Electronic Supplementary Information

Molybdenum based metallomicellar catalyst for controlled and selective sulfoxidation reactions in aqueous medium

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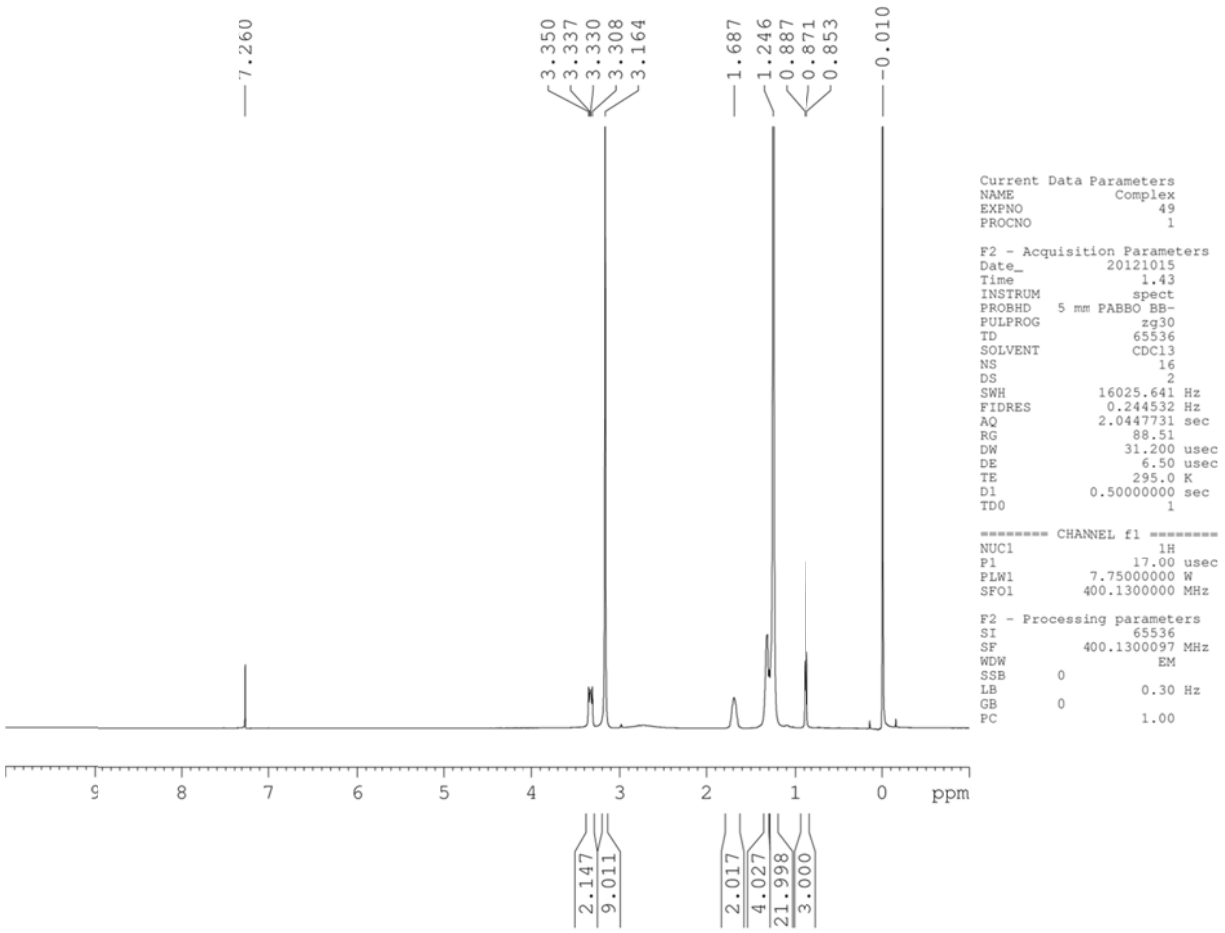


Figure S1: ^{1}H-NMR spectrum of complex $(C_{19}H_{42}N)_2[MoO(O_2)_2(C_2O_4)]\cdot H_2O$

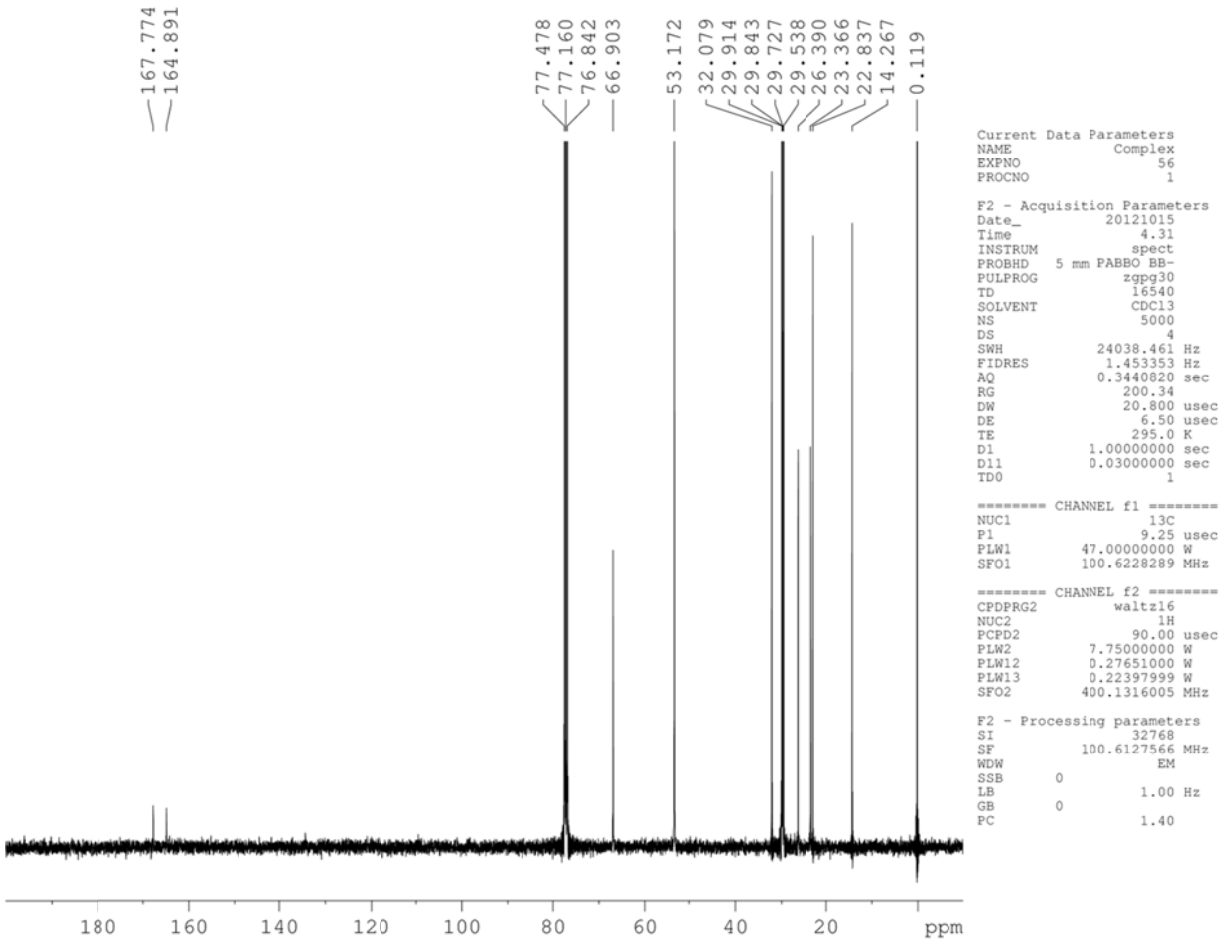


Figure S2: ^{13}C-NMR spectrum of complex $(C_{19}H_{42}N)_2[MoO(O_2)_2(C_2O_4)]\cdot H_2O$

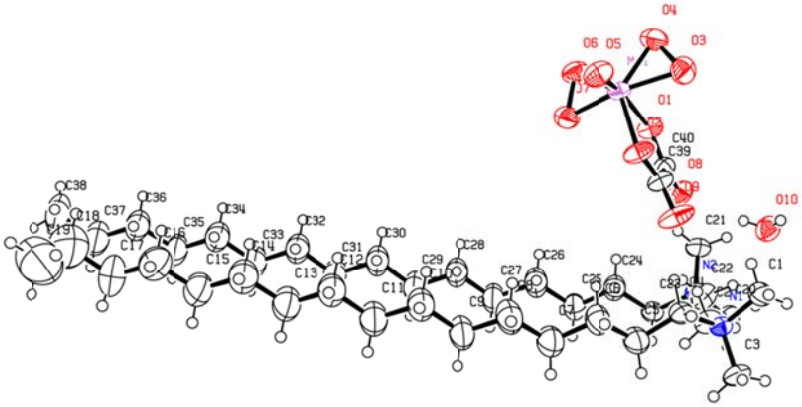


Figure S3 : ORTEP diagram of the complex$(C_{19}H_{42}N)_2[MoO(O_2)_2(C_2O_4)]\cdot H_2O$ with 50% thermal ellipsoids

Table S1: Crystallographic data and parameters for complex $(C_{19}H_{42}N)_2[MoO(O_2)_2(C_2O_4)]\cdot H_2O$

