Amino-benzo-cinnolines "ABCDyes" as versatile cinnoline-based green emitting fluorophores.

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Supporting Information

I. Additional figures

Solvatochromism of 4a

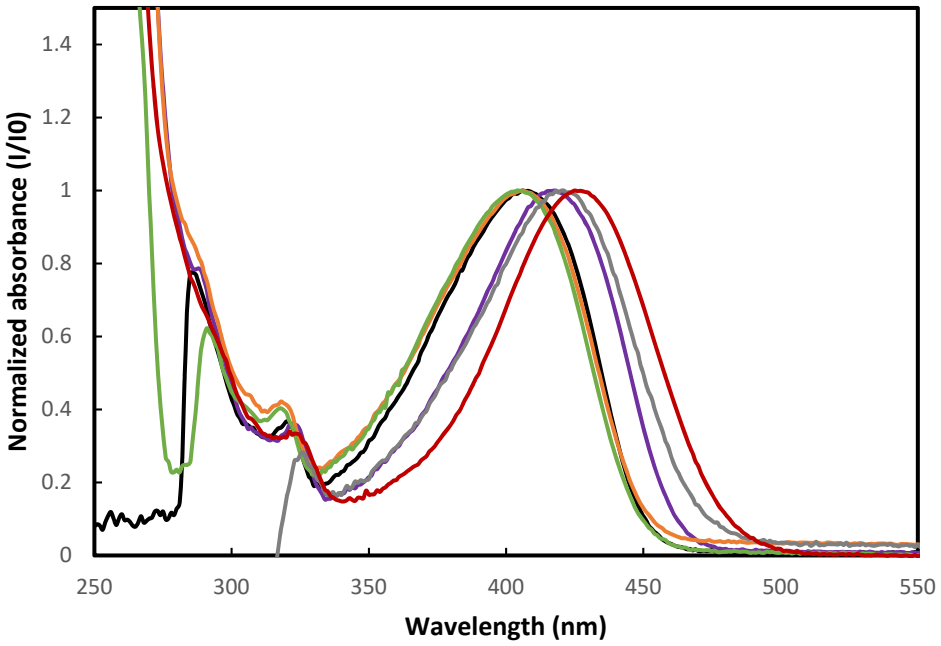


Figure S1. Absorbance spectra of **4a** in toluene (black), dioxane (orange), THF (green), CHCl3 (violet), DMSO (grey) and MeOH (red). [c] ~ 1 x 10-5M.

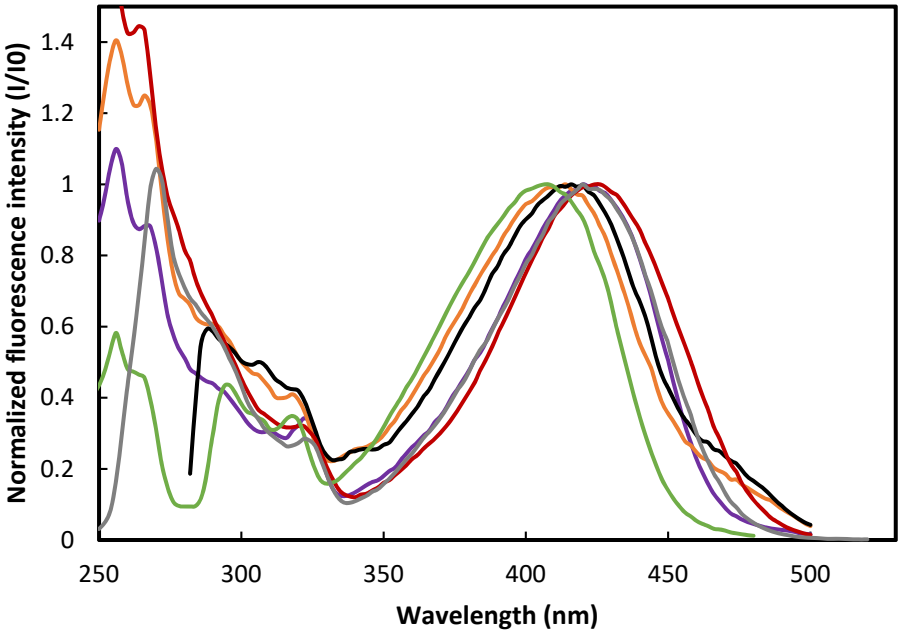


Figure S2. excitation spectra of **4a** in toluene (black), dioxane (orange),THF (green), CHCl3 (violet), DMSO (grey) and MeOH (red). [c] ~ 1 x 10-5M.

$E_T(30)$ analysis for 4a

solvent	λ(em, nm)	ν (em, cm^{-1})	$E_T(30)$
Toluene	472	21 186	33,9
Dioxane	482	20 746	36
THF	488	20 491	37,4
$CHCl_3$	490	20 408	39,1
DMSO	526	19 011	45,1
MeOH	529	18 903	55,4

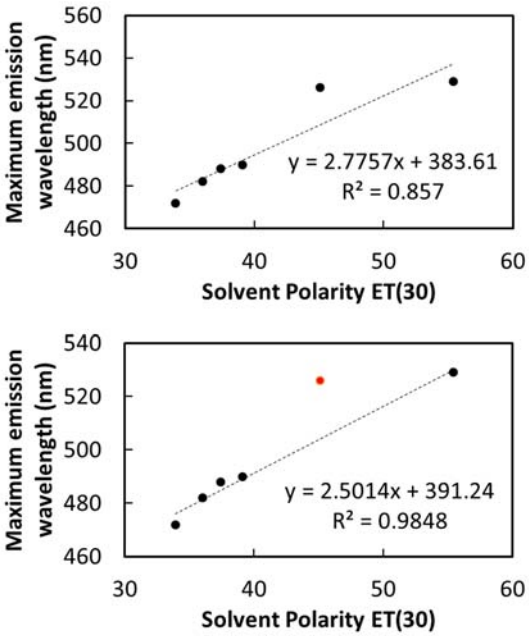


Figure S3. Correlation between Maximum emission wavelength and corresponding solvent polarity coefficient ET(30) for ABCDye 4a

Catalan analysis for 4a

In the Catalan methodology, the description of the solvent effect relies on solute–solvent interactions with four independent parameters: polarizability (SP), dipolarity (SdP), acidity(SA) and basicity (SB).

The solvent-dependent maximum emission wavenumber ($\bar{\nu}$) is formulated as:

$$\bar{\nu} = \bar{\nu}_0 + a \times SP + b \times SdP + c \times SA + d \times SB$$

where $\bar{\nu}_0$ is the value of maximum emission wavenumber in the gas phase, and the coefficients *a*–*d* are the regression coefficients describing the sensitivity of the wavenumber to the different solute–solvent interactions.

Solvent	**λ(em, nm)**	**ν (em, cm^{-1})**	**ν_0 (em, cm^{-1})**	**a**	**SP**	**b**	**SdP**	**c**	SA	d
Tol	472	21186	25861	-5306	0,782	-1363	0,284	-2908	0	-1082
Dioxane	482	20747	25693	-5433	0,737	-1413	0,312	-2908	0	-1129
THF	488	20492	25809	-5348	0,714	-1365	0,634	-2908	0	-1072
CHCL3	490	20408	25728	-5410	0,783	-1416	0,614	-2910	0,047	-1096
DMSO	526	19011	25774	-5373	0,83	-1387	1	-2908	0,072	-1092
MeOH	529	18904	25776	-5372	0,608	-1386	0,904	-2906	0,605	-1092
		Mean value	25774	-5374		-1388		-2908		-1094
		Standard deviation	59	45		23		1		19

Figure S4. Experimental emission wavenumber and Catalan parameters use for the Catalan method for **4a**.

Simulated absorption spectra

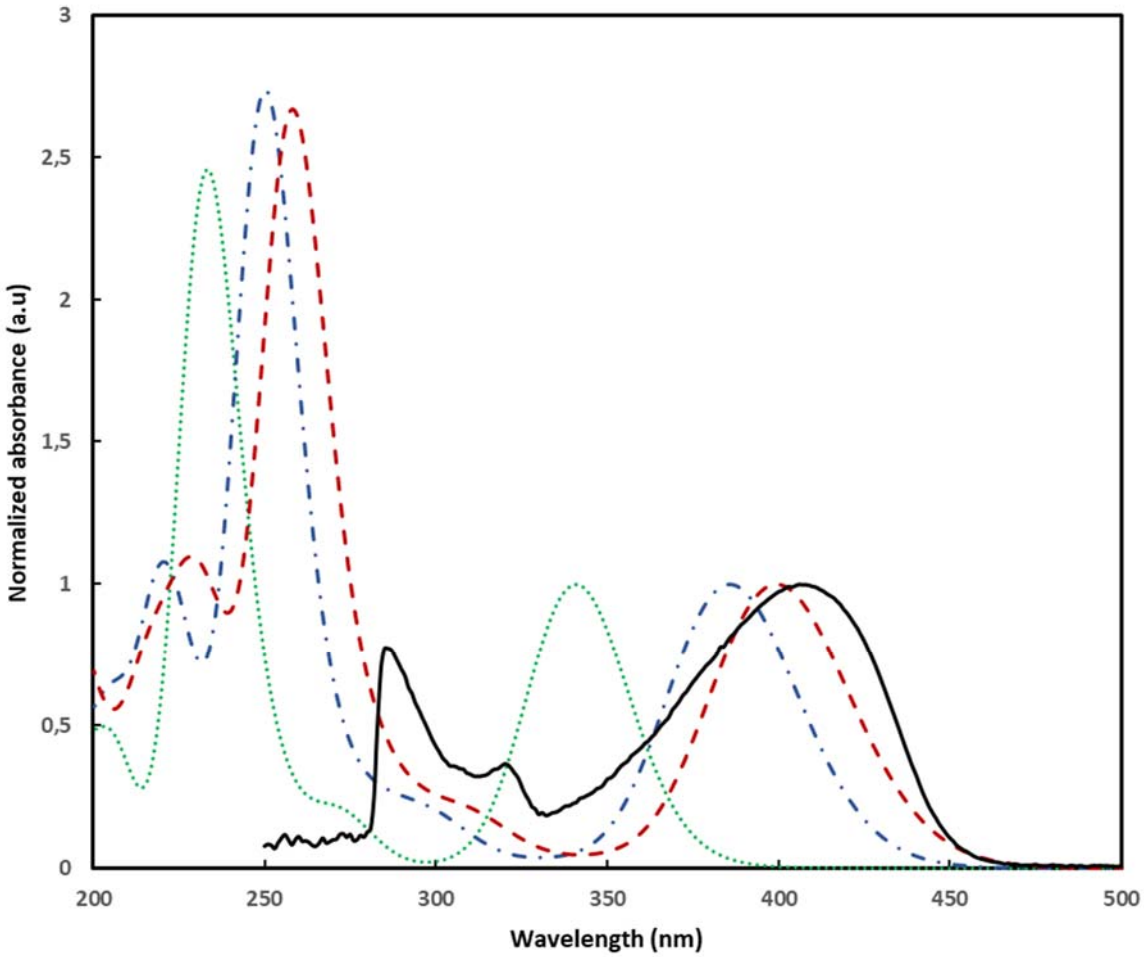


Figure S5. Normalized absorbance spectra of 4a in toluene. Experimental spectrum is depicted in black, PBE0-calculated spectra in blue dotted blue, B3LYP-D3BJ spectra in red dotted red and CAM-B3LYP spectra in green dotted line (FWHM=3000 cm-1).

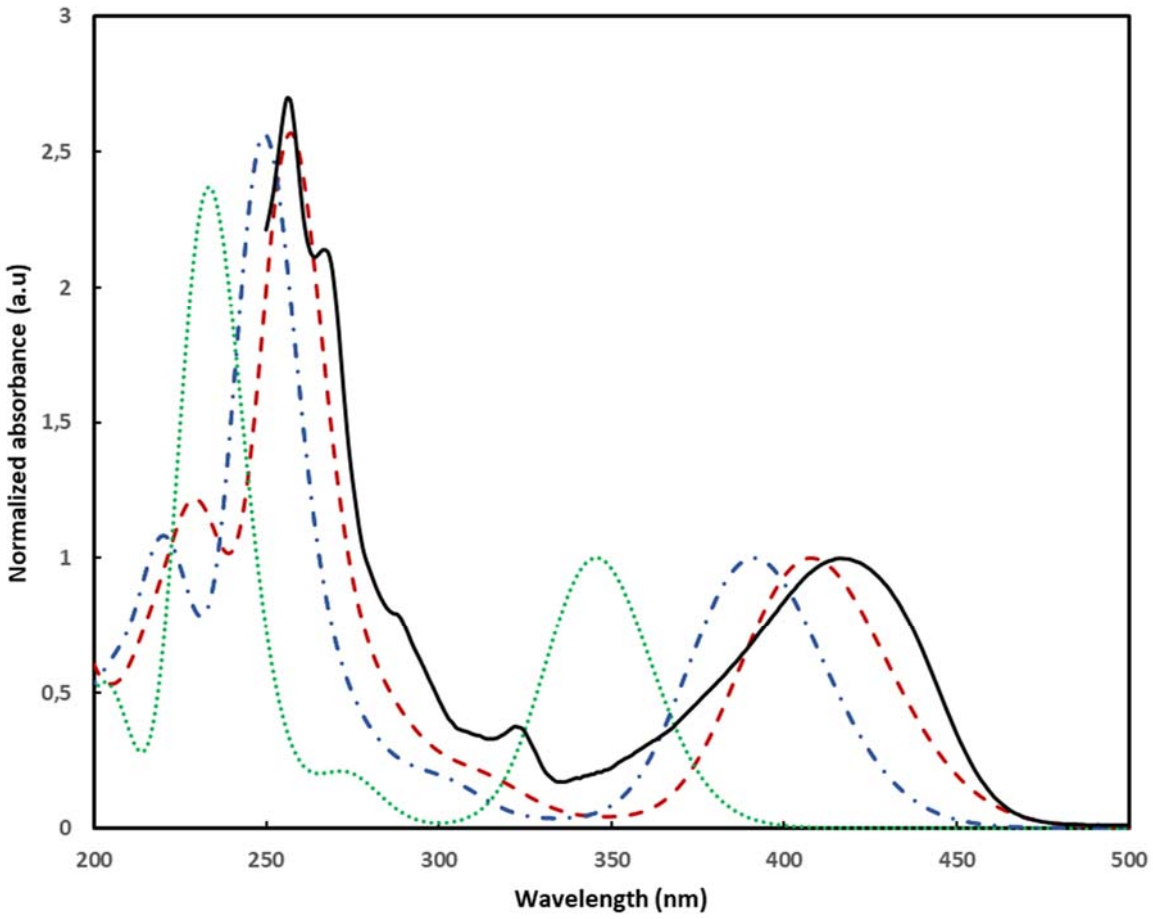


Figure S6. Normalized absorbance spectra of 4a in chloroform. Experimental spectrum is depicted in black, PBE0-calculated spectra in blue dotted blue, B3LYP-D3BJ spectra in red dotted red and CAM-B3LYP spectra in green dotted line (FWHM=3000 cm-1).

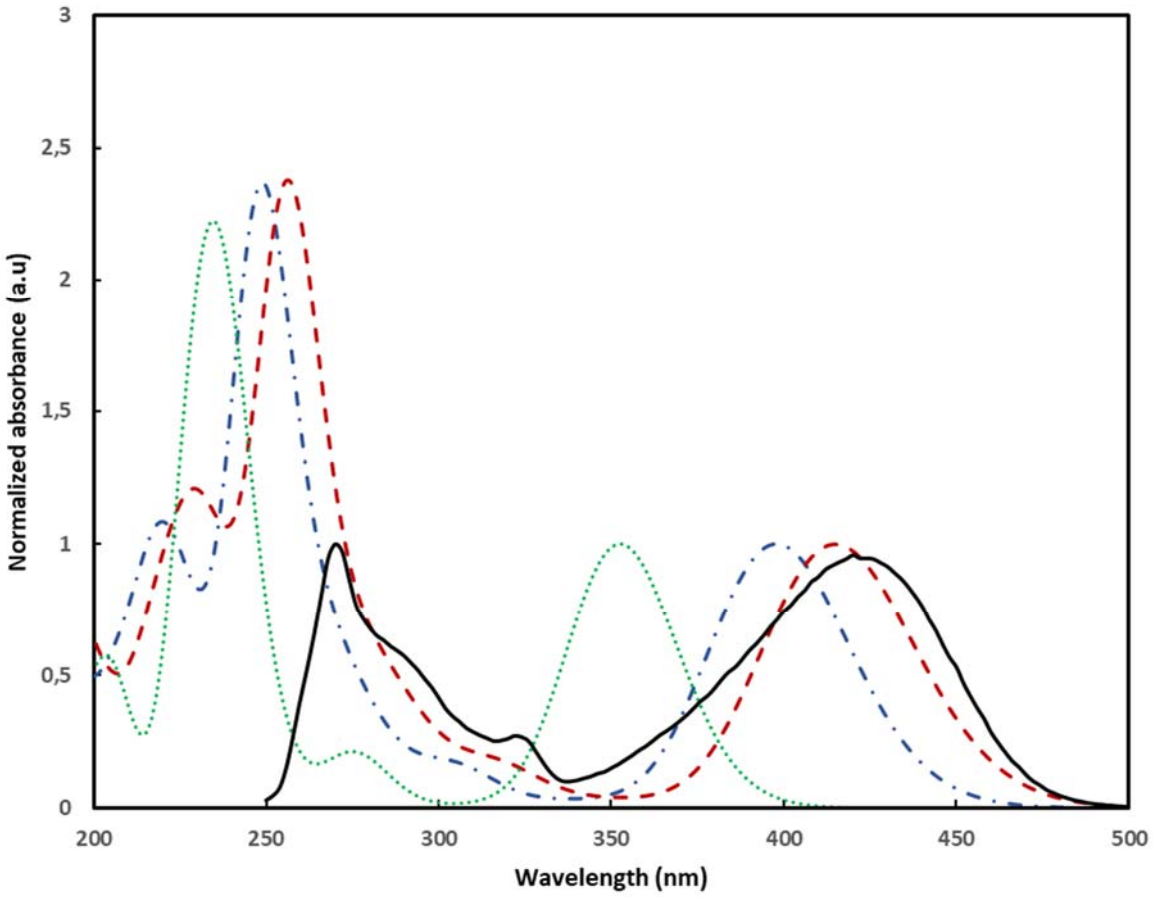


Figure S7. Normalized absorbance spectra of 4a in DMSO. Experimental spectrum is depicted in black, PBE0-calculated spectra in blue dotted blue, B3LYP-D3BJ spectra in red dotted red and CAM-B3LYP spectra in green dotted line (FWHM=3000 cm-1).

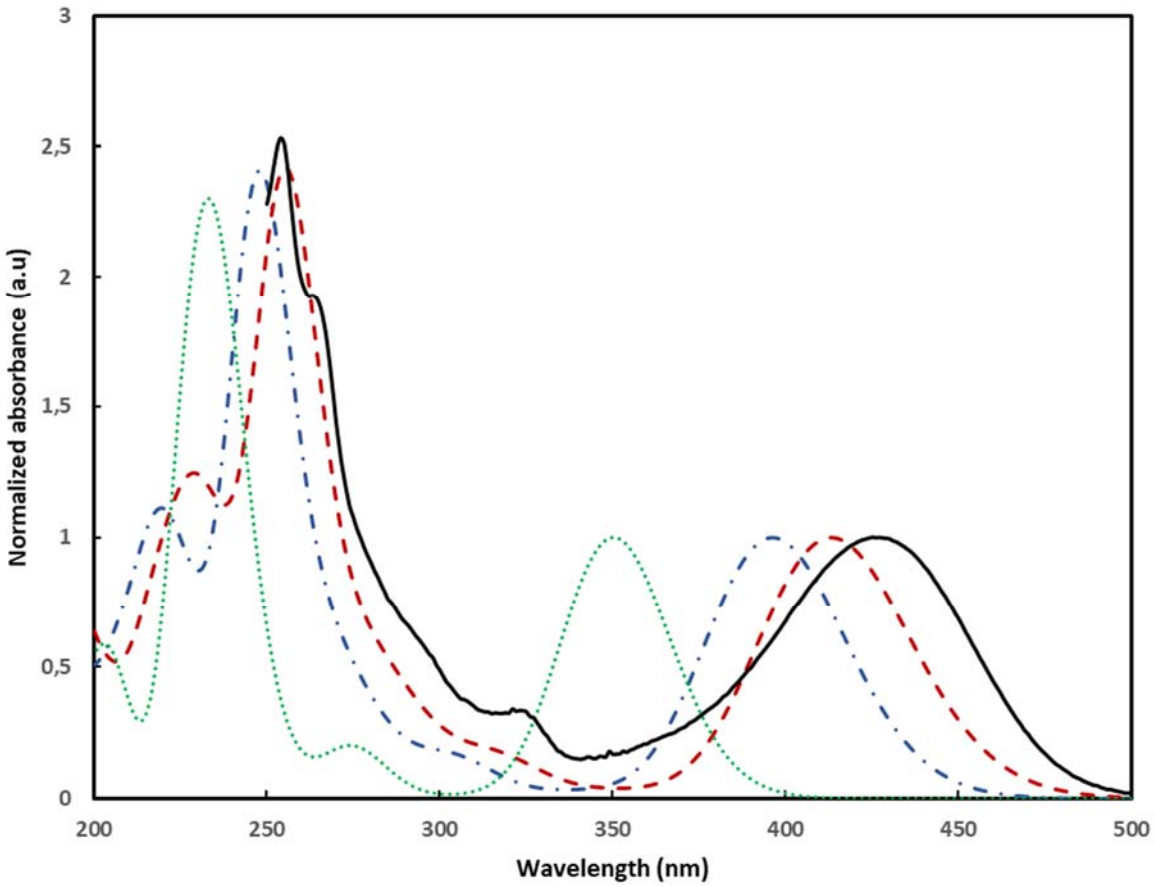


Figure S8. Normalized absorbance spectra of 4a in methanol. Experimental spectrum is depicted in black, PBE0-calculated spectra in blue dotted blue, B3LYP-D3BJ spectra in red dotted red and CAM-B3LYP spectra in green dotted line (FWHM=3000 cm-1).

Natural Transition Orbitals with PBE0/6-31+G(d,p)

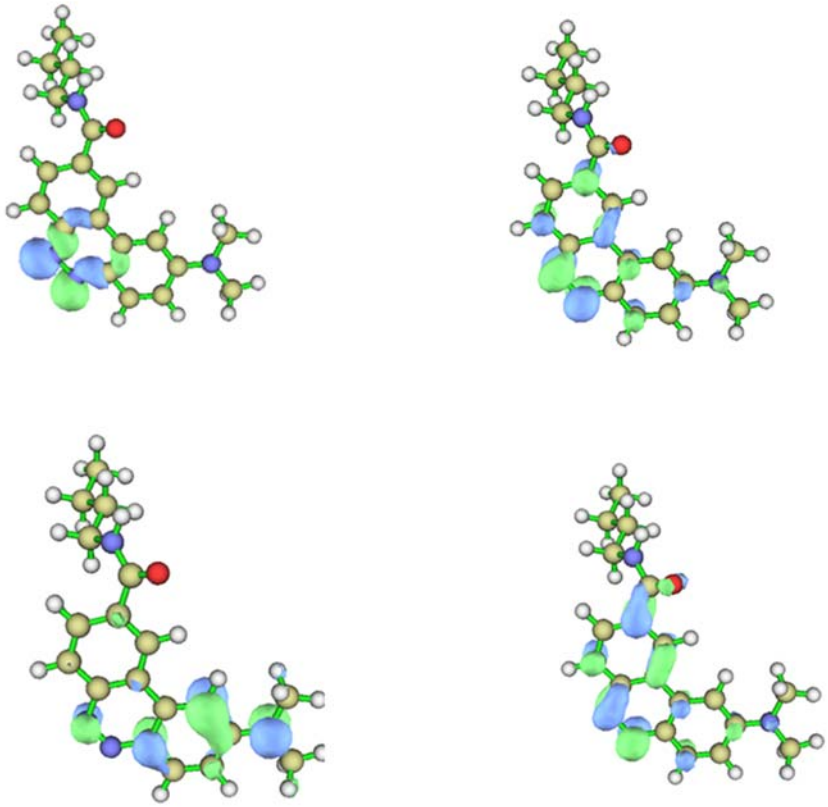


Figure S9. Natural transition orbitals pairs for the first excited states (top) and the second excited state (bottom) of **4a** in toluene based on the ground state geometry, calculated at the PBE0/6-31+G(d,p) level of theory, for each state, the hole is on the left, the electron on the right

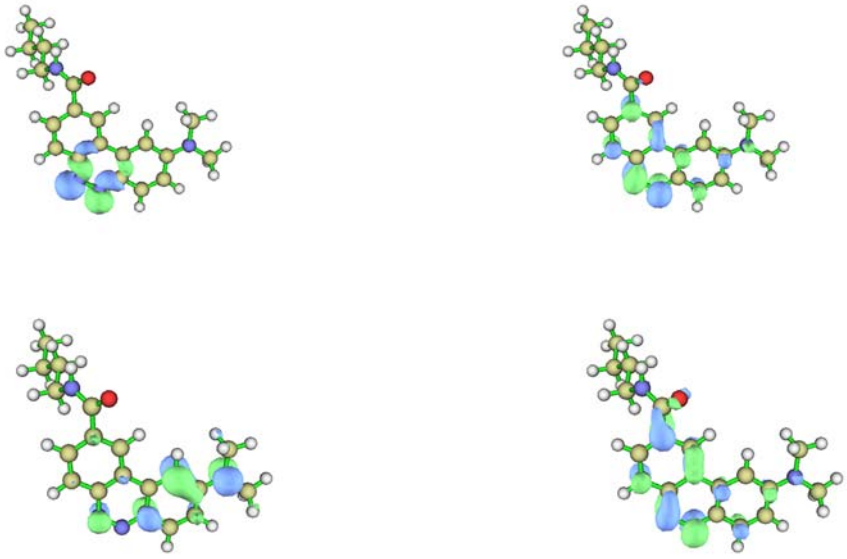


Figure S10. Natural transition orbitals pairs for the first excited states (top) and the second excited state (bottom) of **4a** in chloroform based on the ground state geometry, calculated at

the PBE0/6-31+G(d,p) level of theory, for each state, the hole is on the left, the electron on the right

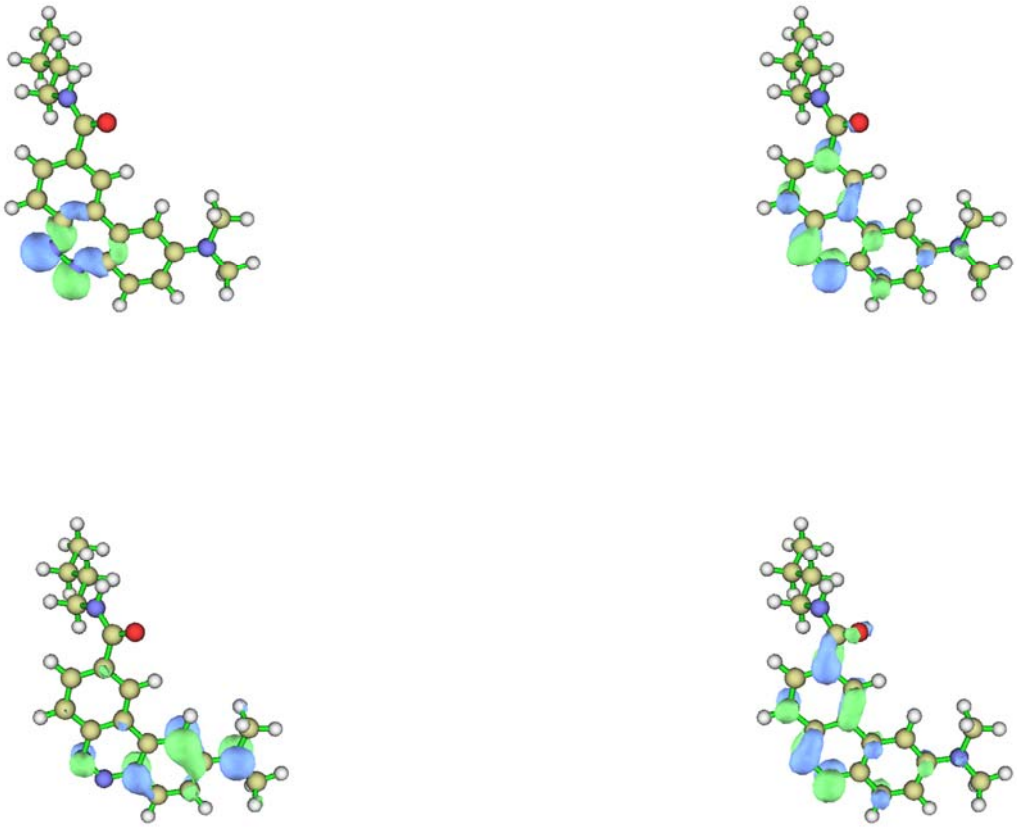


Figure S11. Natural transition orbitals pairs for the first excited states (top) and the second excited state (bottom) of **4a** in DMSO based on the ground state geometry , calculated at the PBE0/6-31+G(d,p) level of theory, for each state, the hole is on the left, the electron on the right

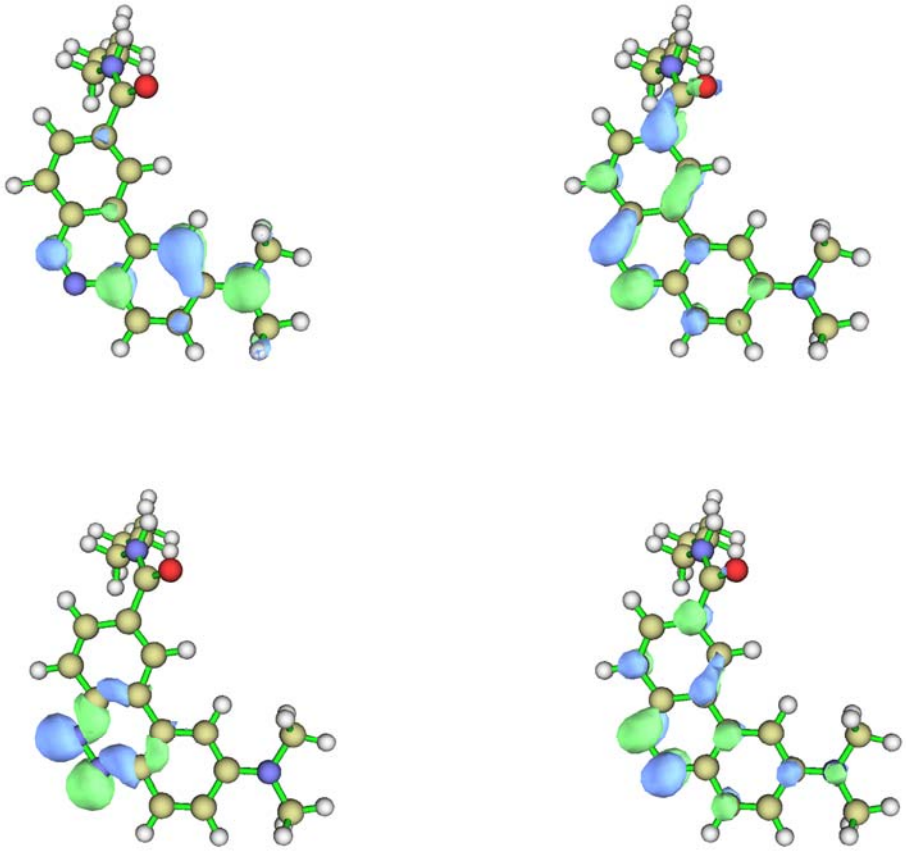


Figure S12. Natural transition orbitals pairs for the first excited states (top) and the second excited state (bottom) of **4a** in methanol based on the ground state geometry , calculated at the PBE0/6-31+G(d,p) level of theory, for each state, the hole is on the left, the electron on the right

Natural Transition Orbitals with B3LYP-D3BJ/6-31+G(d,p)

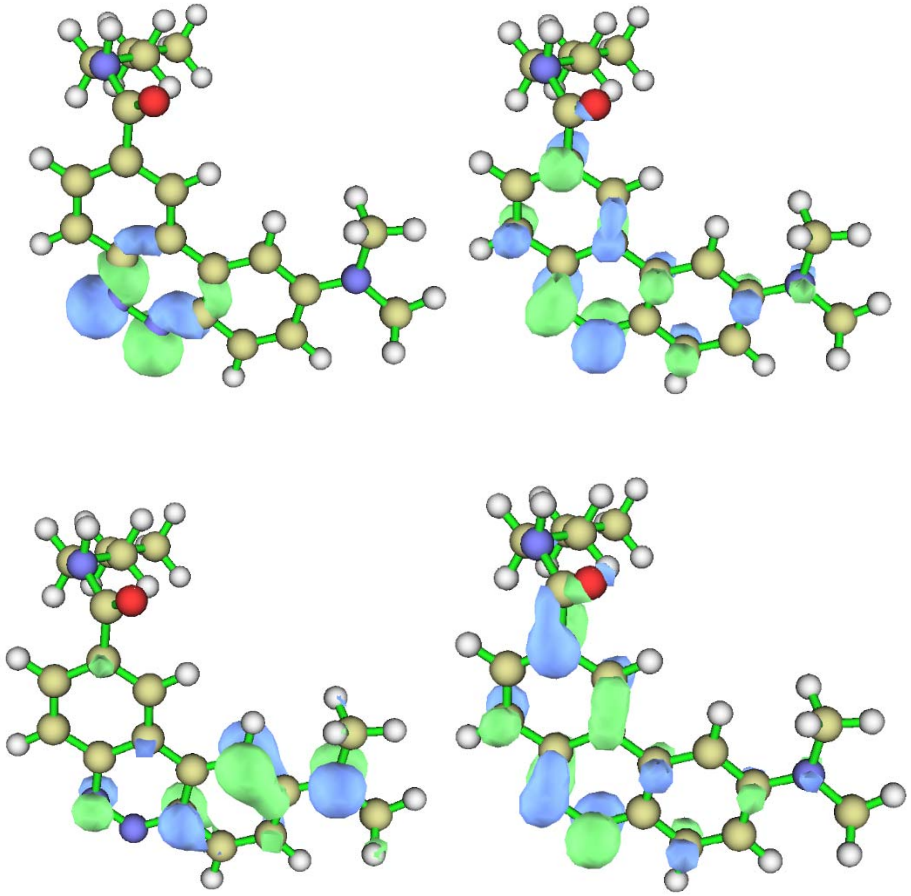


Figure S13. Natural transition orbitals pairs for the first excited states (top) and the second excited state (bottom) of **4a** in toluene based on the ground state geometry ,calculated at the B3LYP-D3BJ/6-31+G(d,p) level of theory, for each state, the hole is on the left, the electron on the right

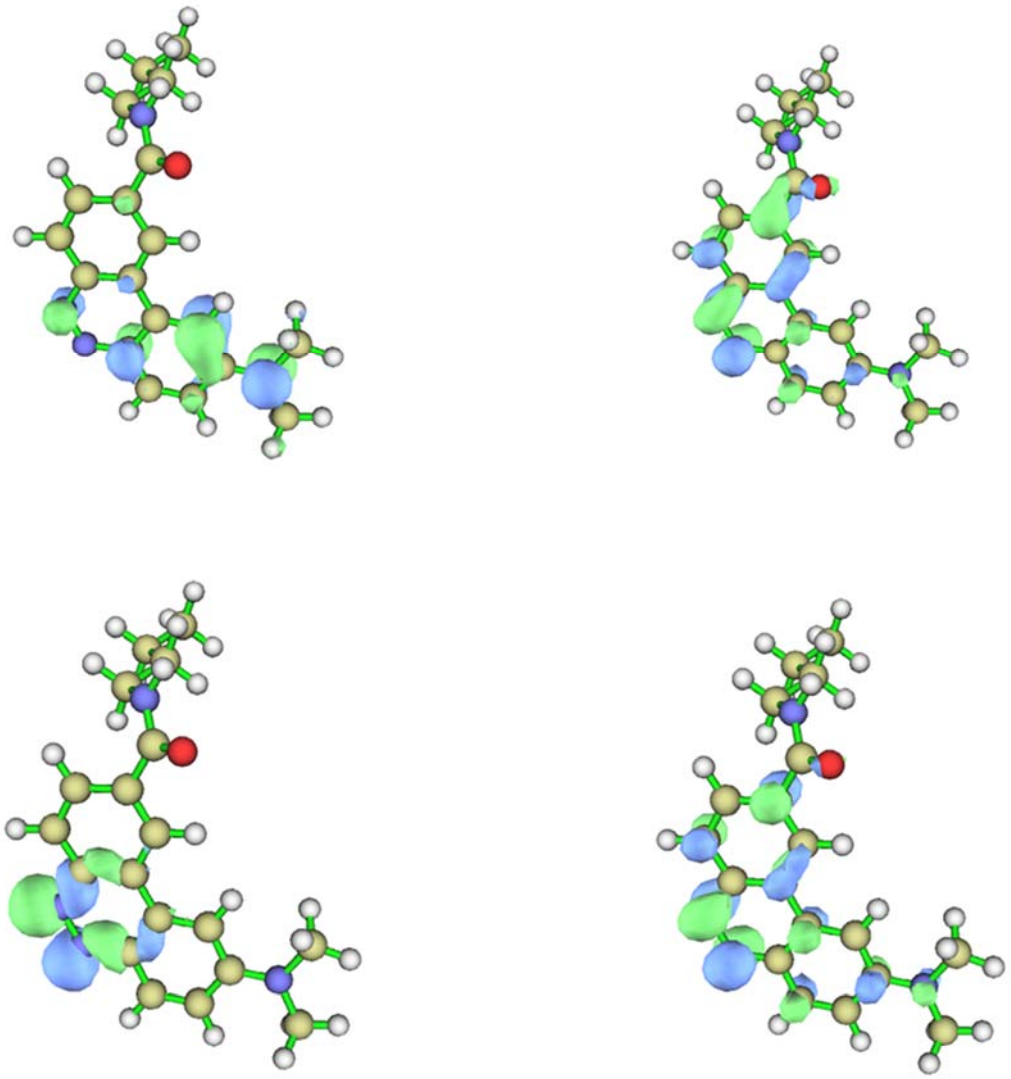


Figure S14. Natural transition orbitals pairs for the first excited states (top) and the second excited state (bottom) of **4a** in chloroform based on the ground state geometry , calculated at the B3LYP-D3BJ/6-31+G(d,p) level of theory, for each state, the hole is on the left, the electron on the right

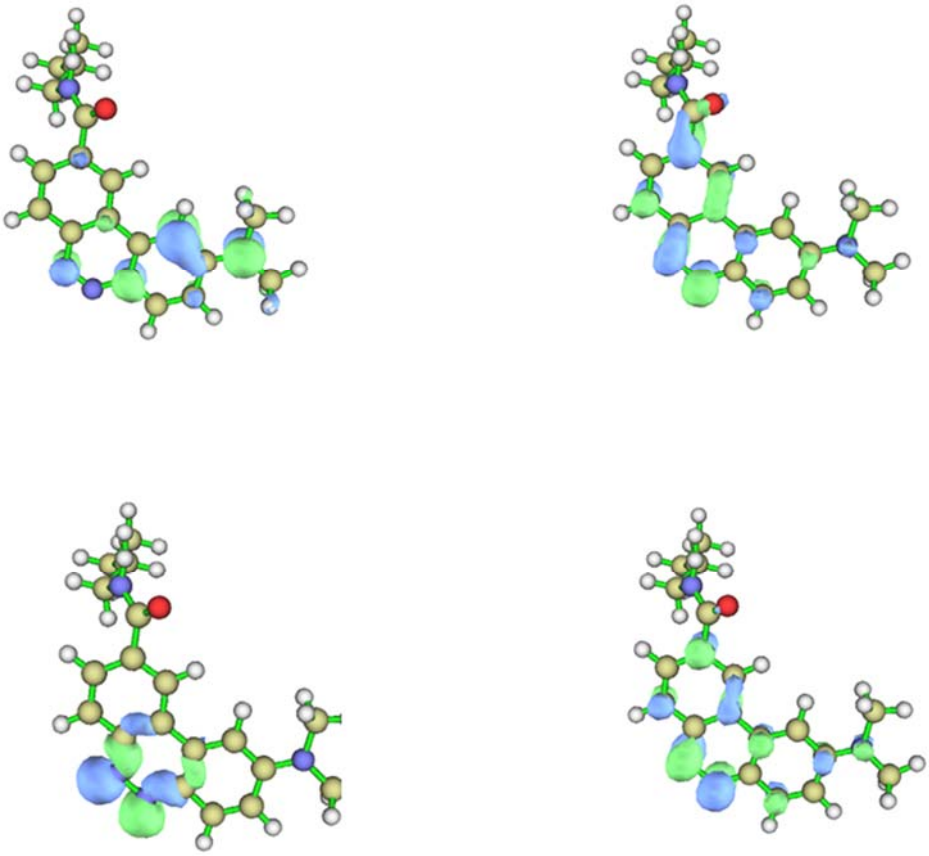


Figure S15. Natural transition orbitals pairs for the first excited states (top) and the second excited state (bottom) of **4a** in DMSO based on the ground state geometry, calculated at the B3LYP-D3BJ/6-31+G(d,p) level of theory, for each state, the hole is on the left, the electron on the right

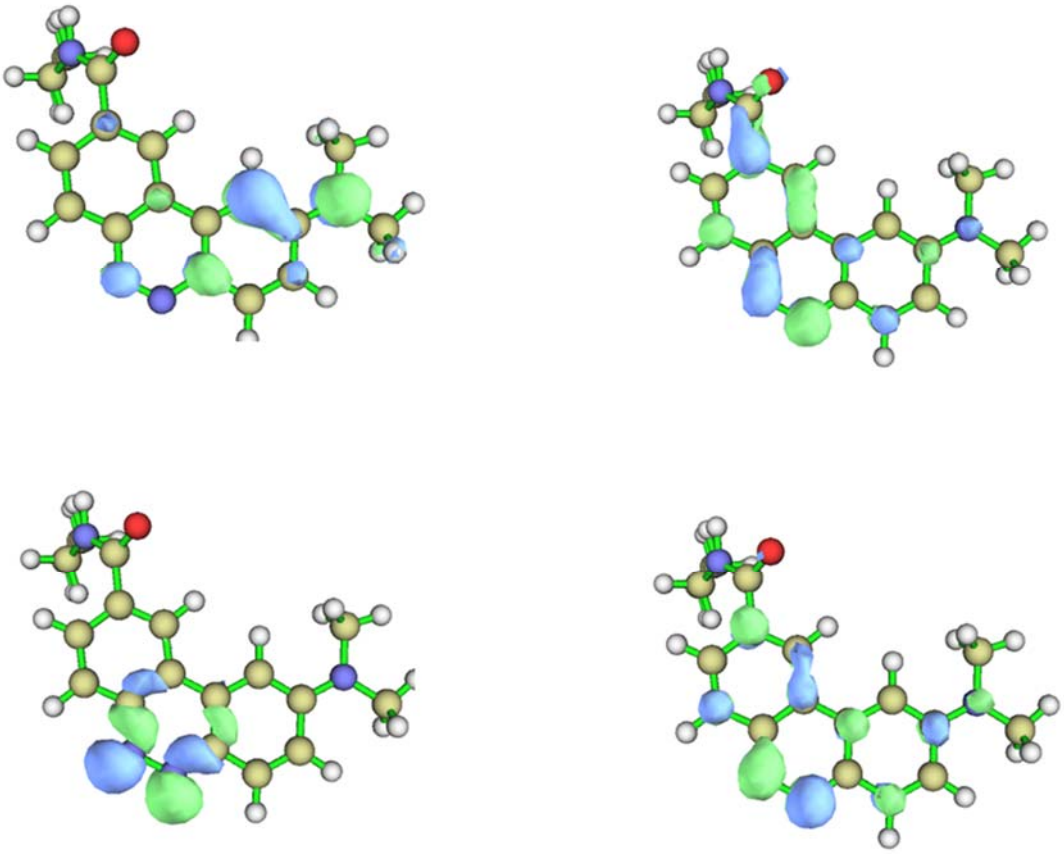


Figure S16. Natural transition orbitals pairs for the first excited states (top) and the second excited state (bottom) of **4a** in methanol based on the ground state geometry. calculated at the B3LYP-D3BJ/6-31+G(d,p) level of theory, for each state, the hole is on the left, the electron on the right

Natural Transition Orbitals with CAM-B3LYP/6-31+G(d,p)

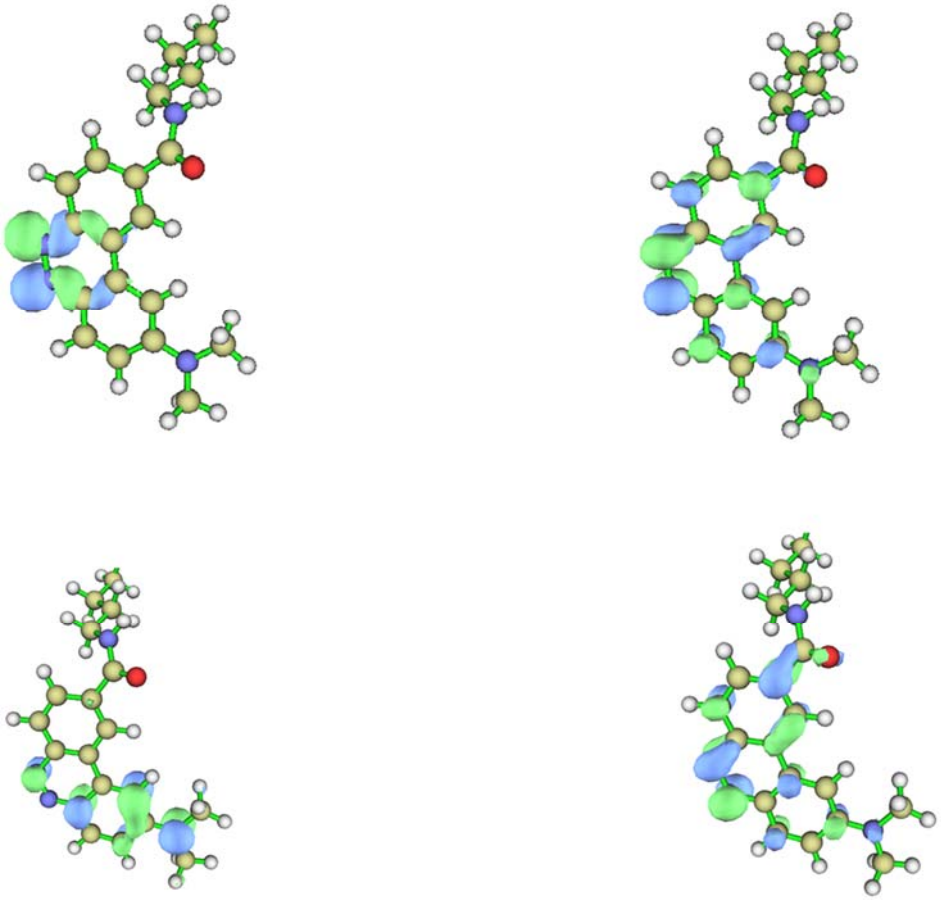


Figure S17. Natural transition orbitals pairs for the first excited states (top) and the second excited state (bottom) of **4a** in toluene based on the ground state geometry. calculated at the CAM-B3LYP/6-31+G(d,p) level of theory, for each state, the hole is on the left, the electron on the right

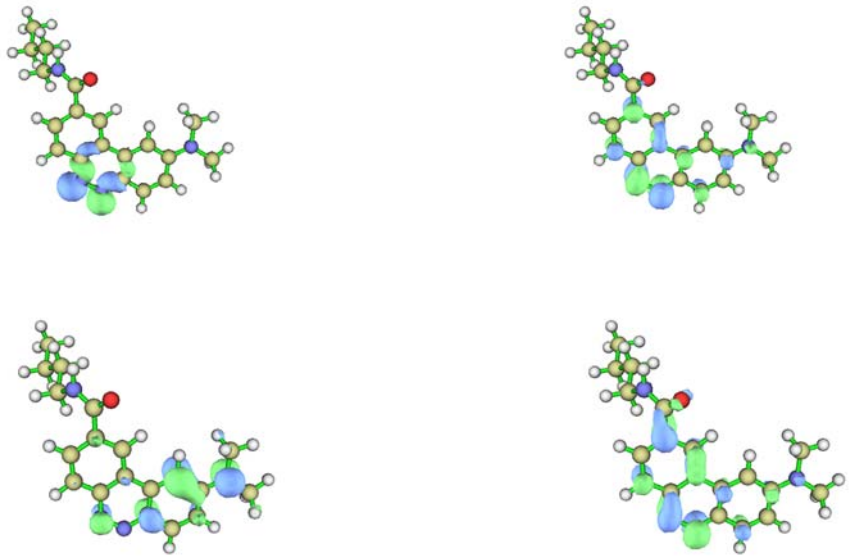


Figure S18. Natural transition orbitals pairs for the first excited states (top) and the second excited state (bottom) of **4a** in chloroform based on the ground state geometry. calculated at the CAM-B3LYP/6-31+G(d,p) level of theory, for each state, the hole is on the left, the electron on the right

