

Electronic Supplementary Information

Selective oxidation of organic sulfides to sulfoxides using sugar derived *cis*-dioxo molybdenum(VI) complexes: it's kinetic and mechanistic studies

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1. Characterization data of sulfoxides

1.1 Diphenyl sulfoxide (**SO2**)

White crystal; m.p. 68-70 °C; IR (KBr; cm⁻¹): 1041 (ν_{S=O}); ¹H NMR (CDCl₃, 400 MHz, ppm): δ 7.65 (4H, m, ArH), 7.46 (6H, m, ArH) ¹³C NMR (100 MHz, CDCl₃, ppm): δ 145.8, 131.2, 129.5, 125.0; ESI-MS: *m/z* calcd for (M+H)⁺ C₁₂H₁₁OS 203.05; found 203.11.

1.2 Benzyl phenyl sulfoxide (**SO3**)

White crystal; m.p. 124-126 °C; IR (KBr; cm⁻¹): 1034 (ν_{S=O}). ¹H NMR (CDCl₃, 400 MHz, ppm): δ 7.41 (5H, m, ArH), 7.24 (3H, m, ArH) 6.99 (2H, m, ArH), 4.0 (2H, m, SOCH₂) ¹³C NMR (100 MHz, CDCl₃, ppm): δ 142.8, 131.1, 130.3, 129.1, 128.8, 128.4, 128.2, 124.4, 63.5; ESI-MS: *m/z* calcd for (M+H)⁺ C₁₃H₁₃OS 217.07; found 216.93.

1.3 2-(Phenylsulfinyl)aniline (**SO4**)

Brown liquid; IR (KBr; cm⁻¹): 1018 (ν_{S=O}). ¹H NMR (CDCl₃, 400 MHz, ppm): δ 7.58 (2H, m, ArH), 7.44 (4H, m, ArH) 7.25 (1H, m, ArH) 6.78 (1H, m, ArH), 6.59 (1H, m, ArH), 4.94 (2H, br, NH₂) ¹³C NMR (100 MHz, CDCl₃, ppm): δ 147.6, 143.2, 133.0, 130.3, 128.9, 128.4, 124.7, 123.5, 117.6, 117.2; ESI-MS: *m/z* calcd for (M+H)⁺ C₁₂H₁₂NOS 218.06; found 218.05.

2. Spectroscopic data

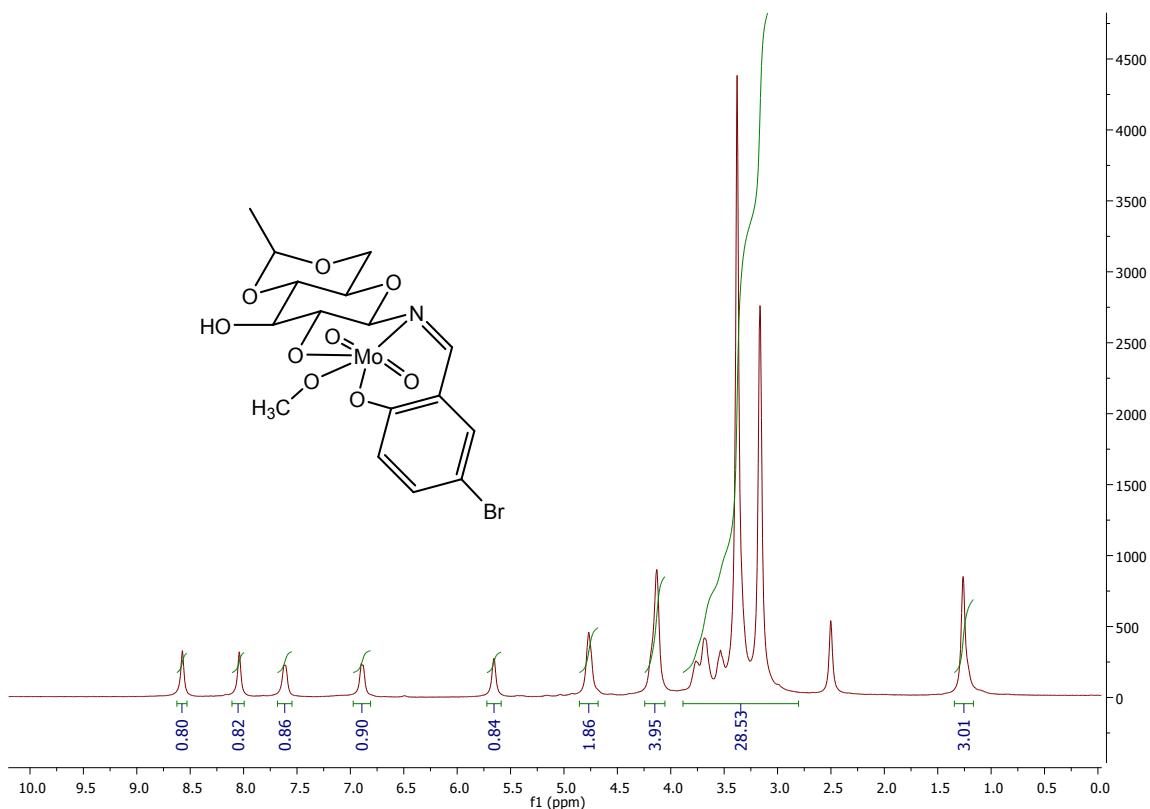


Fig. S1: ^1H NMR of complex **5** recorded in DMSO-d_6 (400 MHz)

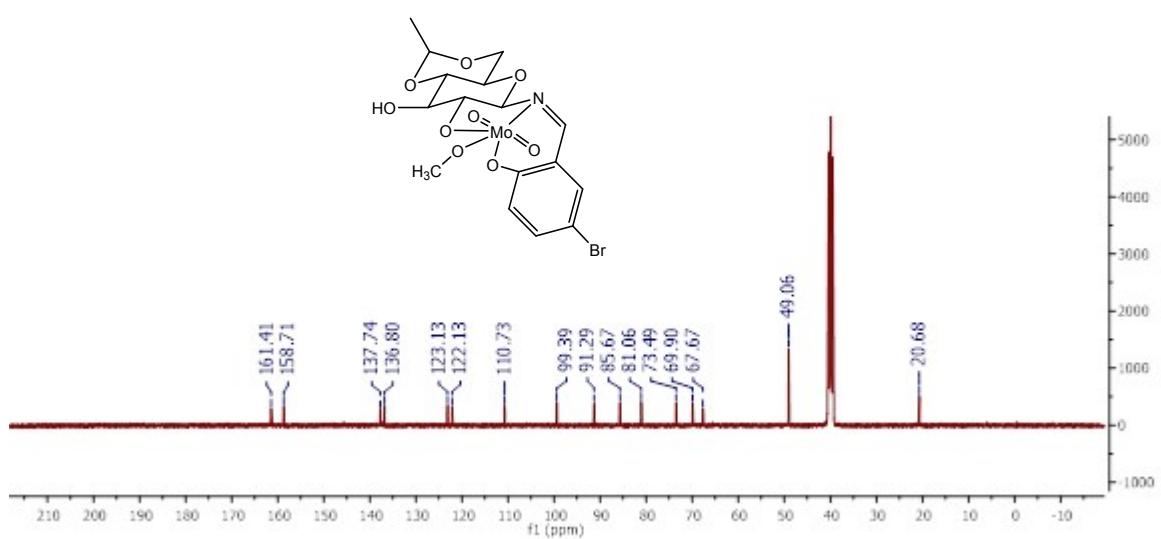


Fig. S2: ^{13}C NMR of complex **5** recorded in DMSO-d_6 (100 MHz)