Compound reference	**1**
Chemical formula	$C_{40}H_{86}MoN_2O_{10}$
Formula mass	851.05
Crystal system	Triclinic
a/Å	9.7003(3)
b/Å	10.0807(4)
c/Å	26.1807(10)
α/°	88.397(2)
β/°	82.0730(10)
γ/°	69.8550(10)
Unit cell volume/Å^3	2379.99(15)
Temperature/ K	298(2)
Space group	*P-1*
No. of formula unit per cell/ *Z*	2
Radiation type	Mo K*a*
Absorption coefficient, *m*/ mm^{-1}	0.326
No. of reflections measured	31760
No. of independent reflections	11050
R_{int}	0.025
Final R_1 values [$I>2\sigma(I)$]	0.0396
Final $wR(F^2)$ values [$I>2\sigma(I)$]	0.1233
Final R_1 values (all data)	0.0551
Final $wR(F^2)$ values (all data)	0.1433
Goodness of fit on F^2	1.046
CCDC number	CCDC 918215

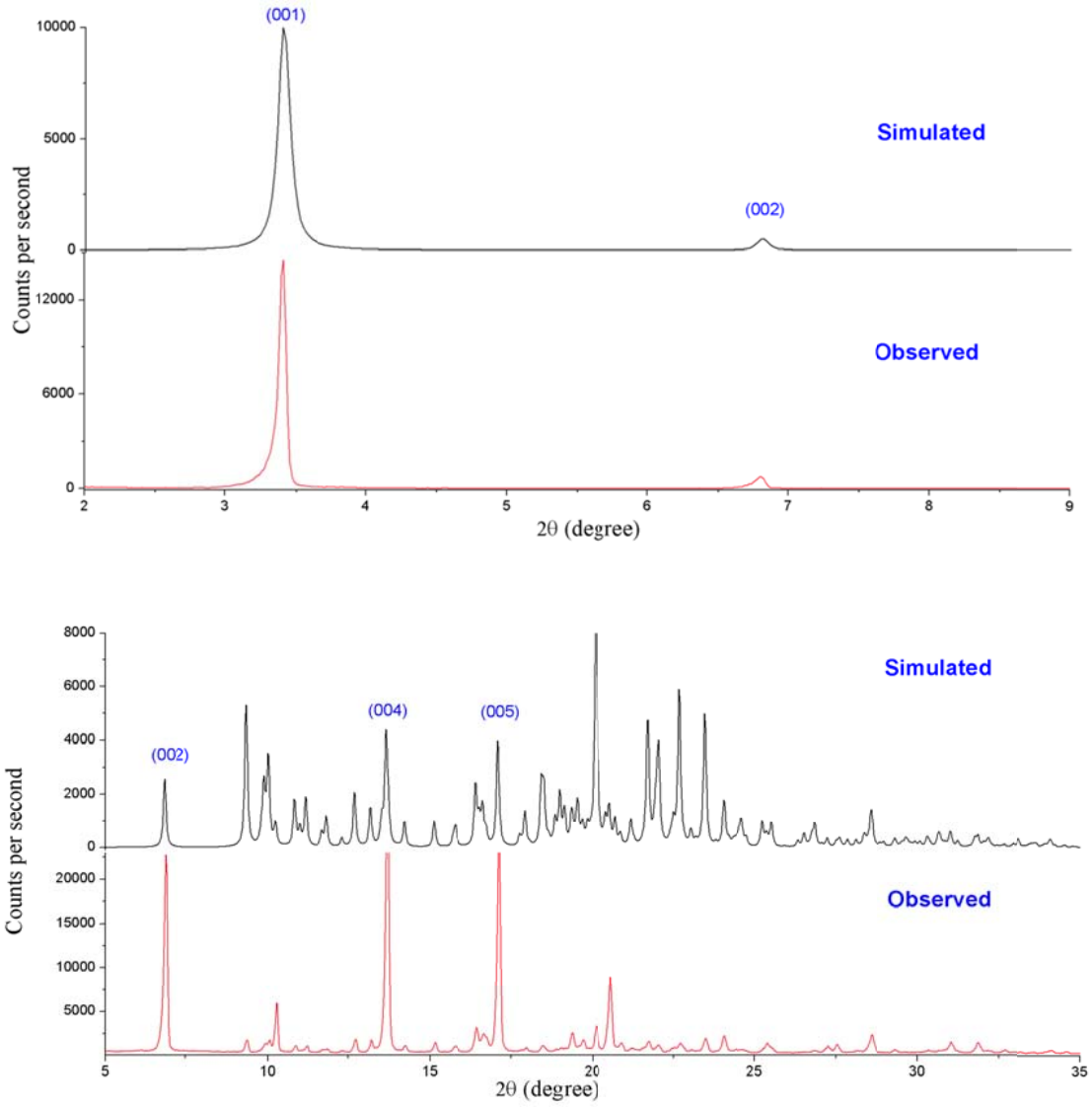


Figure S4: Powder XRD pattern of the bulk complex $(C_{19}H_{42}N)_2[MoO(O_2)_2(C_2O_4)]\cdot H_2O$ compared with the simulated data.

