Electronic Supporting Information (ESI)

Quantum Yield Calculation

Theoretical results for **HL** using LANL2DZ basis set

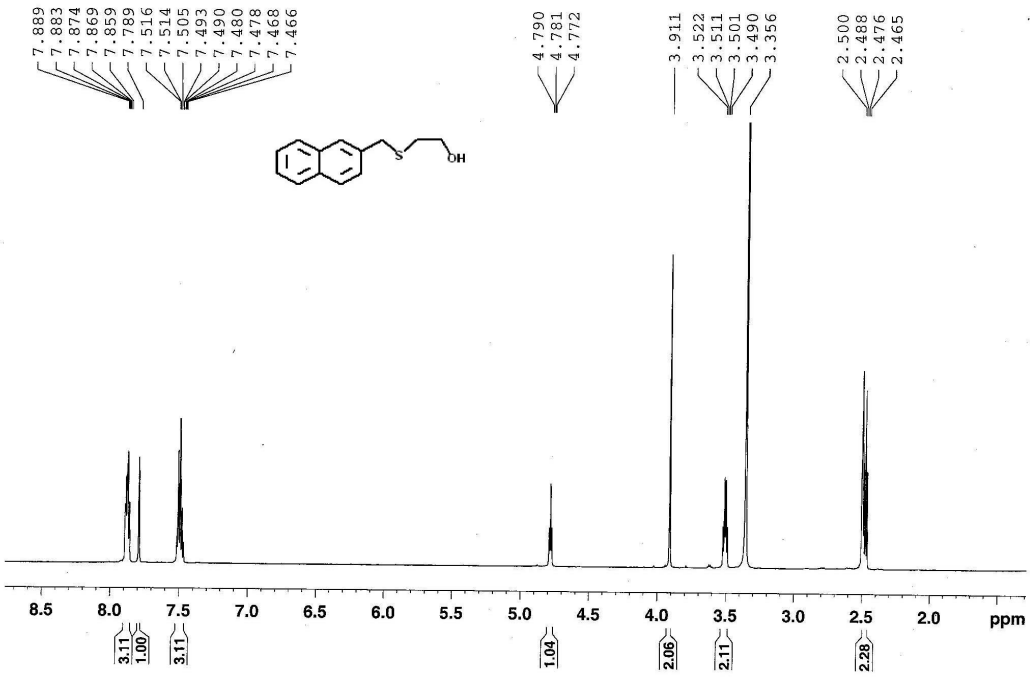


Figure S1a

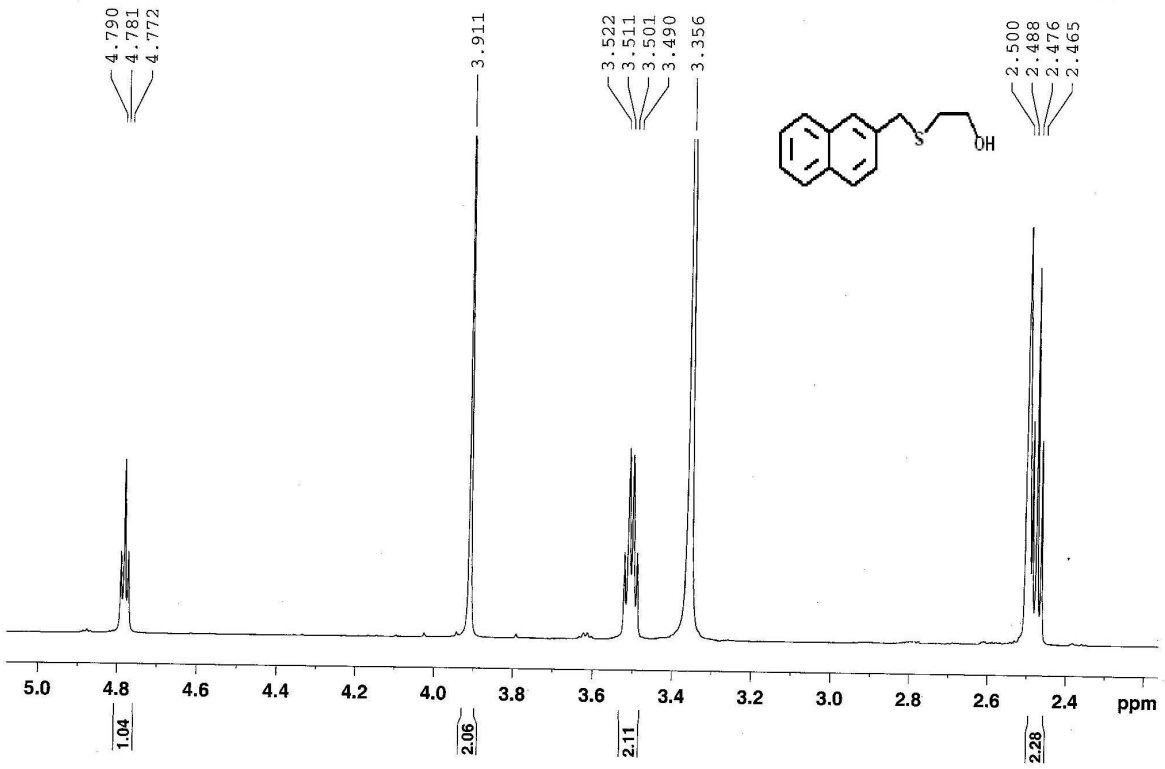


Figure S1b

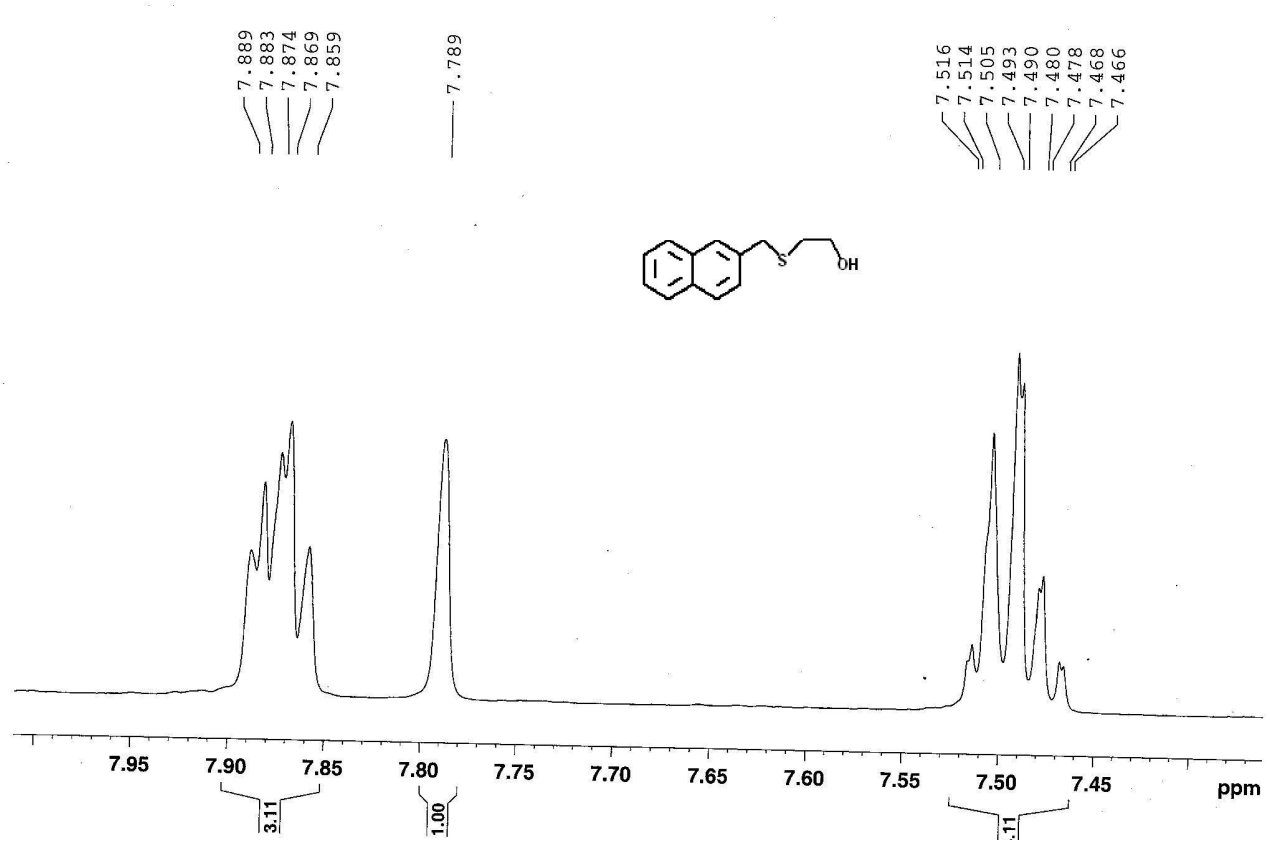
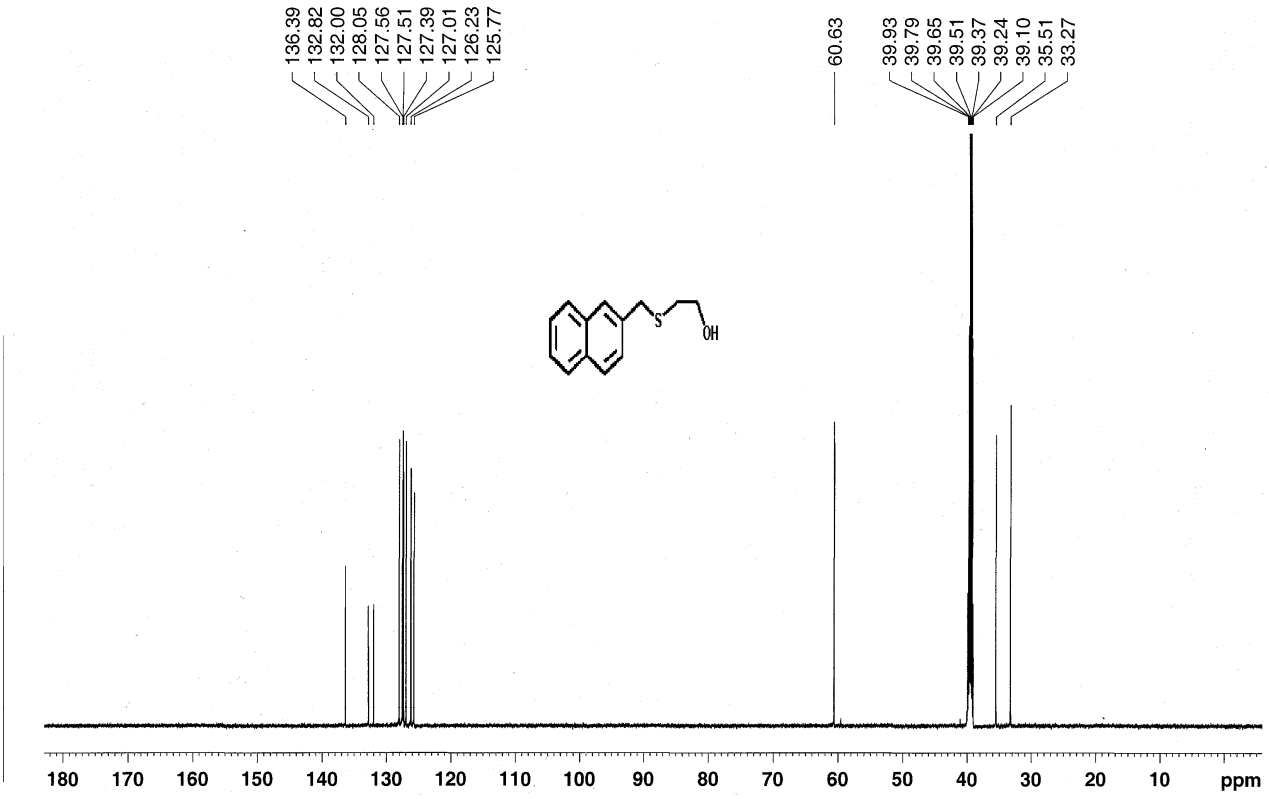


