

# Optical study of solvatochromic isocyanoaminoanthracene dyes and 1,5-diaminoanthracene

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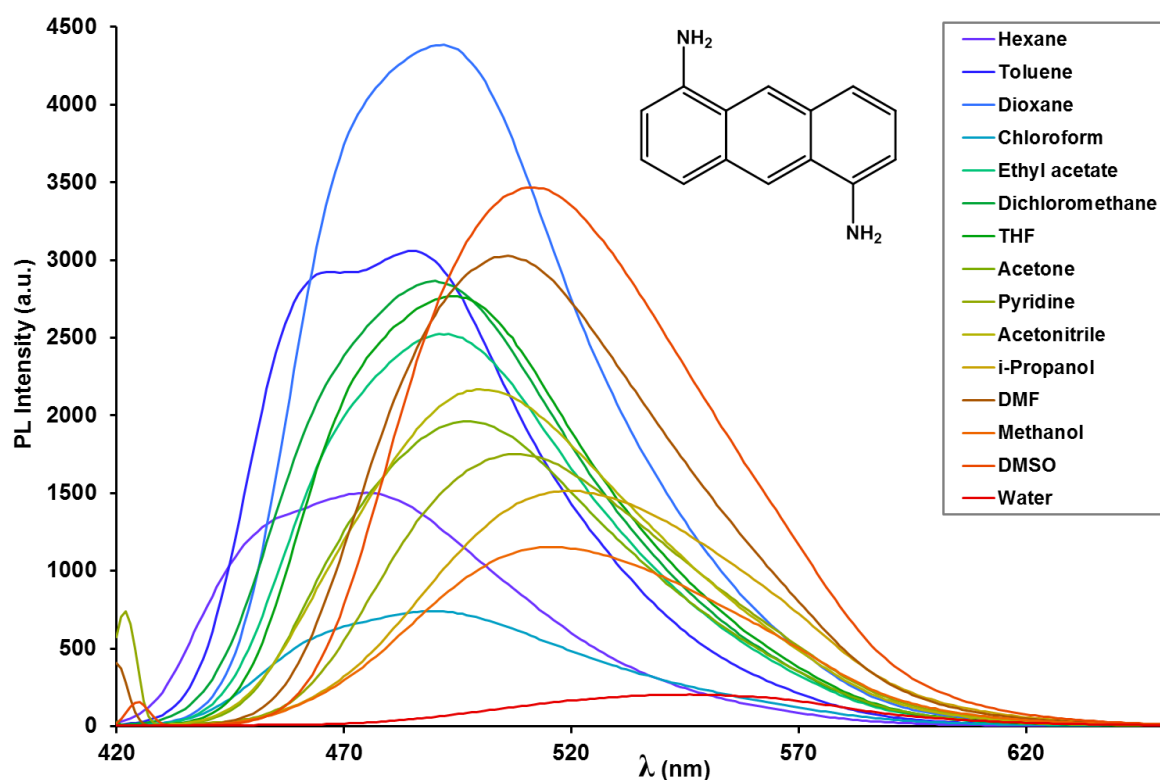
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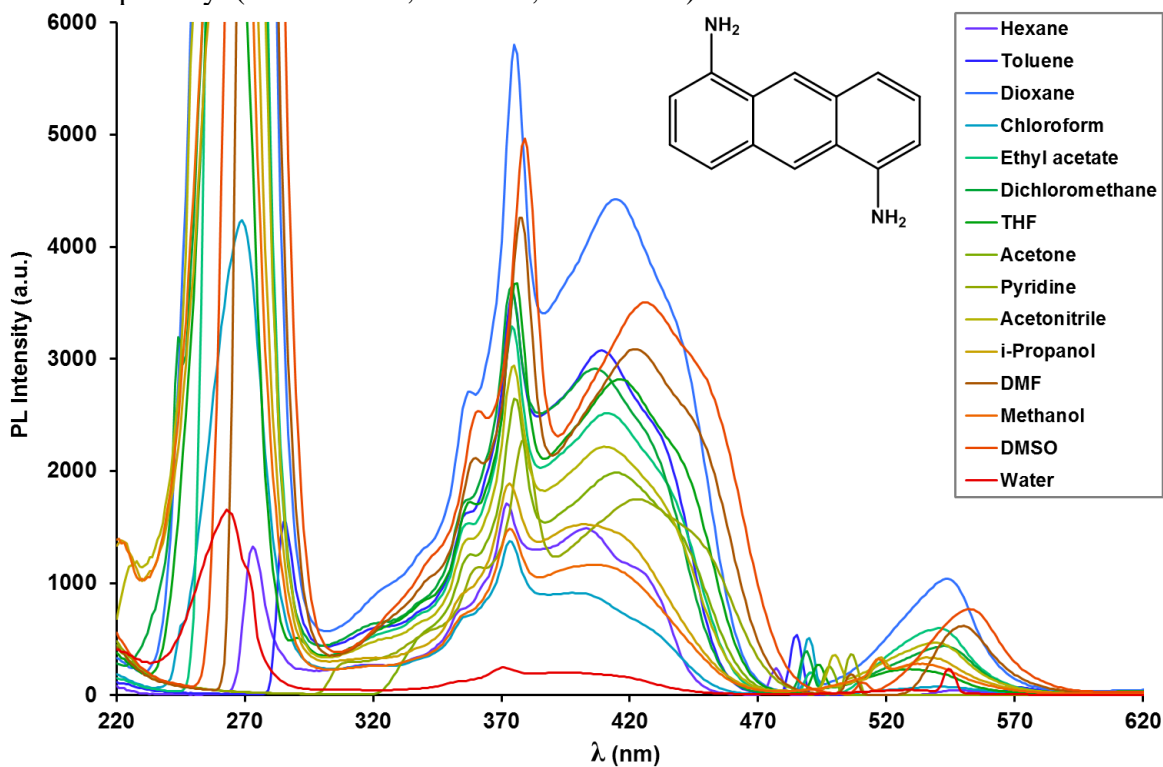
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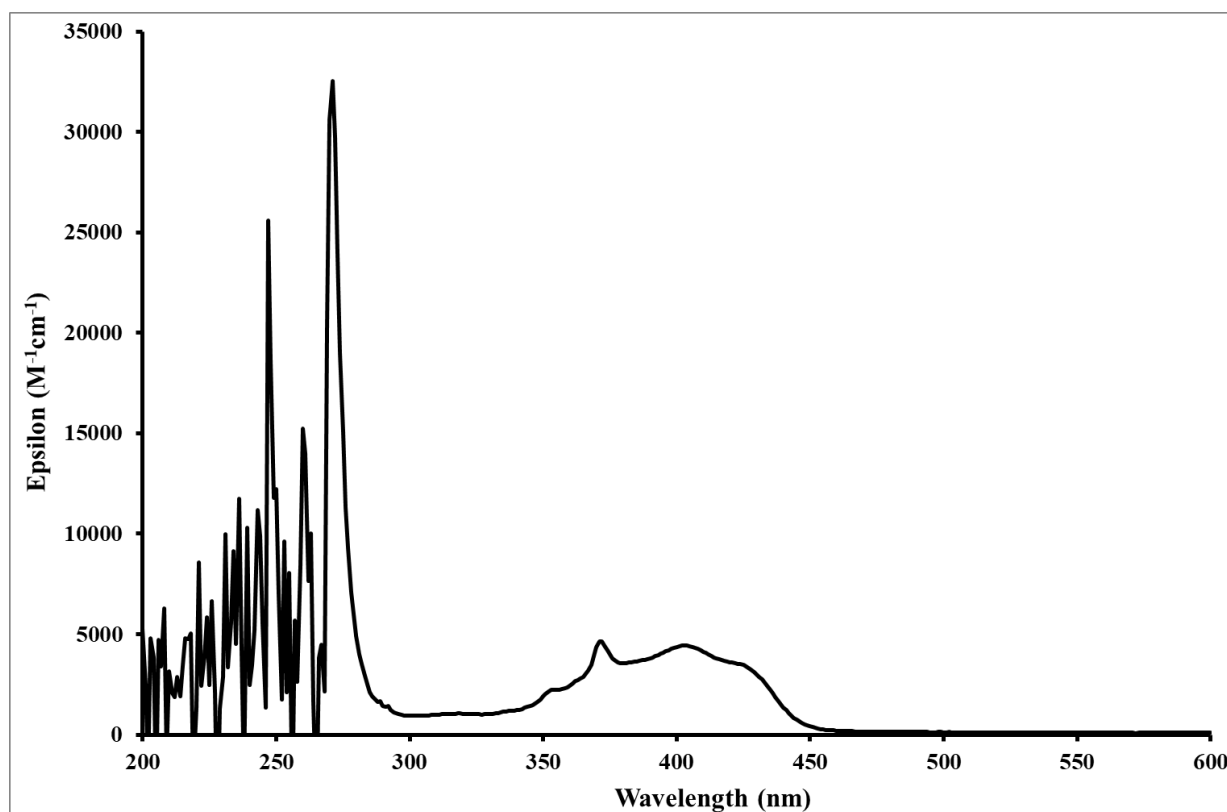
## Chapter 1. 1,5-diaminoanthracene (DAA)



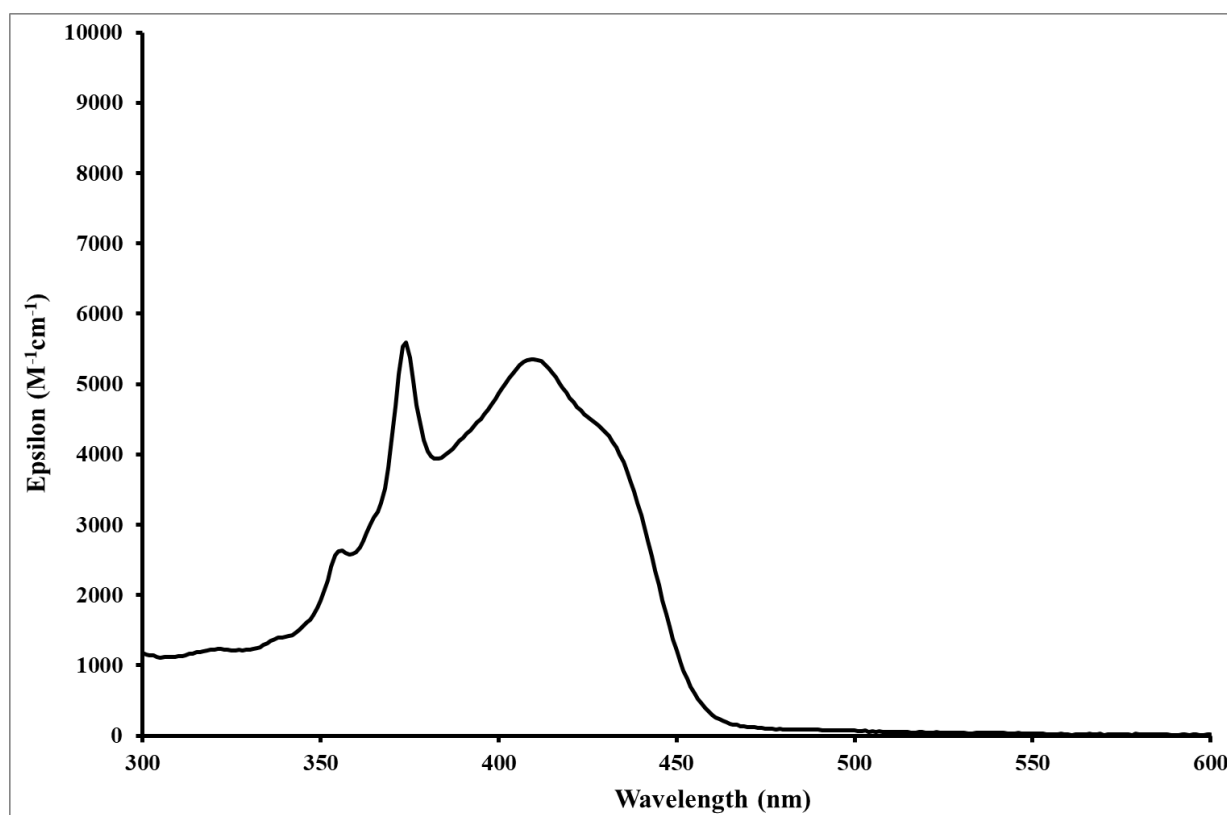
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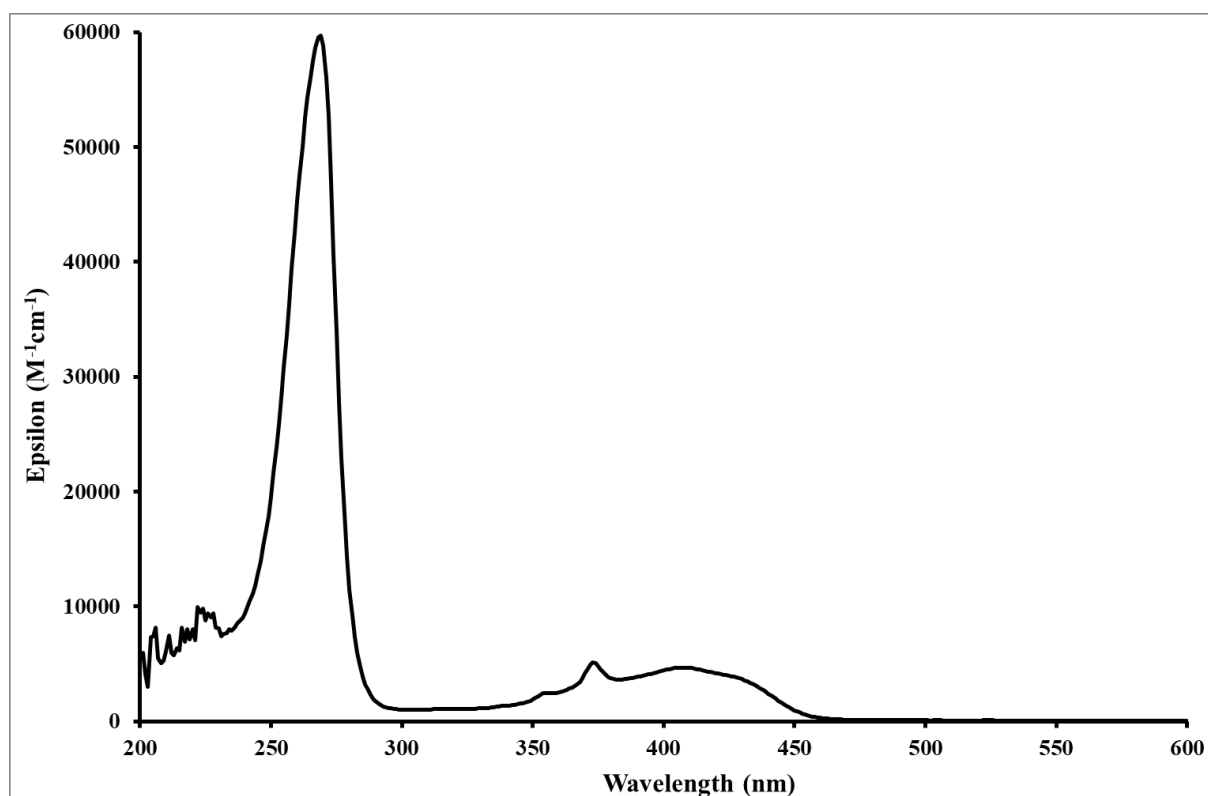
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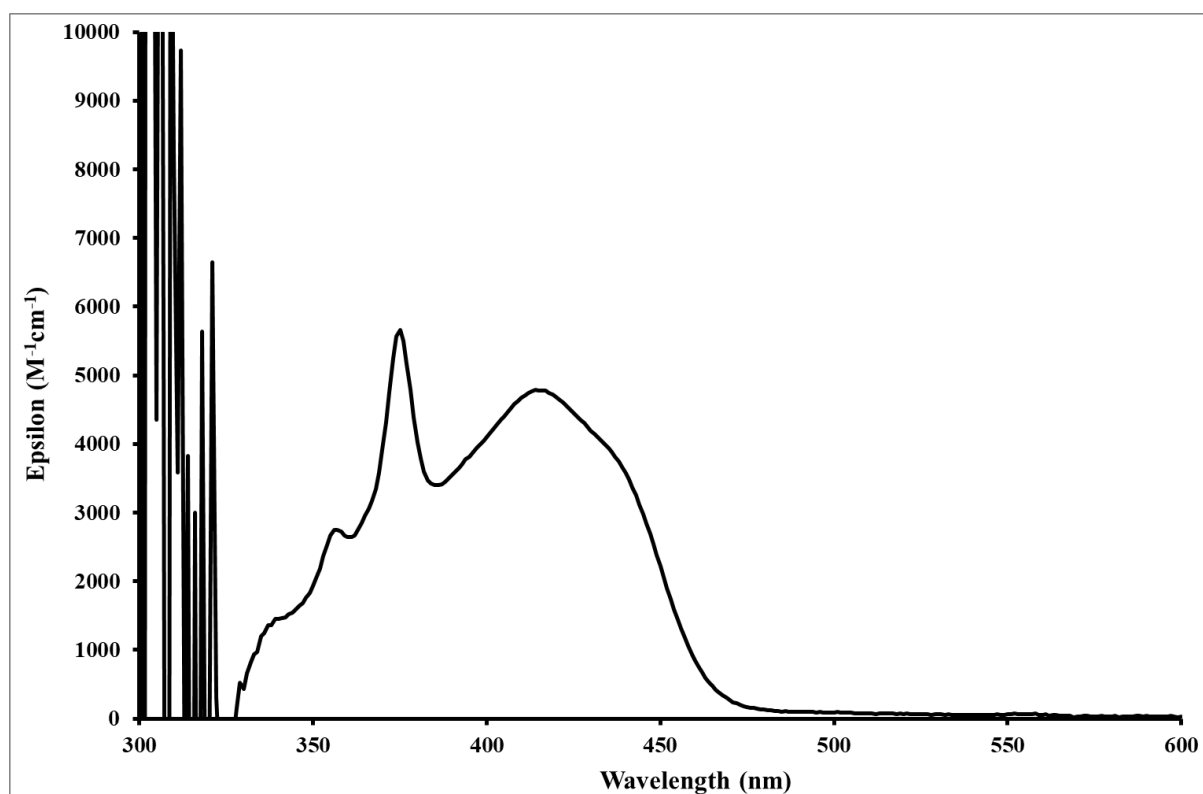
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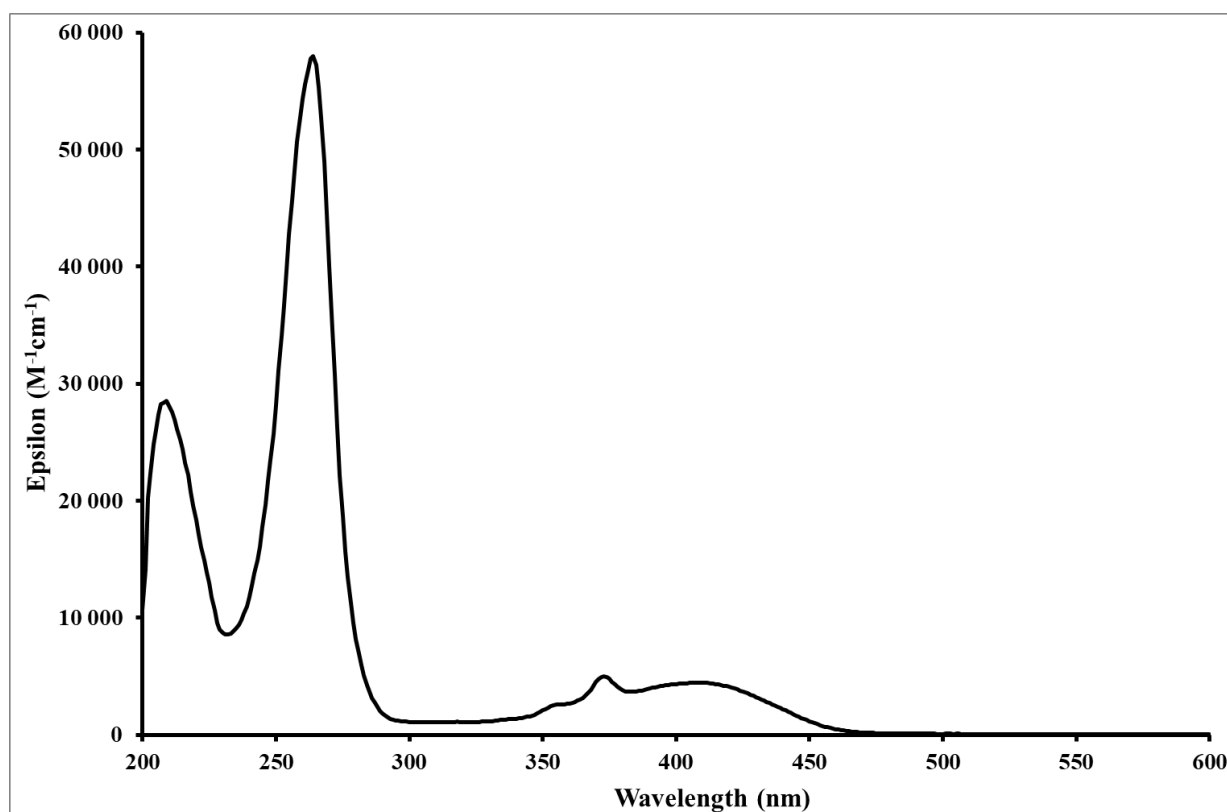
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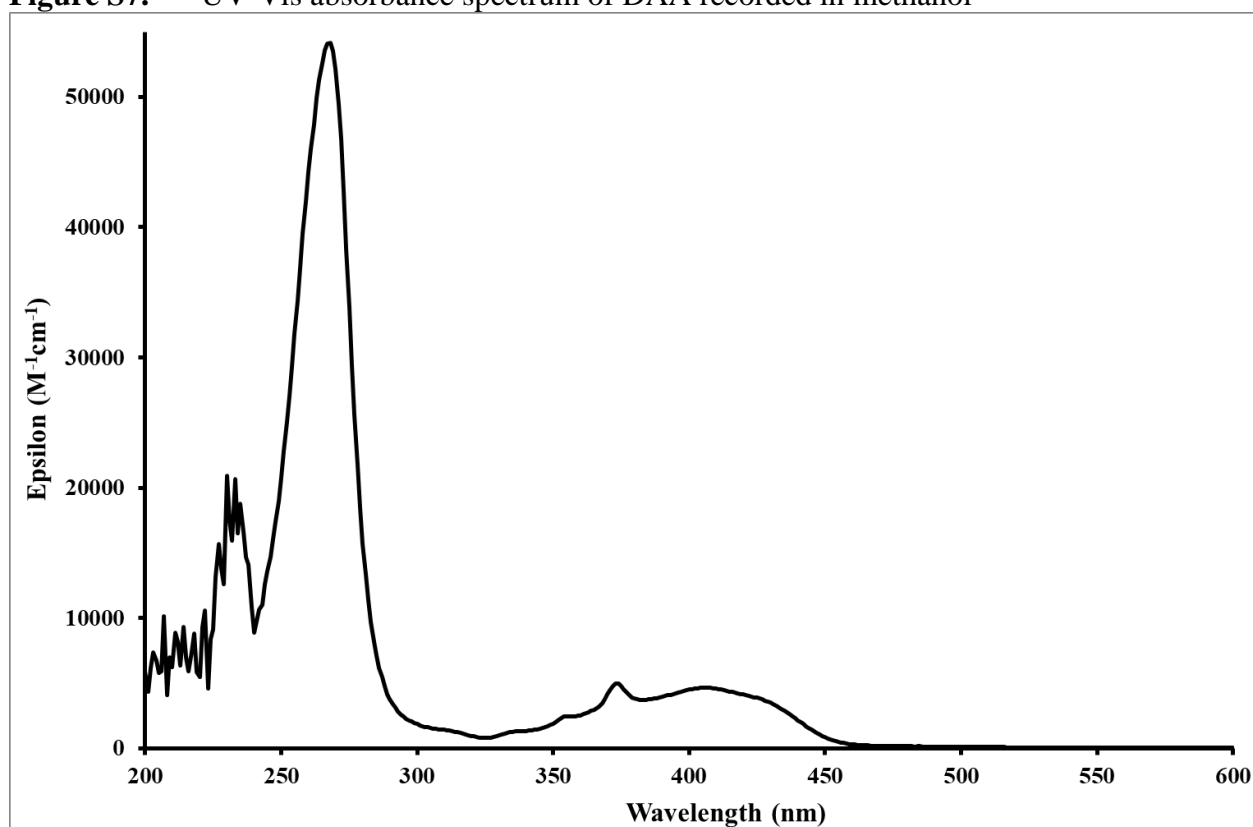
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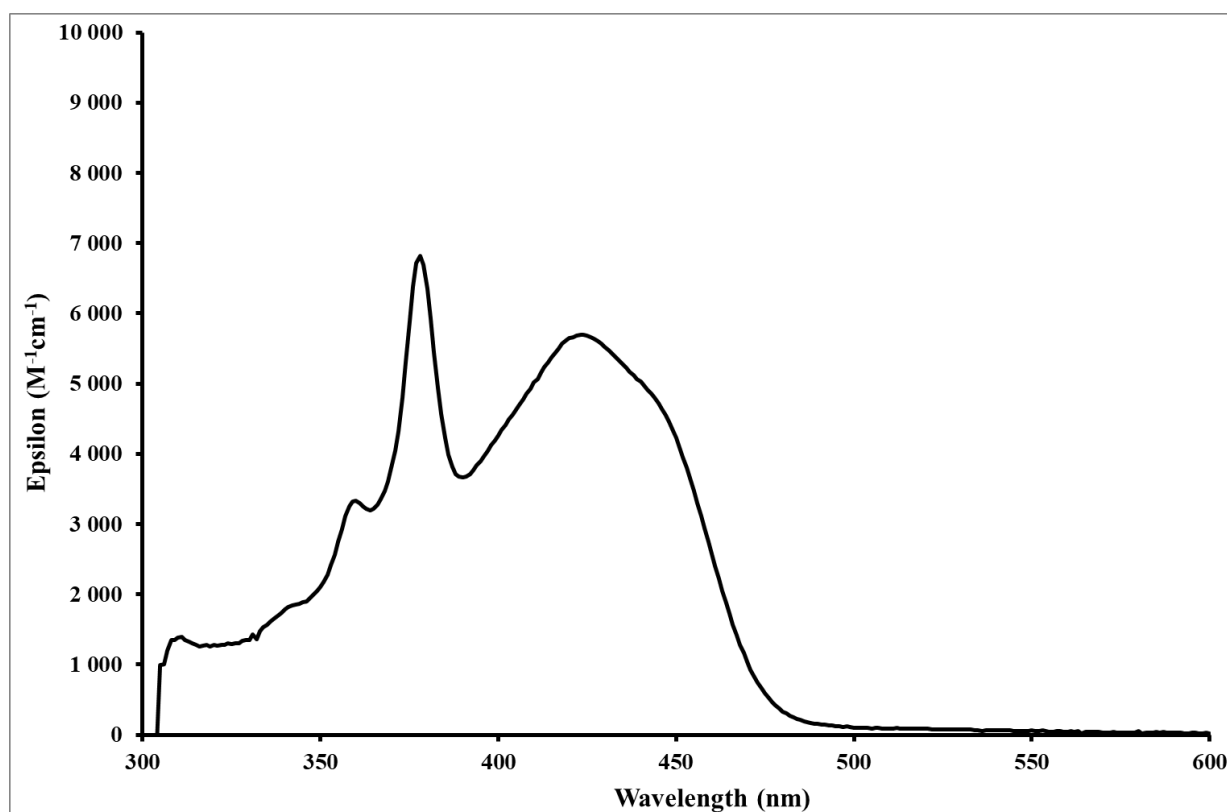


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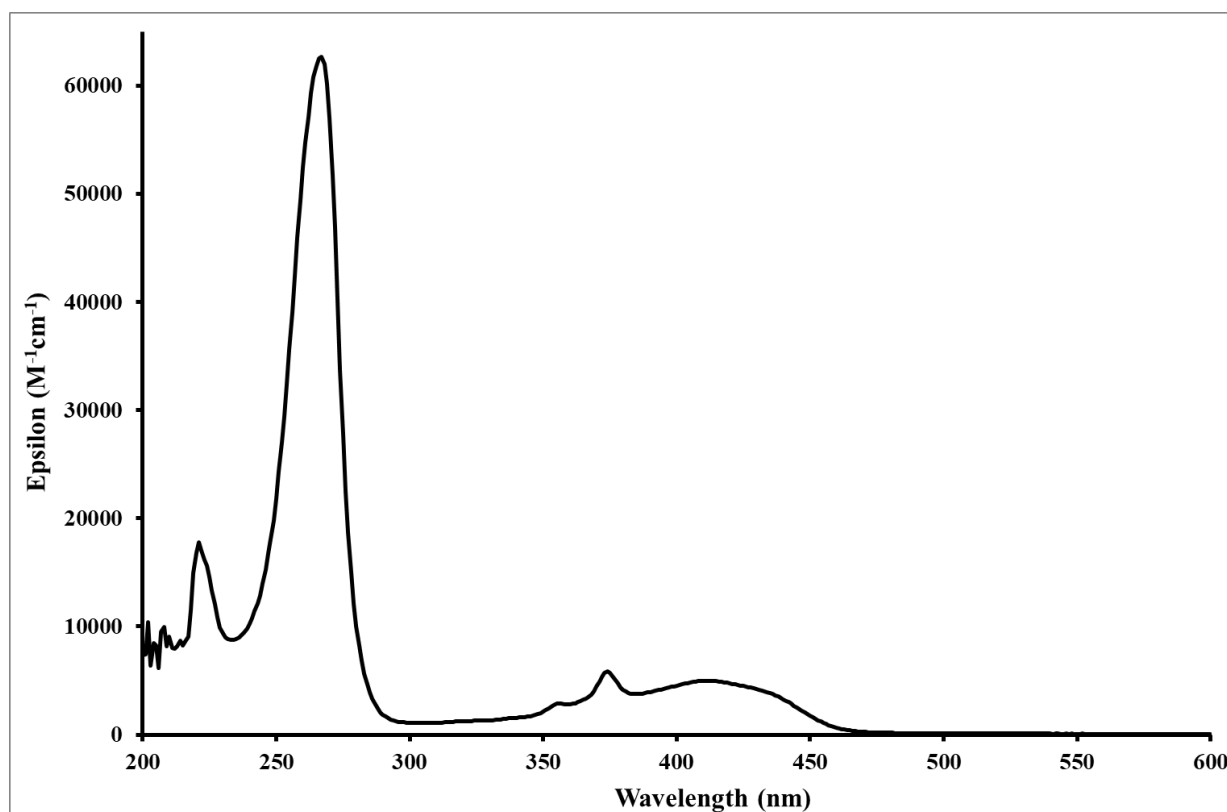


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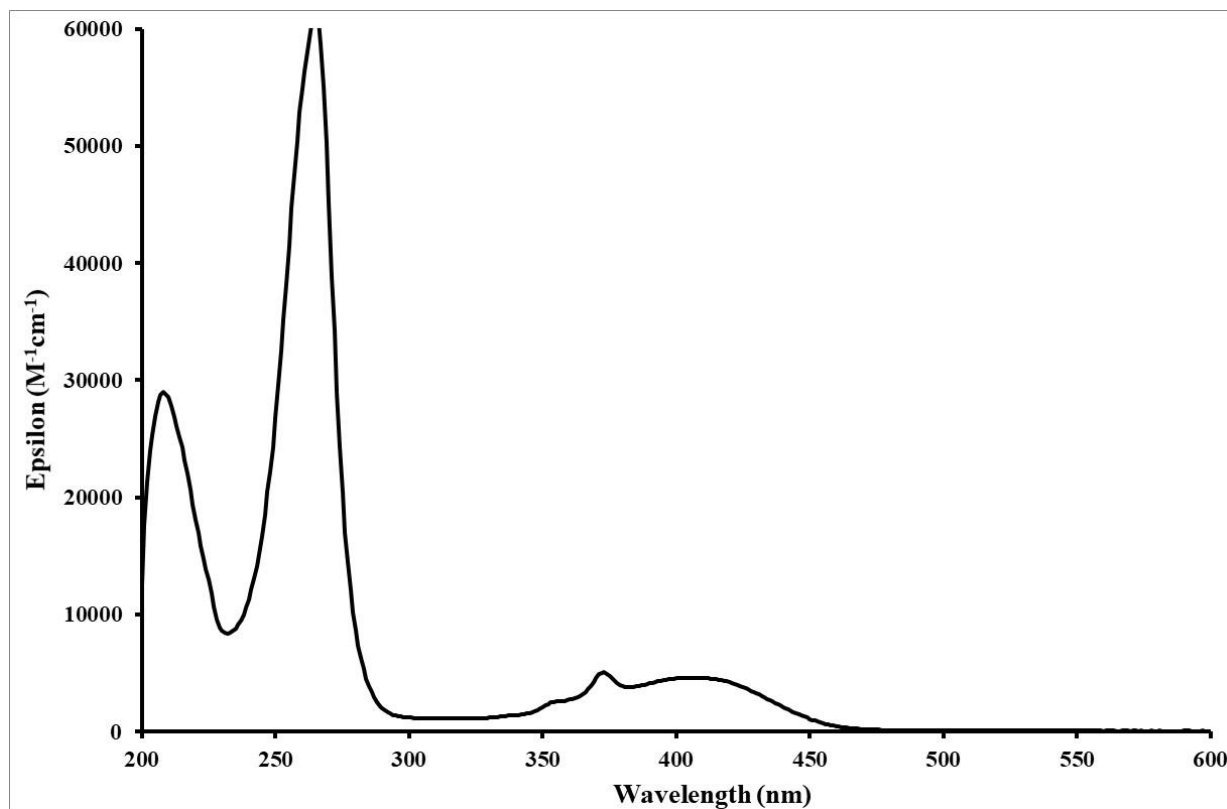




