Supporting Information

Electrophilic Aromatic Substitution of Electron-rich Arenes with *N*-Fluorobenzenesulfonimide (NFSI) as Electrophile

Lina Bai,[†] Dewei Tu,[†] Ping Deng, Yongjie Chen, and Qiang Tang*

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1. General Information

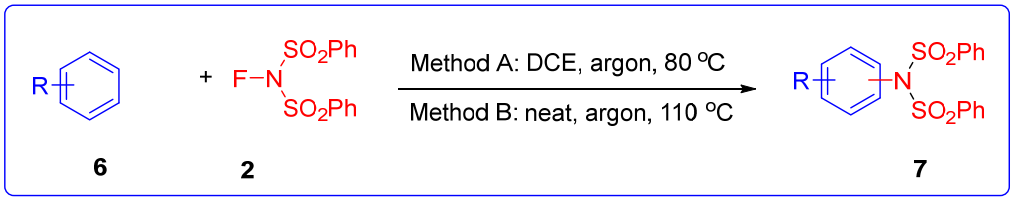
Materials: Unless otherwise specified, the chemicals were obtained commercially and used without further purification. All solvents were of ACS reagent grade or better unless otherwise noted. Flash column chromatography was performed on silica gel (300-400 mesh) or aluminum oxide (pore size 60 Å, activated, neutral) with freshly distilled solvents. TLC analyses were performed on commercial glass plates bearing a 0.25-mm layer of Silica gel GF_{254}. Visualization was performed using a UV lamp or chemical stains like $KMnO_4$ and I_2.

NMR Spectroscopy: ^{1}H and ^{13}C NMR spectra for all compounds were acquired in DMSO-d_6 or $CDCl_3$ solution on a Bruker Avance III HD -600 MHz or JEOL ECA400 (400 MHz), Spectrometer. The splitting patterns are designated as singlet (s), doublet (d), triplet (t), quartet (q), dd (doublet of doublets); m (multiplets), and etc. All first-order splitting patterns were assigned on the basis of the appearance of the multiplet. Splitting patterns that could not be easily interpreted are designated as multiplet (m) or broad (br).

Mass Spectrometry: High resolution mass spectral analysis (HRMS) was performed on ESI-QTOP massspectrometer. LC-MS was performed on a Shimadzu LCMS-IT-TOF under the conditions of electrospray ionization (ESI) in both positive and negative mode.

Melting points: Melting points (mp) were measured in open glass capillaries on a YIDIAN WUGUANG WRS-2C melting point apparatus and are uncorrected.

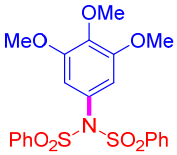
2. Procedure for the preparation of product 7



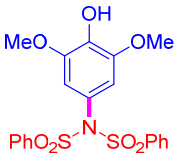
6 2 7

Method A: To a round bottom flask equipped with a reflux condenser, was added arene **6** (1.0 mmol), NFSI (2.0 mmol) and 5 mL of DCE. The resulting solution was stirred under argon at 80 ºC for 1-10 hours until complete consumption of the arene, as monitored by TLC. The reaction mixture was concentrated under reduced pressure. Then, the residue was purified by flash column chromatography using a mixture of hexane and EtOAc as eluent to obtain the desired product.

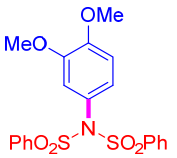
Method B: A mixture of arene **6** (1.0 mmol) and NFSI (2.0 mmol) was stirred under argon at 110 ºC for 1-4 hours until complete consumption of the arene, as monitored by TLC. After completion of the reaction, the reaction mixture was cooled to room temperature. Then, the residue was purified by flash column chromatography using a mixture of hexane and EtOAc as eluent to obtain the desired product.



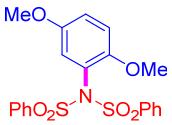
***N*-(phenylsulfonyl)-*N*-(3,4,5-trimethoxyphenyl)benzenesulfonamide (7a).** The title compound was obtained as brownish solid (95% yield in method A and 91% yield in method B, mp: 95-96 ºC). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.0 Hz, 4H), 7.69 (t, *J* = 7.4 Hz, 2H), 7.57 (t, *J* = 7.7 Hz, 4H), 6.16 (s, 2H), 3.87 (s, 3H), 3.65 (s, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 153.14, 139.42, 134.03, 128.98, 128.73, 108.99, 60.96, 56.12; HRMS (ESI) m/z: $[M+H]^+$calcd for $C_{21}H_{22}NO_7S_2$: 464.0832; Found: 464.0828.



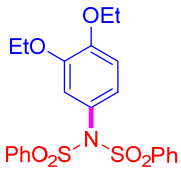
***N*-(4-hydroxy-3,5-dimethoxyphenyl)-*N*-(phenylsulfonyl)benzenesulfonamide (7b).** The title compound was obtained as brown solid (67% yield in method A and 74% yield in method B, mp: 178-179 ºC). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.07 – 7.89 (m, 4H), 7.68 (t, *J* = 7.5 Hz, 2H), 7.56 (t, *J* = 7.9 Hz, 4H), 6.17 (s, 2H), 5.70 (s, 1H), 3.70 (s, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 146.77, 139.42, 136.74, 133.98, 128.96, 128.69, 125.06, 108.81, 56.34; HRMS (ESI) m/z: $[M+H]^+$calcd for $C_{20}H_{20}NO_7S_2$: 450.0676; Found: 450.0685.



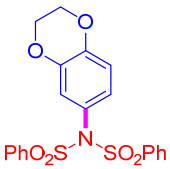
***N*-(3,4-dimethoxyphenyl)-*N*-(phenylsulfonyl)benzenesulfonamide (7c).** The title compound was obtained as brown solid (91% yield in method A and 92% yield in method B, mp: 140-141 ºC). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.96 (d, *J* = 7.7 Hz, 4H), 7.68 (t, *J* = 7.4 Hz, 2H), 7.55 (t, *J* = 7.8 Hz, 4H), 6.80 (d, *J* = 8.6 Hz, 1H), 6.63 (dd, *J* = 8.5, 2.1 Hz, 1H), 6.38 (d, *J* = 2.0 Hz, 1H), 3.89 (s, 3H), 3.66 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.63, 148.96, 139.49, 133.94, 128.98, 128.63, 126.38, 124.37, 114.35, 110.73, 55.98, 55.91; HRMS (ESI) m/z: $[M+H]^+$calcd for $C_{20}H_{20}NO_6S_2$: 434.0727; Found: 434.0734.



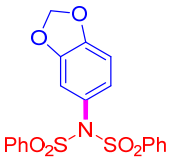
***N*-(2,5-dimethoxyphenyl)-*N*-(phenylsulfonyl)benzenesulfonamide (7d).** The title compound was obtained as white solid (82% yield in method A and 86% yield in method B, mp: 156-157 °C). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.02 – 7.91 (m, 4H), 7.69 – 7.59 (m, 2H), 7.57 – 7.44 (m, 4H), 6.95 (dd, *J* = 9.0, 3.1 Hz, 1H), 6.76 (d, *J* = 9.1 Hz, 1H), 6.66 (d, *J* = 3.1 Hz, 1H), 3.68 (s, 3H), 3.33 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 153.16, 151.98, 139.99, 133.71, 128.88, 128.62, 122.73, 118.34, 117.56, 112.54, 55.82, 55.45; HRMS (ESI) m/z: $[M+H]^+$calcd for $C_{20}H_{20}NO_6S_2$: 434.0727; Found: 434.0738.



***N*-(3,4-diethoxyphenyl)-*N*-(phenylsulfonyl)benzenesulfonamide (7e).** The title compound was obtained as white solid (88% yield in method A and 83% yield in method B, mp: 116-117 °C). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.95 (d, *J* = 7.5 Hz, 4H), 7.66 (t, *J* = 7.5 Hz, 2H), 7.54 (t, *J* = 7.9 Hz, 4H), 6.78 (d, *J* = 8.6 Hz, 1H), 6.59 (dd, *J* = 8.6, 2.4 Hz, 1H), 6.40 (d, *J* = 2.4 Hz, 1H), 4.10 (q, *J* = 7.0 Hz, 2H), 3.86 (q, *J* = 7.0 Hz, 2H), 1.46 (t, *J* = 7.0 Hz, 3H), 1.35 (t, *J* = 7.0 Hz, 3H) ; ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.42, 148.48, 139.57, 133.84, 128.94, 128.60, 126.13, 124.32, 116.27, 112.26, 64.53, 14.72, 14.55; ^{1}H NMR (400 MHz, DMSO-*d6*) δ 7.85 – 7.79 (m, 6H), 7.73 – 7.65 (m, 4H), 6.97 (d, *J* = 8.7 Hz, 1H), 6.58 (dd, *J* = 8.6, 2.5 Hz, 1H), 6.30 (d, *J* = 2.5 Hz, 1H), 4.04 (q, *J* = 7.0 Hz, 2H), 3.77 (q, *J* = 7.0 Hz, 2H), 1.33 (t, *J* = 7.0 Hz, 3H), 1.22 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, DMSO-*d6*) δ 150.40, 148.24, 139.10, 135.15, 130.08, 128.57, 128.56, 125.70, 124.80, 116.09, 113.06, 64.41, 64.36, 15.13, 14.96; HRMS (ESI) m/z: $[M+H]^+$calcd for $C_{22}H_{24}NO_6S_2$: 462.1040; Found: 462.1048.

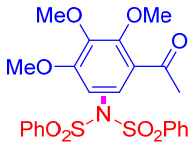


***N*-(2,3-dihydrobenzo[*b*][1,4]dioxin-6-yl)-*N*-(phenylsulfonyl)benzenesulfonamide (7f).** The title compound was obtained as white solid (80% yield in method A and 87% yield in method B, mp: 181-182 °C). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.00 – 7.91 (m, 4H), 7.67 (t, *J* = 7.5 Hz, 2H), 7.55 (t, *J* = 7.9 Hz, 4H), 6.79 (d, *J* = 8.6 Hz, 1H), 6.60 (d, *J* = 2.5 Hz, 1H), 6.45 (dd, *J* = 8.6, 2.5 Hz, 1H), 4.27 (dd, *J* = 5.7, 2.4 Hz, 2H), 4.23 (dd, *J* = 5.7, 2.4 Hz, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 145.47, 143.65, 139.52, 133.95, 129.01, 128.57, 126.79, 124.77, 120.45, 117.48, 64.35, 64.07; ^{1}H NMR (400 MHz, DMSO-*d6*) δ 7.87 – 7.78 (m, 6H), 7.73 – 7.66 (m, 4H), 6.88 (d, *J* = 8.6 Hz, 1H), 6.48 (d, *J* = 2.5 Hz, 1H), 6.40 (dd, *J* = 8.6, 2.6 Hz, 1H), 4.27 (ddd, *J* = 12.1, 3.5, 1.6 Hz, 4H); ^{13}C NMR (101 MHz, DMSO-*d6*) δ 145.80, 143.91, 139.04, 135.20, 130.12, 130.10, 128.52, 128.51, 126.28, 124.95, 120.28, 117.97, 64.71, 64.45; HRMS (ESI) m/z: $[M+H]^+$calcd for $C_{20}H_{18}NO_6S_2$: 432.0570; Found: 432.0560.

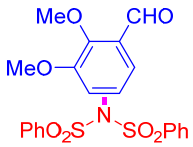


***N*-(phenylsulfonyl)-*N*-(benzo[*d*][1,3]dioxol-5-yl)benzenesulfonamide (7g).** The title compound was obtained as white solid (92% yield in method A and 90% yield in method B, mp: 178-179 °C). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.03 – 7.92 (m, 4H), 7.68 (t, *J* = 7.5 Hz, 2H), 7.56 (t, *J* = 7.9 Hz, 4H), 6.73 (d, *J* = 8.2 Hz, 1H), 6.49 (d, *J* = 2.1 Hz, 1H), 6.45 (dd, *J* = 8.2, 2.1 Hz, 1H), 6.02 (s, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.37, 148.07, 139.40, 134.01, 129.04, 128.58, 127.29, 125.96, 111.84, 108.16, 102.14; ^{1}H NMR (400 MHz, DMSO-*d6*) δ 7.89 – 7.79 (m, 6H), 7.74 – 7.64 (m, 4H), 6.92 (d, *J* = 8.3 Hz, 1H), 6.58 (d, *J* = 2.1 Hz, 1H), 6.39 (dd, *J* =

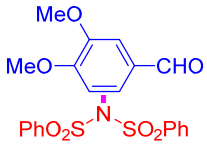
8.3, 2.2 Hz, 1H), 6.13 (s, 2H); ^{13}C NMR (101 MHz, DMSO-*d6*) δ 154.32, 153.03, 143.71, 139.98, 134.87, 133.31, 131.63, 131.10, 116.65, 113.55, 107.67; HRMS (ESI) m/z: $[M+H]^+$calcd for $C_{19}H_{16}NO_6S_2$: 418.0414; Found: 418.0409.



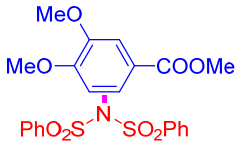
***N*-(5-acetyl-2,3,4-trimethoxyphenyl)-*N*-(phenylsulfonyl)benzenesulfonamide (7h).** The title compound was obtained as yellow solid (51% yield in method A and 54% yield in method B, mp: 200-201 °C). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.16 – 8.01 (m, 4H), 7.68 (d, *J* = 7.5 Hz, 2H), 7.57 (t, *J* = 7.9 Hz, 4H), 5.99 (s, 1H), 3.92 (d, *J* = 7.2 Hz, 6H), 3.50 (s, 3H), 2.46 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 199.51, 153.34, 151.37, 143.51, 138.39, 134.16, 131.34, 129.94, 128.57, 125.25, 112.26, 61.79, 61.00, 55.88, 32.06; HRMS (ESI) m/z: $[M+H]^+$calcd for $C_{23}H_{24}NO_8S_2$: 506.0938; Found: 506.0930.



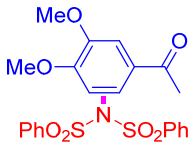
***N*-(3-formyl-4,5-dimethoxyphenyl)-*N*-(phenylsulfonyl)benzenesulfonamide (7i).** The title compound was obtained as white solid (68% yield in method A and 55% yield in method B, mp: 171-172 °C). ^{1}H NMR (600 MHz, $CDCl_3$) δ 10.34 (s, 1H), 7.99 – 7.86 (m, 4H), 7.70 (t, *J* = 7.5 Hz, 2H), 7.57 (t, *J* = 7.9 Hz, 4H), 7.06 (d, *J* = 2.5 Hz, 1H), 6.69 (d, *J* = 2.5 Hz, 1H), 4.04 (s, 3H), 3.72 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 188.53, 153.91, 153.31, 139.14, 134.24, 129.91, 129.58, 129.13, 128.63, 122.33, 120.63, 62.36, 56.19; HRMS (ESI) m/z: $[M+H]^+$calcd for $C_{21}H_{20}NO_7S_2$: 462.0676; Found: 462.0683.



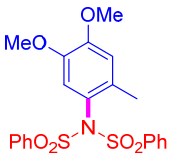
***N*-(5-formyl-2,3-dimethoxyphenyl)-*N*-(phenylsulfonyl)benzenesulfonamide (7j).** The title compound was obtained as white solid (49% yield in method A and 43% yield in method B, mp: 203-204 °C). ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.31 (s, 1H), 7.95 (dt, *J* = 3.1, 2.1 Hz, 4H), 7.72 (t, *J* = 7.5 Hz, 2H), 7.58 (t, *J* = 7.9 Hz, 4H), 7.44 (s, 1H), 6.32 (s, 1H), 3.96 (s, 3H), 3.70 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 187.36, 153.49, 150.78, 138.18, 134.61, 130.22, 129.66, 129.32, 128.98, 128.84, 128.63, 114.65, 109.03, 56.32, 56.30; HRMS (ESI) m/z: $[M+H]^+$calcd for $C_{21}H_{20}NO_7S_2$: 462.0676; Found: 462.0670.



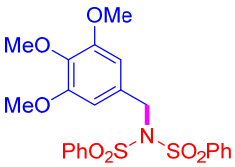
***N*-(5-methoxycarbonyl-2,3-dimethoxyphenyl)-*N*-(phenylsulfonyl)benzenesulfonamide (7k).** The title compound was obtained as brown oil (46% yield in method A and 58% yield in method B,). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.02 – 7.93 (m, 4H), 7.71 – 7.64 (m, 2H), 7.58 – 7.51 (m, 5H), 6.42 (s, 1H), 3.96 (s, 3H), 3.71 (s, 3H), 3.30 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.95, 151.47, 149.95, 139.81, 133.83, 129.18, 128.76, 126.71, 124.47, 116.06, 113.85, 56.26, 56.19, 51.69; HRMS (ESI) m/z: $[M+H]^+$calcd for $C_{22}H_{22}NO_8S_2$: 492.0781; Found: 492.0773.



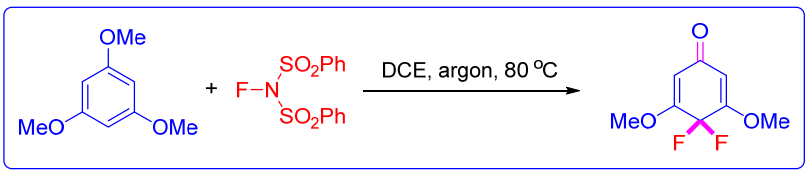
***N*-(5-acetyl-2,3-dimethoxyphenyl)-*N*-(phenylsulfonyl)benzenesulfonamide (7l).** The title compound was obtained as yellow solid (57% yield in method A and 51% yield in method B, mp: 136-137 °C). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.03 – 7.92 (m, 4H), 7.74 – 7.58 (m, 2H), 7.58 – 7.48 (m, 4H), 7.17 (s, 1H), 6.25 (s, 1H), 3.93 (s, 3H), 3.59 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 197.15, 150.62, 149.83, 138.69, 134.20, 133.59, 129.53, 128.78, 124.65, 115.67, 111.81, 56.21, 56.00, 29.47; HRMS (ESI) m/z: $[M+H]^+$calcd for $C_{22}H_{22}NO_7S_2$: 476.0832; Found: 476.0837.



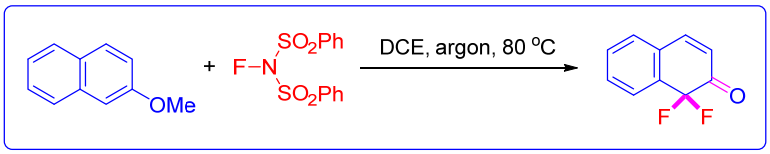
***N*-(4,5-dimethoxy-2-methylphenyl)-*N*-(phenylsulfonyl)benzenesulfonamide (7m).** The title compound was obtained as white solid (78% yield in method A and 59% yield in method B, mp: 143-144 °C). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.96 (d, J = 7.5 Hz, 4H), 7.68 (t, J = 7.5 Hz, 2H), 7.55 (t, J = 7.9 Hz, 4H), 6.68 (s, 1H), 6.23 (s, 1H), 3.88 (s, 3H), 3.59 (s, 3H), 1.88 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.33, 146.78, 139.56, 134.00, 133.49, 128.95, 128.93, 124.60, 114.64, 113.05, 55.89, 55.85, 17.77; HRMS (ESI) m/z: $[M+H]^+$calcd for $C_{21}H_{22}NO_6S_2$: 448.0883; Found: 448.0891.



***N*-(phenylsulfonyl)-*N*-(3,4,5-trimethoxybenzyl)benzenesulfonamide (7n).[1]** The title compound was obtained as yellow solid (53% yield in method A, mp: 109-110 °C), and the analytical data are consistent with those in the literature. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.76 (dd, J = 8.5, 1.1 Hz, 4H), 7.56 – 7.47 (m, 2H), 7.43 – 7.34 (m, 4H), 6.46 (s, 2H), 4.82 (s, 2H), 3.75 (s, 3H), 3.62 (s, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 153.10, 140.11, 137.65, 133.70, 129.84, 128.80, 128.10, 105.90, 60.88, 56.00, 52.88; MS (ESI) m/z: $[M+H]^+$calcd for $C_{22}H_{24}NO_7S_2$: 478.1; Found: 478.2.



4,4-Difluoro-3,5-dimethoxycyclohexa-2,5-dien-1-one (7o).[2] The title compound was obtained as brown oil (48% yield in method A) and the analytical data are consistent with those in the literature. ^{1}H NMR (600 MHz, $CDCl_3$) δ 5.48 (s, 2H), 3.82 (s, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 184.56, 161.19, 161.04, 160.90, 102.48, 102.46, 102.43, 56.75; ^{19}F NMR (565 MHz, $CDCl_3$) δ -112.50, -112.51.



1,1-Difluoronaphthalen-2(1*H*)-one (7p).[3] The title compound was obtained as yellowish solid (47% yield in method A, mp: 52-53 °C) and the analytical data are consistent with those in the literature. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.88 – 7.77 (m, 1H), 7.53 (dd, J = 6.2, 2.6 Hz, 2H), 7.44 (d, J = 10.1 Hz, 1H), 7.40 – 7.33 (m, 1H), 6.22 (dt, J = 10.1, 2.7 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 187.70, 187.54, 187.38, 145.70, 133.42, 133.26, 133.10, 132.14, 132.13, 132.12, 131.01, 131.00, 130.98, 130.33, 130.29, 130.25, 129.94, 127.75, 127.72, 127.70, 123.49, 123.48, 123.46, 107.18, 105.56, 103.94; ^{19}F NMR (565 MHz, $CDCl_3$) δ -101.16.

3. DFT Calculations

All reported structures were optimized at Density Functional Theory level as implemented in Gaussian 09.[4] The geometry optimizations and single point electronic energies for those structures were calculated at B97XD /6-311++ level.[5] The transition states were located and confirmed by frequency calculations (single imaginary frequency). Intrinsic Reaction Coordinate (IRC) calculations were performed to confirm that the first-order saddle points found were real transition states connecting the reactants and the products. All geometry optimizations were carried out without any symmetry constraints. The stationary points were characterized as minima by full vibration frequencies calculations (no imaginary frequency). Distortion energies were obtained by performing a single point calculation for each fragment of the optimized ground state and transition state structures. Reported energy values correspond to Gibbs Free (G) energies in kcal/mol^{-1}.

Table S1. Data of calculated enthalpies, free energies, and imaginary frequencies.

	H [hartree]	H-correction	G [hartree]	G-correction	Frequency
TMB	-575.376305	0.212378	-575.428296	0.160387	
NFSI	-1714.104871	0.225294	-1714.174121	0.156044	
TS1	-2289.458622	0.438217	-2289.555028	0.341810	-357.3532
Int1	-2289.520764	0.439503	-2289.617848	0.342419	
TS2	-2289.51463	0.438506	-2289.611147	0.341990	-95.2605
TS2`	-2289.510762	0.439484	-2289.606152	0.344095	-179.8377
Adduct I	-2289.552996	0.443051	-2289.647906	0.348140	
Adduct II	-2289.537162	0.442039	-2289.634194	0.345007	
Adduct II`	-2389.466451	0.443908	-2389.567190	0.343169	
TS3	-2289.512146	0.437590	-2289.611207	0.338529	-492.3781
TS3`	-2389.441430	0.439544	-2389.540556	0.340417	-104.6049
Products	-2289.607421	0.439238	-2289.709151	0.337508	

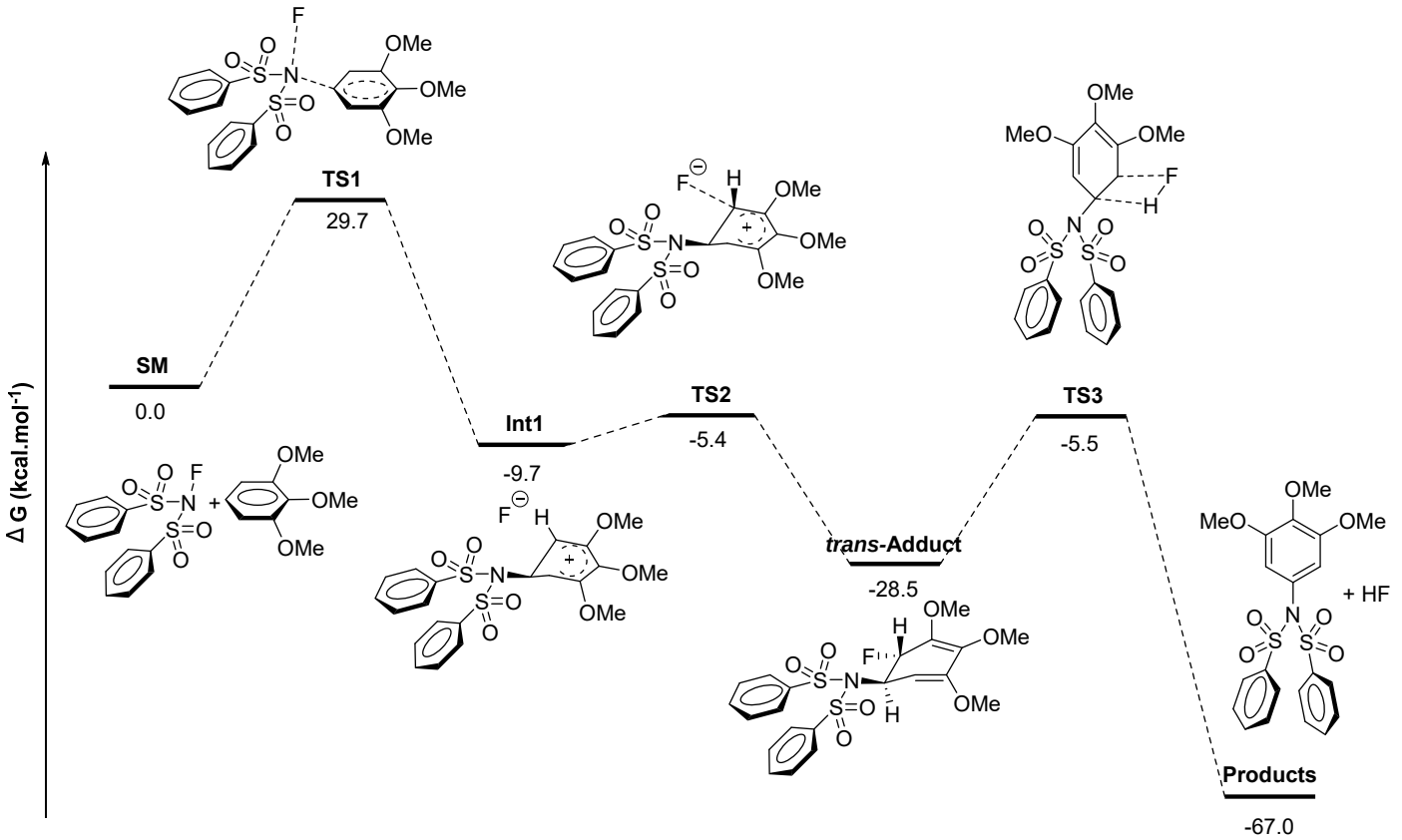


Figure S1. Computed Gibbs energy profile for the amidation reaction through *trans*-addition pathway.