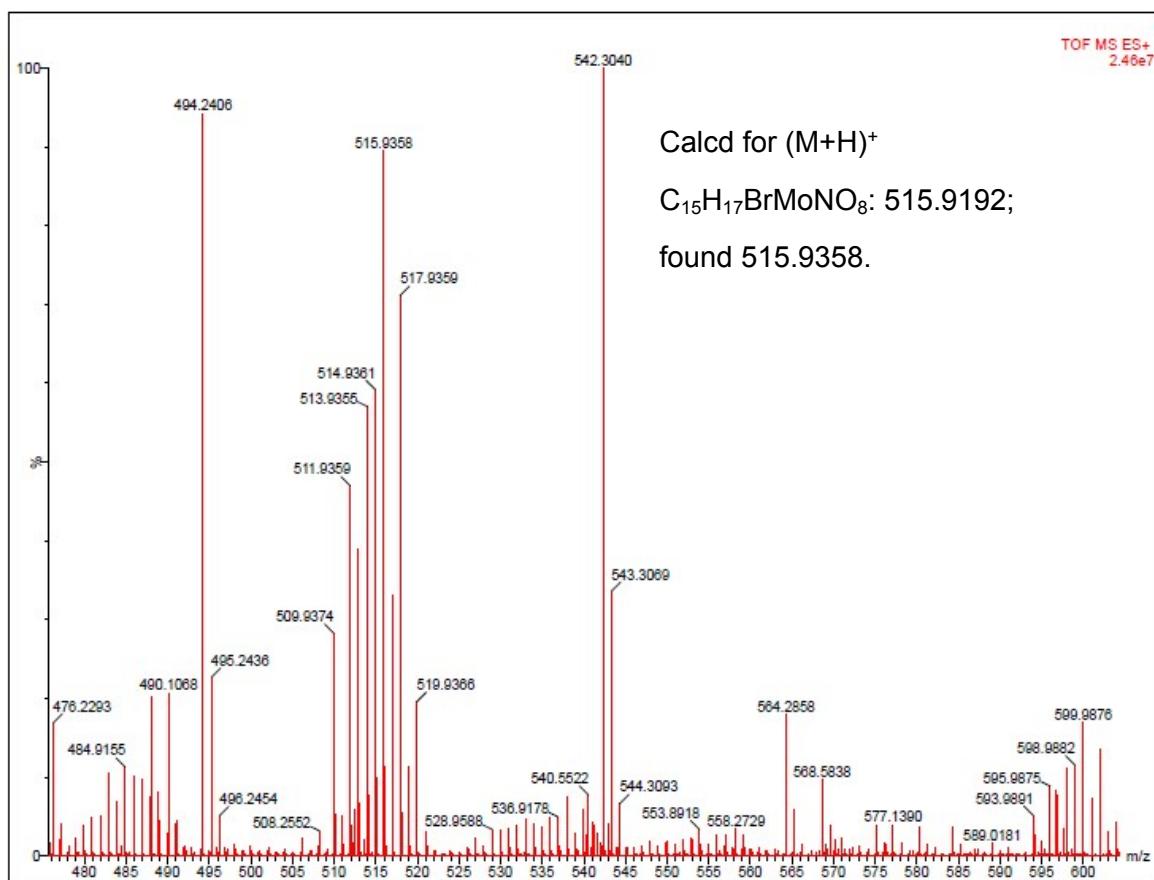


Fig. S3: HRMS of complex 5

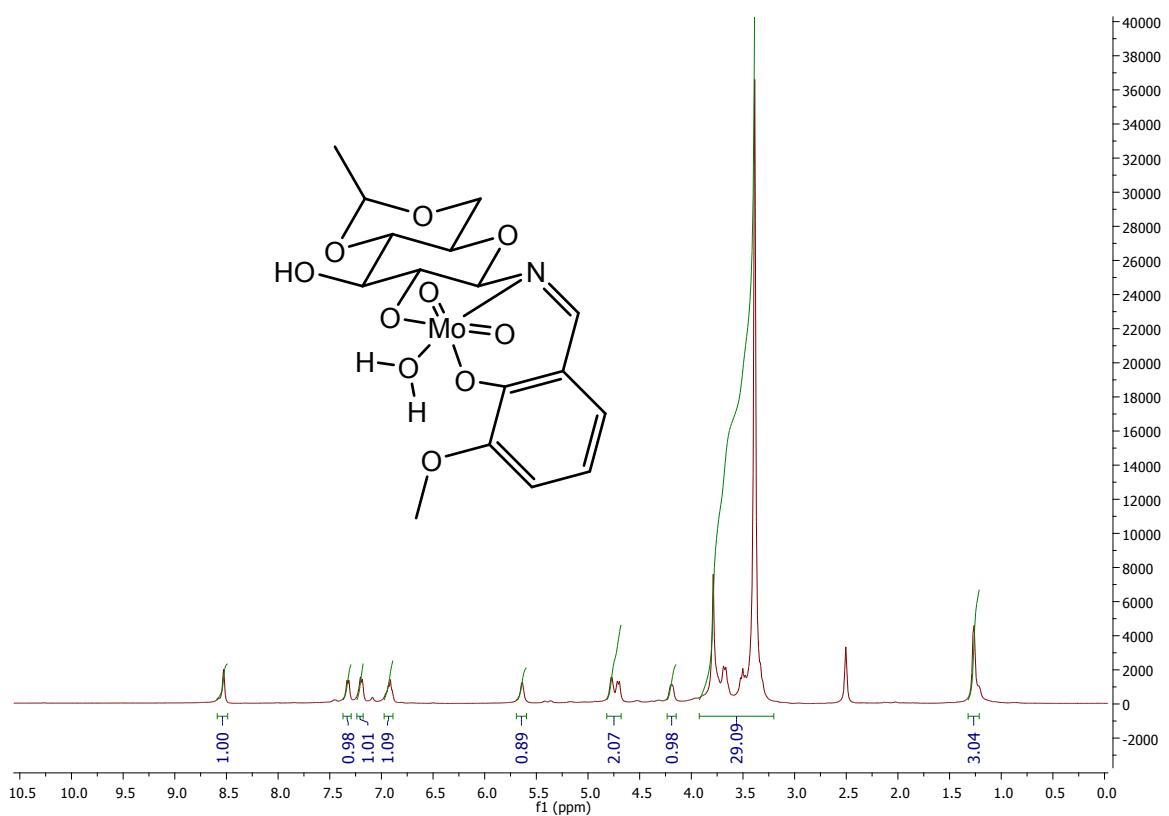


Fig. S4: ^1H NMR of complex **6** recorded in DMSO-d_6 (400 MHz)

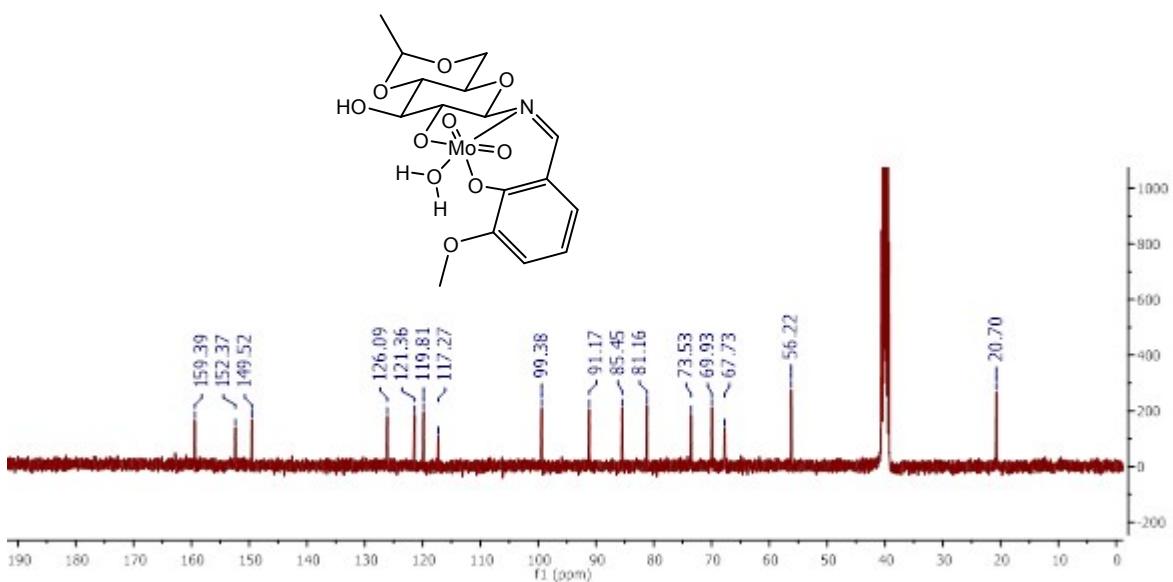


Fig. S5: ^{13}C NMR of complex **6** recorded in DMSO-d_6 (100 MHz)