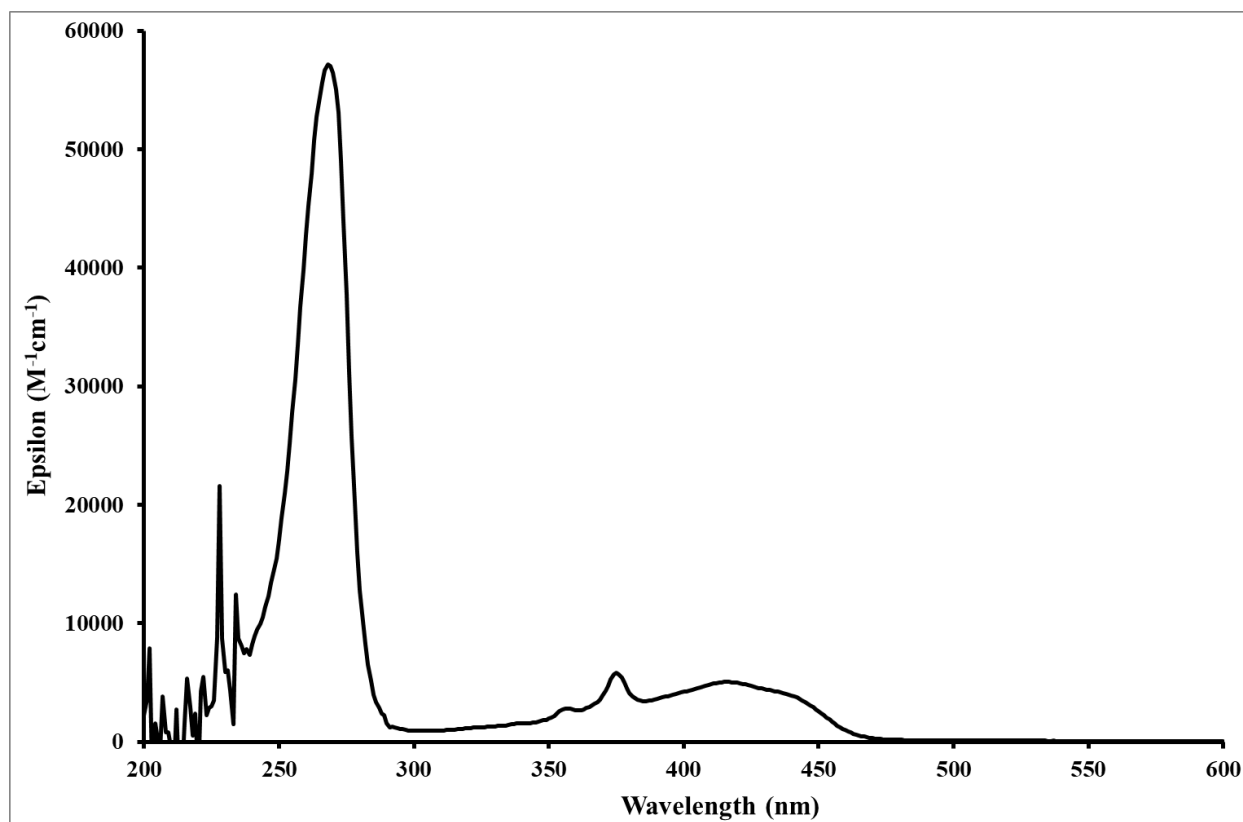
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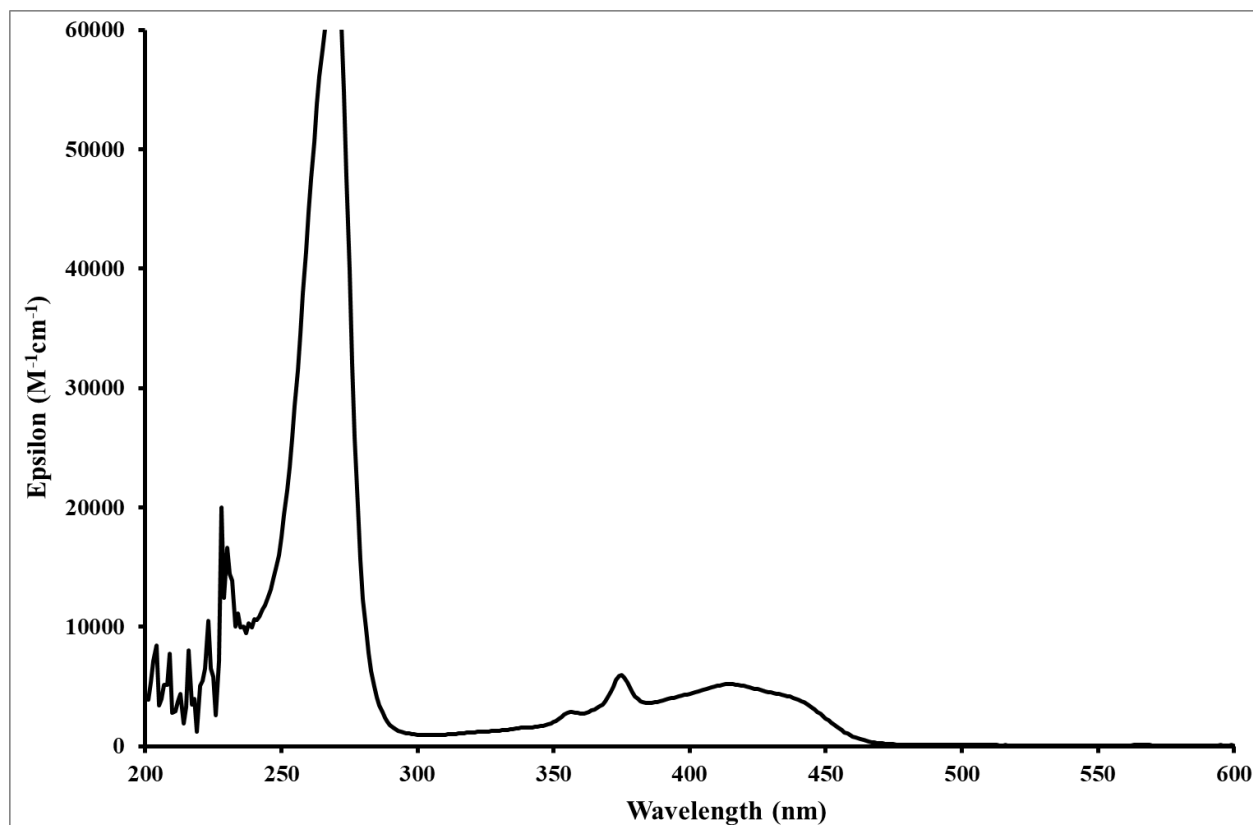
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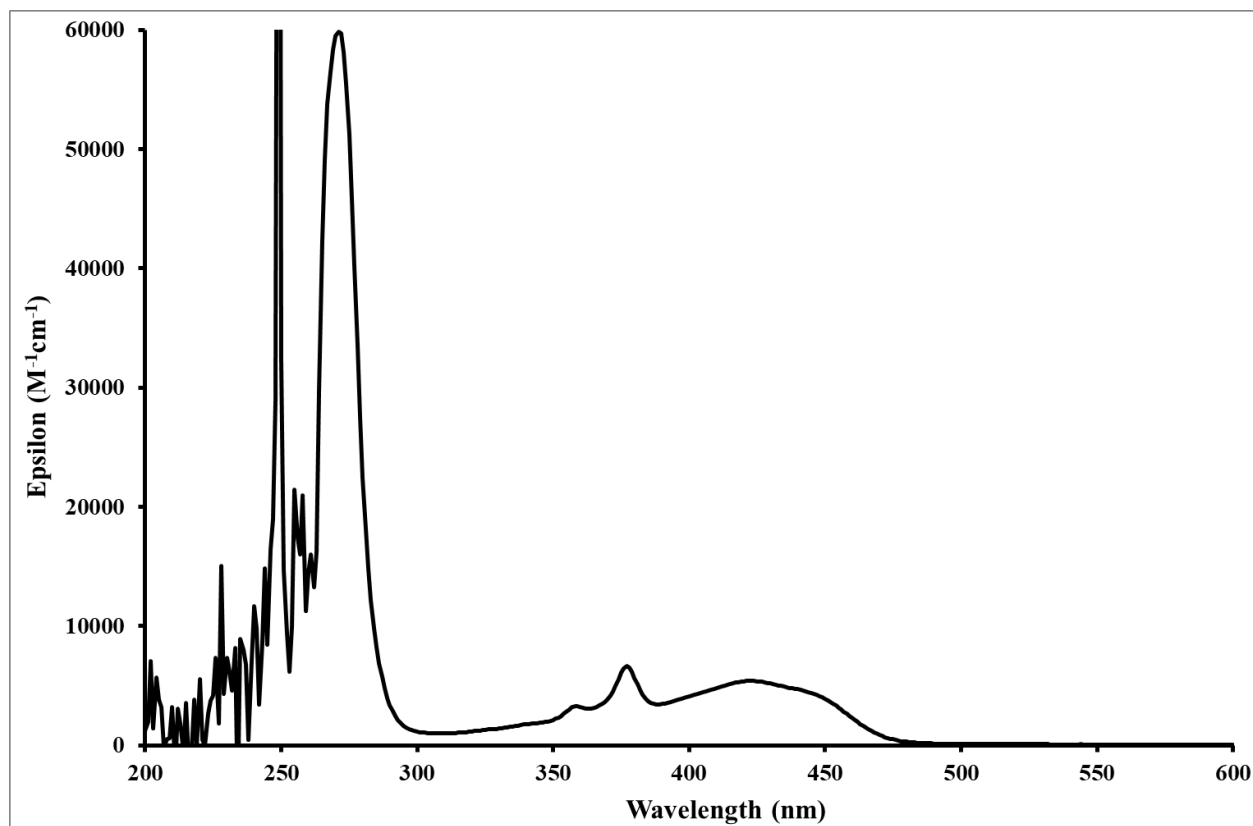
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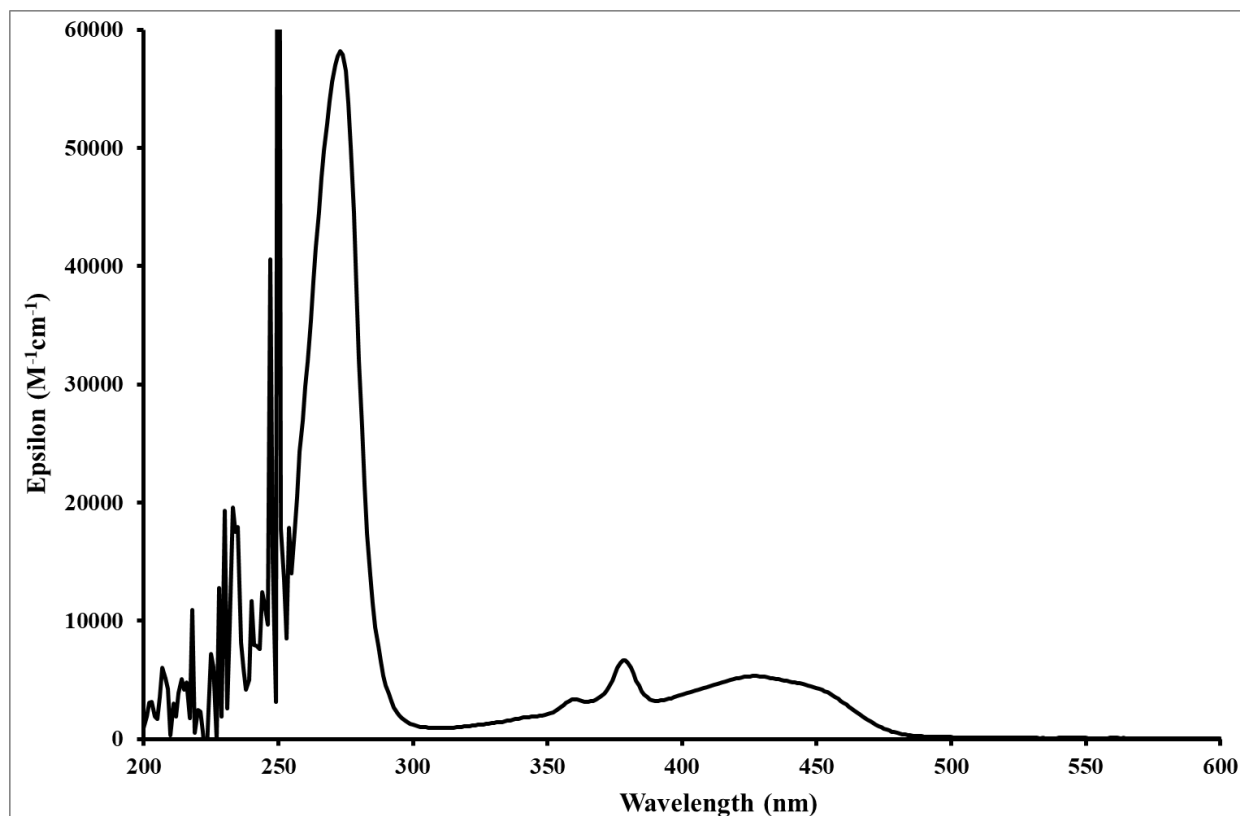
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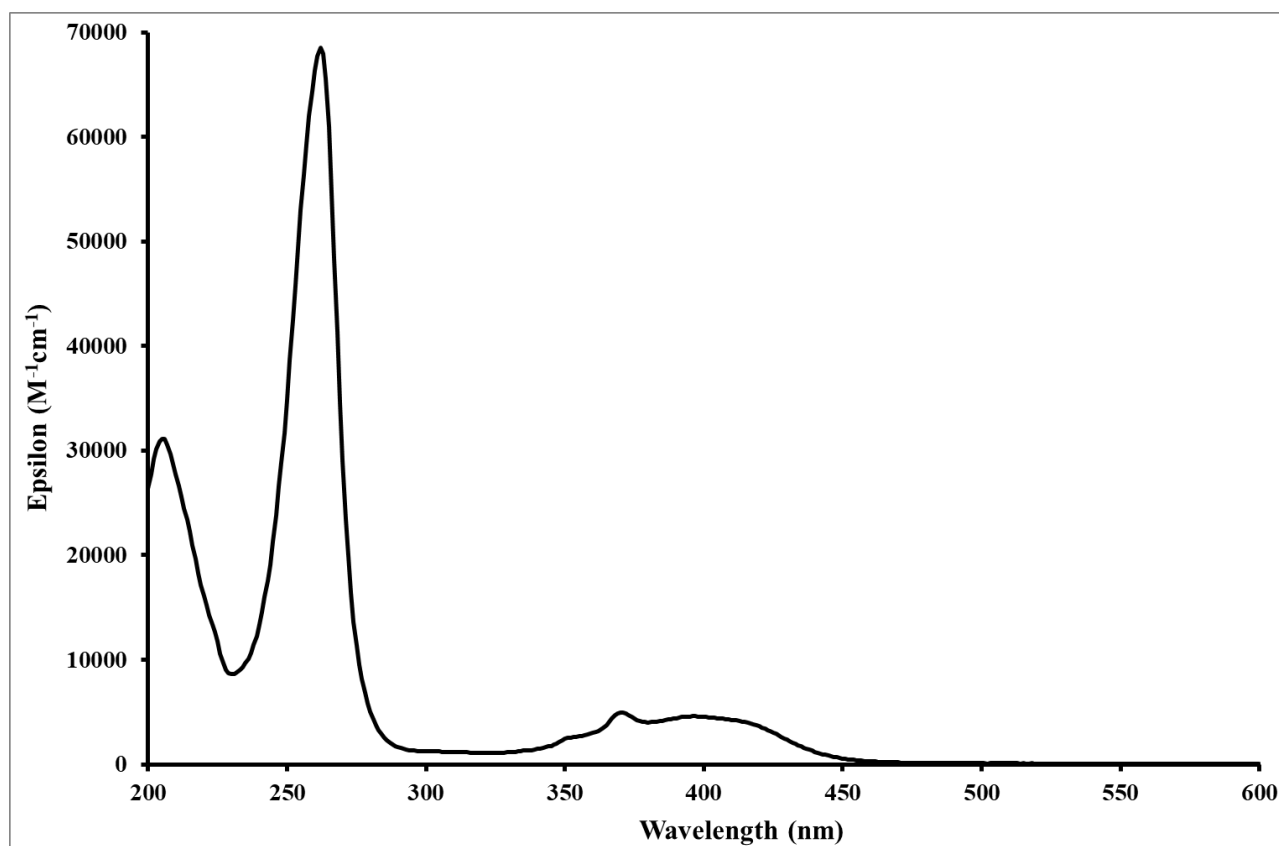
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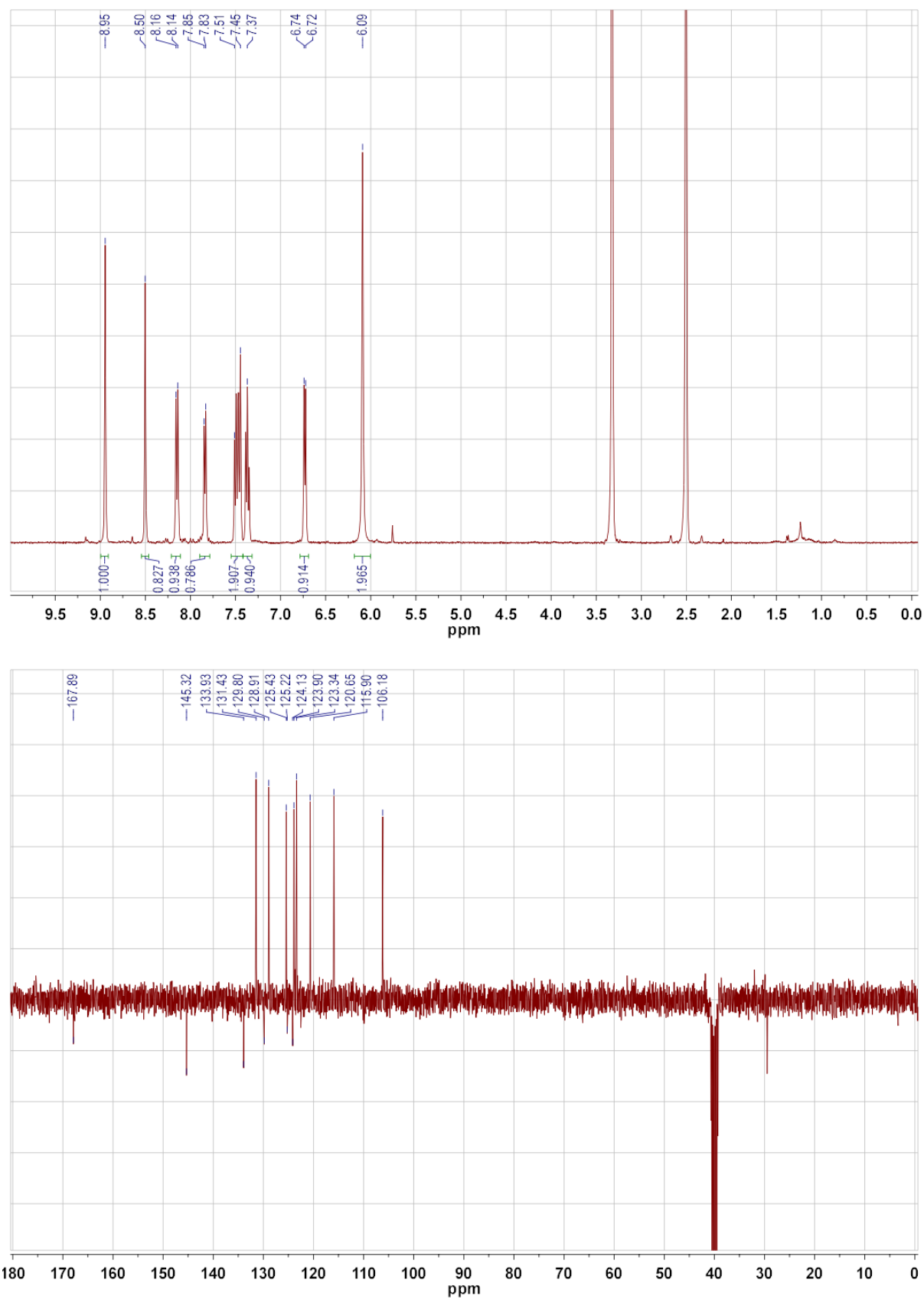


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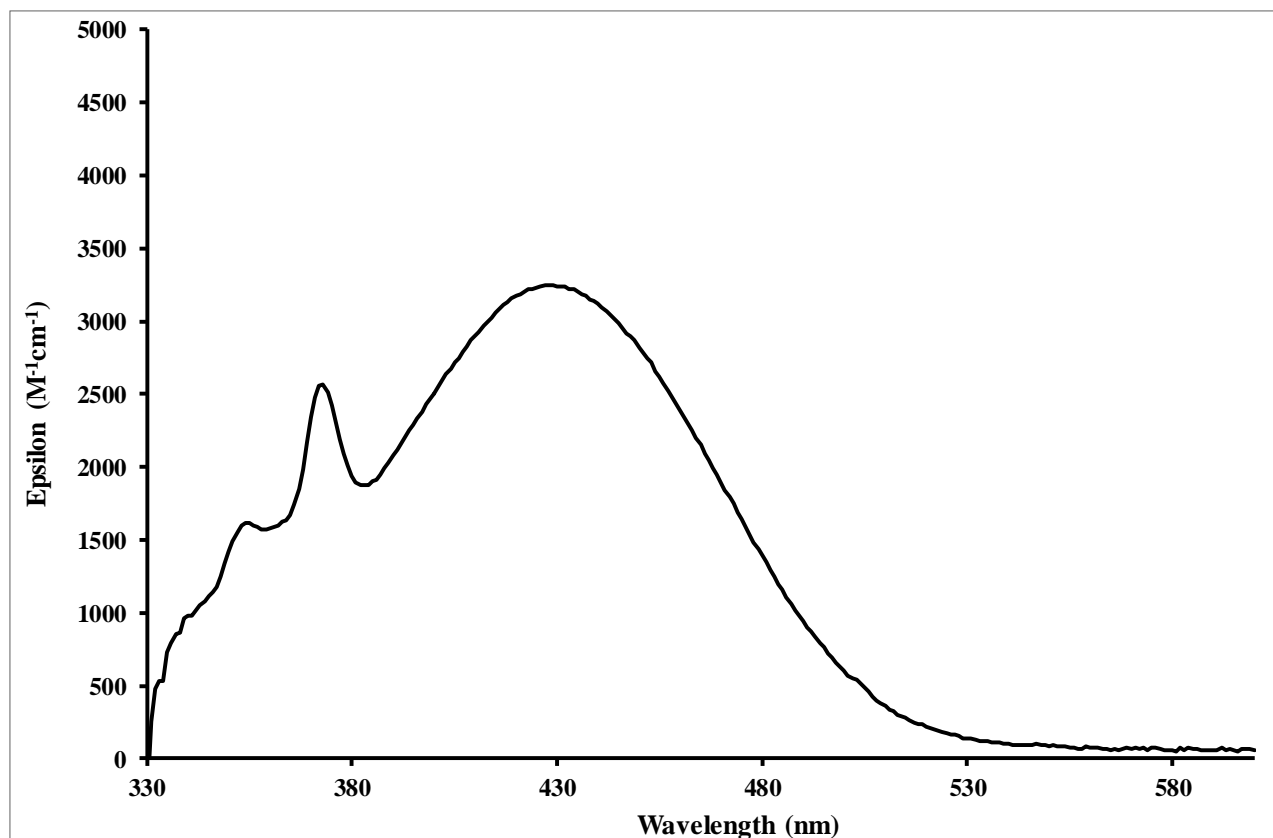


**Figure S16.** UV-Vis absorbance spectrum of DAA recorded in water

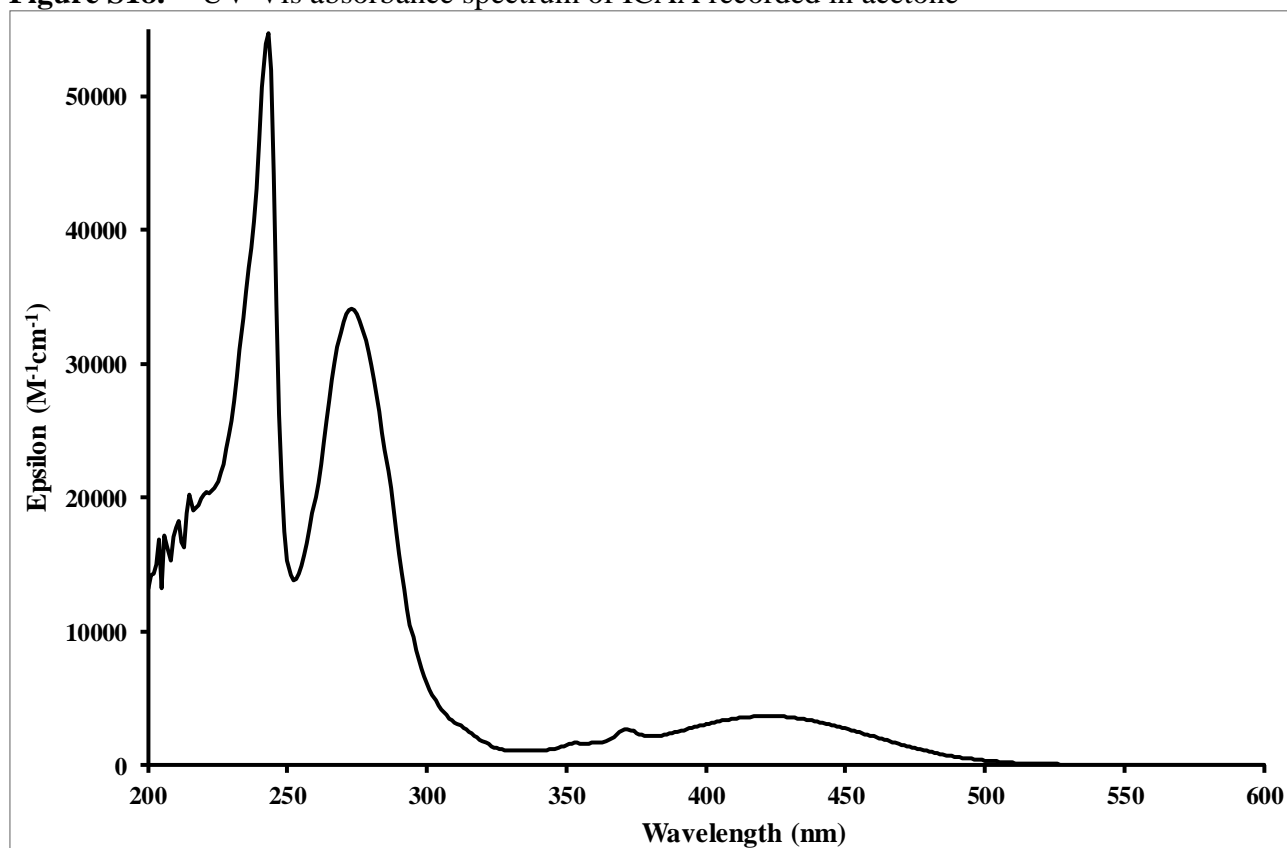
## Chapter 2. 1-amino-5-isocyanoanthracene (ICAA)



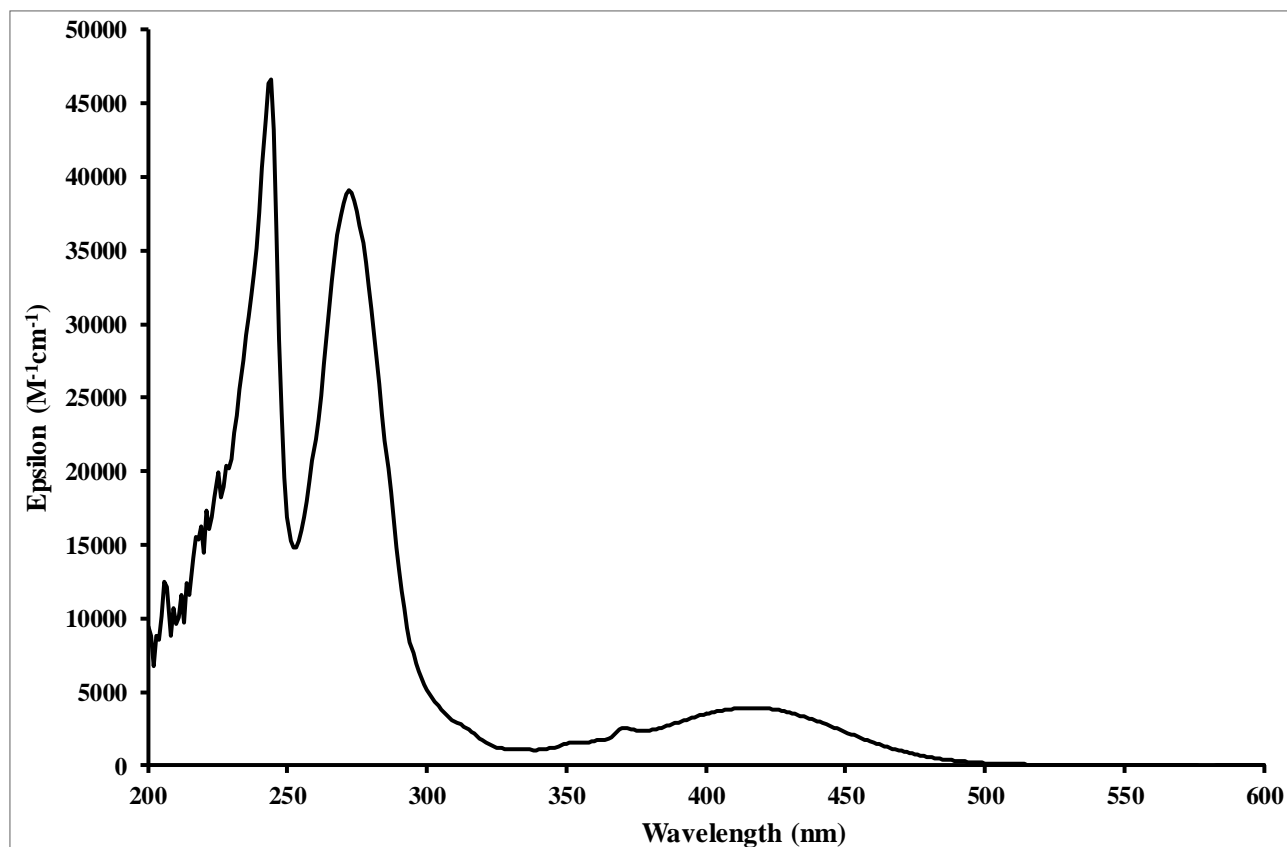
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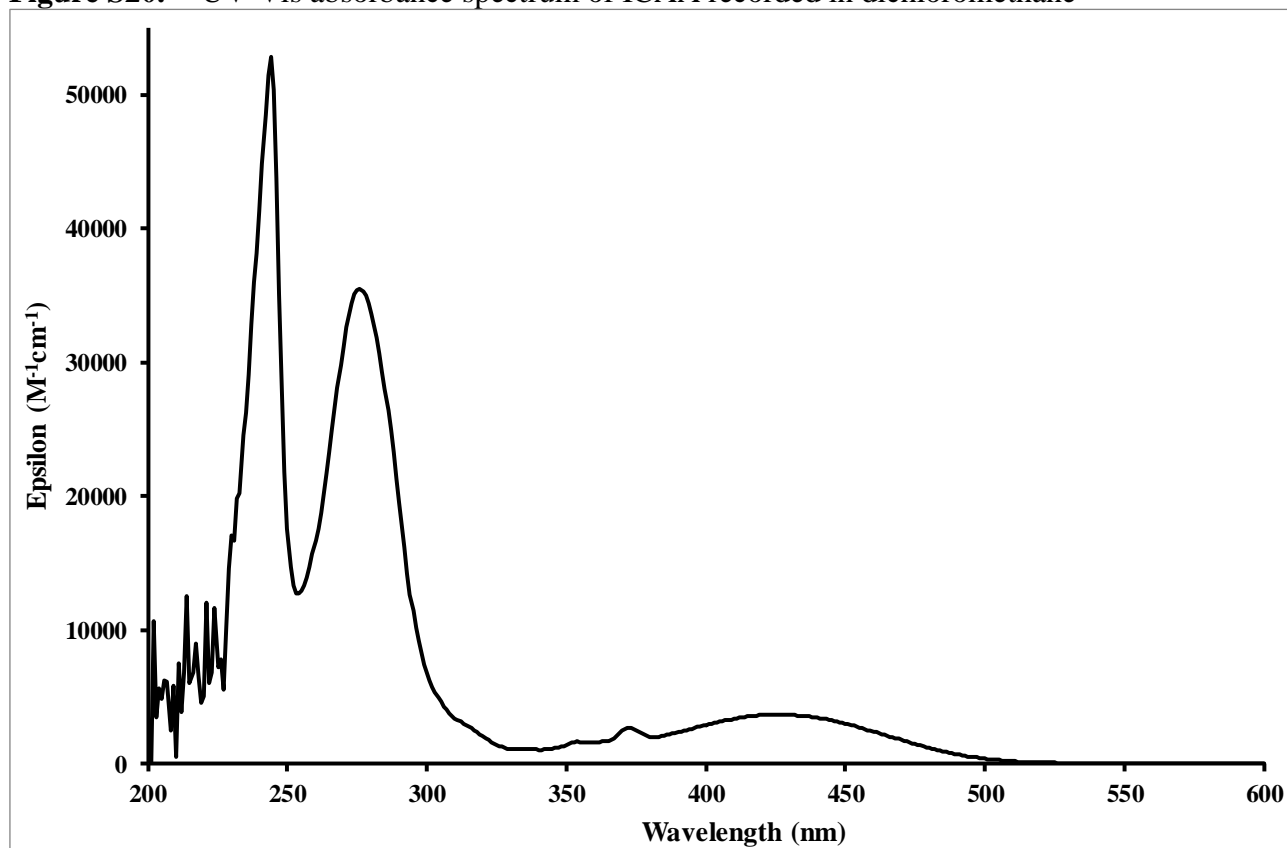
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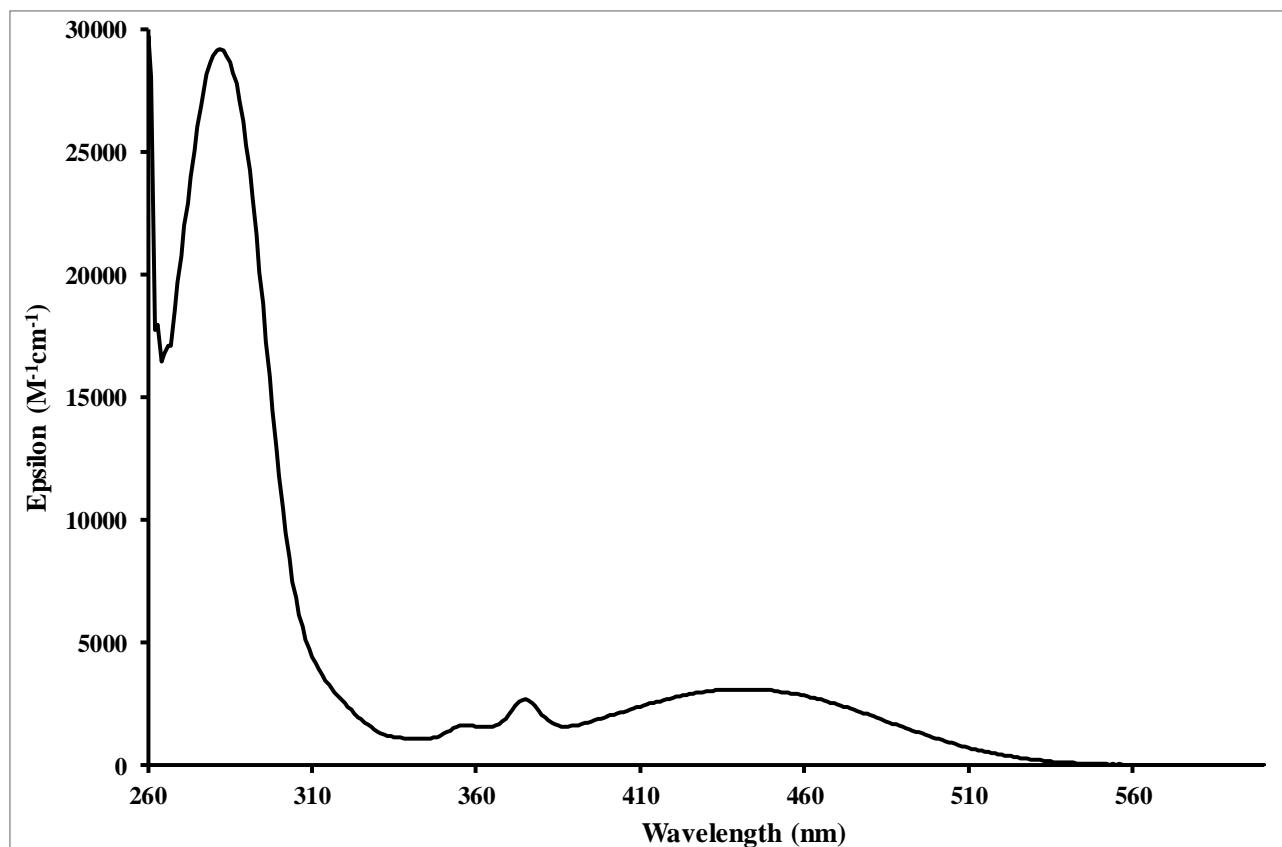
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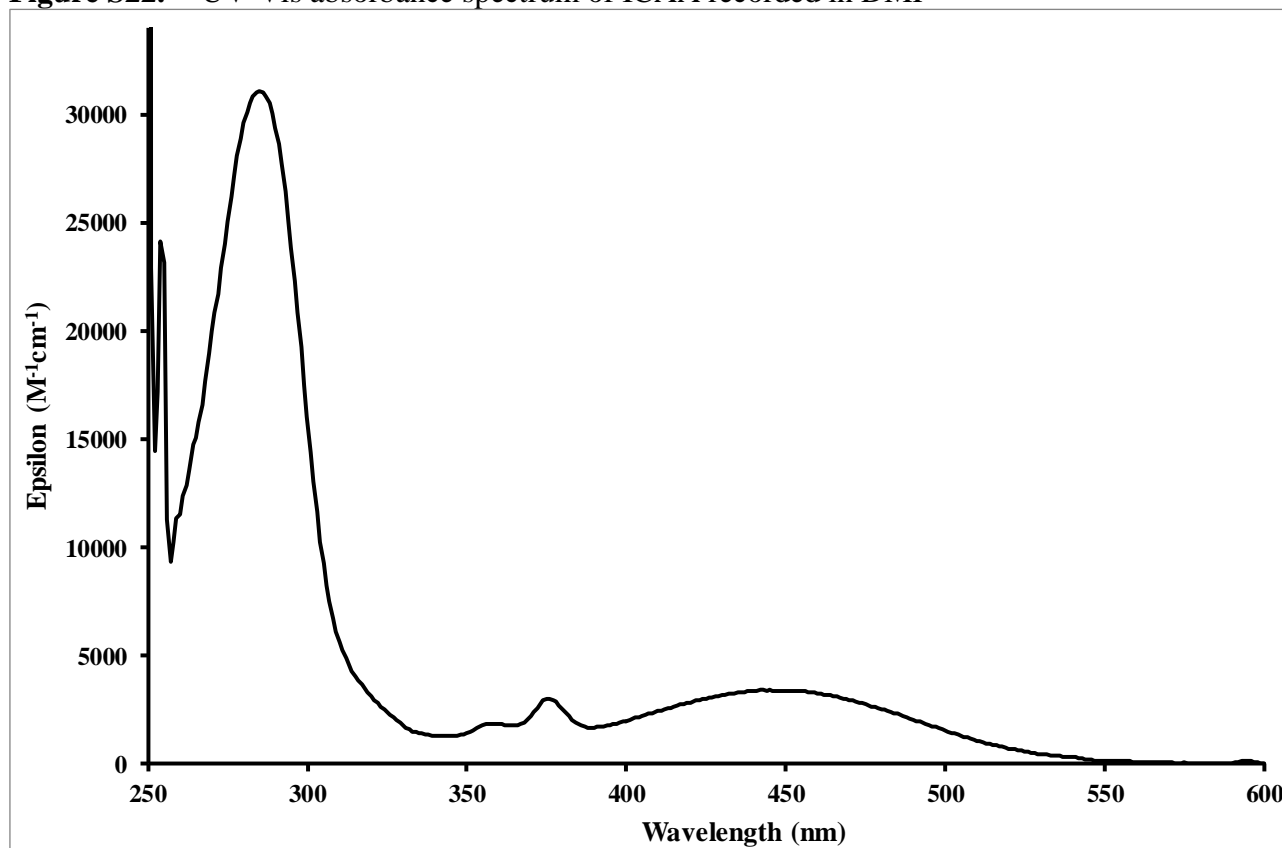
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**Figure S21.** UV-Vis absorbance spectrum of ICAA recorded in 1,4-dioxane

