Supporting Information

D-A Diads and A-D-A Triads based on Ferrocene: Push-pull Dyes of Unusual Behaviours in Solution

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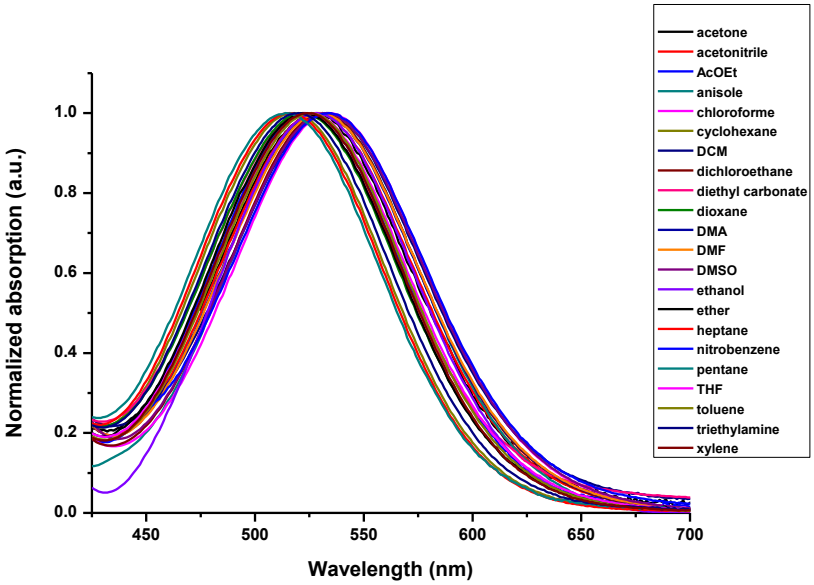
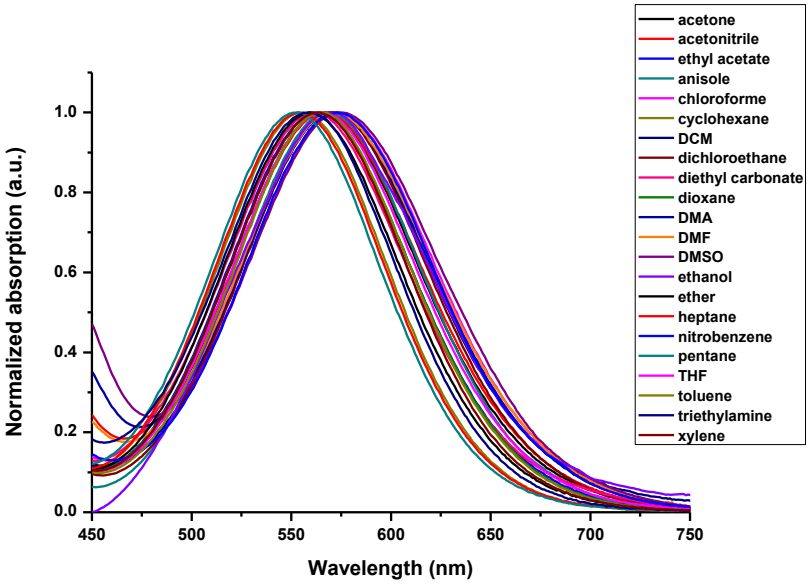
UV-visible absorption spectra of the different dyes recorded in solvents of different polarities.

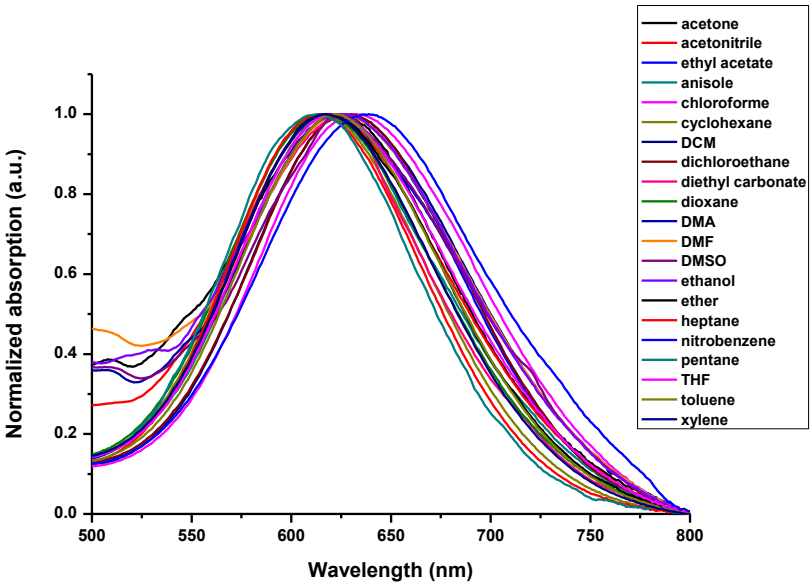
Solvatochromism of **D-A0** in solvents of different polarities.



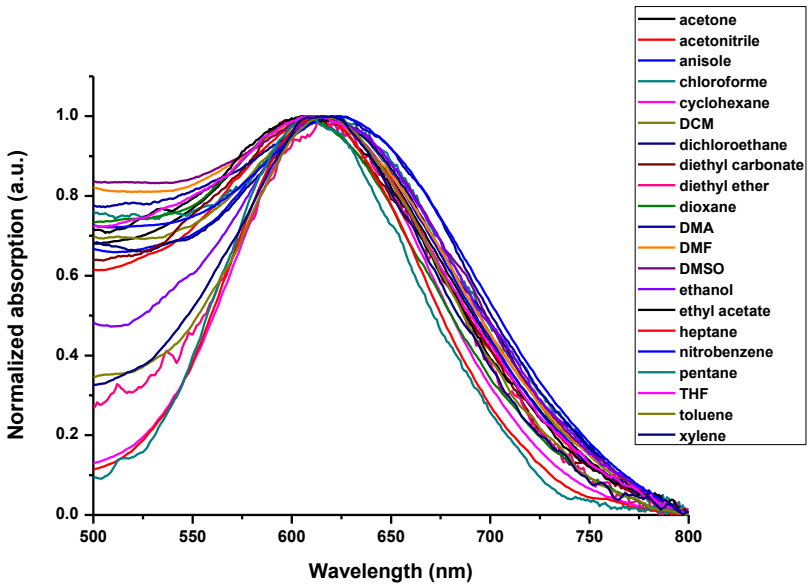
Solvatochromism of **D-A1** in solvents of different polarities.



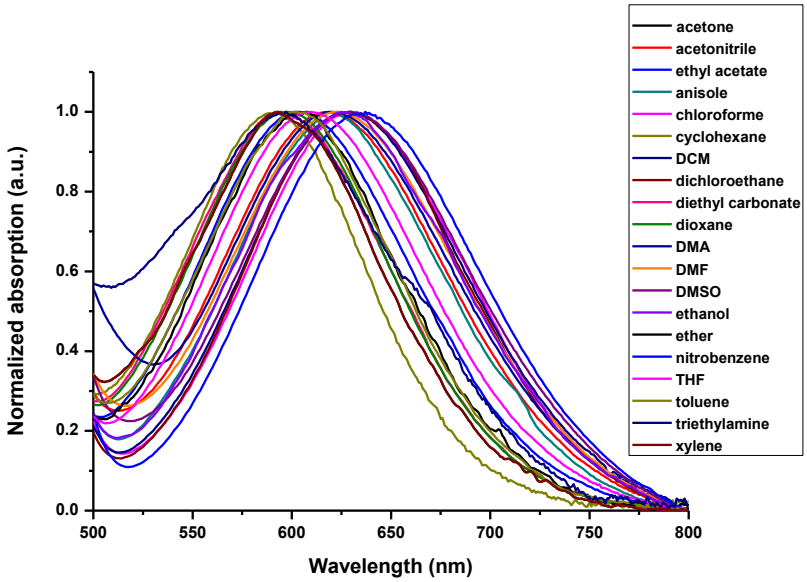
Solvatochromism of **D-A2** in solvents of different polarities.



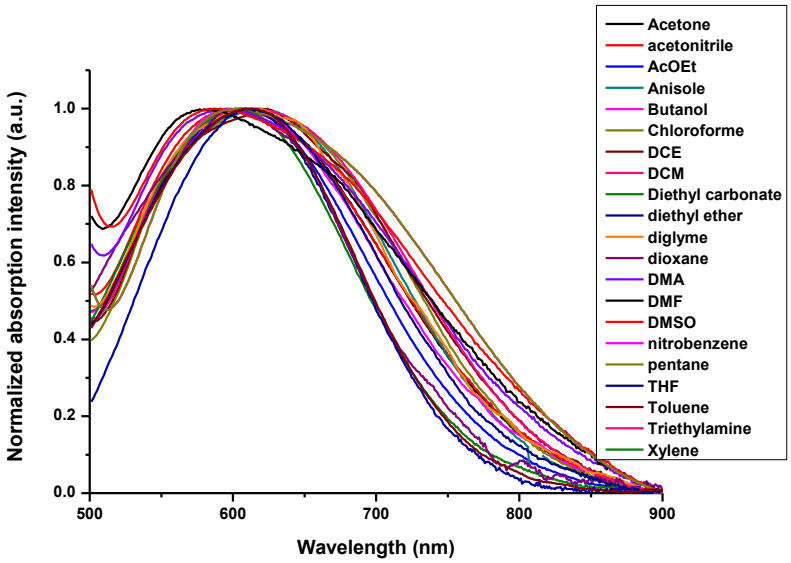
Solvatochromism of **D-A3** in solvents of different polarities.



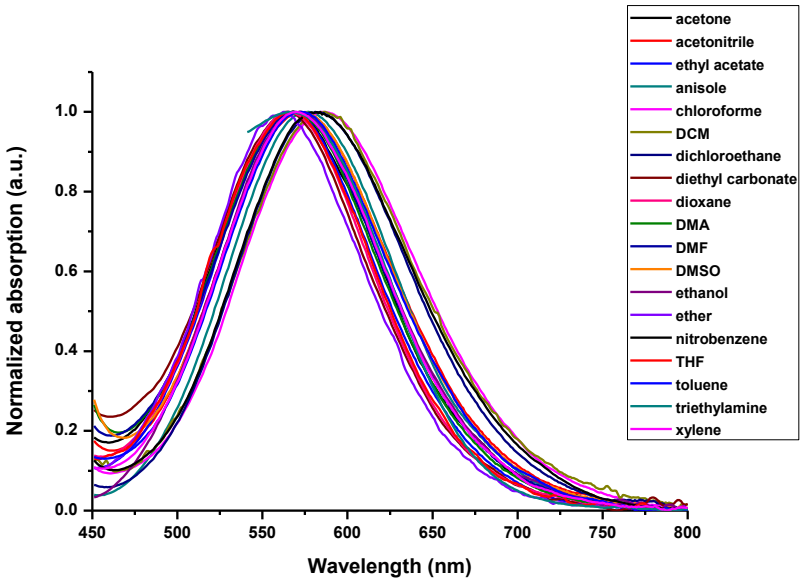
Solvatochromism of **D-A4** in solvents of different polarities.



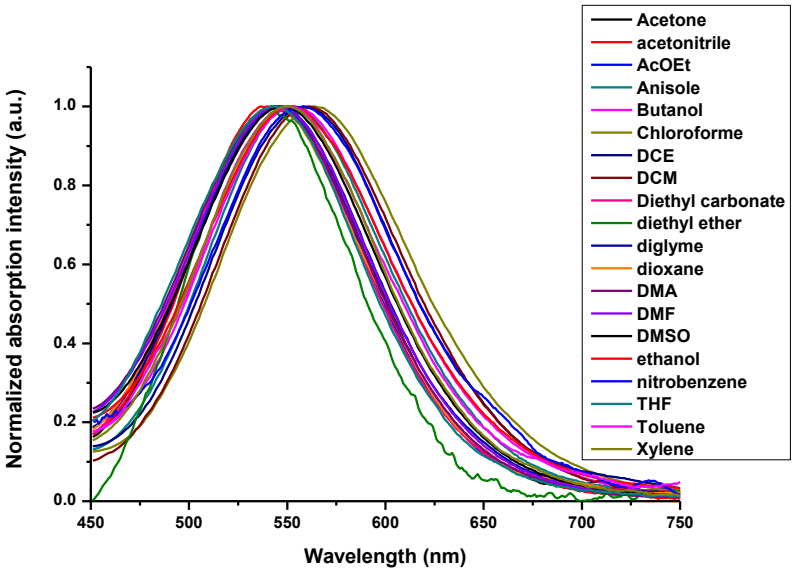
Solvatochromism of **D-A5** in solvents of different polarities.



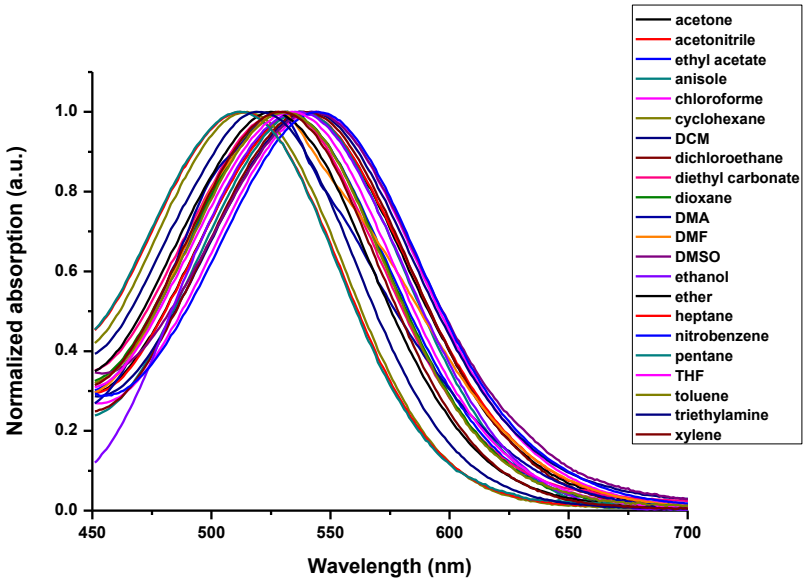
Solvatochromism of **D-A6** in solvents of different polarities.



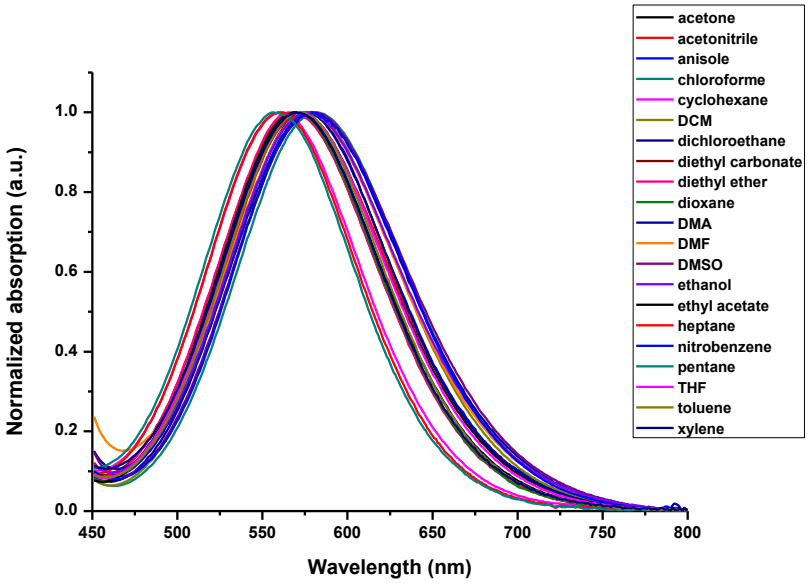
Solvatochromism of **D-A7** in solvents of different polarities.



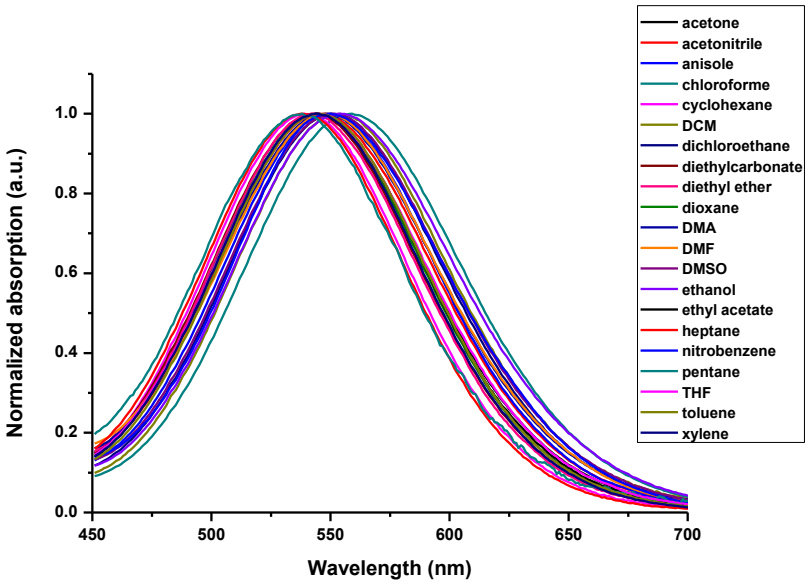
Solvatochromism of **D-A8** in solvents of different polarities.



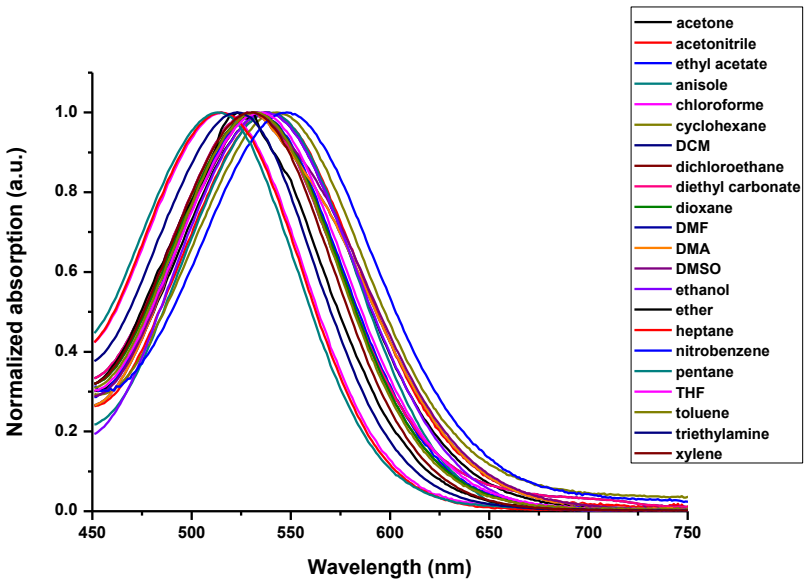
Solvatochromism of **D-A9** in solvents of different polarities.



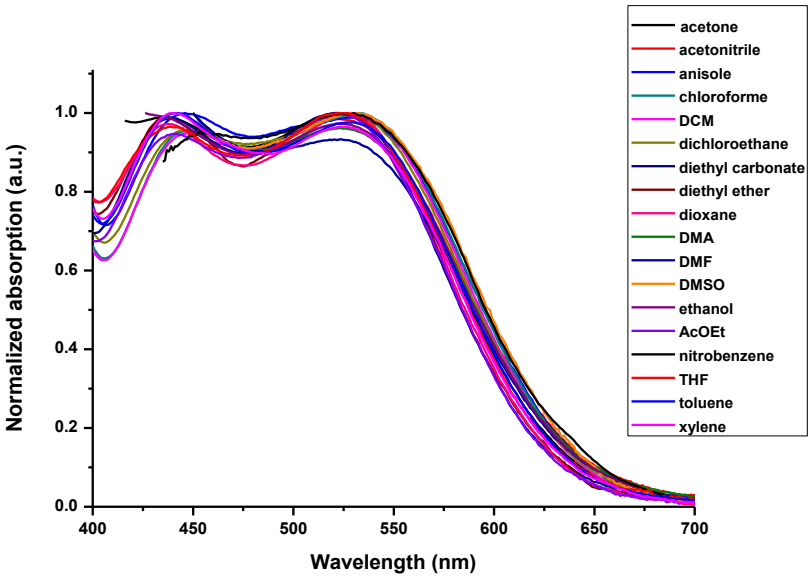
Solvatochromism of **D-A10** in solvents of different polarities.



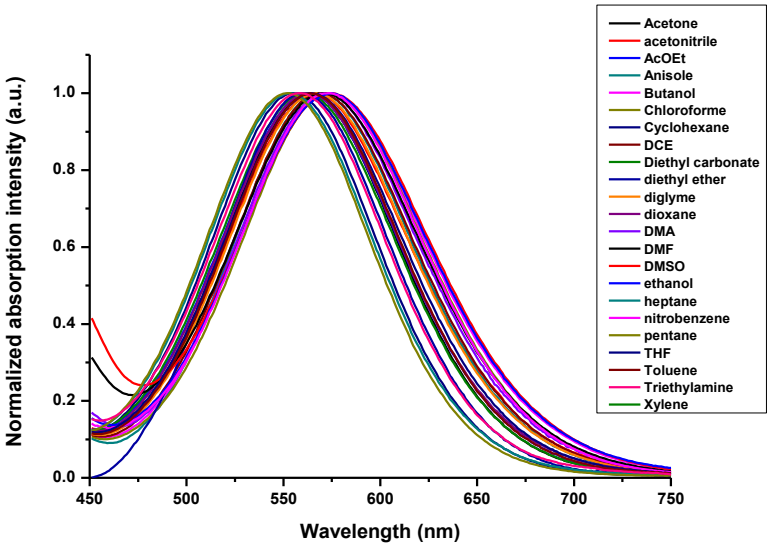
Solvatochromism of **D-A11** in solvents of different polarities.



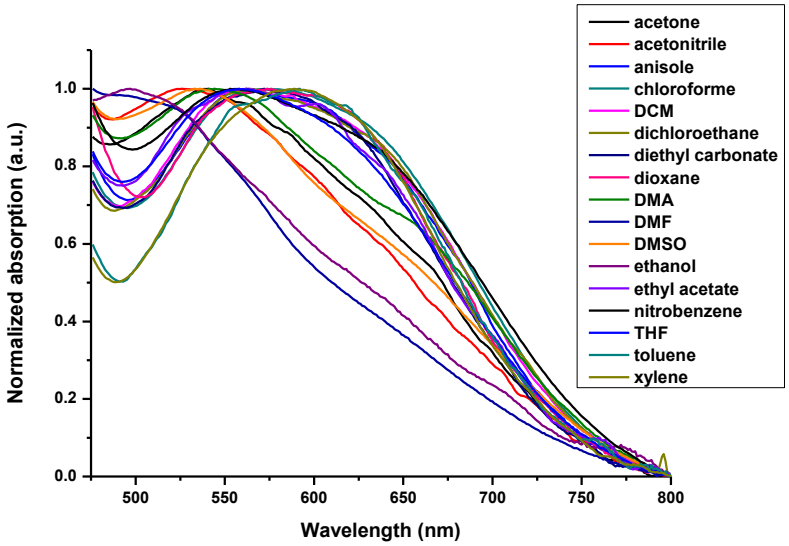
Solvatochromism of **A-D-A0** in solvents of different polarities.



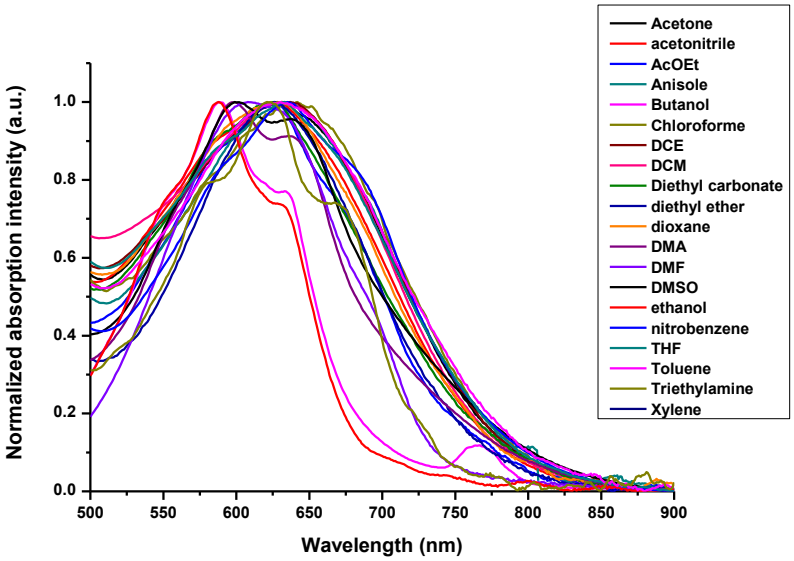
Solvatochromism of **A-D-A1** in solvents of different polarities.



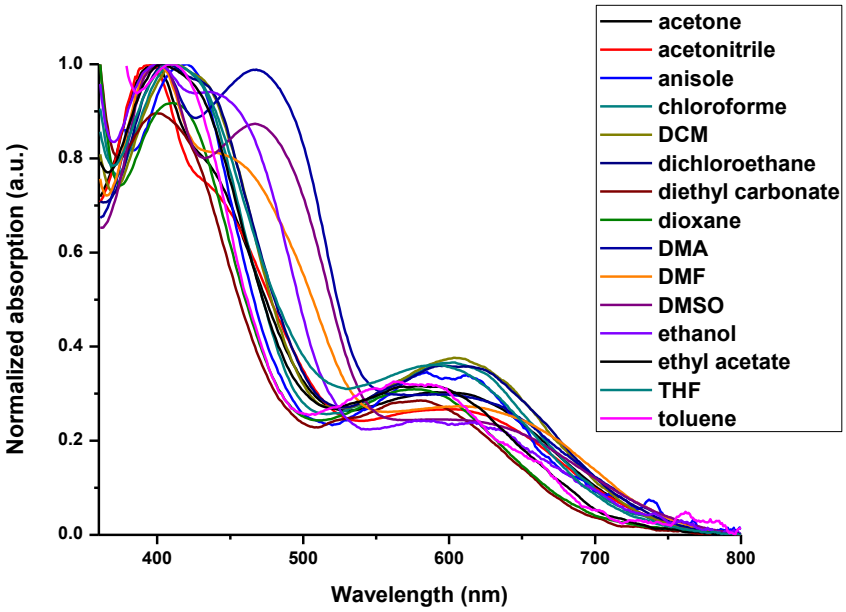
Solvatochromism of **A-D-A2** in solvents of different polarities.



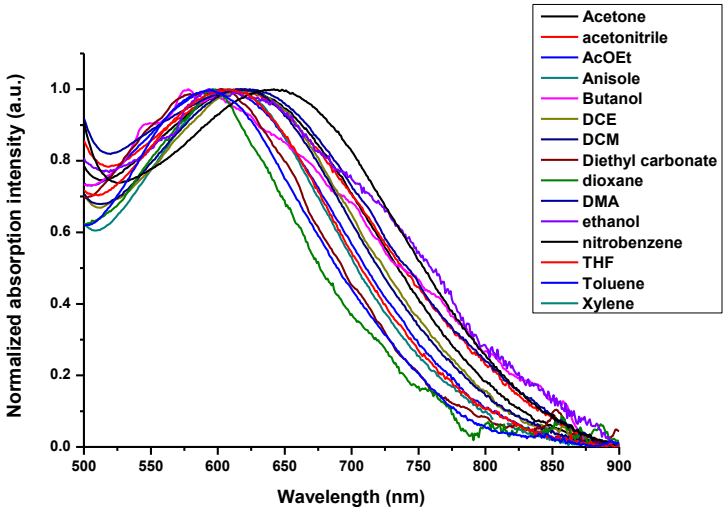
Solvatochromism of **A-D-A3** in solvents of different polarities.



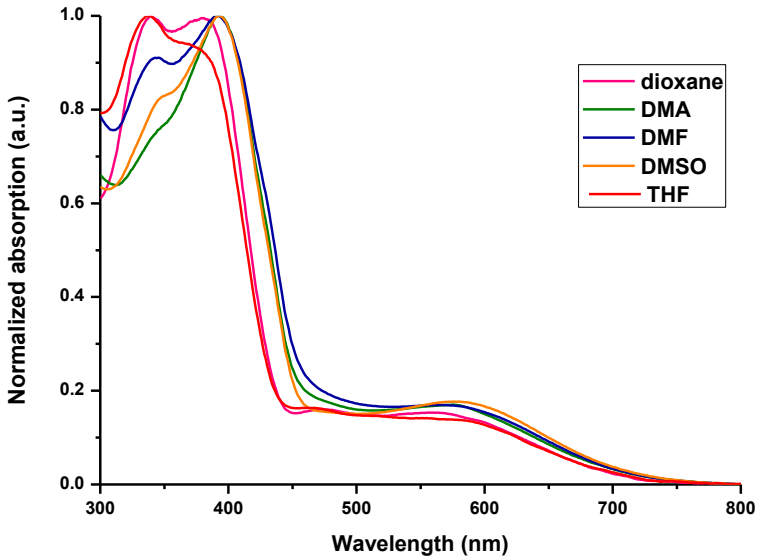
Solvatochromism of **A-D-A4** in solvents of different polarities.



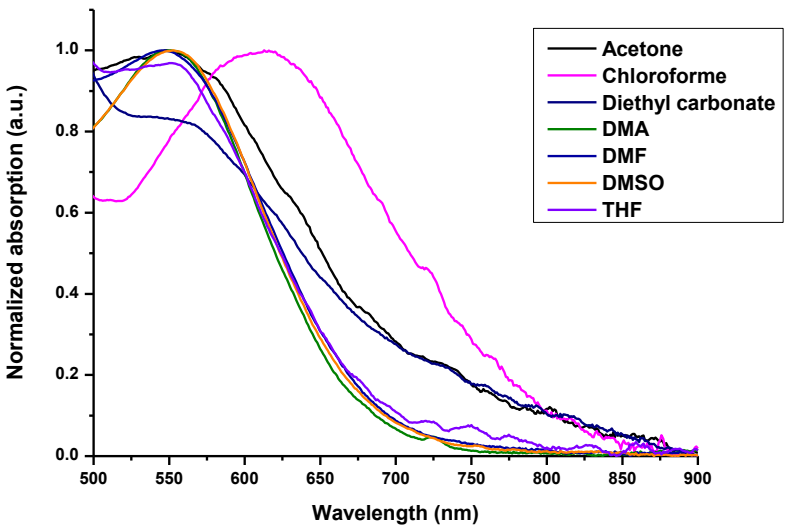
Solvatochromism of **A-D-A5** in solvents of different polarities.



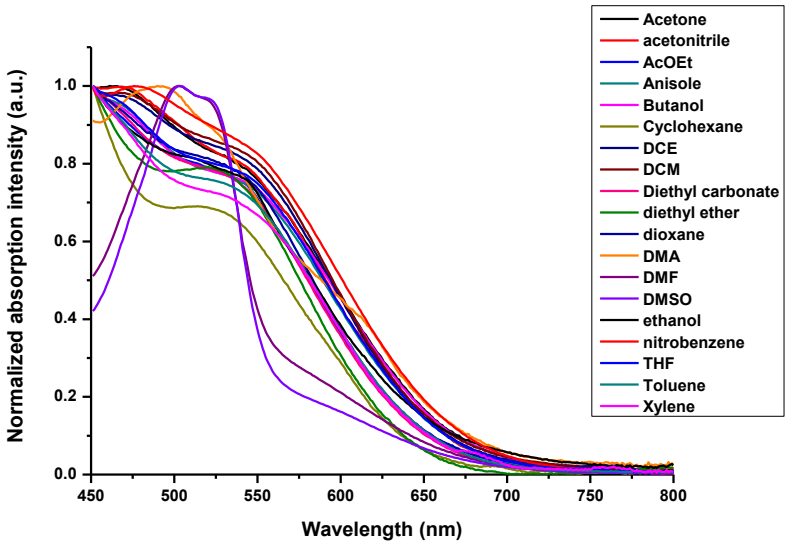
Solvatochromism of **A-D-A6** in solvents of different polarities.



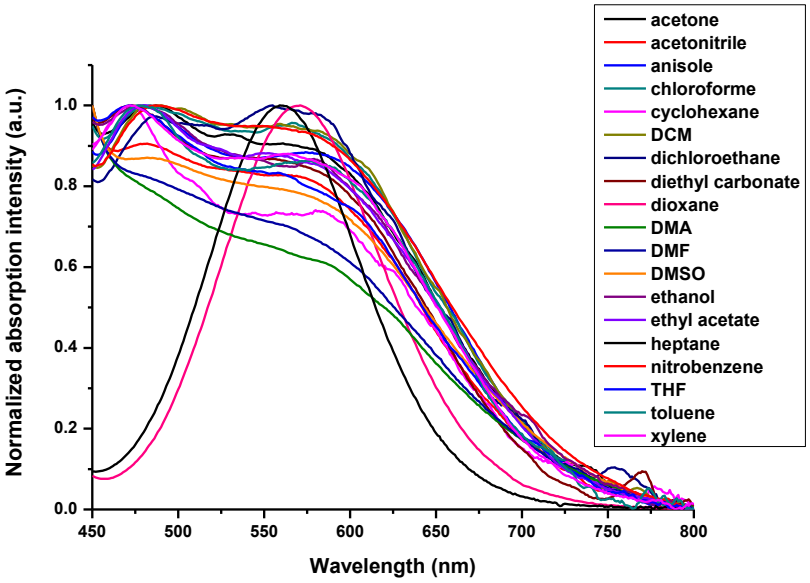
Solvatochromism of **A-D-A7** in solvents of different polarities.



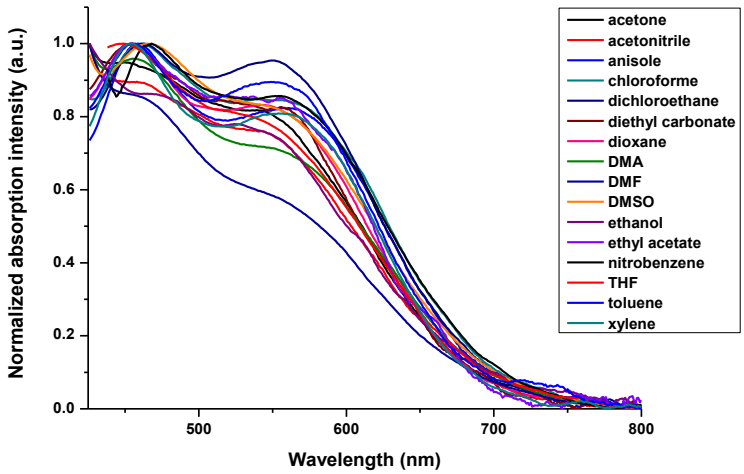
Solvatochromism of **A-D-A8** in solvents of different polarities.



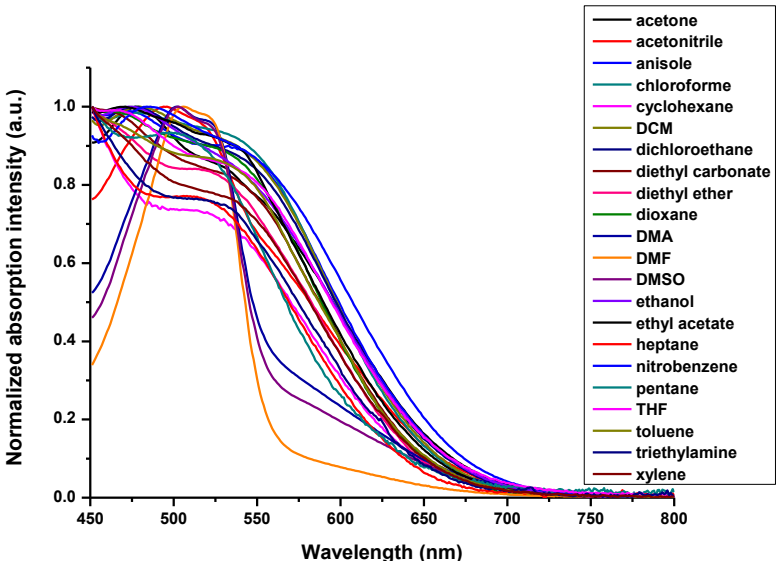
Solvatochromism of **A-D-A9** in solvents of different polarities.



Solvatochromism of **A-D-A10** in solvents of different polarities.



Solvatochromism of **A-D-A11** in solvents of different polarities.



Results of the multiple linear regression analyses

The position of the UV/Vis absorption maxima with regard to the dipolarity/polarizability π* and the hydrogen bonding capacity (α and β) of the solvent can be interpreted using the Kamlet–Taft equation :

$$\nu_{max}\,(cm^{-1}) = \nu_{max,0}\,(cm^{-1}) + a\alpha + b\beta + s\pi^*$$

Table S1. Solvent-independent correlation coefficients *a*, *b* and *s* of the Kamlet-Taft parameters α, β and π* respectively, correlation coefficient (*R*), significance (*F*), standard deviation (*SD*), and number of solvents (*n*) calculated for the solvatochromism.

Compounds	$\nu_{max,0}$	a	b	s	n	F	R^2	SD
D-A0	19397.985	-152.220	14.752	-615.842	22	2.16E-8	0.876	83.76
D-A1	18065.274	-145.299	-54.148	-584.088	22	2.905E-11	0.941	55.10
D-A2	16335.463	-141.341	119.959	-472.699	22	4.746E-4	0.640	117.08
D-A3	16359.532	174.111	141 .007	-161.85	22	0.273	0.199	141.48
D-A4	17075.671	-583.742	37.301	-1144.067	22	1.344E-6	0.822	187.01
D-A5	5.10634E6	-451512.60	-329497.42	-112394.43	22	1.93298E-4	0.745	60287.28
D-A6	18271.698	-1558.188	-297.845	-748.356	22	0.00305	0.570	298.39
D-A7	4.37842E6	-269114.210	-229795.710	205991.17	22	9.56595E-4	0.704	37578.50
D-A8	19302.557	-651.297	373.900	-871.147	22	3.929E-6	0.779	170.45
D-A9	17778.037	-258.40	341.029	-602.977	22	0.00606	0.529	169.71
D-A10	18549.04	-610.744	-262.648	-217.354	22	0.07316	0.328	208.07
D-A11	19258.929	-472.581	315.295	-872.447	22	3.555E-6	0.782	163.25

Results of the linear correlation analyses

The position of the UV/Vis absorption maxima with regard to the dipolarity/polarizability π* can be interpreted using a simplified version of the Kamlet–Taft equation :

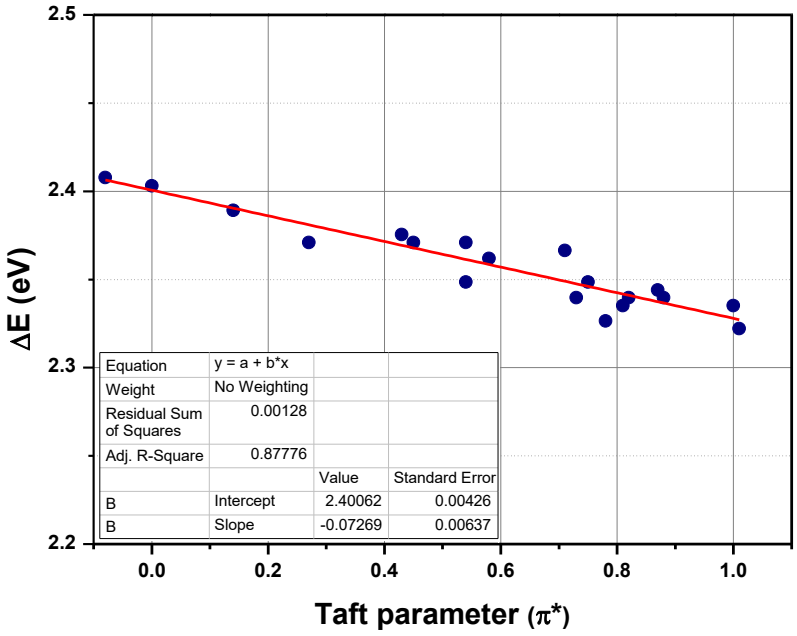
$$\nu_{max}\,(cm^{-1}) = \nu_{max,0}\,(cm^{-1}) + s\pi^*$$

Table S2. Solvent-independent correlation coefficient *s* of the Kamlet-Taft parameters π*

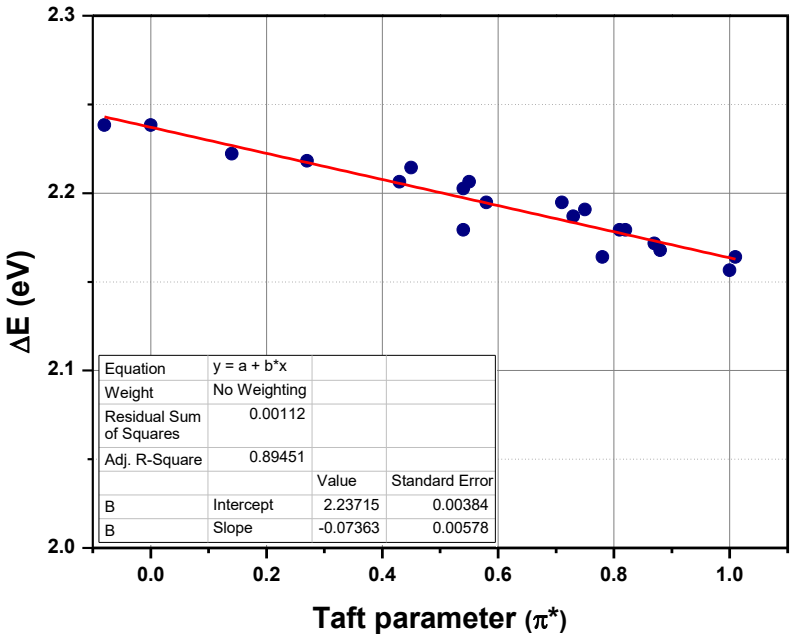
Compounds	s	$\nu_{max,0}$	R^2
D-A0	-0.07269	2.40062	0.878
D-A1	-0.07363	2.23715	0.894
D-A2	-0.05404	2.02674	0.523
D-A3	-0.02134	2.02604	0.073
D-A4	-0.14885	2.11821	0.826
D-A5	0.10006	1.98072	0.278
D-A6	-0.08202	2.22742	0.307
D-A7	-0.06049	2.30174	0.102
D-A8	-0.13460	2.40843	0.926
D-A9	-0.07534	2.21322	0.794
D-A10	-0.04924	2.30534	0.821
D-A11	-0.13447	2.400346	0.950

Position of the absorption maxima of dyes in 22 solvents of different polarities vs. the Kamlet–Taft parameters π*

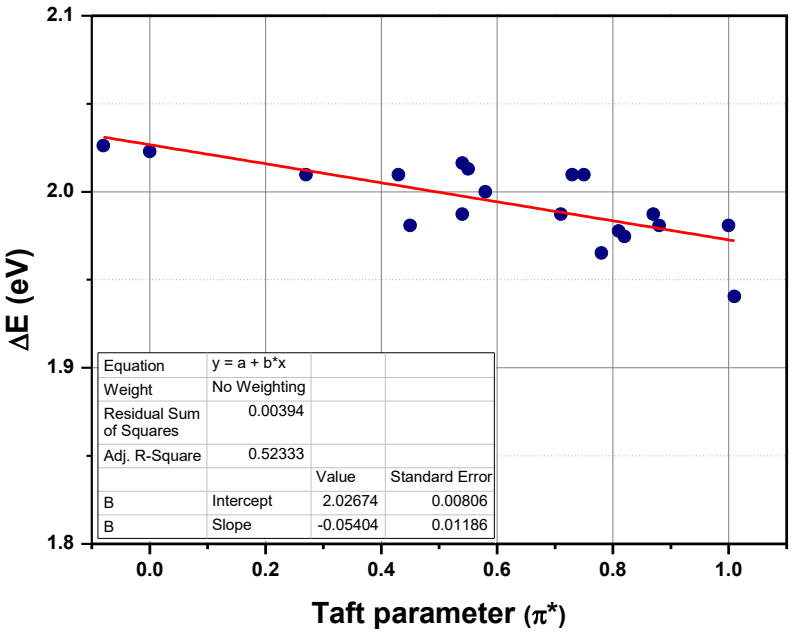
Compound D-A0



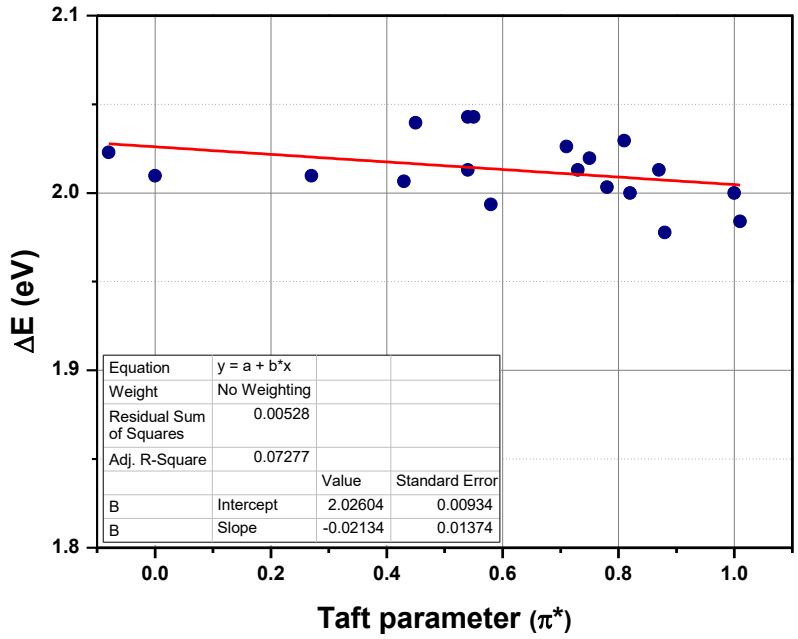
Compound D-A1



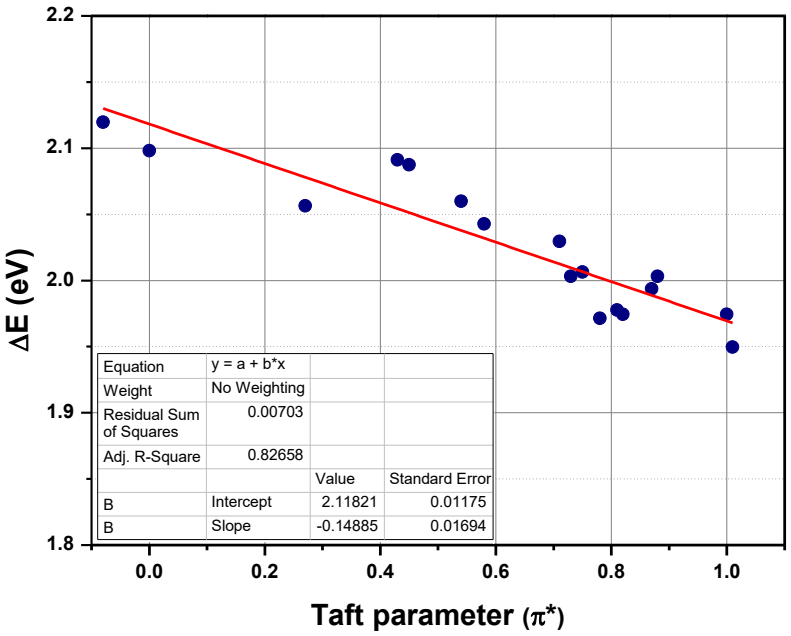
Compound D-A2



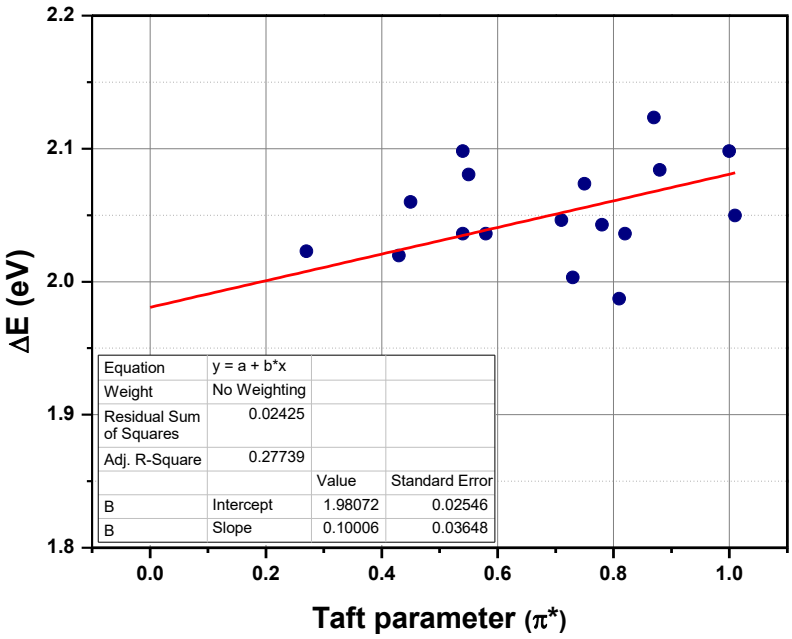
Compound D-A3



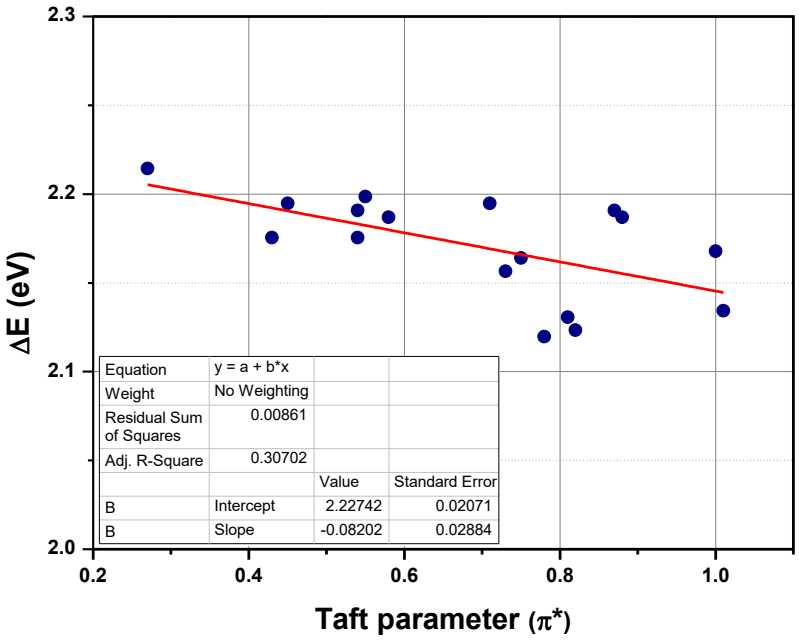
Compound D-A4



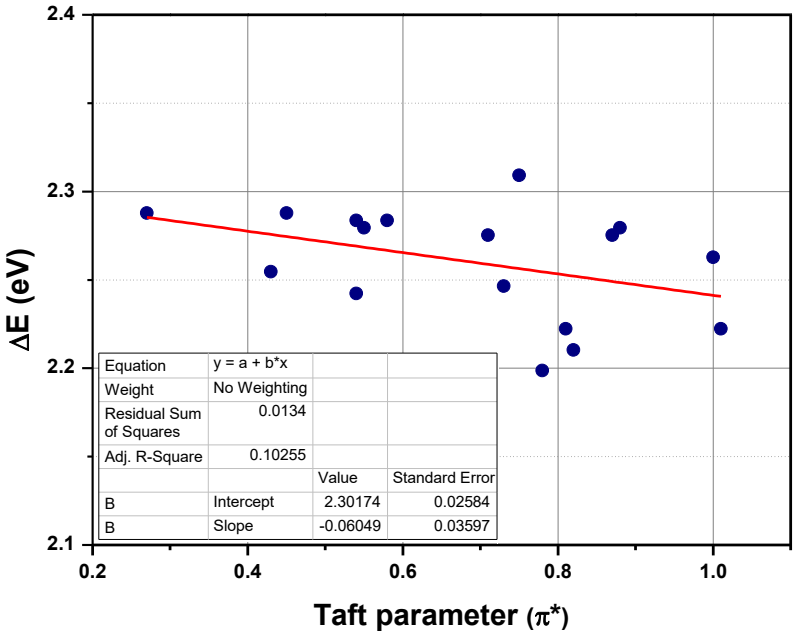
Compound D-A5



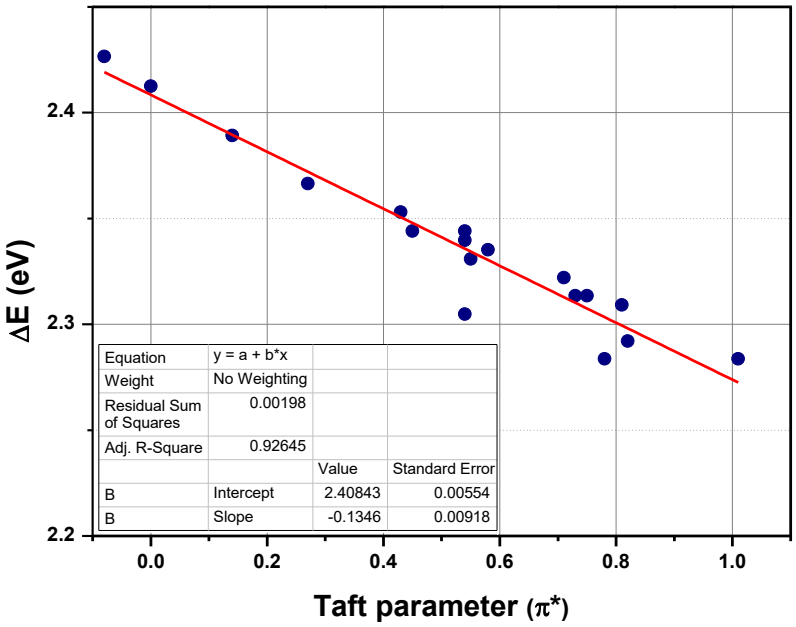
Compound D-A6



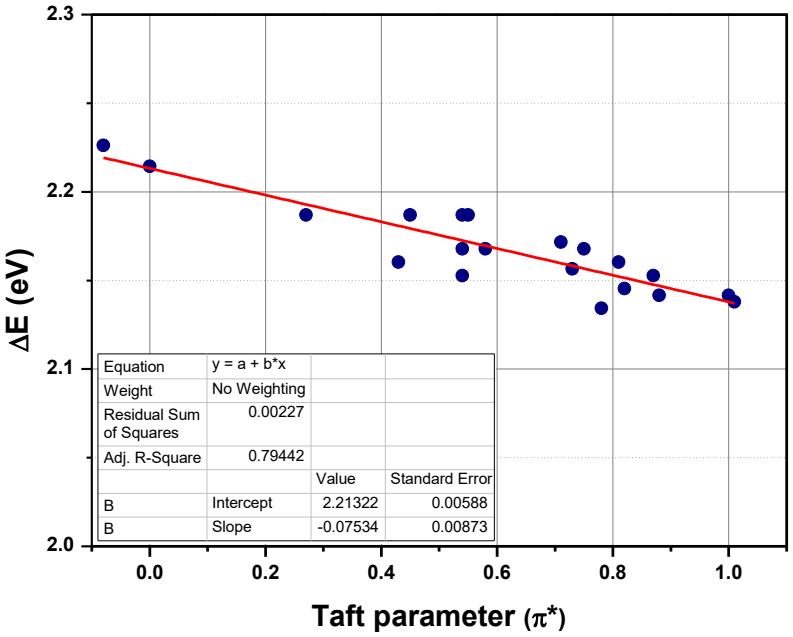
Compound D-A7



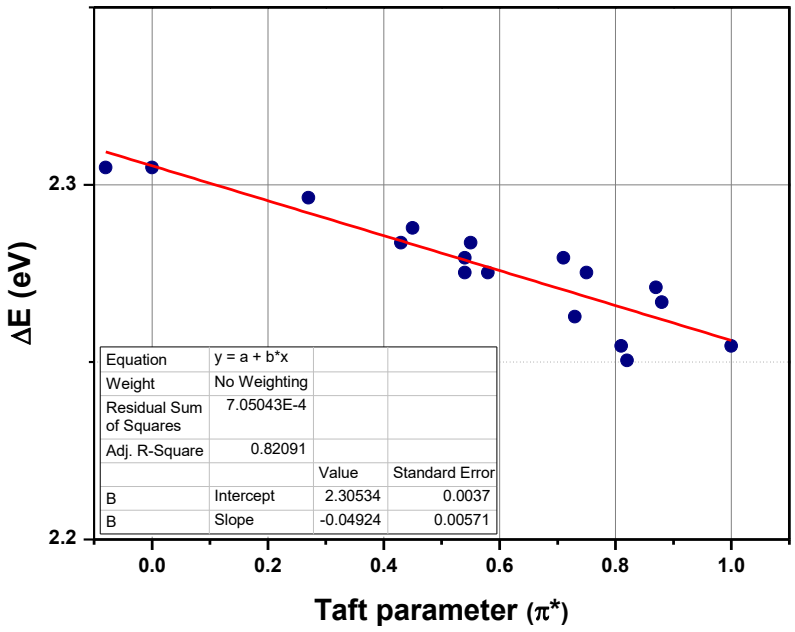
Compound D-A8



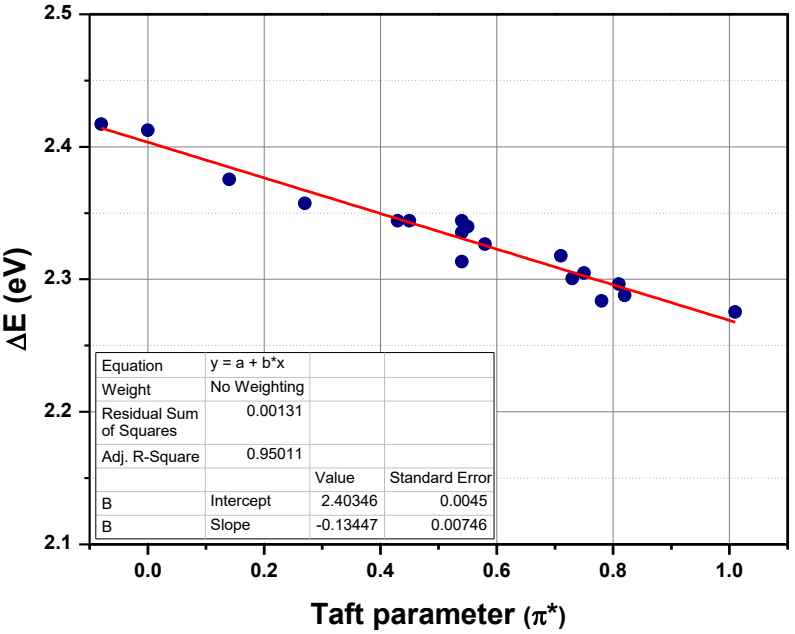
Compound D-A9



Compound D-A10



Compound D-A11



Results of the linear correlation analyses

The position of the UV/Vis absorption maxima with regard to the dipolarity/polarizability π* can also be interpreted using a Catalan parameters, namely, the solvent dipolarity (SdP) and the solvent polarity/polarizability (SPP) using the following equations :

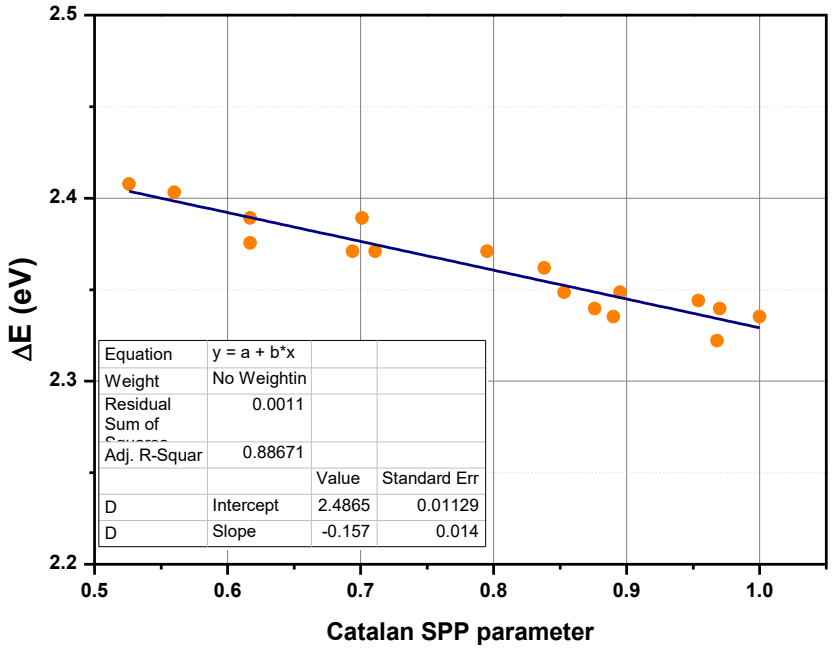
$$\nu_{max}\,(cm^{-1}) = \nu_{max,02}\,(cm^{-1}) + b \times SPP$$

Table S3. Solvent-independent correlation coefficients a and b of the Catalan parameters SdP and SPP.