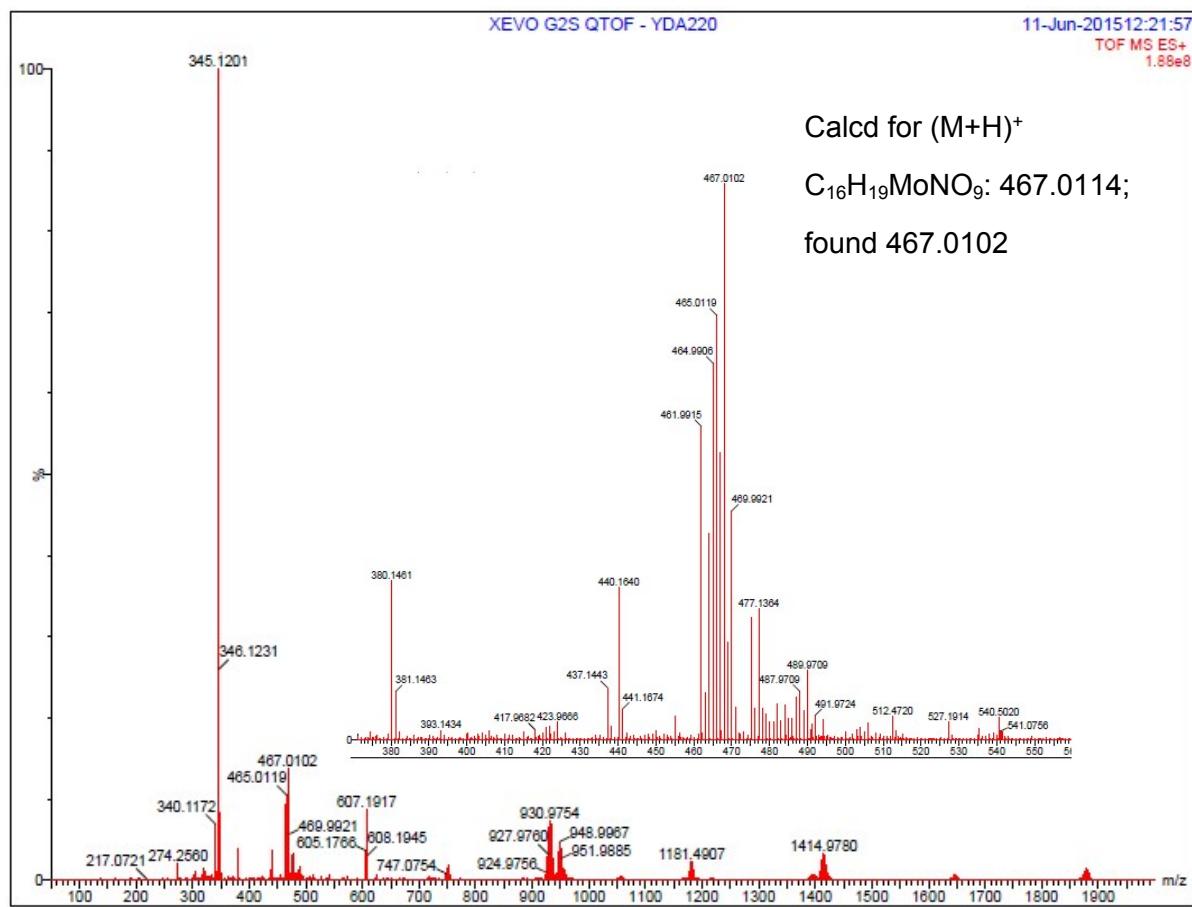
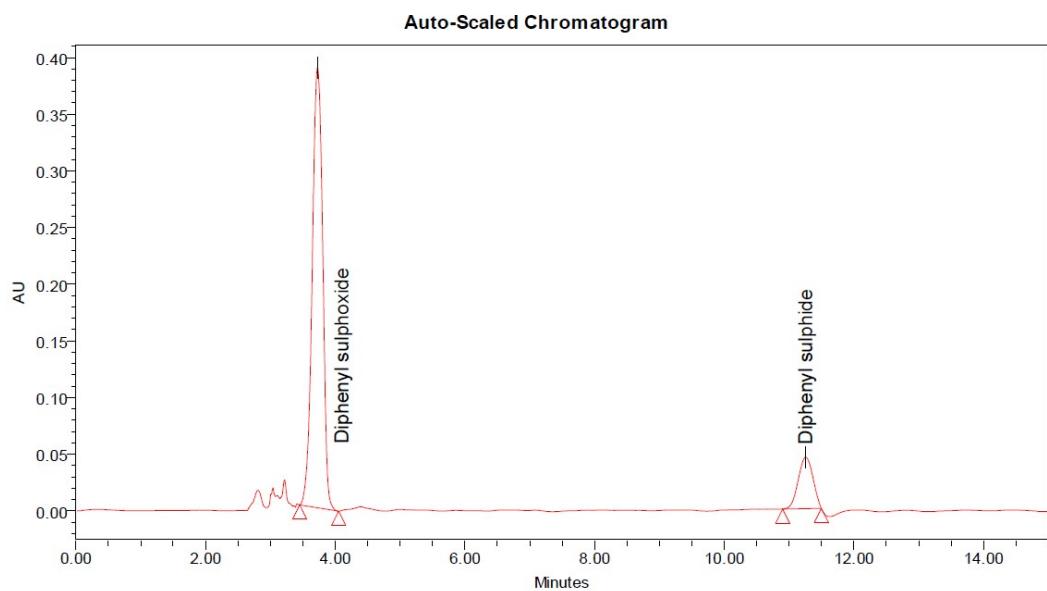
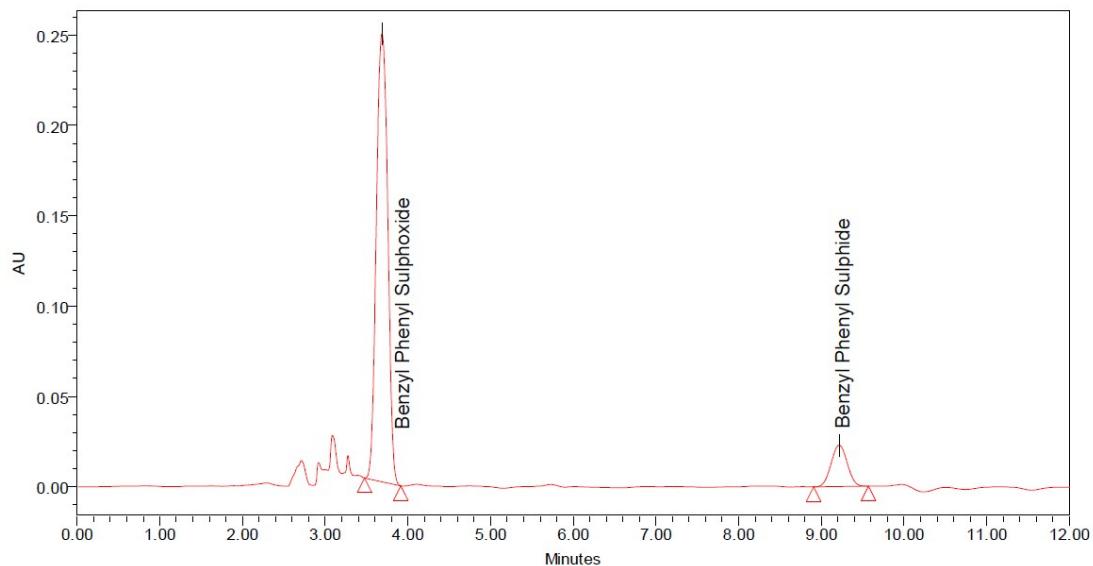