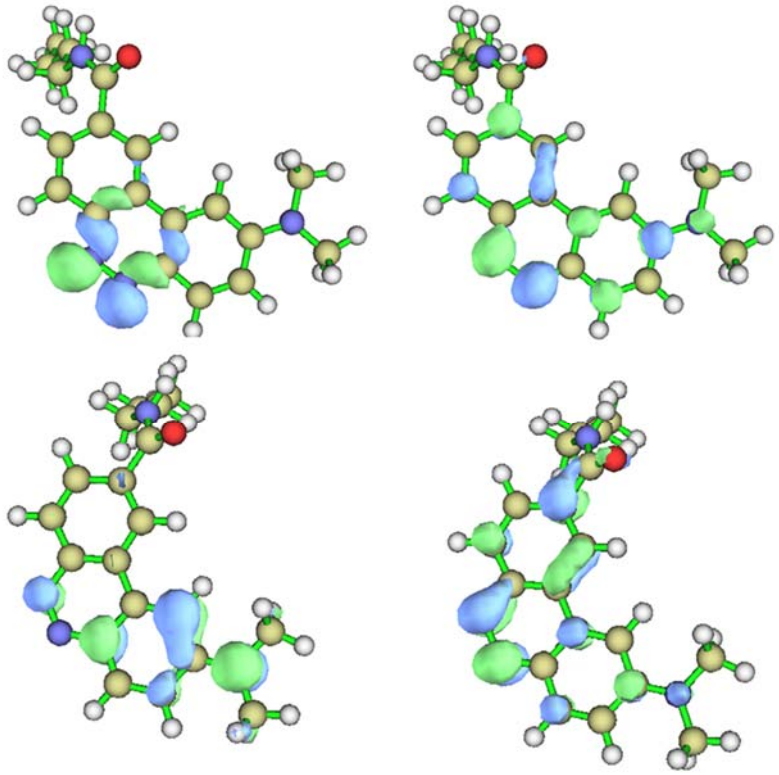


Figure S19. Natural transition orbitals pairs for the first excited states (top) and the second excited state (bottom) of **4a** in DMSO based on the ground state geometry. calculated at the CAM-B3LYP/6-31+G(d,p) level of theory, for each state, the hole is on the left, the electron on the right

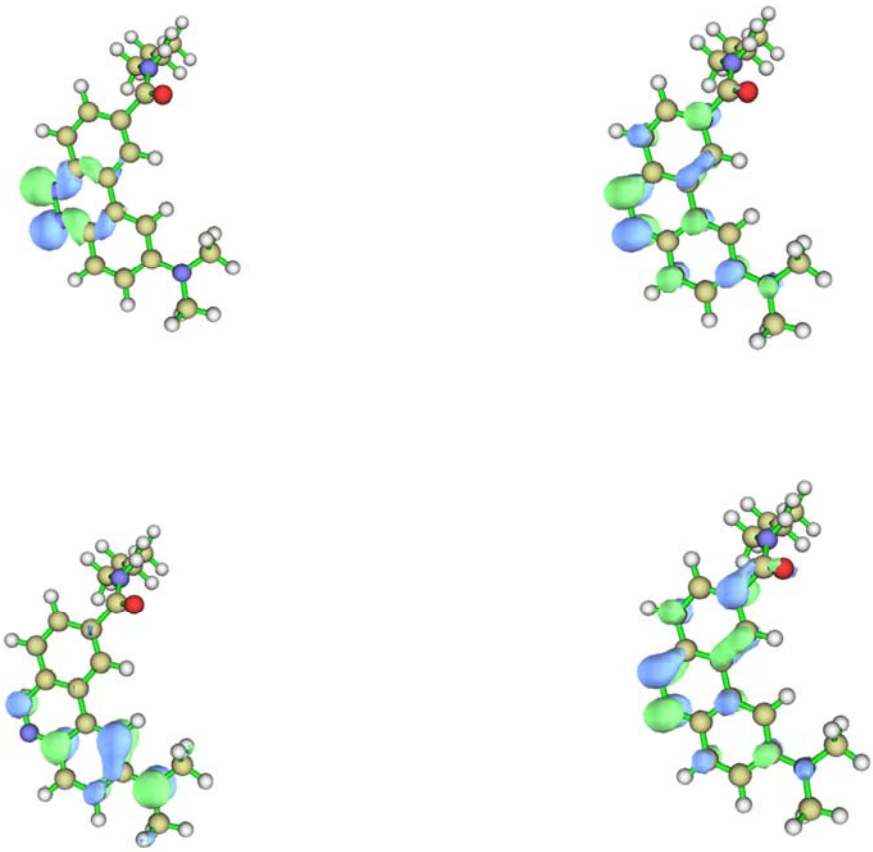


Figure S20. Natural transition orbitals pairs for the first excited states (top) and the second excited state (bottom) of **4a** in methanol based on the ground state geometry. calculated at the CAM-B3LYP/6-31+G(d,p) level of theory, for each state, the hole is on the left, the electron on the right

Functionnal	*Solvent*	*nature*		*Wavelength*	*fosc*
PBE0	Toluene	exc n°1 :	n -> π*	400,91	0,0025
		exc n°2 :	π -> π*	385,32	0,4186
	Chloroform	exc n°1 :	n -> π*	393,11	0,0053
		exc n°2 :	π -> π*	390,92	0,4118
	DMSO	exc n°1 :	π -> π*	397,68	0,4085
		exc n°2 :	n -> π*	383,78	0,0026
	Methanol	exc n°1 :	π -> π*	396,06	0,3981
		exc n°2 :	n -> π*	384,15	0,0026
B3LYP-D3BJ	Toluene	exc n°1 :	n -> π*	405,52	0,0026
		exc n°2 :	π -> π*	399	0,3766
	Chloroform	exc n°1 :	π -> π*	407,62	0,3807
		exc n°2 :	n -> π*	398,43	0,0024
	DMSO	exc n°1 :	π -> π*	414,67	0,3838
		exc n°2 :	n -> π*	388,1	0,0025
	Methanol	exc n°1 :	π -> π*	413,03	0,3667
		exc n°2 :	n -> π*	388,57	0,0024
CAM-B3LYP	Toluene	exc n°1 :	n -> π*	374,97	0,0035
		exc n°2 :	π -> π*	340,57	0,55
	Chloroform	exc n°1 :	n -> π*	368,53	0,0036
		exc n°2 :	π -> π*	345,31	0,5442
	DMSO	exc n°1 :	n -> π*	361,05	0,0041
		exc n°2 :	π -> π*	352,23	0,5571
	Methanol	exc n°1 :	n -> π*	361,17	0,0037
		exc n°2 :	π -> π*	350	0,5214

Figure S21. electron-hole densities distribution maps for **4a** in toluene, chloroform, DMSO and methanol (from left to right). PBE0/6-31+G(d,p). isovalue surface = 0.002. Blue and green isosurfaces represent hole and electron distributions, respectively.

Electron-hole densities maps at the S1 excited state geometry

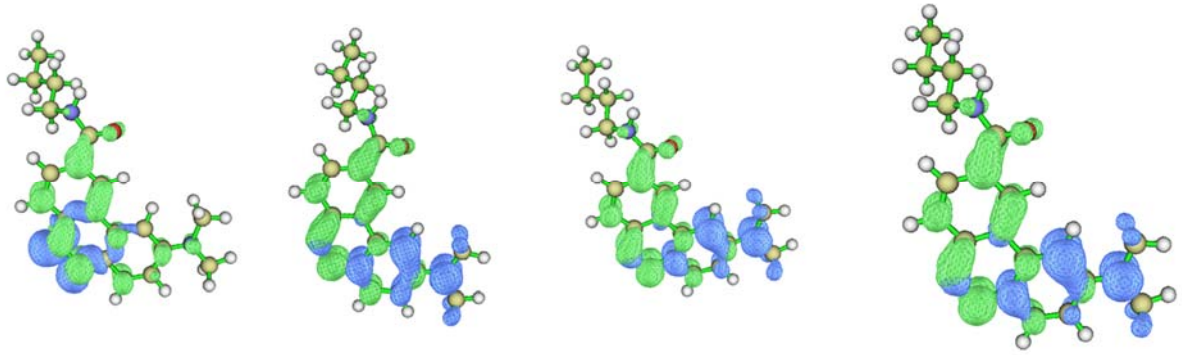


Figure S22. electron-hole densities distribution maps for **4a** in toluene, chloroform, DMSO and methanol (from left to right). PBE0/6-31+G(d,p). isovalue surface = 0.002. Blue and green isosurfaces represent hole and electron distributions, respectively.

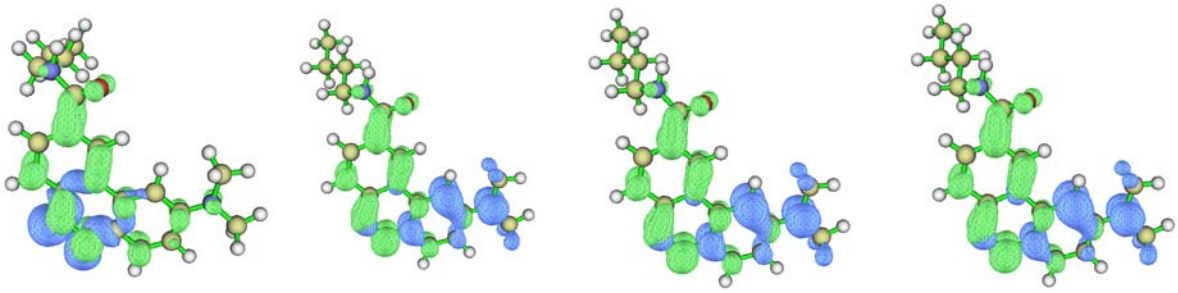


Figure S23. electron-hole densities distribution maps for **4a** in toluene, chloroform, DMSO and methanol (from left to right). B3LYP-D3BJ/6-31+G(d,p). isovalue surface = 0.002. Blue and green isosurfaces represent hole and electron distributions, respectively.

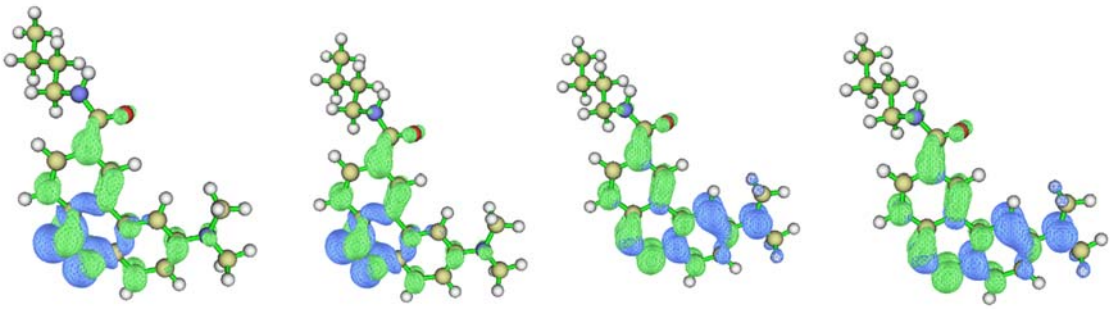


Figure S24. electron-hole densities distribution maps for **4a** in toluene, chloroform, DMSO and methanol (from left to right). CAM-B3LYP/6-31+G(d,p). isovalue surface = 0.002. Blue and green isosurfaces represent hole and electron distributions, respectively.

Photophysical properties in $CHCl_3$

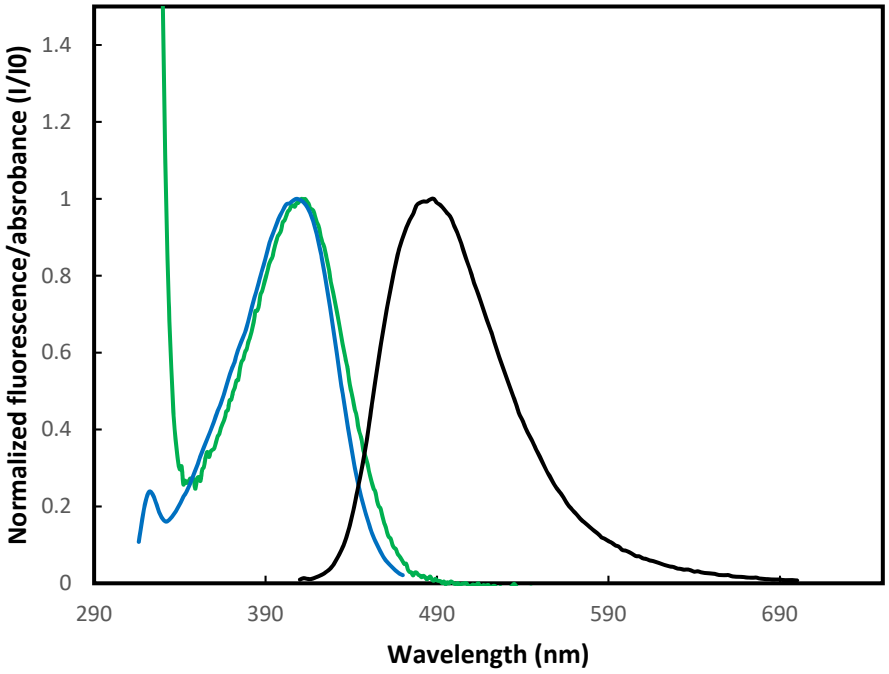


Figure S25. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **3** in $CHCl_3$. λ_{exc} = 400 nm. λ_{em} = 480 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm

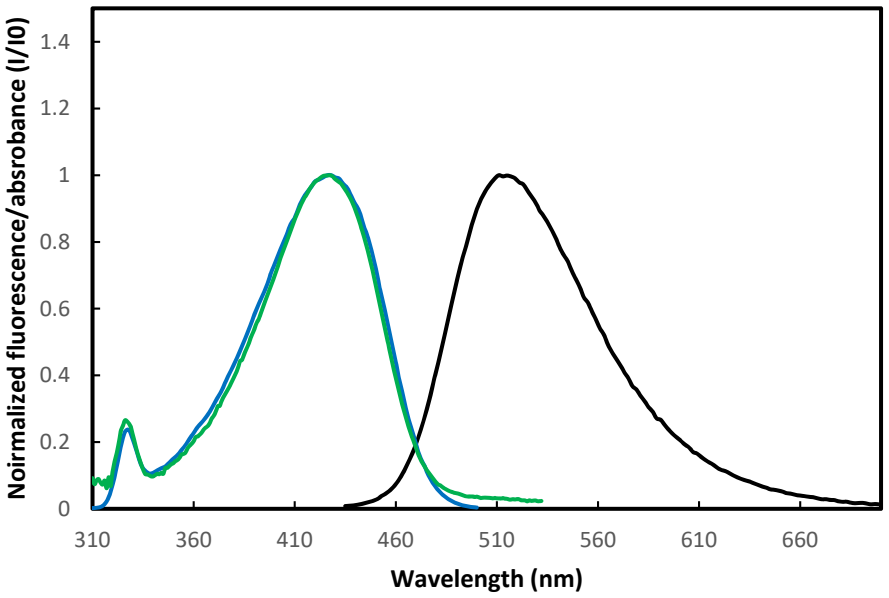


Figure S26. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **4b** in $CHCl_3$. λ_{exc} = 400 nm. λ_{em} = 500 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm

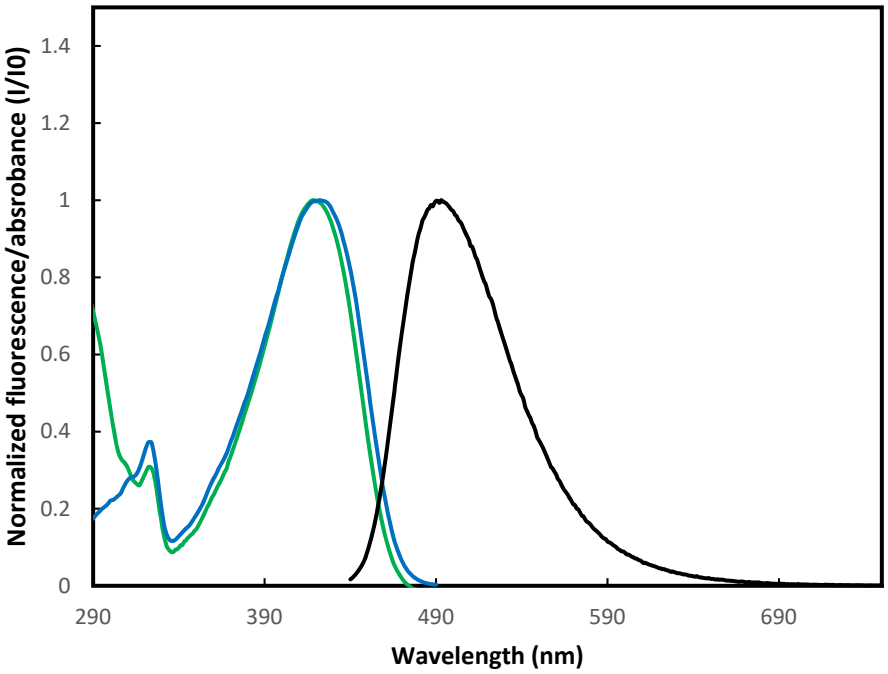


Figure S27. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **4c** in $CHCl_3$. λ_{exc} = 430 nm. λ_{em} = 500 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm.

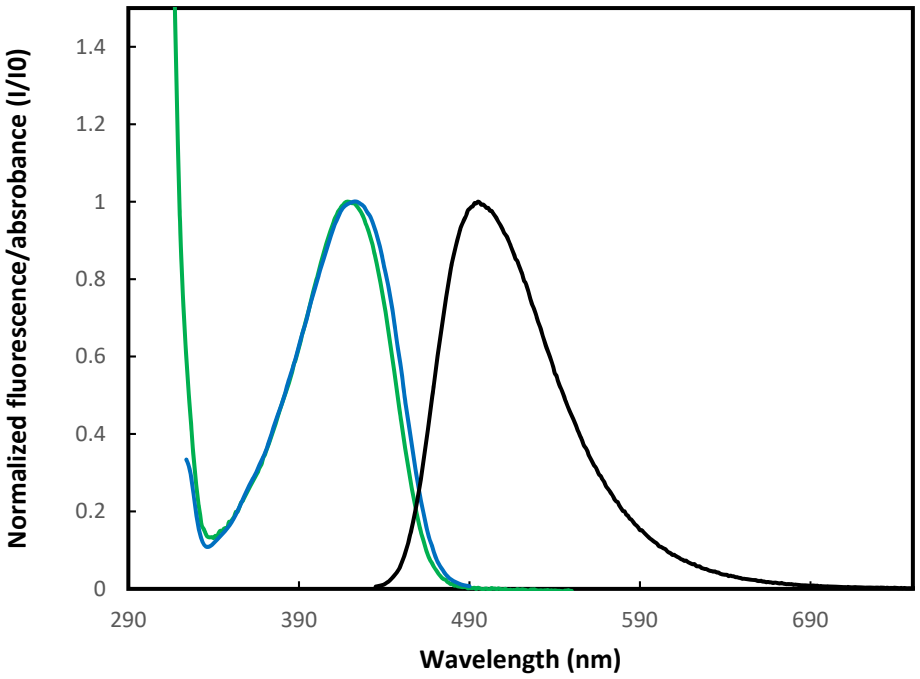


Figure S28. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **4d** in $CHCl_3$. λ_{exc} = 430 nm. λ_{em} = 500 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm

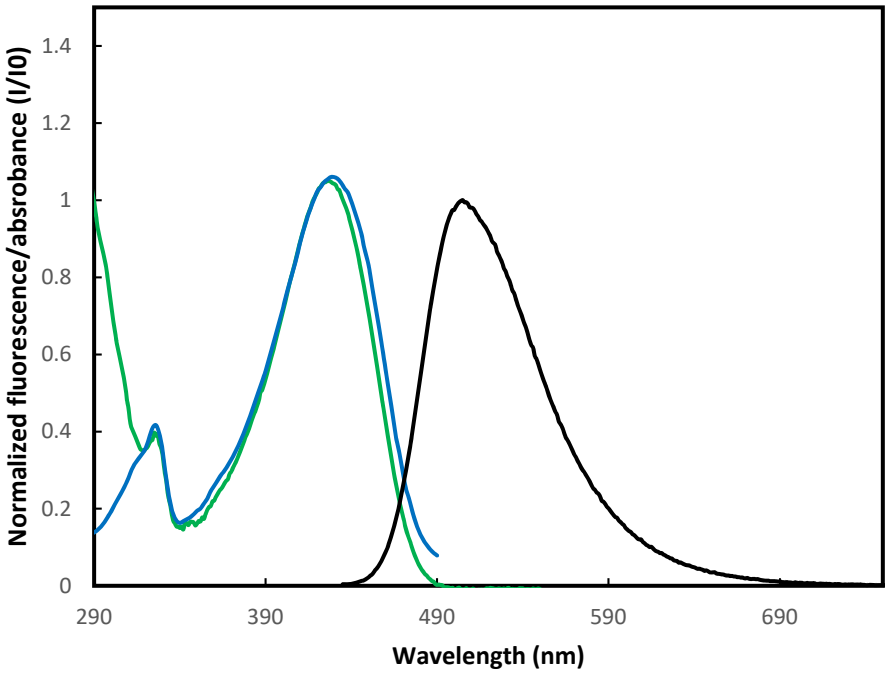


Figure S29. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **4e** in $CHCl_3$. λ_{exc} = 400 nm. λ_{em} = 500 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm

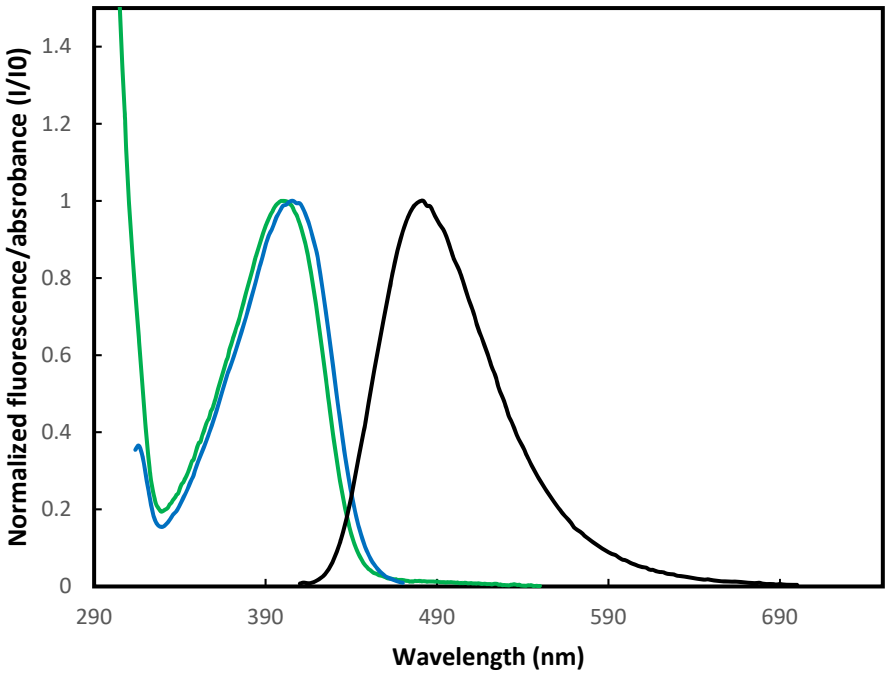


Figure S30. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **7a** in $CHCl_3$. λ_{exc} = 400 nm. λ_{em} = 480 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm

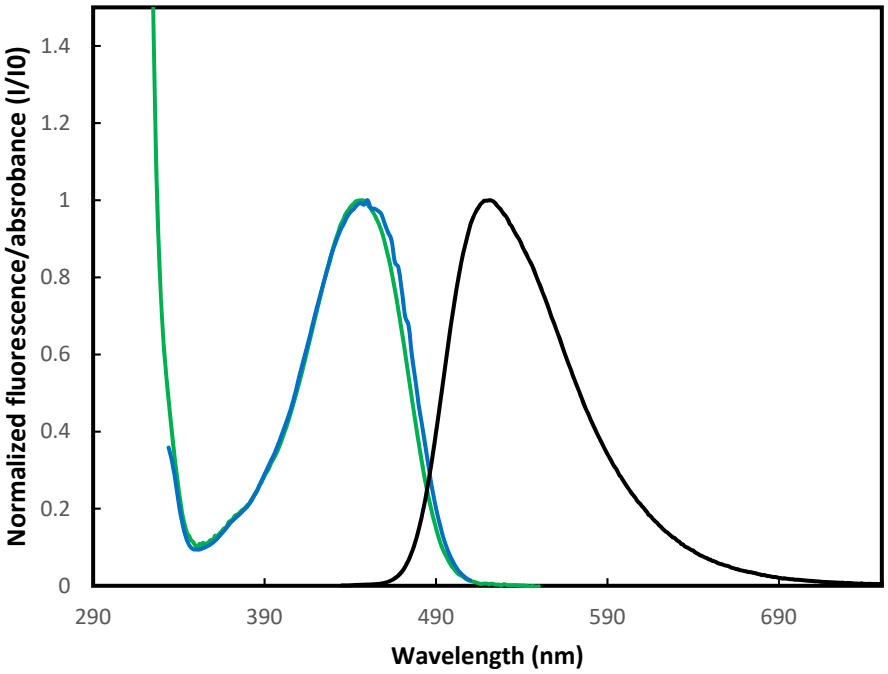


Figure S31. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **7b** in $CHCl_3$. λ_{exc} = 430 nm. λ_{em} = 520 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm

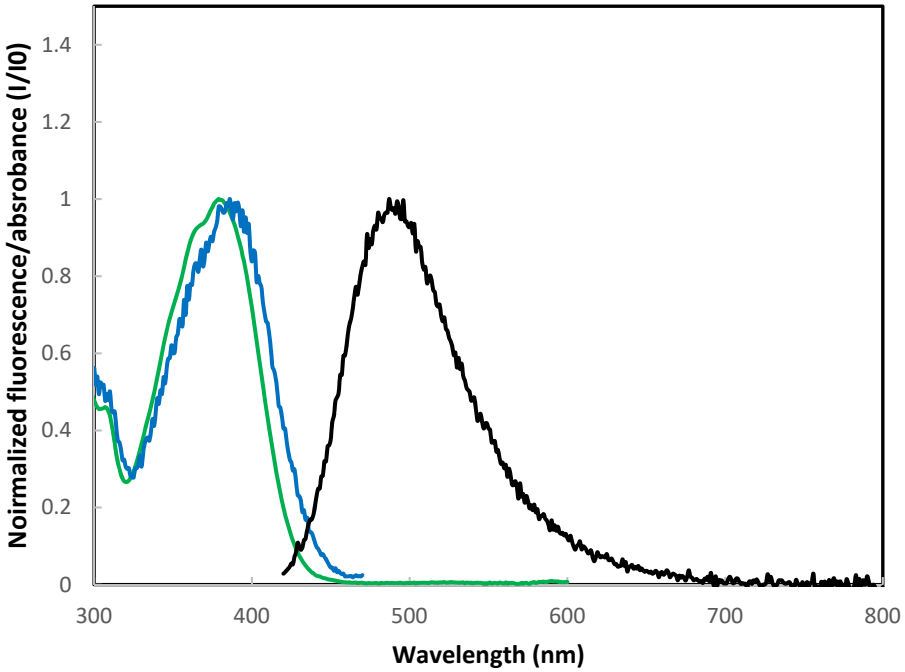


Figure S32. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **7d** in $CHCl_3$. λ_{exc} = 430 nm. λ_{em} = 540 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm

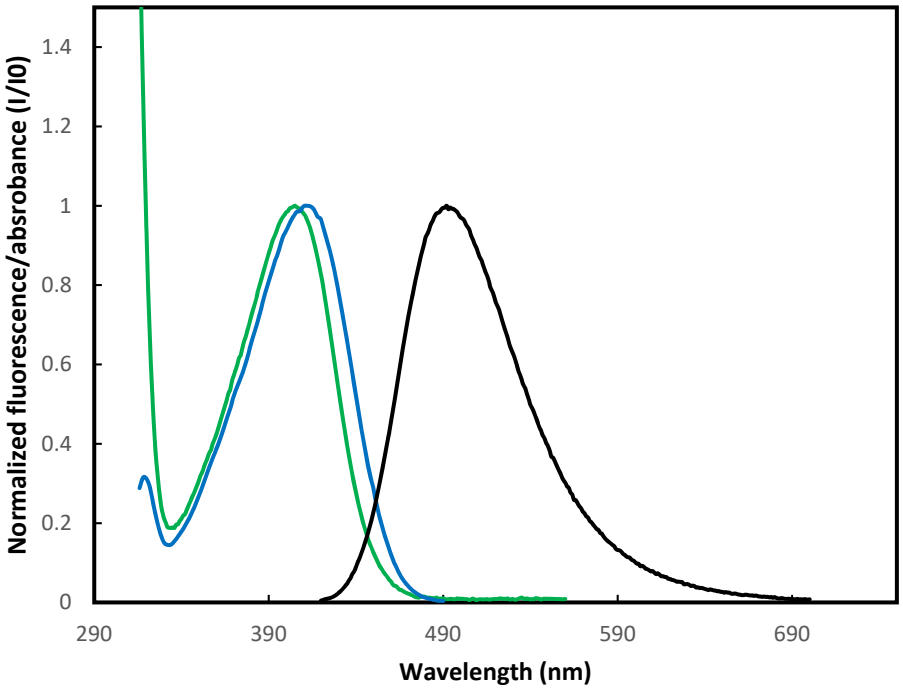


Figure S33. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **11a** in $CHCl_3$. λ_{exc} = 410 nm. λ_{em} = 500 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm.

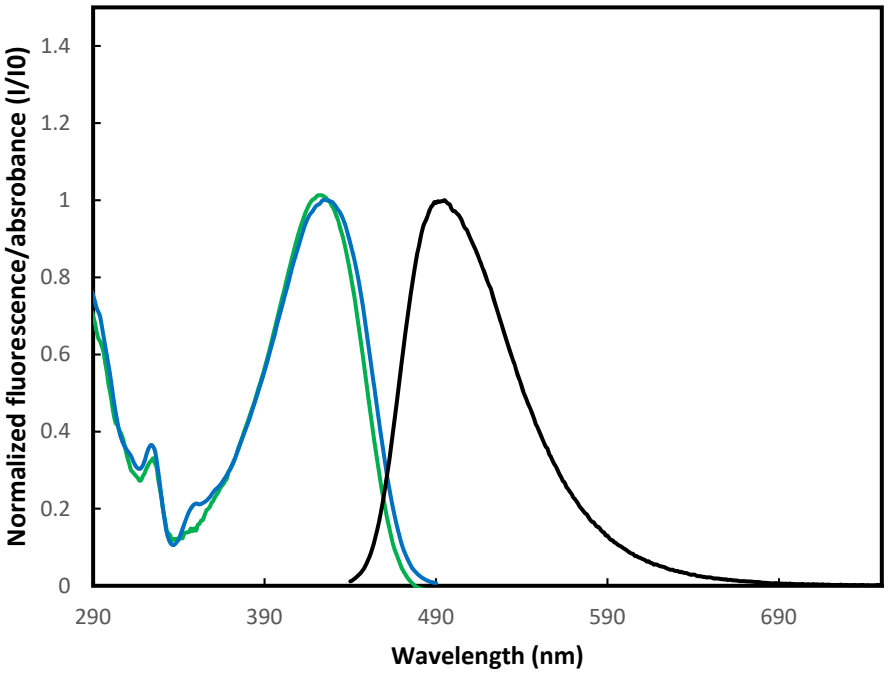


Figure S34. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **11b** in $CHCl_3$. λ_{exc} = 430 nm. λ_{em} = 500 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm.

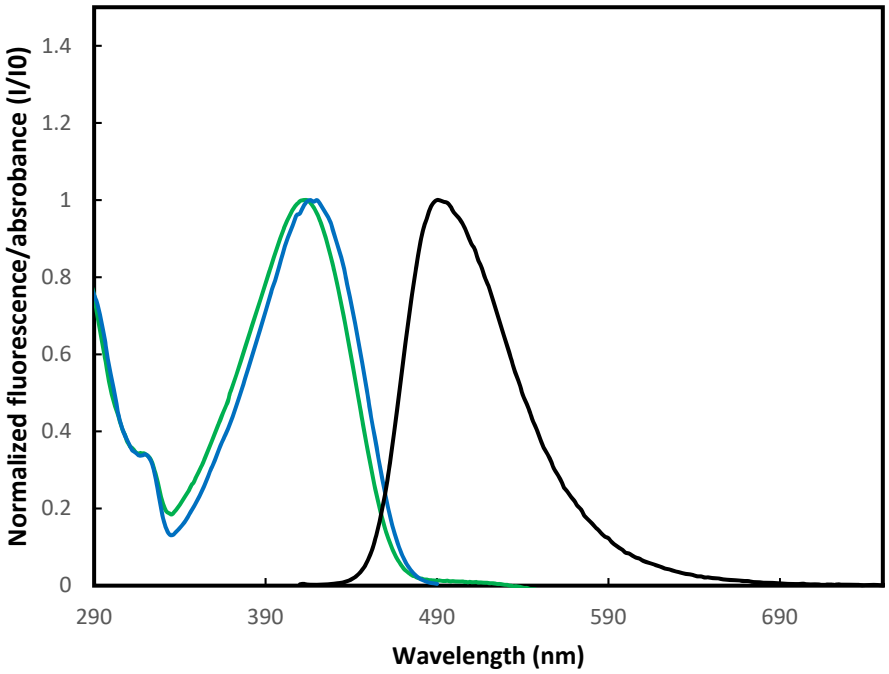


Figure S35. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **11c** in $CHCl_3$. λ_{exc} = 400 nm. λ_{em} = 500 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm

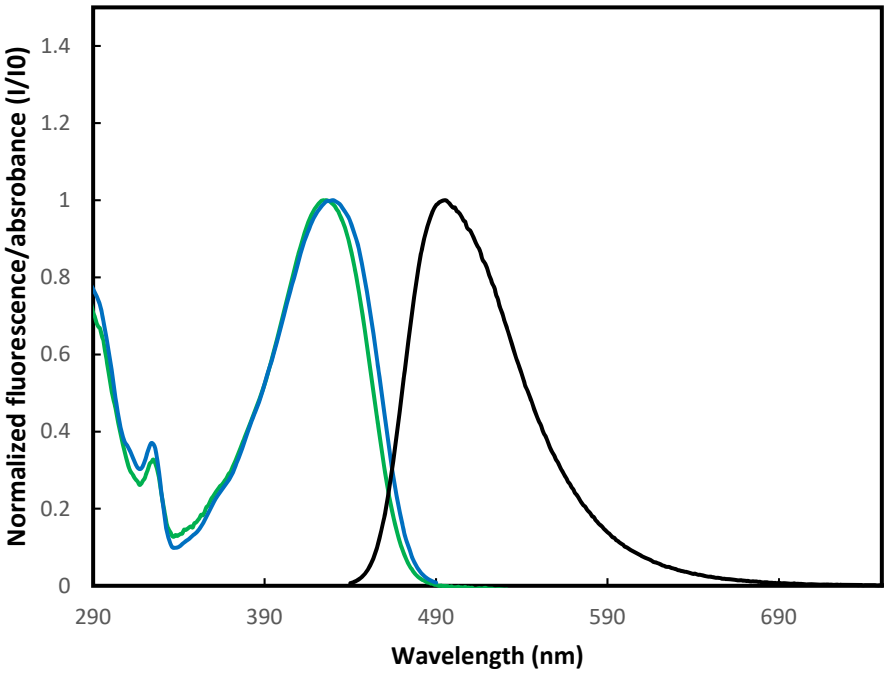


Figure S36. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **11d** in $CHCl_3$. λ_{exc} = 430 nm. λ_{em} = 500 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm.

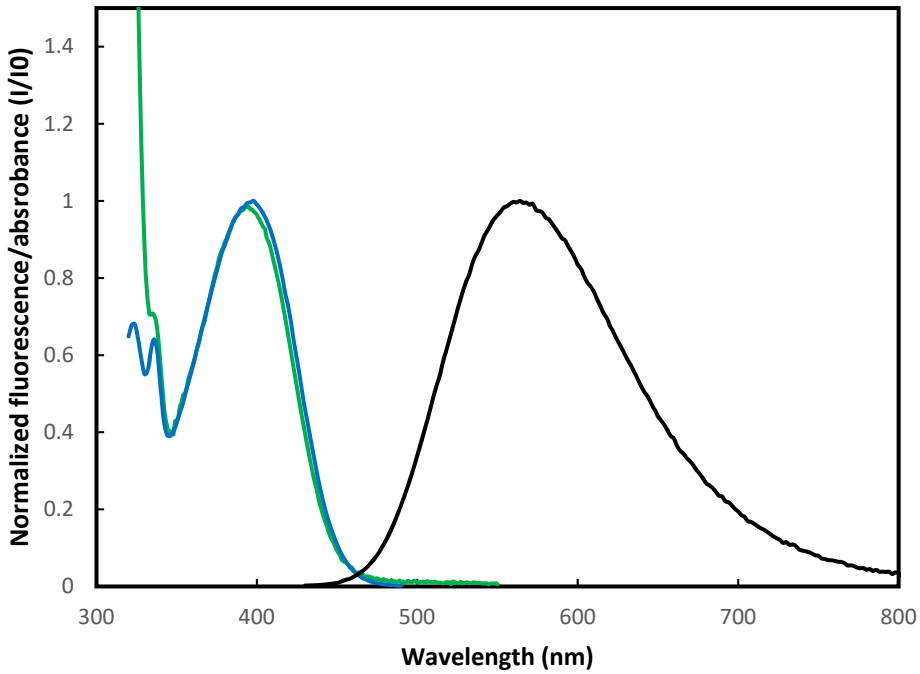


Figure S37. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **11e** in $CHCl_3$. λ_{exc} = 400 nm. λ_{em} = 550 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm.

Photophysical properties DMSO

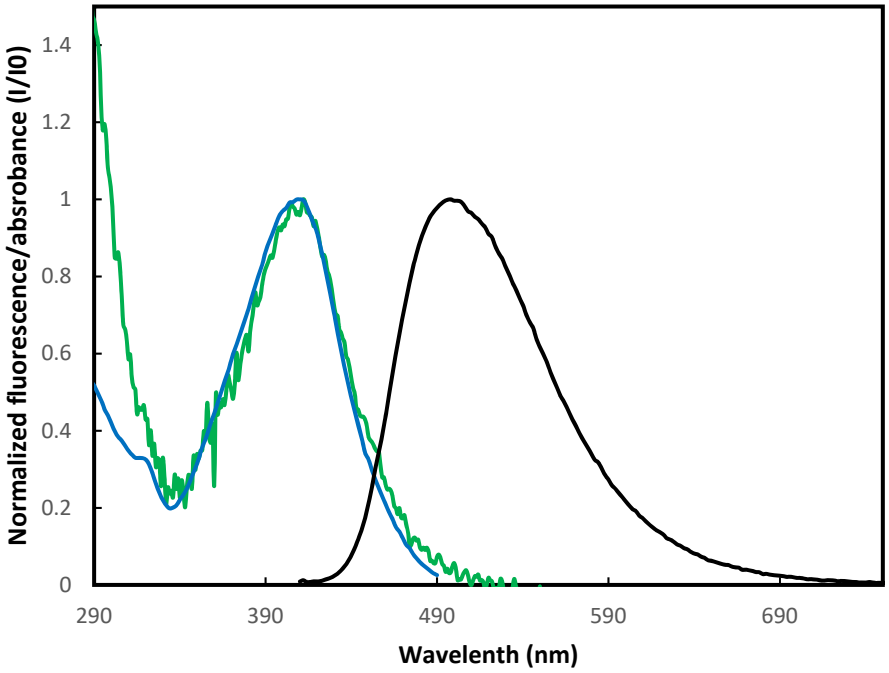


Figure S38. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **3** in DMSO. λ_{exc} = 400 nm. λ_{em} = 510 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm

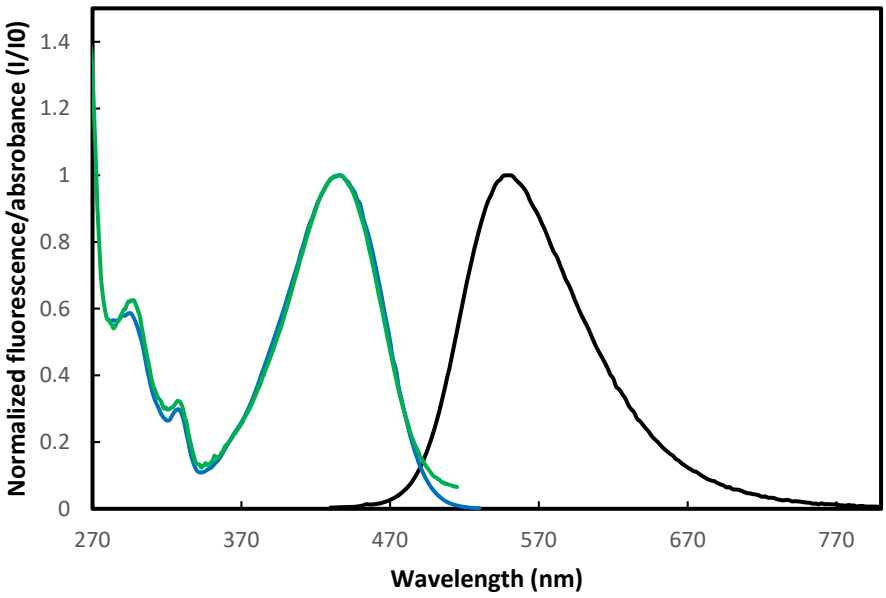


Figure S39. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **4b** in DMSO. λ_{exc} = 430 nm. λ_{em} = 540 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm

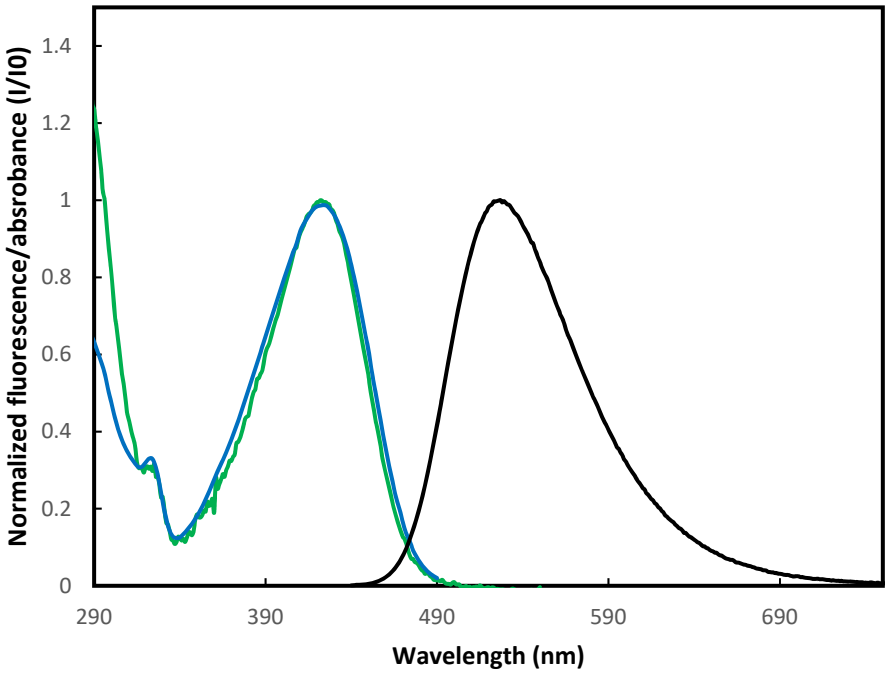


Figure S40. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **4c** in DMSO. λ_{exc} = 430 nm. λ_{em} = 540 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm

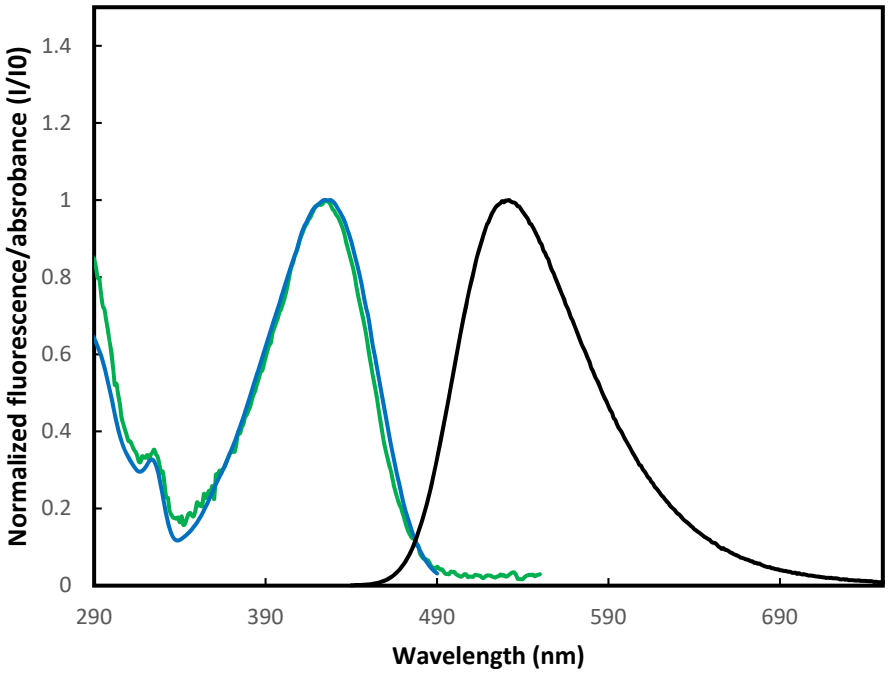


Figure S41. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **4d** in DMSO. λ_{exc} = 430 nm. λ_{em} = 540 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm

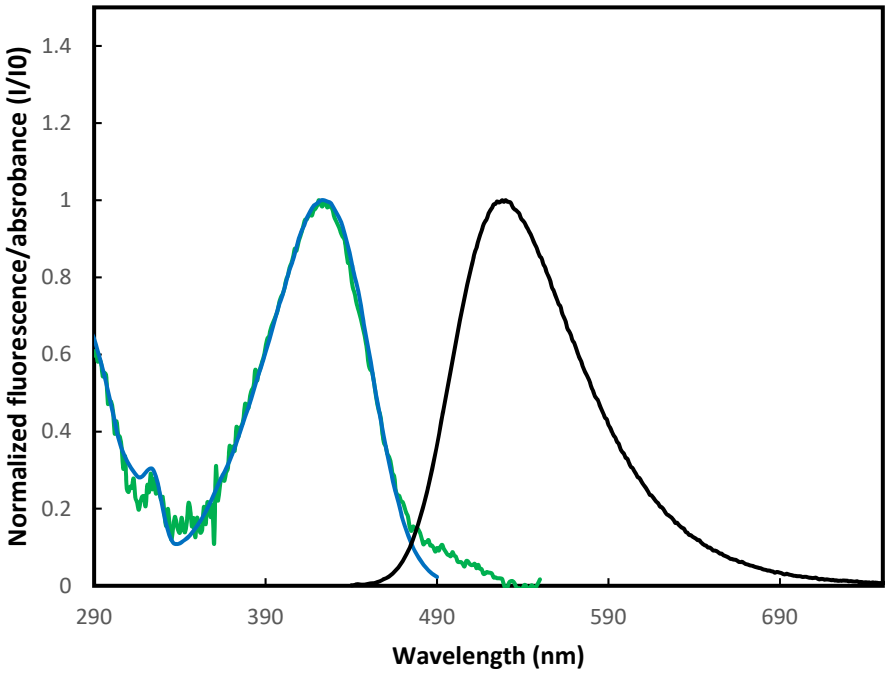


Figure S42. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **4e** in DMSO. λ_{exc} = 430 nm. λ_{em} = 540 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm

