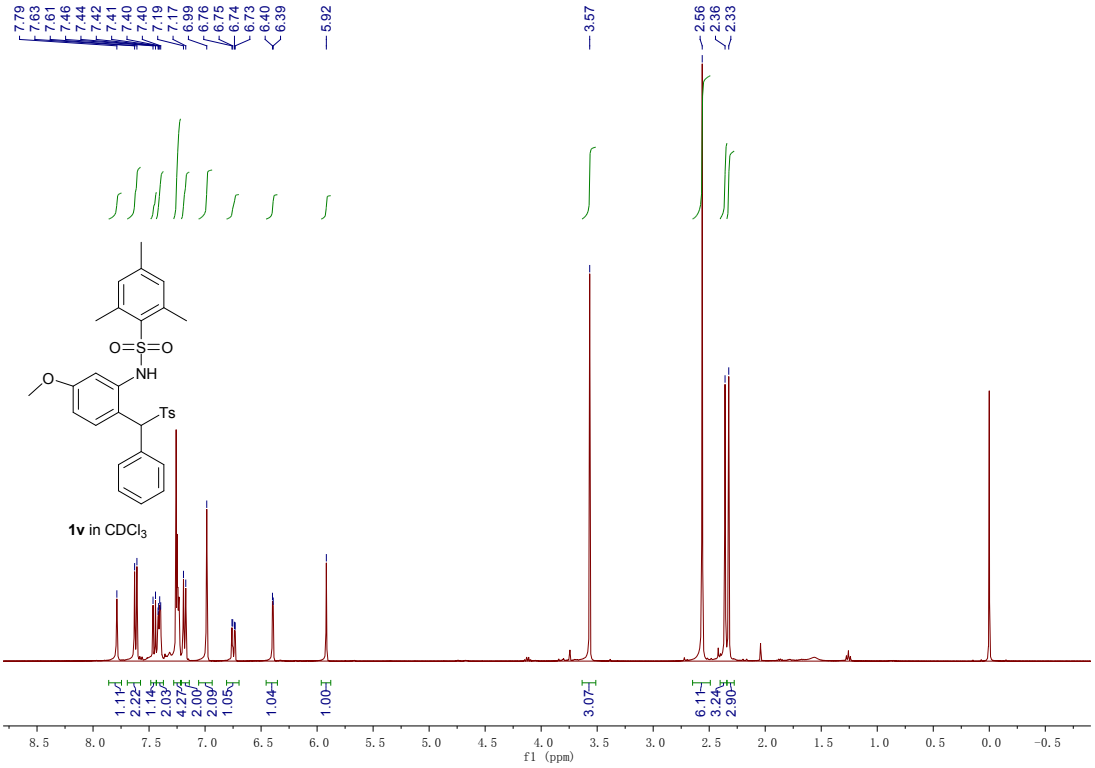

155.14
148.14
147.34
145.02
142.82
139.25
134.80
134.40
132.16
131.47
129.69
129.48
129.41
128.89
125.65
123.82
122.68
111.86
110.17
109.62
102.06
68.62
56.12
23.12
21.65
21.06
O=S=O
NH
O
O
Ts
Cl
O
1s in CDCl3
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