Figure S1c



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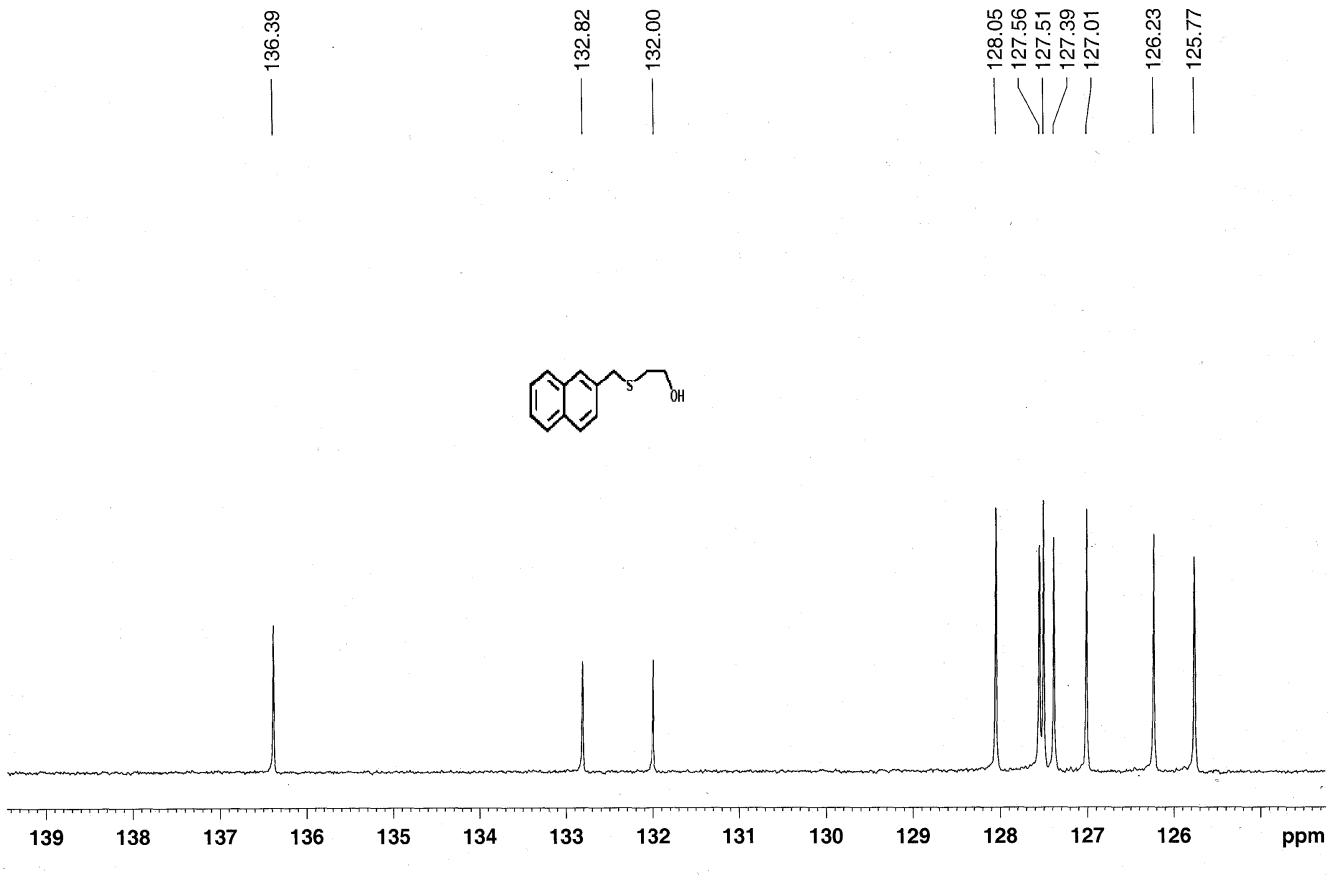

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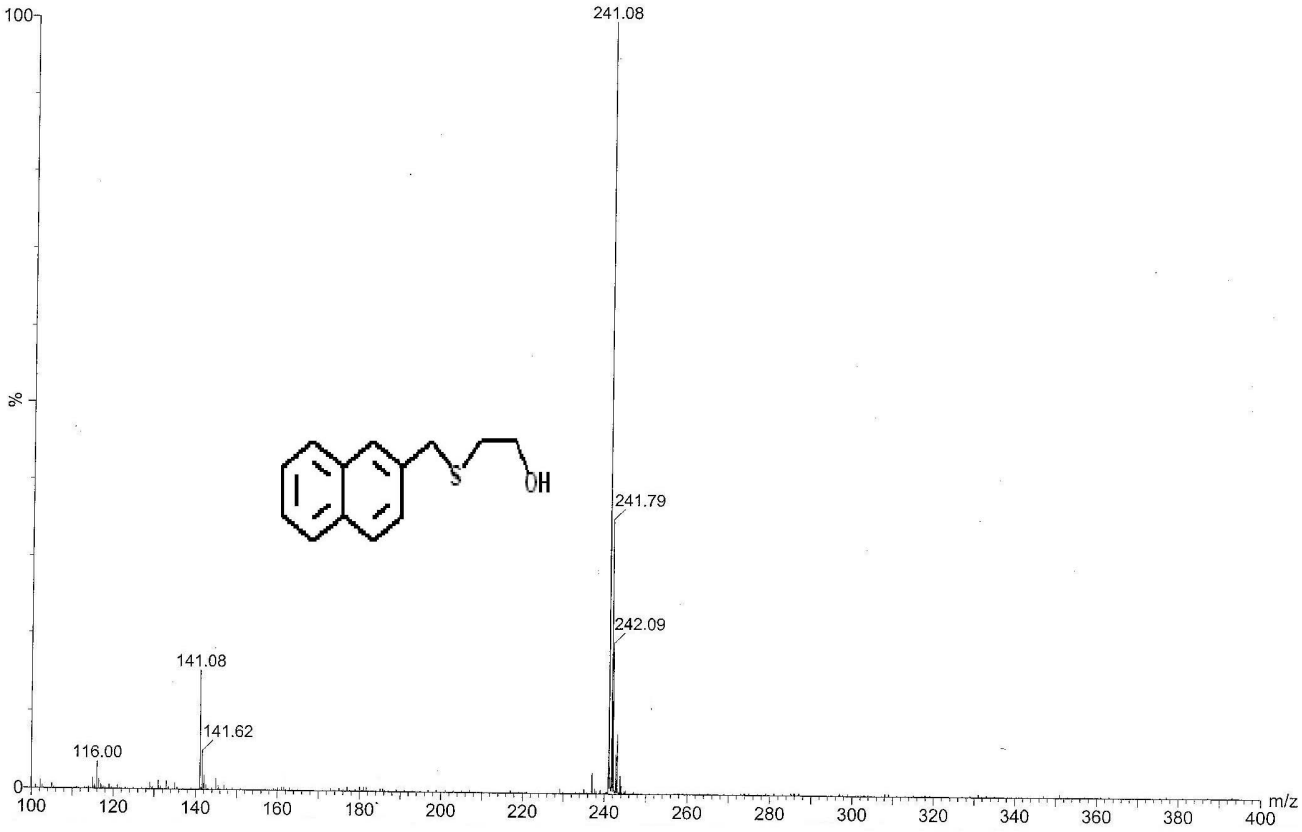

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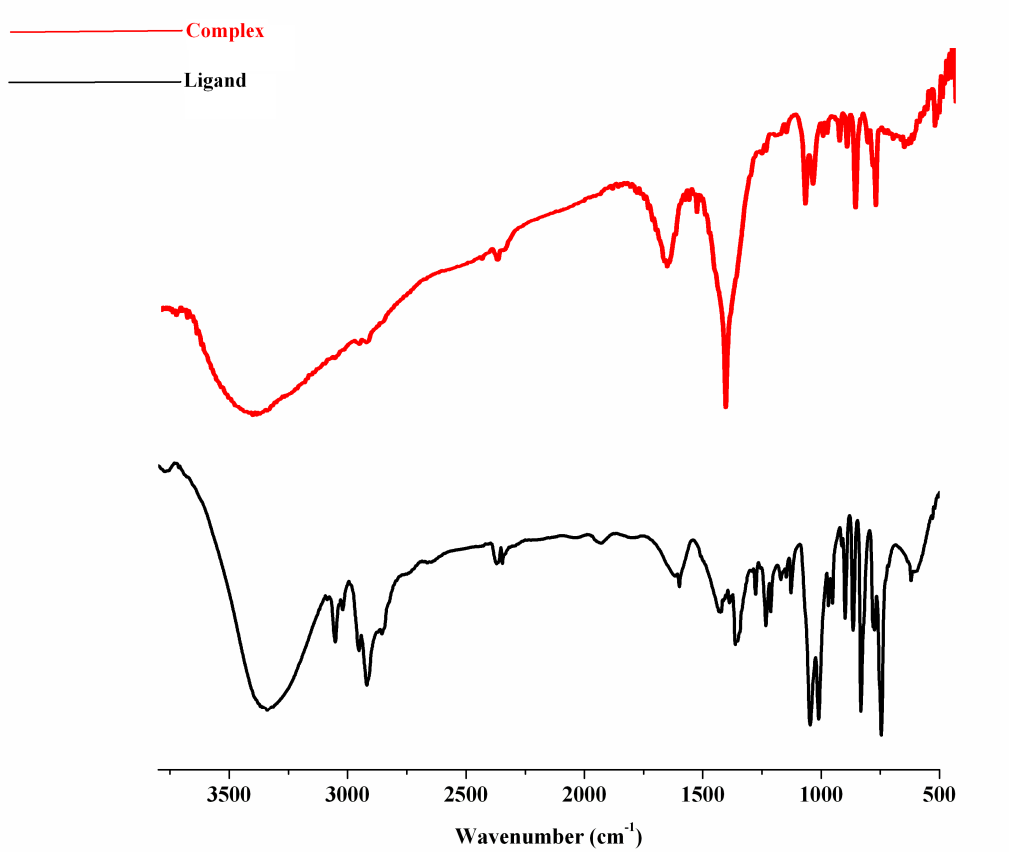