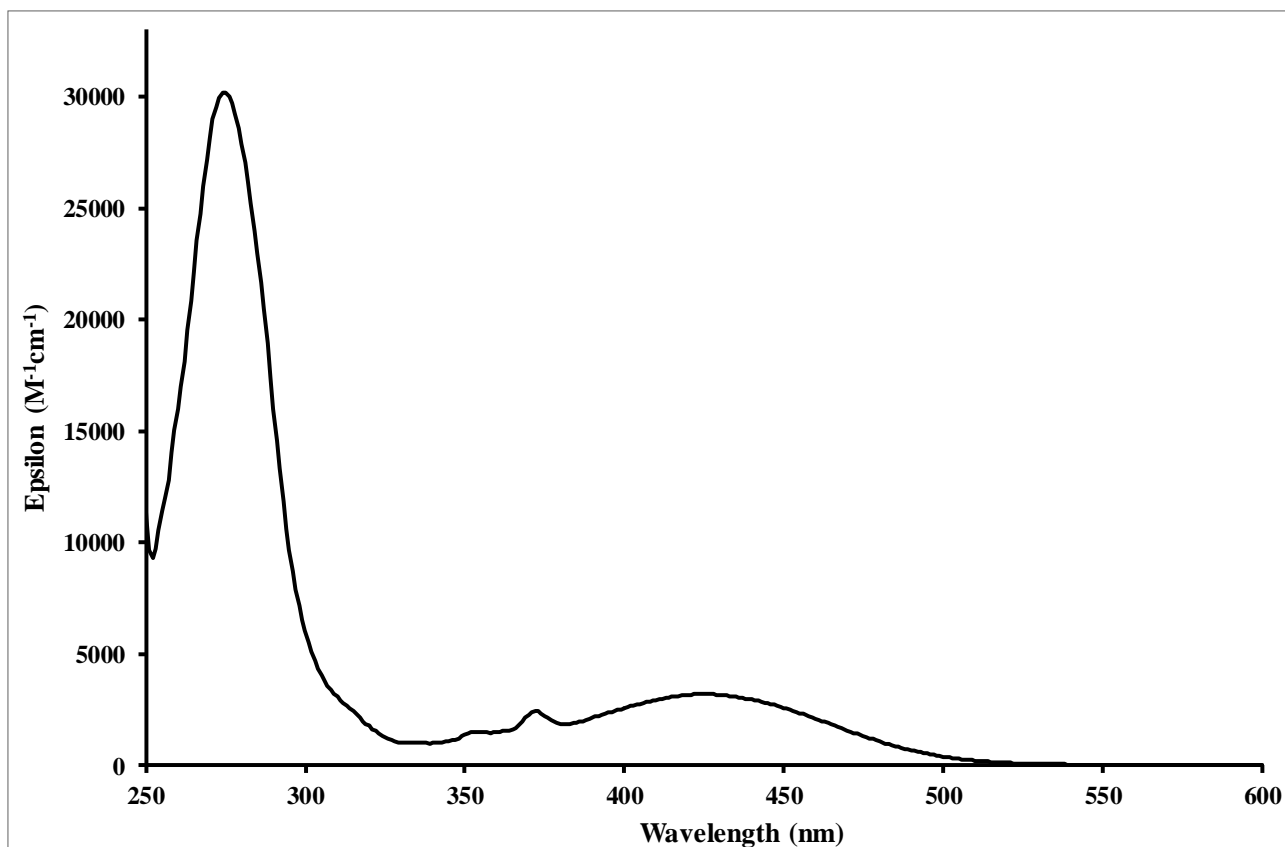


**Figure S22.** UV-Vis absorbance spectrum of ICAA recorded in DMF

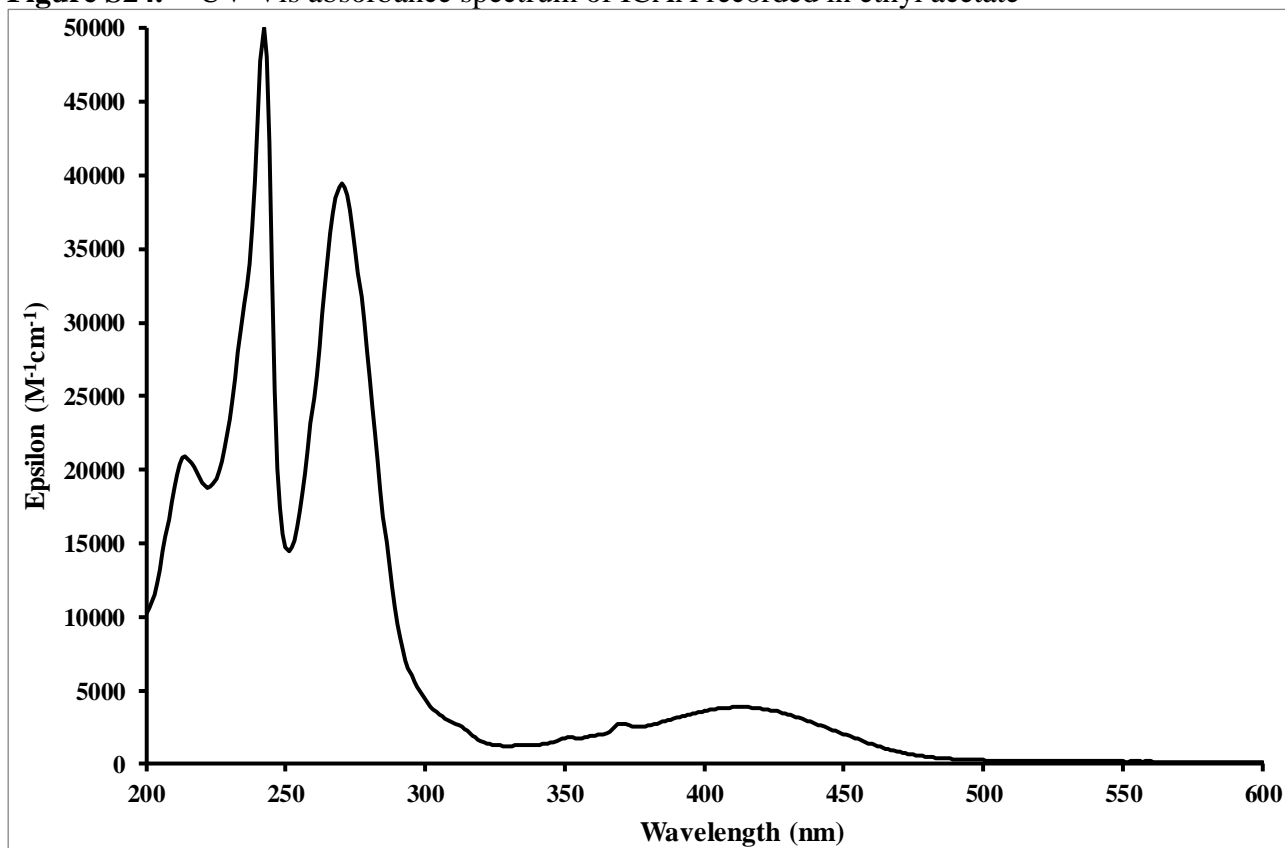


**Figure S23.** UV-Vis absorbance spectrum of ICAA recorded in DMSO

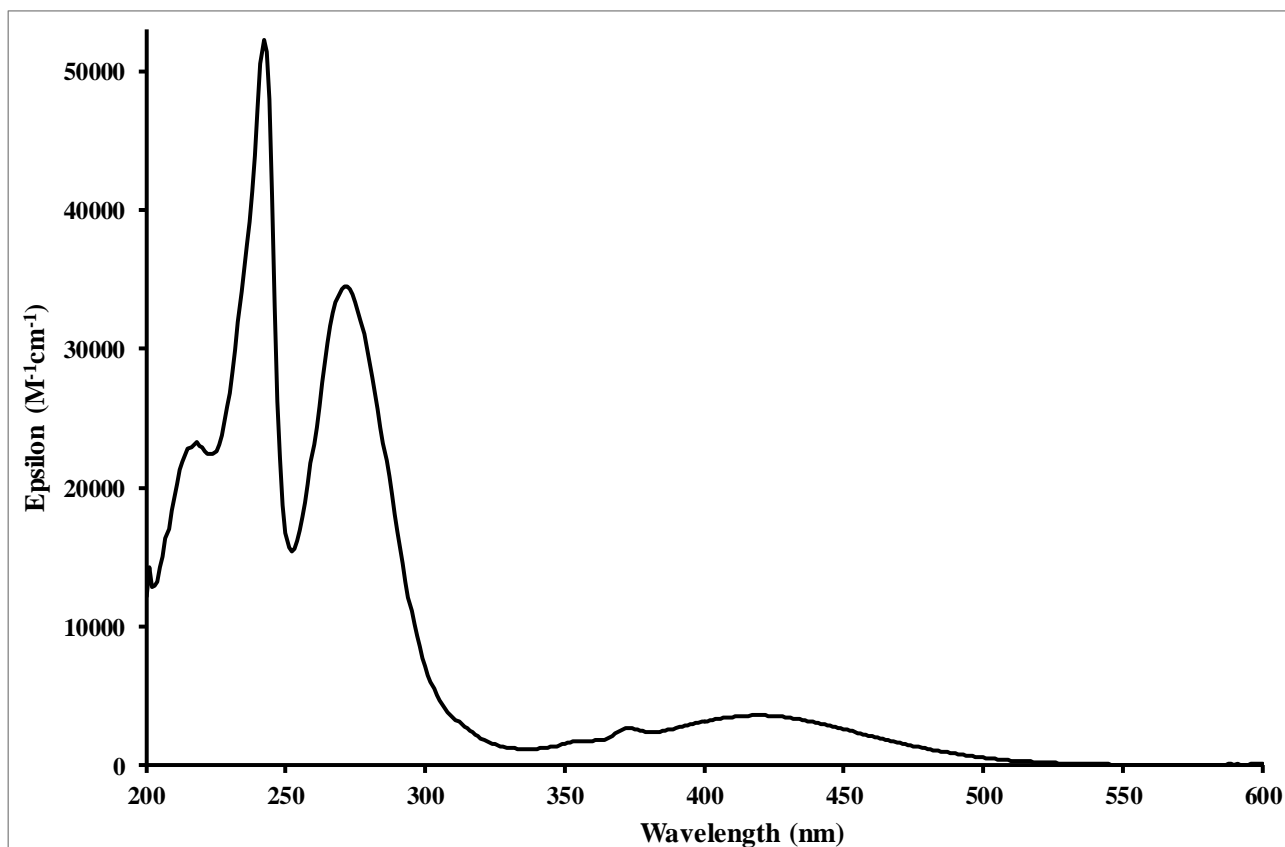




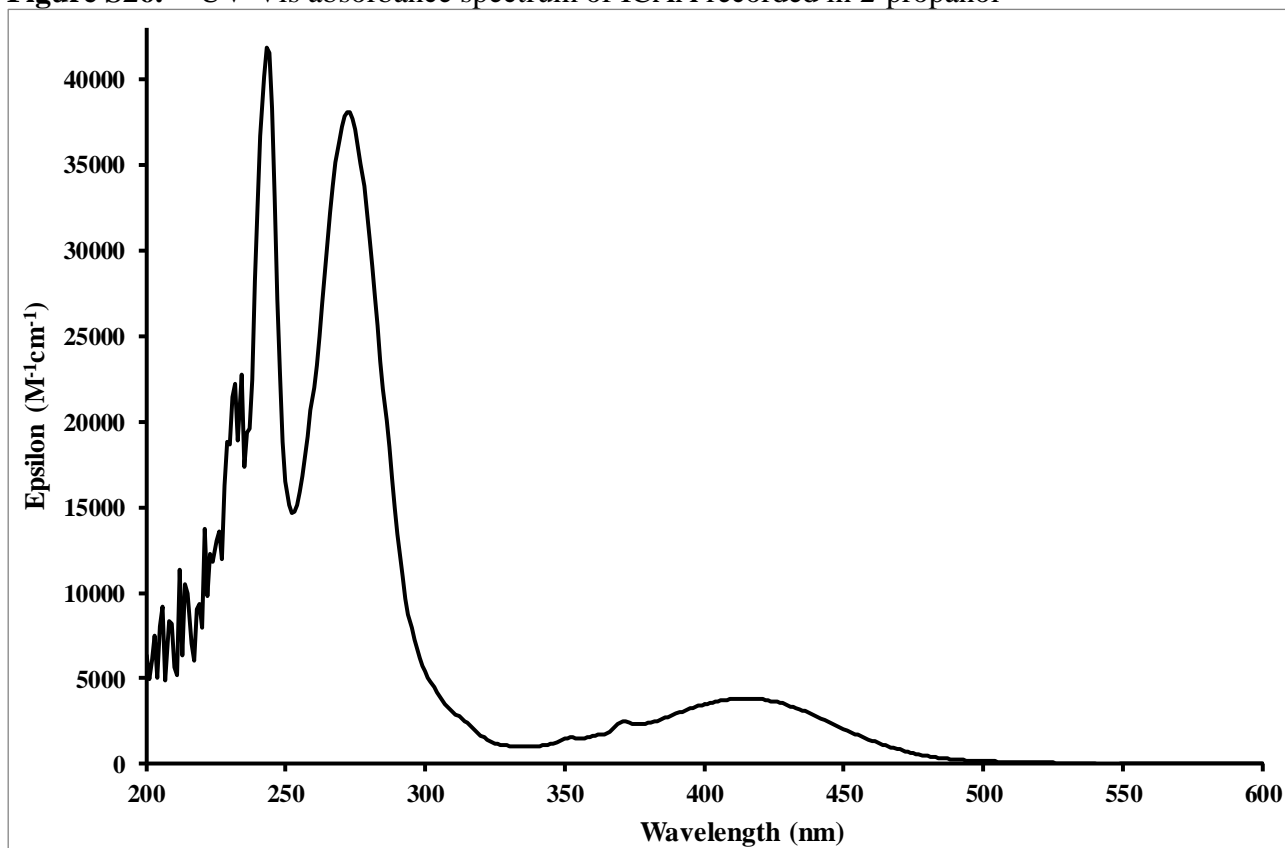
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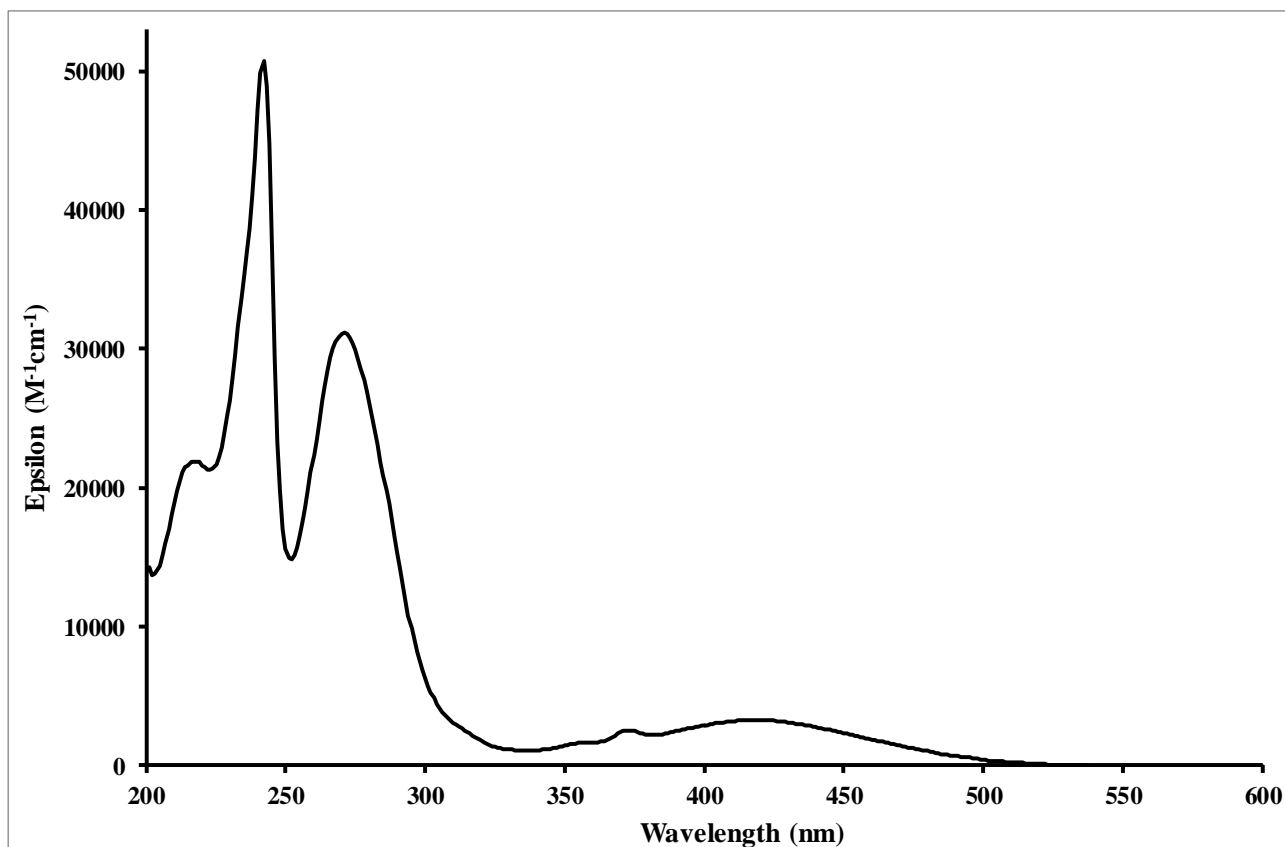
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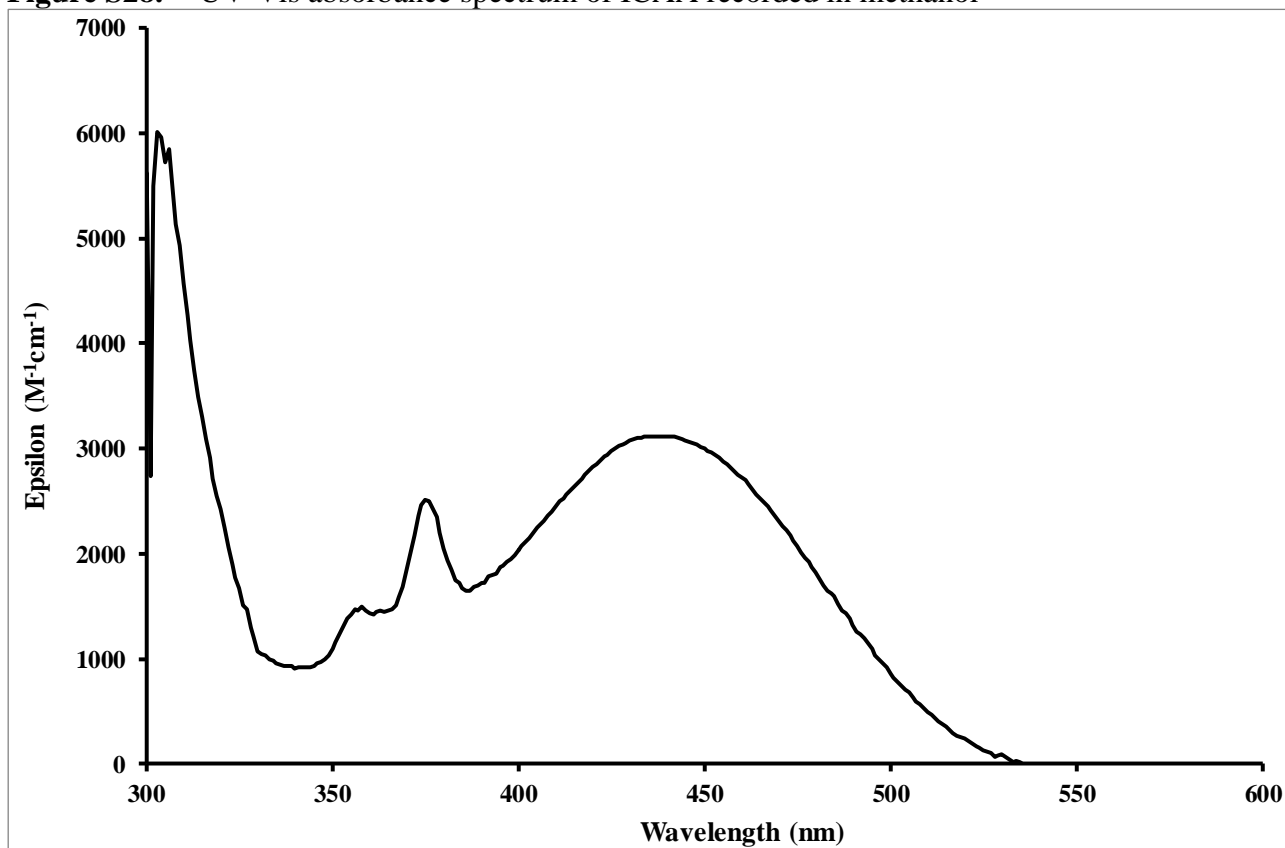
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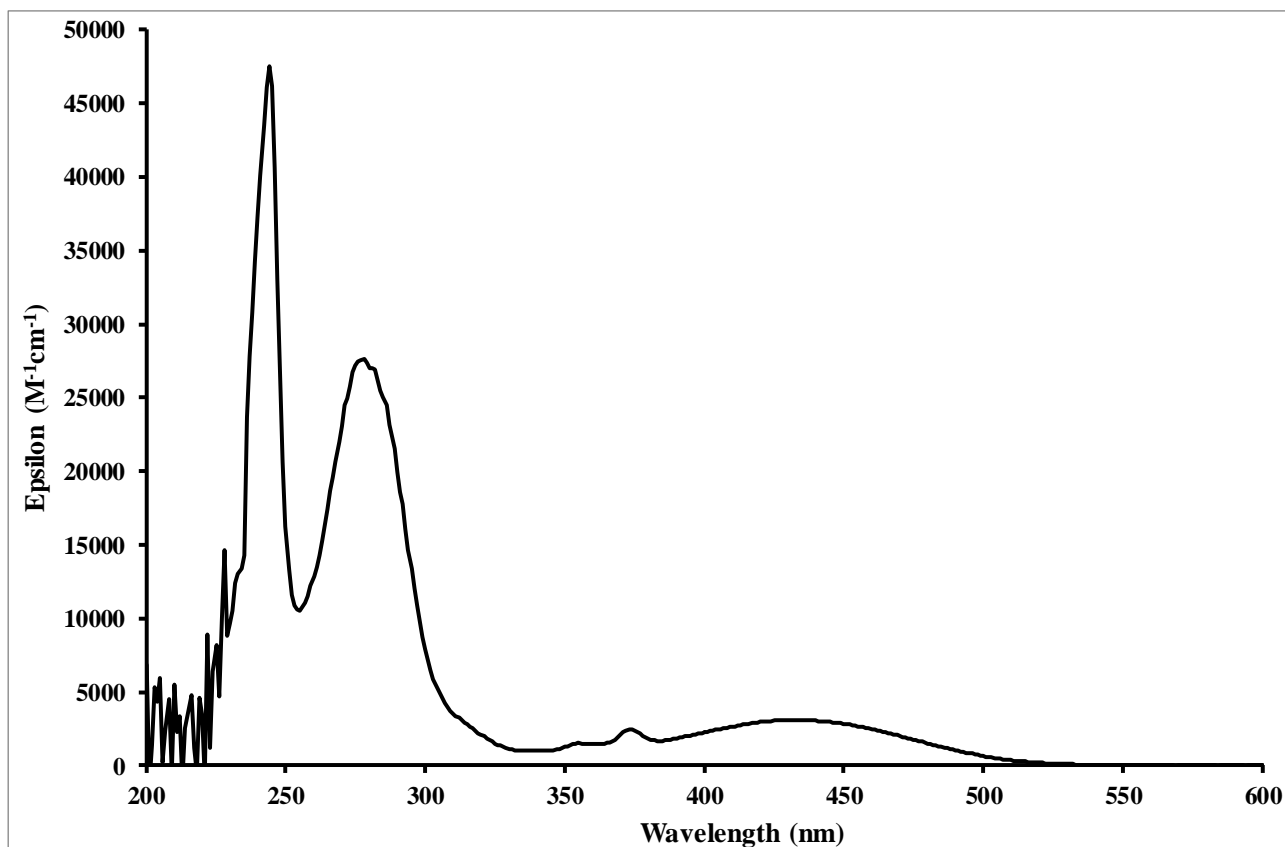
**Figure S27.** UV-Vis absorbance spectrum of ICAA recorded in chloroform



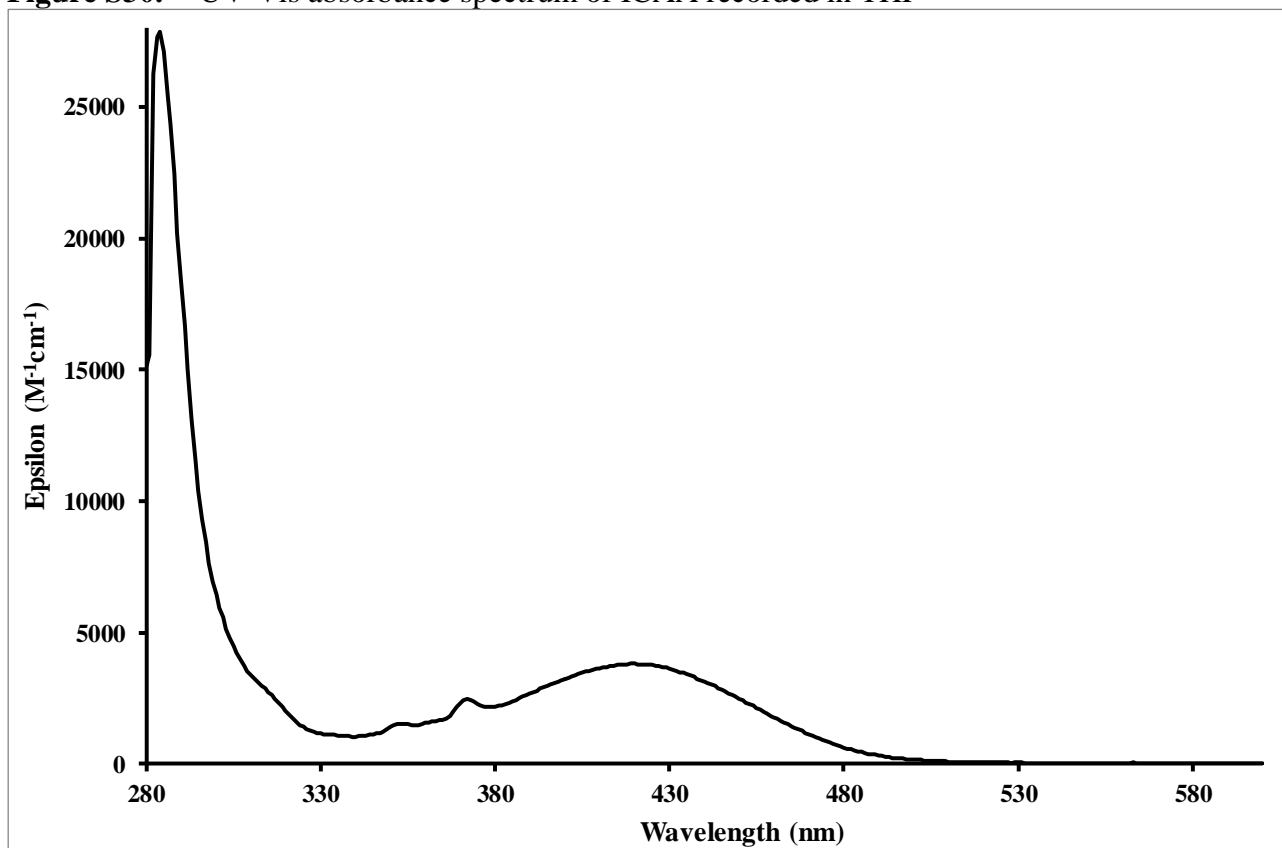
**Figure S28.** UV-Vis absorbance spectrum of ICAA recorded in methanol



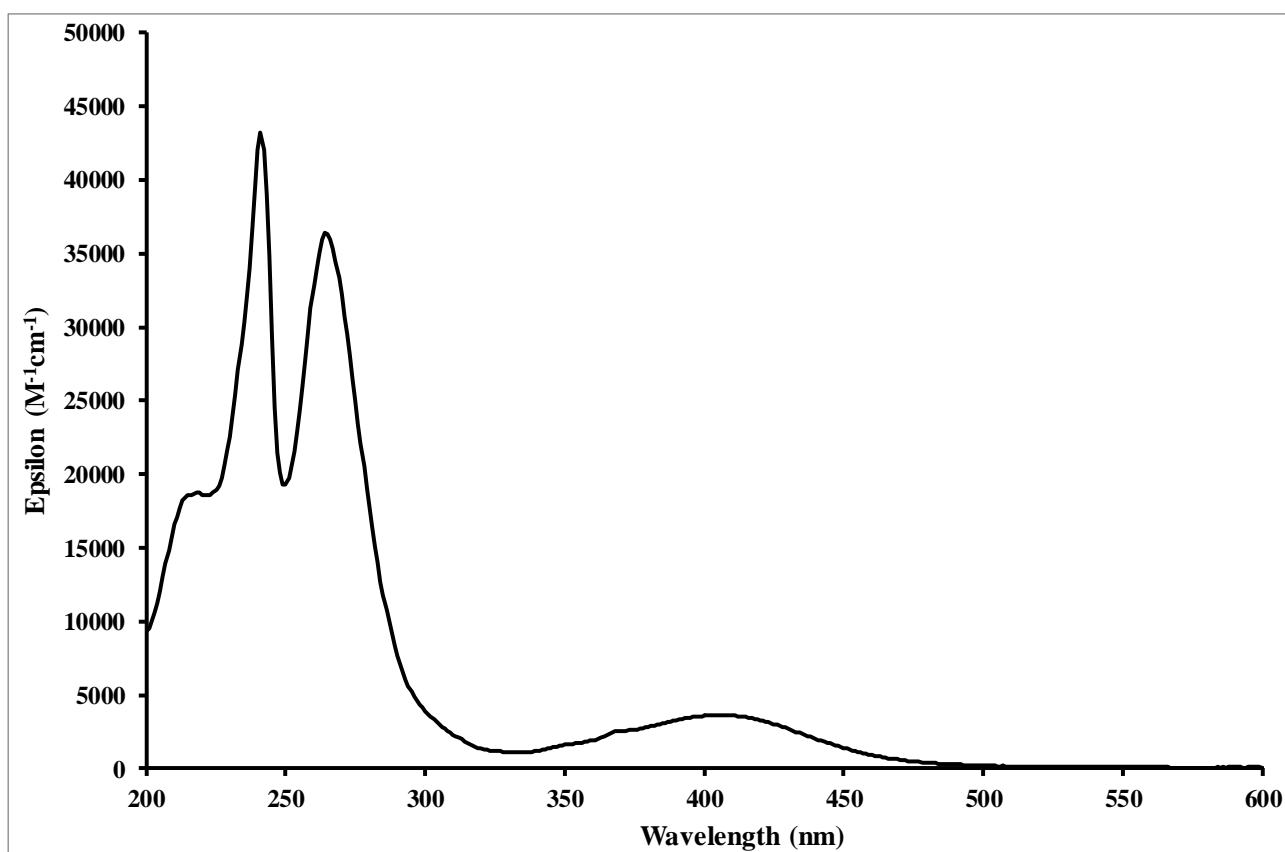
**Figure S29.** UV-Vis absorbance spectrum of ICAA recorded in pyridine



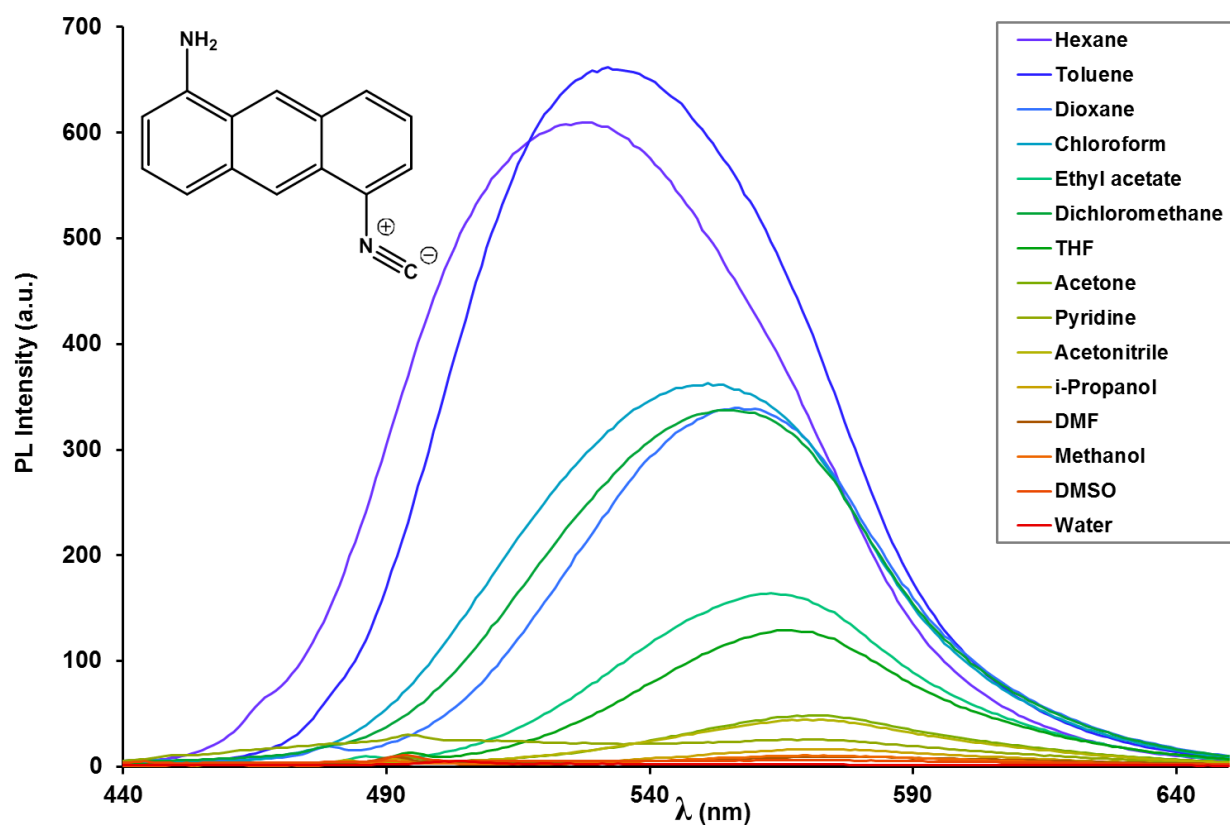
**Figure S30.** UV-Vis absorbance spectrum of ICAA recorded in THF



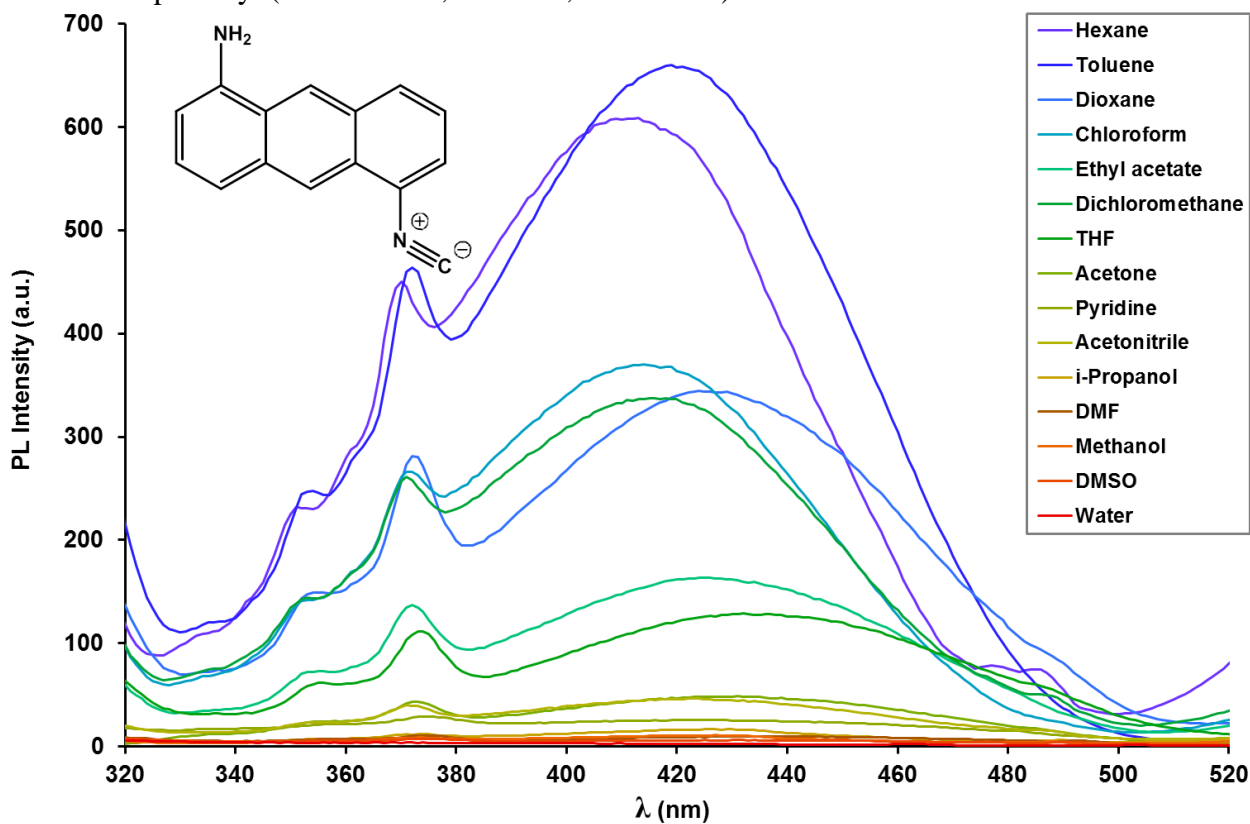
**Figure S31.** UV-Vis absorbance spectrum of ICAA recorded in toluene



**Figure S32.** UV-Vis absorbance spectrum of ICAA recorded in water

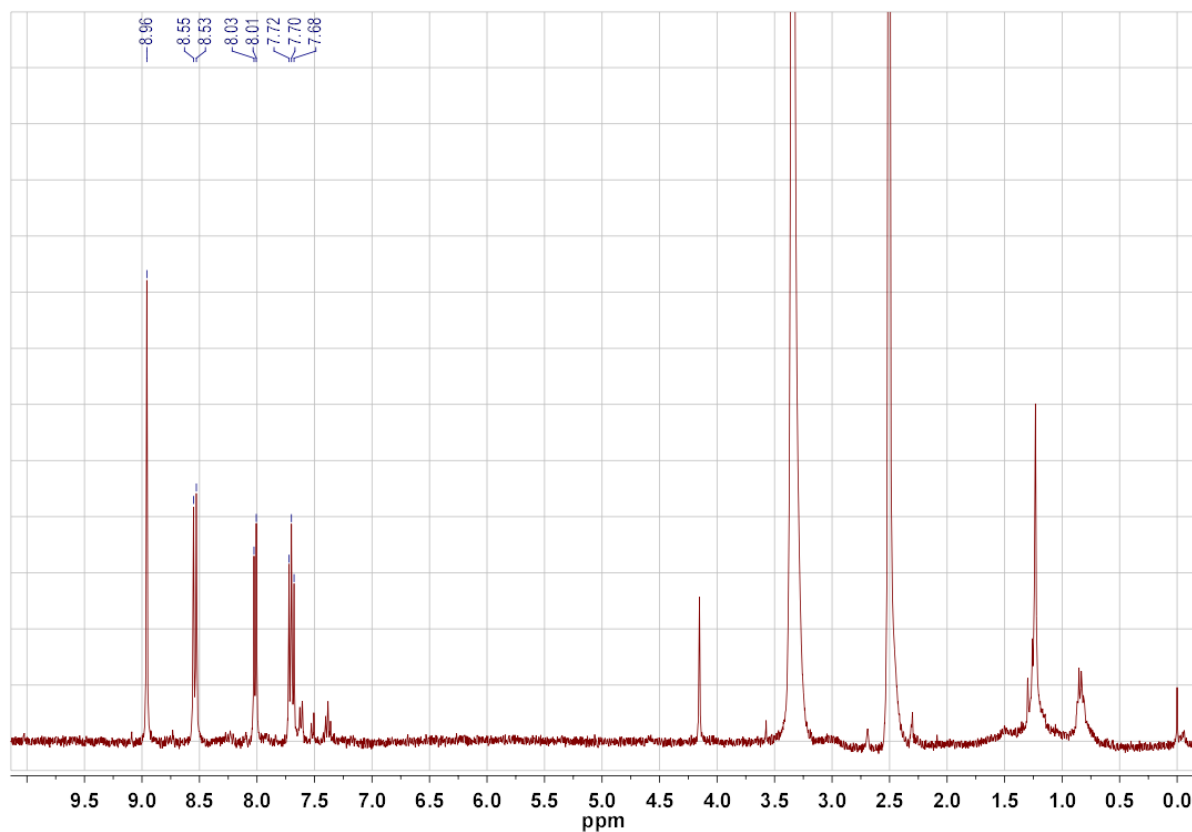


**Figure S33.** The emission spectra of 1-amino-5-isocyanoanthracene (ICAA) recorded in solvents of different polarity. ( $c=5\times10^{-5}$  M,  $T=20$  °C,  $V=3.00$  ml).