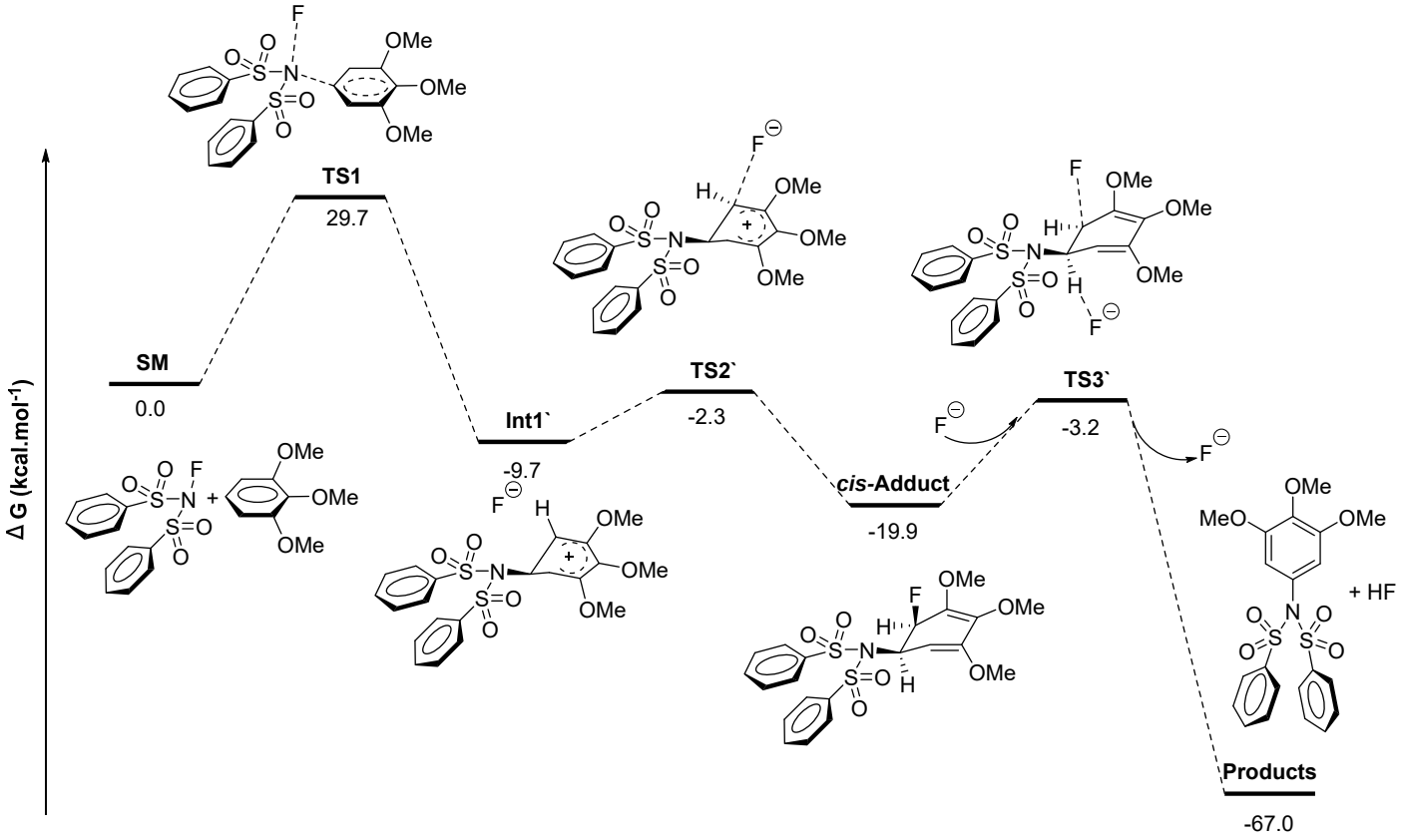
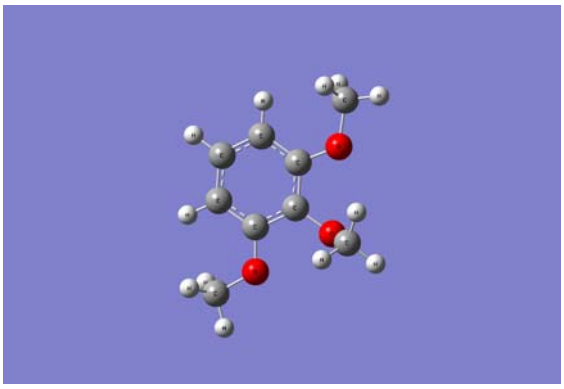


Figure S2. Computed Gibbs energy profile for the amidation reaction through *cis*-addition pathway.

Cartesian Coordinates

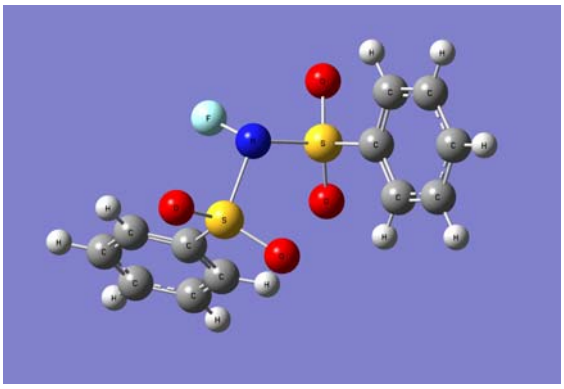
TMB



Symbolic Z-matrix: Charge = 0 Multiplicity = 1

C	-0.93536	-1.77774	0.00009
C	0.33233	-2.34295	0.00014
C	1.46449	-1.53398	0.00009
C	1.32203	-0.14646	0.
C	0.04056	0.45373	-0.00004
C	-1.08993	-0.3858	-0.00001
H	-1.80559	-2.41833	0.00012
H	0.44004	-3.42103	0.00021
H	2.4474	-1.98319	0.00012
O	0.0681	1.8144	-0.00013
O	2.36728	0.72756	-0.00005
O	-2.32176	0.22357	-0.0001
C	-3.48611	-0.58775	-0.00013
H	-4.32783	0.10377	-0.00023
H	-3.53724	-1.21873	-0.89418
H	-3.53737	-1.21861	0.894
C	3.68547	0.20323	-0.00003
H	3.87959	-0.40008	-0.89405
H	4.34662	1.06863	-0.00008
H	3.87961	-0.39999	0.89405
C	-1.09628	2.64138	0.00016
H	-1.70601	2.48117	0.89059
H	-0.70507	3.65889	0.00015
H	-1.70638	2.48129	-0.89004

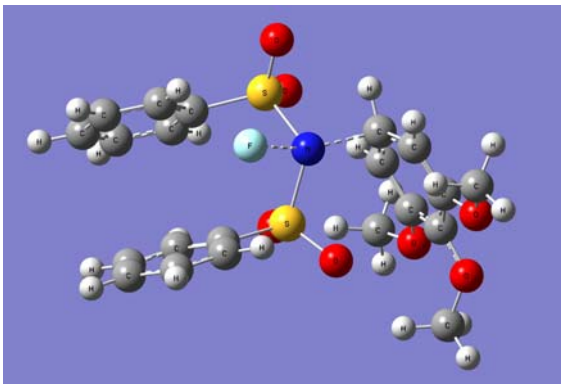
NFSI



Symbolic Z-matrix: Charge = 0 Multiplicity = 1

C	-3.88995	-1.83987	-0.02095
C	-2.66227	-1.34454	0.40986
C	-2.48215	0.0356	0.44585
C	-3.4828	0.93034	0.06866
C	-4.70207	0.41691	-0.36102
C	-4.90363	-0.9632	-0.40508
H	-4.05145	-2.91049	-0.05781
H	-1.8587	-2.00625	0.70132
H	-3.30923	1.99745	0.12027
H	-5.4943	1.09409	-0.65696
H	-5.8561	-1.35668	-0.74139
S	-0.93117	0.69929	1.0342
N	-0.13209	1.01619	-0.58883
O	-1.13189	2.03454	1.56626
O	-0.2066	-0.31959	1.78195
F	0.68133	2.15539	-0.41785
S	0.90613	-0.24671	-1.32595
C	2.40572	-0.35417	-0.35732
C	2.48576	-1.28431	0.67748
C	3.4717	0.48107	-0.69295
C	3.67395	-1.37314	1.3966
H	1.63913	-1.91357	0.91155
C	4.64855	0.38311	0.04275
H	3.37853	1.17866	-1.51466
C	4.74841	-0.54145	1.08253
H	3.7581	-2.09175	2.203
H	5.48749	1.02386	-0.20103
H	5.6691	-0.61506	1.65009
O	1.23793	0.30235	-2.62729
O	0.09599	-1.44621	-1.16873

TS1

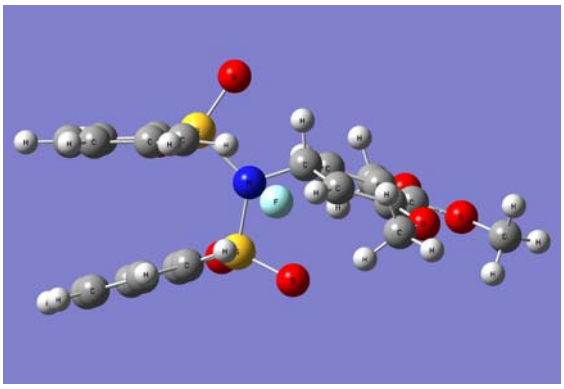


Symbolic Z-matrix: Charge = 0 Multiplicity = 1

C	5.19487	-0.70779	0.95901
C	3.87783	-0.82671	1.38951
C	2.93922	-1.34953	0.50253
C	3.27418	-1.75502	-0.78608
C	4.59718	-1.6152	-1.20404
C	5.55326	-1.0957	-0.33352
H	5.94158	-0.30455	1.6331
H	3.56534	-0.51415	2.37435
H	2.51882	-2.17385	-1.4366
H	4.878	-1.92599	-2.20379
H	6.58268	-0.99661	-0.66004
S	1.27654	-1.71661	1.08864
N	0.11153	-0.29784	0.92873
O	0.77223	-2.79081	0.22091
O	1.27896	-1.93879	2.52914
F	1.74422	0.78956	1.59561
S	0.07694	0.62528	-0.6349
C	1.32599	1.92289	-0.63133
C	2.43223	1.77666	-1.4579
C	1.07439	3.10028	0.0686
C	3.3206	2.84455	-1.57921
H	2.58863	0.85515	-2.00049
C	1.96764	4.15532	-0.06353
H	0.20624	3.17908	0.70738
C	3.09116	4.02837	-0.8835
H	4.18806	2.74697	-2.22158
H	1.79157	5.07679	0.47928
H	3.78479	4.85607	-0.98049
O	-1.22246	1.29998	-0.56107
O	0.37321	-0.27112	-1.75833
C	-3.0519	-1.27863	-0.9205
C	-3.85741	-0.27412	-0.2964
C	-3.55448	0.15544	1.04324
C	-2.43622	-0.31538	1.66556

C	-1.56365	-1.25326	1.00981
C	-1.95136	-1.77355	-0.26925
H	-2.1579	0.0199	2.65386
H	-1.11643	-1.97728	1.68383
H	-1.31553	-2.5246	-0.71063
O	-3.45349	-1.63472	-2.15957
O	-4.85091	0.16774	-1.04088
O	-4.44162	1.02888	1.59099
C	-2.66872	-2.60896	-2.85452
H	-2.72944	-3.58493	-2.36281
H	-3.10561	-2.67581	-3.84875
H	-1.62602	-2.28801	-2.92159
C	-4.78615	1.28505	-1.95653
H	-3.89585	1.21326	-2.57873
H	-5.68315	1.17788	-2.56263
H	-4.79638	2.22788	-1.41485
C	-4.19041	1.49308	2.91813
H	-4.99227	2.19408	3.14114
H	-4.21799	0.66564	3.6336
H	-3.22458	2.00268	2.97783

Int1

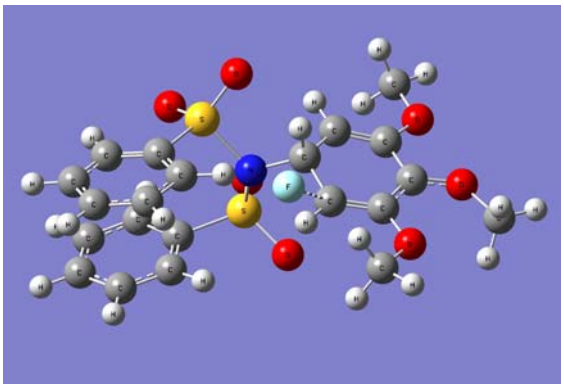


Symbolic Z-matrix: Charge = 0 Multiplicity = 1

C	-3.52399	1.86933	-1.94346
C	-2.4233	1.07778	-1.61332
C	-2.60827	-0.30116	-1.56811
C	-3.84167	-0.90313	-1.82753
C	-4.92109	-0.09201	-2.16229
C	-4.76041	1.29269	-2.22538
H	-3.39973	2.94571	-1.96151
H	-1.4913	1.57155	-1.33045
H	-3.95106	-1.97797	-1.76256
H	-5.88528	-0.54236	-2.3679
H	-5.60507	1.92178	-2.48419
S	-1.23505	-1.4351	-1.32306
N	-0.13001	-0.62664	-0.25043
O	-1.74186	-2.63609	-0.67438
O	-0.48036	-1.54465	-2.57676
F	-0.38523	2.77289	-0.29198
S	-0.20407	-0.80849	1.49796
C	-1.79011	-0.11552	1.93596
C	-2.72188	-0.95705	2.54291
C	-2.00995	1.24813	1.73596
C	-3.92255	-0.40413	2.97905
H	-2.50293	-2.00934	2.66797
C	-3.22141	1.77363	2.18018
H	-1.2907	1.87867	1.20486
C	-4.16688	0.95797	2.80227
H	-4.66235	-1.03613	3.45616
H	-3.4226	2.82789	2.03027
H	-5.10337	1.38406	3.14541
O	0.8764	0.07373	1.93641
O	-0.16547	-2.21694	1.86615
C	3.51611	-1.08927	-0.26959
C	3.92478	0.3078	-0.1706
C	2.9685	1.35879	-0.31175
C	1.65018	1.05468	-0.51431

C	1.22524	-0.33457	-0.77244
C	2.22499	-1.40324	-0.52176
H	0.82659	1.83404	-0.50126
H	1.08243	-0.35802	-1.87407
H	1.89055	-2.42683	-0.61423
O	4.52655	-1.96265	-0.07849
O	5.19983	0.44384	0.07208
O	3.44576	2.61855	-0.14424
C	4.20495	-3.35563	-0.08624
H	3.81705	-3.66209	-1.06263
H	5.1413	-3.8713	0.11421
H	3.47596	-3.59109	0.69453
C	5.93929	1.6882	0.2107
H	5.55606	2.2615	1.04988
H	6.95877	1.35698	0.39258
H	5.87476	2.26831	-0.70606
C	2.5513	3.71967	-0.43104
H	3.11192	4.61243	-0.16084
H	2.31419	3.73056	-1.49832
H	1.61803	3.64557	0.12914

TS2

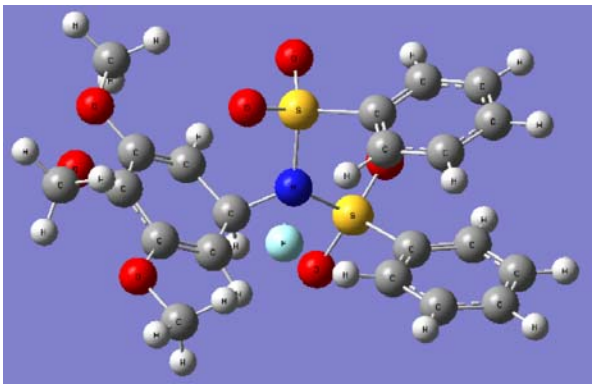


Symbolic Z-matrix: Charge = 0 Multiplicity = 1

C	-3.1147	3.11202	-0.8733
C	-2.11327	2.16507	-1.08902
C	-2.51554	0.85943	-1.36756
C	-3.85593	0.47808	-1.44116
C	-4.83353	1.44639	-1.23041
C	-4.4622	2.76104	-0.94796
H	-2.82196	4.1307	-0.64697
H	-1.06296	2.477	-0.99546
H	-4.11984	-0.54822	-1.659
H	-5.88056	1.17218	-1.28848
H	-5.22687	3.51296	-0.7853
S	-1.2954	-0.39519	-1.7691
N	-0.17172	-0.38042	-0.42159
O	-1.95478	-1.69533	-1.77759
O	-0.49285	0.04281	-2.90833
F	0.50572	3.18801	-0.39746
S	-0.28985	-1.53555	0.87728
C	-1.96193	-1.32269	1.47834
C	-2.88931	-2.33428	1.24417
C	-2.27068	-0.18534	2.22316
C	-4.16917	-2.19568	1.77573
H	-2.60798	-3.19723	0.65594
C	-3.55535	-0.0607	2.74161
H	-1.52356	0.57887	2.39439
C	-4.49947	-1.0643	2.52037
H	-4.90578	-2.97229	1.60701
H	-3.81694	0.81724	3.31999
H	-5.49785	-0.96239	2.93053
O	0.65402	-1.00506	1.86215
O	-0.12557	-2.89794	0.38869
C	3.45942	-0.90347	-0.71029
C	3.9252	0.19865	0.13127
C	3.01941	1.19035	0.59624
C	1.6868	1.07366	0.29583

C	1.20769	0.09124	-0.69402
C	2.16415	-0.97594	-1.08702
H	0.96271	1.83889	0.58397
H	1.09213	0.72394	-1.59708
H	1.79636	-1.75833	-1.73449
O	4.43574	-1.77436	-1.04176
O	5.20613	0.13214	0.38584
O	3.54208	2.17796	1.36541
C	4.06696	-2.90902	-1.82807
H	3.68908	-2.5998	-2.80755
H	4.98065	-3.48565	-1.95353
H	3.31382	-3.51222	-1.31261
C	5.99376	1.09112	1.14113
H	5.64567	1.13833	2.16935
H	7.0026	0.6889	1.08781
H	5.93948	2.07257	0.67759
C	2.64953	3.22781	1.81259
H	3.30515	4.00377	2.20352
H	2.03039	3.59427	0.98702
H	2.01186	2.84674	2.6158

TS2`



Symbolic Z-matrix: Charge = 0 Multiplicity = 1

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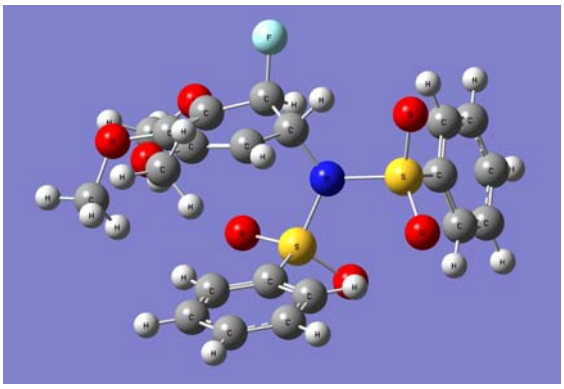
C	-2.16559	2.03089	-1.14542
C	-2.5799	0.729	-1.35253
C	-3.88473	0.27258	-1.27099
C	-4.86271	1.21308	-0.95907
C	-4.50397	2.54466	-0.73908
H	-2.89373	3.97873	-0.65916
H	-1.1085	2.35569	-1.18624
H	-4.11975	-0.76935	-1.43424
H	-5.89639	0.90399	-0.88699
H	-5.26952	3.27106	-0.49881
S	-1.28898	-0.54168	-1.76087
N	-0.12886	-0.30808	-0.34325
O	-1.95716	-2.00622	-1.68876
O	-0.38043	-0.14739	-3.03354
F	0.00849	1.67443	1.9746
S	-0.24902	-1.4105	1.09053
C	-2.02201	-1.1443	1.5268
C	-2.90306	-2.19083	1.33725
C	-2.37468	0.1064	2.00516
C	-4.24062	-1.96011	1.65707
H	-2.55678	-3.13275	0.93795
C	-3.71457	0.31644	2.31444
H	-1.63378	0.88425	2.12261
C	-4.63932	-0.71562	2.14344
H	-4.96408	-2.75186	1.52292
H	-4.03312	1.28229	2.67939
H	-5.67978	-0.54493	2.38508
O	0.74031	-0.66021	2.13103
O	0.03182	-2.96021	0.7683
C	3.45176	-0.98325	-0.58421
C	3.94838	0.20024	0.11003
C	3.06518	1.24561	0.46122

C	1.73328	1.12211	0.19169
C	1.2369	0.06673	-0.70438
C	2.1631	-1.0624	-0.96702
H	1.00309	1.87225	0.46045
H	1.10765	0.61332	-1.66739
H	1.76942	-1.90568	-1.51345
O	4.40487	-1.93924	-0.78923
O	5.23795	0.15824	0.36773
O	3.60427	2.32295	1.13034
C	3.98091	-3.19204	-1.38013
H	3.63032	-3.03694	-2.40271
H	4.86856	-3.81438	-1.38355
H	3.19611	-3.65294	-0.77676
C	6.05133	1.20269	1.00744
H	5.69075	1.3875	2.01268
H	7.04511	0.77012	1.00995
H	6.01247	2.11178	0.41719
C	2.7372	3.48563	1.32809
H	3.41373	4.29578	1.58
H	2.16682	3.7003	0.4205
H	2.05543	3.29459	2.15821

trans-Adduct



Symbolic Z-matrix: Charge = 0 Multiplicity = 1

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C	-3.75538	-1.44739	0.74119
C	-3.50492	-0.13886	0.33005
C	-4.22812	0.46922	-0.69286
C	-5.2302	-0.2639	-1.32296
C	-5.49207	-1.57668	-0.93219
H	-4.96491	-3.18587	0.40103
H	-3.18632	-1.88789	1.54964
H	-4.00064	1.4837	-0.98841
H	-5.80428	0.19243	-2.12067
H	-6.27227	-2.14167	-1.42959
S	-2.22483	0.79387	1.17531
N	-0.7231	0.38072	0.39452
O	-2.45263	2.21597	0.96182
O	-2.09078	0.25478	2.52467
S	-0.28152	1.08979	-1.11304
C	0.71163	2.54648	-0.74213
C	0.10238	3.68279	-0.21236
C	2.06642	2.519	-1.06463
C	0.88367	4.81346	0.01104
H	-0.95265	3.67558	0.02676
C	2.83157	3.66244	-0.84392
H	2.50064	1.62356	-1.48845
C	2.24277	4.80502	-0.30401
H	0.42586	5.70377	0.42598
H	3.88483	3.66001	-1.09985
H	2.84184	5.69253	-0.13405
O	0.59186	0.11033	-1.75051
O	-1.51696	1.52144	-1.75118
C	1.4125	-2.53434	-0.27156
C	2.58386	-1.94904	0.03771
C	2.62268	-0.78261	0.94459
C	1.50579	-0.16472	1.36729
C	0.14425	-0.67997	1.01243

C	0.10962	-2.01534	0.2379
H	1.53499	0.66404	2.06038
H	-0.37216	-0.89195	1.95092
H	-0.59346	-1.96507	-0.59309
O	1.26614	-3.58512	-1.12714
O	3.76212	-2.45424	-0.44262
O	3.89108	-0.43855	1.28685
C	1.95133	-4.80874	-0.81031
H	1.63911	-5.52306	-1.57109
H	3.03298	-4.67521	-0.83708
H	1.64159	-5.16458	0.17643
C	4.3998	-1.66549	-1.45911
H	4.71505	-0.69846	-1.06005
H	5.27619	-2.2318	-1.77244
H	3.7272	-1.52305	-2.31005
C	4.06543	0.63498	2.20632
H	5.14012	0.73009	2.35112
H	3.66176	1.56959	1.80427
H	3.58348	0.41022	3.1631
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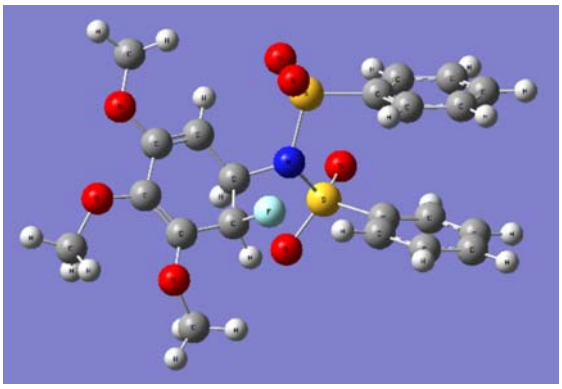
cis-Adduct