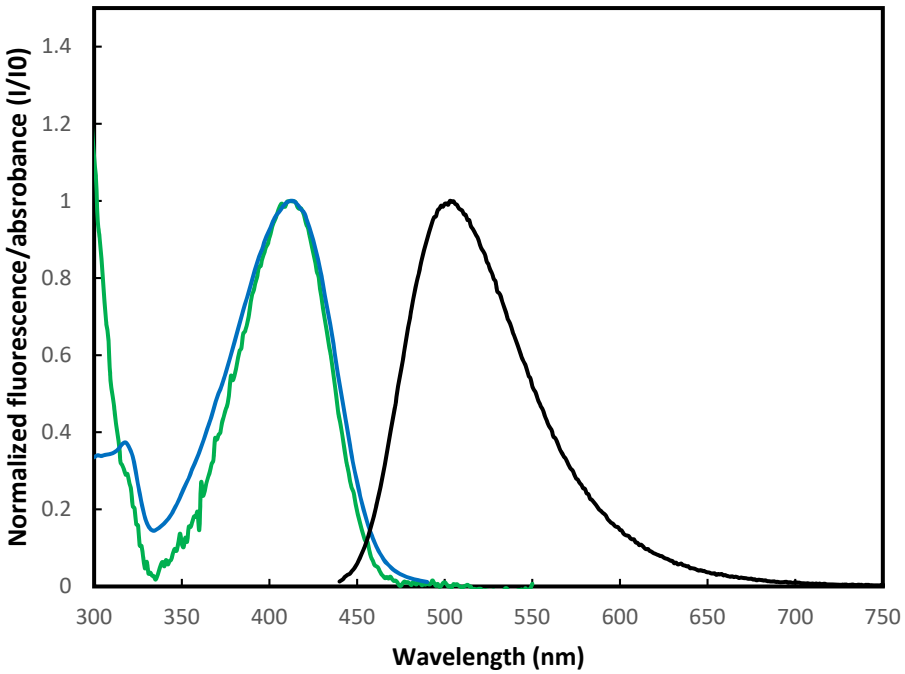


Figure S43. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **7a** in DMSO. λ_{exc} = 430 nm. λ_{em} = 510 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm

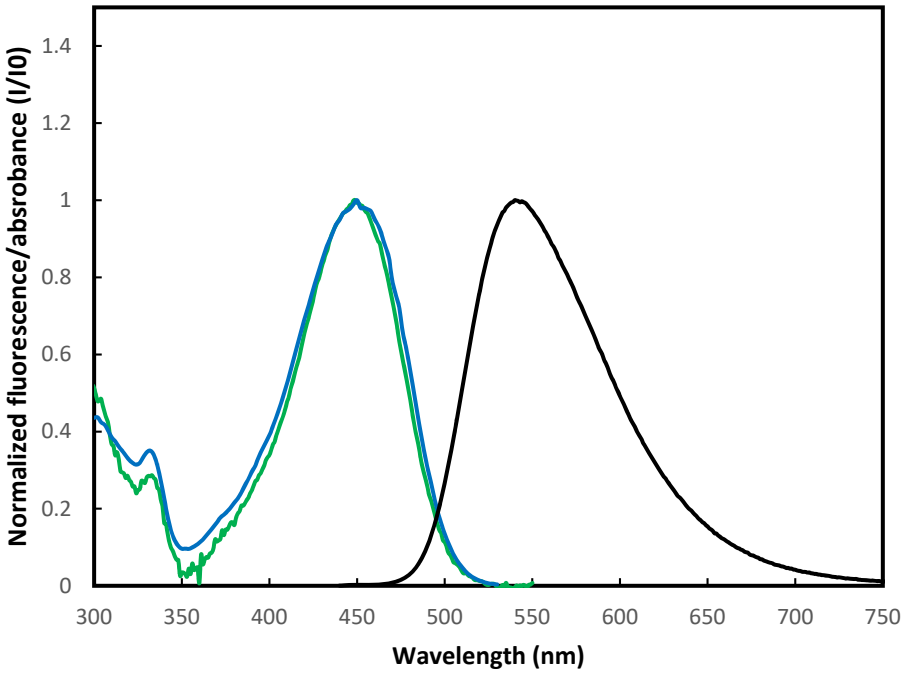


Figure S44. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **7b** in DMSO. λ_{exc} = 430 nm. λ_{em} = 540 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm

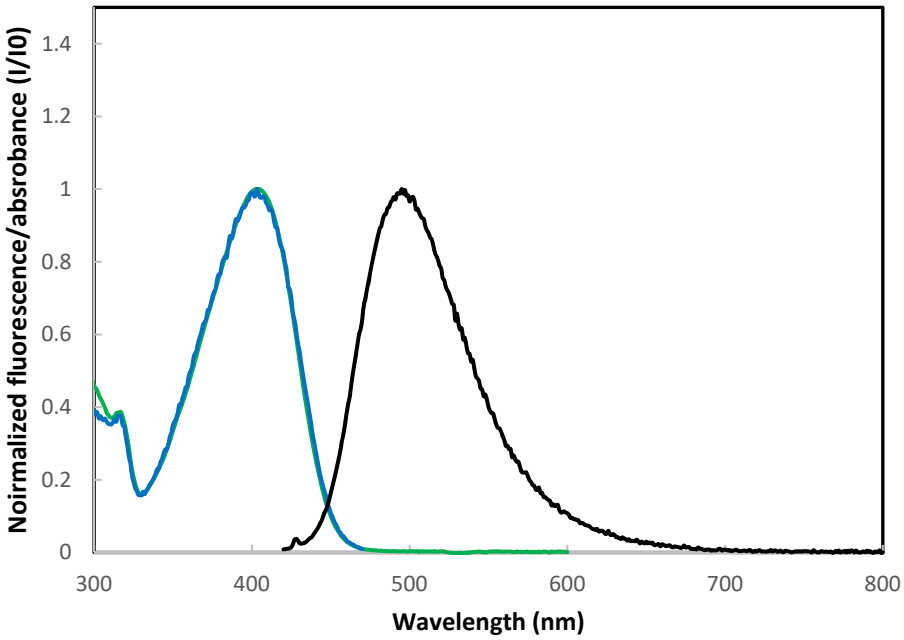


Figure S45. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **7d** in DMSO. λ_{exc} = 430 nm. λ_{em} = 540 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm

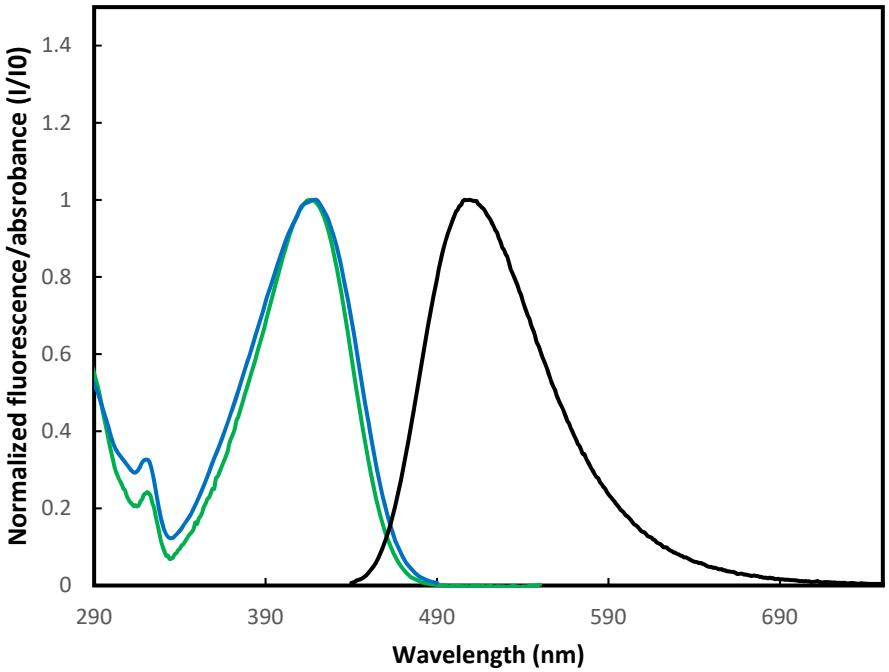


Figure S46. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **11a** in DMSO. λ_{exc} = 430 nm. λ_{em} = 510 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm

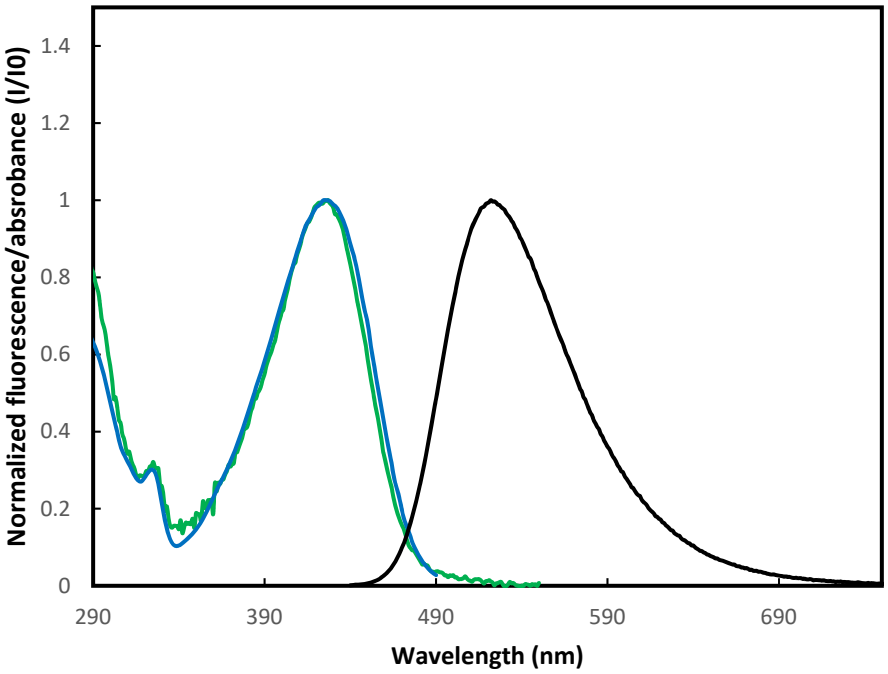


Figure S47. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **11b** in DMSO. λ_{exc} = 430 nm. λ_{em} = 540 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm

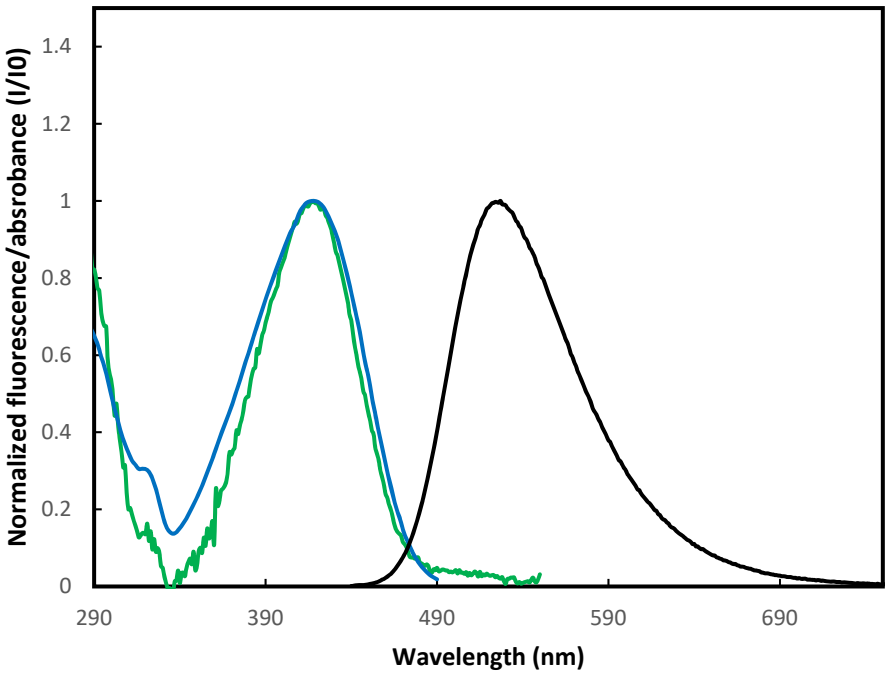


Figure S48. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **11c** in DMSO. λ_{exc} = 430 nm. λ_{em} = 510 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm

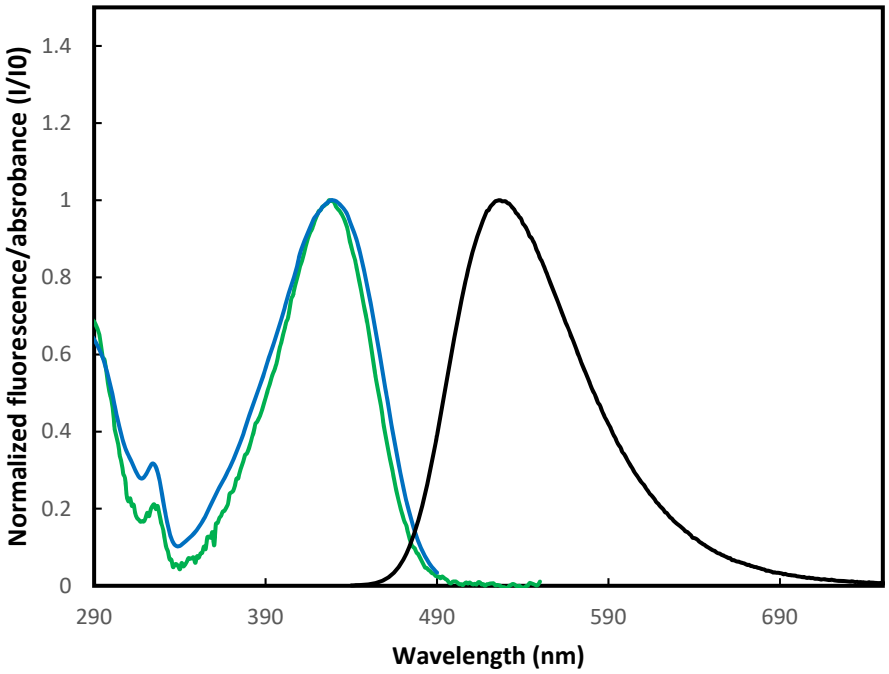


Figure S49. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **11d** in DMSO. λ_{exc} = 430 nm. λ_{em} = 540 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm

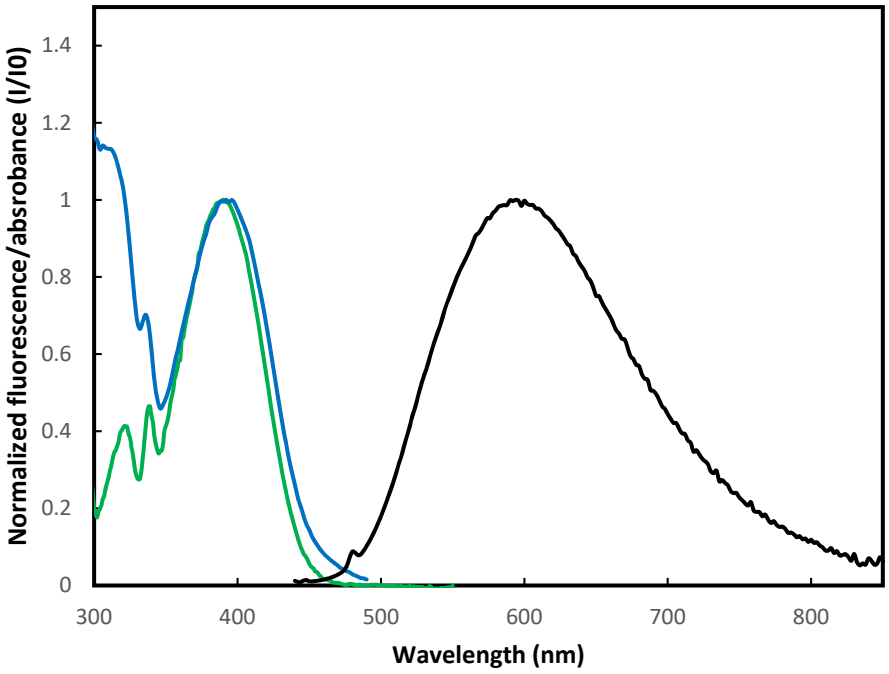


Figure S50. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **11e** in DMSO. λ_{exc} = 420 nm. λ_{em} = 580 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm

Photophysical properties PBS Buffer pH = 7.4

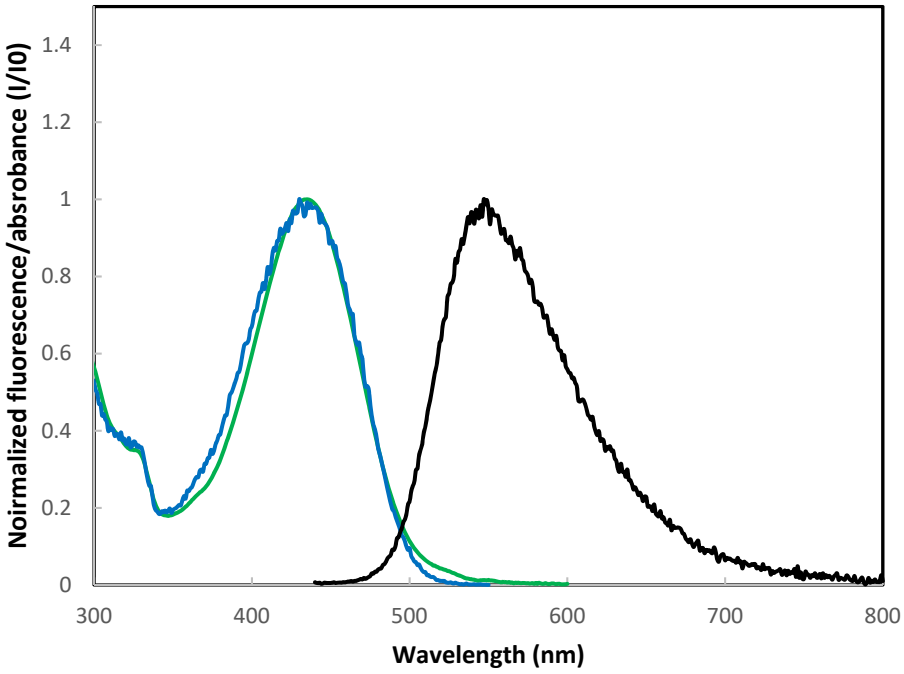


Figure S51. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **3** in PBS buffer pH = 7.4. λ_{exc} = 430 nm. λ_{em} = 540 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm

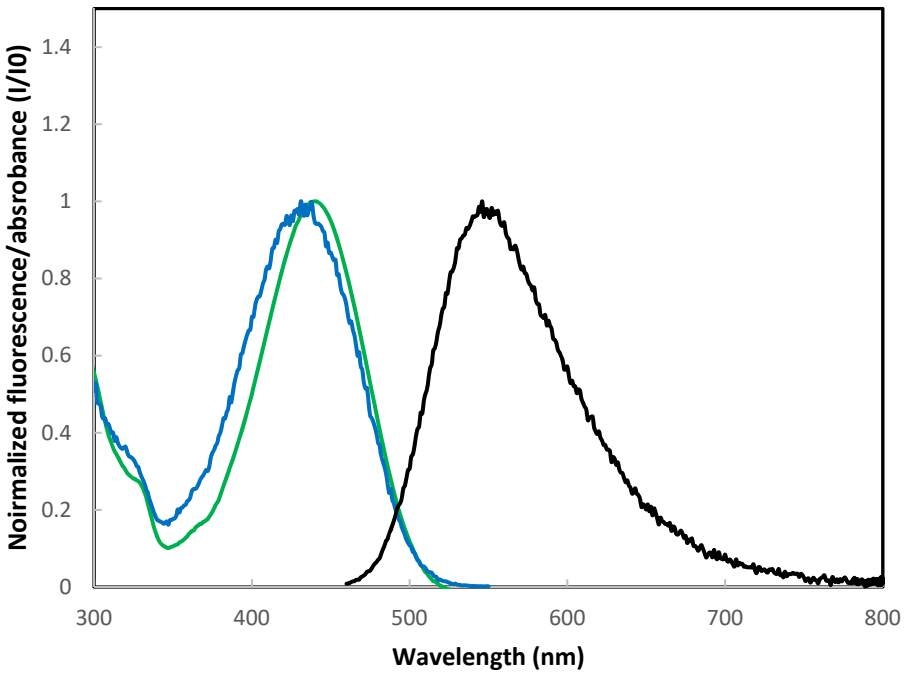


Figure S52. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **4a** in PBS buffer pH = 7.4. λ_{exc} = 430 nm. λ_{em} = 540 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm

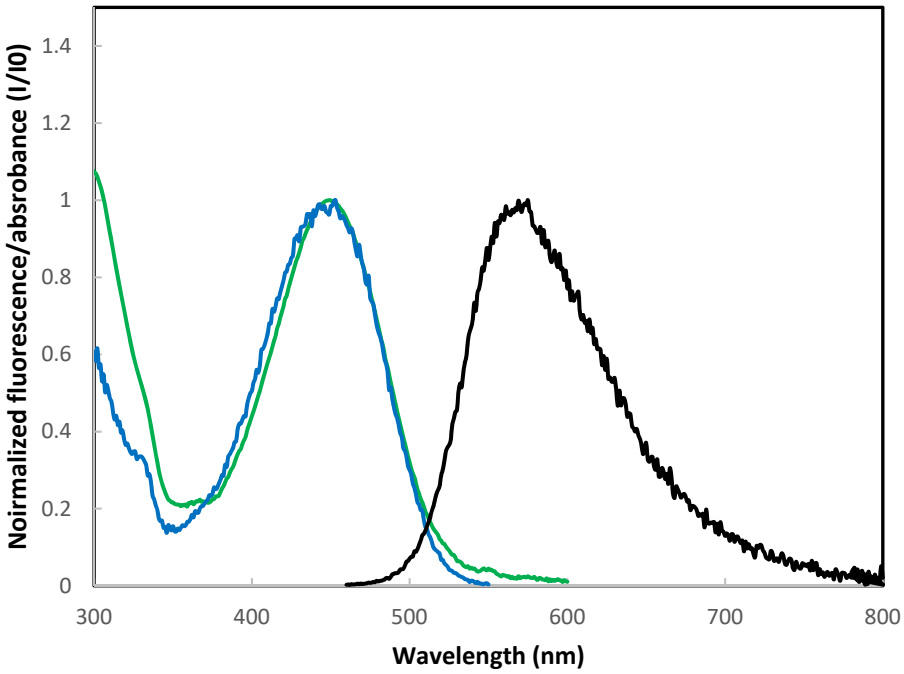


Figure S53. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **4b** in PBS buffer pH = 7.4. λ_{exc} = 430 nm. λ_{em} = 540 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm

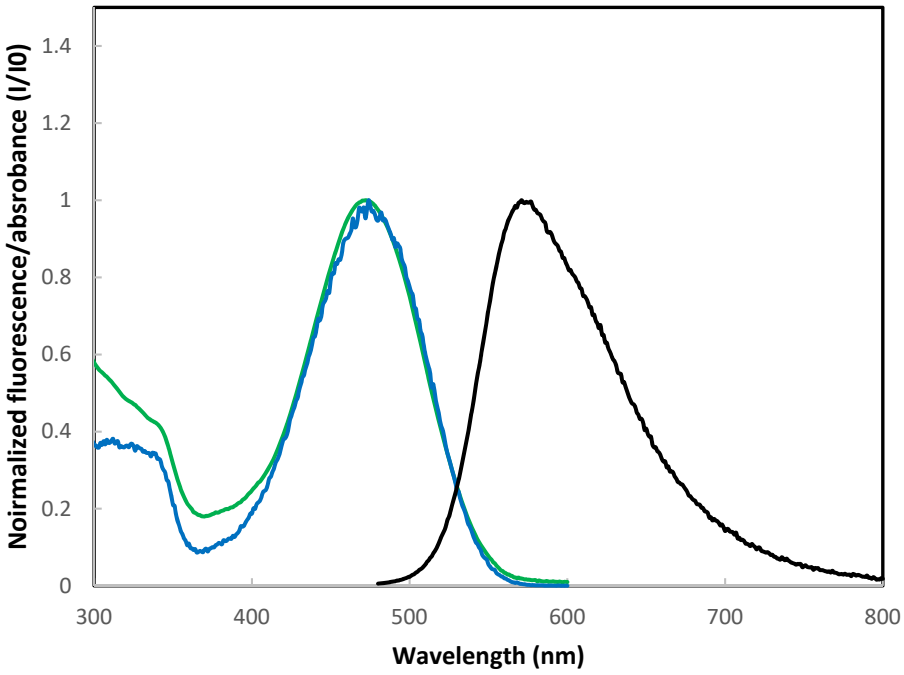


Figure S54. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **7b** in PBS buffer pH = 7.4. λ_{exc} = 430 nm. λ_{em} = 540 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm

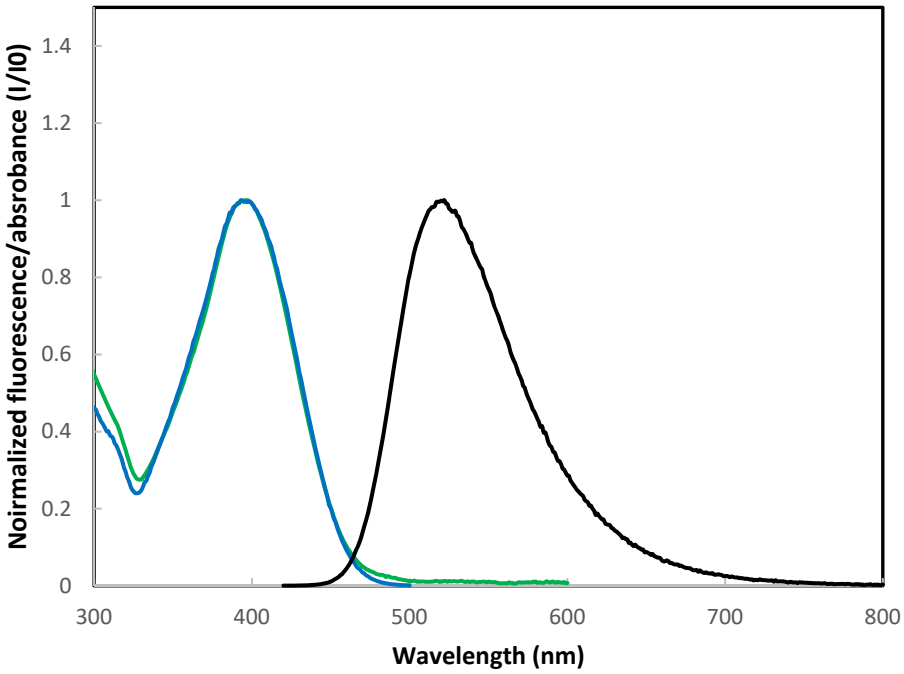


Figure S55. Absorbance (green), fluorescence (black) and excitation spectra (blue) for **7d** in PBS buffer pH = 7.4. λ_{exc} = 430 nm. λ_{em} = 540 nm. [c] = 1 x 10^{-5}M. Optical pathway = 10 mm