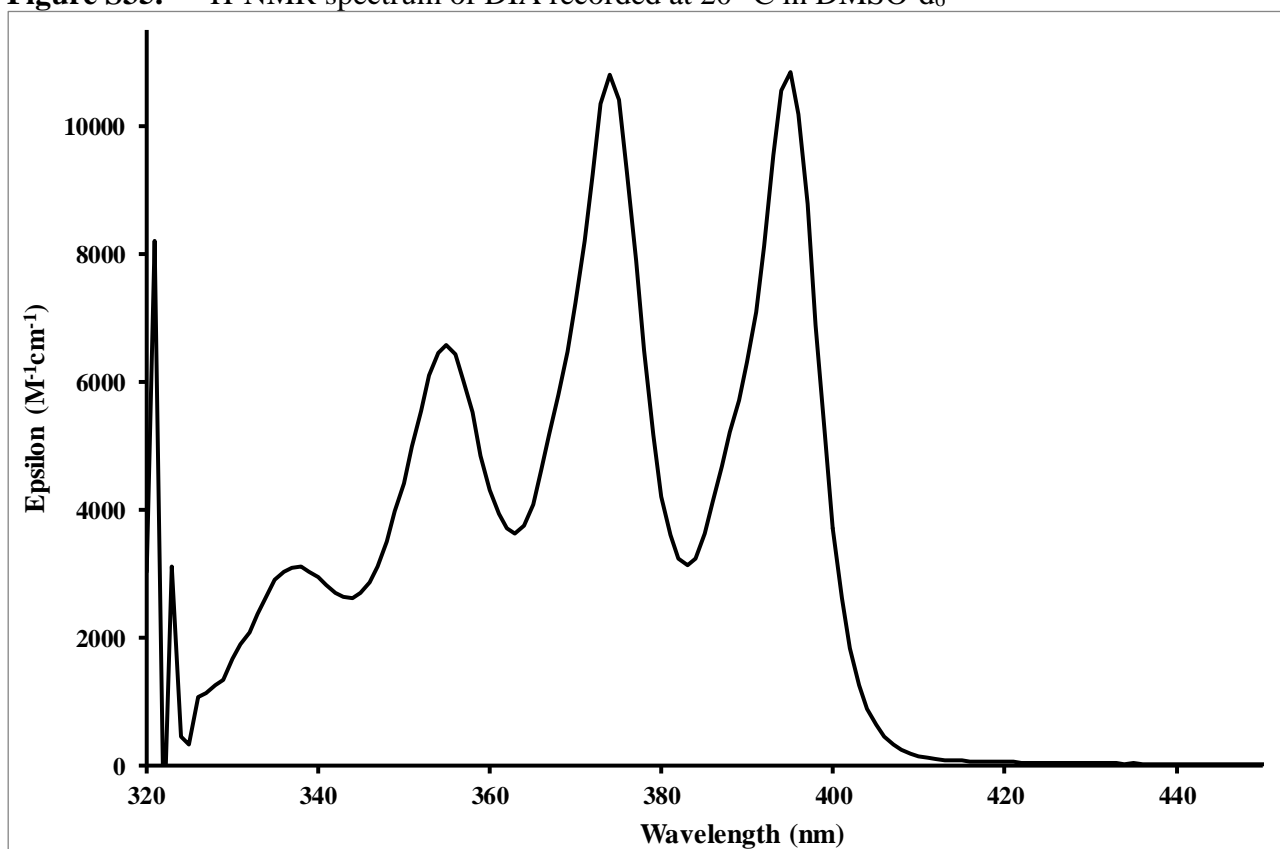


**Figure S34.** The excitation spectra of 1-amino-5-isocyanoanthracene (ICAA) recorded in solvents of different polarity. ( $c=5\times10^{-5}$  M,  $T=20$  °C,  $V=3.00$  ml).

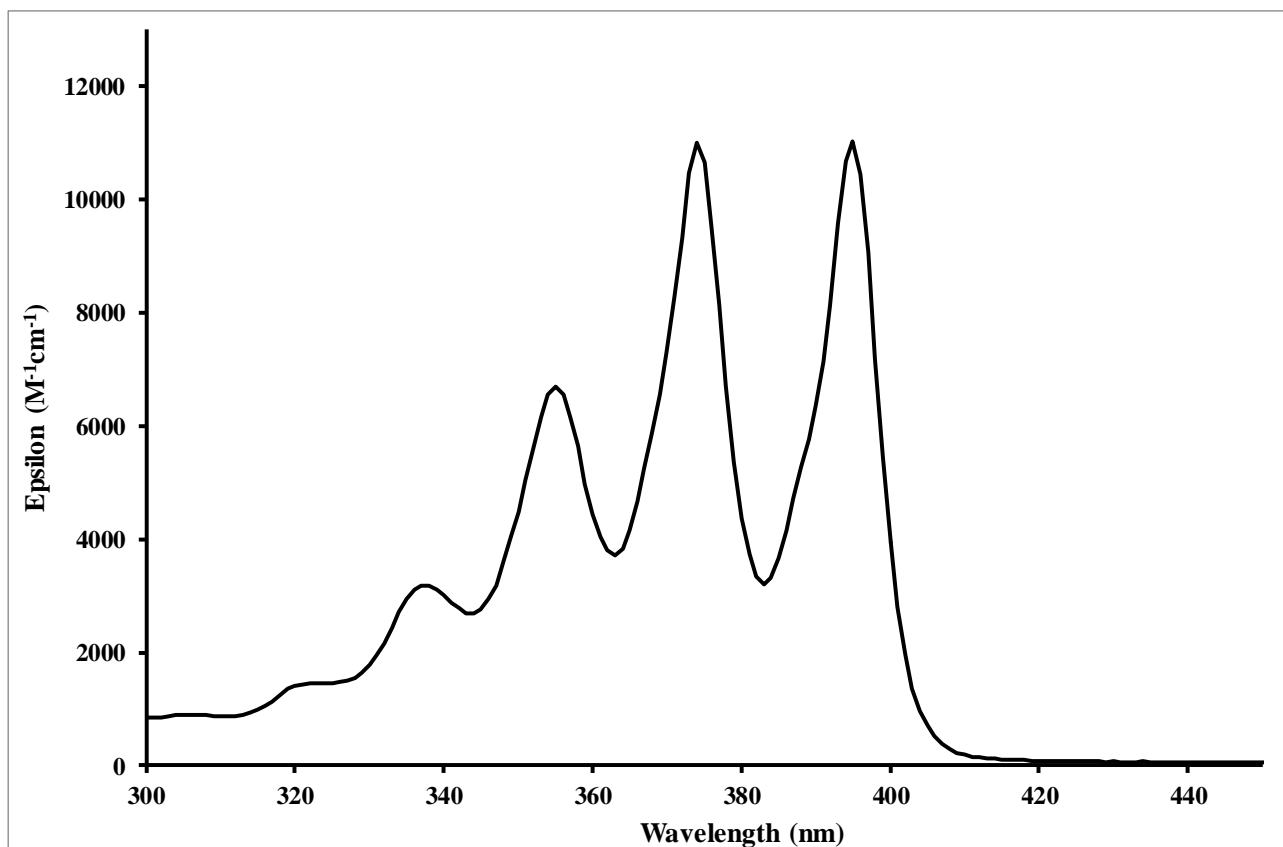
### Chapter 3. 1,5-diisocyanoanthracene (DIA)



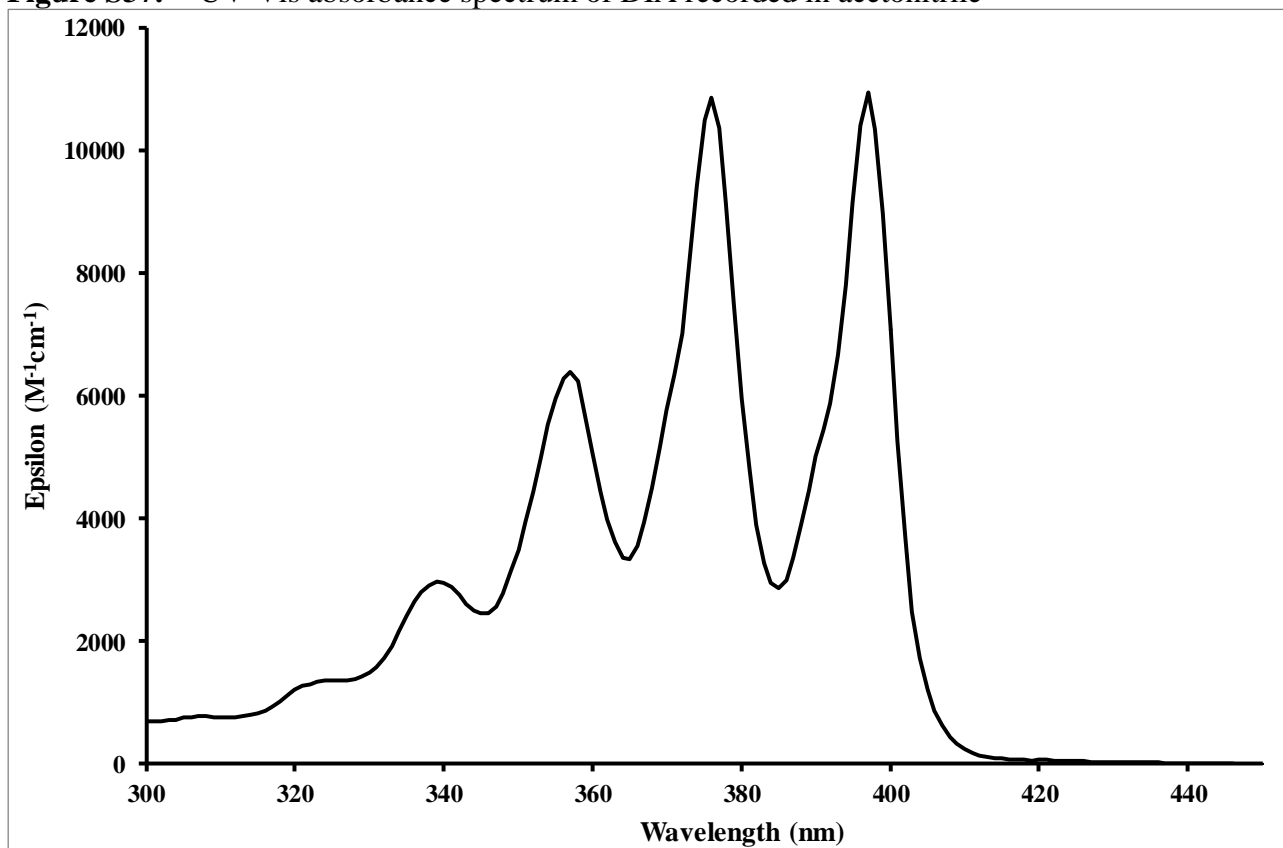
**Figure S35.** <sup>1</sup>H-NMR spectrum of DIA recorded at 20 °C in DMSO-d<sub>6</sub>



**Figure S36.** UV-Vis absorbance spectrum of DIA recorded in acetone

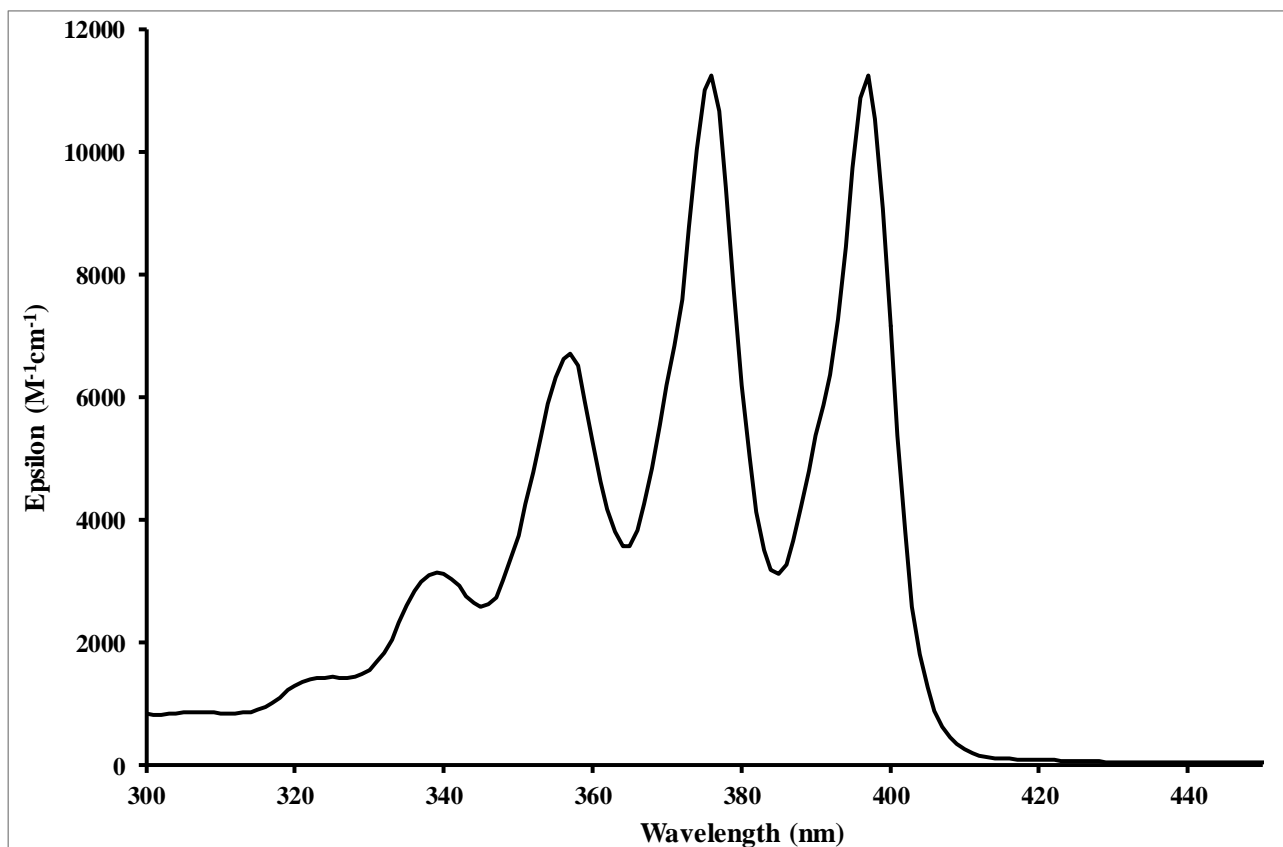


**Figure S37.** UV-Vis absorbance spectrum of DIA recorded in acetonitrile

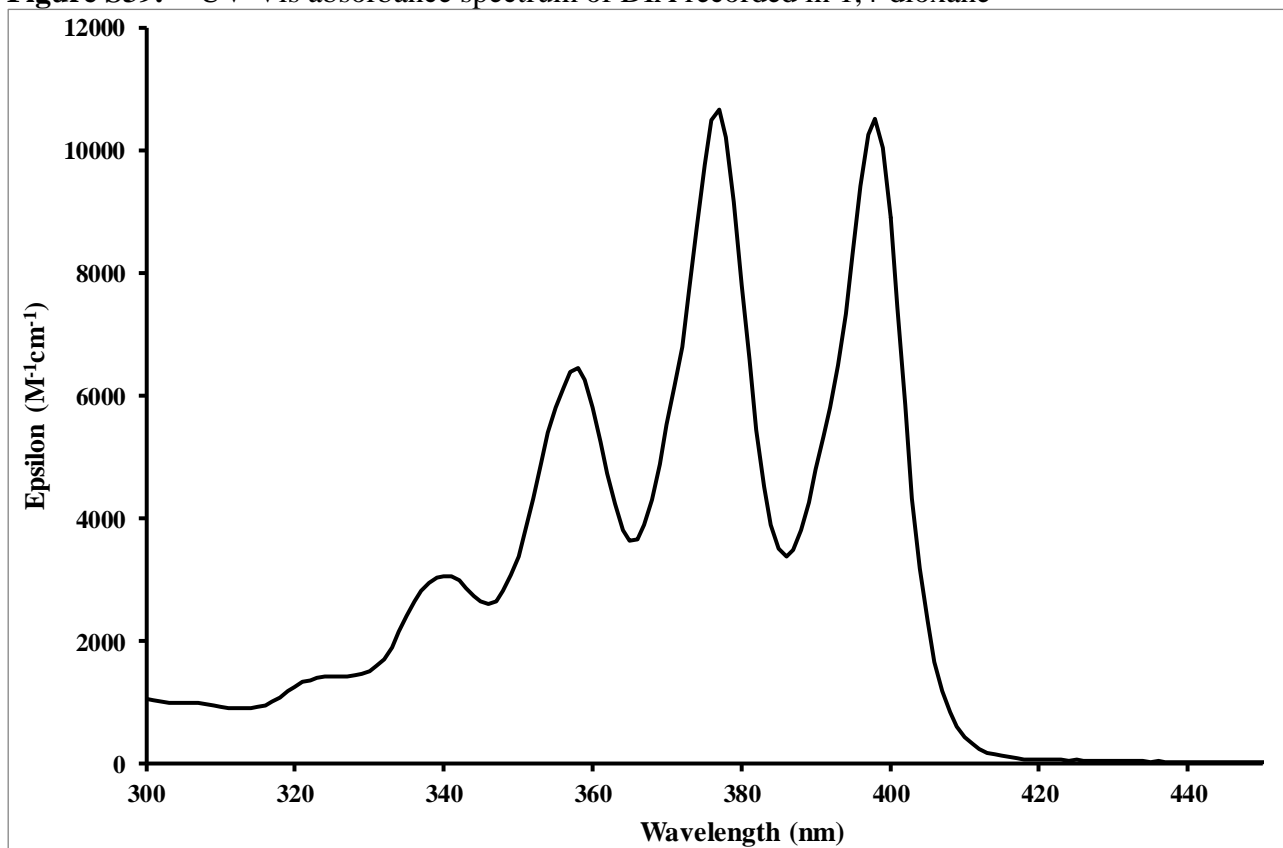


**Figure S38.** UV-Vis absorbance spectrum of DIA recorded in dichloromethane

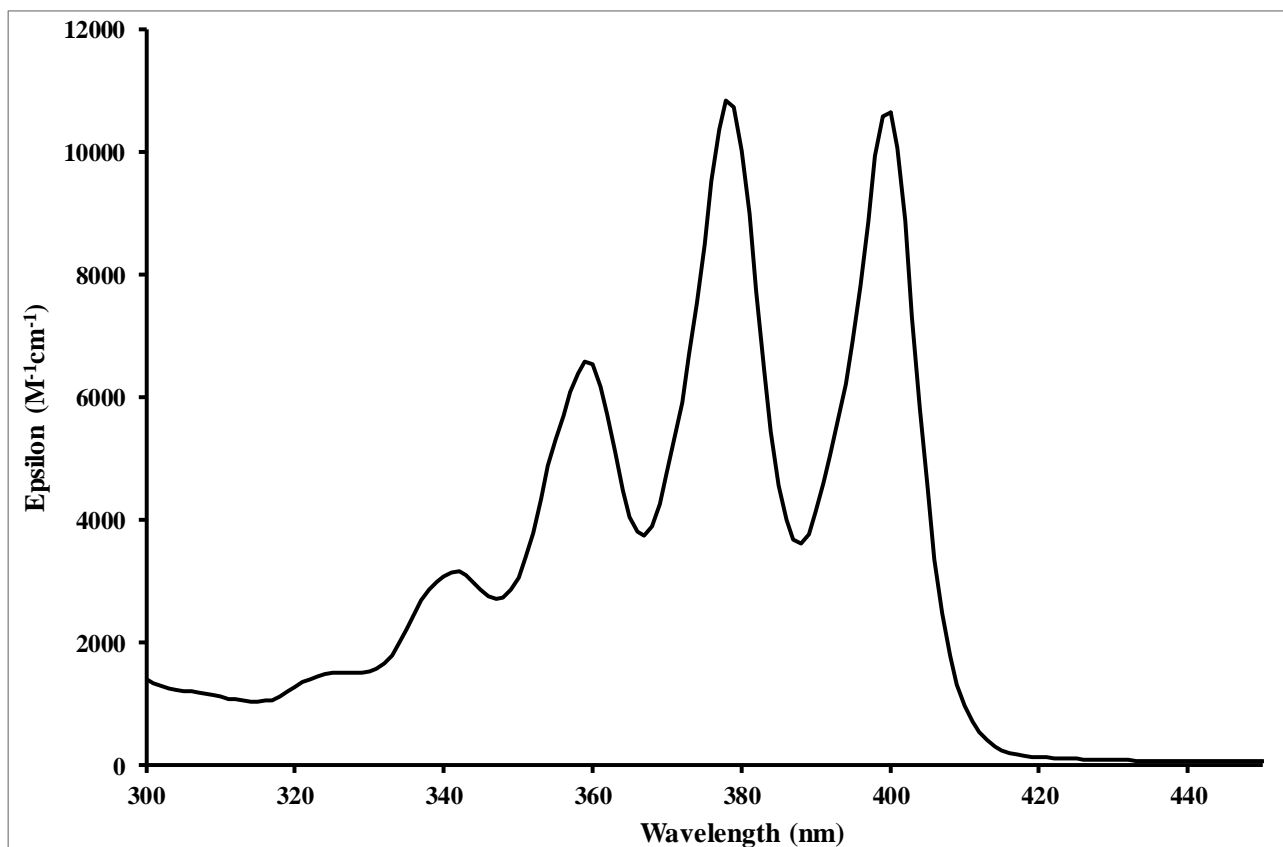




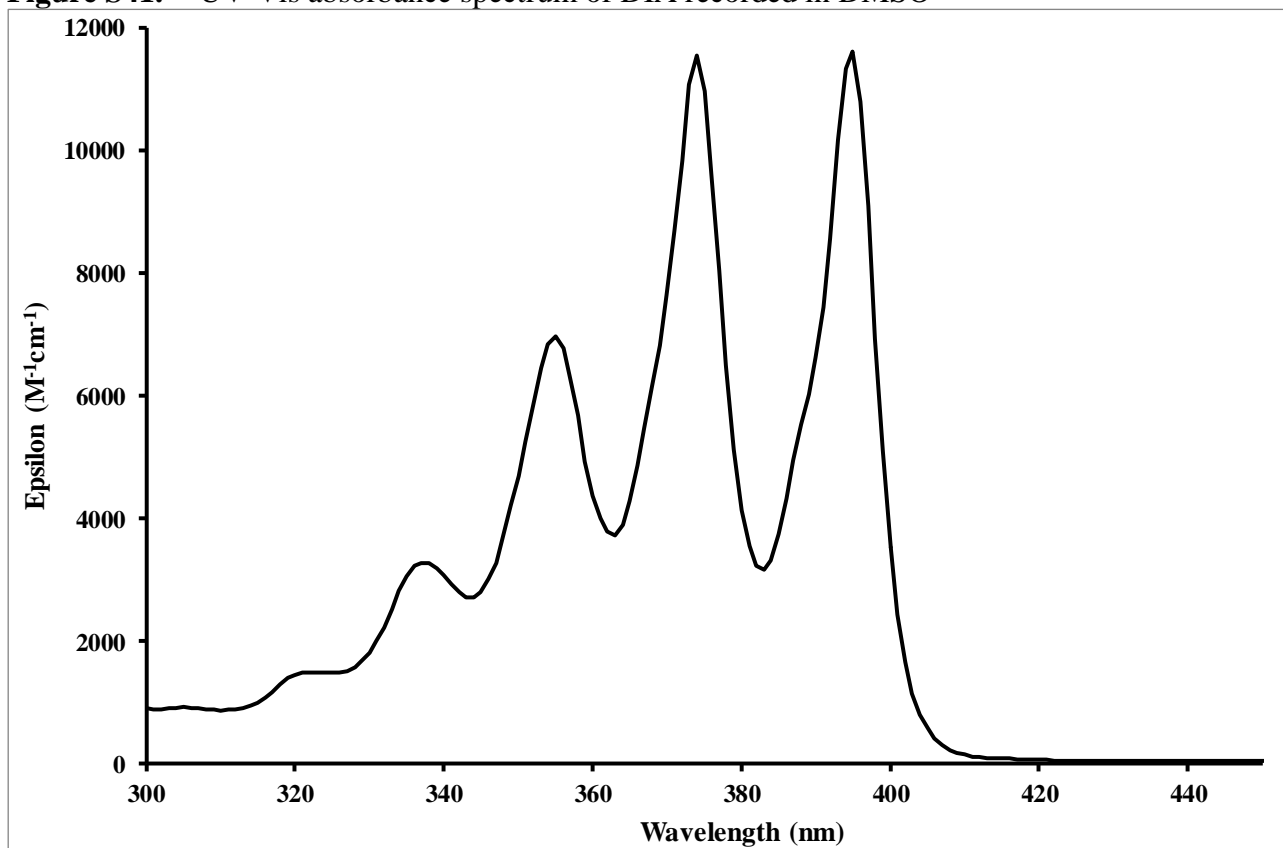
**Figure S39.** UV-Vis absorbance spectrum of DIA recorded in 1,4-dioxane



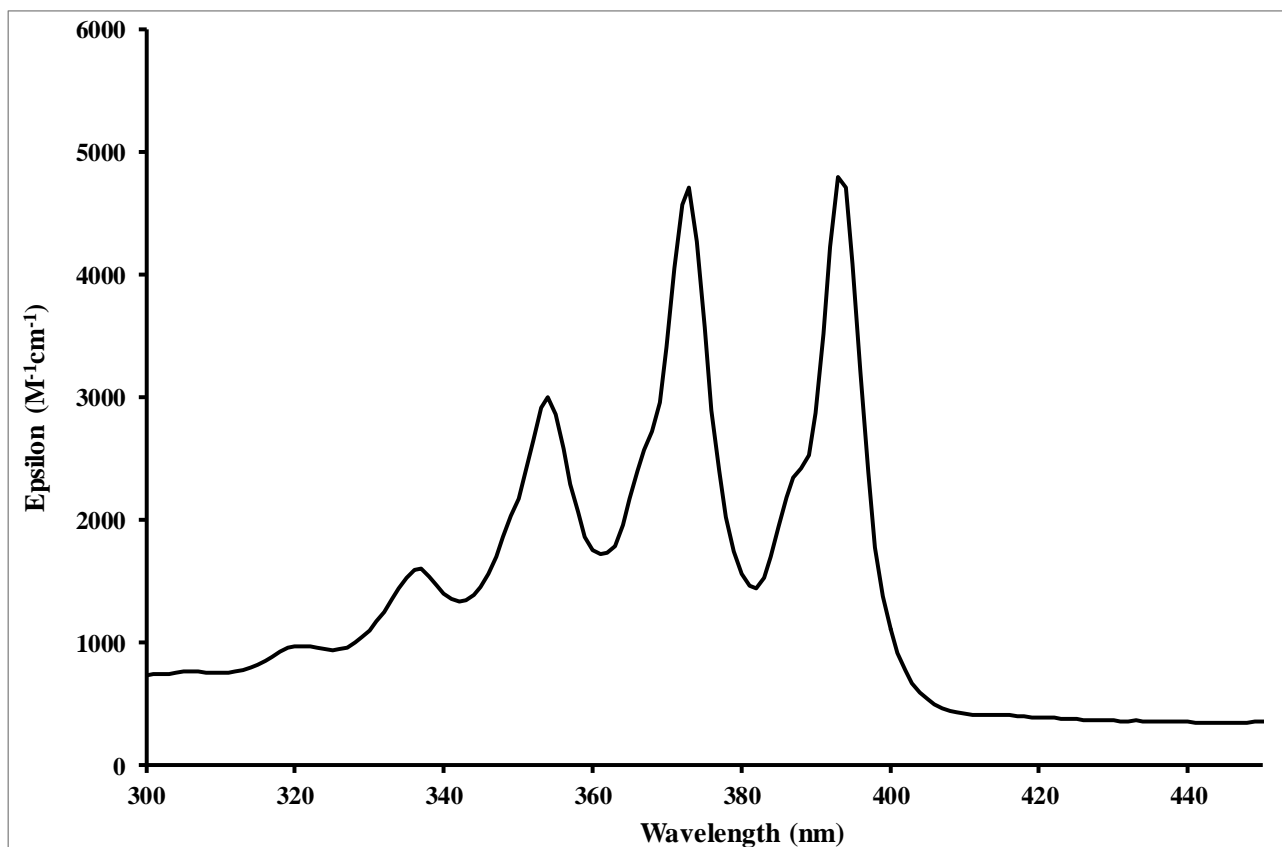
**Figure S40.** UV-Vis absorbance spectrum of DIA recorded in DMF



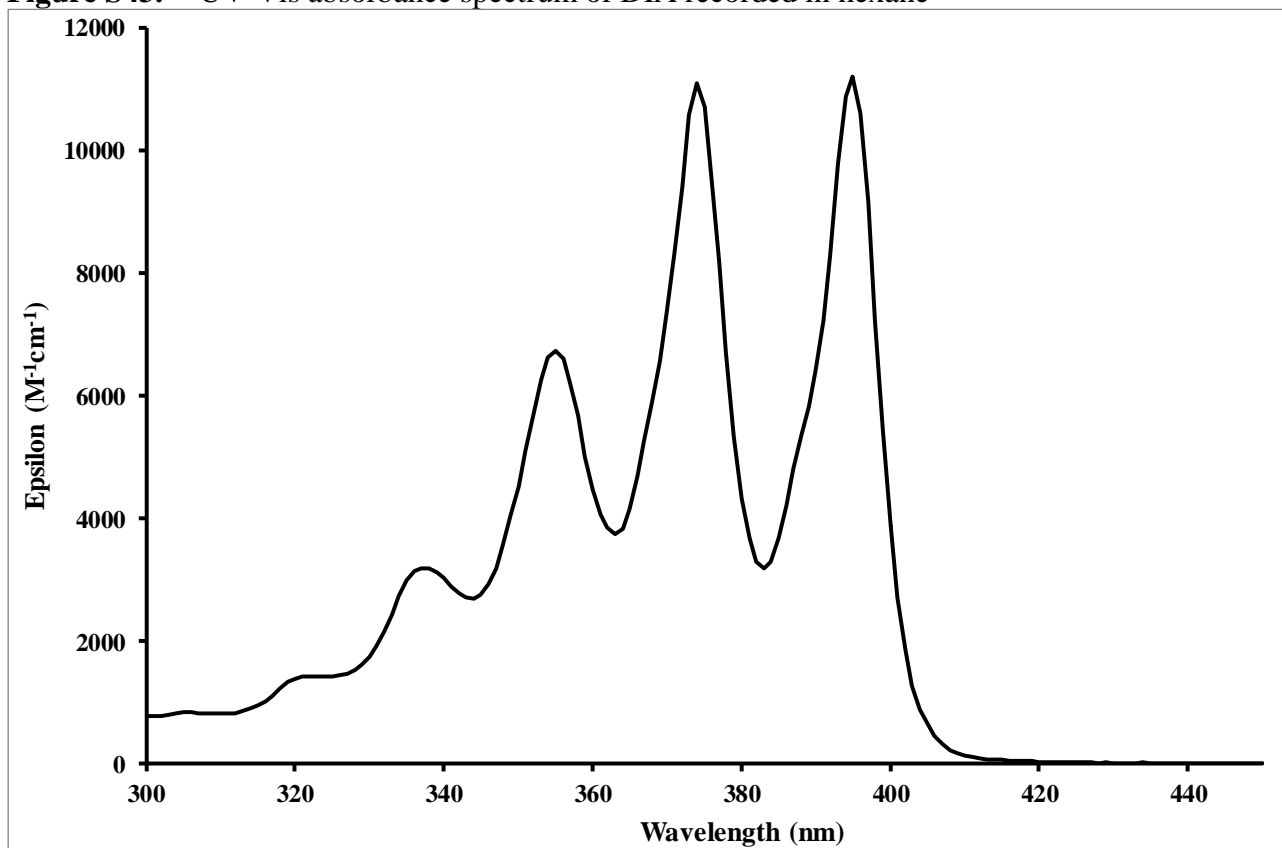
**Figure S41.** UV-Vis absorbance spectrum of DIA recorded in DMSO



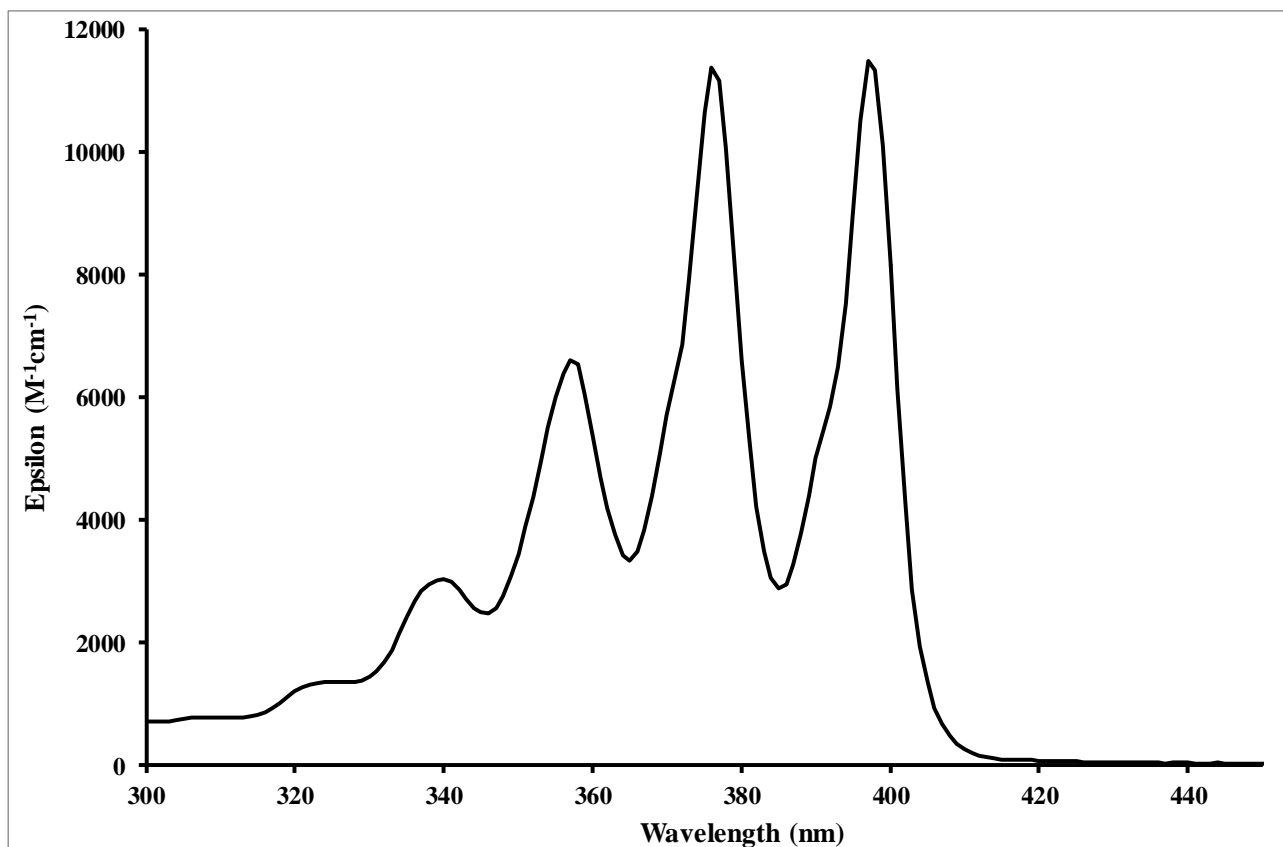
**Figure S42.** UV-Vis absorbance spectrum of DIA recorded in ethyl acetate