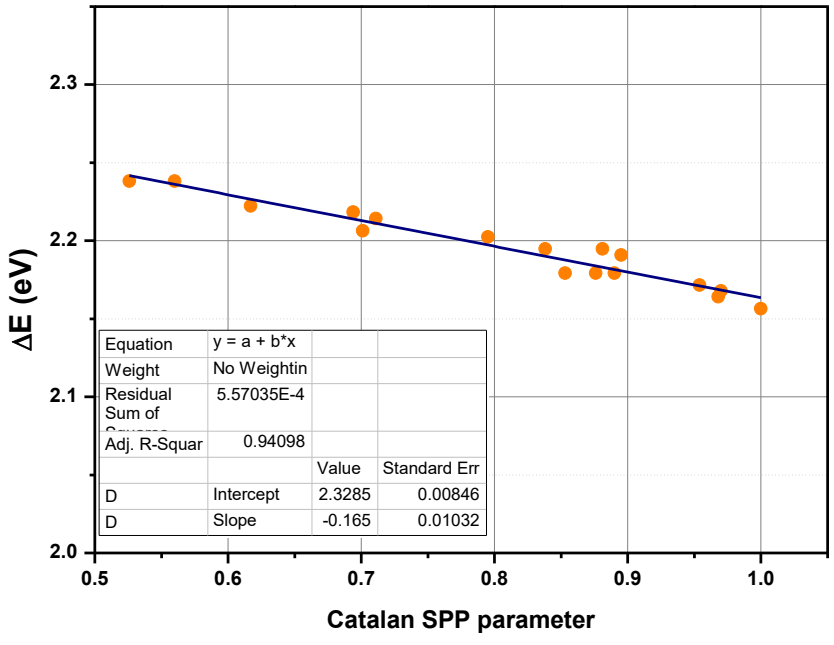
Compounds	$\nu_{max,02}$	b	R^2
D-A0	2.4865	-0.157	0.887
D-A1	2.3285	-0.165	0.940
D-A2	2.0749	-0.099	0.821
D-A3	2.052	-0.048	0.092
D-A4	2.2856	-0.316	0.817
D-A5	1.8327	0.2513	0.046
D-A6	2.2418	-0.080	0.081
D-A7	2.3053	-0.053	0.071
D-A8	2.5457	-0.270	0.809
D-A9	2.3121	-0.172	0.900
D-A10	2.3476	-0.089	0.646
D-A11	2.5440	-0.274	0.860

Position of the absorption maxima of dyes in 22 solvents of different polarities vs. the Catalan parameter SPP

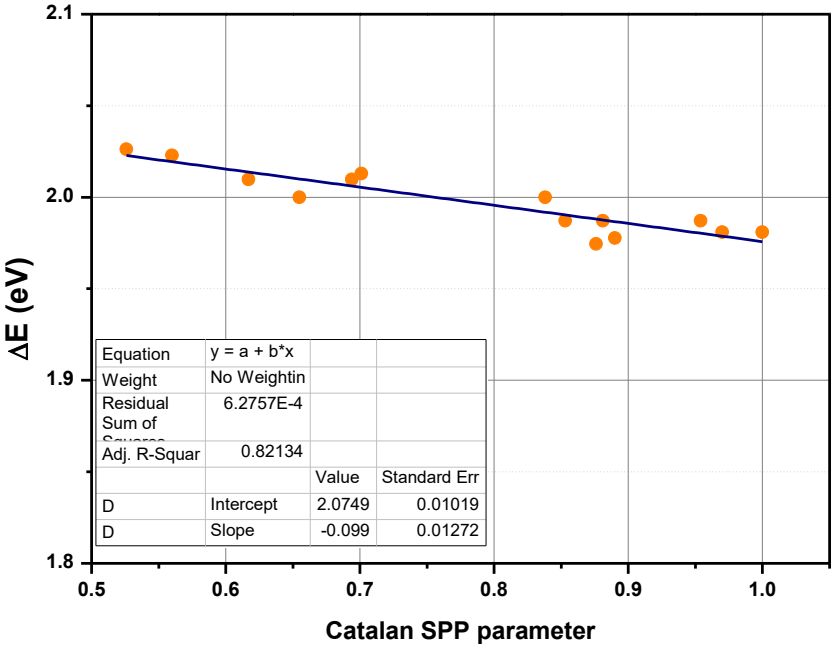
Compound D-A0



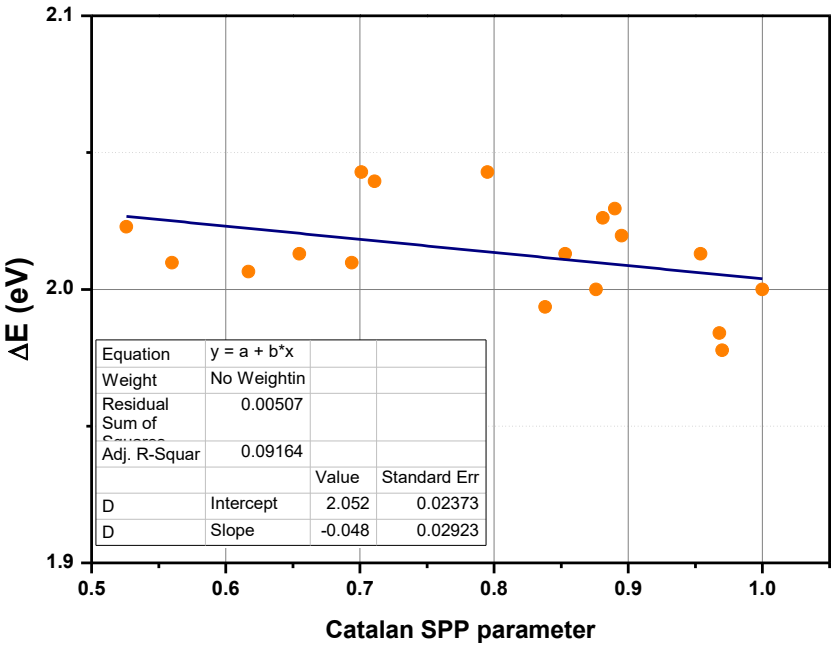
Compound D-A1



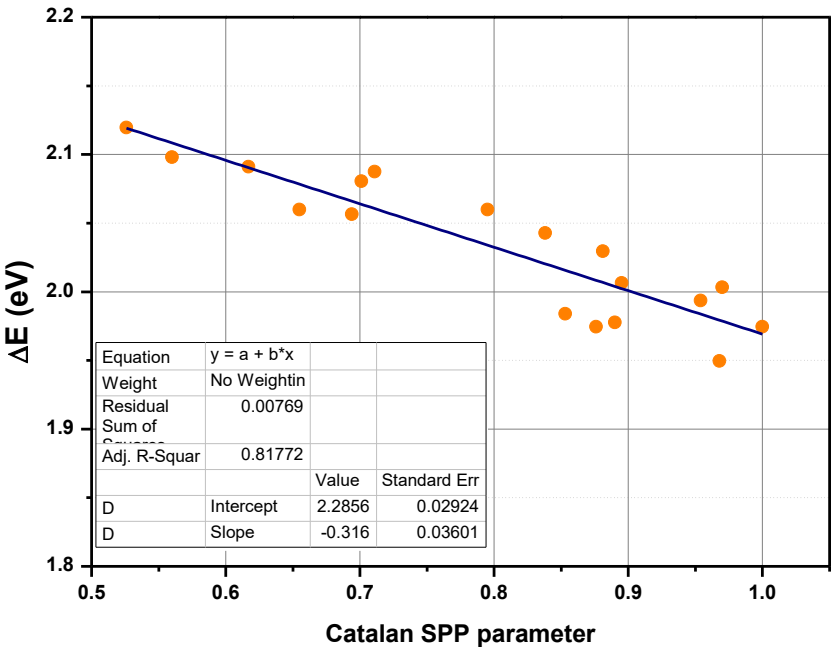
Compound D-A2



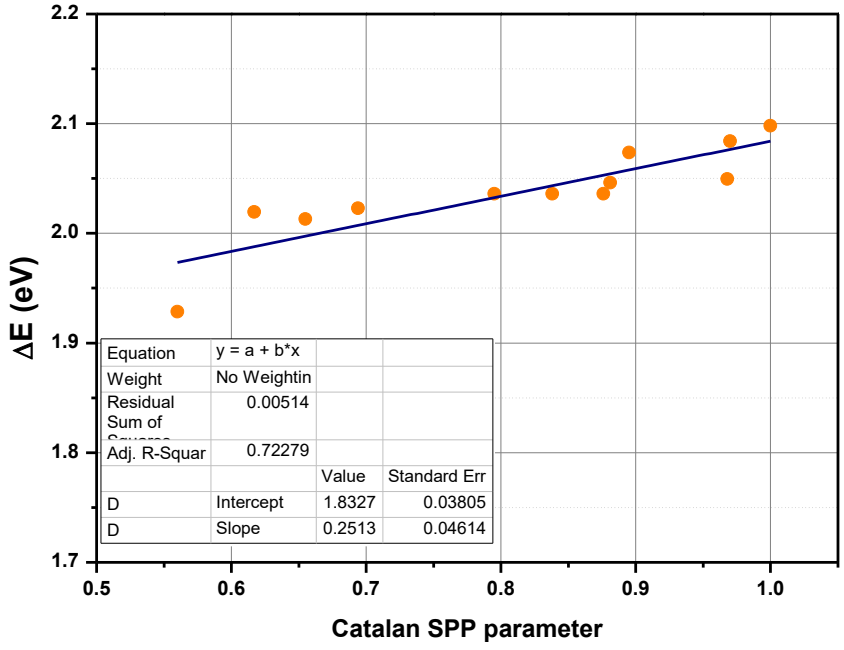
Compound D-A3



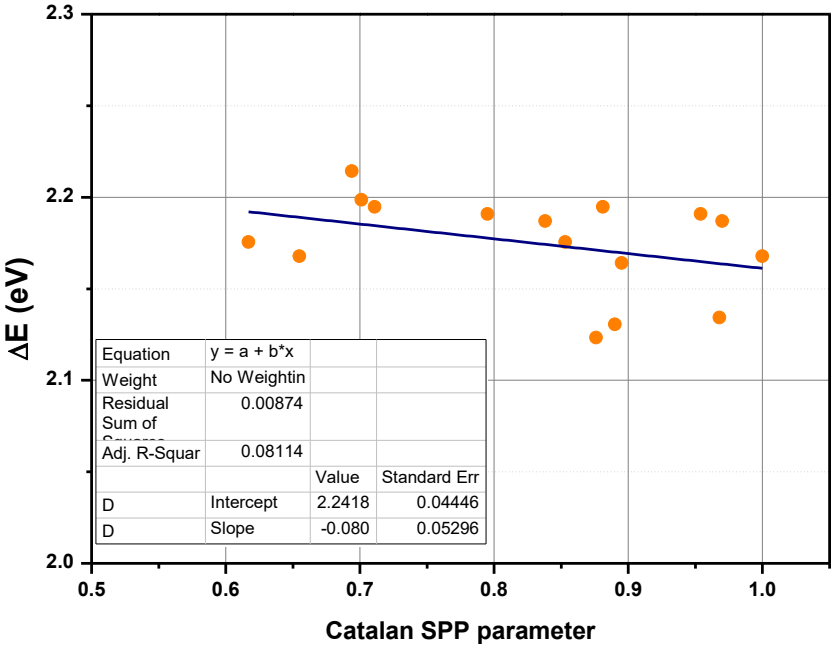
Compound D-A4



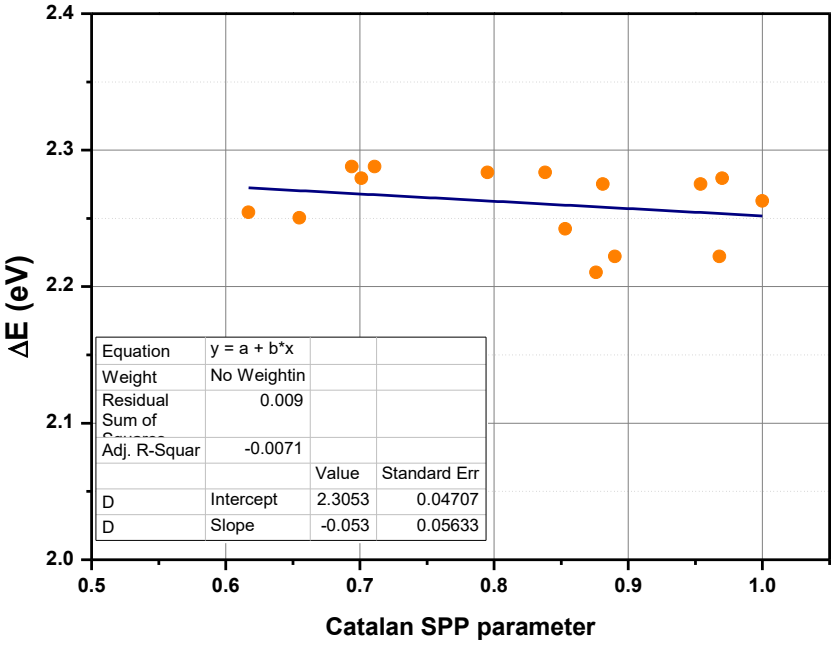
Compound D-A5



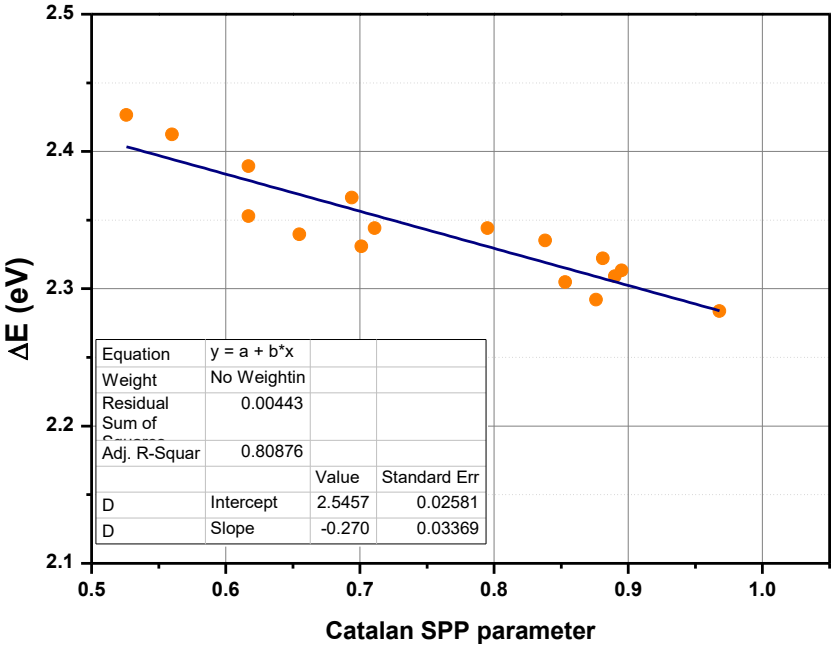
Compound D-A6



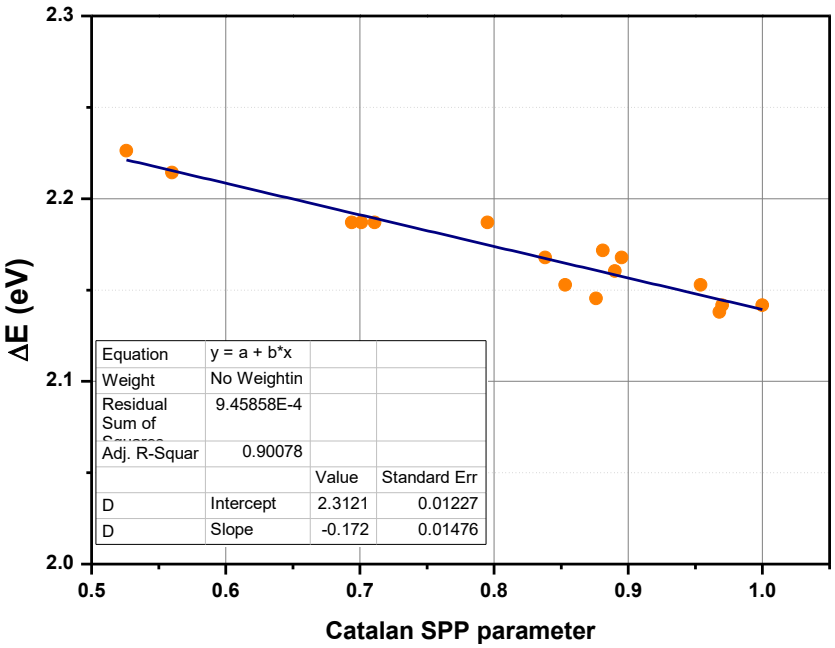
Compound D-A7



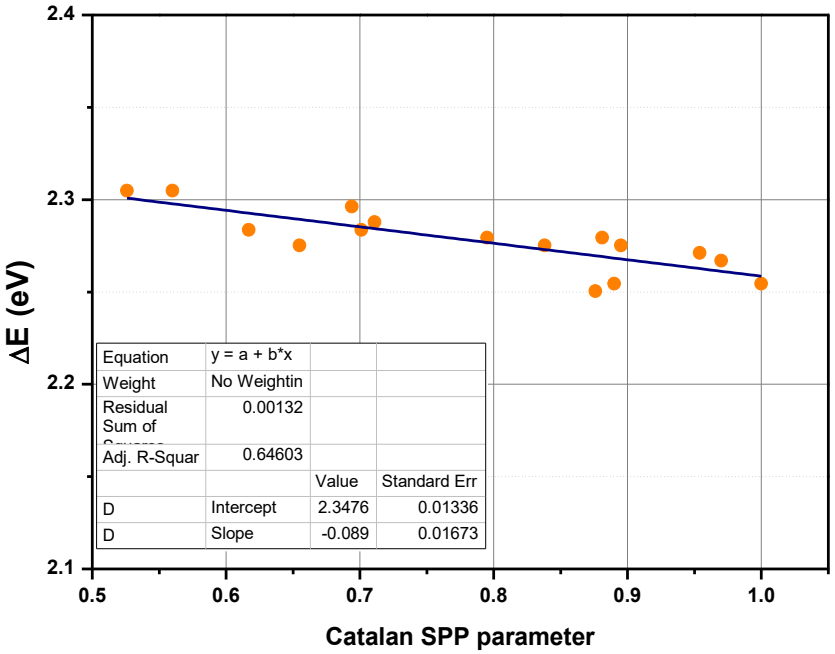
Compound D-A8



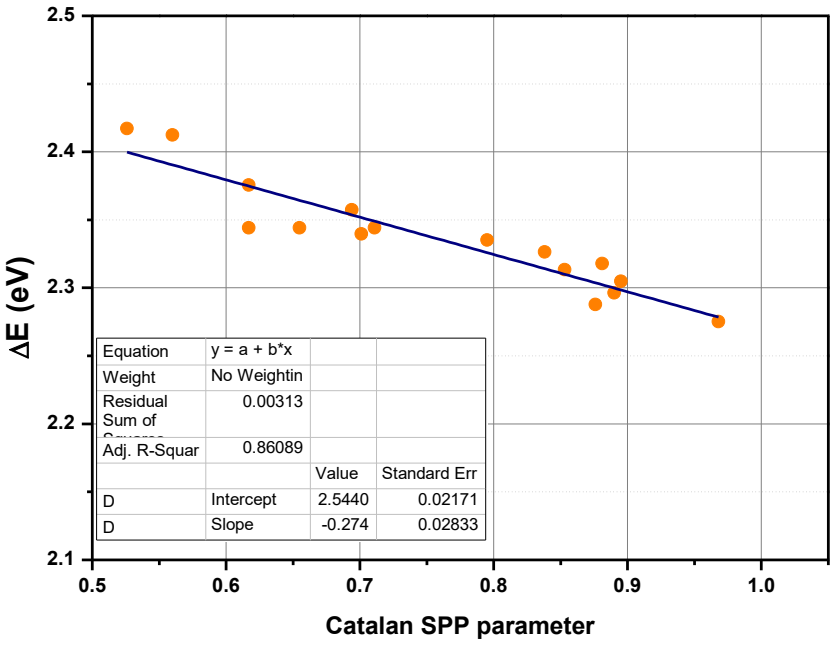
Compound D-A9



Compound D-A10



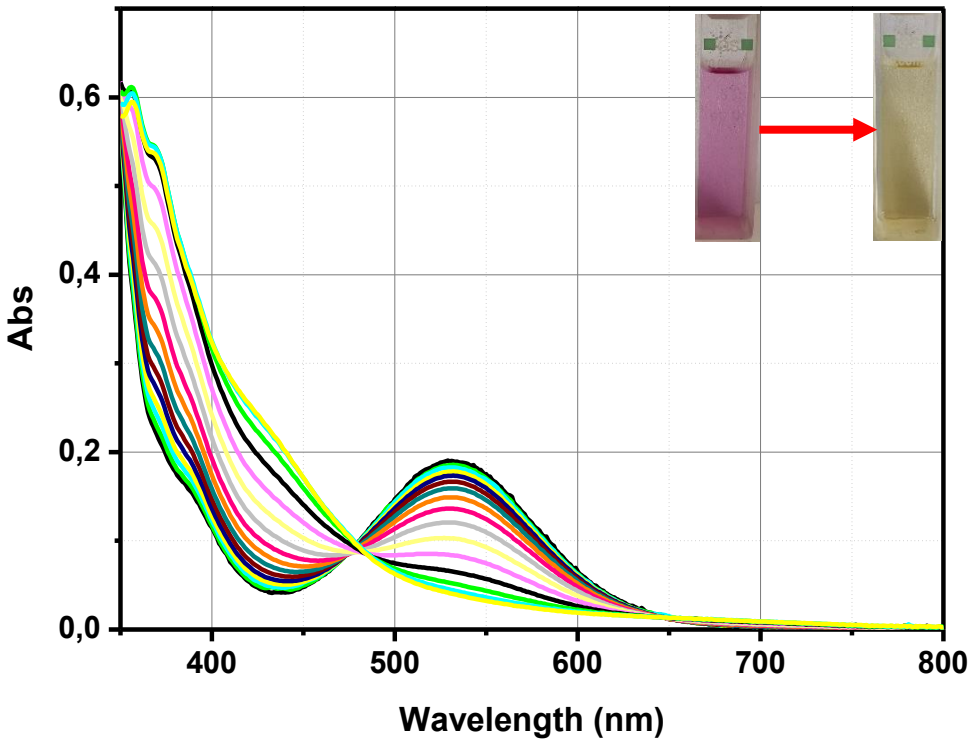
Compound D-A11



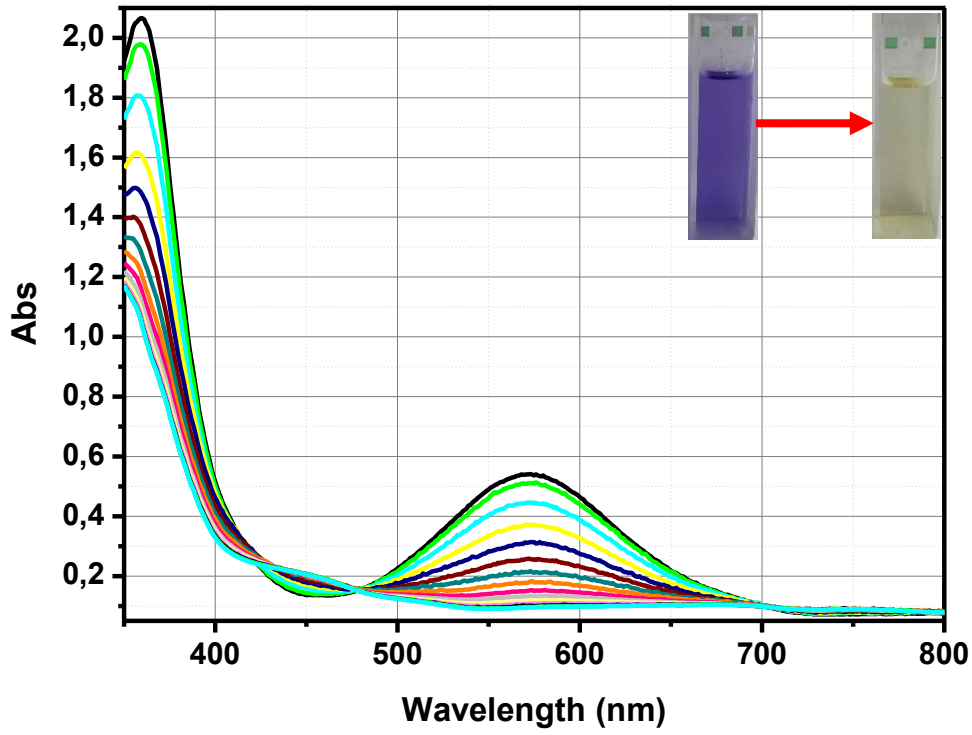
UV-visible absorption spectra of dyes recorded during the kinetics of discoloration in dichloromethane while using nitrosonium cation as the oxidizing agent.

UV-visible absorption spectra presented in the following figures have been recorded with a delay of 1 minute between each spectrum.

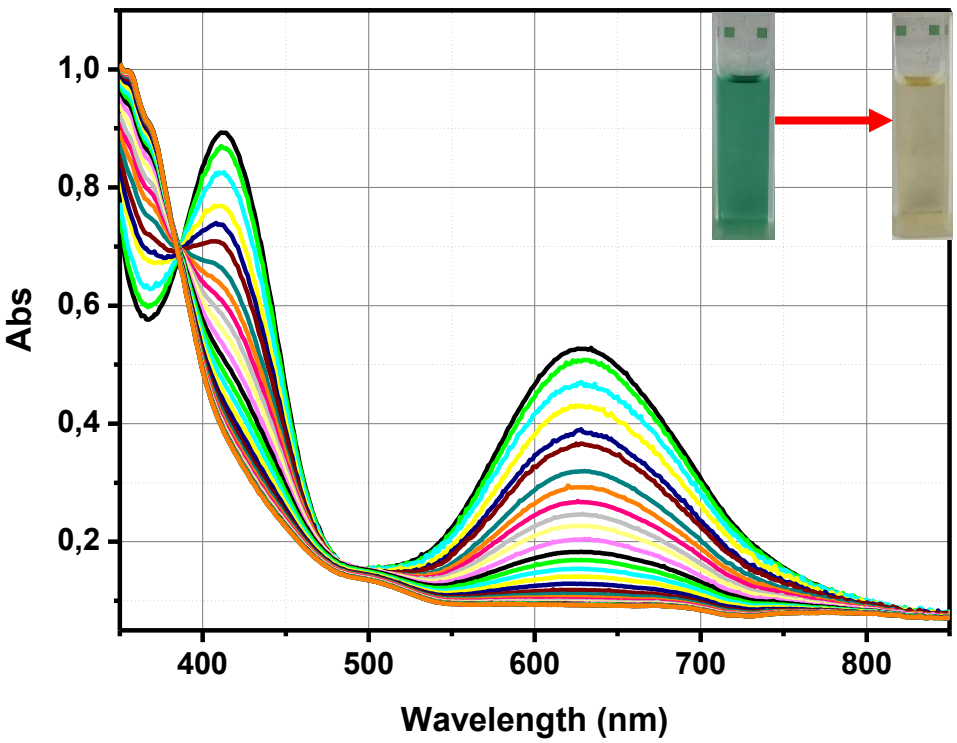
Compound D-A0



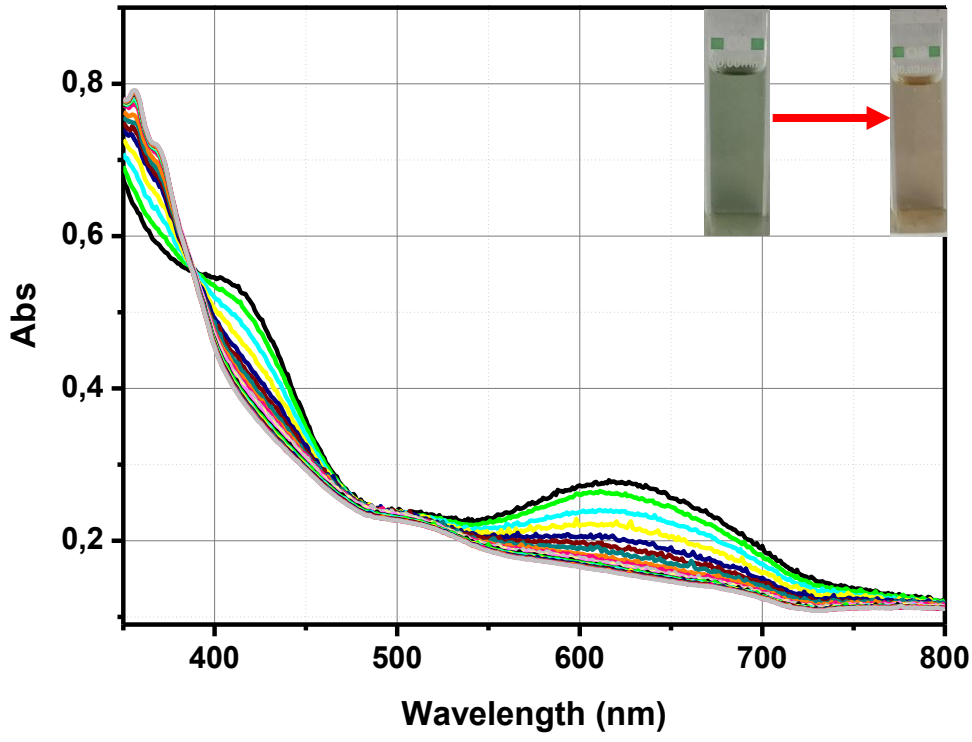
Compound D-A1



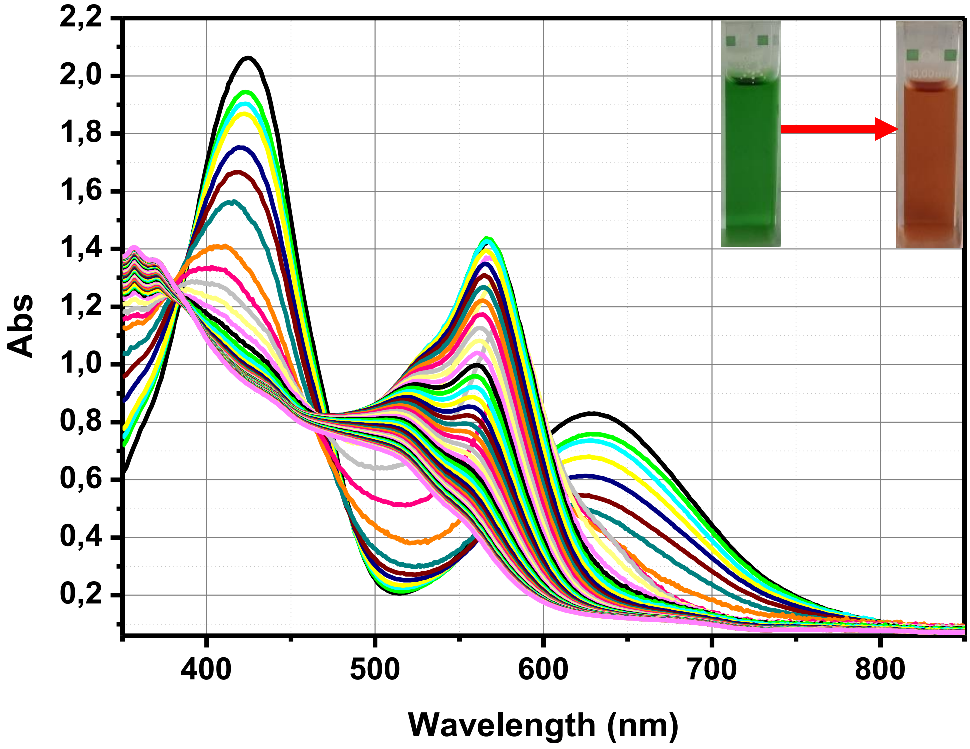
Compound D-A2

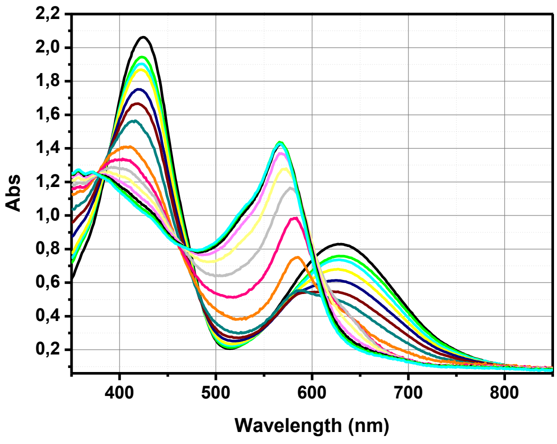


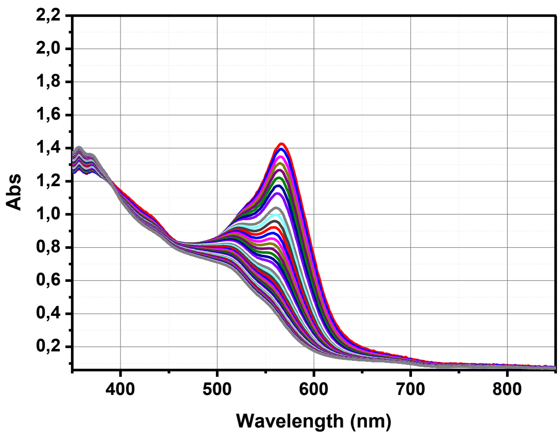
Compound D-A3



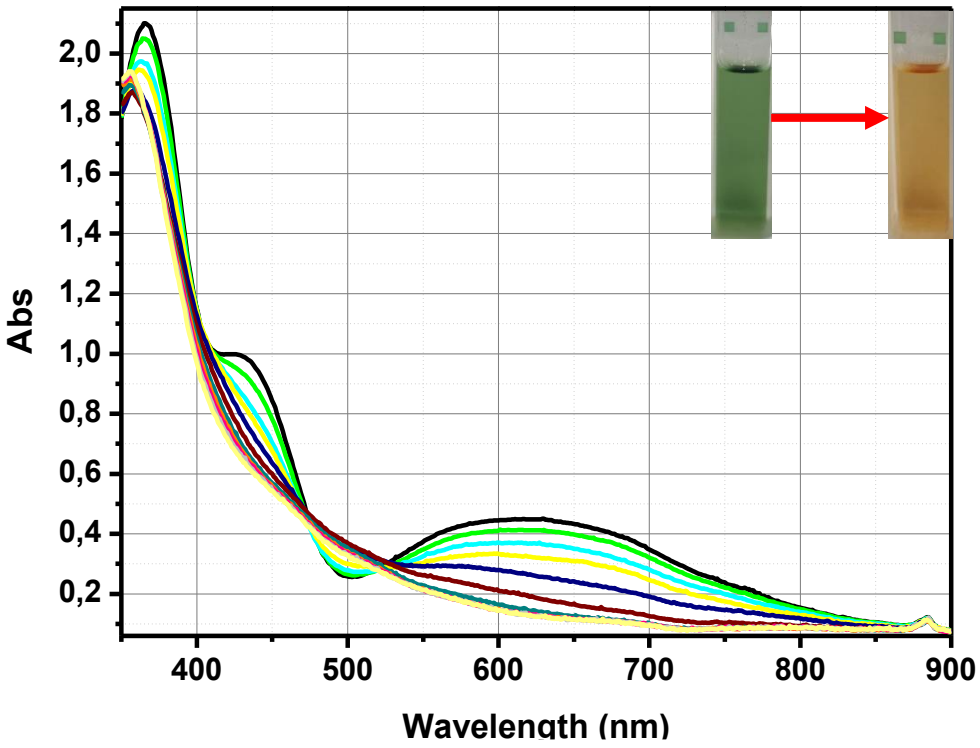
Compound D-A4



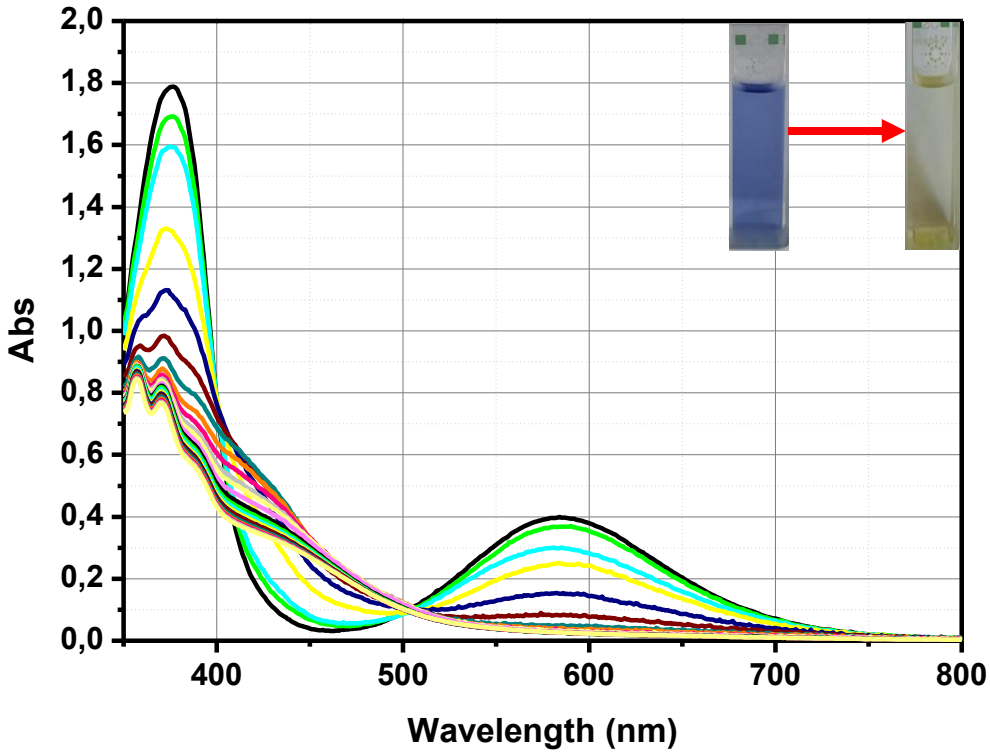




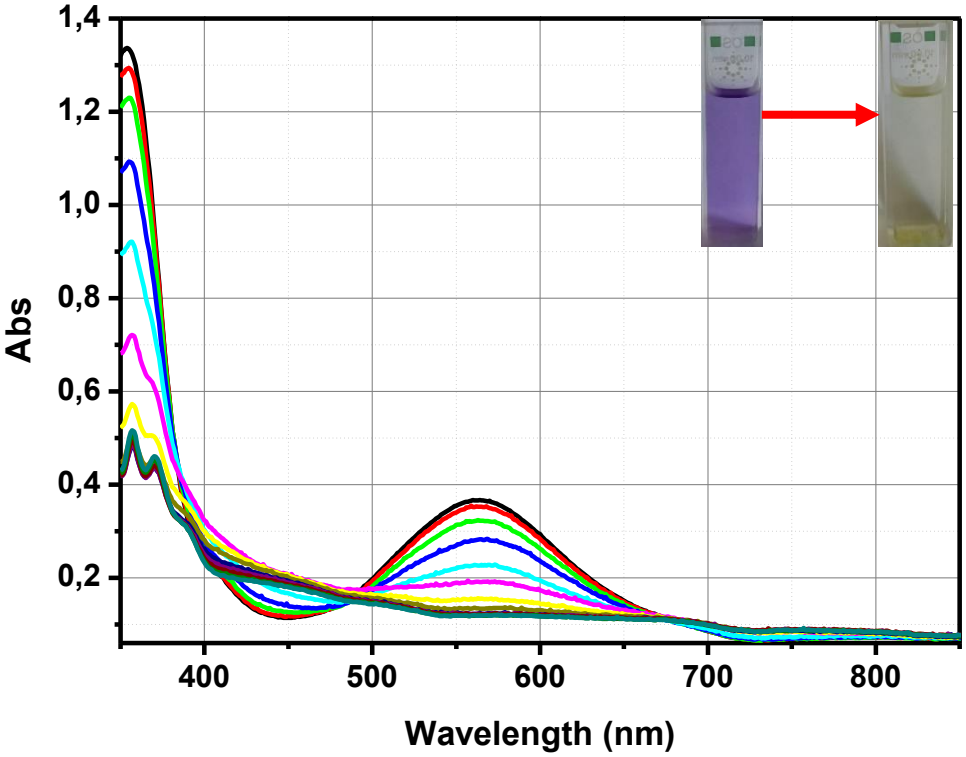
Compound D-A5



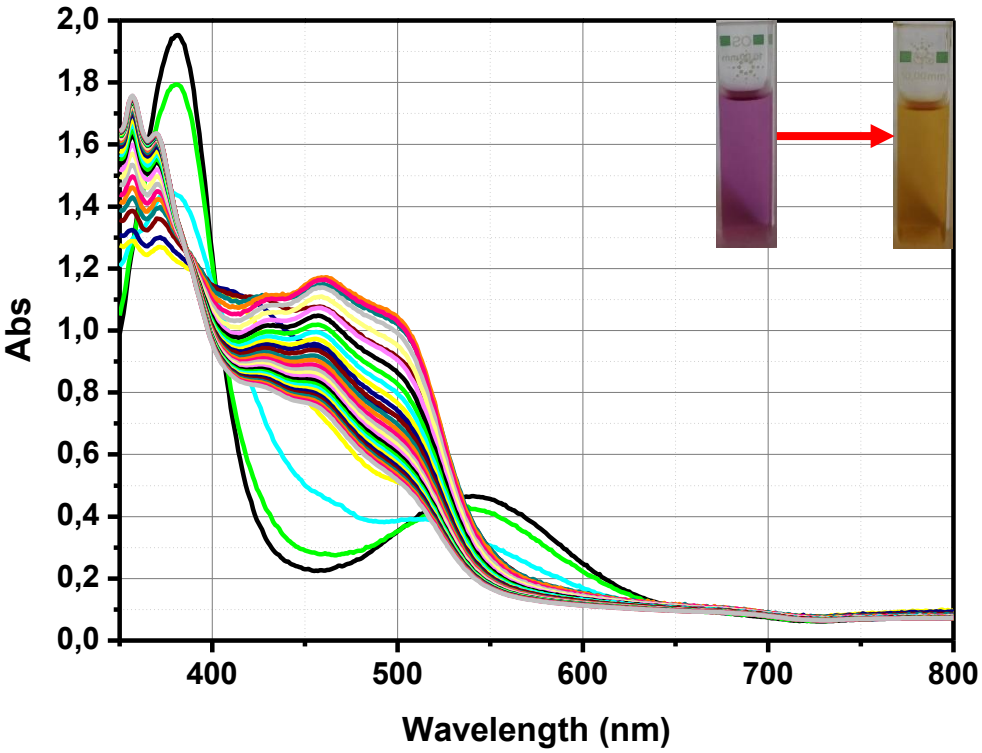
Compound D-A6



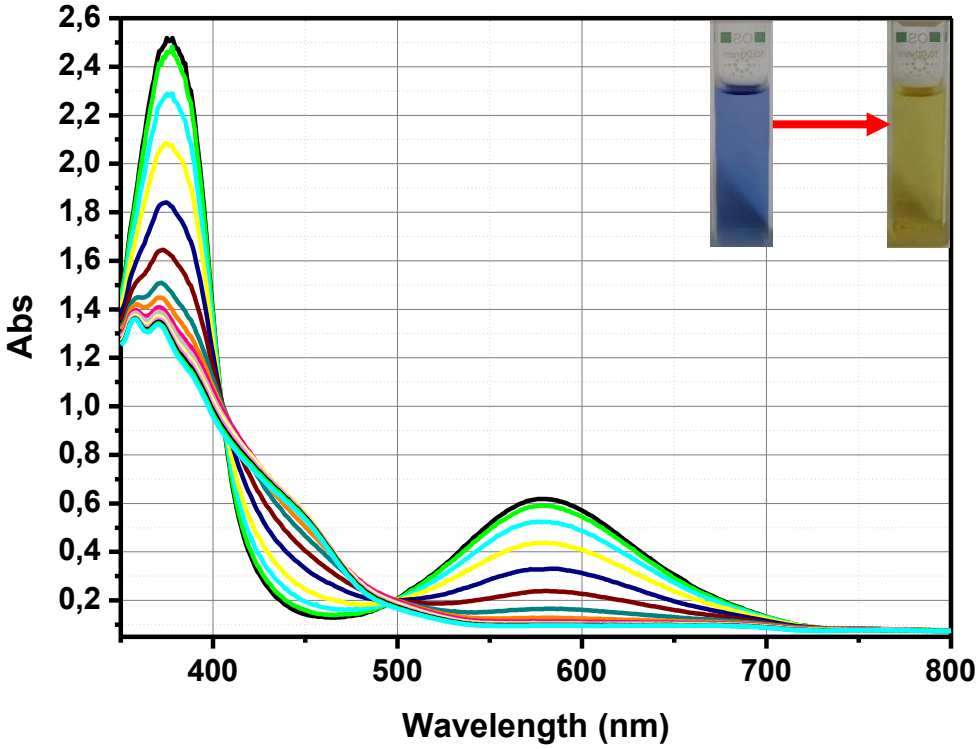
Compound D-A7



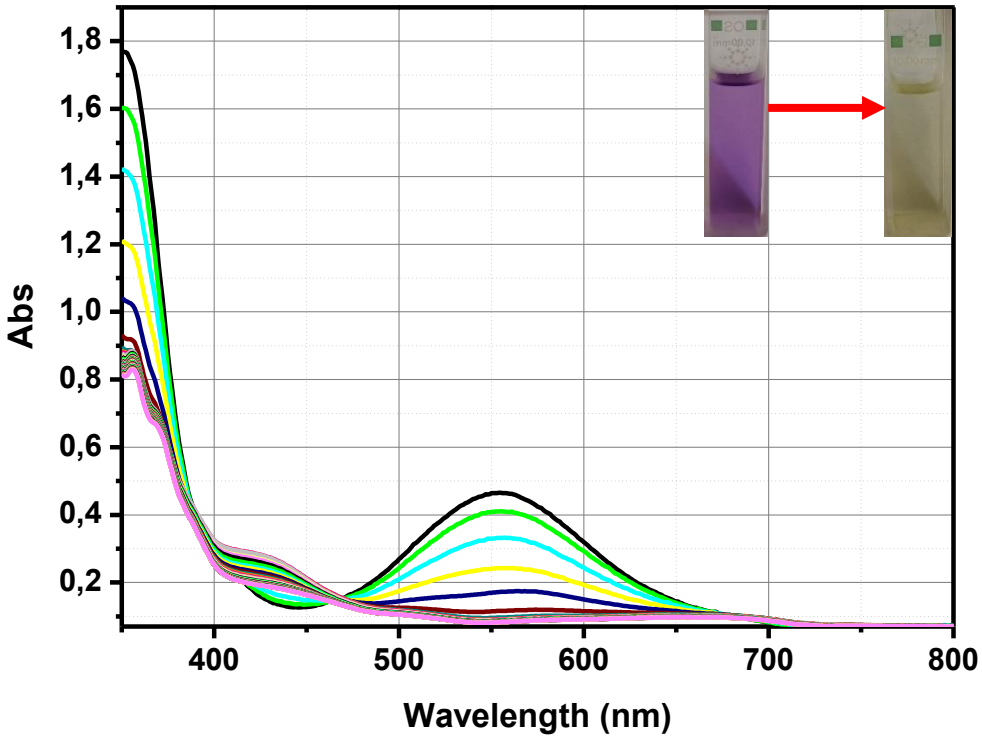
Compound D-A8



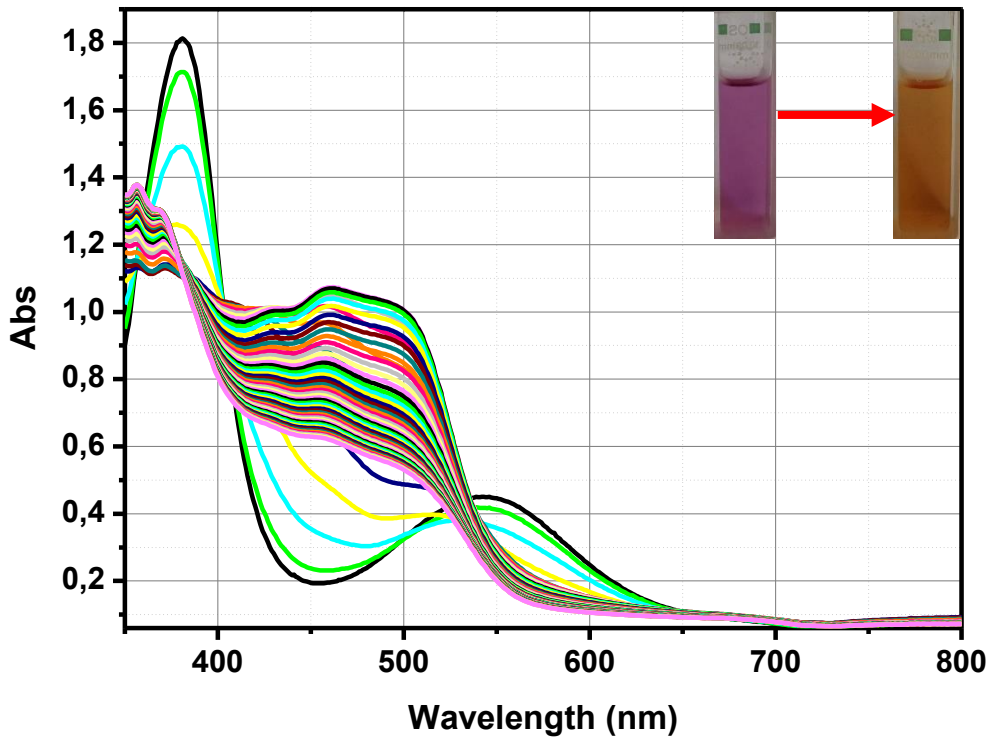
Compound D-A9



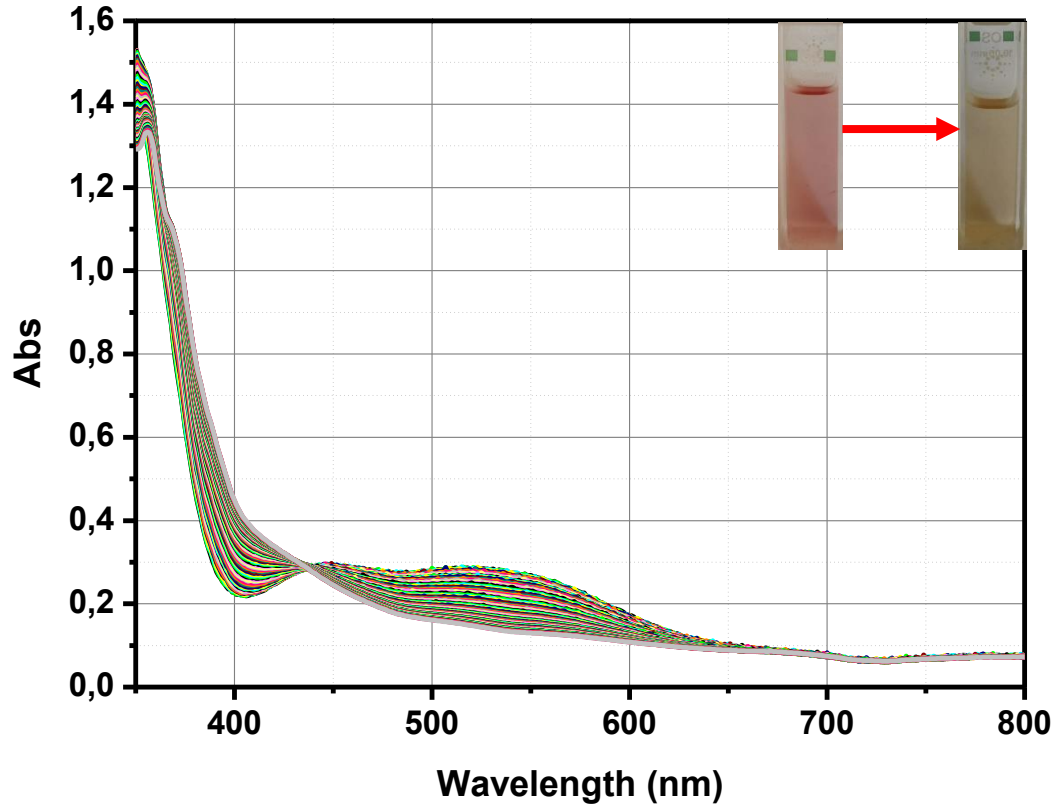
Compound D-A10



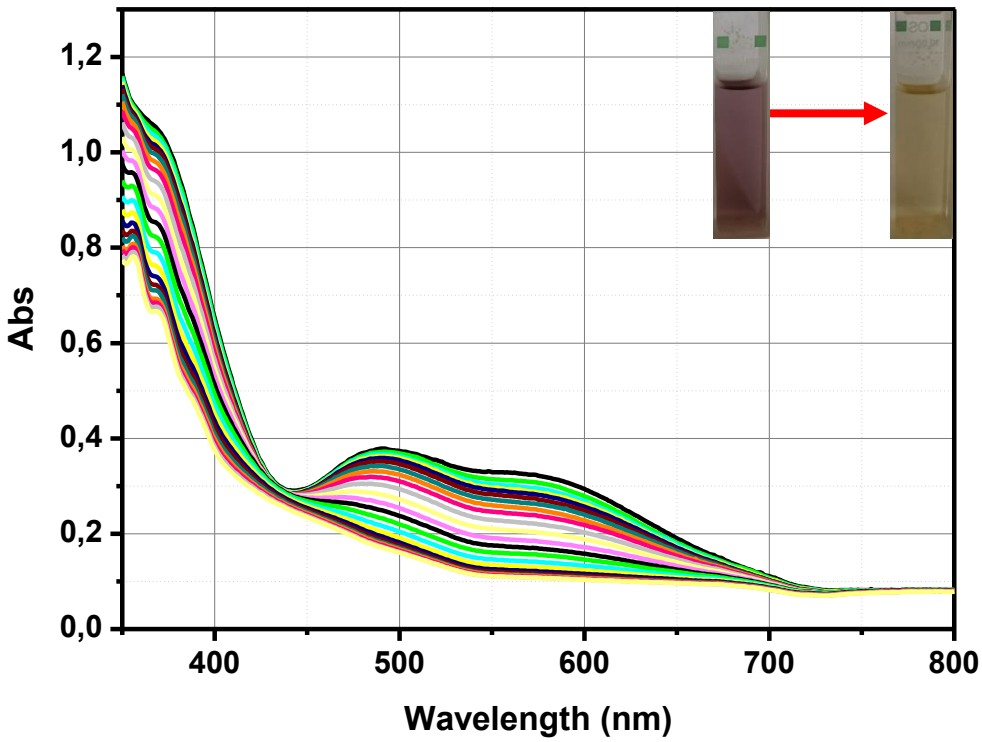
Compound D-A11



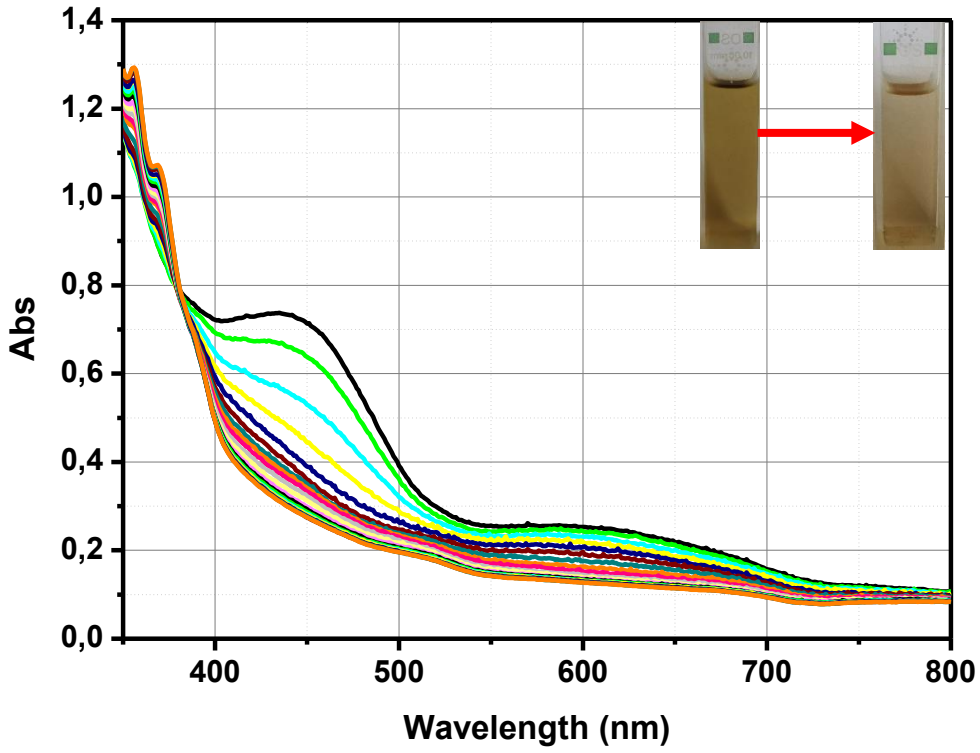
Compound A-D-A0



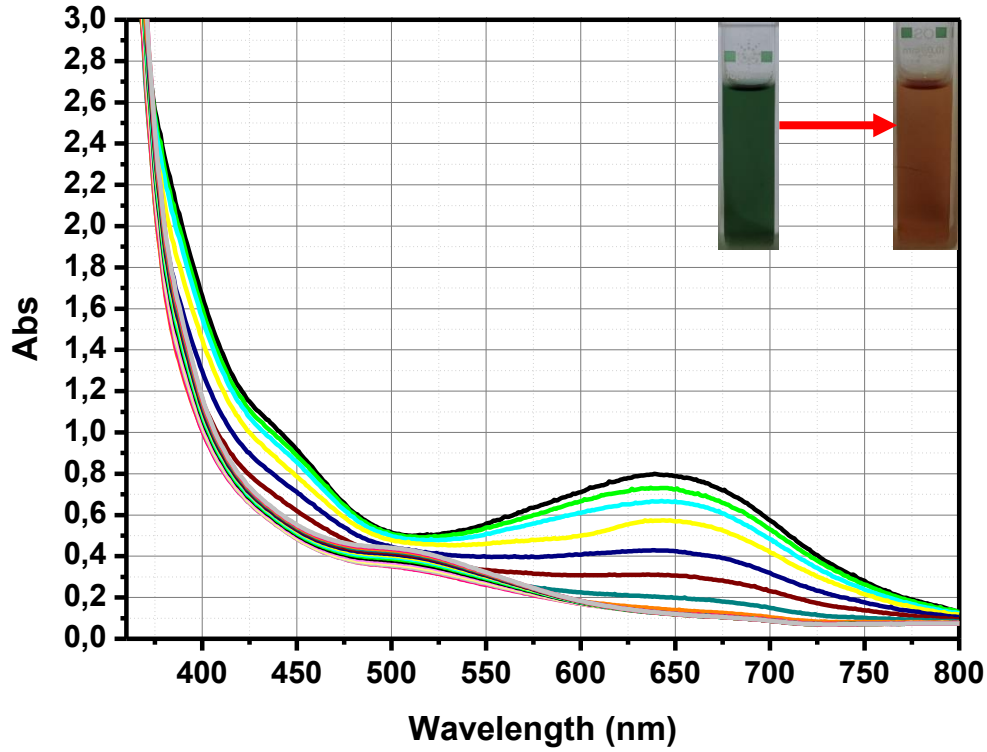
Compound A-D-A1



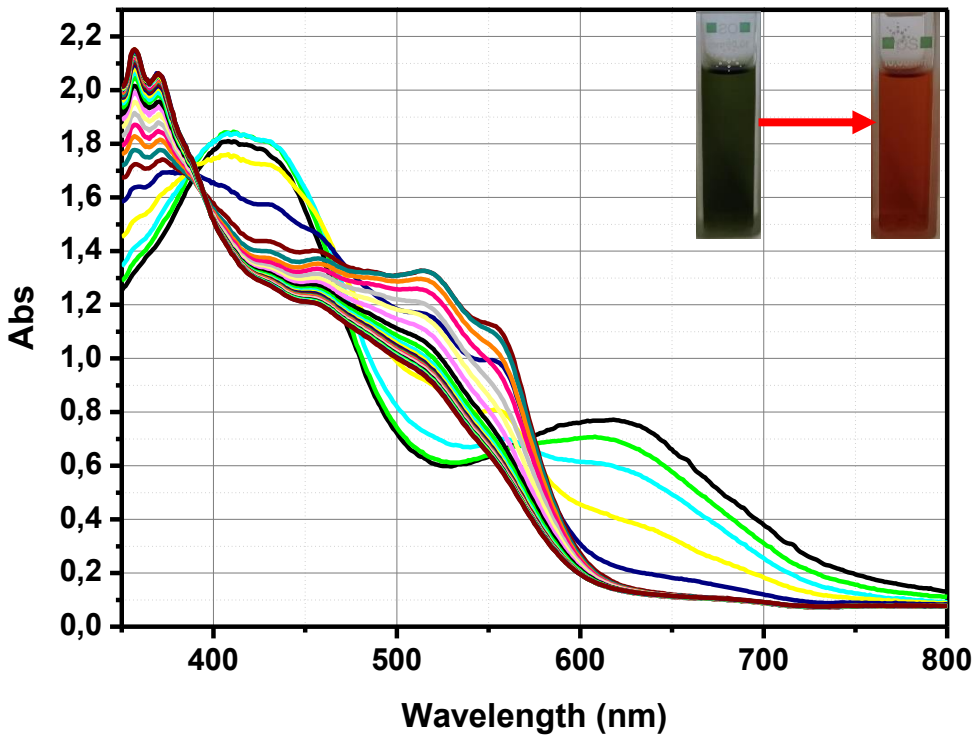
Compound A-D-A2



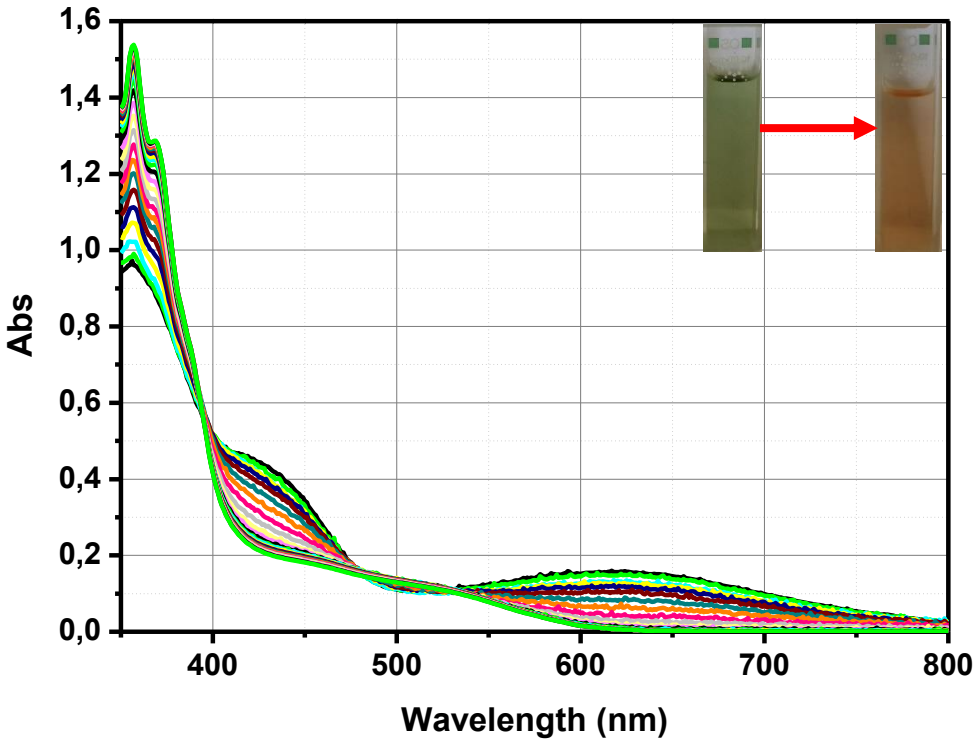
Compound A-D-A3



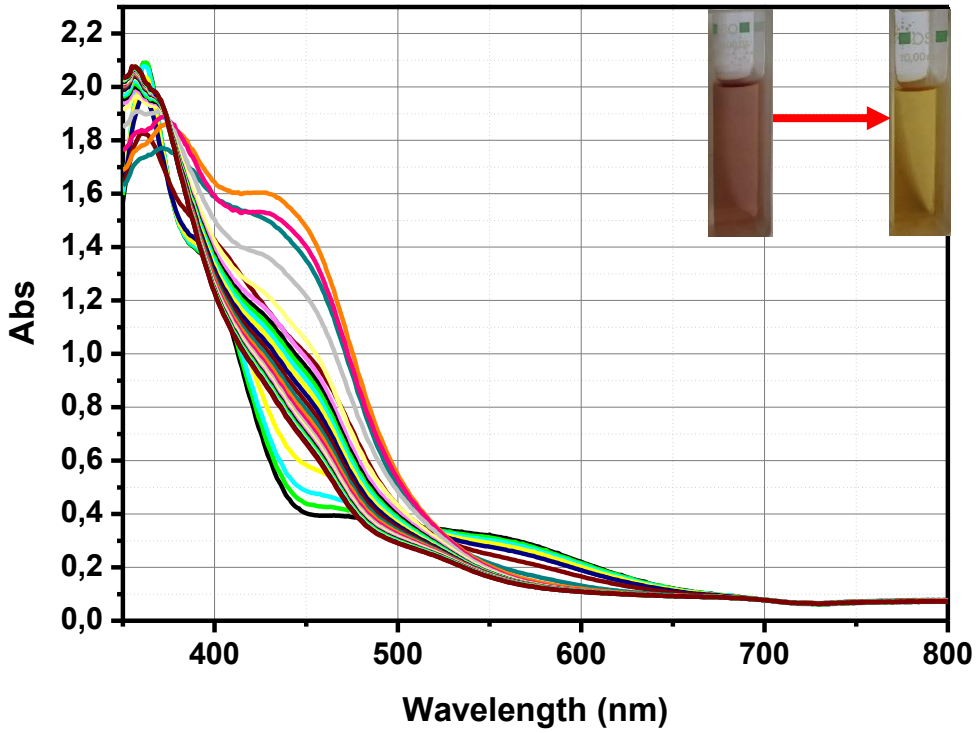
Compound A-D-A4



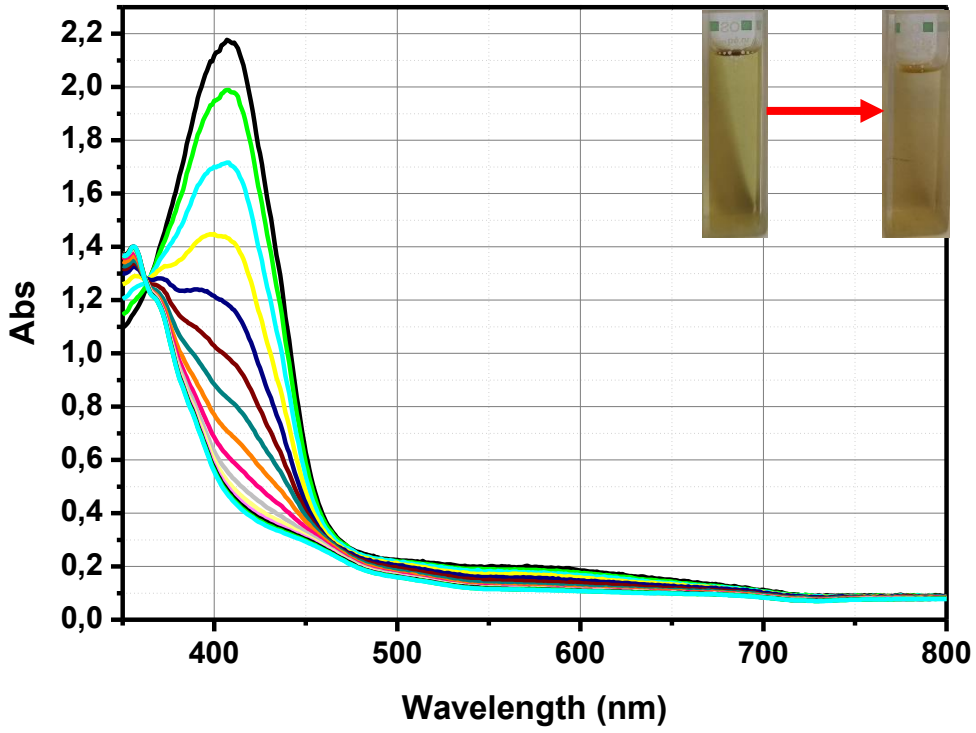
Compound A-D-A5



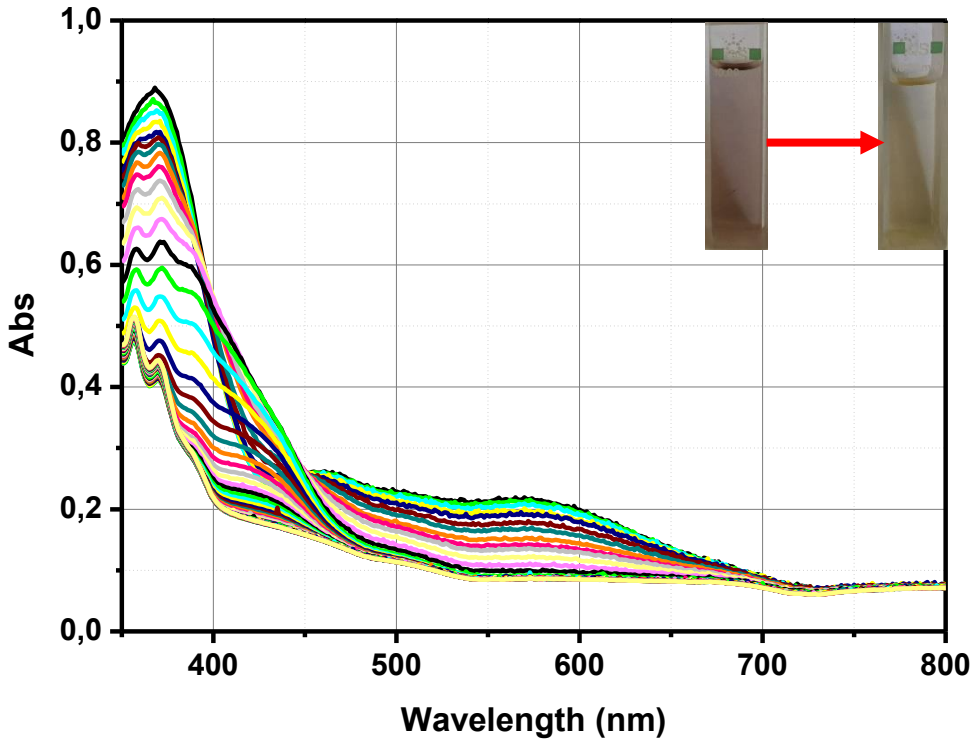
Compound A-D-A8



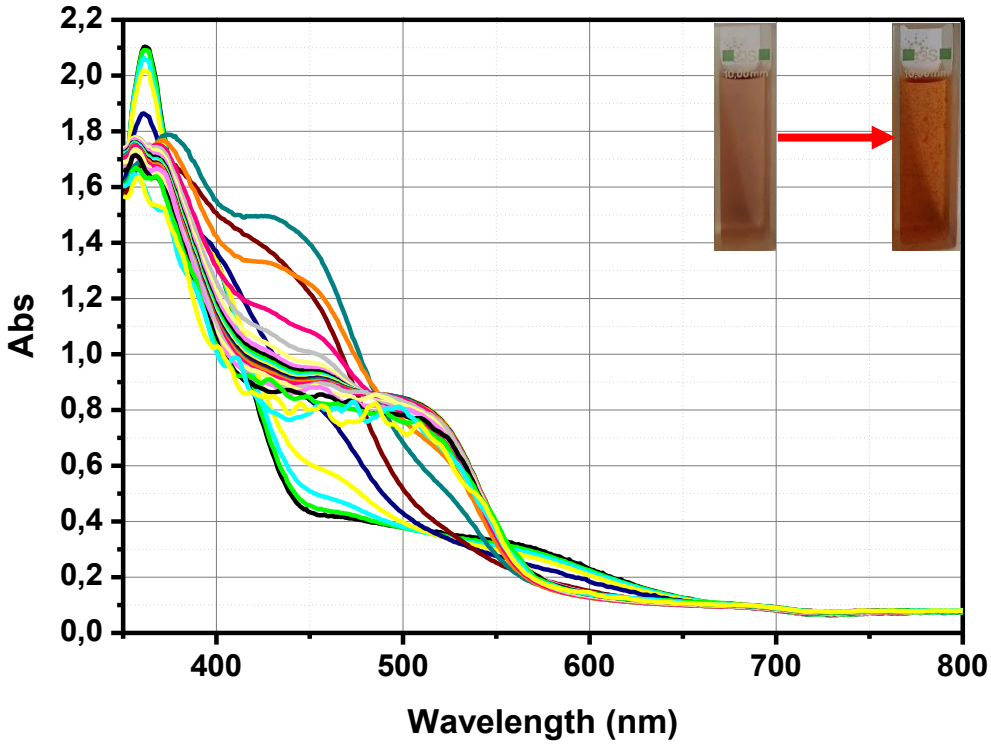
Compound A-D-A9



Compound A-D-A10



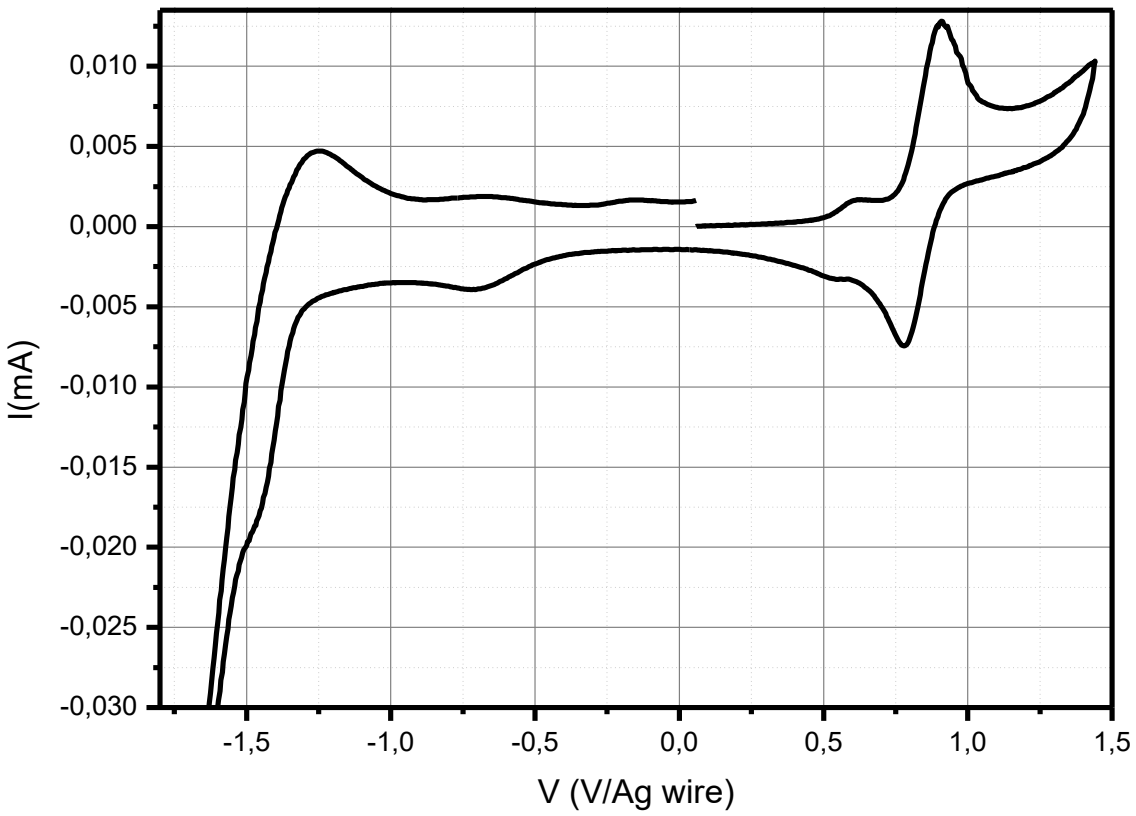
Compound A-D-A11



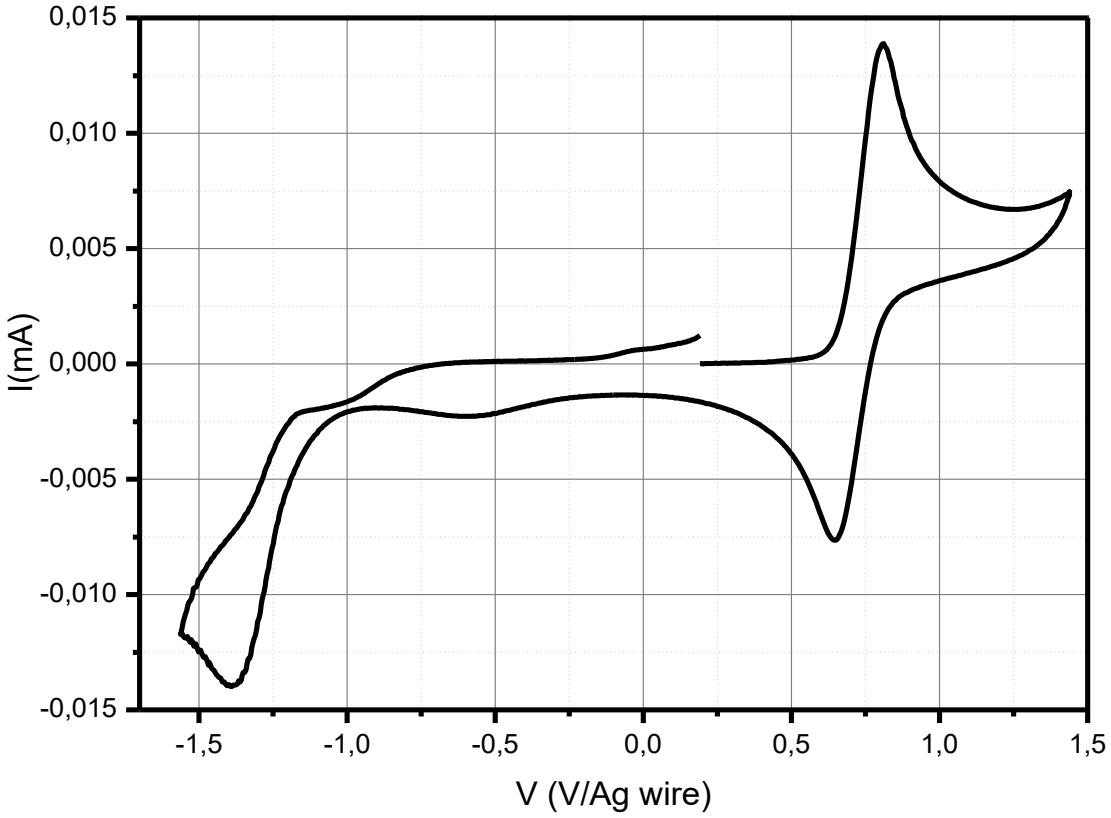
Cyclic voltammograms of the different dyes

The electrochemical properties of the investigated compounds were measured in dichloromethane by cyclic voltammetry, scan rate 100 $mV.s^{-1}$, with tetrabutylammonium perchlorate (0.1M) as the supporting electrolyte in a standard one-compartment, three-electrode electrochemical cell under an argon stream using a VSP BioLogic potentiostat. The working, pseudo-reference and counter electrodes were platinum disk (Ø = 1 mm), Ag wire, and Au wire gauze, respectively. Ferrocene was used as an internal standard.