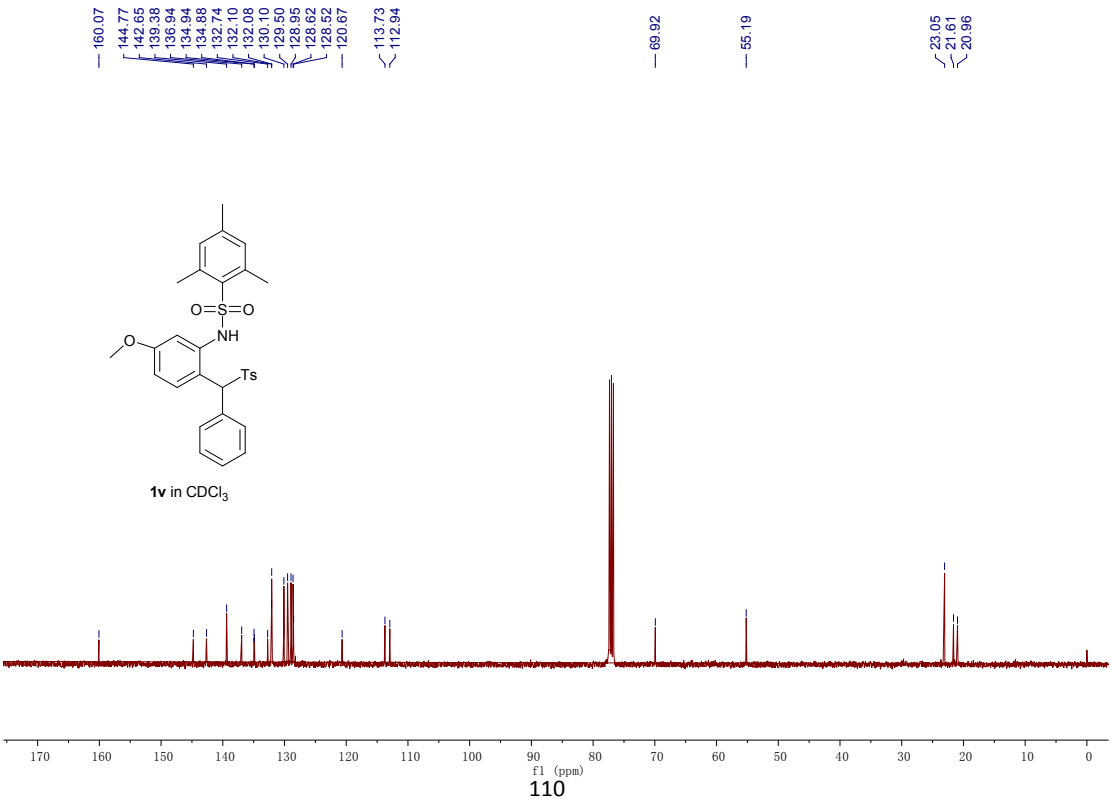

7.97
7.88
7.70
7.68
7.26
7.21
7.19
7.14
7.02
6.90
6.34
6.15
5.90
5.89
2.64
2.37
2.36
2.34
2.05
O=S=O
NH
O
O
Ts
1t in CDCl3
1.07
1.05
2.06
2.18
1.07
2.10
2.16
1.00
1.02
1.99
6.23
9.33
2.96
f1 (ppm)