Epsilon measurement in CHCl3

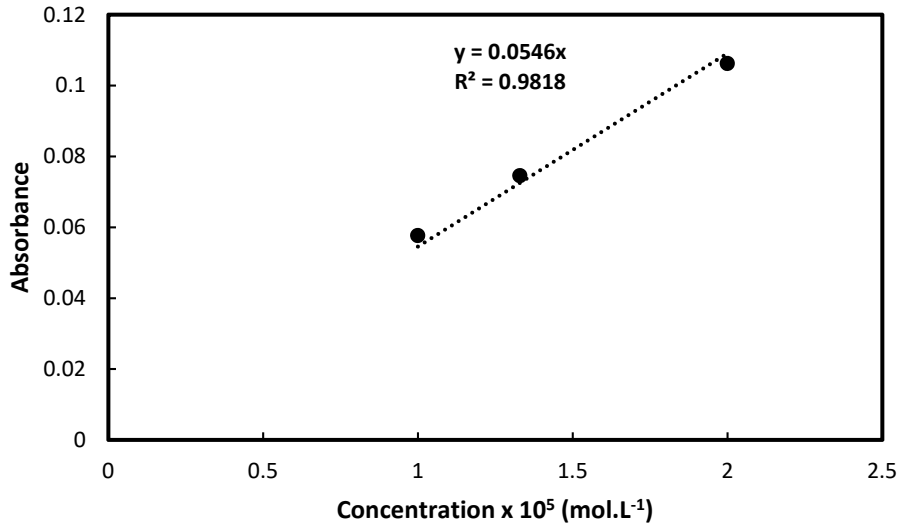


Figure S56. Absorbance at maximum absorption wavelength for **3** in $CHCl_3$

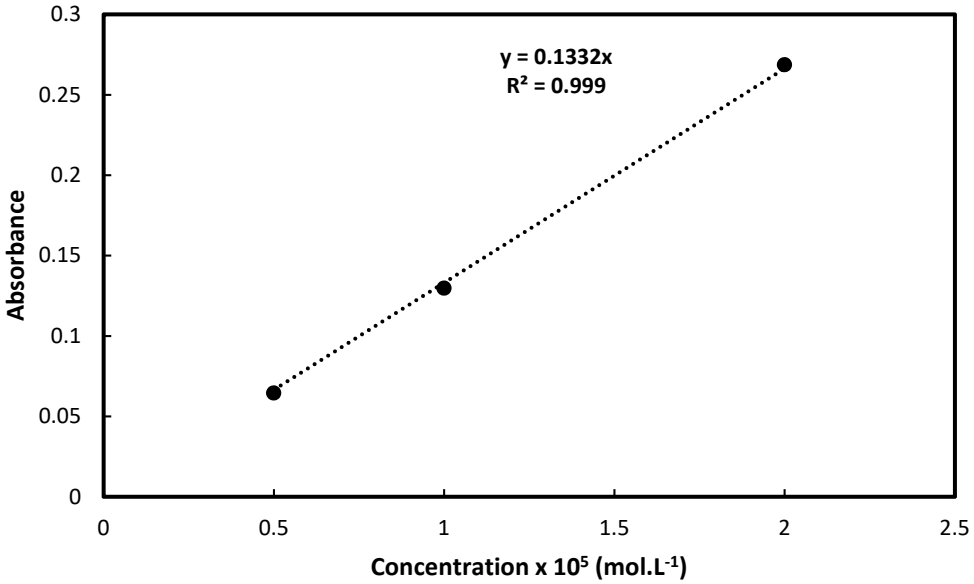


Figure S57. Absorbance at maximum absorption wavelength for **4a** in $CHCl_3$

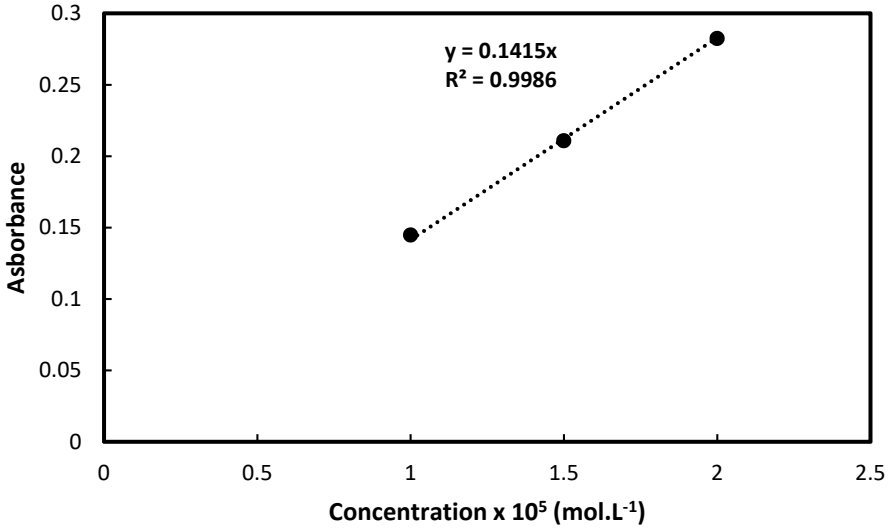


Figure S58. Absorbance at maximum absorption wavelength for **4b** in $CHCl_3$

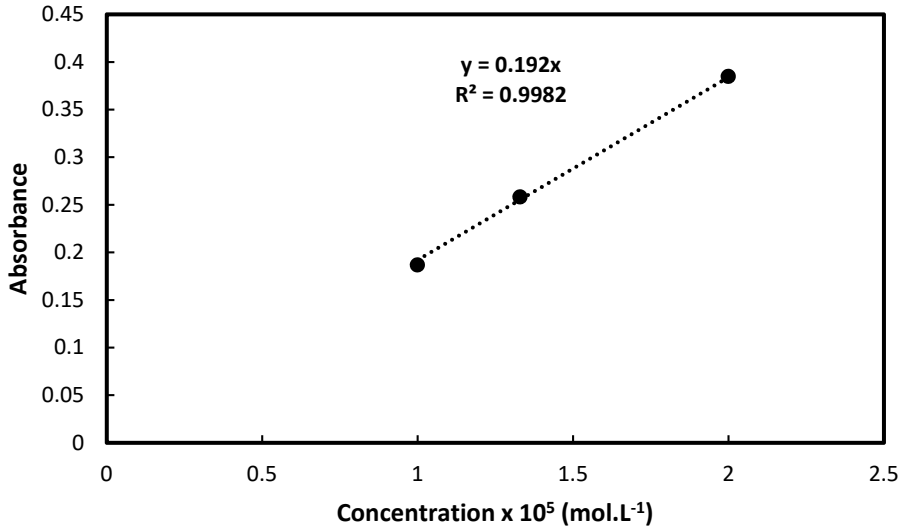


Figure S59. Absorbance at maximum absorption wavelength for **4c** in $CHCl_3$

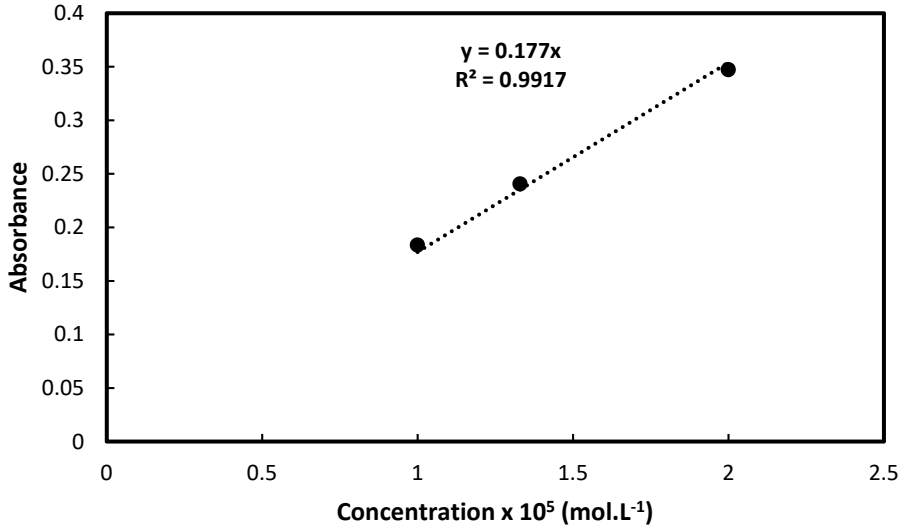


Figure S60. Absorbance at maximum absorption wavelength for **4d** in $CHCl_3$

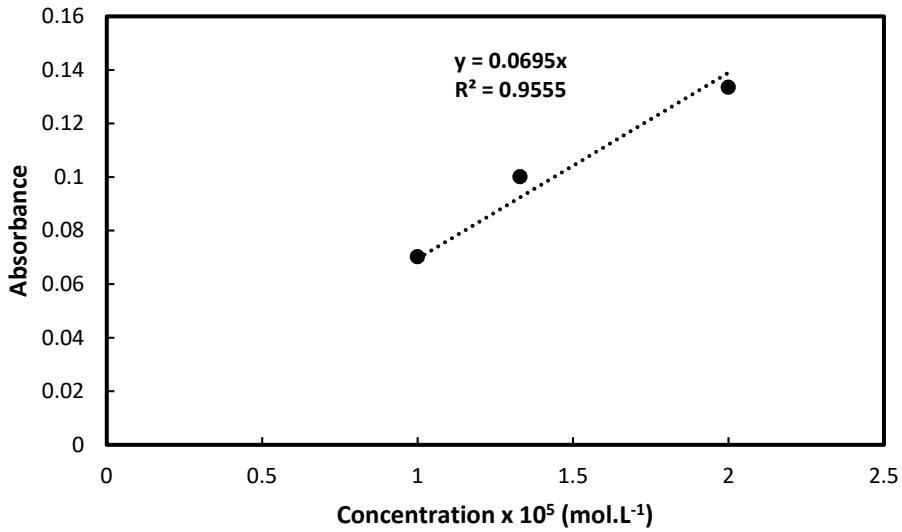


Figure S61. Absorbance at maximum absorption wavelength for **4e** in $CHCl_3$

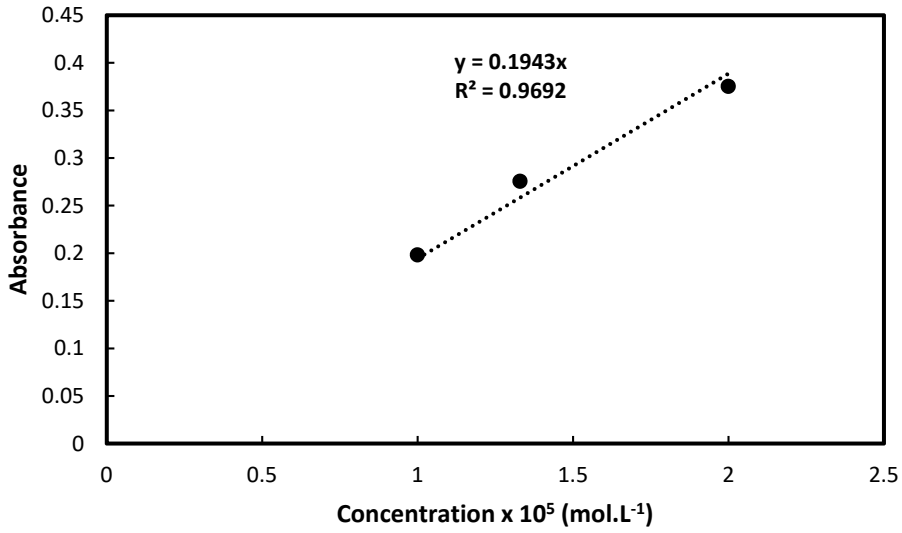


Figure S62. Absorbance at maximum absorption wavelength for **7a** in $CHCl_3$

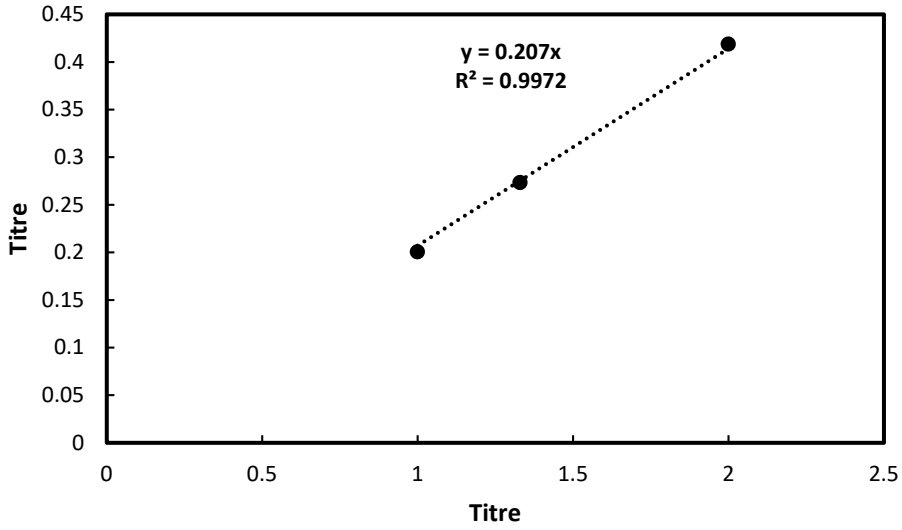


Figure S63. Absorbance at maximum absorption wavelength for **7b** in $CHCl_3$

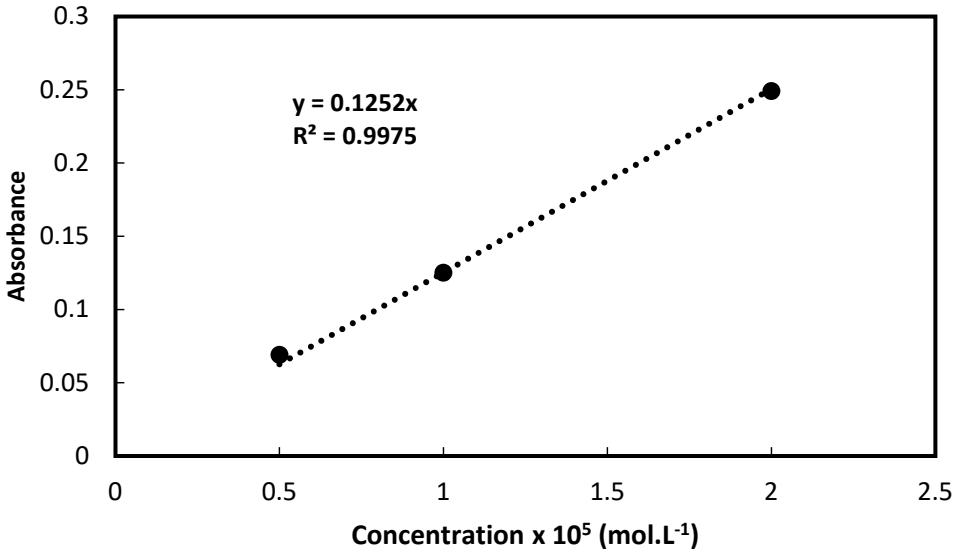


Figure S64. Absorbance at maximum absorption wavelength for **7d** in $CHCl_3$

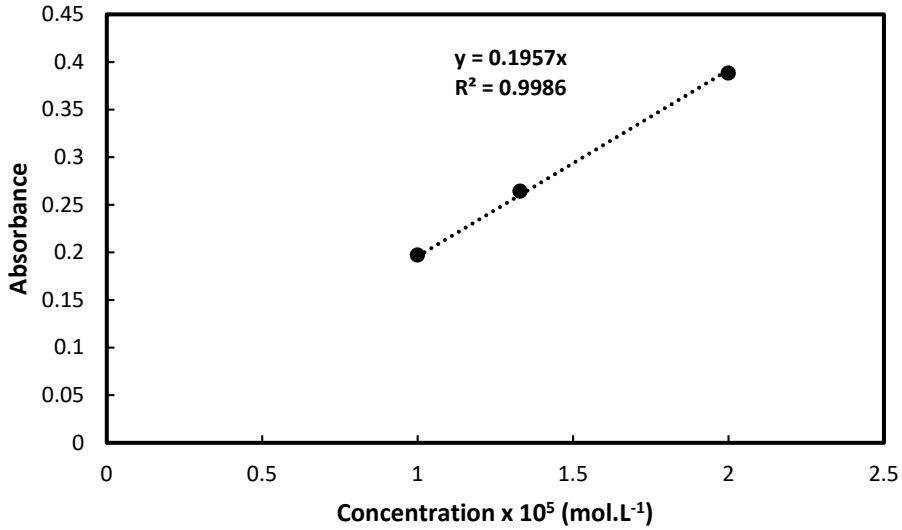


Figure S65. Absorbance at maximum absorption wavelength for **11a** in $CHCl_3$

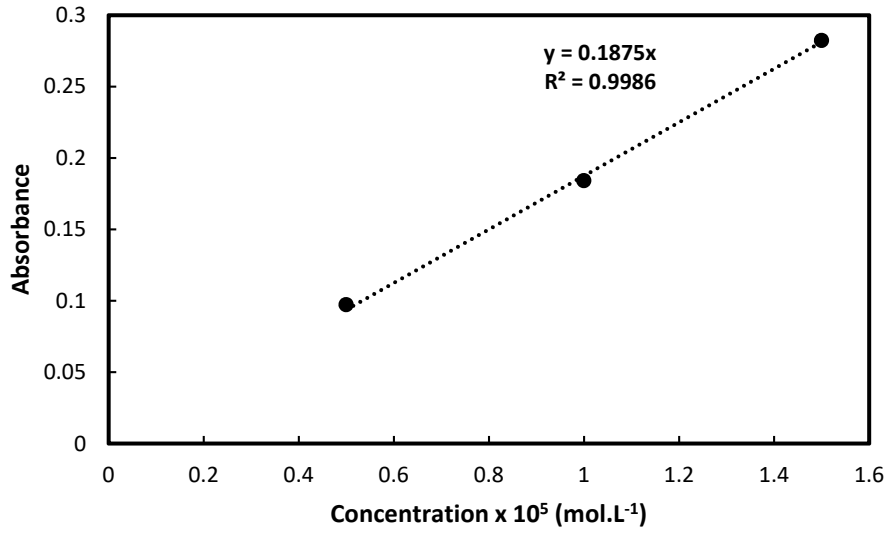


Figure S66. Absorbance at maximum absorption wavelength for **11b** in $CHCl_3$

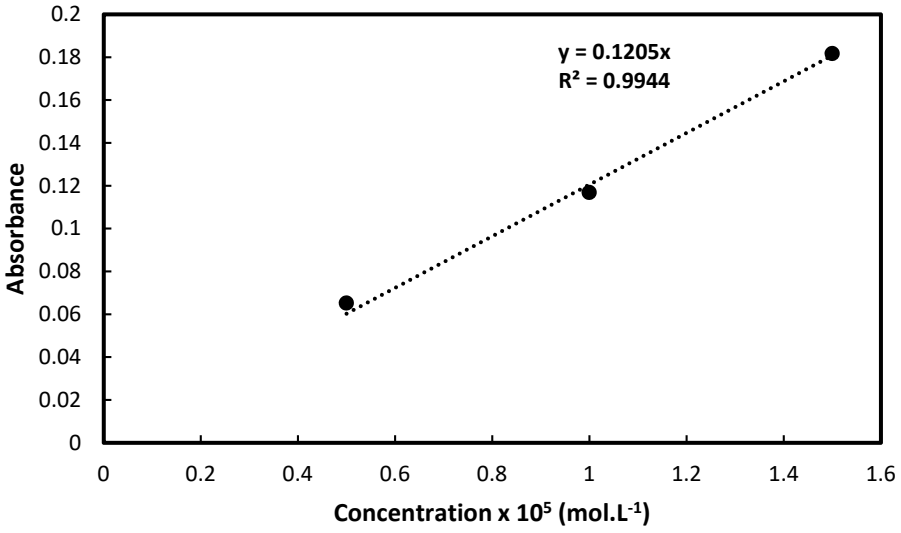


Figure S67. Absorbance at maximum absorption wavelength for **11c** in $CHCl_3$

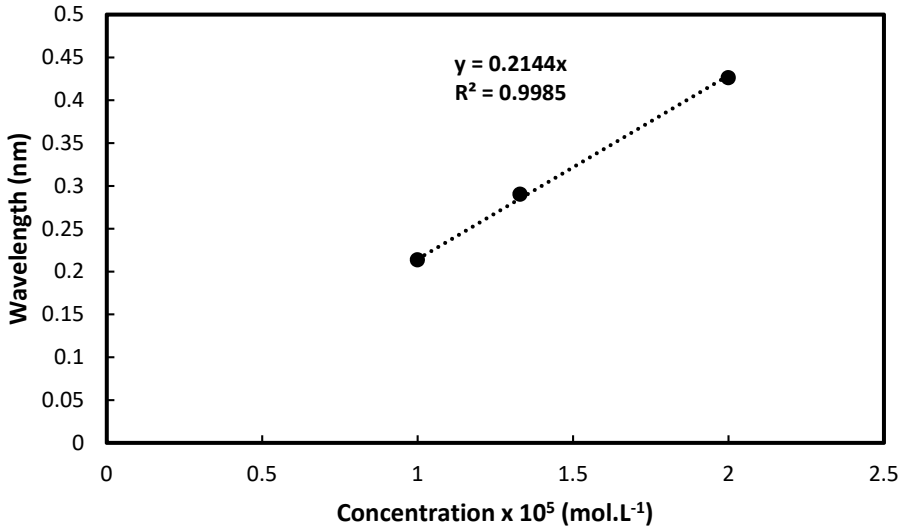


Figure S68. Absorbance at maximum absorption wavelength for **11d** in $CHCl_3$

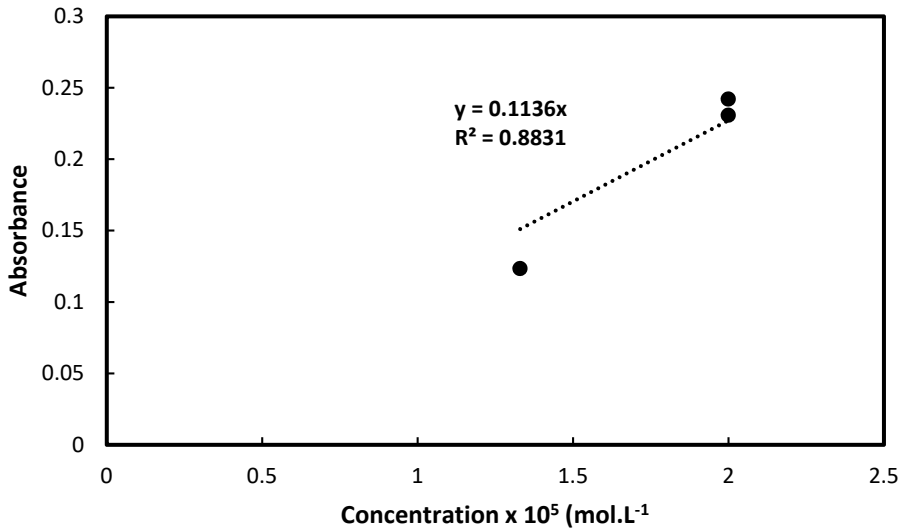


Figure S69. Absorbance at maximum absorption wavelength for **11e** in $CHCl_3$

Epsilon measurement in DMSO

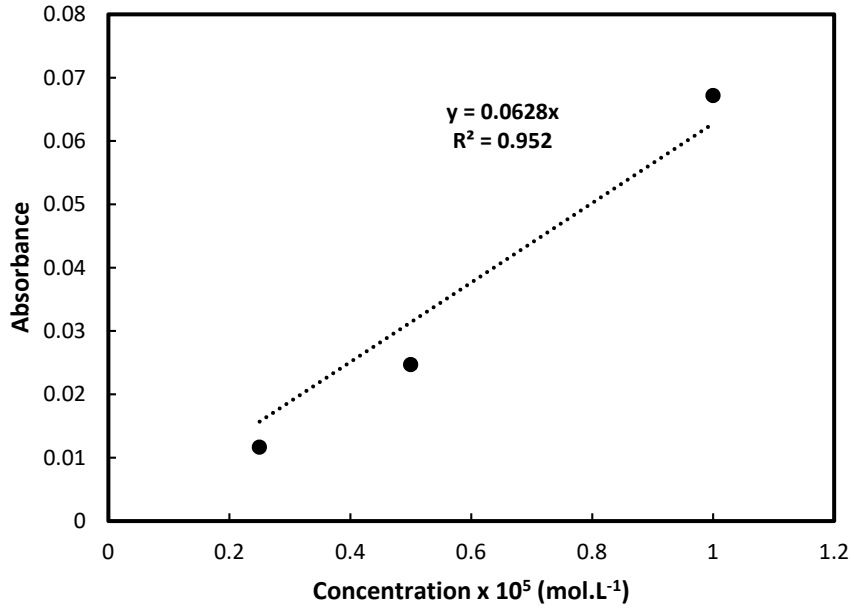


Figure S70. Absorbance at maximum absorption wavelength for **3** in DMSO

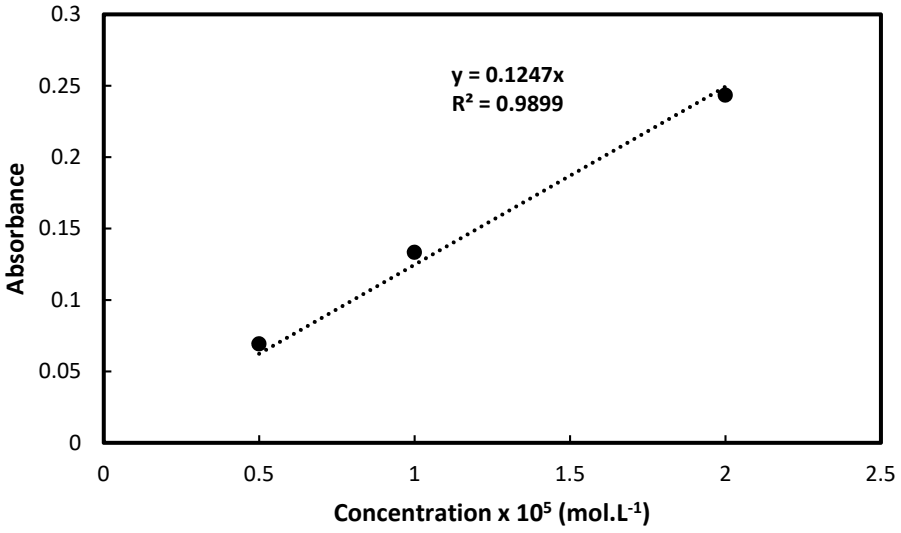


Figure S71. Absorbance at maximum absorption wavelength for **4a** in DMSO

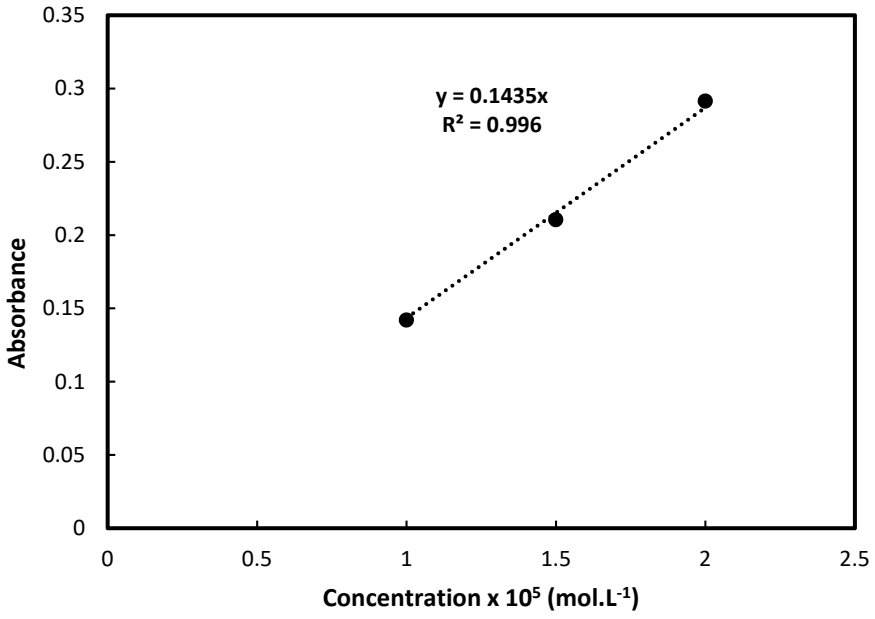


Figure S72. Absorbance at maximum absorption wavelength for **4b** in DMSO

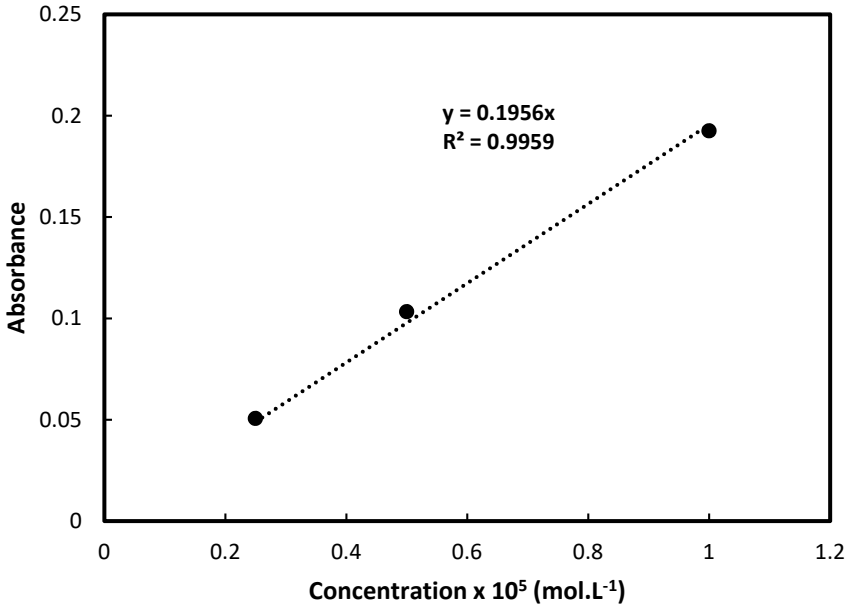


Figure S73. Absorbance at maximum absorption wavelength for **4c** in DMSO

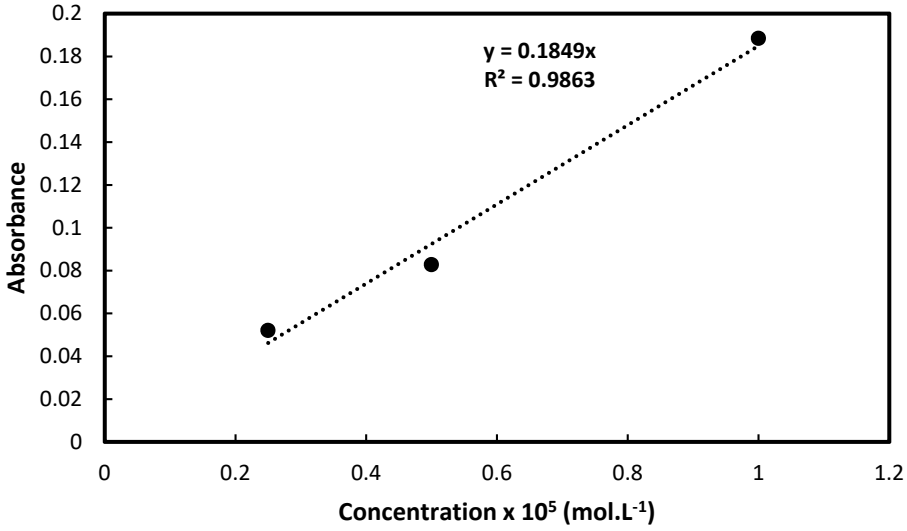


Figure S74. Absorbance at maximum absorption wavelength for **4d** in DMSO

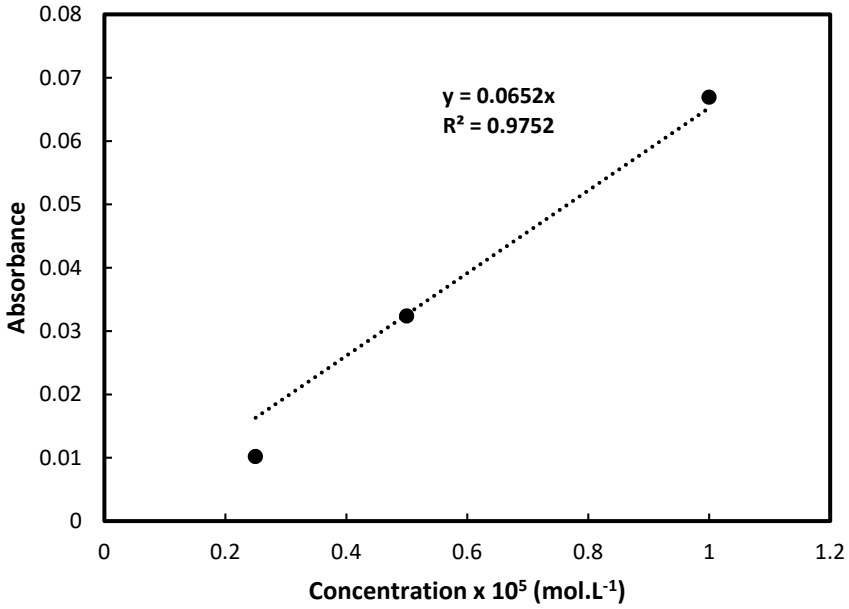


Figure S75. Absorbance at maximum absorption wavelength for **4e** in DMSO

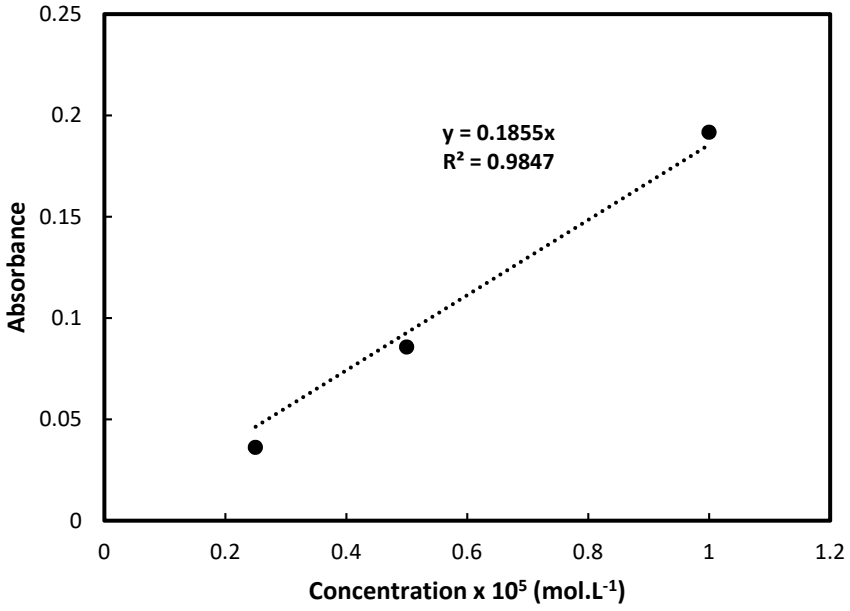


Figure S76. Absorbance at maximum absorption wavelength for **7a** in DMSO

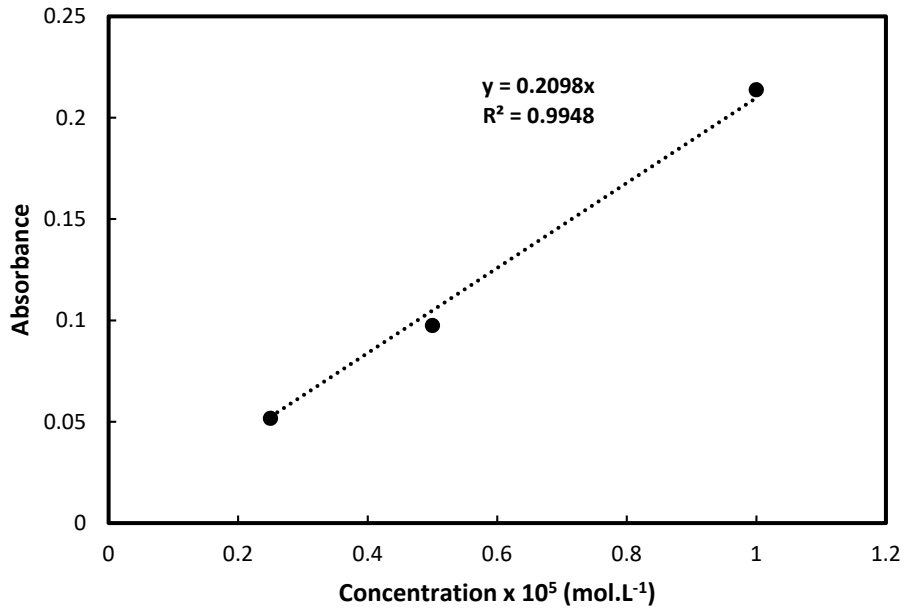


Figure S77. Absorbance at maximum absorption wavelength for **7b** in DMSO

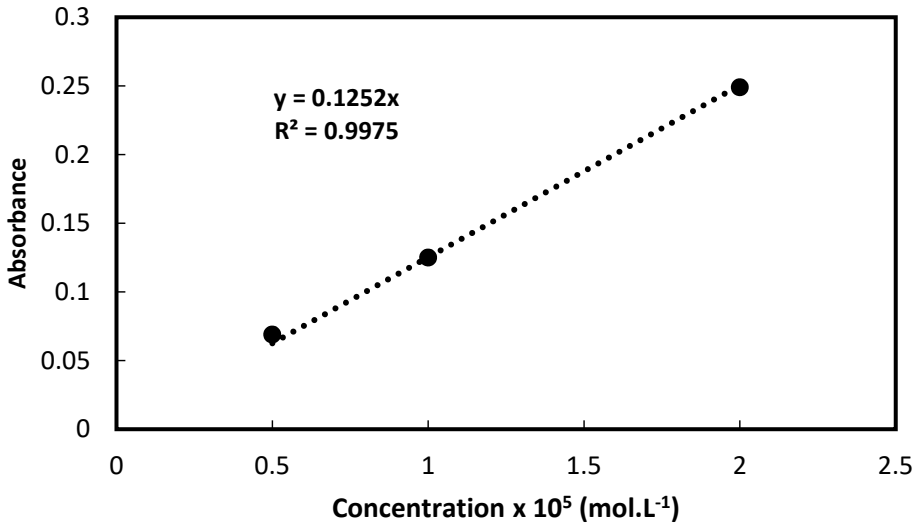


Figure S78. Absorbance at maximum absorption wavelength for **7d** in DMSO

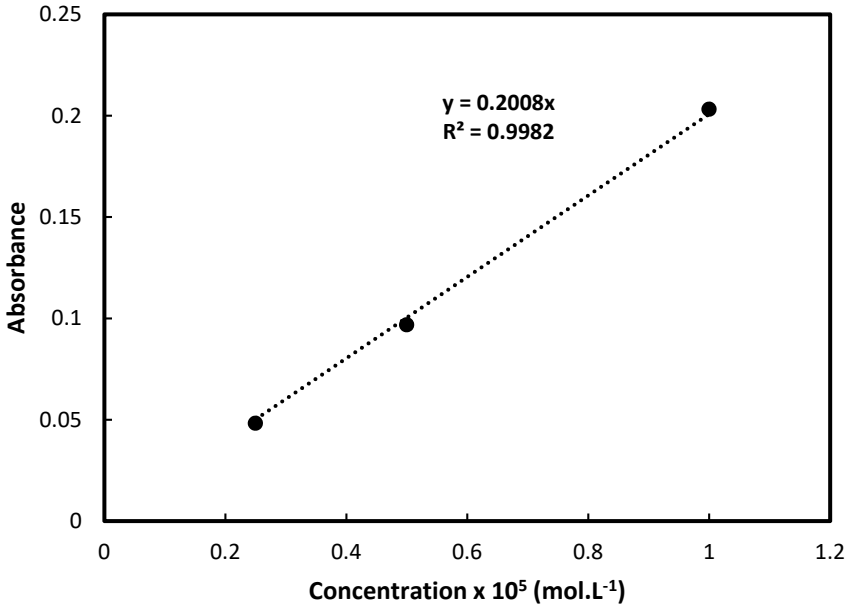


Figure S79. Absorbance at maximum absorption wavelength for **11a** in DMSO

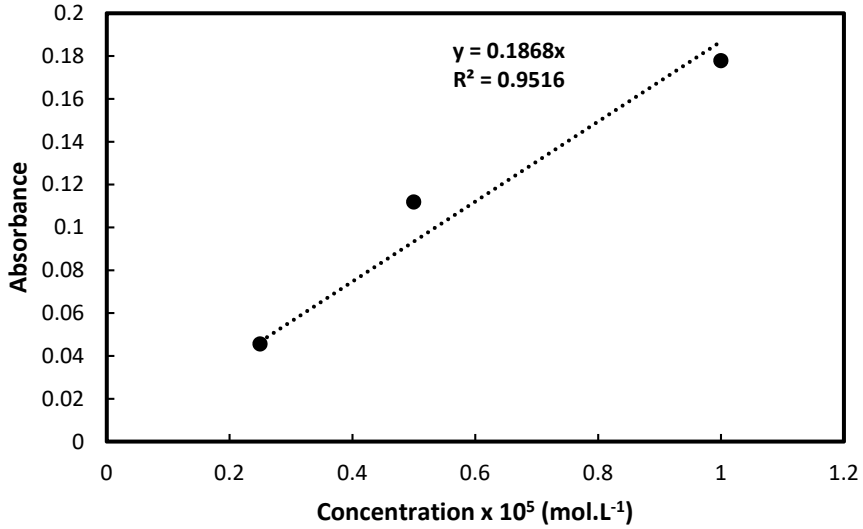


Figure S80. Absorbance at maximum absorption wavelength for **11b** in DMSO

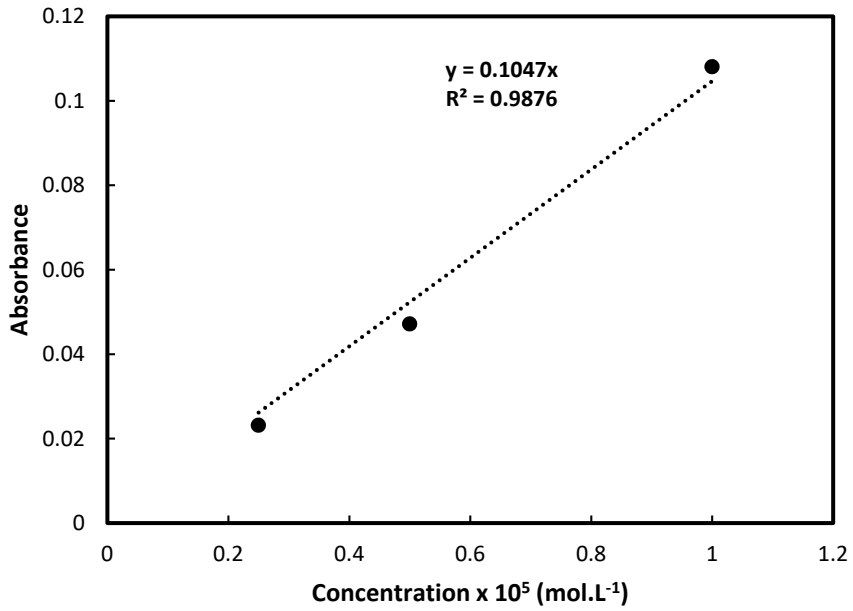


Figure S81. Absorbance at maximum absorption wavelength for **11c** in DMSO

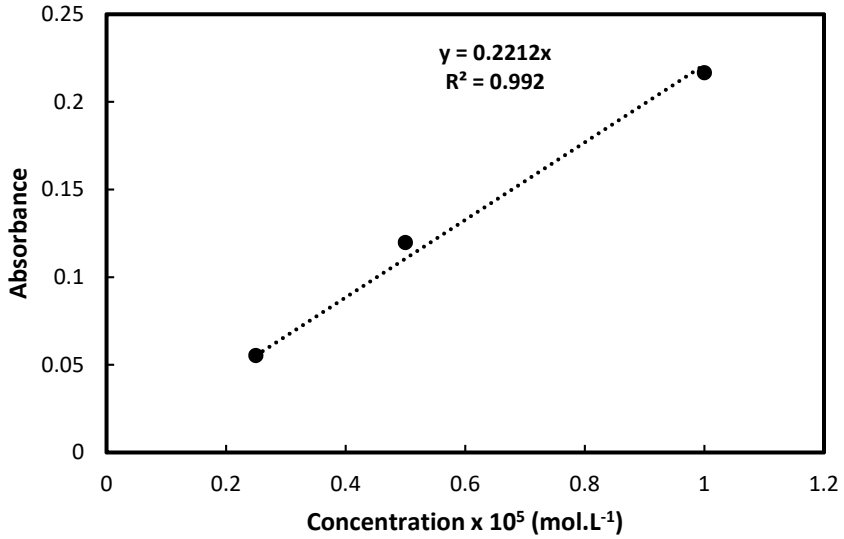


Figure S82. Absorbance at maximum absorption wavelength for **11d** in DMSO

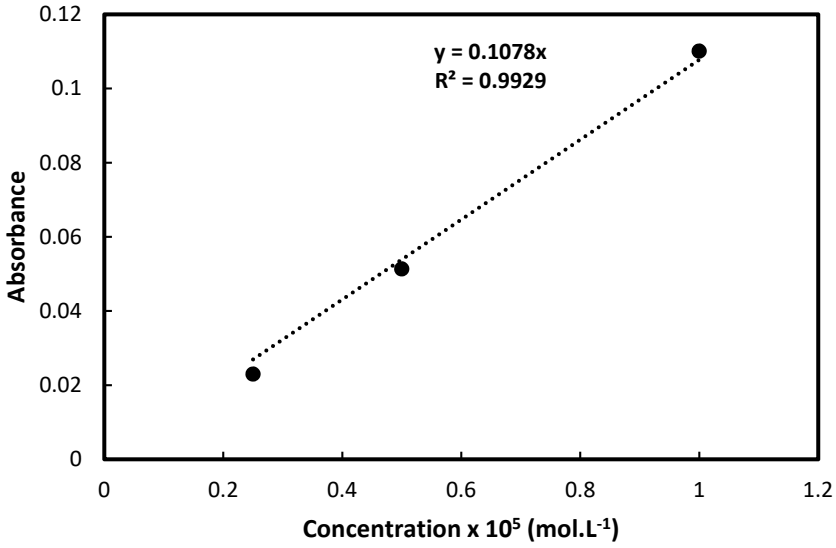


Figure S83. Absorbance at maximum absorption wavelength for **11e** in DMSO

Epsilon measurement in PBS buffer pH = 7.4

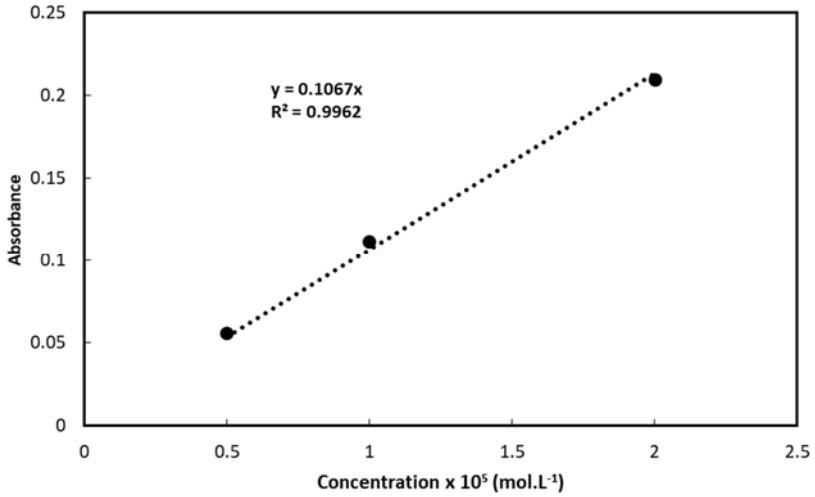


Figure S84. Absorbance at maximum absorption wavelength for **3** in PBS buffer pH = 7.4

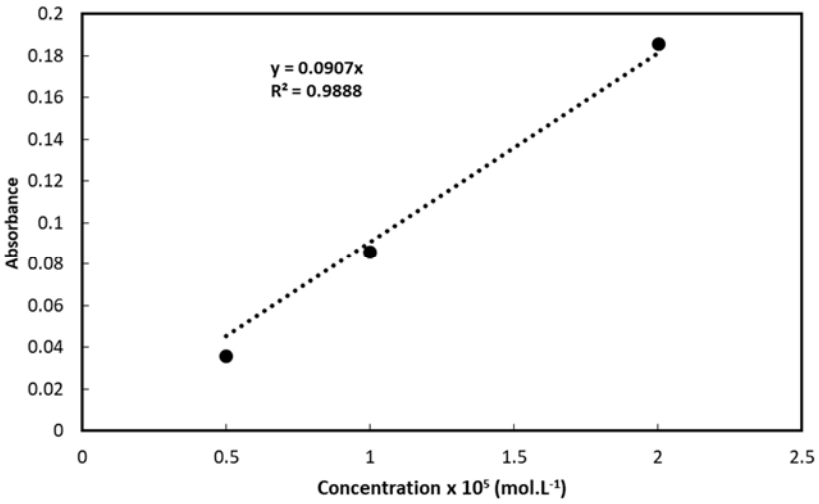


Figure S85. Absorbance at maximum absorption wavelength for **4a** in PBS buffer pH = 7.4

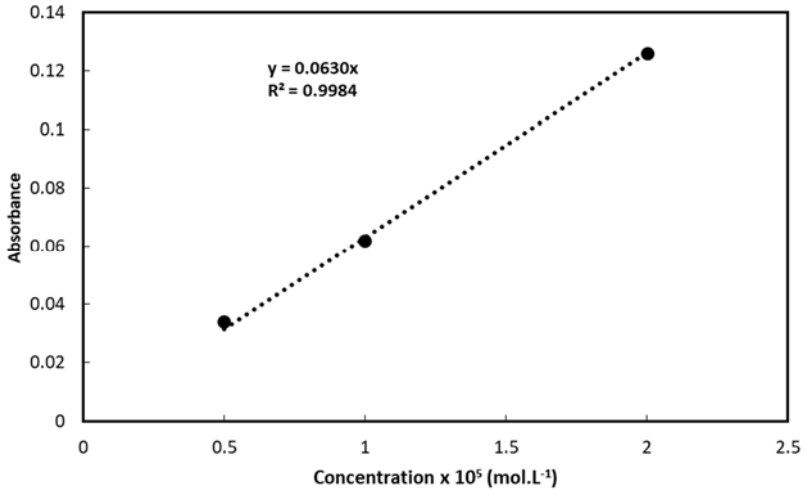


Figure S86. Absorbance at maximum absorption wavelength for **4b** in PBS buffer pH = 7.4

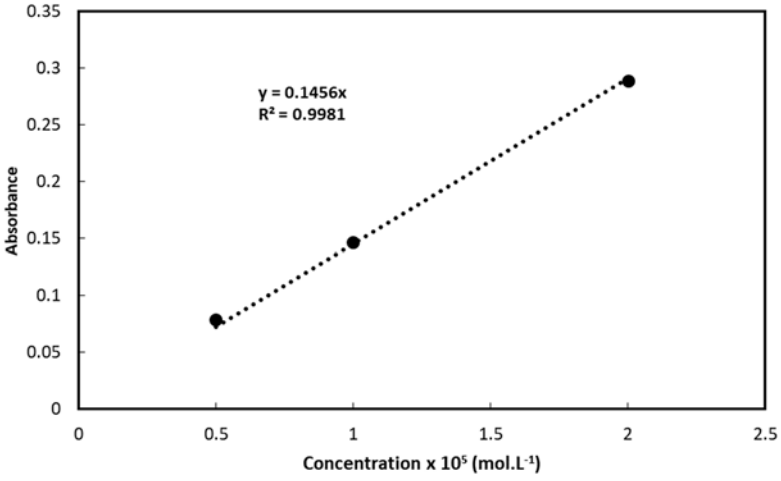


Figure S87. Absorbance at maximum absorption wavelength for **7b** in PBS buffer pH = 7.4

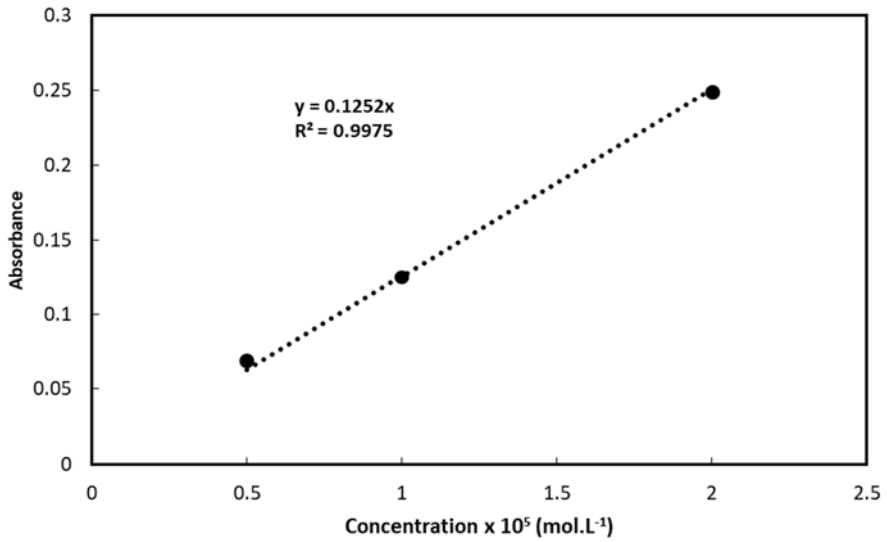


Figure S88. Absorbance at maximum absorption wavelength for **7d** in PBS buffer pH = 7.4

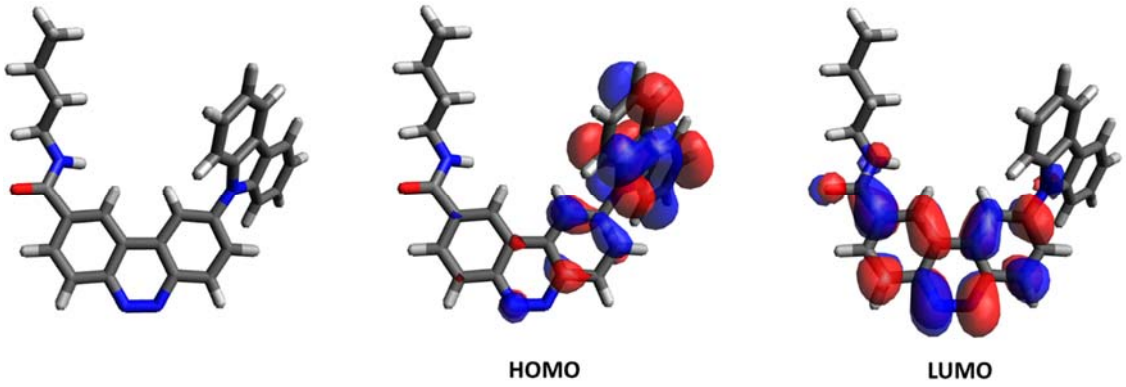


Figure S89. Optimized geometry and frontier molecular orbitals distributions of 11e calculated at the B3LYP/6-31G(d,p) level

pH-dependent behavior of ABCDye 4a

Absorbance and emissions spectra of ABCDye **4a** (λ_{exc} = 440 nm), were recorded at different pH by diluting DMSO 10^{-3} M stock solution of **4** in corresponding buffers to obtain 10^{-5} M solutions (1% DMSO.

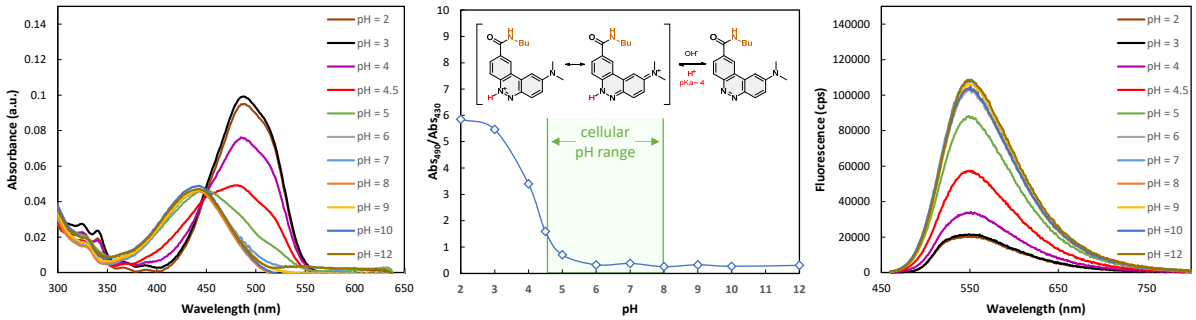


Figure S90. Influence of pH on the photophysical properties of ABCDye **4a**.

Photostability assays

ABCDyes **4b**, **7b** and **coumarin 153** were irradiated using a LED Array Driver (LAD-1 at 10.0 V, 40 mW cm^{-2}) and a LED plate (λ=470 nm LED Array LEDA-B). Emissions spectra were collected at different times over a 2h period.

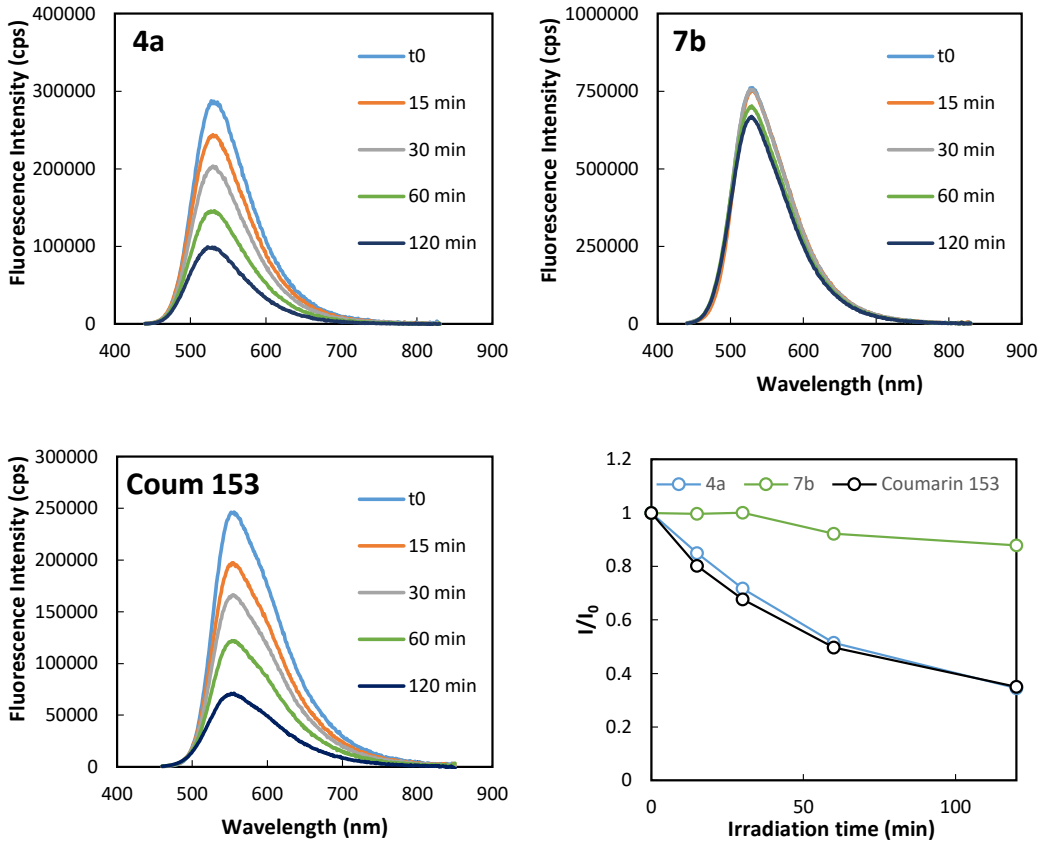


Figure S91. Photostability of CinNApht **4a** and **7b** compared with **coumarin 153** upon continuous irradiation at 470 nm

Co-localisation experiments

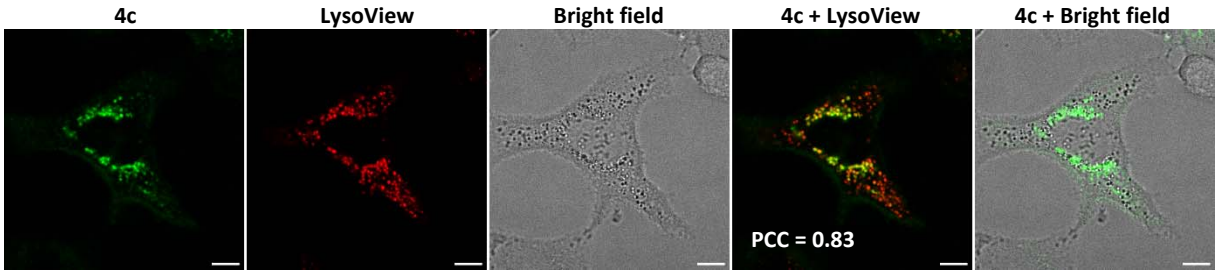


Figure S92. Confocal microscopy experiments with ABCDye **4c**

A549 live cells were incubated with ABCDye **4c** at 5 µM for 2 h at 37 °C. (λ_{Exc}: 440 nm, λ_{Em}: 485 to 600 nm); The Lysosome was stained with LisoView 633 at 37 °C for 30 min (λ_{Exc}: 630 nm, λ_{Em}: 650 to 700 nm), Scale Bar 10 µm.

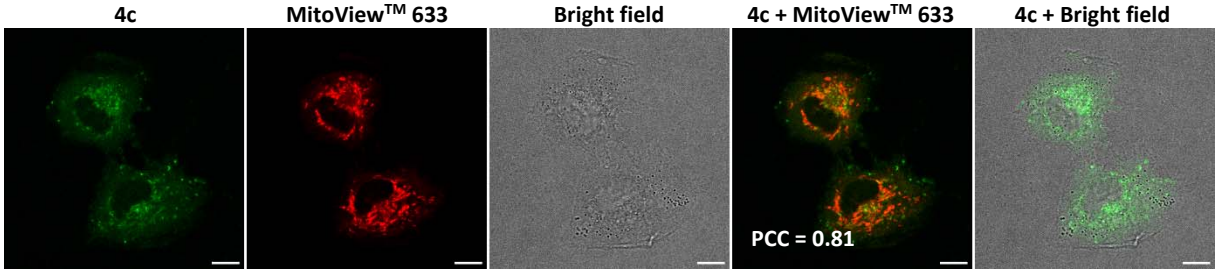


Figure S93. Confocal microscopy experiments with ABCDye **4e**

A549 live cells were incubated with ABCDye **4e** at 5 µM for 2 h at 37 °C. (λ_{Exc}: 440 nm, λ_{Em}: 485 to 600 nm); The mitochondria were stained with MitoView™ 633 at 0.1 µM for 15 min (λ_{Exc}: 630 nm, λ_{Em}: 650 to 750 nm), Scale Bar 10 µm.

II. Experimental section

Abbreviations

Abs, absorption; aq., aqueous; Ar, argon; DCM, dichloromethane; DMSO, dimethylsulfoxide; Em., emission; EtOAc, ethyl acetate; EtOH, Ethanol; Et_2O, Diethyl Ether; Ex., excitation; H_2O, water; Hept, Heptane; HRMS, high-resolution mass spectrum; IR, infrared; MeCN, acetonitrile; MeOH, methanol; min, minutes; NMR, nuclear magnetic resonance; PBS, phosphate buffered saline; MS, mass spectrometry; PLC, preparative layer plate; RP, reversed phase; RPMI, Roswell park memorial institute medium; RT, room temperature; TFA, trifluoroacetic acid; THF, Tetrahydrofuran; TLC, Thin Layer Chromatography, UV, ultraviolet; vis, visible.

General

Unless otherwise noted, all commercially available reagents and solvents were used without further purification. TLC were carried out on silica gel aluminum plates with F-254 indicator; Spots were directly visualized or through illumination with UV lamp (λ = 254/365 nm). Flash-column chromatography purifications were performed on silica gel (40-63 µm) from Macherey-Nagel. Organic solvents for spectroscopy were purchased from Acros Organics or Sigma Aldrich. Absolute EtOH was provided by Carlo Erba. The HPLC grade MeCN used for RP-HPLC analyses was obtained from Carlo Erba. Formic acid (FA, puriss p.a., ACS reagent, reag. Ph. Eur., ≥98%) was provided by Merck-Millipore (brand Sigma-Aldrich). Aq. mobile-phases for HPLC were prepared using water purified with a Milli-Q Integral 3 system from Merck-Millipore (purified to 18.2 MW.cm). RPMI 1640 (1X) used for cell culture were purchased from Life technologies.

Instrument and methods

^{1}H NMR spectra were recorded on a Bruker Avance 500 or 300 MHz and proton-decoupled carbon ^{13}C NMR spectra were recorded at 126 MHz. NMR experiments were carried out in appropriate deuterated solvent and chemical shifts are expressed in parts per million (ppm) from the residual nondeuterated solvent signal. Calibration was made by using residual signals of partially deuterated solvent summarized in 2010 by Fulmer et al.[1] The following abbreviations are used for the multiplicities: s: singlet; d: doublet; t: triplet; q: quadruplet; qt: quintuplet; m: multiplet or overlap of nonequivalent resonances; br: broad singlet; Coupling constants (J) are reported in hertz (Hz).

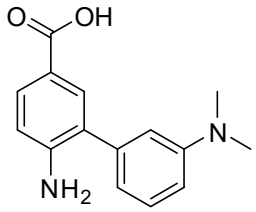
High-resolution mass spectra were determined on an AEI MS-9 using electrospray ionization (ESI) and a time-offlight (TOF) analyzer. IR spectra were recorded with a PerkinElmer Spectrum BX FT-IR spectrometer directly from the substance via attenuated total reflectance (ATR-IR) and bond vibration frequencies are expressed in reciprocal centimeters (cm^{-1}). HPLC-MS analyses were performed on an Alliance W2690 system (Waters, USA). UV-Visible absorption spectra were recorded on a Varian Cary 60 UV-Vis Spectrophotometer using a 10 mm path quartz cell. Emission spectra experiments were performed on an Edimburgh FS-5 spectrofluorimeter with a SC-20 module. Aright angle configuration

was used. The relative fluorescence quantum yields were determined using Coumarin 153 (ϕ_{FL} = 0.53 in EtOH) as reference with the following formula:

$$\Phi_F(x) = \Phi_F(0) \frac{1-10^{-A_0}}{1-10^{-A_x}} \frac{S_x}{S_0} \left(\frac{n_x}{n_0}\right)^2$$

Synthesis protocols

Compound 2

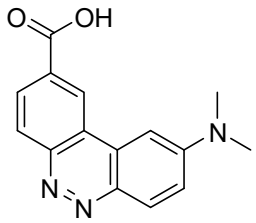


Chemical Formula: $C_{15}H_{16}N_2O_2$
Molecular Weight: 256,31

To a 50 mL schlenck tube, 4-amino-3-bromobenzoic acid (430 mg, 2.0 mmol, 1 eq), (3-(dimethylamino)phenyl)boronic acid (430 mg, 2.3 mmol mmol, 1.15 eq), Na_2CO_3 (620 mg, 6 mmol, 3.0 eq) and $PdCl_2$dppf (150 mg, 10 mol%) were dissolved dioxane (20 mL). The suspensions was deoxygenated with freeze-pump-thaw cycling 3 times and stirred at 80°c overnight under argon atmosphere. The reaction mixture was cooled down and filtered through celite and concentrated under vacuum. The crude product was purified by flash chromatography (Hephtane/AcOEt : 7/3 -> 5/5) to afford **2** as a white solid. 320 mg, 63%.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.93 (d, 1H, *J* = 1.58 Hz), 7.90 (dd, 1H, *J* = 8.42, 1.64 Hz), 7.32 (t, 1H, *J* = 7.76 Hz), 6.78 (d, 1H, *J* = 8.00 Hz), 6.74 (m, 3H), 7.29 (s, 2H), 2.99 (s, 6H)
^{13}C NMR (126 MHz, $CDCl_3$) δ 172.1, 151.3, 149.1 ,139.2 ,133.2 ,131.3 ,129.9 ,127.7 ,118.8 ,117.2 ,114.5 ,113.3, 112.1 ,40.8 (2C).
ESI-HRMS calculated for $C_{17}H_{20}N_3O_2$ $[M+CH_3CN+H]^+$ 298.1556, found 298.1551
IR: ν = 3491, 3391, 2884, 2806, 2602, 2535, 1662, 1605, 1569, 1496, 1409, 1307, 1281, 1141, 993, 837, 771 cm^{-1}

Compound 3

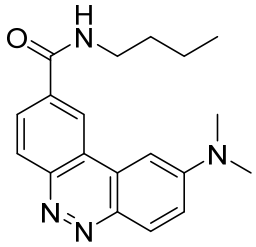


Chemical Formula: $C_{15}H_{13}N_3O_2$
Molecular Weight: 267,29

In a 100 mL round bottom flask, nitrosonium tetrafluoroborate (56.0 mg, 0.48 mmol, 1.25 eq) was added slowly to a solution of **1** (97.0 mg, 0.38 mmol, 1 eq), in acetonitrile (40.0 mL) at 0 °C. The reaction was stirred for 1h30 at 0 °C. A Red precipitate appeared and the reaction was quenched by adding MeOH until complete dissolution of the precipitate. The reaction mixture was concentrated under vacuum and purified by flash chromatography (DCM/MeOH : 98/2 -> 95/5 -> 90/10) to afford **3** as a red solid. 87 mg, 91%.