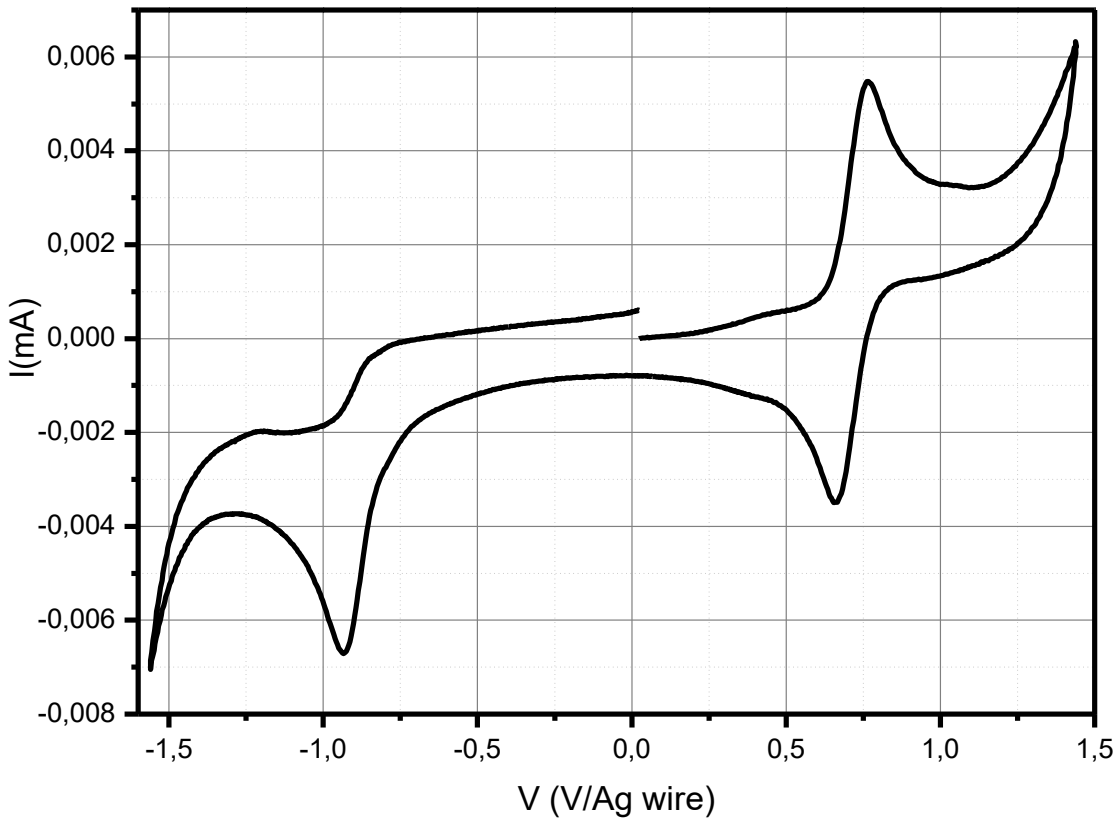
Compound D-A0



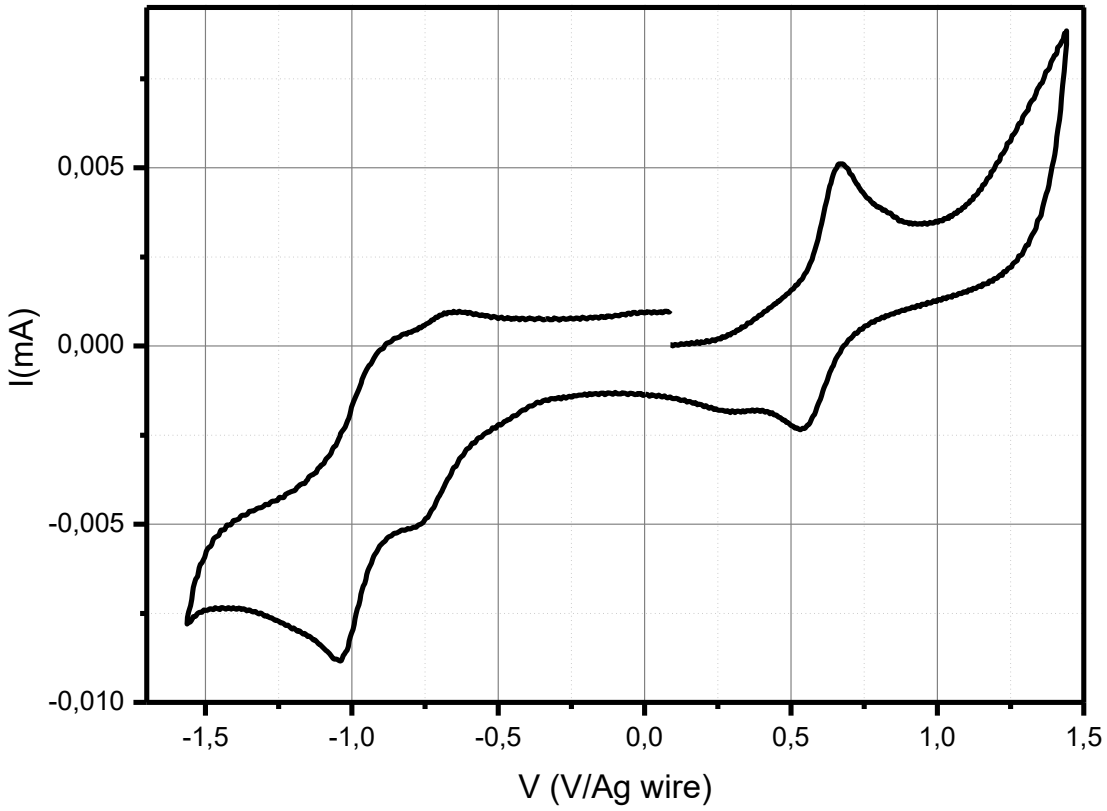
Compound D-A1



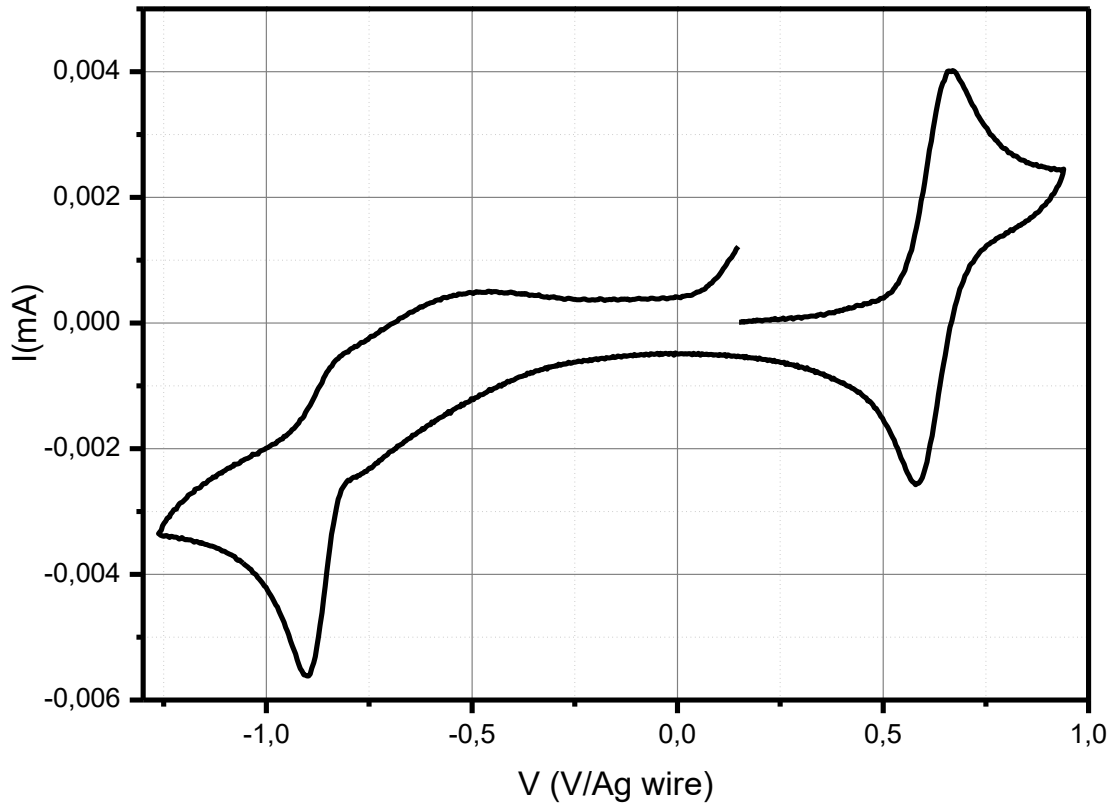
Compound D-A2



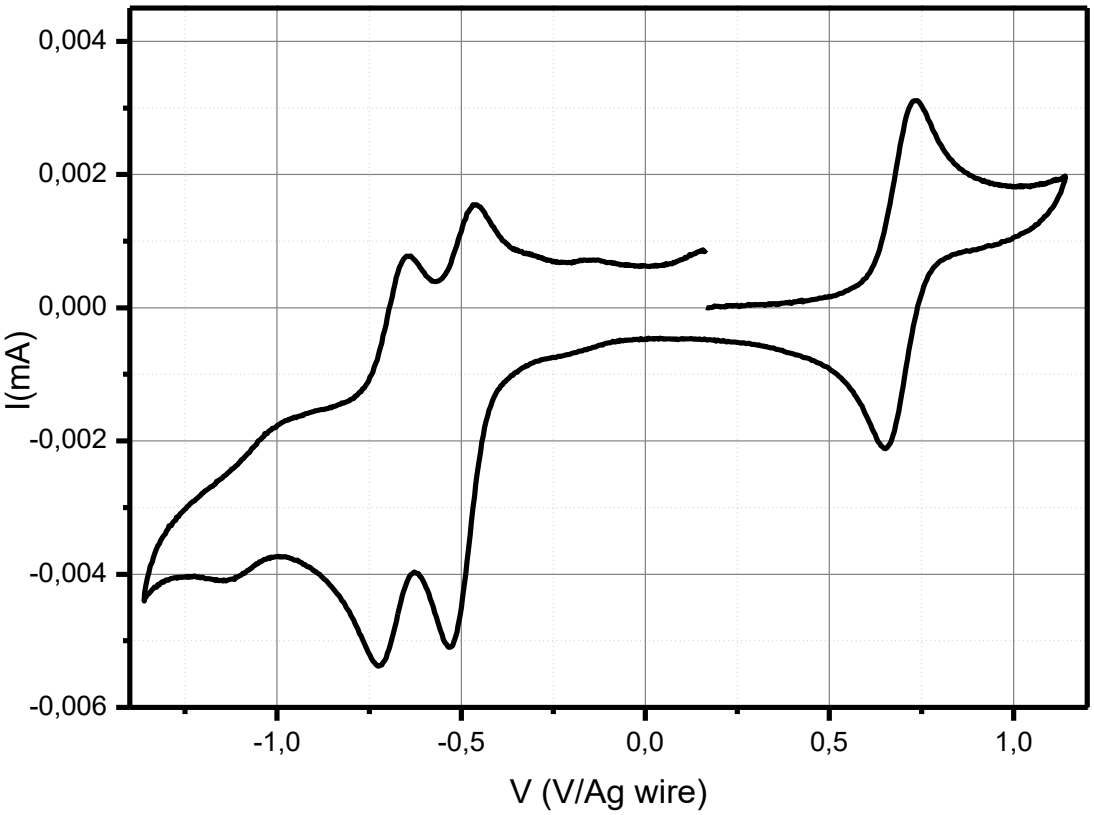
Compound D-A3



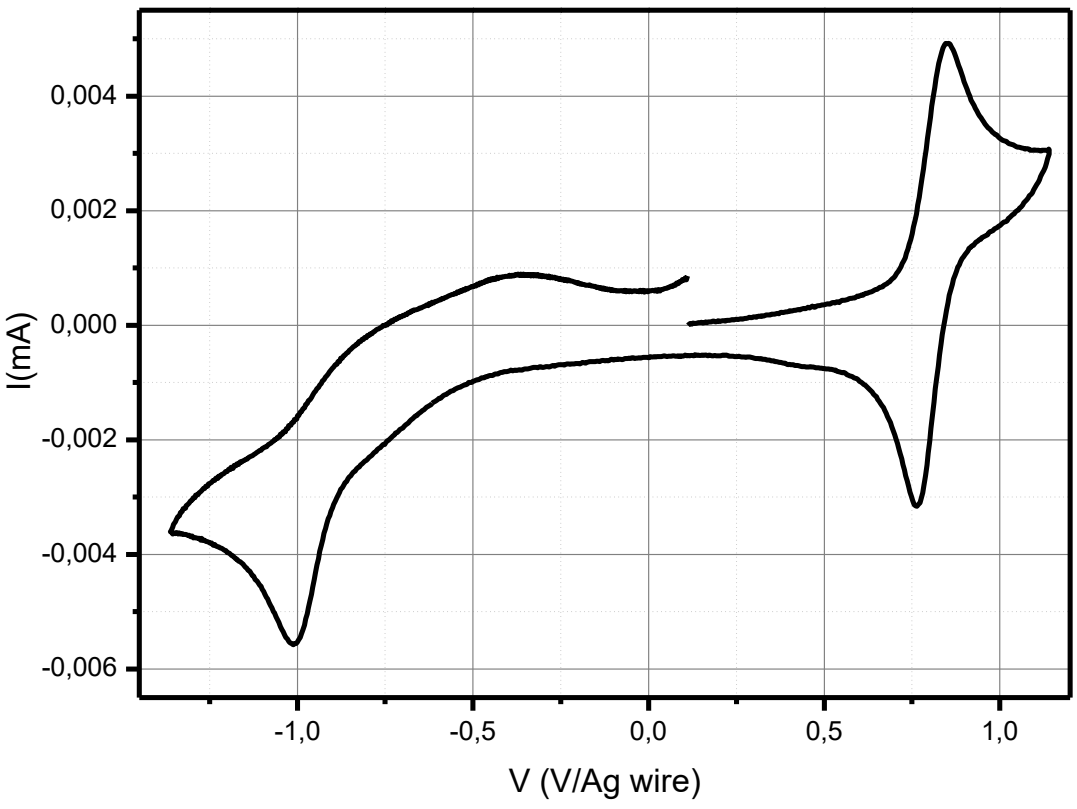
Compound D-A4



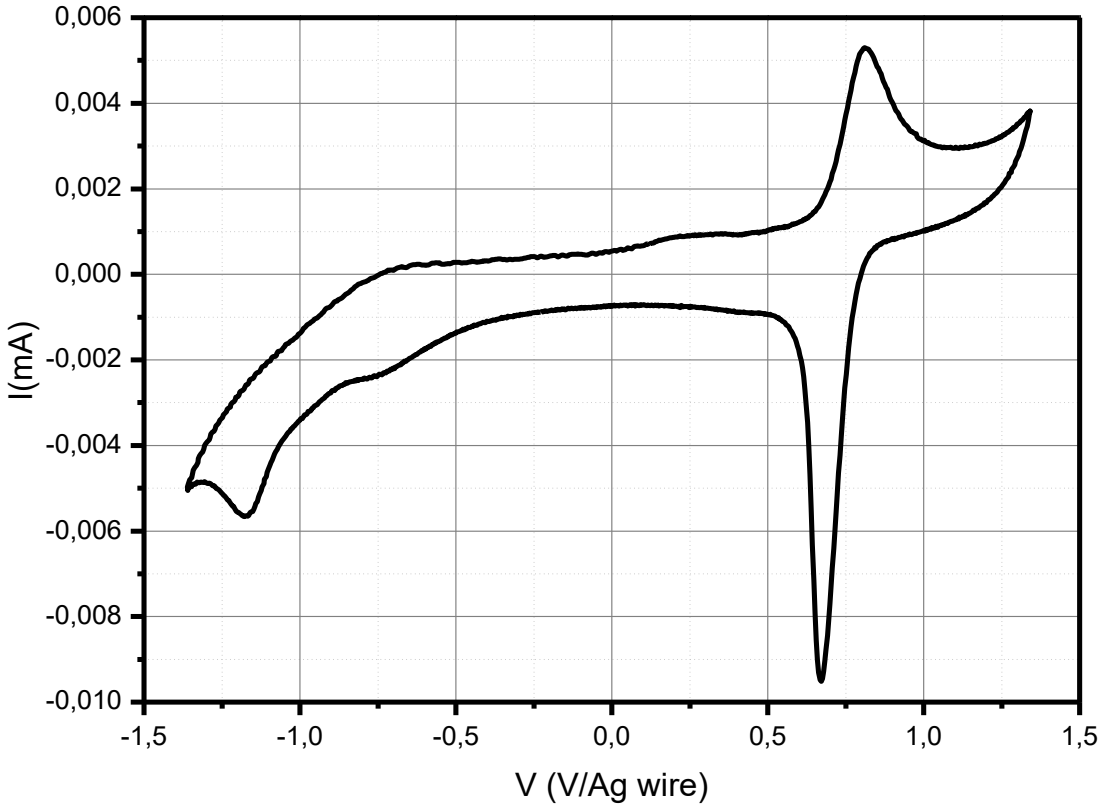
Compound D-A5



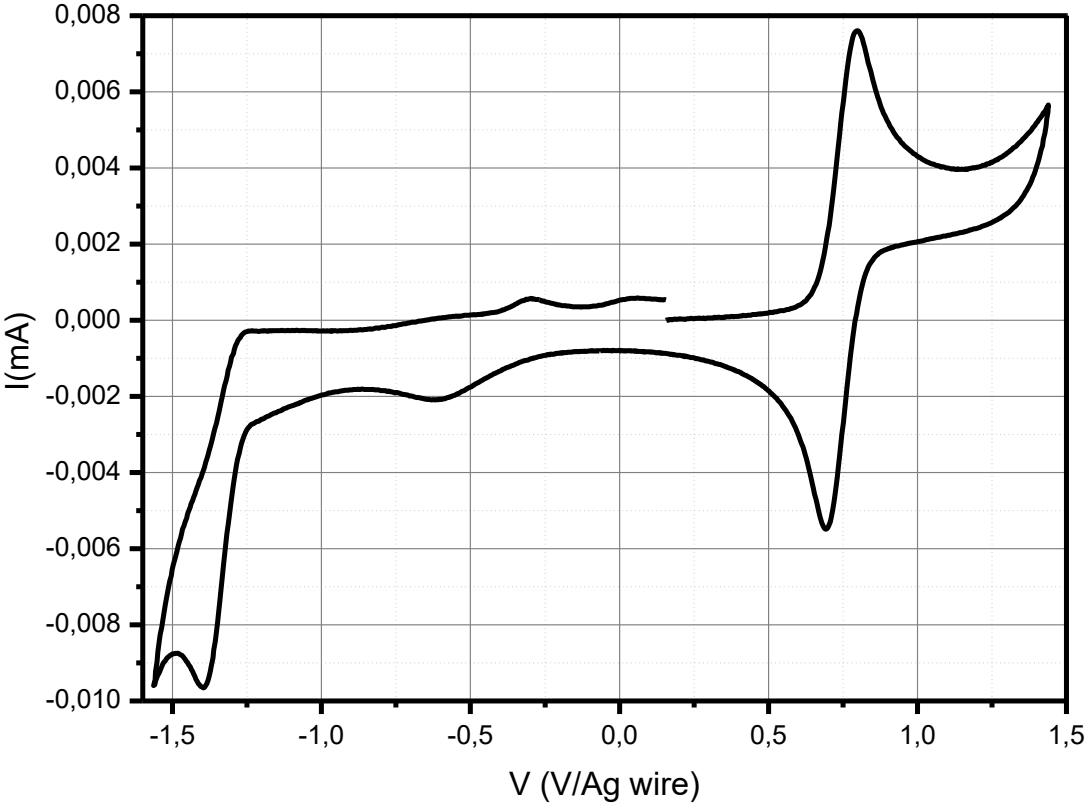
Compound D-A6



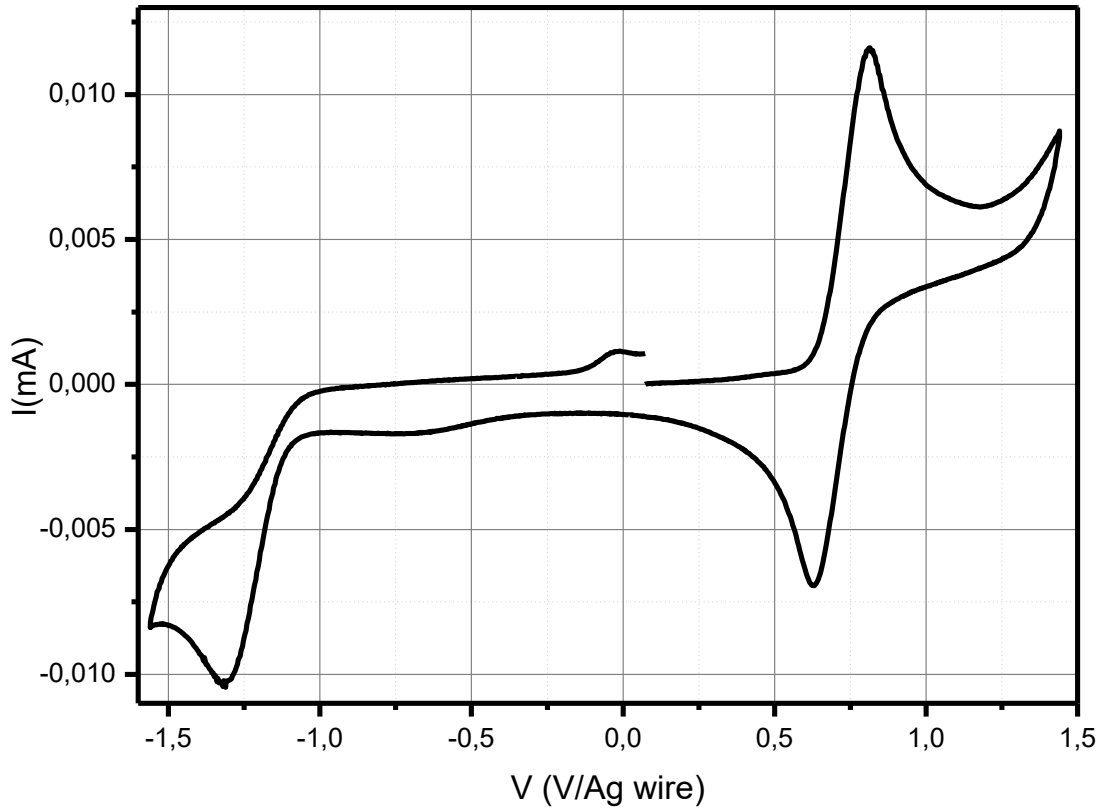
Compound D-A7



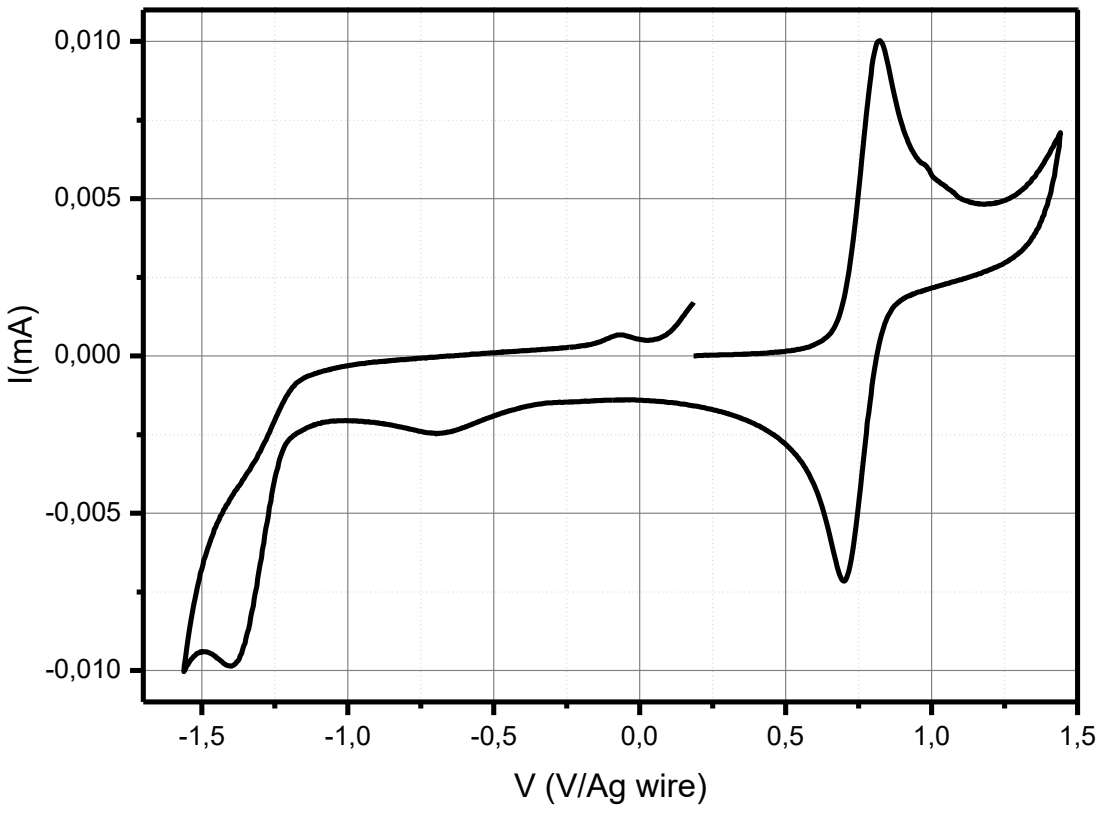
Compound D-A8



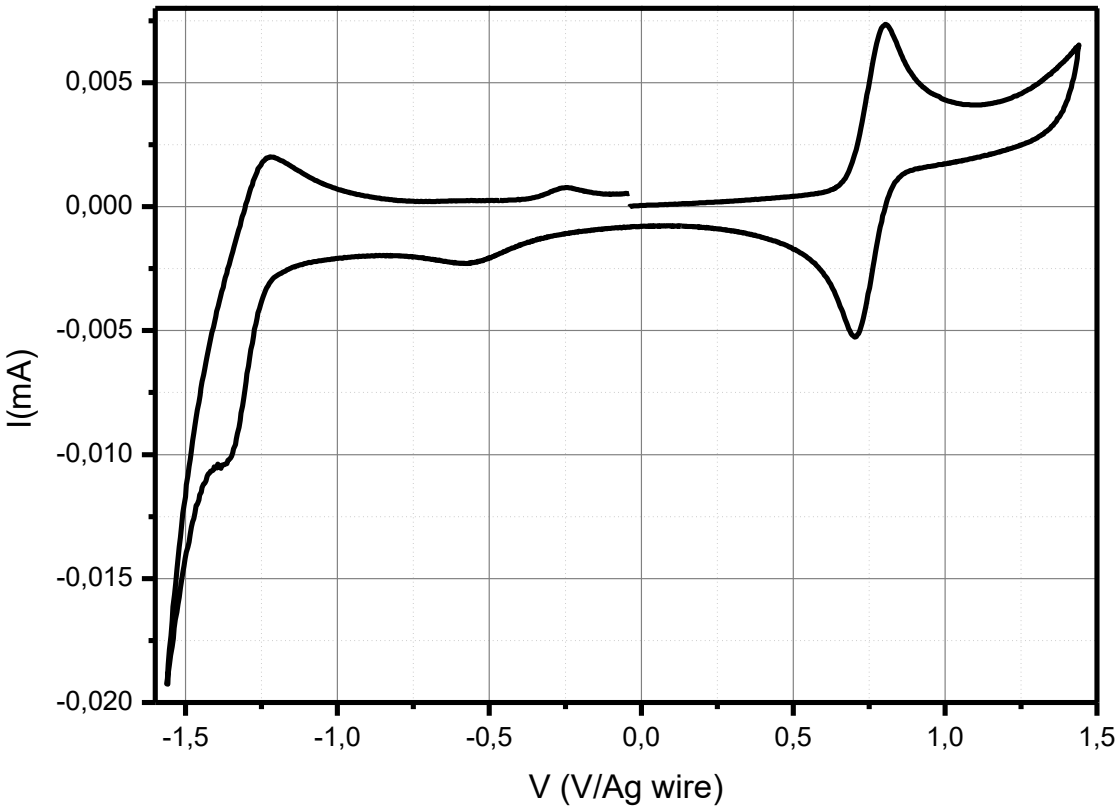
Compound D-A9



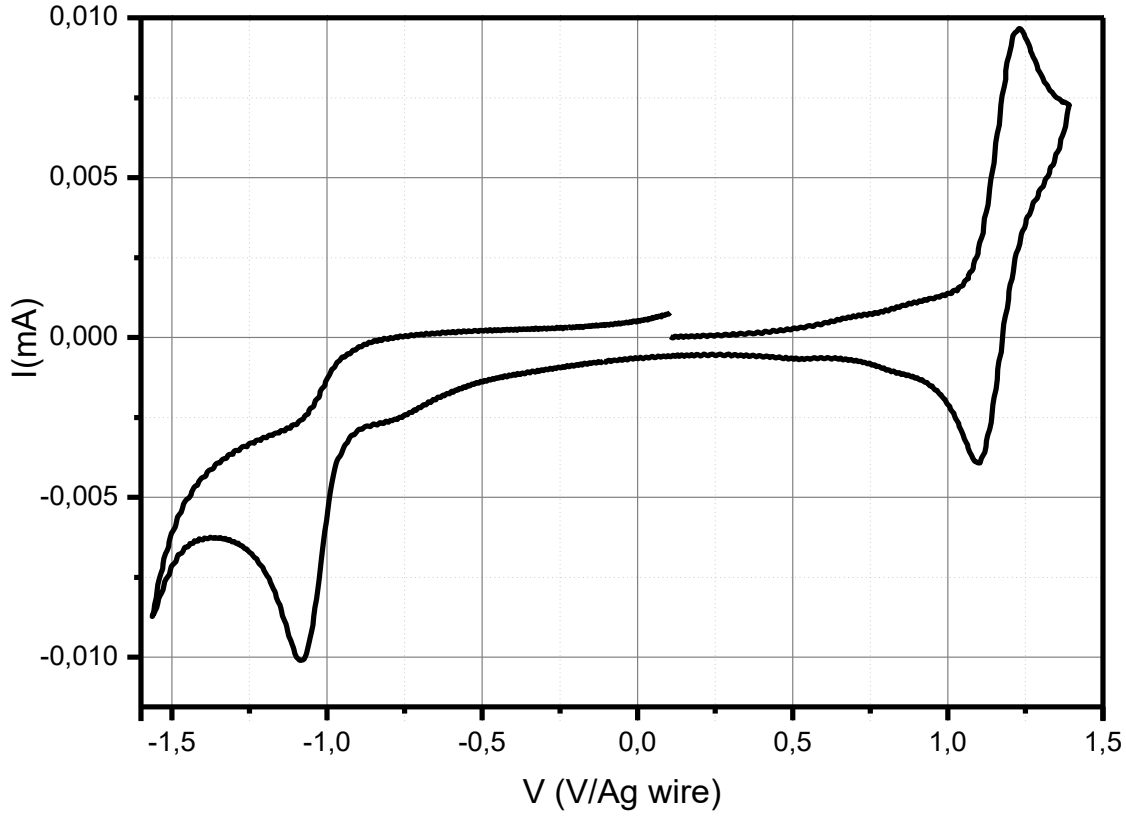
Compound D-A10



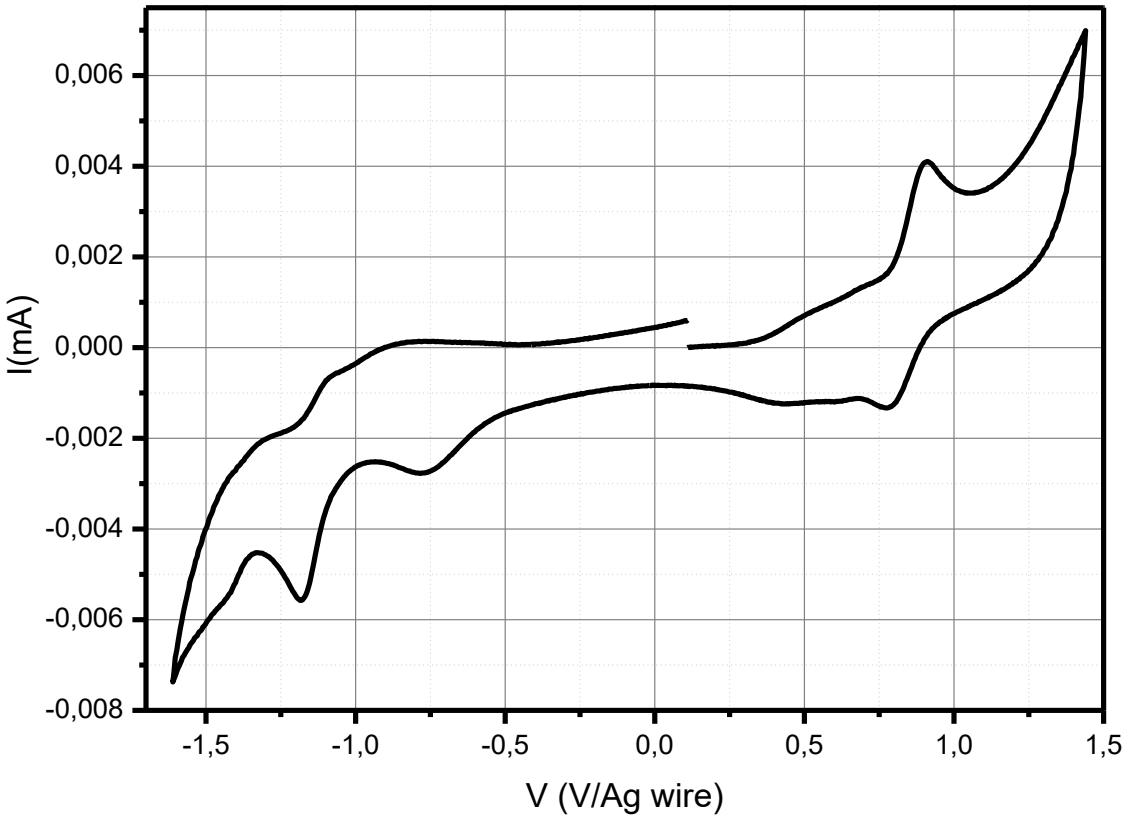
Compound D-A11



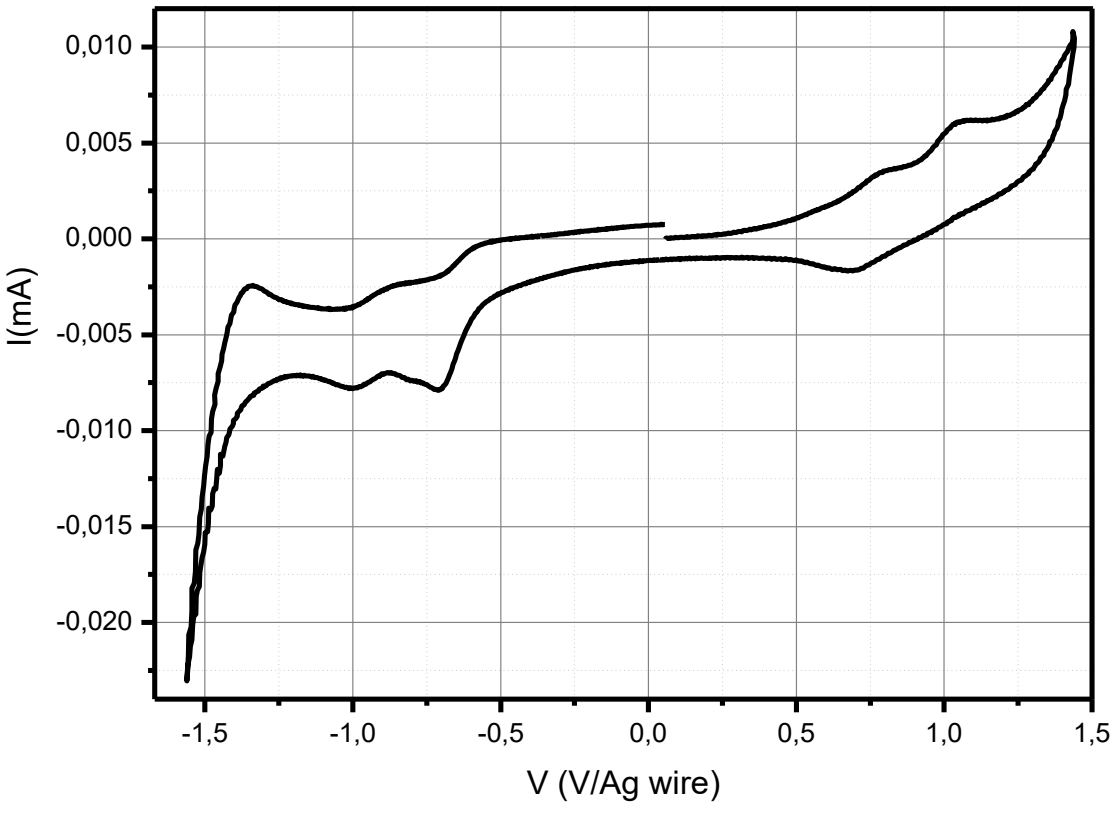
Compound A-D-A0



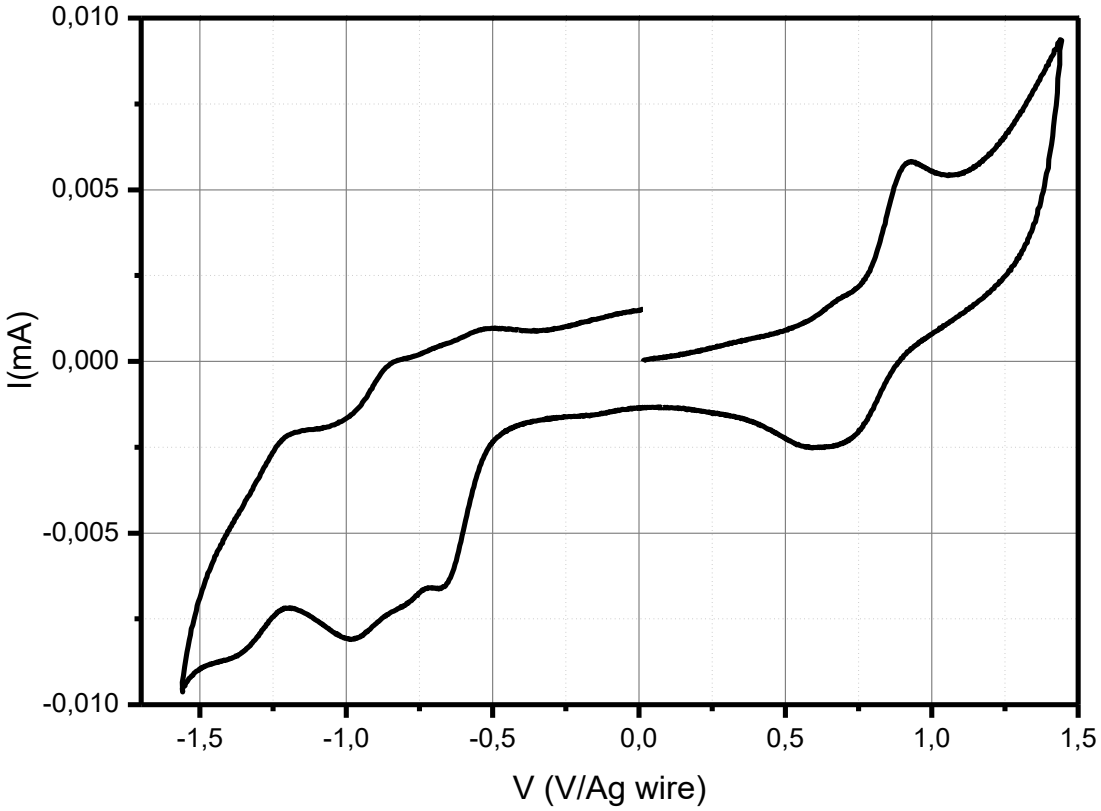
Compound A-D-A1



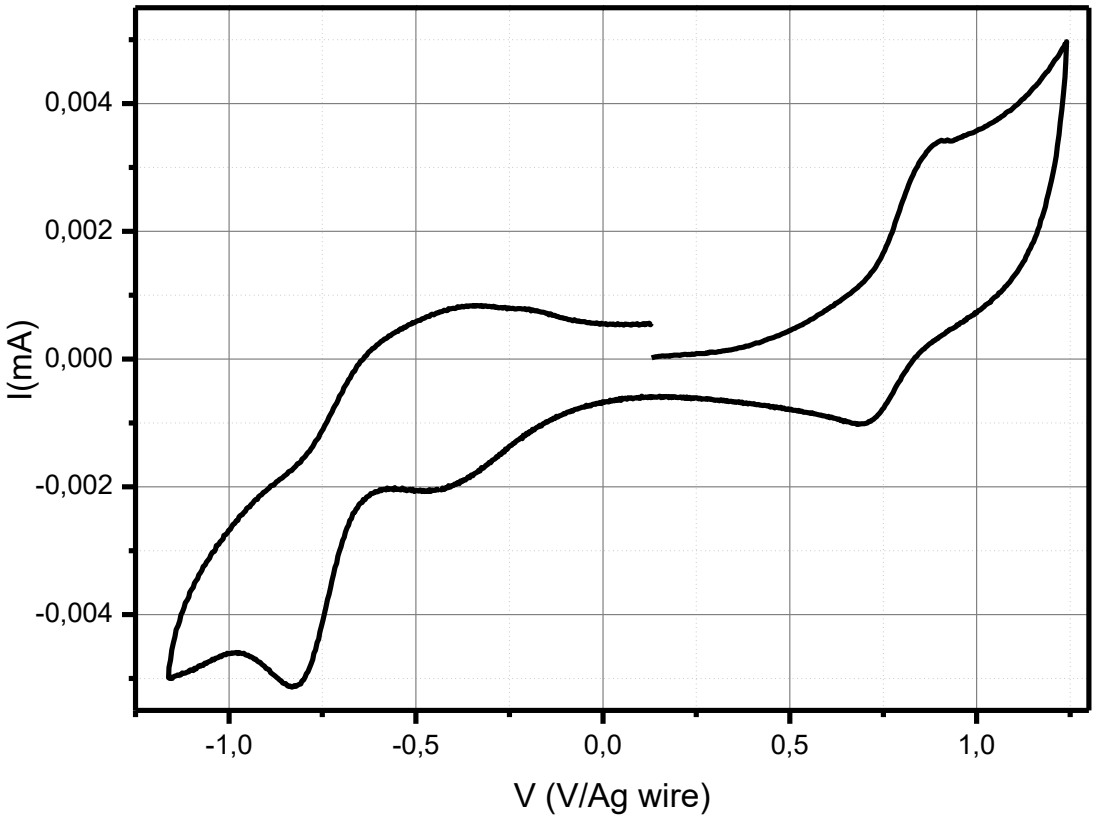
Compound A-D-A2



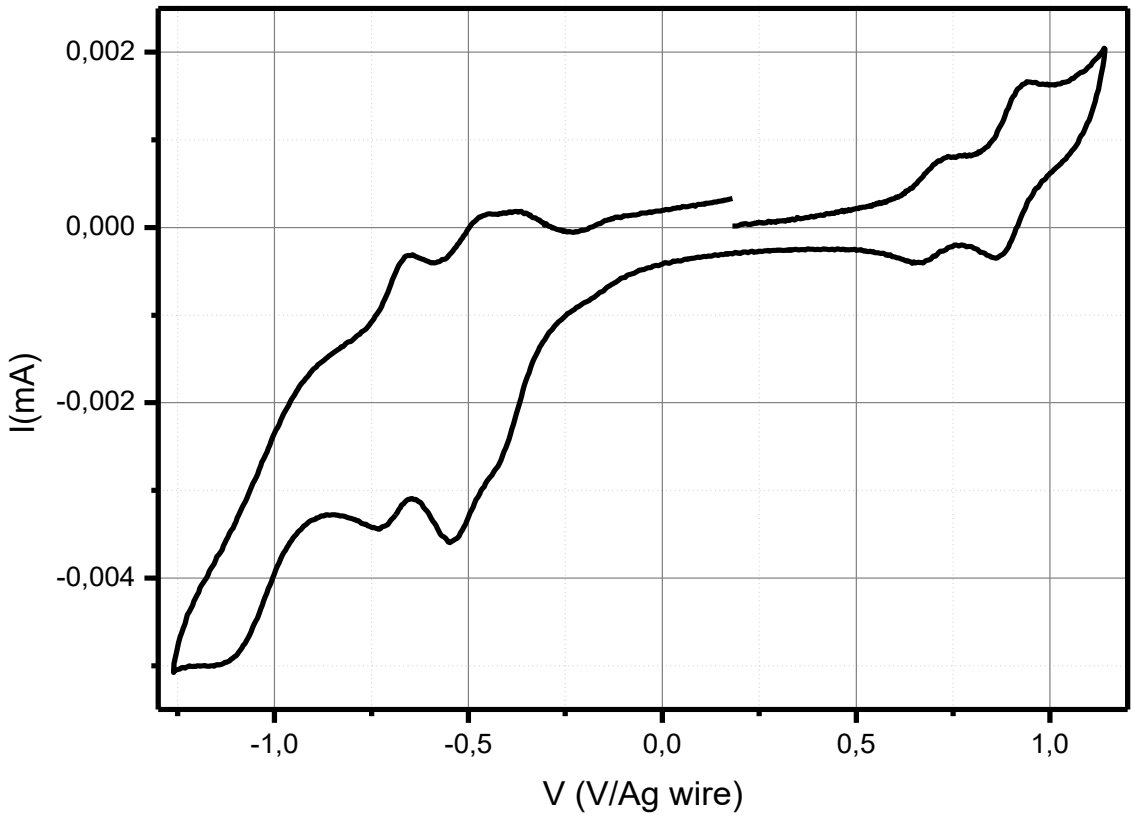
Compound A-D-A3



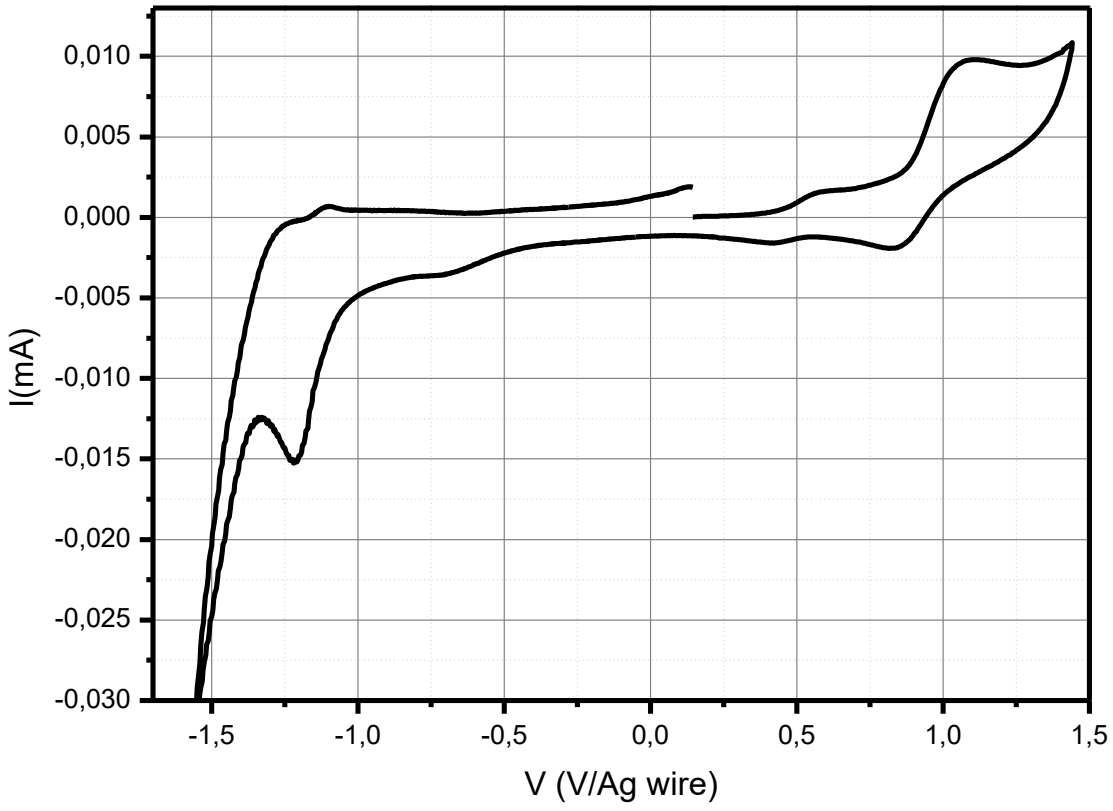
Compound A-D-A4



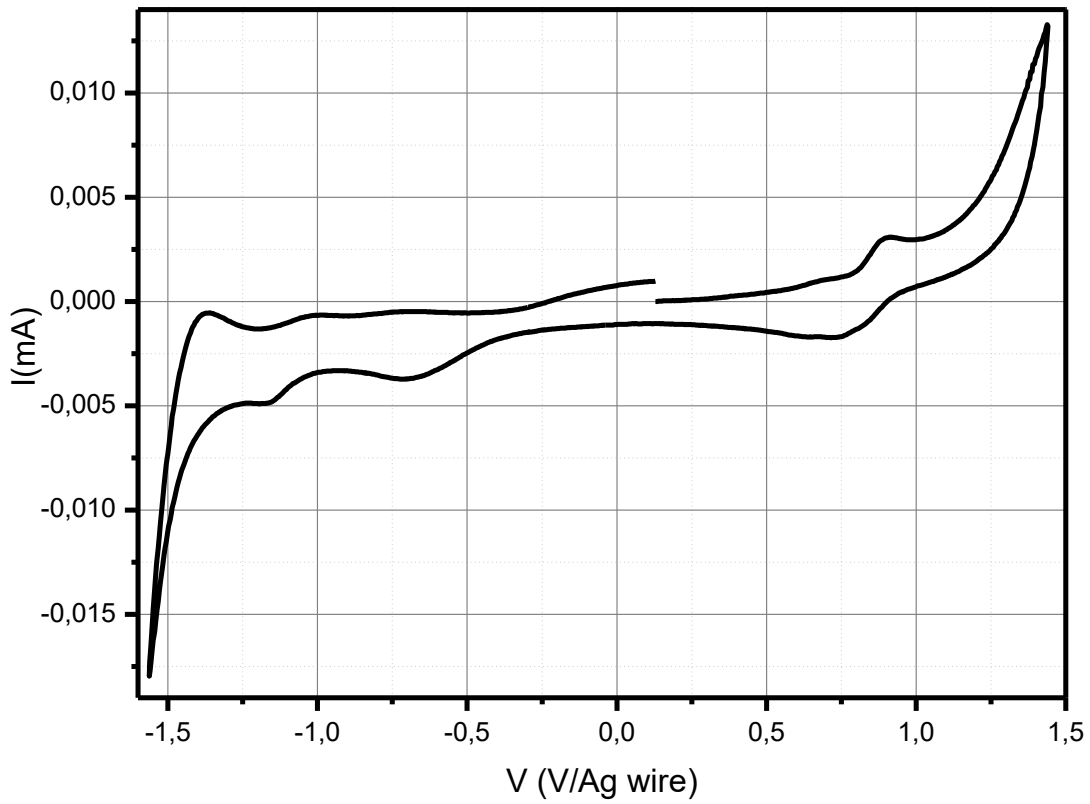
Compound A-D-A5



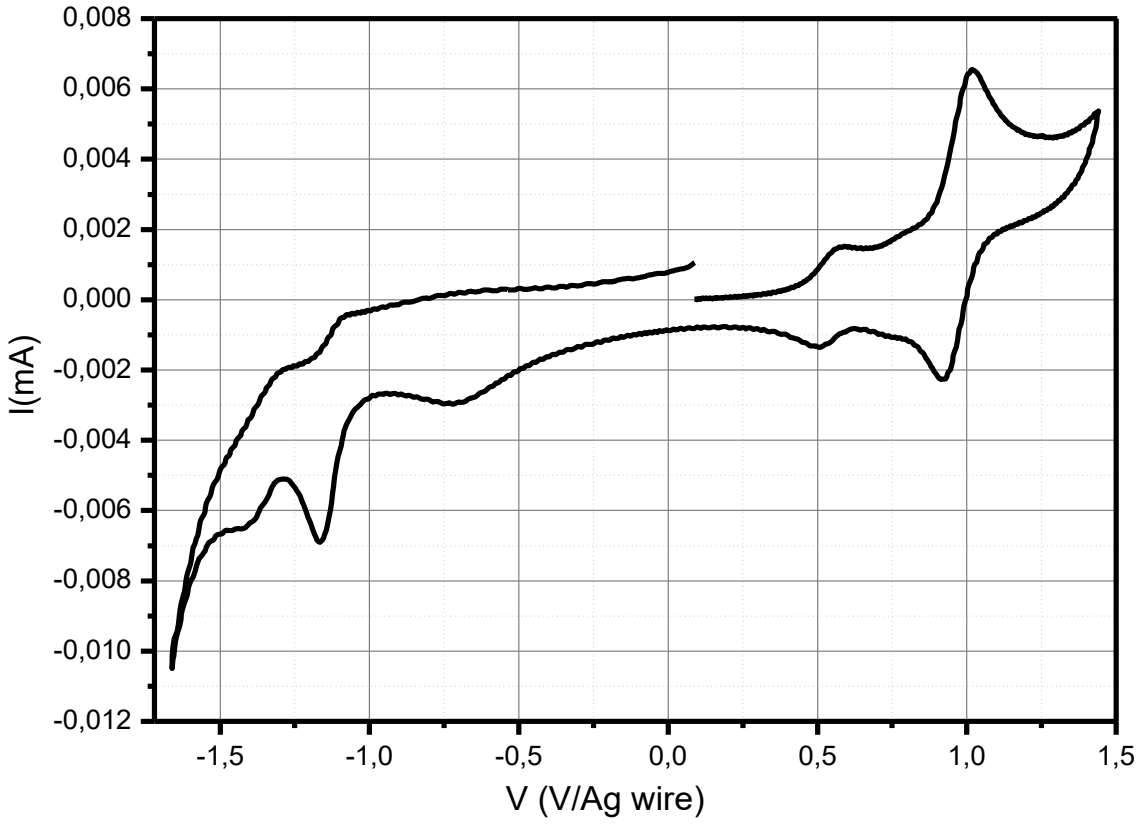
Compound A-D-A8



Compound A-D-A10



Compound A-D-A11



Optimized geometries and HOMO LUMO electronic distributions of all compounds

Computational details: All quantum mechanical calculations were computed using Gaussian Package [1]. All geometry optimizations were performed using density functional theory (DFT) with the global hybrid exchange-correlation functional B3LYP [2] and all minima on the potential energy surface were verified via a calculation of vibrational frequencies, ensuring no imaginary frequencies were present. The Pople double-zeta basis set with a double set of polarization functions on non-hydrogen atoms (6-3111G(d,p))[3,4] was used throughout. This computational approach was chosen in consistency with previous works, as it provides good agreement with experimental data. Excited states were probed using time dependent density functional theory (TD-DFT) using the same functional. All transitions (singlet-singlet) were calculated vertically with respect to the singlet ground state geometry. Solvent effects were taken into account by using the implicit polarizable continuum model (PCM) [5,6]. DCM where chosen in analogy with the experiments. Computed spectra were simulated by convoluting each transition with Gaussians functions-centered on each absorption maximum- using a constant full width at half maximum (FWHM) value of 0.2 eV. The assignment of electronic transitions for λ_{max} has been determined with GaussSum 3.0 software [7]

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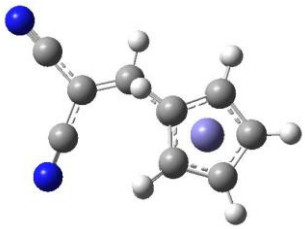
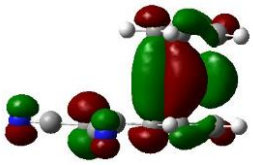
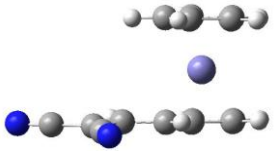
Compound D-A0

D-A0

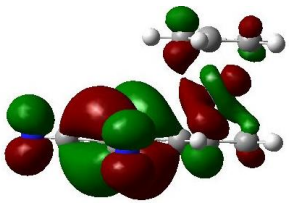


Homo



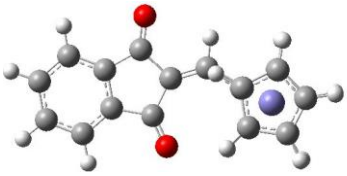


Lumo

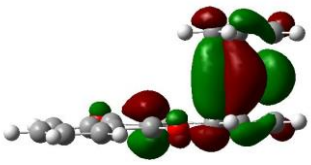


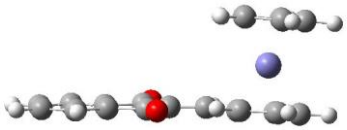
Compound D-A1

D-A1



Homo





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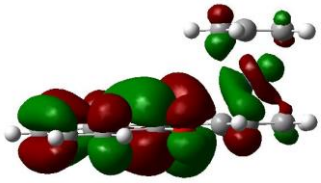
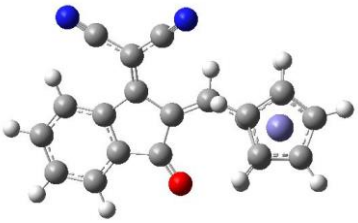


Compound D-A2

D-A2



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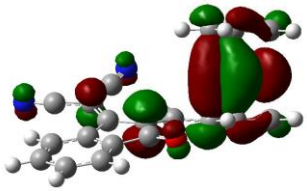
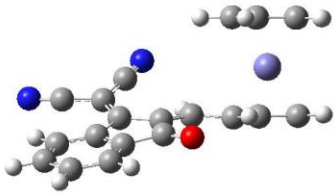
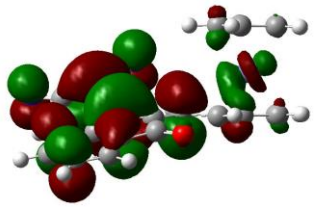


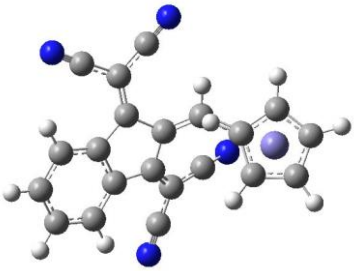
Lumo



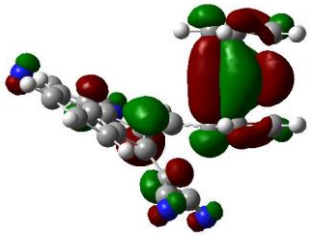


Compound D-A3

D-A3



Homo



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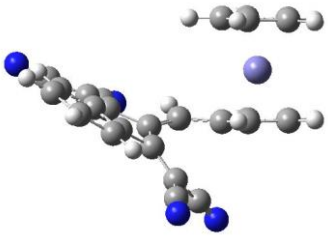
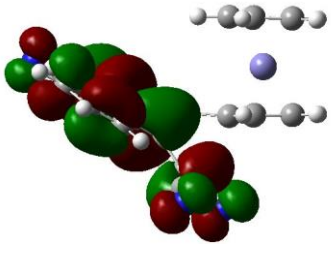
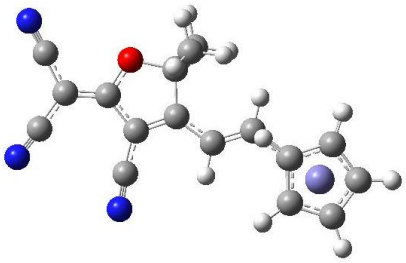


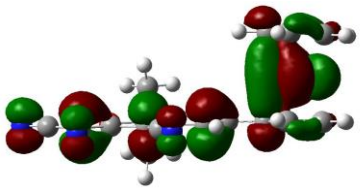


Compound D-A4

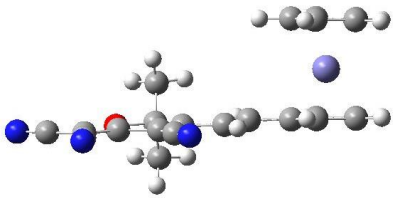
D-A4

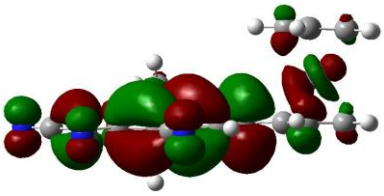


Homo



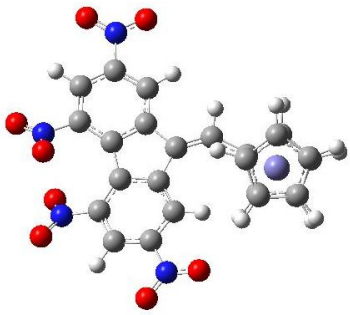
Lumo



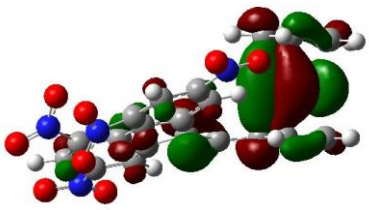


Compound D-A5

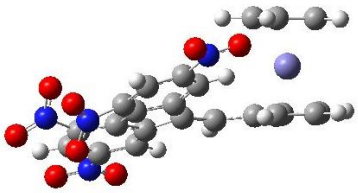
D-A5

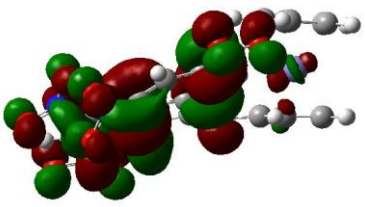


Homo



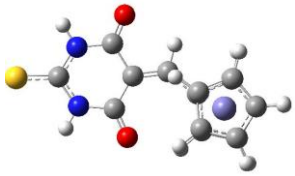
Lumo



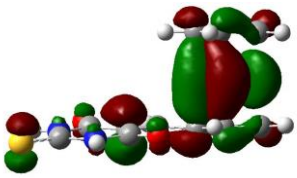


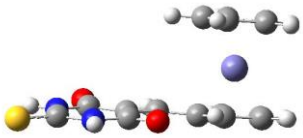
Compound D-A6

D-A6

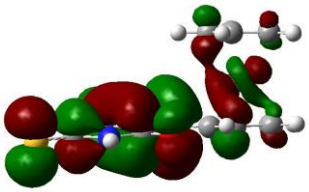


Homo



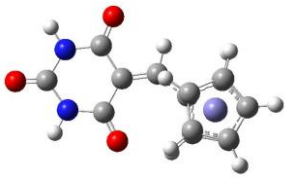


Lumo

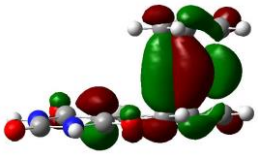


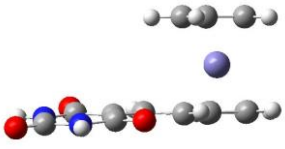
Compound D-A7

D-A7



Homo





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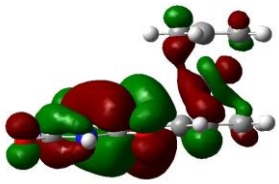
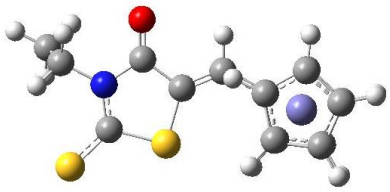
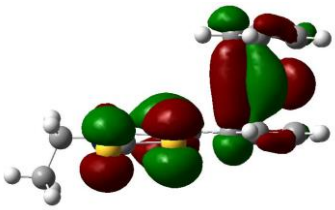


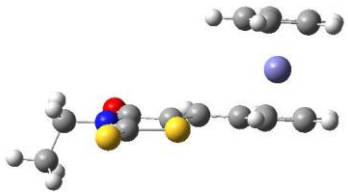
Compound D-A8

D-A8



Homo





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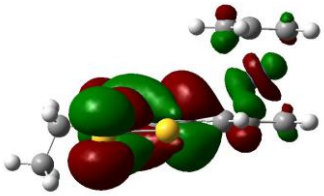
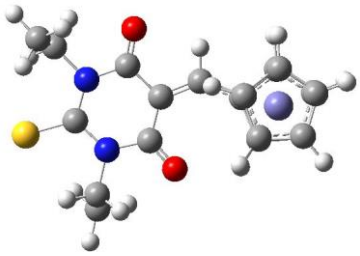
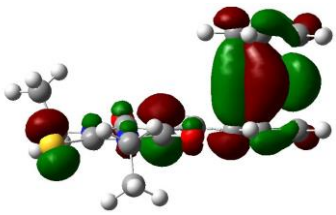


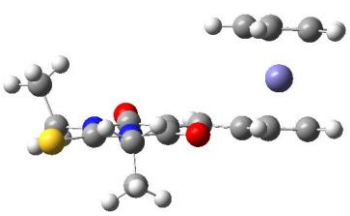
Compound D-A9

D-A9

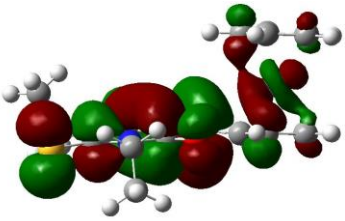


Homo



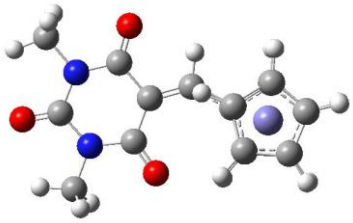


Lumo

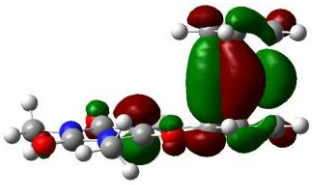


Compound D-A10

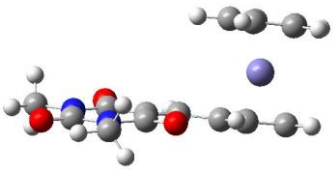
D-A10

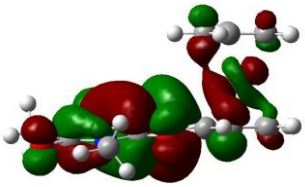


Homo



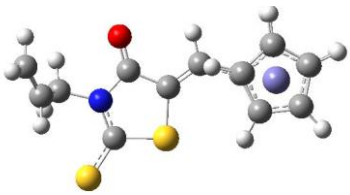
Lumo



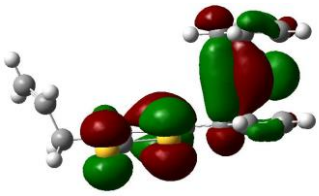


Compound D-A11

D-A11



Homo



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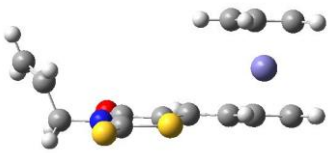
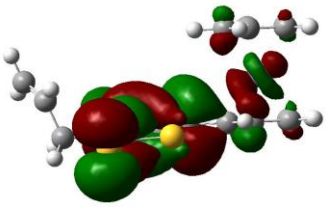
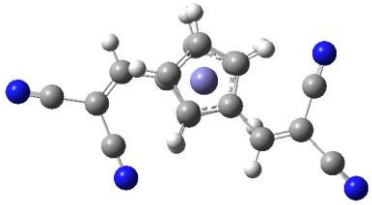
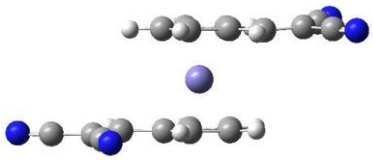