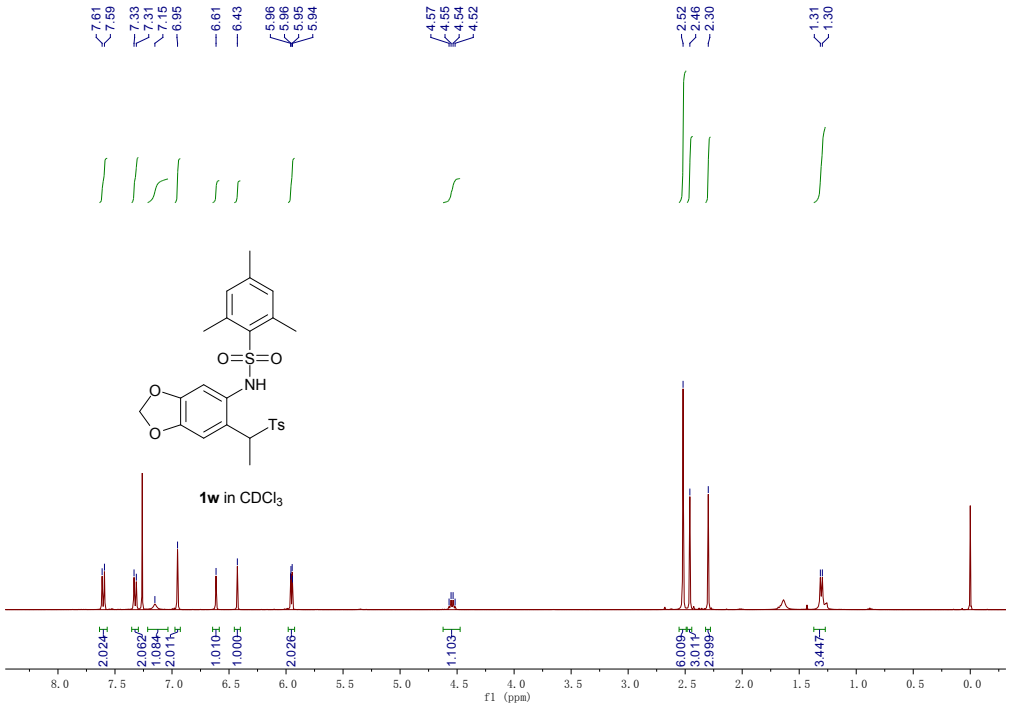

148.16
146.45
144.75
142.54
138.65
135.81
135.38
135.34
134.82
132.22
131.07
130.85
130.46
130.00
129.53
129.32
128.73
121.45
110.81
106.55
101.86
66.01
22.85
21.63
21.26
21.01
19.28
O=S=O
NH
O
O
Ts
1t in CDCl3
f1 (ppm)