Fig. S6: HRMS of complex 6



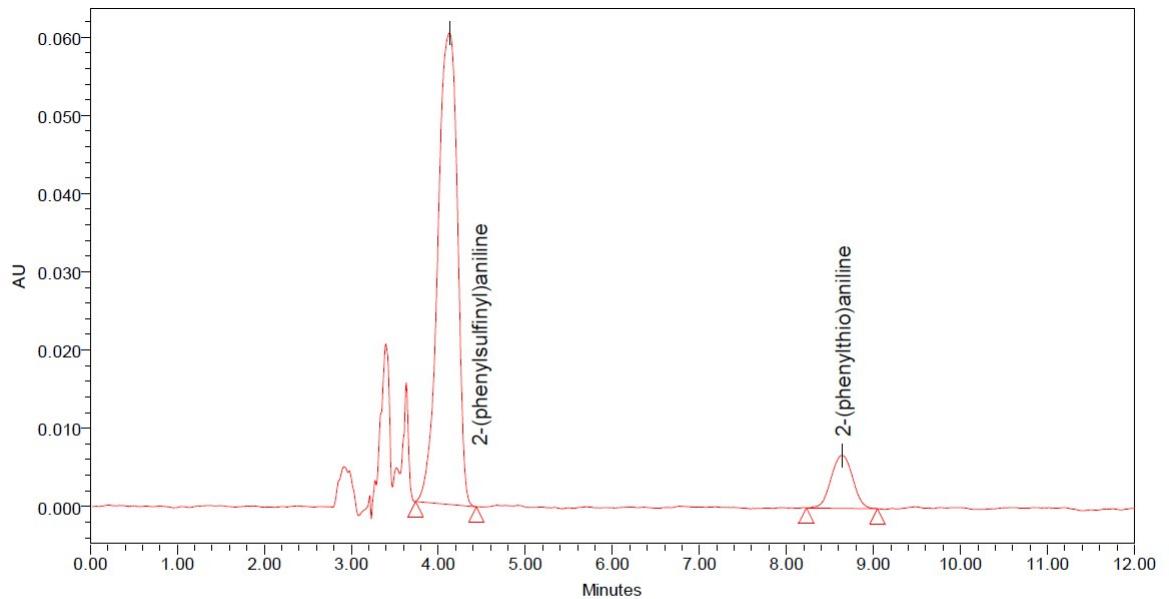
Peak Results							
	Name	Peak Label	RT	Area	Height	% Area	Processed Channel Descr.
1	Diphenyl Sulfoxide	Diphenyl Sulfoxide	3.727	4363479	388417	85.94	PDA 242.0 nm
2	Diphenyl Sulfide	Diphenyl Sulfide	11.257	713624	45435	14.06	PDA 242.0 nm

Fig. S7: Representative HPLC of diphenyl sulfoxide (**SO2**), formed from catalyst **5**; (peaks in the range of 2.5-3.5 RT are from the blank)



Peak Results							
	Name	Peak Label	RT	Area	Height	% Area	Processed Channel Descr.
1	BENZYLPHENYLSULFOXIDE	BENZYLPHENYLSULFOXIDE	3.687	2379131	247949	88.45	PDA 250.0 nm
2	BENZYL PHENYL SULFIDE	BENZYL PHENYL SULFIDE	9.215	310775	22938	11.55	PDA 250.0 nm

Fig. S8: Representative HPLC of benzyl phenyl sulfoxide (**SO3**), formed from catalyst **1**; (peaks in the range of 2.5-3.5 RT are from the blank)



Peak Results

	Name	Peak Label	RT	Area	Height	% Area	Processed Channel Descr.
1	2-(phenylsulfinyl)aniline	2-(phenylsulfinyl)aniline	4.128	939724	60275	88.94	PDA 315.0 nm
2	2-(phenylthio)aniline	2-(phenylthio)aniline	8.638	116843	6787	11.06	PDA 315.0 nm

Fig. S9: Representative HPLC of 2-(phenylsulfinyl)aniline (**S04**), formed from catalyst **3**; (peaks in the range of 2.5-3.5 RT are from the blank)

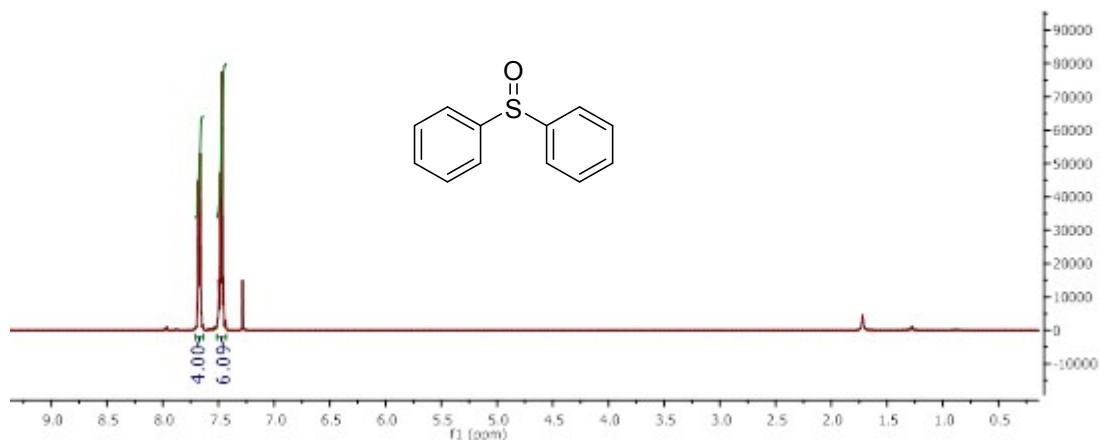


Fig. S10: ^1H NMR of **SO2** recorded in CDCl_3 (400 MHz)

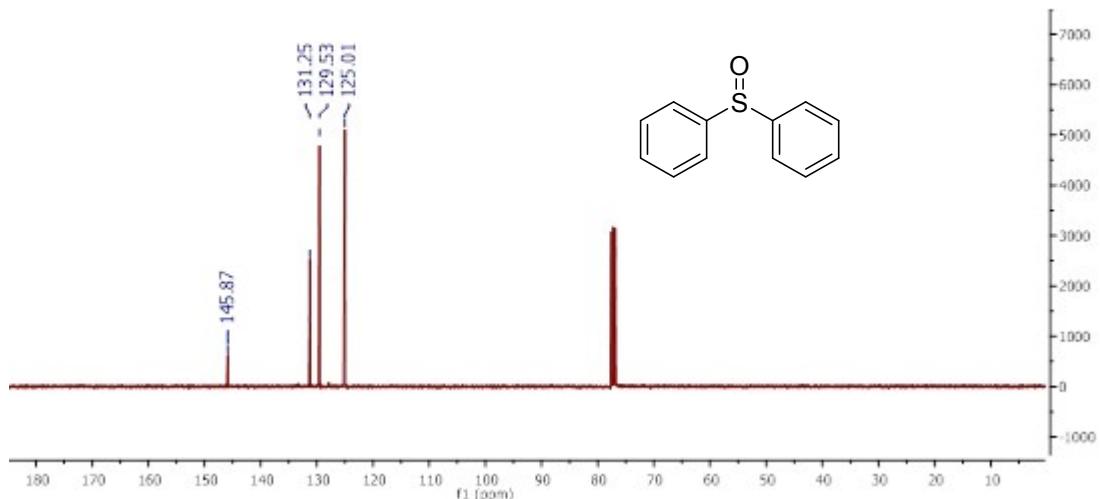


Fig. S11: ^{13}C NMR of **SO2** recorded in CDCl_3 (100 MHz)