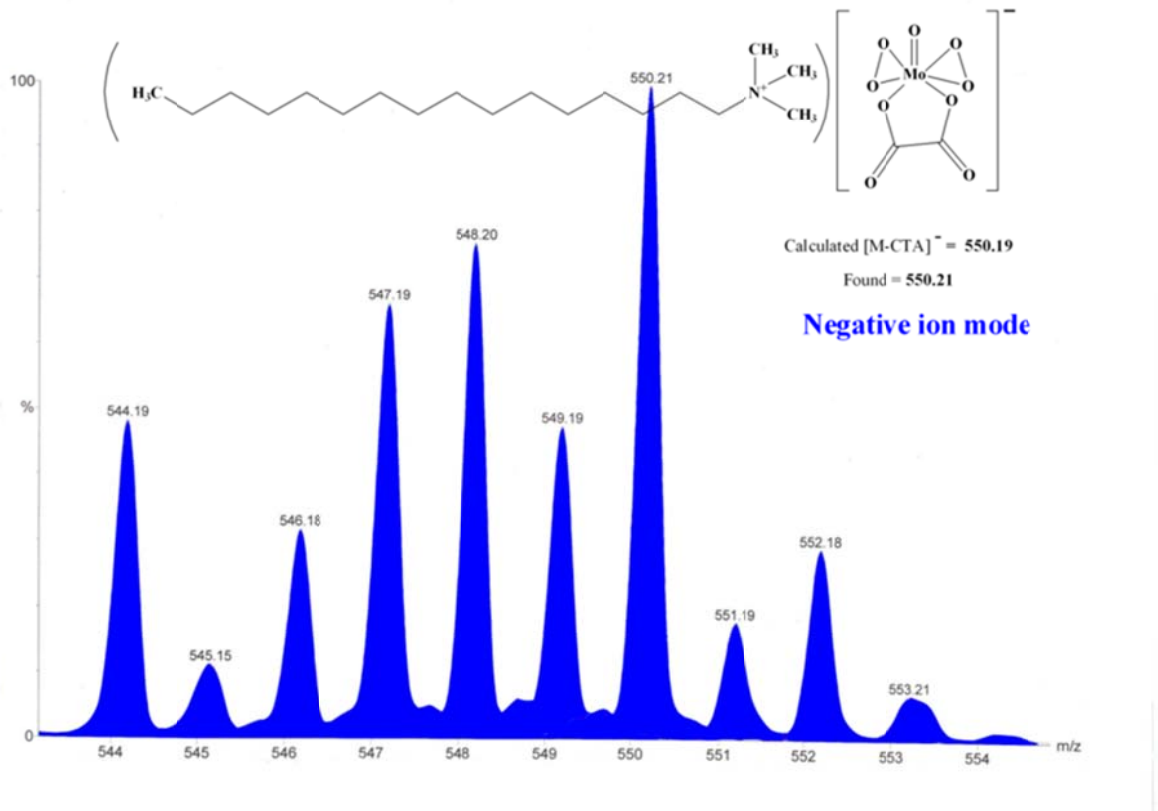


Figure S5:ESI-MS of complex $(C_{19}H_{42}N)_2[MoO(O_2)_2(C_2O_4)]\cdot H_2O$

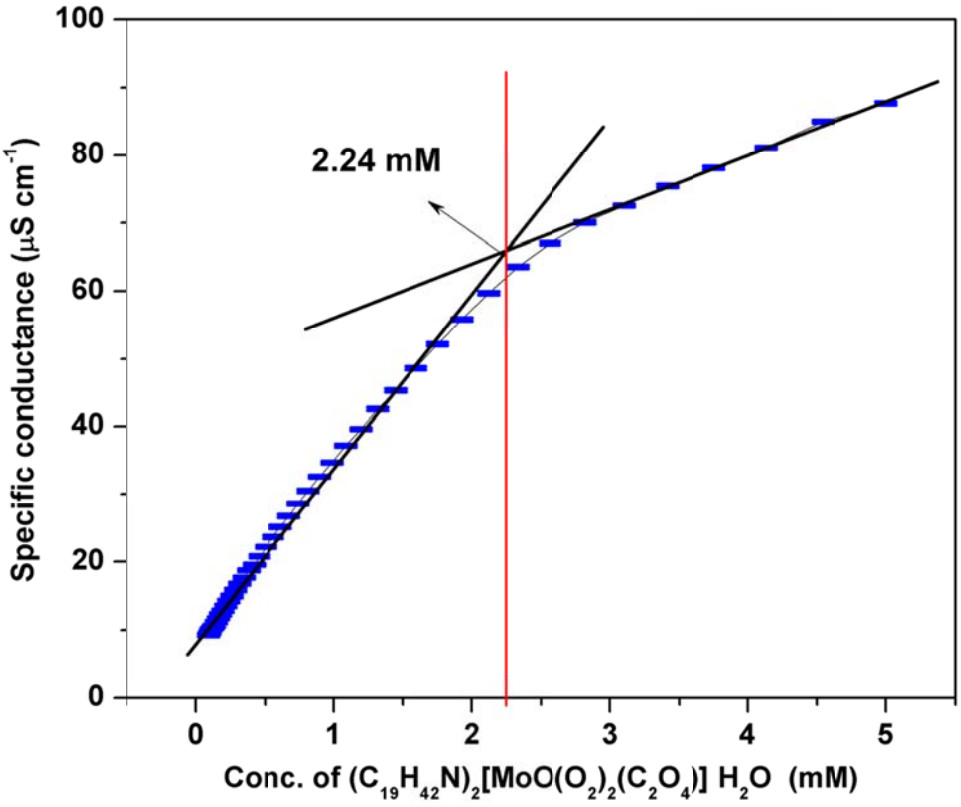


Figure S6: Critical micellar concentration (CMC) of metallo-micelle obtained from a plot of specific conductance against concentration. (Standard Deviation = 0.23)