^{1}H NMR (500 MHz, DMSO-d6) δ 13.50 (s, 1H), 9.30 (s, 1H), 8.52 (d, *J* = 8.54 Hz, 1H), 8.43 (d, *J* = 9.23 Hz, 1H), 8.34 (dd, *J* = 8.55, 1.49 Hz, 1H), 7.65 (d, *J* = 2.51 Hz, 1H), 7.55 (dd, *J* = 9.31, 2.59 Hz, 1H), 3.28 (s, 6H)
^{13}C NMR (126 MHz, DMSO-d6) δ 166.9, 152.2, 145.6, 140.2, 132.1, 131.4, 130.0, 128.9, 124.8, 122.9, 119.8, 117.4, 98.0, 40.1 (2C)
ESI-HRMS calculated for $C_{15}H_{14}N_3O_2$ $[M+H]^+$ 268.1086, found 268.1082
IR: ν = 3374, 3029, 2918, 2849, 2421, 1980, 1610 ,1543, 1519, 1428, 1351, 1239, 1051 cm^{-1}

Compound 4a

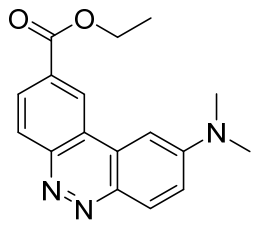


Chemical Formula: $C_{19}H_{22}N_4O$
Molecular Weight: 322,41

To a 5 mL round bottom flask, **2** (73.0 mg, 0.27 mmol, 1 eq) and BOP (133 mg, 0.30 mmol, 1.1 eq) were dissolved into 2 mL of dry DMF followed by the addition of butylamine (60.0 µL, 0.60 mmol, 2.2 eq) and DIEA (150 µL, 0.87 mmol, 3.2 eq). The reaction was stirred at room temperature for 2 hours. The reaction mixture was then diluted with DCM, saturated NH_4Cl was added extracted 3 times with DCM and washed 2 times with brine. The organic layers was dried over $MgSO_4$ and concentrated under vacuum. The crude mixture was purified by flash chromatography (DCM/MeOH 10/0 -> 95/5) to afford **3a** as a yellow solid. 52 mg, 6 0%.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.91 (s, 1H), 8.52 (d, *J* = 8.5 Hz, 1H), 8.43 (d, *J* = 9.1 Hz, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.32 (s, 1H), 7.30 (d, *J* = 9.2 Hz, 1H), 6.64 (s, 1H), 3.56 (dd, *J* = 13.3, 6.7 Hz, 2H), 3.21 (s, 6H), 1.74 – 1.65 (m, 2H), 1.52 – 1.44 (m, 2H), 0.99 (t, *J* = 7.3 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 167.1, 152.1, 145.7, 140.8, 135.2, 132.8, 130.8, 125.93, 123.7, 122.3, 120.9, 116.9, 98.1, 40.6, 40.4, 31.9, 20.4, 14.0.
ESI-HRMS calculated for $C_{19}H_{23}N_4O$ $[M+H]^+$ 323.1872, found 323.1880
IR (neat) : ν = 3250, 3071, 2954, 2930, 2867, 1647, 1613, 1546, 1517, 1303, 1107, 840 cm^{-1}

Compound 4b



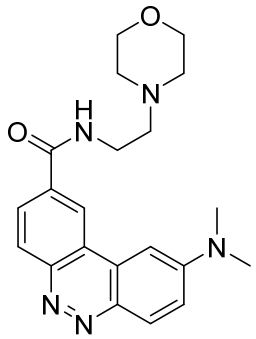
Chemical Formula: $C_{17}H_{17}N_3O_2$
Molecular Weight: 295,34

To a 5 mL round bottom flask, **3e** (25 mg, 0.09 mmol, 1 eq) and BOP (44 mg, 0.1 mmol, 1.1 eq) were dissolved into 1 mL of dry DMF followed by the addition of ethanol (52 µL, 0.9 mmol, 9 eq) and DIEA

(52.0 µL, 0.30 mmol, 3.3 eq). The reaction was stirred at room temperature for 2 hours. The reaction mixture was then diluted with DCM, saturated NH_4Cl was added extracted 3 times with DCM and washed 2 times with brine. The organic layers was dried over $MgSO_4$ and concentrated under vacuum. The crude mixture was purified by flash chromatography (DCM/MeOH 95/5 -> 90/10) to afford **3e** as a yellow solid. 15.8 mg, 57%.

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.16 (s, 1H), 8.59 (d, *J* = 8.6 Hz, 1H), 8.50 (d, *J* = 9.2 Hz, 1H), 8.38 (dd, *J* = 8.6, 1.4 Hz, 1H), 7.43 (d, *J* = 2.4 Hz, 1H), 7.35 (dd, *J* = 9.2, 2.5 Hz, 1H), 4.51 (q, *J* = 7.1 Hz, 2H), 3.27 (s, 6H), 1.49 (t, *J* = 7.1 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 166.3, 152.2, 146.4, 141.0, 135.1, 133.0, 130.8, 128.7, 124.7, 123.7, 120.5, 116.9, 98.0, 61.8, 40.7, 14.5.
ESI-HRMS calculated for $C_{17}H_{18}N_3O_2$ $[M+H]^+$ 296.1399, found 296.1389
IR (neat) : ν = 3273, 2922, 2852, 1644, 1619, 1544, 1437, 1369, 1323, 1111, 815 cm^{-1}

Compound 4c

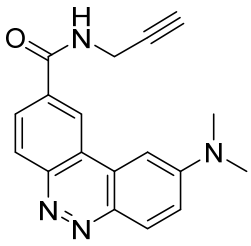


Chemical Formula: $C_{21}H_{25}N_5O_2$
Molecular Weight: 379,46

To a 5 mL round bottom flask, **2** (20.0 mg, 0.074 mmol, 1.00 eq) and PyBOP (41.0 mg, 0.079 mmol, 1.00 eq) were dissolved into 0.75 mL of dry DMF followed by the addition of 4-(2-Aminoethyl)morpholine (10.3 mg, 0.079 mmol, 1.00 eq) and DIEA (46.0 µL, 0.26 mmol, 3.00 eq). The reaction was stirred at room temperature for 3 hours. The reaction mixture was then diluted with DCM, saturated NH_4Cl was added extracted 3 times with DCM and washed twice with brine. The organic layers was dried over $MgSO_4$ and concentrated under vacuum. The crude mixture was purified by flash chromatography (DCM/MeOH 95/5 -> 90/10) to afford **3b** as a yellow solid. 17 mg, 60%.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.98 (m, 1H), 8.58 (m, 1H), 8.48 (m, 1H), 8.01 (d, 1H, *J* = 8.44 hz), 7.37 (m, 2H), 7.15 (m, 1H), 4.06 (t, 4H, *J* = 4.90 Hz), 3.67 (q, 2H, *J* = 5.62 Hz), 3.25 (m, 6H), 2.70 (t, 2H, *J* = 5.95 Hz), 2.57 (q, 4H, *J* = 4.60 Hz)
^{13}C NMR (126 MHz, $CDCl_3$) δ 166.7, 152.0, 145.8, 140.8, 134.7, 132.8, 130.9, 125.7, 123.5, 122.3, 120.8, 116.8, 98.0, 67.0, 56.8, 53.4, 40.5, 36.4
ESI-HRMS calculated for $C_{21}H_{25}N_6O_2$ $[M+H]^+$ 380.2087, found 380.2070
IR (neat) : ν = 3267, 3077, 2954, 2847, 1638, 1620, 1543, 1513, 1422, 1297, 1140, 1112,31, 1065, 811 cm^{-1}

Compound 4d

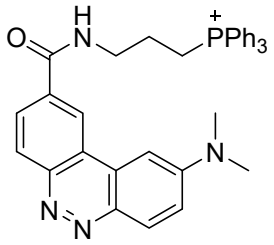


Chemical Formula: $C_{18}H_{16}N_4O$
Molecular Weight: 304,35

To a 5 mL round bottom flask, **2** (17.0 mg, 0.063 mmol, 1 eq) and BOP (30.0 mg, 0.067 mmol, 1 eq) were dissolved into 1 mL of dry DMF followed by the addition of propargylamine (9.00 µL, 0.13 mmol, 1.90 eq) and DIEA (35.0 µL, 0.20 mmol, 3.00 eq). The reaction was stirred overnight at room temperature under argon atmosphere. The reaction mixture was dileted with brine, extracted 3 times with DCM and washed with brine. The organic layer was dried over $MgSO_4$ and concentrated under vacuum. The crude mixture was purified by flash chromatography (DCM/MeOH 9/1 -> 7/3) to afford **3c** as a yellow solid. 12.5 mg, 66%.

^{1}H NMR (500 MHz, MeOD) δ 9.17 (s, 1H), 8.46 (d, 1H, *J* = 8.6 Hz), 8.38 (d, 1H, *J* = 9.3 Hz), 8.32 (dd, 1H, *J* = 8.60, 1.3 Hz), 7.66 (d, 1H, *J* = 2.2 Hz), 7.57 (dd, 1H, *J* = 9.3 Hz, 2.5 Hz), 4.32 (d, 2H, *J* = 2.4 Hz), 2.72 (t, 1H, *J* = 2.4 Hz), 3.35 (s, 6H)
^{13}C NMR (126 MHz, $CDCl_3$/MeOD : 9/1) δ 170.8, 167.0, 152.6, 145.5, 140.5, 134.4, 132.3, 129.6, 127.1, 124.5, 122.5, 121.1, 117.3, 98.0, 71.4, 40.4, 29.7.
ESI-HRMS calculated for $C_{18}H_{17}N_4O$ $[M+H]^+$ 305.1402, found 305.1388
IR (neat) : ν = 3293, 3245, 3054, 2918, 2850, 1653, 1620, 1539, 1518, 1495, 1371, 1297, 1255, 1111, 813 cm^{-1}

Compound 4e

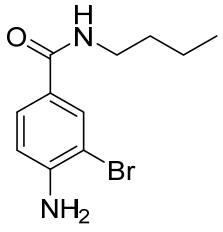


Chemical Formula:
$C_{36}H_{34}N_4OP^+$
Molecular Weight: 569,67

To a 5 mL round bottom flask, **2** (25.6 mg, 0.10 mmol, 1.00 eq) and BOP (44 mg, 0.10 mmol, 1.00 eq) were dissolved into 1 mL of dry DMF followed by the addition of (3-Aminopropyl)(triphenyl)phosphonium bromide (48.0 mg, 0.10 mmol, 1.00 eq) and DIEA (52.0 µL, 0.30 mmol, 3.00 eq). The reaction was stirred at room temperature for 2 hours. The reaction mixture was then diluted with DCM, saturated NH_4Cl was added extracted 3 times with DCM and washed 2 times with brine. The organic layers was dried over $MgSO_4$ and concentrated under vacuum. The crude mixture was purified by flash chromatography (DCM/MeOH 95/5 -> 90/10) to afford **3d** as an orange solid. 15 mg, 24%.

^{1}H NMR (500 MHz, $CDCl_3$) δ 10.34 (s, 1H), 9.84 (s, 1H), 8.56 (d, *J* = 8.61 Hz, 1H), 8.48 (d, *J* = 8.70 Hz, 1H), 8.44 (d, *J* = 9.25 Hz, 1H), 8.14 (s, 1H), 7.71 (m, 9H), 7.55 (m, 6H), 7.30 (dd, *J* = 9.30, 2.04 Hz, 1H), 3.97 (m, 2H), 3.81 (m, 2H), 3.33 (s, 6H), 2.03 (m, 2H)
^{13}C NMR (126 MHz, $CDCl_3$) δ 166.9, 152.5, 146.2, 141.1, 135.2 (d, *J* = 2.4 Hz), 133.5 (d, *J* = 9.9 Hz), 132.4, 130.6 (d, *J* = 12.5 Hz), 130.1, 128.3, 124.6, 123.1, 121.1, 118.8, 118.1, 116.6, 100.4, 41.1, 39.6 (d, *J* = 15.63 Hz), 22.8 (d, *J* = 3.24 Hz), 20.6 (d, *J* = 51.25 Hz)
^{31}P NMR (122 MHz, $CDCl_3$) δ 24.28
ESI-HRMS calculated for $C_{36}H_{34}N_4OP$ $[M]^+$ 569.2470, found 569.2491
IR (neat) : ν = 3273, 2922, 2852, 1644, 1619, 1544, 1437, 1369, 1323, 1111, 815 cm^{-1}

Compound 5



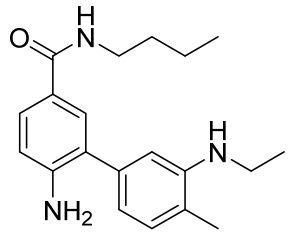
Chemical Formula: $C_{11}H_{15}BrN_2O$
Exact Mass: 270,04

To a 50 mL round bottom flask, 4-amino-3-bromobenzoic acid (860 mg, 4.00 mmol, 1.00 eq) and BOP (1.80 g, 4.00 mmol, 1.00 eq) were dissolved into 20 mL of dry DMF followed by the addition of butylamine (0,80 mL, 8.00 mmol, 2.00 eq) and DIEA (2.10 mL, 12.0 mmol, 3.00 eq). The reaction was stirred at room temperature for 3 hours and monitored by TLC (heptane/AcOEt : 5/5) until full conversion of the starting material.

The reaction mixture was then diluted with DCM, saturated NH_4Cl was added extracted 3 times with DCM and washed 2 times with brine. The organic layers was dried over $MgSO_4$ and concentrated under vacuum. The crude mixture was purified by flash chromatography (Heptane/AcOEt 8/2 to 5/5) to afford **5** as a colorless oil wich slowly crystallize to a white solid over the course of the weekend. 1.08g, 97%.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (d, *J* = 1.6 Hz, 1H), 7.52 (dd, *J* = 8.3, 1.7 Hz, 1H), 6.72 (d, *J* = 8.4 Hz, 1H), 6.09 (s, 1H), 4.42 (s, 2H), 3.40 (q, *J* = 6.9 Hz, 2H), 1.63 – 1.50 (m, 2H), 1.45 – 1.32 (m, 2H), 0.93 (t, *J* = 7.3 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 166.0, 146.8, 131.7, 127.3, 125.6, 114.6, 108.4, 39.8, 31.8, 20.2, 13.8.
ESI-HRMS calculated for $C_{11}H_{16}N_2OBr$ $[M+H]^+$ 271.0446, found 271.0444
IR (neat) : ν = 3477, 3457, 3342, 2953, 2930, 2966, 1608, 1594, 1553, 1490, 1295, 1242, 816, 760 cm^{-1}

Compound 6a

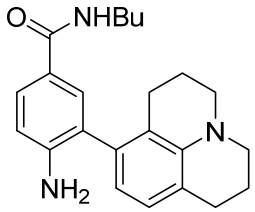


Chemical Formula: $C_{20}H_{27}N_3O$
Molecular Weight: 325,46

To a 10 mL schlenck tube, **5** (118 mg, 0.43 mmol, 1.00 eq), N-ethyl-2-methyl-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)aniline (170 mg, 0.65 mmol mmol, 1.50 eq), Na_2CO_3 (136 mg, 1.28 mmol, 3.00 eq) and $Pd(PPh_3)_4$ (90.0 mg, 20 mol%) were dissolved in a mixture of H_2O, EtOH, and toluene (0.90 mL/0.9 mL/3 mL). The suspensions was deoxygenated three times with freeze-pump-thaw cycling and stirred at 80°c overnight. The reaction mixture was cooled down and filtered through celite and concentrated under vacuum. The crude product was purified by flash chromatography (DCM/AcOEt : 9/1) to afford **6a** as a solid. 70.0 mg, 51%.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 (dd, *J* = 8.3, 1.8 Hz, 1H), 7.55 (d, *J* = 1.8 Hz, 1H), 7.11 (d, *J* = 7.5 Hz, 1H), 6.71 (d, *J* = 8.4 Hz, 1H), 6.69 (d, *J* = 7.6 Hz, 1H), 6.64 (s, 1H), 6.05 (s, 1H), 4.13 (s, 2H), 3.50 (s, 1H), 3.41 (dd, *J* = 13.1, 6.9 Hz, 2H), 3.20 (q, *J* = 7.1 Hz, 2H), 2.18 (s, 3H), 1.61 – 1.51 (m, 2H), 1.43 – 1.34 (m, 2H), 1.30 (t, *J* = 7.1 Hz, 3H), 0.93 (t, *J* = 7.34 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 167.5, 146.88, 146.84, 137.6, 130.6, 129.2, 127.7, 127.5, 124.3, 121.2, 117.2, 114.7, 110.2, 39.7, 38.5, 32.0, 20.3, 17.3, 15.0, 13.9.
ESI-HRMS calculated for $C_{20}H_{28}N_3O$ $[M+H]^+$ 326.2232, found 326.2234
IR (neat) : ν = 3465, 3310, 3189, 2928, 2855, 1611, 1563, 1499, 1439, 1319, 1293, 1153, 833 cm^{-1}

Compound 6b

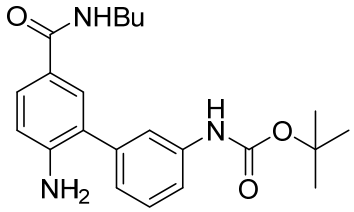


Chemical Formula: $C_{23}H_{29}N_3O$
Molecular Weight: 363,51

To a 10 mL schlenck tube, **5** (75.0 mg, 0.27 mmol, 1.00 eq), 8-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-julolidine (110 mg, 0.36 mmol, 1.30 eq), Na_2CO_3 (85.0 mg, 0.80 mmol, 3.00 eq) and $Pd(PPh_3)_4$ (31.0 mg, 10 mol%) were dissolved in a mixture of H_2O/EtOH/toluene (0.6 mL/0.6 mL/2 mL). The suspensions was deoxygenated three times with freeze-pump-thaw cycling and stirred at 80 °C overnight. The reaction mixture was cooled down and filtered through celite and concentrated under vacuum. The crude product was purified by flash chromatography (DCM/AcOEt : 9/1) to afford **6b** as a solid. 68 mg, 70%.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.64 (dd, *J* = 8.32, 1.85 Hz, 1H), 7.38 (d, *J* = 1.81 Hz, 1H), 6.85 (d, *J* = 7.51 Hz, 1H), 6.71 (d, *J* = 8.35 Hz, 1H), 6.39 (d, *J* = 7.49 Hz, 1H), 5.97 (s, 1H), 3.88 (s, 2H), 3.41 (q, *J* = 7.34 Hz, 2H), 3.18 (t, *J* = 5.50 Hz, 2H), 3.12 (t, *J* = 5.02 Hz, 2H), 2.80 (m, 2H), 2.44 (m, 2H), 2.02 (m, 2H), 1.87 (m, 2H), 1.55 (m, 2H), 1.37 (m, 2H), 0.93 (t, *J* = 7.34 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 167.4, 147.0, 143.5, 135.5, 128.7, 127.8, 127.3, 127.1, 124.0, 121.4, 120.4, 117.3, 114.2, 50.4, 50.0, 39.7, 31.9, 28.0, 25.2, 22.1, 22.0, 21.0, 13.9.
IR: ν = 3227, 2927, 2858, 1614, 1541, 1440, 1352, 1301, 1248, 1198, 1151, 1073, 950, 830, 300, 768 cm^{-1}

Compound 6c



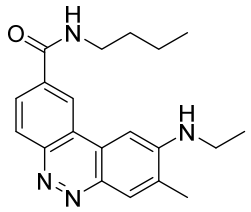
Chemical Formula: $C_{22}H_{29}N_3O_3$
Molecular Weight: 383,49

To a schlenck tube, **5** (271 mg, 1.00 mmol, 1.00 eq), tert-butyl N-[3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]carbamate (382 mg, 1.20 mmol, 1.20 eq), Na_2CO_3 (316 mg, 3.00 mmol, 3.00 eq) were dissolved in a mixture of H_2O/EtOH/toluene (1.5 mL/1.5 mL/5 mL). The suspensions was deoxygenated with freeze-pump-thaw cycling 3 times. $Pd(PPh_3)_4$ (111 mg, 10 mol%) was added to the mixture and an additional freeze-pump-thaw was performed. The resulting reaction mixture was stirred at 80 °C overnight. The reaction mixture was cooled down and filtered through celite and concentrated under vacuum. The crude product was purified by flash chromatography (DCM/MeOH : 10/0 to 9/1) to afford **6c** as beige solid. 376 mg, 98%.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 (dd, *J* = 8.35, 1.96 Hz, 1H), 7.48 (d, *J* = 1.95 Hz, 1H), 7.43 (brs, 1H), 7.36 (m, 2H) 7.07 (m, 1H), 6.72 (brs, 1H), 6.70 (d, *J* = 8.39 Hz, 1H), 6.09 (t, *J* = 4.76 Hz, 1H), 4.08 (brs, 2H), 3.41 (q, *J* = 7.35 Hz, 2H), 1.56 (qt, *J* = 7.35 Hz, 2H), 1.50 (s, 9H), 1.38 (sx, *J* = 7.35 Hz, 2H), 0.93 (t, *J* = 7.35 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 167.3, 152.9, 146.7, 139.5, 139.1, 129.8, 128.2, 128.0, 126.4, 124.6, 123.8, 119.3, 117.9, 114.9, 80.9, 39.8, 32.0, 28.5, 20.3, 14.0.
ESI-HRMS calculated for $C_{22}H_{30}N_3O_3$ $[M+H]^+$ 384.2287, found 384.2293

IR: ν = 3326, 2961, 2930, 2871, 1704, 1610, 1534, 1496, 1431, 1366, 1307, 1276, 1239, 1153, 1053, 1026, 888, 844, 766, 702, 631 cm^{-1}

Compound 7a

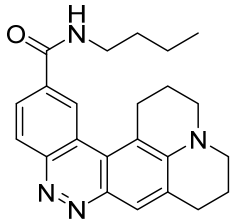


Chemical Formula: $C_{20}H_{24}N_4O$
Molecular Weight: 336,44

To a 50 mL round bottom flask, **8a** (40.0 mg, 0.14 mmol, 1.00 eq) was dissolved in acetonitrile (15.0 mL) and cooled down in an ice bath. $NOBF_4$ (22.0 mg, 0.19 mmol, 1.30 eq) was added and the reaction mixture was stirred at 0 °C for 2 hours. The reaction mixture was quenched with $NaHCO_3$ (sat) and extracted 3 times with DCM. The crude product was purified by flash chromatography (DCM/MeOH : 98/2 -> 95/5 -> 90/10) to afford **9a** as a yellow solid. 5.5 mg, 15%.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.98 (s, 1H), 8.57 (d, *J* = 8.5 Hz, 1H), 8.32 (s, 1H), 7.97 (d, *J* = 8.6 Hz, 1H), 7.36 (s, 1H), 6.45 (s, 1H), 4.36 (s, 1H), 3.57 (dd, *J* = 13.3, 6.8 Hz, 2H), 3.49 – 3.41 (m, 2H), 2.42 (s, 3H), 1.69 (m, 2H), 1.47 (m, 5H), 1.01 (t, *J* = 7.4 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 167.0, 149.8, 145.6, 141.4, 135.0, 132.1, 130.8, 127.2, 125.3, 122.8, 122.4, 120.8, 95.6, 40.2, 38.5, 31.8, 20.2, 17.7, 14.5, 13.8.
ESI-HRMS calculated for $C_{20}H_{25}N_4O$ $[M+H]^+$ 337.2028, found 337.2032
IR (neat) : ν = 3390, 3311, 2957, 2918, 2850, 1647, 1618, 1530, 1447, 1369, 1322, 1175, 1145, 841 cm^{-1}

Compound 7b

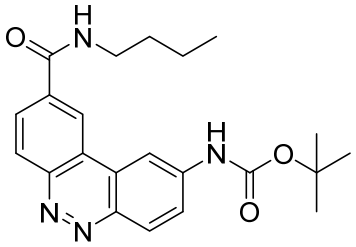


Chemical Formula: $C_{23}H_{26}N_4O$
Molecular Weight: 374,49

To a 50 mL round bottom flask, **8b** (40.0 mg, 0.13 mmol, 1.00 eq) was dissolved in acetonitrile (15 mL) and cooled down in an ice bath. $NOBF_4$ (15 mg, 0.15 mmol, 1.20 eq) was added and the reaction mixture was stirred at 0 °C for 30 minute. The reaction mixture was quenched with $NaHCO_3$ (sat) and extracted 3 times with DCM. The crude product was purified by flash chromatography (DCM/MeOH : 96/4) to afford **9b** as an orange solid. 19 mg, 46%.

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.04 (s, 1H), 8.44 (d, *J* = 8.5 Hz, 1H), 7.95 (s, 1H), 7.92 (d, *J* = 8.5 Hz, 1H), 6.73 (s, 1H), 3.55 (dd, *J* = 13.2, 6.9 Hz, 2H), 3.41 (t, *J* = 5.8 Hz, 2H), 3.34 (t, *J* = 5.7 Hz, 4H), 2.98 (t, *J* = 6.1 Hz, 2H), 2.06 – 1.94 (m, 4H), 1.74 – 1.63 (m, 2H), 1.53 – 1.42 (m, 2H), 0.99 (t, *J* = 7.4 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 167.4, 147.0, 146.6, 141.1, 133.4, 130.4, 129.7, 127.3, 126.9, 124.6, 121.6, 121.0, 111.8, 51.2, 49.9, 40.3, 31.9, 29.0, 28.8, 22.6, 21.1, 20.4, 14.0.
ESI-HRMS calculated for $C_{23}H_{27}N_4O$ $[M+H]^+$ 375.2185, found 375.2173
IR (neat) : ν = 3267, 2918, 2850, 1644, 1610, 1515, 1285, 1141, 1107, 818 cm^{-1}

Compound 7c

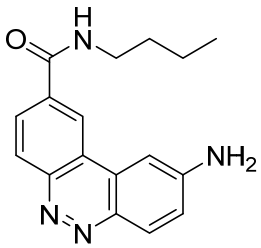


Chemical Formula: $C_{22}H_{26}N_4O_3$
Molecular Weight: 394,47

To a solution of **6c** (200 mg, 0.52 mmol, 1.00 eq) in dry CH_3CN (20.0 mL) at 0 °C under argon was slowly added $NOBF_4$ (67.0 mg, 0.57 mmol, 1.10 eq) and the resulting reaction mixture was stirred under argon for 1h. After the reaction was complete, it was quenched by adding 40.0 mL of a $NaHCO_3$ saturated solution and extracted 3 times with 20.0 mL DCM. The crude product was directly used for the next step

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.96 (d, *J* = 2.1 Hz, 1H), 8.89 (d, *J* = 1.8 Hz, 1H), 8.73 (d, *J* = 8.5 Hz, 1H), 8.66 (d, *J* = 8.9 Hz, 1H), 8.18 (dd, *J* = 1.8 and 8.5 Hz, 1H), 7.69 (dd, *J* = 2.1 and 8.9 Hz, 1H), 7.02 (brs, 1H), 6.40 (t, *J* = 6.4 Hz, 1H), 3.55 (q, *J* = 7.3 Hz, 2H), 1.71 (qt, *J* = 7.35 Hz, 2H), 1.60 (s, 9H), 1.48 (sx, *J* = 7.35 Hz, 2H), 1.01 (t, *J* = 7.35 Hz, 3H).

Compound 7d

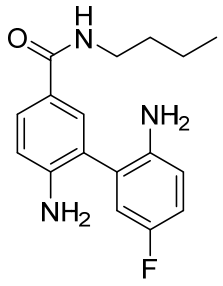


Chemical Formula: $C_{17}H_{18}N_4O$
Molecular Weight: 294,36

The crude **7c** was dissolved in 5.00 mL of DCM and cooled down to 0 °C. 1.00 mL of TFA was slowly added dropwise and the resulting mixture was stirred at room temperature for 6h. After the reaction was completed, it was poured in 50.0 mL of cold stirring Et_2O. The solid was isolated by filtration and purified by flash chromatography (DCM/MeOH : 90/10) to afford **7c** as pale yellow solid. 199 mg, 94%.

^{1}H NMR (500 MHz, DMSO-d6) δ 8.92 (d, *J* = 1.6 Hz, 1H), 8.87 (t, *J* = 5.5 Hz, 1H), 8.56 (d, *J* = 8.6 Hz, 1H), 8.30 (d, *J* = 8.9 Hz, 1H), 8.24 (dd, *J* = 1.8 and 8.6 Hz, 1H), 7.59 (d, *J* = 2.3, 1H), 7.30 (dd, *J* = 2.3 and 8.9 Hz, 1H), 6.66 (brs, 2H), 3.36 (q, *J* = 7.4 Hz, 2H), 1.58 (qt, *J* = 7.4 Hz, 2H), 1.39 (sx, *J* = 7.4 Hz, 2H), 0.94 (t, *J* = 7.34 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 165.5, 152.8, 145.0, 140.6, 135.1, 132.5, 129.6, 127.5, 123.6, 121.5, 119.8, 119.5, 98.9, 39.02, 31.3, 19.7, 13.8.
ESI-HRMS calculated for $C_{23}H_{27}N_4O$ $[M+H]^+$ 295.1559, found 295.1562
IR: ν = 3317, 3105, 2961, 2933, 2873, 1601, 1514, 1465, 1403, 1358, 1277, 1197, 1174, 1123, 904, 829, 794, 757, 718, 626, 611, 562 cm^{-1}

Compound 9

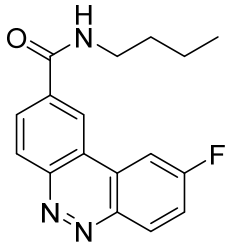


Chemical Formula: $C_{17}H_{20}FN_3O$
Exact Mass: 301,16

To a 50 mL schlenck tube, **4** (400 mg, 1.45 mmol, 1.00 eq), 4-fluoro-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)aniline (512 mg 2.16 mmol, 1.50 eq), Na_2CO_3 (440 mg, 4.15 mmol, 2.90 eq) and $Pd(PPh_3)_4$ (170 mg, 10 mol%) were dissolved in a mixture of H_2O, EtOH, and toluene (2.4 mL/2.4mL/8 mL). The suspensions was deoxygenated with freeze-pump-thaw cycling 3 times and stirred at 80°c overnight. The reaction mixture was cooled down and filtered through celite and concentrated under vacuum. The crude product was purified by flash chromatography (DCM/AcOEt 8/2 -> 7/3 -> 6/4) to afford the desired product as a white solid. 292 mg, 70%.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 (dd, *J* = 8.4, 2.1 Hz, 1H), 7.48 (d, *J* = 2.0 Hz, 1H), 6.89 (td, *J* = 8.5, 3.0 Hz, 1H), 6.82 (dd, *J* = 9.0, 2.9 Hz, 1H), 6.74 (d, *J* = 8.4 Hz, 1H), 6.70 (dd, *J* = 8.8, 4.8 Hz, 1H), 6.18 (t, *J* = 4.8 Hz, 1H), 3.68 (s, 4H), 3.42 – 3.35 (m, 2H), 1.59 – 1.51 (m, 2H), 1.41 – 1.32 (m, 2H), 0.92 (t, *J* = 7.4 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 167.2, 156.2 (d, *J* = 237.29 Hz), 147.1, 140.3, 129.8, 128.6, 124.7, 124.7 (d, *J* = 7.52 Hz), 122.6, 117.3 (d, *J* = 22.05 Hz), 116.7 (d, *J* = 7.47 Hz), 115.8 (d, *J* = 22.27 Hz), 115.1, 39.8, 31.9, 20.2, 13.9
^{19}F NMR (282 MHz, $CDCl_3$) δ – 126.28
ESI-HRMS calculated for $C_{17}H_{21}N_3OF$ [M+H]+ 302.1669, found 302.1672
IR (neat) ν = 3325, 3061, 2959, 2930, 2872, 1621, 1542, 1494, 1312, 1266, 1179, 917, 873 cm^{-1}

Compound 10



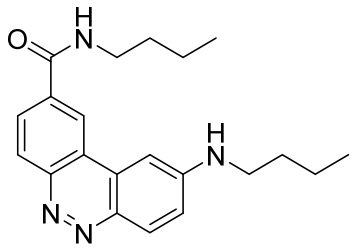
Chemical Formula: $C_{17}H_{16}FN_3O$
Exact Mass: 297,13

To a 250 mL round bottom flask, **5** (290 mg, 0.96 mmol, 1.00 eq) was dissolved in $CHCl_3$ (100 mL) and cooled down to 0 °C in an ice bath. *m*CPBA (344 mg, 2.00 mmol, 2.00 eq) was added portion wise over the course of 10 minute. The reaction mixture was stired 2 hours at 0 °C and washed with $Na_2S_2O_3$ (10%) 2 times and $NaHCO_3$ (saturated), dried over $MgSO_4$ and concentrated under vacuum.

The crude product was purified by flash chromatography (heptane/AcOEt 8/2 -> 65/35 -> 5/5) to afford **6** as an off-white solid. 163 mg, 56%.

^{1}H NMR (500 MHz, CDCl3) δ 8.92 (s, 1H), 8.82 – 8.73 (m, 2H), 8.19 (dd, *J* = 8.55, 1.43 Hz, 2H), 7.66 (m, 1H), 6.52 (s, 1H), 3.58 (dd, *J* = 13.5, 6.6 Hz, 2H), 1.69 (m, 2H), 1.54 – 1.41 (m, 2H). 1.00 (t, *J* = 7.34 Hz, 3H)
^{13}C NMR (126 MHz, CDCl3) δ 166.4, 164.3 (d, *J* = 265.4 Hz), 145.4, 143.3, 137.3, 134.8 (d, *J* = 10.0 Hz), 13.6, 131.9, 127.5, 123.0, 121.9, 119.6 (d, *J* = 25.1 Hz), 106.6 (d, *J* = 23.6 H), 40.5, 31.9, 20.4, 13.9
^{19}F NMR (282 MHz, $CDCl_3$) δ -102.6
ESI-HRMS calculated for $C_{17}H_{17}N_3OF$ [M+H]+ 298.1356, found 298.1361
IR (neat) : ν = 3299, 3068, 2958, 2936, 2872, 1633, 1610, 1539, 1441, 1610, 1194, 869 cm^{-1}

Compound 11a

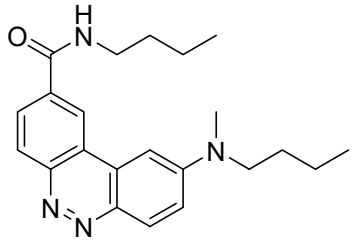


Chemical Formula: $C_{21}H_{26}N_4O$
Exact Mass: 350,21

To a 5 mL round bottom flask, **6** (22.0 mg, 0.07 mmol, 1.00 eq) was dissolved in dry DMF (1.00 mL). Cs_2CO_3 (32.0 mg, 0.10 mmol, 1.40 eq) and butylamine (30.0 µL, 0.30 mmol, 4.20 eq) were added and the reaction mixture was stirred overnight at 80 °C. After cooling down, the reaction mixture was quenched with brine, extracted with DCM and washed with brine. The organic layer was dried over $MgSO_4$ and concentrated under vacuum. The crude product was purified by flash chromatography (DCM/MeOH 98/2 -> 95/5) to afford **7a** as a yellow solid. 14 mg, 55%.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.95 (d, *J* = 1.05 Hz, 1H), 8.55 (d, *J* = 8.54 Hz, 1H), 8.40 (d, *J* = 8.96 Hz, 1H), 7.99 (dd, *J* = 8.57, 1.39 Hz, 1H), 7.33 (d, *J* = 1.94 Hz, 1H), 7.13 (dd, *J* = 8.97, 2.22 Hz, 1H), 6.48 (s, 1H), 4.57 (t, *J* = 4.72 Hz, 1H), 3.57 (m, 2H), 3.34 (m, 2H), 1.78 – 1.62 (m, 4H), 1.57 – 1.43 (m, 4H), 1.02 (t, *J* = 7.46 Hz, 3H), 1.01 (t, *J* = 1.32 Hz, 3H)
^{13}C NMR (126 MHz, $CDCl_3$) δ 166.9, 151.0, 145.8, 141.6, 135.1, 132.9, 130.8, 125.8, 124.2, 122.4, 120.8, 119.3, 96.8, 43.4, 40.2, 31.8, 31.3, 20.3, 20.2, 13.9, 13.8.
ESI-HRMS calculated for $C_{21}H_{27}N_4O$ [M+H]+ 351.2185, found 351.2173
IR (neat) : ν = 3222, 3058, 2956, 2932, 2862, 1632, 1605, 1536, 1473, 1291, 1143, 1103, 849 cm^{-1}

Compound 11b



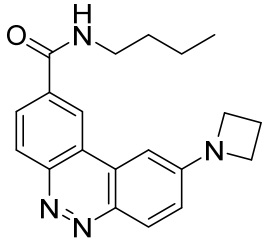
Chemical Formula: $C_{22}H_{28}N_4O$
Exact Mass: 364,23

To a 5 mL round bottom flask, **6** (30.0 mg, 0.10 mmol, 1.00 eq) was dissolved in dry DMF (1.00 mL). Cs_2CO_3 (32.0 mg, 0.10 mmol, 1.00 eq) and *n*-methylbutylamine (28.0 µL, 0.23 mmol, 2.30 eq) were added and the reaction mixture was stirred overnight at 80 °C. After cooling down, the reaction mixture was quenched with brine, extracted with DCM and washed with brine. The organic layer was dried over $MgSO_4$ and concentrated under vacuum. The crude product was purified by flash chromatography (DCM/MeOH 98/2 -> 95/5) to afford **7b** as a yellow solid. 16 mg, 46%.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.89 (s, 1H), 8.48 (d, *J* = 8.5 Hz, 1H), 8.40 (d, *J* = 9.0 Hz, 1H), 7.98 (t, *J* = 8.5 Hz, 1H), 7.31 – 7.23 (m, 2H), 6.69 (s, 1H), 3.60 – 3.49 (m, 4H), 3.15 (s, 3H), 1.73 – 1.61 (m, 4H), 1.50 – 1.37 (m, 4H), 0.98 (m, 6H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 167.0, 151.2, 145.7, 140.6, 135.0, 132.7, 130.6, 125.8, 123.7, 122.1, 120.7, 116.7, 97.6, 52.5, 40.2, 38.9, 31.7, 29.3, 20.26, 20.24, 14.0, 13.8.
ESI-HRMS calculated for $C_{22}H_{29}N_4O$ $[M+H]^+$ 365.2341, found 365.2334

IR (neat) : ν = 3289, 3071, 2956, 2925, 2870, 1637, 1610, 1542, 1510, 1494, 1364, 1254, 1143, 1100, 813 cm^{-1}

Compound 11c

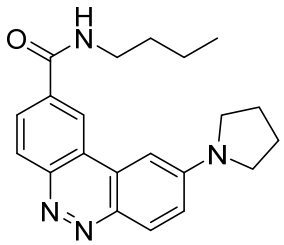


Chemical Formula: $C_{20}H_{22}N_4O$
Exact Mass: 334,18

To a 5 mL round bottom flask, **6** (13 mg, 0.04 mmol, 1.00 eq) was dissolved in dry DMF (1.00 mL). Cs_2CO_3 (44.0 mg, 0.13 mmol, 3.00 eq) and azetidine hydrochloride (8.50 mg, 0.09 mmol, 2.00 eq) were added and the reaction mixture was stirred overnight at 100 °C. After cooling down, the reaction mixture was quenched with brine, extracted with DCM and washed with brine. The organic layer was dried over $MgSO_4$ and concentrated under vacuum. The crude product was purified by flash chromatography (DCM/MeOH 98/2 -> 95/5) to afford **7c** as a yellow solid. 4 mg, 31%.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.89 (s, 1H), 8.50 (d, *J* = 8.5 Hz, 1H), 8.39 (d, *J* = 9.0 Hz, 1H), 7.92 (d, *J* = 8.2 Hz, 1H), 7.05 (s, 1H), 6.91 (d, *J* = 9.0 Hz, 1H), 6.34 (s, 1H), 4.13 (t, *J* = 7.4 Hz, 4H), 3.50 (q, *J* = 6.8 Hz, 2H), 2.51 – 2.43 (m, 2H), 1.62 (m, 2H), 1.42 (m, 2H), 0.94 (t, *J* = 7.4 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 166.9, 152.6, 145.7, 141.2, 135.0, 132.0, 130.7, 125.7, 123.7, 122.5, 120.6, 115.4, 96.6, 51.7, 40.2, 31.8, 29.7, 20.2, 16.4, 13.8.
ESI-HRMS calculated for $C_{20}H_{23}N_4O$ $[M+H]^+$ 335.1872, found 335.1858
IR (neat) : ν = 3272, 2918, 2850, 1644, 1610, 1515, 1436, 1302, 1142, 1107, 895, 815 cm^{-1}

Compound 11d



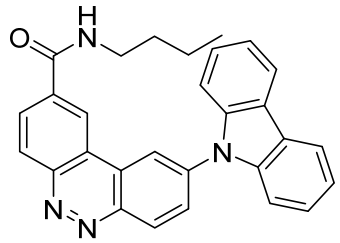
Chemical Formula: $C_{21}H_{24}N_4O$
Exact Mass: 348,20

To a 5 mL round bottom flask, **6** (20.0 mg, 0.07 mmol, 1.00 eq) was dissolved in dry DMF (1.00 mL). Cs_2CO_3 (32.0 mg, 0.1 mmol, 1.40 eq) and pyrrolidine (100 µL, 1.20 mmol, 15 eq) were added and the reaction mixture was stirred overnight at 80°c. After cooling down, the reaction mixture was quenched with brine, extracted with DCM and washed with brine. The organic layer was dried over $MgSO_4$ and concentrated under vacuum. The crude product was purified by flash chromatography (DCM/MeOH 98/2 -> 95/5) to afford **7d** as a yellow solid. 16.7 mg, 73%.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.76 (s, 1H), 8.43 (d, *J* = 8.5 Hz, 1H), 8.31 (d, *J* = 9.1 Hz, 1H), 7.97 (dd, *J* = 8.5 Hz ; 1.0 Hz, 1H), 7.06 (dd, *J* = 15.1, 13.1 Hz, 1H), 7.00 (s, 1H), 6.83 (s, 1H), 3.55 (q, *J* = 7.1 Hz, 2H),

3.40 (d, *J* = 6.0 Hz, 4H), 2.09 (t, *J* = 6.3 Hz, 4H), 1.73 – 1.65 (m, 2H), 1.46 (qt, 7.4 Hz, 2H), 0.98 (t, *J* = 7.4 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 167.3, 149.6, 145.7, 140.8, 135.1, 132.8, 130.5, 126.1, 123.9, 122.1, 120.7, 117.3, 97.7, 48.1, 40.4, 31.9, 25.6, 20.4, 14.0.
ESI-HRMS calculated for $C_{21}H_{25}N_4O$ $[M+H]^+$ 349.2028, found 349.2019
IR (neat) : ν = 3311, 3067, 2956, 2927, 2860, 1640, 1620, 1541, 1493, 1452, 1313, 1291, 1148, 1104, 849 cm^{-1}

Compound 11e



Chemical Formula: $C_{29}H_{24}N_4O$
Exact Mass: 444,20

To a 5 mL round bottom flask, **6** (30.0 mg, 0.10 mmol, 1.00 eq) was dissolved in dry DMF (1.00 mL). Cs_2CO_3 (32 mg, 0.10 mmol, 1.00 eq) and carbazole (26.0 mg, 1.60 mmol, 1.60 eq) were added and the reaction mixture was stirred overnight at 80 °C. After cooling down, the reaction mixture was quenched with brine, extracted with DCM and washed with brine. The organic layer was dried over $MgSO_4$ and concentrated under vacuum. The crude product was purified by flash chromatography (DCM/MeOH 98/2 -> 95/5 -> 90/10) and another flash chromatography (DCM/AcOEt) to afford **7e** as a yellow solid. 34 mg, 77%.

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.00 – 8.96 (m, 2H), 8.83 (s, 1H), 8.80 (d, *J* = 8.55 Hz, 1H), 8.20 (d, *J* = 8.60 Hz, 1H), 8.17 (d, *J* = 7.76 Hz, 3H), 7.55 (d, *J* = 8.17 Hz, 2H), 7.44 (t, *J* = 7.63 Hz, 2H), 7.35 (t, *J* = 7.43 Hz, 2H), 6.50 (s, 1H), 3.53 (q, *J* = 6.57 Hz, 2H), 1.68 – 1.61 (m, 2H), 1.47 – 1.37 (m, 2H), 0.95 (t, *J* = 7.32 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 166.3, 145.8, 144.3, 141.3, 140.4, 137.4, 133.7, 131.9, 128.6, 127.6, 126.6, 124.2, 122.6, 121.5, 121.3, 120.8, 120.5, 118.7, 109.7, 40.4, 31.8, 20.3, 13.9.
ESI-HRMS calculated for $C_{29}H_{25}N_4O$ $[M+H]+$ 445.2028, found 445.2023
IR (neat) : ν = 3400, 3053, 2949, 2924, 2865, 1668, 1652, 1611, 1526, 1542, 1364, 1232, 1150, 832 cm^{-1}

Cell Culture and Confocal Microscopy

Cell Culture

A549 Human lung carcinoma cell lines were obtained from the American type Culture Collection (ATCC, Rockville, USA) and were cultured according to the supplier's instructions, in RPMI 1640 containing 10% FCS and 1% glutamine. All cell lines were maintained at 37 °C in a humidified atmosphere containing 5% CO2.

Sample preparation for confocal microscopy with live cell

An Ibidi® µSlide 8 Well high Glass Bottom plate was seeded with 20 000 cells/well and then maintain ed at 37 °C in a humidified atmosphere containing 5% CO_2 for 24h. After adequate confluence was o

btained, the medium was removed and replaced by a solution of fluorophore at desired concentration in RPMI, prepared from a stock solution of fluorophore in DMSO (final concentration of DMSO was kept under 1% v/v). After 3h of incubation with ABCDye, the medium was removed, cells were washed once with warmed PBS (1X). Organelle staining was performed following instruction from the supplier (see Co-localization experiment section). The stain-containing medium was removed, cells were washed once with warmed PBS (1X) then fresh RPMI 1640 medium was added before imaging.

Confocal fluorescence microscopy

Fluorescence images were acquired using a Leica SP8-X inverted confocal microscope with a 63× oil immersion objective (HC PL APO CS2 Leica). Excitation was performed using a White light laser pulsed at 80MHz and a Diode 440 nm LDH-P-C-440B pulsed at 40 MHz. Detection was carried out by using PMT detector (Hamamatsu 6357) collecting photons, or GaAsP Hybrid (Hamamatsu) collecting photons over the appropriate emission wavelength window.

Colocalization experiments:

MitoView™ 633, LysoView™ 633 and NucSpot® live 650 were purchased from Biotium.