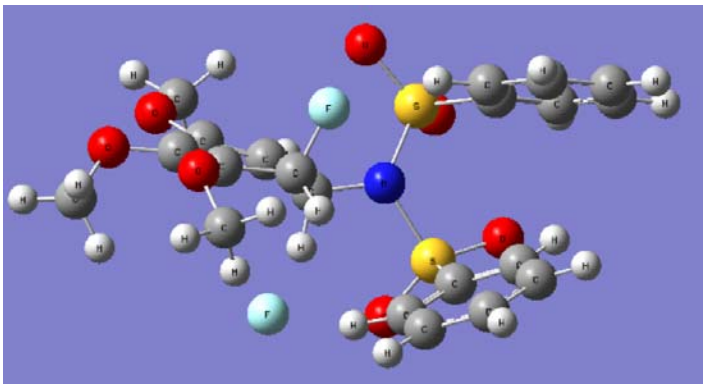


Symbolic Z-matrix: Charge = 0 Multiplicity = 1

C	-3.17156	2.94792	-0.82971
C	-2.16559	2.03089	-1.14542
C	-2.5799	0.729	-1.35253
C	-3.88473	0.27258	-1.27099
C	-4.86271	1.21308	-0.95907
C	-4.50397	2.54466	-0.73908
H	-2.89373	3.97873	-0.65916
H	-1.1085	2.35569	-1.18624
H	-4.11975	-0.76935	-1.43424
H	-5.89639	0.90399	-0.88699
H	-5.26952	3.27106	-0.49881
S	-1.28898	-0.54168	-1.76087
N	-0.12886	-0.30808	-0.34325
O	-1.95716	-2.00622	-1.68876
O	-0.38043	-0.14739	-3.03354
F	1.85711	0.95509	1.49012
S	-0.24902	-1.4105	1.09053
C	-2.02201	-1.1443	1.5268
C	-2.90306	-2.19083	1.33725
C	-2.37468	0.1064	2.00516
C	-4.24062	-1.96011	1.65707
H	-2.55678	-3.13275	0.93795
C	-3.71457	0.31644	2.31444
H	-1.63378	0.88425	2.12261
C	-4.63932	-0.71562	2.14344
H	-4.96408	-2.75186	1.52292
H	-4.03312	1.28229	2.67939
H	-5.67978	-0.54493	2.38508
O	0.74031	-0.66021	2.13103
O	0.03182	-2.96021	0.7683
C	3.45176	-0.98325	-0.58421
C	3.94838	0.20024	0.11003
C	3.06518	1.24561	0.46122

C	1.73328	1.12211	0.19169
C	1.2369	0.06673	-0.70438
C	2.1631	-1.0624	-0.96702
H	1.00309	1.87225	0.46045
H	1.10765	0.61332	-1.66739
H	1.76942	-1.90568	-1.51345
O	4.40487	-1.93924	-0.78923
O	5.23795	0.15824	0.36773
O	3.60427	2.32295	1.13034
C	3.98091	-3.19204	-1.38013
H	3.63032	-3.03694	-2.40271
H	4.86856	-3.81438	-1.38355
H	3.19611	-3.65294	-0.77676
C	6.05133	1.20269	1.00744
H	5.69075	1.3875	2.01268
H	7.04511	0.77012	1.00995
H	6.01247	2.11178	0.41719
C	2.7372	3.48563	1.32809
H	3.41373	4.29578	1.58
H	2.16682	3.7003	0.4205
H	2.05543	3.29459	2.15821

Adduct II`

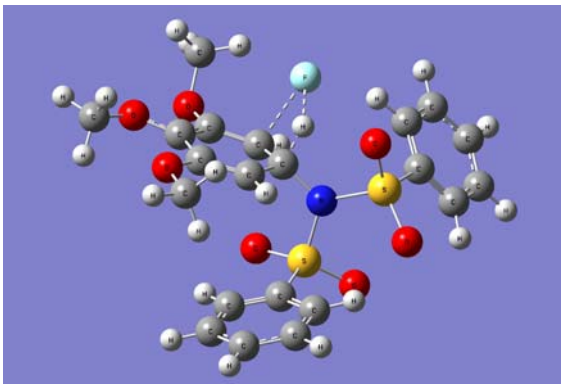


Symbolic Z-matrix: Charge = -1 Multiplicity = 1

C	-3.17156	2.94792	-0.82971
C	-2.16559	2.03089	-1.14542
C	-2.5799	0.729	-1.35253
C	-3.88473	0.27258	-1.27099
C	-4.86271	1.21308	-0.95907
C	-4.50397	2.54466	-0.73908
H	-2.89373	3.97873	-0.65916
H	-1.1085	2.35569	-1.18624
H	-4.11975	-0.76935	-1.43424
H	-5.89639	0.90399	-0.88699
H	-5.26952	3.27106	-0.49881
S	-1.28898	-0.54168	-1.76087
N	-0.12886	-0.30808	-0.34325
O	-1.95716	-2.00622	-1.68876
O	-0.38043	-0.14739	-3.03354
F	1.85711	0.95509	1.49012
S	-0.24902	-1.4105	1.09053
C	-2.02201	-1.1443	1.5268
C	-2.90306	-2.19083	1.33725
C	-2.37468	0.1064	2.00516
C	-4.24062	-1.96011	1.65707
H	-2.55678	-3.13275	0.93795
C	-3.71457	0.31644	2.31444
H	-1.63378	0.88425	2.12261
C	-4.63932	-0.71562	2.14344
H	-4.96408	-2.75186	1.52292
H	-4.03312	1.28229	2.67939
H	-5.67978	-0.54493	2.38508
O	0.74031	-0.66021	2.13103
O	0.03182	-2.96021	0.7683
C	3.45176	-0.98325	-0.58421
C	3.94838	0.20024	0.11003
C	3.06518	1.24561	0.46122

C	1.73328	1.12211	0.19169
C	1.2369	0.06673	-0.70438
C	2.1631	-1.0624	-0.96702
H	1.00309	1.87225	0.46045
H	1.10765	0.61332	-1.66739
H	1.76942	-1.90568	-1.51345
O	4.40487	-1.93924	-0.78923
O	5.23795	0.15824	0.36773
O	3.60427	2.32295	1.13034
C	3.98091	-3.19204	-1.38013
H	3.63032	-3.03694	-2.40271
H	4.86856	-3.81438	-1.38355
H	3.19611	-3.65294	-0.77676
C	6.05133	1.20269	1.00744
H	5.69075	1.3875	2.01268
H	7.04511	0.77012	1.00995
H	6.01247	2.11178	0.41719
C	2.7372	3.48563	1.32809
H	3.41373	4.29578	1.58
H	2.16682	3.7003	0.4205
H	2.05543	3.29459	2.15821
F	0.91055	1.44682	-3.13587

TS3

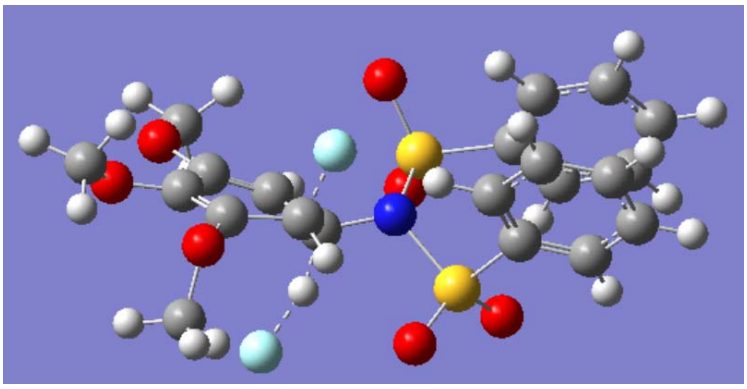


Symbolic Z-matrix: Charge = 0 Multiplicity = 1

C	-4.08278	-3.03984	0.15337
C	-3.07957	-2.20247	0.63692
C	-3.29507	-0.8255	0.57093
C	-4.45776	-0.26841	0.0425
C	-5.44792	-1.12652	-0.42777
C	-5.26095	-2.50734	-0.37022
H	-3.93634	-4.11301	0.18862
H	-2.14475	-2.61394	1.01328
H	-4.57569	0.80577	0.00125
H	-6.3615	-0.71464	-0.84013
H	-6.03514	-3.17076	-0.73956
S	-2.04595	0.27995	1.22486
N	-0.72156	0.23531	0.07874
O	-2.5626	1.64278	1.21294
O	-1.47322	-0.28769	2.43771
S	-0.70226	1.23571	-1.32862
C	-0.0315	2.83329	-0.83451
C	-0.86585	3.77923	-0.24188
C	1.30817	3.10226	-1.11102
C	-0.3315	5.02016	0.09513
H	-1.90124	3.54165	-0.0426
C	1.8262	4.34959	-0.76912
H	1.91786	2.35534	-1.60213
C	1.00909	5.30458	-0.16512
H	-0.96706	5.76634	0.55724
H	2.86291	4.57813	-0.98808
H	1.41509	6.27557	0.09525
O	0.28851	0.60664	-2.19873
O	-2.0843	1.41098	-1.74302
C	2.02233	-2.11825	-0.80017
C	3.09001	-1.51683	-0.11647
C	2.84406	-0.41985	0.81195
C	1.58454	0.04331	0.99559
C	0.43004	-0.61885	0.36589

C	0.72925	-1.65801	-0.62431
H	1.36669	0.83292	1.70002
H	0.07116	-1.42644	1.11783
H	-0.05413	-2.019	-1.2707
O	2.2706	-3.11978	-1.68982
O	4.27827	-2.05507	-0.34791
O	3.94796	0.03112	1.47269
C	2.08544	-4.4505	-1.1499
H	2.06038	-5.11841	-2.00965
H	2.93014	-4.71133	-0.50508
H	1.15461	-4.50326	-0.58117
C	5.55245	-1.40499	-0.15041
H	5.83498	-1.42085	0.89963
H	6.24616	-1.99763	-0.74362
H	5.52459	-0.37981	-0.51673
C	3.76055	1.02574	2.47914
H	4.74694	1.20781	2.90118
H	3.36824	1.95231	2.04892
H	3.08459	0.66588	3.26063
F	-0.13814	-3.03637	0.8523

TS3`

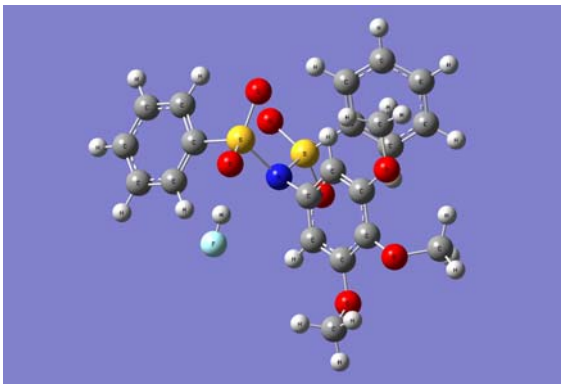


Symbolic Z-matrix: Charge = -1 Multiplicity = 1

C	-2.6502	-2.56936	-1.92613
C	-1.79512	-1.96975	-1.00311
C	-2.34185	-1.5642	0.20261
C	-3.67395	-1.72198	0.53739
C	-4.51272	-2.3263	-0.39757
C	-4.00071	-2.7497	-1.62355
H	-2.25386	-2.89104	-2.87974
H	-0.75214	-1.79041	-1.23663
H	-4.03731	-1.36405	1.49021
H	-5.56175	-2.45909	-0.16858
H	-4.65621	-3.21869	-2.34649
S	-1.21138	-0.85374	1.49817
N	-0.17703	0.22439	0.35221
O	-2.1618	-0.09615	2.5722
O	-0.2267	-2.01769	2.00797
F	1.08175	-1.11578	-1.814
S	-0.88891	1.8845	0.03143
C	-2.68963	1.55071	-0.23585
C	-3.57164	1.83013	0.78941
C	-3.06952	1.09947	-1.48811
C	-4.9288	1.62699	0.54102
H	-3.20036	2.17105	1.74384
C	-4.42687	0.89763	-1.71673
H	-2.32286	0.91873	-2.24826
C	-5.35078	1.16256	-0.70399
H	-5.64917	1.82966	1.3217
H	-4.75855	0.52971	-2.67776
H	-6.40566	1.00203	-0.88663
O	-0.30815	2.35421	-1.40271
O	-0.75422	2.90048	1.2807
C	3.27295	1.3315	-0.25462
C	3.93828	0.04884	-0.50274
C	3.23988	-1.09642	-0.4048

C	1.77073	-1.08298	-0.26022
C	1.29087	0.10942	0.52728
C	2.03187	1.37591	0.24414
H	1.41143	-2.00892	0.1788
H	1.66186	-0.2172	1.6272
H	1.59228	2.31132	0.54938
O	4.05966	2.44127	-0.52034
O	5.29242	0.13086	-0.72212
O	3.85399	-2.35144	-0.37332
C	3.4607	3.72652	-0.28414
H	3.2439	3.86963	0.77844
H	4.20002	4.4533	-0.60955
H	2.53815	3.83968	-0.86064
C	5.9308	-0.87515	-1.54355
H	5.29469	-1.13009	-2.39277
H	6.85576	-0.41373	-1.88243
H	6.13761	-1.7812	-0.97769
C	4.24735	-2.74017	0.99572
H	4.13884	-3.82185	1.04751
H	5.29163	-2.45708	1.15598
H	3.61355	-2.22533	1.72983
F	2.5563	-0.71918	2.64179

Products



Symbolic Z-matrix: Charge = 0 Multiplicity = 1

C	-0.60514	-0.38169	-0.36246
C	0.39955	0.4198	0.17376
C	0.22204	1.80349	0.16062
C	-0.92282	2.40095	-0.36282
C	-1.91664	1.58184	-0.89073
C	-1.75756	0.19656	-0.89332
H	-0.48685	-1.45868	-0.35571
H	1.28509	-0.02896	0.60478
H	-1.02258	3.47705	-0.36206
H	-2.8143	2.02908	-1.30078
H	-2.53569	-0.43479	-1.30694
S	1.49612	2.85561	0.85925
N	2.66387	3.11833	-0.39188
O	0.91476	4.13578	1.23018
O	2.22895	2.08563	1.8719
S	2.38132	4.26848	-1.66557
C	3.15737	5.78979	-1.10663
C	2.49215	6.59778	-0.18529
C	4.39822	6.13773	-1.63657
C	3.09984	7.78323	0.21862
H	1.52993	6.29796	0.20815
C	4.99099	7.32892	-1.2222
H	4.87482	5.49378	-2.36408
C	4.34447	8.14747	-0.29723
H	2.59718	8.42456	0.933
H	5.95261	7.61861	-1.6295
H	4.80835	9.0749	0.01912
O	3.13336	3.77834	-2.80945
O	0.93902	4.45721	-1.7231
C	5.31839	0.59633	-1.04859
C	6.36684	1.08911	-0.26027
C	6.16608	2.25119	0.51589
C	4.94575	2.9204	0.46468
C	3.92278	2.42086	-0.34647

C	4.09621	1.26723	-1.09809
H	4.76481	3.80632	1.05525
H	2.90963	0.53812	2.07733
H	3.30867	0.88924	-1.73543
O	5.48333	-0.51481	-1.82956
O	7.544	0.39812	-0.20443
O	7.22269	2.64092	1.28029
C	5.62941	-1.76079	-1.12491
H	5.69455	-2.52932	-1.89418
H	6.53481	-1.76215	-0.5162
H	4.75475	-1.9427	-0.493
C	8.66507	1.01547	-0.85556
H	8.91221	1.96975	-0.38601
H	9.49737	0.32257	-0.73853
H	8.4542	1.15911	-1.91972
C	7.04406	3.73441	2.17528
H	7.98492	3.8304	2.71424
H	6.83821	4.66414	1.63455
H	6.23562	3.53476	2.88541
F	3.17717	-0.36395	2.10299

4. References

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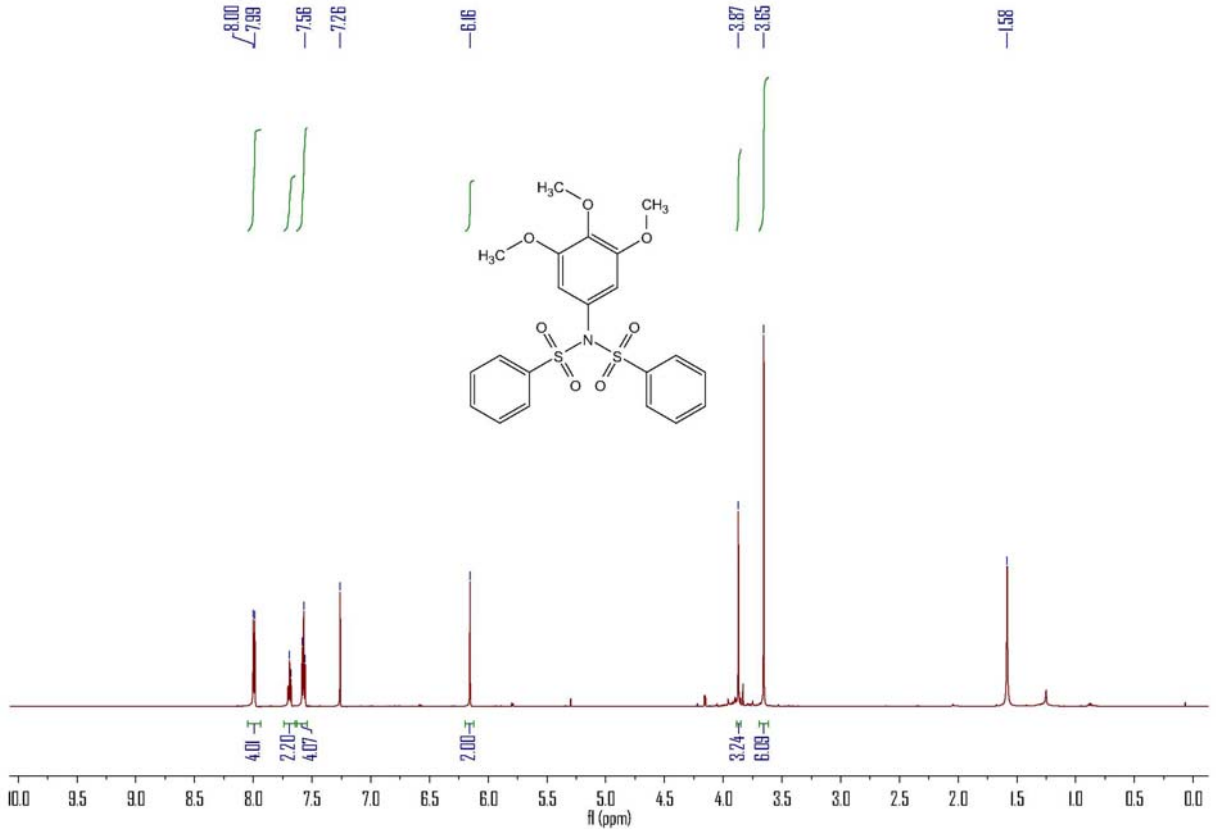
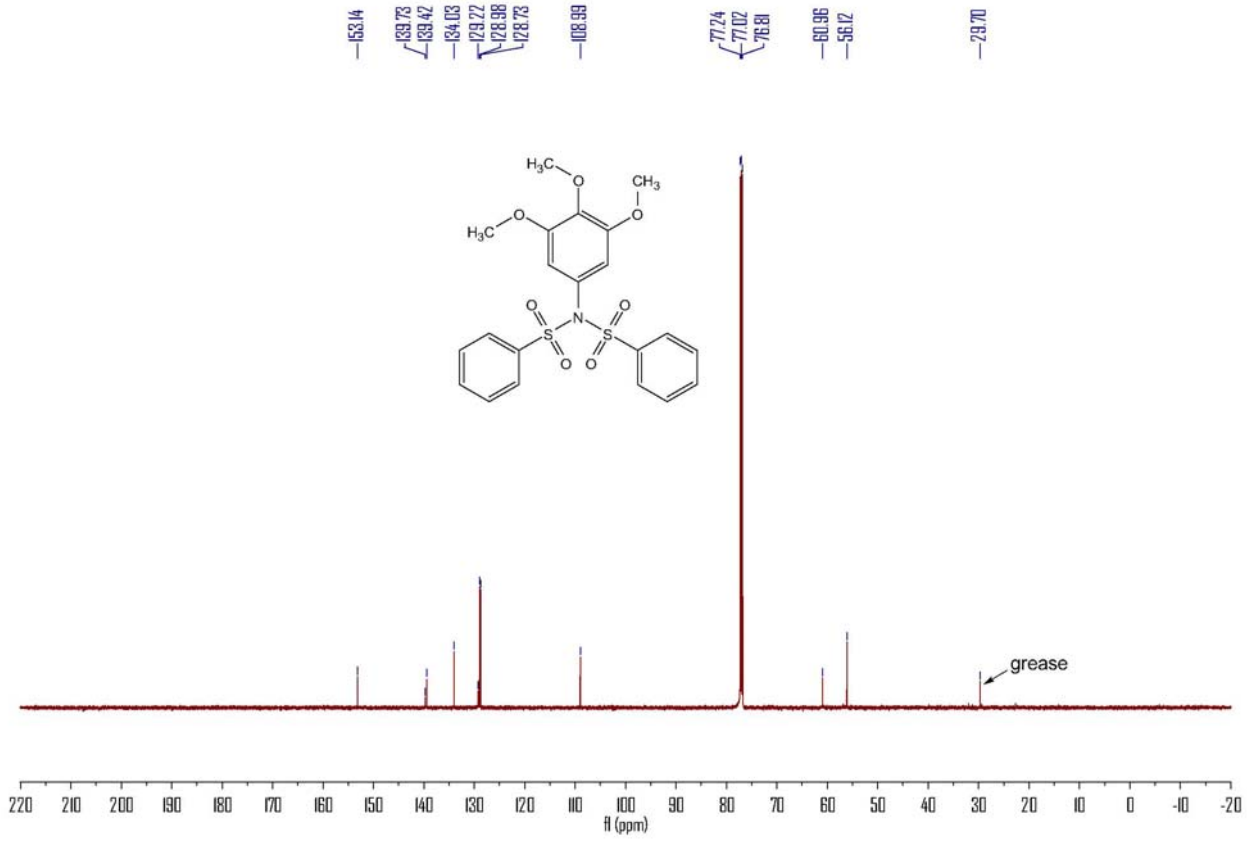
(5) Lu, T.; Chen, Q., Shermo: A general code for calculating molecular thermochemistry properties. *Computational and Theoretical Chemistry* **2021,** *1200*, 113249.