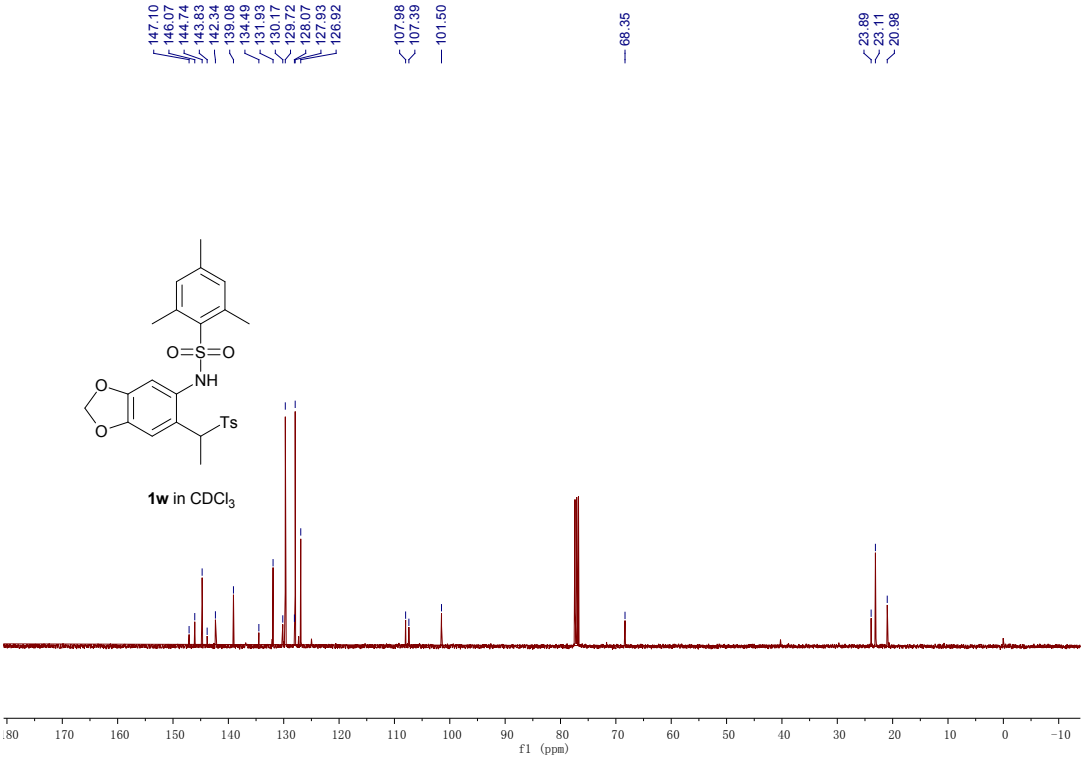

7.63
7.61
7.45
7.44
7.43
7.42
7.27
7.26
7.25
7.20
7.18
7.18
7.10
6.96
6.23
6.00
3.77
3.49
2.49
2.37
2.31
O=S=O
NH
O
O
Ts
1u in CDCl3
2.04
2.16
4.55
1.19
1.84
1.04
2.06
1.02
1.00
2.97
2.98
5.97
3.10
3.05
f1 (ppm)

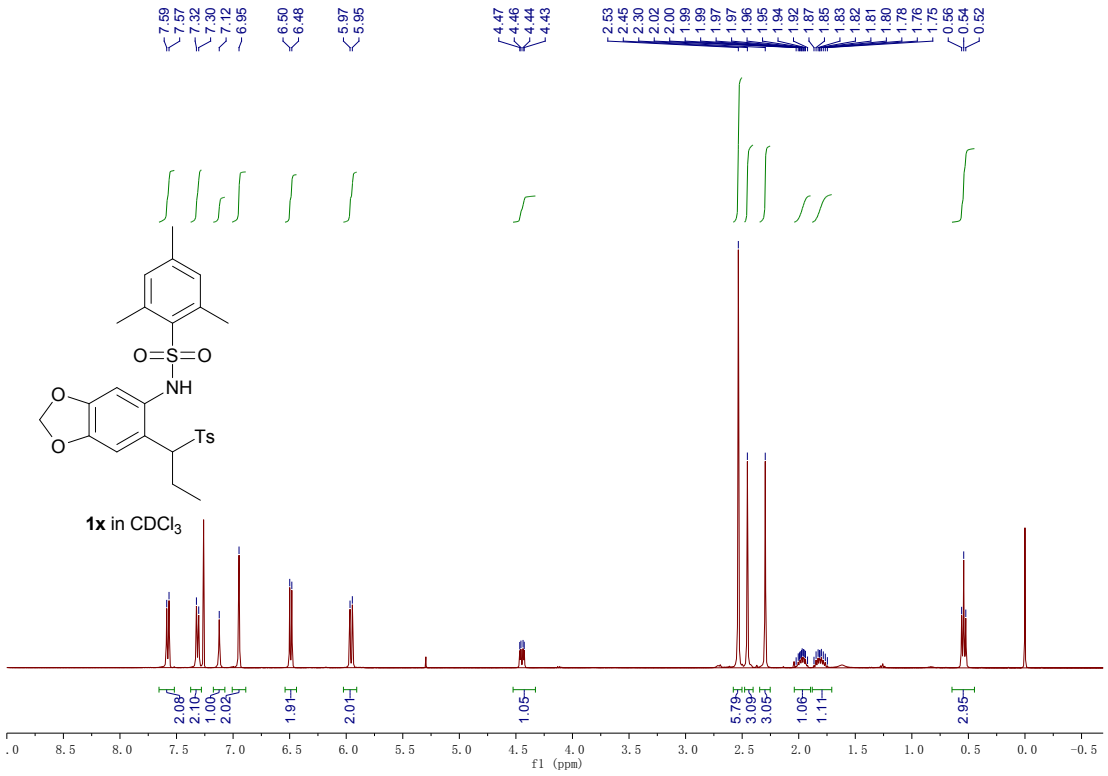

149.12
148.30
144.74
142.67
139.70
131.96
130.00
129.49
128.97
128.65
113.02
111.97
69.73
55.91
55.55
23.12
21.61
20.91
O=S=O
NH
O
O
Ts
1u in CDCl3
f1 (ppm)