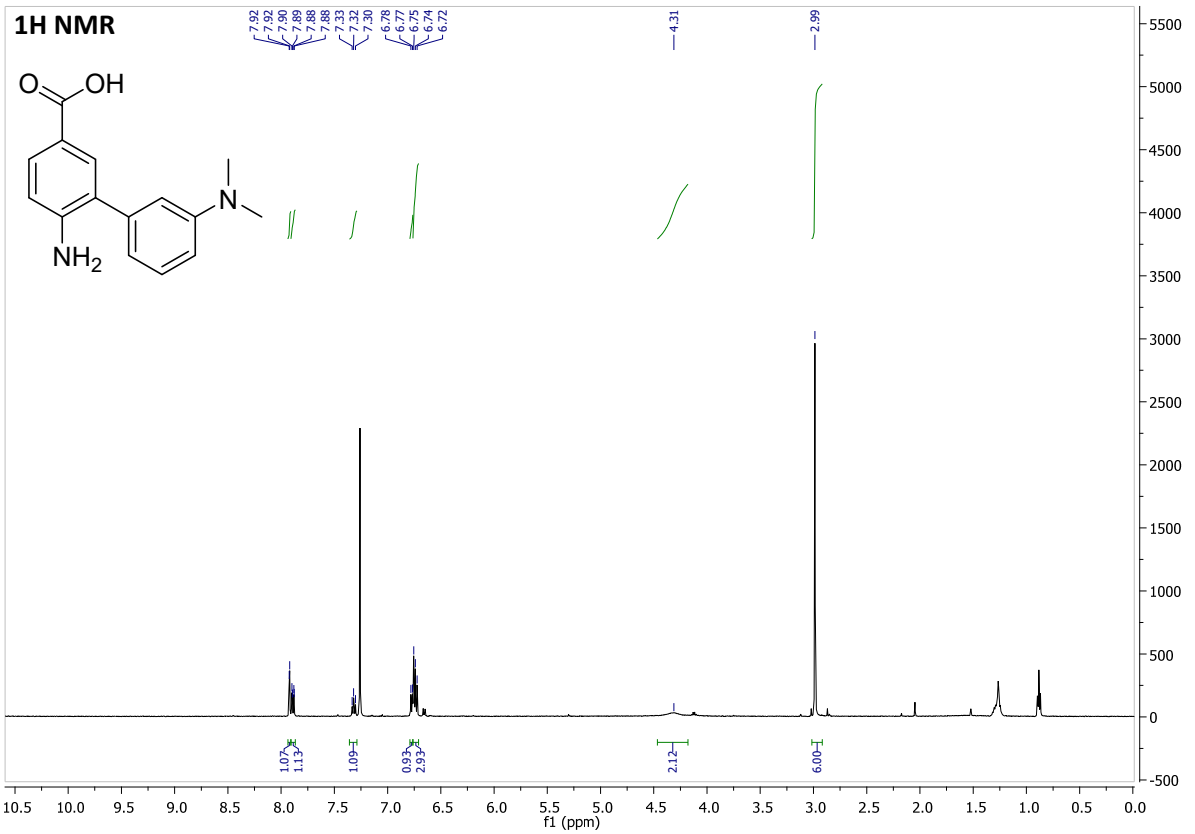
- *Protocol for* MitoView™ *633 staining:* After incubation with ABCDye, the medium was removed. A 100 nM MitoView™ 633 solution in appropriate medium was then added, and cells were incubated for 15 minutes at 37 °C. The medium was removed, cells were washed once with warmed PBS (1X) then fresh RPMI was added before imaging.

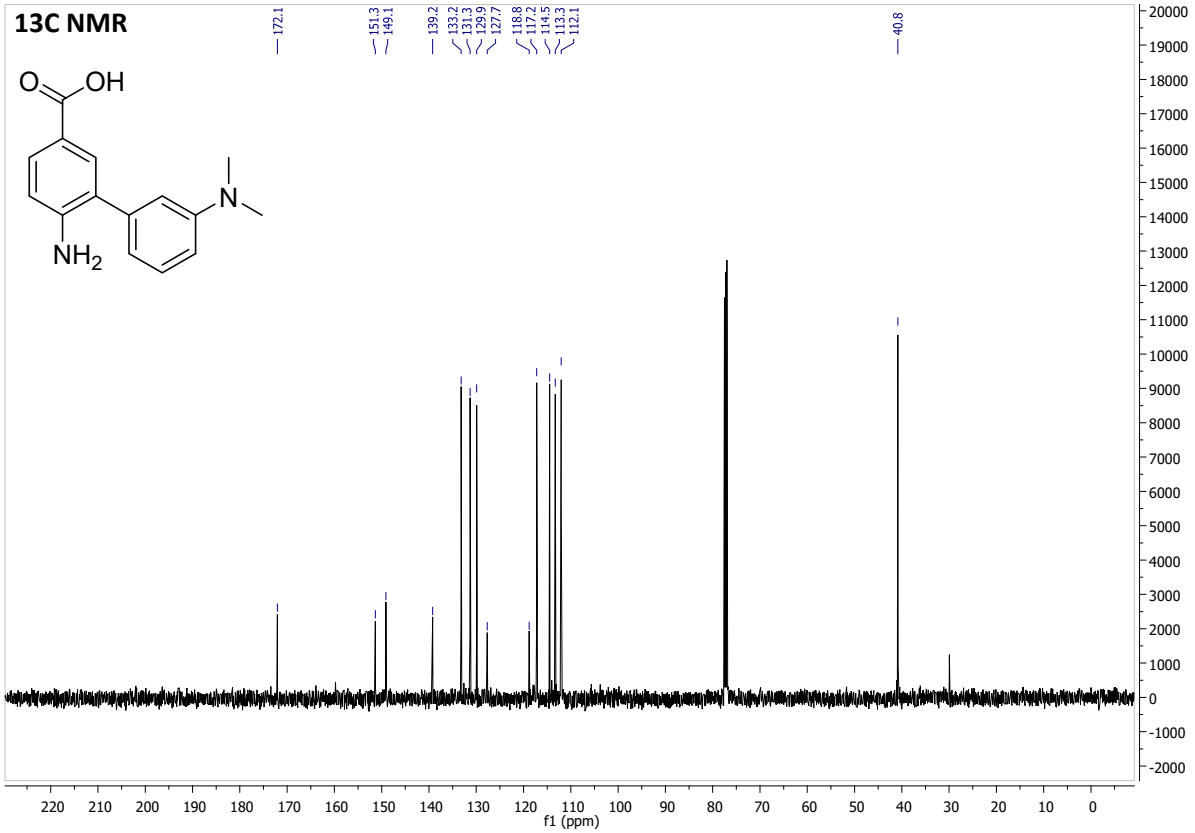
- *Protocol for* LysoView™ *633 staining:* After incubation with ABCDye, the medium was removed. A 1X solution of LysoView™ 633 in RPMI (prepared following Biotium instructions) was then added, and cells were incubated for 30 minutes at 37 °C. The medium was removed, cells were washed once with warmed PBS (1X) then fresh RPMI was added before imaging.

- *Protocol for* NucSpot® live 650 *staining:* After incubation with ABCDye, the medium was removed. A 1X solution of NucSpot® live 650 in RPMI (prepared following Biotium instructions) was then added, and cells were incubated for 15 minutes at 37 °C. The medium was removed, cells were washed once with warmed PBS (1X) then fresh RPMI was added before imaging.

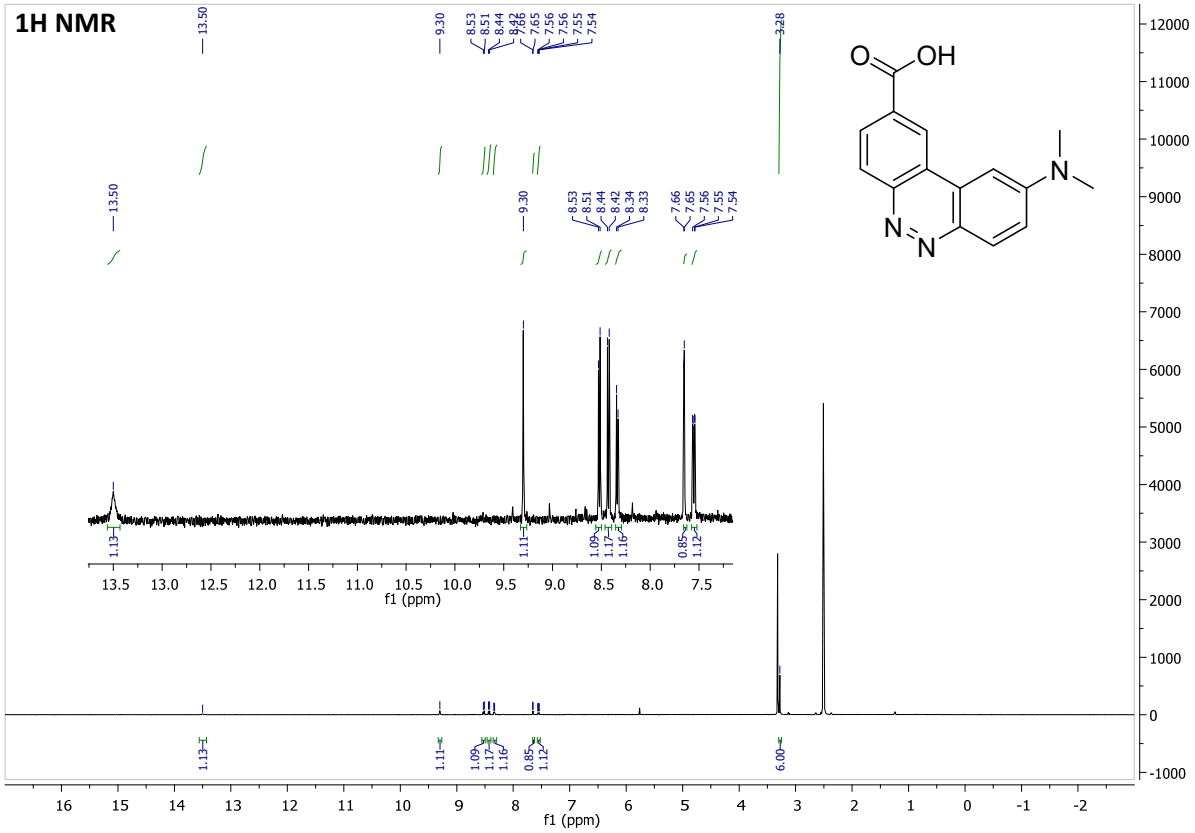
III. NMR spectra

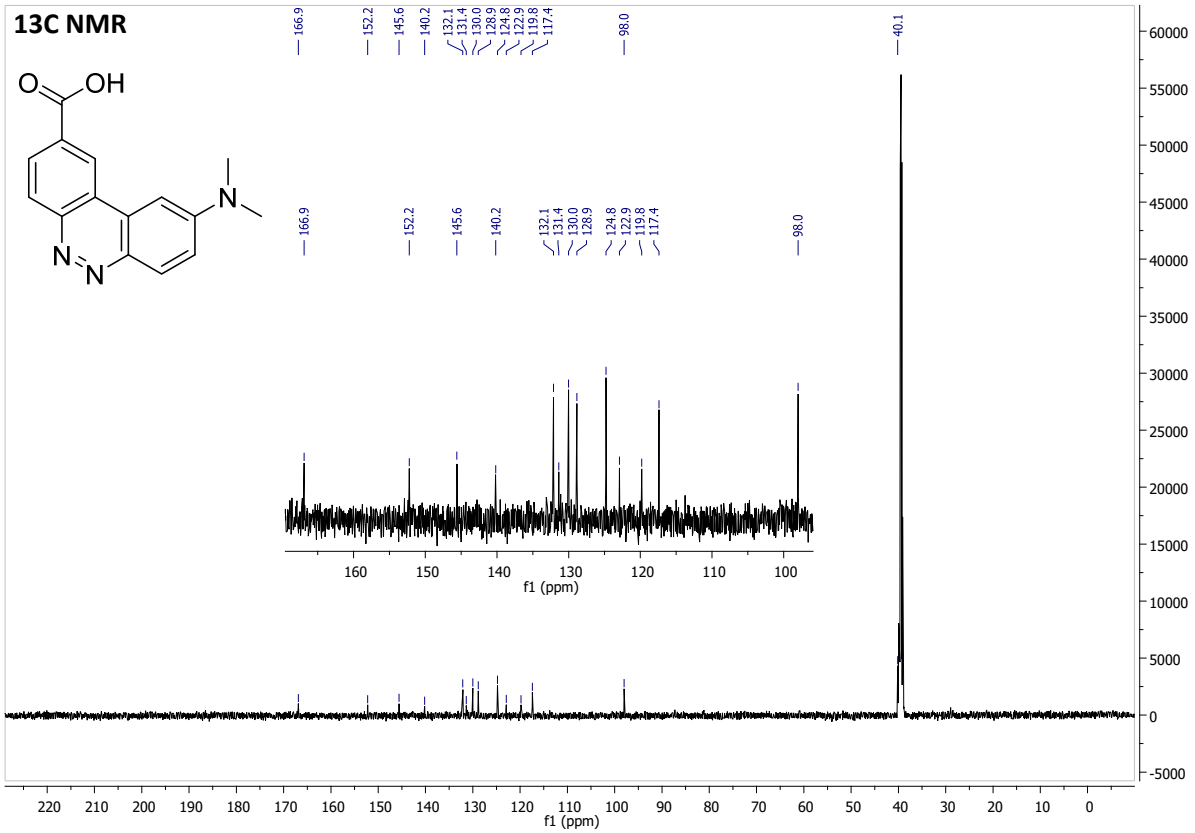
Compound 2



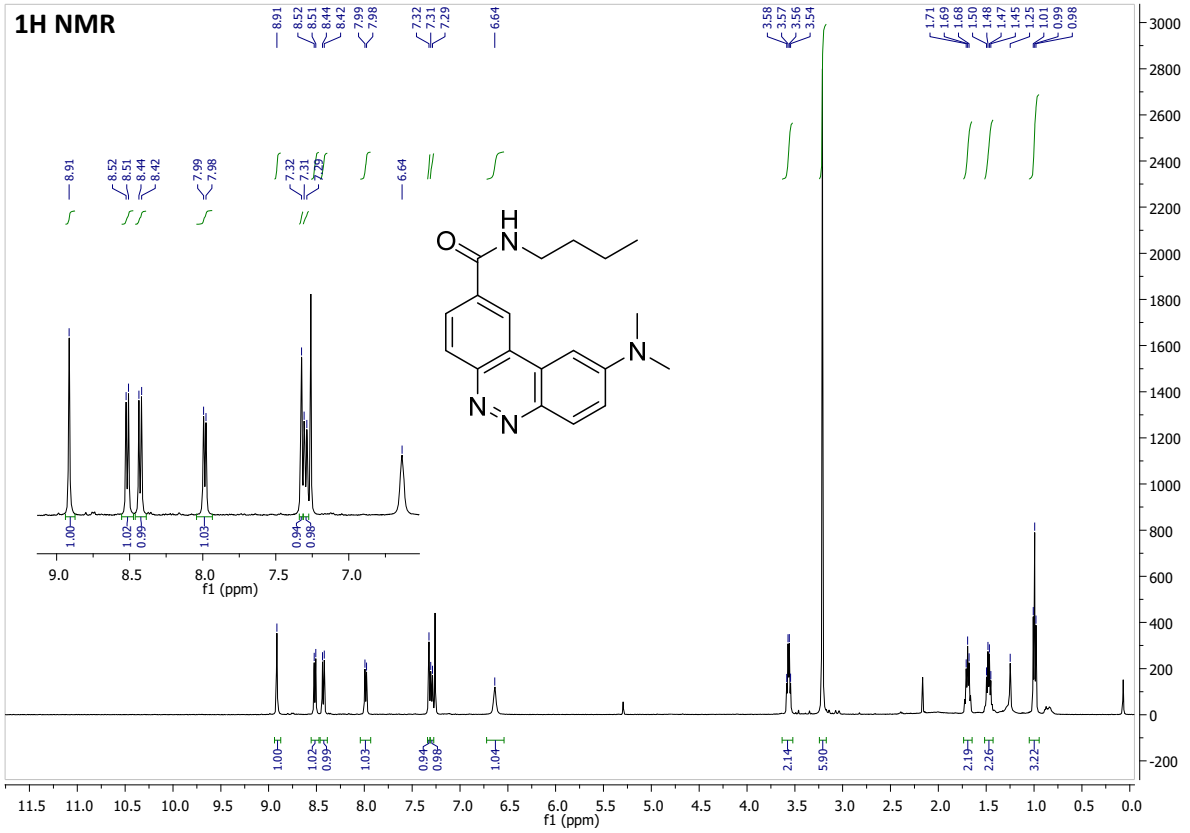


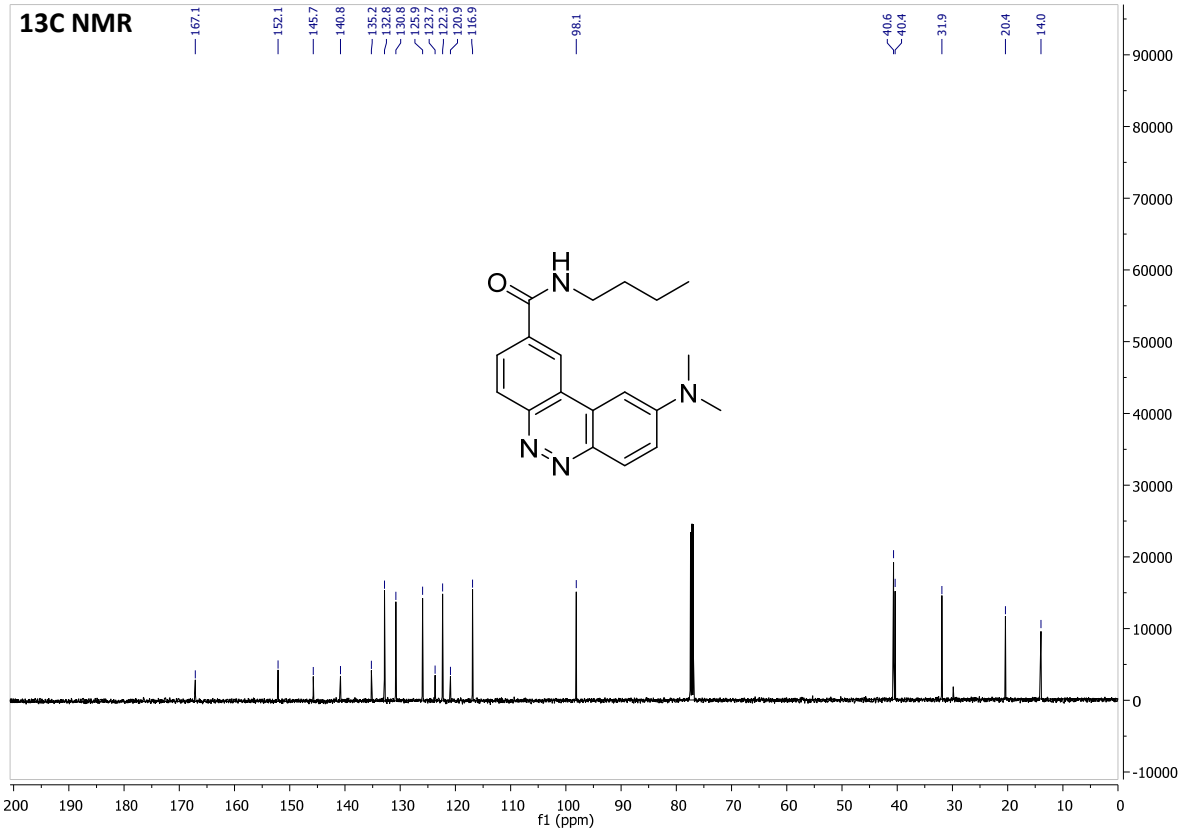
Compound 3


1H NMR
13.50
9.30
8.53
8.51
8.44
8.42
8.34
8.33
7.66
7.65
7.56
7.55
7.54
3.28
O
OH
N
N
N
f1 (ppm)


13C NMR
166.9
152.2
145.6
140.2
132.1
131.4
130.0
128.9
124.8
122.9
119.8
117.4
98.0
40.1
O
OH
N
N
N
f1 (ppm)

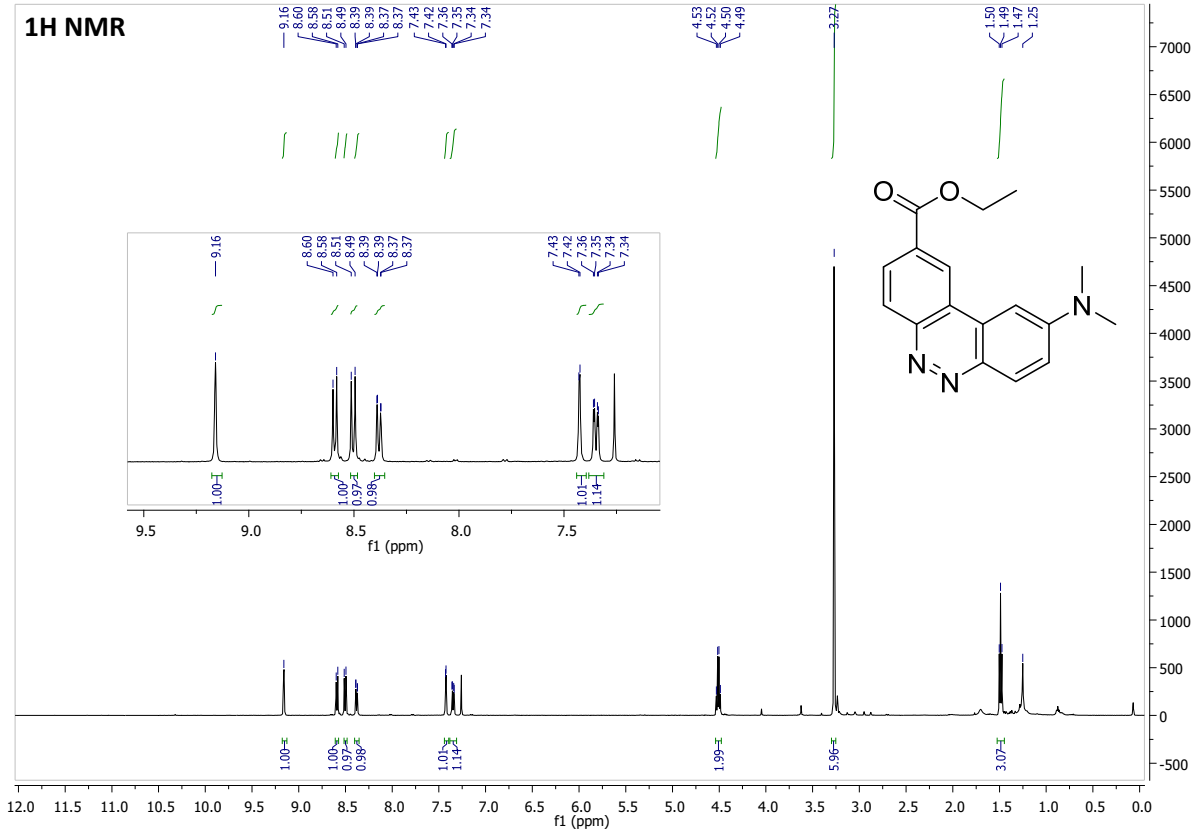
Compound 4a



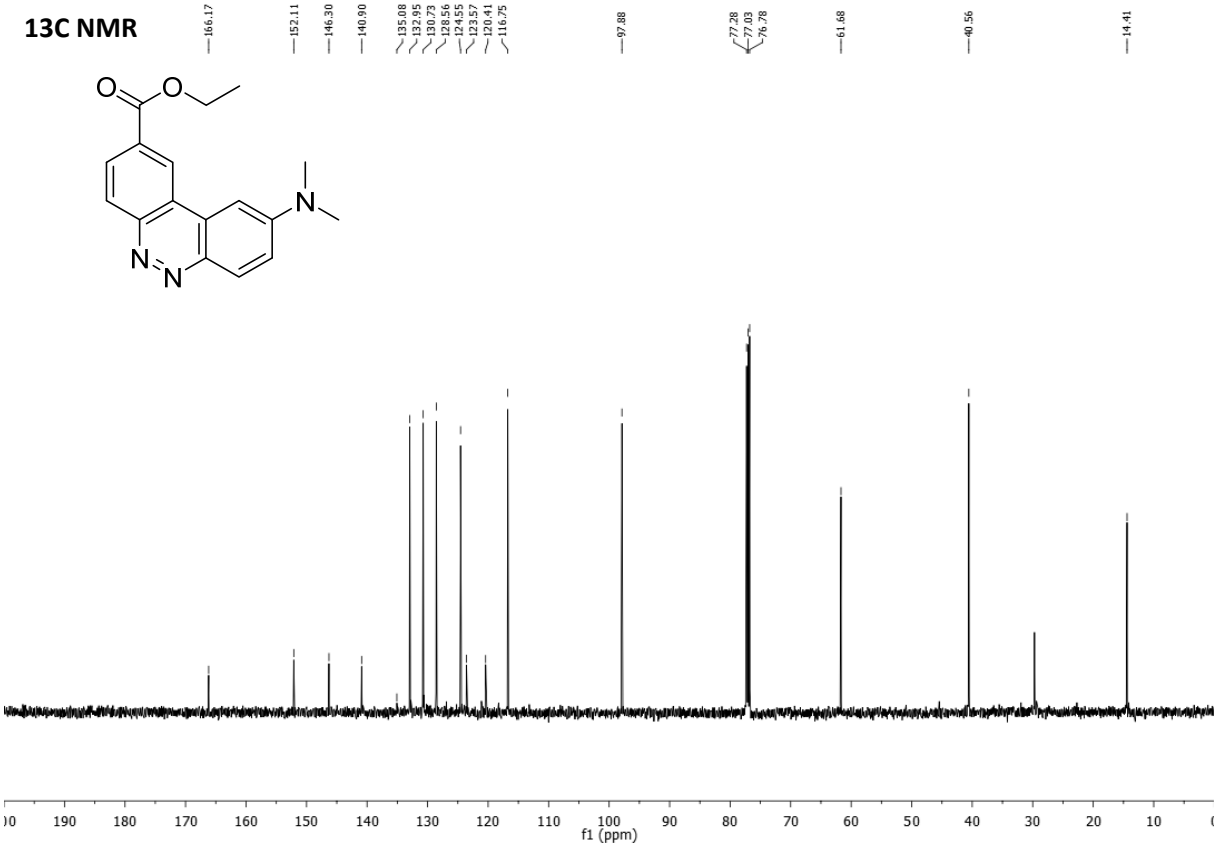


Compound 4b

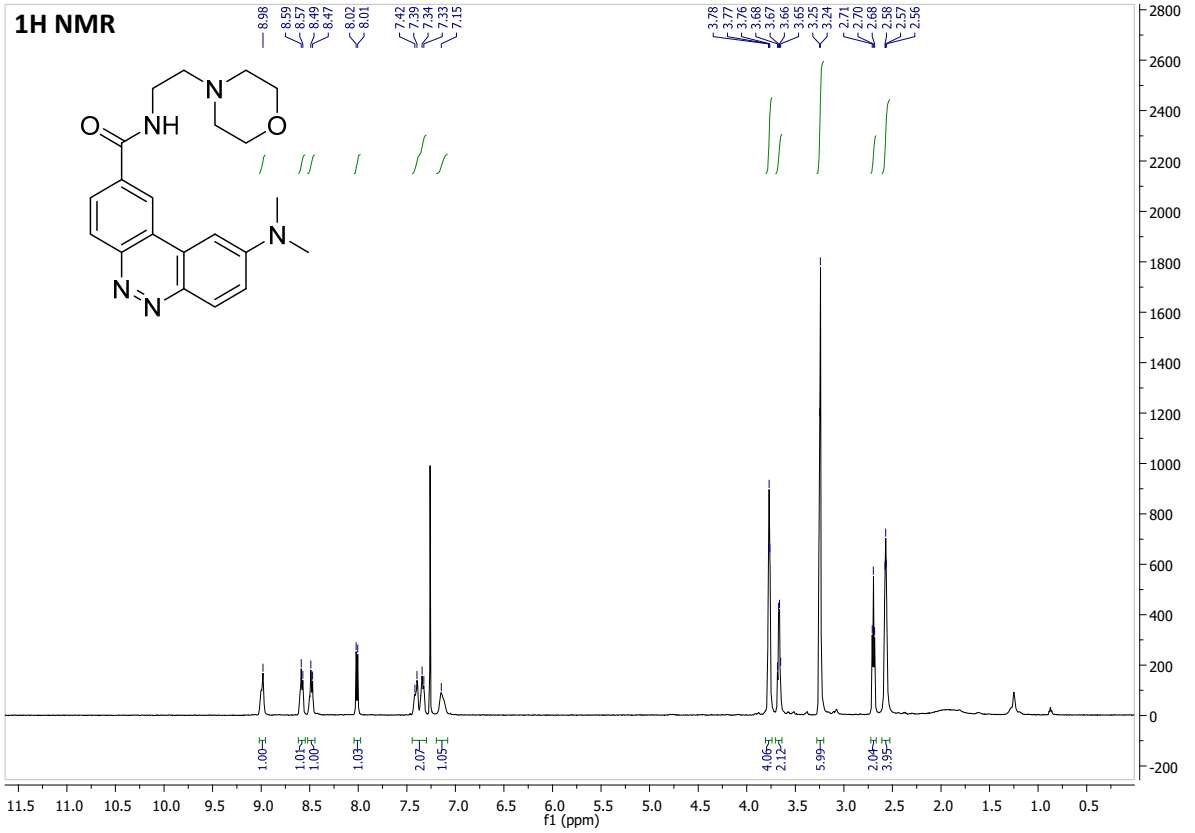
1H NMR



13C NMR



Compound 4c


1H NMR
8.98
8.59
8.57
8.49
8.47
8.02
8.01
7.42
7.39
7.34
7.33
7.15
3.78
3.77
3.76
3.68
3.67
3.66
3.65
3.25
3.24
2.71
2.70
2.68
2.58
2.57
2.56
1.00
1.01
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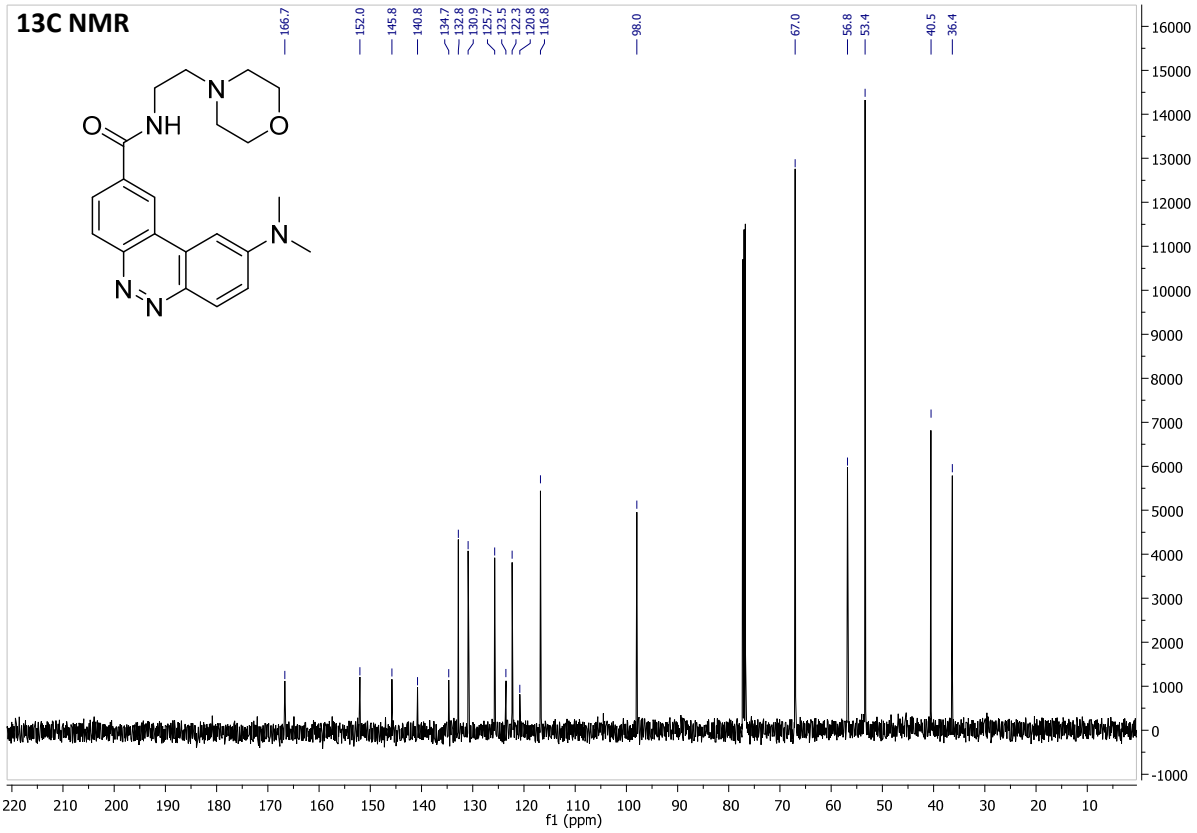
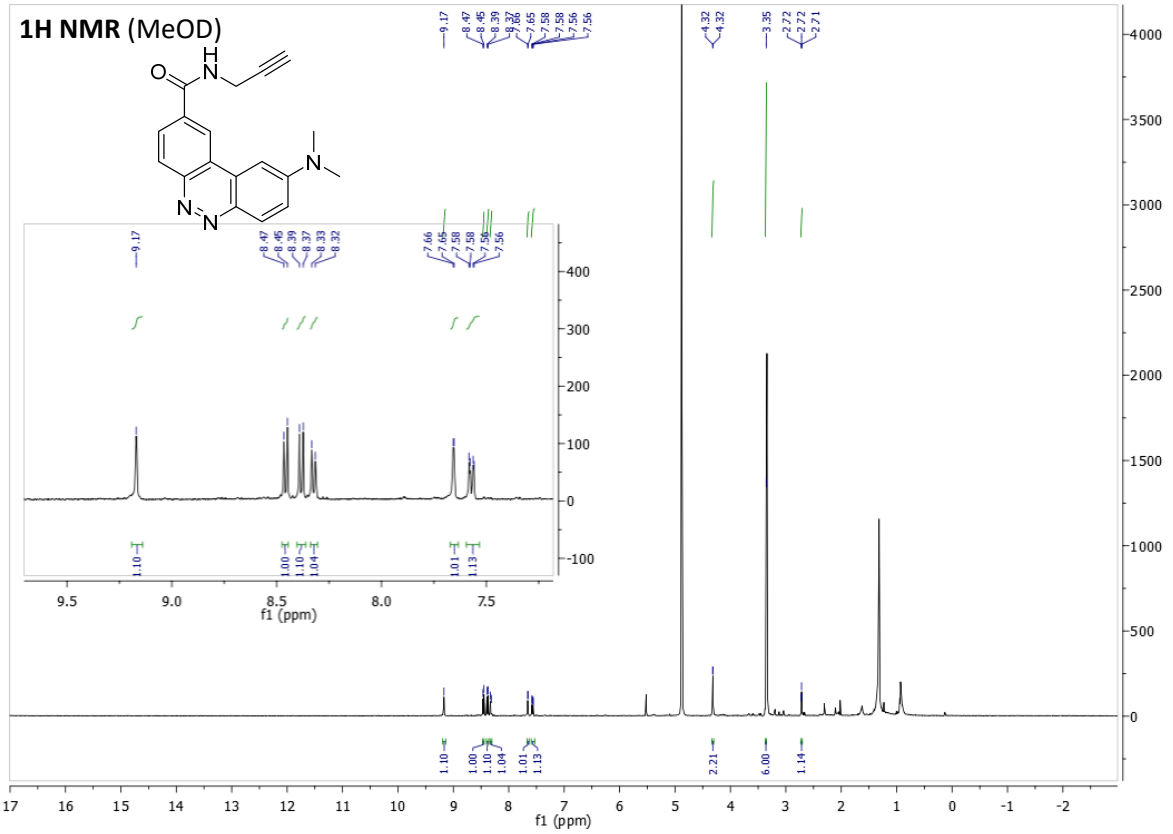
1.03
2.07
1.05
4.06
2.12
5.99
2.04
3.95
f1 (ppm)

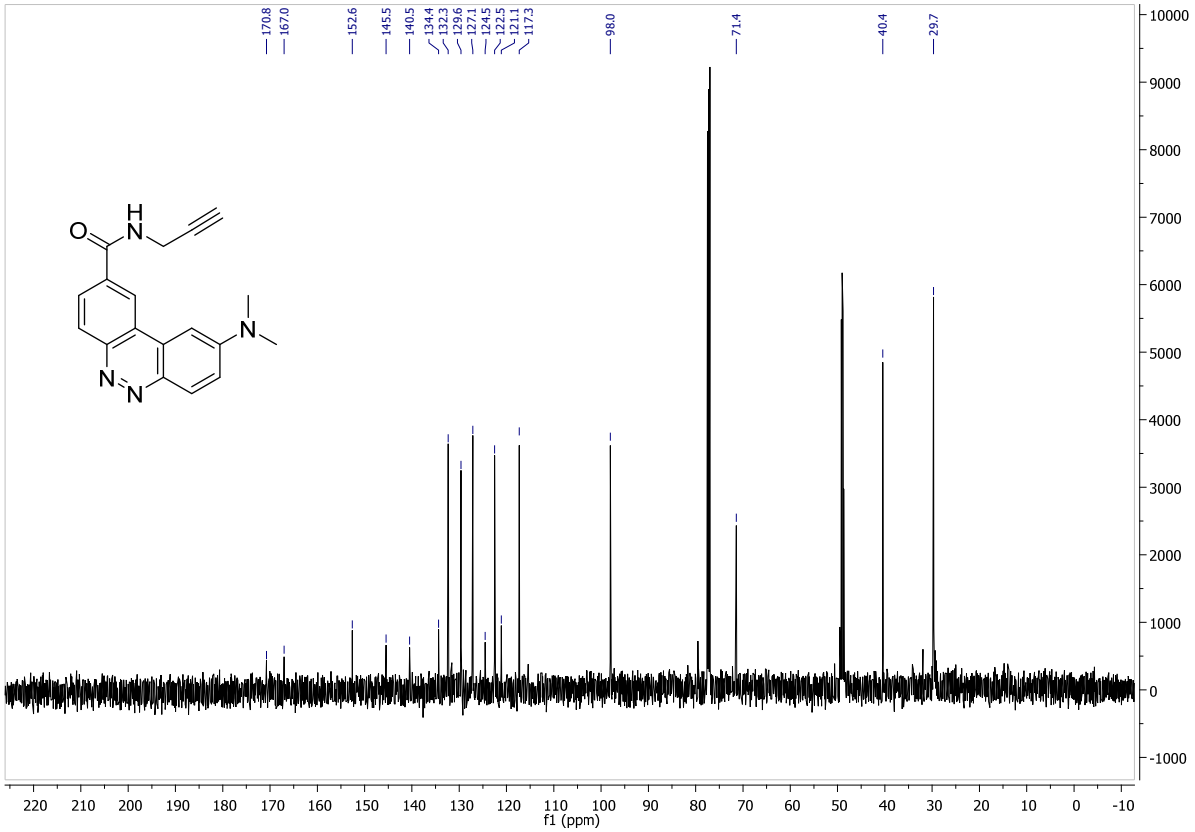

13C NMR
166.7
152.0
145.8
140.8
134.7
132.8
130.9
125.7
123.5
122.3
120.8
116.8
98.0
67.0
56.8
53.4
40.5
36.4
f1 (ppm)

Compound 4d

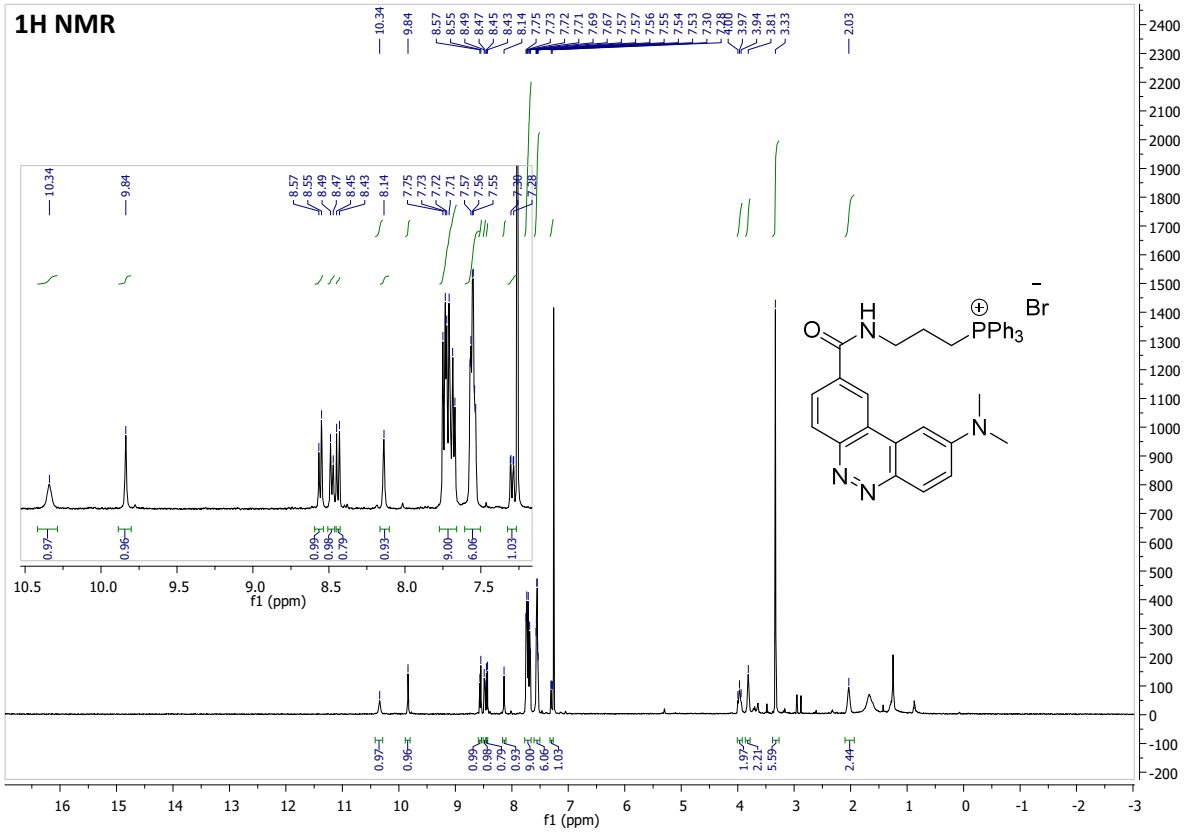
1H NMR (MeOD)

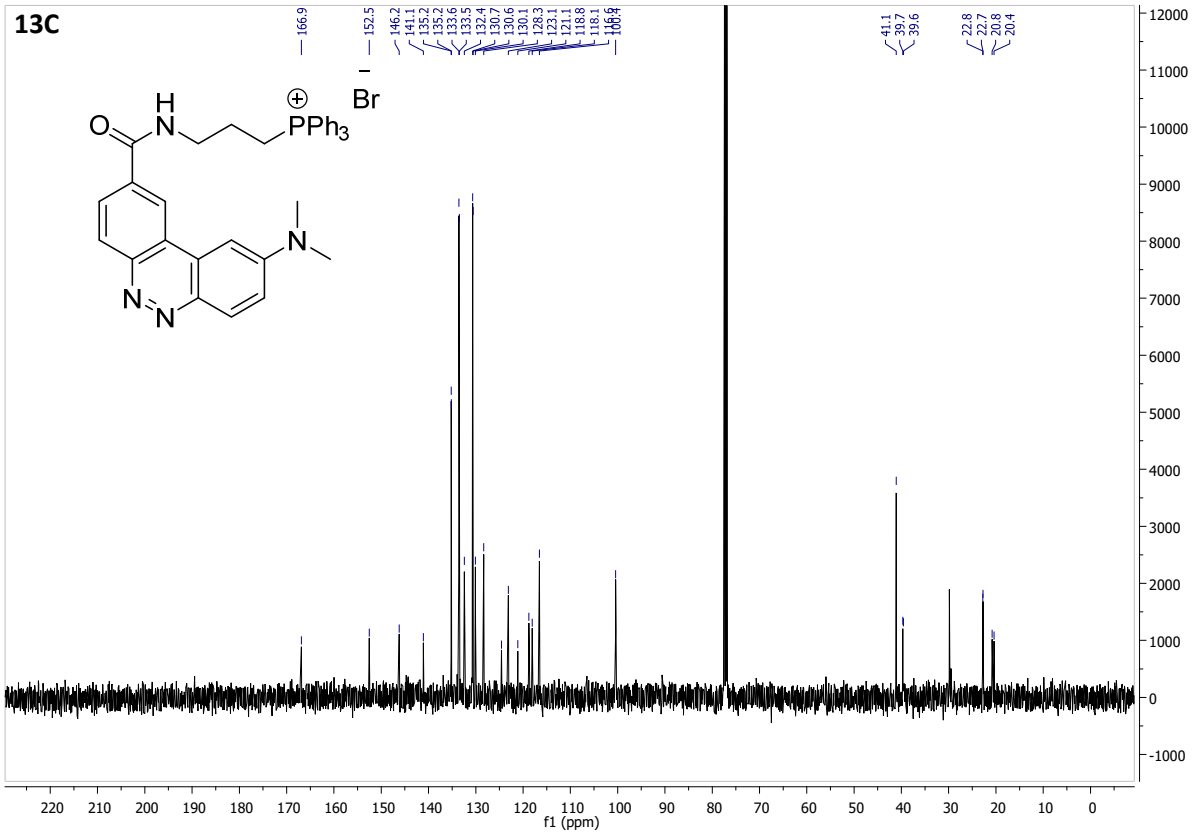


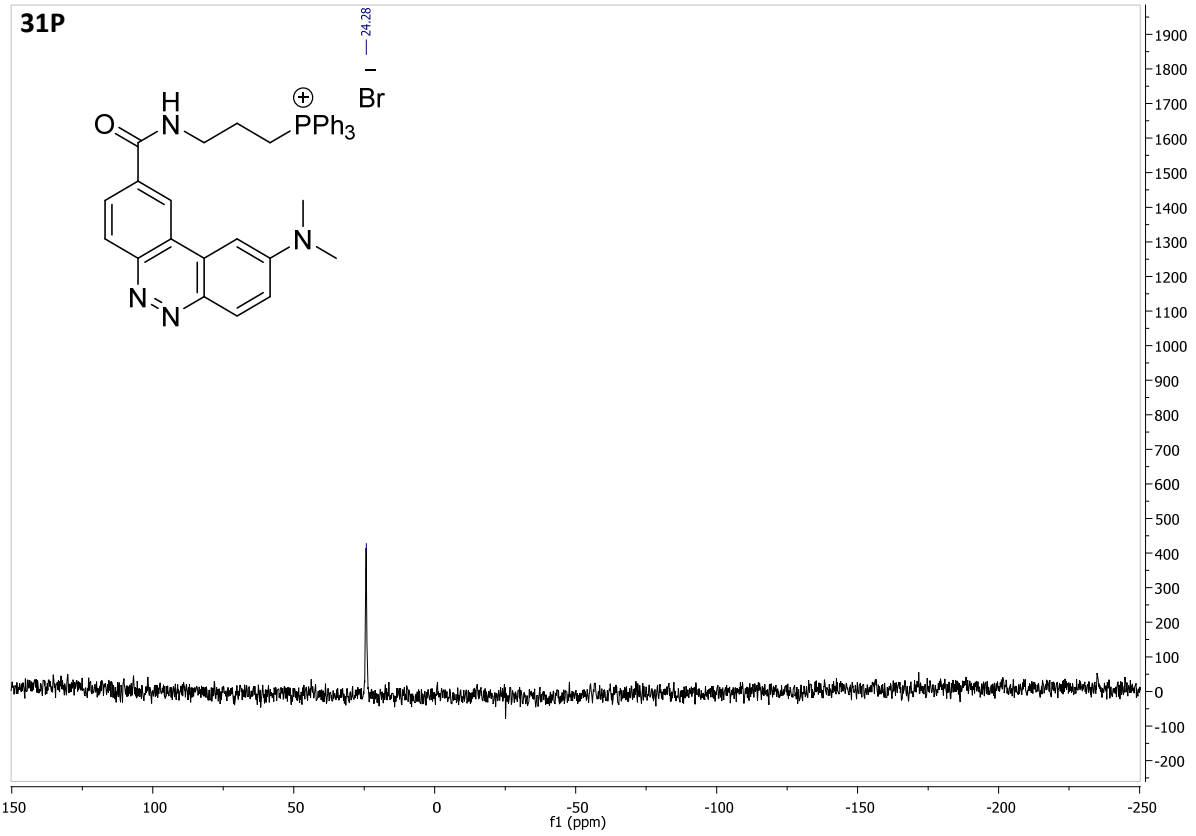
13C NMR ($CDCl_3$/MeOD 9/1)