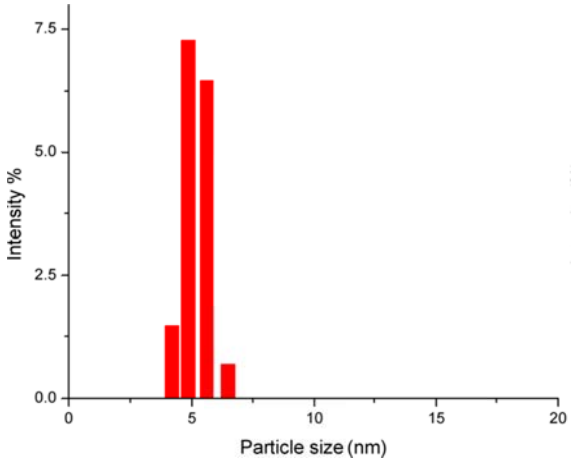


Figure S7: Dynamic light scattering (DLS) histogram of CTAB

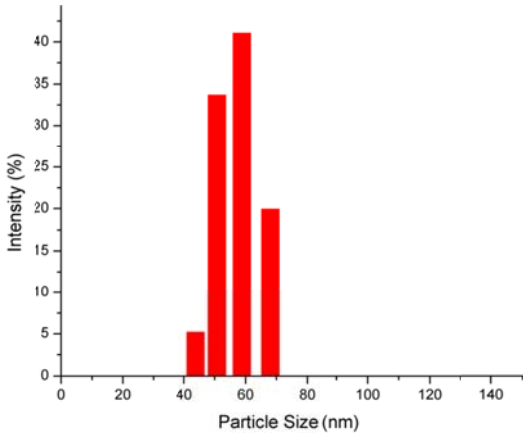


Figure S8: Dynamic light scattering (DLS) histogram of complex **1**

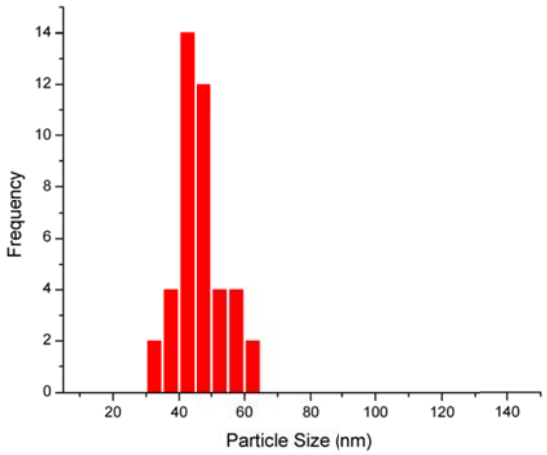


Figure S9: Particle size distribution histogram from TEM image

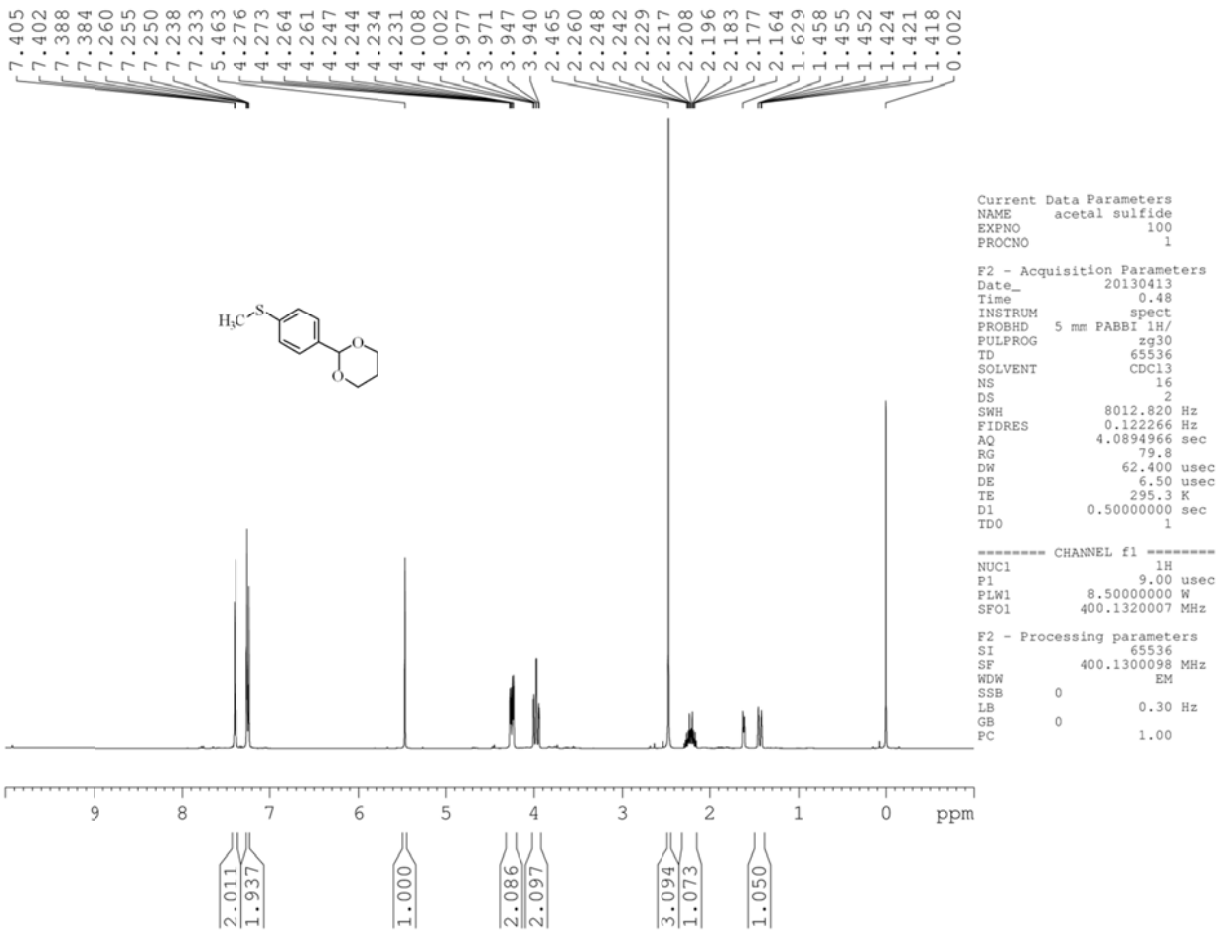


Figure S10: ^{1}H-NMR spectrum of 2-(4-(methylthio)phenyl)-1,3-dioxane

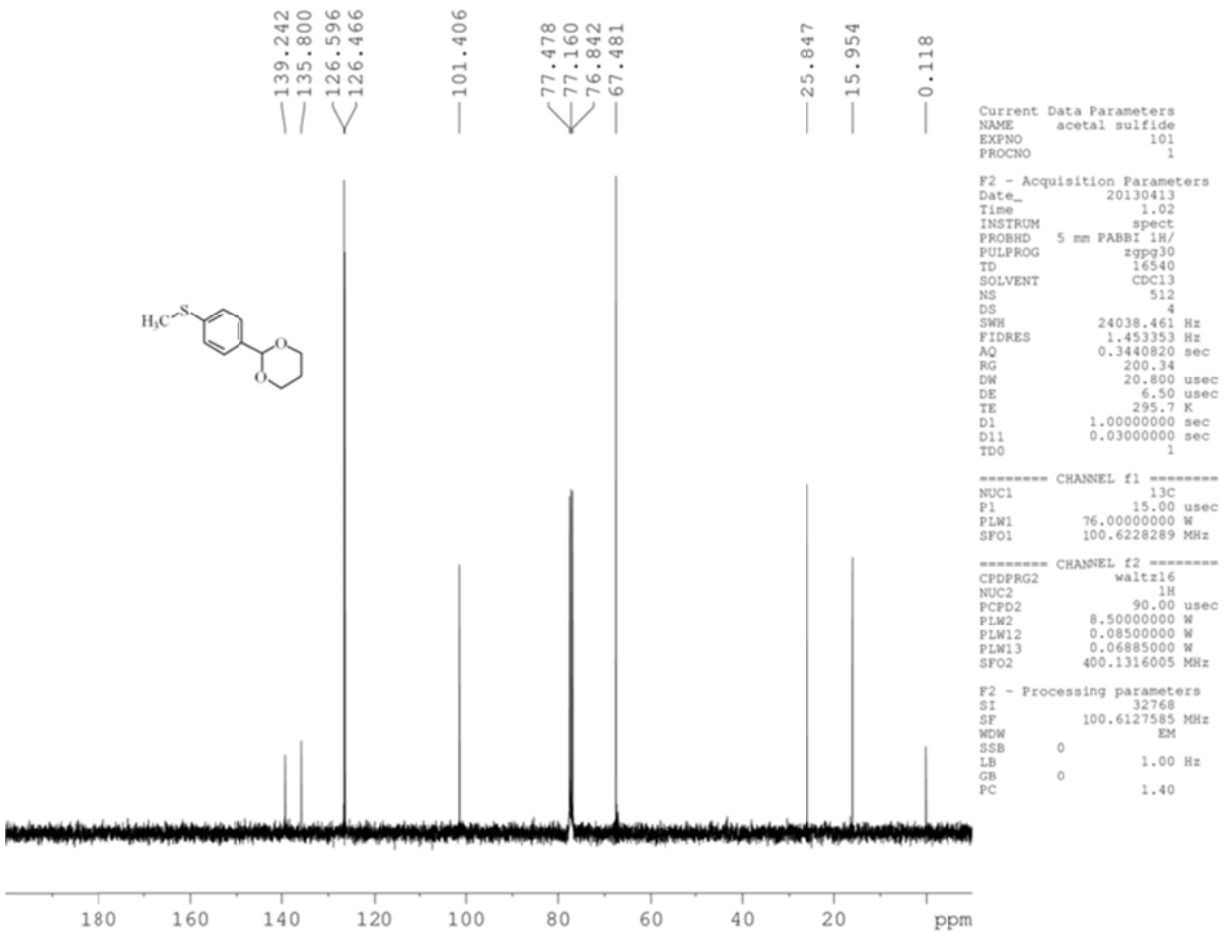