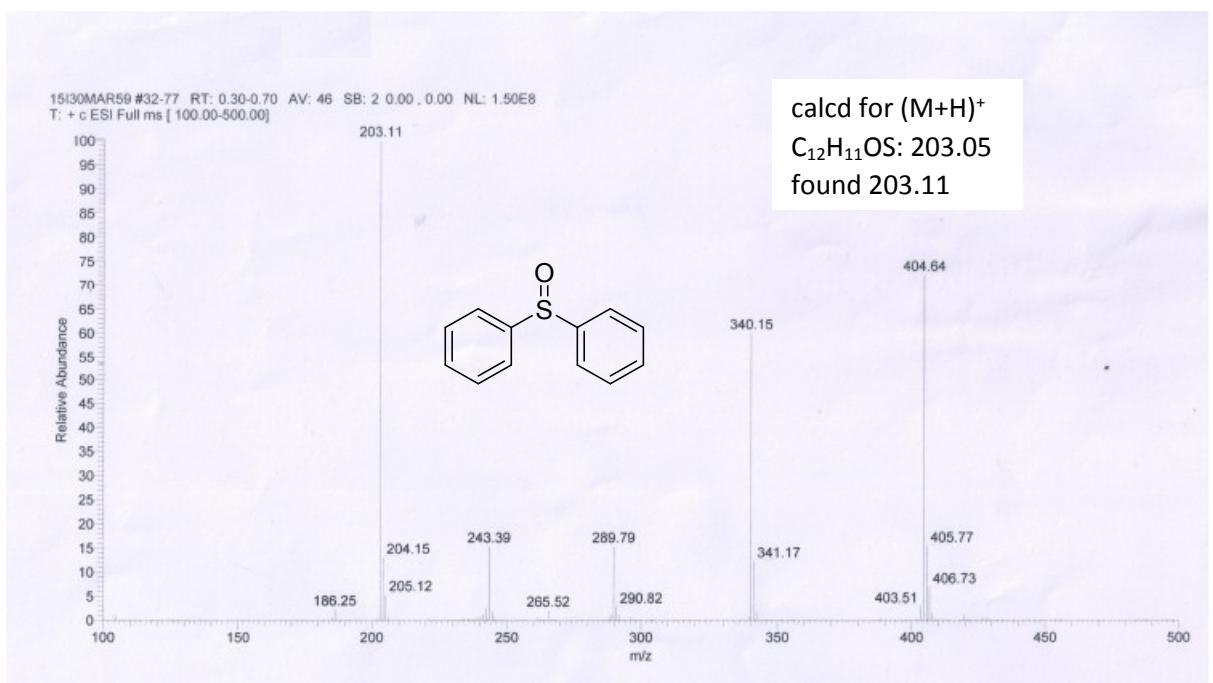


Fig. S12: ESI-MS of **SO2**

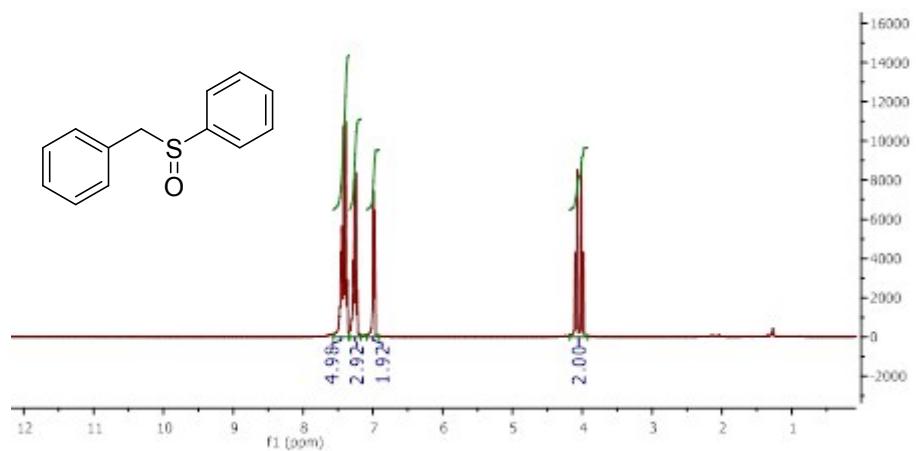


Fig. S13: 1H NMR of **SO3** recorded in $CDCl_3$ (400 MHz)

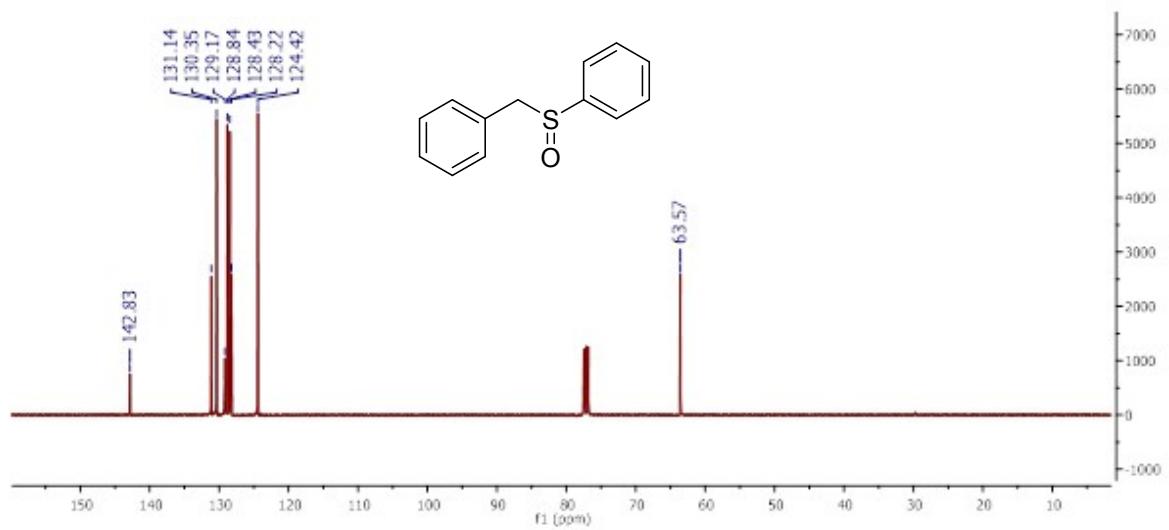


Fig. S14: ^{13}C NMR of **SO3** recorded in CDCl_3 (100 MHz)