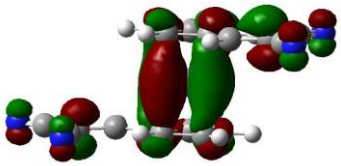
Compound A-D-A0

A-D-A0

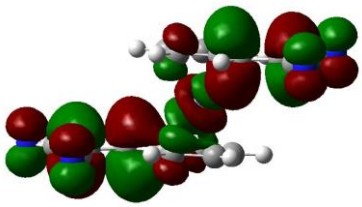




Homo

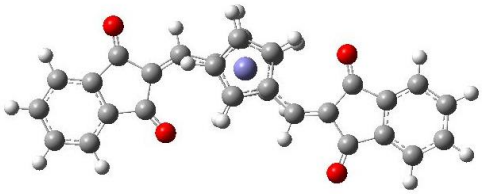


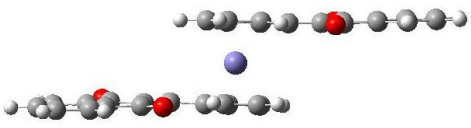
Lumo



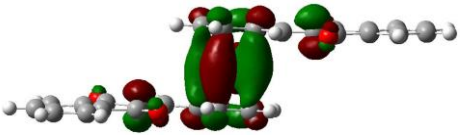
Compound A-D-A1

A-D-A1

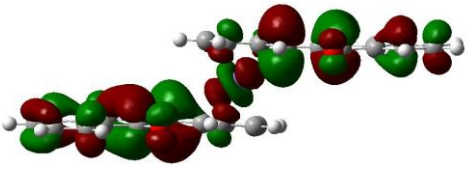




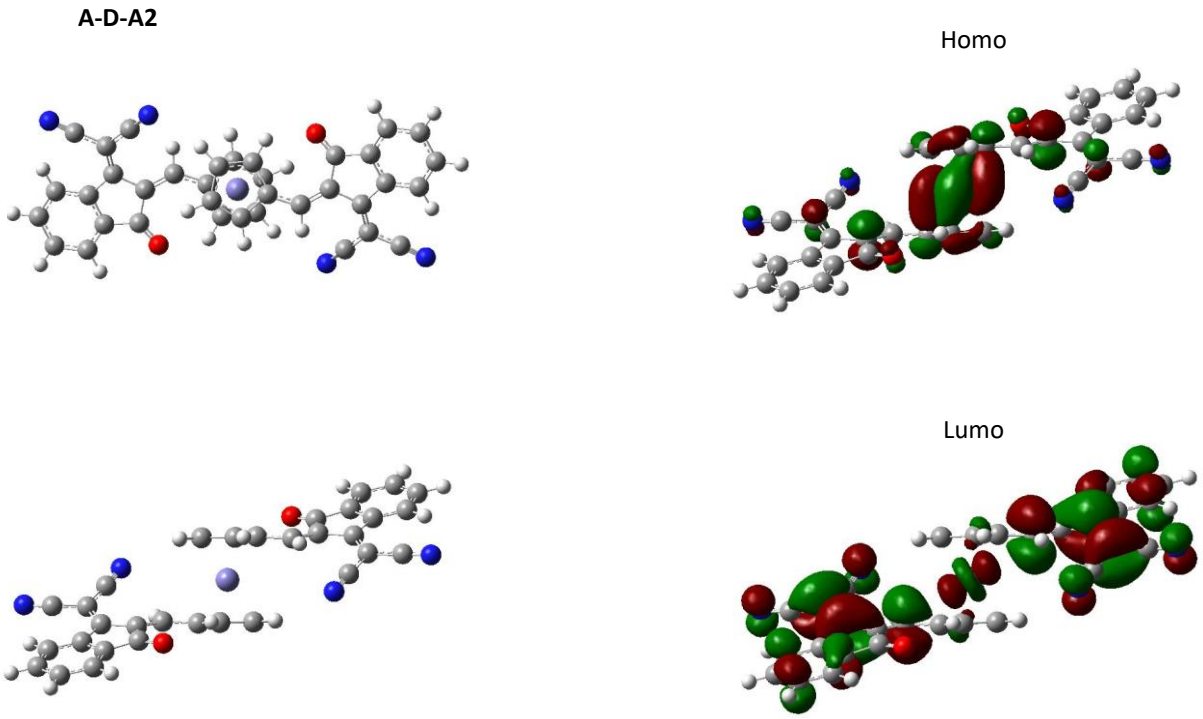
Homo



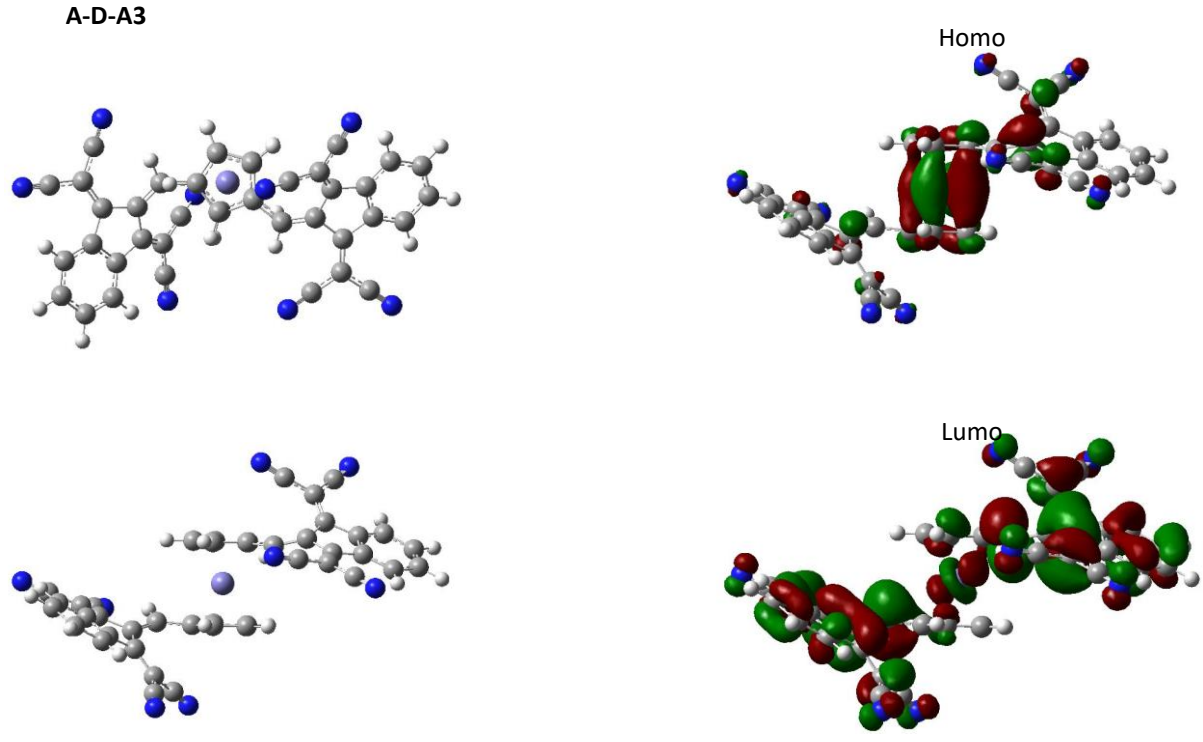
Lumo



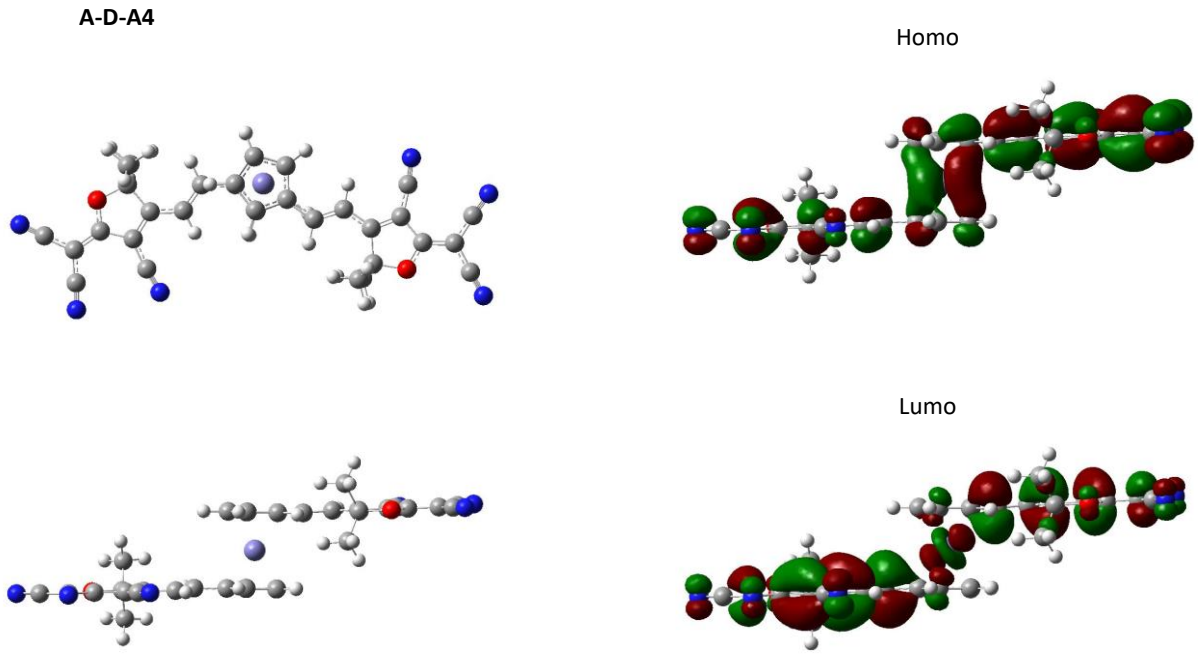
Compound A-D-A2



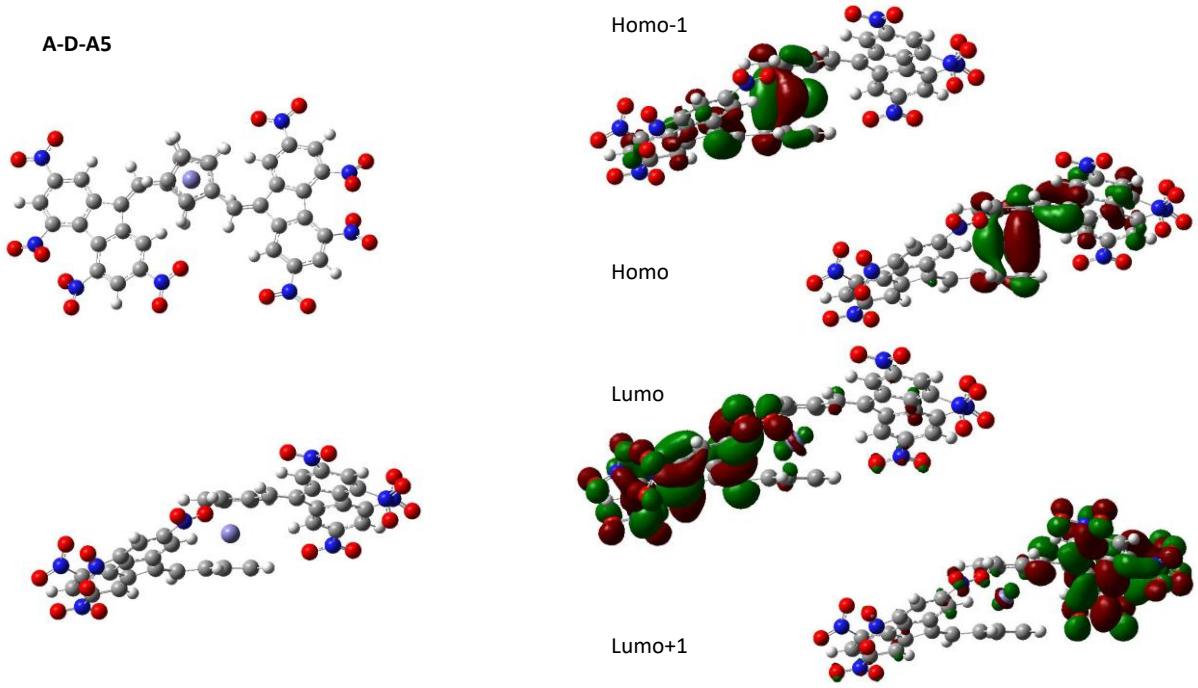
Compound A-D-A3



Compound A-D-A4

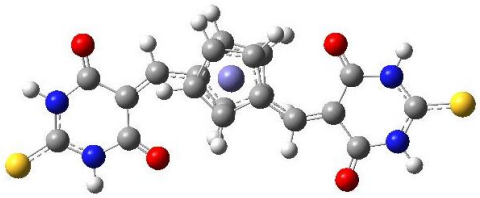


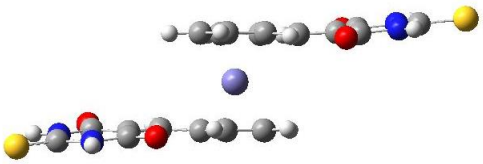
Compound A-D-A5



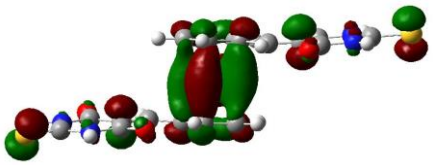
Compound A-D-A6

A-D-A6

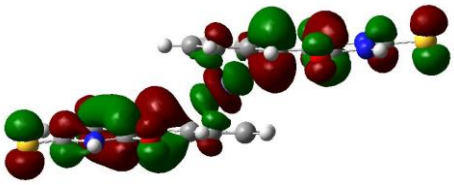




Homo

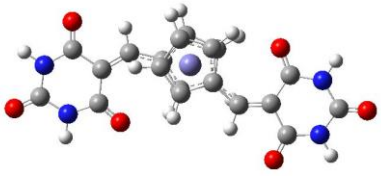


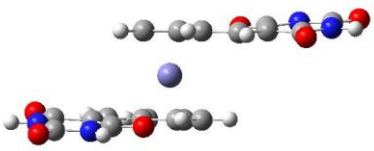
Lumo



Compound A-D-A7

A-D-A7





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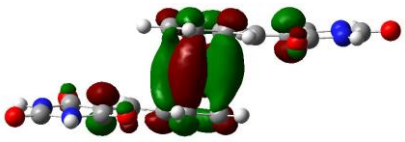

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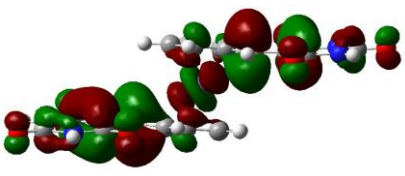

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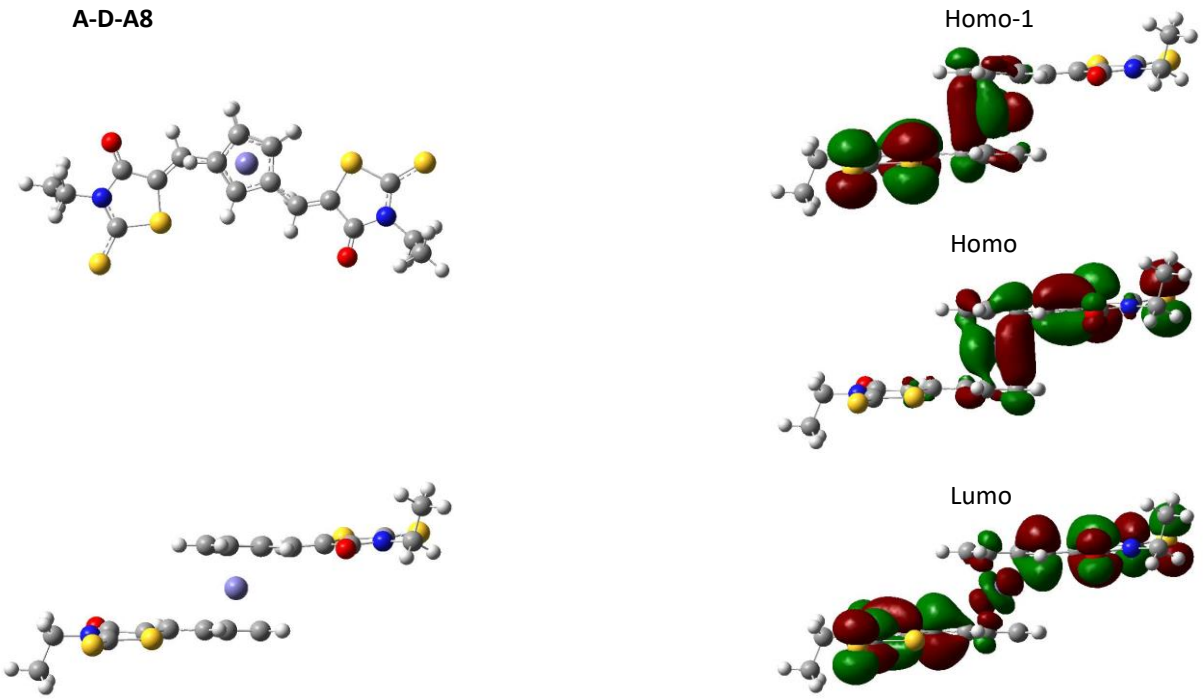

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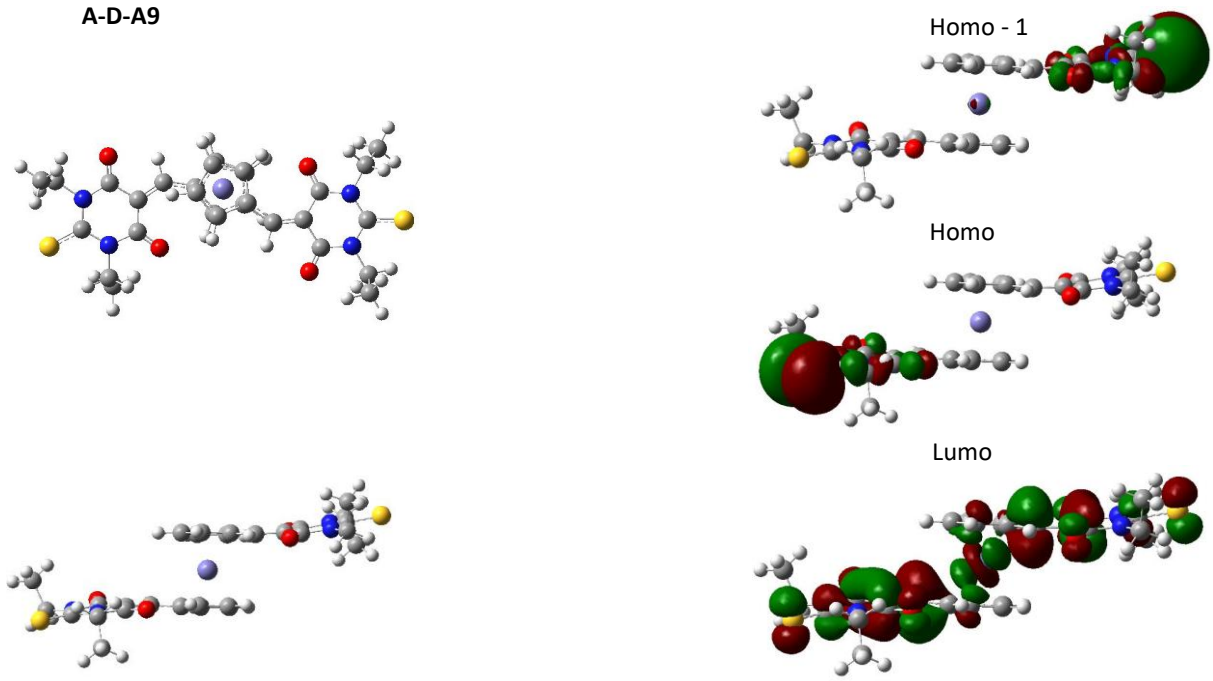
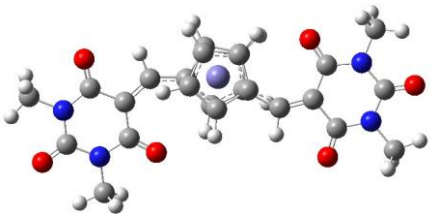
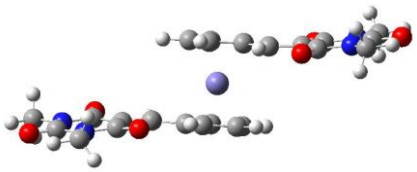


Compound A-D-A10

A-D-A10





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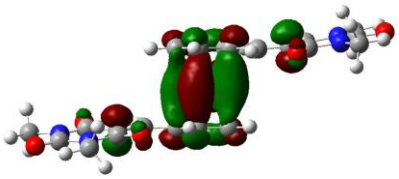

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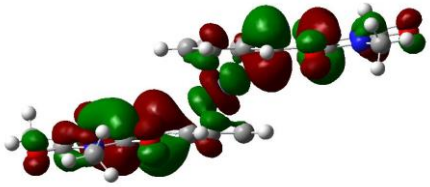
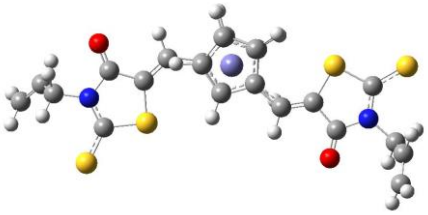
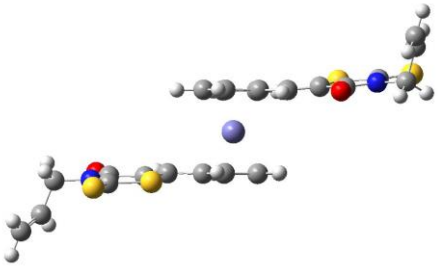


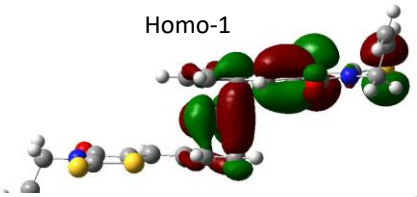
Compound A-D-A11

A-D-A11





Homo-1



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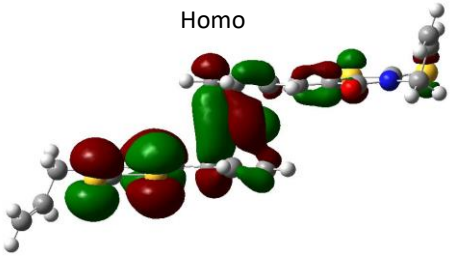

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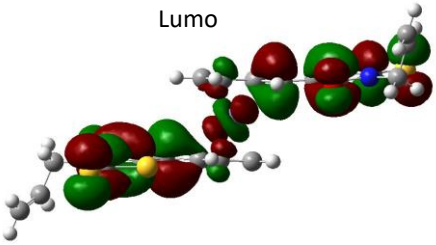


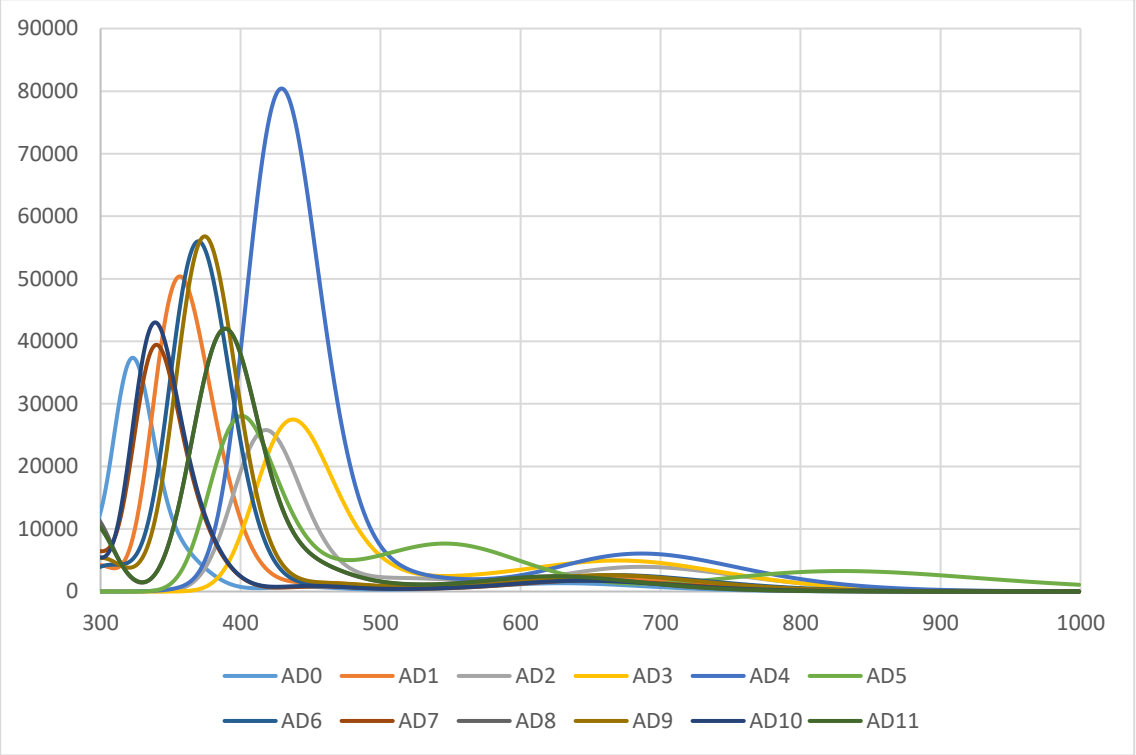
Energy levels of D-A0-D-A-11

	Homo-1	Homo	Lumo	Lumo+1
AD0	-6,400	-6,326	-2,773	-1,208
AD1	-5,961	-5,887	-2,657	-2,240
AD2	-6,170	-6,071	-3,291	-2,789
AD3	-6,478	-6,360	-3,613	-3,549
AD4	-6,493	-6,336	-3,459	-1,437
AD5	-6,573	-6,474	-4,150	-3,479
AD6	-6,283	-6,207	-3,020	-1,260
AD7	-6,210	-6,145	-2,793	-1,011
AD8	-6,056	-5,908	-2,586	-1,202
AD9	-6,107	-6,063	-2,840	-1,083
AD10	-6,074	-6,009	-2,613	-0,886
AD11	-6,065	-5,920	-2,602	-1,234

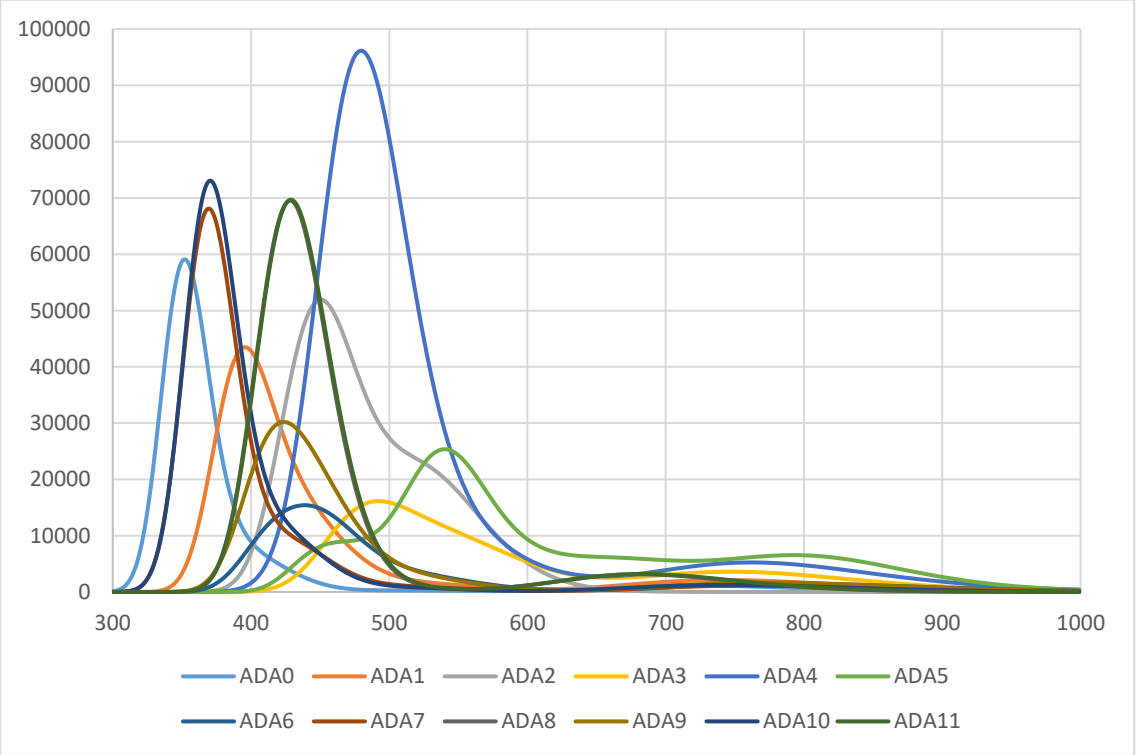
Energy levels of A-D-A0-A-D-A-11

	Homo-1	Homo	Lumo	Lumo+1
ADA0	-7,065	-7,015	-3,465	-3,060
ADA1	-6,249	-6,185	-2,983	-2,675
ADA2	-6,561	-6,401	-3,577	-3,423
ADA3	-6,933	-6,901	-3,963	-3,889
ADA4	-6,930	-6,877	-3,983	-3,749
ADA5	-6,573	-6,474	-4,150	-3,479
ADA6	-6,771	-6,709	-3,531	-3,185
ADA7	-6,697	-6,629	-3,312	-2,922
ADA8	-6,275	-6,273	-2,934	-2,695
ADA9	-6,306	-6,299	-3,264	-2,921
ADA10	-6,459	-6,392	-3,049	-2,664
ADA11	-6,291	-6,289	-2,951	-2,711

Simulated absorption spectra of D-A0-D-A-11 in the 300-1000 nm range



Simulated absorption spectra of A-D-A0-A-D-A-11 in the 300-1000 nm range



Main transitions involved in the different absorption bands observed in the simulated UV-visible absorption spectra of D-A dyads **D-Ax, x = 0-11** and A-D-A triads **A-D-Ax, x = 0-11**.

AD 0

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	669.316524575	0.0004	H-1->LUMO (64%), H-1->L+2 (24%)	HOMO->L+1 (9%)
2	632.15312809	0.019	H-1->L+1 (13%), HOMO->LUMO (51%), HOMO->L+2 (31%)	
3	536.333404041	0.0039	H-3->LUMO (11%), H-3->L+2 (10%), H-2->LUMO (24%), H-2->L+2 (20%), H-1->L+1 (29%)	
4	500.299382666	0.0001	H-2->L+1 (24%), HOMO->L+1 (62%)	H-3->L+1 (5%), H-1->LUMO (6%)
5	443.243933263	0.011	H-2->LUMO (20%), H-1->L+1 (41%), HOMO->LUMO (27%)	H-3->LUMO (3%), H-2->L+2 (3%), HOMO->L+2 (3%)
6	422.505343371	0.0005	H-3->L+1 (10%), H-2->L+1 (22%), H-1->LUMO (27%), H-1->L+2 (34%)	HOMO->L+1 (4%)
7	359.27033617	0.0717	H-1->L+1 (11%), HOMO->LUMO (15%), HOMO->L+2 (58%)	H-3->LUMO (5%), H-2->LUMO (8%)
8	352.227821057	0.0005	H-3->L+1 (12%), H-2->L+1 (22%), H-1->L+2 (39%), HOMO->L+1 (21%)	
9	324.684944776	0.391	H-3->LUMO (32%), H-2->LUMO (40%), H-2->L+2 (10%)	H-5->LUMO (4%), H-4->LUMO (4%), H-3->L+2 (5%)
10	319.934438656	0.0315	H-4->LUMO (38%), H-3->LUMO (20%), H-2->L+2 (25%)	H-3->L+2 (7%), H-2->LUMO (3%), HOMO->L+2 (2%)
11	317.720813398	0.138	H-4->LUMO (55%), H-3->LUMO (26%), H-2->L+2 (11%)	H-3->L+2 (3%)
12	285.316288142	0.0244	H-6->LUMO (63%), H-5->LUMO (29%)	H-6->L+2 (3%)
13	284.19793933	0.1047	H-6->LUMO (30%), H-5->LUMO (60%)	H-2->LUMO (2%)
14	260.695542405	0.0001	HOMO->L+3 (94%)	H-3->L+3 (2%), H-2->L+3 (3%)
15	251.892877049	0.0007	H-1->L+3 (99%)	
16	246.788735867	0.0004	H-3->L+1 (68%), H-2->L+1 (26%)	
17	241.684586768	0.0	HOMO->L+4 (97%)	
18	239.462671918	0.0174	H-4->L+1 (39%), H-3->L+2 (40%), H-2->L+2 (15%)	
19	238.499938467	0.0002	H-1->L+4 (97%)	
20	236.900399366	0.0005	H-5->L+1 (72%), H-4->L+2 (11%)	H-7->L+1 (2%), H-6->L+2 (6%)

AD 1				
No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	689.222263673	0.0003	H-1->LUMO (64%), H-1->L+2 (18%)	H-1->L+4 (8%), HOMO->L+3 (7%)
2	653.063961086	0.0347	H-1->L+3 (10%), HOMO->LUMO (54%), HOMO->L+2 (19%), HOMO->L+4 (11%)	
3	542.481702088	0.007	H-3->LUMO (15%), H-2->LUMO (19%), H-2->L+2 (11%), H-1->L+3 (29%)	H-3->L+2 (9%), H-3->L+4 (5%), H-2->L+4 (7%)
4	505.913383981	0.0001	H-2->L+3 (19%), HOMO->L+3 (63%)	H-3->L+3 (6%), H-1->LUMO (7%)
5	460.257602688	0.0188	H-2->LUMO (15%), H-1->L+3 (37%), HOMO->LUMO (29%)	H-3->LUMO (4%), HOMO->L+2 (3%), HOMO->L+4 (5%)
6	437.10274286	0.0003	H-3->L+3 (14%), H-2->L+3 (18%), H-1->LUMO (25%), H-1->L+2 (17%), H-1->L+4 (20%)	
7	417.975906052	0.0022	HOMO->L+1 (98%)	
8	403.135077263	0.0	H-1->L+1 (98%)	
9	381.70122841	0.0086	H-4->LUMO (84%)	H-10->L+1 (3%), H-9->L+1 (2%), H-4->L+1 (4%)
10	378.415923002	0.2201	H-2->LUMO (21%), H-1->L+3 (13%), HOMO->LUMO (14%), HOMO->L+2 (28%), HOMO->L+4 (19%)	
11	363.078929988	0.0003	H-4->L+1 (79%)	H-10->LUMO (5%), H-9->LUMO (5%), H-4->LUMO (5%)
12	356.153605114	0.0001	H-3->L+3 (19%), H-2->L+3 (19%), H-1->L+2 (19%), H-1->L+4 (15%), HOMO->L+3 (23%)	
13	353.331983506	0.6318	H-3->LUMO (57%), H-2->LUMO (31%)	H-4->LUMO (2%), HOMO->L+4 (2%)
14	338.87499115	0.0176	H-2->L+1 (85%)	H-3->L+1 (8%)
15	332.272586729	0.0033	H-5->LUMO (91%)	
16	330.74799395	0.0072	H-3->LUMO (15%), H-3->L+4 (10%), H-2->L+2 (17%), H-2->L+4 (18%)	H-6->LUMO (3%), H-5->LUMO (5%), H-3->L+2 (8%), H-2->LUMO (9%), H-1->L+3 (5%), HOMO->L+2 (3%)
17	313.764881721	0.0008	H-3->L+1 (86%), H-2->L+1 (10%)	
18	302.267767839	0.0021	H-10->LUMO (39%), H-9->LUMO (49%), H-4->L+1 (11%)	
19	297.902864106	0.0566	H-6->LUMO (84%)	H-7->L+1 (4%)
20	295.989765594	0.0026	H-10->LUMO (32%), H-10->L+1 (10%), H-9->LUMO (25%), H-8->LUMO (14%)	H-9->L+1 (9%)

AD 2

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	744.963005541	0.0004	H-1->LUMO (57%), H-1->L+1 (19%), H-1->L+2 (12%)	H-1->L+5 (6%), HOMO->L+3 (4%)
2	688.342177505	0.0577	HOMO->LUMO (53%), HOMO->L+1 (14%), HOMO->L+2 (12%), HOMO->L+5 (10%)	H-1->L+3 (6%)
3	557.232328145	0.0121	H-3->LUMO (18%), H-3->L+2 (11%), H-2->LUMO (15%), H-1->L+3 (19%)	H-3->L+1 (9%), H-3->L+5 (8%), H-2->L+1 (6%), H-2->L+2 (6%), H-2->L+5 (4%)
4	515.934388965	0.0183	H-1->L+3 (10%), HOMO->LUMO (37%), HOMO->L+1 (24%)	H-1->LUMO (2%), HOMO->L+2 (5%), HOMO->L+3 (8%), HOMO->L+5 (6%)
5	512.861191364	0.0023	H-1->LUMO (18%), HOMO->L+3 (45%)	H-3->L+3 (2%), H-2->L+3 (7%), H-1->L+1 (3%), H-1->L+2 (3%), H-1->L+3 (4%), H-1->L+5 (5%), HOMO->LUMO (5%)
6	482.35369208	0.0003	H-3->L+3 (12%), H-2->L+3 (12%), H-1->LUMO (22%), H-1->L+1 (30%), HOMO->L+3 (11%)	H-1->L+2 (6%), H-1->L+5 (5%)
7	463.630966316	0.0098	H-2->LUMO (15%), H-1->L+3 (34%), HOMO->L+1 (40%)	H-3->LUMO (2%)
8	433.026659026	0.0003	H-3->L+3 (14%), H-1->L+1 (45%), H-1->L+2 (10%), H-1->L+5 (17%)	H-2->L+3 (8%)
9	418.102761895	0.3765	H-3->LUMO (14%), H-2->LUMO (63%), HOMO->L+1 (10%)	
10	388.458166533	0.0093	H-3->LUMO (41%), HOMO->L+2 (17%), HOMO->L+5 (16%)	H-3->L+5 (3%), H-1->L+3 (7%), HOMO->L+1 (6%)

AD 3

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	746.892728989	0.0004	H-1->L+1 (76%), H-1->L+2 (11%)	H-1->L+4 (3%), HOMO->L+3 (3%)
2	683.108501445	0.065	HOMO->L+1 (67%), HOMO->L+2 (11%)	H-1->L+3 (4%), HOMO->L+4 (5%), HOMO->L+6 (3%)
3	597.571780471	0.0205	HOMO->LUMO (97%)	
4	563.359655635	0.004	H-1->LUMO (85%)	H-3->L+1 (4%), H-1->L+3 (3%)
5	553.007105318	0.01	H-3->L+1 (27%), H-3->L+2 (11%), H-2->L+1 (16%), H-1->LUMO (13%), H-1->L+3 (10%)	H-3->L+4 (4%), H-3->L+6 (3%), H-2->L+2 (3%), H-1->L+4 (2%)

6	507.1757875	0.001	HOMO->L+3 (48%)	H-3->L+3 (4%), H-2->L+3 (8%), H-1->L+1 (9%), H-1->L+2 (4%), H-1->L+4 (2%), H-1->L+6 (3%), HOMO->L+4 (9%), HOMO->L+5 (3%)
7	492.371998778	0.021	H-1->L+3 (33%), HOMO->L+1 (20%)	H-3->L+1 (5%), H-2->L+1 (5%), H-1->L+4 (7%), H-1->L+5 (2%), HOMO->L+2 (9%), HOMO->L+4 (5%), HOMO->L+6 (4%)
8	462.420531897	0.0067	H-3->L+3 (20%), H-2->LUMO (10%), H-1->L+1 (11%), H-1->L+2 (15%), H-1->L+4 (10%)	H-3->L+4 (3%), H-2->L+3 (9%), H-1->L+5 (4%), H-1->L+6 (8%)
9	452.860665542	0.0881	H-2->LUMO (77%)	H-4->LUMO (5%), H-3->L+3 (2%)
10	433.072035391	0.3293	H-2->L+1 (67%)	H-3->L+1 (6%), H-2->LUMO (4%), H-1->L+3 (3%), HOMO->L+1 (6%), HOMO->L+2 (3%)

AD 4

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	736.160747015	0.0005	H-1->LUMO (74%), H-1->L+3 (12%)	H-1->L+1 (4%), H-1->L+2 (4%), HOMO->L+2 (3%)
2	687.578710139	0.089	HOMO->LUMO (62%), HOMO->L+3 (14%)	H-2->LUMO (4%), H-1->L+2 (4%), HOMO->L+1 (4%), HOMO->L+2 (4%)
3	553.179819802	0.0187	H-3->LUMO (36%), H-3->L+3 (18%), H-1->L+2 (18%)	H-3->L+1 (5%), H-3->L+2 (5%), H-2->LUMO (6%), H-1->L+3 (5%)
4	512.140910456	0.0001	HOMO->L+2 (48%), HOMO->L+3 (14%)	H-3->L+2 (7%), H-3->L+3 (2%), H-2->L+2 (9%), H-2->L+3 (3%), H-1->LUMO (9%), H-1->L+3 (4%)
5	488.453661948	0.0367	H-3->LUMO (10%), H-1->L+2 (31%), HOMO->LUMO (22%), HOMO->L+3 (13%)	H-2->LUMO (6%), H-1->L+3 (9%), HOMO->L+2 (3%)
6	457.793423964	0.0001	H-3->L+2 (26%), H-1->LUMO (15%), H-1->L+3 (29%)	H-3->L+3 (8%), H-2->L+2 (4%), H-1->L+1 (4%), H-1->L+2 (7%), H-1->L+6 (4%)
7	429.456851445	1.1775	H-2->LUMO (76%), HOMO->LUMO (11%)	H-1->L+2 (2%), HOMO->L+3 (3%)
8	395.35775833	0.0309	H-3->LUMO (35%), H-1->L+2 (11%), HOMO->L+3 (23%)	H-3->L+3 (3%), H-2->LUMO (6%), H-1->L+3 (4%), HOMO->LUMO (3%), HOMO->L+1 (6%), HOMO->L+2 (6%)
9	362.951384696	0.0017	H-5->LUMO (51%), H-3->L+2 (14%)	H-4->LUMO (4%), H-3->L+3 (4%), H-1->L+2 (2%), H-1->L+3 (8%), HOMO->L+2 (8%), HOMO->L+3 (3%)
10	357.622639858	0.002	H-5->LUMO (39%), H-3->L+2 (17%), H-1->L+3 (10%), HOMO->L+2 (10%)	H-7->LUMO (3%), H-4->LUMO (4%), H-3->L+3 (4%), H-1->L+1

				(3%), H-1->L+2 (4%), HOMO->L+3 (4%)

AD 5

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	833.507179914	0.0162	H-1->LUMO (47%), HOMO->LUMO (32%)	H-1->L+1 (4%), H-1->L+4 (7%), H-1->L+8 (4%)
2	828.660560167	0.0323	H-1->LUMO (27%), HOMO->LUMO (57%)	H-1->L+1 (2%), H-1->L+4 (4%), H-1->L+8 (2%), HOMO->L+8 (3%)
3	642.338581557	0.0025	HOMO->LUMO (10%), HOMO->L+1 (25%), HOMO->L+4 (29%), HOMO->L+8 (20%)	H-2->LUMO (3%), H-1->L+7 (8%)
4	629.713002246	0.0004	H-1->LUMO (25%), H-1->L+1 (17%), H-1->L+4 (30%), H-1->L+8 (18%)	HOMO->L+7 (8%)
5	580.722215514	0.0392	H-3->LUMO (14%), H-3->L+4 (10%), H-3->L+8 (12%), H-2->LUMO (45%)	H-3->L+1 (4%), H-2->L+8 (2%), H-1->L+7 (6%)
6	547.294928102	0.0489	H-3->LUMO (11%), H-2->LUMO (40%), H-1->L+7 (20%)	H-3->L+4 (3%), H-3->L+8 (5%), HOMO->L+1 (8%), HOMO->L+4 (2%), HOMO->L+8 (2%)
7	536.914052539	0.0225	H-2->LUMO (10%), HOMO->L+1 (58%)	H-3->LUMO (5%), H-3->L+8 (2%), HOMO->L+2 (7%), HOMO->L+4 (9%), HOMO->L+8 (4%)
8	520.3298347	0.0001	H-1->L+1 (50%), HOMO->L+7 (32%)	H-3->L+7 (3%), H-2->L+7 (5%), H-1->L+2 (3%), H-1->L+8 (5%)
9	502.978470638	0.0148	HOMO->L+2 (85%)	H-1->L+7 (4%), HOMO->L+1 (5%)
10	500.279195466	0.0	H-3->L+7 (13%), H-1->L+1 (17%), H-1->L+2 (15%), H-1->L+4 (15%), HOMO->L+7 (24%)	H-2->L+7 (9%)
11	481.1743432	0.0299	H-3->LUMO (48%), H-1->L+7 (24%), HOMO->L+4 (14%)	H-3->L+8 (3%), H-1->L+2 (3%), HOMO->L+2 (2%)
12	476.917309737	0.0017	H-1->L+2 (76%)	H-3->LUMO (2%), H-3->L+7 (3%), H-1->L+1 (8%), H-1->L+8 (3%)
13	457.236292271	0.0004	HOMO->L+3 (94%)	
14	447.564049571	0.0011	H-3->LUMO (13%), H-2->L+1 (23%), H-1->L+7 (13%), HOMO->L+4 (16%)	H-3->L+1 (3%), H-3->L+4 (8%), H-3->L+8 (5%), H-2->L+4 (5%), HOMO->L+3 (2%), HOMO->L+8 (5%)
15	434.209543364	0.0001	H-1->L+3 (81%)	H-3->L+7 (3%), H-1->L+2 (2%), H-1->L+4 (7%), H-1->L+8 (4%)
16	429.055587127	0.0011	H-4->LUMO (42%), H-3->L+7 (10%), H-1->L+3 (10%),	H-2->L+1 (7%), H-2->L+7 (2%)

			H-1->L+4 (14%), H-1->L+8 (10%)	
17	428.595799959	0.0015	H-4->LUMO (48%), H-3->L+7 (10%), H-1->L+4 (16%), H-1->L+8 (11%)	H-1->L+3 (7%)
18	425.433870954	0.0678	H-2->L+1 (61%), HOMO->L+4 (10%)	H-4->LUMO (7%), H-3->L+1 (5%), H-3->L+4 (3%), H-3->L+8 (2%), H-2->L+2 (2%)
19	407.159676241	0.1097	H-5->LUMO (51%), H-2->L+2 (42%)	
20	394.992491039	0.2802	H-5->LUMO (39%), H-2->L+2 (50%)	H-6->LUMO (2%), H-3->L+1 (2%), H-2->L+3 (3%)

AD 6

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	727.222670023	0.0005	H-1->LUMO (70%), H-1->L+1 (12%), H-1->L+3 (10%)	HOMO->L+2 (5%)
2	669.714217103	0.0379	HOMO->LUMO (60%), HOMO->L+1 (12%), HOMO->L+3 (15%)	H-1->L+2 (8%)
3	554.739118623	0.0079	H-4->LUMO (21%), H-3->LUMO (21%), H-1->L+2 (21%)	H-4->L+1 (8%), H-4->L+3 (9%), H-3->L+1 (6%), H-3->L+3 (8%)
4	503.386898141	0.0001	H-3->L+2 (15%), HOMO->L+2 (65%)	H-4->L+2 (7%), H-1->LUMO (6%)
5	469.352638599	0.015	H-3->LUMO (10%), H-1->L+2 (46%), HOMO->LUMO (24%)	H-4->LUMO (5%), HOMO->L+1 (3%), HOMO->L+3 (7%)
6	441.256292306	0.0003	H-4->L+2 (17%), H-3->L+2 (15%), H-1->LUMO (20%), H-1->L+1 (12%), H-1->L+3 (31%)	
7	424.865303996	0.0003	H-2->LUMO (95%)	H-2->L+1 (3%)
8	382.218980863	0.3503	H-3->LUMO (27%), H-1->L+2 (12%), HOMO->LUMO (14%), HOMO->L+1 (19%), HOMO->L+3 (23%)	
9	363.984948514	0.5669	H-5->LUMO (10%), H-4->LUMO (44%), H-3->LUMO (32%)	H-1->L+2 (3%), HOMO->L+1 (3%), HOMO->L+3 (6%)
10	355.683610684	0.0022	H-4->L+2 (21%), H-3->L+2 (15%), H-1->L+1 (11%), H-1->L+3 (17%), HOMO->L+2 (22%)	H-8->LUMO (3%), H-6->LUMO (7%)
11	346.034588368	0.0036	H-6->LUMO (89%)	
12	336.556890828	0.0128	H-4->LUMO (19%), H-4->L+3 (17%), H-3->L+1 (10%), H-3->L+3 (20%)	H-7->LUMO (6%), H-4->L+1 (6%), H-3->LUMO (4%), H-1->L+2 (6%), HOMO->L+1 (3%), HOMO->L+3 (3%)
13	327.195505798	0.0254	H-5->LUMO (83%)	H-4->LUMO (6%), H-3->LUMO (3%), H-3->L+3 (2%)

14	310.286283128	0.0011	H-9->LUMO (81%)	H-8->LUMO (4%), H-7->LUMO (8%), H-2->L+1 (4%)
15	304.989159235	0.0026	H-8->LUMO (87%)	H-9->LUMO (3%), H-8->L+1 (3%)
16	304.002042498	0.0485	H-7->LUMO (80%)	H-9->LUMO (8%)
17	284.217483924	0.0052	H-10->LUMO (92%)	H-9->L+4 (3%)
18	279.911936181	0.0148	HOMO->L+1 (52%), HOMO->L+3 (36%)	H-2->L+1 (5%)
19	279.508077488	0.0014	H-1->L+1 (56%), H-1->L+3 (32%)	H-2->L+1 (5%)
20	278.103703316	0.001	H-2->L+1 (74%)	H-9->LUMO (4%), H-2->LUMO (3%), H-2->L+3 (6%), H-1->L+1 (4%), H-1->L+3 (2%), HOMO->L+1 (3%), HOMO->L+3 (2%)

AD 7

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	699.408771999	0.0004	H-1->LUMO (68%), H-1->L+2 (23%)	HOMO->L+1 (7%)
2	652.548384275	0.0253	H-1->L+1 (10%), HOMO->LUMO (56%), HOMO->L+2 (29%)	
3	546.42658886	0.0051	H-2->LUMO (31%), H-2->L+2 (23%), H-1->L+1 (25%)	H-3->LUMO (9%), H-3->L+2 (8%)
4	502.285662827	0.0001	H-2->L+1 (23%), HOMO->L+1 (64%)	H-3->L+1 (3%), H-1->LUMO (6%)
5	456.49555601	0.0115	H-2->LUMO (18%), H-1->L+1 (45%), HOMO->LUMO (25%)	HOMO->L+2 (6%)
6	430.754935247	0.0005	H-2->L+1 (25%), H-1->LUMO (23%), H-1->L+2 (37%)	H-3->L+1 (8%), HOMO->L+1 (3%)
7	367.916534652	0.1126	H-2->LUMO (14%), H-1->L+1 (11%), HOMO->LUMO (14%), HOMO->L+2 (53%)	
8	353.291710869	0.0001	H-3->L+1 (10%), H-2->L+1 (27%), H-1->L+2 (32%), HOMO->L+1 (21%)	H-7->LUMO (3%), HOMO->L+2 (2%)
9	339.431634167	0.5129	H-3->LUMO (64%), H-2->LUMO (25%)	
10	332.254778144	0.0165	H-4->LUMO (91%)	H-5->LUMO (3%)
11	327.01427708	0.0383	H-3->LUMO (20%), H-2->L+2 (43%)	H-6->LUMO (4%), H-5->LUMO (5%), H-3->L+2 (8%), H-2->LUMO (8%), H-1->L+1 (4%), HOMO->L+2 (4%)
12	325.477628468	0.0016	H-5->LUMO (88%)	H-4->LUMO (4%), H-2->L+2 (3%)

13	295.650975325	0.0022	H-7->LUMO (92%)	H-7->L+2 (4%)
14	293.808367526	0.0881	H-6->LUMO (90%)	
15	273.08692102	0.0081	H-10->LUMO (86%)	H-9->LUMO (4%), H-8->LUMO (3%), H-5->L+3 (5%)
16	258.284259343	0.0087	H-8->LUMO (75%), HOMO->L+3 (19%)	H-10->LUMO (2%)
17	251.117398198	0.0318	H-8->LUMO (19%), HOMO->L+3 (78%)	
18	248.764432208	0.0012	H-1->L+3 (96%)	
19	244.940916299	0.0	H-3->L+1 (73%), H-2->L+1 (20%)	
20	243.737109798	0.0047	HOMO->L+4 (89%)	H-9->LUMO (3%), HOMO->L+6 (3%)

AD 8

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	646.121178864	0.0003	H-1->LUMO (49%), H-1->L+1 (15%), H-1->L+3 (20%), HOMO->L+2 (11%)	
2	627.545644644	0.0344	H-1->L+2 (15%), HOMO->LUMO (39%), HOMO->L+1 (13%), HOMO->L+3 (22%)	H-2->LUMO (3%), H-2->L+3 (2%)
3	528.446820443	0.0102	H-4->LUMO (19%), H-4->L+1 (12%), H-4->L+3 (21%), H-1->L+2 (37%)	HOMO->LUMO (3%)
4	506.016623183	0.0001	H-4->L+2 (20%), H-2->L+2 (14%), H-1->LUMO (10%), HOMO->L+2 (52%)	
5	450.802432506	0.0536	H-4->LUMO (13%), H-1->L+2 (22%), HOMO->LUMO (39%)	H-4->L+1 (4%), H-4->L+3 (6%), H-2->LUMO (6%), HOMO->L+1 (2%), HOMO->L+3 (7%)
6	437.735464667	0.0006	H-4->L+2 (27%), H-1->LUMO (36%), H-1->L+3 (24%)	H-1->L+1 (6%)
7	413.777175985	0.0003	H-3->LUMO (94%)	H-3->L+1 (5%)
8	393.750612971	0.5032	H-2->LUMO (49%), H-1->L+2 (10%), HOMO->LUMO (17%), HOMO->L+3 (10%)	H-4->LUMO (3%), HOMO->L+1 (9%)
9	371.532747033	0.1928	H-4->LUMO (24%), H-2->LUMO (39%), HOMO->L+3 (15%)	H-1->L+2 (9%), HOMO->L+1 (9%)
10	360.38773657	0.0	H-4->L+2 (38%), H-1->L+1 (13%), H-1->L+3 (20%), HOMO->L+2 (24%)	H-1->LUMO (2%)
11	331.384489796	0.0005	H-4->LUMO (36%), H-4->L+1 (10%), H-4->L+3 (32%)	H-2->L+1 (3%), H-2->L+3 (6%), H-1->L+2 (4%), HOMO->L+1 (2%)
12	319.184926919	0.001	H-5->LUMO (96%)	

13	301.84830922	0.0647	H-6->LUMO (47%), HOMO->L+1 (32%), HOMO->L+3 (16%)	
14	297.195917859	0.0259	H-7->LUMO (56%), H-6->LUMO (16%), HOMO->L+1 (12%)	HOMO->L+3 (9%)
15	293.398156591	0.0023	H-1->L+1 (61%), H-1->L+3 (30%)	H-7->LUMO (3%)
16	290.933435827	0.0589	H-10->LUMO (30%), H-9->LUMO (10%), H-7->LUMO (18%), H-6->LUMO (14%), HOMO->L+1 (12%)	H-3->L+1 (3%), HOMO->L+3 (7%)
17	286.967232987	0.0403	H-10->LUMO (44%), H-8->LUMO (14%), H-6->LUMO (12%)	H-7->LUMO (9%), H-3->L+1 (7%), H-2->L+1 (3%), HOMO->L+1 (4%), HOMO->L+3 (3%)
18	284.106766756	0.0138	H-8->LUMO (76%)	H-10->LUMO (7%), H-8->L+1 (3%), H-7->LUMO (3%)
19	277.599339525	0.0021	H-10->LUMO (10%), H-3->L+1 (79%)	H-3->LUMO (5%), H-3->L+3 (3%)
20	272.54065113	0.0207	H-9->LUMO (33%), H-2->L+1 (54%)	H-10->LUMO (4%), HOMO->L+3 (2%)

AD 9

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	712.675708526	0.0004	H-1->LUMO (68%), H-1->L+1 (14%), H-1->L+3 (10%)	HOMO->L+2 (6%)
2	663.194399637	0.038	HOMO->LUMO (57%), HOMO->L+1 (14%), HOMO->L+3 (14%)	H-1->L+2 (9%)
3	550.209430249	0.008	H-4->LUMO (28%), H-4->L+1 (12%), H-4->L+3 (11%), H-3->LUMO (10%), H-1->L+2 (23%)	H-5->LUMO (3%), H-3->L+1 (3%), H-3->L+3 (3%)
4	504.000784603	0.0001	H-4->L+2 (13%), H-3->L+2 (11%), HOMO->L+2 (64%)	H-1->LUMO (6%)
5	468.607578094	0.0002	H-2->LUMO (89%)	H-2->L+1 (3%), H-1->L+2 (4%)
6	465.091878656	0.0179	H-1->L+2 (40%), HOMO->LUMO (23%)	H-4->LUMO (9%), H-3->LUMO (8%), H-2->LUMO (7%), HOMO->L+1 (3%), HOMO->L+3 (6%)
7	438.773376552	0.0004	H-4->L+2 (23%), H-1->LUMO (22%), H-1->L+1 (13%), H-1->L+3 (27%)	H-5->L+2 (2%), H-3->L+2 (7%)
8	382.101186551	0.4823	H-3->LUMO (34%), H-1->L+2 (10%), HOMO->LUMO (14%), HOMO->L+1 (18%), HOMO->L+3 (19%)	
9	366.188767831	0.4337	H-4->LUMO (28%), H-3->LUMO (42%)	H-5->LUMO (8%), H-1->L+2 (5%), HOMO->L+1 (7%), HOMO->L+3 (8%)

10	355.469460169	0.0003	H-4->L+2 (29%), H-1->L+1 (14%), H-1->L+3 (17%), HOMO->L+2 (23%)	H-10->LUMO (3%), H-6->LUMO (2%), H-5->L+2 (3%), H-3->L+2 (6%)
11	340.410172457	0.0019	H-6->LUMO (95%)	
12	334.866152633	0.0057	H-5->LUMO (10%), H-4->LUMO (27%), H-4->L+3 (19%)	H-7->LUMO (4%), H-4->L+1 (9%), H-3->L+1 (7%), H-3->L+3 (7%), H-1->L+2 (5%), HOMO->L+3 (3%)
13	329.894348541	0.0178	H-5->LUMO (70%)	H-9->LUMO (5%), H-4->L+1 (4%), H-4->L+3 (6%), H-3->LUMO (4%), H-3->L+3 (4%)
14	319.217798693	0.0034	H-9->LUMO (75%)	H-8->LUMO (7%), H-5->LUMO (6%), H-2->L+1 (5%)
15	303.503446702	0.0277	H-8->LUMO (78%)	H-11->LUMO (5%), H-9->LUMO (4%), H-7->LUMO (9%)
16	301.386049424	0.0084	H-10->LUMO (81%)	H-10->L+1 (2%), H-7->LUMO (8%)
17	301.012874826	0.0306	H-7->LUMO (70%)	H-11->LUMO (4%), H-10->LUMO (6%), H-9->LUMO (4%), H-8->LUMO (5%)
18	293.412043289	0.0005	H-2->L+1 (80%)	H-9->LUMO (6%), H-2->LUMO (3%), H-2->L+3 (9%)
19	288.388986351	0.0143	H-11->LUMO (84%)	H-8->LUMO (7%)
20	275.367447001	0.0152	HOMO->L+1 (50%), HOMO->L+3 (43%)	

AD 9

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	685.905028835	0.0004	H-1->LUMO (65%), H-1->L+2 (25%)	HOMO->L+1 (8%)
2	646.424363984	0.0249	H-1->L+1 (11%), HOMO->LUMO (54%), HOMO->L+2 (30%)	
3	542.268163979	0.0053	H-3->LUMO (11%), H-3->L+2 (10%), H-2->LUMO (25%), H-2->L+2 (21%), H-1->L+1 (27%)	
4	502.794894409	0.0001	H-2->L+1 (23%), HOMO->L+1 (63%)	H-3->L+1 (4%), H-1->LUMO (6%)
5	451.936257973	0.0128	H-2->LUMO (18%), H-1->L+1 (42%), HOMO->LUMO (27%)	H-3->LUMO (3%), H-2->L+2 (2%), HOMO->L+2 (5%)
6	427.915348285	0.0006	H-3->L+1 (10%), H-2->L+1 (22%), H-1->LUMO (25%), H-1->L+2 (35%)	HOMO->L+1 (3%)
7	366.795435218	0.1266	H-2->LUMO (13%), H-1->L+1 (11%), HOMO->LUMO (15%), HOMO->L+2 (53%)	H-3->LUMO (2%)

8	353.331983506	0.0003	H-3->L+1 (13%), H-2->L+1 (24%), H-1->L+2 (34%), HOMO->L+1 (21%)	
9	338.50490898	0.5328	H-3->LUMO (56%), H-2->LUMO (28%)	H-5->LUMO (7%)
10	332.183562888	0.0674	H-5->LUMO (80%)	H-4->LUMO (9%), H-3->LUMO (7%)
11	325.999666103	0.0007	H-4->LUMO (79%)	H-5->LUMO (8%), H-2->L+2 (4%)
12	324.31125559	0.0164	H-3->LUMO (16%), H-3->L+2 (11%), H-2->L+2 (39%)	H-6->LUMO (3%), H-5->LUMO (3%), H-4->LUMO (8%), H-2->LUMO (9%), H-1->L+1 (3%), HOMO->L+2 (3%)
13	292.064245865	0.0038	H-8->LUMO (72%), H-7->LUMO (18%)	H-8->L+2 (4%), H-6->LUMO (3%)
14	290.531207996	0.0694	H-6->LUMO (88%)	H-8->LUMO (3%)
15	285.191592704	0.0148	H-8->LUMO (18%), H-7->LUMO (79%)	
16	276.140210277	0.0146	H-10->LUMO (92%)	H-5->L+4 (4%)
17	252.559925469	0.0987	H-9->LUMO (98%)	
18	247.142928643	0.0042	HOMO->L+3 (79%)	H-3->L+1 (8%), H-2->L+1 (3%), HOMO->L+5 (4%)
19	246.59240043	0.0001	H-3->L+1 (60%), H-2->L+1 (24%), HOMO->L+3 (10%)	
20	244.945755403	0.0195	HOMO->L+4 (94%)	

AD 10

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	685.905028835	0.0004	H-1->LUMO (65%), H-1->L+2 (25%)	HOMO->L+1 (8%)
2	646.424363984	0.0249	H-1->L+1 (11%), HOMO->LUMO (54%), HOMO->L+2 (30%)	
3	542.268163979	0.0053	H-3->LUMO (11%), H-3->L+2 (10%), H-2->LUMO (25%), H-2->L+2 (21%), H-1->L+1 (27%)	
4	502.794894409	0.0001	H-2->L+1 (23%), HOMO->L+1 (63%)	H-3->L+1 (4%), H-1->LUMO (6%)
5	451.936257973	0.0128	H-2->LUMO (18%), H-1->L+1 (42%), HOMO->LUMO (27%)	H-3->LUMO (3%), H-2->L+2 (2%), HOMO->L+2 (5%)
6	427.915348285	0.0006	H-3->L+1 (10%), H-2->L+1 (22%), H-1->LUMO (25%), H-1->L+2 (35%)	HOMO->L+1 (3%)
7	366.795435218	0.1266	H-2->LUMO (13%), H-1->L+1 (11%), HOMO->LUMO (15%), HOMO->L+2 (53%)	H-3->LUMO (2%)
8	353.331983506	0.0003	H-3->L+1 (13%), H-2->L+1 (24%), H-1->L+2	

			(34%), HOMO->L+1 (21%)	
9	338.50490898	0.5328	H-3->LUMO (56%), H-2->LUMO (28%)	H-5->LUMO (7%)
10	332.183562888	0.0674	H-5->LUMO (80%)	H-4->LUMO (9%), H-3->LUMO (7%)
11	325.999666103	0.0007	H-4->LUMO (79%)	H-5->LUMO (8%), H-2->L+2 (4%)
12	324.31125559	0.0164	H-3->LUMO (16%), H-3->L+2 (11%), H-2->L+2 (39%)	H-6->LUMO (3%), H-5->LUMO (3%), H-4->LUMO (8%), H-2->LUMO (9%), H-1->L+1 (3%), HOMO->L+2 (3%)
13	292.064245865	0.0038	H-8->LUMO (72%), H-7->LUMO (18%)	H-8->L+2 (4%), H-6->LUMO (3%)
14	290.531207996	0.0694	H-6->LUMO (88%)	H-8->LUMO (3%)
15	285.191592704	0.0148	H-8->LUMO (18%), H-7->LUMO (79%)	
16	276.140210277	0.0146	H-10->LUMO (92%)	H-5->L+4 (4%)
17	252.559925469	0.0987	H-9->LUMO (98%)	
18	247.142928643	0.0042	HOMO->L+3 (79%)	H-3->L+1 (8%), H-2->L+1 (3%), HOMO->L+5 (4%)
19	246.59240043	0.0001	H-3->L+1 (60%), H-2->L+1 (24%), HOMO->L+3 (10%)	
20	244.945755403	0.0195	HOMO->L+4 (94%)	

AD 11

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	647.403232271	0.0003	H-1->LUMO (50%), H-1->L+1 (15%), H-1->L+3 (20%), HOMO->L+2 (11%)	
2	628.2133817	0.0348	H-1->L+2 (15%), HOMO->LUMO (39%), HOMO->L+1 (12%), HOMO->L+3 (22%)	H-2->LUMO (3%)
3	528.762337991	0.0103	H-4->LUMO (19%), H-4->L+1 (11%), H-4->L+3 (21%), H-1->L+2 (37%)	HOMO->LUMO (3%)
4	506.181893575	0.0001	H-4->L+2 (20%), H-2->L+2 (13%), H-1->LUMO (10%), HOMO->L+2 (53%)	
5	451.90331321	0.0527	H-4->LUMO (12%), H-1->L+2 (22%), HOMO->LUMO (39%)	H-4->L+1 (4%), H-4->L+3 (5%), H-2->LUMO (6%), HOMO->L+1 (2%), HOMO->L+3 (7%)
6	438.633669469	0.0005	H-4->L+2 (27%), H-1->LUMO (36%), H-1->L+3 (24%)	H-1->L+1 (6%)

7	412.332279132	0.001	H-3->LUMO (94%)	H-3->L+1 (5%)
8	394.151173106	0.4965	H-2->LUMO (48%), H-1->L+2 (10%), HOMO->LUMO (16%), HOMO->L+3 (10%)	H-4->LUMO (3%), HOMO->L+1 (9%)
9	371.967457735	0.2011	H-4->LUMO (25%), H-2->LUMO (39%), HOMO->L+3 (14%)	H-1->L+2 (9%), HOMO->L+1 (9%)
10	360.513486122	0.0	H-4->L+2 (38%), H-1->L+1 (12%), H-1->L+3 (19%), HOMO->L+2 (24%)	H-1->LUMO (2%)
11	332.094586737	0.0005	H-4->LUMO (36%), H-4->L+3 (31%)	H-4->L+1 (9%), H-2->L+1 (3%), H-2->L+3 (6%), H-1->L+2 (4%), HOMO->L+1 (2%)
12	320.116167959	0.001	H-5->LUMO (96%)	
13	303.555462277	0.0552	H-6->LUMO (39%), HOMO->L+1 (37%), HOMO->L+3 (17%)	
14	298.347313358	0.0226	H-7->LUMO (33%), H-6->LUMO (25%), HOMO->L+1 (12%)	H-11->LUMO (2%), H-8->LUMO (9%), H-1->L+1 (3%), HOMO->L+3 (8%)
15	296.039237392	0.0043	H-11->LUMO (16%), H-8->LUMO (34%), H-7->LUMO (34%)	H-1->L+1 (8%), H-1->L+3 (3%)
16	295.763819209	0.0021	H-8->LUMO (10%), H-1->L+1 (54%), H-1->L+3 (23%)	H-11->LUMO (4%)
17	290.211584224	0.0881	H-10->LUMO (10%), H-7->LUMO (21%), H-6->LUMO (24%), HOMO->L+1 (10%)	H-11->LUMO (9%), H-9->LUMO (5%), H-8->LUMO (5%), H-3->L+1 (2%), H-2->L+1 (4%), HOMO->L+3 (6%)
18	284.93598008	0.0101	H-9->LUMO (86%)	H-9->L+1 (3%)
19	279.899297933	0.005	H-3->L+1 (73%)	H-11->LUMO (3%), H-8->LUMO (8%), H-3->LUMO (5%), H-2->L+1 (6%)
20	274.198184338	0.0072	H-11->LUMO (10%), H-10->LUMO (26%), H-3->L+1 (12%), H-2->L+1 (40%)	H-8->LUMO (6%)

ADA 0

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	716.298994813	0.016	H-1->LUMO (71%), H-1->L+3 (18%)	HOMO->L+2 (7%)
2	684.844194721	0.002	HOMO->LUMO (61%), HOMO->L+3 (21%)	H-1->L+1 (4%), H-1->L+2 (8%)
3	563.052647649	0.0002	H-3->LUMO (39%), H-3->L+3 (19%), H-1->L+2 (20%)	H-4->LUMO (9%), H-4->L+3 (4%), H-1->L+1 (4%)

4	515.977331609	0.0038	H-3->L+2 (22%), HOMO->L+1 (21%), HOMO->L+2 (46%)	H-3->L+1 (3%), H-1->LUMO (4%)
5	447.725671718	0.0003	H-3->LUMO (22%), H-1->L+1 (22%), H-1->L+2 (35%), HOMO->LUMO (16%)	H-3->L+3 (2%)
6	419.972200434	0.0344	H-3->L+2 (26%), HOMO->L+1 (51%)	H-4->L+2 (5%), H-3->L+1 (5%), H-1->LUMO (5%), H-1->L+3 (4%)
7	397.984762341	0.0009	H-1->L+1 (62%), H-1->L+2 (21%), HOMO->L+3 (12%)	HOMO->LUMO (4%)
8	393.325908928	0.0717	H-1->LUMO (12%), H-1->L+3 (14%), HOMO->L+1 (25%), HOMO->L+2 (28%)	H-4->L+2 (2%), H-3->L+1 (6%), H-3->L+2 (9%)
9	352.628535302	0.791	H-2->LUMO (95%)	
10	343.598805599	0.0898	H-3->L+1 (21%), H-1->L+3 (53%), HOMO->L+2 (10%)	H-6->LUMO (3%), H-3->L+2 (2%), H-1->LUMO (6%)

ADA 1

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	745.142093949	0.0292	H-1->LUMO (69%), H-1->L+4 (15%)	H-1->L+7 (4%), HOMO->L+5 (5%)
2	711.326408561	0.0026	HOMO->LUMO (61%), HOMO->L+4 (17%)	H-1->L+1 (3%), H-1->L+5 (7%), HOMO->L+7 (6%)
3	573.390339047	0.0005	H-3->LUMO (36%), H-3->L+4 (14%), H-1->L+5 (17%)	H-6->LUMO (8%), H-6->L+4 (4%), H-3->L+7 (5%), H-1->L+1 (4%)
4	529.078232535	0.0184	H-3->L+5 (14%), HOMO->L+1 (32%), HOMO->L+5 (38%)	H-3->L+1 (2%), H-1->LUMO (4%), HOMO->L+6 (2%)
5	467.900192513	0.0009	H-3->LUMO (18%), H-1->L+1 (39%), H-1->L+5 (22%), HOMO->LUMO (13%)	
6	449.169267877	0.1265	H-3->L+5 (17%), HOMO->L+1 (58%)	H-6->L+5 (3%), H-3->L+1 (3%), HOMO->L+5 (9%), HOMO->L+6 (3%)
7	428.092649031	0.0004	H-1->L+1 (47%), H-1->L+5 (24%)	H-1->L+6 (6%), HOMO->LUMO (7%), HOMO->L+4 (6%), HOMO->L+7 (5%)
8	415.427016292	0.1343	H-3->L+5 (14%), H-1->LUMO (19%), H-1->L+4 (13%), H-1->L+7 (10%), HOMO->L+5 (15%)	H-6->L+5 (3%), H-3->L+1 (7%), HOMO->L+1 (6%), HOMO->L+6 (2%)
9	391.586738084	0.5402	H-5->LUMO (28%), H-4->L+1 (11%), H-2->LUMO (46%)	H-5->L+1 (3%), H-4->LUMO (2%)
10	389.973242576	0.012	H-5->L+1 (12%), H-4->LUMO (35%), HOMO->L+2 (30%)	H-4->L+1 (5%), H-2->LUMO (2%), HOMO->L+3 (5%)