Figure S11: ^{13}C-NMR spectrum of 2-(4-(methylthio)phenyl)-1,3-dioxane

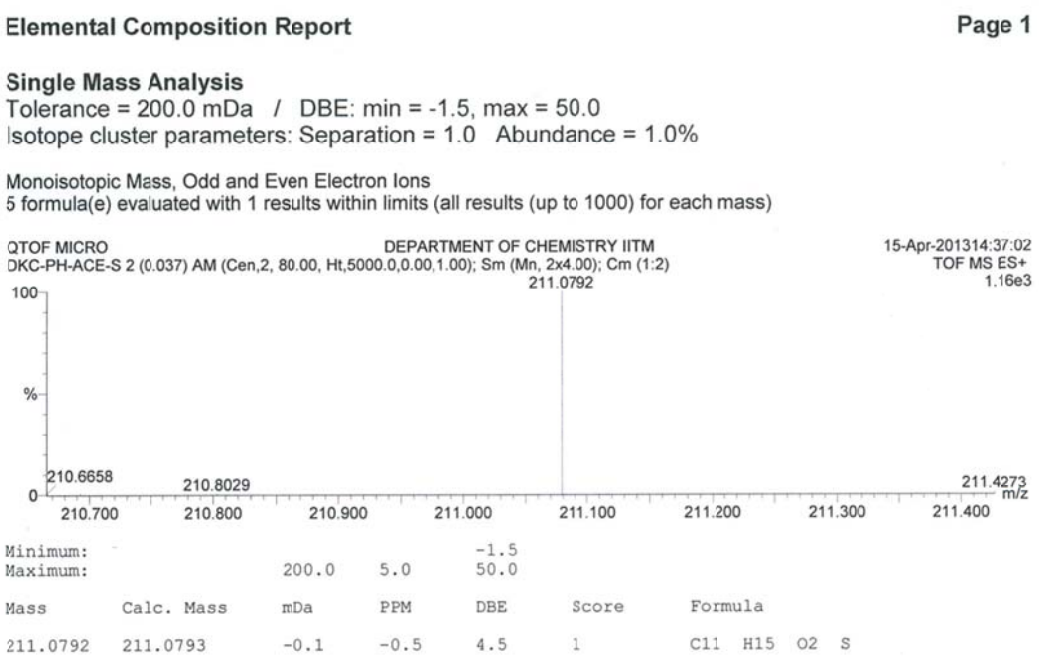


Figure S12:ESI-HRMS of 2-(4-(methylthio)phenyl)-1,3-dioxane

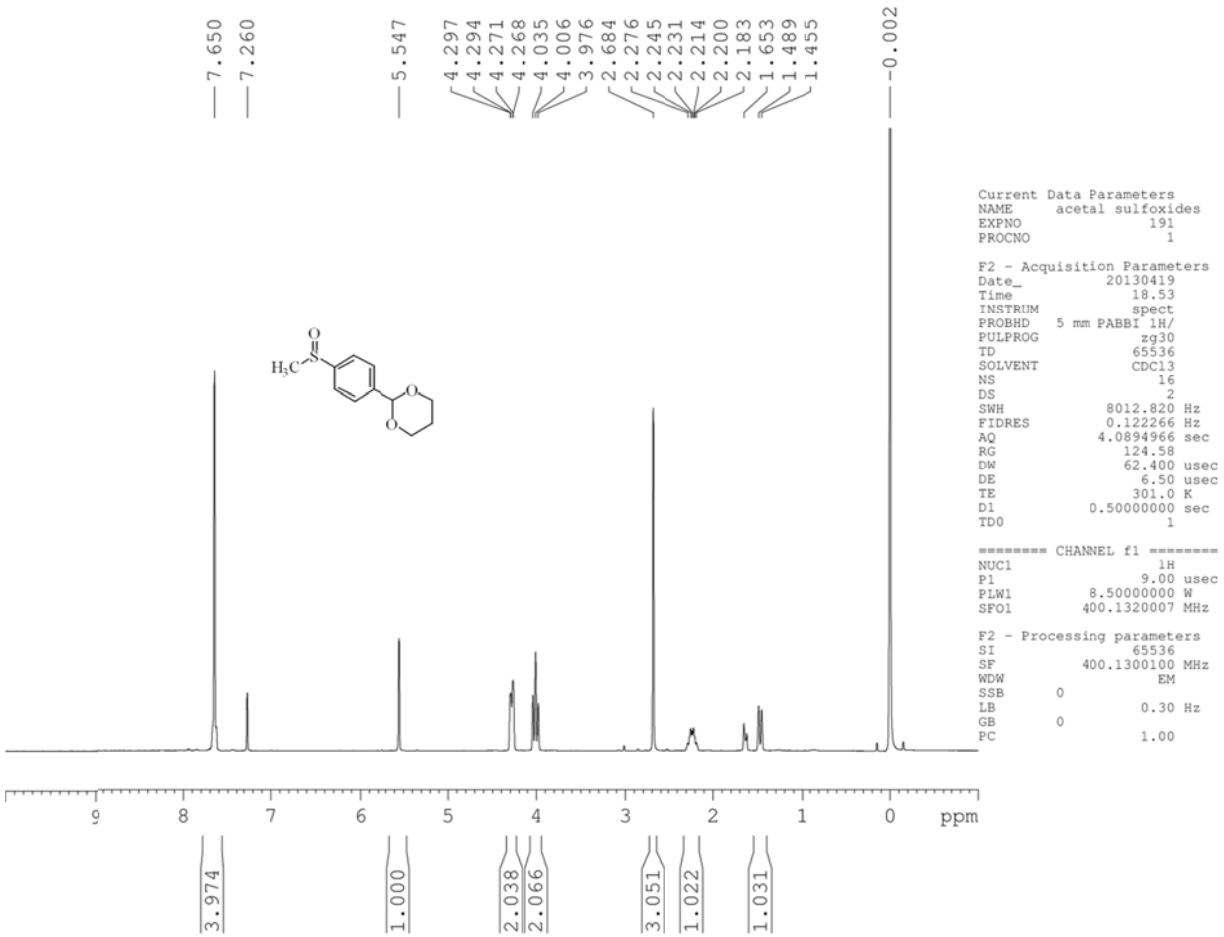


Figure S13: ^{1}H-NMR spectrum of 2-(4-(methylsulfinyl)phenyl)-1,3-dioxane

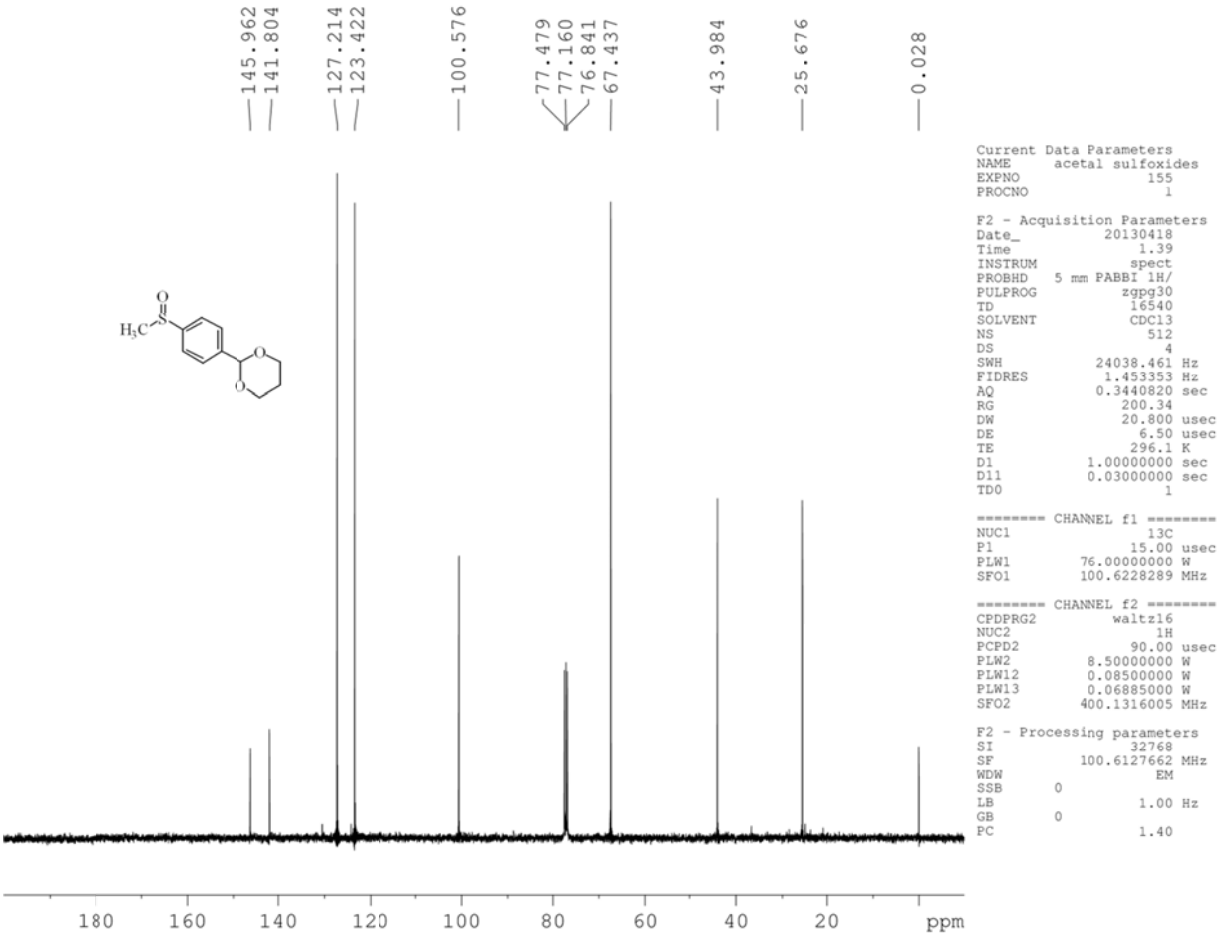


Figure S14: ^{13}C-NMR spectrum of 2-(4-(methylsulfinyl)phenyl)-1,3-dioxane

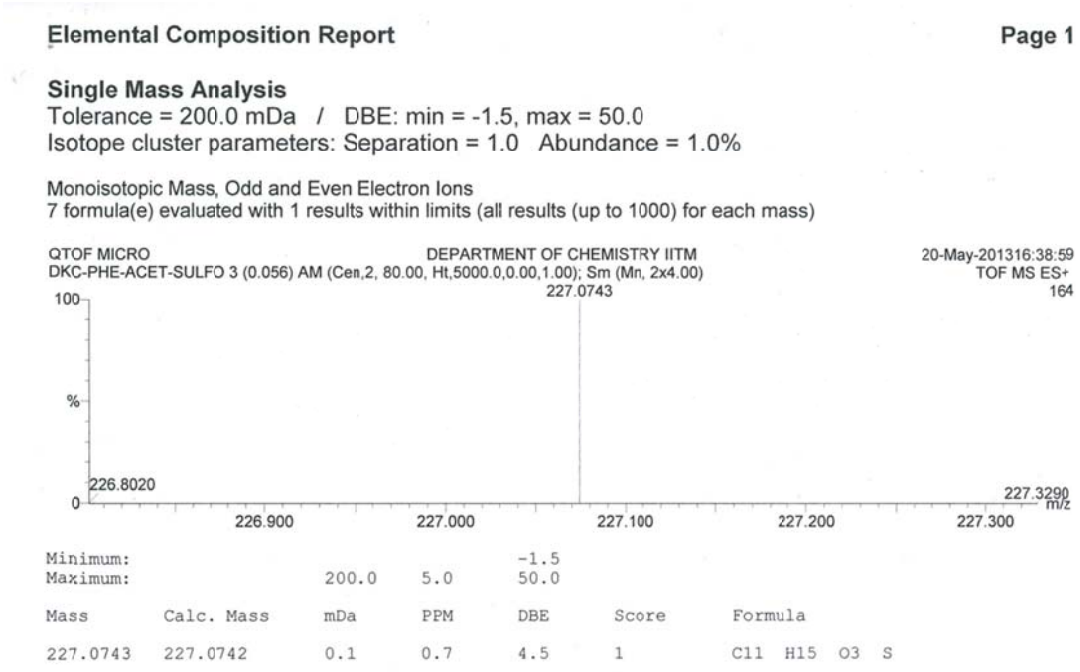