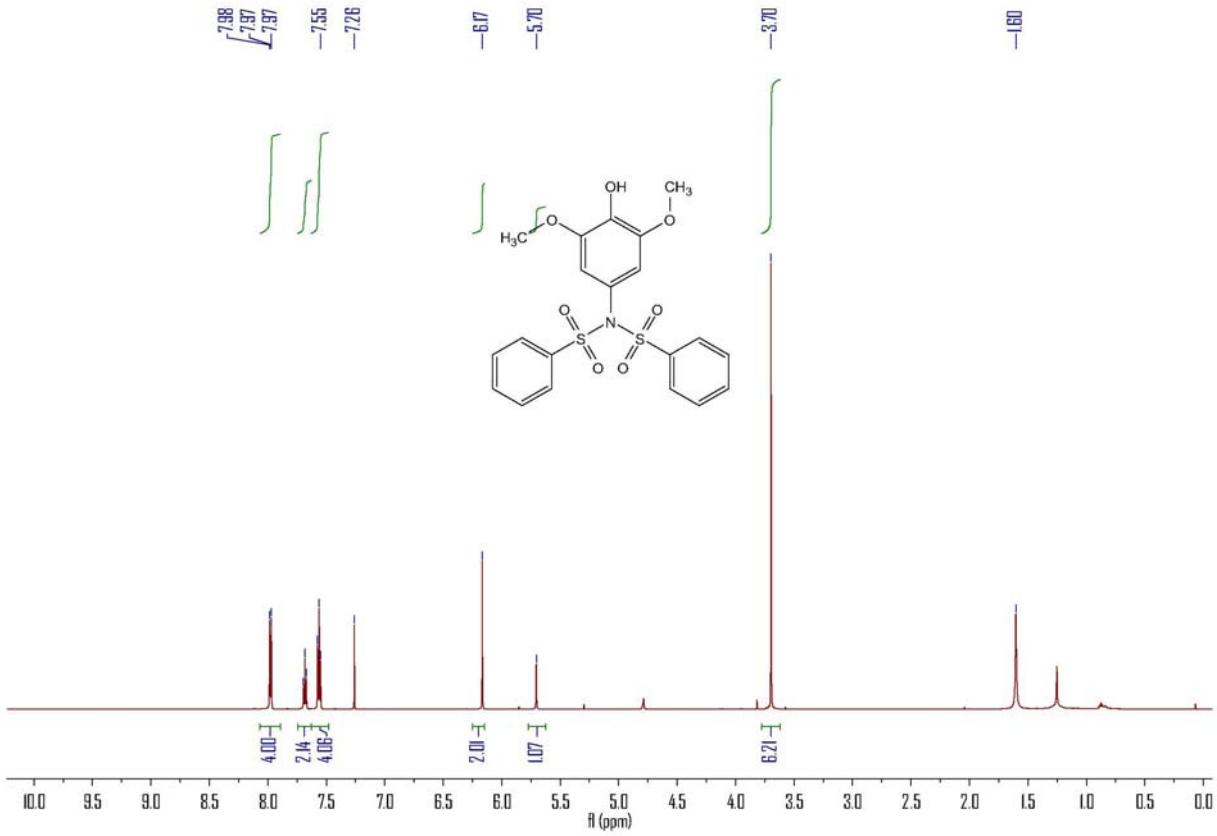
^{1}H NMR of **7a**



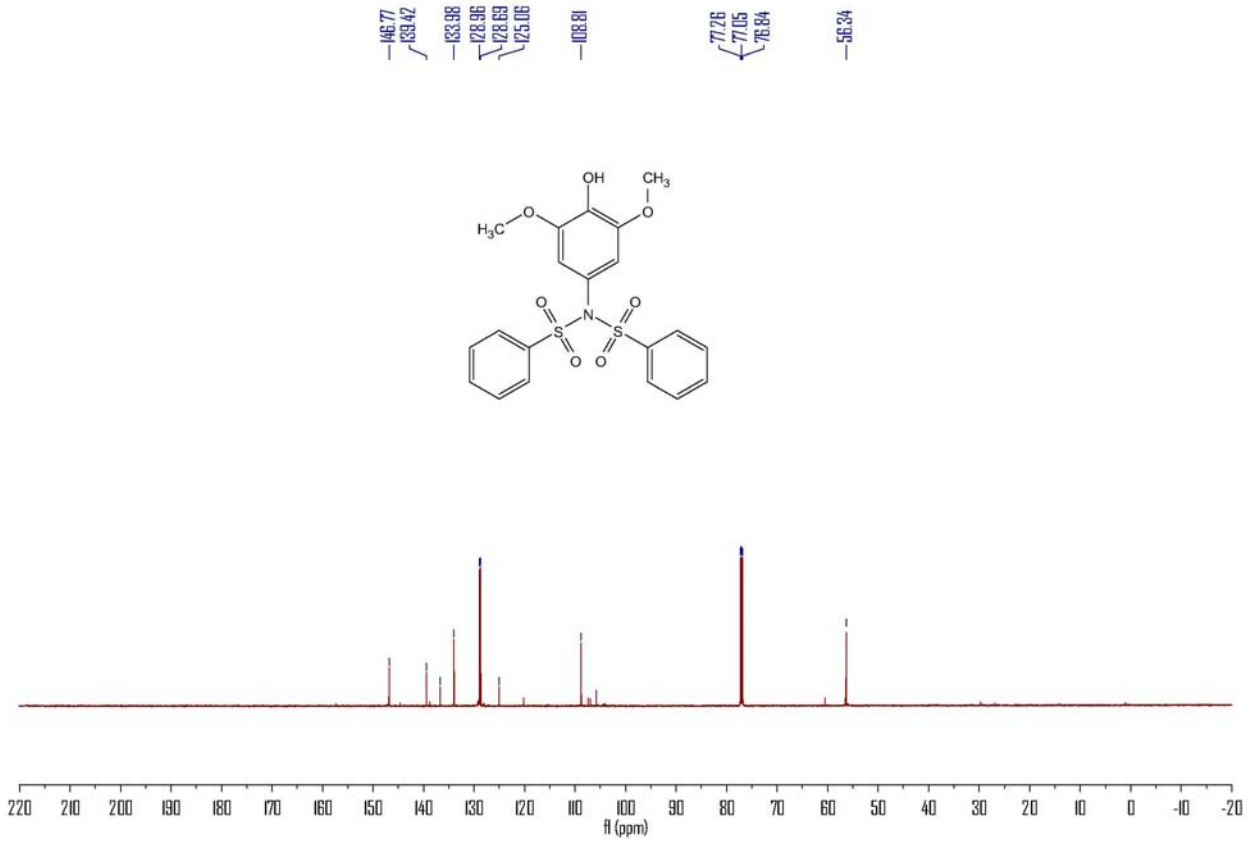
^{13}C NMR of **7a**



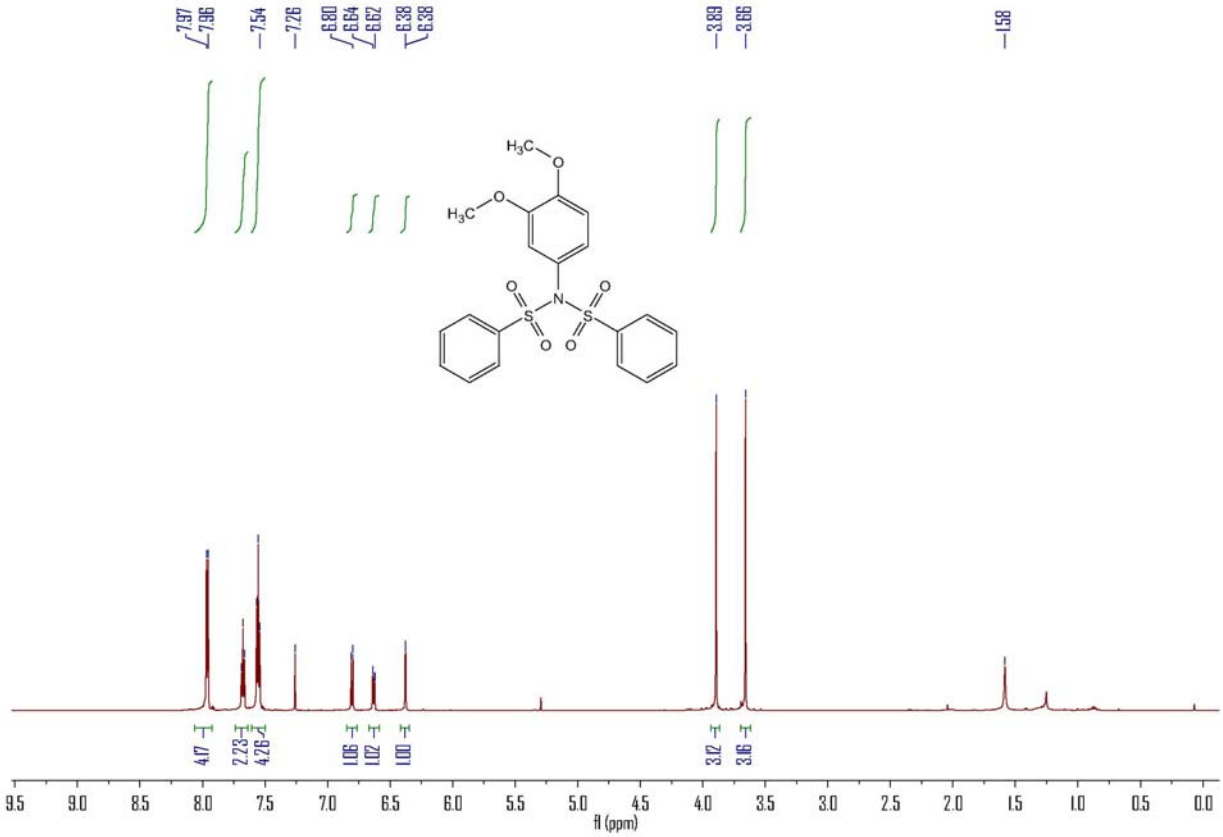
^{1}H NMR of **7b**



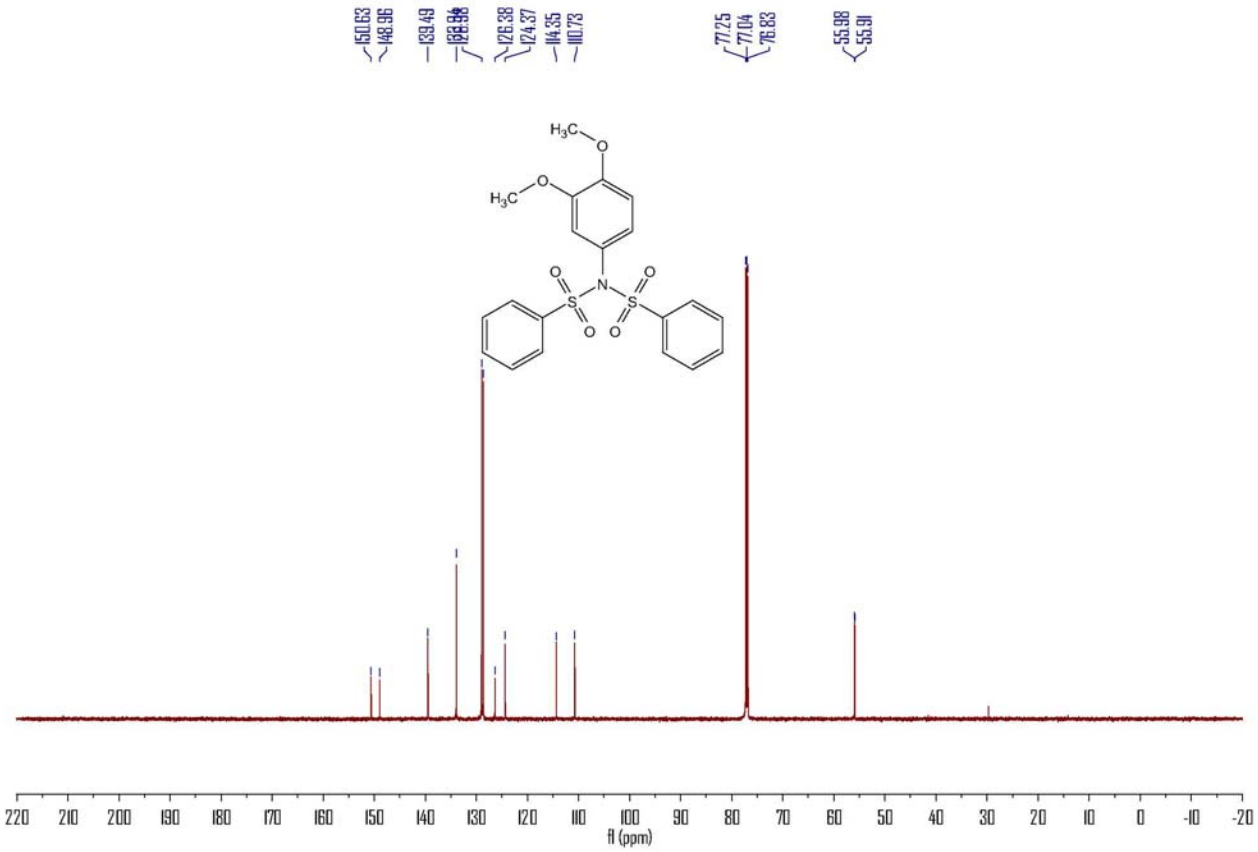
^{13}C NMR of **7b**



^{1}H NMR of **7c**



^{13}C NMR of **7c**



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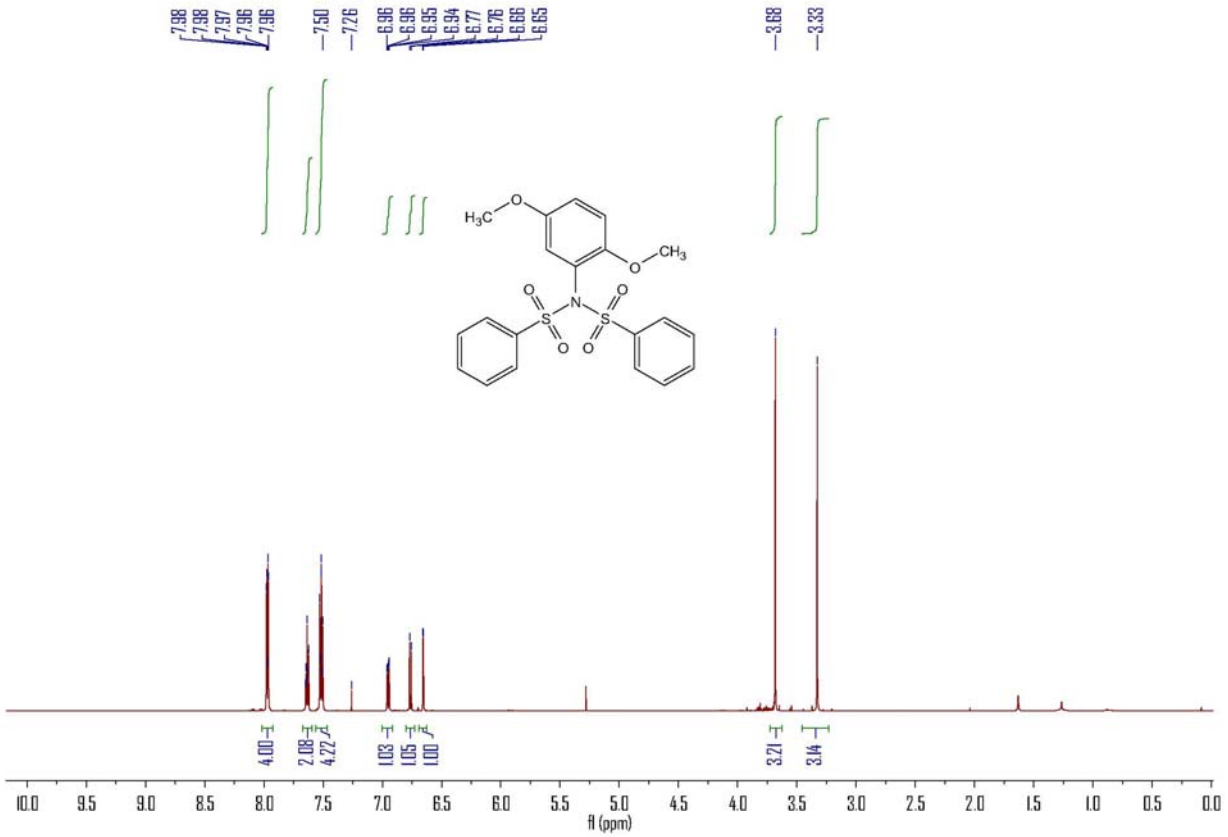

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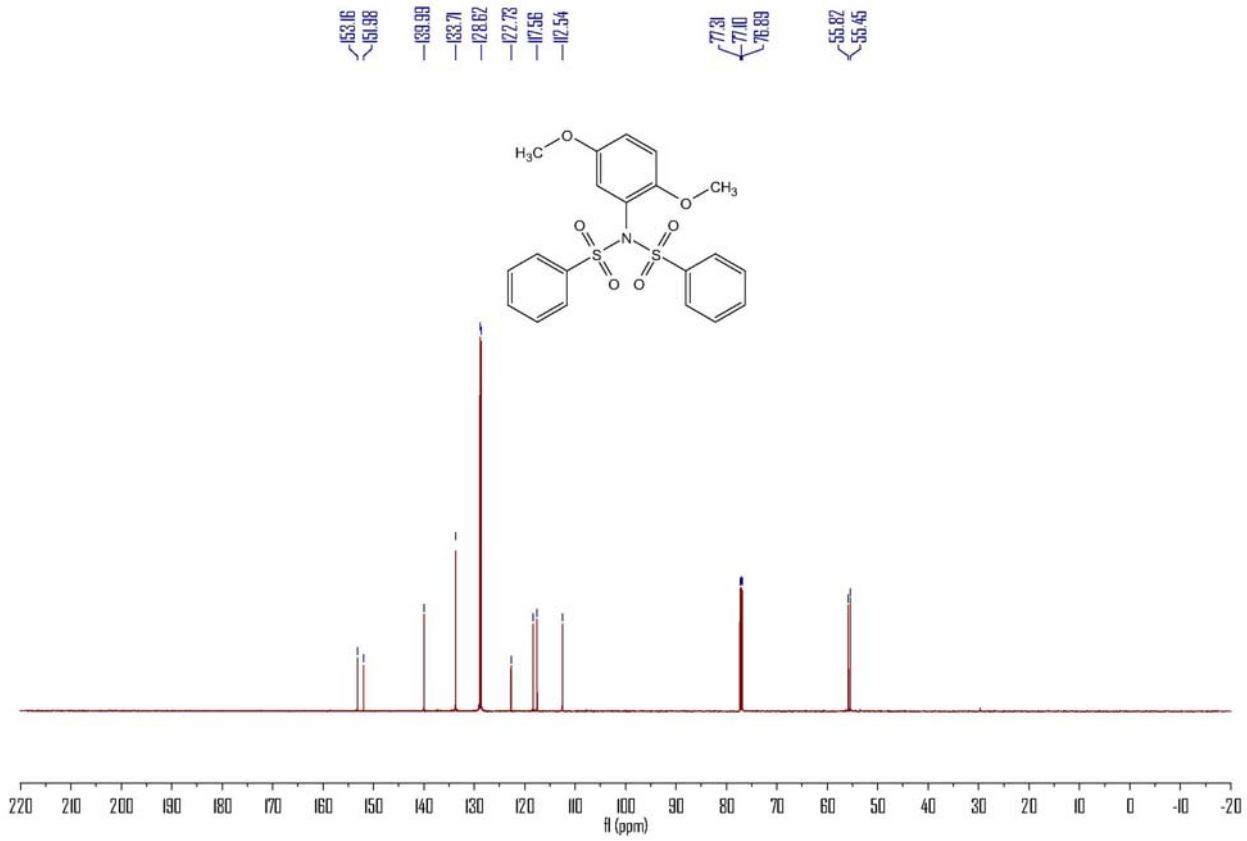
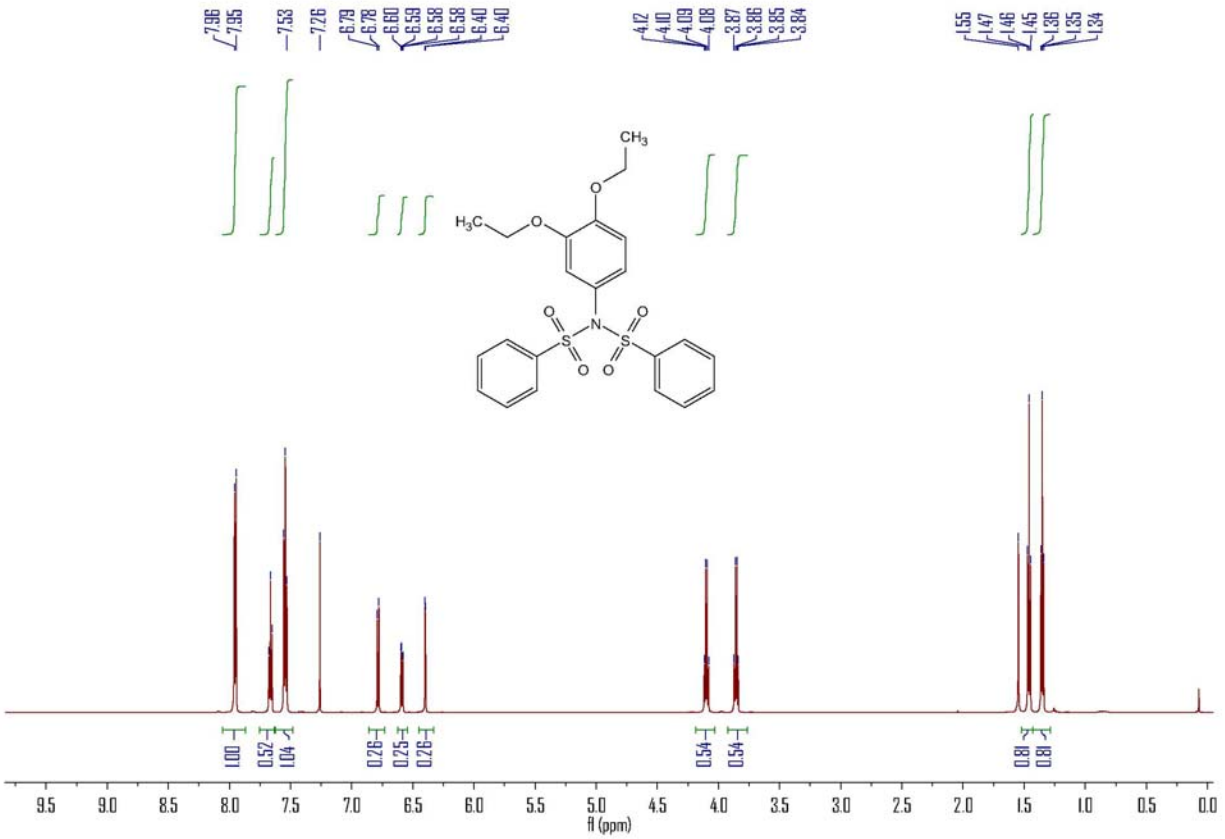
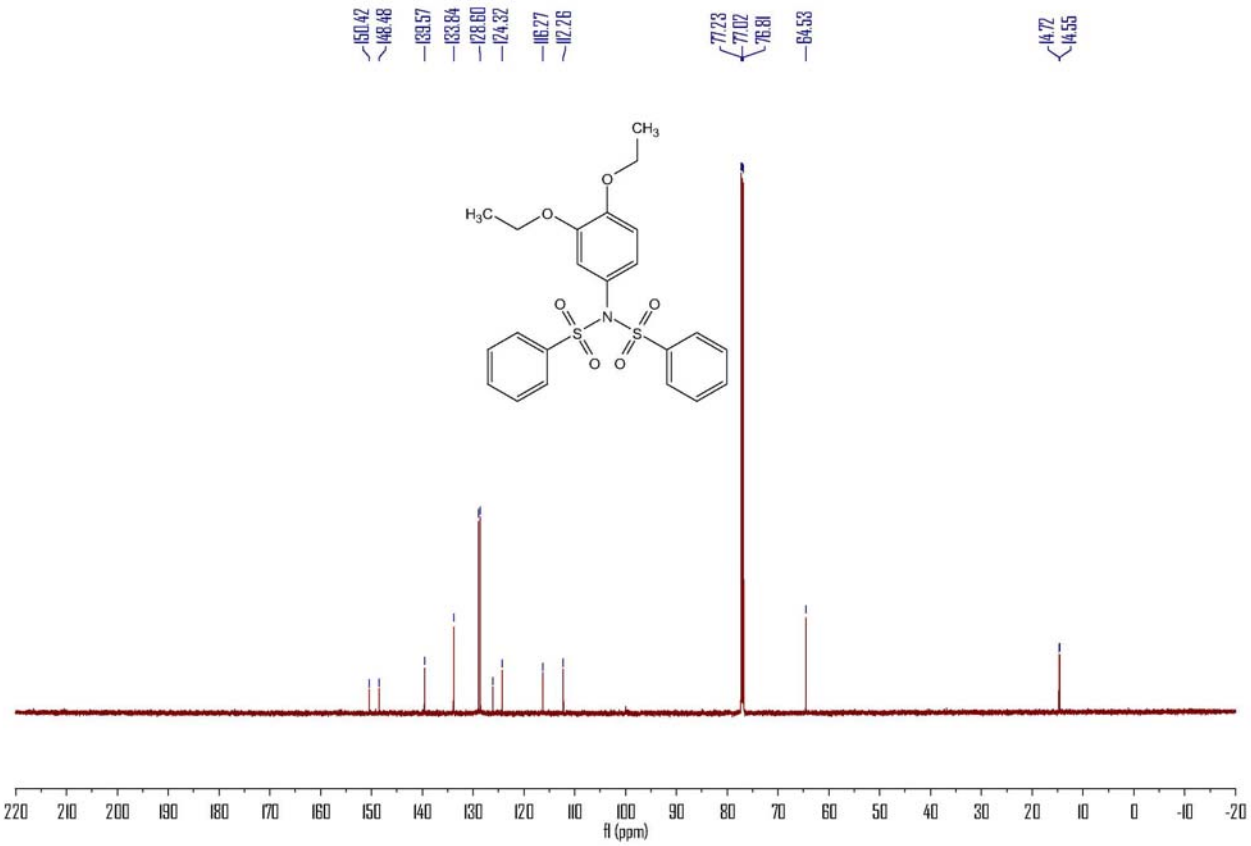