ADA 2

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	827.720094881	0.0	H-1->LUMO (62%), H-1->L+2 (15%), H-1->L+4 (14%)	H-1->L+9 (3%), HOMO->L+5 (3%)
2	731.383866283	0.0	HOMO->LUMO (55%), HOMO->L+2 (12%), HOMO->L+4 (15%)	H-1->L+5 (5%), HOMO->L+9 (6%)
3	596.450632666	0.0	H-4->LUMO (13%), H-3->LUMO (30%), H-3->L+4 (11%), H-1->L+5 (13%)	H-7->LUMO (3%), H-4->L+2 (4%), H-4->L+4 (6%), H-4->L+9 (2%), H-3->L+2 (8%), H-3->L+9 (4%)
4	528.739788529	0.292	HOMO->L+1 (95%)	HOMO->L+3 (4%)
5	505.027262779	0.0	H-3->L+5 (23%), HOMO->L+5 (63%)	H-4->L+5 (3%), H-1->LUMO (5%)
6	503.305159585	0.0024	H-1->L+1 (93%)	H-1->L+3 (7%)
7	484.124142961	0.0	H-1->L+5 (33%), HOMO->LUMO (32%), HOMO->L+2 (20%)	H-3->LUMO (4%), HOMO->L+4 (5%), HOMO->L+9 (3%)
8	451.557682967	0.0001	H-1->LUMO (30%), H-1->L+2 (34%), H-1->L+4 (11%)	H-4->L+5 (4%), H-3->L+5 (9%), H-1->L+9 (6%)
9	448.97408297	0.7539	H-2->LUMO (94%)	
10	448.454418245	0.0	H-1->L+5 (31%), HOMO->L+2 (48%)	H-3->LUMO (9%), H-2->L+1 (2%), H-1->L+2 (2%), HOMO->LUMO (3%)

ADA 3

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	752.605275053	0.0502	H-1->LUMO (57%), H-1->L+2 (12%), H-1->L+4 (15%)	H-2->LUMO (3%), H-1->L+7 (2%), HOMO->L+5 (3%)
2	714.853511371	0.003	HOMO->LUMO (49%), HOMO->L+2 (11%), HOMO->L+4 (17%)	H-1->L+3 (5%), H-1->L+5 (5%), HOMO->L+7 (3%)
3	570.82961792	0.0087	H-4->LUMO (21%), H-4->L+4 (15%), H-3->LUMO (10%), H-1->L+5 (10%)	H-4->L+2 (5%), H-4->L+7 (3%), H-3->L+2 (2%), H-3->L+4 (5%), H-1->L+3 (4%), HOMO->L+3 (5%), HOMO->L+5 (2%)
4	561.726137243	0.0827	HOMO->L+1 (10%), HOMO->L+3 (60%), HOMO->L+5 (11%)	H-3->L+5 (2%), H-1->LUMO (3%)
5	523.117982415	0.0065	HOMO->LUMO (21%), HOMO->L+2 (62%)	H-1->L+1 (3%), H-1->L+2 (2%), HOMO->L+1 (6%), HOMO->L+3 (3%)

6	522.324611418	0.0276	HOMO->L+1 (70%), HOMO->L+2 (10%)	H-1->LUMO (3%), H-1->L+1 (6%), H-1->L+2 (2%), HOMO->L+3 (4%)
7	511.844911911	0.0059	H-1->L+1 (45%), H-1->L+2 (14%), H-1->L+3 (22%)	H-3->LUMO (2%), HOMO->L+1 (4%), HOMO->L+2 (3%), HOMO->L+3 (2%)
8	508.090291829	0.0076	H-1->LUMO (18%), H-1->L+1 (11%), H-1->L+2 (56%)	HOMO->L+1 (6%), HOMO->L+2 (2%)
9	500.178283896	0.0021	H-1->L+1 (31%), H-1->L+3 (48%)	H-4->LUMO (2%), H-3->LUMO (4%), H-1->L+5 (2%), HOMO->LUMO (5%)
10	482.222367906	0.1944	HOMO->L+3 (20%), HOMO->L+5 (29%)	H-4->L+3 (2%), H-4->L+5 (9%), H-3->L+3 (2%), H-3->L+5 (9%), HOMO->L+6 (8%)

ADA 4

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	766.896721793	0.0688	H-2->LUMO (15%), H-1->LUMO (58%)	H-2->L+5 (3%), H-1->L+2 (5%), H-1->L+5 (9%), HOMO->L+4 (4%)
2	733.287159997	0.0095	HOMO->LUMO (59%), HOMO->L+5 (12%)	H-3->LUMO (4%), H-1->L+1 (4%), H-1->L+4 (4%), HOMO->L+2 (6%)
3	577.826317809	0.0036	H-4->LUMO (38%), H-4->L+5 (15%), H-1->L+4 (11%)	H-6->LUMO (2%), H-4->L+2 (7%), H-3->LUMO (4%), H-2->L+4 (4%), H-1->L+1 (5%)
4	560.887550383	0.0941	HOMO->L+1 (64%), HOMO->L+4 (15%)	H-4->L+4 (4%), H-3->L+1 (3%), H-3->L+4 (4%), H-1->LUMO (3%), HOMO->L+3 (3%)
5	502.346716147	0.007	H-4->LUMO (10%), H-2->L+1 (12%), H-1->L+1 (55%)	H-3->LUMO (9%), H-1->L+4 (3%), HOMO->LUMO (6%)
6	484.294336206	0.6827	H-4->L+4 (11%), HOMO->L+1 (27%), HOMO->L+4 (26%)	H-4->L+1 (3%), H-3->L+4 (8%), H-2->LUMO (9%), H-1->LUMO (7%)
7	474.835100196	0.7398	H-2->LUMO (55%), H-1->LUMO (20%)	H-4->L+1 (2%), H-4->L+4 (7%), H-3->L+4 (2%), HOMO->L+1 (3%), HOMO->L+4 (3%)
8	458.504467336	0.0011	H-2->L+4 (10%), H-1->L+1 (16%), H-1->L+4 (32%), HOMO->LUMO (13%), HOMO->L+5 (10%)	H-4->LUMO (5%), HOMO->L+2 (3%)
9	436.02670305	0.0129	H-4->L+1 (10%), H-4->L+4 (16%), H-2->LUMO (16%), H-1->L+5 (15%), HOMO->L+4 (11%)	H-3->L+1 (4%), H-2->L+5 (4%), H-1->LUMO (7%), H-1->L+2 (4%)
10	421.413932267	0.005	H-3->LUMO (39%), H-2->L+1 (47%)	H-6->LUMO (2%), H-1->L+1 (2%), HOMO->LUMO (4%)

ADA 5

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	804.517507055	0.0657	H-1->LUMO (44%), H-1->L+2 (12%), H-1->L+6 (16%), H-1->L+15 (10%)	HOMO->L+12 (3%)
2	784.114552316	0.0028	HOMO->LUMO (44%), HOMO->L+2 (10%), HOMO->L+6 (14%), HOMO->L+15 (12%)	H-1->L+1 (3%), H-1->L+12 (3%)
3	676.695737432	0.048	HOMO->L+1 (89%)	HOMO->LUMO (2%)
4	656.24407459	0.0038	H-1->L+1 (80%)	H-1->LUMO (5%), HOMO->LUMO (8%)
5	605.864899395	0.0336	H-1->LUMO (31%), HOMO->LUMO (18%)	H-2->LUMO (4%), H-1->L+2 (5%), H-1->L+6 (7%), H-1->L+15 (3%), HOMO->L+2 (5%), HOMO->L+6 (7%), HOMO->L+12 (3%), HOMO->L+15 (4%)
6	600.088054848	0.0064	H-1->LUMO (16%), HOMO->LUMO (24%), HOMO->L+6 (10%)	H-1->L+1 (9%), H-1->L+2 (4%), H-1->L+6 (6%), H-1->L+15 (3%), HOMO->L+2 (8%), HOMO->L+12 (3%), HOMO->L+15 (5%)
7	583.427570525	0.0007	H-4->LUMO (13%), H-4->L+6 (13%), H-4->L+15 (15%), H-1->L+12 (13%)	H-4->L+2 (8%), H-3->LUMO (6%), H-3->L+2 (3%), H-3->L+6 (5%), H-3->L+15 (4%), H-1->L+1 (5%), H-1->L+9 (3%), H-1->L+14 (2%)
8	540.424518404	0.2432	H-2->LUMO (83%)	HOMO->L+12 (3%)
9	537.915714401	0.0212	H-2->L+1 (58%)	H-4->L+12 (2%), H-3->LUMO (3%), H-3->L+1 (2%), H-3->L+12 (2%), H-1->L+2 (3%), HOMO->L+3 (5%), HOMO->L+9 (5%), HOMO->L+12 (6%)
10	532.029664488	0.0056	H-2->L+1 (28%), HOMO->L+12 (14%)	H-4->L+12 (5%), H-3->LUMO (4%), H-3->L+12 (5%), H-1->L+2 (4%), H-1->L+6 (3%), HOMO->L+1 (2%), HOMO->L+3 (7%), HOMO->L+9 (8%), HOMO->L+14 (2%)
11	494.769116933	0.0001	H-3->LUMO (27%), H-2->L+1 (11%), H-1->L+3 (25%), HOMO->L+2 (14%)	H-1->L+9 (6%), H-1->L+12 (7%)
12	484.521446763	0.0401	HOMO->L+3 (70%)	H-4->L+12 (3%), H-3->L+1 (4%), H-3->L+12 (2%), H-1->L+2 (3%), HOMO->L+12 (5%)

13	479.833557848	0.0038	H-3->L+1 (59%), H-1->L+2 (14%)	H-3->LUMO (4%), HOMO->L+2 (5%)
14	472.392718937	0.0039	H-3->LUMO (17%), H-1->L+3 (55%)	H-1->L+2 (5%), H-1->L+4 (2%), H-1->L+12 (5%), HOMO->L+2 (5%)
15	471.781556363	0.0051	H-3->LUMO (22%), H-3->L+1 (10%), HOMO->L+2 (42%), HOMO->L+6 (10%)	HOMO->L+4 (4%), HOMO->L+5 (3%)
16	465.913317847	0.0172	H-3->L+1 (17%), H-1->L+2 (41%), H-1->L+6 (11%)	H-4->L+12 (3%), H-1->L+3 (6%), H-1->L+4 (3%), H-1->L+5 (4%), H-1->L+15 (3%)
17	453.191728241	0.0036	H-4->LUMO (15%), HOMO->L+4 (13%), HOMO->L+5 (10%)	H-3->LUMO (9%), H-3->L+2 (3%), H-2->L+3 (3%), H-1->L+3 (2%), H-1->L+4 (6%), H-1->L+5 (4%), H-1->L+9 (7%), H-1->L+12 (8%), HOMO->L+6 (8%)
18	447.128252055	0.0306	HOMO->L+4 (31%), HOMO->L+5 (47%)	H-1->L+4 (2%), HOMO->L+9 (7%)
19	441.617784549	0.0253	H-4->L+1 (20%), H-1->L+4 (53%)	H-4->L+12 (2%), H-1->L+5 (3%), HOMO->L+4 (2%), HOMO->L+5 (2%), HOMO->L+9 (4%)
20	439.504406282	0.0001	HOMO->L+4 (19%), HOMO->L+5 (19%), HOMO->L+6 (14%)	H-4->LUMO (8%), H-2->L+3 (4%), H-1->L+4 (8%), H-1->L+5 (9%), H-1->L+9 (2%), H-1->L+12 (3%), HOMO->L+2 (4%)

ADA 6

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	794.974307593	0.02	H-1->LUMO (74%), H-1->L+2 (12%)	H-1->L+5 (6%), HOMO->L+3 (2%)
2	734.460002442	0.0027	HOMO->LUMO (64%), HOMO->L+2 (13%)	H-1->L+1 (3%), H-1->L+3 (4%), HOMO->L+5 (8%)
3	592.772007134	0.0004	H-6->LUMO (43%), H-6->L+2 (13%)	H-8->LUMO (3%), H-6->L+5 (8%), H-5->LUMO (7%), H-1->L+1 (2%), H-1->L+3 (8%), H-1->L+4 (5%)
4	526.472157164	0.0349	HOMO->L+1 (37%), HOMO->L+3 (28%), HOMO->L+4 (11%)	H-6->L+3 (7%), H-6->L+4 (4%), H-5->L+3 (3%), H-1->LUMO (3%)
5	476.038368256	0.0012	H-1->L+1 (46%), H-1->L+3 (18%), HOMO->LUMO (10%)	H-6->LUMO (9%), H-5->LUMO (4%), H-1->L+4 (7%)
6	454.587493628	0.1615	H-6->L+3 (10%), HOMO->L+1 (56%), HOMO->L+4 (10%)	H-6->L+1 (2%), H-6->L+4 (5%), H-5->L+3 (2%), HOMO->L+3 (8%)

7	444.738478414	0.002	H-3->LUMO (36%), H-3->L+1 (17%), H-2->LUMO (37%)	H-2->L+1 (6%)
8	444.164910125	0.0001	H-3->LUMO (37%), H-2->LUMO (36%), H-2->L+1 (18%)	H-3->L+1 (6%)
9	434.148725444	0.0004	H-1->L+1 (41%), H-1->L+3 (18%), H-1->L+4 (18%)	HOMO->LUMO (6%), HOMO->L+2 (4%), HOMO->L+5 (6%)
10	415.566257792	0.136	H-6->L+3 (13%), H-1->LUMO (17%), H-1->L+2 (12%), H-1->L+5 (15%)	H-6->L+1 (8%), H-6->L+4 (6%), HOMO->L+1 (3%), HOMO->L+3 (8%), HOMO->L+4 (6%)

ADA 7

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	766.091158009	0.0148	H-1->LUMO (74%), H-1->L+3 (17%)	HOMO->L+2 (5%)
2	714.153522333	0.0022	HOMO->LUMO (64%), HOMO->L+3 (21%)	H-1->L+1 (3%), H-1->L+2 (7%)
3	582.058086532	0.0002	H-3->LUMO (48%), H-3->L+3 (21%), H-1->L+2 (15%)	H-4->LUMO (5%), H-4->L+3 (2%), H-1->L+1 (2%)
4	518.653808878	0.012	H-3->L+2 (19%), HOMO->L+1 (26%), HOMO->L+2 (46%)	H-3->L+1 (2%), H-1->LUMO (3%)
5	462.248128448	0.0005	H-3->LUMO (16%), H-1->L+1 (32%), H-1->L+2 (35%), HOMO->LUMO (13%)	
6	436.318246805	0.0972	H-3->L+2 (19%), HOMO->L+1 (63%)	H-3->L+1 (3%), HOMO->L+2 (8%)
7	418.3143595	0.0006	H-1->L+1 (56%), H-1->L+2 (26%), HOMO->L+3 (10%)	HOMO->LUMO (4%)
8	405.415581101	0.0519	H-3->L+2 (18%), H-1->LUMO (15%), H-1->L+3 (22%), HOMO->L+2 (20%)	H-3->L+1 (9%), HOMO->L+1 (8%)
9	369.572531931	0.9676	H-2->LUMO (97%)	
10	352.568370051	0.0471	H-3->L+1 (42%), H-1->L+3 (37%)	H-8->LUMO (4%), H-1->LUMO (4%), HOMO->L+2 (8%)

ADA 8

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	682.206410324	0.0439	H-2->LUMO (14%), H-1->LUMO (43%), H-1->L+2 (11%)	H-2->L+2 (5%), H-2->L+5 (4%), H-1->L+5 (9%), HOMO->L+3 (3%), HOMO->L+4 (6%)
2	668.198291631	0.0026	HOMO->LUMO (45%), HOMO->L+2 (14%),	H-3->LUMO (4%), H-2->L+4 (2%), H-1->L+1 (3%), H-1->L+3 (3%), H-1->L+4 (5%)

			HOMO->L+5 (13%)	
3	547.802734999	0.0009	H-6->LUMO (27%), H-6->L+2 (14%), H-6->L+5 (14%), H-1->L+4 (13%)	H-3->LUMO (3%), H-2->L+3 (3%), H-2->L+4 (5%), H-1->L+1 (3%), H-1->L+3 (6%)
4	522.390633742	0.0045	H-6->L+4 (10%), HOMO->L+1 (19%), HOMO->L+3 (14%), HOMO->L+4 (23%)	H-6->L+3 (4%), H-3->L+3 (5%), H-3->L+4 (9%), H-1->LUMO (6%)
5	448.421979139	0.0131	H-6->LUMO (12%), H-3->LUMO (12%), H-1->L+1 (20%), HOMO->LUMO (12%)	H-6->L+2 (4%), H-6->L+5 (3%), H-2->L+1 (5%), H-2->L+3 (2%), H-2->L+4 (3%), H-1->L+3 (5%), H-1->L+4 (9%), HOMO->L+1 (8%)
6	444.499311699	0.129	H-6->L+4 (10%), HOMO->L+1 (59%)	H-6->L+1 (2%), H-6->L+3 (5%), H-3->L+4 (4%), H-1->L+1 (4%), HOMO->L+4 (5%)
7	426.604937592	0.7574	H-2->LUMO (18%), H-1->LUMO (37%)	H-6->L+3 (2%), H-6->L+4 (5%), H-2->L+5 (2%), H-1->L+1 (8%), H-1->L+2 (3%), H-1->L+5 (4%), HOMO->LUMO (3%), HOMO->L+1 (4%), HOMO->L+4 (3%)
8	425.185847093	0.1501	H-1->L+1 (42%), H-1->L+4 (11%)	H-2->LUMO (3%), H-2->L+1 (4%), H-2->L+4 (4%), H-1->LUMO (8%), HOMO->LUMO (8%), HOMO->L+2 (3%), HOMO->L+5 (5%)
9	420.370899207	0.008	H-5->LUMO (41%), H-5->L+1 (25%), H-4->LUMO (18%)	H-4->L+1 (7%)
10	419.787347257	0.0028	H-5->LUMO (16%), H-4->LUMO (40%), H-4->L+1 (29%)	H-5->L+1 (8%)

ADA 9

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	779.627699253	0.0227	H-3->LUMO (63%), H-3->L+2 (12%)	H-3->L+5 (4%), H-2->LUMO (2%), H-1->LUMO (7%), HOMO->L+3 (3%)
2	725.435568499	0.0026	HOMO->LUMO (62%), HOMO->L+2 (14%)	H-3->L+1 (3%), H-3->L+3 (4%), HOMO->L+5 (8%)
3	586.490979244	0.0005	H-6->LUMO (44%), H-6->L+2 (14%), H-3->L+3 (10%)	H-8->LUMO (3%), H-6->L+5 (8%), H-5->LUMO (4%), H-3->L+1 (2%), H-3->L+4 (3%)

4	524.423454074	0.0308	H-6->L+3 (10%), HOMO->L+1 (33%), HOMO->L+3 (33%)	H-6->L+4 (3%), H-5->L+3 (4%), H-3->LUMO (3%), HOMO->L+4 (7%)
5	489.93990758	0.0016	H-2->LUMO (59%), H-2->L+1 (15%)	H-3->LUMO (6%), H-3->L+1 (3%), H-1->LUMO (9%), H-1->L+1 (5%)
6	489.630333355	0.0015	H-2->LUMO (12%), H-1->LUMO (58%), H-1->L+1 (18%)	H-3->LUMO (3%), H-2->L+1 (6%)
7	471.351098739	0.0018	H-6->LUMO (11%), H-3->L+1 (36%), H-3->L+3 (20%), HOMO->LUMO (11%)	H-5->LUMO (4%), H-3->L+4 (4%), H-2->L+1 (2%), H-1->L+1 (3%), H-1->L+3 (2%)
8	452.002161911	0.1907	H-6->L+3 (12%), HOMO->L+1 (59%)	H-6->L+1 (2%), H-6->L+4 (3%), H-5->L+3 (2%), HOMO->L+3 (9%), HOMO->L+4 (6%)
9	431.714868248	0.0005	H-3->L+1 (40%), H-3->L+3 (18%), H-3->L+4 (10%)	H-1->L+1 (4%), HOMO->LUMO (6%), HOMO->L+2 (5%), HOMO->L+5 (6%)
10	415.413097273	0.3607	H-6->L+3 (15%), H-3->LUMO (17%), H-3->L+2 (10%), H-3->L+5 (11%)	H-6->L+1 (7%), H-6->L+4 (3%), H-4->LUMO (9%), HOMO->L+1 (3%), HOMO->L+3 (9%), HOMO->L+4 (3%)

ADA 10

No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	750.010241439	0.0169	H-1->LUMO (72%), H-1->L+3 (18%)	HOMO->L+2 (5%)
2	705.417575172	0.0022	HOMO->LUMO (63%), HOMO->L+3 (22%)	H-1->L+1 (3%), H-1->L+2 (7%)
3	575.626505466	0.0003	H-3->LUMO (44%), H-3->L+3 (21%), H-1->L+2 (17%)	H-4->LUMO (6%), H-4->L+3 (3%), H-1->L+1 (3%)
4	518.111964113	0.0099	H-3->L+2 (20%), HOMO->L+1 (23%), HOMO->L+2 (46%)	H-3->L+1 (2%), H-1->LUMO (4%)
5	458.40275451	0.0006	H-3->LUMO (18%), H-1->L+1 (28%), H-1->L+2 (35%), HOMO->LUMO (14%)	
6	432.981292168	0.1007	H-3->L+2 (19%), HOMO->L+1 (63%)	H-4->L+2 (2%), H-3->L+1 (3%), HOMO->L+2 (6%)
7	414.648985025	0.0005	H-1->L+1 (59%), H-1->L+2 (24%), HOMO->L+3 (10%)	HOMO->LUMO (4%)
8	404.081064473	0.0749	H-3->L+2 (17%), H-1->LUMO (16%), H-1->L+3 (21%), HOMO->L+1 (10%), HOMO->L+2 (21%)	H-4->L+2 (2%), H-3->L+1 (7%)
9	370.301036414	1.0402	H-2->LUMO (97%)	
10	350.812611092	0.0402	H-3->L+1 (36%), H-1->L+3 (40%)	H-10->LUMO (3%), H-1->LUMO (4%), HOMO->L+2 (9%)

ADA 11				
No.	Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
1	684.01298142	0.0447	H-2->LUMO (14%), H-1->LUMO (44%), H-1->L+2 (11%)	H-2->L+2 (5%), H-2->L+5 (4%), H-1->L+5 (9%), HOMO->L+3 (3%), HOMO->L+4 (7%)
2	669.858949766	0.0027	HOMO->LUMO (46%), HOMO->L+2 (14%), HOMO->L+5 (14%)	H-2->L+4 (2%), H-1->L+1 (3%), H-1->L+3 (3%), H-1->L+4 (5%)
3	548.602623948	0.001	H-6->LUMO (27%), H-6->L+2 (14%), H-6->L+5 (14%), H-1->L+4 (14%)	H-4->LUMO (2%), H-2->L+3 (2%), H-2->L+4 (5%), H-1->L+1 (3%), H-1->L+3 (6%)
4	523.405070129	0.0052	H-6->L+4 (10%), HOMO->L+1 (20%), HOMO->L+3 (13%), HOMO->L+4 (24%)	H-6->L+3 (4%), H-4->L+3 (3%), H-4->L+4 (6%), H-3->L+4 (4%), H-1->LUMO (6%)
5	449.543847035	0.0137	H-6->LUMO (12%), H-1->L+1 (21%), HOMO->LUMO (12%)	H-6->L+2 (3%), H-6->L+5 (3%), H-4->LUMO (8%), H-3->LUMO (5%), H-2->L+1 (5%), H-2->L+3 (2%), H-2->L+4 (3%), H-1->L+3 (5%), H-1->L+4 (9%), HOMO->L+1 (7%)
6	445.5215531	0.1359	H-6->L+4 (10%), HOMO->L+1 (59%)	H-6->L+1 (2%), H-6->L+3 (5%), H-4->L+4 (3%), H-1->L+1 (4%), HOMO->L+4 (6%)
7	427.148739104	0.7308	H-2->LUMO (18%), H-1->LUMO (35%)	H-6->L+3 (2%), H-6->L+4 (5%), H-2->L+5 (2%), H-1->L+1 (8%), H-1->L+2 (3%), H-1->L+5 (4%), HOMO->LUMO (3%), HOMO->L+1 (3%), HOMO->L+4 (3%)
8	425.88689548	0.1416	H-1->L+1 (41%), H-1->L+4 (12%)	H-2->LUMO (3%), H-2->L+1 (3%), H-2->L+4 (4%), H-1->LUMO (7%), HOMO->LUMO (9%), HOMO->L+2 (3%), HOMO->L+5 (5%)
9	421.91585453	0.0433	H-4->LUMO (25%), H-4->L+1 (14%), H-3->LUMO (33%), H-3->L+1 (18%)	H-1->LUMO (2%)
10	418.554429182	0.0009	H-5->LUMO (58%), H-5->L+1 (37%)	H-5->L+2 (3%)

Cartesian coordinates of the optimized structures

AD 0

H	1.82875800	-0.90121900	-3.32031100
C	1.57287800	-0.04668500	-2.71244600
H	3.46612900	1.14713200	-2.71766800
C	2.44316100	1.03924200	-2.39088200
H	-0.51824800	-0.50316300	-2.10650400
C	0.33028300	0.15930100	-2.06356400
C	1.74912500	1.92489000	-1.53415400
C	0.41203200	1.40421000	-1.33396900
H	2.13077700	2.84048400	-1.10767700
Fe	1.83423500	0.06646700	-0.64079300
H	4.54596900	-0.54078300	-0.12997300
C	2.66012100	-1.74237700	-0.05178500
C	3.54902800	-0.67244200	0.26293500
C	1.43507000	-1.51880800	0.64533000
C	2.87484100	0.21486500	1.15379000
H	3.27327100	1.13225900	1.55990400
C	1.57066400	-0.31145400	1.39079700
H	0.80441200	0.14540800	1.99935600
C	-0.53411600	2.03977000	-0.46886000
H	-0.14802600	2.88721000	0.08912100
C	-1.85781600	1.75310000	-0.25884900
H	0.55393800	-2.14060300	0.59820900
C	-2.56892200	0.70882900	-0.91759400
N	-3.16617900	-0.13117500	-1.44274000
C	-2.61402600	2.52933700	0.66934800
N	-3.23120800	3.15659600	1.42053700
H	2.86743200	-2.56170900	-0.72351500

AD 1

H	2.44166000	-1.30727800	-3.01944100
C	1.98861600	-0.41895100	-2.60537500
H	3.62770700	1.09697200	-2.78483900
C	2.62058100	0.85684300	-2.47922500
H	-0.04506900	-1.12466600	-1.99058800
C	0.68476500	-0.33600200	-2.05719400
C	1.71233100	1.73701300	-1.84521500
C	0.48150200	1.01497800	-1.59004100
H	1.88836400	2.77317100	-1.59663200
Fe	2.07944100	0.13790300	-0.59310500
H	4.81381800	0.16686300	0.12264700
C	3.17155000	-1.33070600	0.38257300
C	3.83053100	-0.07118700	0.49974100
C	1.87948900	-1.21067900	0.97688800
C	2.94693000	0.82959500	1.16623200
H	3.14518600	1.86729400	1.38824500
C	1.74388900	0.12319200	1.46199800
H	0.86632100	0.53807500	1.93525300
C	-0.62149200	1.62049200	-0.90124000
H	-0.41522600	2.63251800	-0.55324900

H	1.12924100	-1.98505800	1.02918900
C	-1.88625100	1.20078900	-0.61085800
C	-2.81628400	2.09961600	0.12586700
C	-2.61331500	-0.05569200	-0.90444800
C	-4.10886500	1.36979000	0.26032200
C	-3.98985100	0.11315600	-0.34344200
C	-5.29690000	1.77093200	0.86088100
C	-5.05682500	-0.77774600	-0.36324900
C	-6.37091600	0.87923200	0.84353100
H	-5.38401000	2.74530800	1.32674300
C	-6.25212600	-0.37988200	0.23863400
H	-4.96079300	-1.74993100	-0.83192100
H	-7.31113100	1.16101500	1.30312700
H	-7.10263500	-1.05170400	0.24016700
O	-2.21766600	-1.05759400	-1.48390100
O	-2.57770400	3.22304400	0.54409000
H	3.56936800	-2.21165000	-0.09837900

AD 2

H	-0.11376000	-3.65258200	-0.40198300
C	-0.26870500	-2.61344800	-0.65075200
H	0.40154200	-2.51445700	-2.78536400
C	0.00847700	-2.00982200	-1.91586200
H	-1.02197200	-1.74978300	1.26551100
C	-0.73642200	-1.61520300	0.23787100
C	-0.27495200	-0.62900300	-1.81587700
C	-0.77384200	-0.35992000	-0.47747000
H	-0.16180700	0.10838200	-2.59673900
Fe	1.16516300	-1.10887900	-0.42359300
H	3.01988500	0.65843700	-1.64501800
C	3.14828800	-1.45797400	-0.92237300
C	2.90918700	-0.05356700	-0.84132100
C	2.85431100	-2.03065100	0.35029500
C	2.47111500	0.23868400	0.48370400
H	2.17779900	1.21040900	0.85202700
C	2.43340900	-0.98105200	1.22084500
H	2.12105000	-1.09350100	2.24797400
C	-1.05277000	0.98300100	-0.06200700
H	-0.73959200	1.69905700	-0.81277300
H	2.91071800	-3.07915000	0.60138700
C	-1.67221300	1.51559700	1.04189000
C	-1.87552500	2.94825900	1.27894800
C	-2.41538200	0.78231600	2.10558700
C	-2.87600400	3.08453800	2.36254200
C	-3.17363100	1.80617000	2.86332500
C	-3.50526900	4.20056300	2.92158600
C	-4.06402100	1.60799200	3.90835000
C	-4.40903800	4.00405500	3.96736900
C	-4.68619900	2.72597200	4.46331500
H	-4.26591400	0.60823000	4.27389400
H	-5.38922300	2.60757900	5.27923800

H	-4.90516800	4.86376900	4.40198400
H	-3.32237200	5.20278700	2.56561500
C	-1.21112000	4.00227000	0.68110800
C	-1.48473900	5.37123400	0.96603700
N	-1.66193600	6.49978100	1.15187100
C	-0.13985800	3.85625900	-0.24775300
N	0.74756500	3.80956300	-0.98968800
O	-2.44088300	-0.41779800	2.32533500
H	3.46556600	-1.99803100	-1.80176200

AD 3

H	0.98585200	-2.80815500	-1.57806900
C	0.70420200	-1.77062000	-1.67455300
H	1.91183100	-1.09186800	-3.43197100
C	1.19950300	-0.85904700	-2.65523700
H	-0.68201800	-1.49209500	0.04096600
C	-0.18076400	-1.07217700	-0.81581000
C	0.63733100	0.41449900	-2.40190700
C	-0.26089400	0.29606700	-1.27033700
H	0.81887300	1.32028100	-2.96069600
Fe	1.68592400	-0.18566100	-0.73550100
H	4.41139200	-0.36455400	-1.45971800
C	3.25172000	-1.03020400	0.33394300
C	3.75830700	-0.11651600	-0.63659300
C	2.39695000	-0.30650700	1.21840500
C	3.21614900	1.17281700	-0.35563300
H	3.39271500	2.07436700	-0.92242100
C	2.37930500	1.05353200	0.79326100
H	1.80178300	1.84877800	1.24055400
C	-0.88684500	1.44103700	-0.67331400
H	-0.41794100	2.37155000	-0.97000600
H	1.84503400	-0.71979000	2.04897200
C	-1.88567600	1.53649400	0.26231200
C	-2.07774400	2.71728700	1.12280800
C	-2.74682900	0.48221800	0.81236800
C	-2.66808700	2.22045900	2.37518200
C	-3.05396500	0.86841500	2.19419800
C	-2.87080600	2.84779100	3.60462000
C	-3.63454900	0.15007600	3.23779400
C	-3.44156500	2.11708700	4.64627400
C	-3.81653900	0.78399400	4.46654700
H	-3.92351800	-0.88413300	3.12047700
H	-4.25001600	0.23166900	5.29145400
H	-3.58949500	2.59165900	5.60871100
H	-2.58385800	3.87509000	3.77147400
C	-1.80898200	4.03260300	0.81134700
C	-2.01343900	5.11248700	1.71758500
N	-2.16178700	6.02392800	2.41471600
C	-1.36004900	4.46089700	-0.47155200
N	-1.00604300	4.85530600	-1.50012900
C	-3.33745300	-0.53452800	0.09708200

C	-3.23927700	-0.64017100	-1.32077200
N	-3.23133300	-0.73737900	-2.47308200
C	-4.20828300	-1.49768300	0.68405900
N	-4.91495700	-2.30223700	1.12167700
H	3.45612100	-2.08948800	0.37429200

AD 4

H	0.82778100	-1.18342600	-3.34483500
C	0.81946100	-0.25875700	-2.78782200
H	2.82248100	0.62157700	-3.26133900
C	1.87932900	0.69804700	-2.74202800
H	-1.15371800	-0.33355700	-1.75788500
C	-0.22696600	0.18772900	-1.94156200
C	1.49631500	1.74196100	-1.86430300
C	0.16923800	1.45242200	-1.37030200
H	2.08037800	2.61395100	-1.60998300
Fe	1.50367300	-0.04544300	-0.82643700
H	4.15374000	-1.02853700	-0.77082400
C	2.17270100	-1.91533300	-0.22700200
C	3.24564000	-0.97657400	-0.18919000
C	1.15292700	-1.45699800	0.66017200
C	2.89053600	0.06398400	0.72006100
H	3.48503600	0.93431800	0.95349800
C	1.59916100	-0.23647000	1.24583000
H	1.03937400	0.37449200	1.93828700
C	-0.54023400	2.27298300	-0.42991900
H	0.02432600	3.11545200	-0.04661600
H	0.20296000	-1.93749600	0.83906400
C	-1.83025900	2.08139800	-0.02563900
H	-2.38116300	1.24183800	-0.43693400
C	-2.54666700	2.88452400	0.89897400
C	-3.85580800	2.65667100	1.29070300
C	-2.05520500	4.12391600	1.62959800
C	-4.65278000	1.58556400	0.82402200
N	-5.25555700	0.69044900	0.40745000
C	-4.24714900	3.67347400	2.23066400
O	-3.23473400	4.51239300	2.43213800
C	-5.43783100	3.88822400	2.90641600
C	-0.93452000	3.84626200	2.63381100
H	-1.20342200	3.02183700	3.29587600
H	-0.00834000	3.59122900	2.11882600
H	-0.76148600	4.74153500	3.23328400
C	-1.76293900	5.30953800	0.70748000
H	-0.87189100	5.12291900	0.10804900
H	-2.60268100	5.49368200	0.03570300
H	-1.59084800	6.20012400	1.31412200
C	-5.55059100	4.99017100	3.79353400
N	-5.65445700	5.88574400	4.52034000
C	-6.57300200	3.05372100	2.76210500
N	-7.52618000	2.40132600	2.67814300
H	2.12778700	-2.80202500	-0.84127400

AD 5

H	0.85871900	-1.99622300	-2.94610900
C	0.70822400	-0.99259800	-2.57811100
H	2.12724600	0.21617600	-3.81639200
C	1.37480300	0.17989900	-3.04347500
H	-0.83385300	-1.30627500	-1.02112300
C	-0.16664800	-0.62770600	-1.52434800
C	0.90306200	1.27921300	-2.28974700
C	-0.07415000	0.80421500	-1.33420400
H	1.21396500	2.30833900	-2.39450700
Fe	1.77399900	-0.10801700	-1.01309300
H	4.51299900	-0.12030100	-1.69783000
C	3.23912900	-1.46064400	-0.43844000
C	3.83798800	-0.23843200	-0.86355300
C	2.38684600	-1.17353400	0.66963500
C	3.35452600	0.80691700	-0.02177300
H	3.60437900	1.85410000	-0.10140100
C	2.46024400	0.22704000	0.92602000
H	1.90734700	0.76278800	1.68339600
C	-0.78918600	1.72058900	-0.48388600
H	-0.66426900	2.74580100	-0.82234100
H	1.78201100	-1.88998400	1.20495500
C	-1.62525300	1.59478100	0.59181800
C	-2.39742800	2.72804200	1.10846100
C	-1.99950600	0.46622600	1.43898300
C	-2.40831000	4.04972200	0.66506900
C	-3.21544900	2.30728100	2.19476500
C	-1.44569600	-0.81009200	1.52500300
C	-3.03849100	0.86575400	2.33523300
C	-3.20910800	4.95937000	1.33380900
H	-1.81393000	4.38294400	-0.17352600
C	-3.92919500	3.30243700	2.89042000
C	-1.99591300	-1.71401700	2.41940100
H	-0.58928200	-1.09784800	0.93787900
C	-3.63760500	-0.13732000	3.12075100
C	-3.95790800	4.61526400	2.45815200
C	-3.11739800	-1.41665800	3.18951100
H	-4.51533000	5.36278000	3.00184700
H	-3.58361100	-2.16860700	3.80787600
N	-1.40263800	-3.05722600	2.53023800
O	-1.93116500	-3.85615200	3.29383300
O	-0.40777300	-3.30150900	1.85544300
N	-4.93522700	0.05451900	3.79151700
O	-5.17119600	-0.59816400	4.79635700
O	-5.72999800	0.82031400	3.25512700
N	-4.54772900	3.06578800	4.20664600
O	-5.55333500	3.69508300	4.49550400
O	-3.96982800	2.28881600	4.96021400
N	-3.23552300	6.35984600	0.87535300
O	-3.95213000	7.14709500	1.48211200

O	-2.54291200	6.65940800	-0.09052900
H	3.38409500	-2.42933500	-0.89251800

AD 6

H	2.08885900	-0.87661600	-3.32916100
C	1.73751400	-0.05073200	-2.72903400
H	3.57974500	1.20078000	-2.49363600
C	2.53167500	1.05076600	-2.28344000
H	-0.40120900	-0.57516900	-2.36601800
C	0.42656700	0.09375700	-2.21757300
C	1.71980900	1.88193300	-1.48191400
C	0.37894200	1.31639900	-1.44470100
H	2.02218900	2.79301300	-0.98729800
Fe	1.76956500	0.00436000	-0.63607900
H	4.43435100	-0.56432100	0.10881200
C	2.57745500	-1.80497100	-0.02547100
C	3.40854400	-0.72812900	0.40290400
C	1.28789400	-1.62832300	0.55952200
C	2.63465900	0.11651500	1.25364500
H	2.97238600	1.02783900	1.72336800
C	1.32705700	-0.44333700	1.35123900
H	0.49675200	-0.01978900	1.89660000
C	-0.61923500	1.90892500	-0.61257400
H	-0.22804700	2.73411900	-0.02223900
H	0.42944600	-2.26572000	0.41174800
C	-1.96327300	1.71267700	-0.38555200
C	-2.56839800	2.61496300	0.61628200
C	-2.81724000	0.73172900	-1.05676000
N	-3.94067800	2.45716500	0.83625000
O	-1.96880900	3.46918700	1.25216100
N	-4.17168100	0.75188500	-0.68279300
O	-2.47042600	-0.08147700	-1.89932000
H	-4.35306800	3.07465300	1.52470600
C	-4.77449500	1.56213700	0.23234200
H	-4.76173400	0.07391100	-1.14937400
S	-6.40476400	1.46796200	0.58725400
H	2.86519700	-2.59745800	-0.69977500

AD 7

H	2.08586900	-0.86581400	-3.33698200
C	1.73241600	-0.04460100	-2.73163900
H	3.56808800	1.21708100	-2.49785800
C	2.52178100	1.05945600	-2.28432400
H	-0.40268400	-0.58181300	-2.36188900
C	0.42217300	0.09083100	-2.21432100
C	1.70702500	1.88247100	-1.47629800
C	0.37081300	1.30844100	-1.43539500
H	2.00599100	2.79309900	-0.97868800
Fe	1.77359200	0.00104600	-0.63974700
H	4.44251500	-0.55321400	0.10385700
C	2.59323800	-1.80497600	-0.03456400

C	3.41753900	-0.72407500	0.39691400
C	1.30251300	-1.63792600	0.55079300
C	2.63813500	0.11339100	1.24974600
H	2.97014100	1.02556500	1.72195800
C	1.33377700	-0.45458300	1.34542600
H	0.50084400	-0.03790500	1.89205100
C	-0.63197500	1.90045600	-0.60383400
H	-0.24055500	2.72499800	-0.01252700
H	0.44807100	-2.28025700	0.40095900
C	-1.97386400	1.70791800	-0.37843200
C	-2.57802700	2.62063400	0.62195100
C	-2.82932900	0.72160000	-1.04950600
N	-3.94402900	2.47195600	0.84112400
O	-1.96554700	3.47335100	1.24972900
N	-4.17806700	0.74318000	-0.68345200
O	-2.46847700	-0.09316500	-1.88622200
H	-4.36412200	3.09075400	1.52376300
C	-4.79256900	1.56779300	0.23510000
H	-4.77574900	0.06760300	-1.14383300
O	-5.98144900	1.50429300	0.49079800
H	2.88610300	-2.59410000	-0.71063600

AD 8

H	-3.40142800	-2.11378100	1.84751100
C	-2.84713900	-1.19482300	1.73080500
H	-4.30341500	0.35814900	2.42106600
C	-3.32577700	0.11557300	2.03305100
H	-0.92529600	-1.90933600	0.87193400
C	-1.53071300	-1.08329400	1.21018400
C	-2.31022300	1.04532500	1.69658900
C	-1.16967700	0.31328400	1.19744700
H	-2.36345600	2.11909800	1.79826000
Fe	-2.84207000	-0.02124700	0.00763100
H	-5.53460800	0.57053300	-0.62533300
C	-4.07778400	-0.95472200	-1.37355700
C	-4.57676300	0.34678000	-1.07056400
C	-2.76491600	-0.80952300	-1.91405300
C	-3.57294100	1.29775500	-1.42283400
H	-3.63866100	2.36779700	-1.29550900
C	-2.45533300	0.58205100	-1.94565700
H	-1.52215900	1.01587700	-2.27299800
H	-2.11229100	-1.61231800	-2.22235800
C	1.22945000	0.41450000	0.39618800
S	1.70664400	-1.28977600	0.37471800
C	2.36314000	1.25460000	-0.02449900
C	3.34039500	-0.89647100	-0.16752500
O	2.37793400	2.46861400	-0.12331600
N	3.48715700	0.45420700	-0.31583200
S	4.48106900	-2.06831800	-0.44532700
C	4.74670600	1.08818300	-0.74546700
H	4.46179000	1.98482800	-1.29465400

H	5.23382800	0.39494500	-1.42944800
C	5.65702300	1.43501600	0.43061200
H	5.16889800	2.13435700	1.11237000
H	5.93999600	0.53924100	0.98665600
H	6.56846700	1.90556800	0.05398700
C	0.03942400	0.95358500	0.74829200
H	0.00818500	2.03927600	0.70130400
H	-4.59224700	-1.88758600	-1.19817000

AD 9

H	2.09393000	-0.84769000	-3.31982600
C	1.73848700	-0.03655800	-2.70213200
H	3.58118900	1.20331900	-2.41296900
C	2.53037200	1.05032500	-2.21904600
H	-0.40519700	-0.56339900	-2.37773100
C	0.42152400	0.09952000	-2.20226700
C	1.70983800	1.86265100	-1.40633900
C	0.36726400	1.30070700	-1.39773300
H	2.00907400	2.75943800	-0.88429400
Fe	1.74771300	-0.03694600	-0.60963500
H	4.40022700	-0.62658600	0.16489800
C	2.54519800	-1.86191800	-0.03196600
C	3.36942100	-0.79675900	0.43717700
C	1.24607200	-1.69895100	0.53576300
C	2.58159900	0.02687200	1.29578000
H	2.91177900	0.92593300	1.79370900
C	1.27214100	-0.53409100	1.35740800
H	0.43295200	-0.12370200	1.89919500
C	-0.63638500	1.88976900	-0.56437400
H	-0.23640300	2.69697800	0.04376800
H	0.38996400	-2.33176900	0.35765200
C	-1.98446500	1.71702400	-0.34682500
C	-2.57603500	2.61998600	0.65309900
C	-2.83767500	0.75517500	-1.03013600
N	-3.96477800	2.52783900	0.86006700
O	-1.92671600	3.43807500	1.29202600
N	-4.20332700	0.73850400	-0.66244200
O	-2.44575600	-0.02679900	-1.88488800
C	-4.78741200	1.60273300	0.24345900
C	-4.52644300	3.49247500	1.84167900
C	-4.49146000	2.96522900	3.27353400
H	-5.54400000	3.70675600	1.52985300
H	-3.92835400	4.39577500	1.75283400
H	-4.90682100	3.72101500	3.94547300
H	-5.08844900	2.05684200	3.37357200
H	-3.46817500	2.75461600	3.59016300
C	-5.02988600	-0.28399000	-1.35545900
C	-5.60684600	0.21973900	-2.67573500
H	-5.82056300	-0.57167200	-0.66948500
H	-4.37758800	-1.13675100	-1.52480100
H	-6.19326000	-0.57763600	-3.14001300

H	-6.26430100	1.07651700	-2.51673700
H	-4.81295000	0.50528000	-3.36848300
S	-6.43464500	1.53381900	0.58614300
H	2.84398700	-2.63776300	-0.72069800

AD 10

H	2.07391400	-0.87355700	-3.33755300
C	1.71880400	-0.05186300	-2.73374200
H	3.54600500	1.22575800	-2.51900700
C	2.50251100	1.06032600	-2.29754000
H	-0.40944700	-0.60320000	-2.34554700
C	0.41058100	0.07697000	-2.20779900
C	1.68536600	1.88098000	-1.48842100
C	0.35464300	1.29697400	-1.43428800
H	1.98067500	2.79630700	-0.99716100
Fe	1.77575600	0.00384800	-0.64394300
H	4.45256300	-0.51434000	0.10040700
C	2.61837400	-1.78916500	-0.03069300
C	3.42973700	-0.69597000	0.39458800
C	1.32614700	-1.63484200	0.55498500
C	2.64064800	0.13629700	1.24364100
H	2.96191700	1.05485100	1.71095600
C	1.34313400	-0.44685400	1.34317000
H	0.50554100	-0.03759300	1.88826600
C	-0.64871200	1.89852800	-0.60492900
H	-0.25165500	2.72665400	-0.02297100
H	0.47946300	-2.28828300	0.40896000
C	-1.98968400	1.71871500	-0.37316600
C	-2.58339800	2.64724100	0.61351900
C	-2.84595100	0.72843600	-1.02794500
N	-3.95319900	2.53881400	0.84367300
O	-1.94147800	3.49278500	1.22627100
N	-4.20479800	0.74981500	-0.69144800
O	-2.45758400	-0.09940500	-1.84224800
C	-4.79536000	1.61906300	0.22174400
O	-5.98923400	1.57749600	0.46804100
C	-4.53734300	3.46924300	1.82228100
H	-4.06875100	3.32118500	2.79497700
H	-4.36495900	4.49580400	1.50020500
H	-5.60115600	3.27025000	1.88555000
C	-5.06276900	-0.23850000	-1.36356900
H	-5.01888200	-0.09013200	-2.44226900
H	-4.71542700	-1.24516000	-1.13205700
H	-6.07797000	-0.10262800	-1.00844700
H	2.92048600	-2.57851000	-0.70246200

AD 11

H	2.16276800	-0.16092900	-3.38558500
C	1.78402100	0.51048800	-2.62989400
H	3.55460500	1.80222000	-2.17663700
C	2.52222500	1.54988100	-1.98772000

H	-0.29719500	-0.21901500	-2.35165300
C	0.47655100	0.48036000	-2.07685200
C	1.67747800	2.16512600	-1.03029600
C	0.38503500	1.52259000	-1.08367100
H	1.93897300	2.98069400	-0.37257300
Fe	1.86912000	0.15760400	-0.57670200
H	4.56927700	-0.36653900	0.08297200
C	2.79860100	-1.67822700	-0.30787400
C	3.55554700	-0.64829100	0.32532500
C	1.49976400	-1.69857300	0.28322300
C	2.72546600	-0.03053100	1.30788900
H	3.00124400	0.79780100	1.94296800
C	1.45674200	-0.68184600	1.28201900
H	0.60009300	-0.42460600	1.88708700
H	0.68614400	-2.35221500	0.00710400
C	-2.00492500	1.49569800	-0.24970700
S	-2.79641500	0.37621700	-1.36982200
C	-2.98509200	2.00541500	0.72328700
C	-4.36229200	0.58688500	-0.58382700
O	-2.77923800	2.79351600	1.62783300
N	-4.25958800	1.45482400	0.46780400
S	-5.72764000	-0.19288700	-1.11071400
C	-5.40344600	1.82313600	1.32491900
H	-6.28796400	1.80884700	0.68623800
H	-5.22454900	2.84153200	1.66715100
C	-0.71100600	1.89097400	-0.22571800
H	-0.47789500	2.61340500	0.55252900
C	-5.57052800	0.88428400	2.48964100
H	-5.70347700	-0.16500000	2.24013000
C	-5.59262000	1.28120800	3.75917100
H	-5.74842100	0.57592900	4.56770800
H	-5.46202800	2.32358300	4.03334100
H	3.13966300	-2.31221600	-1.11249500

ADA 0

H	1.72776000	-0.91708700	-3.37467100
C	1.50162000	-0.06230100	-2.75518900
H	3.41468700	1.09831300	-2.80161100
C	2.39988300	1.00329100	-2.44727200
H	-0.57745100	-0.49439900	-2.09383200
C	0.28154200	0.15521500	-2.06871300
C	1.74151800	1.89139100	-1.56410600
C	0.40587000	1.38888700	-1.32964800
H	2.15105500	2.79324300	-1.13441700
Fe	1.82757700	0.02500900	-0.68615000
H	4.55391300	-0.39124300	-0.07836300
C	2.73985600	-1.73319800	-0.07496200
C	3.55671400	-0.59577600	0.27465600
C	1.46759600	-1.56321000	0.59267000
C	2.80753400	0.22650500	1.15214200
H	3.14038700	1.16292000	1.57302800

C	1.52601400	-0.37171800	1.35086100
H	0.72328800	0.03755600	1.94533900
C	-0.51487200	2.04647100	-0.44512700
H	-0.10050500	2.88180000	0.11031000
C	-1.83838400	1.78906100	-0.22314700
C	3.00398700	-2.83777900	-0.95404000
H	2.14816800	-3.47086000	-1.16595800
C	4.17918400	-3.22043400	-1.53709600
H	0.63050400	-2.24127700	0.52252600
C	5.42363800	-2.54681800	-1.35878900
N	6.44265800	-2.01690900	-1.22655600
C	4.21230400	-4.36913100	-2.38531000
N	4.24535400	-5.29822300	-3.07287400
C	-2.57877100	0.75902000	-0.87503500
N	-3.19775400	-0.06880600	-1.39294000
C	-2.57047400	2.58216400	0.71240300
N	-3.16786600	3.22103600	1.46872000

ADA 1

H	1.85832800	-1.30332400	-3.39385300
C	1.48077700	-0.41631900	-2.90727100
H	3.16350100	1.03859900	-3.16893300
C	2.17868400	0.82400000	-2.78305300
H	-0.51639800	-1.07276100	-2.13864700
C	0.23721000	-0.31028600	-2.23722700
C	1.36769700	1.70716900	-2.03080400
C	0.13781400	1.02228300	-1.69364600
H	1.61171800	2.72070900	-1.74893400
Fe	1.78183300	0.04061400	-0.88612400
H	4.54823200	0.16802600	-0.28693400
C	2.99218200	-1.42195600	-0.04263800
C	3.59277100	-0.12026800	0.11728400
C	1.70562800	-1.37639700	0.62056600
C	2.70606300	0.68314000	0.87646000
H	2.86598300	1.71597200	1.14684700
C	1.54695900	-0.09182000	1.18995300
H	0.68045200	0.25766900	1.73092800
C	-0.88099900	1.64562100	-0.89188100
H	-0.60360300	2.63312300	-0.52364800
C	3.43572900	-2.58746300	-0.75961900
H	2.69369600	-3.38469500	-0.79738800
H	0.99980700	-2.19213100	0.66845300
C	4.60330200	-2.90920700	-1.37973400
C	4.75797700	-4.24324700	-2.02838100
C	5.87842500	-2.17232700	-1.56026800
C	6.13849800	-4.29597900	-2.58426500
C	6.79131900	-3.08900600	-2.30879700
C	6.77715800	-5.31900800	-3.27659100
C	8.10213000	-2.87180500	-2.71887300
C	8.09281800	-5.10486900	-3.68981000
H	6.26723200	-6.25153100	-3.48695300

C	8.74734300	-3.89568200	-3.41413900
H	8.60425100	-1.93611300	-2.50379900
H	8.61931900	-5.88188900	-4.23163800
H	9.76934100	-3.75774600	-3.74749300
C	-2.13327200	1.26470500	-0.52092900
C	-2.96992600	2.17213100	0.31634700
C	-2.93438600	0.04741300	-0.80103900
C	-4.27747100	1.48911900	0.51976600
C	-4.25624300	0.25190300	-0.13425000
C	-5.40085900	1.91445900	1.22053800
C	-5.35895200	-0.59463400	-0.10558900
C	-6.50960100	1.06749800	1.25182100
H	-5.41229200	2.87321700	1.72507600
C	-6.48880500	-0.17206800	0.59637900
H	-5.33846000	-1.55150500	-0.61339600
H	-7.40125900	1.36868300	1.78920600
H	-7.36485000	-0.80879700	0.63776800
O	-2.62252900	-0.94695800	-1.43956900
O	-2.65156400	3.26697600	0.75361200
O	6.17209600	-1.04424800	-1.19243100
O	3.91935000	-5.12842600	-2.09379000

ADA 2

H	-0.14668100	-3.60925400	-0.56788100
C	-0.30350300	-2.56074200	-0.77411100
H	0.31292300	-2.38464600	-2.92269400
C	-0.05370000	-1.91053800	-2.02483400
H	-0.98429600	-1.76028100	1.19285400
C	-0.73490800	-1.59183900	0.16047000
C	-0.31924300	-0.53404500	-1.86471700
C	-0.76933200	-0.31033300	-0.50350000
H	-0.20835900	0.23302100	-2.61676700
Fe	1.16462900	-1.08464600	-0.53415500
H	3.31231300	-0.40318100	-2.26047900
C	3.09901700	-1.85760700	-0.56774000
C	3.06349300	-0.57442600	-1.22842300
C	2.64948300	-1.63764300	0.79426300
C	2.63197800	0.39180200	-0.29114400
H	2.47439000	1.44071700	-0.49473500
C	2.38312800	-0.26172000	0.95803700
H	2.01675100	0.20988500	1.85731300
C	-1.02872900	1.02045700	-0.02585500
H	-0.70097400	1.76820600	-0.73898500
C	3.35869500	-3.18704800	-1.04897600
H	3.03181100	-3.93674800	-0.33750400
H	2.53940500	-2.40669700	1.54440200
C	-1.64558100	1.50010200	1.09786200
C	-1.83326400	2.92345900	1.40676800
C	-2.42856000	0.72482200	2.10647600
C	-2.88256700	3.01935000	2.44430300
C	-3.21165400	1.72194800	2.87370400

C	-3.52852500	4.11631800	3.02192200
C	-4.14986700	1.48728300	3.86858700
C	3.97476800	-3.66355400	-2.17445600
C	4.75658100	-2.88535200	-3.18172800
C	4.16248200	-5.08603200	-2.48739500
C	5.53899100	-3.88021500	-3.95258000
C	5.21060800	-5.17885400	-3.52639800
C	6.47605300	-3.64264100	-4.94785900
C	5.85608500	-6.27410800	-4.10779300
C	7.11398800	-4.73976000	-5.52534400
C	6.80692300	-6.03740000	-5.10157700
H	5.65045900	-7.28958800	-3.80523800
H	7.31714300	-6.88000400	-5.55294600
H	7.85331300	-4.59052700	-6.30317200
H	6.70130800	-2.62932200	-5.25807100
C	-4.48052500	3.88251300	4.01528100
C	-4.78827500	2.58610400	4.44230400
H	-4.37562500	0.47486100	4.18135800
H	-5.52850000	2.43915100	5.21971000
H	-4.99112600	4.72644600	4.46372700
H	-3.32239700	5.13092300	2.71678100
C	3.43599700	-6.14926700	-1.99119400
C	-1.10589400	3.98512100	0.90851200
C	3.68798800	-7.50776400	-2.34037200
N	3.84826500	-8.62743900	-2.58424800
C	2.31163300	-6.01277800	-1.12522400
N	1.37764100	-5.96328900	-0.44339300
C	-1.35800600	5.34466300	1.25350300
N	-1.51833400	6.46506900	1.49396300
C	0.01954100	3.84586000	0.04438400
N	0.95441800	3.79409900	-0.63606400
O	-2.46234400	-0.48232100	2.27345600
O	4.78997000	-1.67774600	-3.34541700

ADA 3

H	0.48274200	-2.93153500	-2.05473000
C	0.23441800	-1.88164800	-2.09152600
H	1.18272800	-1.21558800	-4.00553200
C	0.61280500	-0.97144400	-3.12227100
H	-0.85292700	-1.58421200	-0.17437300
C	-0.47366300	-1.16661800	-1.09280400
C	0.14807900	0.31772400	-2.76354700
C	-0.56257100	0.21022600	-1.50900100
H	0.28284700	1.22871200	-3.32696300
Fe	1.42587700	-0.35576100	-1.29386800
H	3.97244900	-0.41473300	-2.47756600
C	3.16578600	-1.19277700	-0.52245400
C	3.47709800	-0.22107900	-1.53982600
C	2.42611000	-0.49981300	0.50946800
C	2.97383300	1.03625400	-1.11991600
H	3.03303600	1.95732300	-1.67928100

C	2.33828700	0.86495900	0.14661900
H	1.83772900	1.63649300	0.71171100
C	-1.07797900	1.36600700	-0.81667600
H	-0.60460300	2.28783800	-1.13345500
C	3.35164500	-2.62269000	-0.50644700
H	2.63143600	-3.12942400	0.12488800
H	2.03237700	-0.95326200	1.40648800
C	-1.97239200	1.46613400	0.20943600
C	-2.05753200	2.64327200	1.09930400
C	-2.78877400	0.41785300	0.84445800
C	-2.48864000	2.13263800	2.40734500
C	-2.91045600	0.78657800	2.25816600
C	-2.52509300	2.74369000	3.66120300
C	-3.36073800	0.05758600	3.35761500
C	4.20490900	-3.42036700	-1.21310600
C	5.30029900	-3.04457900	-2.12247100
C	3.97453500	-4.86431600	-1.42825500
C	5.34823100	-4.07627400	-3.16304900
C	4.56462100	-5.17884900	-2.73625600
C	6.01542400	-4.11072000	-4.38645800
C	4.45686700	-6.31480200	-3.53926000
C	5.88655400	-5.24536300	-5.18594600
C	5.11869400	-6.33447100	-4.76594200
H	3.86313300	-7.16586400	-3.24086200
H	5.02983800	-7.20570800	-5.40337000
H	6.38508200	-5.27866200	-6.14704000
H	6.60633000	-3.27491200	-4.73180500
C	-2.96674700	2.00251500	4.75605100
C	-3.37698800	0.67517700	4.60721900
H	-3.67282000	-0.97235800	3.26348800
H	-3.70756000	0.11504700	5.47343000
H	-2.98520400	2.46299300	5.73629800
H	-2.20574800	3.76523800	3.80365800
C	3.38047400	-5.74898400	-0.55858200
C	-1.83457000	3.95754300	0.76068500
C	3.19435300	-7.13121300	-0.85161200
N	3.02282600	-8.25903000	-1.04253200
C	2.94972800	-5.38955500	0.75223800
N	2.59543400	-5.14384100	1.82563700
C	-1.93719700	5.03410900	1.68891000
N	-2.00974000	5.94044800	2.40383400
C	-1.54320800	4.38630000	-0.56755600
N	-1.31418000	4.77852900	-1.63140300
C	-3.48568800	-0.56827700	0.18914900
C	6.23239300	-2.06028300	-1.89783400
C	-3.55306300	-0.65324800	-1.23249700
N	-3.67627600	-0.73259000	-2.37934700
C	-4.30742000	-1.51912400	0.86237900
N	-4.97902100	-2.31105100	1.37142900
C	7.30832100	-1.78877500	-2.79300800
N	8.19078400	-1.53422700	-3.49574400

C	6.28465800	-1.30665000	-0.68875600
N	6.39522600	-0.70589800	0.29287900

ADA 4

H	1.49498800	-0.59001700	-3.49365800
C	1.41496400	0.23503800	-2.80194700
H	3.47553700	1.10882400	-2.83451300
C	2.46824600	1.13108600	-2.44773700
H	-0.68686500	0.05975400	-2.08662700
C	0.26153900	0.57292500	-2.04951900
C	1.96982900	2.03224500	-1.47310300
C	0.58518900	1.71078000	-1.22636600
H	2.52067500	2.82769200	-0.99355200
Fe	1.81339200	0.10123800	-0.75145600
H	4.45573500	-0.79886900	-0.31713900
C	2.45064700	-1.82826400	-0.31282500
C	3.45187700	-0.86587600	0.07302800
C	1.25002700	-1.50856800	0.42330900
C	2.88208400	-0.00078700	1.04149100
H	3.37763400	0.83604100	1.50969100
C	1.52811500	-0.40068500	1.25986900
H	0.82446000	0.08543300	1.91857800
C	-0.25365100	2.40466100	-0.28216100
H	0.25664400	3.14781500	0.31987500
C	2.54957500	-2.89220100	-1.27753600
H	1.61373600	-3.38322100	-1.51842600
H	0.31127500	-2.03640000	0.34713800
C	3.70731300	-3.32464900	-1.85232500
H	4.63460600	-2.84358100	-1.56154400
C	-1.59167600	2.20689800	-0.12935700
H	-2.08132100	1.47018000	-0.75783200
C	3.83744900	-4.38425000	-2.79690300
C	2.90498600	-5.17422600	-3.44244600
C	5.21502500	-4.82249800	-3.26011500
C	3.60509600	-6.10952400	-4.29307900
C	3.13955300	-7.10514700	-5.13555600
O	4.91731000	-5.91815400	-4.19578800
C	1.76602200	-7.40178500	-5.31515200
N	0.65901200	-7.68700700	-5.49929400
C	4.06948300	-7.88774600	-5.86960200
N	4.81729800	-8.53287600	-6.47389100
C	5.95164600	-3.74183100	-4.05408900
H	5.33470500	-3.37284200	-4.87490900
H	6.20995200	-2.90474700	-3.40359800
H	6.87412700	-4.15939500	-4.46097300
C	6.06253800	-5.41116200	-2.13081700
H	6.31235400	-4.63559900	-1.40492800
H	5.52624100	-6.21148400	-1.61871300
H	6.99038400	-5.81012500	-2.54402100
C	-2.44133100	2.88244200	0.79196400
C	-3.79626700	2.64823200	0.92383000

C	-2.05683500	3.96528600	1.78640300
C	1.49969700	-5.08361200	-3.31799200
N	0.35504600	-4.97448700	-3.19147200
C	-4.52247700	1.70274900	0.16142900
N	-5.06354700	0.91587500	-0.49065300
C	-4.32345600	3.51393000	1.94969500
O	-3.34533800	4.26480400	2.44644000
C	-5.60477000	3.66170100	2.45144200
C	-1.11633900	3.48487500	2.89380200
H	-1.49749300	2.57449700	3.35894300
H	-0.12194300	3.28316800	2.49564700
H	-1.03247800	4.26377600	3.65336200
C	-1.60379600	5.27117300	1.12978800
H	-0.63203900	5.14661000	0.65204700
H	-2.32340500	5.59570400	0.37669300
H	-1.51629400	6.04418800	1.89489700
C	-5.84796200	4.60829500	3.48124800
N	-6.05756900	5.37722000	4.32101700
C	-6.71144100	2.90721400	1.98955300
N	-7.64570900	2.31537900	1.64687500

ADA 5

H	0.77314900	-2.01508600	-2.97878600
C	0.64309700	-1.01202800	-2.60086500
H	2.06350900	0.19360300	-3.84703000
C	1.32707600	0.15230300	-3.05899700
H	-0.88621500	-1.31817100	-1.03030300
C	-0.21390800	-0.64458000	-1.53320500
C	0.88283400	1.24898200	-2.28337100
C	-0.09001100	0.78011300	-1.32515300
H	1.21415400	2.27284300	-2.37591000
Fe	1.74636800	-0.16712300	-1.03193100
H	4.54707200	-0.30435900	-1.61139700
C	3.15538800	-1.54049700	-0.32540000
C	3.80303600	-0.35421300	-0.83510100
C	2.29420600	-1.10492800	0.74944300
C	3.35785700	0.75810100	-0.07627900
H	3.66312900	1.78213400	-0.22838400
C	2.42213900	0.29622200	0.89507300
H	1.88178100	0.91372300	1.59655400
C	-0.79824200	1.70724100	-0.47025700
H	-0.66818000	2.72938900	-0.81468600
C	3.30733800	-2.94636600	-0.62822300
H	2.89872700	-3.55953500	0.17014600
H	1.66802500	-1.76010500	1.33716500
C	-1.63120400	1.58890400	0.60331000
C	-2.38799600	2.73349700	1.12684600
C	-2.02433500	0.46028400	1.44662900
C	-2.37578600	4.05677000	0.69141500
C	-3.21070300	2.31943400	2.20957300
C	-1.49526000	-0.82548400	1.52189400

C	-3.05720200	0.87138300	2.34188600
C	-3.16228600	4.97525800	1.36589500
H	-1.77551000	4.38577000	-0.14465000
C	-3.90751200	3.32020100	2.91236300
C	-2.06104900	-1.72617000	2.41019600
H	-0.64696100	-1.12665300	0.93073100
C	-3.67554700	-0.12533200	3.11872100
C	-3.91543800	4.63641200	2.48762000
C	-3.17726800	-1.41466800	3.18025000
H	-4.46194200	5.38910700	3.03549300
H	-3.65615800	-2.16164800	3.79522200
C	3.88913300	-3.66580700	-1.63065200
C	4.46995700	-3.29964200	-2.92198500
C	4.06183500	-5.12125700	-1.53751800
C	4.43749900	-2.08667300	-3.60486100
C	5.06931000	-4.44995900	-3.51840100
C	3.67997300	-5.97840500	-0.50755100
C	4.72175100	-5.60905200	-2.69801800
C	5.08697400	-1.99297700	-4.82556500
H	3.90219500	-1.23398200	-3.22324400
C	5.82096400	-4.25436800	-4.69130900
C	3.92488100	-7.33272100	-0.65840400
H	3.20074300	-5.62373500	0.39365900
C	4.84784100	-7.00449100	-2.83254800
C	5.82095900	-3.04520400	-5.36390600
C	4.48301800	-7.86903500	-1.81655900
H	6.39261800	-2.91908100	-6.27095300
H	4.59409500	-8.93630500	-1.93453100
N	5.03611800	-0.71838600	-5.56197000
O	5.67370000	-0.63208700	-6.60352300
O	4.35272400	0.18600500	-5.09244700
N	6.77397000	-5.25888300	-5.19625400
O	7.32021400	-5.97367300	-4.36213400
O	7.01129200	-5.28146900	-6.39351400
N	5.20902200	-7.65248400	-4.10584200
O	4.81563300	-7.11156800	-5.13440600
O	5.81607700	-8.71059900	-4.06483200
N	3.53492100	-8.25435400	0.42511600
O	3.74543600	-9.45000600	0.26185300
O	3.02587000	-7.77183300	1.42962300
N	-1.48695100	-3.07878900	2.51309700
O	-2.04483600	-3.88404300	3.24726000
O	-0.47666100	-3.32157400	1.86056400
N	-4.97022000	0.08584300	3.79053000
O	-5.21643600	-0.56707200	4.79217700
O	-5.75084300	0.86725900	3.25651300
N	-4.53054000	3.08388300	4.22682200
O	-5.52587100	3.72693900	4.51909700
O	-3.96474700	2.29235600	4.97416900
N	-3.16714600	6.37930100	0.91469800
O	-3.87150700	7.17352900	1.52580800

O	-2.47179600	6.67140600	-0.05101200

ADA 6

H	2.00385300	-0.91731500	-3.40455000
C	1.67541500	-0.09008900	-2.79312300
H	3.52968500	1.15542900	-2.61860700
C	2.49006800	1.00542600	-2.37095200
H	-0.44818600	-0.61498100	-2.35442300
C	0.38456700	0.05319600	-2.23360700
C	1.70561400	1.83474200	-1.53971700
C	0.36997400	1.26981800	-1.45359400
H	2.02836400	2.73971400	-1.04679400
Fe	1.78875500	-0.04427900	-0.69762500
H	4.44260100	-0.25678200	0.25826200
C	2.78924200	-1.74031500	-0.03887400
C	3.43063000	-0.54972900	0.47018600
C	1.42300700	-1.72058400	0.45609100
C	2.49319200	0.14941800	1.26623200
H	2.67066000	1.08901400	1.76714400
C	1.26100700	-0.57536800	1.26370400
H	0.34967000	-0.27388900	1.75780500
C	-0.60981800	1.88563600	-0.60604700
H	-0.19639600	2.70831500	-0.02741100
C	3.20482100	-2.76789900	-0.94914500
H	2.38060800	-3.41011300	-1.25023200
H	0.67306800	-2.46686200	0.24088400
C	4.39177300	-3.16105300	-1.51273300
C	5.70647500	-2.55239200	-1.27777000
C	4.30156200	-4.33311800	-2.41593400
N	5.50818700	-4.78624800	-2.95358600
H	5.44614100	-5.58817300	-3.56899100
N	6.78469600	-3.17933600	-1.91905800
H	7.69251800	-2.76236300	-1.75214100
O	3.26963700	-4.91415300	-2.71143300
O	5.93945600	-1.57587900	-0.58418300
C	6.75229300	-4.26270700	-2.74788900
C	-1.94847500	1.71278000	-0.36382200
C	-2.53296700	2.64372900	0.63084200
C	-2.82594100	0.72916800	-1.00926500
N	-3.90408400	2.51264100	0.86045800
O	-1.91093200	3.49505300	1.24588200
N	-4.17452700	0.78201500	-0.62784700
O	-2.49366100	-0.10746900	-1.83277400
H	-4.30285100	3.14828400	1.54066900
C	-4.75746100	1.62034700	0.27718500
H	-4.78052600	0.10522600	-1.07576900
S	-6.38429900	1.56048000	0.64321600
S	8.12365000	-4.89716500	-3.45585500