Figure S15:ESI-HRMS of2-(4-(methylsulfinyl)phenyl)-1,3-dioxane

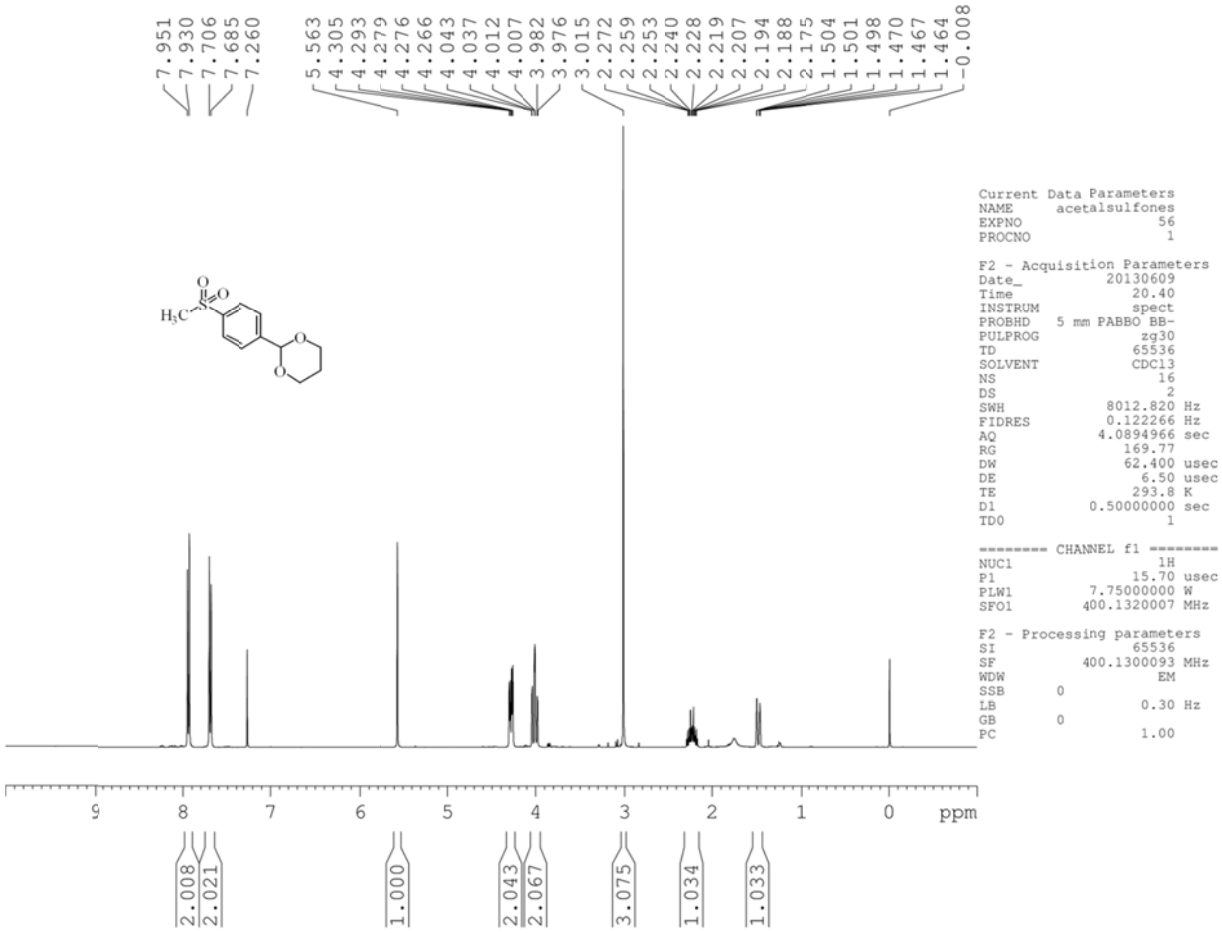


Figure S16: ^{1}H-NMR spectrum of 2-(4-(methylsulfonyl)phenyl)-1,3-dioxane

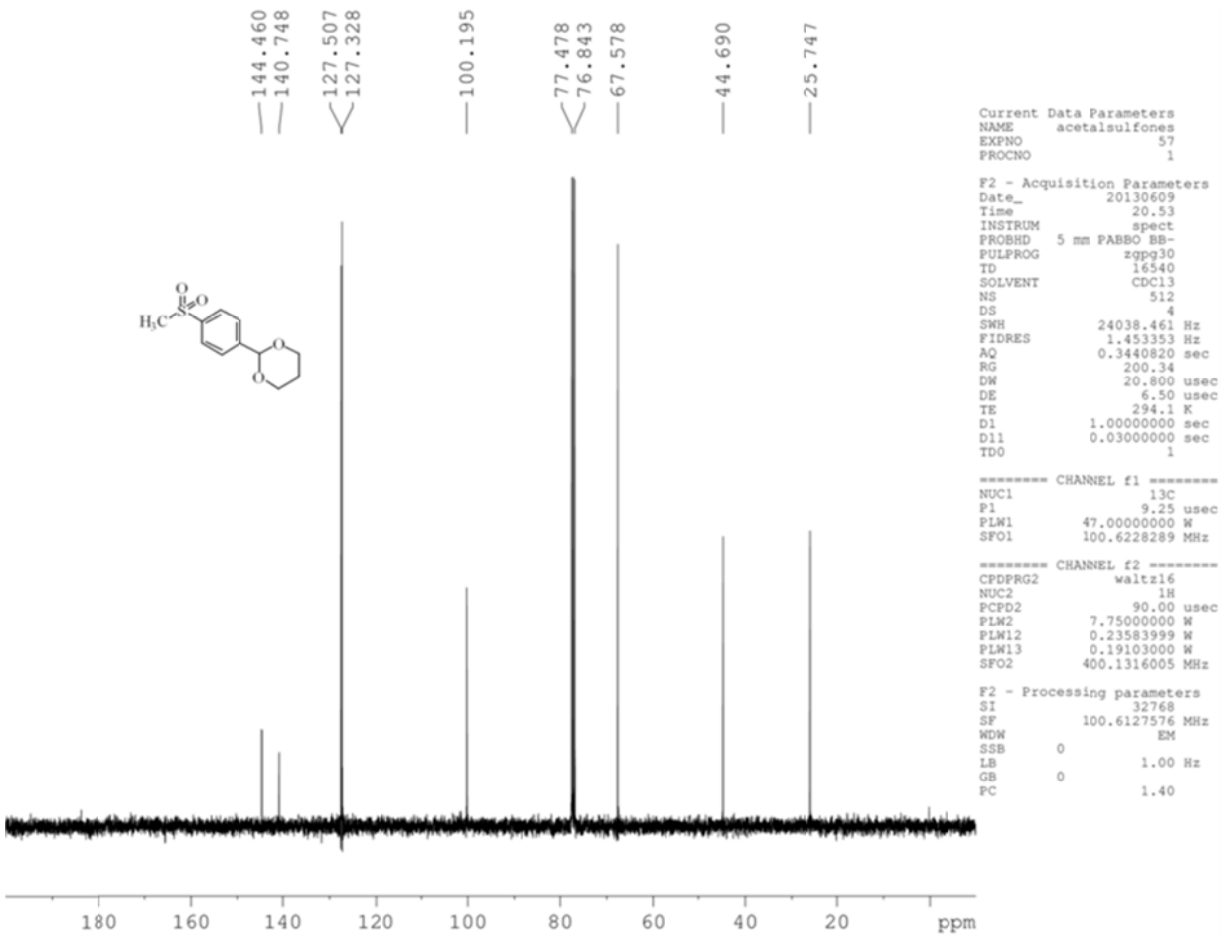


Figure S17: ^{13}C-NMR spectrum of 2-(4-(methylsulfonyl)phenyl)-1,3-dioxane

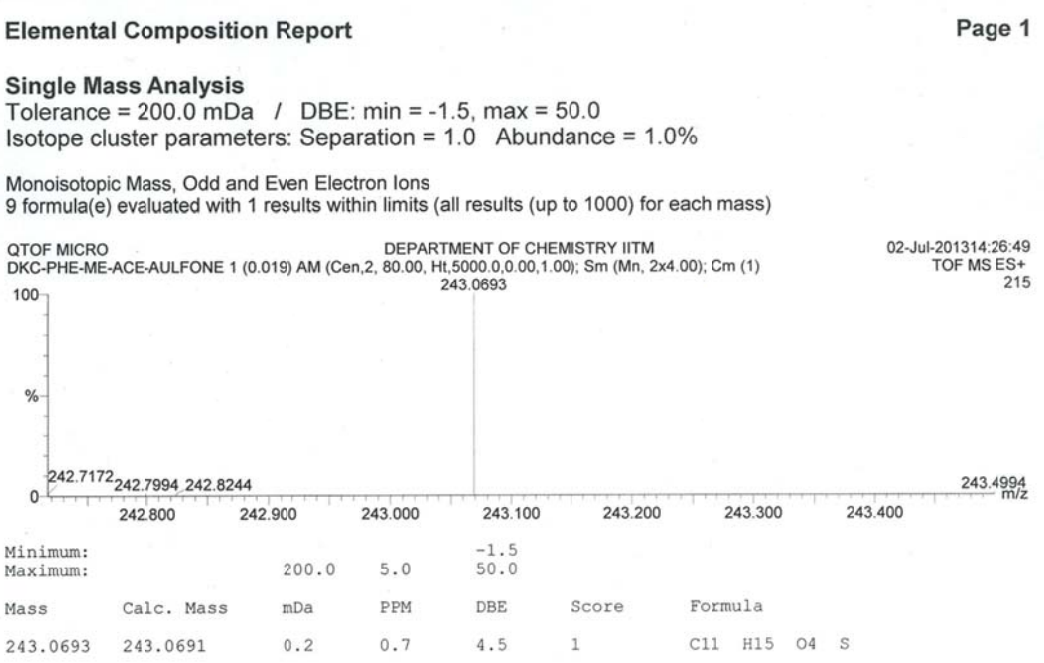


Figure S18:ESI-HRMS of 2-(4-(methylsulfonyl)phenyl)-1,3-dioxane

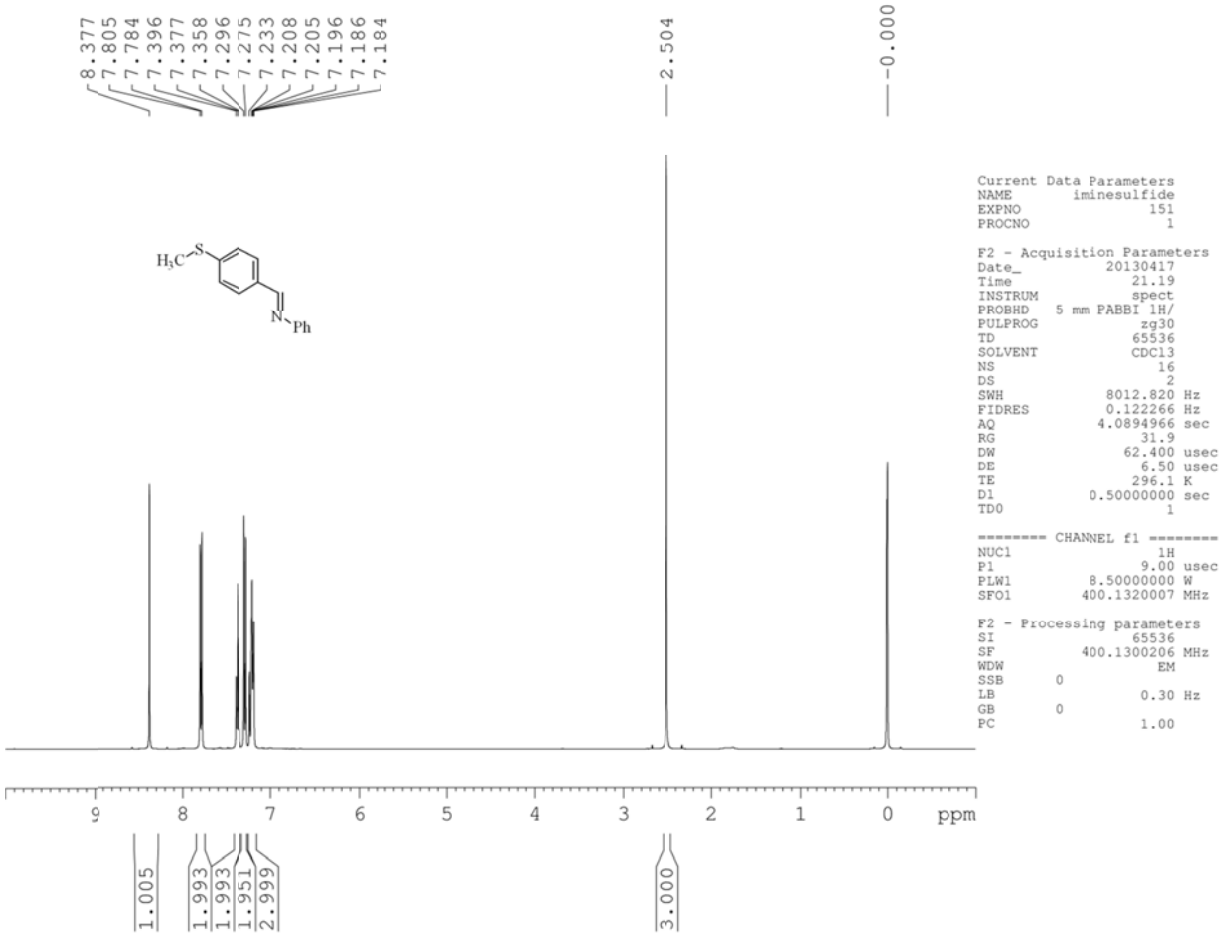


Figure S19: ^{1}H-NMR spectrum of N-(4-(methylthio)benzylidene)aniline