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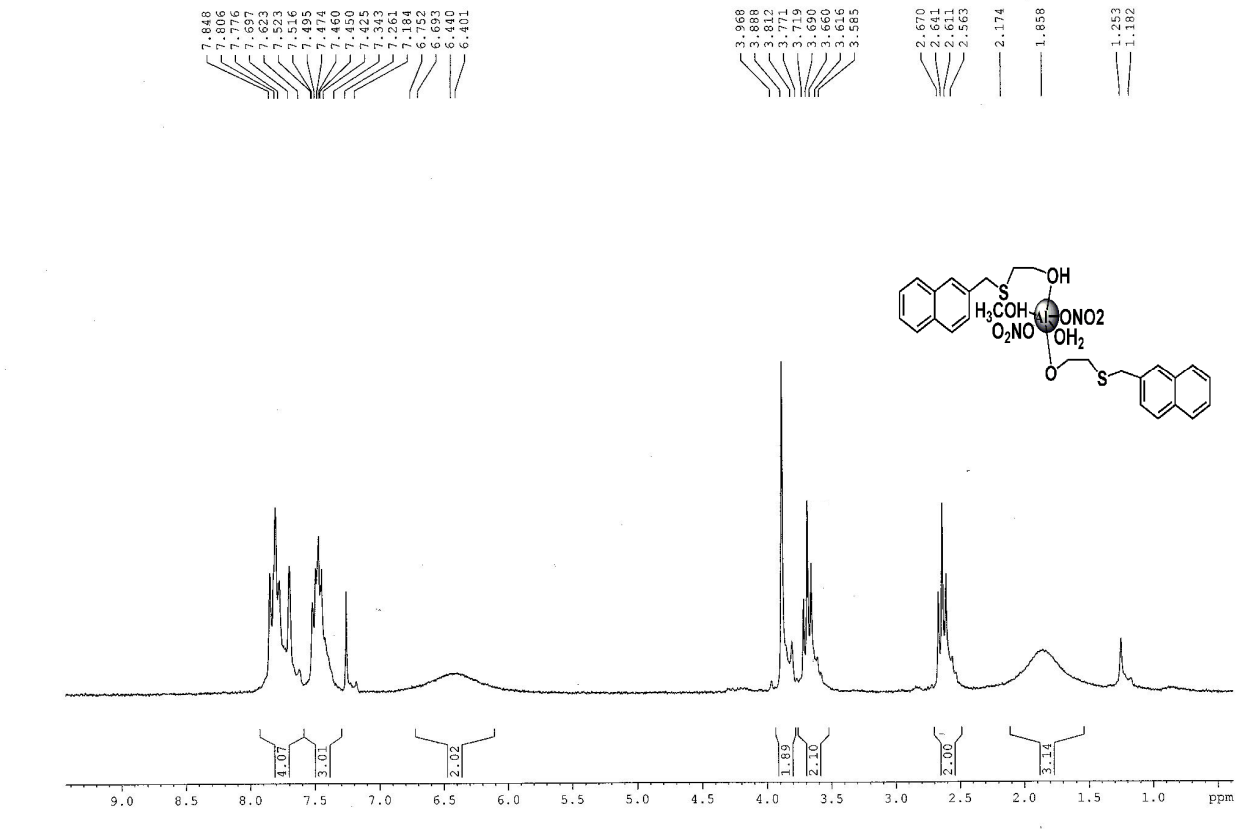

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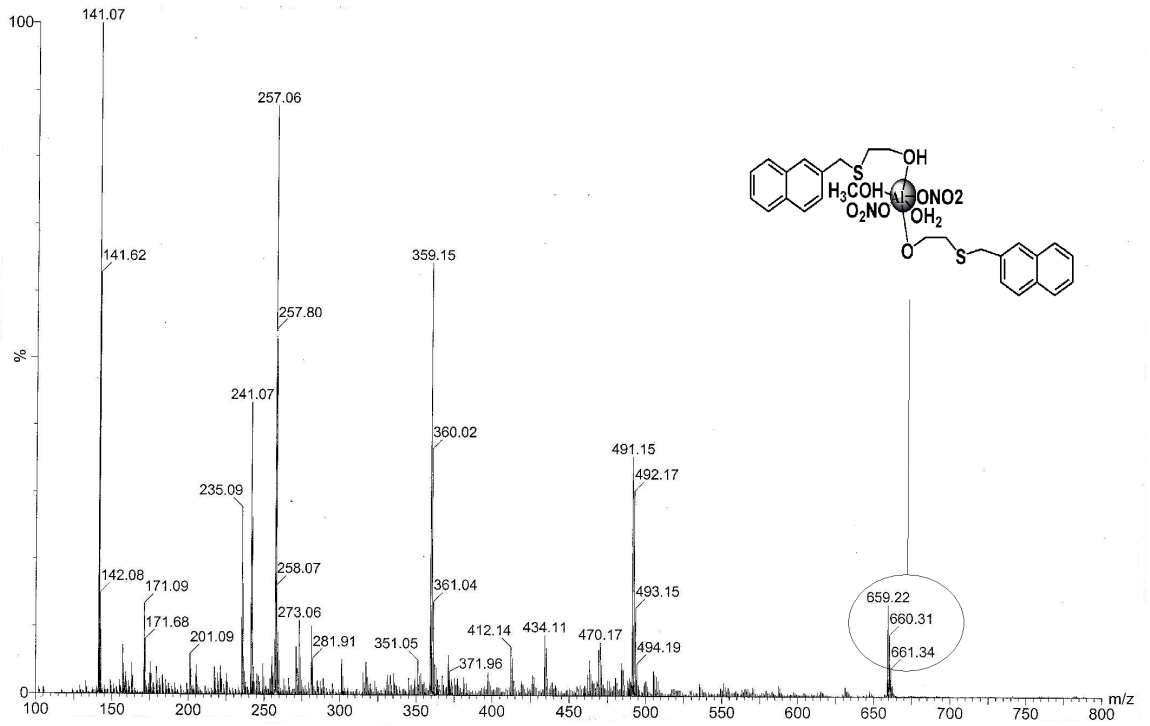

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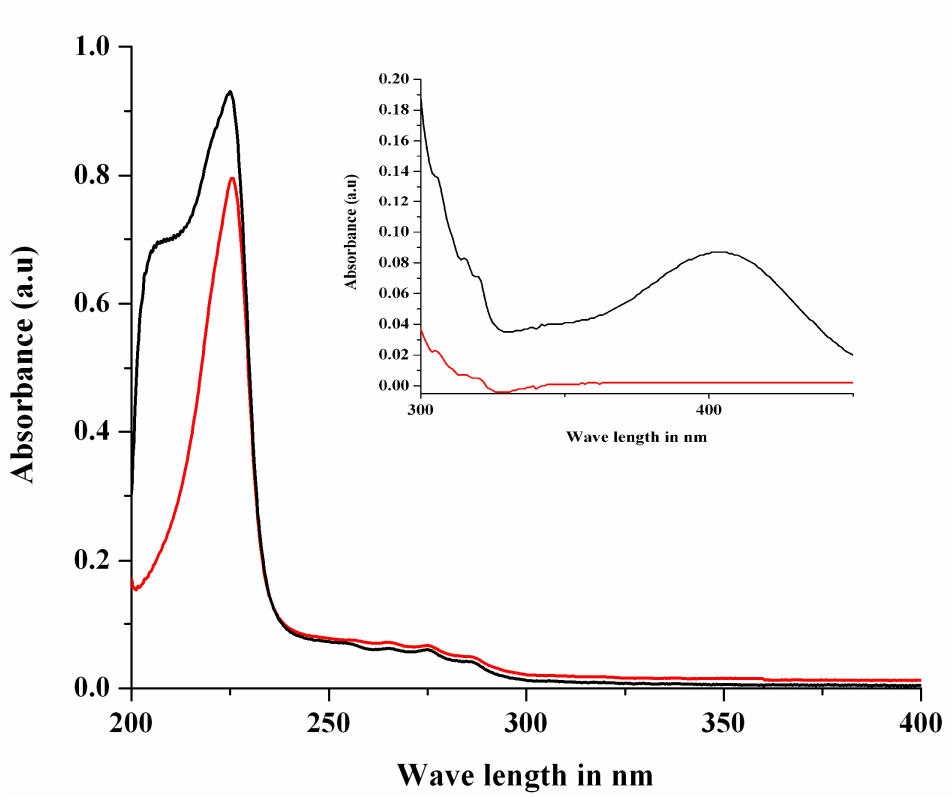

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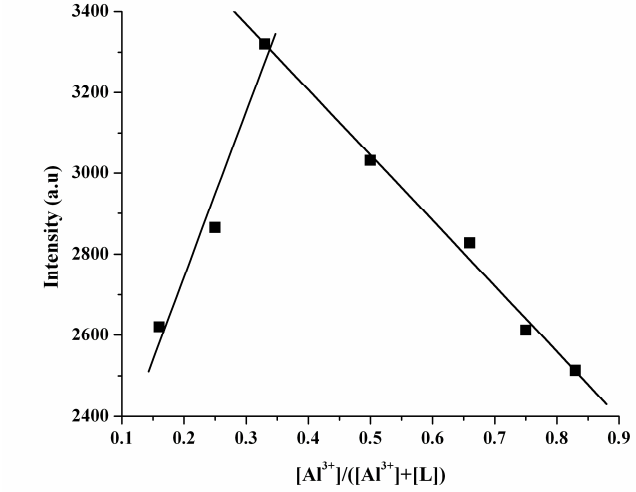