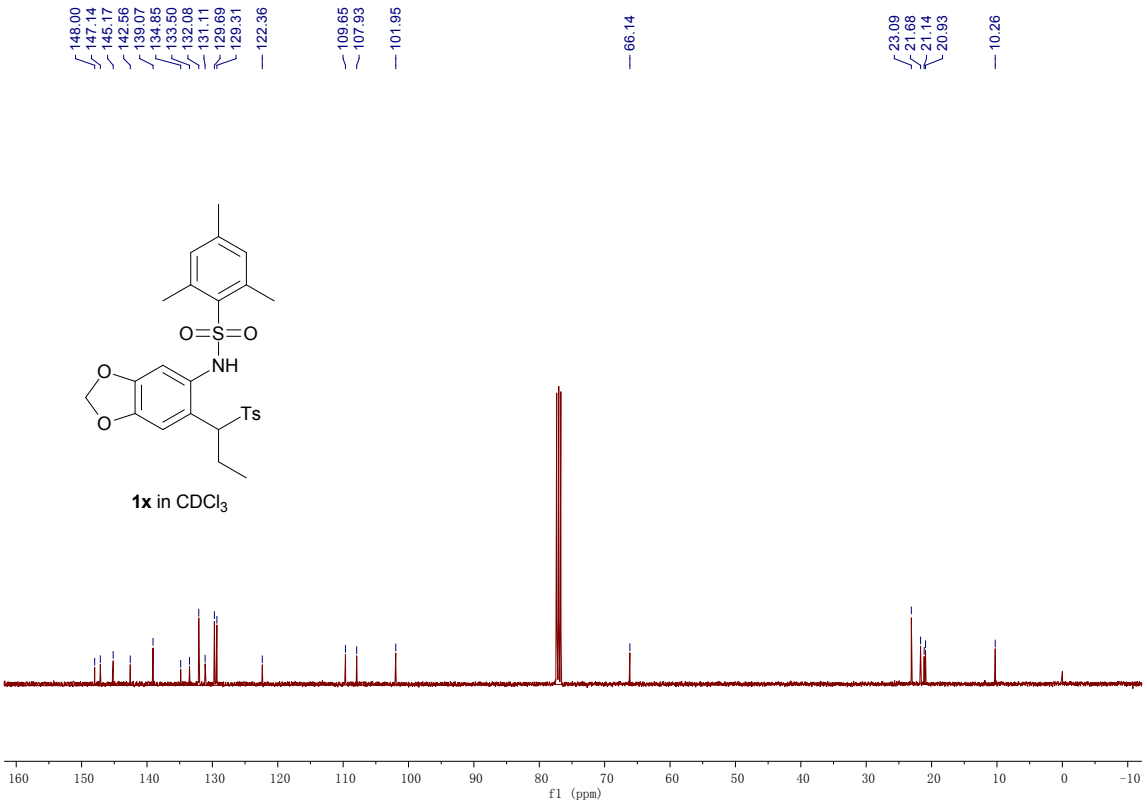

7.79
7.63
7.61
7.46
7.44
7.42
7.41
7.40
7.40
7.19
7.17
6.99
6.76
6.75
6.74
6.73
6.40
6.39
5.92
3.57
2.56
2.36
2.33
O=S=O
NH
O
Ts
1v in CDCl3
1.11
2.22
1.14
2.03
4.27
2.00
2.09
1.05
1.04
1.00
3.07
6.11
3.24
2.90
f1 (ppm)