ADA 7

H	2.00702500	-0.91497000	-3.40052800

C	1.67496500	-0.08996300	-2.78803300
H	3.52274300	1.16517800	-2.61397400
C	2.48411400	1.00932200	-2.36567100
H	-0.44628200	-0.62516400	-2.34701200
C	0.38351300	0.04675700	-2.22701800
C	1.69537700	1.83376900	-1.53283600
C	0.36345900	1.26165200	-1.44550400
H	2.01383800	2.73991800	-1.03921600
Fe	1.79088000	-0.04602800	-0.69396400
H	4.44778900	-0.25139700	0.25570900
C	2.79946900	-1.73926700	-0.04052300
C	3.43719700	-0.54774900	0.46919800
C	1.43471900	-1.72559800	0.45734200
C	2.49834900	0.14777100	1.26765200
H	2.67333300	1.08758500	1.76910400
C	1.26892000	-0.58129200	1.26635700
H	0.35715300	-0.28390200	1.76214900
C	-0.62071400	1.87685500	-0.59939500
H	-0.20778000	2.69975300	-0.02053500
C	3.21727300	-2.76799100	-0.95148300
H	2.39243300	-3.40996300	-1.25170600
H	0.68722300	-2.47443800	0.24232300
C	4.40085300	-3.16250800	-1.51625200
C	5.71883700	-2.55064600	-1.28342500
C	4.30374600	-4.34009100	-2.41895800
N	5.50001800	-4.79420800	-2.96130700
H	5.44387600	-5.59621000	-3.57725700
N	6.79215300	-3.17139500	-1.92370200
H	7.70429900	-2.76023000	-1.76603200
O	3.26319600	-4.91460000	-2.70161000
O	5.94109000	-1.57224600	-0.58706900
C	6.76069800	-4.26704000	-2.76220900
O	7.75850100	-4.72892500	-3.28303500
C	-1.95801200	1.70725500	-0.35904400
C	-2.54135000	2.64831100	0.63350100
C	-2.83624000	0.71912500	-1.00555100
N	-3.90720300	2.52827000	0.85913500
O	-1.90685600	3.49632600	1.24269000
N	-4.18047100	0.77500400	-0.63499300
O	-2.48968300	-0.12005000	-1.82216800
H	-4.31419600	3.16504200	1.53341500
C	-4.77496000	1.62867100	0.27180500
H	-4.79381300	0.10093800	-1.07706600
O	-5.96254600	1.59172300	0.53336200

ADA 8

H	1.94837000	-1.20954400	-3.09674500
C	1.58292600	-0.36633700	-2.53016300
H	3.22145000	1.13925900	-2.76525400
C	2.26081500	0.87580300	-2.34986400
H	-0.33714100	-1.14085200	-1.72171600

C	0.37001900	-0.32974000	-1.79296900
C	1.46992300	1.68810100	-1.49821200
C	0.27408600	0.95855600	-1.15323800
H	1.70922500	2.68481000	-1.15861100
Fe	1.97233800	-0.05304700	-0.50269800
H	4.75617800	0.04826400	-0.05593800
C	3.20964000	-1.57979200	0.18171700
C	3.83145700	-0.29480900	0.38047800
C	1.96716700	-1.56228700	0.91578600
C	2.99778300	0.47395500	1.23530100
H	3.18618400	1.48806800	1.55321200
C	1.85219600	-0.30950400	1.56761500
H	1.02128500	0.01245400	2.17705600
H	1.25720200	-2.37472900	0.95678500
C	4.82972800	-2.93500800	-1.21162500
S	6.27376100	-1.91361000	-1.23612400
C	5.08452600	-4.17686200	-1.96680200
C	7.17063100	-3.08641800	-2.20717900
O	4.30443900	-5.09360100	-2.14659700
N	6.39593900	-4.17918200	-2.48120500
S	8.73393300	-2.81669900	-2.68572100
C	6.87510800	-5.33482900	-3.26172400
H	7.58266700	-4.95086400	-3.99487900
H	6.00416900	-5.72885300	-3.78415300
C	7.51626700	-6.40679700	-2.38327300
H	8.38709600	-6.01379100	-1.85518700
H	6.80391500	-6.79293000	-1.65148800
H	7.84433900	-7.23820500	-3.01179500
C	-1.97720200	1.00568300	0.00115900
S	-2.75263200	-0.46938200	-0.59155000
C	-2.89619200	1.72352600	0.90552700
C	-4.23013400	-0.14118500	0.32108600
O	-2.67682800	2.77024800	1.48657200
N	-4.11328900	1.02489900	1.02555800
S	-5.53227400	-1.16485100	0.28039500
C	-5.19083200	1.56931200	1.87224600
H	-4.69716800	2.10136200	2.68463700
H	-5.73081800	0.71831600	2.28434100
C	-6.12686500	2.49718300	1.10104000
H	-5.58434000	3.35245900	0.69327100
H	-6.61898100	1.96831300	0.28265200
H	-6.89812300	2.87336700	1.77746700
C	3.64250500	-2.70710400	-0.60754100
H	2.91821700	-3.50974100	-0.72016700
C	-0.75010800	1.49192500	-0.28849100
H	-0.51738300	2.44016100	0.18927500

ADA 9

H	2.00242000	-0.89137100	-3.43596800
C	1.66417000	-0.07859900	-2.81061400
H	3.50504300	1.18243700	-2.60794300

C	2.46638000	1.01691900	-2.36605300
H	-0.45435000	-0.63298000	-2.38753600
C	0.36988700	0.04221600	-2.25242500
C	1.66999000	1.82243500	-1.52219900
C	0.33962100	1.24320300	-1.44940800
H	1.98218500	2.72129300	-1.01151300
Fe	1.77256000	-0.07099500	-0.71582300
H	4.42492200	-0.27225300	0.24499100
C	2.79127600	-1.76948900	-0.08677700
C	3.41643600	-0.58170800	0.44741900
C	1.42322000	-1.77285500	0.40397100
C	2.46810500	0.09350500	1.25219900
H	2.63374300	1.02589800	1.77044700
C	1.24422700	-0.64435500	1.23199700
H	0.32758800	-0.36226300	1.72776800
C	-0.64394200	1.84462900	-0.59195800
H	-0.22550900	2.65464000	-0.00015600
C	3.21220200	-2.78156300	-1.01546700
H	2.38533400	-3.41302400	-1.32982000
H	0.68239000	-2.52326500	0.17197900
C	4.39518800	-3.17539000	-1.58722400
C	5.70167600	-2.57299000	-1.34223200
C	4.29504500	-4.32810300	-2.50229800
N	5.49462800	-4.83014000	-3.03368300
N	6.80566800	-3.15541000	-2.00123900
O	3.23361900	-4.85840200	-2.79978200
O	5.88502200	-1.60947200	-0.61289700
C	6.74227900	-4.27188200	-2.81504000
C	-1.98348300	1.68091800	-0.34792800
C	-2.55525700	2.60461500	0.65012900
C	-2.85548400	0.70917600	-0.99996800
N	-3.94182000	2.53750100	0.86433000
O	-1.88576800	3.41617800	1.27425900
N	-4.21659500	0.72302700	-0.62648300
O	-2.47483800	-0.10131500	-1.83170100
C	-4.78357800	1.61734700	0.26328900
C	8.11313300	-2.49594600	-1.74308000
C	8.82014100	-3.05081200	-0.50953600
H	7.89839500	-1.43799500	-1.61668900
H	8.71868700	-2.63184200	-2.63369600
H	9.76577700	-2.52076000	-0.36833600
H	8.21468500	-2.91039400	0.38793700
H	9.04036300	-4.11350600	-0.62648900
C	5.35193700	-6.02361800	-3.90921700
C	5.11082400	-5.65553700	-5.37055200
H	4.51230400	-6.58923100	-3.51359400
H	6.25942700	-6.60898600	-3.79855200
H	5.00472200	-6.57073000	-5.95894400
H	4.19572000	-5.07107400	-5.48342900
H	5.94852500	-5.08569500	-5.77690600
C	-4.48339100	3.52405500	1.83634100

C	-4.45460000	3.01197200	3.27371200
H	-5.49733400	3.75381400	1.52393800
H	-3.86892300	4.41499400	1.73546700
H	-4.85436100	3.78288800	3.93776300
H	-5.06803100	2.11600100	3.38540900
H	-3.43470700	2.78600700	3.59072500
C	-5.06310800	-0.30159900	-1.29327700
C	-5.63380500	0.18073400	-2.62408700
H	-5.85678500	-0.55859900	-0.59876300
H	-4.42619400	-1.16960100	-1.44274600
H	-6.23514300	-0.61715700	-3.06773800
H	-6.27563700	1.05257800	-2.48458600
H	-4.83673700	0.43537400	-3.32519000
S	-6.42929400	1.58744100	0.60629400
S	8.12438900	-4.92413800	-3.51607800

ADA 10

H	2.01294900	-0.91620300	-3.40254900
C	1.67123500	-0.09157300	-2.79481500
H	3.50018800	1.19297500	-2.63837400
C	2.46519300	1.02277700	-2.38421700
H	-0.43962300	-0.65527800	-2.33900800
C	0.37984300	0.03040800	-2.22861000
C	1.66658700	1.84088400	-1.55351700
C	0.34416800	1.24960300	-1.45529200
H	1.97338200	2.75524400	-1.06761900
Fe	1.79735500	-0.03150300	-0.70342100
H	4.46412800	-0.20480600	0.22296700
C	2.82846300	-1.71067100	-0.04411200
C	3.45869300	-0.50858300	0.44864800
C	1.46845400	-1.70403500	0.46587600
C	2.52005600	0.18711700	1.24841600
H	2.69096100	1.13358100	1.73876400
C	1.29756400	-0.55271500	1.26486800
H	0.38702100	-0.25883600	1.76501900
C	-0.64464500	1.86414900	-0.61016300
H	-0.23275800	2.69212800	-0.03841800
C	3.24439700	-2.75220800	-0.94491100
H	2.41776700	-3.40006600	-1.22586200
H	0.72627600	-2.46203400	0.26463300
C	4.42039800	-3.15711700	-1.51638700
C	5.73351200	-2.53720700	-1.31004400
C	4.31305900	-4.34764400	-2.39336300
N	5.49264800	-4.83312700	-2.94965200
N	6.82511500	-3.15901000	-1.92341900
O	3.25569000	-4.91188600	-2.64487100
O	5.92927000	-1.53259100	-0.63936100
C	6.75745200	-4.28422200	-2.74234200
O	7.75334400	-4.76402900	-3.25546200
C	-1.98038500	1.69614700	-0.36453200
C	-2.56019600	2.64267400	0.61821100

C	-2.85162400	0.70204500	-1.00004500
N	-3.92953600	2.55580200	0.84934100
O	-1.90276900	3.48185400	1.22095500
N	-4.20817900	0.75074600	-0.66603000
O	-2.47111600	-0.14721700	-1.79440300
C	-4.78536900	1.64079600	0.23721600
O	-5.97865300	1.61964700	0.48387400
C	-4.50032300	3.50440700	1.81901400
H	-4.03833500	3.35458800	2.79458000
H	-4.30726000	4.52475400	1.48935000
H	-5.56785400	3.32578100	1.87941200
C	-5.08114100	-0.23583700	-1.32218600
H	-5.02255200	-0.11445900	-2.40337900
H	-4.75812700	-1.24368000	-1.06211700
H	-6.09652700	-0.06928400	-0.98110000
C	8.14388300	-2.54794000	-1.69213800
H	8.15889500	-1.53598100	-2.09708500
H	8.34195700	-2.50283200	-0.62197400
H	8.89112000	-3.15802600	-2.18662200
C	5.37887300	-6.01637700	-3.81732300
H	4.96745000	-6.85019700	-3.24897600
H	4.71401400	-5.79507900	-4.65165500
H	6.36879800	-6.26517200	-4.18247000

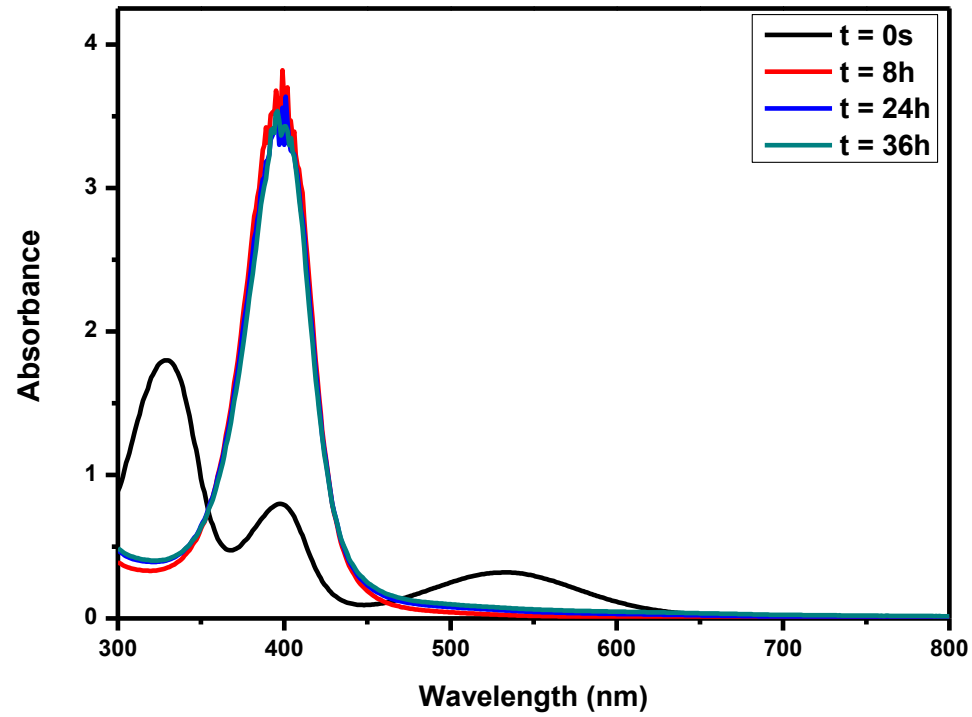
ADA 11

H	2.01294900	-0.91620300	-3.40254900
C	1.67123500	-0.09157300	-2.79481500
H	3.50018800	1.19297500	-2.63837400
C	2.46519300	1.02277700	-2.38421700
H	-0.43962300	-0.65527800	-2.33900800
C	0.37984300	0.03040800	-2.22861000
C	1.66658700	1.84088400	-1.55351700
C	0.34416800	1.24960300	-1.45529200
H	1.97338200	2.75524400	-1.06761900
Fe	1.79735500	-0.03150300	-0.70342100
H	4.46412800	-0.20480600	0.22296700
C	2.82846300	-1.71067100	-0.04411200
C	3.45869300	-0.50858300	0.44864800
C	1.46845400	-1.70403500	0.46587600
C	2.52005600	0.18711700	1.24841600
H	2.69096100	1.13358100	1.73876400
C	1.29756400	-0.55271500	1.26486800
H	0.38702100	-0.25883600	1.76501900
C	-0.64464500	1.86414900	-0.61016300
H	-0.23275800	2.69212800	-0.03841800
C	3.24439700	-2.75220800	-0.94491100
H	2.41776700	-3.40006600	-1.22586200
H	0.72627600	-2.46203400	0.26463300
C	4.42039800	-3.15711700	-1.51638700
C	5.73351200	-2.53720700	-1.31004400
C	4.31305900	-4.34764400	-2.39336300

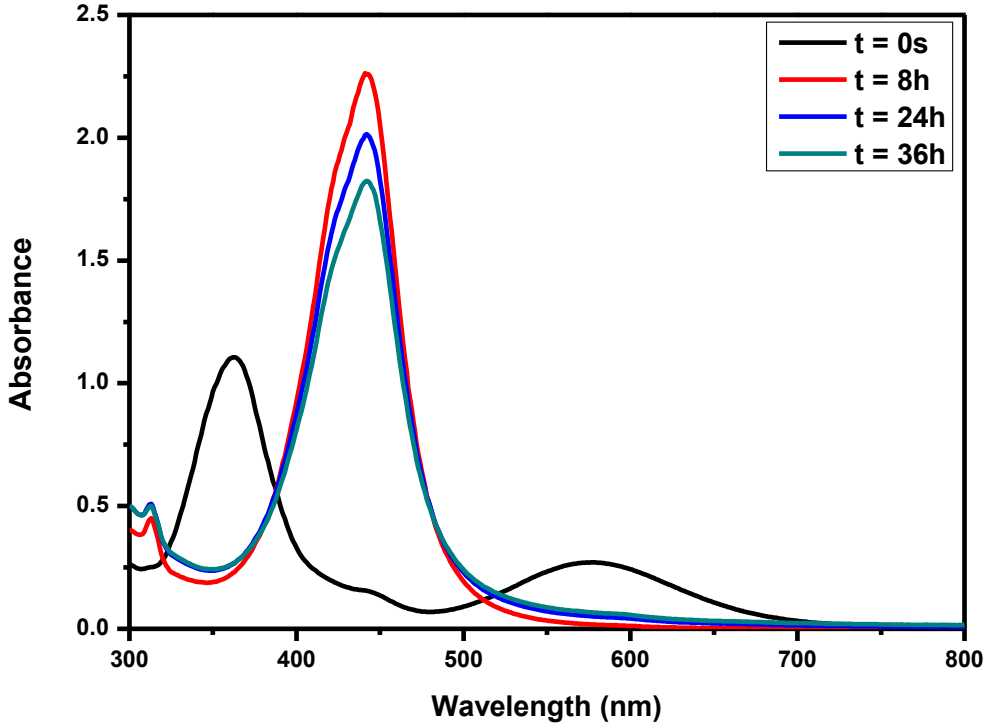
N	5.49264800	-4.83312700	-2.94965200
N	6.82511500	-3.15901000	-1.92341900
O	3.25569000	-4.91188600	-2.64487100
O	5.92927000	-1.53259100	-0.63936100
C	6.75745200	-4.28422200	-2.74234200
O	7.75334400	-4.76402900	-3.25546200
C	-1.98038500	1.69614700	-0.36453200
C	-2.56019600	2.64267400	0.61821100
C	-2.85162400	0.70204500	-1.00004500
N	-3.92953600	2.55580200	0.84934100
O	-1.90276900	3.48185400	1.22095500
N	-4.20817900	0.75074600	-0.66603000
O	-2.47111600	-0.14721700	-1.79440300
C	-4.78536900	1.64079600	0.23721600
O	-5.97865300	1.61964700	0.48387400
C	-4.50032300	3.50440700	1.81901400
H	-4.03833500	3.35458800	2.79458000
H	-4.30726000	4.52475400	1.48935000
H	-5.56785400	3.32578100	1.87941200
C	-5.08114100	-0.23583700	-1.32218600
H	-5.02255200	-0.11445900	-2.40337900
H	-4.75812700	-1.24368000	-1.06211700
H	-6.09652700	-0.06928400	-0.98110000
C	8.14388300	-2.54794000	-1.69213800
H	8.15889500	-1.53598100	-2.09708500
H	8.34195700	-2.50283200	-0.62197400
H	8.89112000	-3.15802600	-2.18662200
C	5.37887300	-6.01637700	-3.81732300
H	4.96745000	-6.85019700	-3.24897600
H	4.71401400	-5.79507900	-4.65165500
H	6.36879800	-6.26517200	-4.18247000

Modification of the UV-visible absorption spectra of DA0-DA11 and ADA0-ADA11 in DMSO at room temperature over time

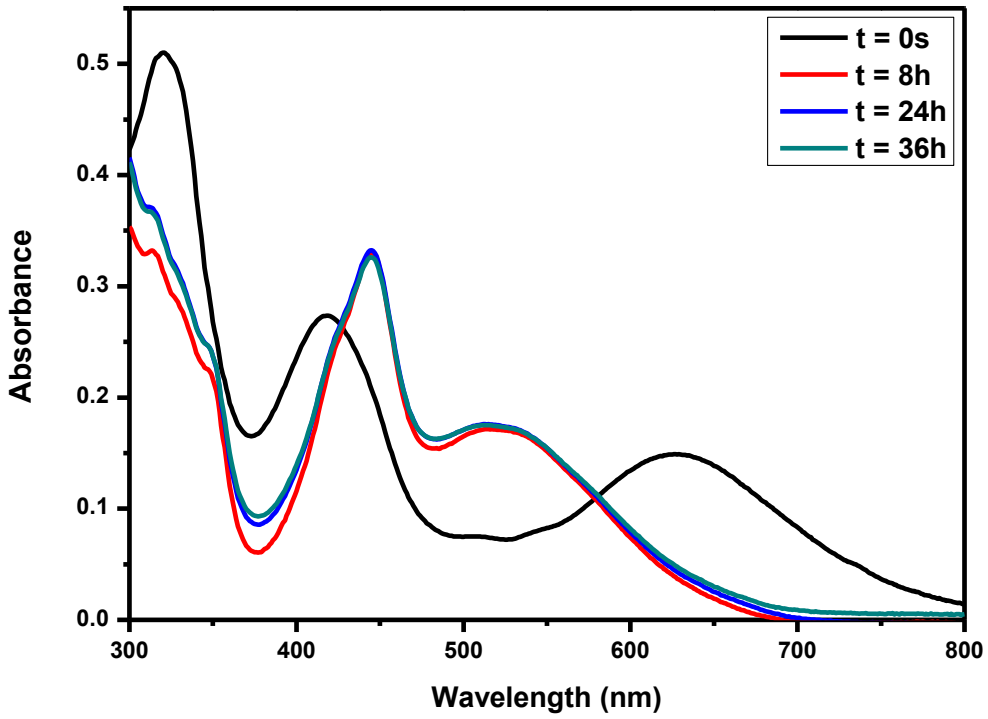
DA0



DA1



DA2


t = 0s
t = 8h
t = 24h
t = 36h
Absorbance
Wavelength (nm)
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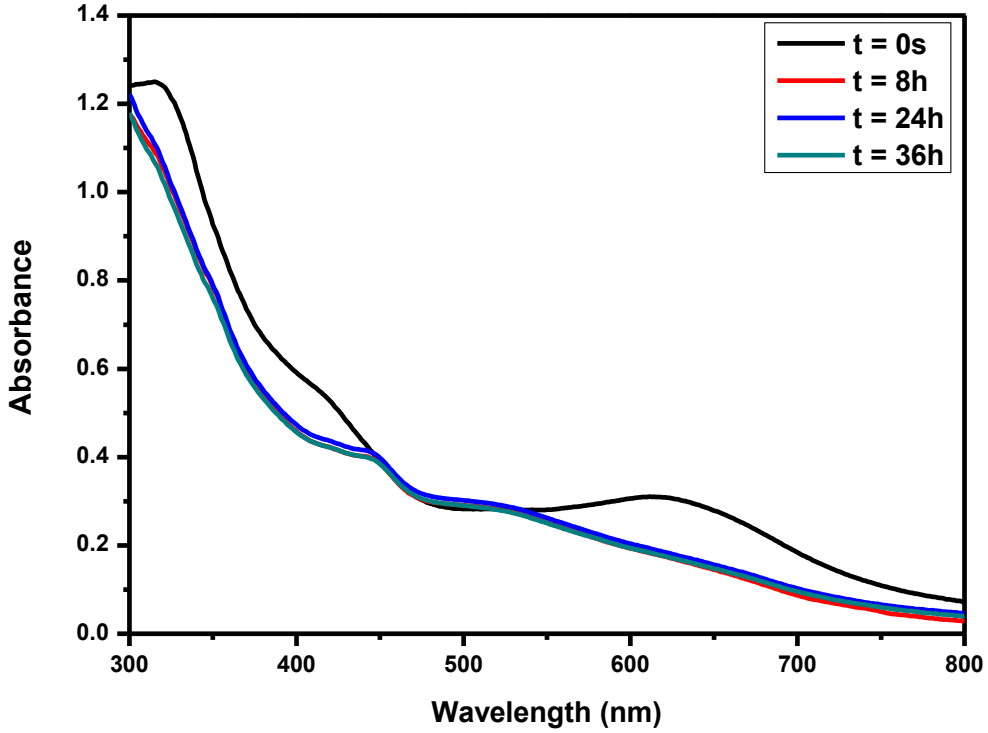
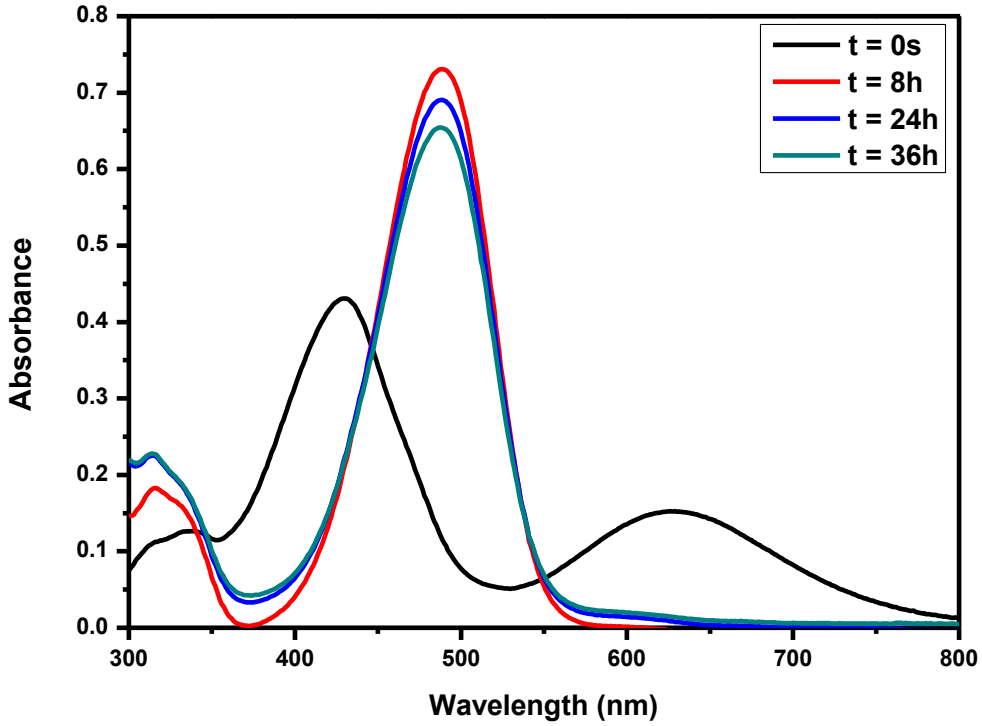
0.1
0.2
0.3
0.4
0.5
300
400
500
600
700
800

DA3


t = 0s
t = 8h
t = 24h
t = 36h
Absorbance
Wavelength (nm)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
300
400
500
600
700
800

DA4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Wavelength (nm)
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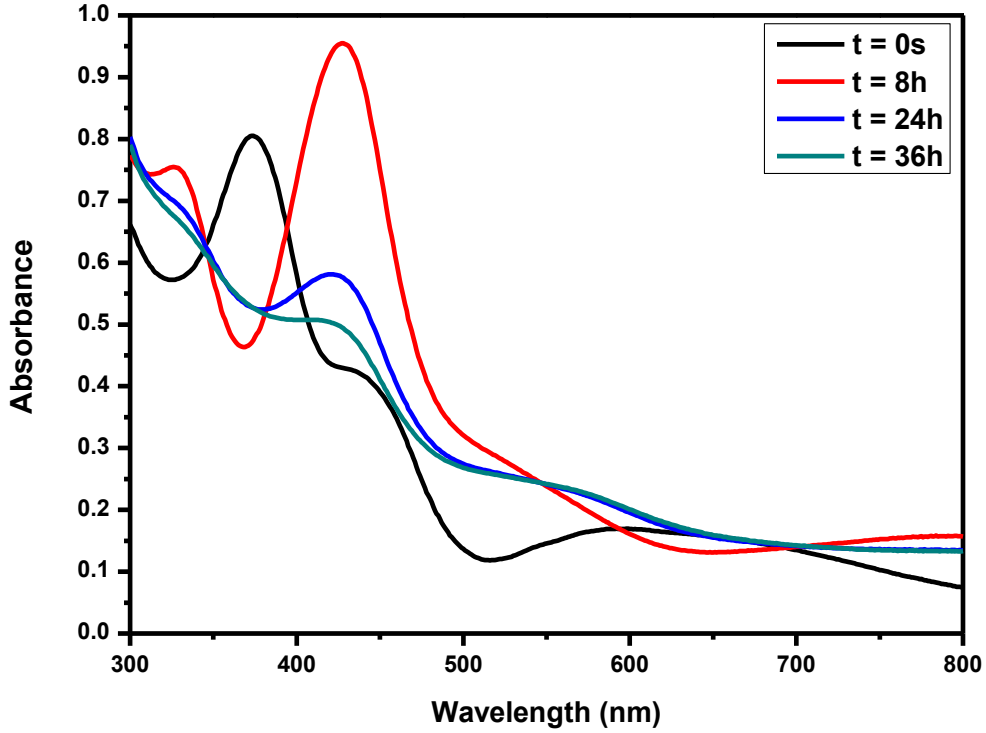
0.4
0.5
0.6
0.7
0.8
300
400
500
600
700
800

DA5


t = 0s
t = 8h
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Absorbance
Wavelength (nm)
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0.7
0.8
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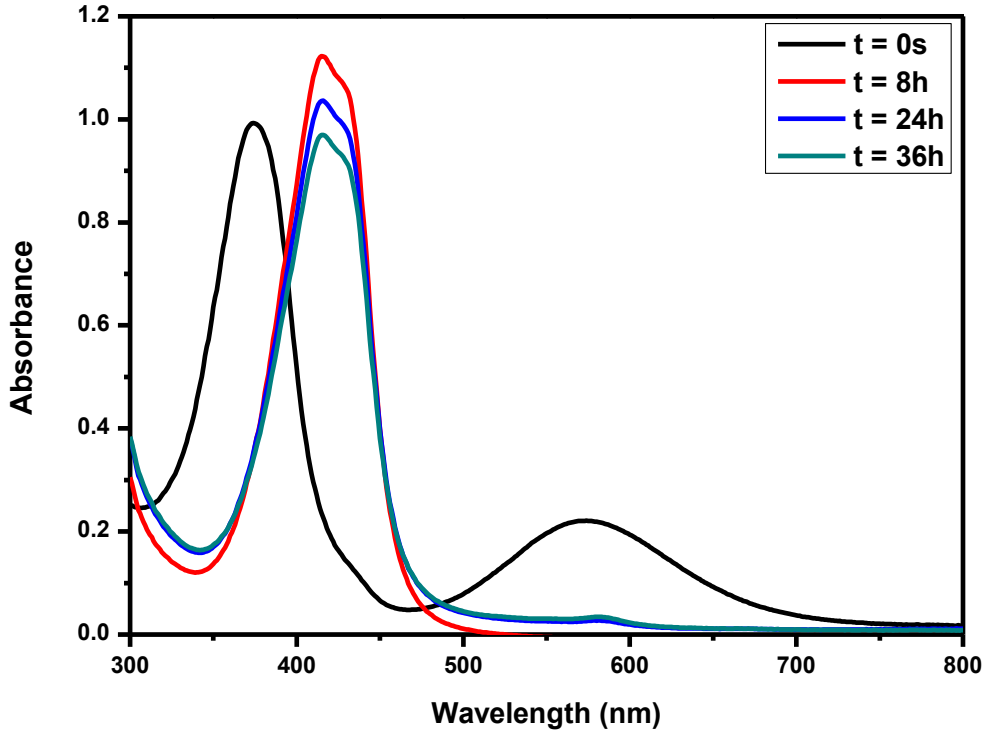
DA6


t = 0s
t = 8h
t = 24h
t = 36h
Absorbance
Wavelength (nm)
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0.8
1.0
1.2
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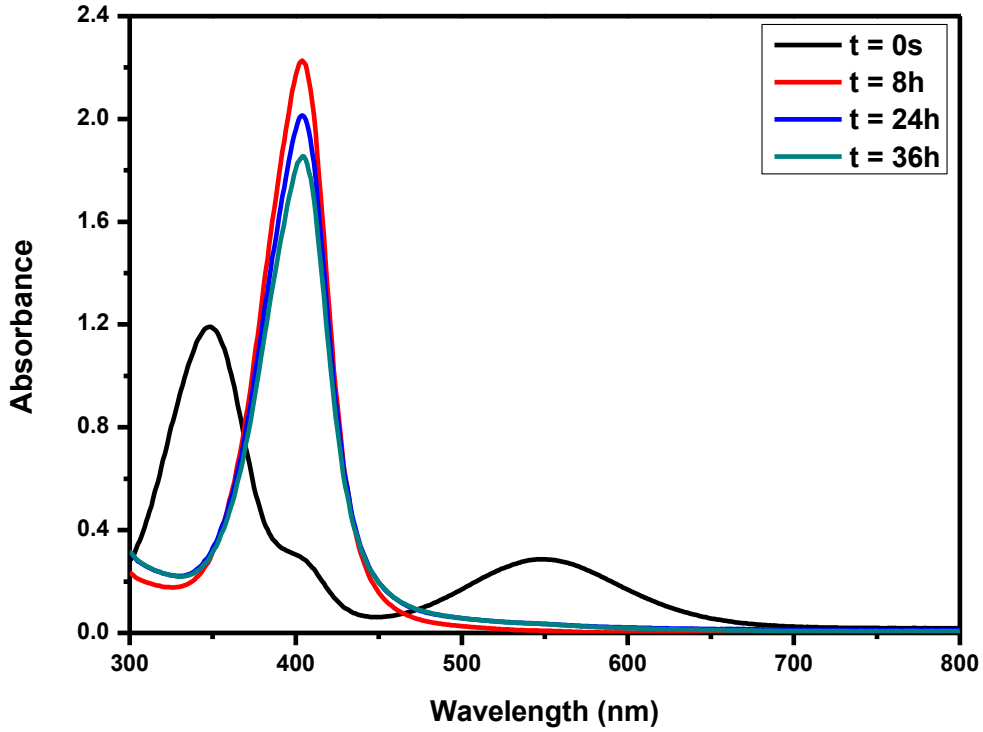
600
700
800

DA7


t = 0s
t = 8h
t = 24h
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Absorbance
Wavelength (nm)
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1.6
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2.4
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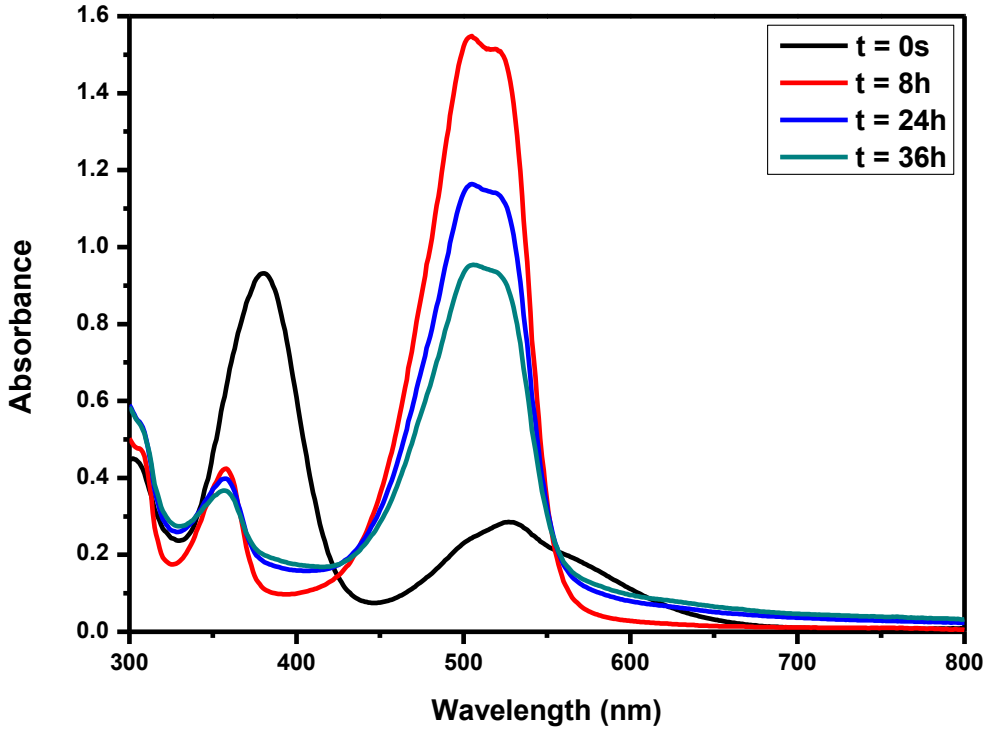
600
700
800

DA8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t = 8h
t = 24h
t = 36h
Absorbance
Wavelength (nm)
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1.2
1.4
1.6
300
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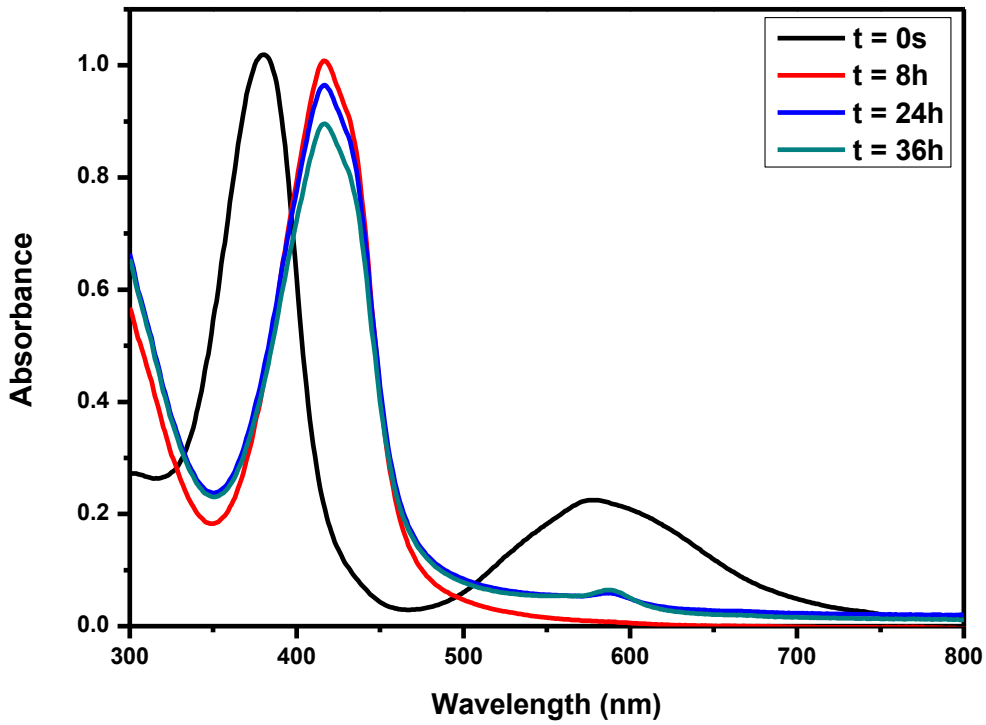
500
600
700
800

DA9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t = 8h
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t = 36h
Absorbance
Wavelength (nm)
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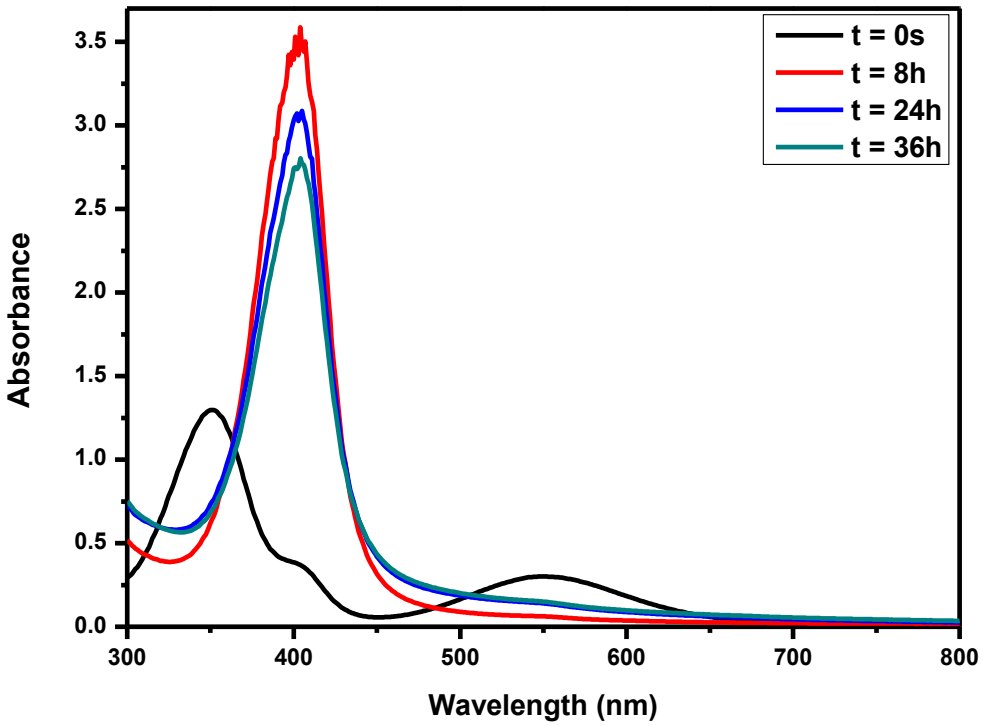
800

DA10


t = 0s
t = 8h
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Absorbance
Wavelength (nm)
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3.5
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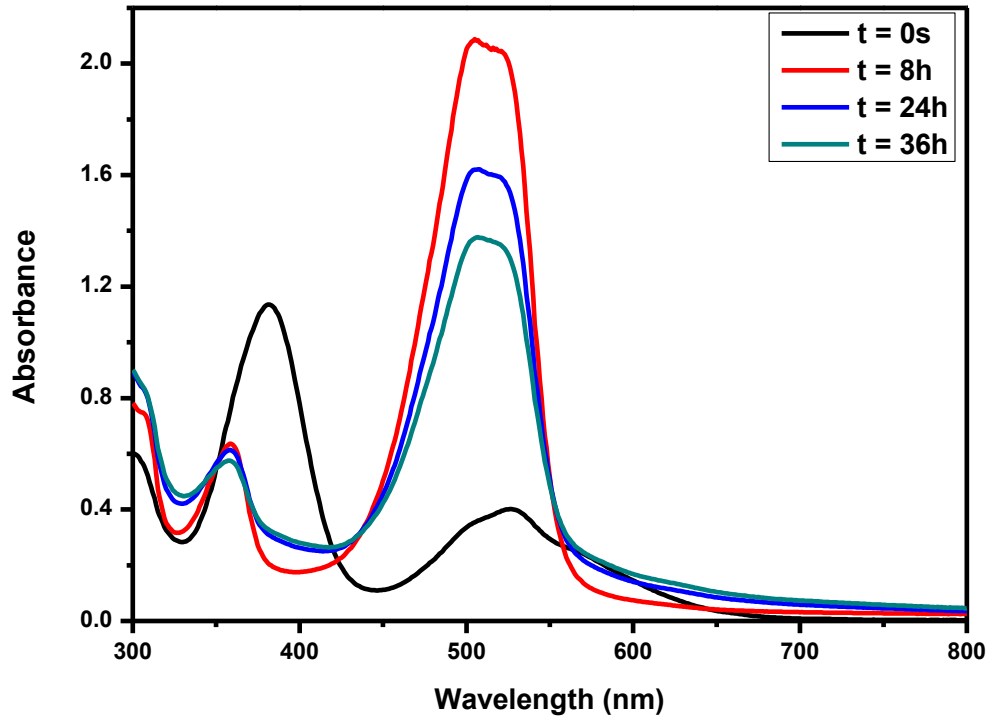
400
500
600
700
800

DA11


t = 0s
t = 8h
t = 24h
t = 36h
Absorbance
Wavelength (nm)
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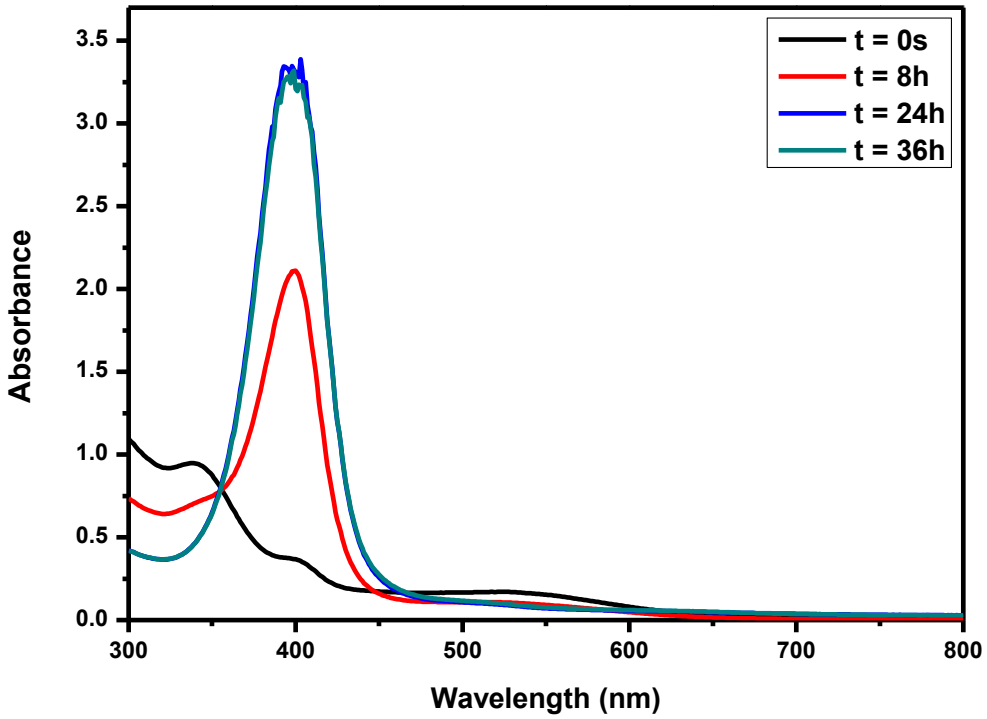
1.6
2.0
300
400
500
600
700
800

ADA0


t = 0s
t = 8h
t = 24h
t = 36h
Absorbance
Wavelength (nm)
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2.0
2.5
3.0
3.5
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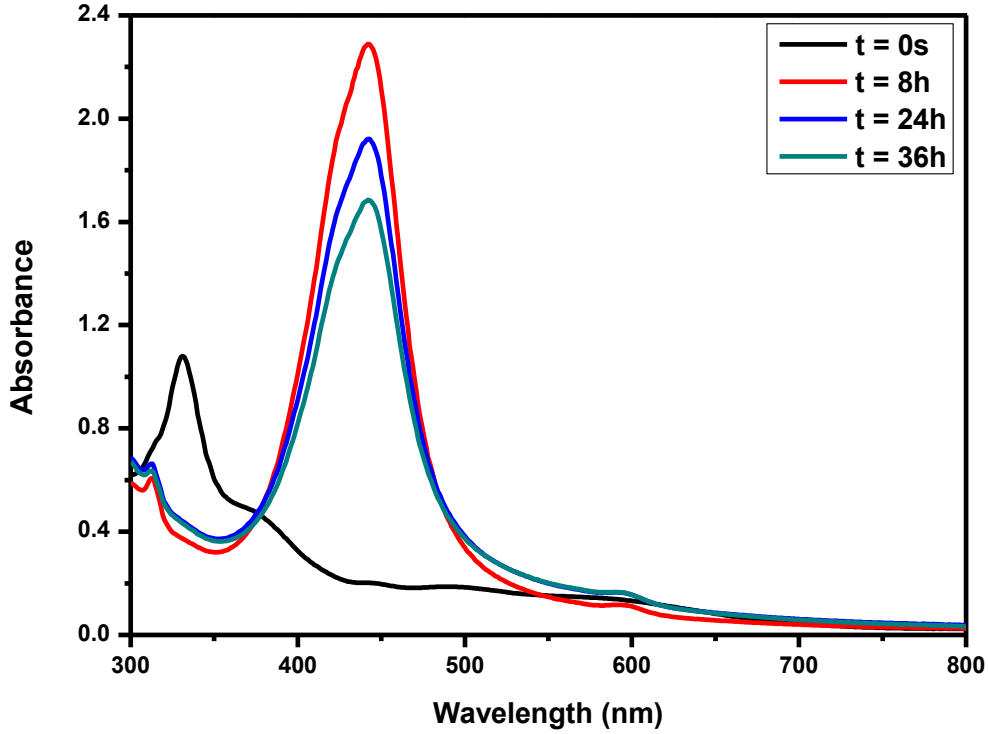
400
500
600
700
800

ADA1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Absorbance
Wavelength (nm)
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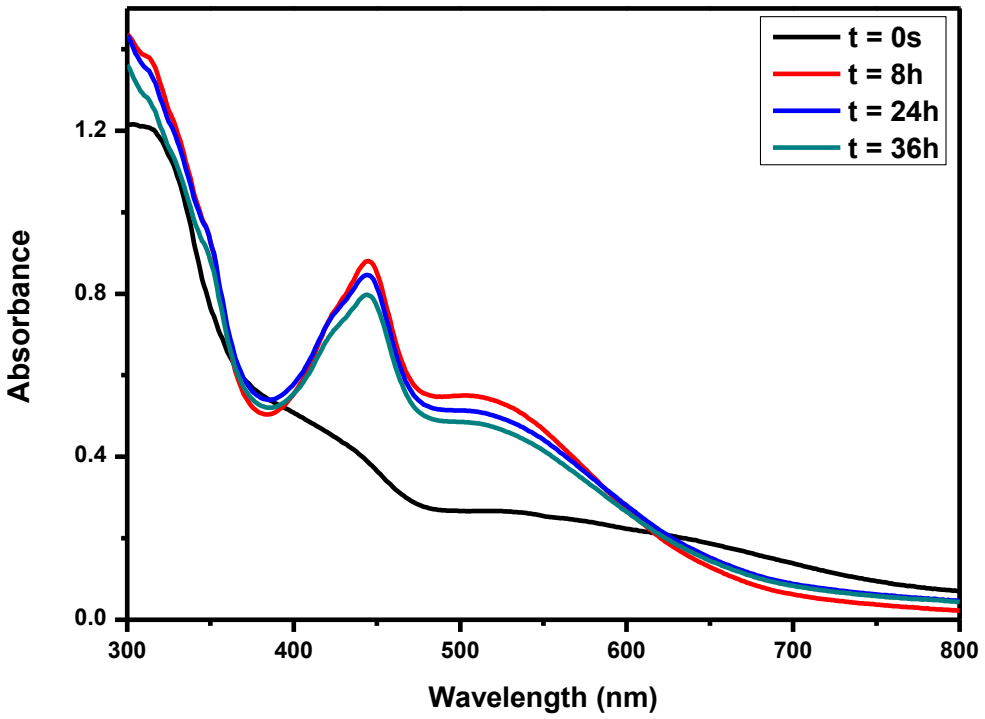
2.0
2.4
300
400
500
600
700
800

ADA2


t = 0s
t = 8h
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t = 36h
Absorbance
Wavelength (nm)
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0.8
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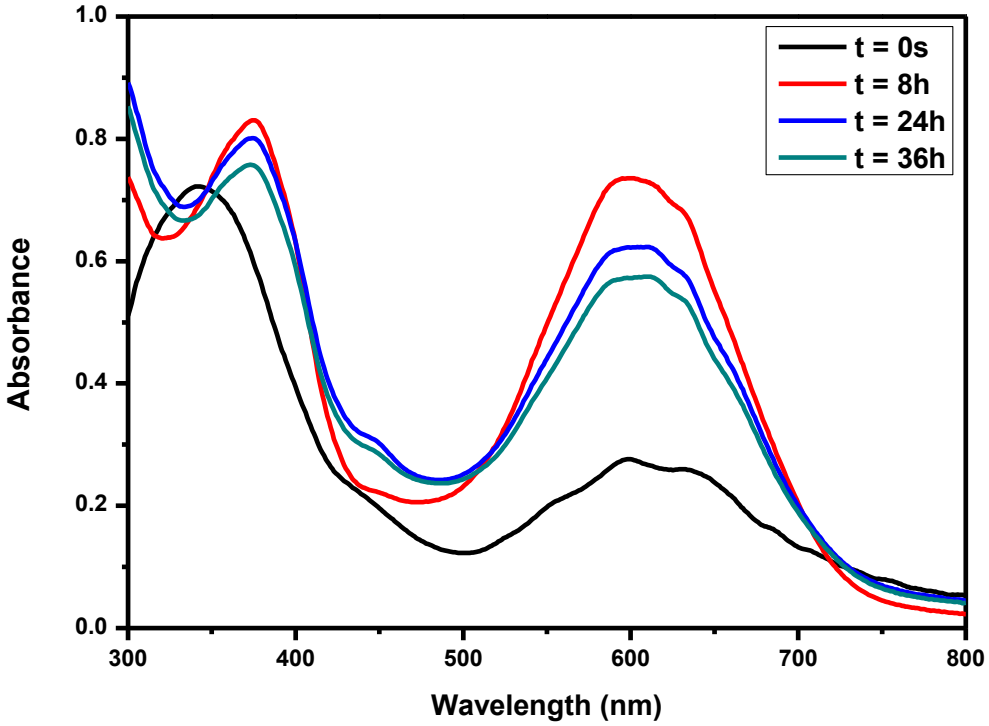
500
600
700
800

ADA3


t = 0s
t = 8h
t = 24h
t = 36h
Absorbance
Wavelength (nm)
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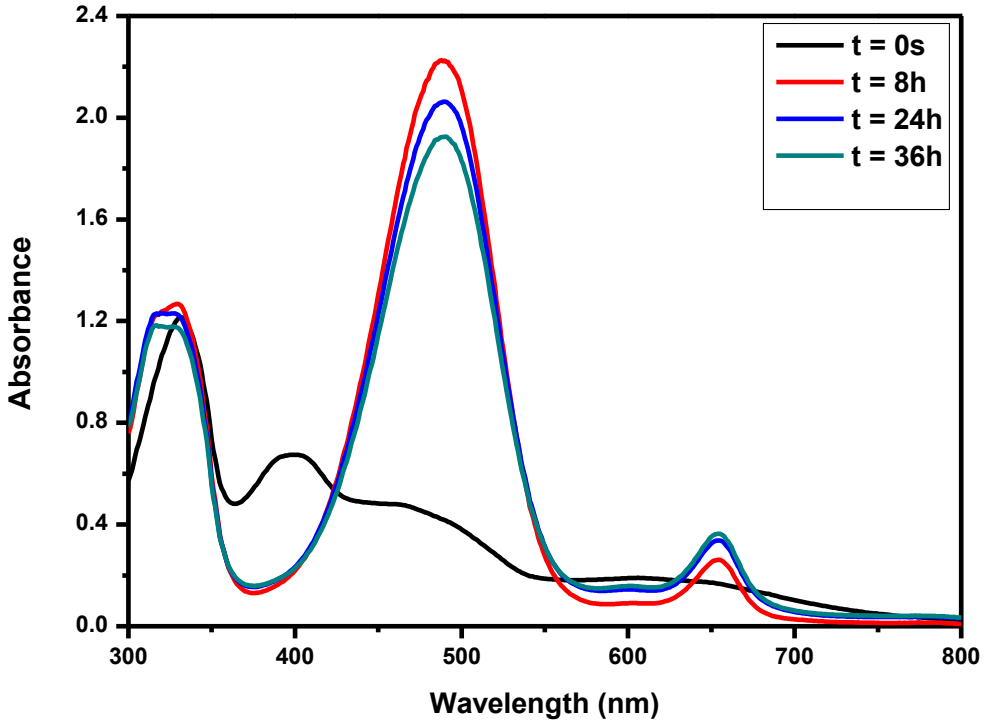
1.0
300
400
500
600
700
800

ADA4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t = 24h
t = 36h
Absorbance
Wavelength (nm)
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1.2
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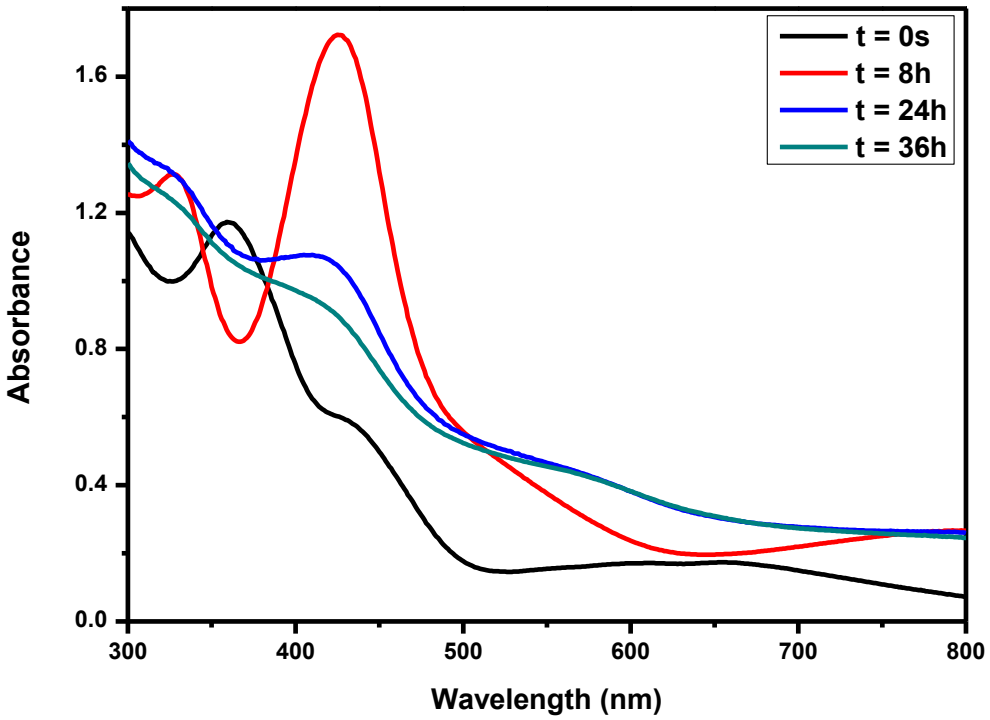
500
600
700
800

ADA5


t = 0s
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t = 24h
t = 36h
Absorbance
Wavelength (nm)
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300
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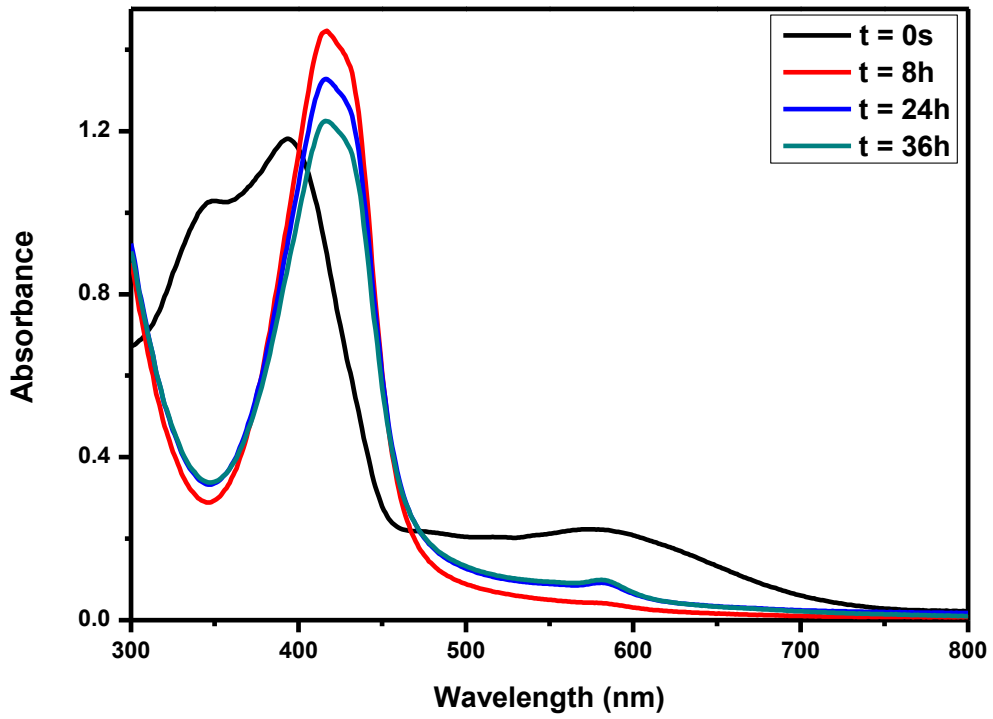
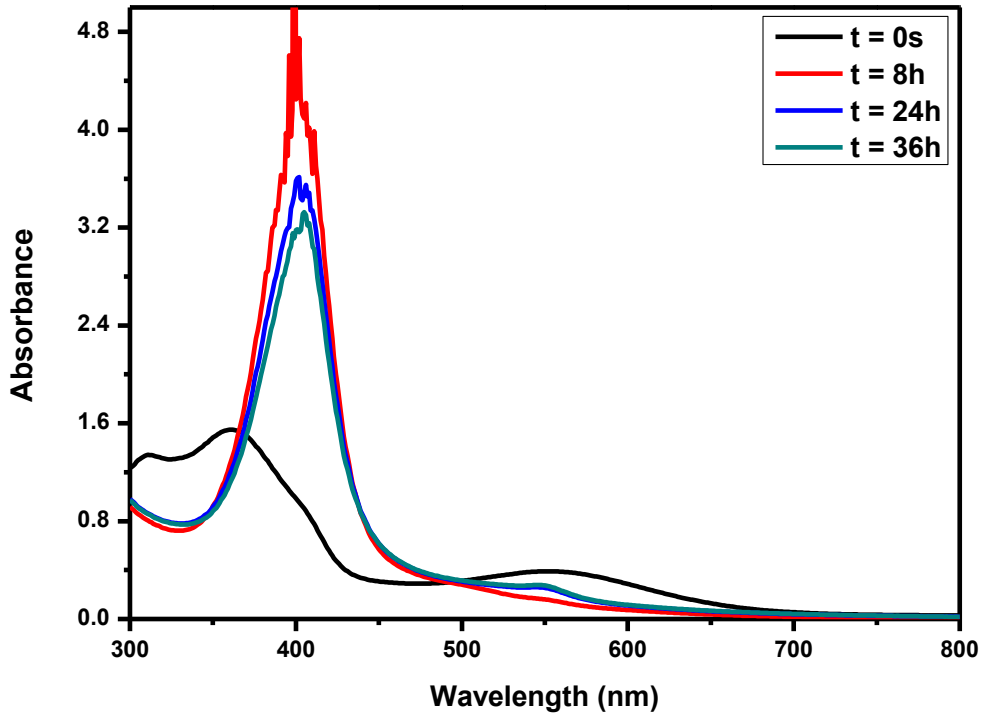
500
600
700
800

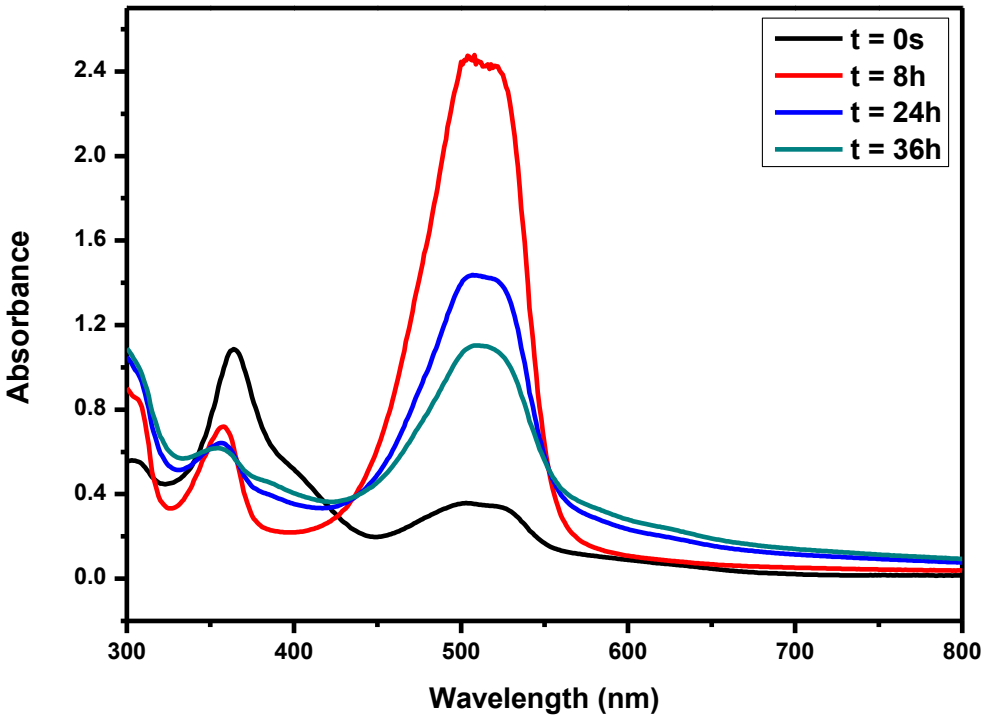
ADA6



ADA7



ADA8


t = 0s
t = 8h
t = 24h
t = 36h
Absorbance
Wavelength (nm)
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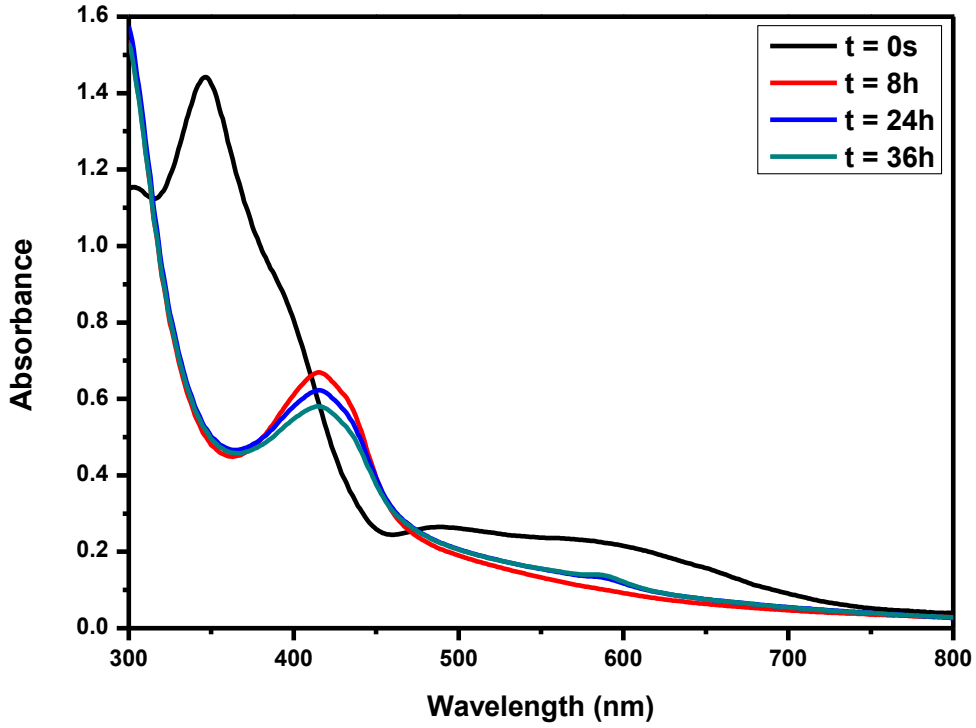
0.8
1.2
1.6
2.0
2.4
300
400
500
600
700
800

ADA9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t = 8h
t = 24h
t = 36h
Absorbance
Wavelength (nm)
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1.0
1.2
1.4
1.6
300
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600
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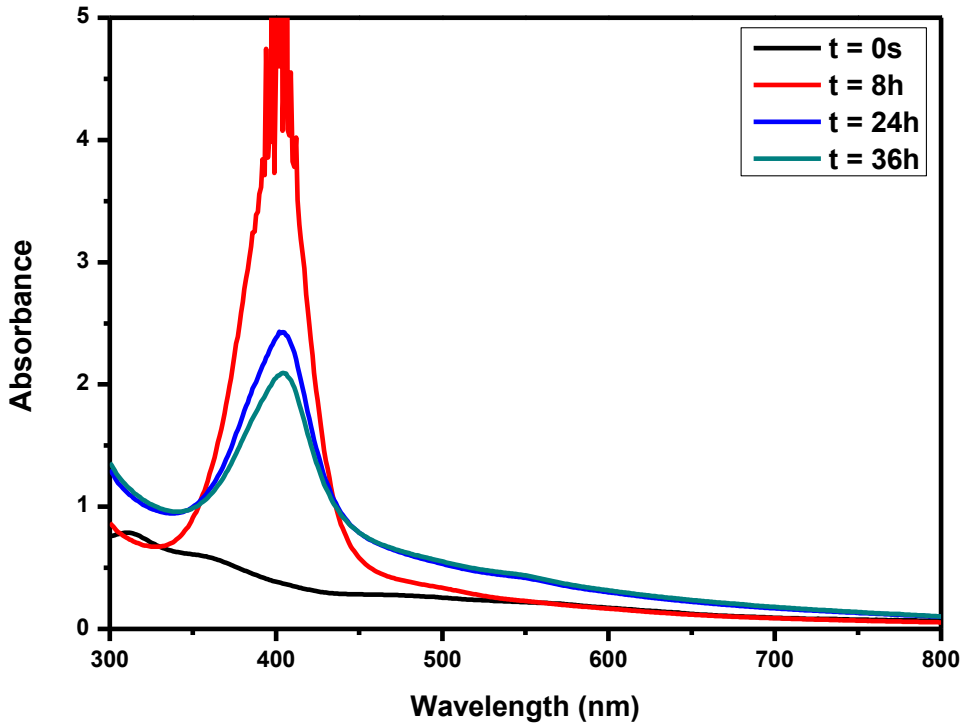
ADA10


t = 0s
t = 8h
t = 24h
t = 36h
Absorbance
Wavelength (nm)
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600
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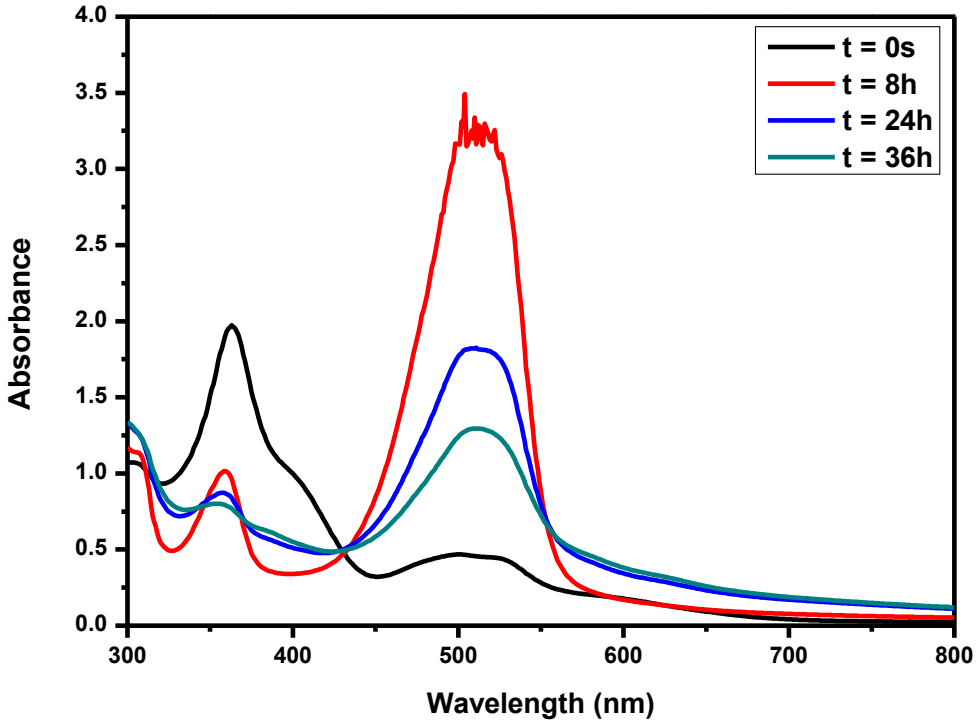
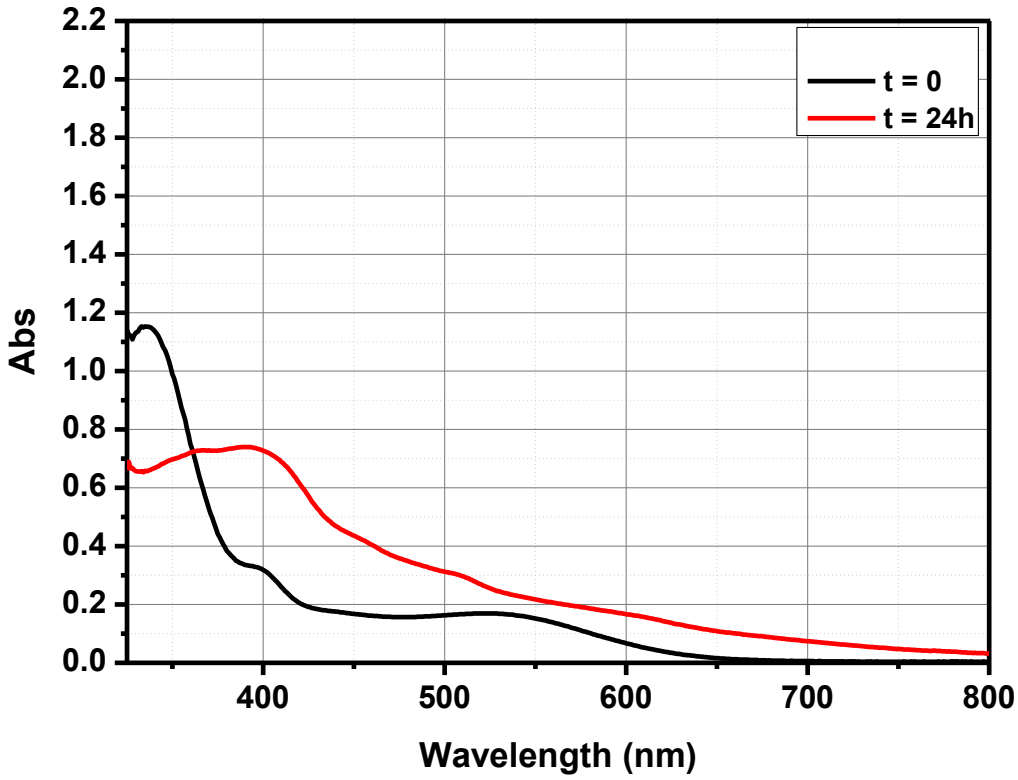
800