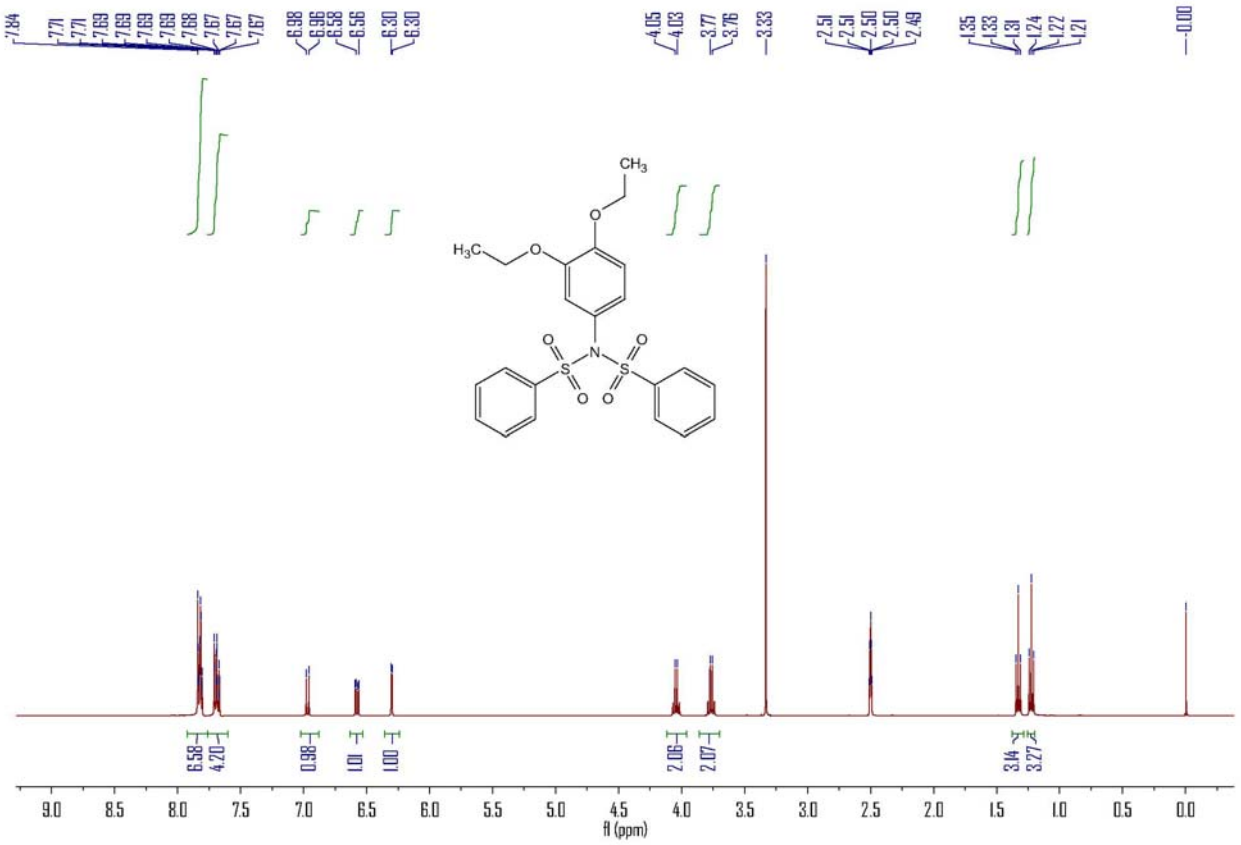
^{1}H NMR of **7e** ($CDCl_3$)



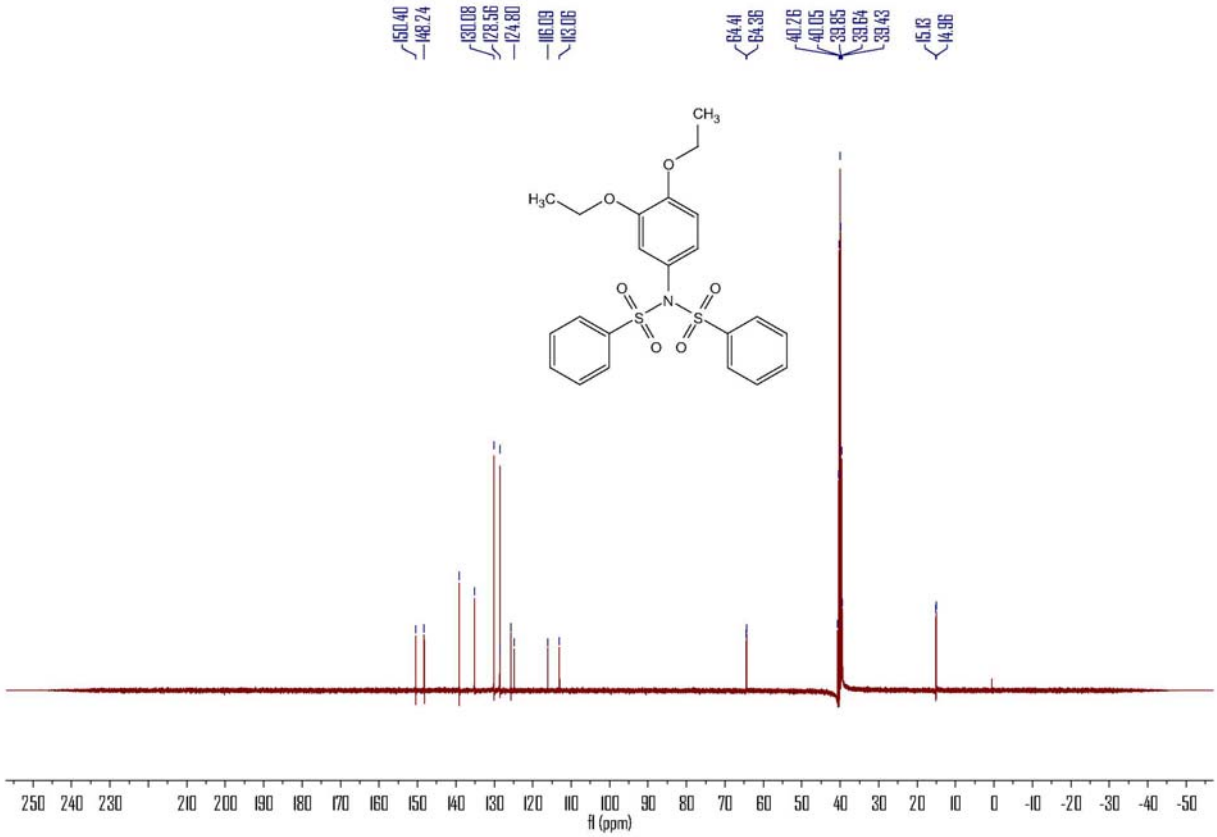
^{13}C NMR of **7e** ($CDCl_3$)



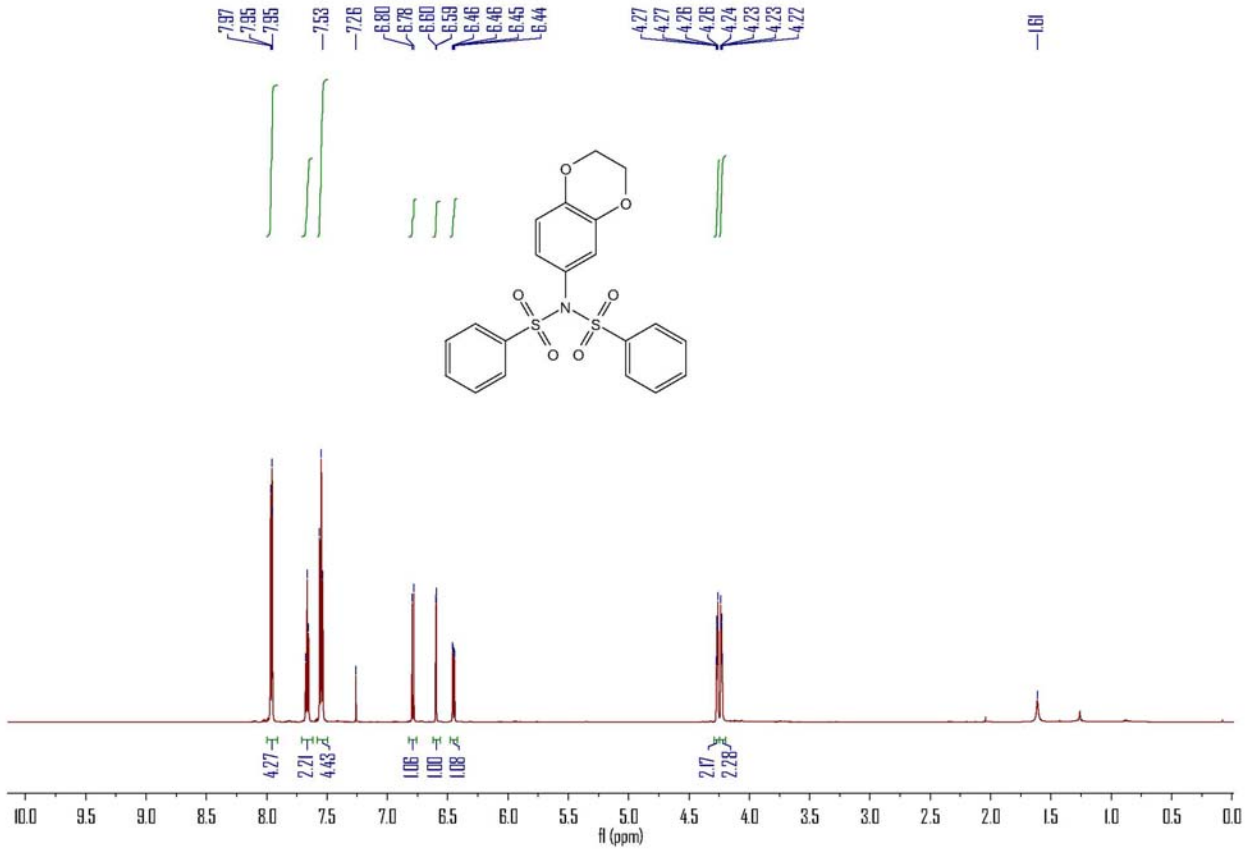
^{1}H NMR of **7e** (DMSO-*d6*)



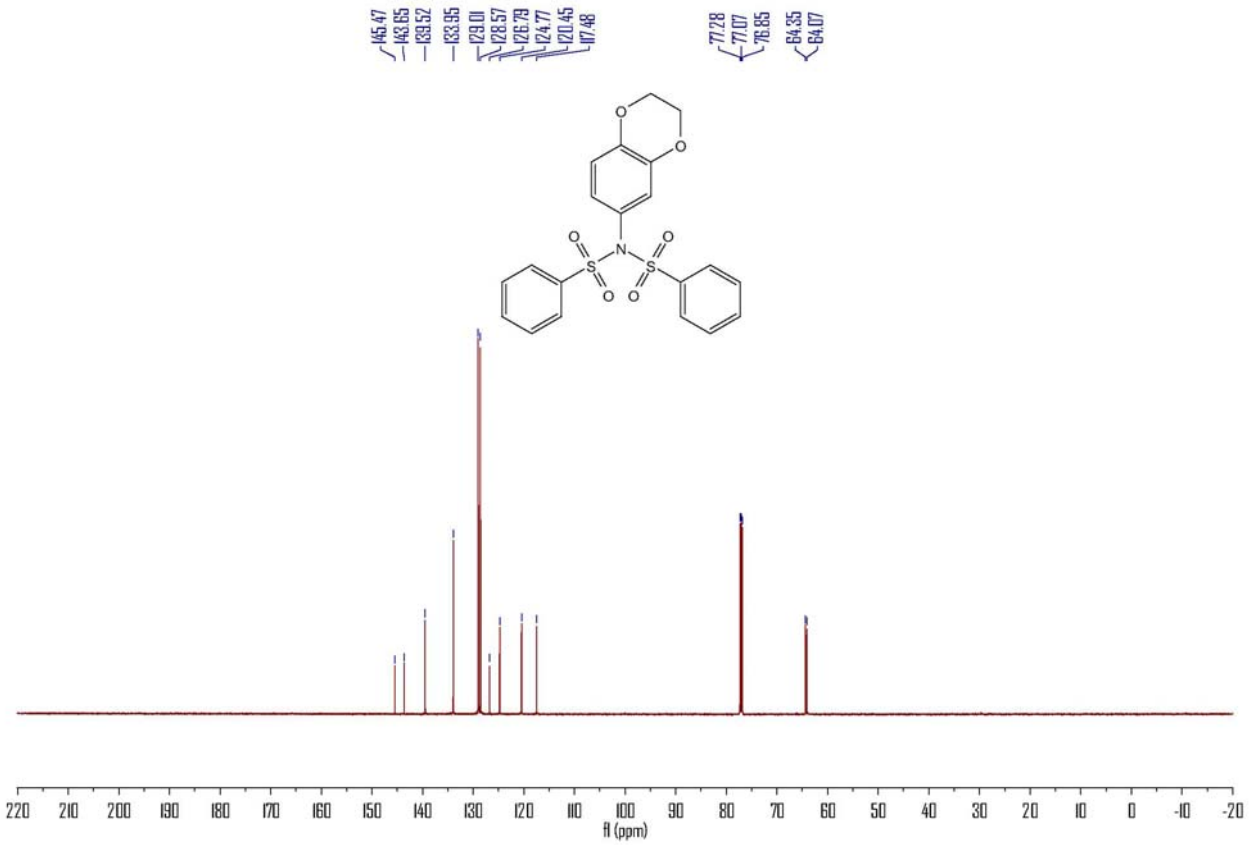
^{13}C NMR of **7e** (DMSO-*d6*)



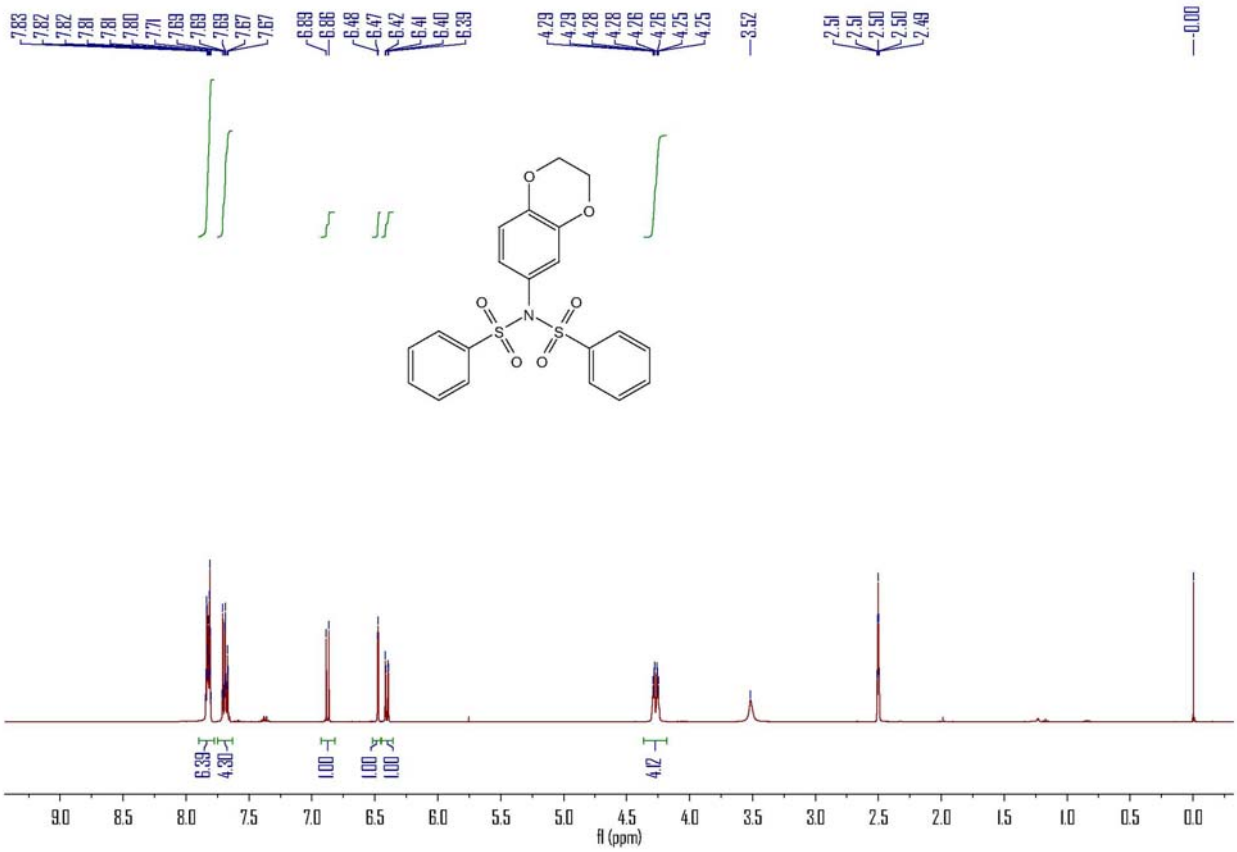
^{1}H NMR of **7f** ($CDCl_3$)



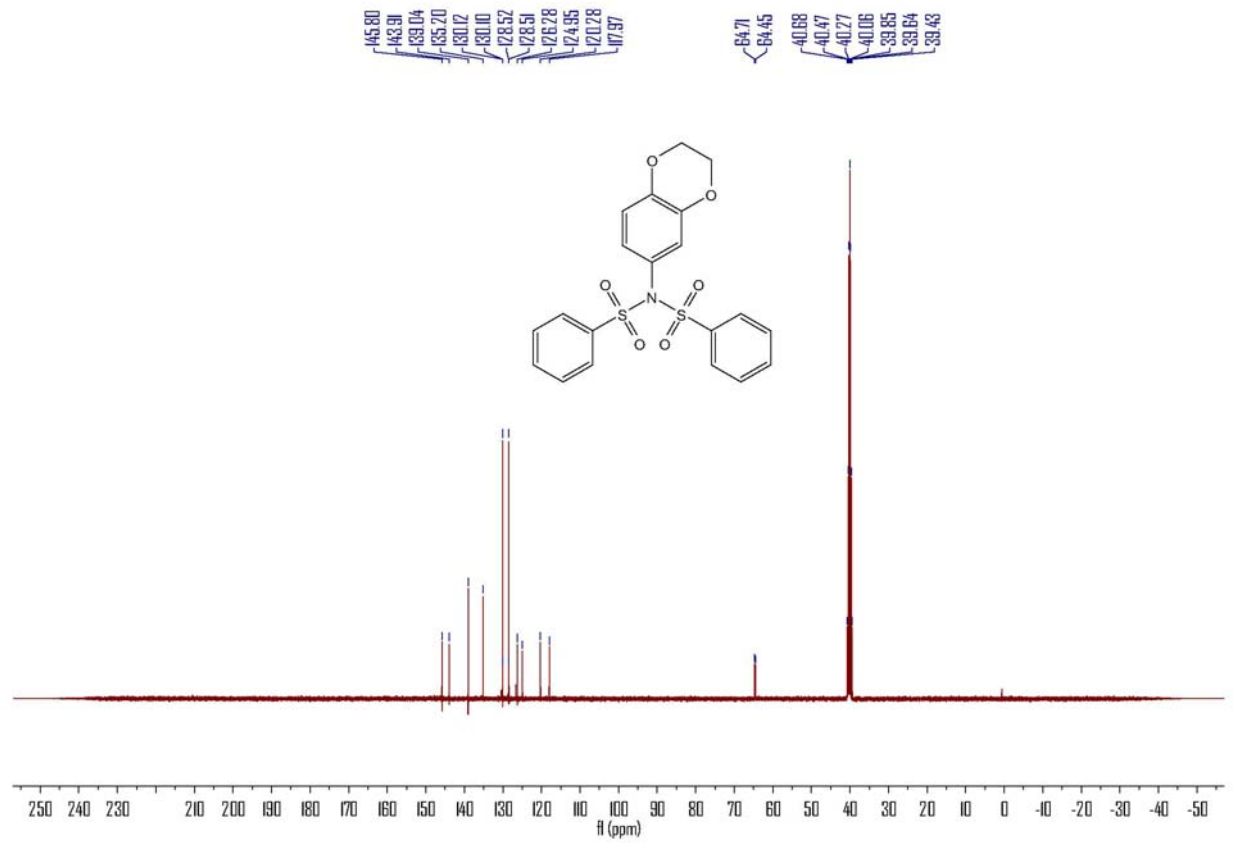
^{13}C NMR of **7f** ($CDCl_3$)



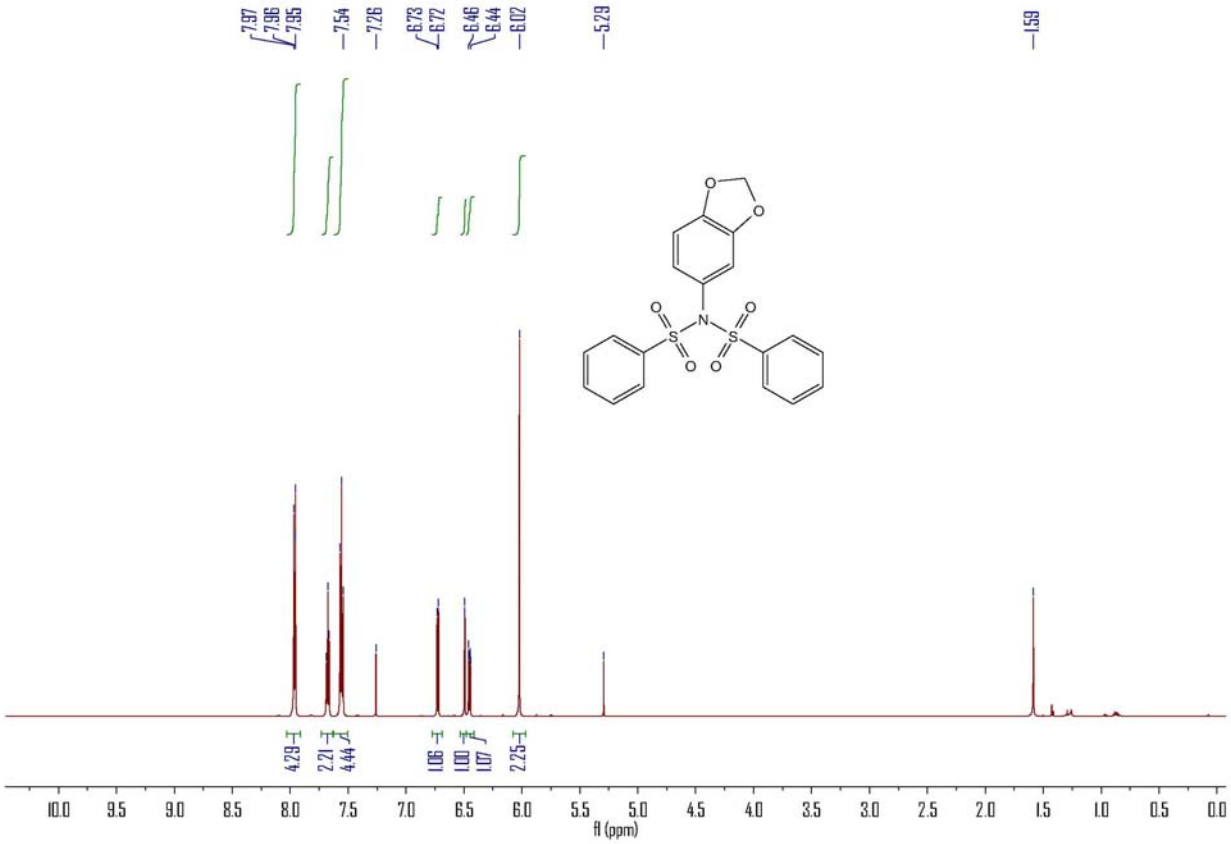
^{1}H NMR of **7f** (DMSO-*d6*)



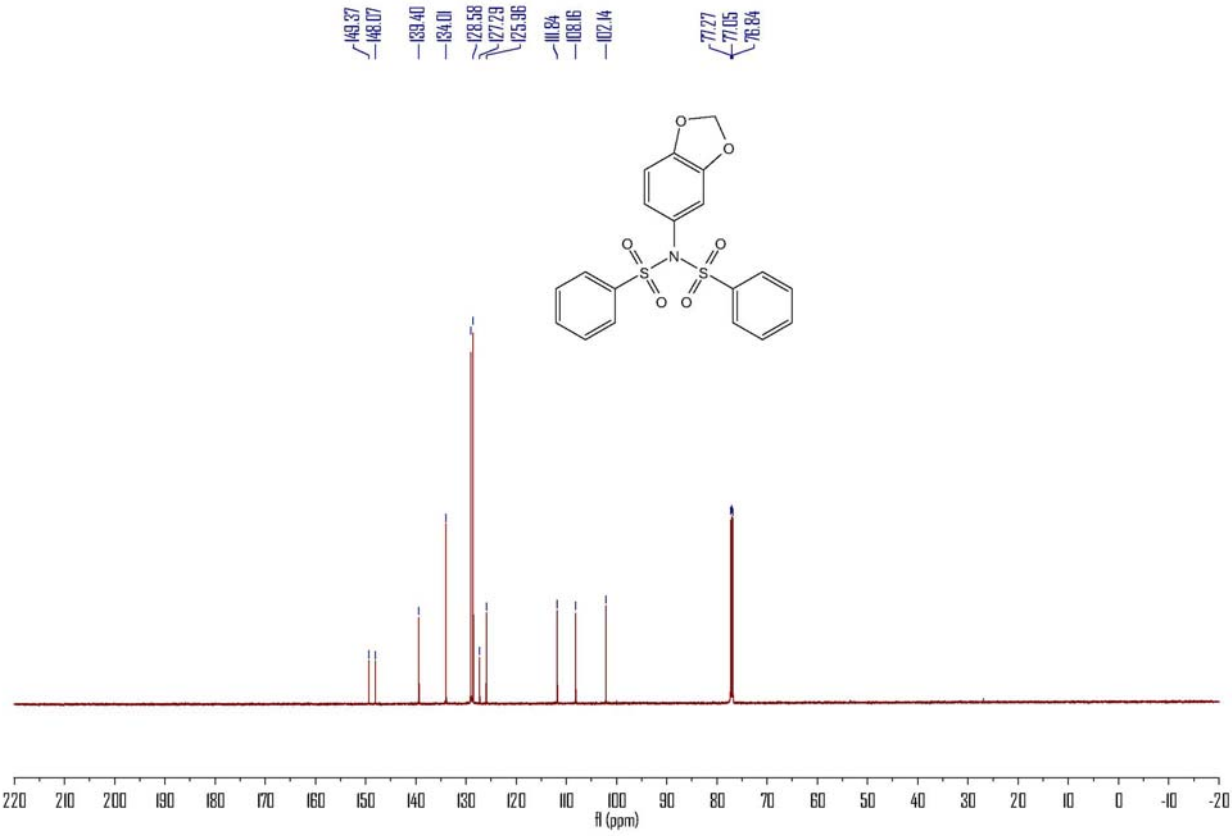
^{13}C NMR of **7f** (DMSO-*d6*)