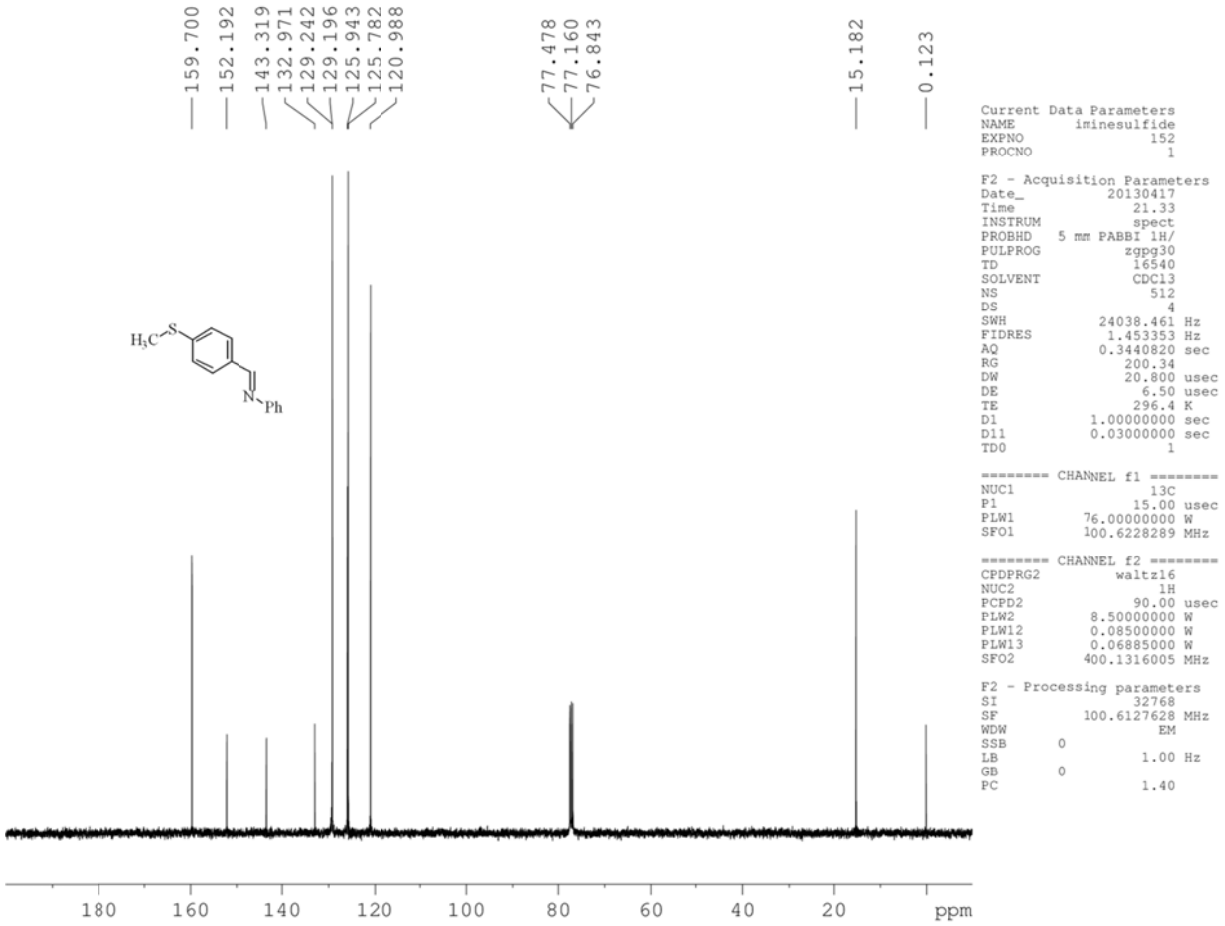
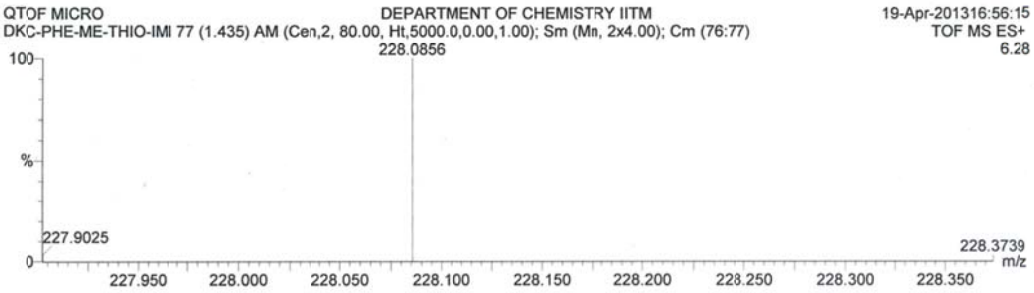


Figure S20: ^{13}C-NMR spectrum of N-(4-(methylthio)benzylidene)aniline

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 200.0 mDa / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
3 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)



Minimum:				-1.5		
Maximum:		200.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
228.0856	228.0847	1.0	4.2	8.5	1	C14 H14 N S