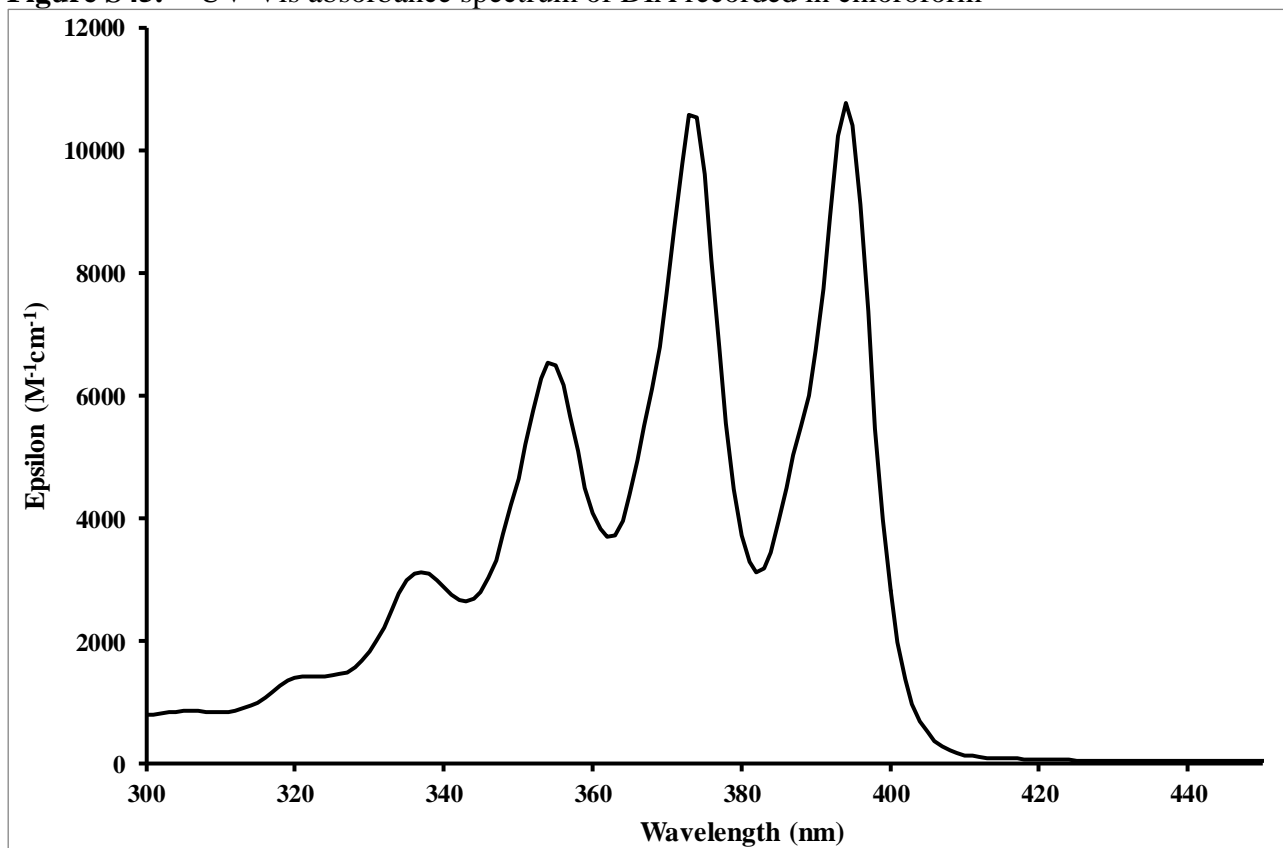
**Figure S43.** UV-Vis absorbance spectrum of DIA recorded in hexane



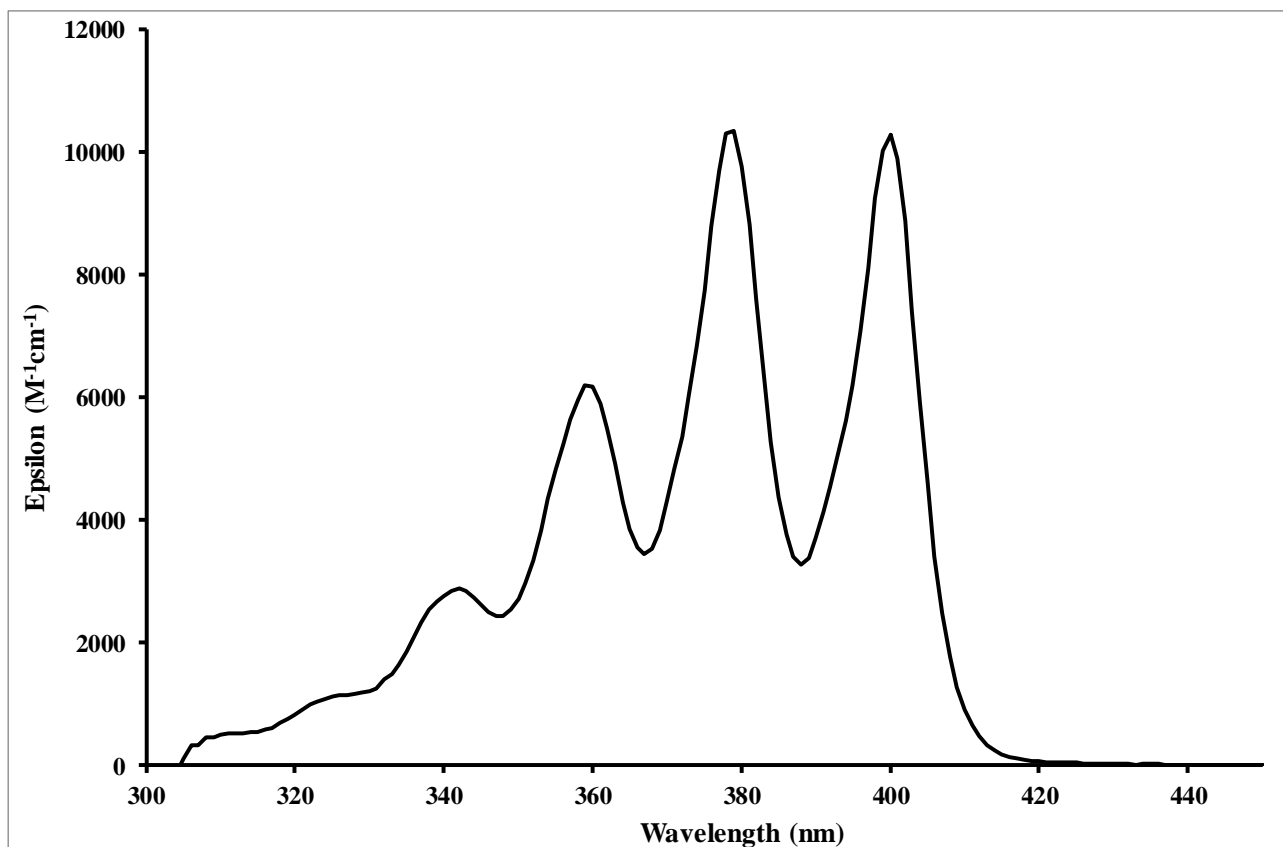
**Figure S44.** UV-Vis absorbance spectrum of DIA recorded in 2-propanol



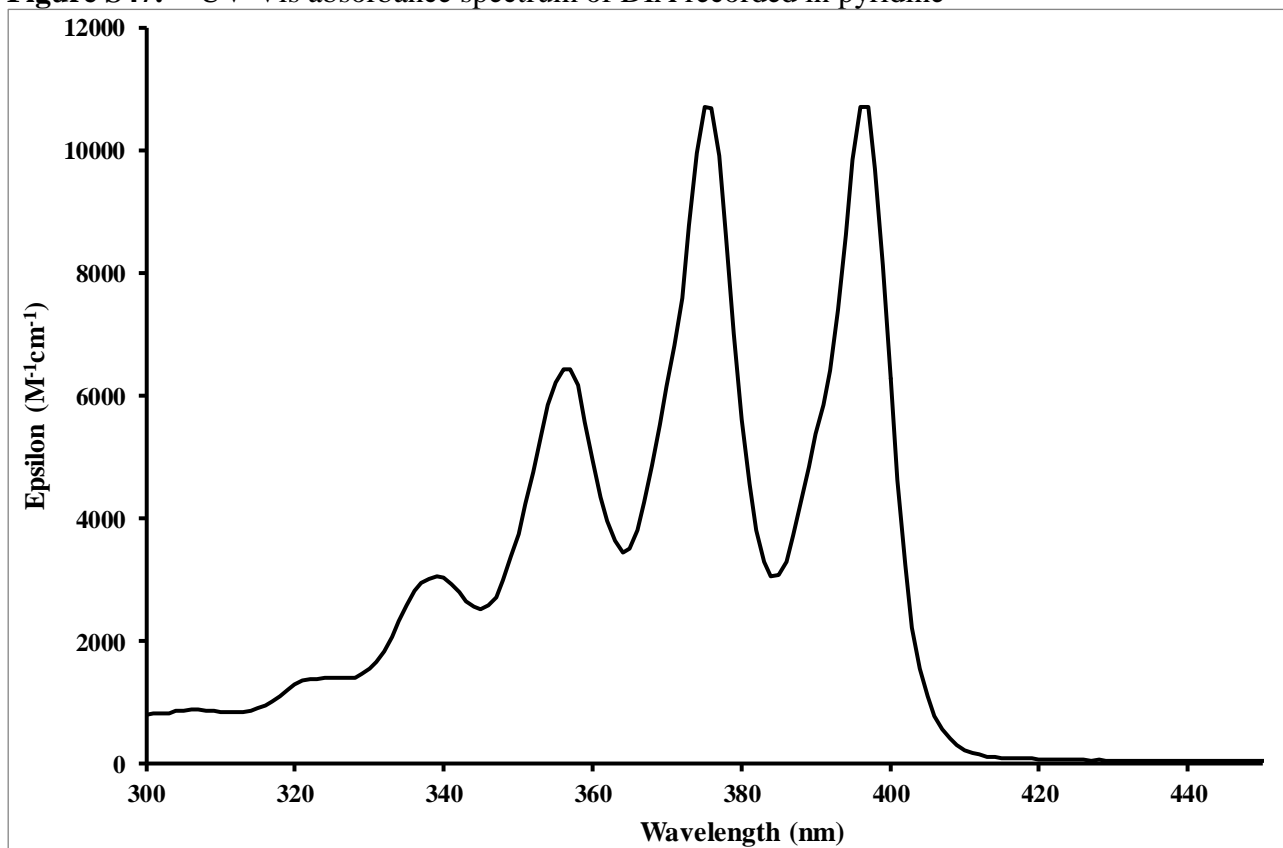
**Figure S45.** UV-Vis absorbance spectrum of DIA recorded in chloroform



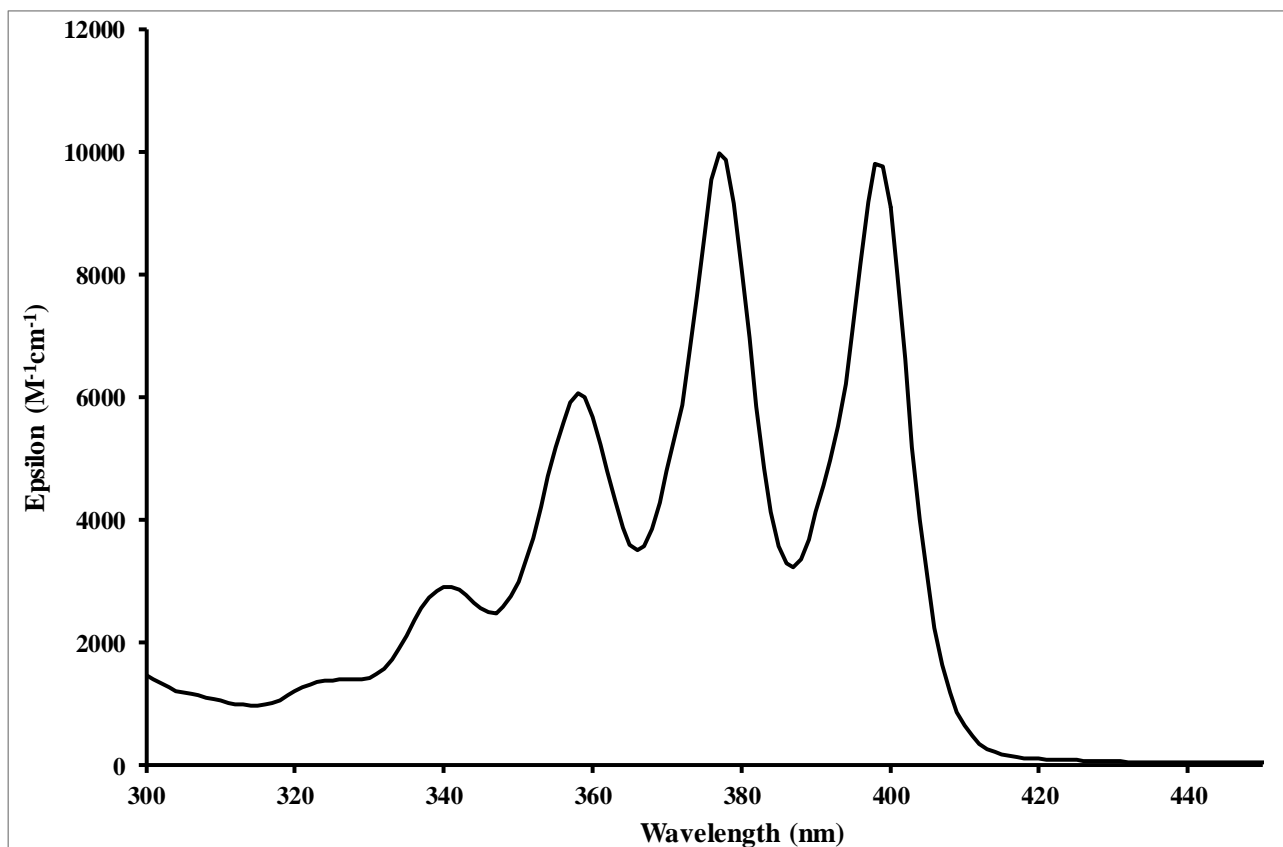
**Figure S46.** UV-Vis absorbance spectrum of DIA recorded in methanol



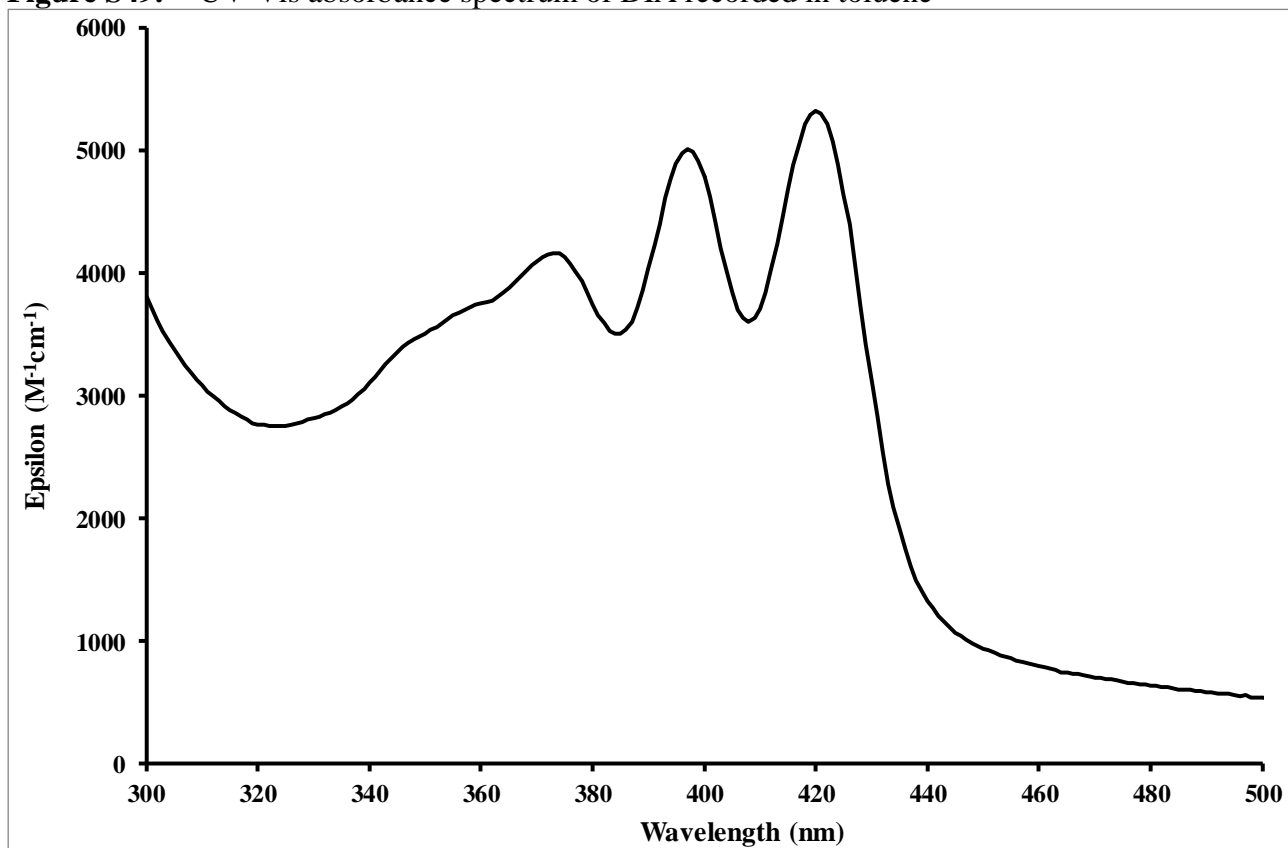
**Figure S47.** UV-Vis absorbance spectrum of DIA recorded in pyridine



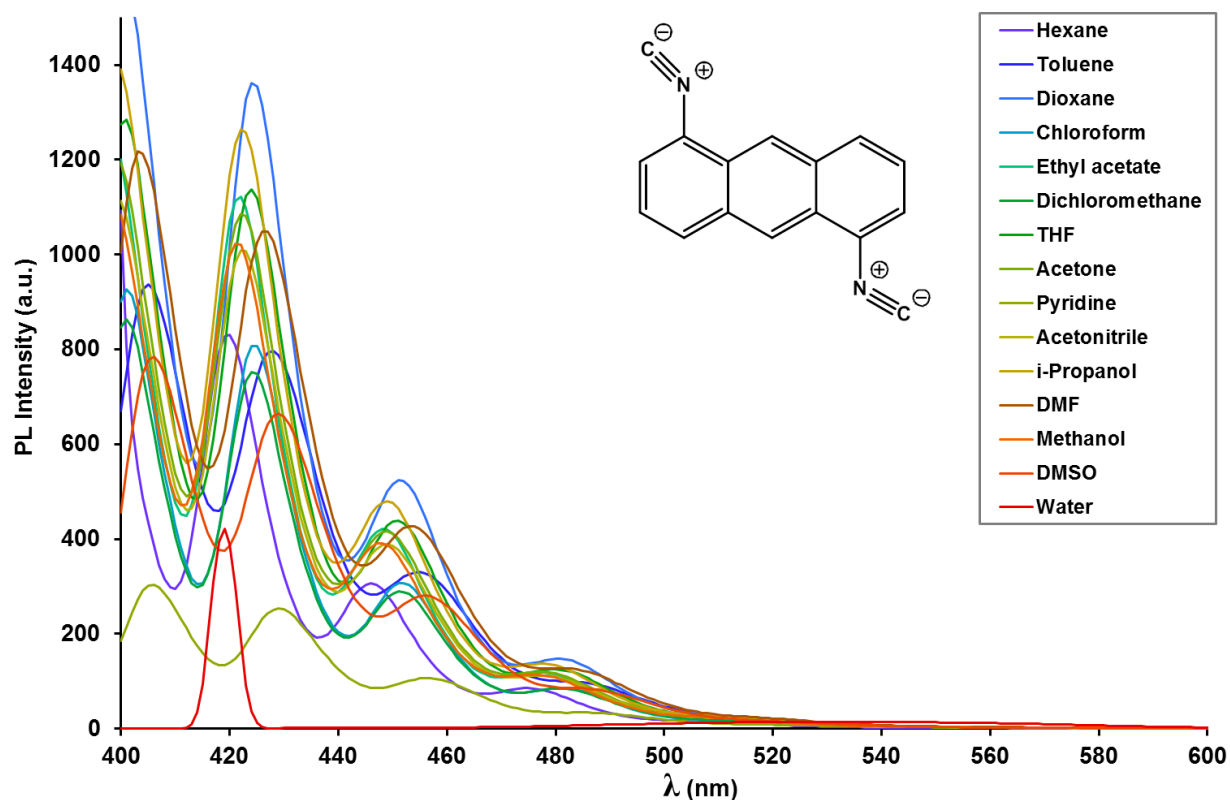
**Figure S48.** UV-Vis absorbance spectrum of DIA recorded in THF



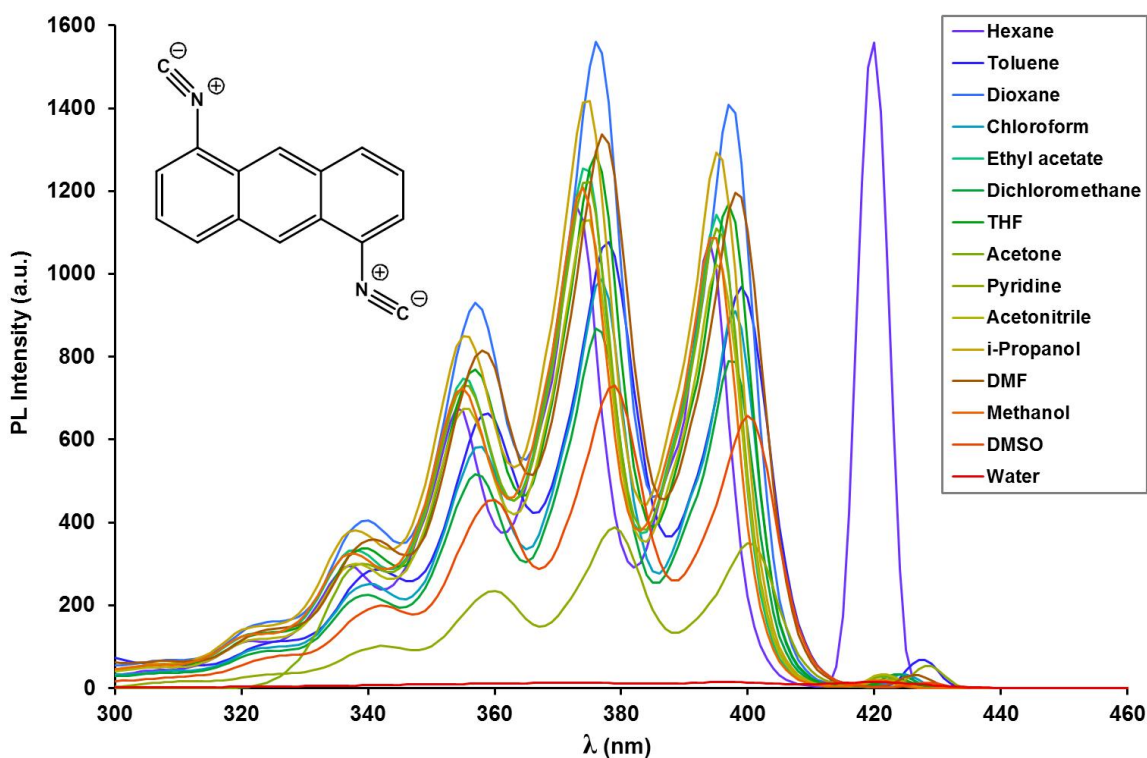
**Figure S49.** UV-Vis absorbance spectrum of DIA recorded in toluene



**Figure S50.** UV-Vis absorbance spectrum of DIA recorded in water



**Figure S51.** The emission spectra of 1,5-diisocyanoanthracene (**DIA**) recorded in solvents of different polarity. ( $c=5\times10^{-5}$  M,  $T=20$  °C,  $V=3.00$  ml).

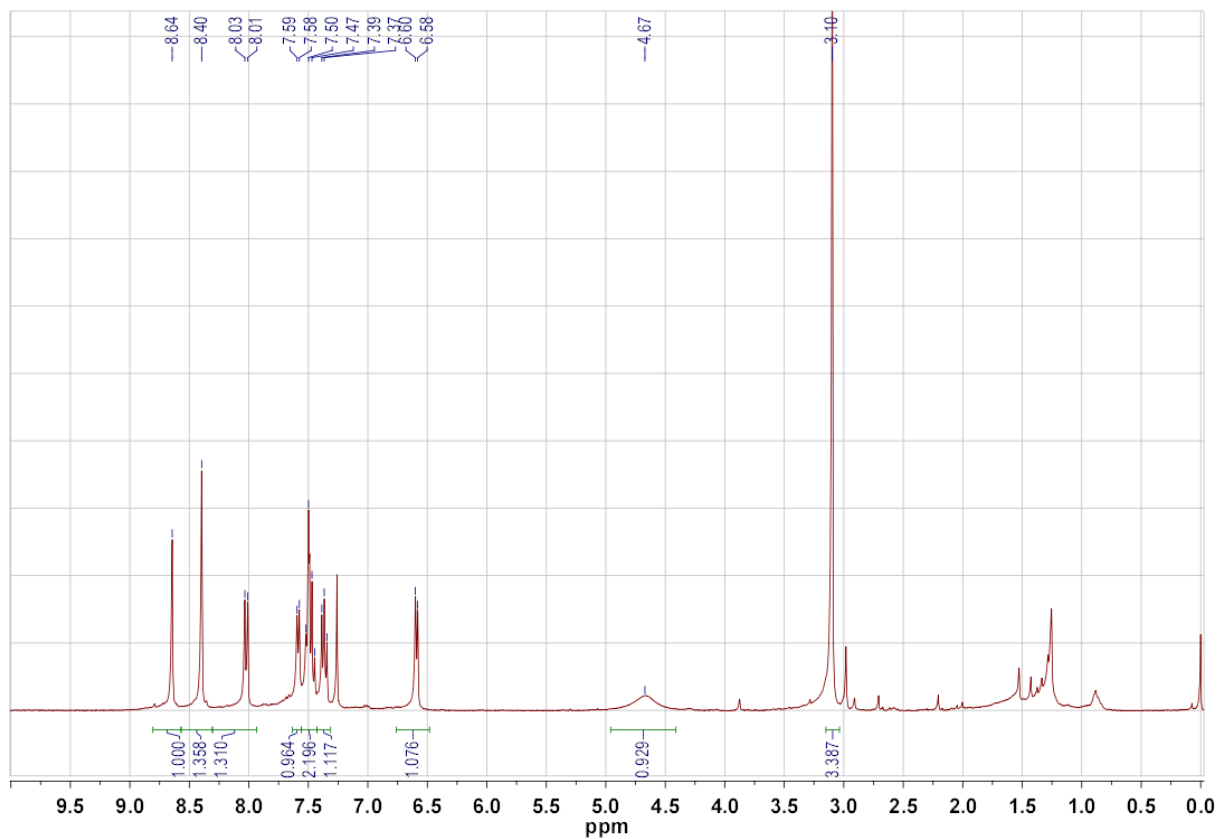


**Figure S52.** The excitation spectra of 1,5-diisocyanoanthracene (**DIA**) recorded in solvents of different polarity. ( $c=5\times10^{-5}$  M,  $T=20$  °C,  $V=3.00$  ml).

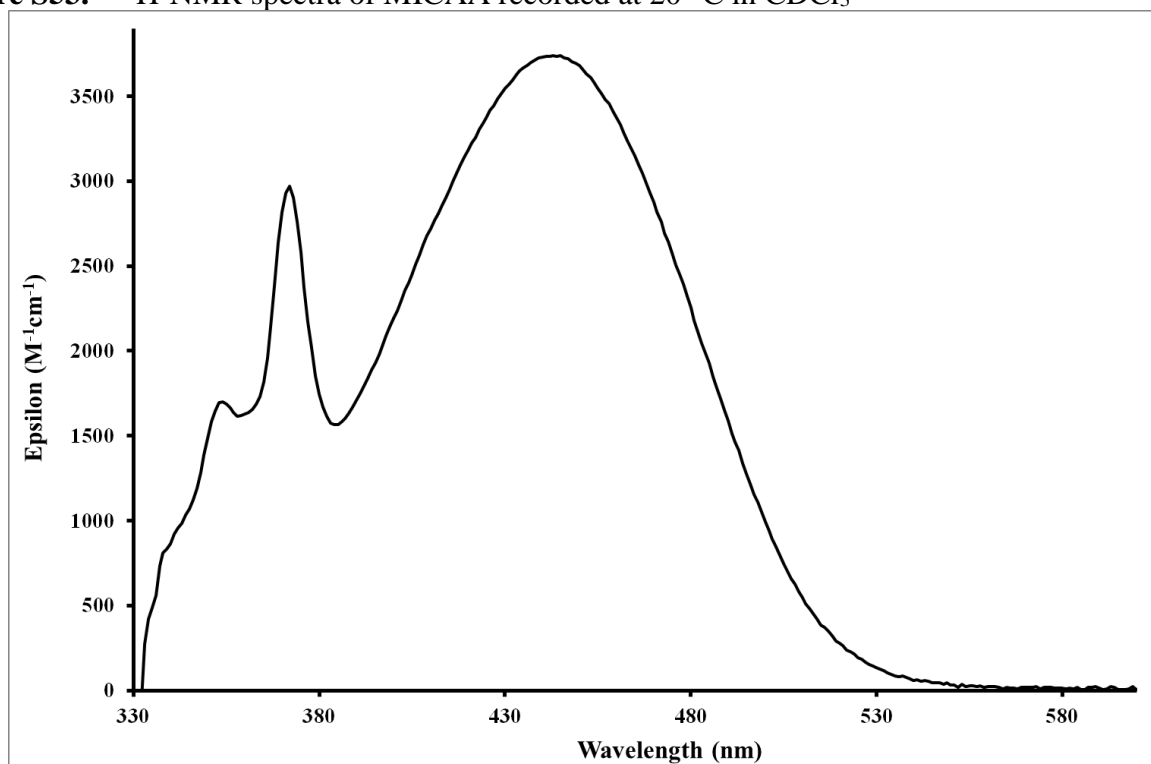
Solvent	Polarity	$\lambda_{em,max,1}$	$\lambda_{em,max,2}$	$\lambda_{em,max,3}$	$\lambda_{ex,max,1}$	$\lambda_{ex,max,2}$	$\lambda_{ex,max,3}$	$\lambda_{ex,max,4}$	Stokes shift	$\epsilon$	$\Phi_F$
	Index	(nm)	(nm)	(nm)	(nm)	(nm)	(nm)	(nm)	(cm <sup>-1</sup> )	(M <sup>-1</sup> )	(%)
Hexane	0.0	397	420	446	337	354	373	394	3000	-	-
Toluene	2.4	405	428	455	341	359	378	399	3091	9989	38
Dichloromethane	3.1	401	424	451	340	357	376	397	3011	10942	25
i-propanol	3.9	398	422	449	338	355	375	395	2970	11217	38
THF	4.0	401	424	451	339	357	376	397	3011	10720	38
Chloroform	4.1	401	425	452	340	358	377	398	2996	11488	26
Ethyl acetate	4.4	397	422	448	338	355	374	395	3041	11618	30
Dioxane	4.8	401	424	451	340	357	376	397	3011	11258	44
Acetone	5.1	397	422	449	339	355	375	395	2970	10852	33
Methanol	5.1	397	421	448	337	355	374	395	2985	10784	30
Pyridine	5.3	406	429	456	342	360	379	400	3075	10360	12
Acetonitrile	5.8	397	422	449	338	356	375	395	2970	11034	31
Dimethyl formamide	6.4	403	427	453	341	358	377	398	3106	10667	42
Dimethyl sulfoxide	7.2	406	429	456	342	360	379	400	3075	10836	30
Water	9.0	-	-	-	-	-	-	-	-	-	-



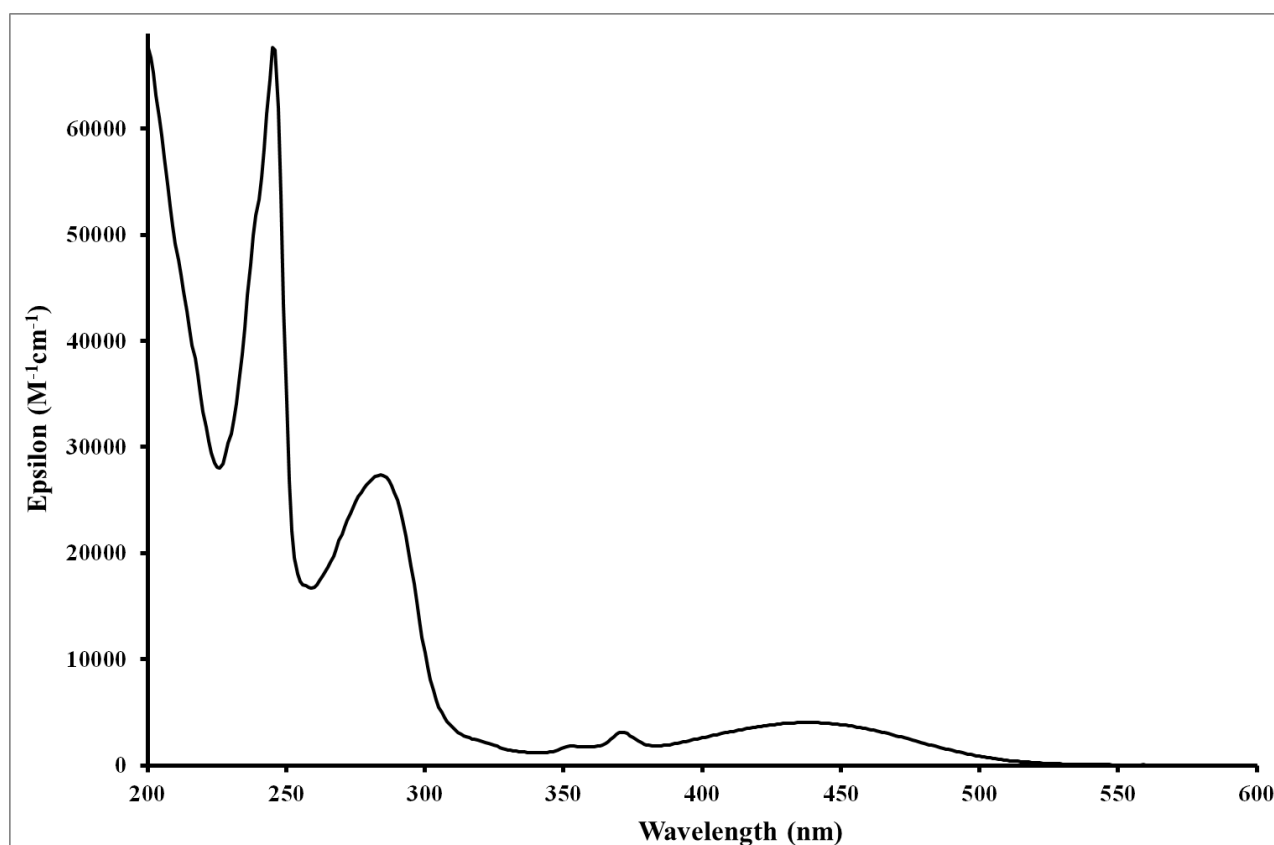
## Chapter IV. 1-N-methylamino-5-isocyanoanthracene (MICAA)



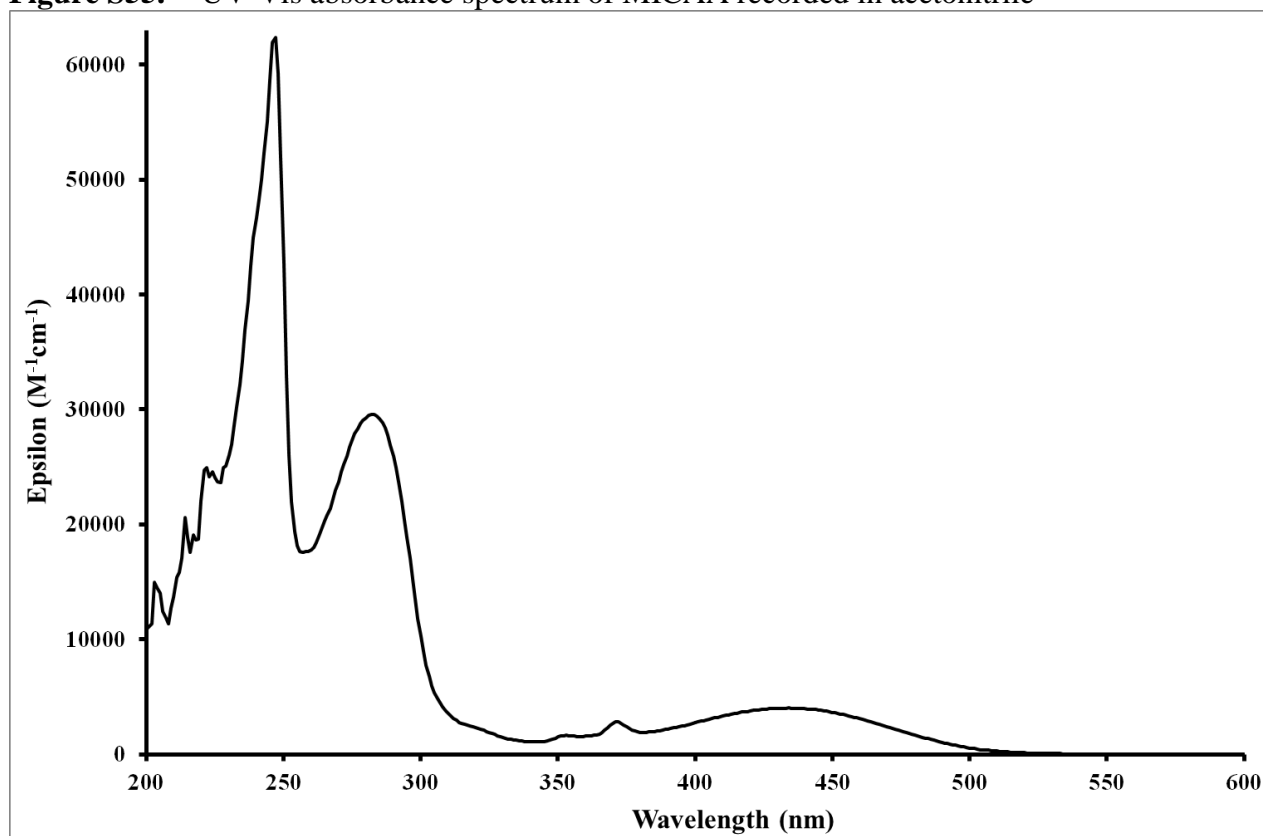
**Figure S53.** <sup>1</sup>H-NMR spectra of MICAA recorded at 20 °C in CDCl<sub>3</sub>