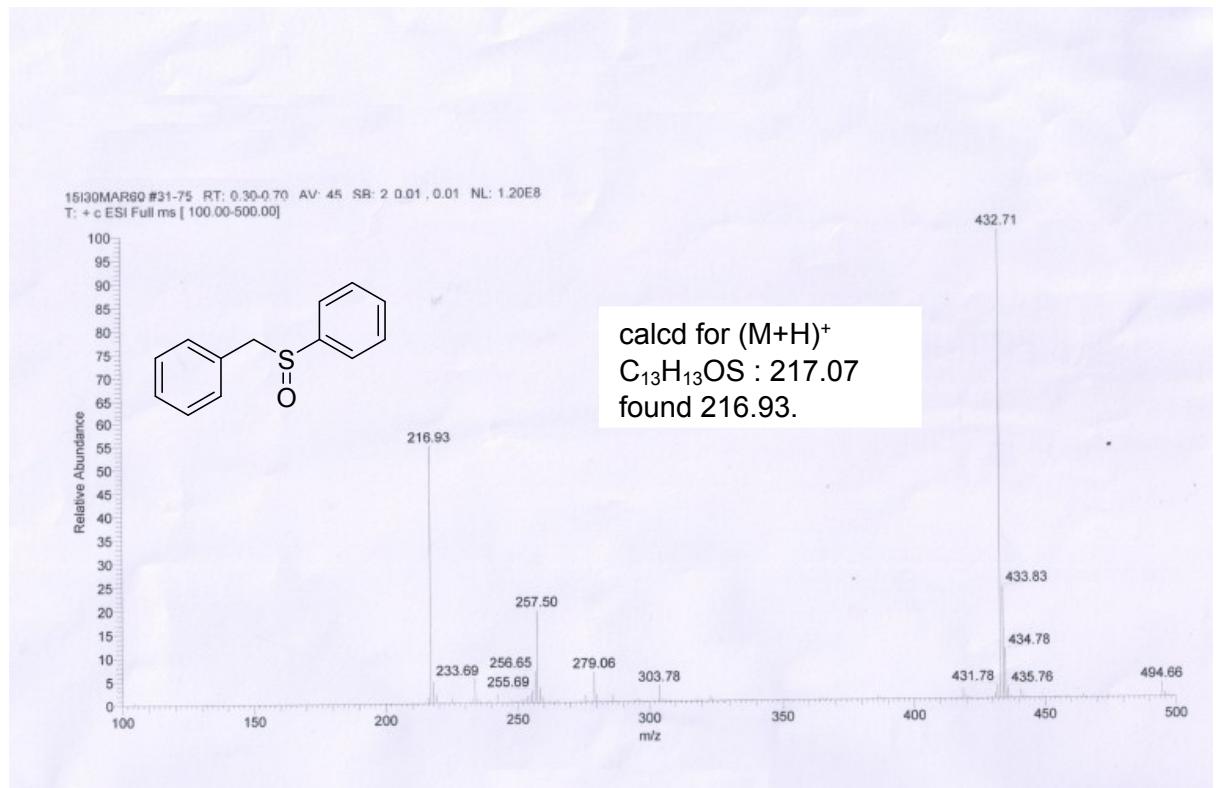


Fig. S15: ESI-MS of **SO3**

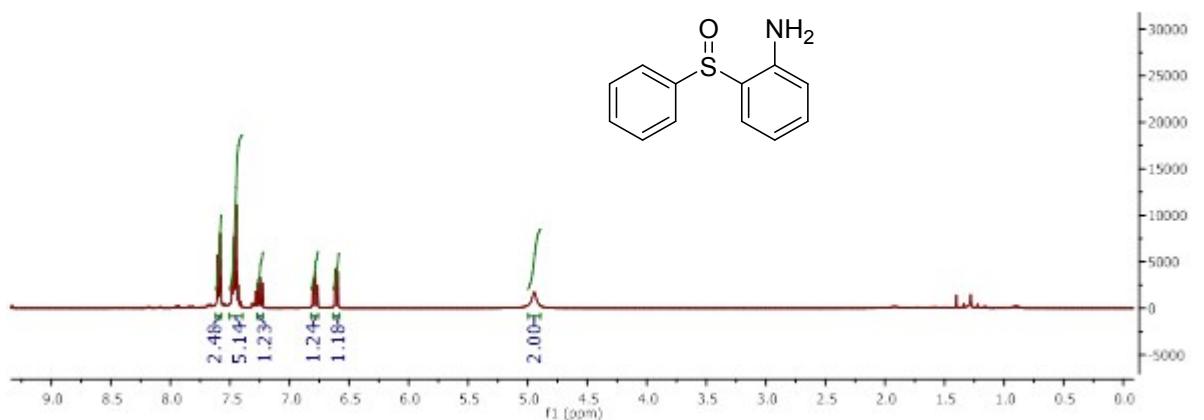


Fig. S16: ¹H NMR of **SO4** recorded in CDCl_3 (400 MHz)

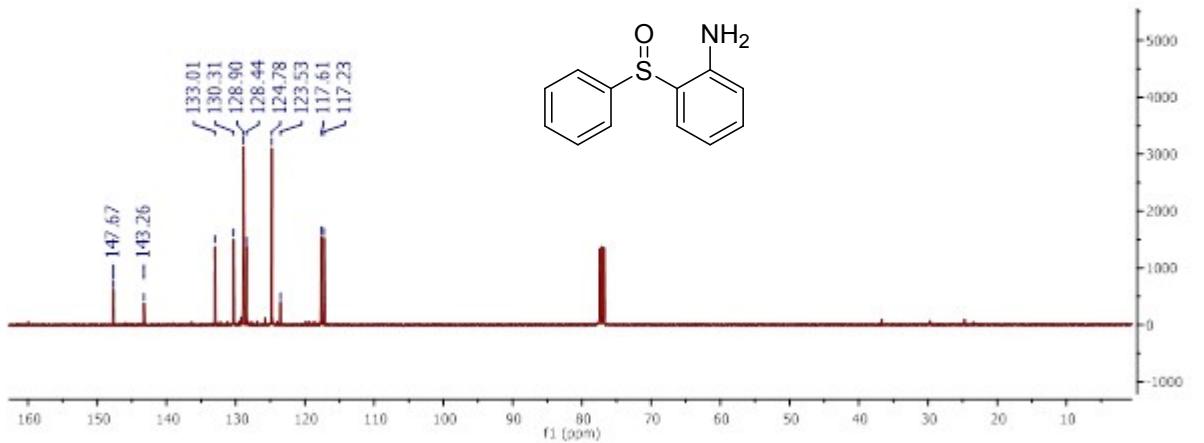


Fig. S17: ¹³C NMR of **SO4** recorded in CDCl_3 (100 MHz)

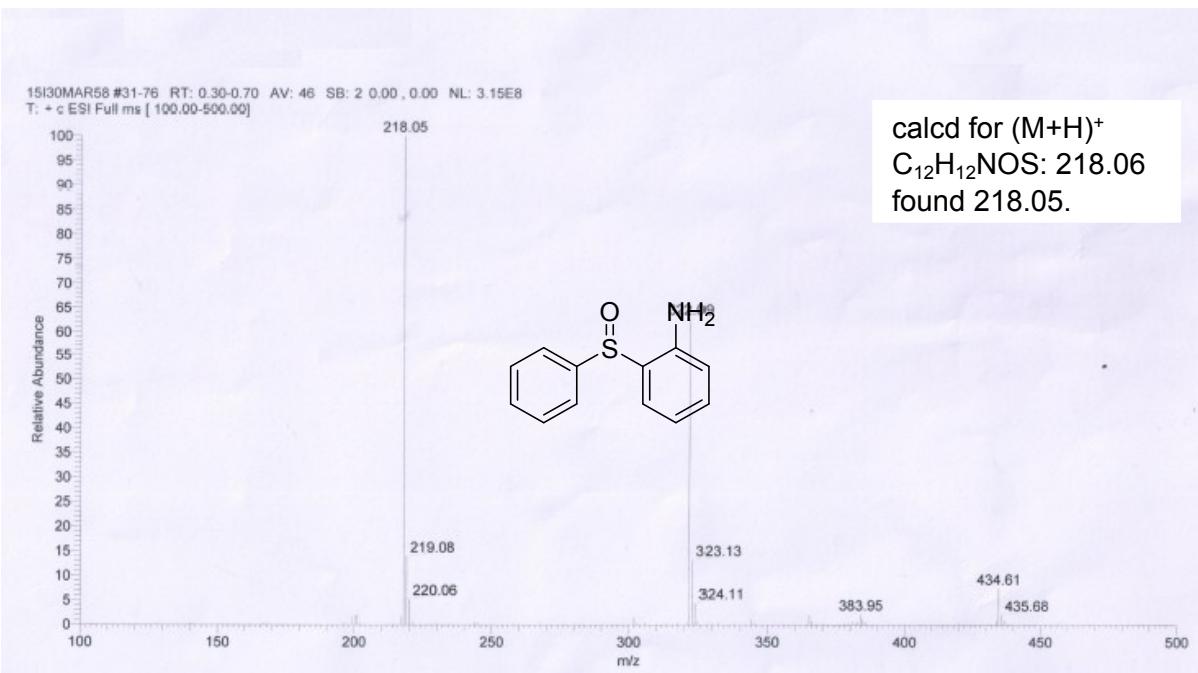


Fig. S18: ESI-MS of **S4**

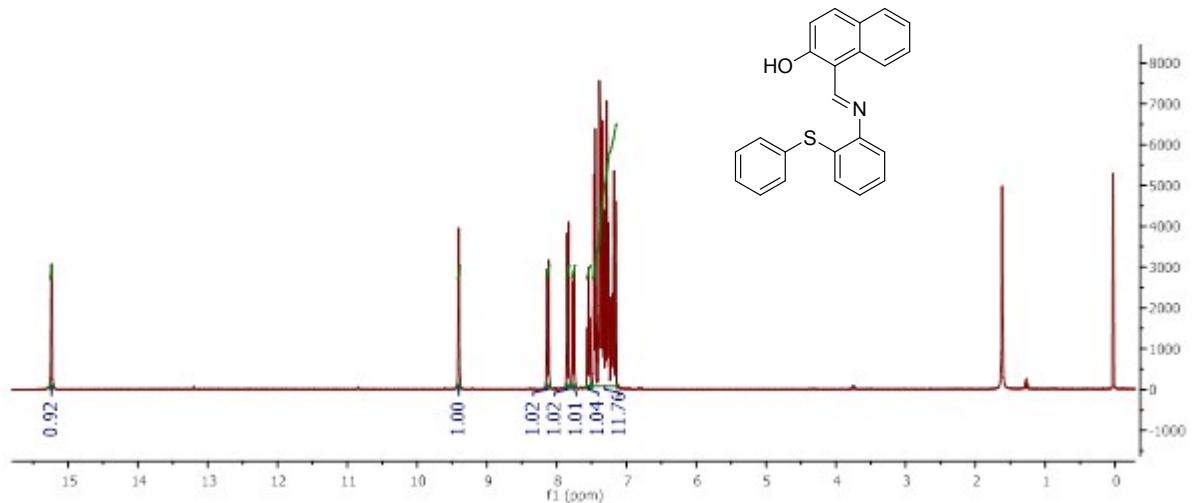


Fig. S19: 1H NMR of **S5** recorded in $CDCl_3$ (400 MHz)