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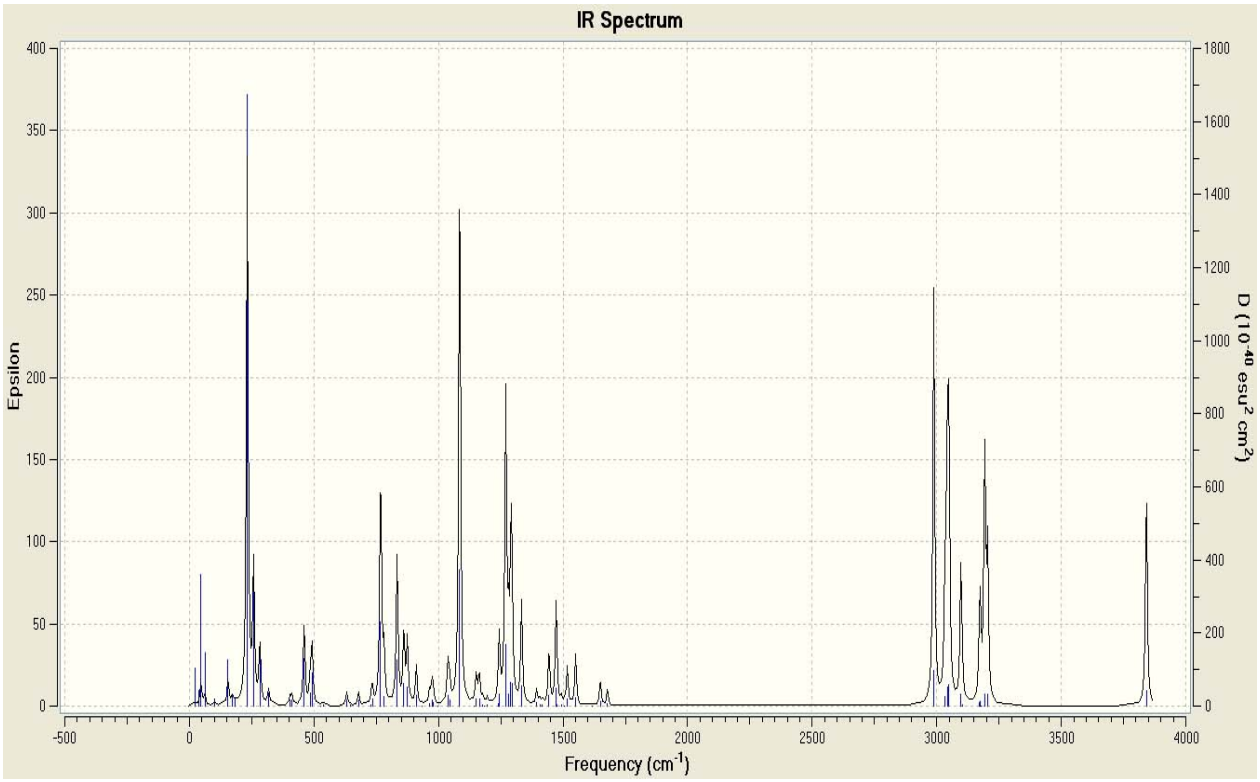

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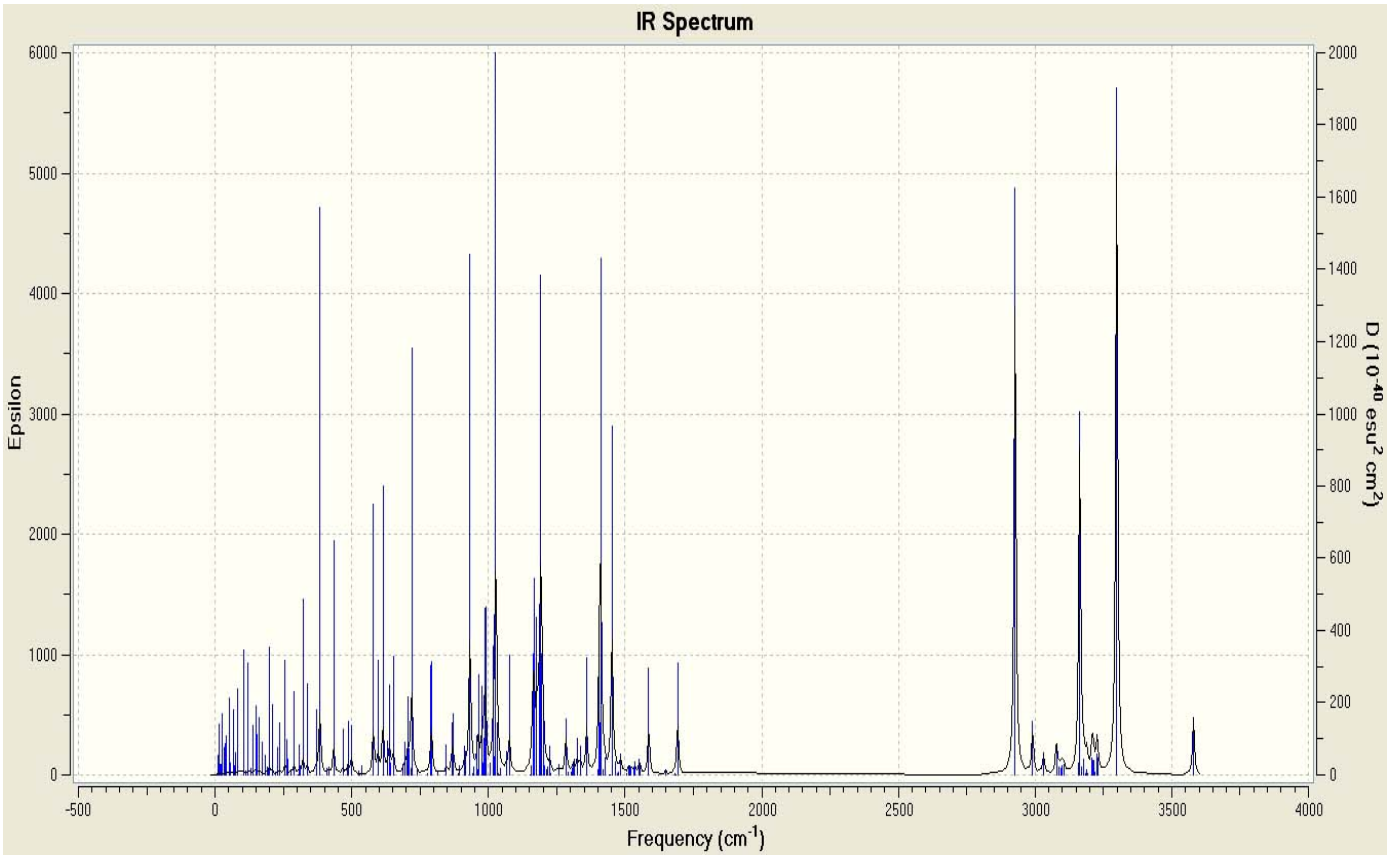

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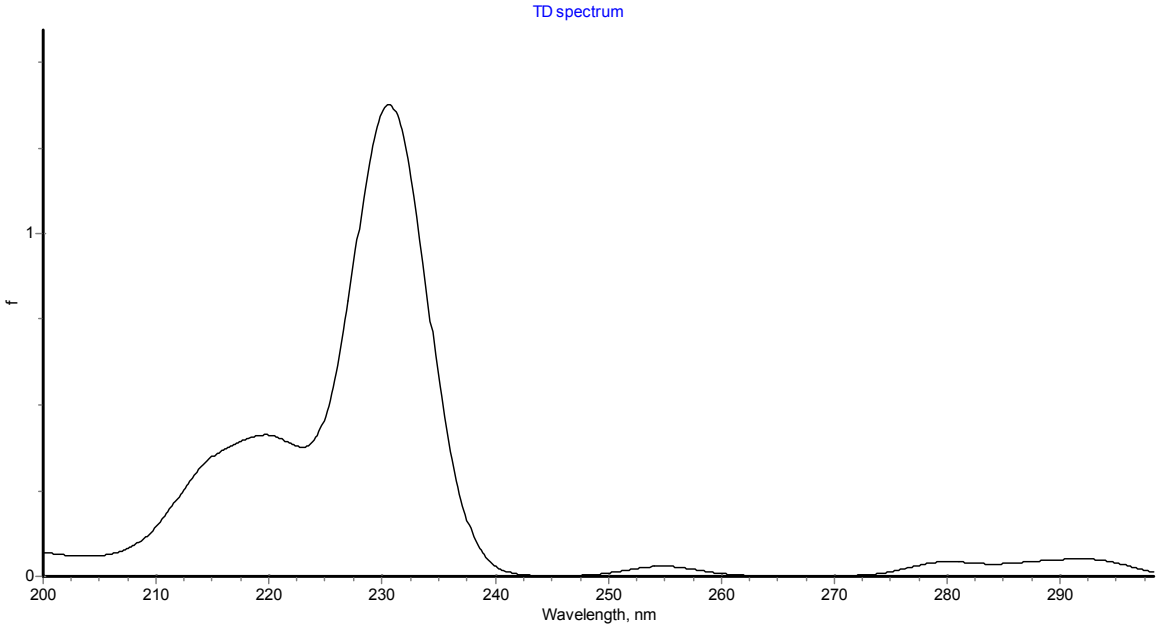

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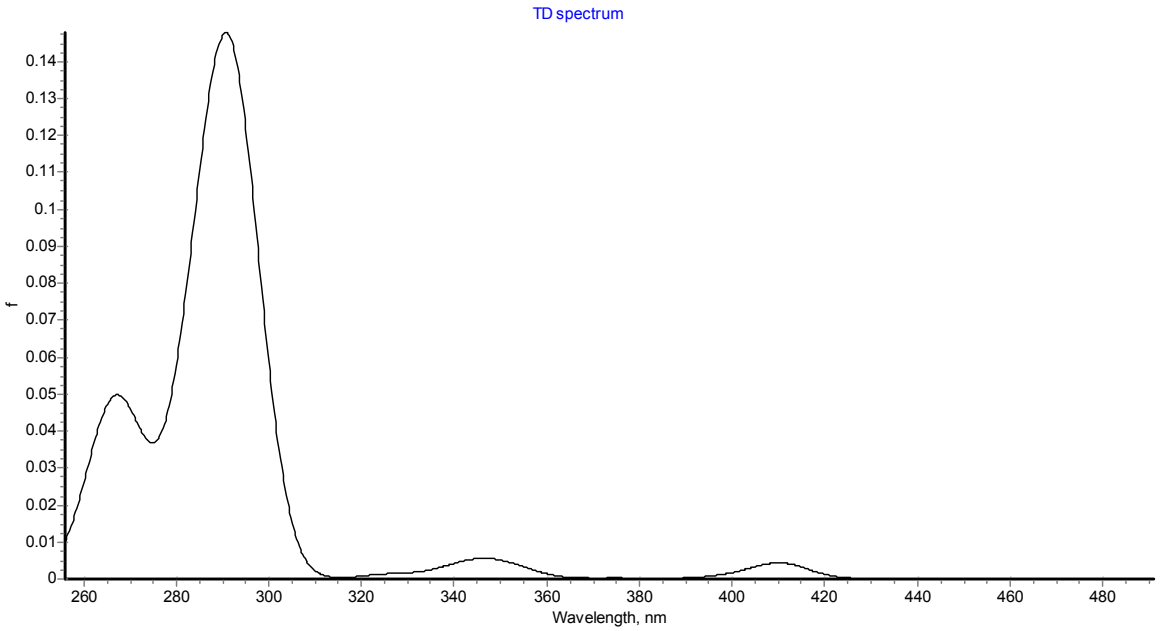