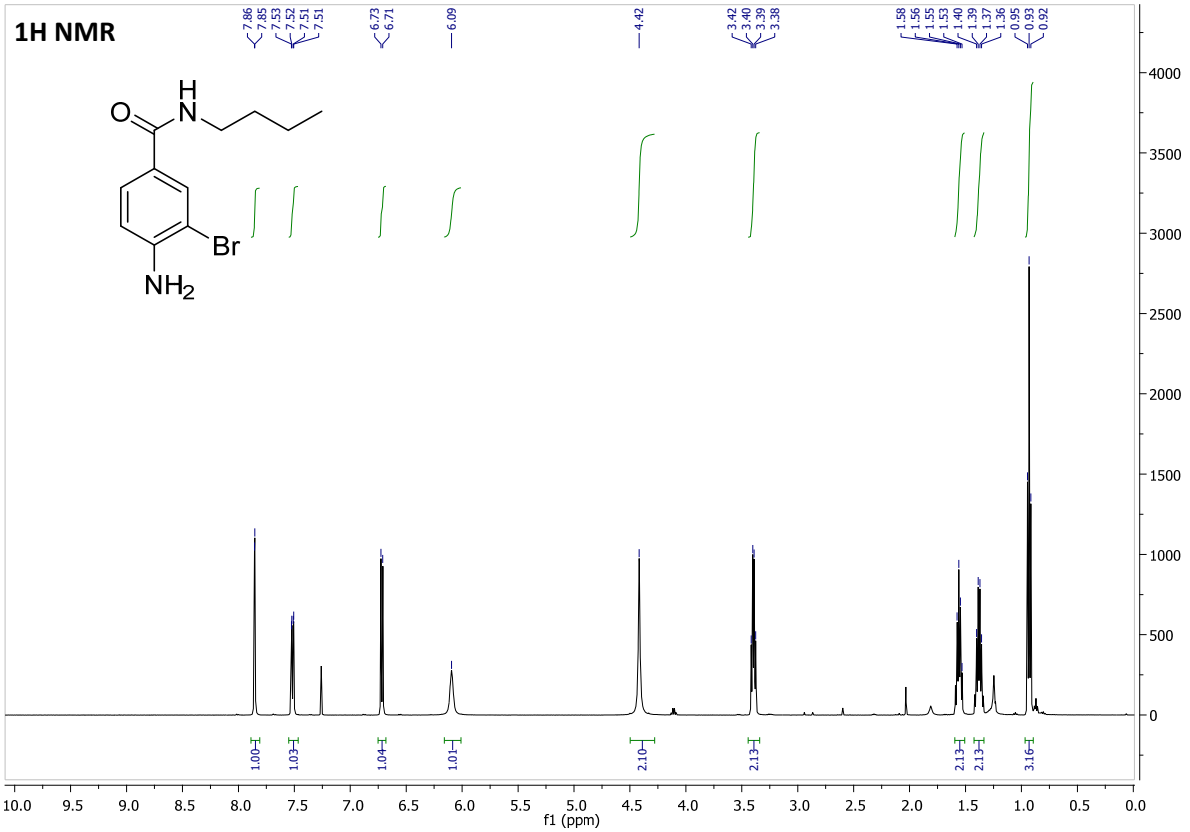
Compound 4e

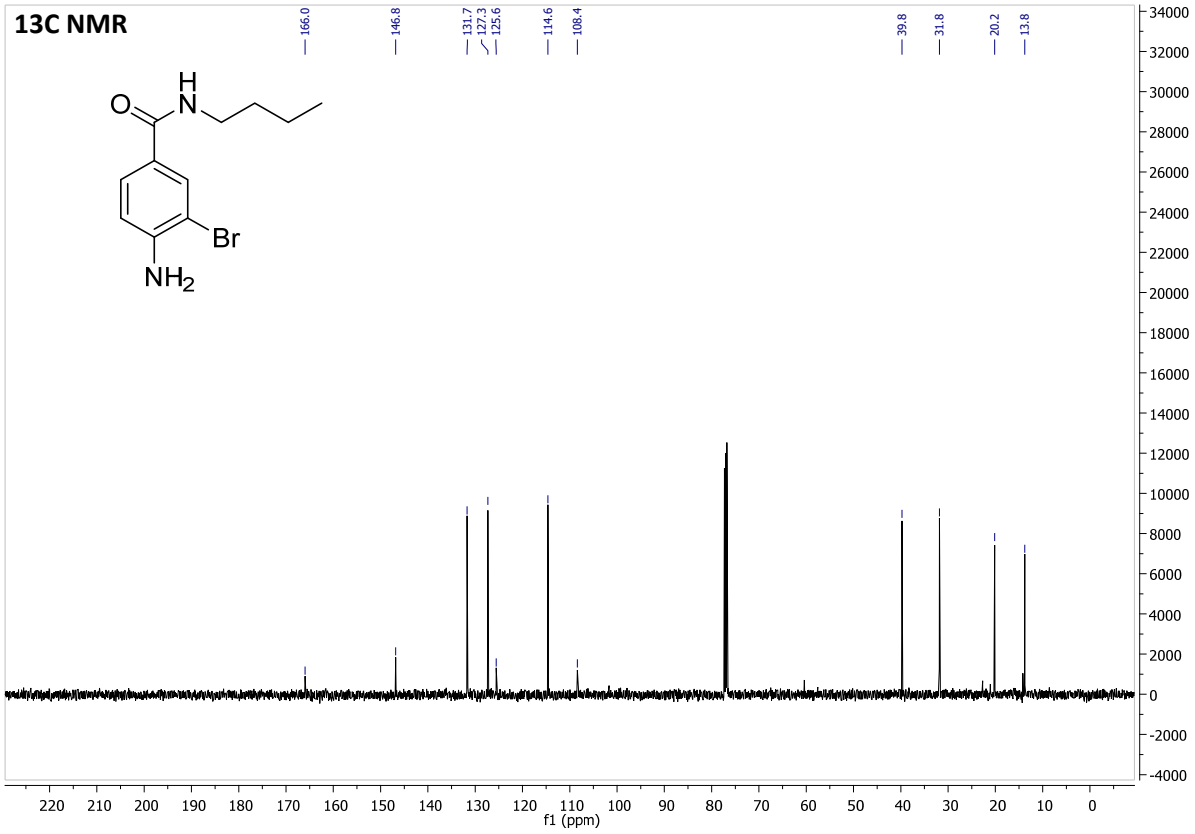




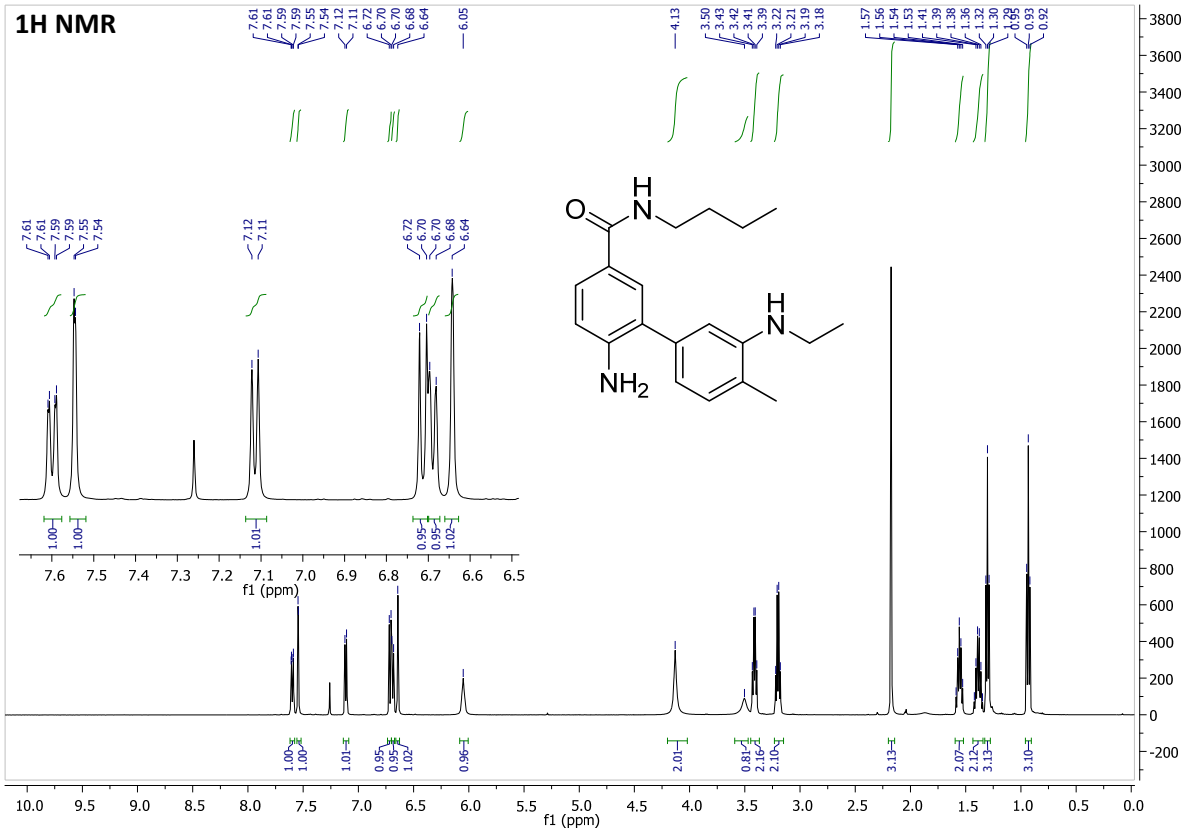

31P
24.28
Br
PPh3
f1 (ppm)

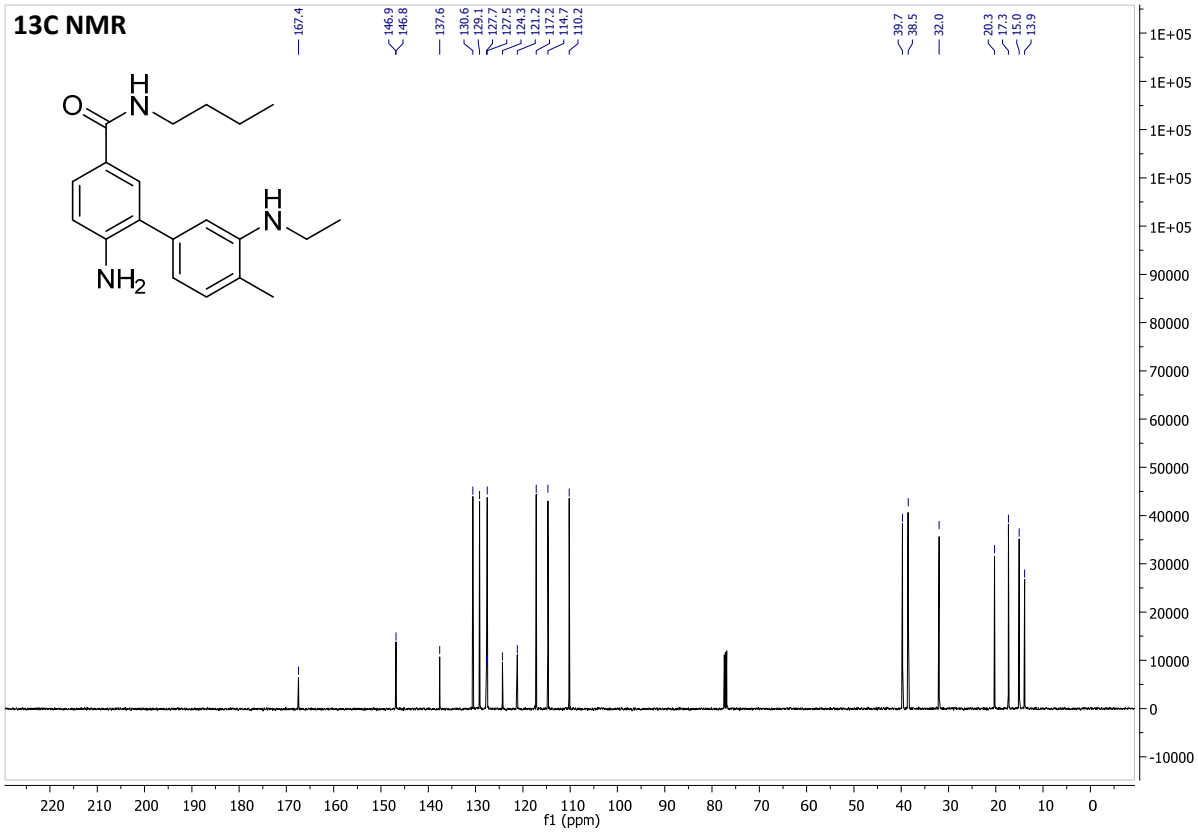
Compound 5


1H NMR
7.86
7.85
7.53
7.52
7.51
7.51
6.73
6.71
6.09
4.42
3.42
3.40
3.39
3.38
1.58
1.56
1.55
1.53
1.40
1.39
1.37
1.36
0.95
0.93
0.92
Br
NH2
f1 (ppm)

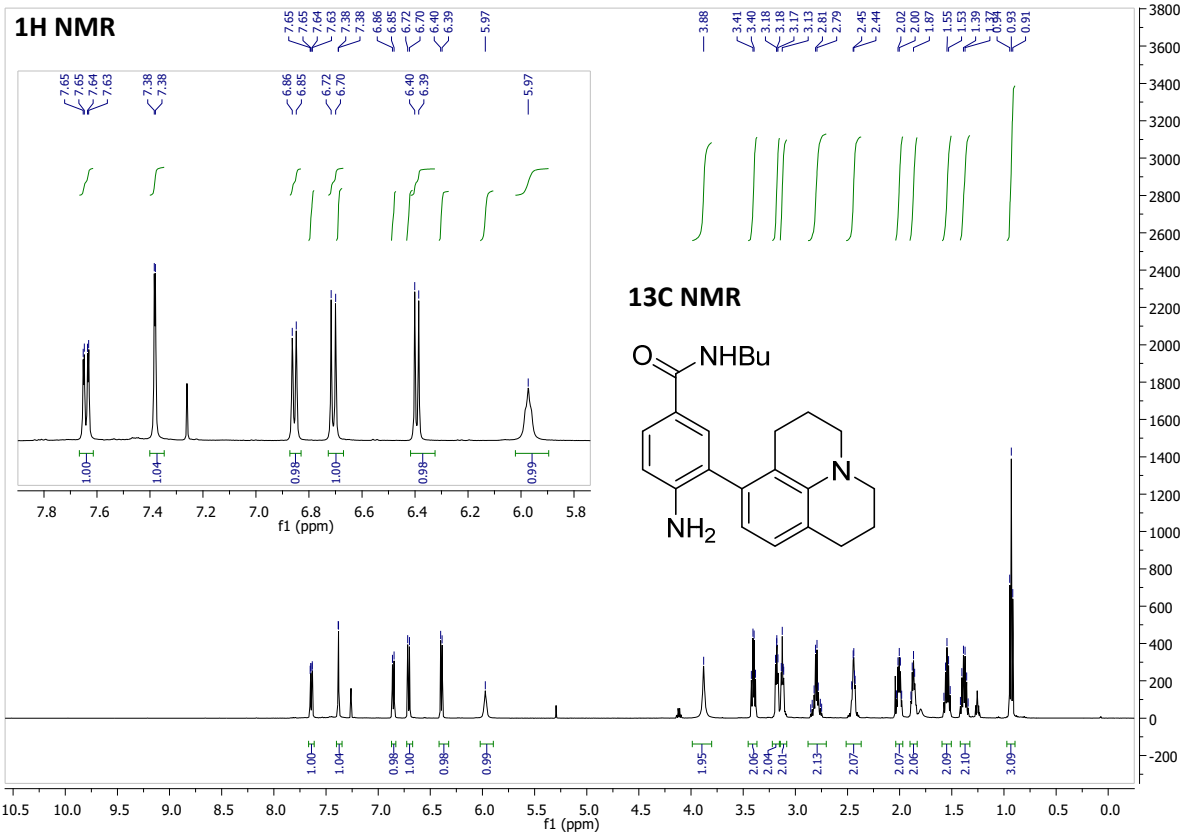

13C NMR
166.0
146.8
131.7
127.3
125.6
114.6
108.4
39.8
31.8
20.2
13.8
Br
NH2
f1 (ppm)

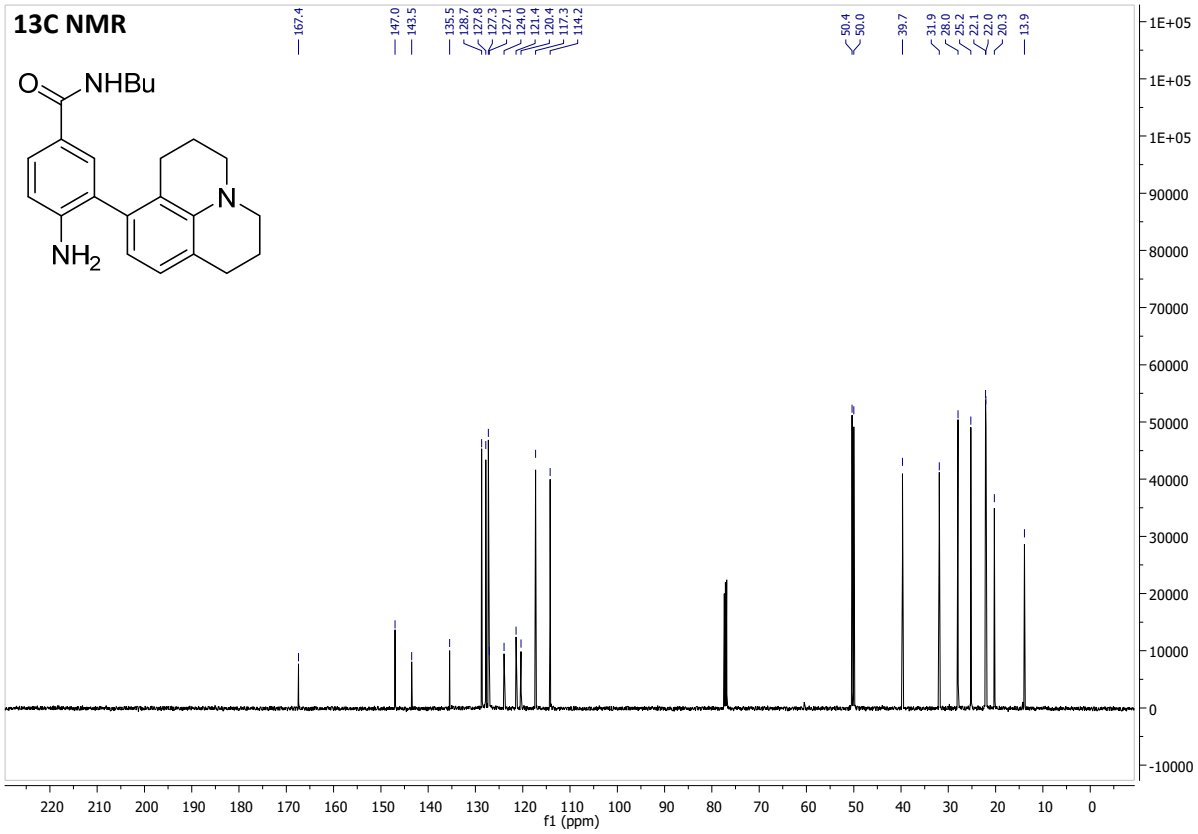
Compound 6a


1H NMR
7.61
7.59
7.55
7.54
7.12
7.11
6.72
6.70
6.68
6.64
6.05
4.13
3.50
3.43
3.42
3.41
3.39
3.22
3.21
3.19
3.18
1.57
1.56
1.54
1.53
1.41
1.39
1.38
1.36
1.32
1.30
0.93
0.92
NH2
f1 (ppm)


13C NMR
167.4
146.9
146.8
137.6
130.6
129.1
127.7
127.5
124.3
121.2
117.2
114.7
110.2
39.7
38.5
32.0
20.3
17.3
15.0
13.9
f1 (ppm)

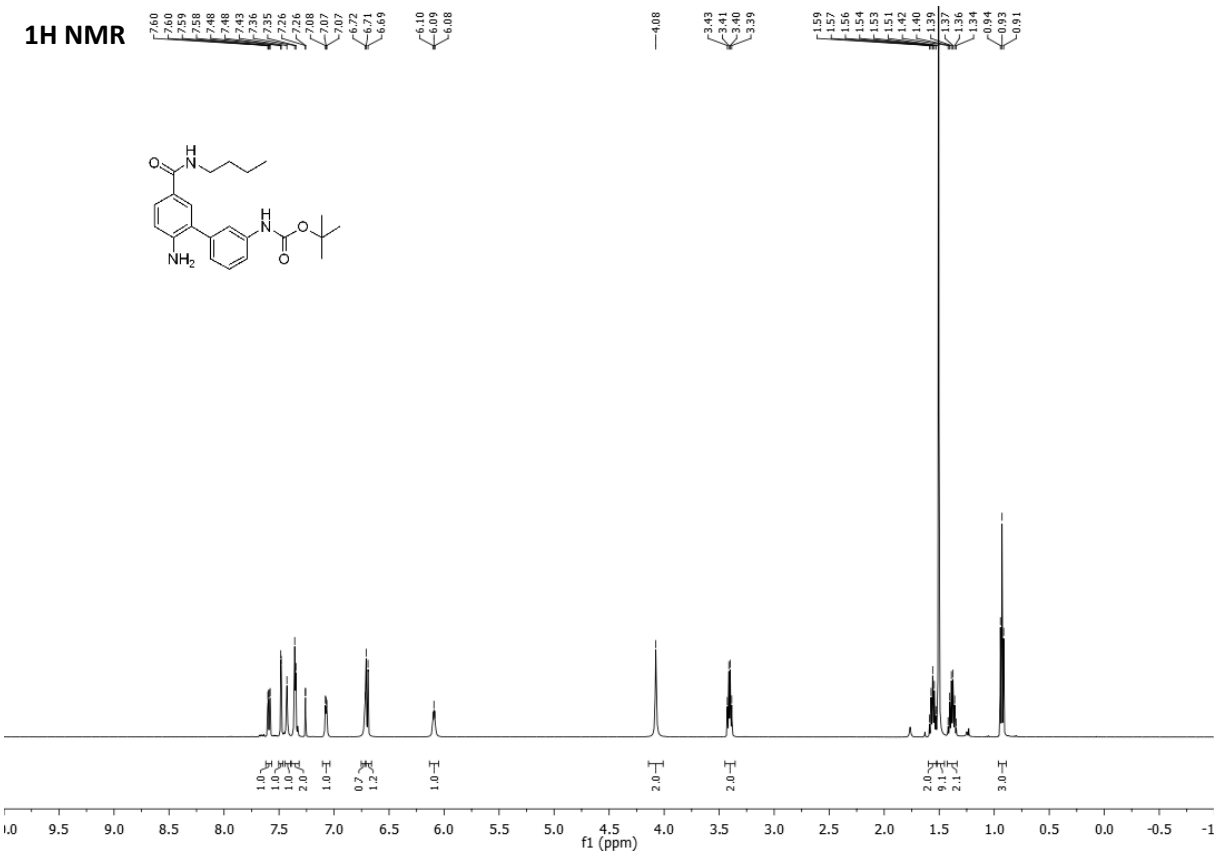
Compound 6b


1H NMR
7.65
7.64
7.63
7.38
6.86
6.85
6.72
6.70
6.40
6.39
5.97
3.88
3.41
3.40
3.18
3.17
3.13
2.81
2.79
2.45
2.44
2.02
2.00
1.87
1.55
1.53
1.39
0.93
0.91
13C NMR
NHBu
NH2
f1 (ppm)

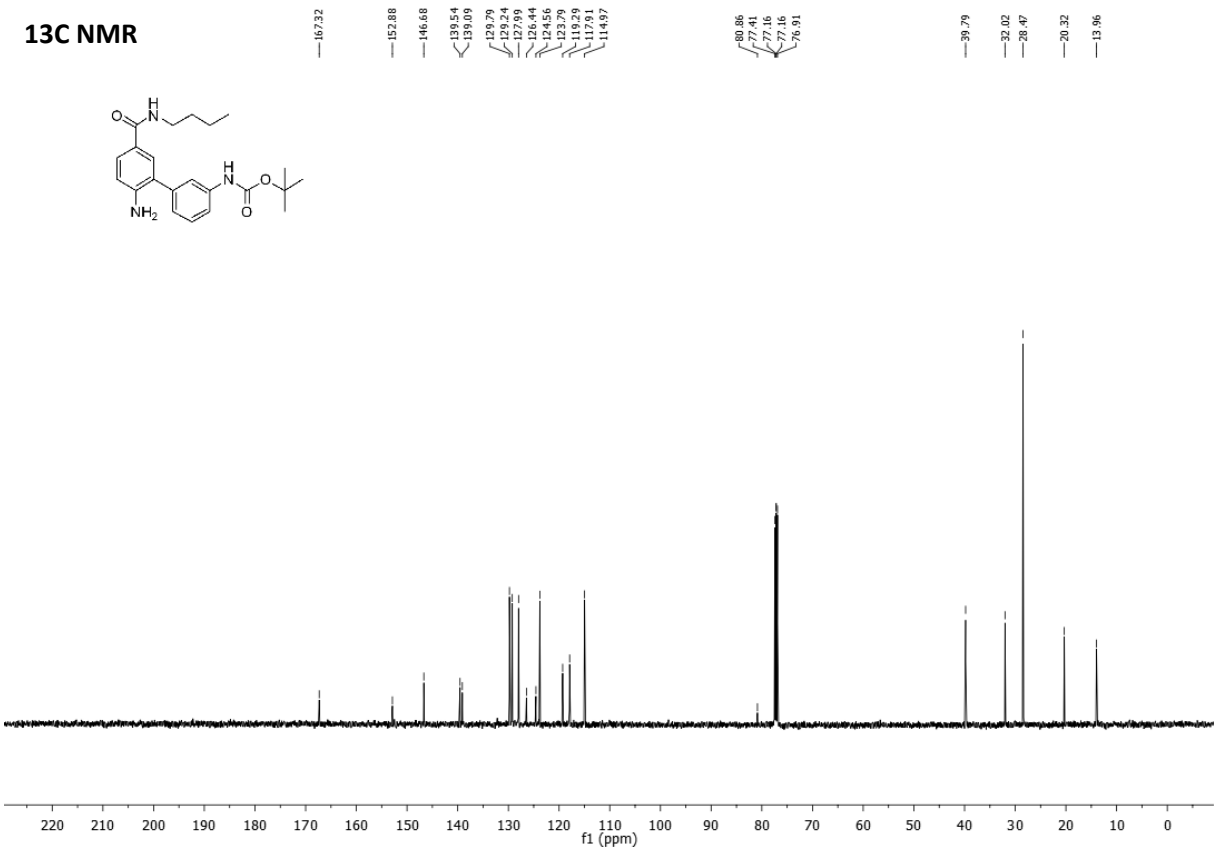

13C NMR
O
NHBu
N
NH2
167.4
147.0
143.5
135.5
128.7
127.8
127.3
127.1
124.0
121.4
120.4
117.3
114.2
50.4
50.0
39.7
31.9
28.0
25.2
22.1
22.0
20.3
13.9
1E+05
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

Compound 6c

1H NMR

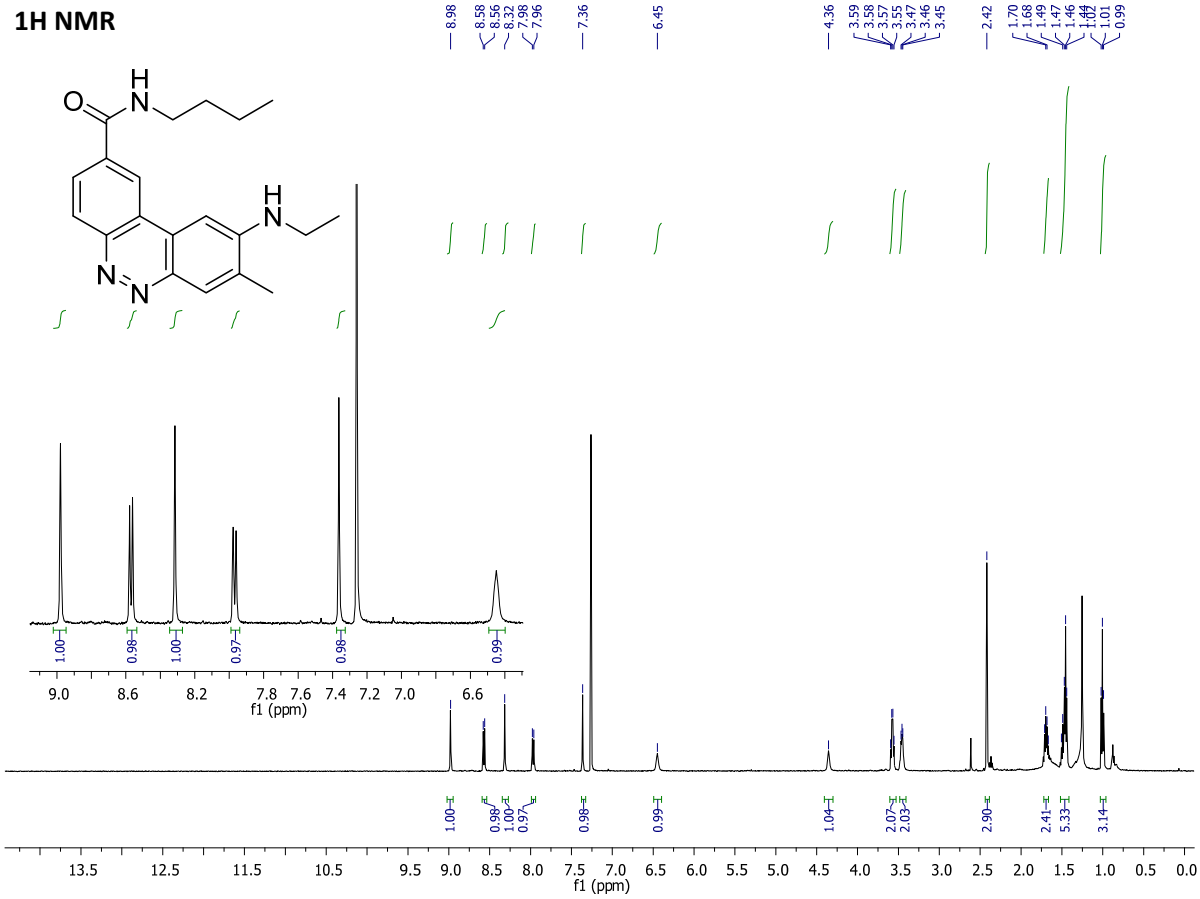


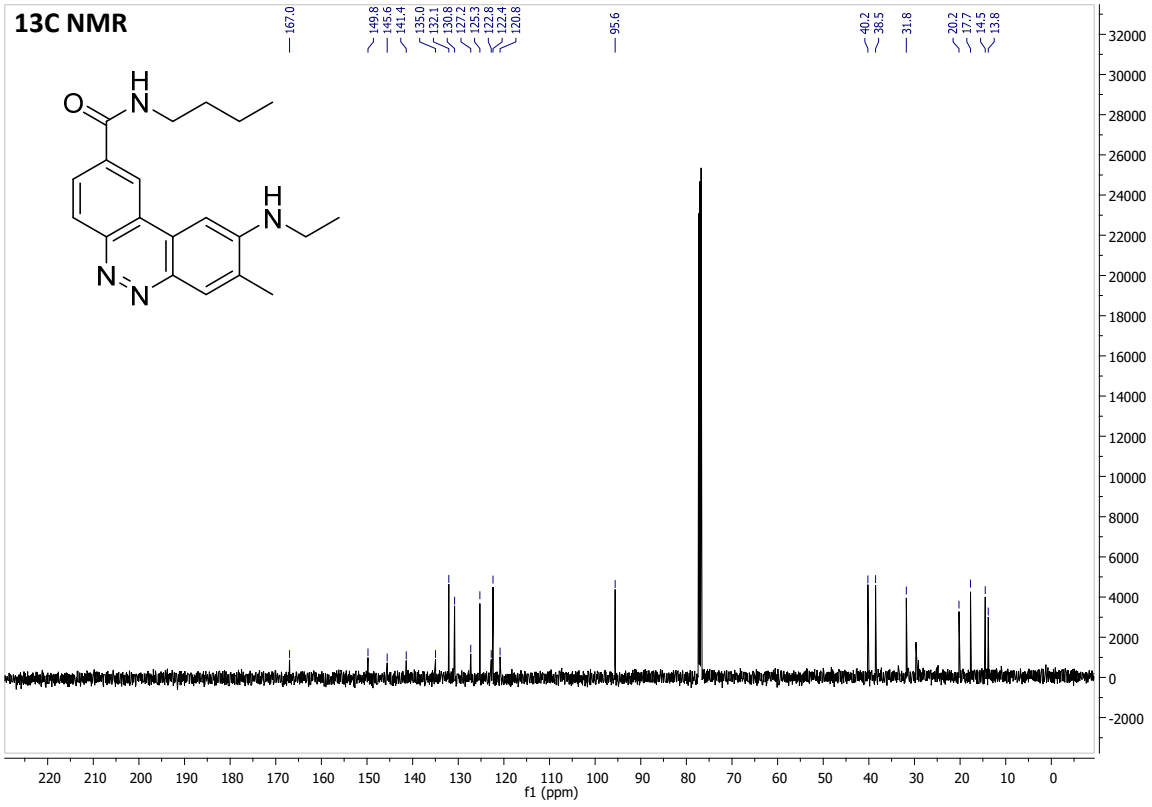
13C NMR



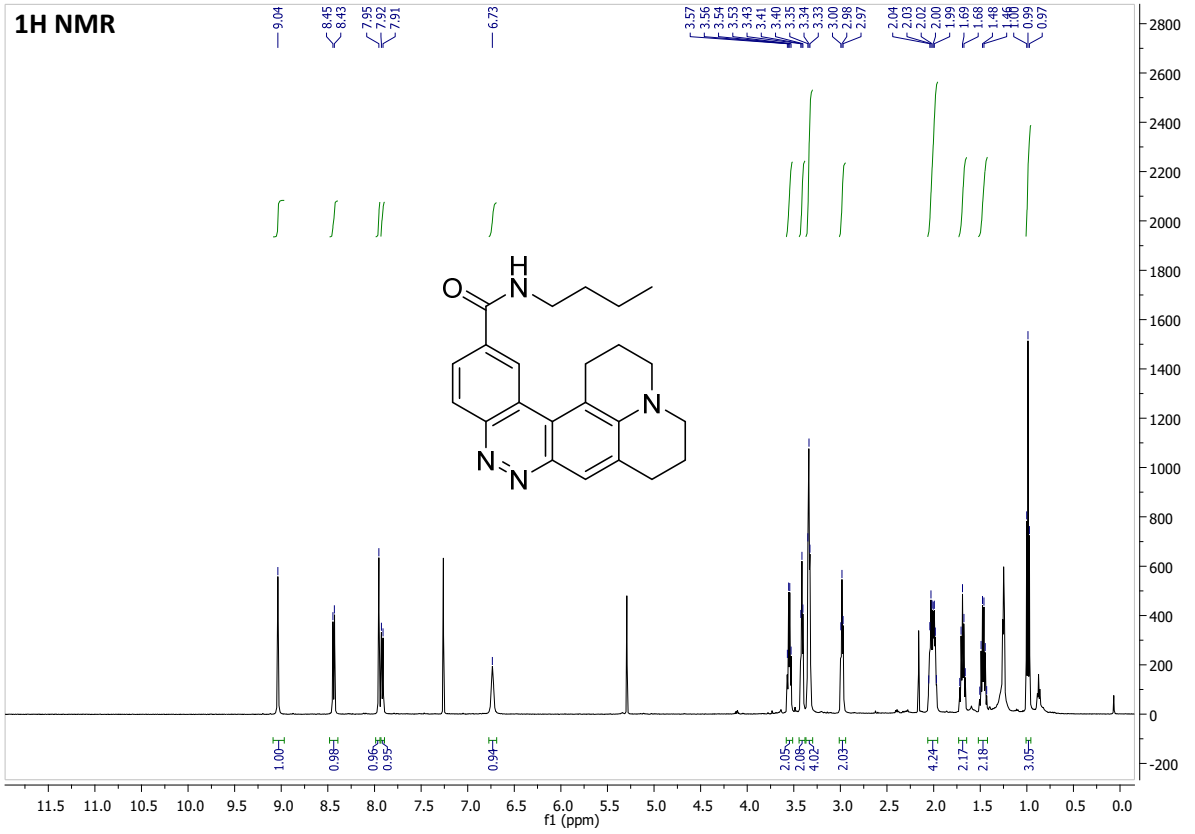
Compound 7a

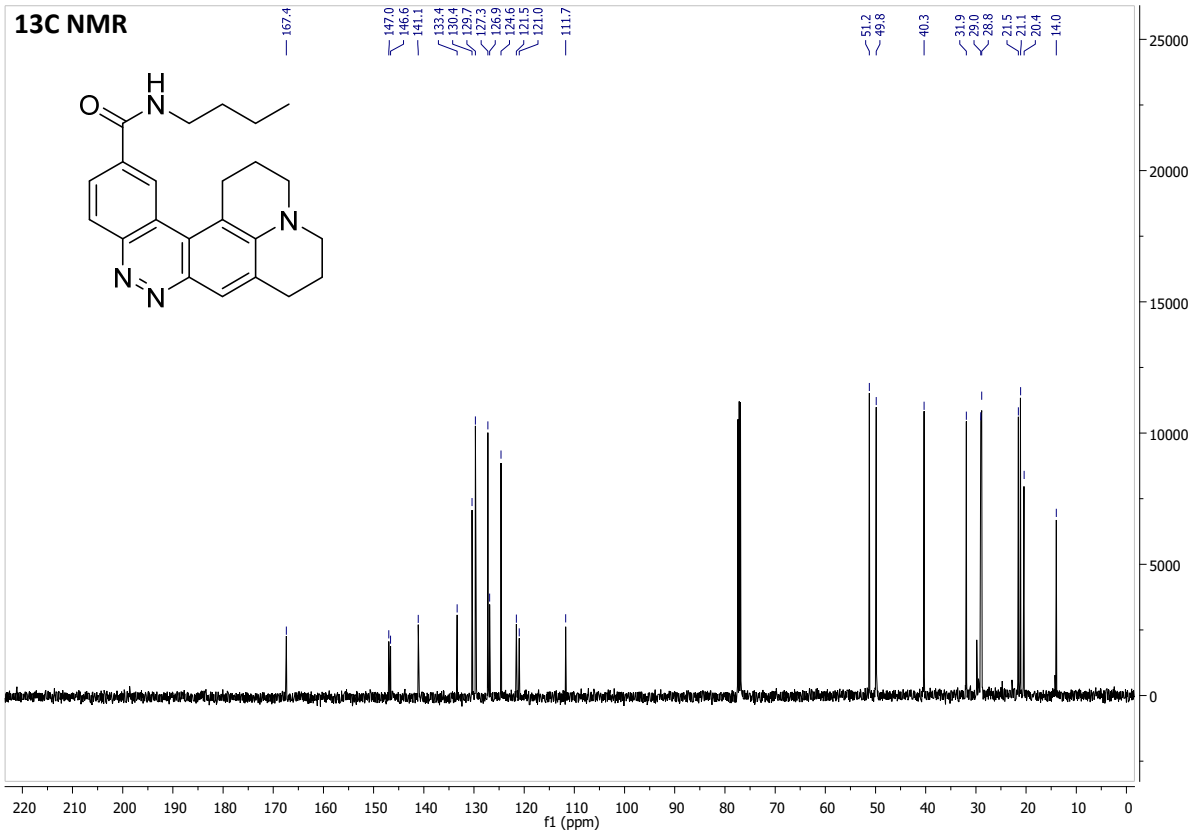
1H NMR




13C NMR
167.0
149.8
145.6
141.4
135.0
132.1
130.8
127.2
125.3
122.8
122.4
120.8
95.6
40.2
38.5
31.8
20.2
17.7
14.5
13.8
f1 (ppm)