ADA11

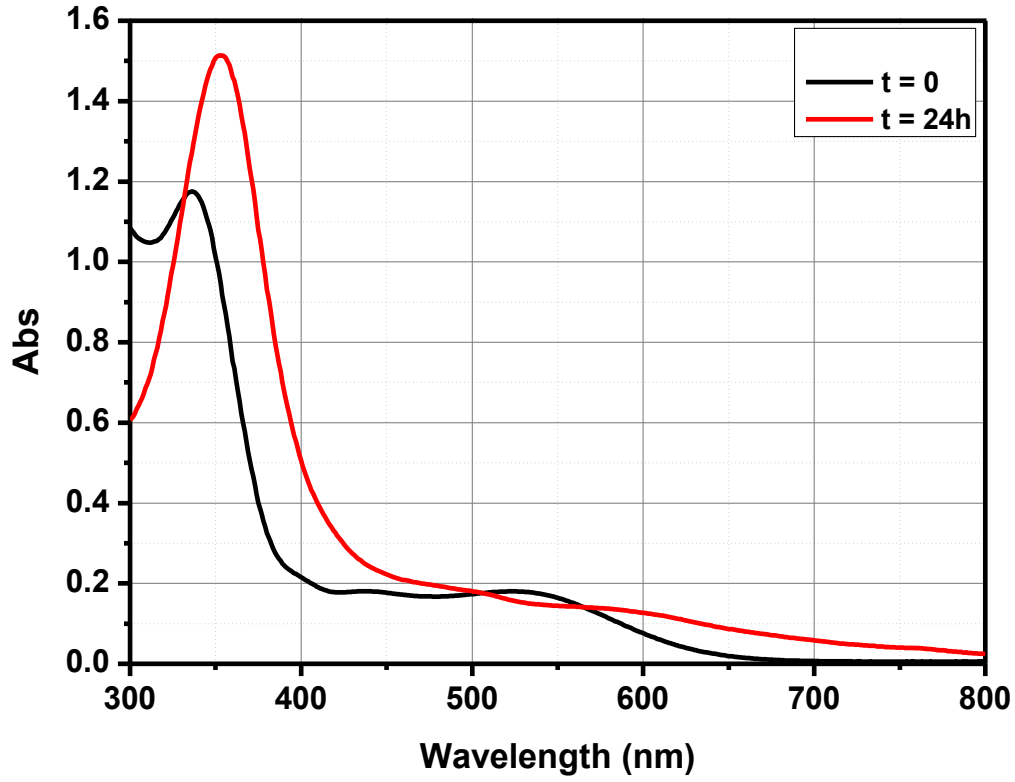

t = 0s
t = 8h
t = 24h
t = 36h
Absorbance
Wavelength (nm)
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
300
400
500
600
700
800

Modification of the UV-visible absorption spectra of A-D-A0 in different solvents at room temperature over time