Figure S12a

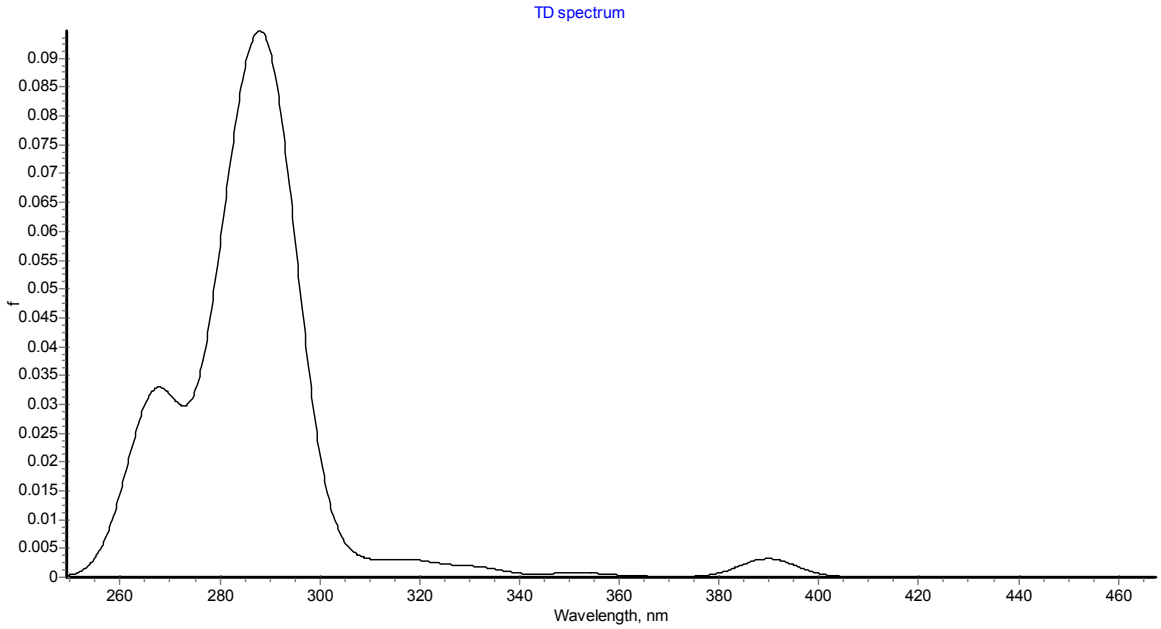


Figure S12b

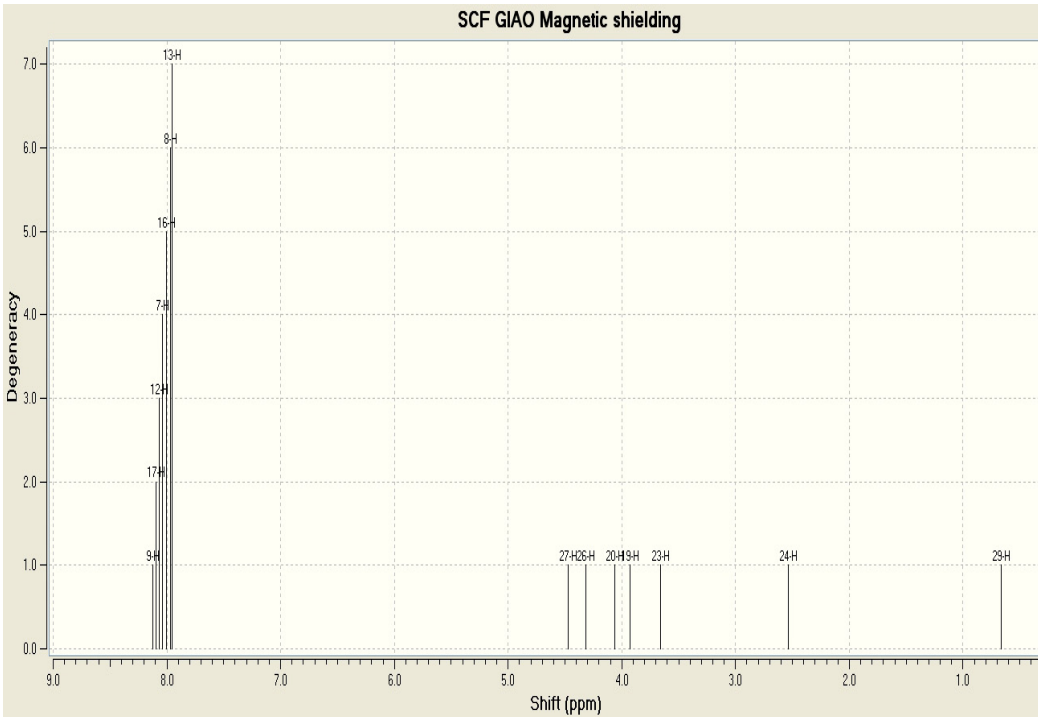
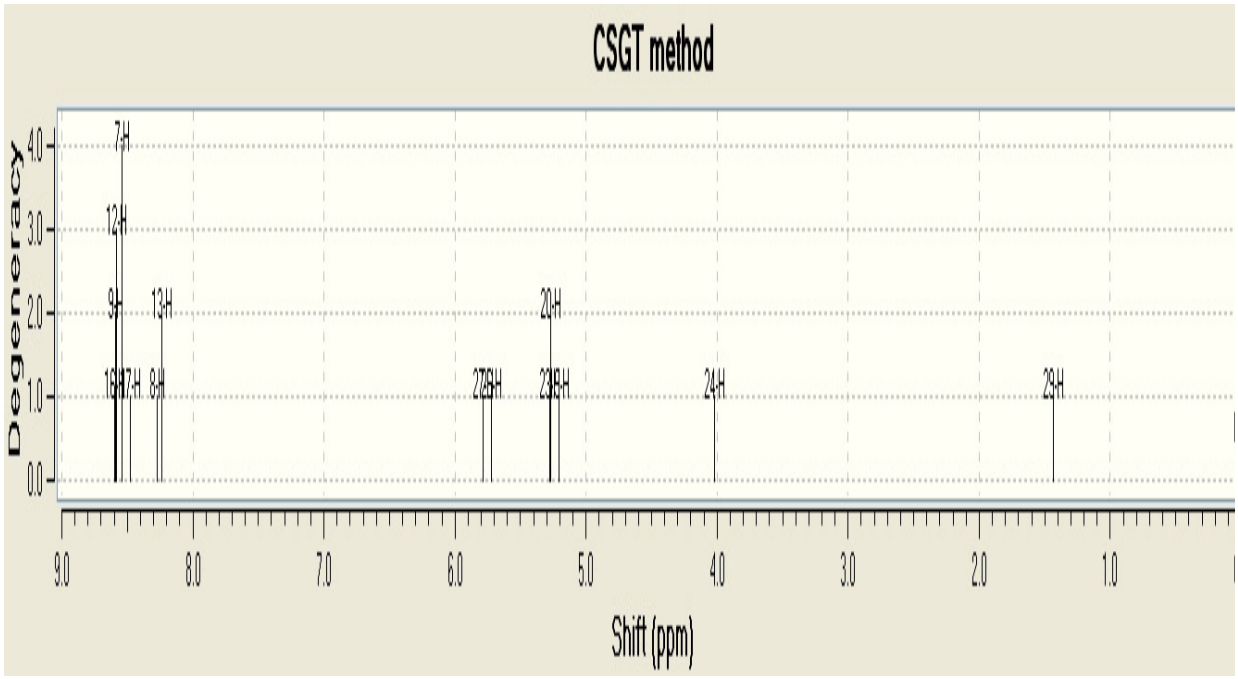


Figure S13a



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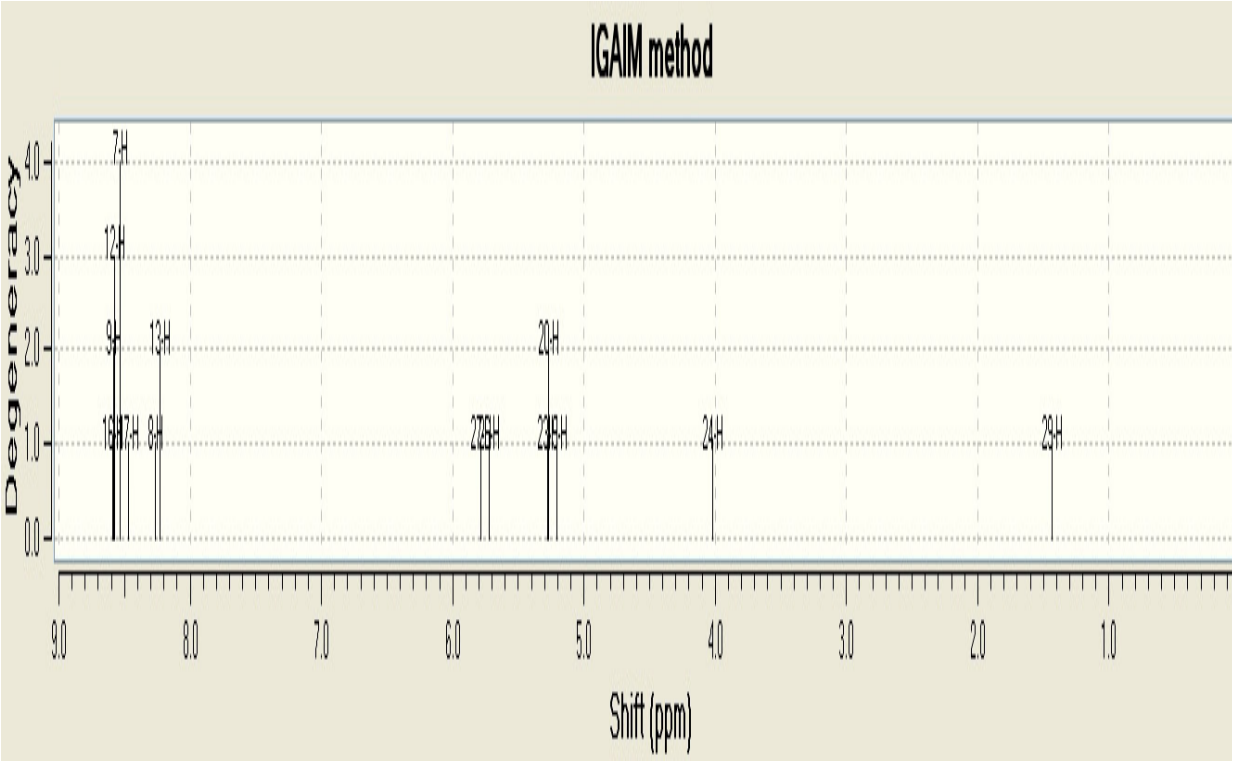