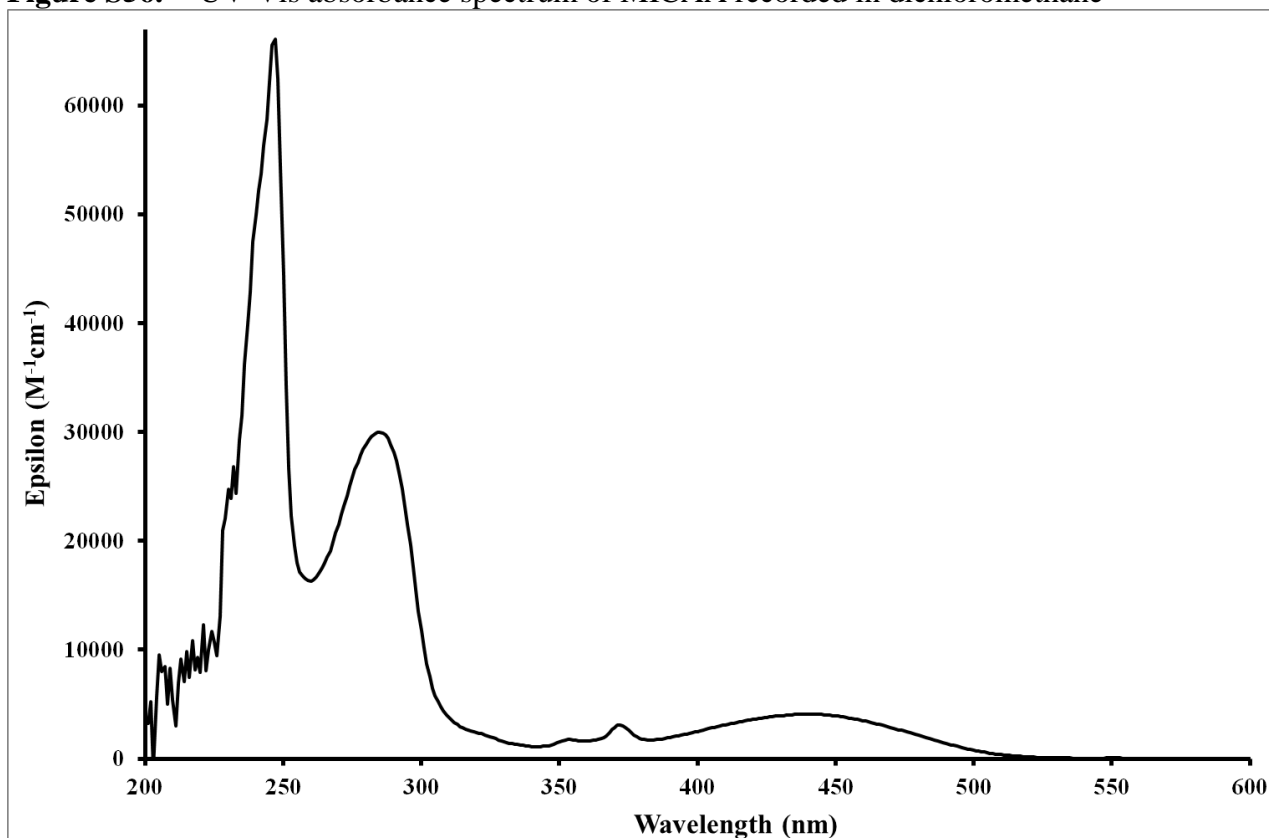
**Figure S54.** UV-Vis absorbance spectrum of MICA A recorded in acetone



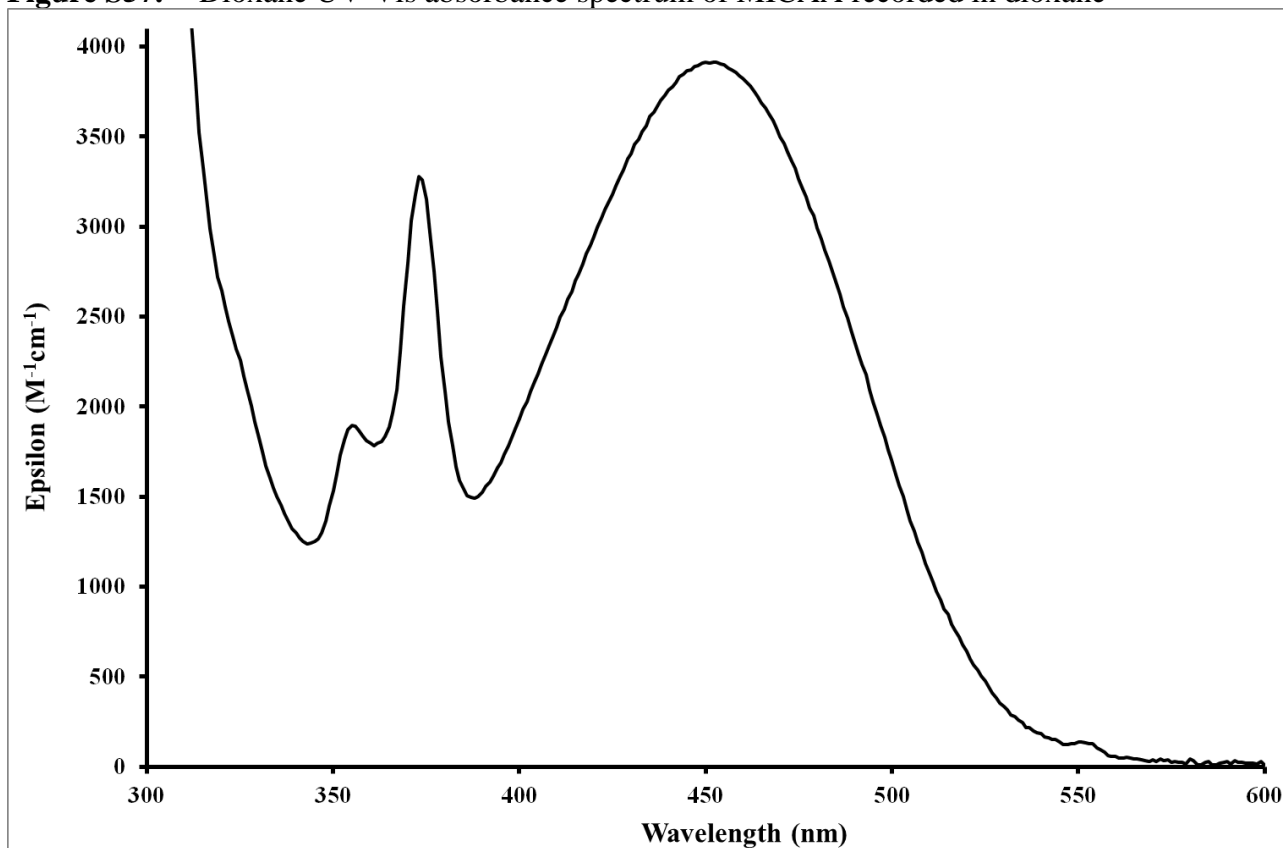
**Figure S55.** UV-Vis absorbance spectrum of MICA A recorded in acetonitrile



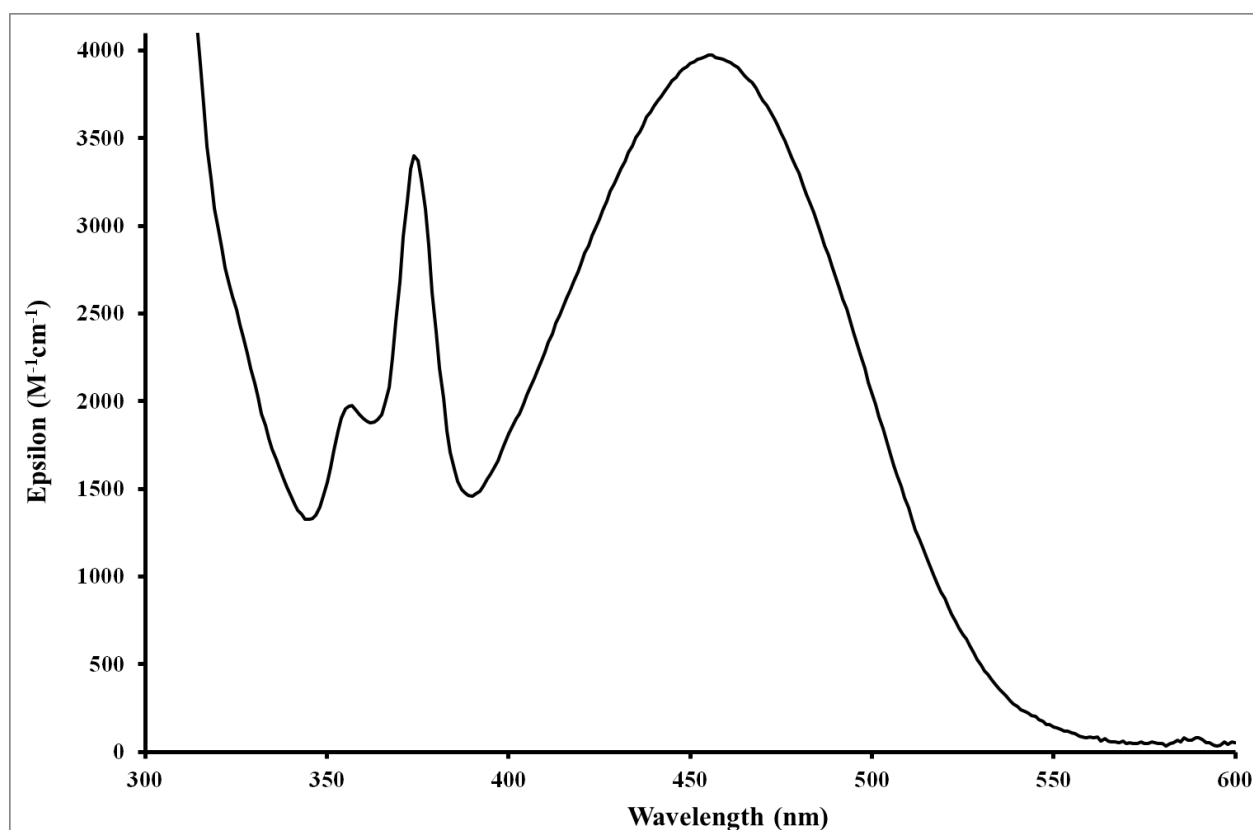
**Figure S56.** UV-Vis absorbance spectrum of MICA A recorded in dichloromethane



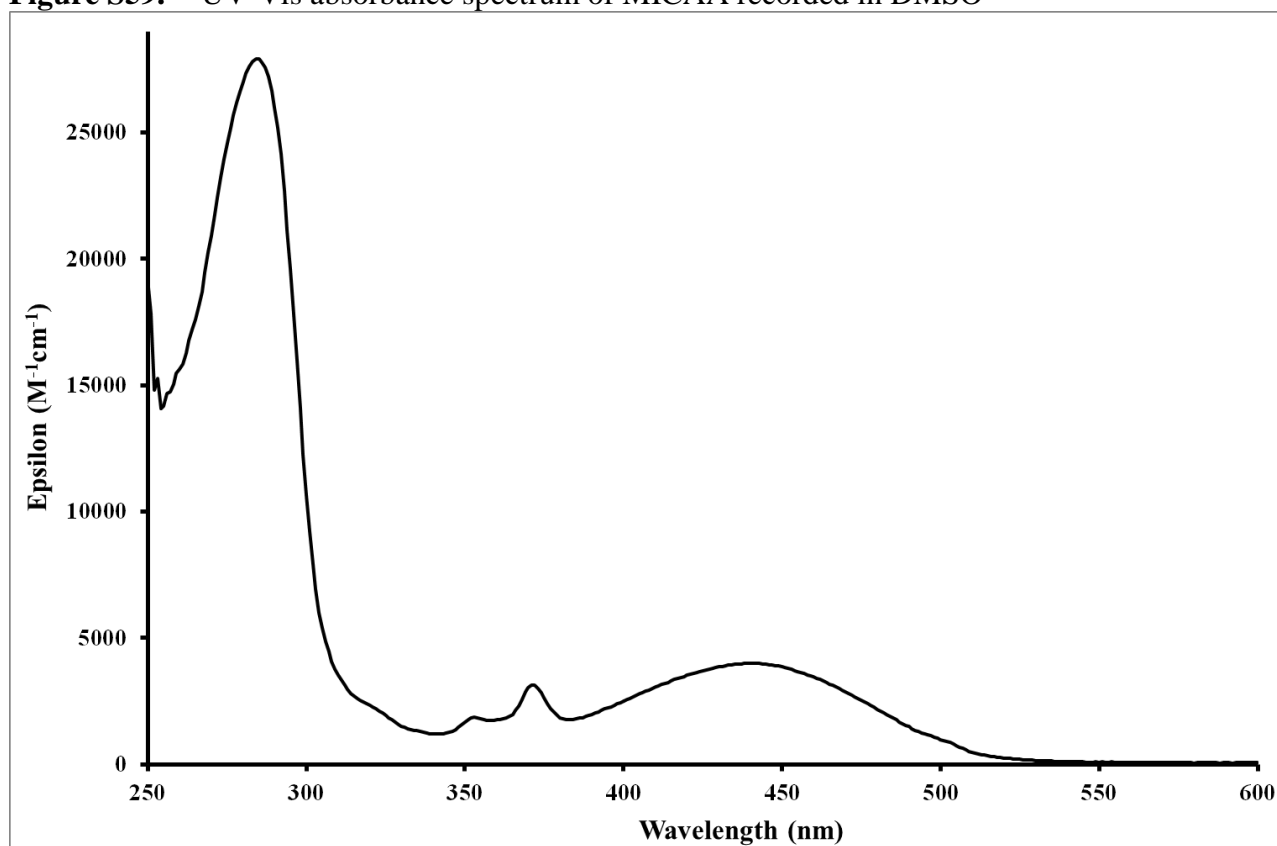
**Figure S57.** Dioxane UV-Vis absorbance spectrum of MICA A recorded in dioxane



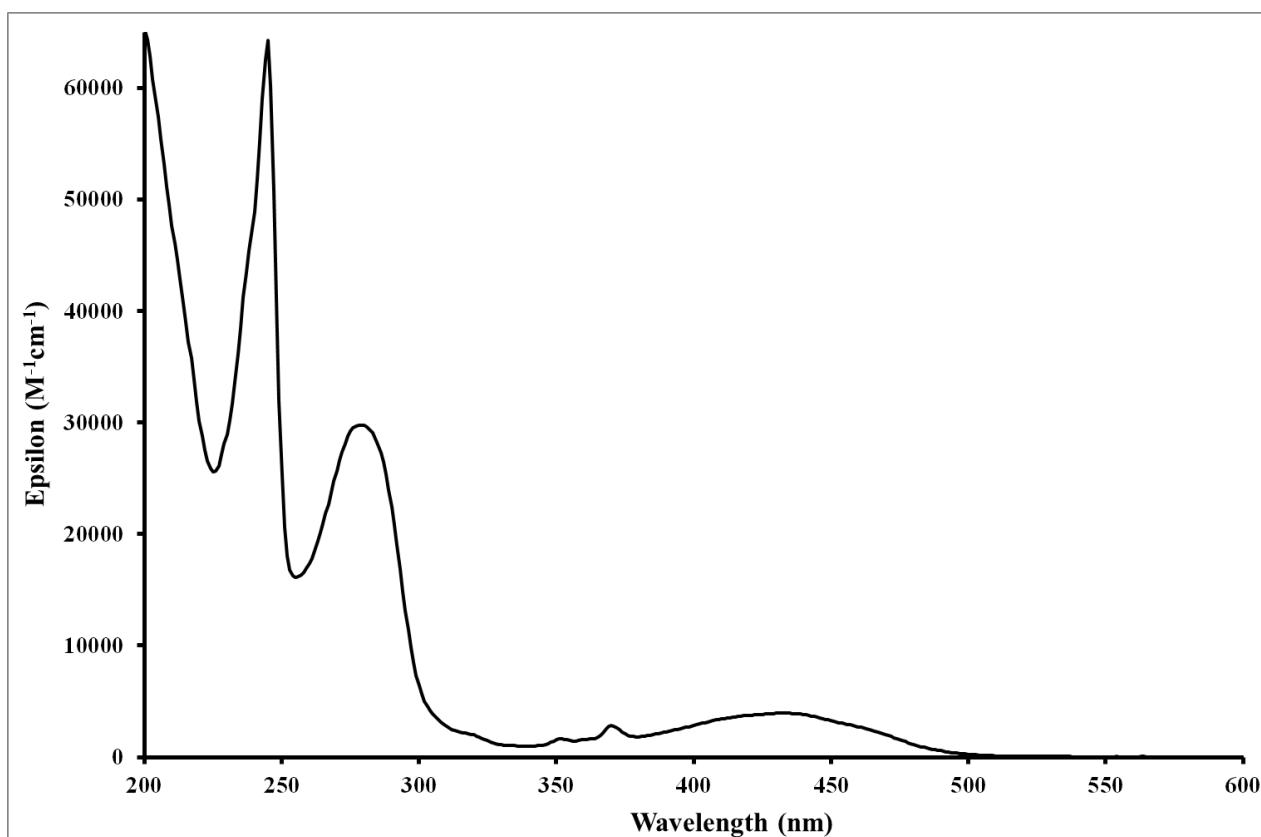
**Figure S58.** UV-Vis absorbance spectrum of MICA A recorded in DMF



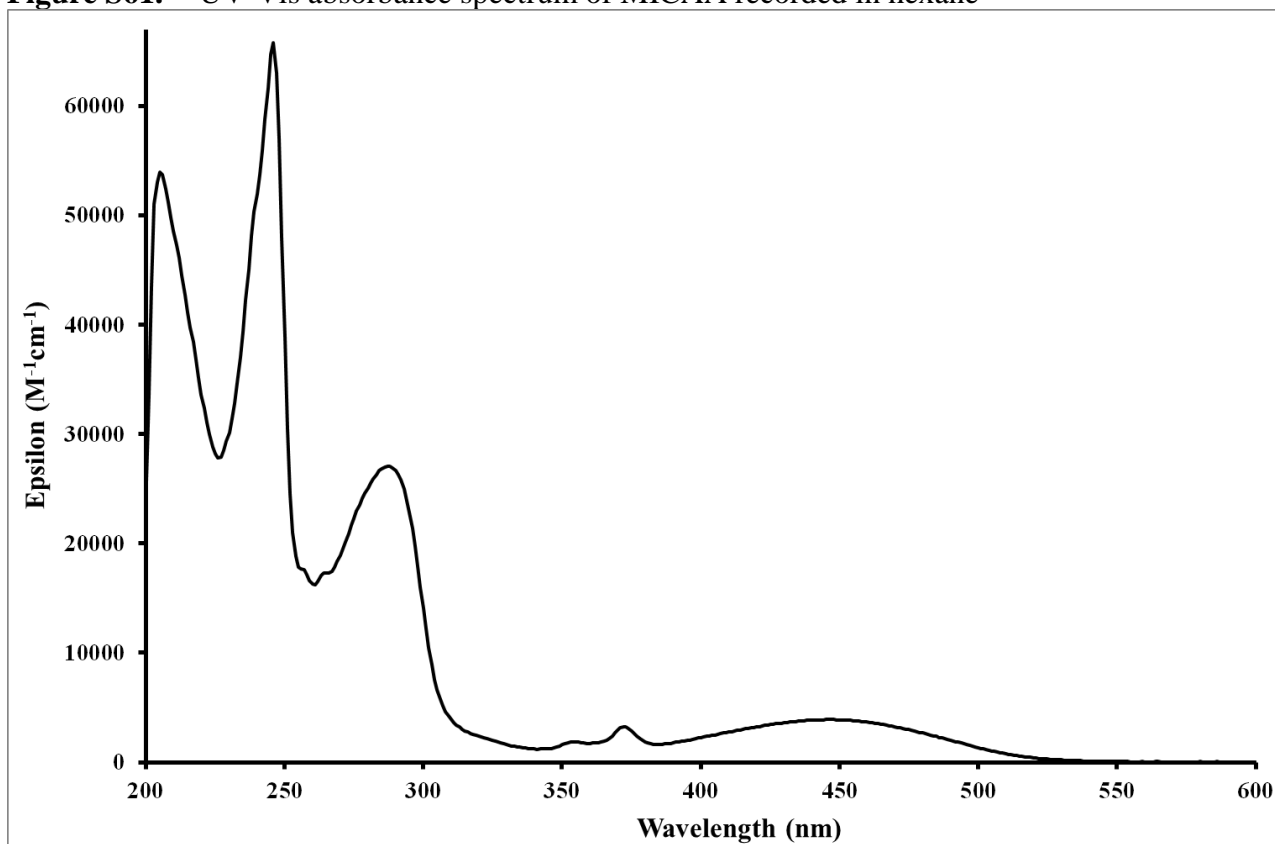
**Figure S59.** UV-Vis absorbance spectrum of MICA in DMSO



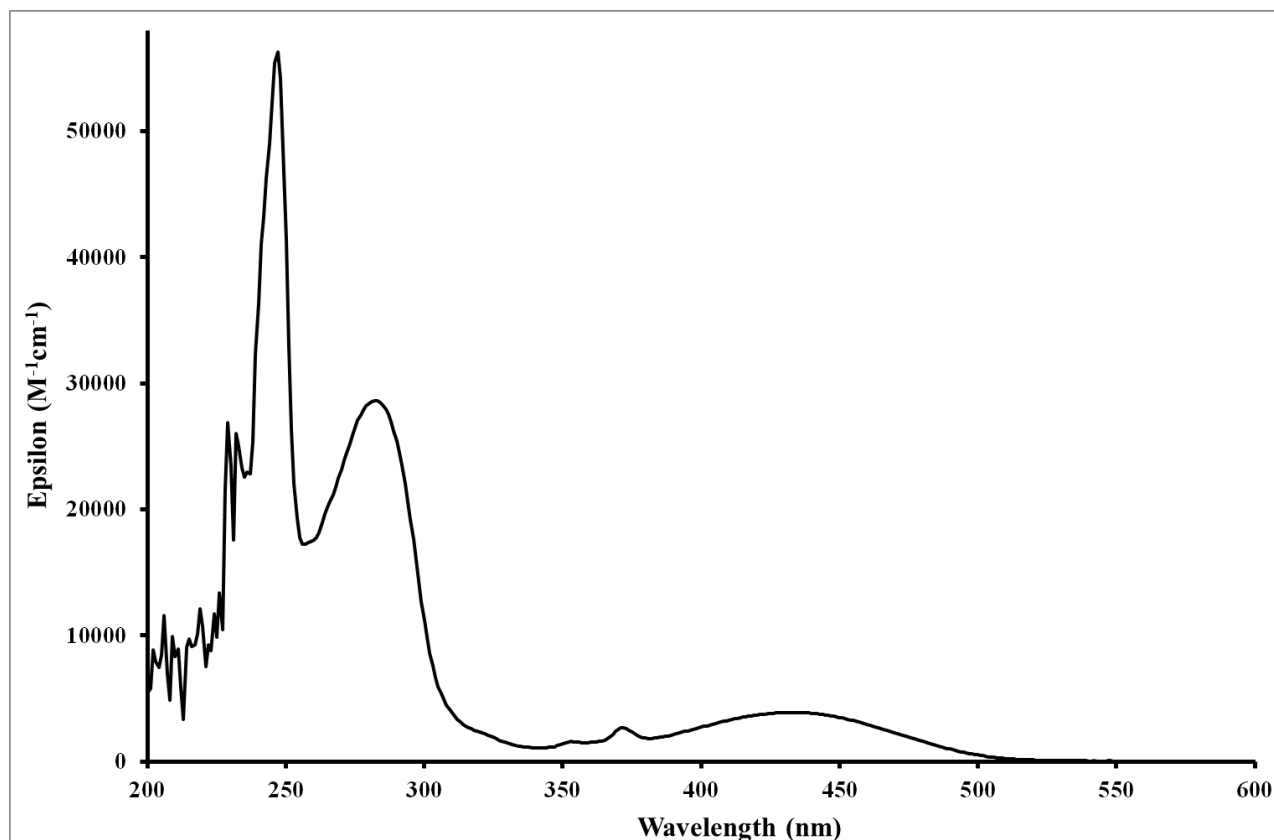
**Figure S60.** UV-Vis absorbance spectrum of MICA A recorded in ethyl-acetate



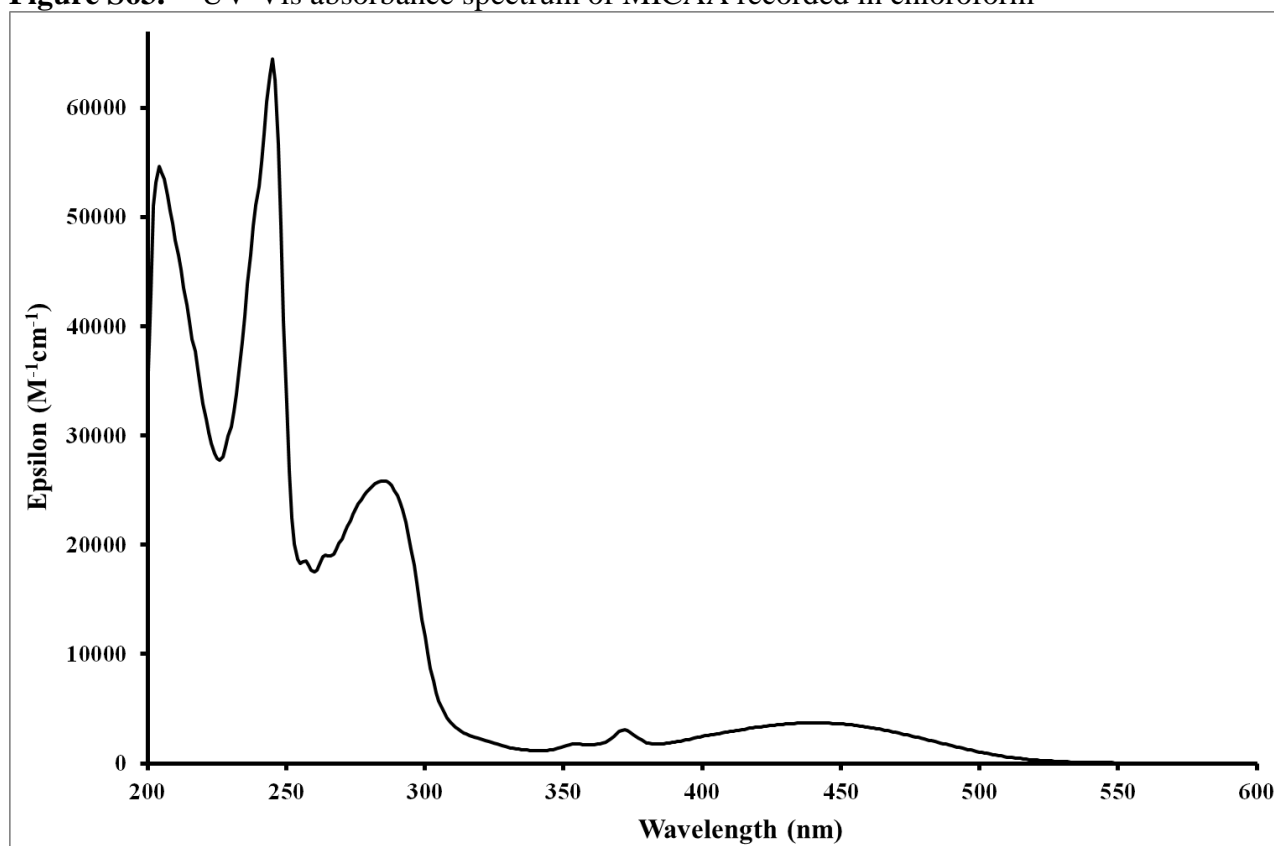
**Figure S61.** UV-Vis absorbance spectrum of MICA A recorded in hexane



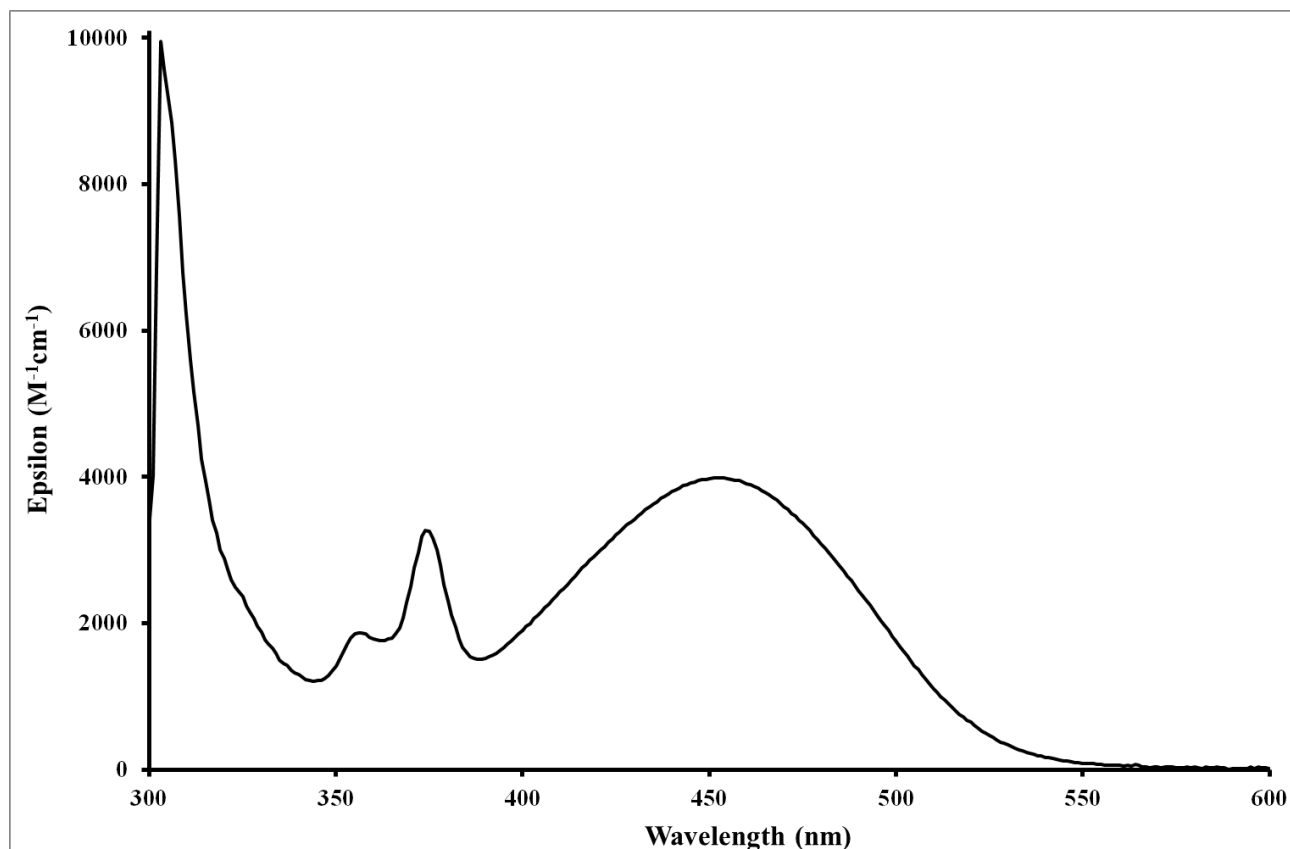
**Figure S62.** UV-Vis absorbance spectrum of MICA A recorded in isopropanole



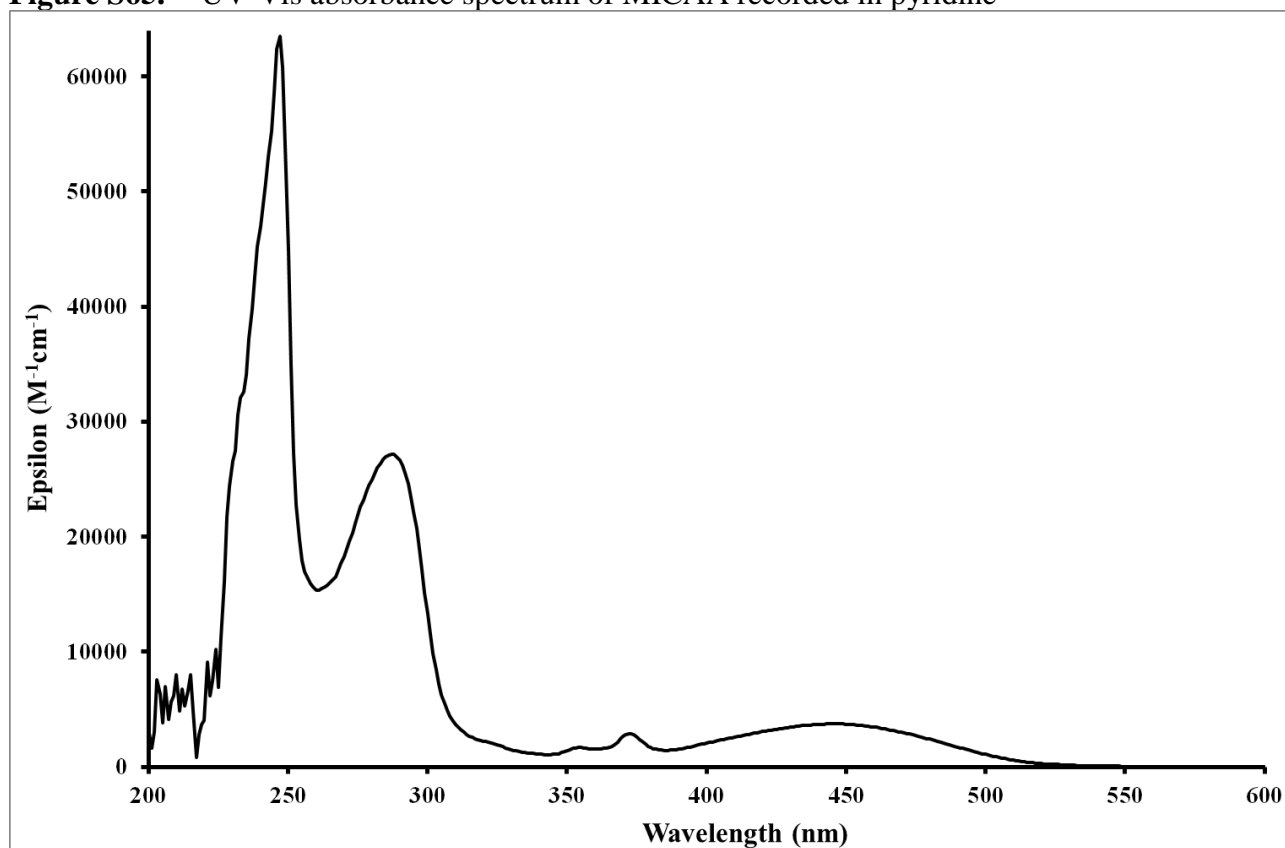
**Figure S63.** UV-Vis absorbance spectrum of MICA recorded in chloroform



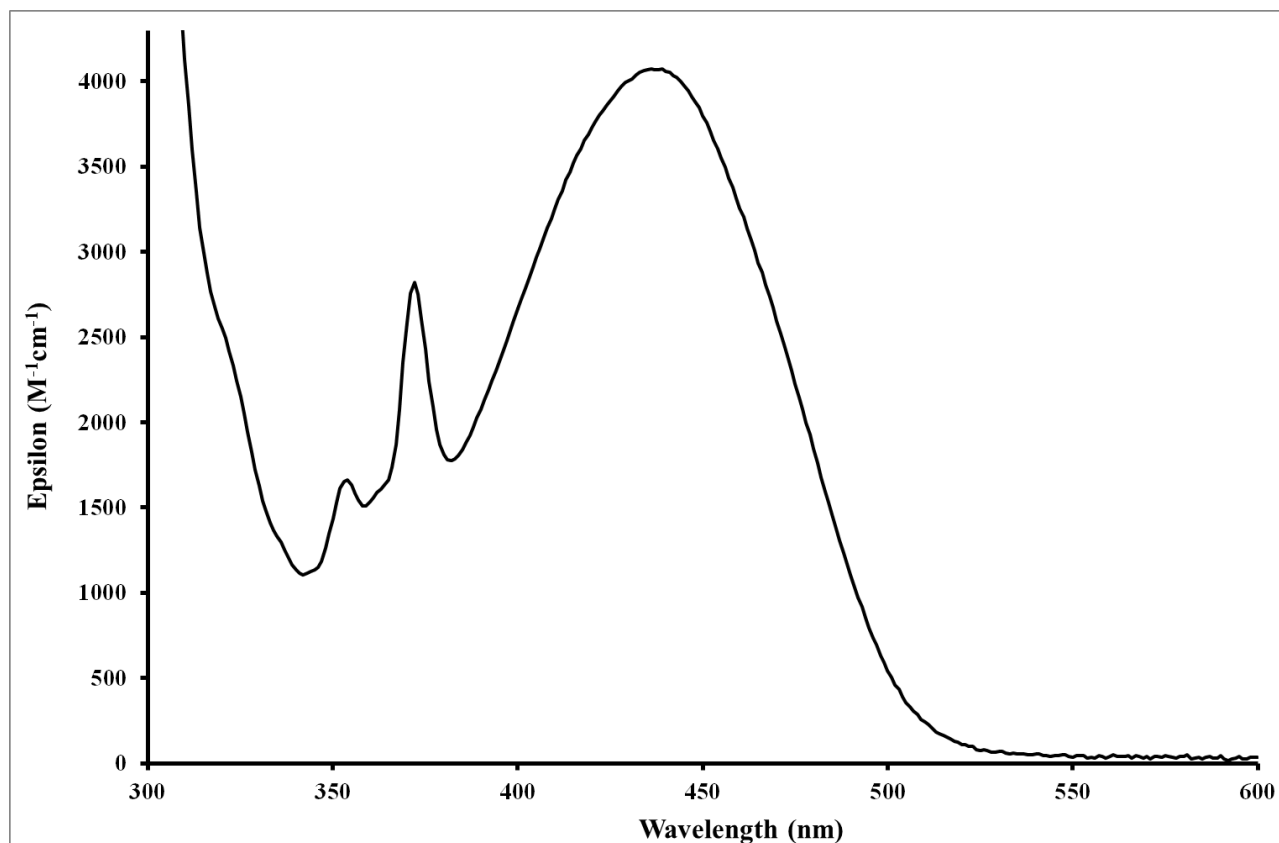
**Figure S64.** UV-Vis absorbance spectrum of MICA recorded in methanol