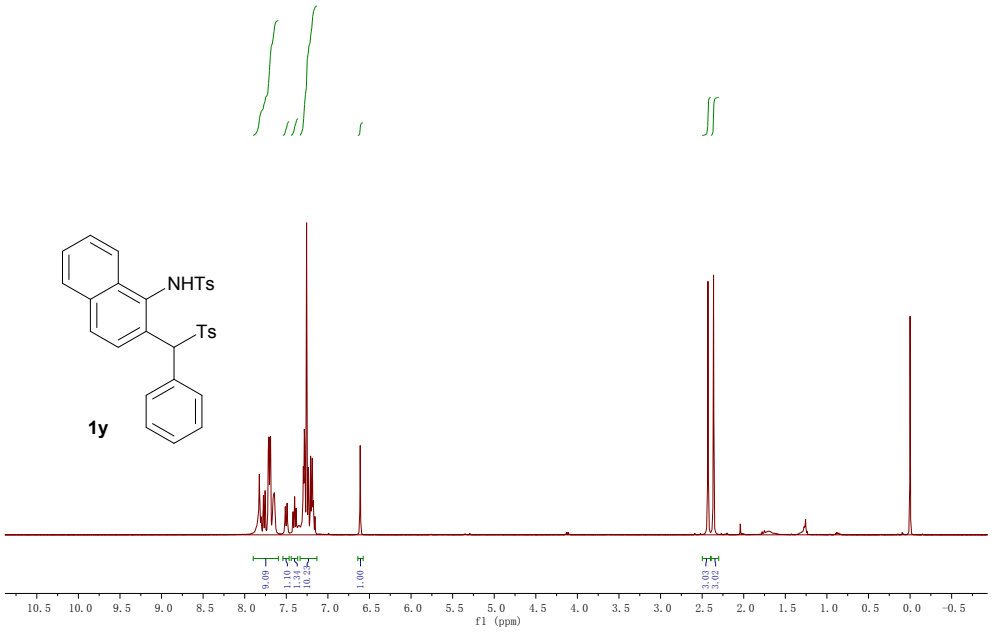

160.07
144.77
142.65
139.38
136.94
134.94
134.88
132.74
132.10
132.08
130.10
129.50
128.95
128.62
128.52
120.67
113.73
112.94
69.92
55.19
23.05
21.61
20.96
O=S=O
NH
O
Ts
1v in CDCl3
f1 (ppm)