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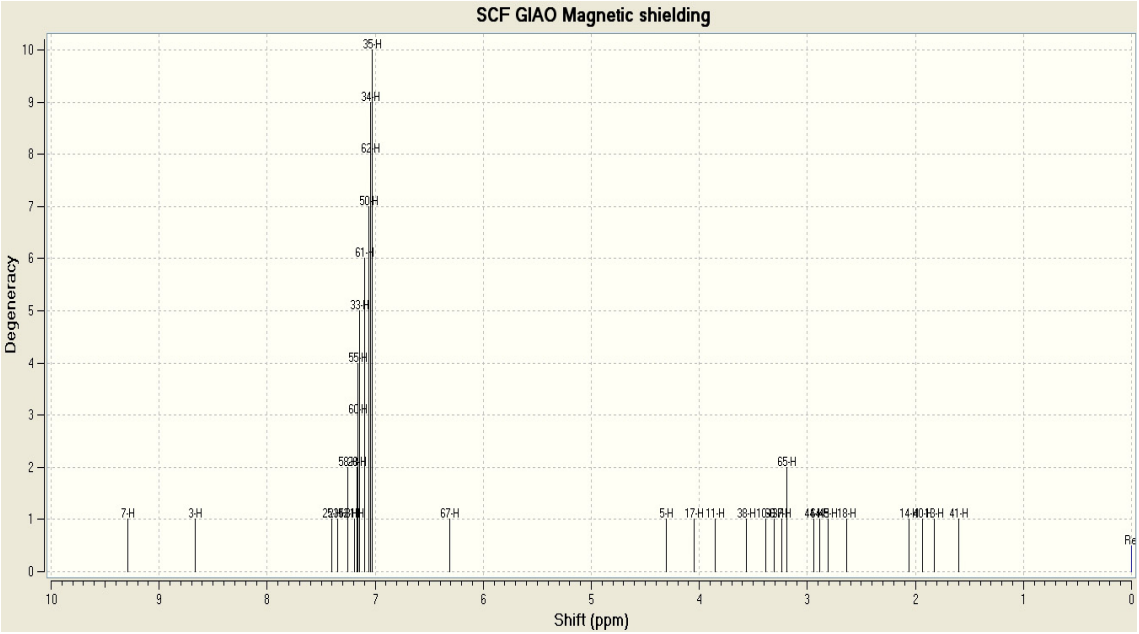


Figure S14a

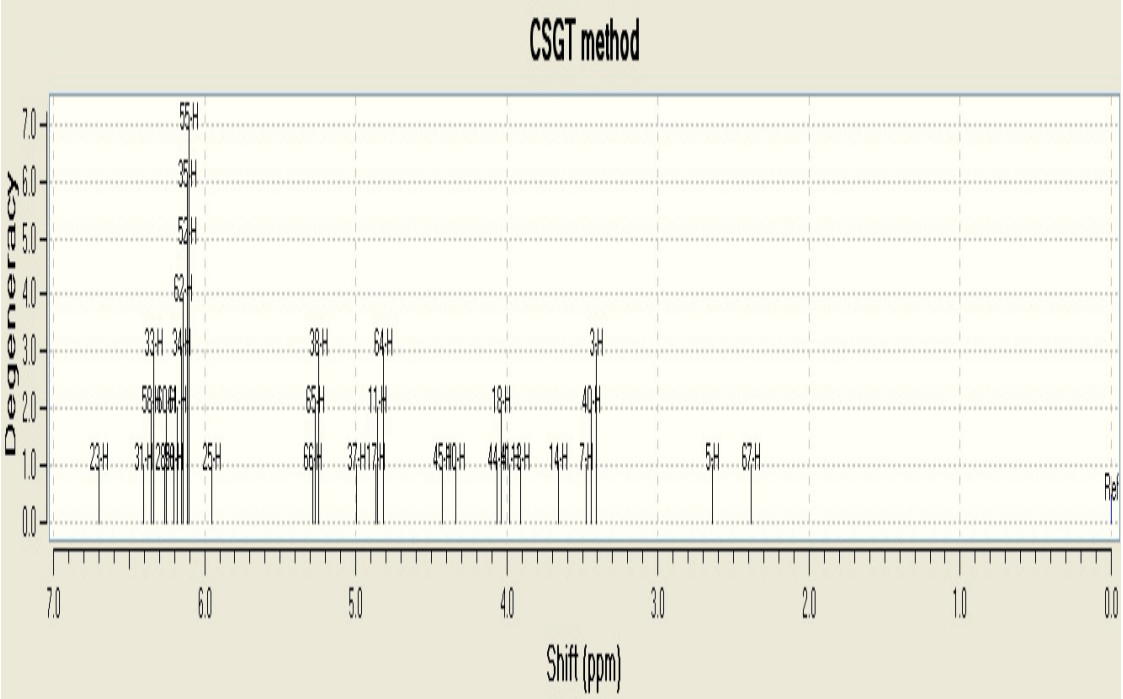


Figure S14b

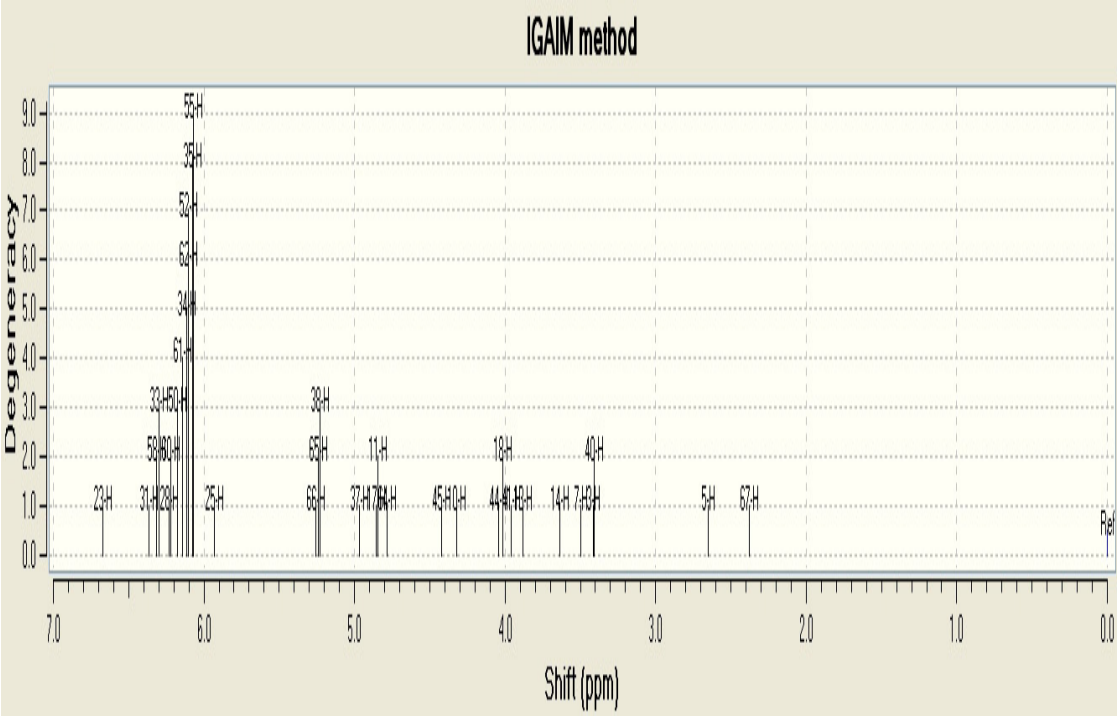


Figure S14c

Table S1

Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.23615	1.99915	4.22077	0.01623	6.23615
C	2	-0.20582	1.99910	4.19154	0.01519	6.20582
C	3	-0.06833	1.99908	4.05302	0.01624	6.06833
C	4	-0.06291	1.99904	4.04817	0.01570	6.06291
C	5	-0.20701	1.99910	4.19260	0.01531	6.20701
C	6	-0.23638	1.99915	4.22103	0.01619	6.23638
H	7	0.23569	0.00000	0.76252	0.00179	0.76431
H	8	0.23895	0.00000	0.75959	0.00146	0.76105
H	9	0.23663	0.00000	0.76172	0.00165	0.76337
C	10	-0.17294	1.99868	4.15669	0.01756	6.17294
C	11	-0.20180	1.99911	4.18696	0.01573	6.20180
H	12	0.23623	0.00000	0.76204	0.00173	0.76377
H	13	0.23883	0.00000	0.75969	0.00147	0.76117
C	14	-0.22037	1.99907	4.20539	0.01591	6.22037
C	15	-0.06697	1.99910	4.04992	0.01795	6.06697
H	16	0.23694	0.00000	0.76129	0.00177	0.76306
H	17	0.24142	0.00000	0.75672	0.00186	0.75858
C	18	-0.57471	1.99925	4.56158	0.01387	6.57471
H	19	0.24161	0.00000	0.75592	0.00247	0.75839
H	20	0.24514	0.00000	0.75280	0.00207	0.75486
S	21	0.19831	9.99932	5.76578	0.03659	15.80169
C	22	-0.60154	1.99932	4.58774	0.01449	6.60154
H	23	0.24631	0.00000	0.75142	0.00227	0.75369
H	24	0.23934	0.00000	0.75862	0.00204	0.76066
C	25	-0.10435	1.99925	4.08718	0.01792	6.10435
H	26	0.20378	0.00000	0.79389	0.00233	0.79622
H	27	0.19980	0.00000	0.79791	0.00229	0.80020
O	28	-0.77346	1.99982	6.75590	0.01773	8.77346
H	29	0.49375	0.00000	0.50195	0.00430	0.50625
* Total *		0.00001	37.98755	77.72035	0.29210	115.99999