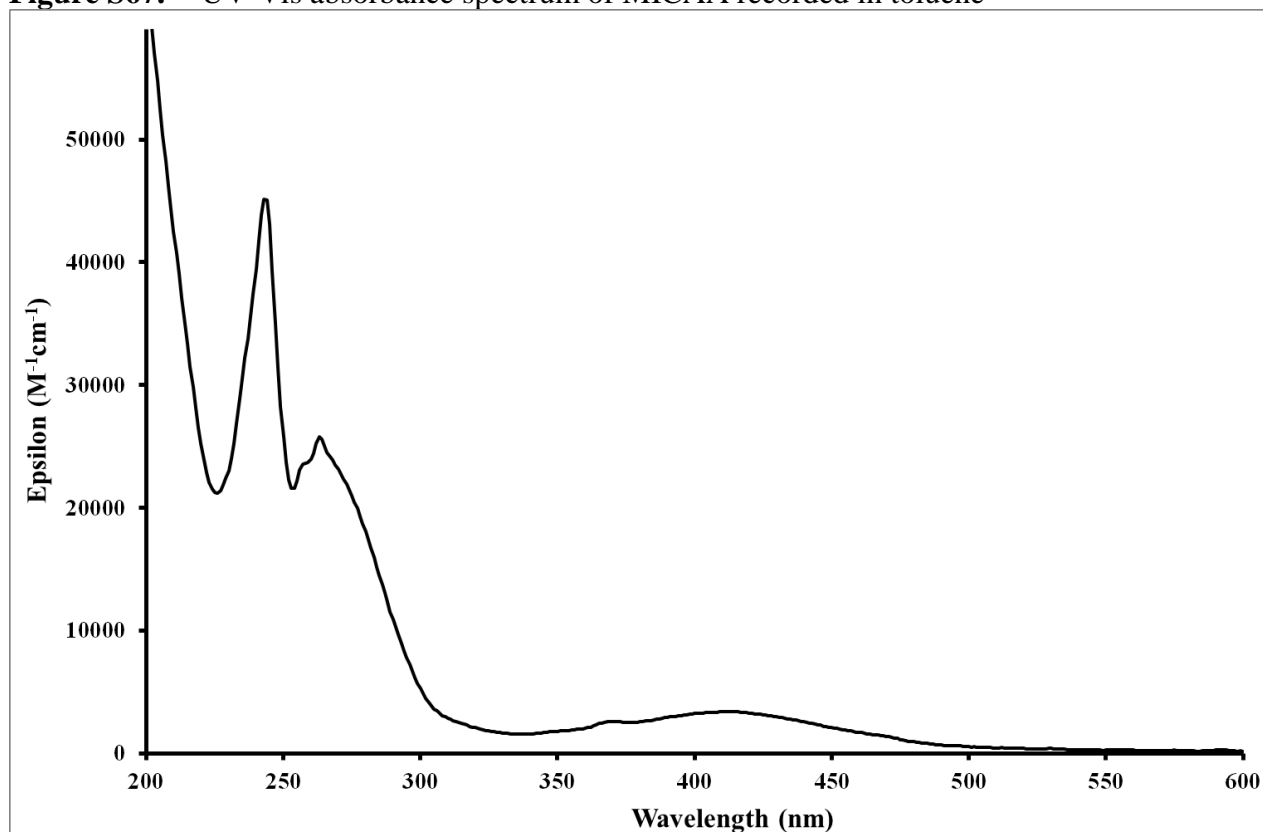
**Figure S65.** UV-Vis absorbance spectrum of MICA in pyridine



**Figure S66.** UV-Vis absorbance spectrum of MICA in tetrahydrofuran

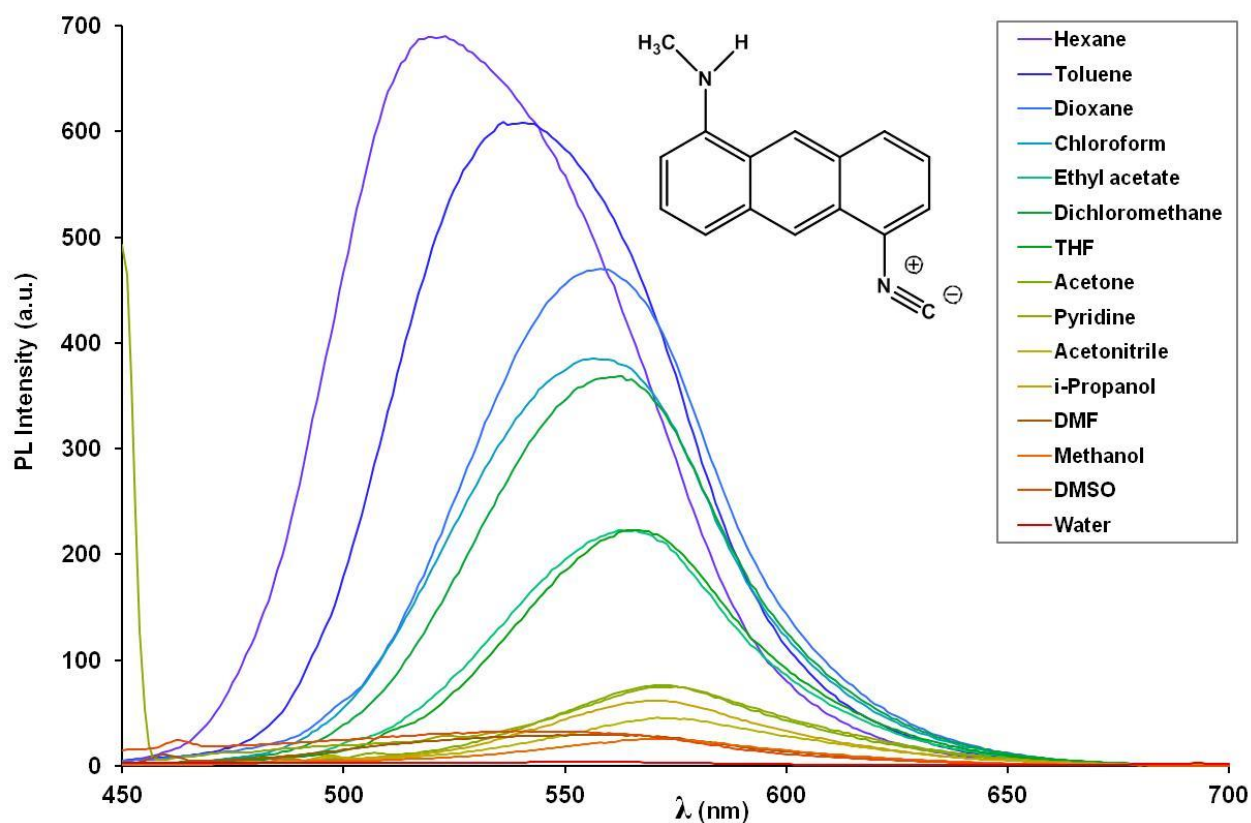


**Figure S67.** UV-Vis absorbance spectrum of MICA in toluene

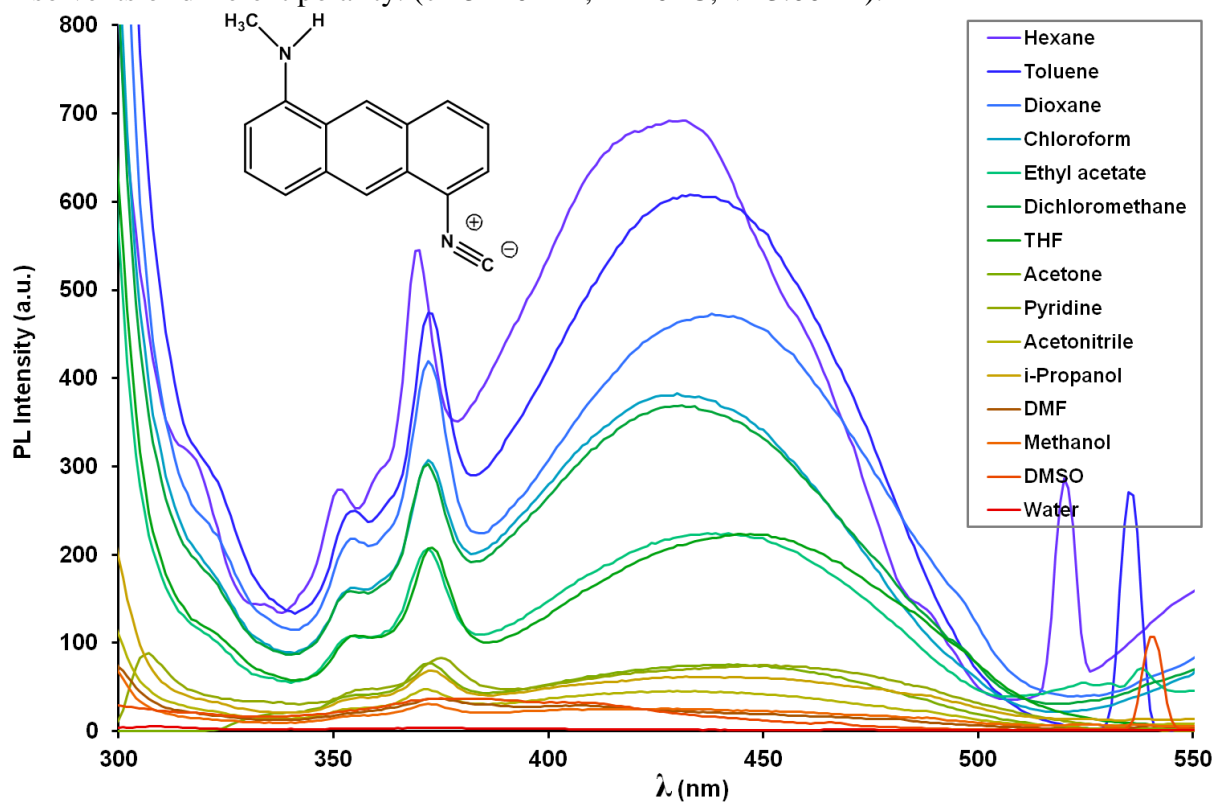


**Figure S68.** UV-Vis absorbance spectrum of MICA in water



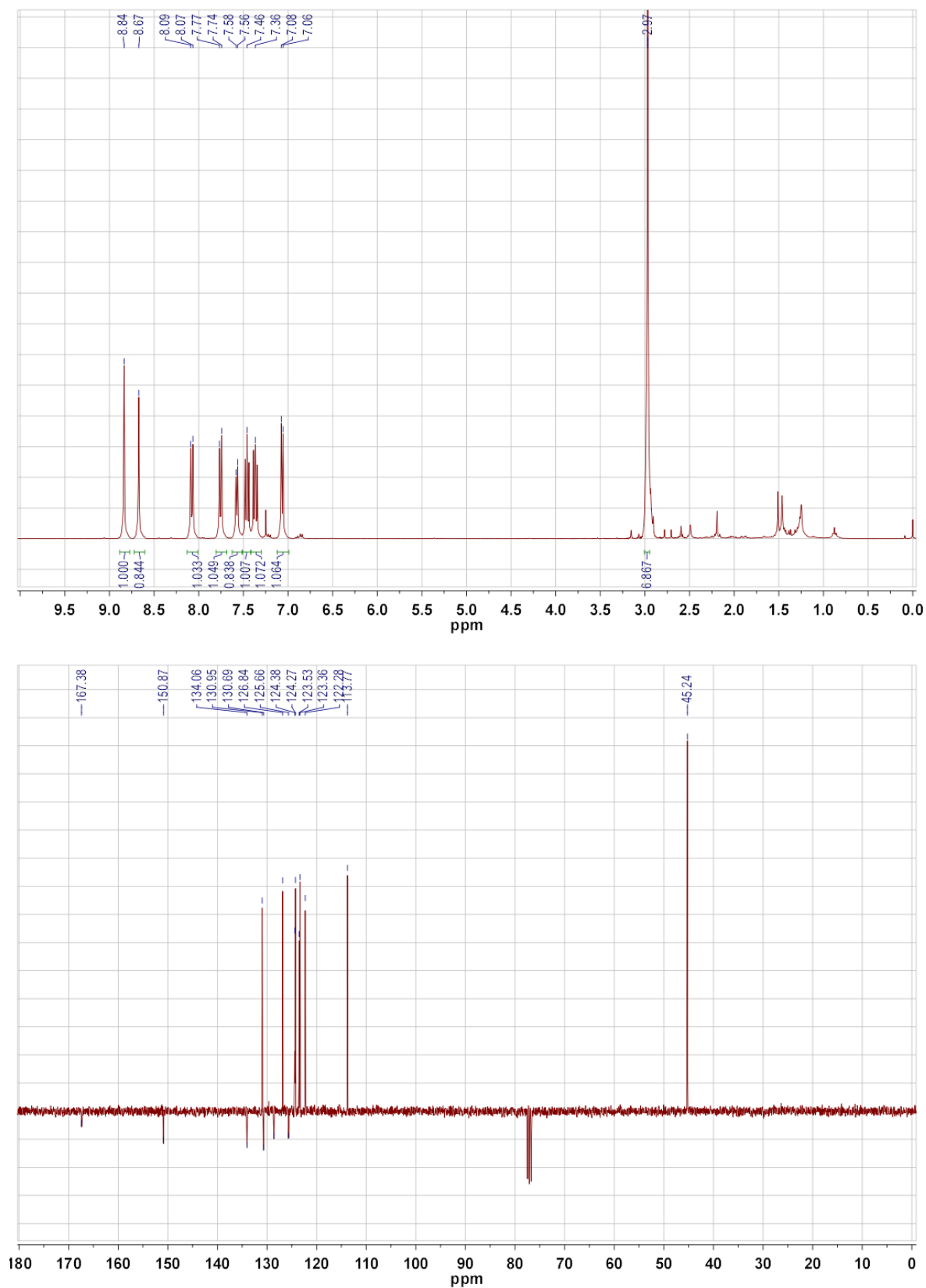


**Figure S69.** The emission spectra of 1-N-methylamino-5-isocyanoanthracene (MICA) recorded in solvents of different polarity. ( $c=5\times10^{-5}$  M,  $T=20$  °C,  $V=3.00$  ml).

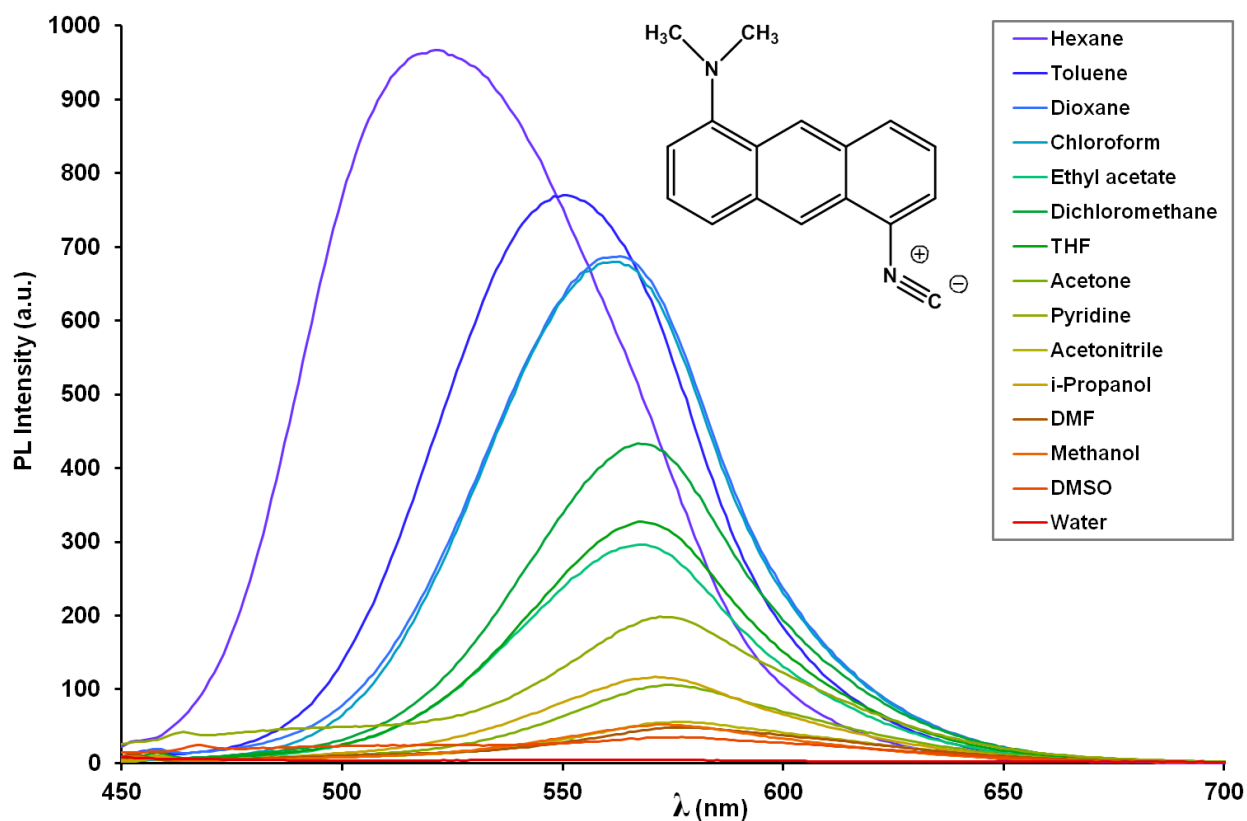


**Figure S70.** The excitation spectra of 1-N-methylamino-5-isocyanoanthracene (MICA) recorded in solvents of different polarity. ( $c=5\times10^{-5}$  M,  $T=20$  °C,  $V=3.00$  ml).

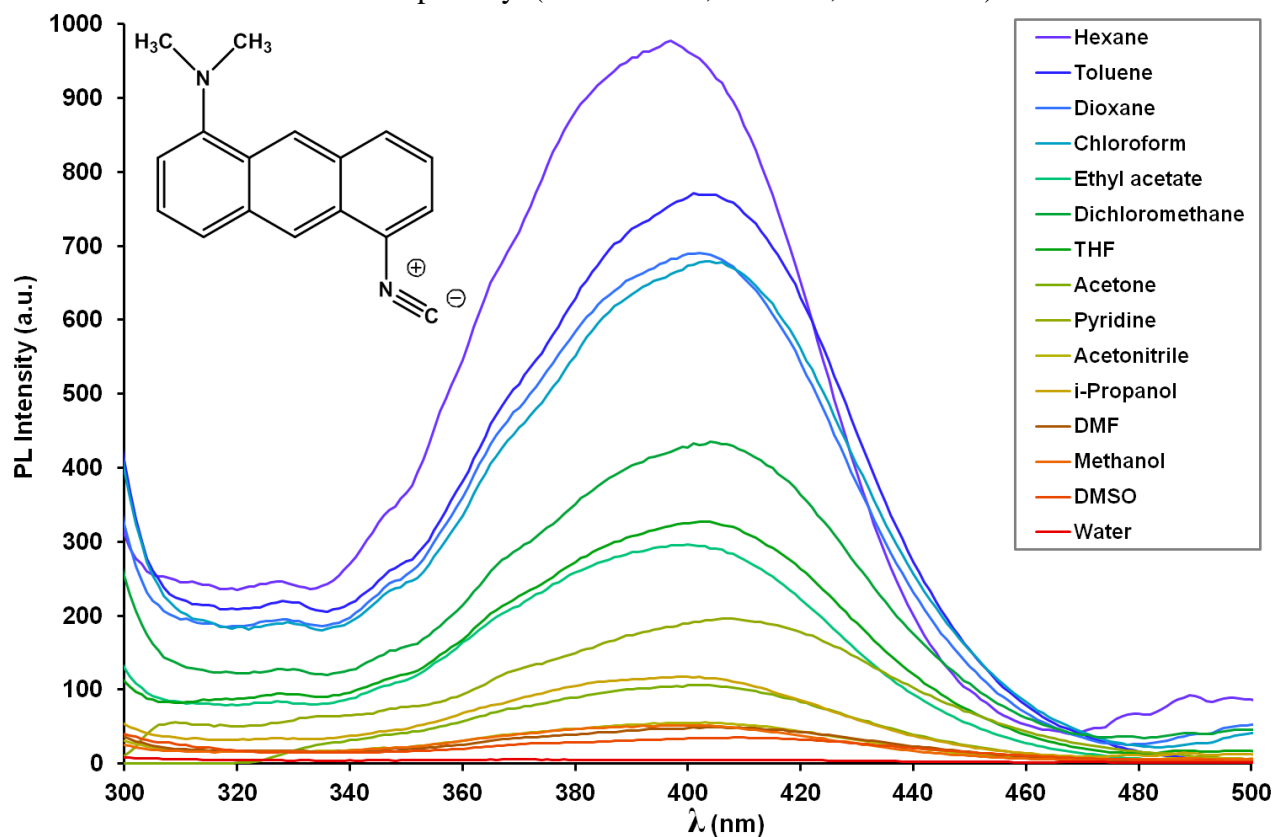
## Chapter V. 1-N,N-dimethylamino-5-isocyanoanthracene (DIMICAA)



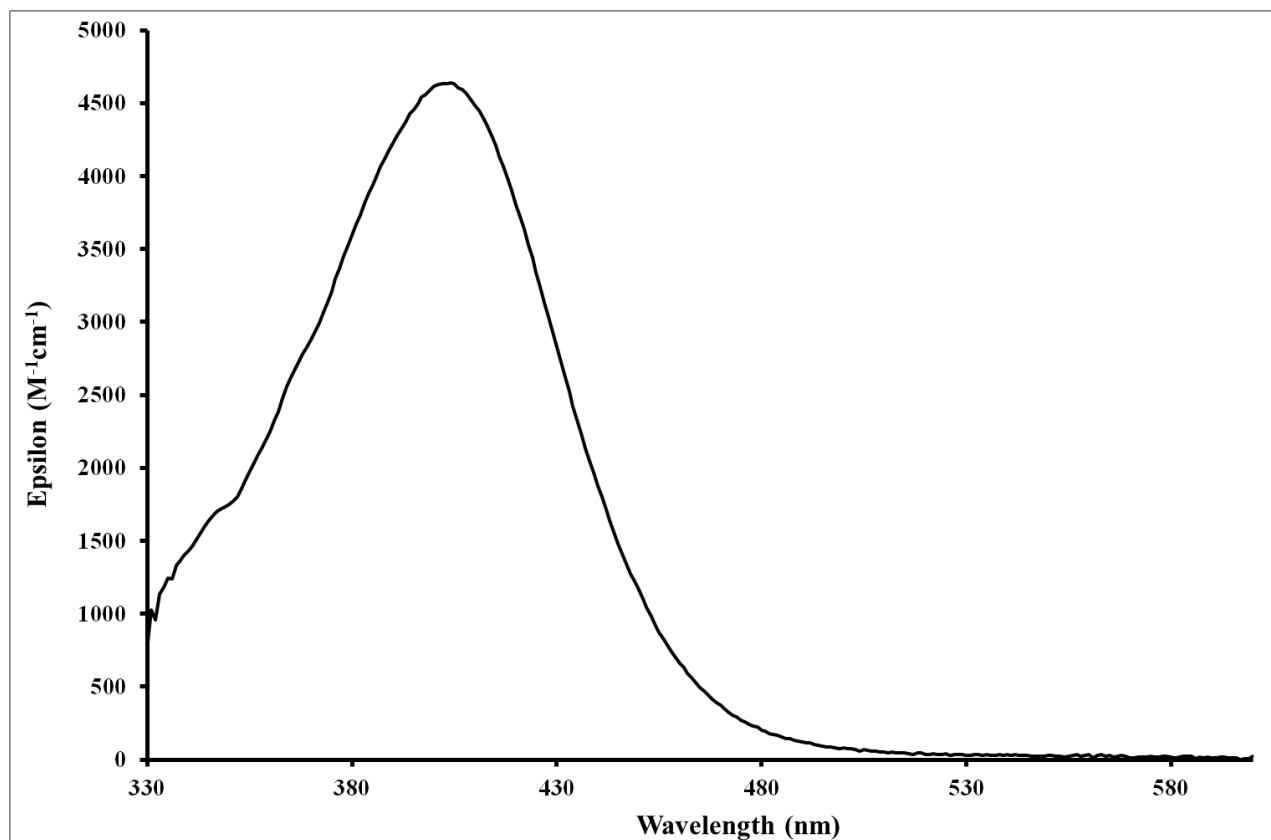
**Figure S71.**  $^1\text{H}$ -NMR (top) and  $^{13}\text{C}$ -NMR (bottom) spectra of 1-N,N-dimethylamino-5-isocyanoanthracene (DIMICAA) recorded at 20 °C in  $\text{CDCl}_3$



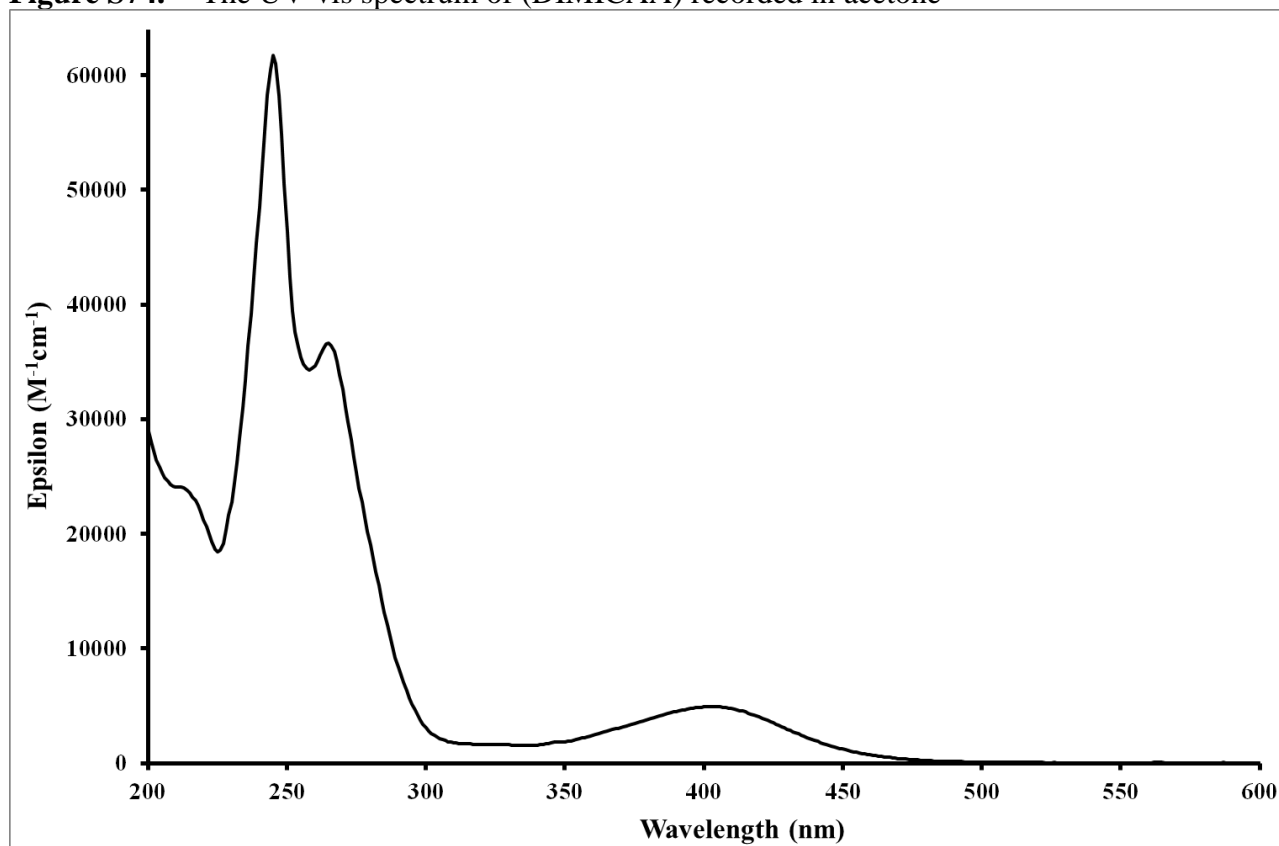
**Figure S72.** The emission spectra of 1-N,N-dimethylamino-5-isocyanoanthracene (DIMICAA) recorded in solvents of different polarity. ( $c=5\times10^{-5}$  M,  $T=20$  °C,  $V=3.00$  ml).



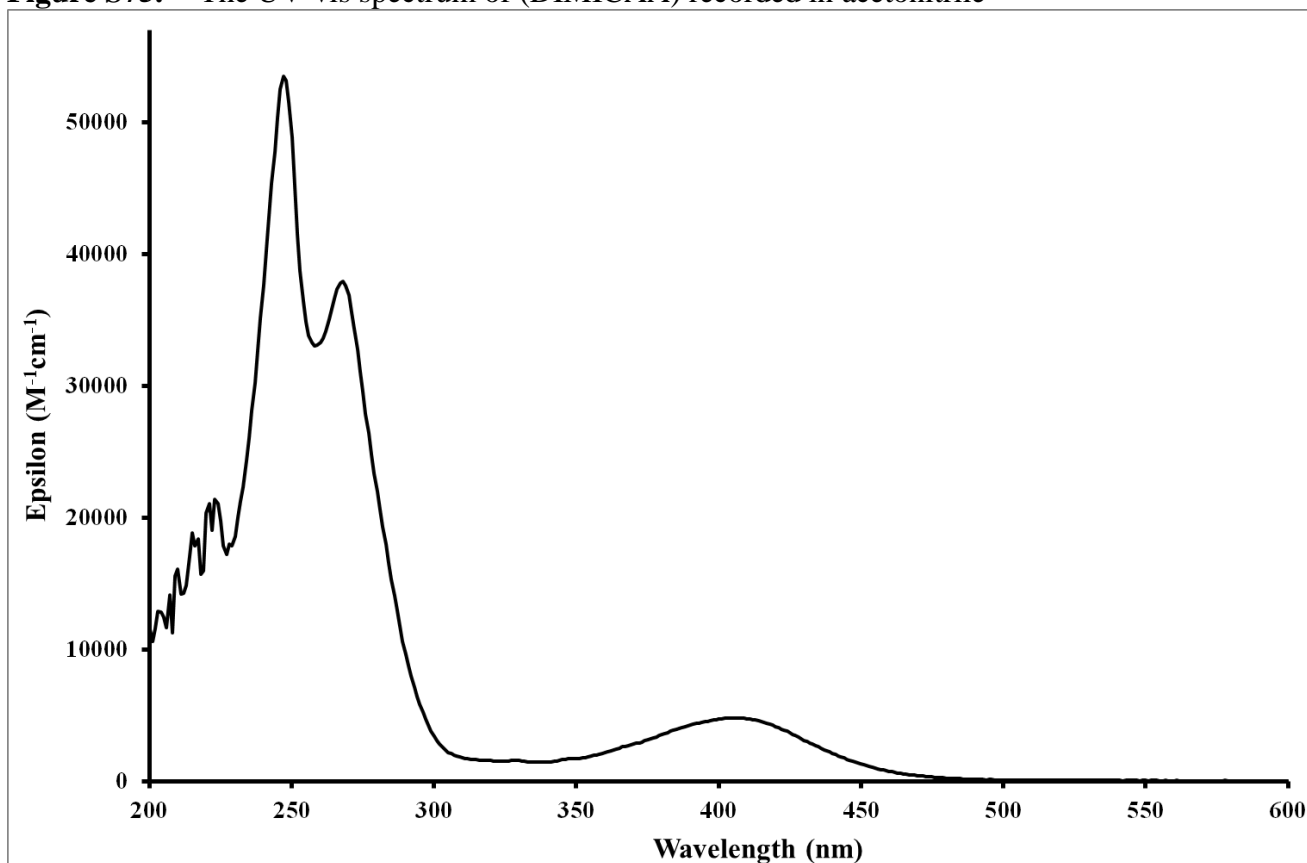
**Figure S73.** The excitation spectra of 1-N,N-dimethylamino-5-isocyanoanthracene (DIMICAA) recorded in solvents of different polarity. ( $c=5\times10^{-5}$  M,  $T=20$  °C,  $V=3.00$  ml).



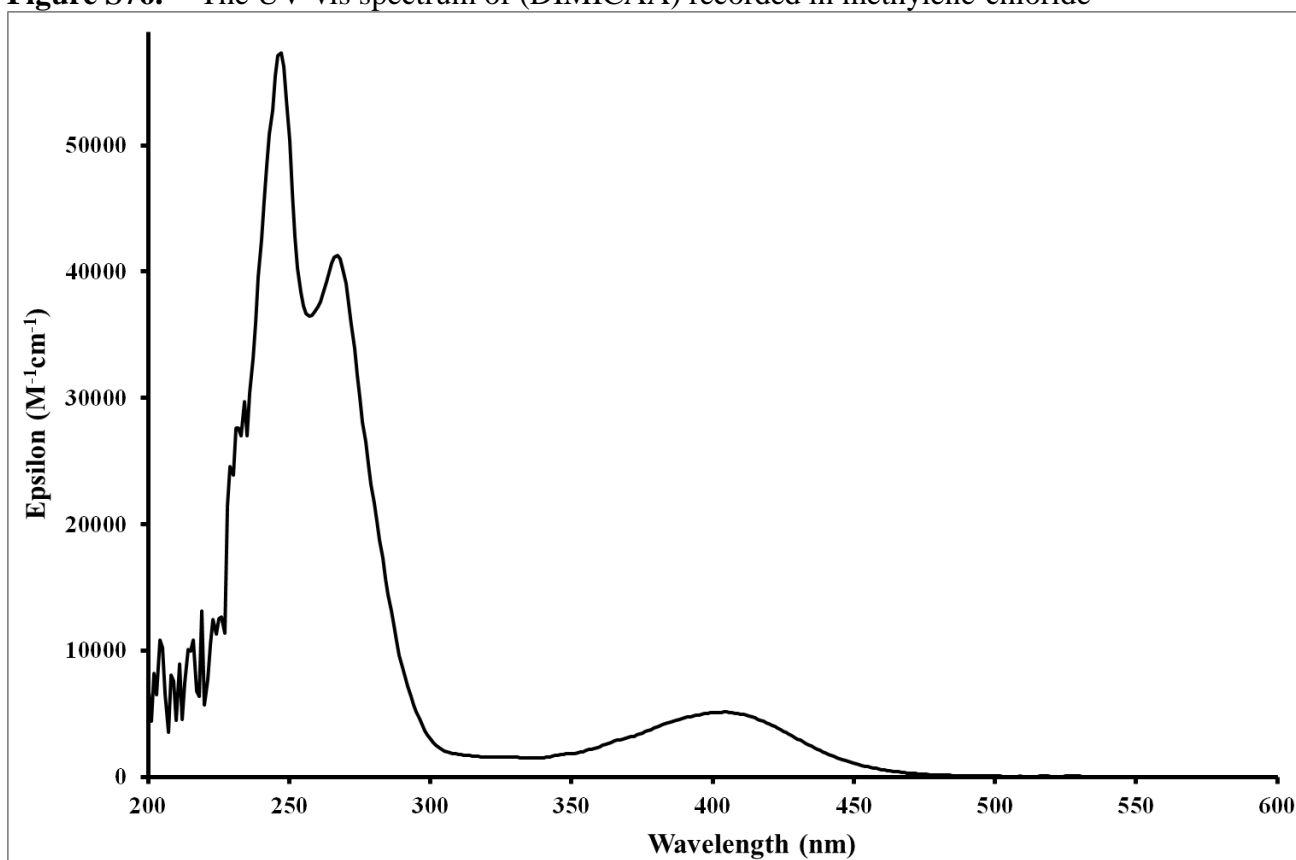
**Figure S74.** The UV-vis spectrum of (DIMICAA) recorded in acetone



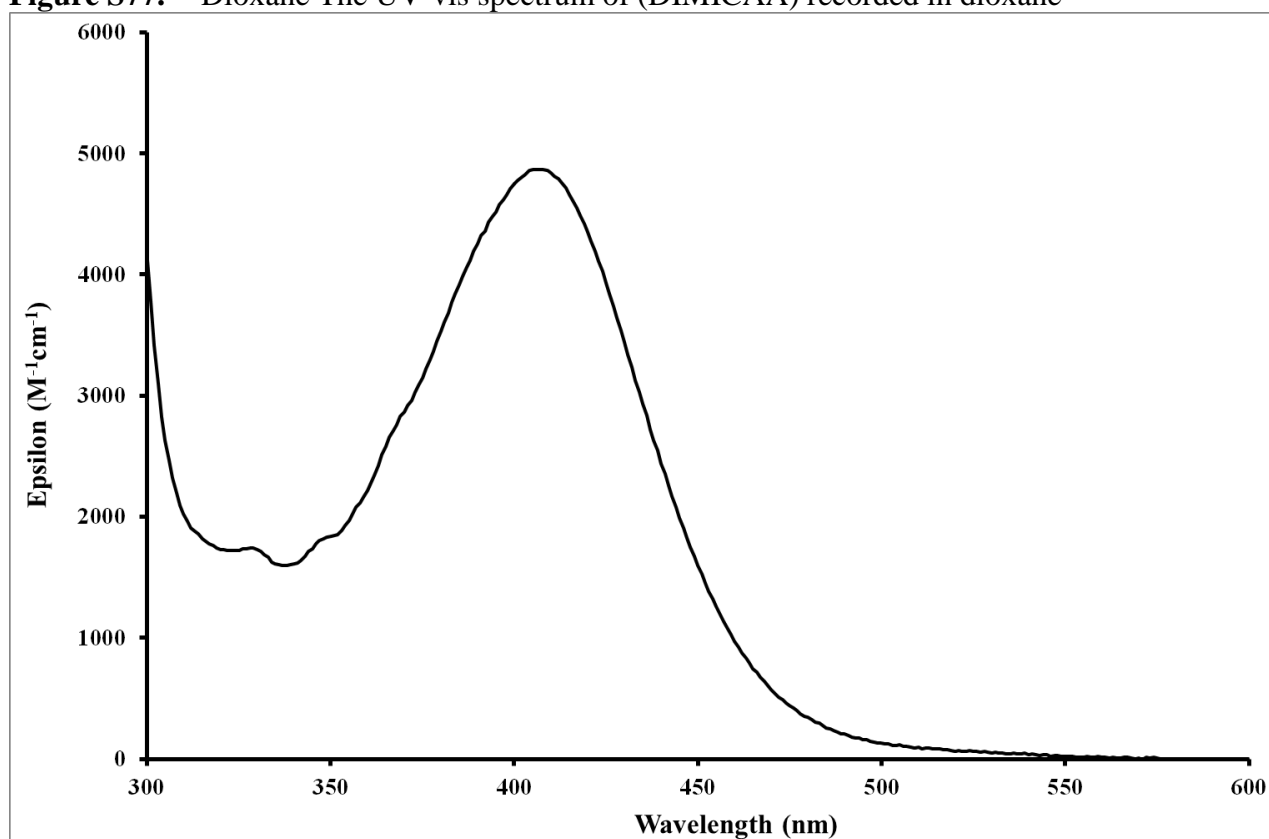
**Figure S75.** The UV-vis spectrum of (DIMICAA) recorded in acetonitrile