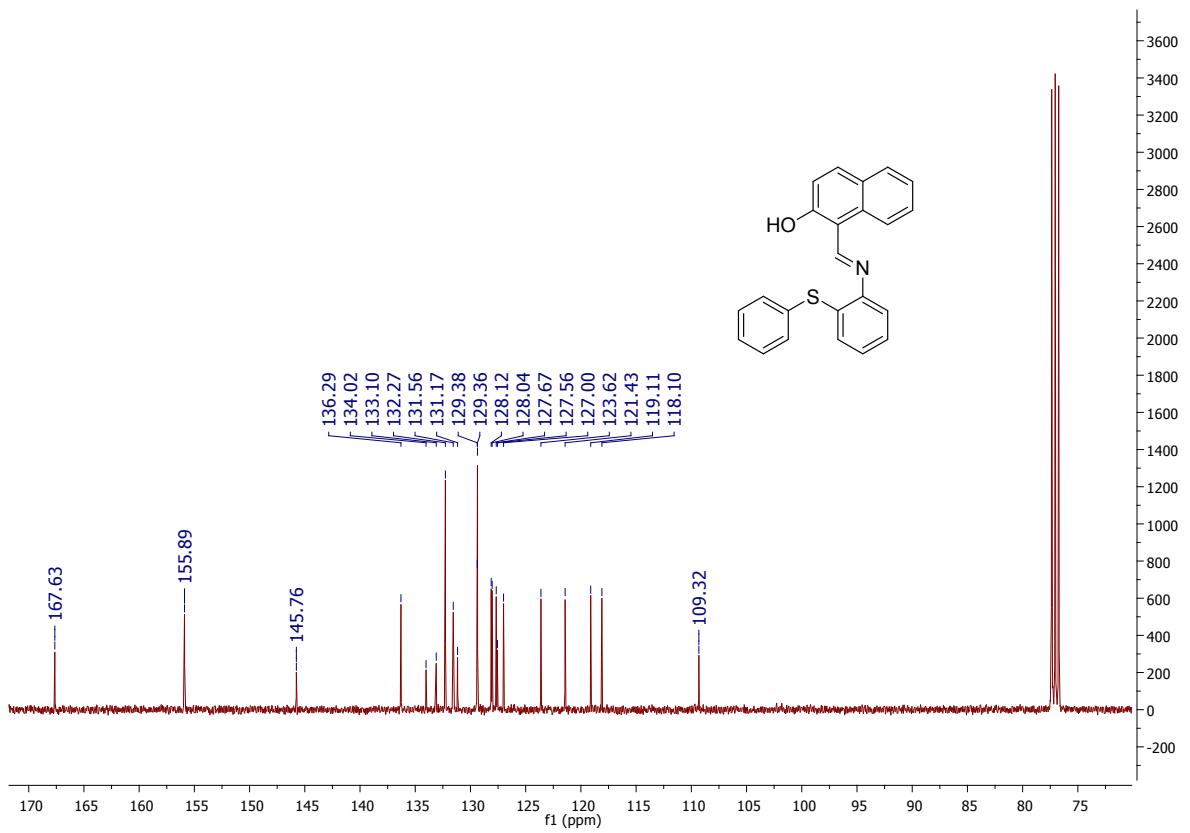


Fig. S20: ^{13}C NMR of **S5** recorded in CDCl_3 (100 MHz)

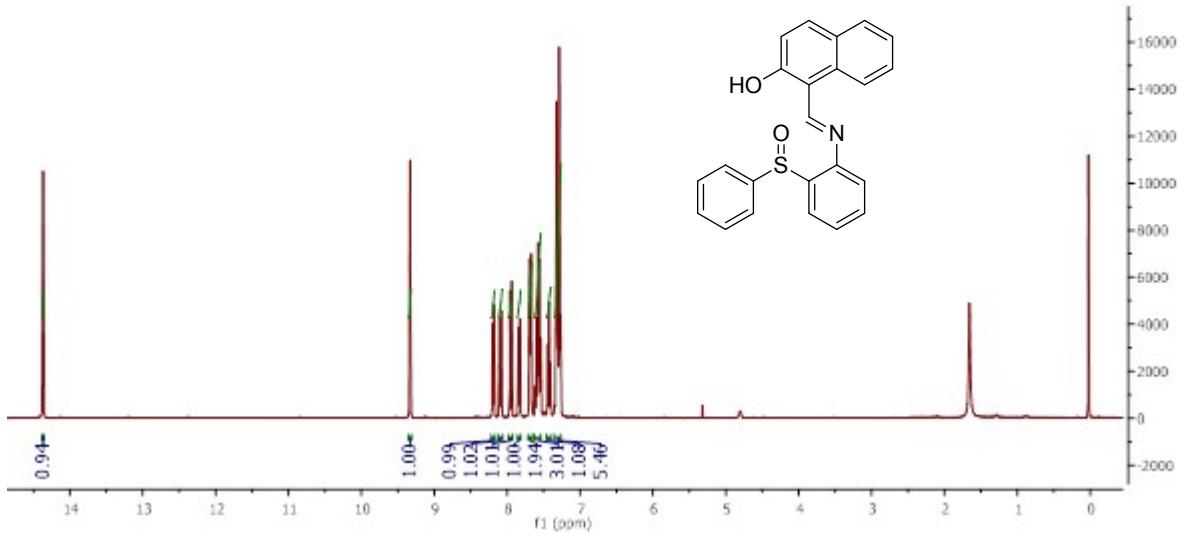


Fig. S21: ^1H NMR of **S05** recorded in CDCl_3 (400 MHz)

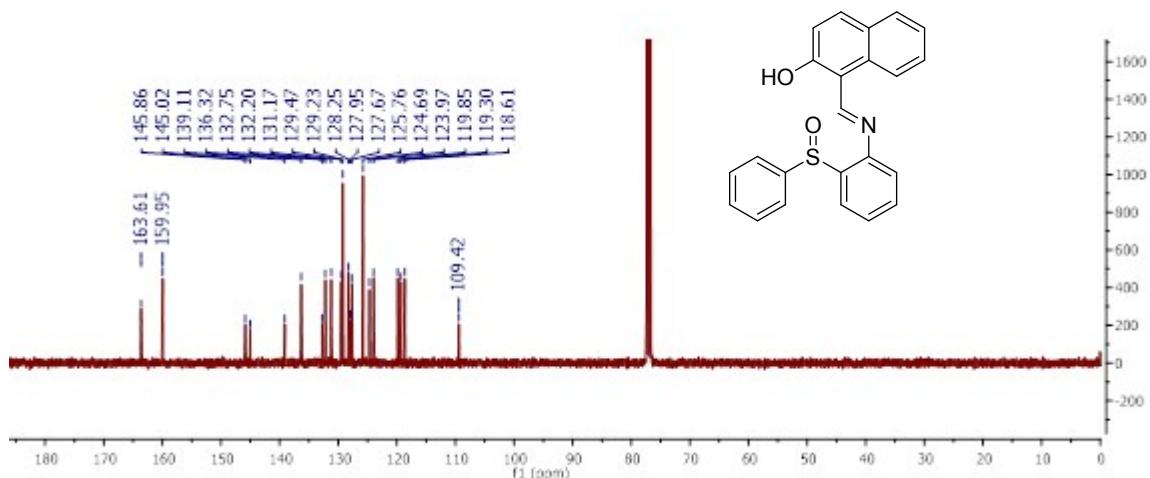


Fig. S22: ^{13}C NMR of **SO5** recorded in CDCl_3 (100 MHz)