Table S2

Atom	No	Charge	Core	Valence	Rydberg	Total
Al	1	2.11620	10.00000	0.87653	0.00727	10.88380
O	2	-1.07800	1.99984	7.07395	0.00420	9.07800
H	3	0.53890	0.00000	0.45702	0.00408	0.46110
O	4	-0.86941	1.99985	6.86065	0.00891	8.86941
H	5	0.55124	0.00000	0.44488	0.00387	0.44876
O	6	-0.89965	1.99983	6.89311	0.00671	8.89965
H	7	0.53355	0.00000	0.46139	0.00506	0.46645
O	8	-1.04940	1.99986	7.04060	0.00894	9.04940
C	9	-0.03556	1.99916	4.02074	0.01567	6.03556
H	10	0.19691	0.00000	0.80056	0.00253	0.80309
H	11	0.18002	0.00000	0.81724	0.00274	0.81998
C	12	-0.52070	1.99927	4.51071	0.01072	6.52070
H	13	0.24682	0.00000	0.75108	0.00210	0.75318
H	14	0.22815	0.00000	0.76980	0.00206	0.77185
S	15	0.08018	10.00000	5.91066	0.00916	15.91982
C	16	-0.50169	1.99916	4.48825	0.01429	6.50169
H	17	0.24822	0.00000	0.74937	0.00241	0.75178
H	18	0.23488	0.00000	0.76299	0.00213	0.76512
C	19	-0.04050	1.99903	4.02074	0.02073	6.04050
C	20	-0.18935	1.99897	4.17356	0.01682	6.18935
C	21	-0.20625	1.99906	4.19184	0.01535	6.20625
C	22	-0.04813	1.99897	4.02920	0.01996	6.04813
H	23	0.21931	0.00000	0.77916	0.00153	0.78069
C	24	-0.18455	1.99908	4.17087	0.01461	6.18455
H	25	0.23163	0.00000	0.76664	0.00173	0.76837
C	26	-0.05354	1.99897	4.03488	0.01968	6.05354
C	27	-0.19208	1.99908	4.17847	0.01454	6.19208
H	28	0.21894	0.00000	0.77983	0.00123	0.78106
C	29	-0.19393	1.99908	4.18011	0.01474	6.19393
C	30	-0.21274	1.99916	4.19963	0.01395	6.21274
H	31	0.21650	0.00000	0.78236	0.00114	0.78350
C	32	-0.21202	1.99916	4.19888	0.01398	6.21202
H	33	0.21675	0.00000	0.78209	0.00116	0.78325
H	34	0.21968	0.00000	0.77941	0.00091	0.78032
H	35	0.21951	0.00000	0.77957	0.00092	0.78049
C	36	-0.05511	1.99916	4.04185	0.01410	6.05511
H	37	0.22249	0.00000	0.77531	0.00220	0.77751
H	38	0.22812	0.00000	0.77004	0.00184	0.77188
C	39	-0.53746	1.99928	4.52624	0.01194	6.53746

H	40	0.24899	0.00000	0.74969	0.00132	0.75101
H	41	0.23316	0.00000	0.76445	0.00239	0.76684
S	42	0.08268	10.00000	5.90884	0.00848	15.91732
C	43	-0.49811	1.99917	4.48553	0.01342	6.49811
H	44	0.23759	0.00000	0.76060	0.00181	0.76241
H	45	0.23759	0.00000	0.76021	0.00220	0.76241
C	46	-0.04290	1.99903	4.02290	0.02097	6.04290
C	47	-0.18488	1.99897	4.16931	0.01661	6.18488
C	48	-0.20648	1.99906	4.19187	0.01555	6.20648
C	49	-0.04712	1.99897	4.02821	0.01994	6.04712
H	50	0.21704	0.00000	0.78154	0.00143	0.78296
C	51	-0.18164	1.99907	4.16802	0.01454	6.18164
H	52	0.21808	0.00000	0.78026	0.00165	0.78192
C	53	-0.05190	1.99897	4.03319	0.01975	6.05190
C	54	-0.19116	1.99908	4.17759	0.01448	6.19116
H	55	0.21839	0.00000	0.78037	0.00124	0.78161
C	56	-0.19318	1.99908	4.17939	0.01471	6.19318
C	57	-0.20942	1.99916	4.19637	0.01389	6.20942
H	58	0.21739	0.00000	0.78147	0.00113	0.78261
C	59	-0.20833	1.99916	4.19524	0.01392	6.20833
H	60	0.21762	0.00000	0.78122	0.00116	0.78238
H	61	0.22133	0.00000	0.77776	0.00091	0.77867
H	62	0.22124	0.00000	0.77785	0.00092	0.77876
C	63	-0.25085	1.99927	4.24460	0.00698	6.25085
H	64	0.20655	0.00000	0.79271	0.00074	0.79345
H	65	0.21776	0.00000	0.78098	0.00125	0.78224
H	66	0.21005	0.00000	0.78860	0.00134	0.78995
H	67	0.52004	0.00000	0.47516	0.00480	0.47996
N	68	0.71127	1.99967	4.26348	0.02558	6.28873
O	69	-0.48330	1.99988	6.47522	0.00820	8.48330
O	70	-0.33003	1.99988	6.32099	0.00915	8.33003
O	71	-0.66761	1.99985	6.65701	0.01074	8.66761
N	72	0.71336	1.99967	4.26235	0.02462	6.28664
O	73	-0.48613	1.99989	6.47778	0.00846	8.48613
O	74	-0.35485	1.99988	6.34555	0.00942	8.35485
O	75	-0.63020	1.99986	6.61932	0.01102	8.63020
* Total *		0.00000	107.97353	225.38586	0.64061	334.00000

Table S3. TDDFT results of HL in methanol.

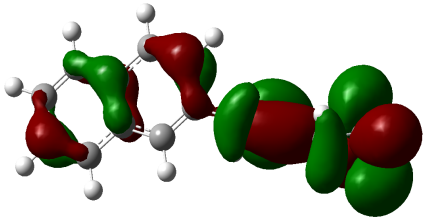
Excited State 1:	Percentage(%)	Excitation energy(nm)	Oscillator strength(f)
HOMO-2 ⟶LUMO	2.6	293.18	0.0428
HOMO-2 ⟶LUMO+1	2.4		
HOMO-1 ⟶LUMO	26.5		
HOMO ⟶LUMO	61.5		
HOMO ⟶LUMO	7.0		
Excited State 2:	Percentage(%)	Excitation energy(nm)	Oscillator strength(f)
HOMO-2 ⟶LUMO	40.0	230.66	1.2766
HOMO-1 ⟶LUMO+1	2.0		
HOMO-1 ⟶LUMO+3	11.0		
HOMO ⟶LUMO+1	35.0		
HOMO ⟶LUMO+2	6.0		
HOMO-2 ⟶LUMO+4	6.0		

Table S4. TDDFT of Al^{3+} complex in methanol.

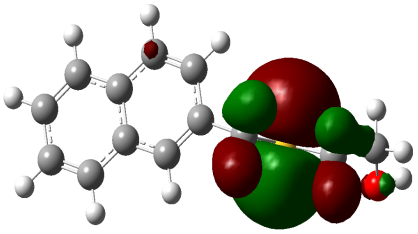
Excited State 1:	Percentage(%)	Excitation energy(nm)	Oscillator strength(f)
HOMO-2 ⟶LUMO	100	410.42	0.0042
Excited State 2:	Percentage(%)	Excitation energy(nm)	Oscillator strength(f)
HOMO-7 ⟶LUMO+1	4.2	352.83	0.0019
HOMO-6 ⟶LUMO+1	26.6		
HOMO-4 ⟶ LUMO+1	68.2		
Excited State 3:	Percentage(%)	Excitation energy(nm)	Oscillator strength(f)
HOMO-6 ⟶ LUMO+1	74.6	348.85	0.0010
HOMO-4 ⟶ LUMO+1	25.4		
Excited State 4:	Percentage(%)	Excitation energy(nm)	Oscillator strength(f)
HOMO-7 ⟶ LUMO	95.0	345.91	0.0020
HOMO-6 ⟶ LUMO	5.0		
Excited State 5:	Percentage(%)	Excitation energy(nm)	Oscillator strength(f)
HOMO-13 ⟶ LUMO+1	5.9	326.62	0.0011
HOMO-12 ⟶ LUMO+1	23.8		
HOMO-11 ⟶ LUMO+1	9.9		

HOMO-10 ⟶ LUMO	2.5		
HOMO-10 ⟶ LUMO+1	49.8		
HOMO-7 ⟶ LUMO+1	8.1		
Excited State 6:	Percentage(%)	Excitation energy(nm)	Oscillator strength(f)
HOMO-4 ⟶ LUMO+5	4.8	293.37	0.0728
HOMO⟶ LUMO+3	95.2		
Excited State 7:	Percentage(%)	Excitation energy(nm)	Oscillator strength(f)
HOMO-4 ⟶ LUMO+3	48.5	285.32	0.0025
HOMO⟶LUMO+3	2.5		
HOMO⟶LUMO+5	49.0		
Excited State 8:	Percentage(%)	Excitation energy(nm)	Oscillator strength(f)
HOMO-5 ⟶ LUMO+2	35.4	266.72	0.0418
HOMO-3 ⟶ LUMO+2	58.3		
HOMO-3 ⟶ LUMO+4	2.9		
HOMO-1 ⟶ LUMO+4	3.4		

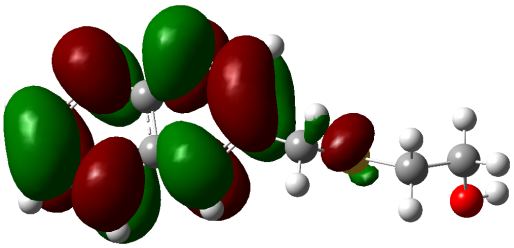
Table S5



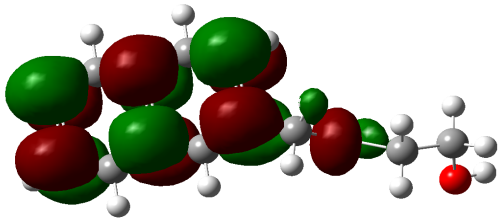
HOMO-2 (HL)



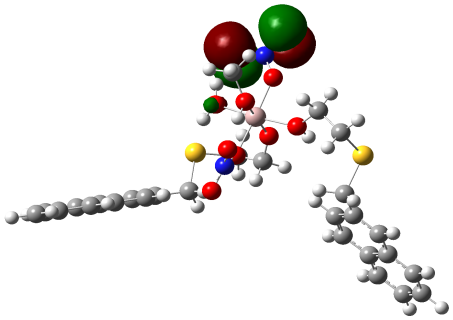
HOMO-1 (HL)



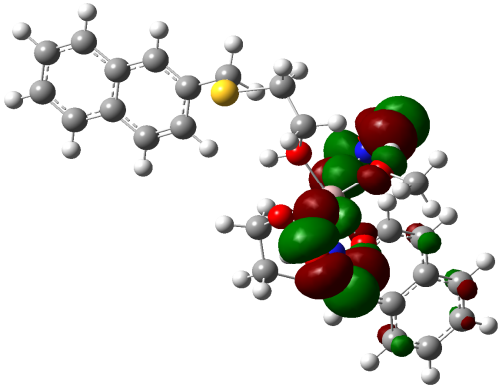
LUMO (HL)



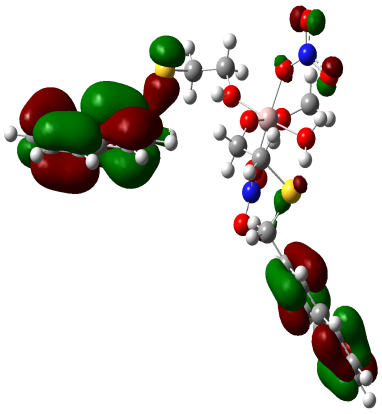
LUMO+1 (HL)