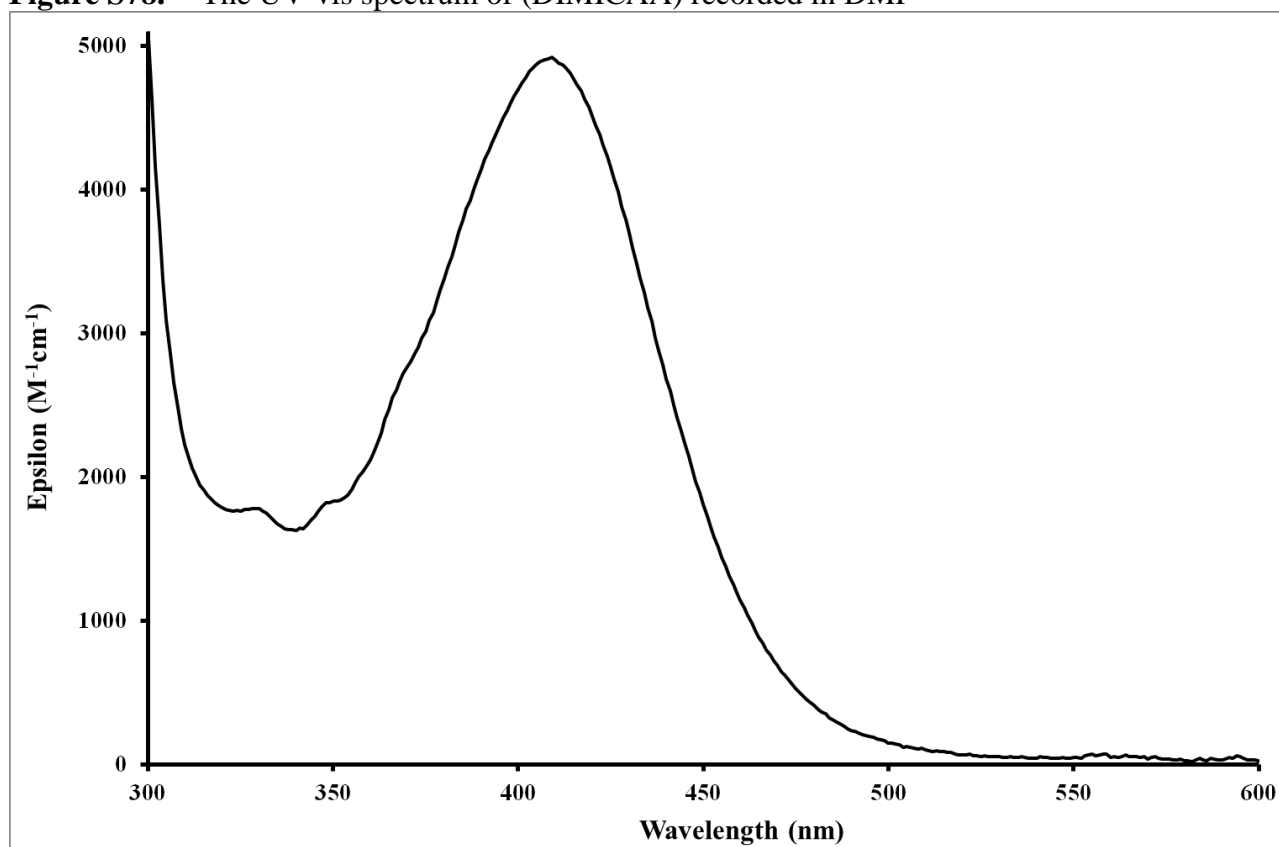
**Figure S76.** The UV-vis spectrum of (DIMICAA) recorded in methylene-chloride



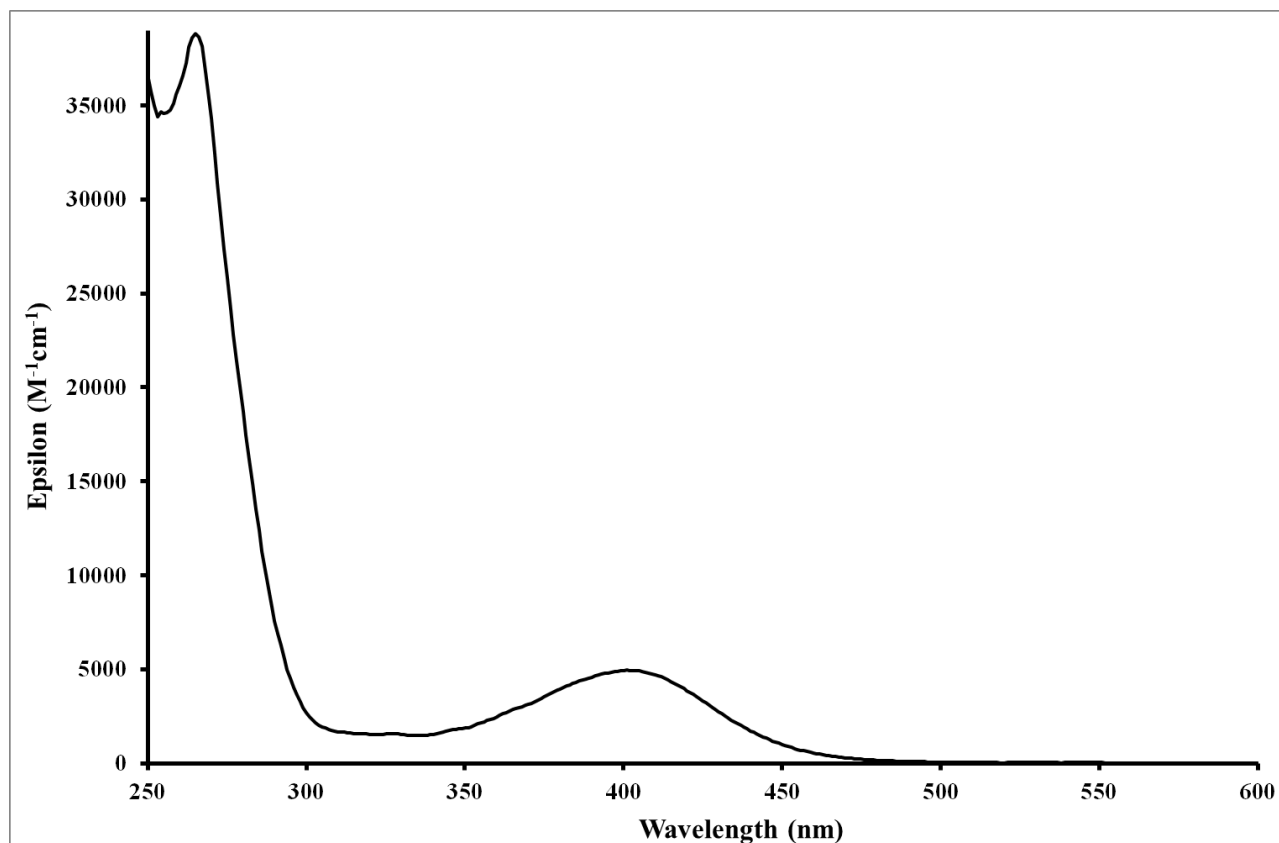
**Figure S77.** Dioxane The UV-vis spectrum of (DIMICAA) recorded in dioxane



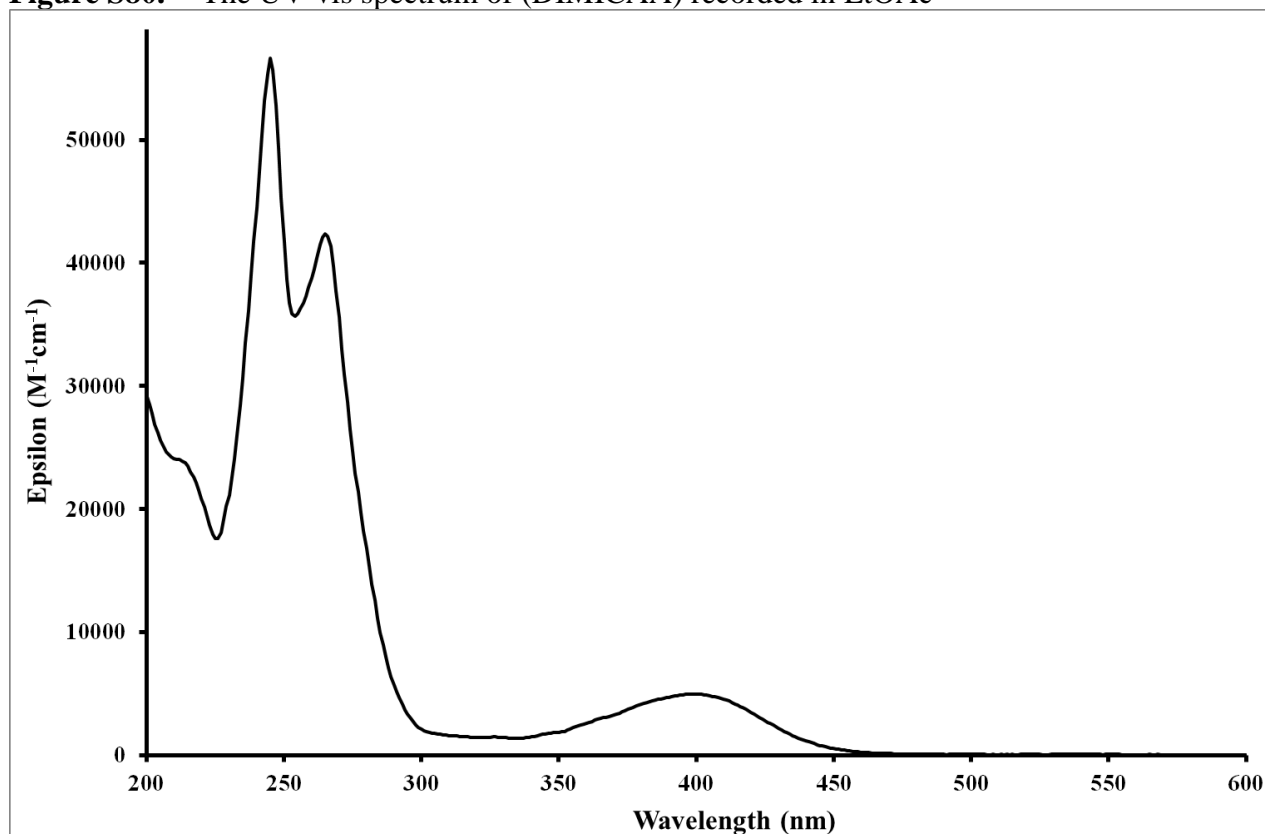
**Figure S78.** The UV-vis spectrum of (DIMICAA) recorded in DMF



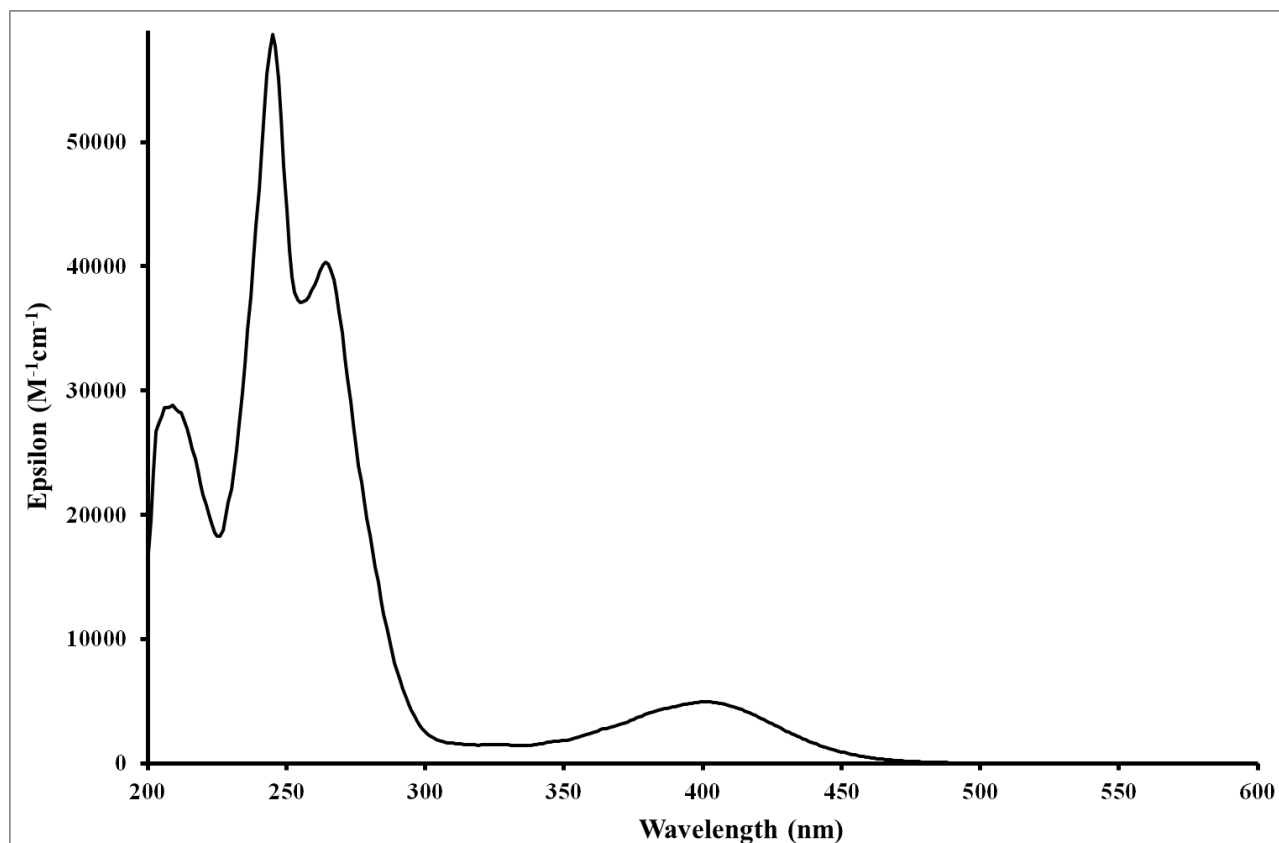
**Figure S79.** The UV-vis spectrum of (DIMICAA) recorded in DMSO



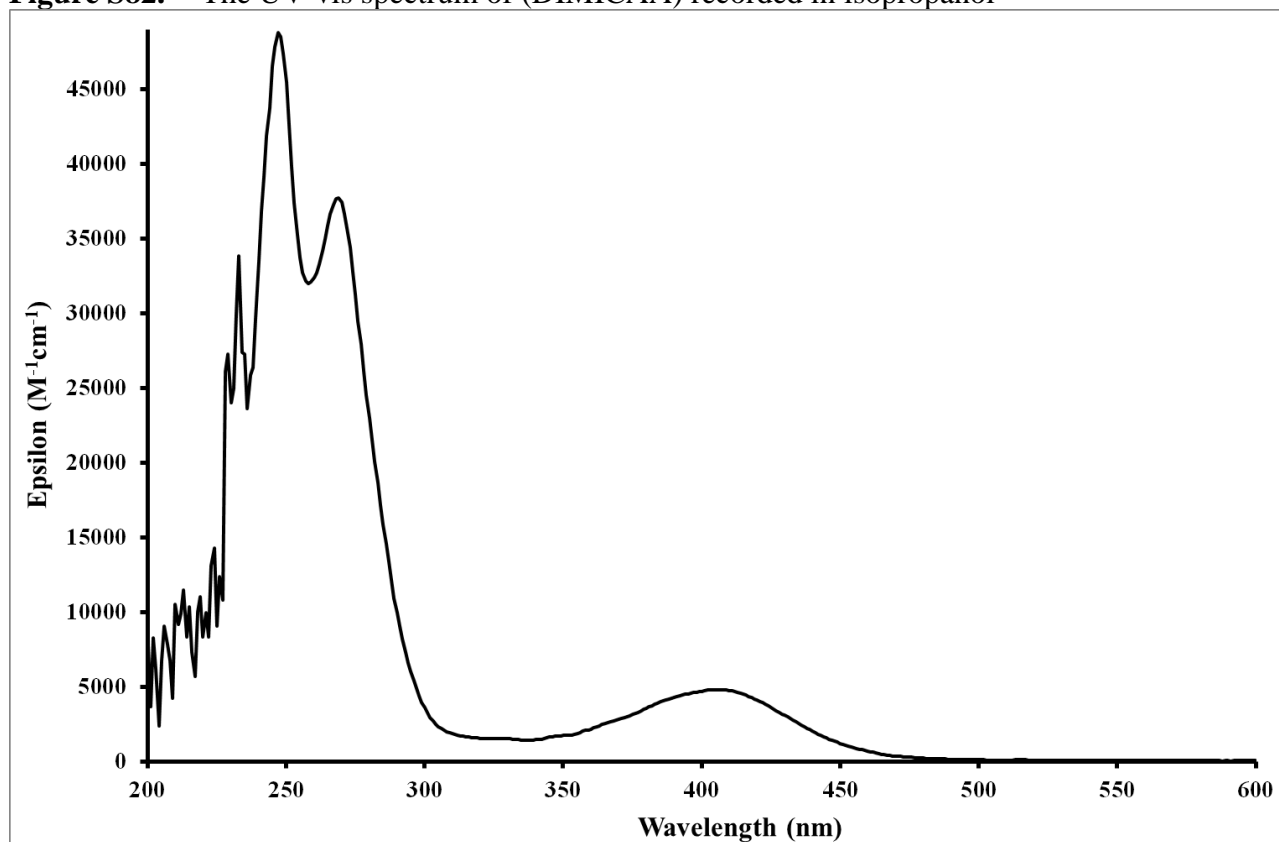
**Figure S80.** The UV-vis spectrum of (DIMICAA) recorded in EtOAc



**Figure S81.** The UV-vis spectrum of (DIMICAA) recorded in hexane

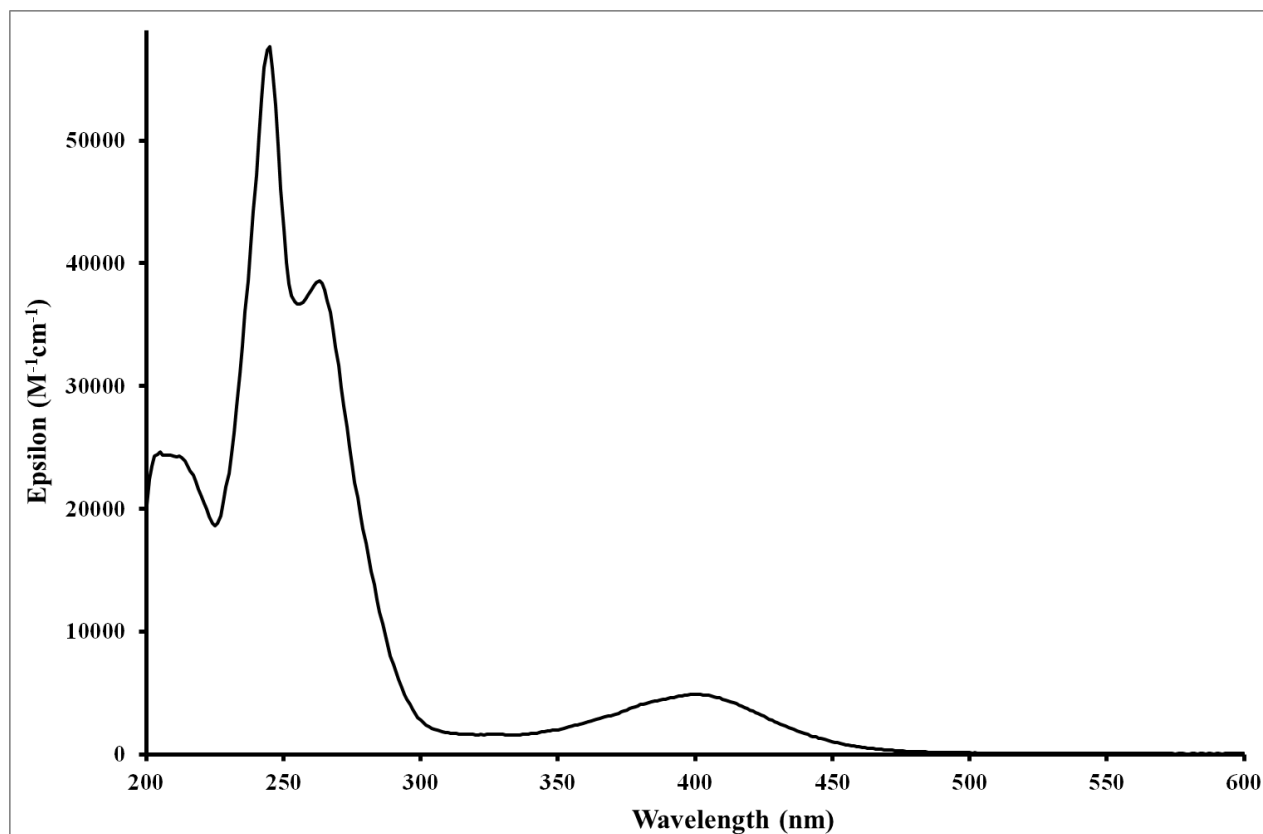


**Figure S82.** The UV-vis spectrum of (DIMICAA) recorded in isopropanol

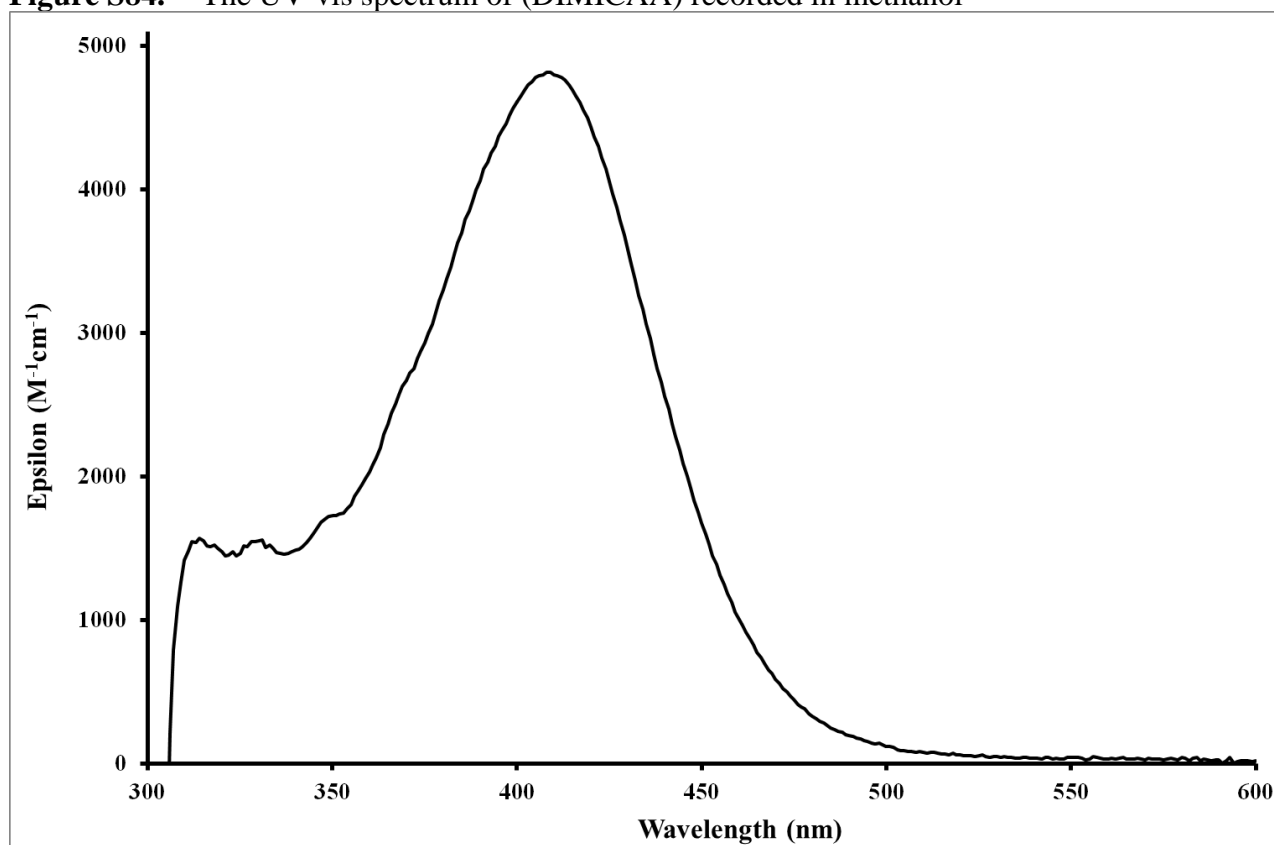


**Figure S83.** The UV-vis spectrum of (DIMICAA) recorded in chloroform

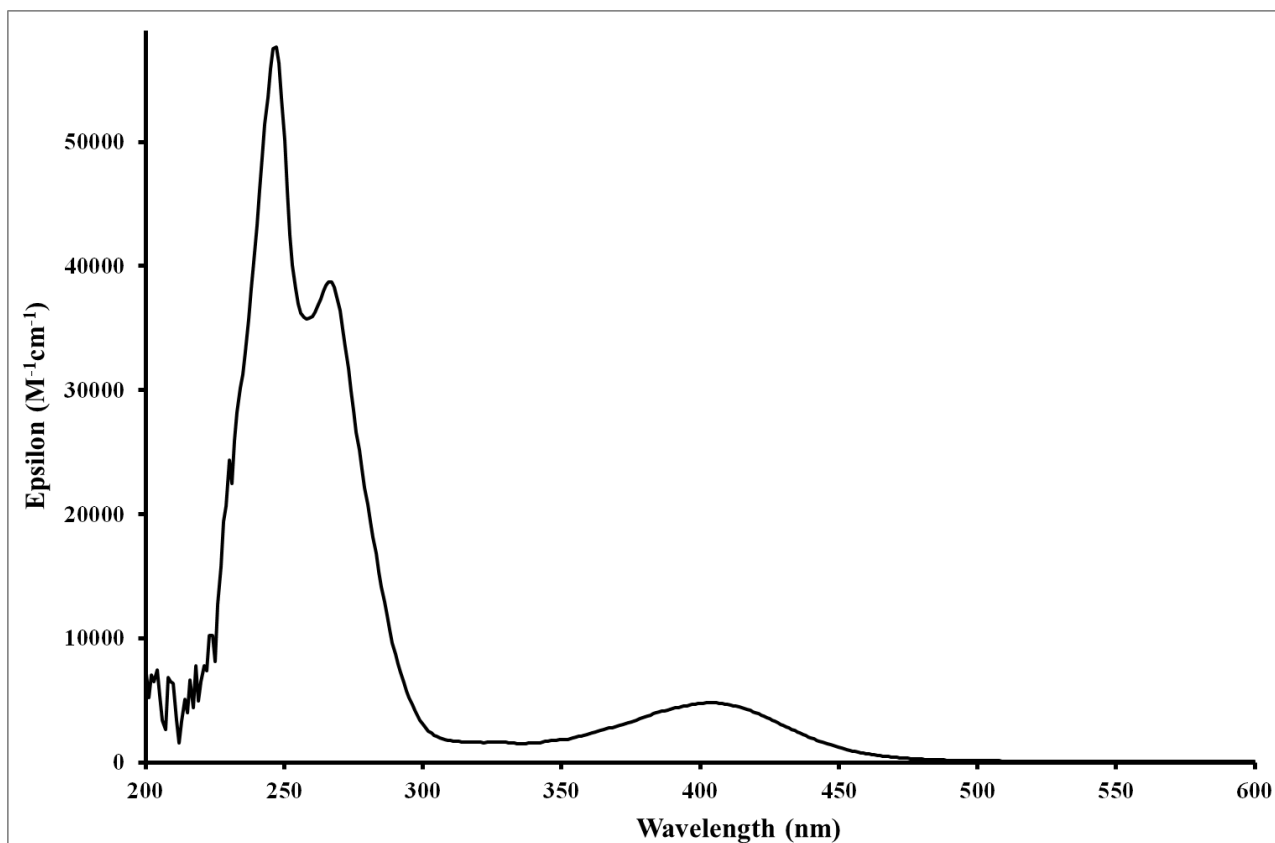




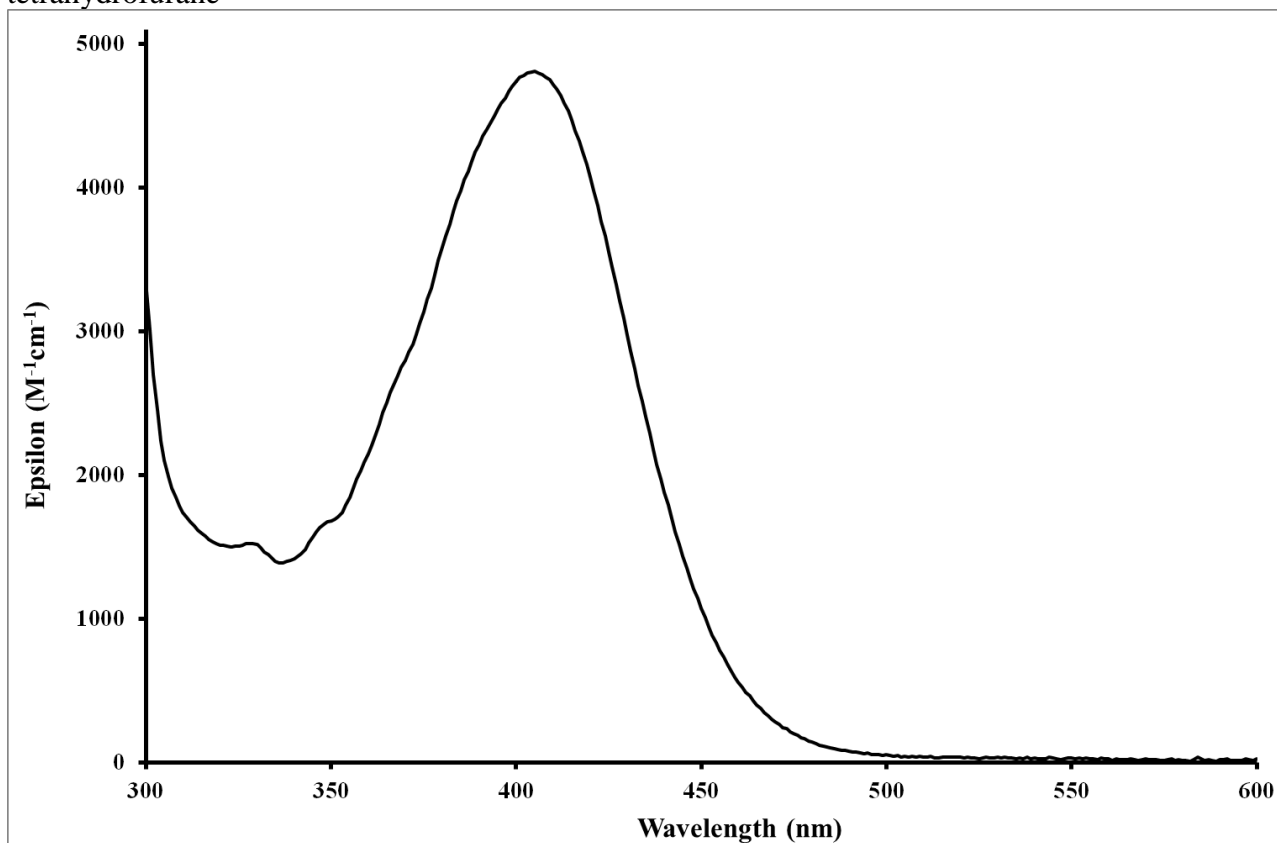
**Figure S84.** The UV-vis spectrum of (DIMICAA) recorded in methanol



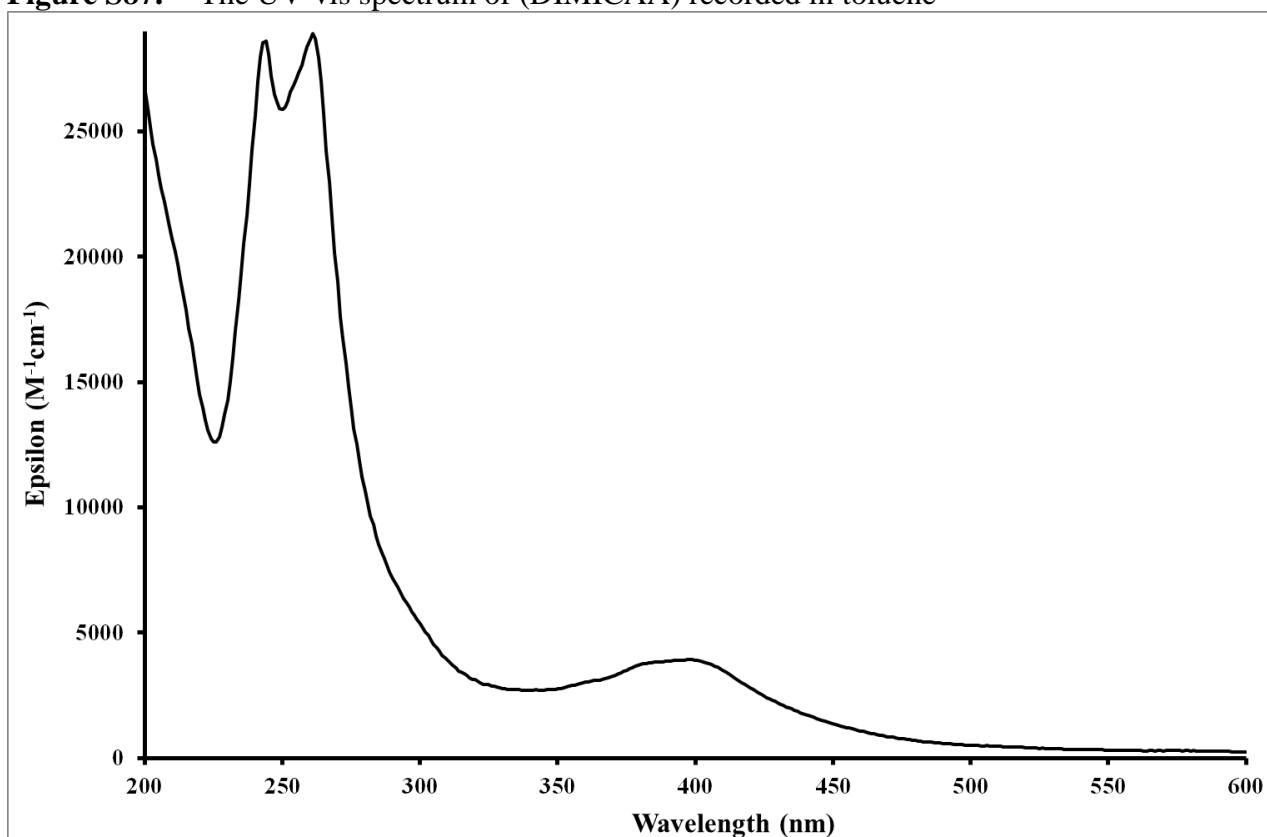
**Figure S85.** The UV-vis spectrum of (DIMICAA) recorded in pyridine



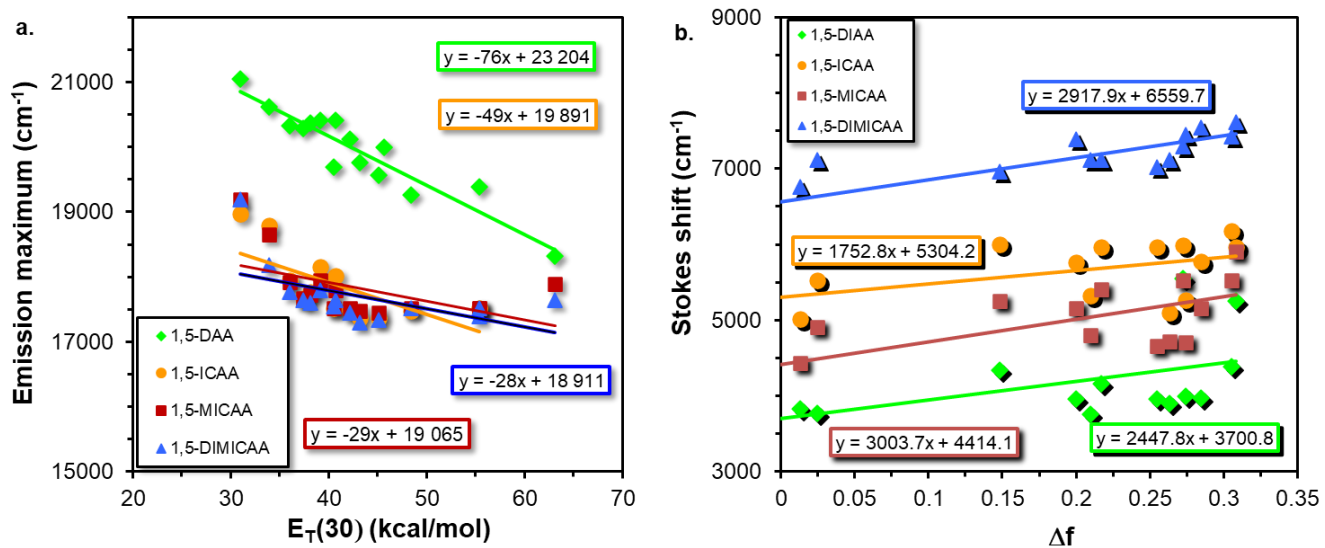
**Figure S86.** The UV-vis spectrum of (DIMICAA) recorded in tetrahydrofuran



**Figure S87.** The UV-vis spectrum of (DIMICAA) recorded in toluene



**Figure S88.** The UV-vis spectrum of (DIMICAA) recorded in water



**Figure S89.** Variation of the fluorescence emission maximum with the empirical solvent polarity parameter  $E_T(30)$  (a) and the Lippert-Mataga (LM) (b) plots for the 1,5-disubstituted anthracene dyes.