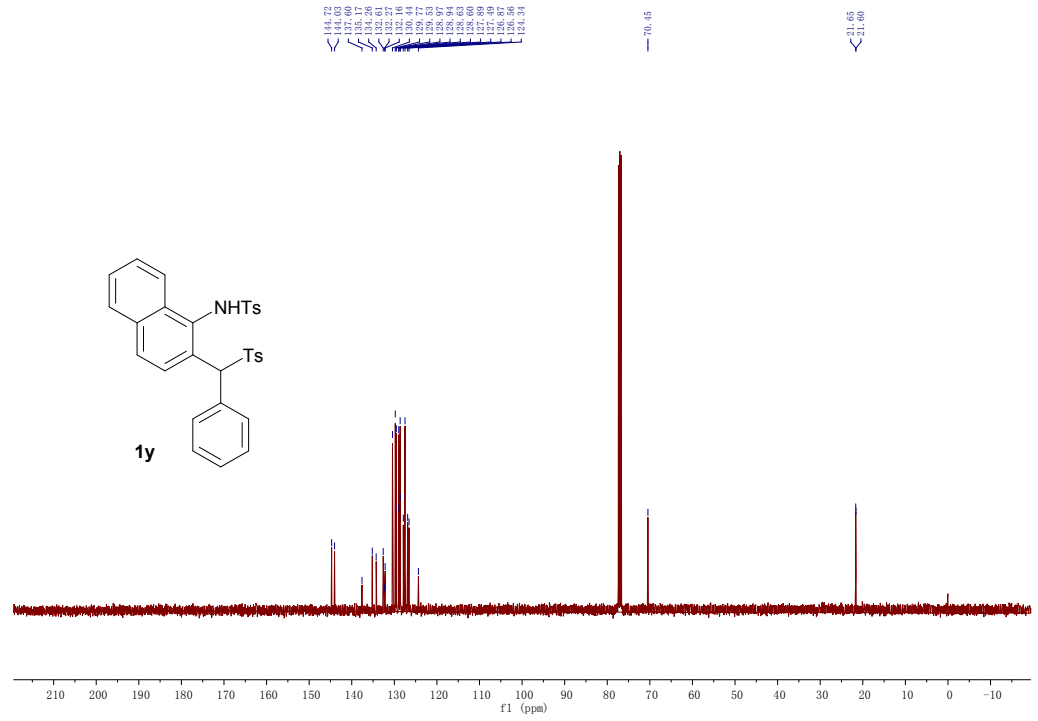

7.61
7.59
7.33
7.31
7.15
6.95
6.61
6.43
5.96
5.96
5.95
5.94
4.57
4.55
4.54
4.52
2.52
2.46
2.30
1.31
1.30
O=S=O
NH
O
O
Ts
1w in CDCl3
2.024
2.062
1.084
2.011
1.010
1.000
2.026
1.103
6.009
3.014
2.999
3.447
f1 (ppm)


147.10
146.07
144.74
143.83
142.34
139.08
134.49
131.93
130.17
129.72
128.07
127.93
126.92
107.98
107.39
101.50
68.35
23.89
23.11
20.98
O=S=O
NH
O
O
Ts
1w in CDCl3
f1 (ppm)


7.59
7.57
7.32
7.30
7.12
6.95
6.50
6.48
5.97
5.95
4.47
4.46
4.44
4.43
2.53
2.45
2.30
2.02
2.00
1.99
1.99
1.97
1.97
1.96
1.95
1.94
1.92
1.87
1.85
1.83
1.82
1.81
1.80
1.78
1.76
1.75
0.56
0.54
0.52
O=S=O
NH
O
O
Ts
1x in CDCl3
2.08
2.10
1.00
2.02
1.91
2.01
1.05
5.79
3.09
3.05
1.06
1.11
2.95
f1 (ppm)


148.00
147.14
145.17
142.56
139.07
134.85
133.50
132.08
131.11
129.69
129.31
122.36
109.65
107.93
101.95
66.14
23.09
21.68
21.14
20.93
10.26
O=S=O
NH
O
O
Ts
1x in CDCl3
f1 (ppm)


NHTs
Ts
1y
9.09
1.10
1.00
3.03
3.02
f1 (ppm)