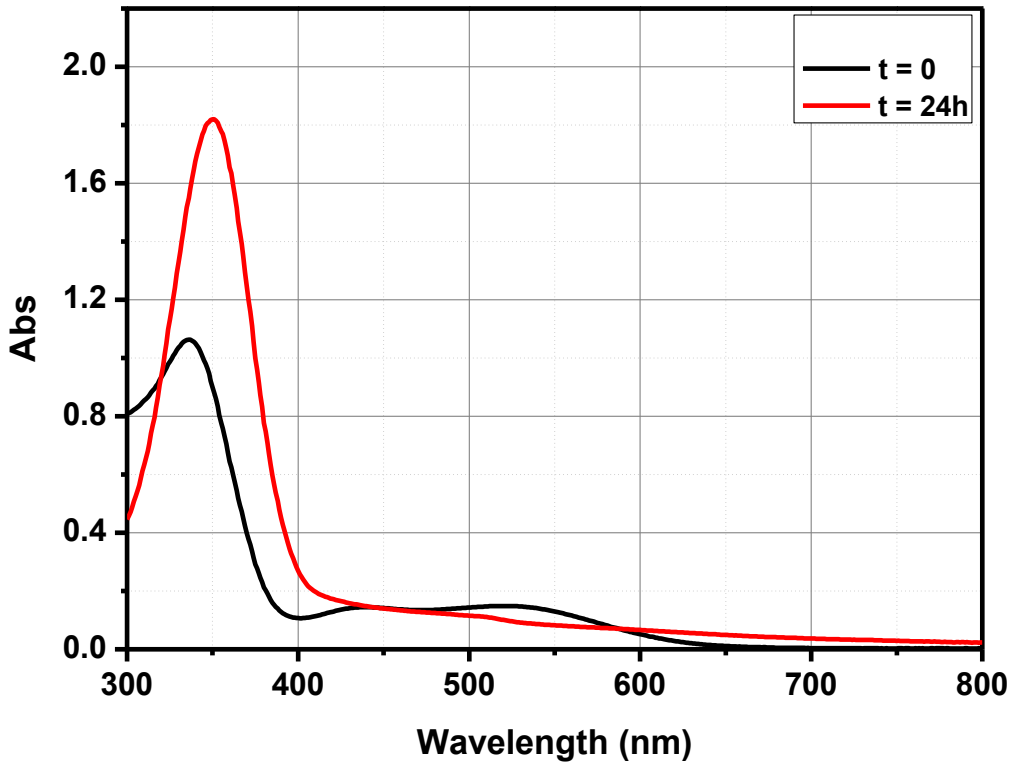
Acetone



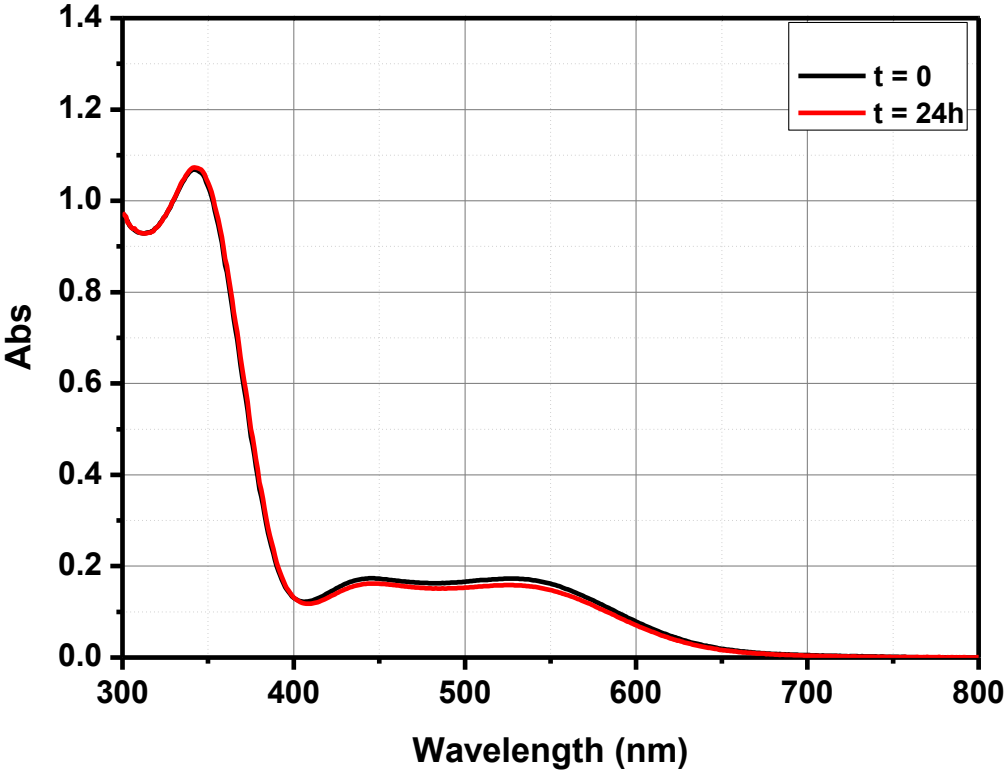
Acetonitrile



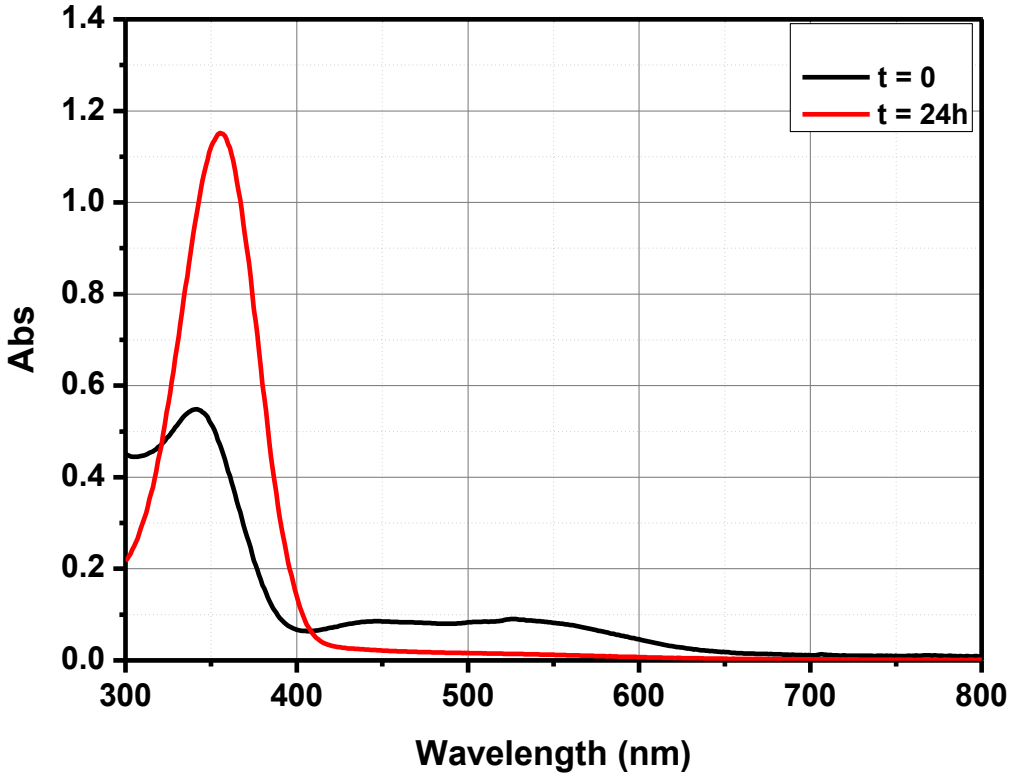
AcOEt



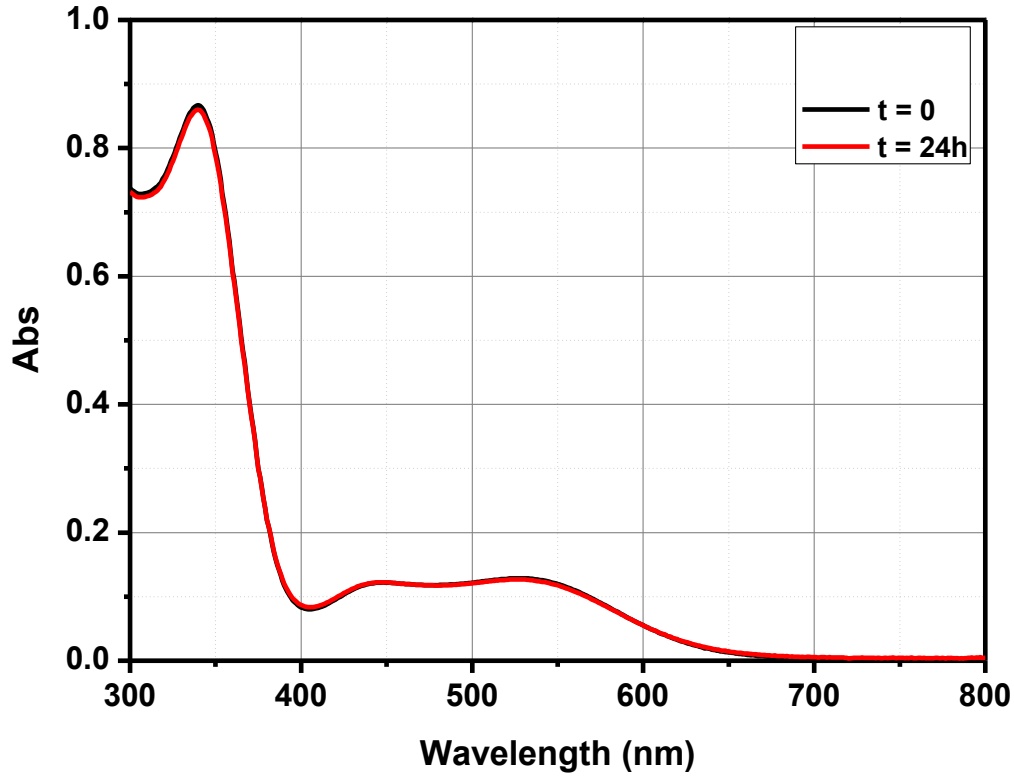
Anisole



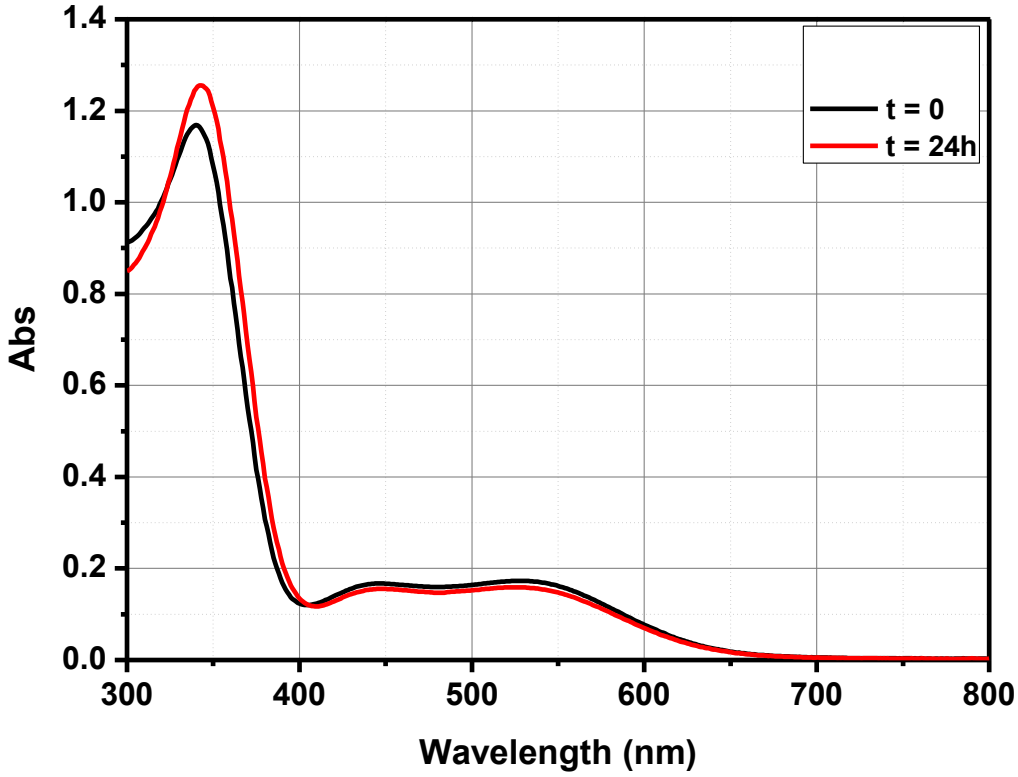
Chloroforme



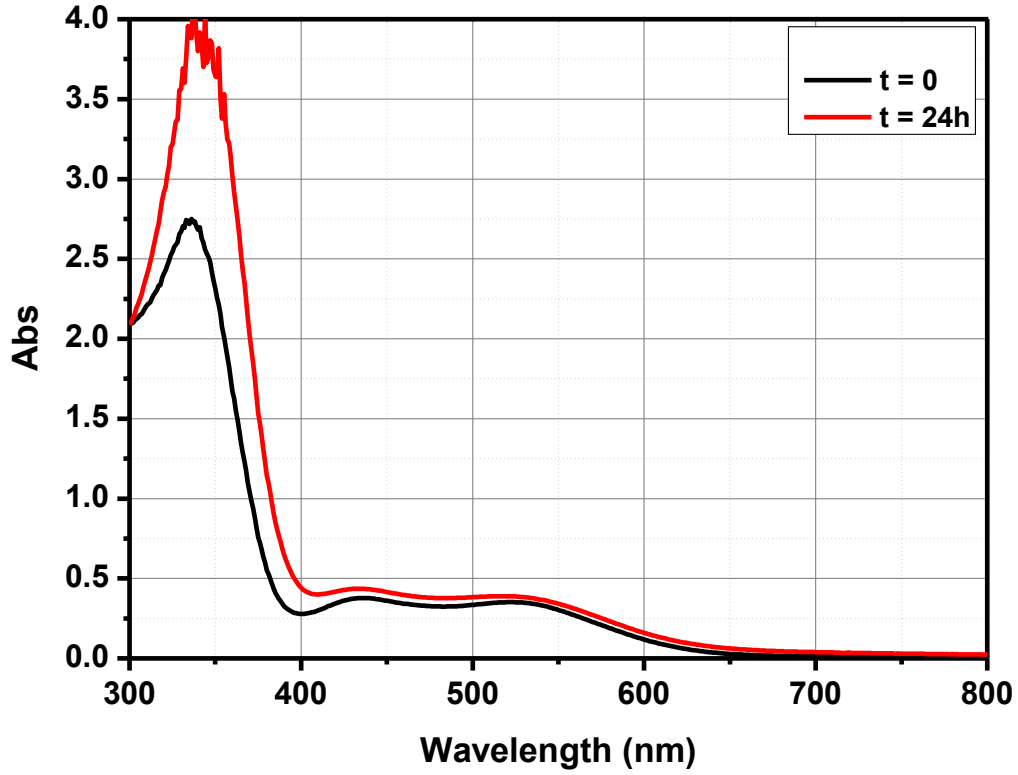
1,2-Dichloroethane



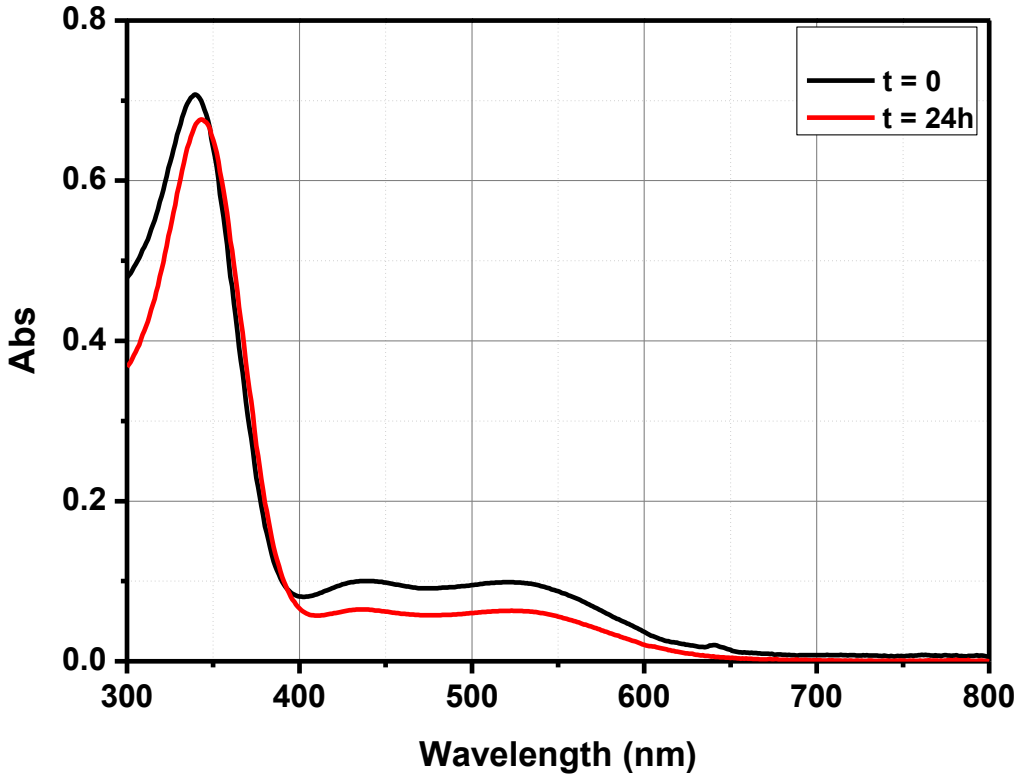
Dichloromethane



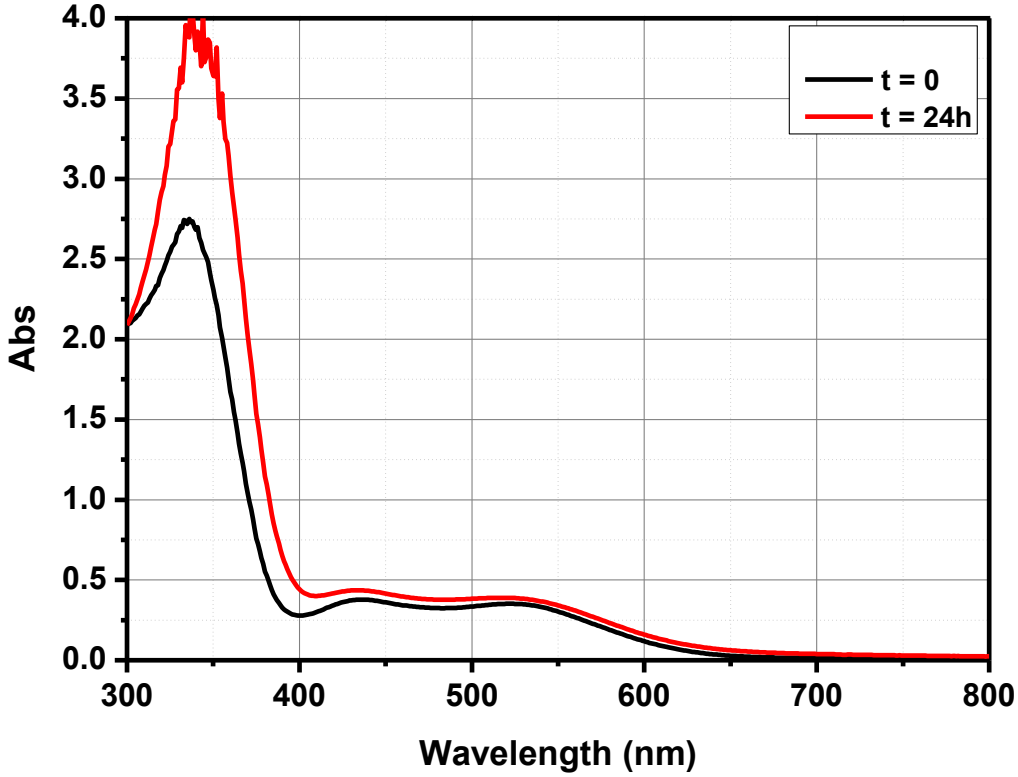
Diethyl carbonate



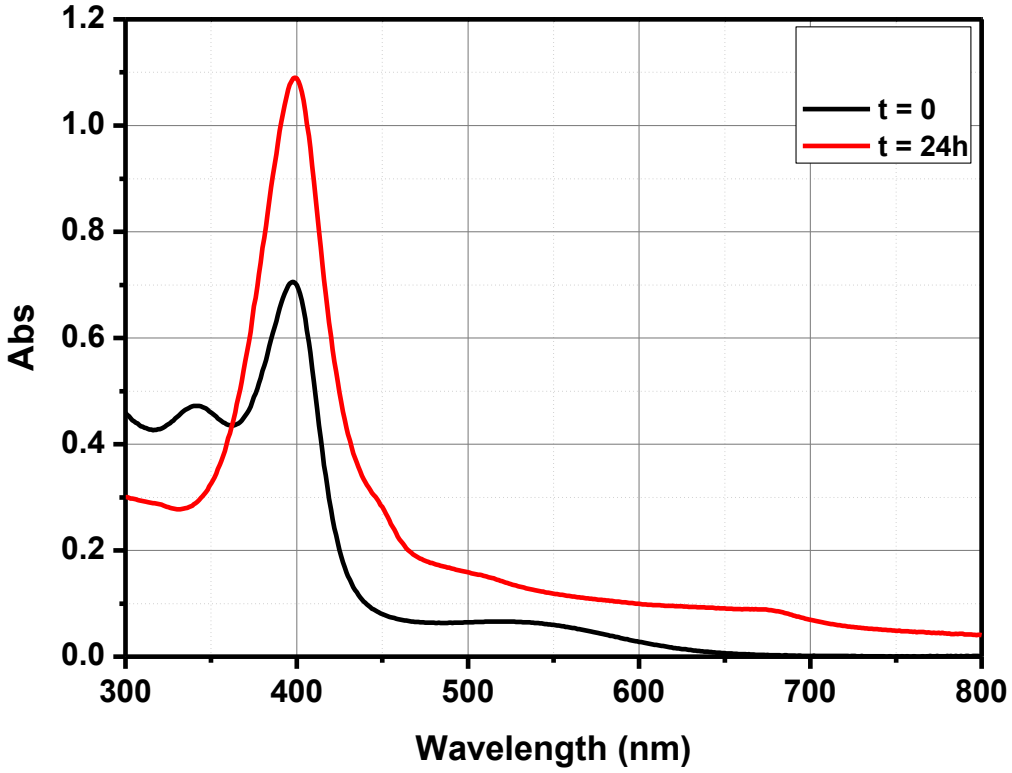
Diglyme



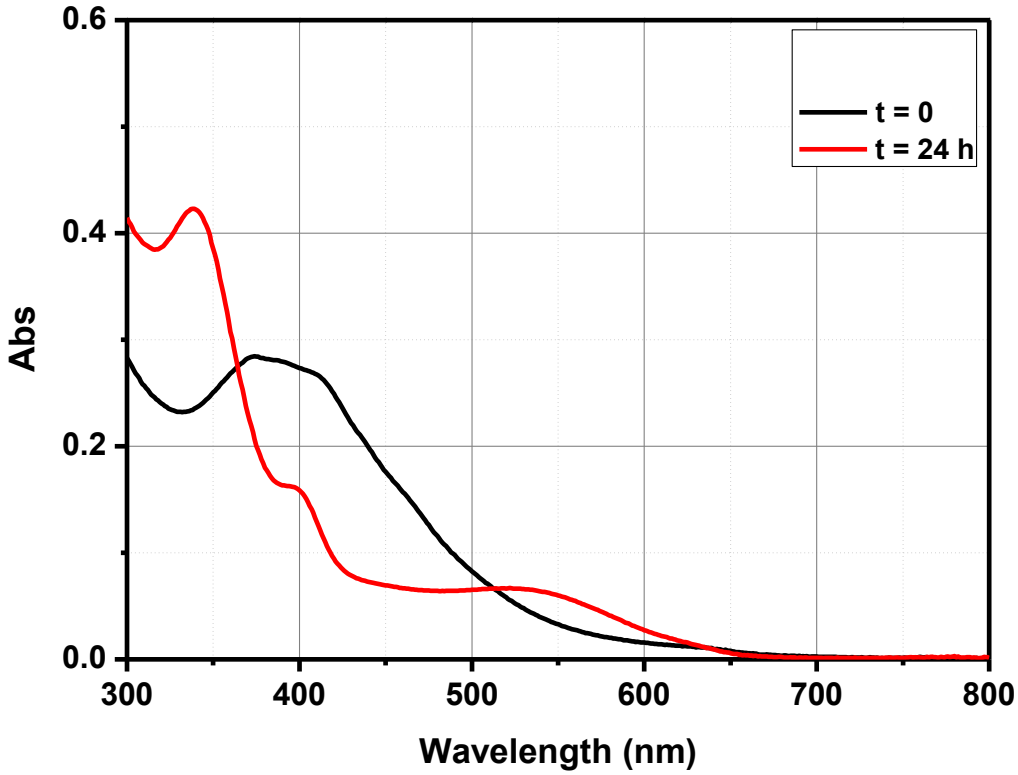
Dioxane



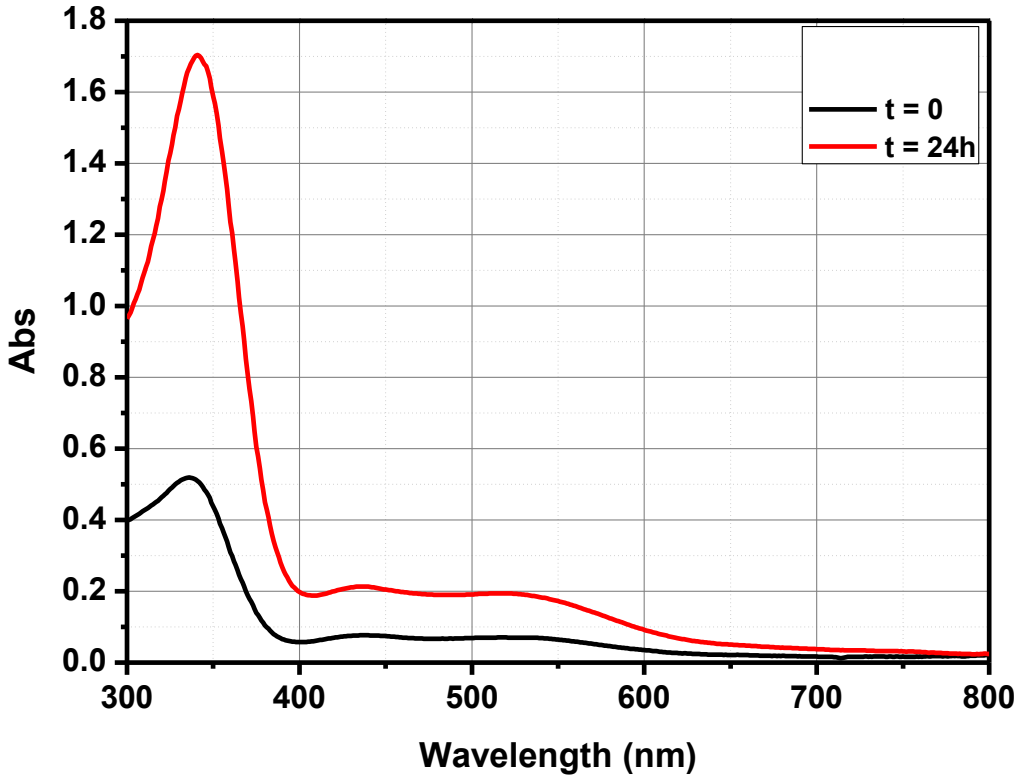
Dimethylacetamide



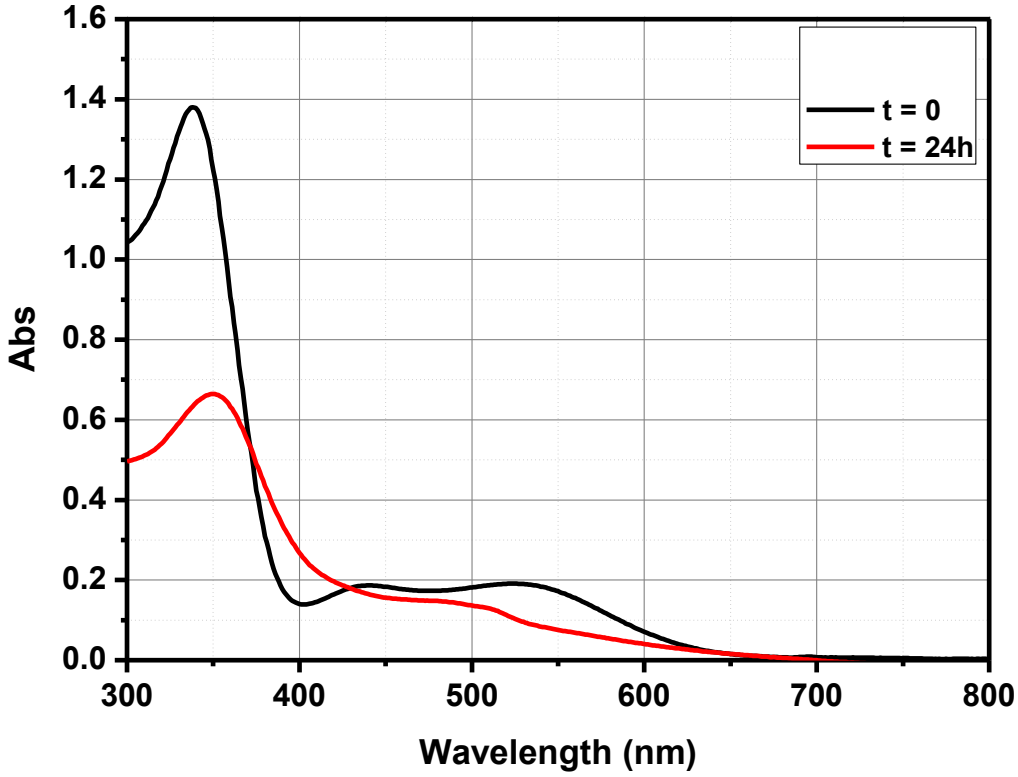
DMF



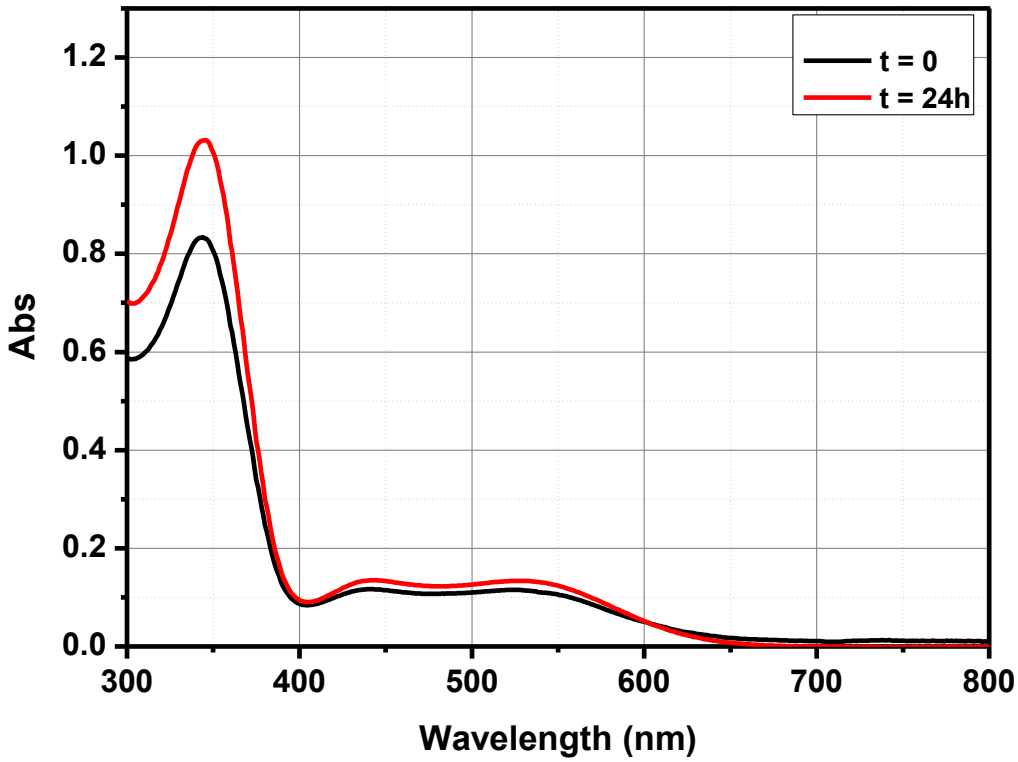
Diethyl ether



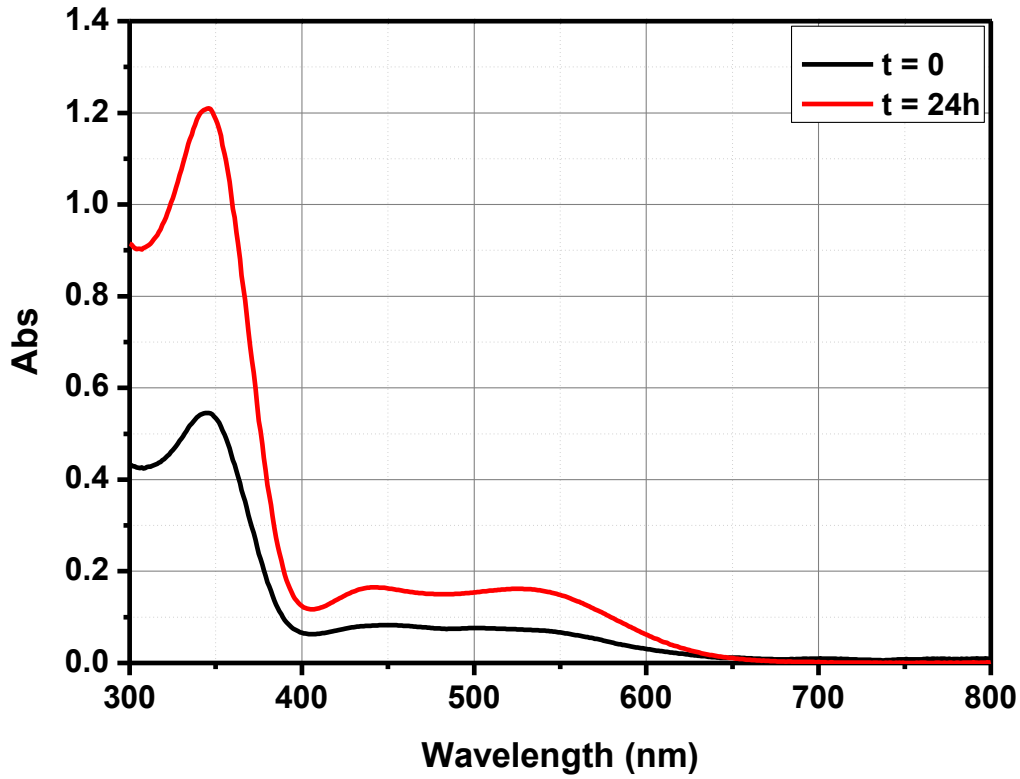
THF



Toluene

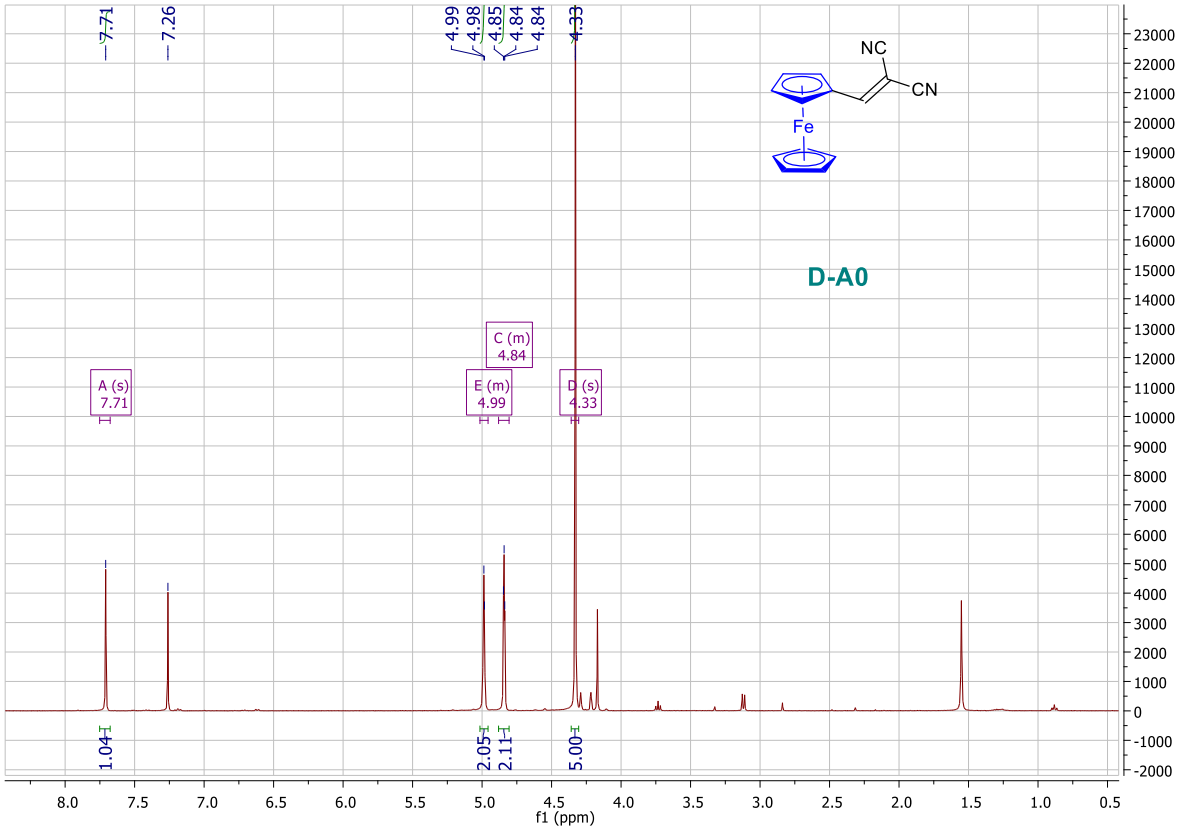


Xylene

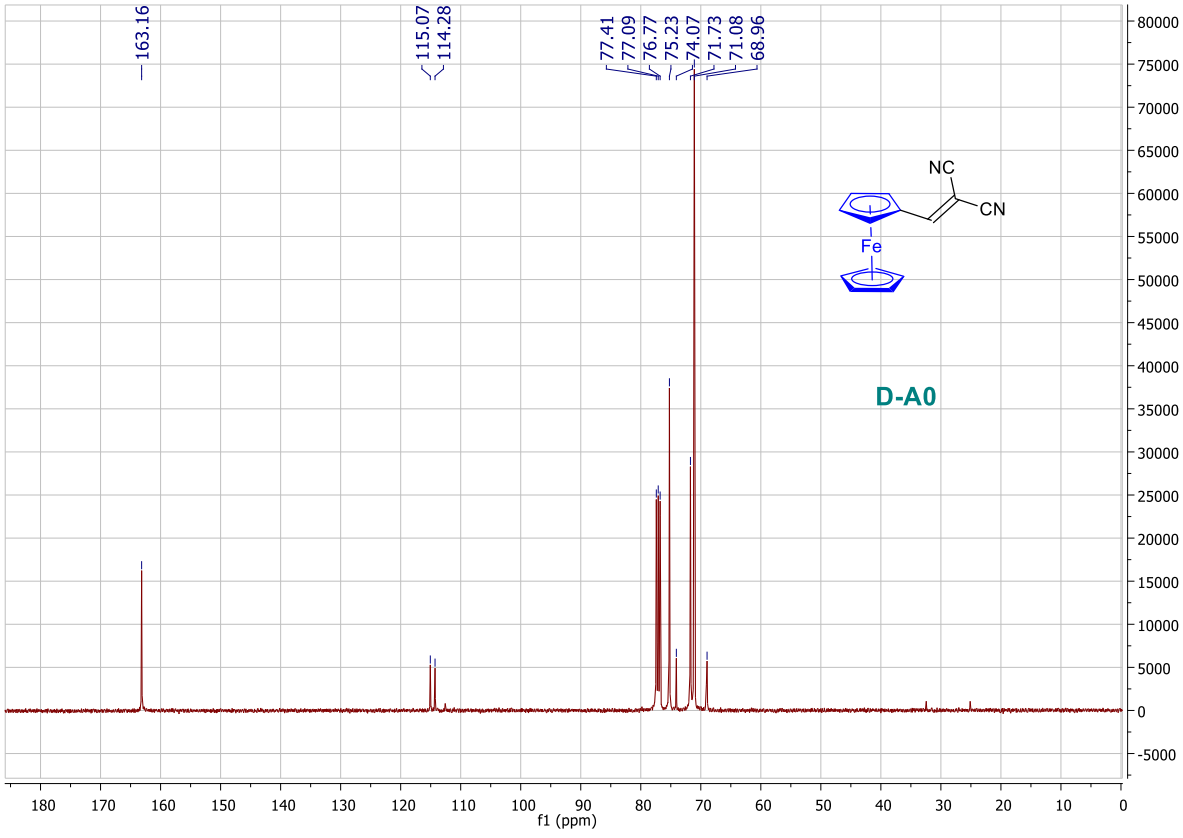


^{1}H and ^{13}C NMR spectra of the different dyes

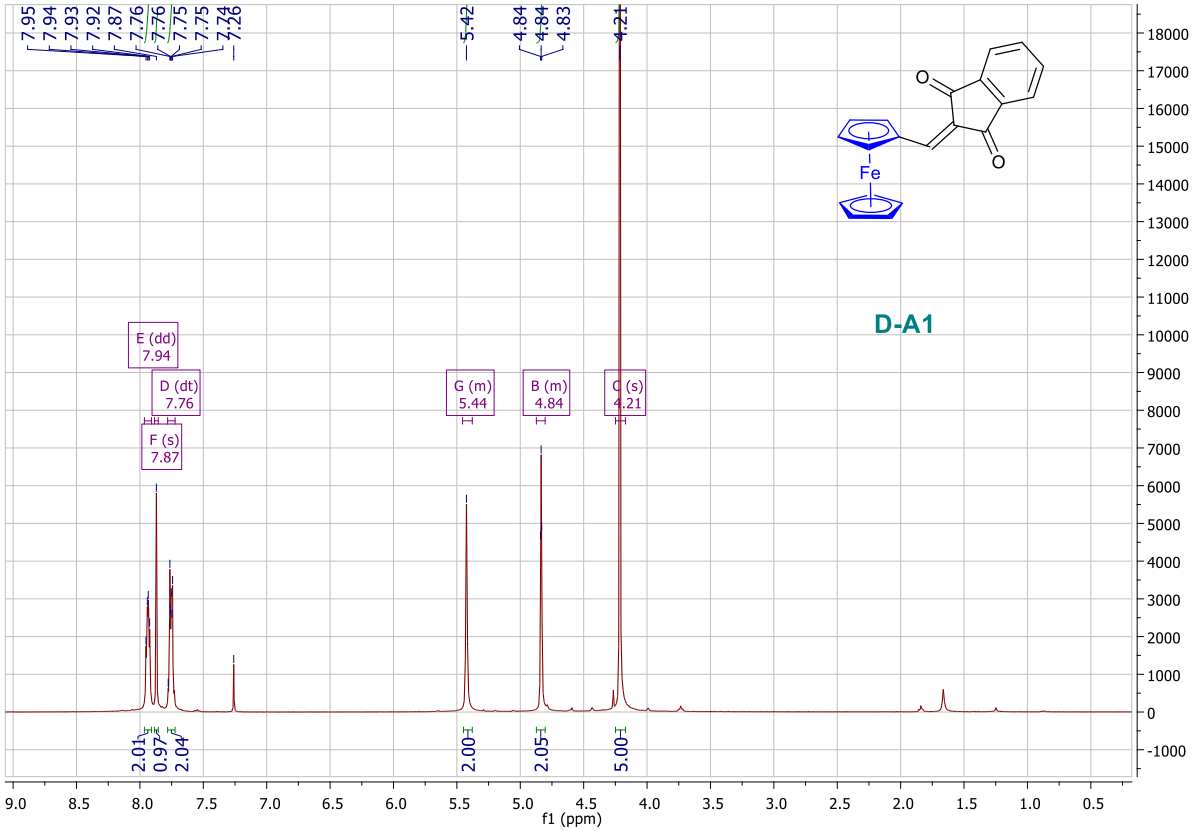
^{1}H NMR spectrum of **D-A0**



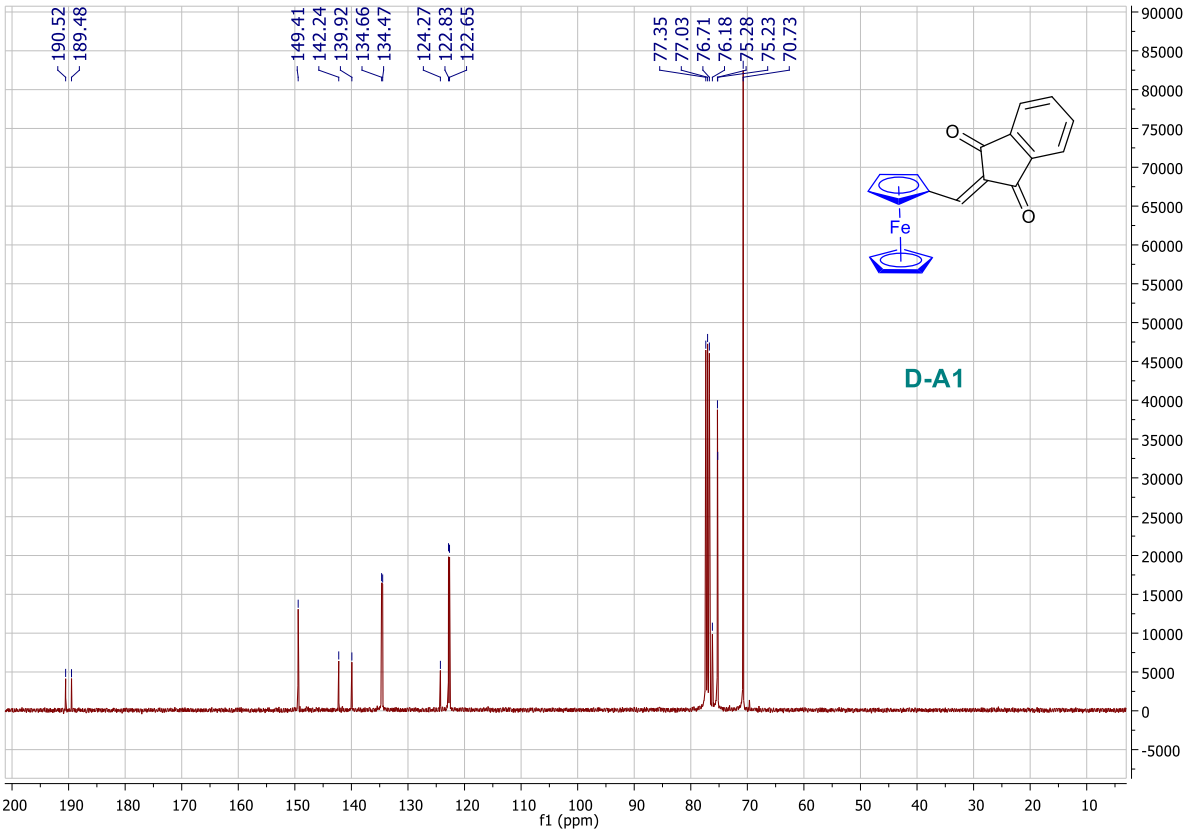
^{13}C NMR spectrum of **D-A0**



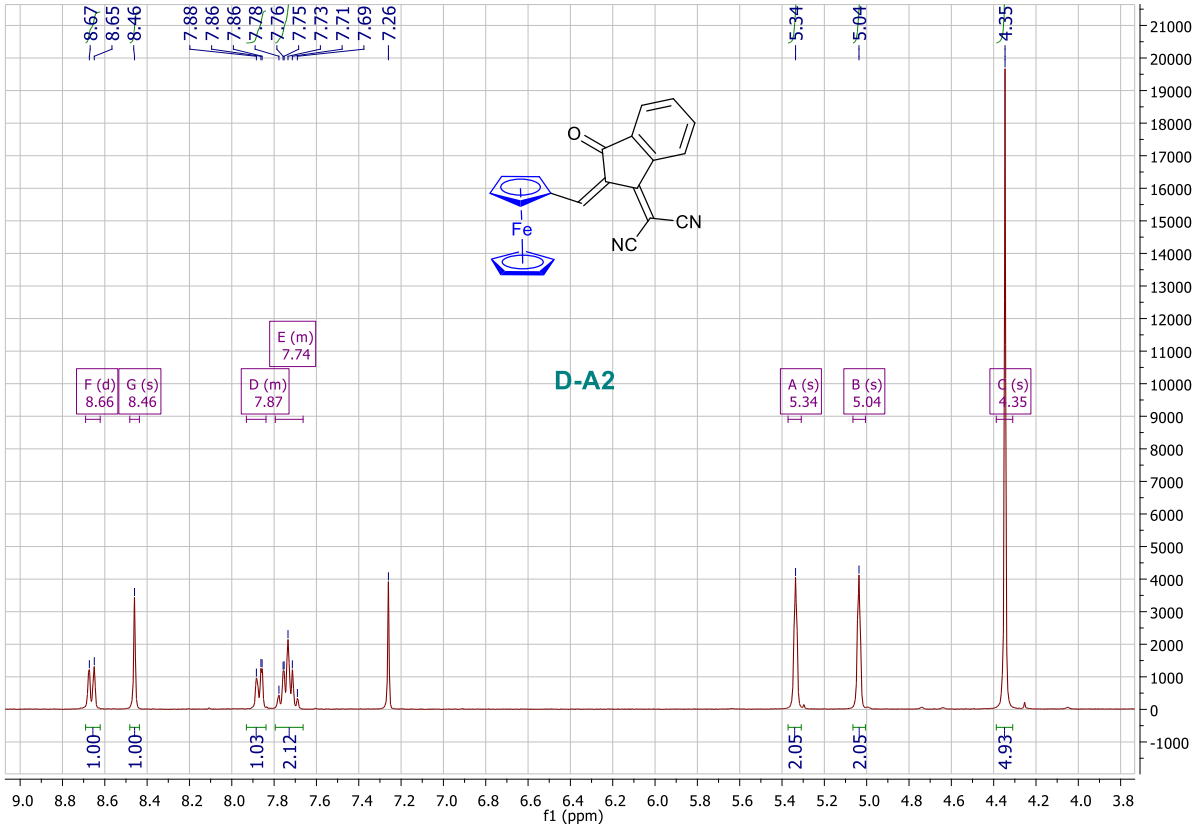
^{1}H NMR spectrum of **D-A1**



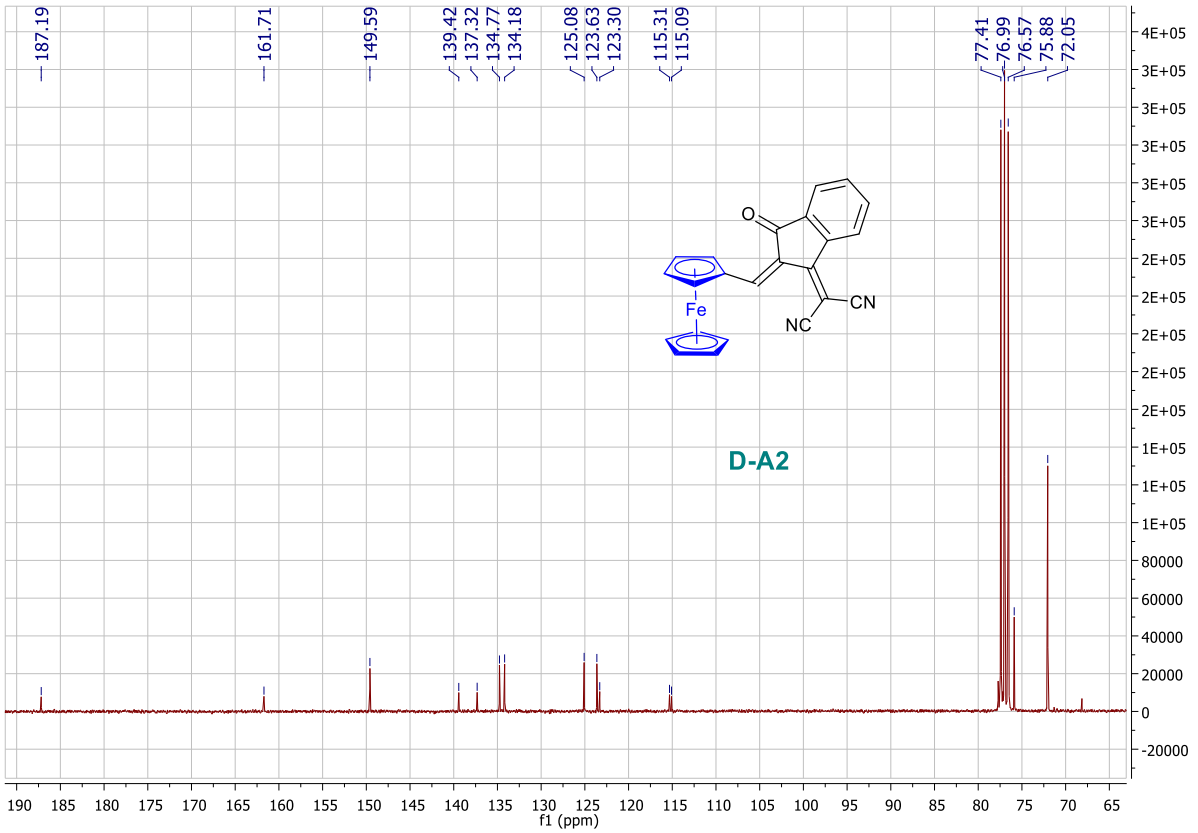
^{13}C NMR spectrum of **D-A1**



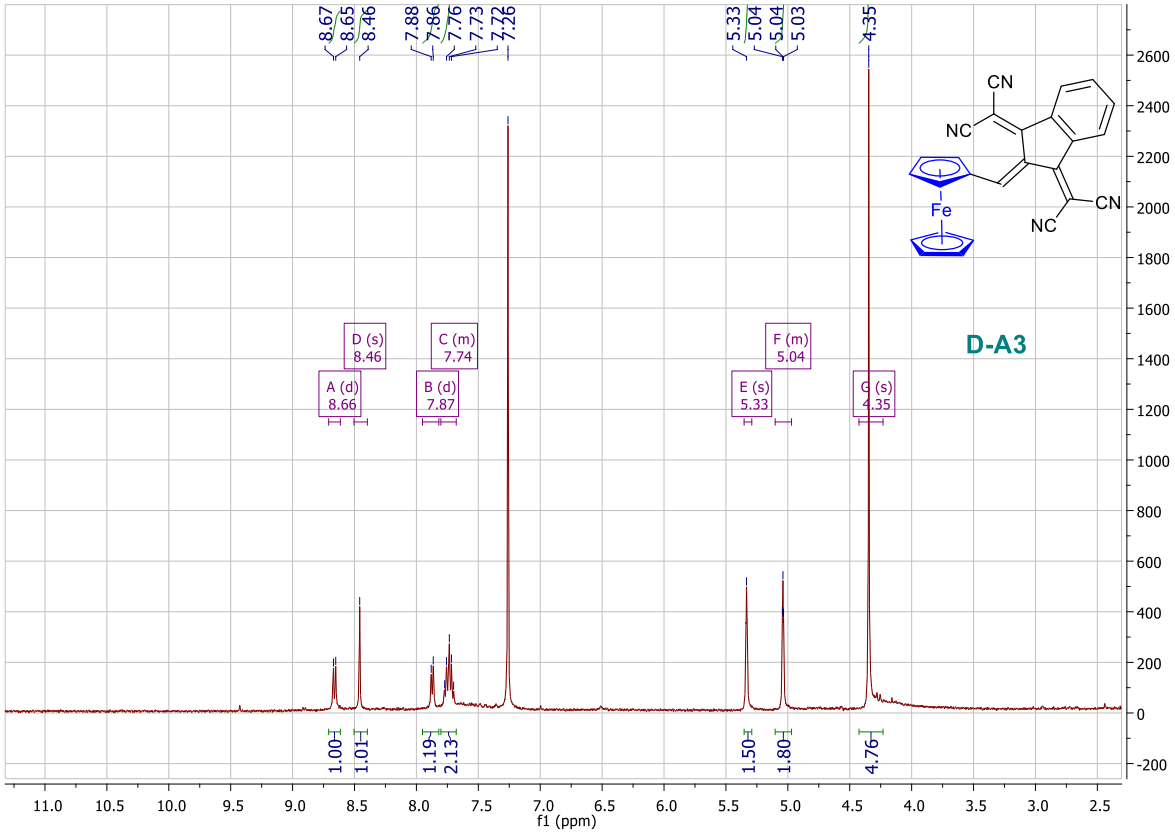
^{1}H NMR spectrum of **D-A2**



^{13}C NMR spectrum of **D-A2**



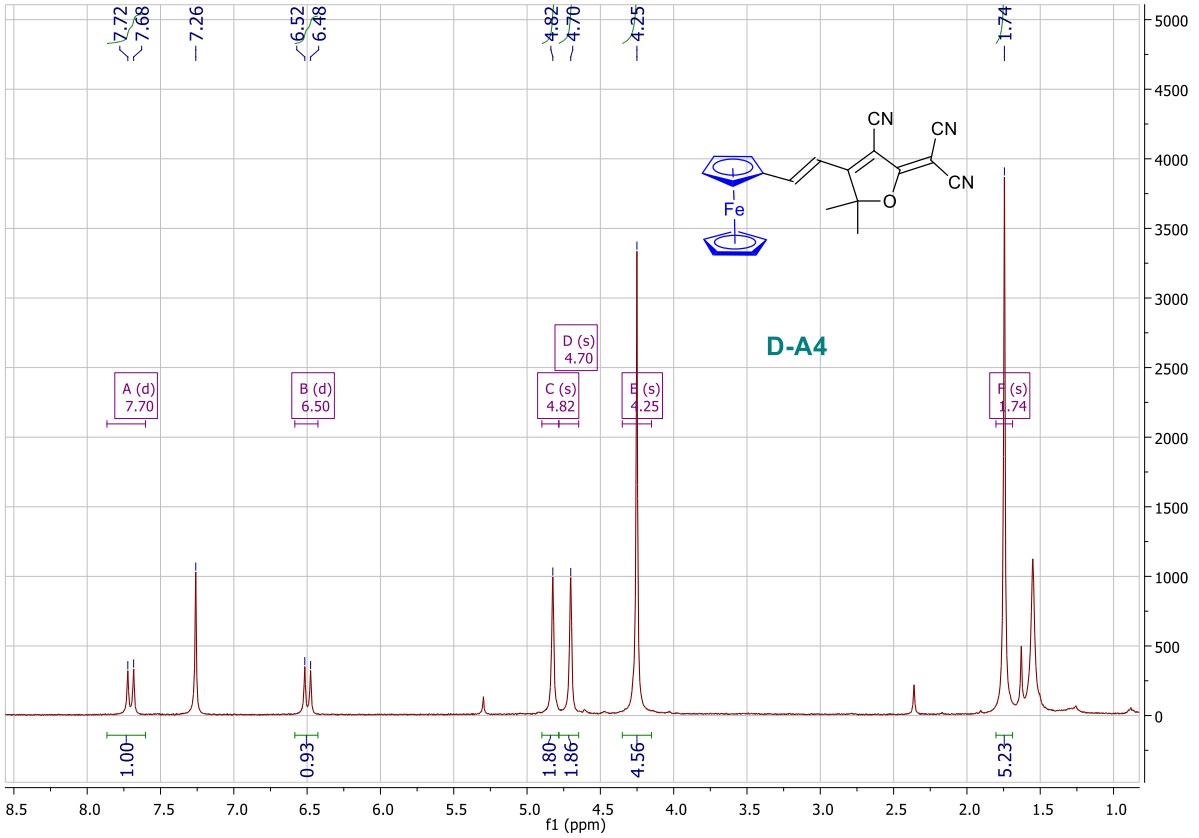
[1]H NMR spectrum of **D-A3**



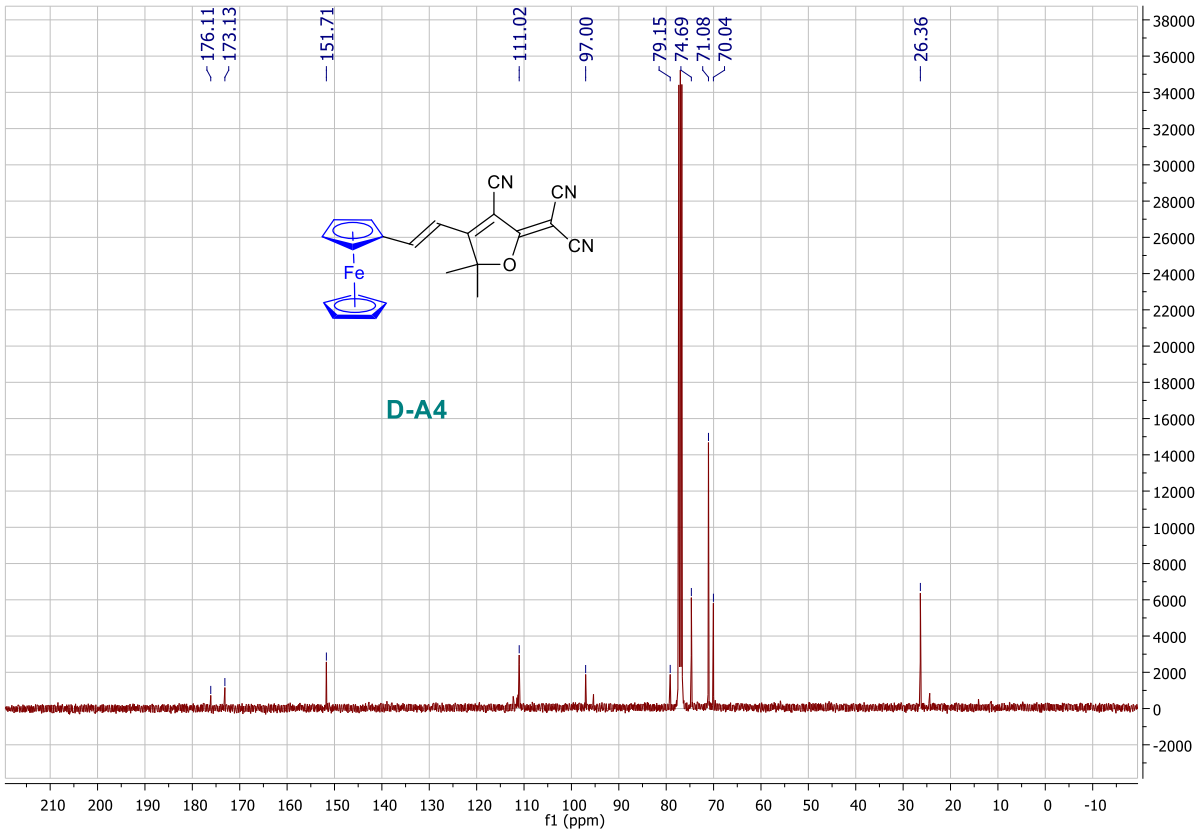
[13]C NMR spectrum of **D-A3**

NOT SUFFICENTLY SOLUBLE

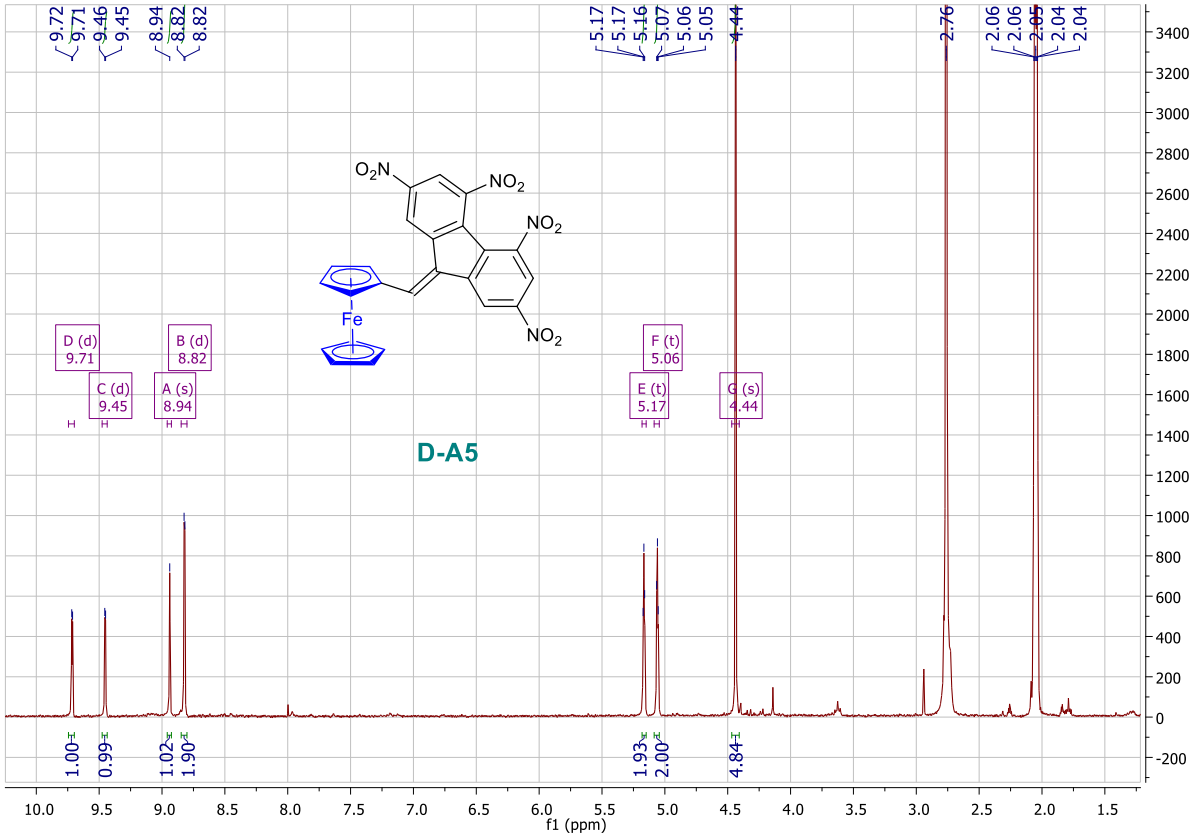
[1]H NMR spectrum of **D-A4**



[13]C NMR spectrum of **D-A4**



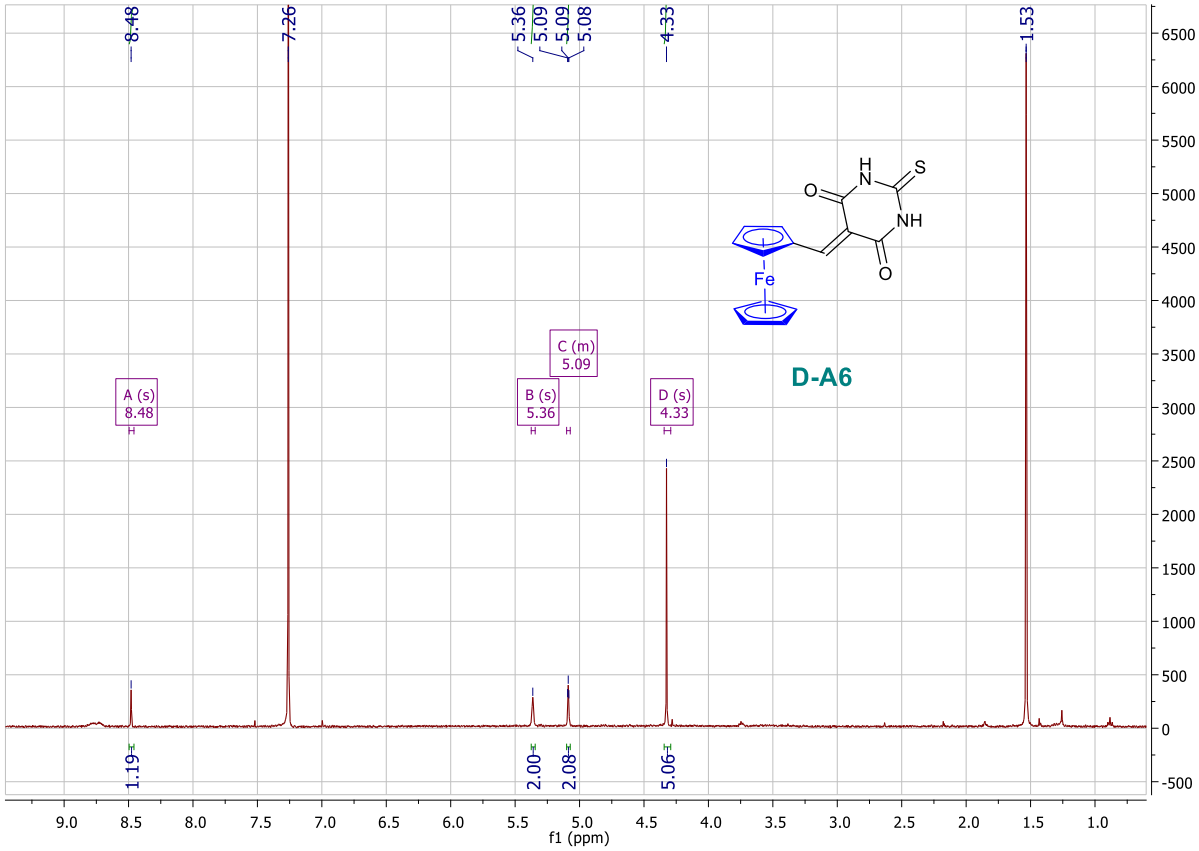
^{1}H NMR spectrum of **D-A5**



^{13}C NMR spectrum of **D-A5**

NOT SUFFICENTLY SOLUBLE

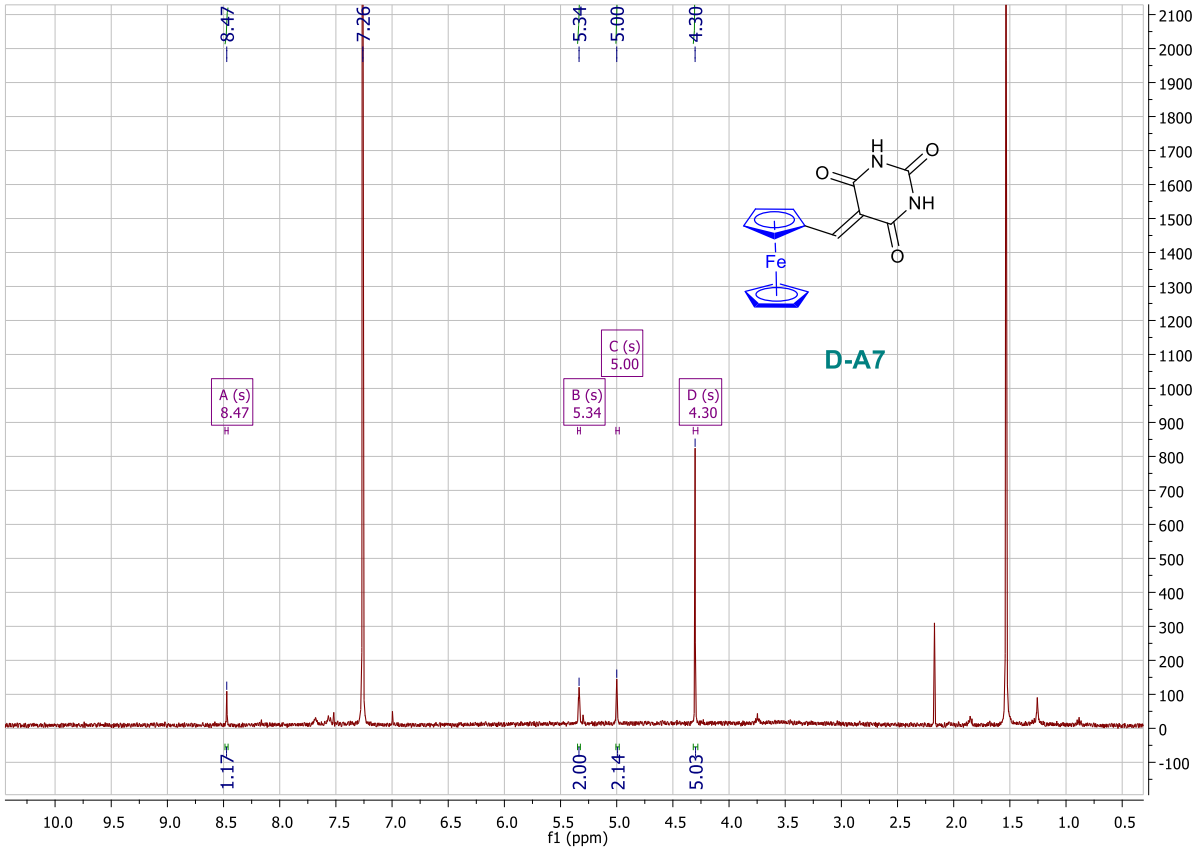
^{1}H NMR spectrum of **D-A6**



^{13}C NMR spectrum of **D-A6**

NOT SUFFICENTLY SOLUBLE

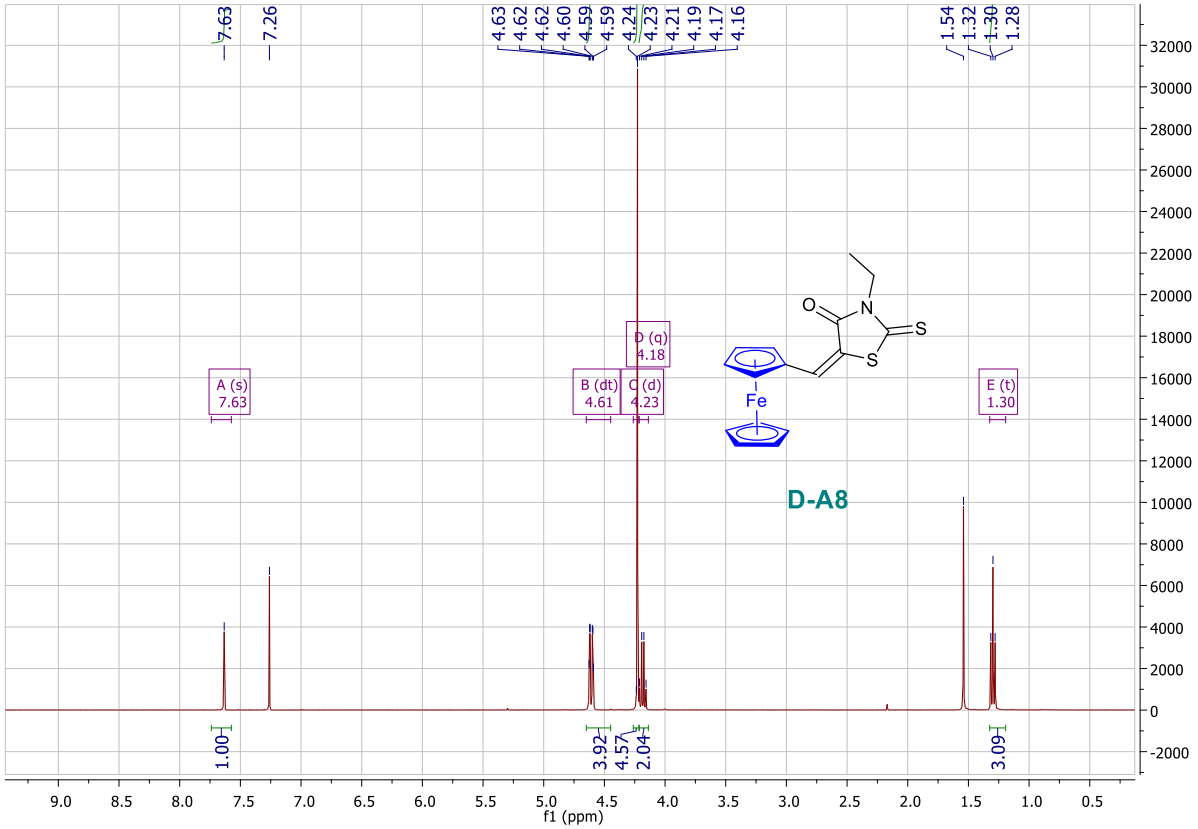
[1]H NMR spectrum of **D-A7**



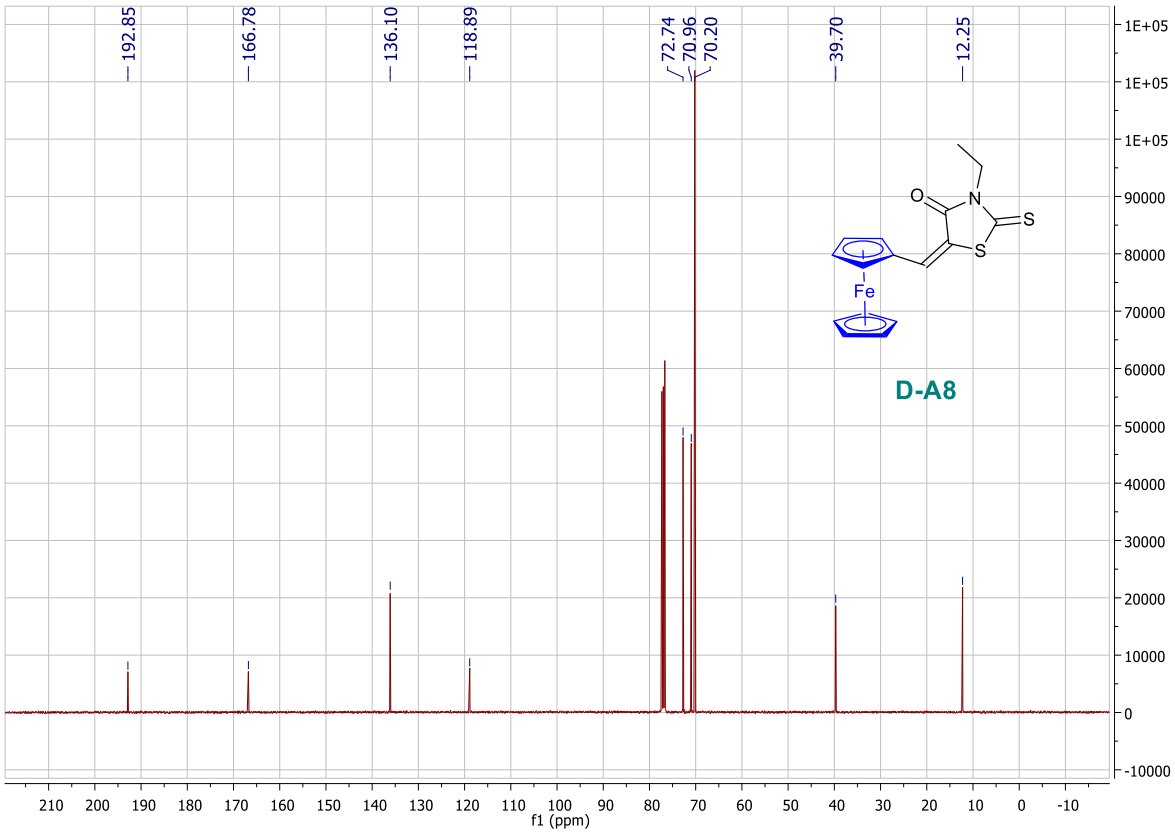
[13]C NMR spectrum of **D-A7**

NOT SUFFICENTLY SOLUBLE

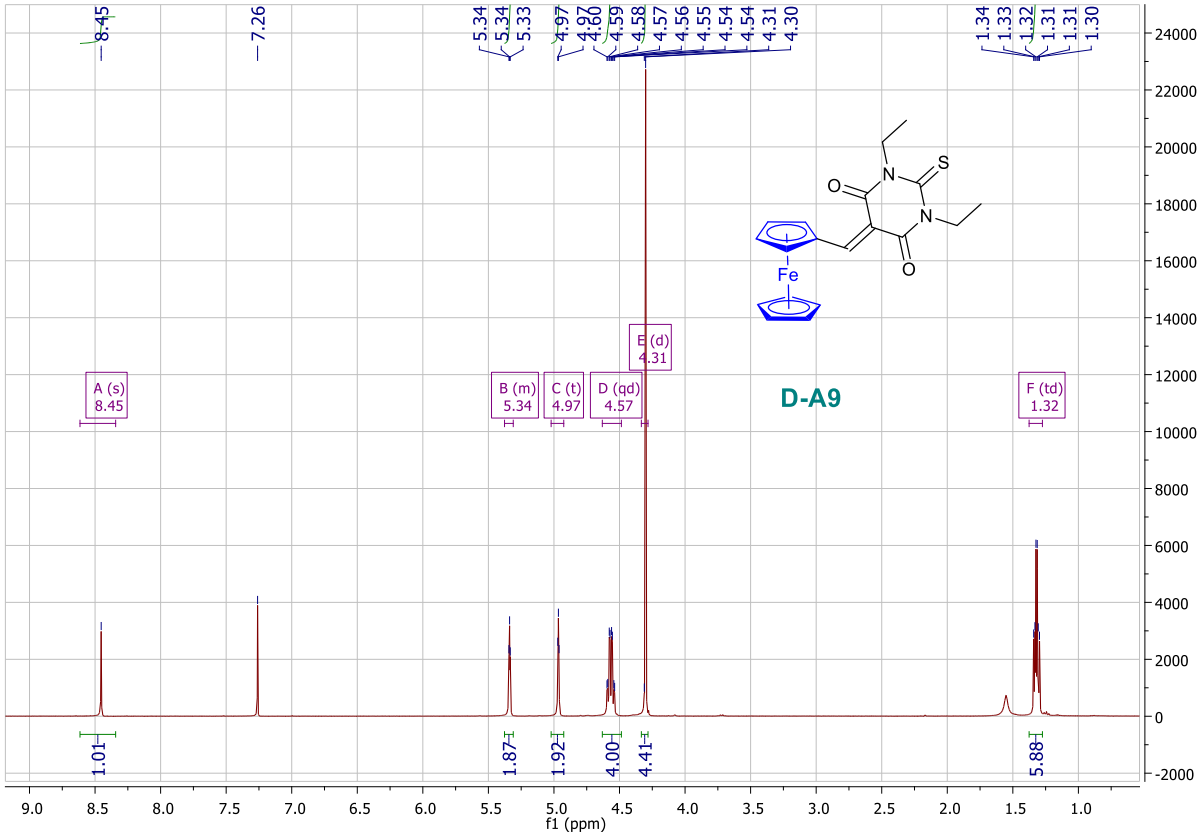
^{1}H NMR spectrum of **D-A8**



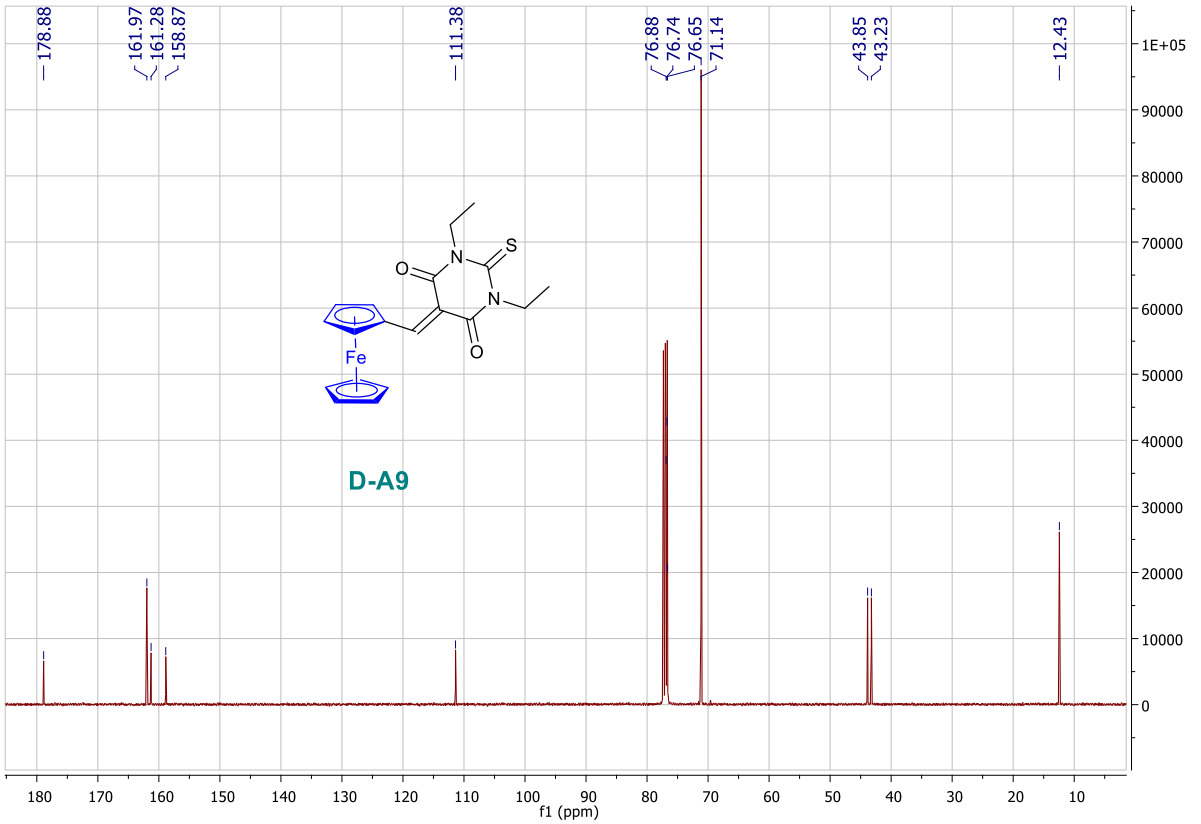
^{13}C NMR spectrum of **D-A8**



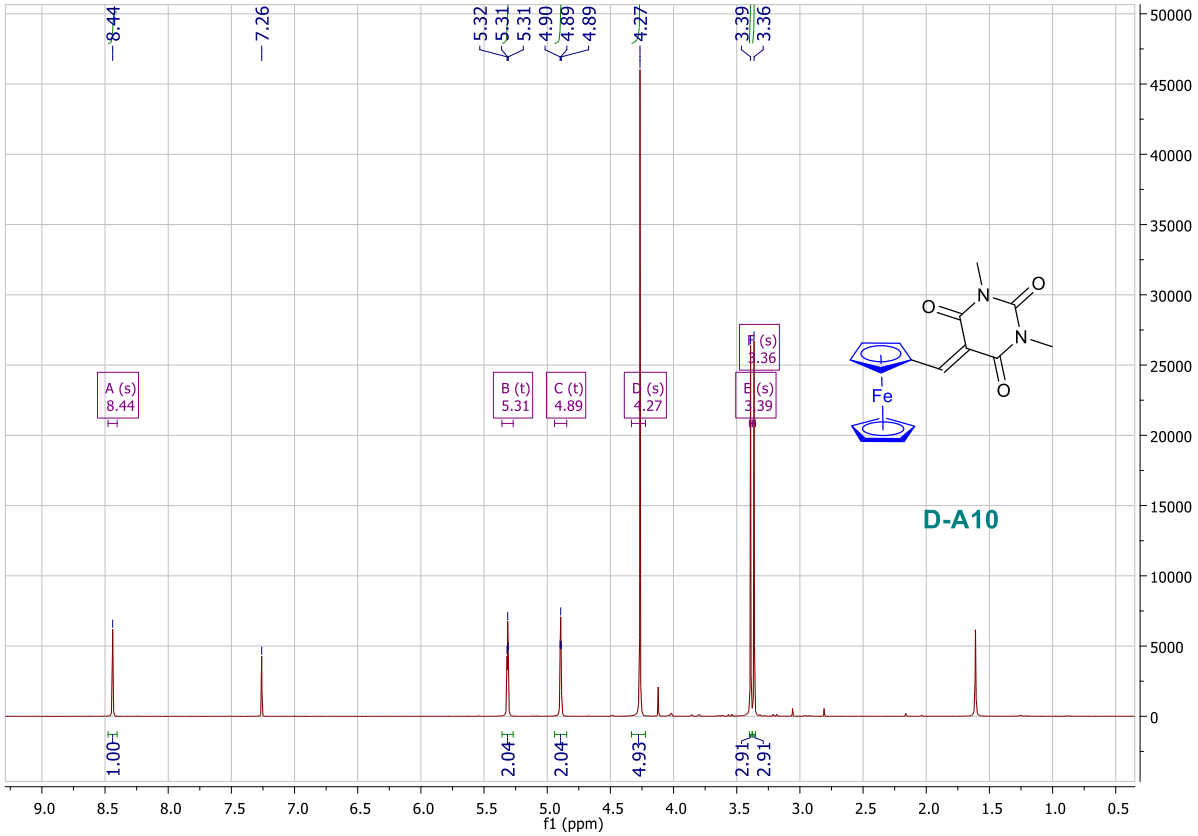
^{1}H NMR spectrum of **D-A9**



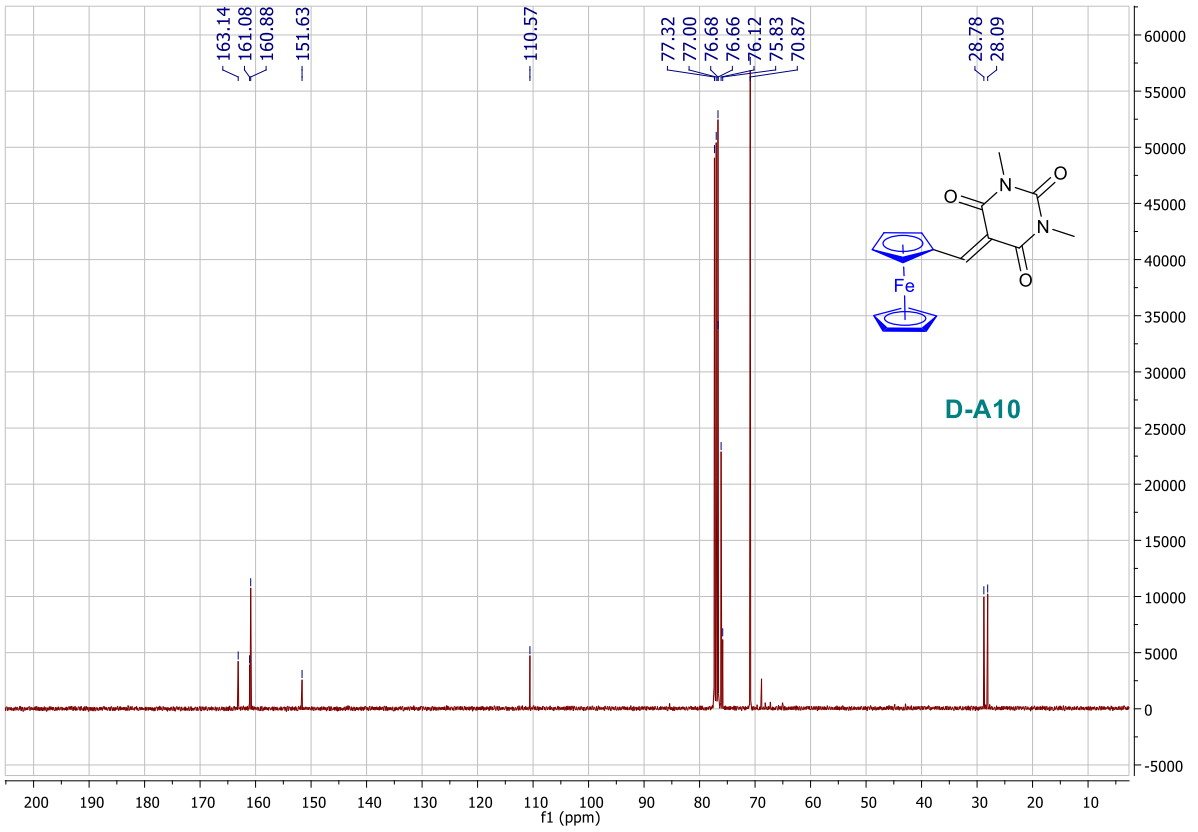
^{13}C NMR spectrum of **D-A9**



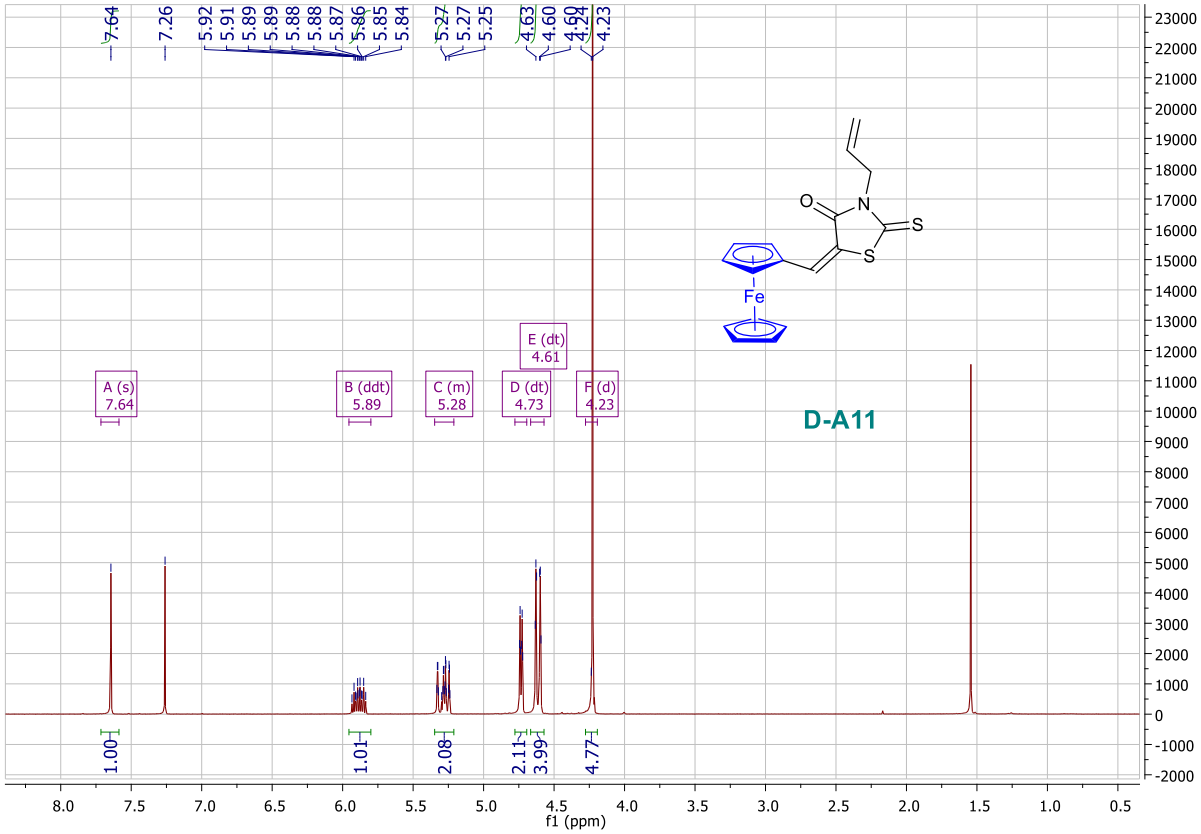
[1]H NMR spectrum of **D-A10**



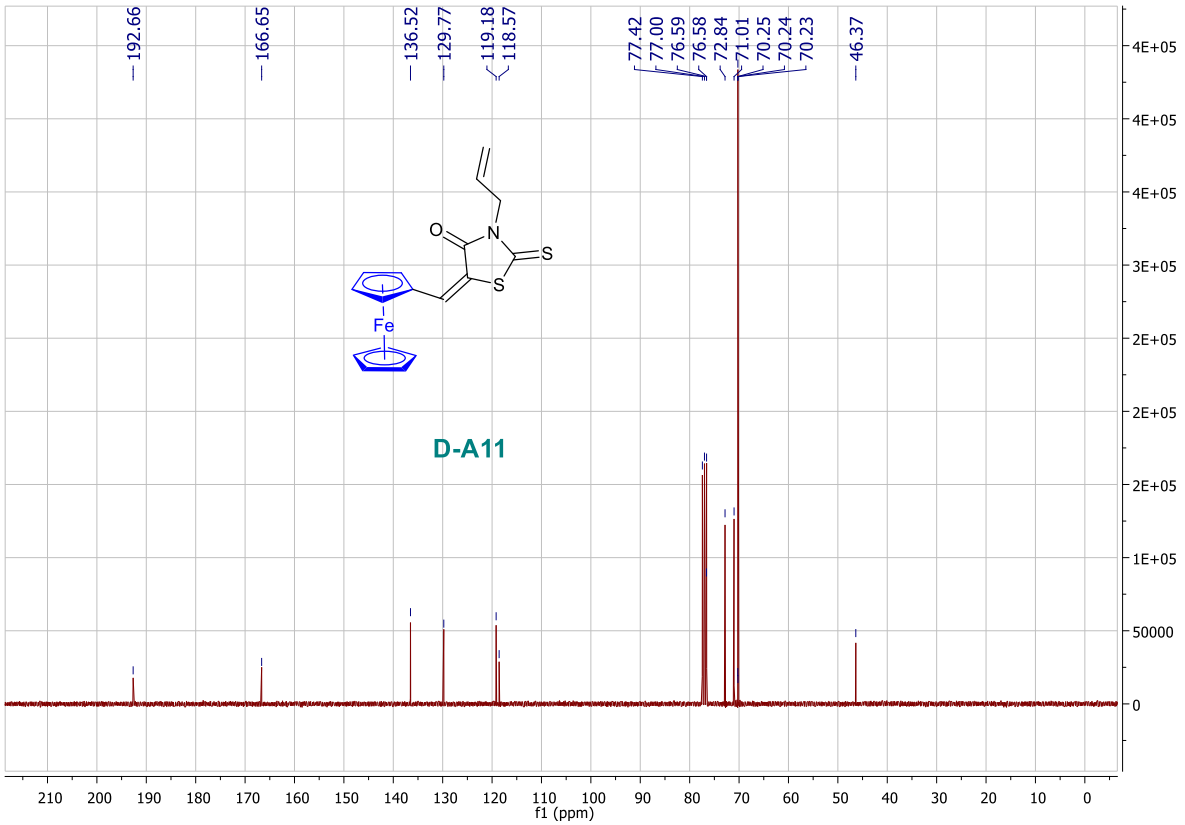
[13]C NMR spectrum of **D-A10**



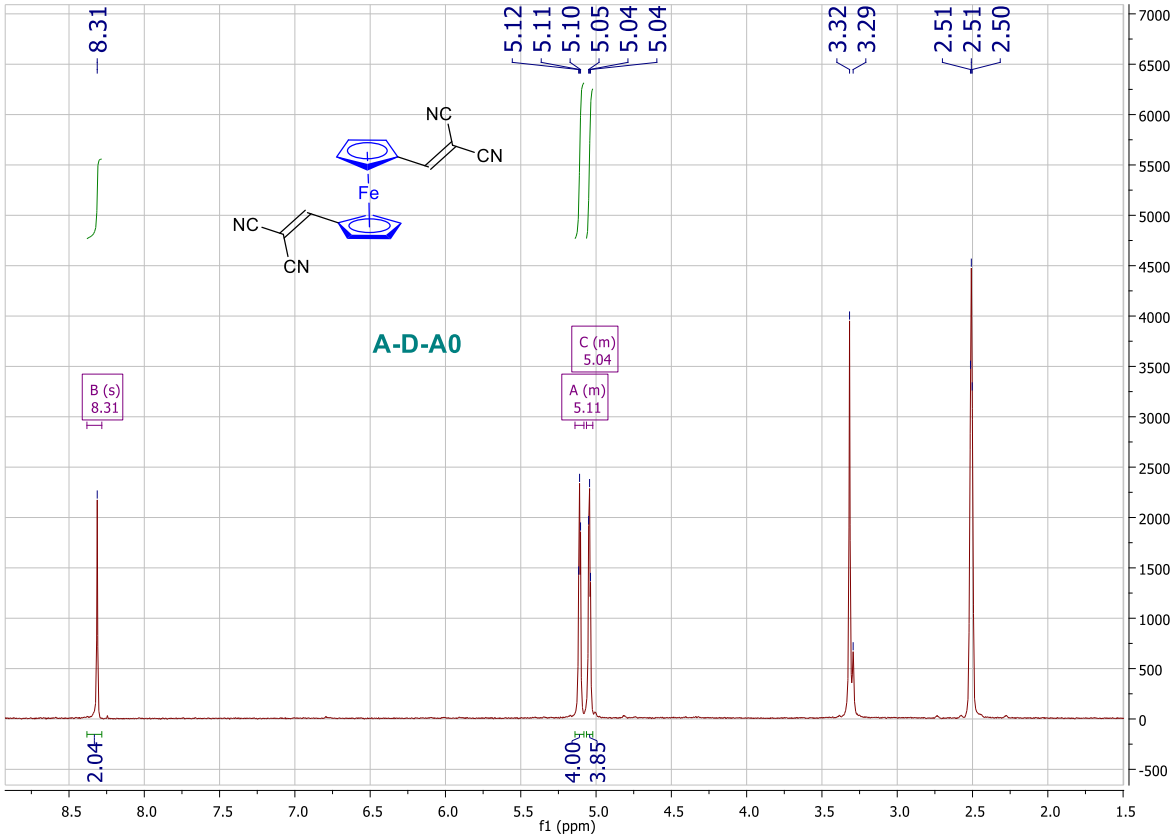
[1]H NMR spectrum of **D-A11**



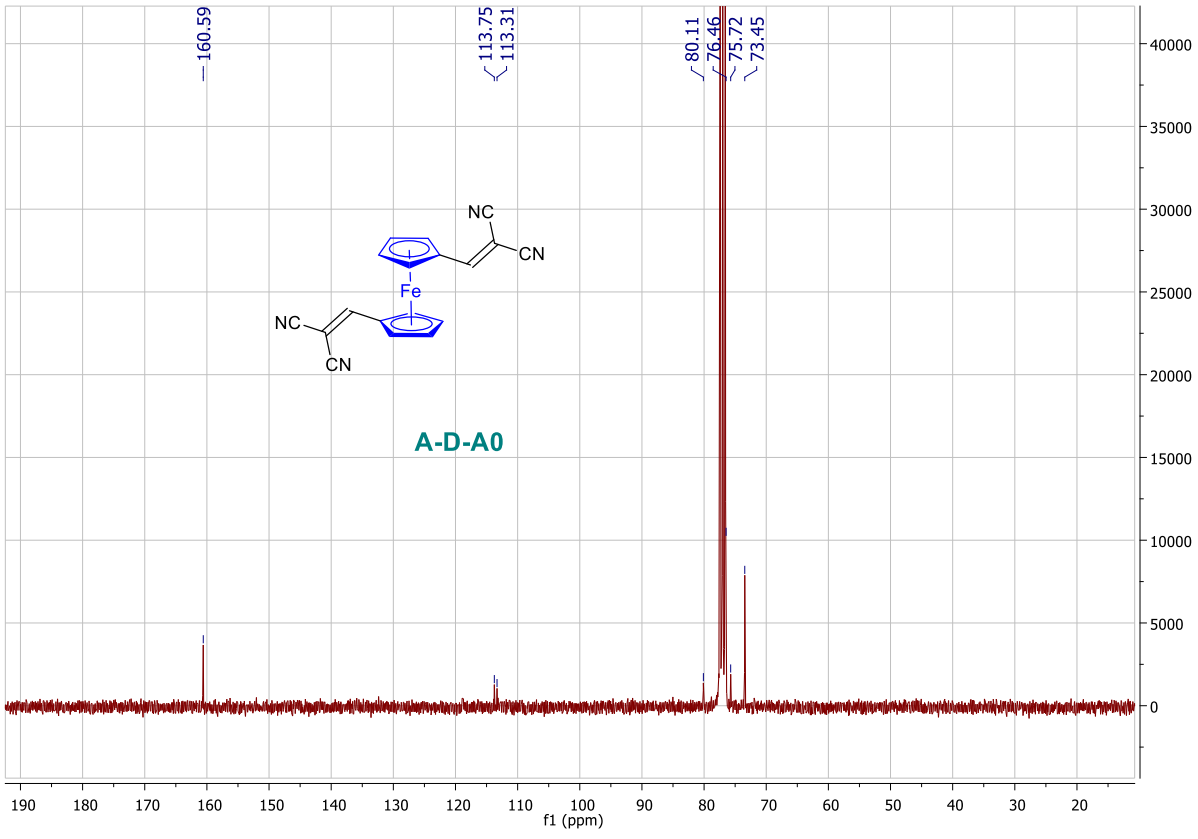
[13]C NMR spectrum of **D-A11**



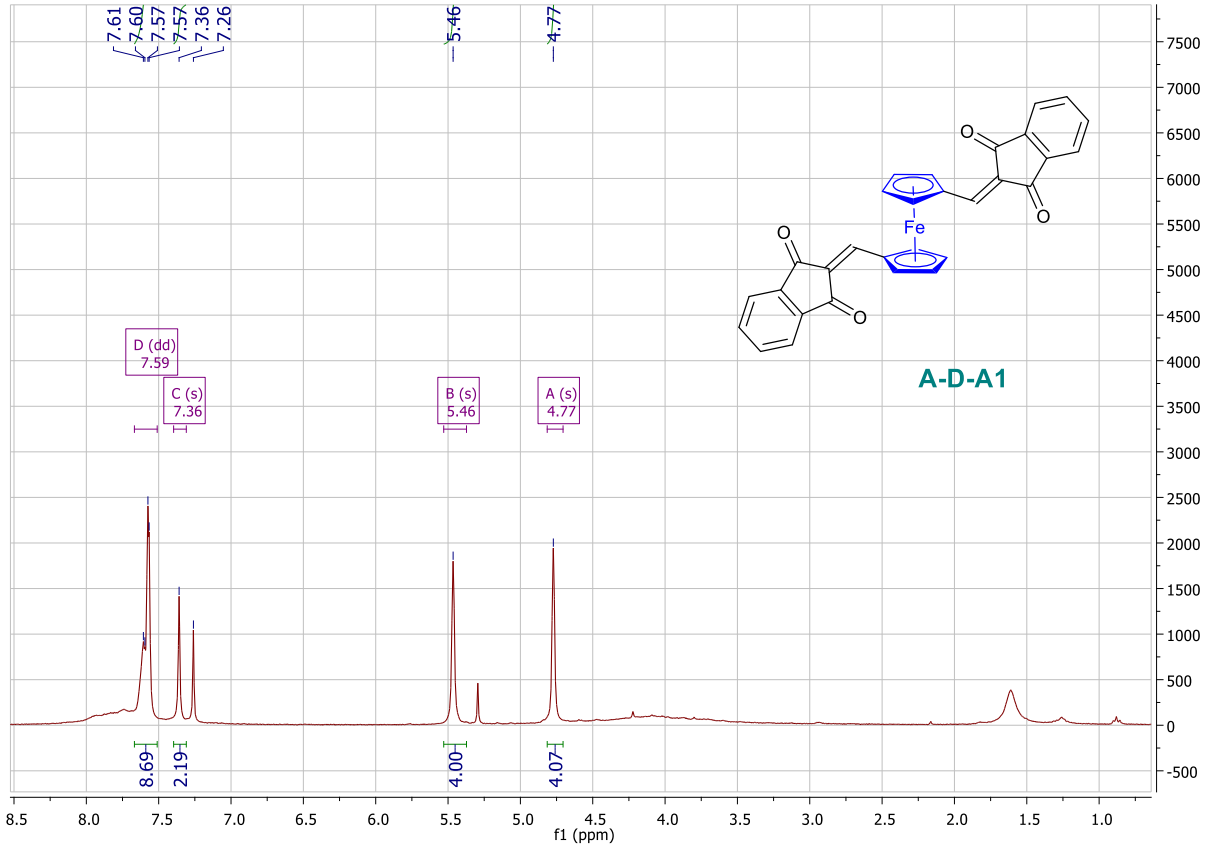
^{1}H NMR spectrum of **A-D-A0**



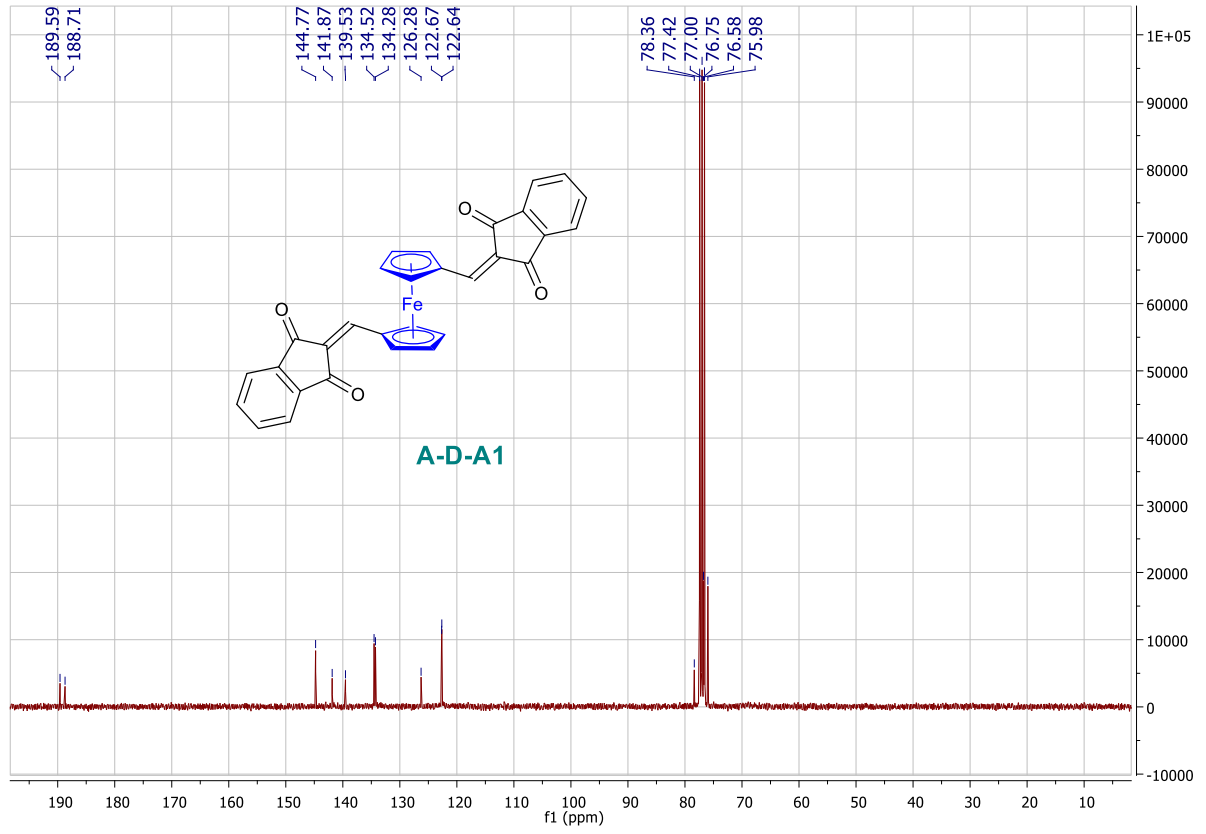
^{13}C NMR spectrum of **A-D-A0**



^{1}H NMR spectrum of **A-D-A1**



^{13}C NMR spectrum of **A-D-A1**



^{1}H NMR spectrum of **A-D-A2**

NOT SUFFICENTLY SOLUBLE

^{13}C NMR spectrum of **A-D-A2**

NOT SUFFICENTLY SOLUBLE

^{1}H NMR spectrum of **A-D-A3**

NOT SUFFICENTLY SOLUBLE

^{13}C NMR spectrum of **A-D-A3**

NOT SUFFICENTLY SOLUBLE

^{1}H NMR spectrum of **A-D-A4**

NOT SUFFICENTLY SOLUBLE

^{13}C NMR spectrum of **A-D-A4**

NOT SUFFICENTLY SOLUBLE

^{1}H NMR spectrum of **A-D-A5**

NOT SUFFICENTLY SOLUBLE

^{13}C NMR spectrum of **A-D-A5**

NOT SUFFICENTLY SOLUBLE

^{1}H NMR spectrum of **A-D-A6**

NOT SUFFICENTLY SOLUBLE

^{13}C NMR spectrum of **A-D-A6**

NOT SUFFICENTLY SOLUBLE

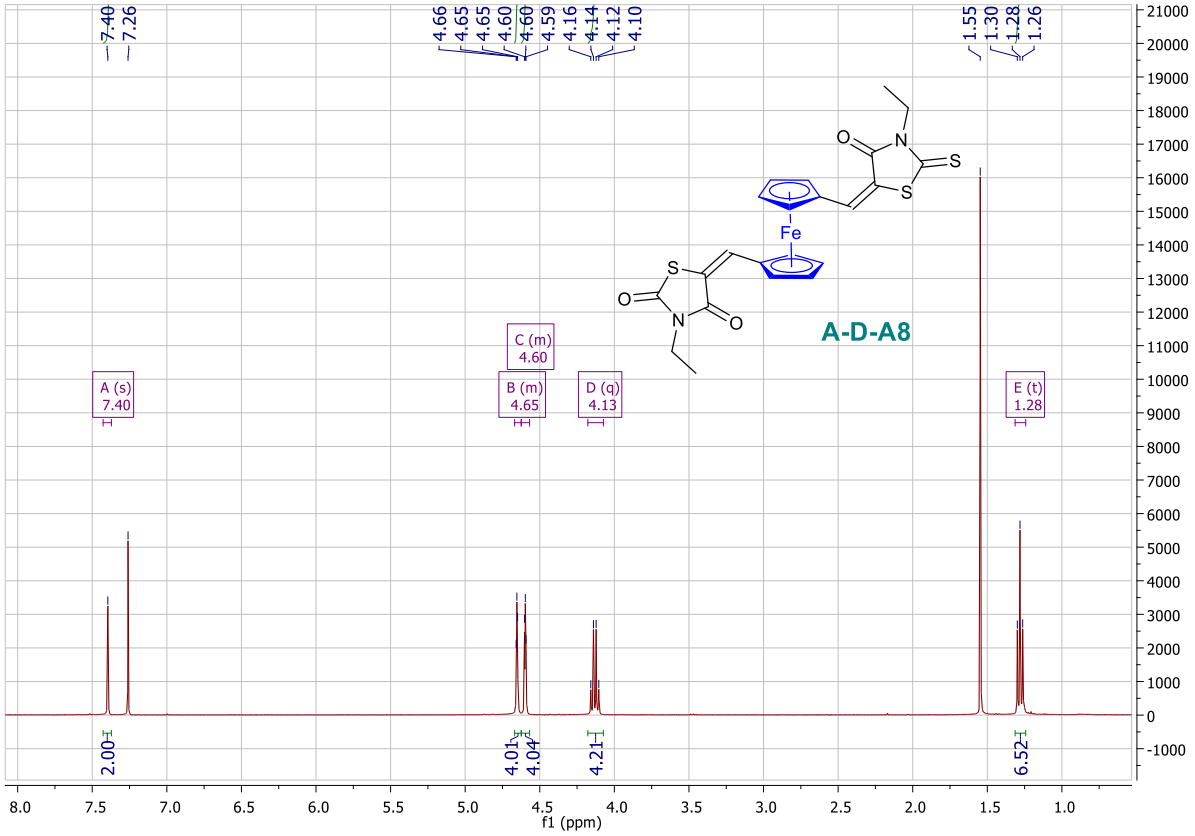
^{1}H NMR spectrum of **A-D-A7**

NOT SUFFICENTLY SOLUBLE

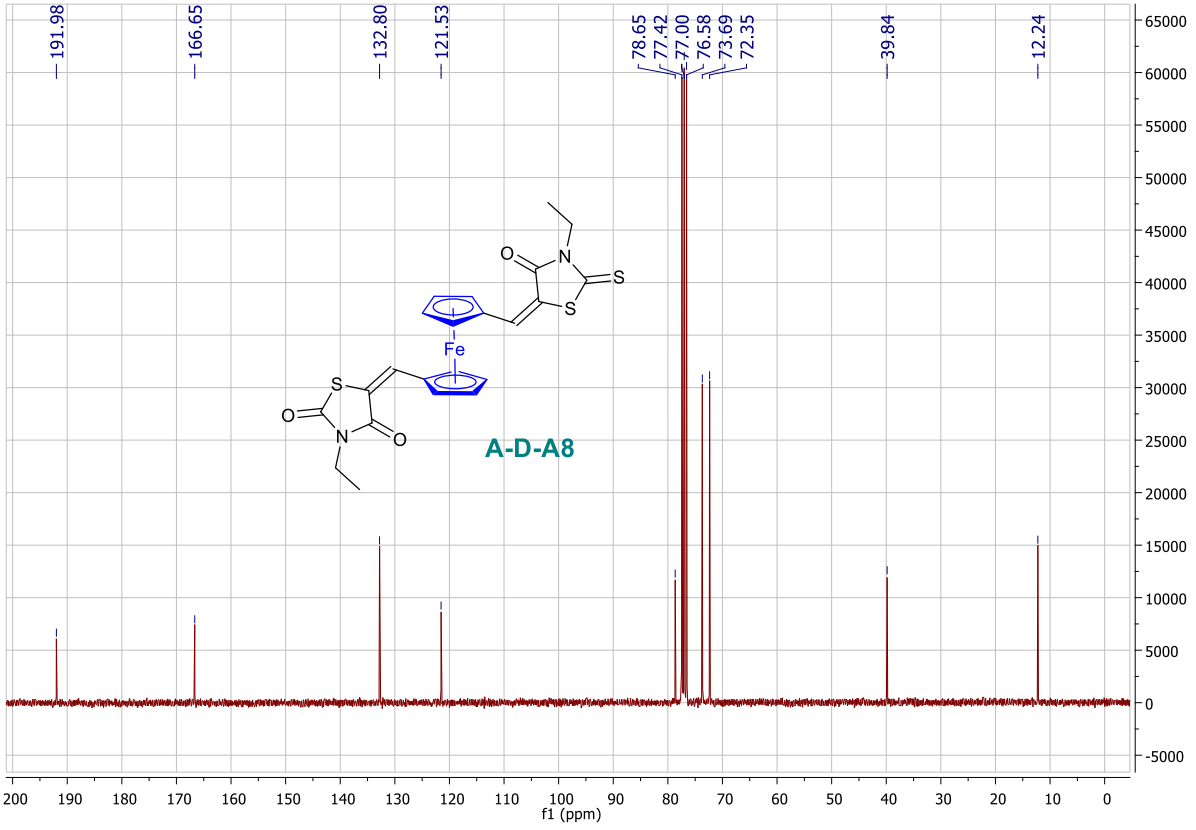
^{13}C NMR spectrum of **A-D-A7**

NOT SUFFICENTLY SOLUBLE

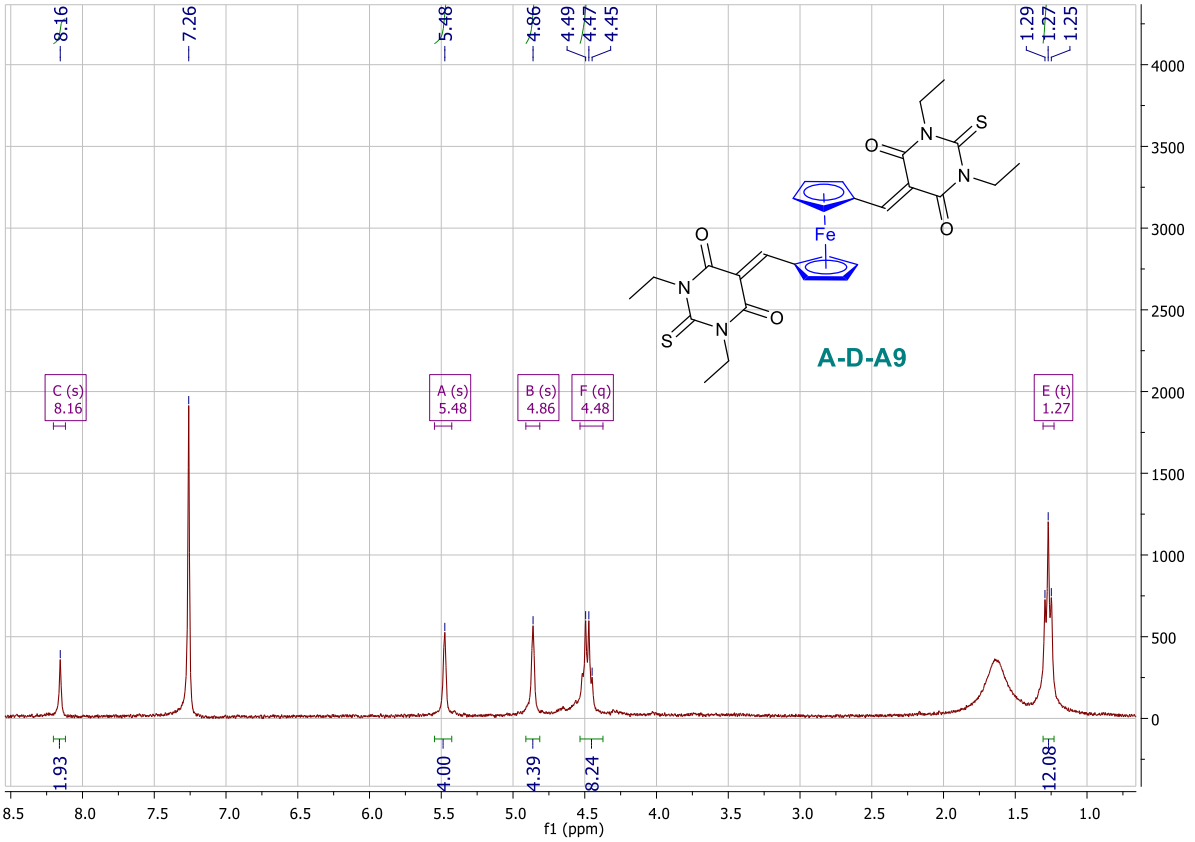
^{1}H NMR spectrum of **A-D-A8**



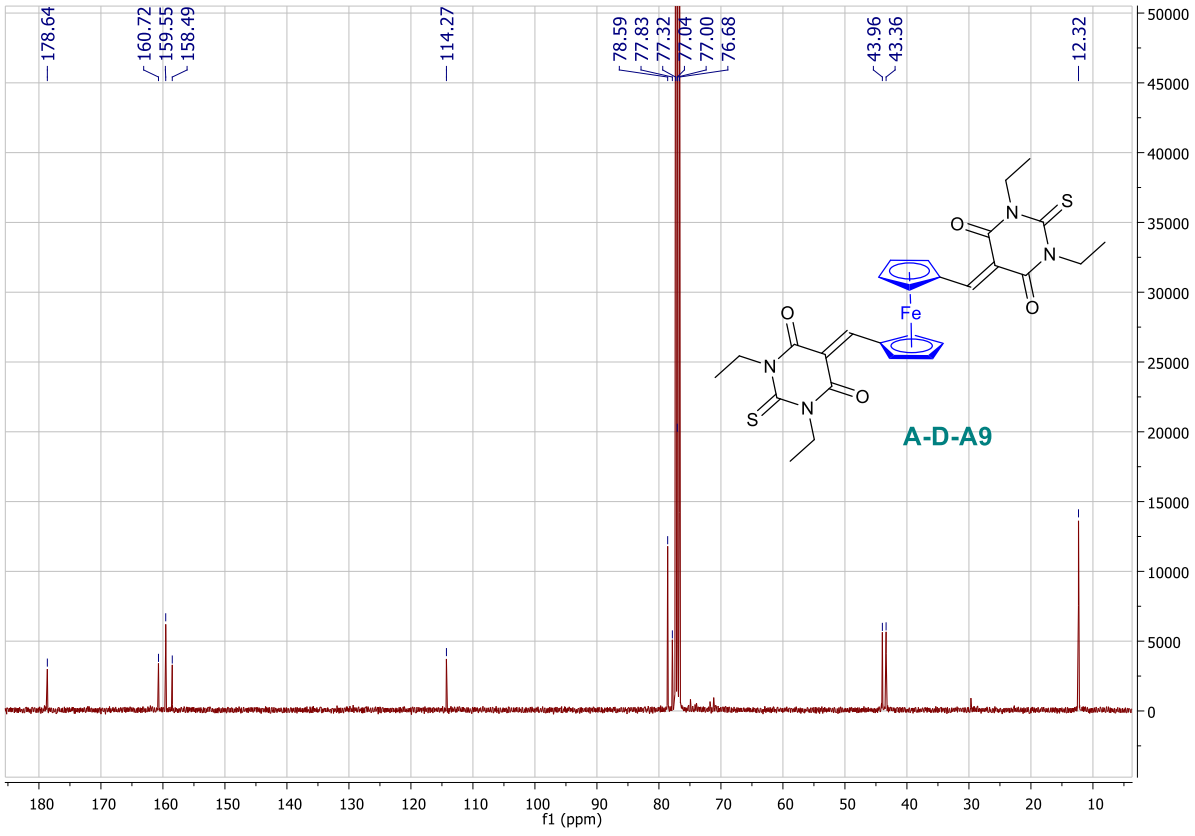
^{13}C NMR spectrum of **A-D-A8**



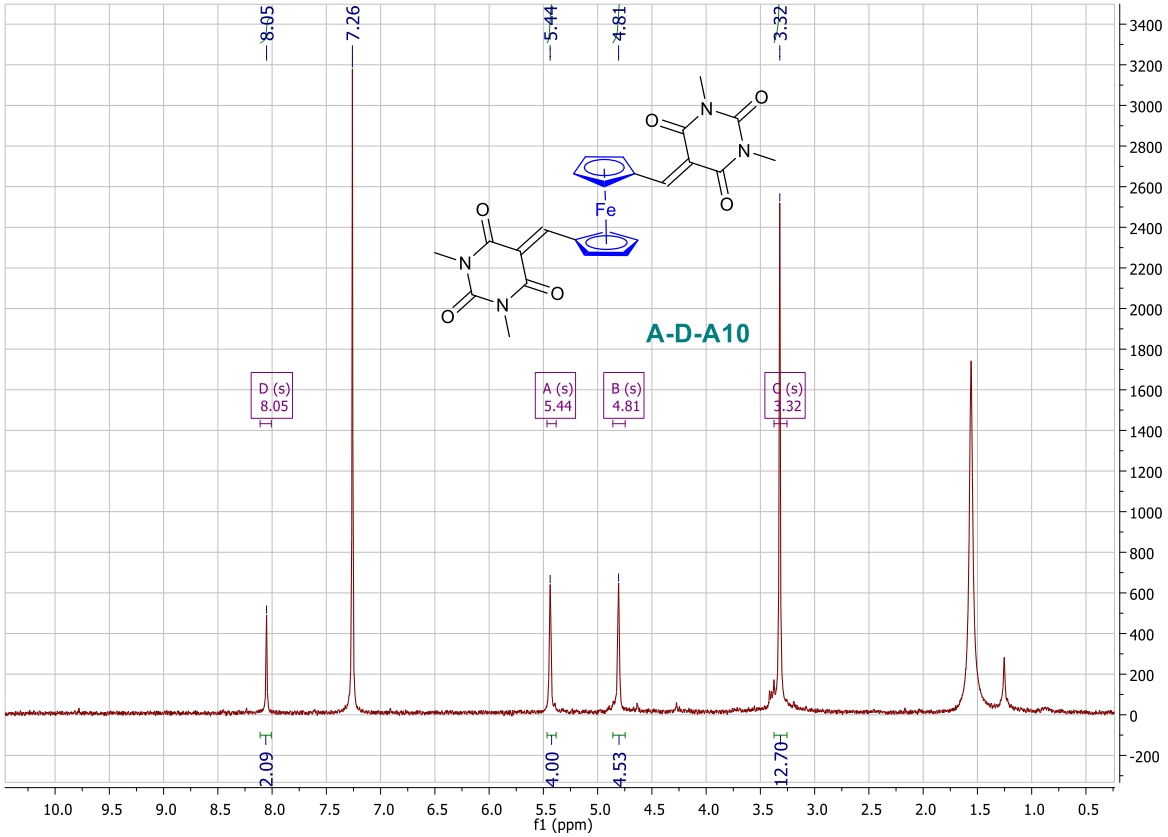
^{1}H NMR spectrum of **A-D-A9**



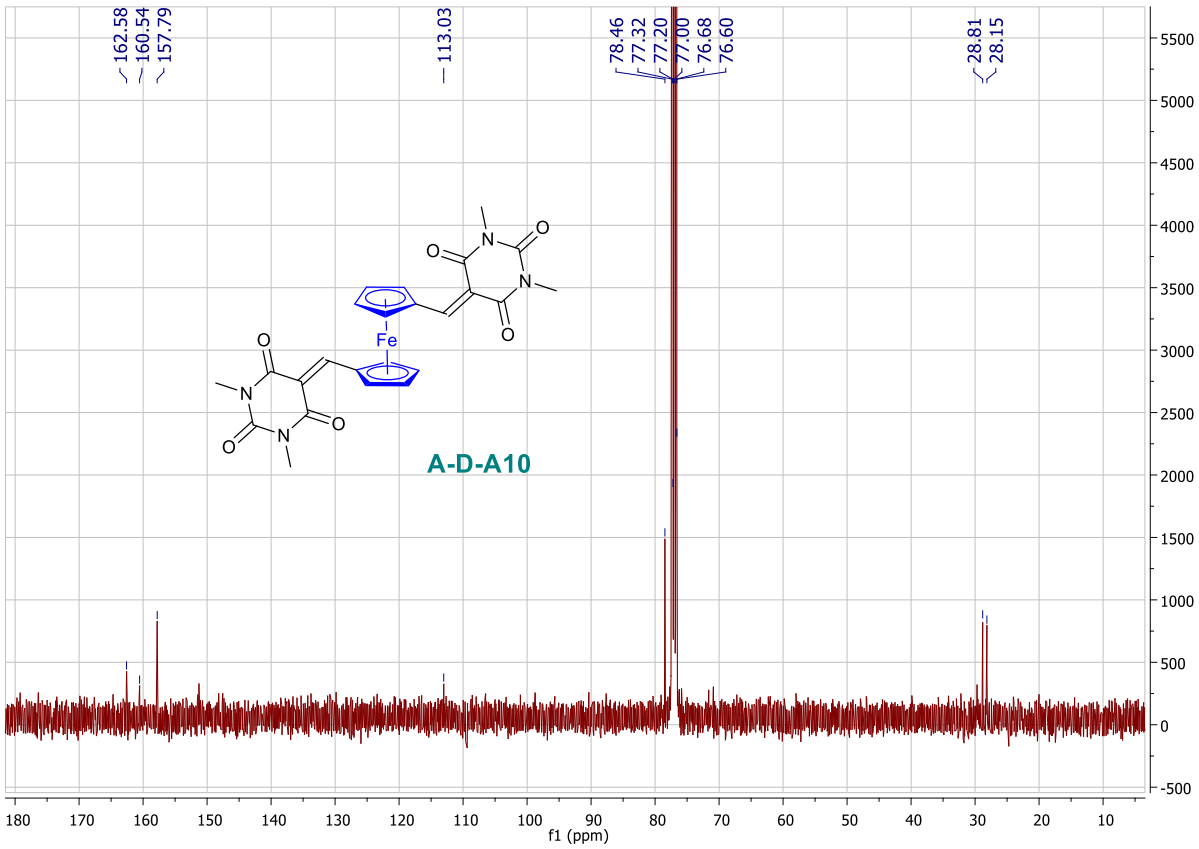
^{13}C NMR spectrum of **A-D-A9**



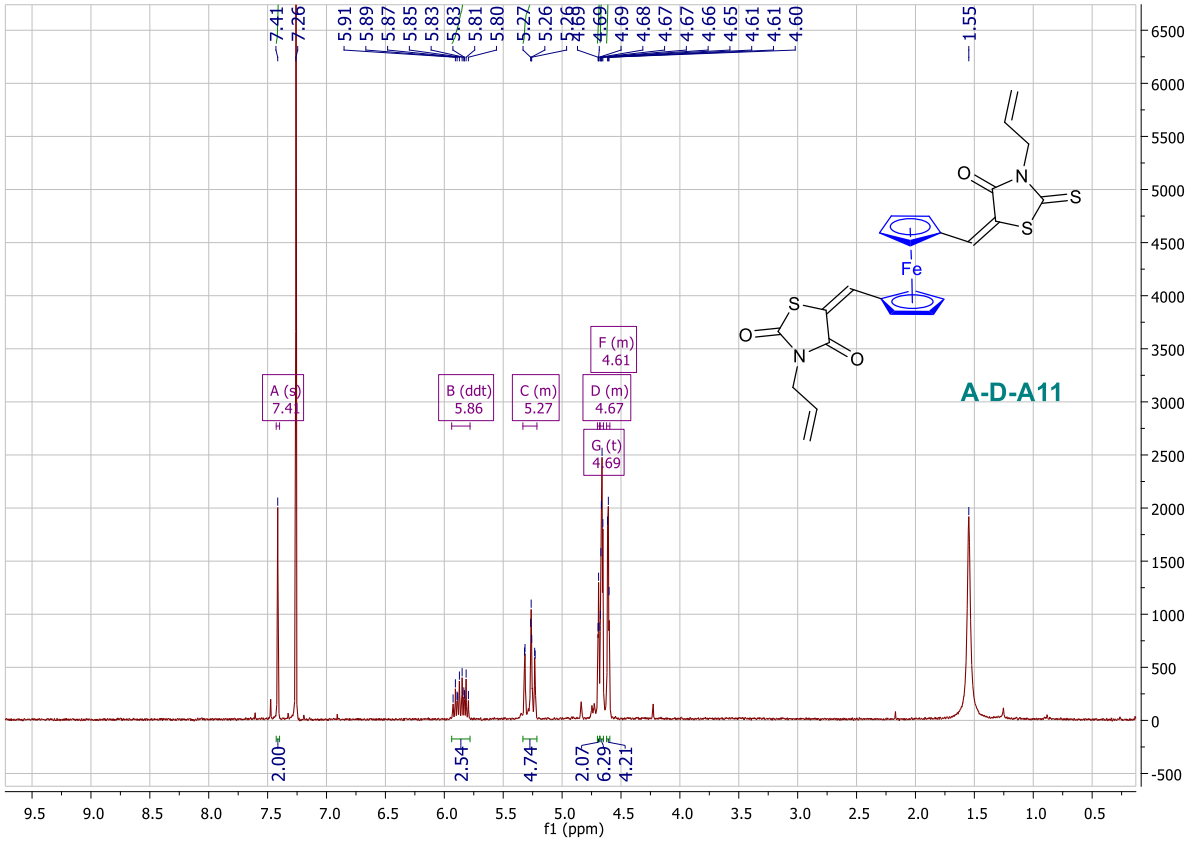
[1]H NMR spectrum of **A-D-A10**



[13]C NMR spectrum of **A-D-A10**



[1]H NMR spectrum of **A-D-A11**



[13]C NMR spectrum of **A-D-A11**