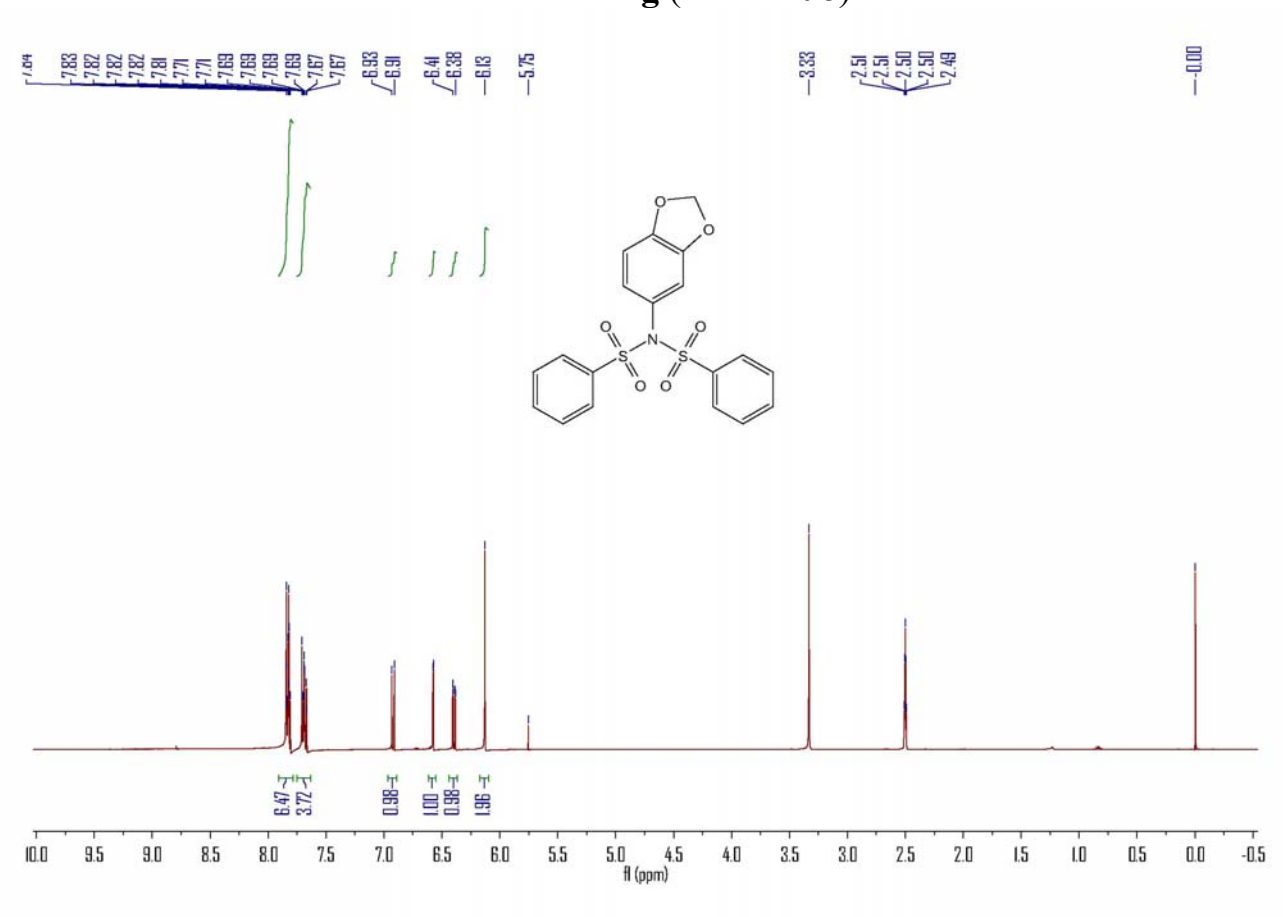
^{1}H NMR of **7g** ($CDCl_3$)



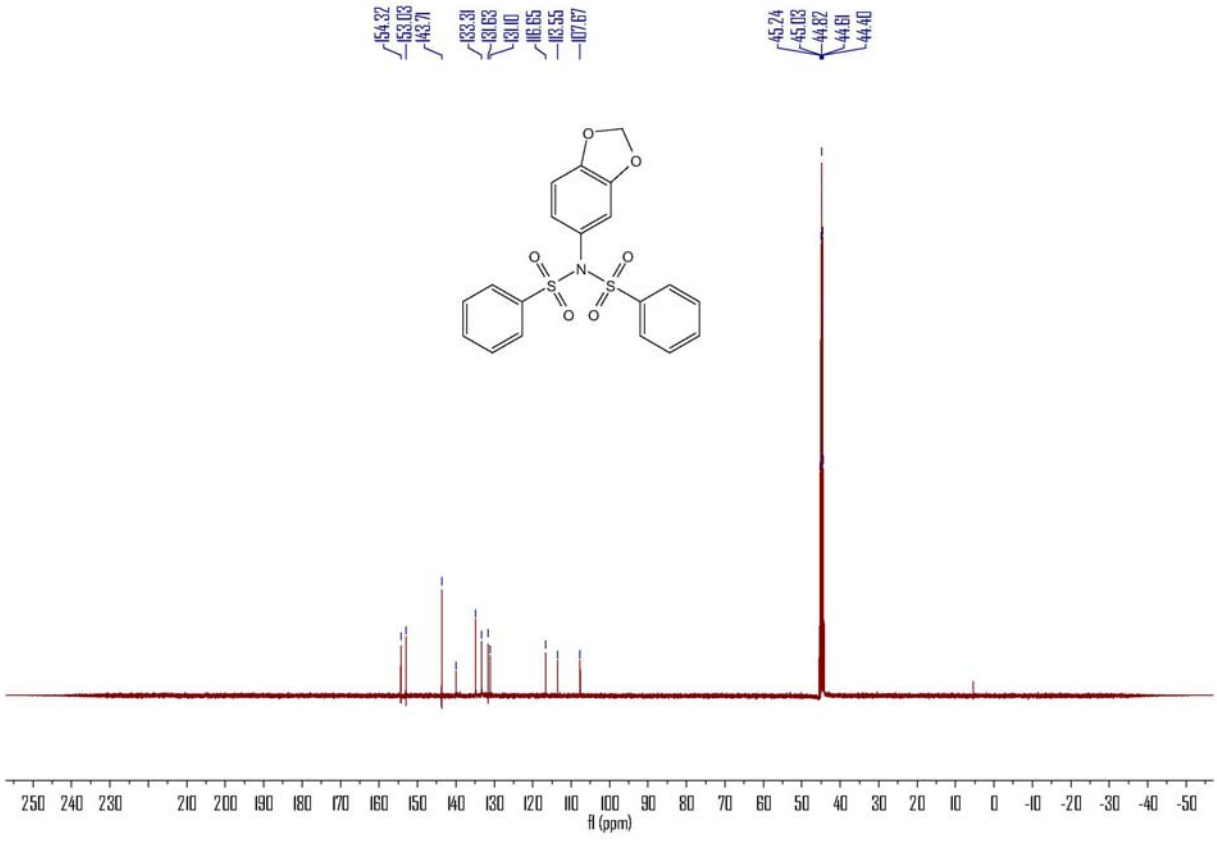
^{13}C NMR of **7g** ($CDCl_3$)



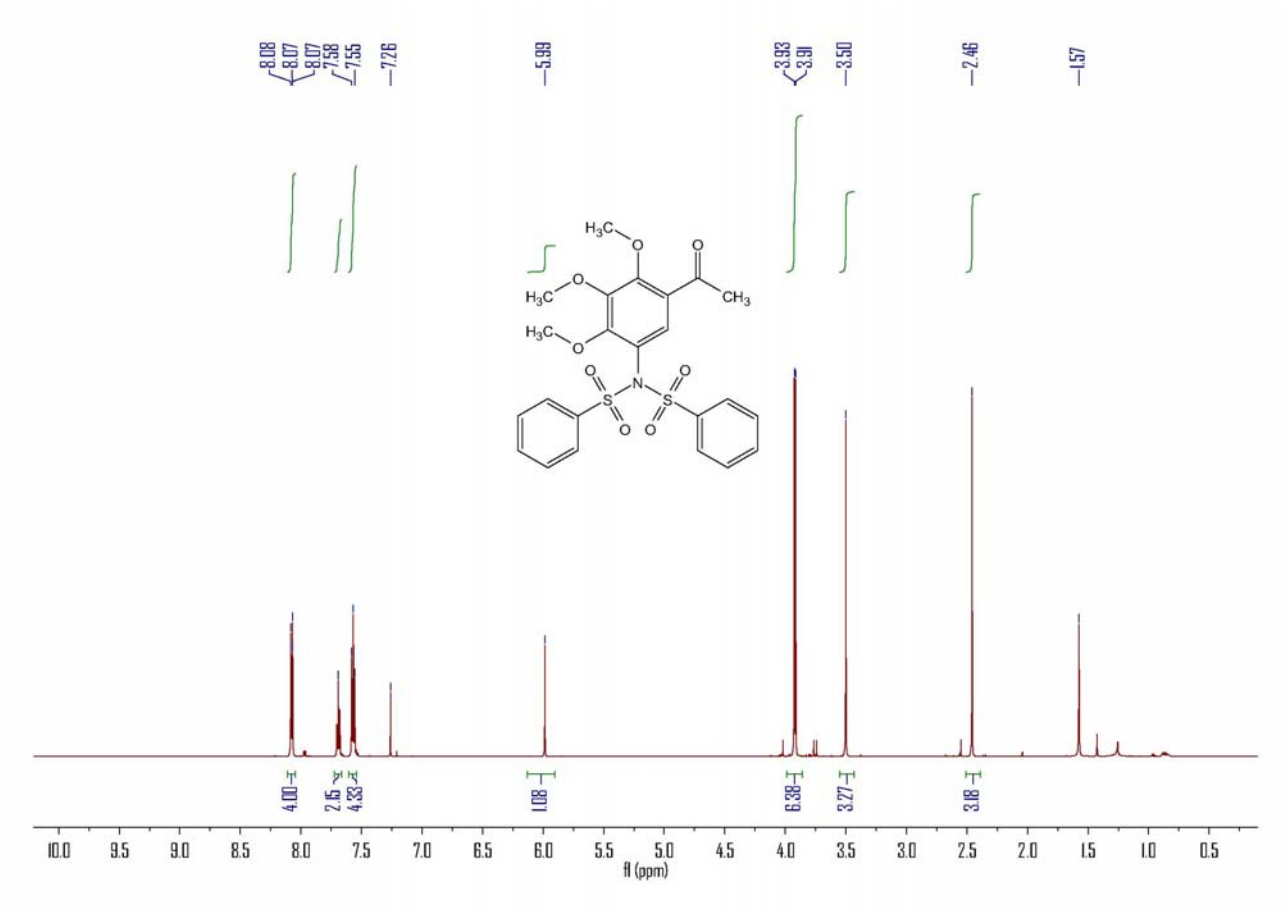
^{1}H NMR of **7g** (DMSO-*d6*)



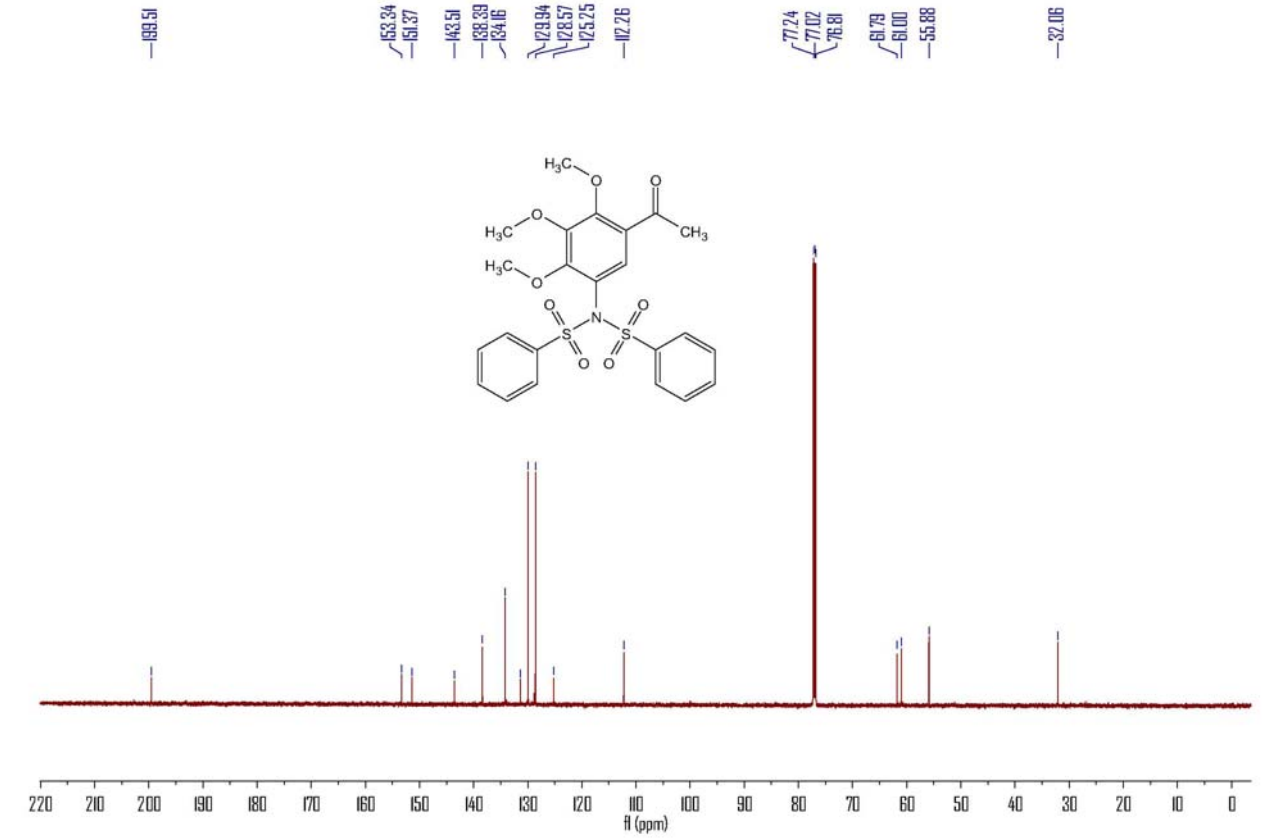
^{13}C NMR of **7g** (DMSO-*d6*)