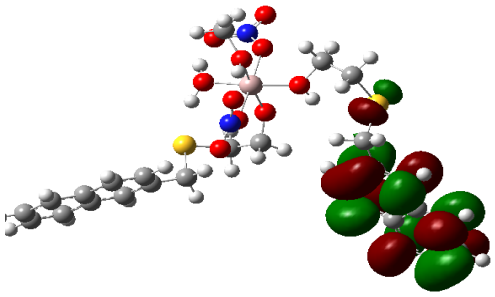
HOMO-6 (COMPLEX)



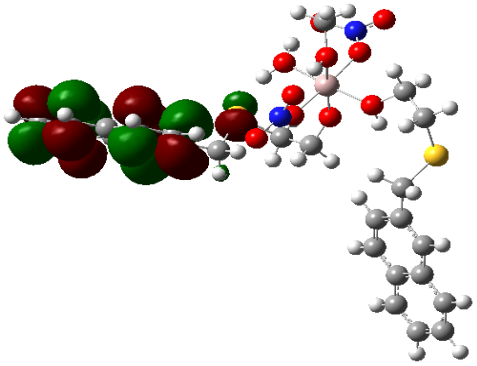
HOMO-2 (COMPLEX)



HOMO-4 (COMPLEX)



LUMO+1 (COMPLEX)



LUMO (COMPLEX)

Table S6

	Theoretical, λ/nm (Solvent Methanol)	**Theoretical, λ/nm (Gas Phase)**
L- Al^{3+} Complex	410, 352, 348, 345, 293, 285, 266	399, 389, 351, 348, 333, 331,291,282, 267

Calculation of Quantum Yield:

Fluorescence quantum yields (Φ) were estimated by integrating the area under the fluorescence curves using the equation,

$$\phi_{sample} = \frac{OD_{standard} \times A_{sample}}{OD_{sample} \times A_{standard}} \times \phi_{standard}$$

where A was the area under the fluorescence spectral curve and OD was optical density of the compound at the excitation wavelength.[1] Anthracene was used as quantum yield standard (quantum yield is 0.27 in ethanol)[2] for measuring the quantum yields of ligand and its Al^{3+} complex. The calculated quantum yield of ligand is 0.013 and its Al^{3+} is 0.083.

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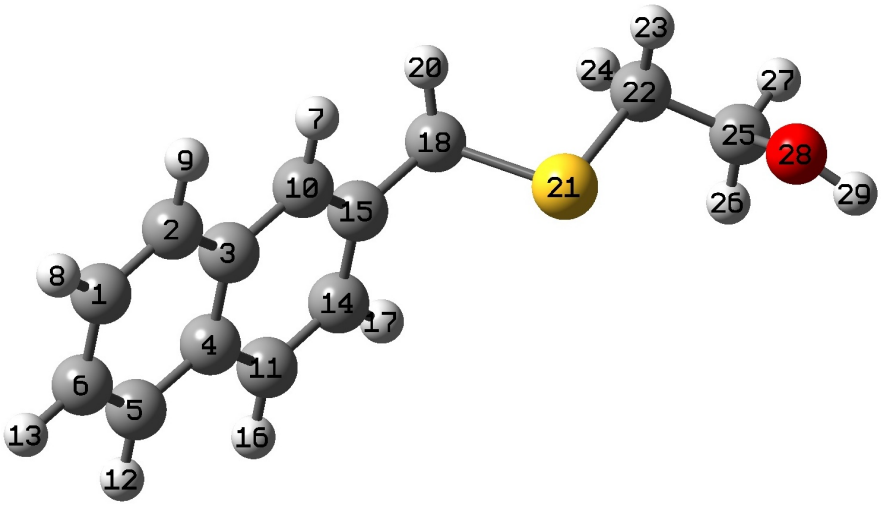
[1] Austin,E.; Gouterman,M. *Bioinorg. Chem.*, **1978,** *9*, 281.

[2] Melhuish W. H. *J. Phys. Chem.*, **1961**, *65*, 229

Computational results for HL using LANL2DZ basis set



Optimized geometry of **HL** using LANLDZ basis set

Natural Population Analysis

Atom	No.	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.21264	1.99916	4.19954	0.01394	6.21264
C	2	-0.19231	1.99908	4.17875	0.01448	6.19231
C	3	-0.04657	1.99897	4.02770	0.01990	6.04657
C	4	-0.05436	1.99897	4.03570	0.01969	6.05436
C	5	-0.19445	1.99908	4.18068	0.01468	6.19445
C	6	-0.21291	1.99916	4.19974	0.01400	6.21291
H	7	0.21591	0.00000	0.78268	0.00141	0.78409
H	8	0.21954	0.00000	0.77955	0.00091	0.78046
H	9	0.21636	0.00000	0.78250	0.00114	0.78364
C	10	-0.18981	1.99897	4.17435	0.01649	6.18981
C	11	-0.18556	1.99908	4.17189	0.01459	6.18556
H	12	0.21610	0.00000	0.78273	0.00116	0.78390
H	13	0.21931	0.00000	0.77977	0.00092	0.78069
C	14	-0.20867	1.99906	4.19469	0.01493	6.20867
C	15	-0.03213	1.99904	4.01240	0.02070	6.03213
H	16	0.21709	0.00000	0.78167	0.00124	0.78291
H	17	0.22150	0.00000	0.77724	0.00127	0.77850

C	18	-0.51717	1.99917	4.50484	0.01316	6.51717
H	19	0.22773	0.00000	0.77003	0.00224	0.77227
H	20	0.23136	0.00000	0.76668	0.00196	0.76864
S	21	0.11389	10.00000	5.87675	0.00937	15.88611
C	22	-0.52984	1.99928	4.51725	0.01331	6.52984
H	23	0.23695	0.00000	0.76029	0.00276	0.76305
H	24	0.22300	0.00000	0.77506	0.00194	0.77700
C	25	-0.05367	1.99918	4.04241	0.01208	6.05367
H	26	0.19092	0.00000	0.80643	0.00265	0.80908
H	27	0.18985	0.00000	0.80776	0.00239	0.81015
O	28	-0.79201	1.99988	6.78288	0.00924	8.79201
H	29	0.48259	0.00000	0.51661	0.00080	0.51741

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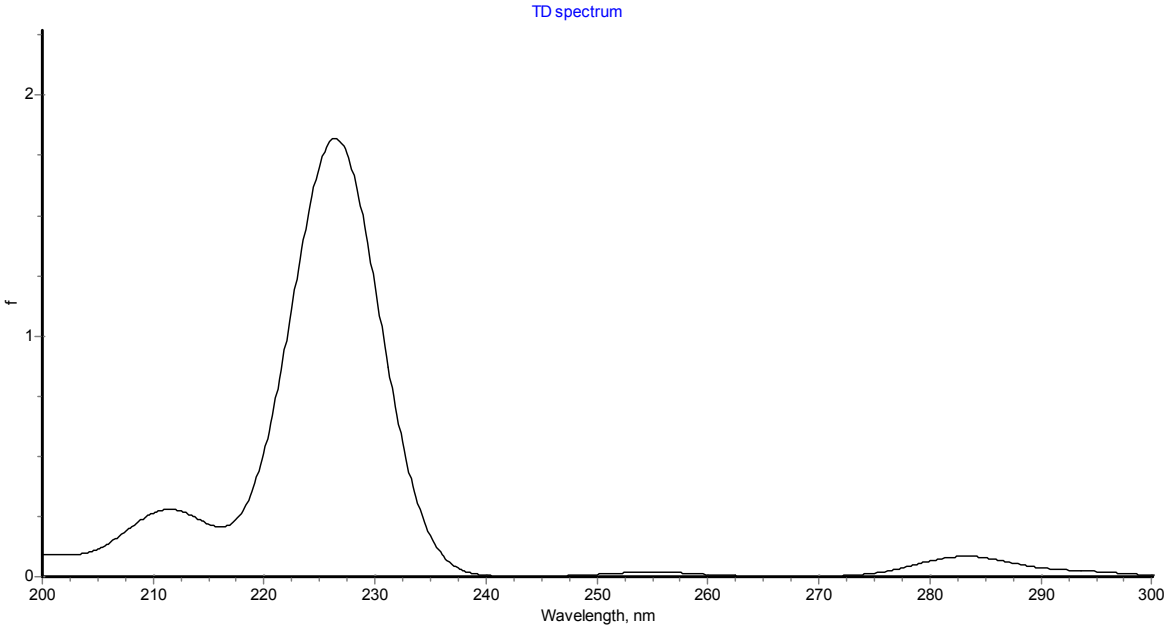
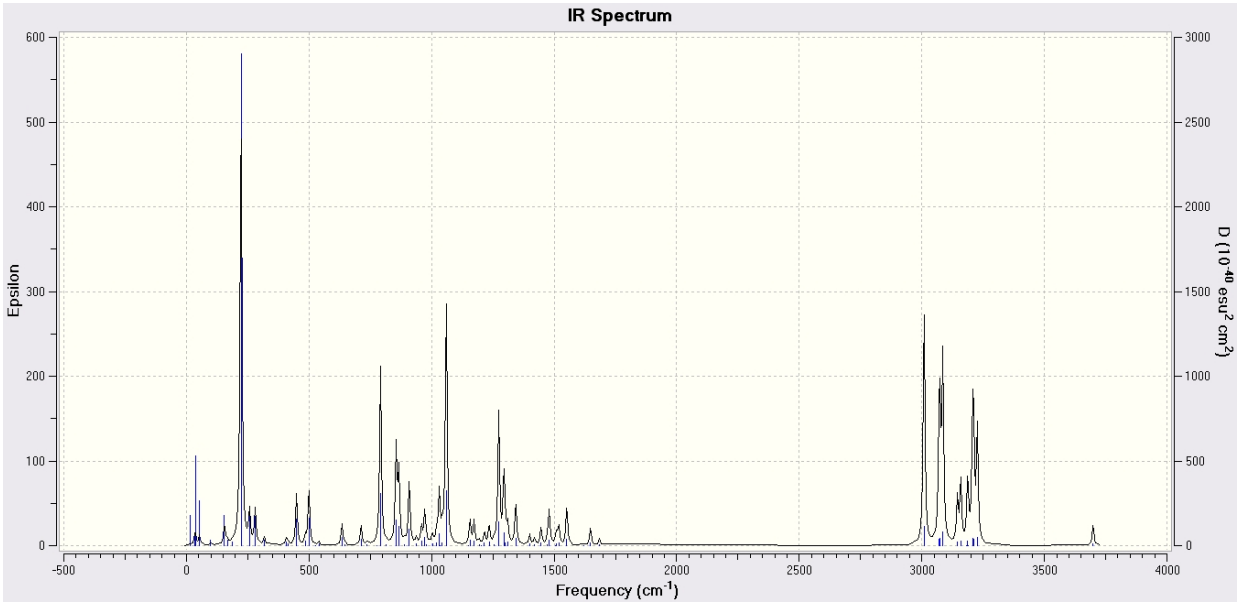
* Total *	0.00000	37.98808	77.76857	0.24335	116.00000

UV-vis spectrum



IR spectrum



NMR spectrum