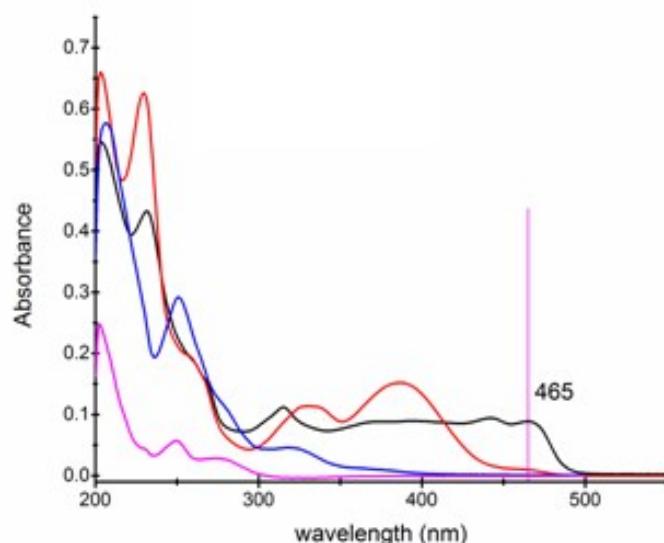


Fig. S23: Comparative UV-visible absorption spectra of reactants **(S5)** (black), **(SO5)** (red), complex **1**(blue), UHP (pink)

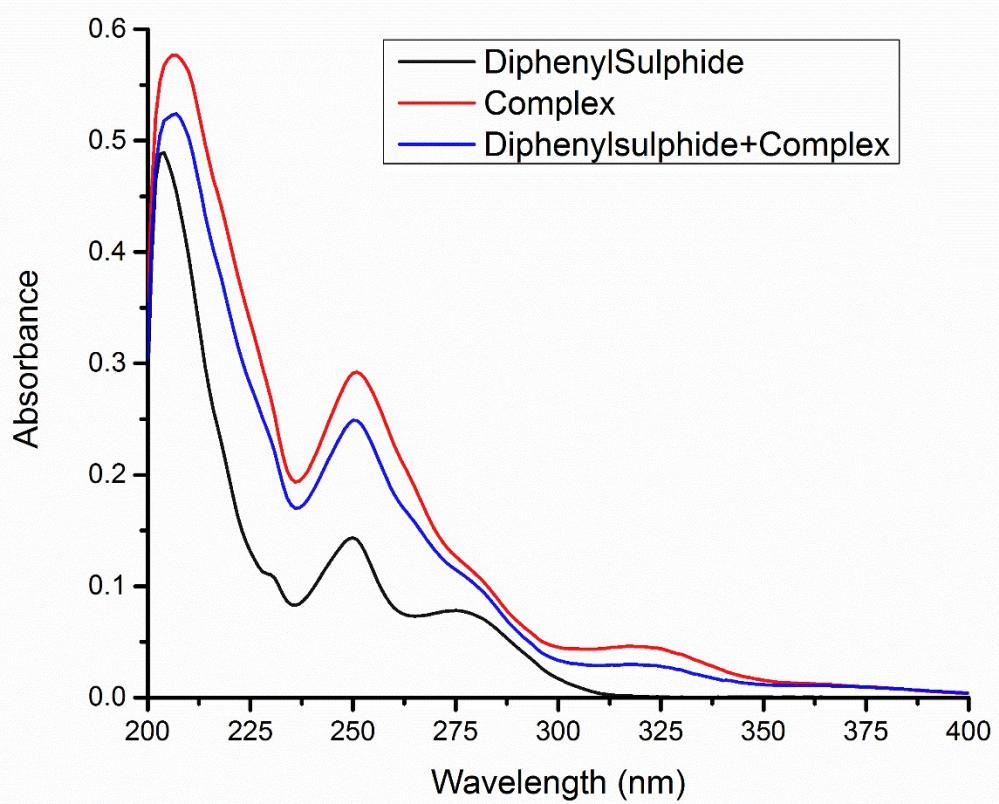


Fig. S24: UV-Vis spectrum of diphenyl sulphide (**S2**) [10^{-5} M], Complex **1** [10^{-5} M] and mixture of **S2** and complex **1**

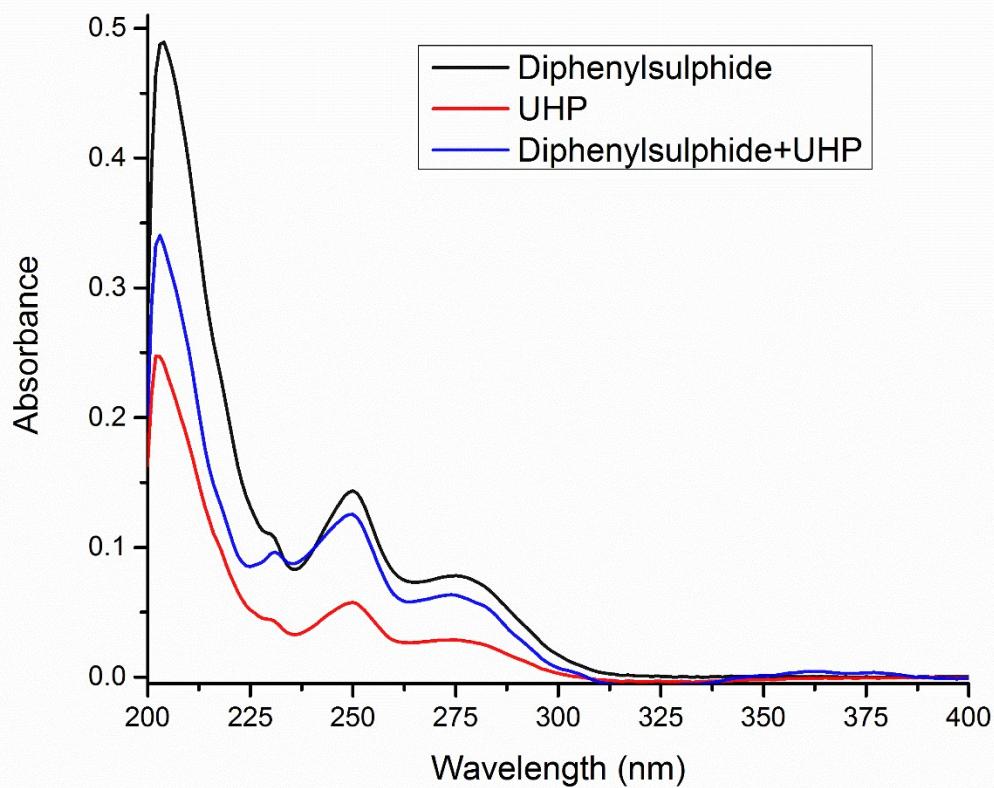


Fig. S25: UV-Vis spectrum of Diphenylsulfide (**S2**) [10^{-5} M], **UHP** [10^{-5} M] and mixture of **S2** and **UHP**

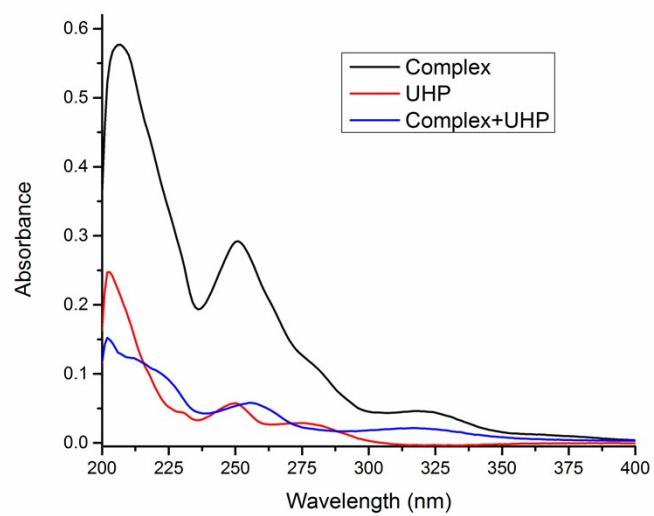


Fig. S26: Absorption spectra of complex **1** [10^{-5} M], UHP [10^{-5} M] and mixture of UHP and complex