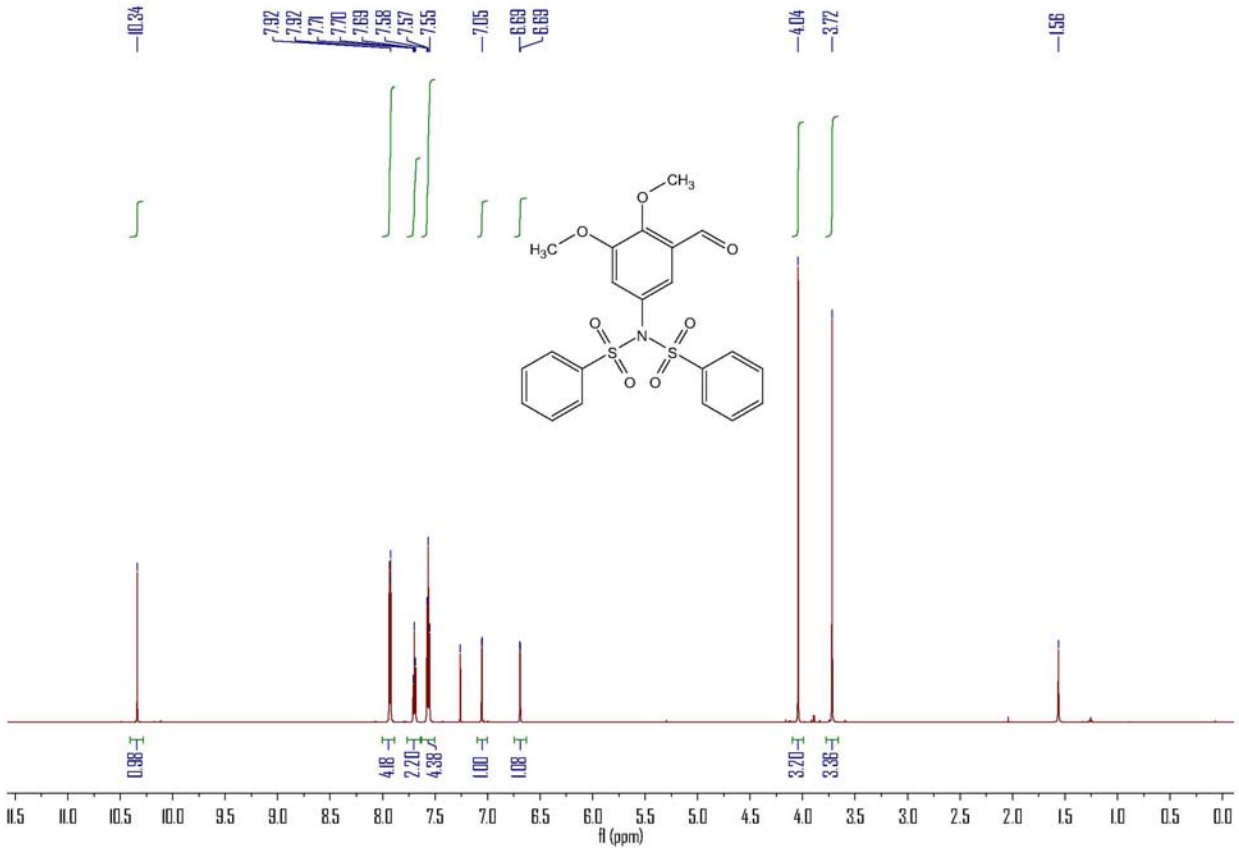
^{1}H NMR of **7h**



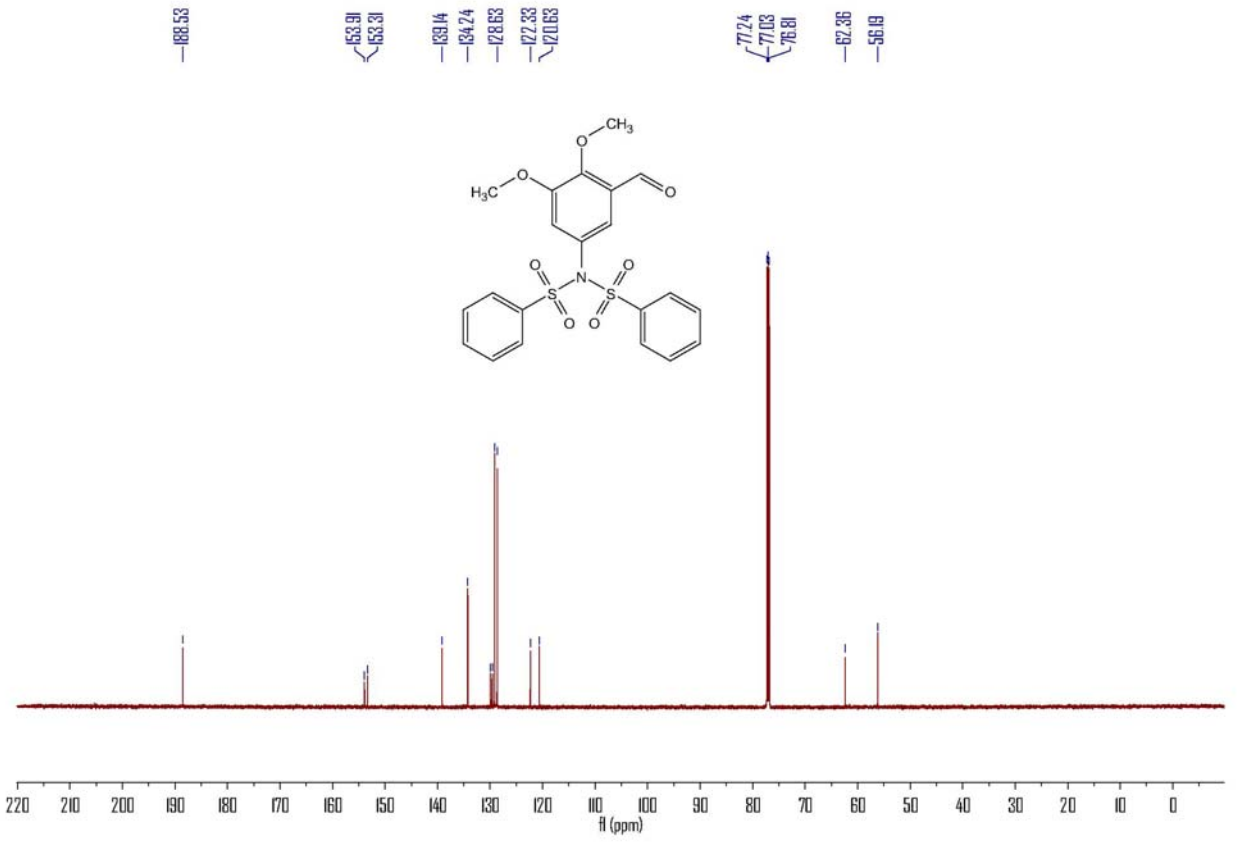
^{13}C NMR of **7h**



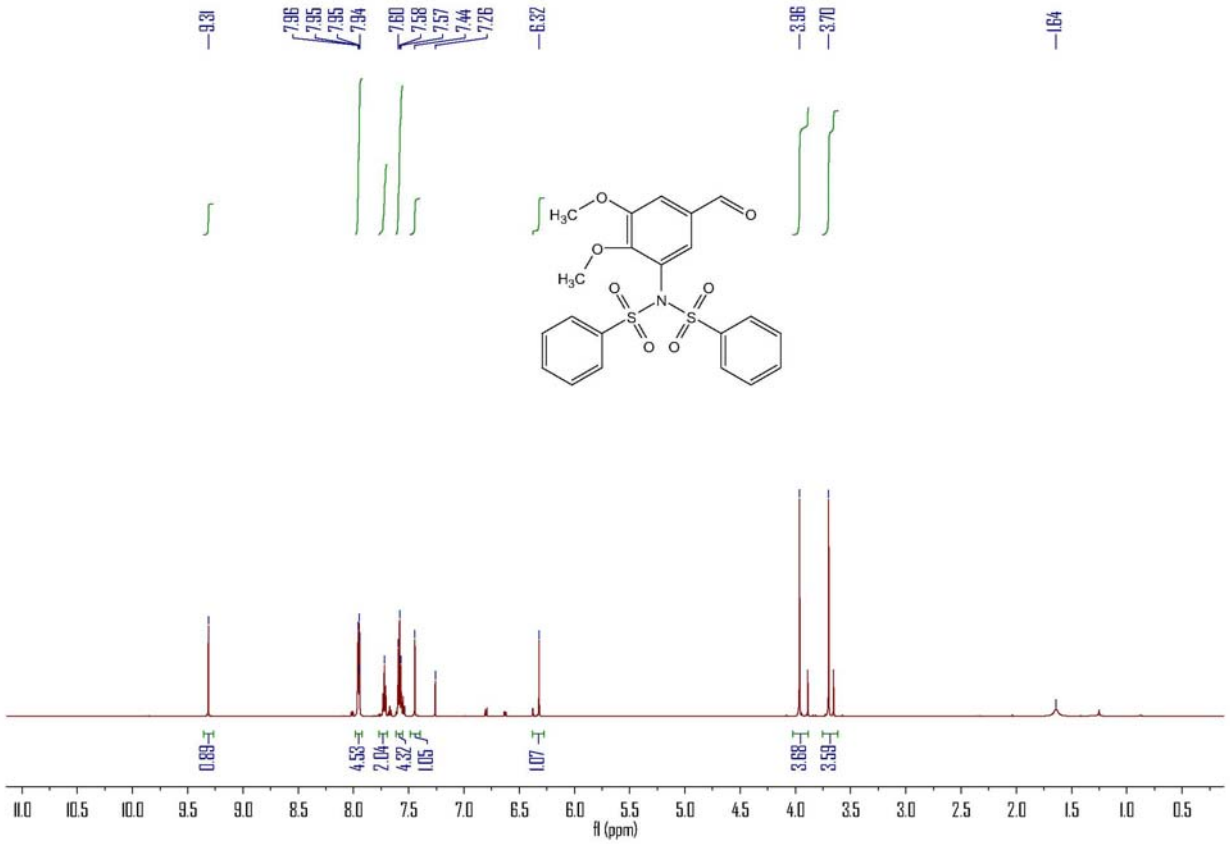
^{1}H NMR of **7i**



^{13}C NMR of **7i**



^{1}H NMR of **7j**



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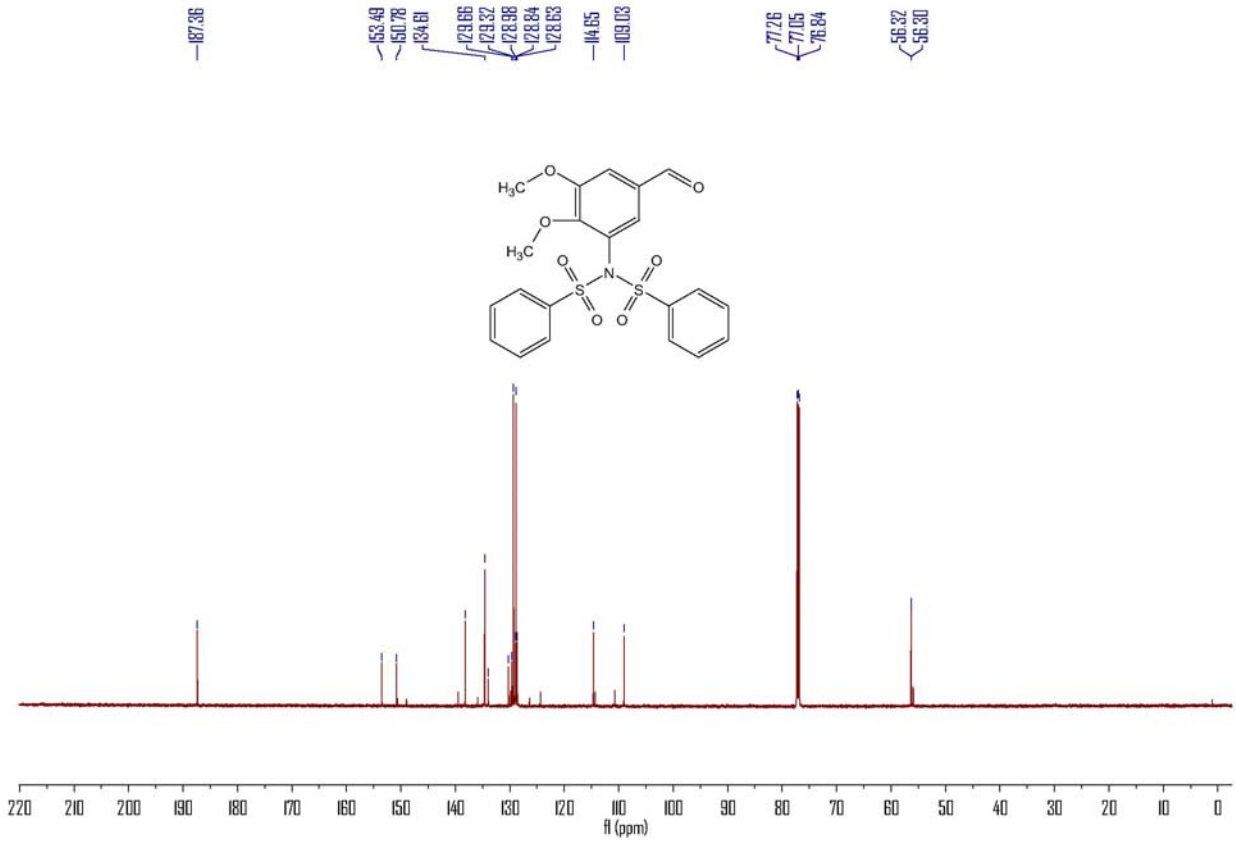
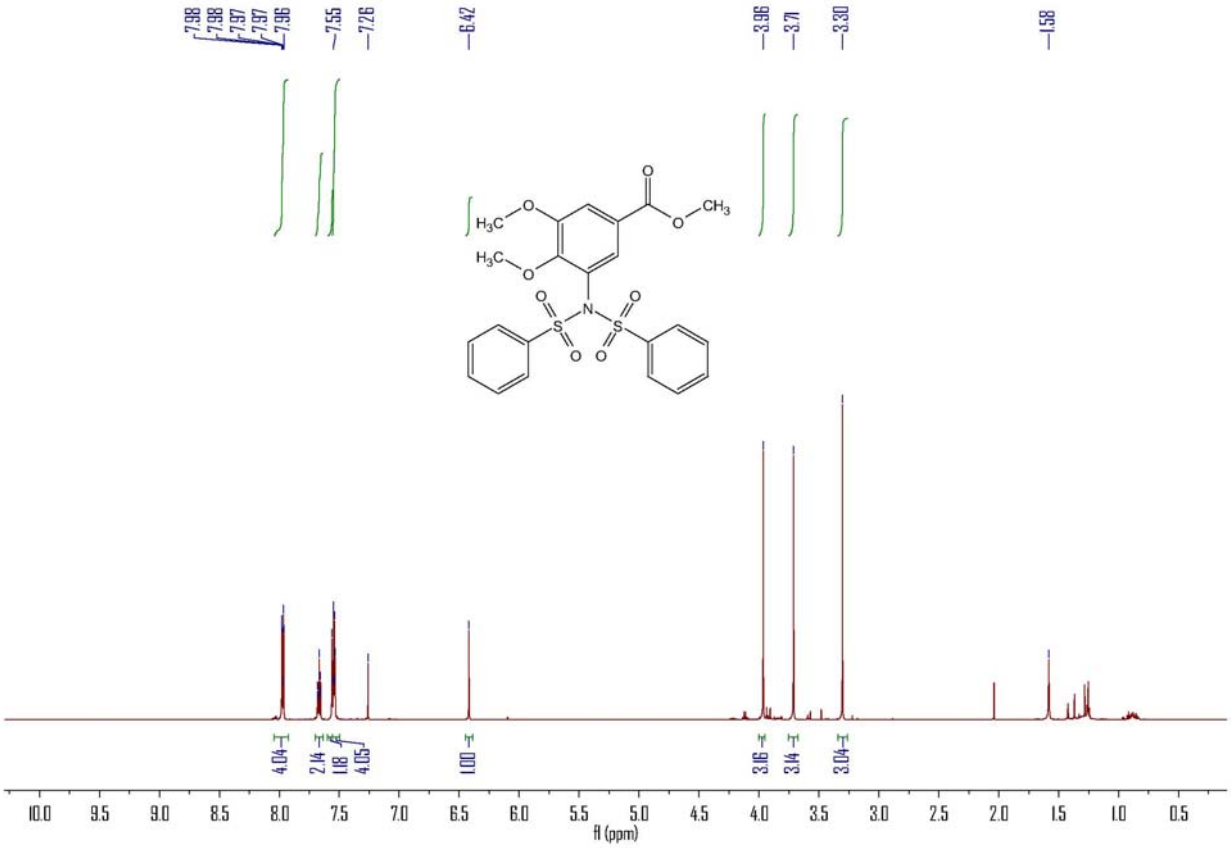


^{1}H NMR of **7k**



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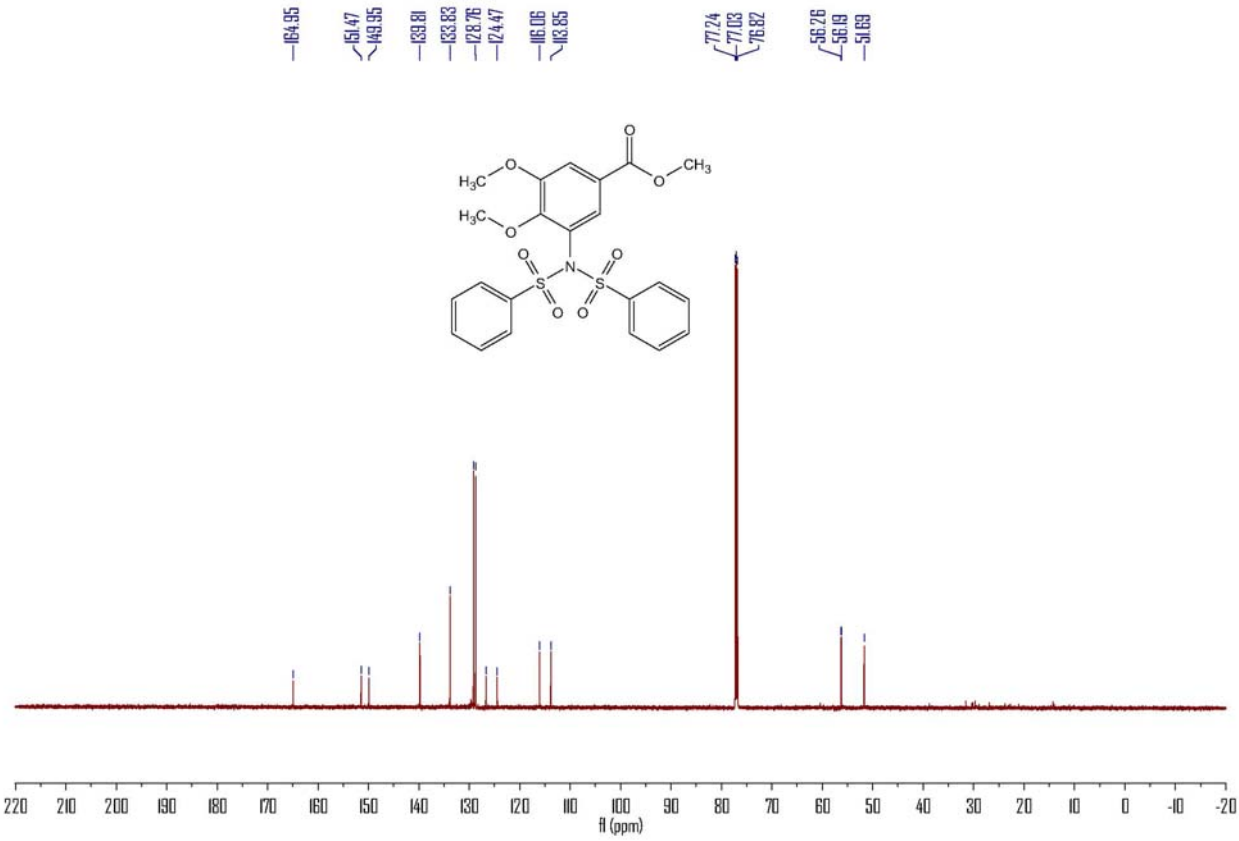
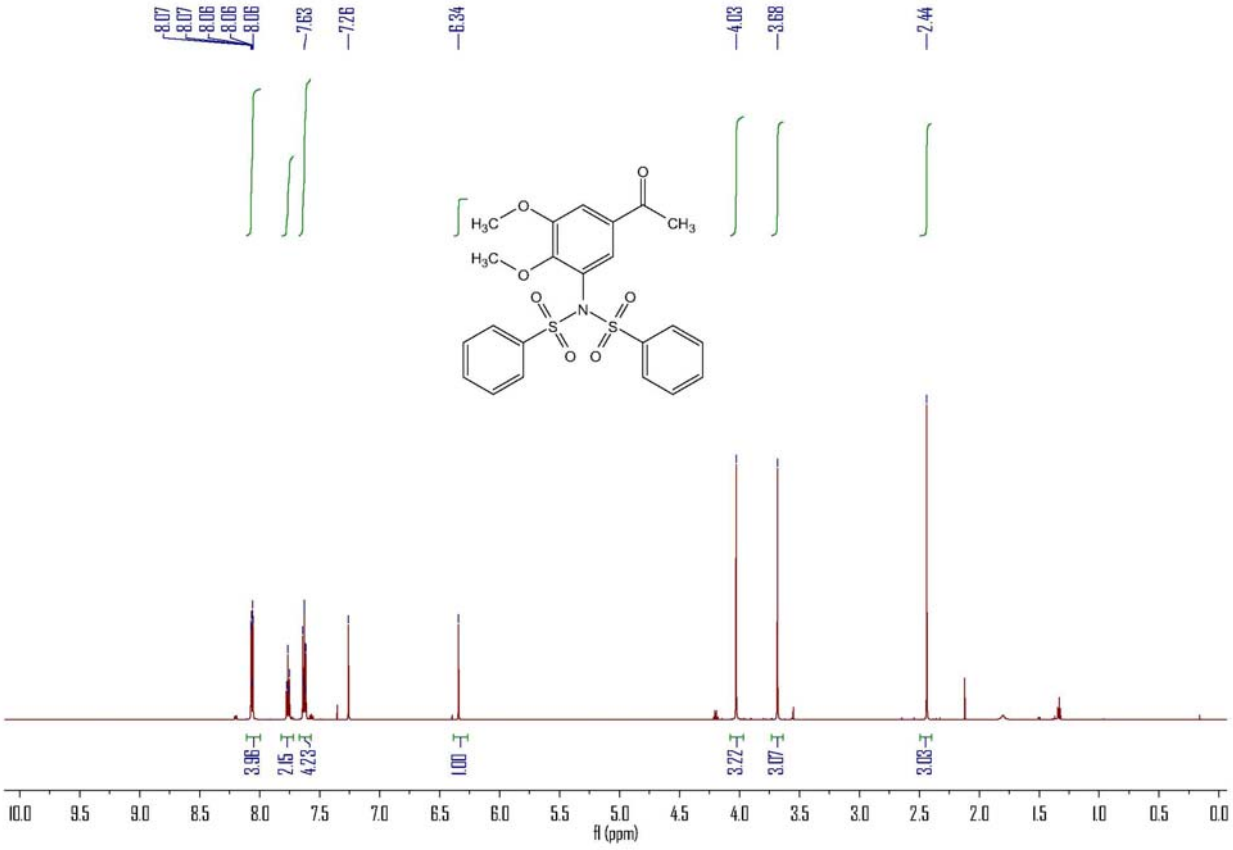
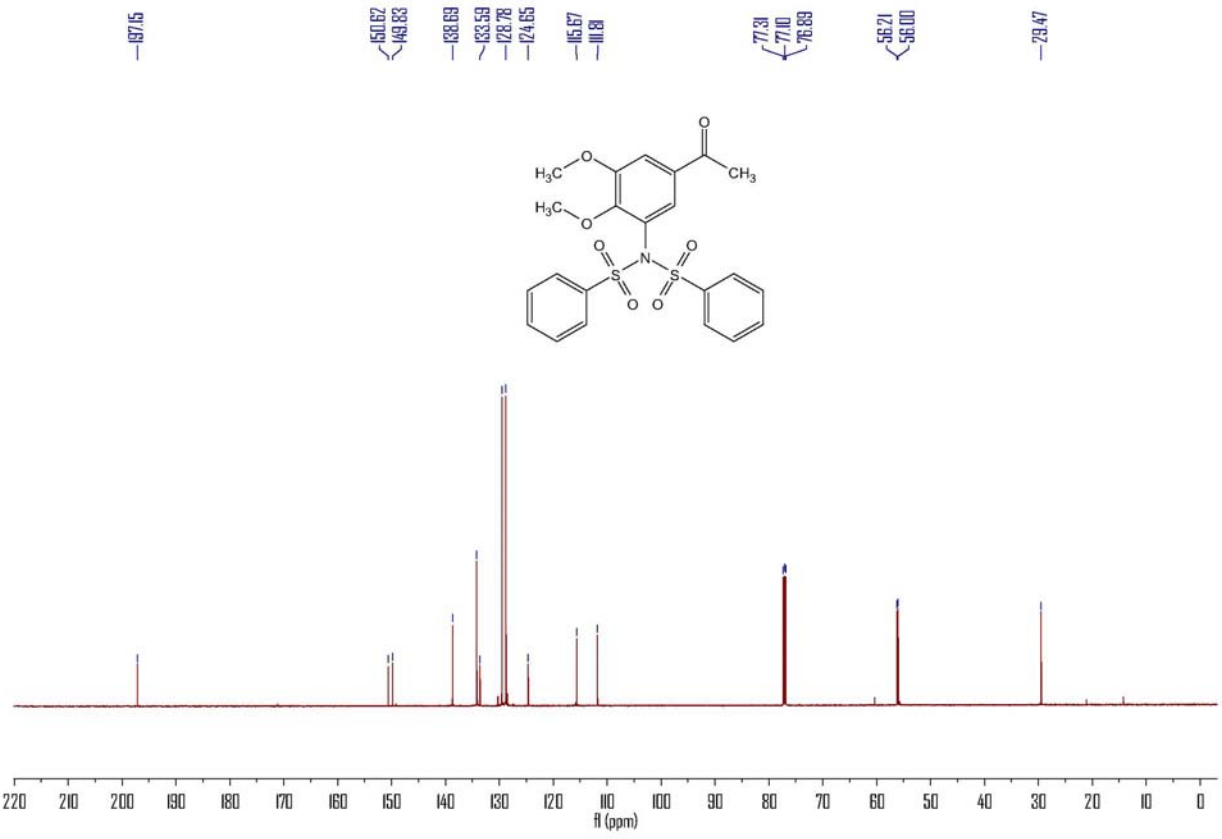


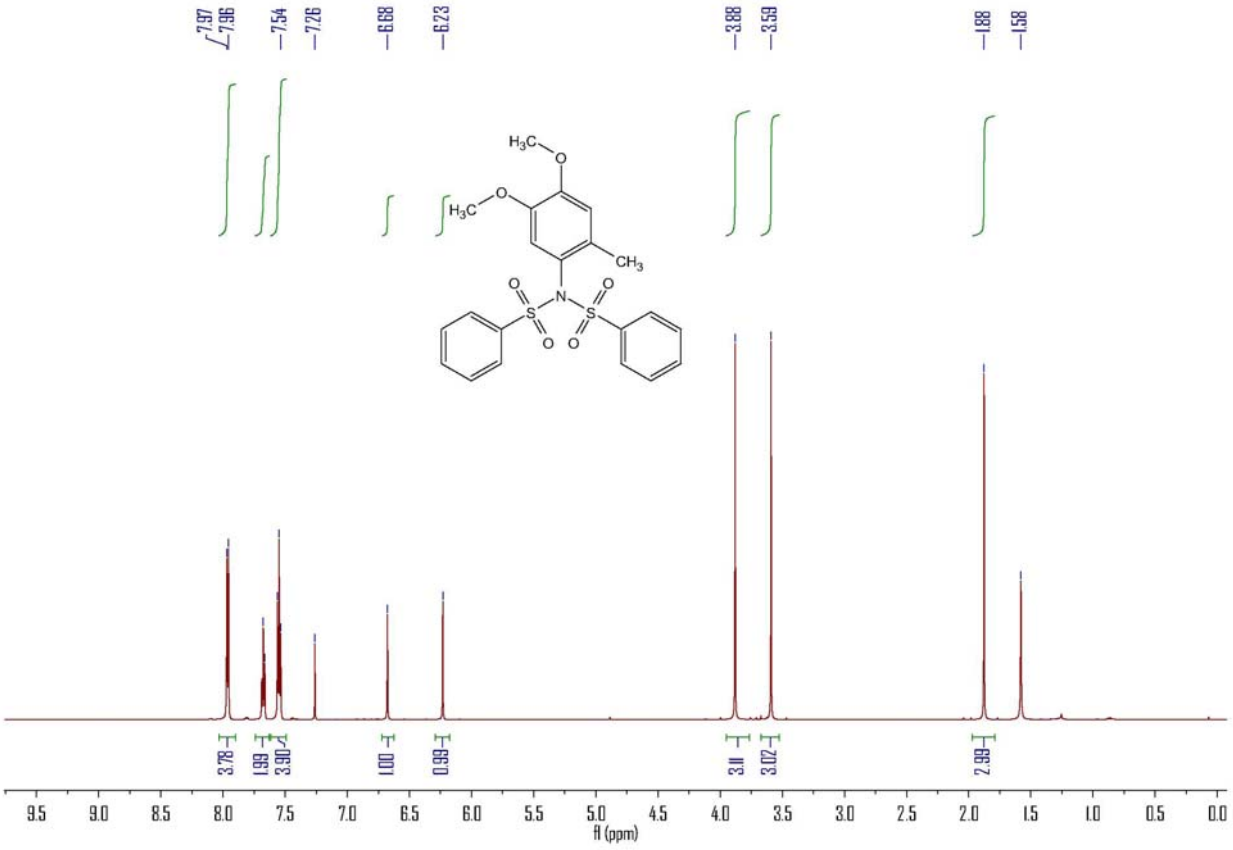
^{1}H NMR of **7l**



^{13}C NMR of **7l**



^{1}H NMR of **m**



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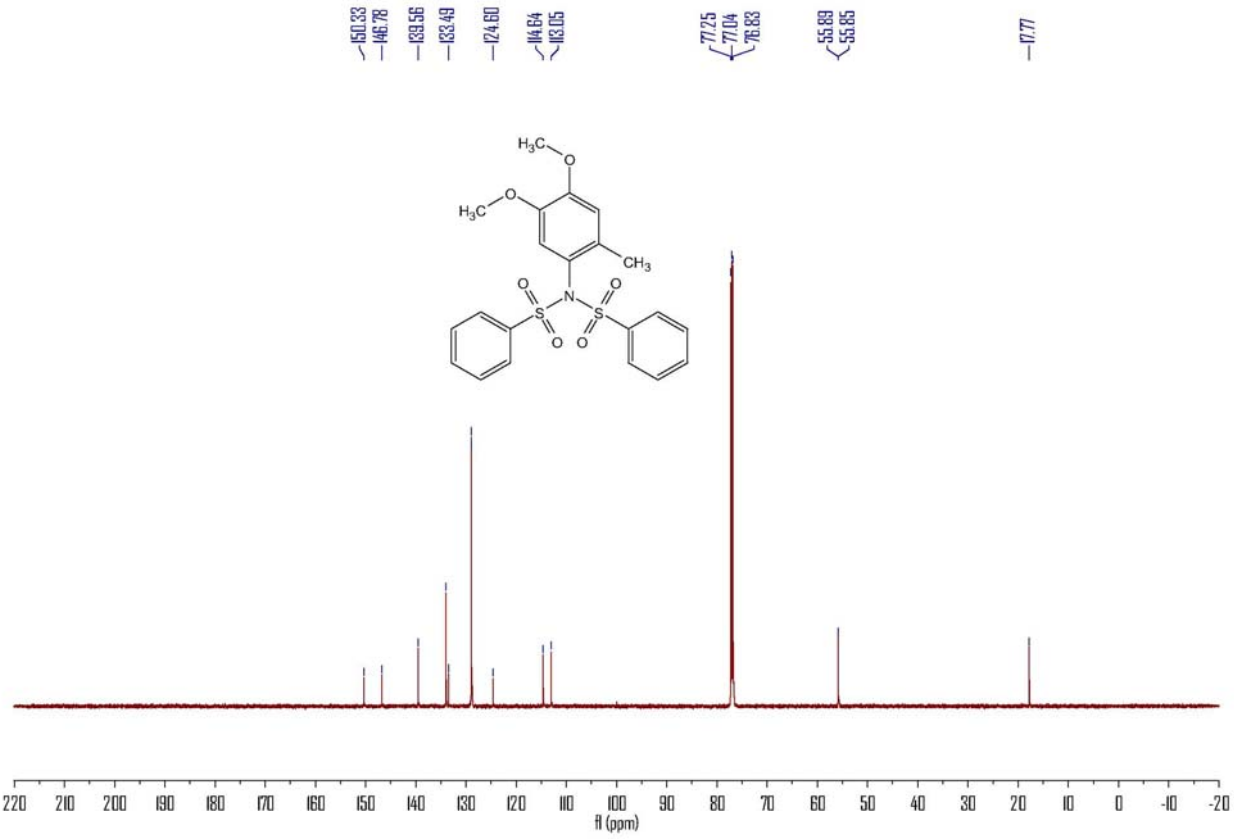

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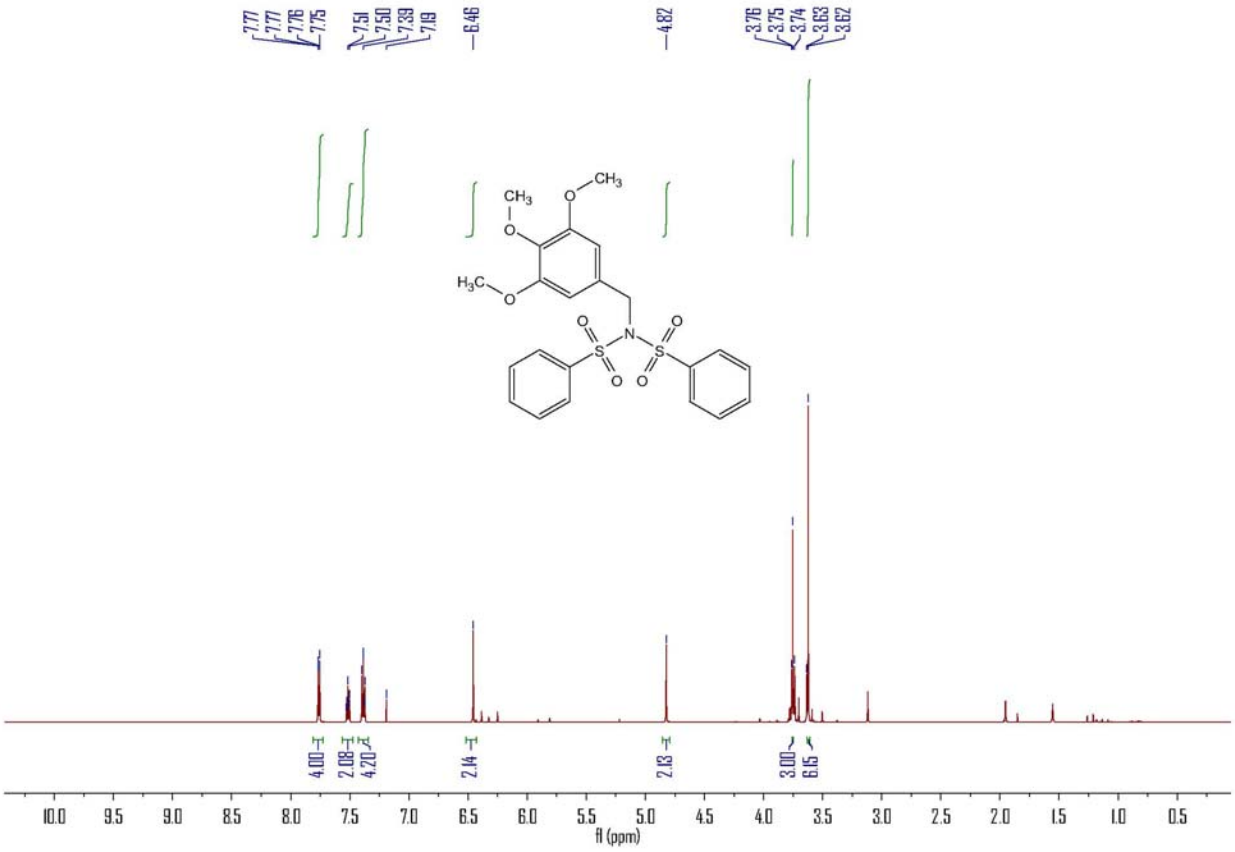