144.72
144.03
137.60
135.17
134.26
132.61
132.27
132.16
130.44
129.77
129.53
128.97
128.94
128.63
128.60
127.98
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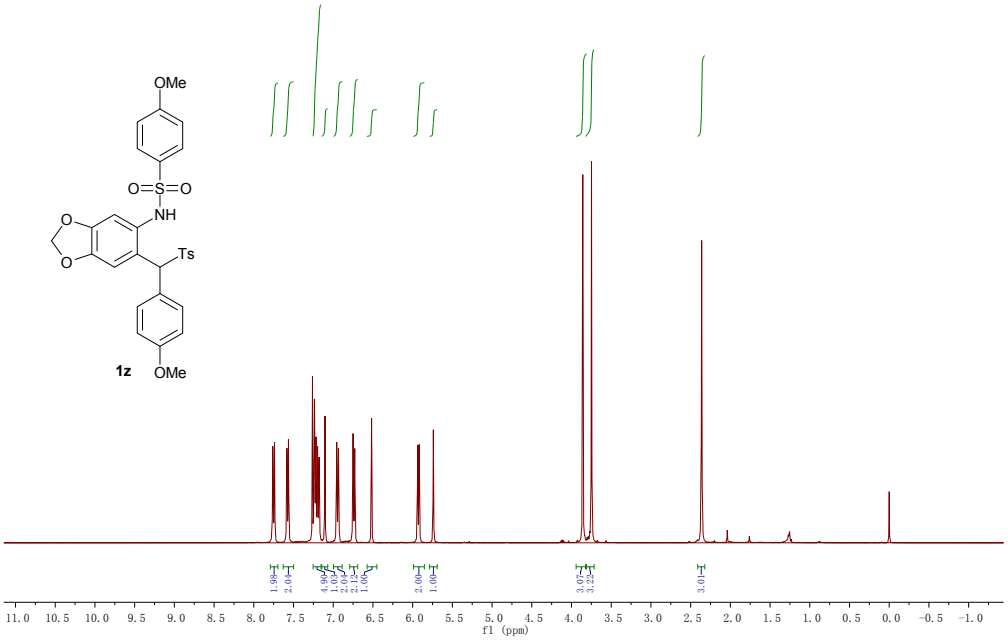
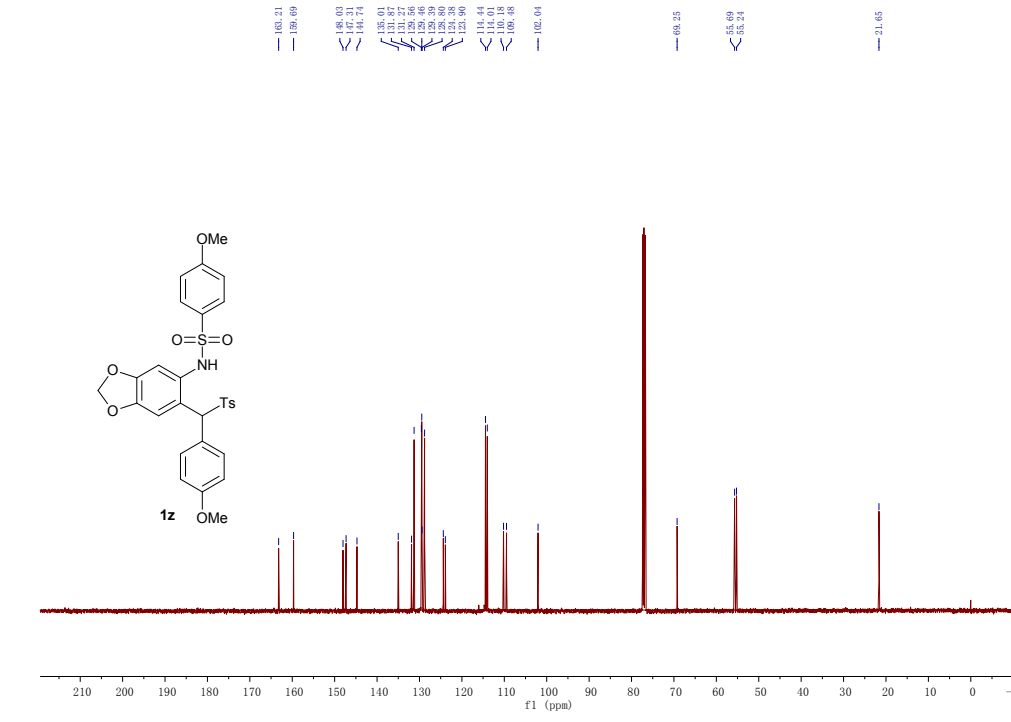
126.87
126.56
124.34
70.45
21.65
21.60
NHTs
Ts
1y
f1 (ppm)


OMe
O=S=O
NH
O
O
Ts
1z
OMe
1.99
2.04
4.90
1.03
2.01
2.15
1.06
2.00
1.00
3.07
3.22
3.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


OMe
O=S=O
NH
O
O
Ts
1z
OMe
163.21
159.69
148.03
147.31
144.74
135.01
131.87
131.27
129.66
129.46
129.39
128.89
128.38
124.38
123.90
114.44
114.01
110.18
109.48
102.04
69.25
55.69
55.24
21.65
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)