Figure S21:ESI-HRMS of N-(4-(methylthio)benzylidene)aniline

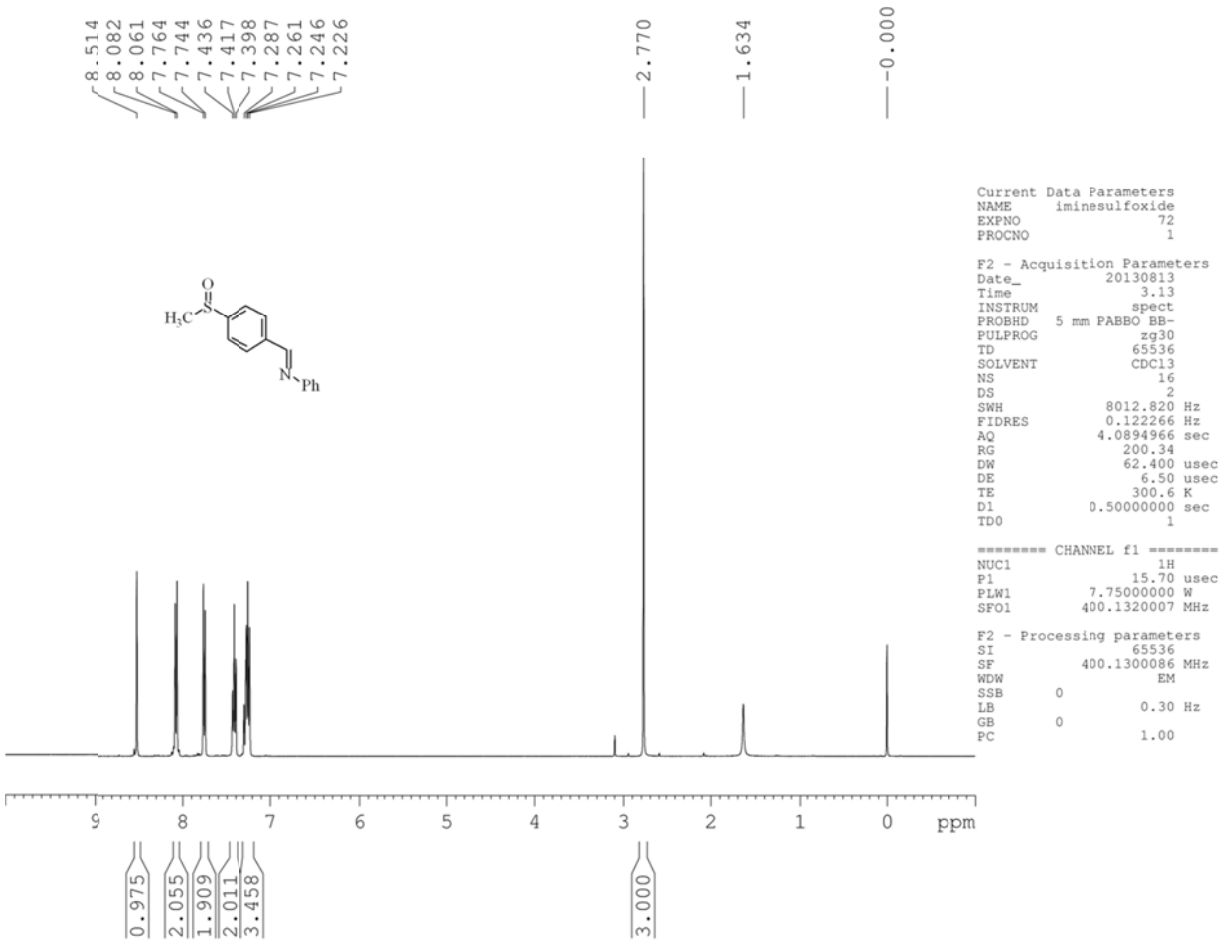


Figure S22: ^{1}H-NMR spectrum of N-(4-(methylsulfinyl)benzylidene)aniline

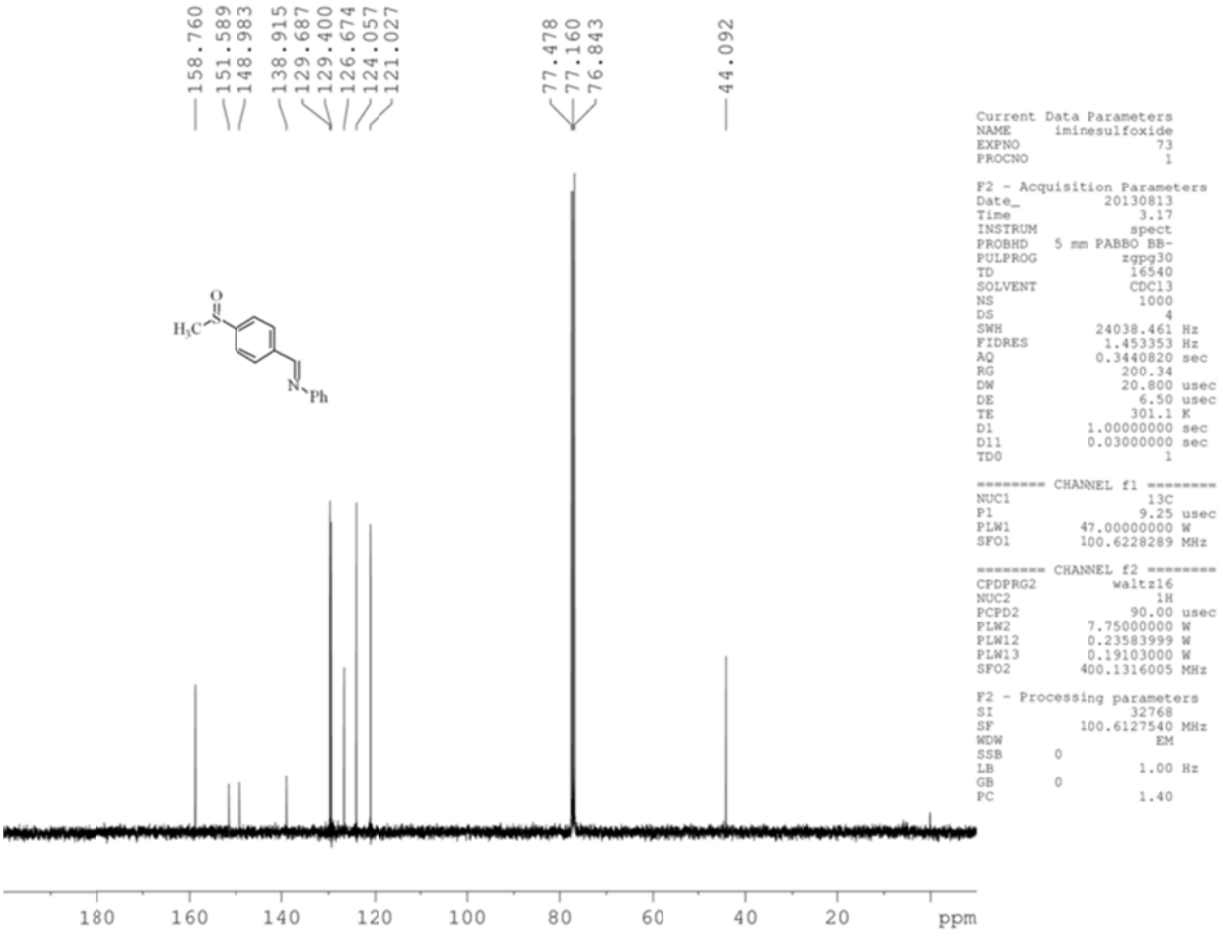


Figure S23: ^{13}C-NMR spectrum of N-(4-(methylsulfinyl)benzylidene)aniline

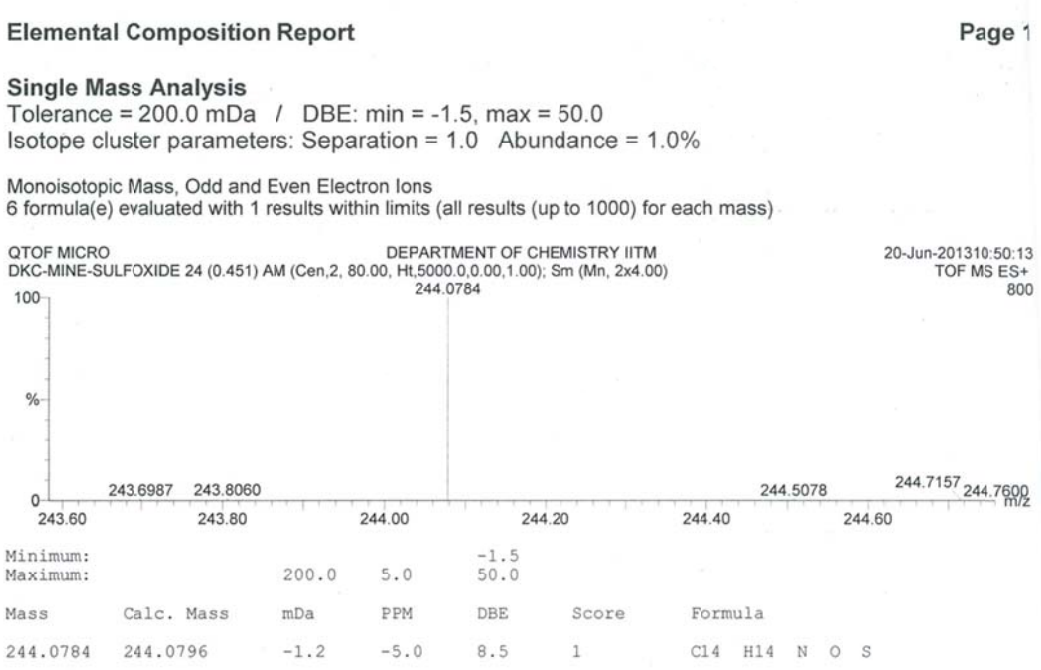


Figure S24:ESI-HRMS of N-(4-(methylsulfinyl)benzylidene)aniline

Determination of critical micelle concentration of $(C_{19}H_{42}N)_2[MoO(O_2)_2(C_2O_4)]\cdot H_2O$

Electrical conductivity method was employed to determine the critical micelle concentration (CMC) of the complex$(C_{19}H_{42}N)_2[MoO(O_2)_2(C_2O_4)]\cdot H_2O$. The conductivity experiments were carried out in a double-jacket flask. The temperature of the flask was maintained at 25 °C by circulating water with Julabo FP50 Refrigerated - Heating Circulators. A SYSTRONICS digital bench top conductivity meter (Model 306) was usedfor the measurements. Solutions were prepared in deionised water which was first filtered with a Millipore Milli-Q system. A step-by-step dilution-extraction method was adopted for the measurements of specific conductance of the complex at various concentrations in order to avoid dilution error.[1]The conductance was plotted as a function of molar concentration and the inflection point gives the value of CMC which is indicated in the **figure S6**.

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1 . (a) A. Jover, F. Meijide, V. Mosquera andJ. V. Tato, *J. Chem. Educ.* 1990, **67**, 530. (b) A. Domínguez, A. Fernández, N. González, E. Iglesias, and L. Montenegro, *J. Chem. Educ.* 1997, **74**, 1227.

Procedure for the recyclability of the catalyst

In a centrifuge tube, molybdenum complex (0.032g, 2.5 mol%) and thioanisole (0.186g, 1.5 mmol) in 2.5 ml of water were taken and stirred at room temperature. Then 40% (w/v) hydrogen peroxide (0.128ml, 1.5 mmol) was added slowly into the reaction mixture.Stirring was continued for 10 min. Reaction progress was monitored by TLC. After completion, ethyl acetate was added to it and the reaction mixture was centrifuged and decanted to separate molybdenum compound. The residual compound obtained was dried and used for second run. The aqueous phase is extracted with ethyl acetate 3-4 times. Then the combined organic extracts were dried over anhydrous sodium sulfate and the solvent was removed under reduced pressure. The crude product thus obtained was purified by column chromatography with Hexane: Ethyl acetate as an eluent.

For the second run: To the residual catalyst in the centrifuge tube, 2.5 ml of water and hydrogen peroxide (0.128ml, 1.5 mmol) was added. The mixture was stirred for 30 min to activate the catalyst. Then thioanisole (0.186g, 1.5 mmol) was added and stirring was continued for 45 min. Reaction progress was monitored by TLC. After completion, ethyl acetate was added to it and the reaction mixture was centrifuged and decanted to separate molybdenum compound. The residual compound was dried and used for the subsequent cycle.

After 4 run, 0.013g of catalyst was recovered. So in each run, on an average of 81 % catalysts can be recovered.