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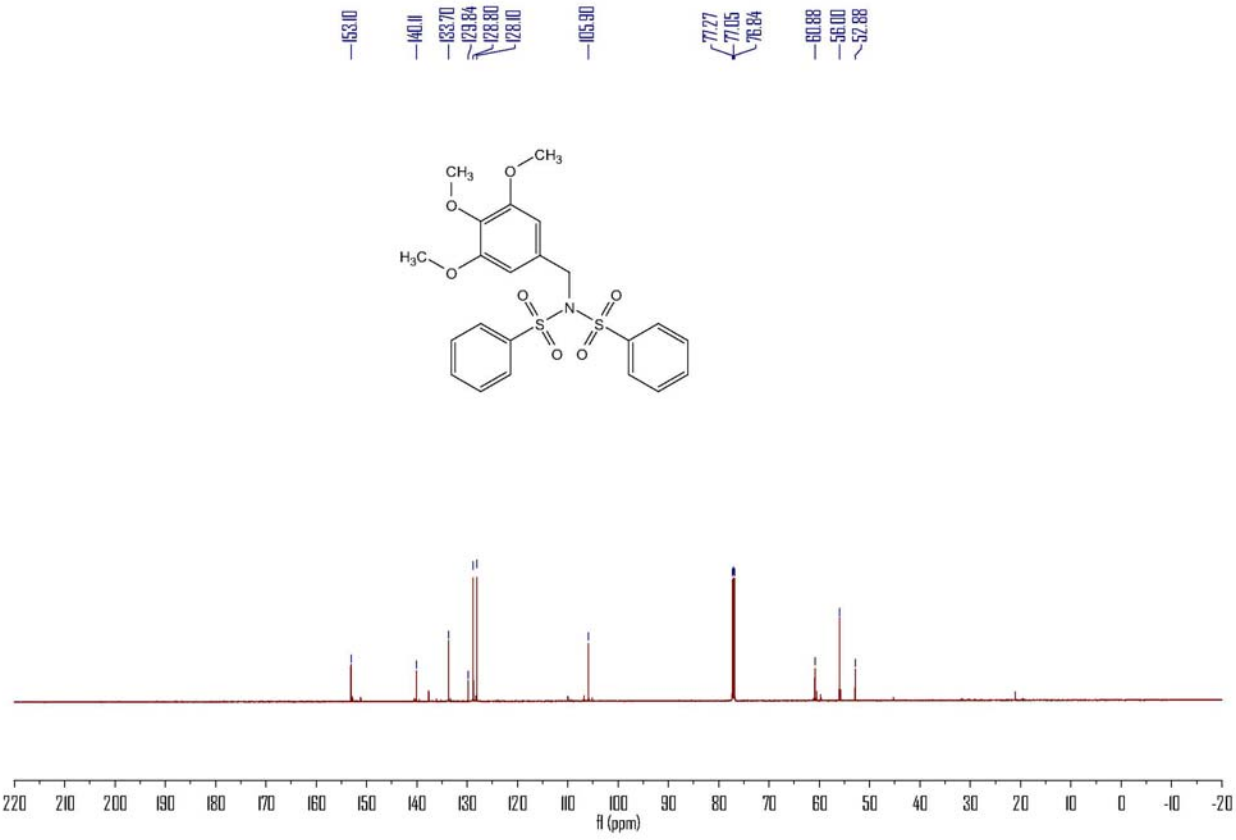
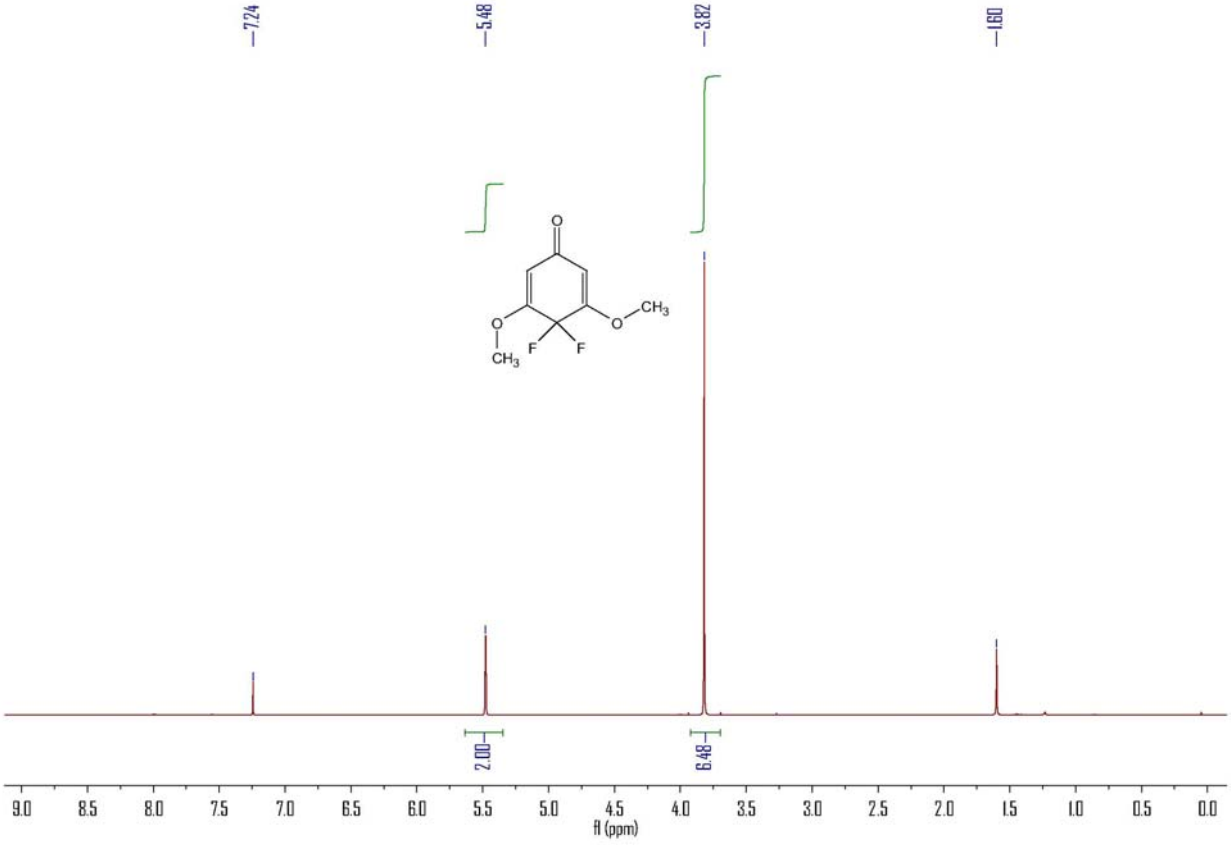
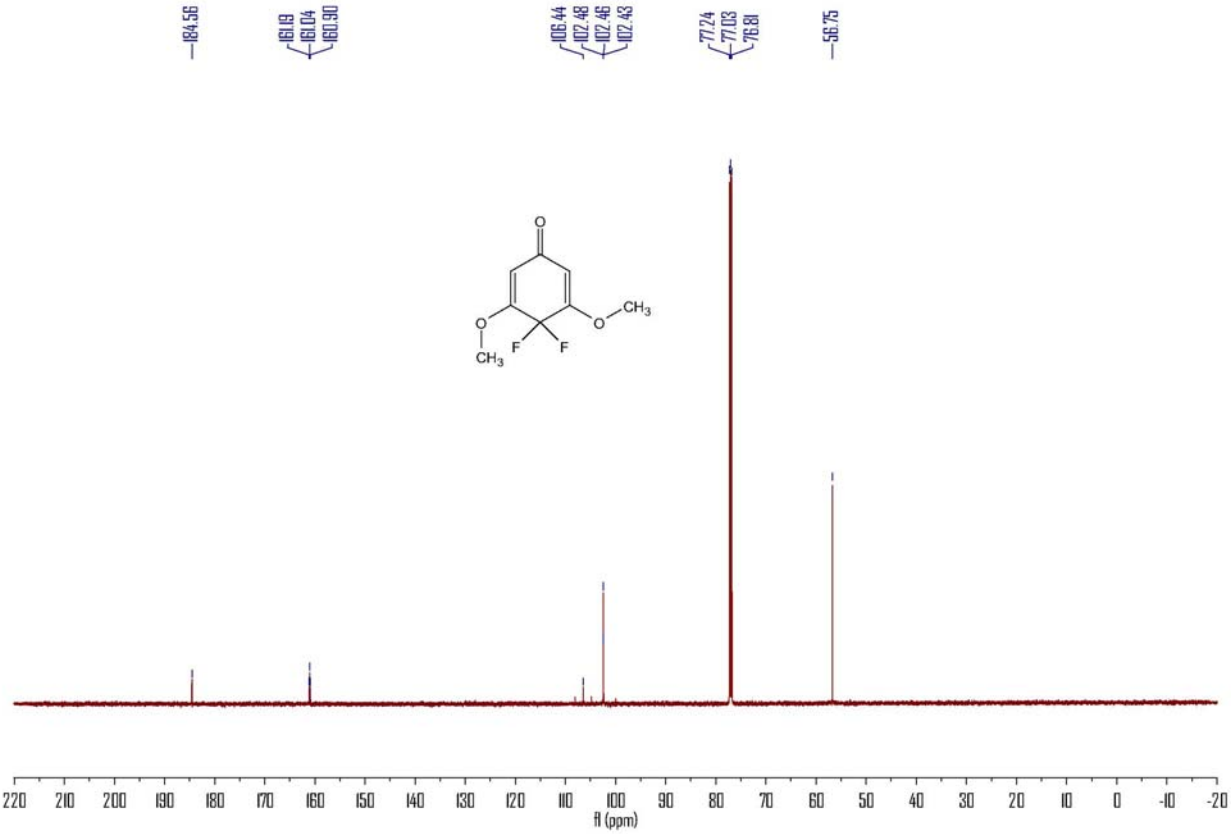


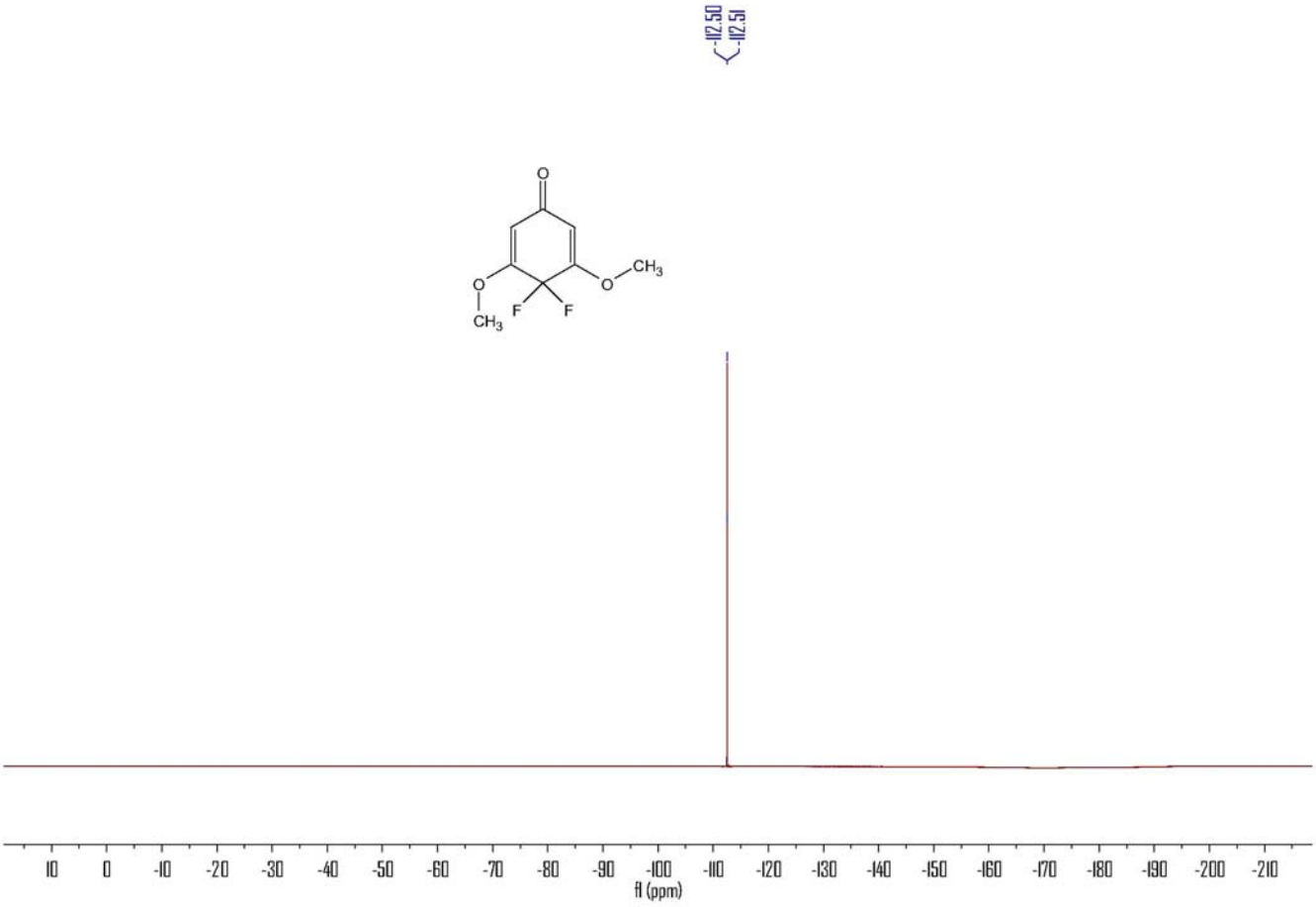
^{1}H NMR of **7o**



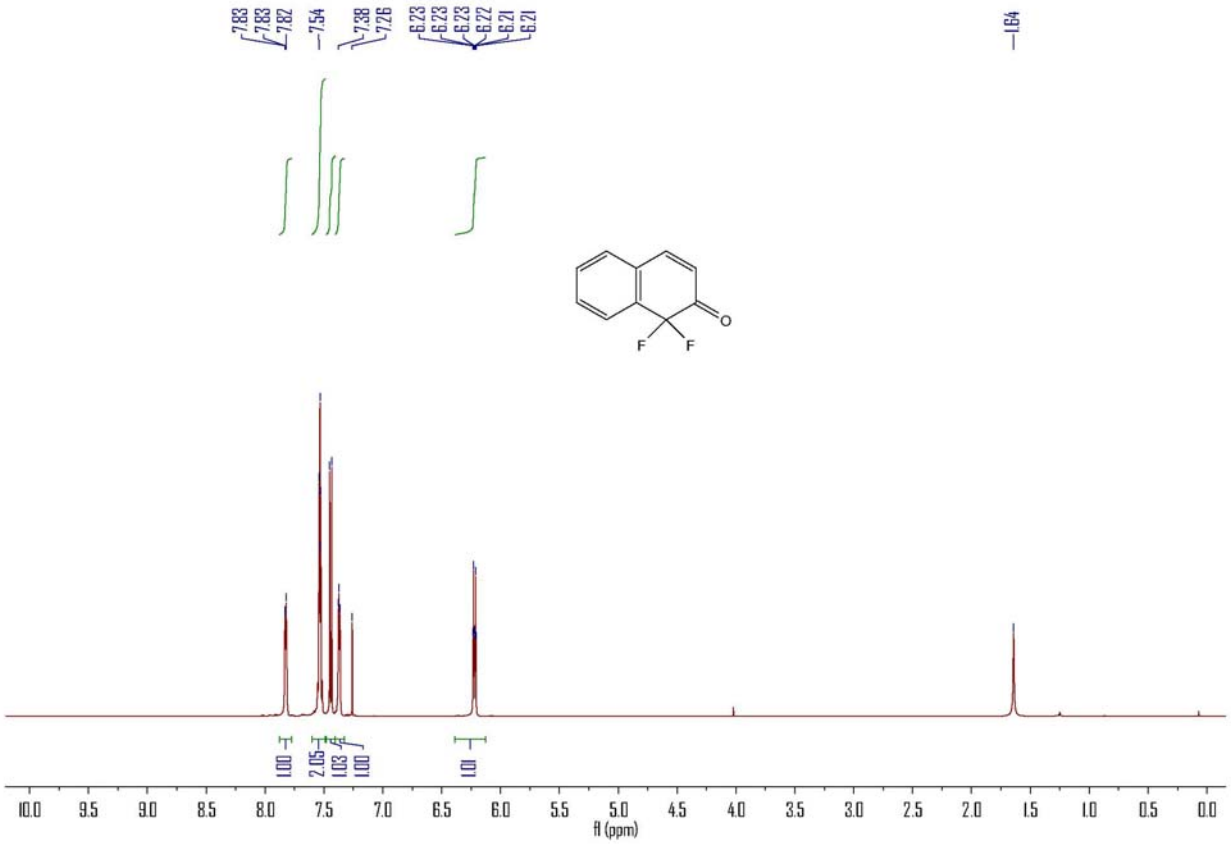
^{13}C NMR of **7o**



^{19}F NMR of **7o**


-112.50
-112.51
O
O
CH3
O
CH3
F
F
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

^{1}H NMR of **7p**



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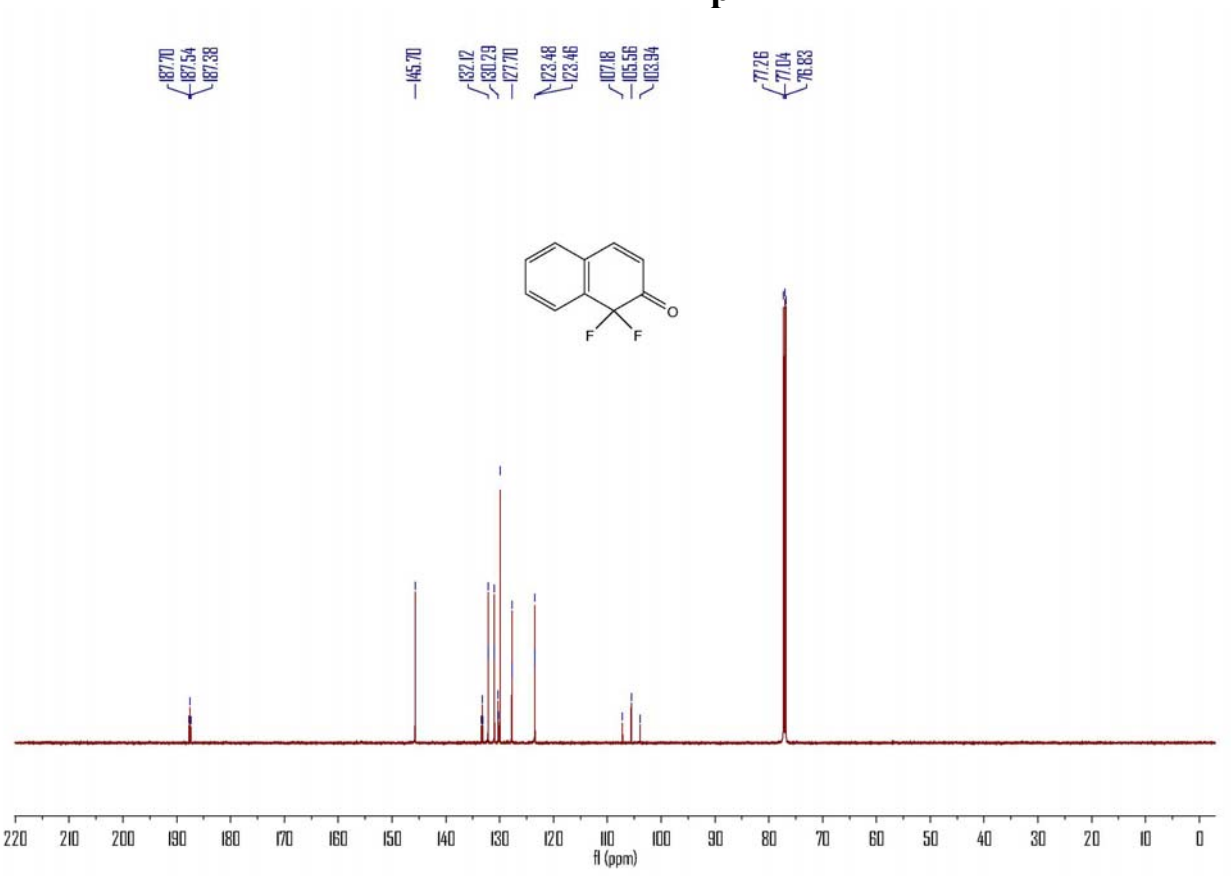
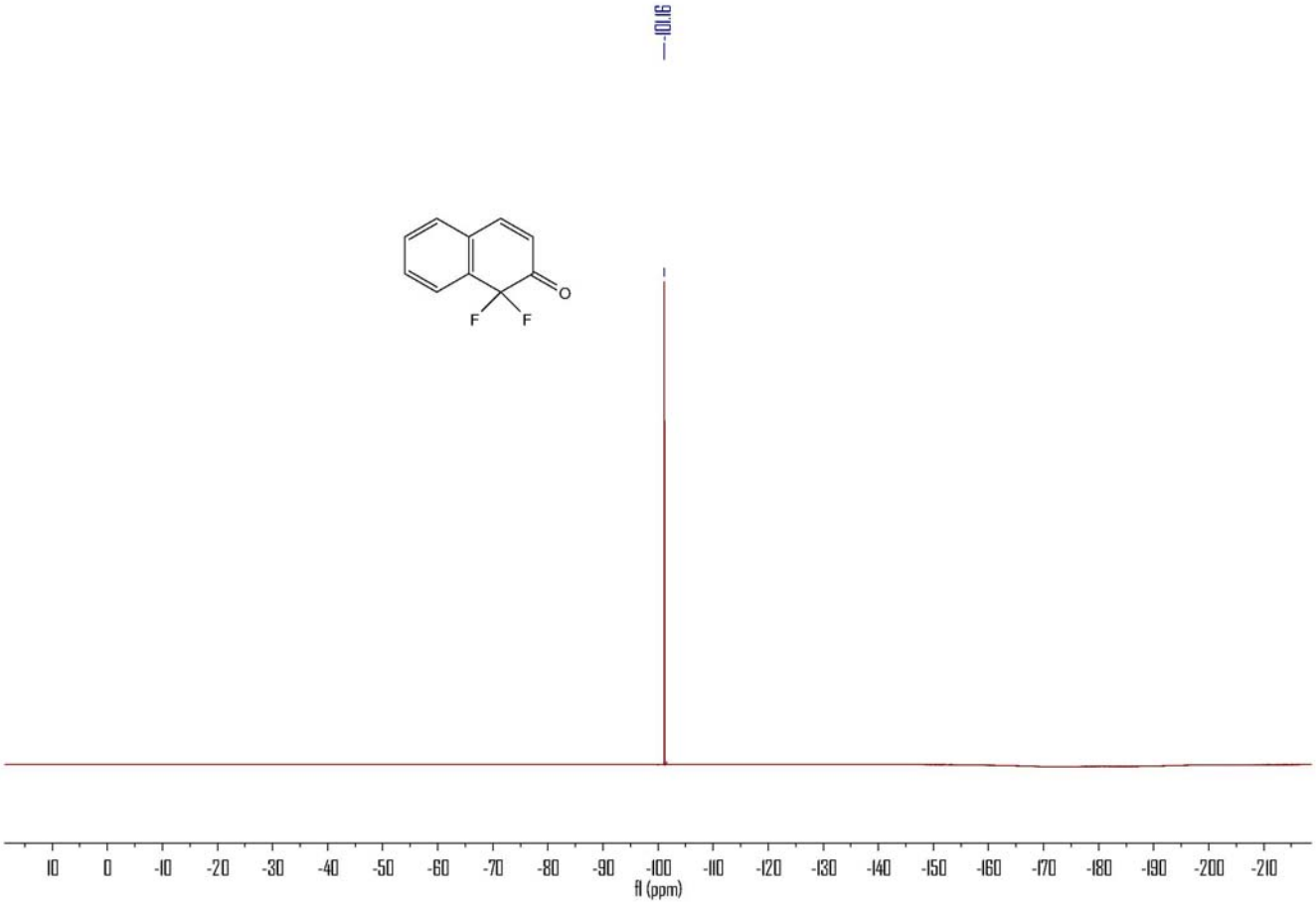


^{19}F NMR of **7p**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f1 (ppm)