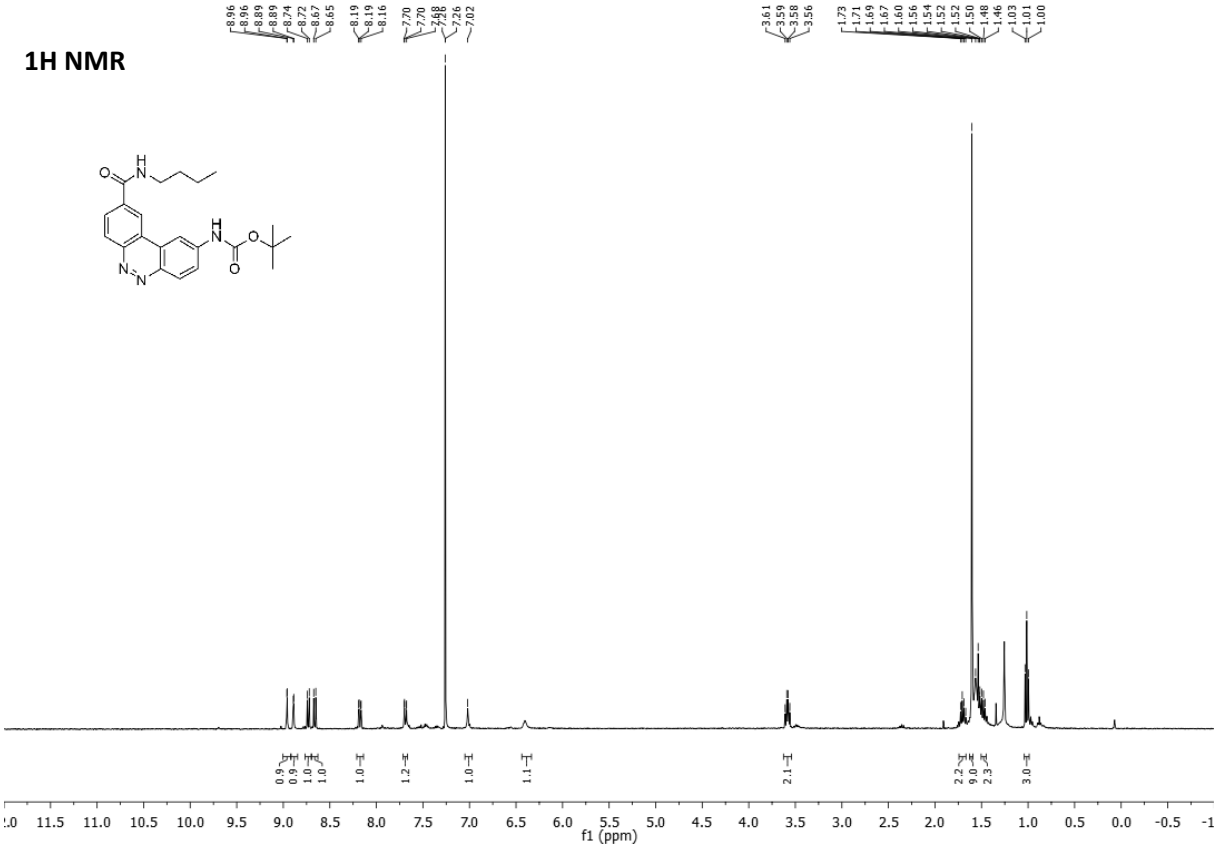
Compound 7b





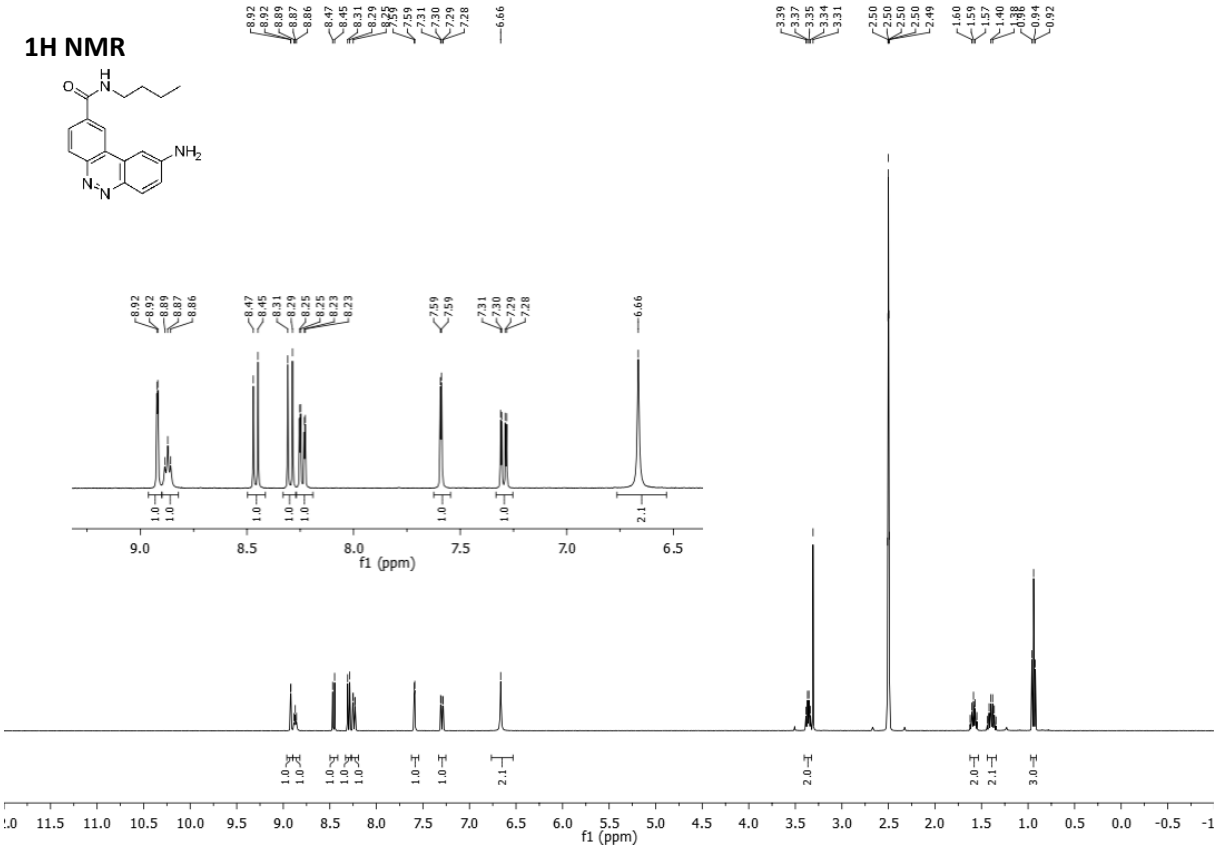
Compound 7c

1H NMR

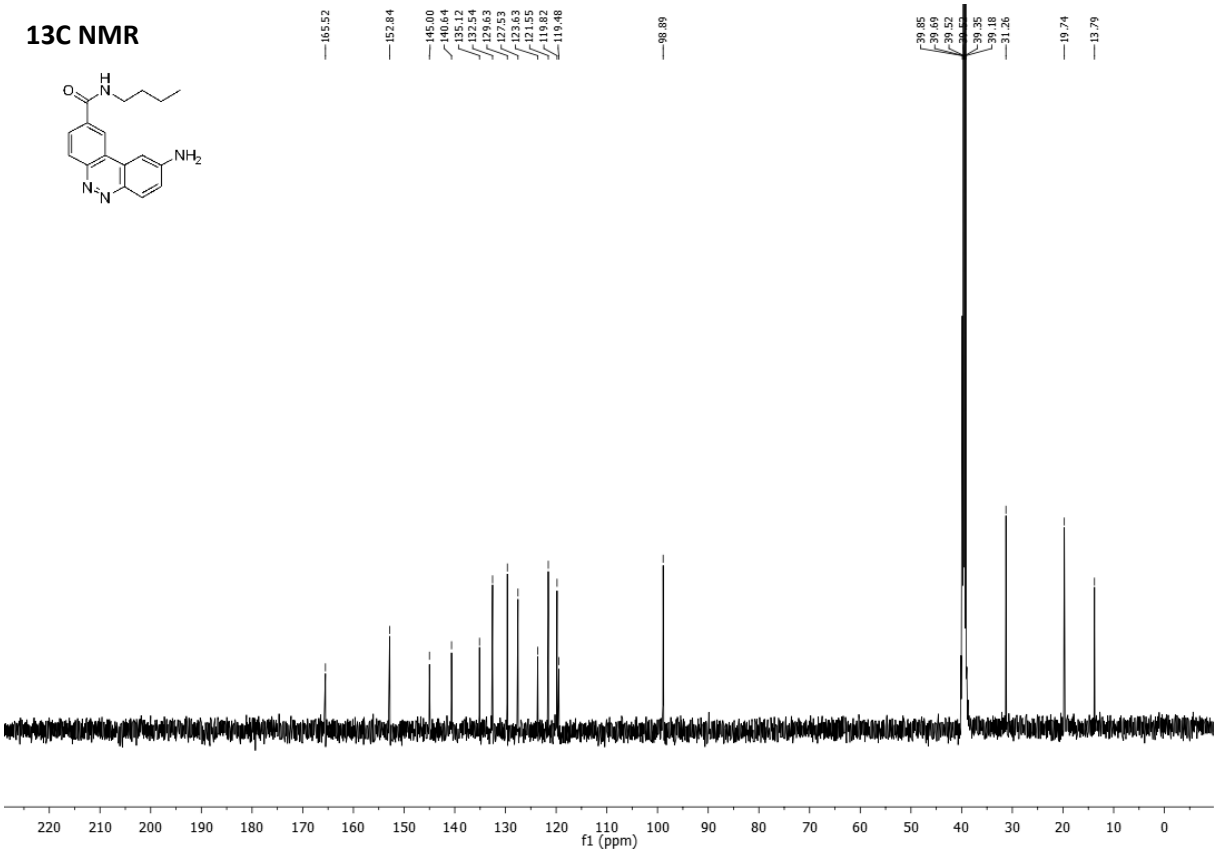


Compound 7d

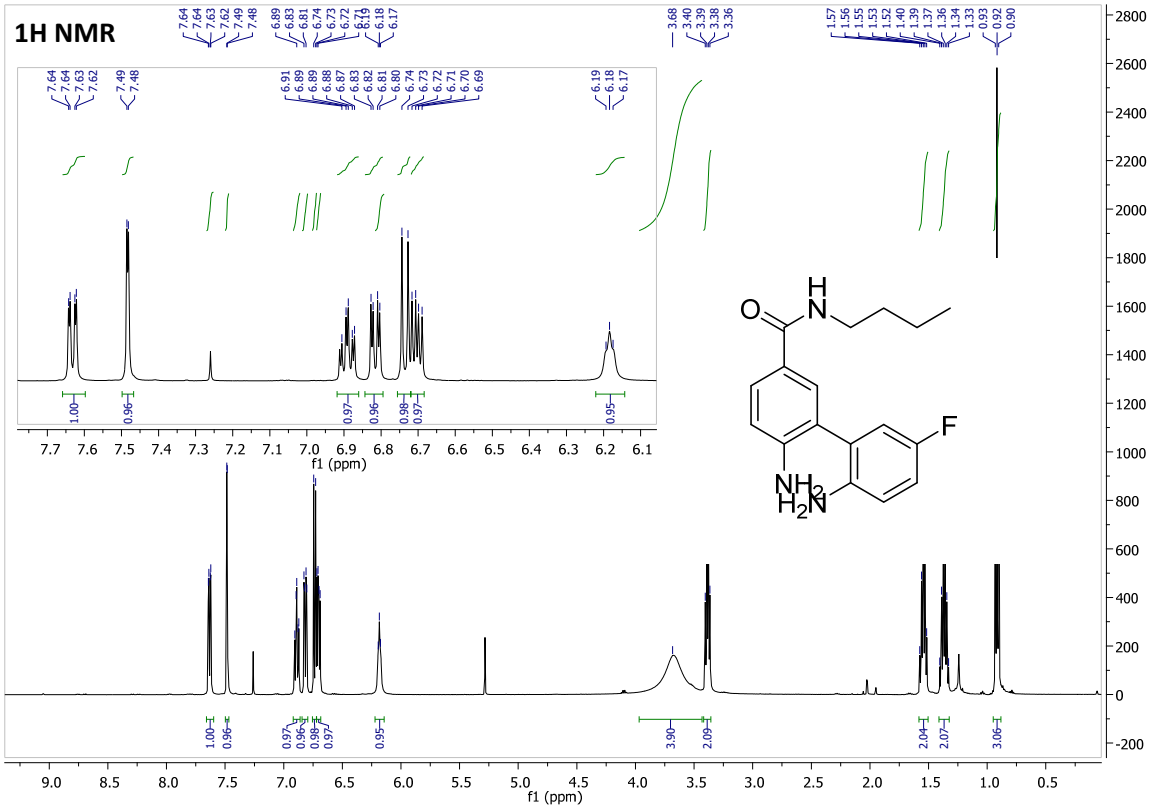
1H NMR

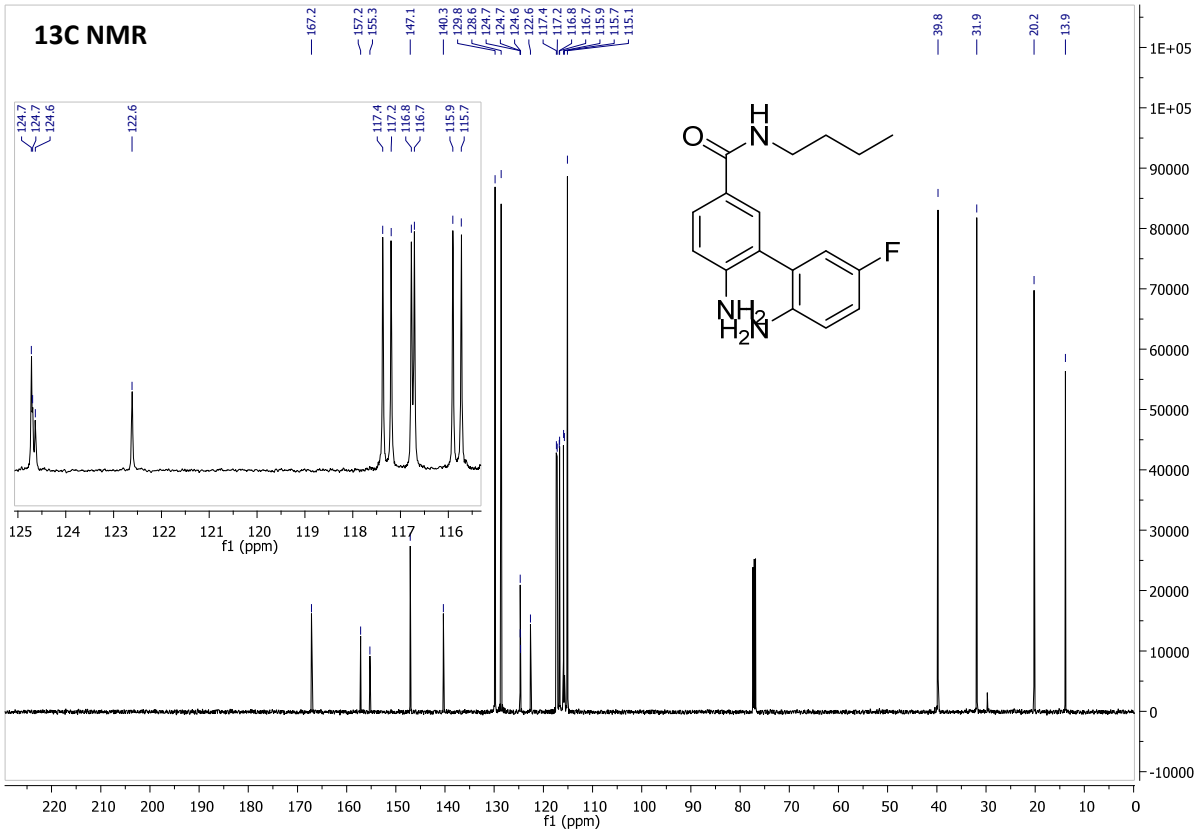


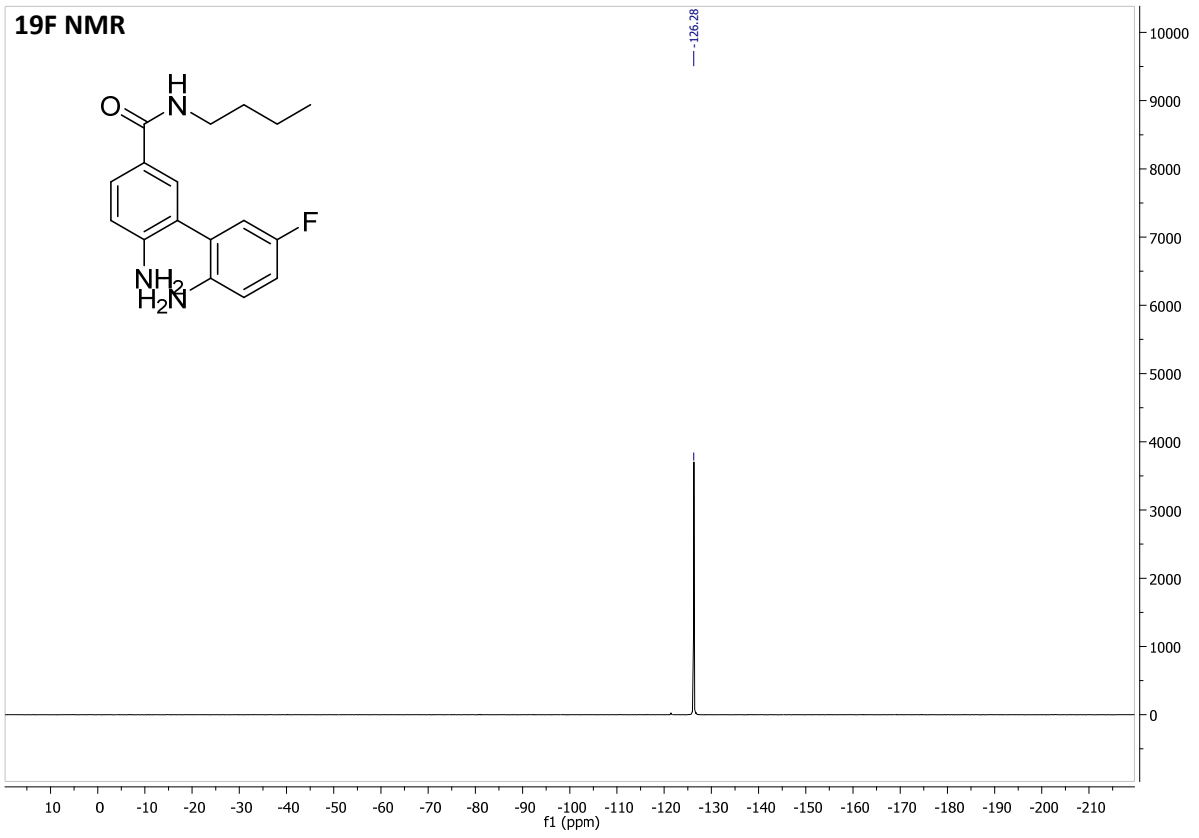
13C NMR



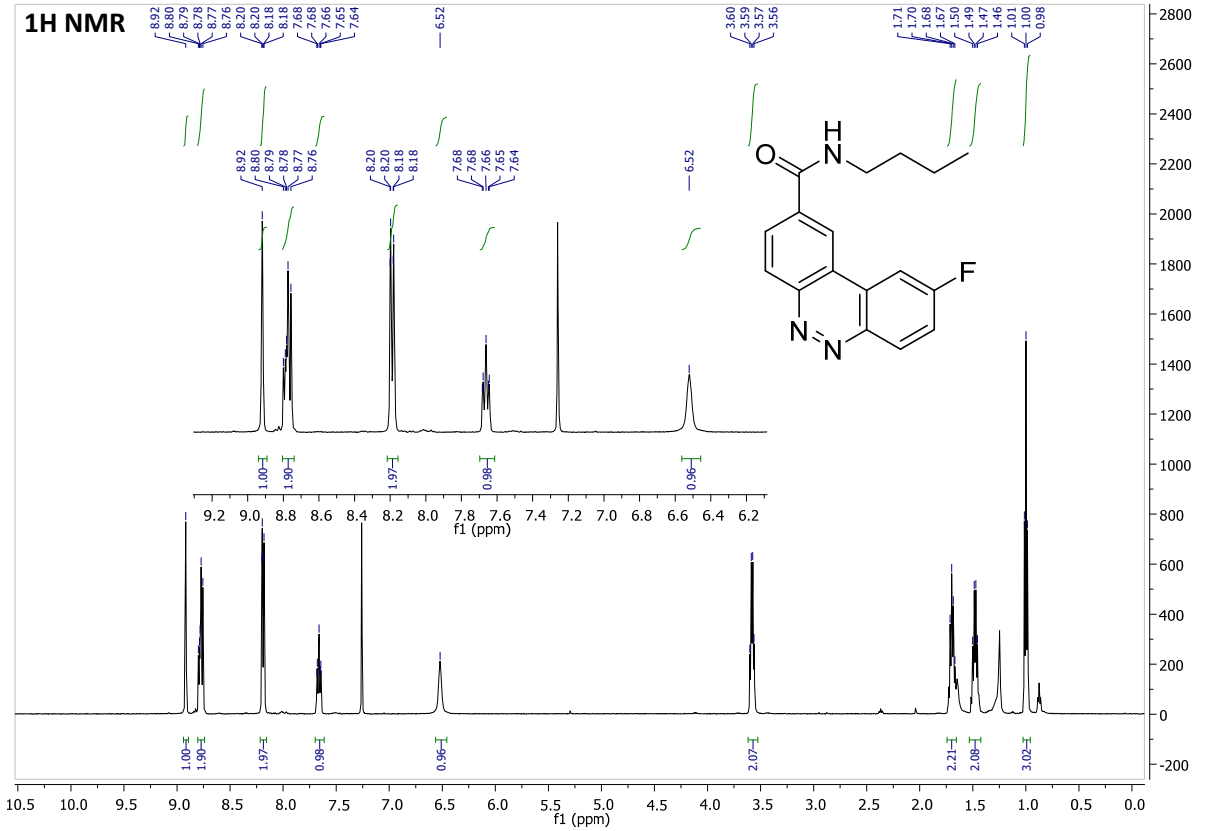
Compound 9

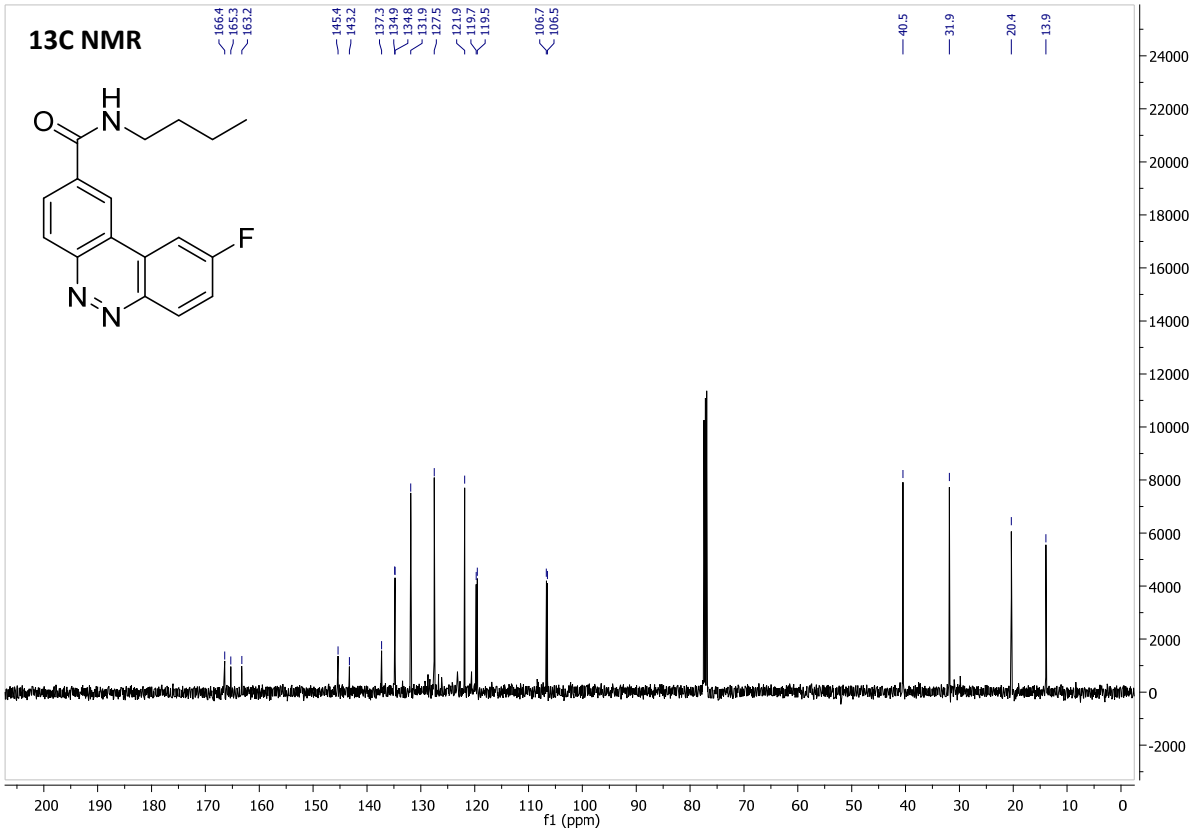


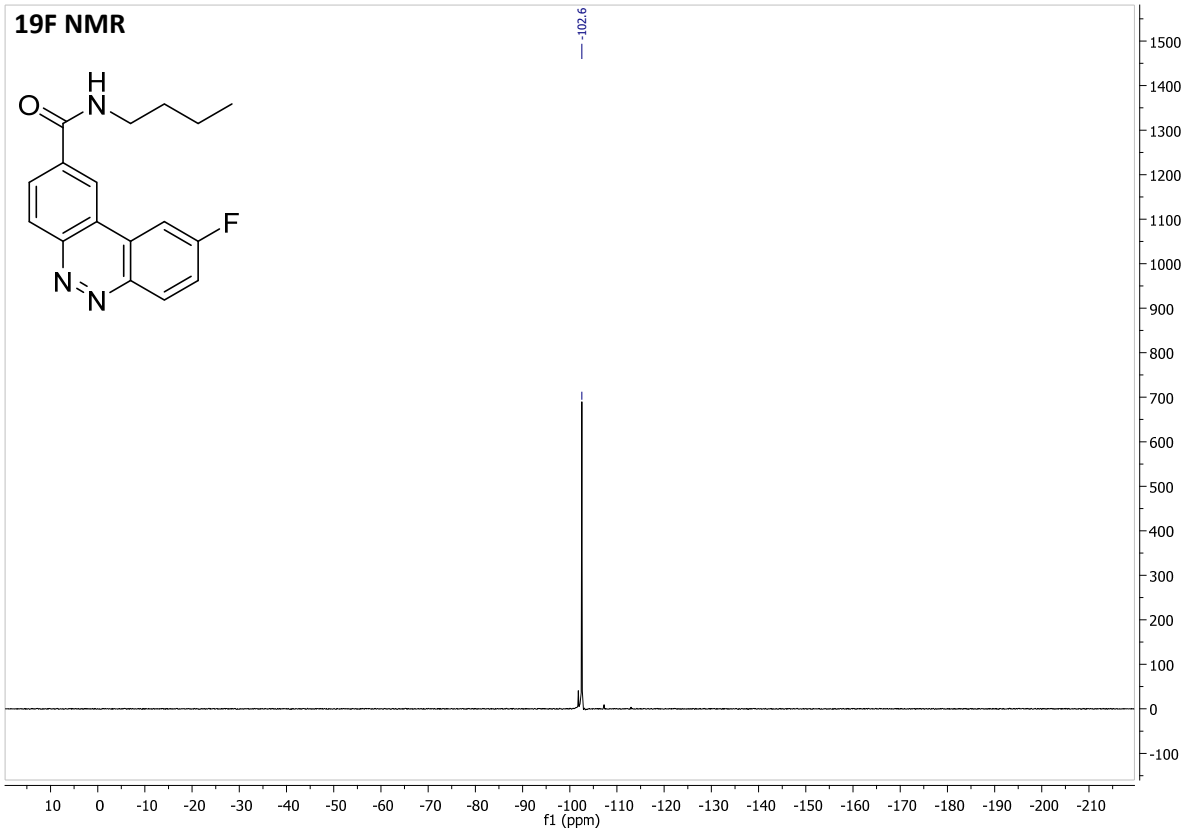

13C NMR
167.2
157.2
155.3
147.1
140.3
129.8
128.6
124.7
124.7
124.6
122.6
117.4
117.2
116.8
116.7
115.9
115.7
115.1
39.8
31.9
20.2
13.9
124.7
124.7
124.6
122.6
117.4
117.2
116.8
116.7
115.9
115.7
O
H
N
F
NH2
H2N
f1 (ppm)
f1 (ppm)


19F NMR
-126.28
O
H
N
F
NH2
H2N
f1 (ppm)

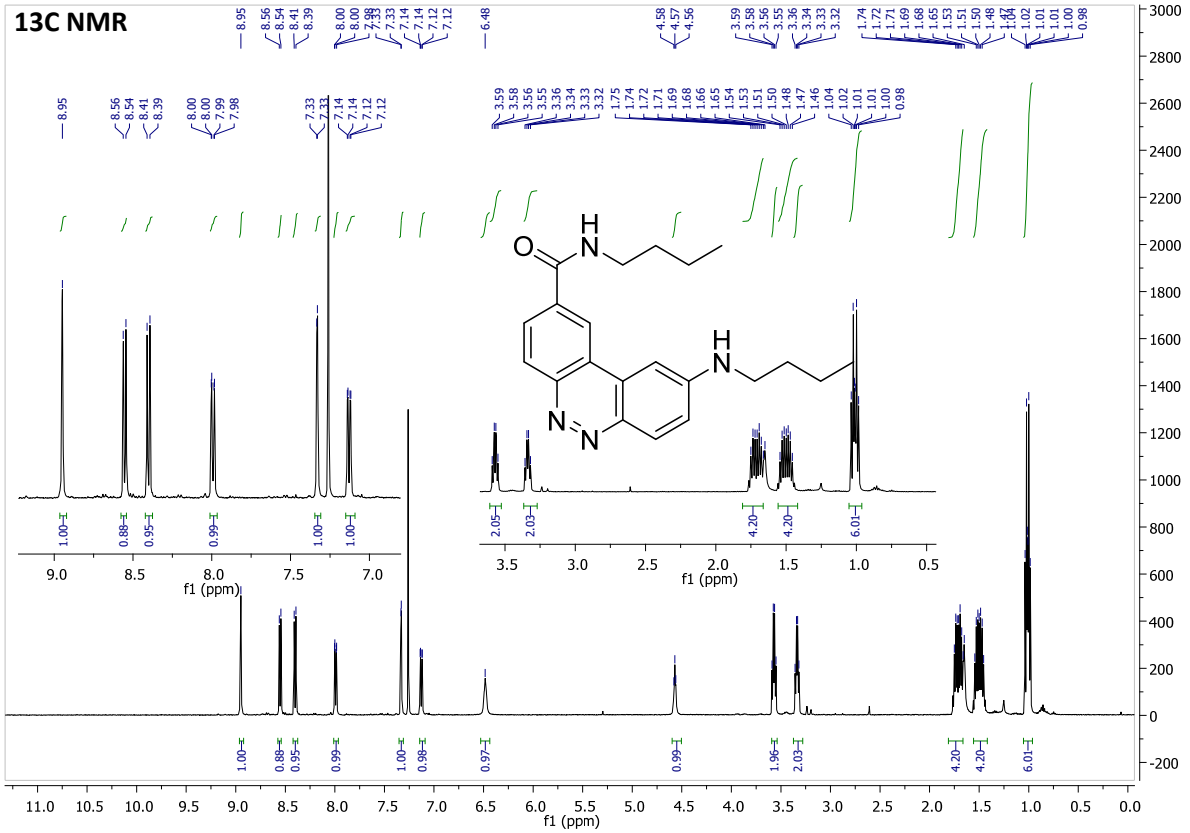
Compound 10

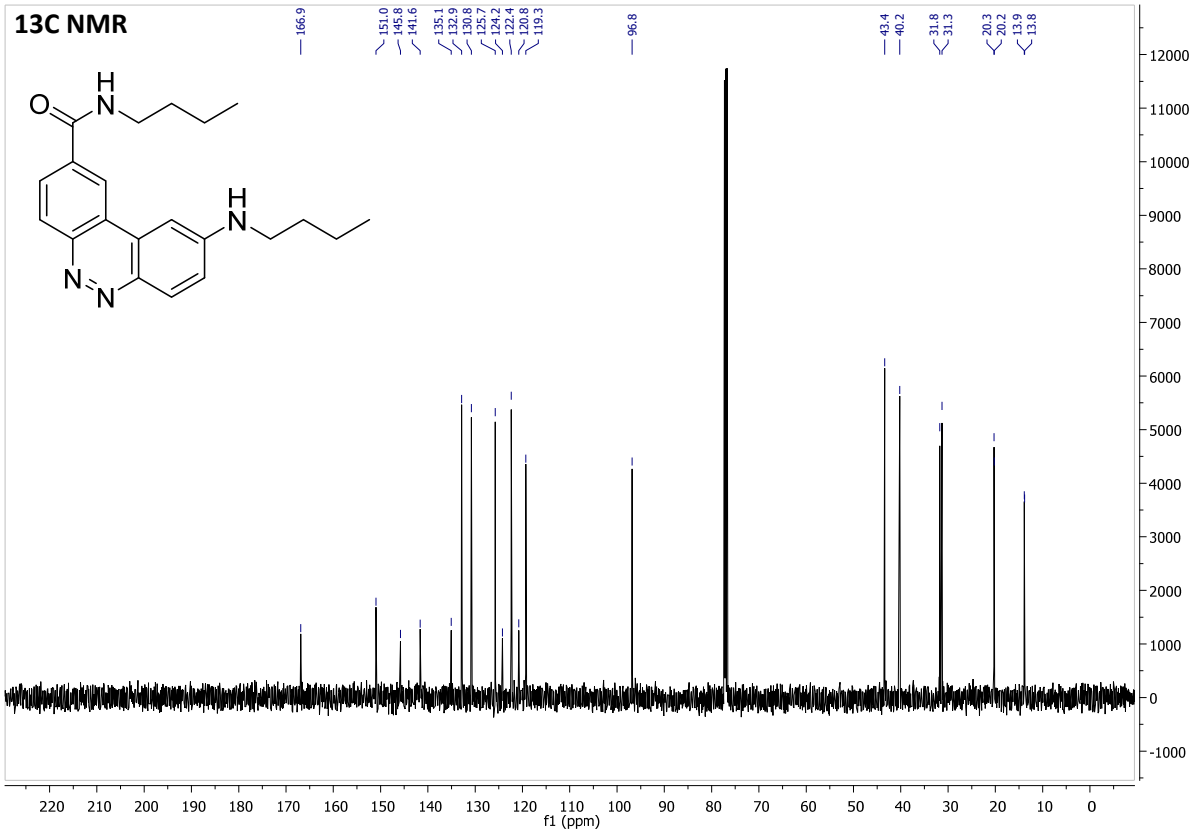




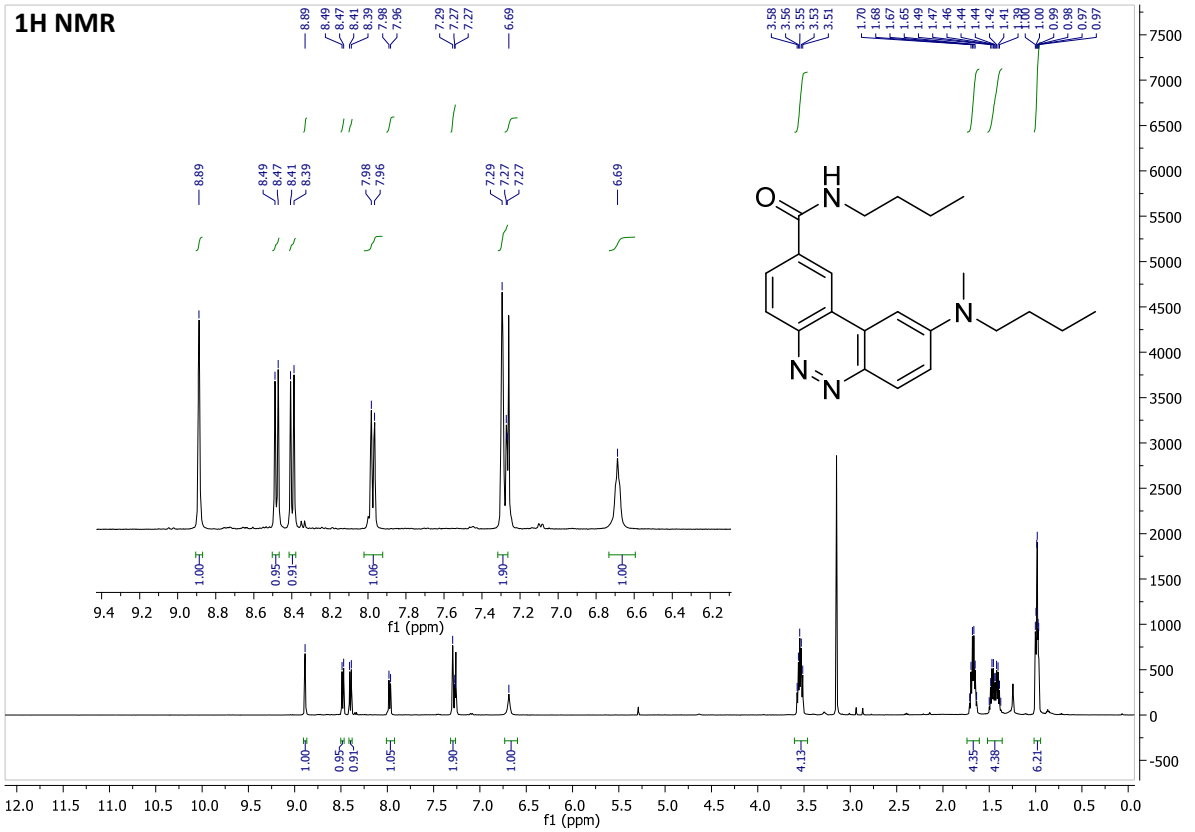


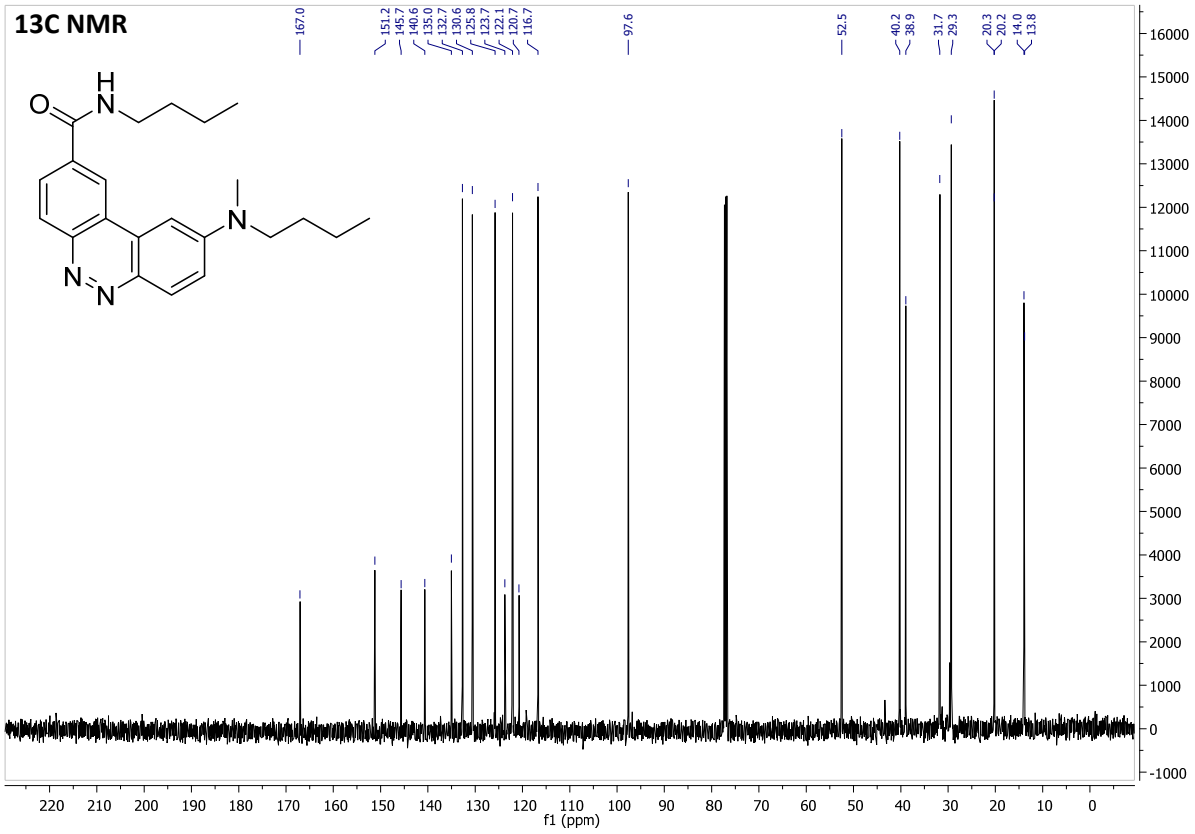
Compound 11a



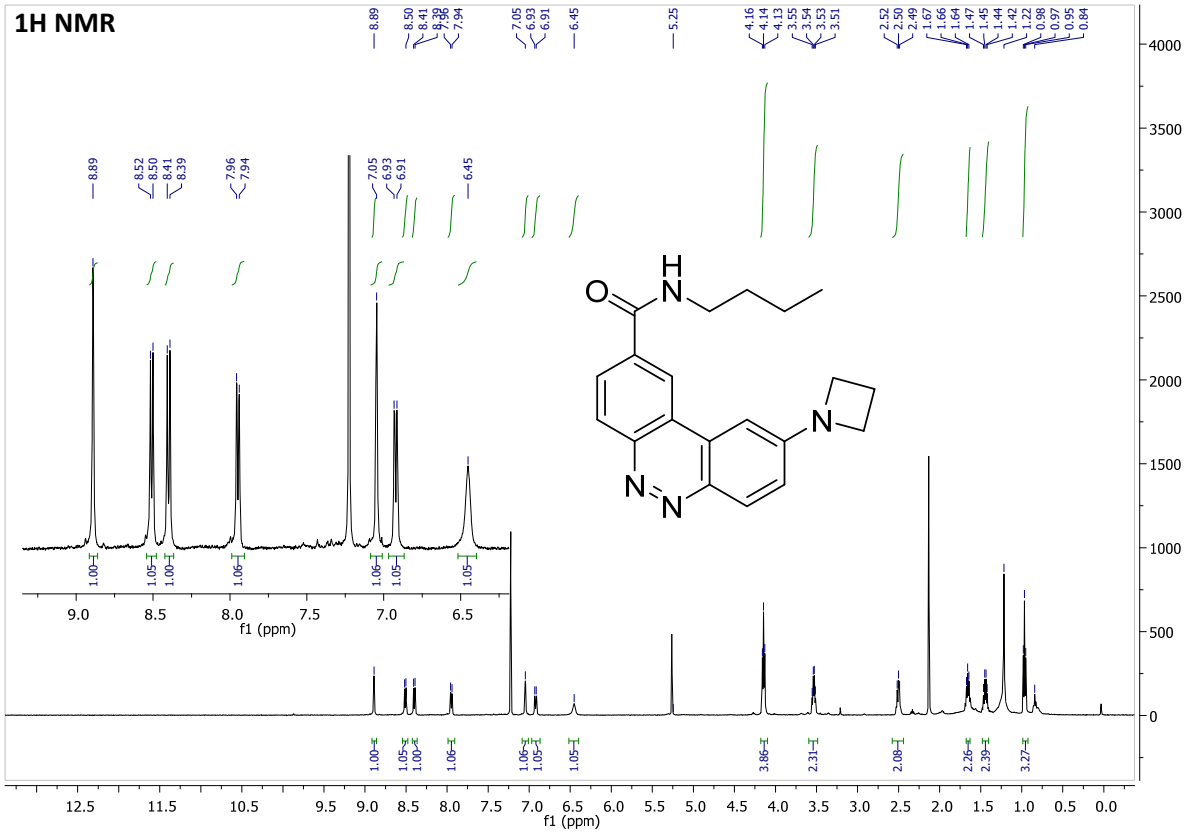


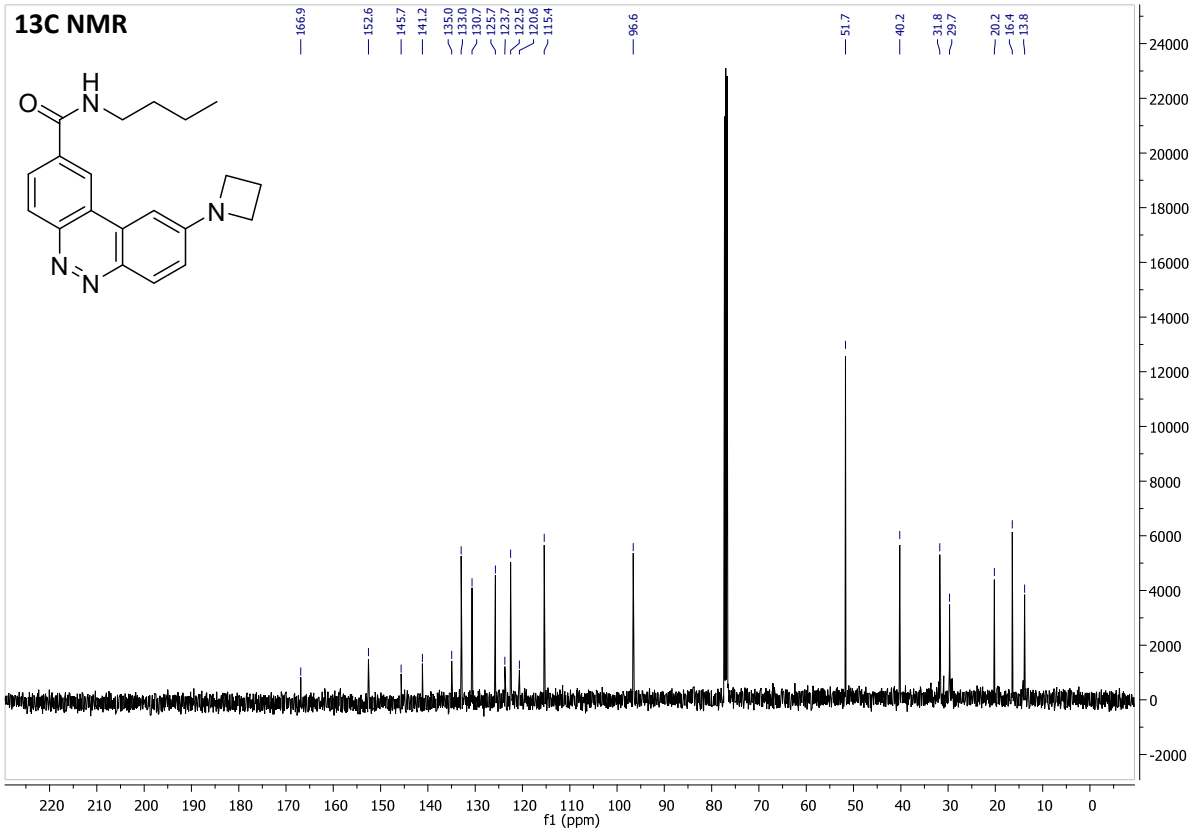
Compound 11b



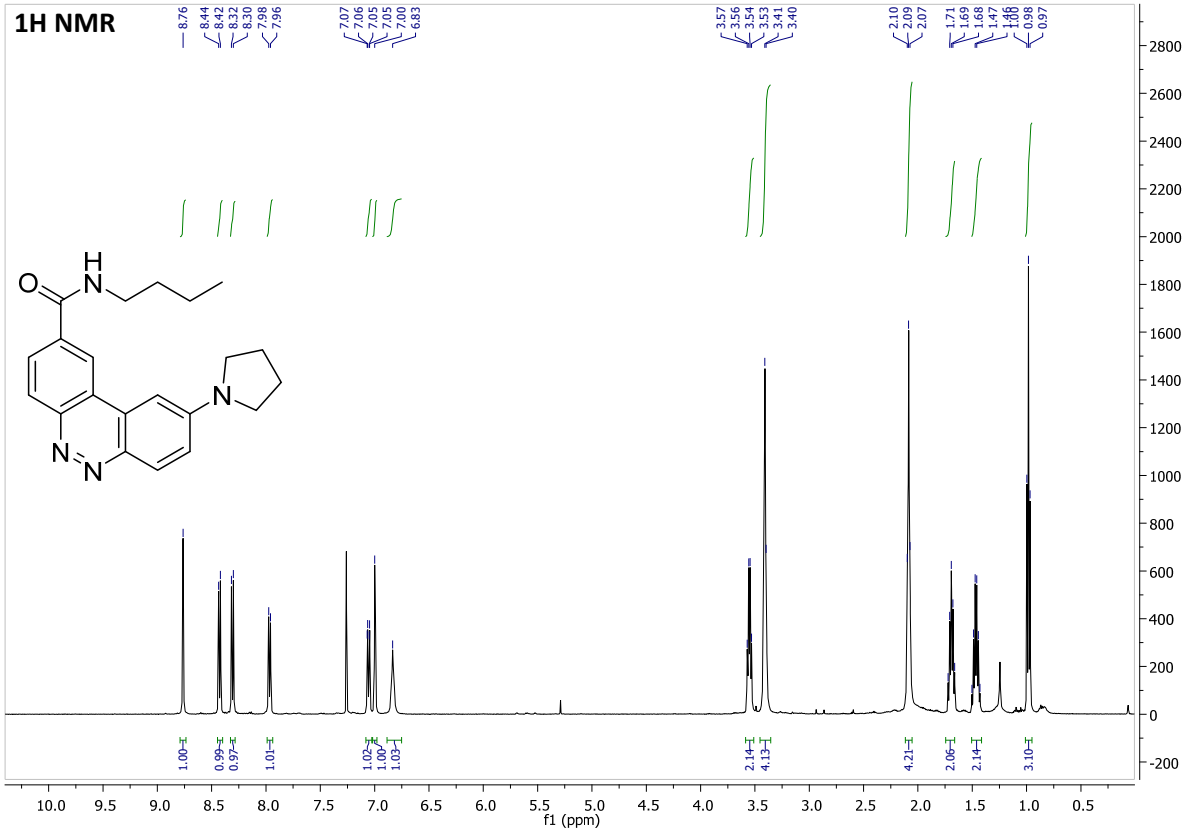


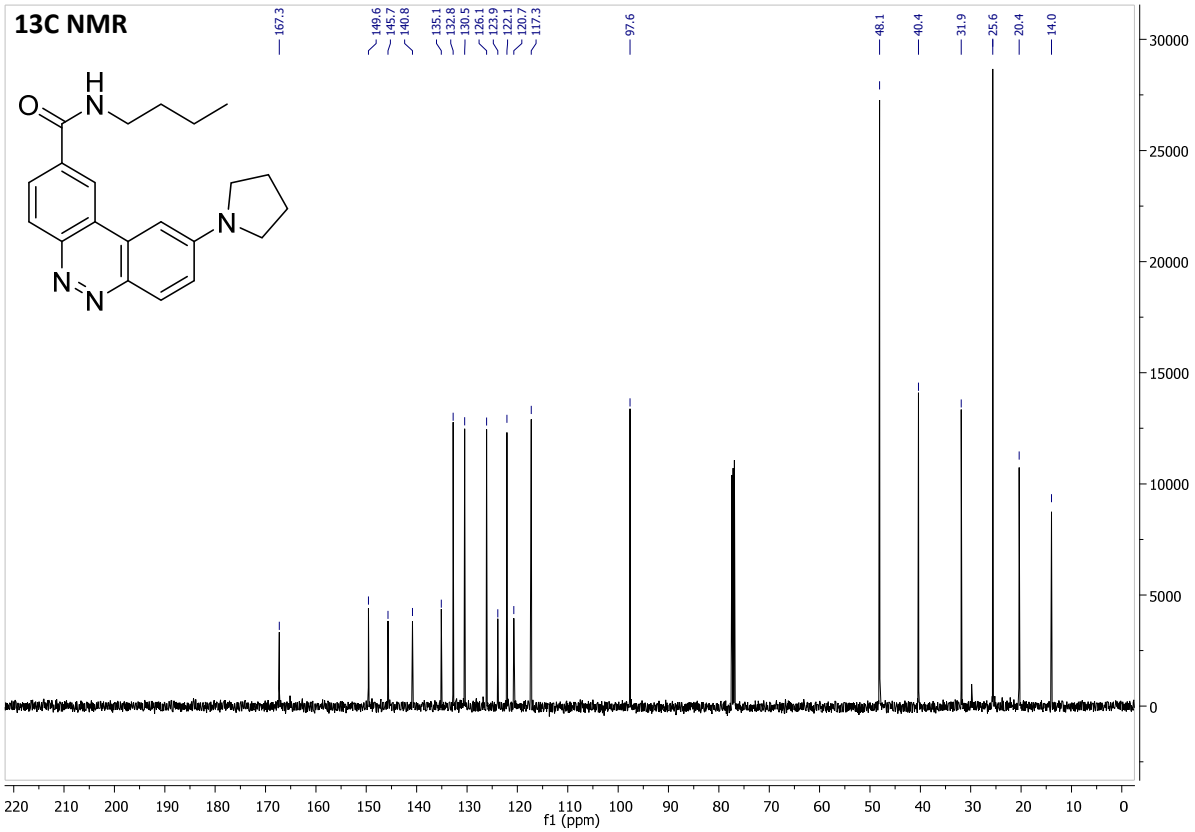
Compound 11c


1H NMR
f1 (ppm)

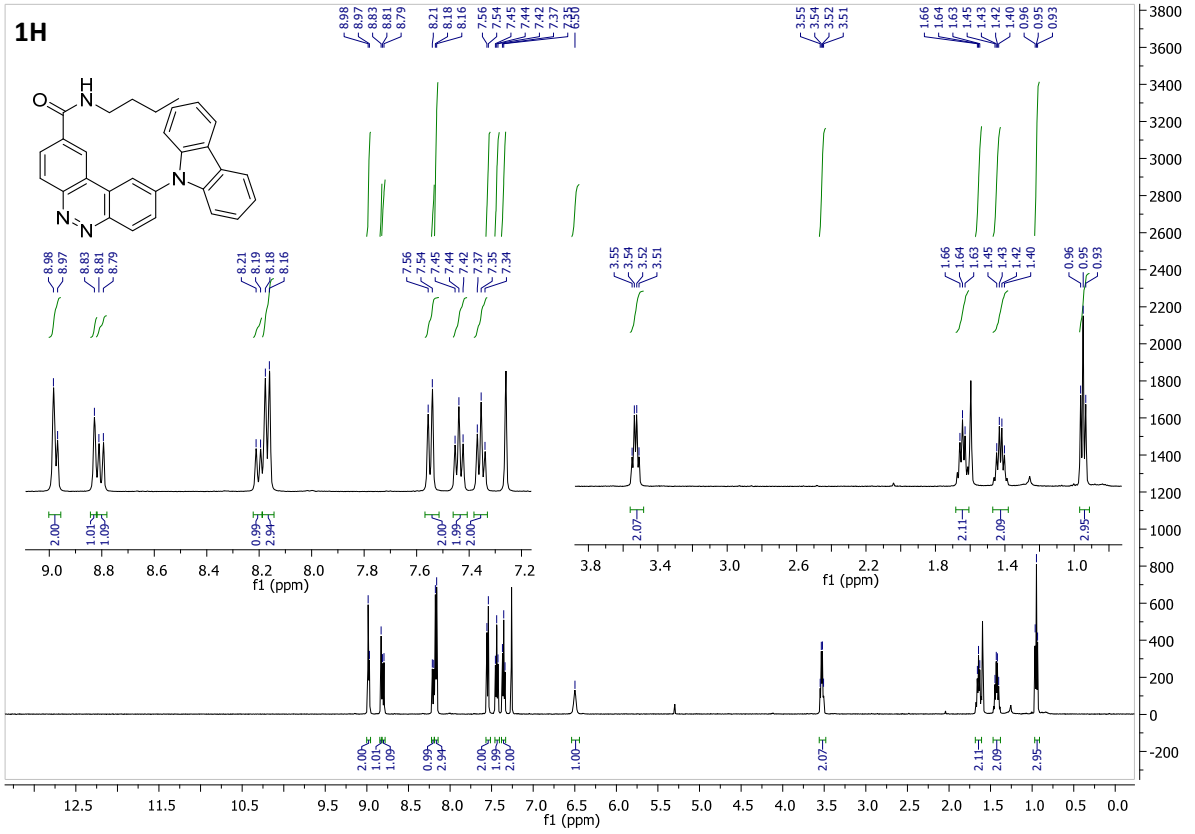

13C NMR
f1 (ppm)

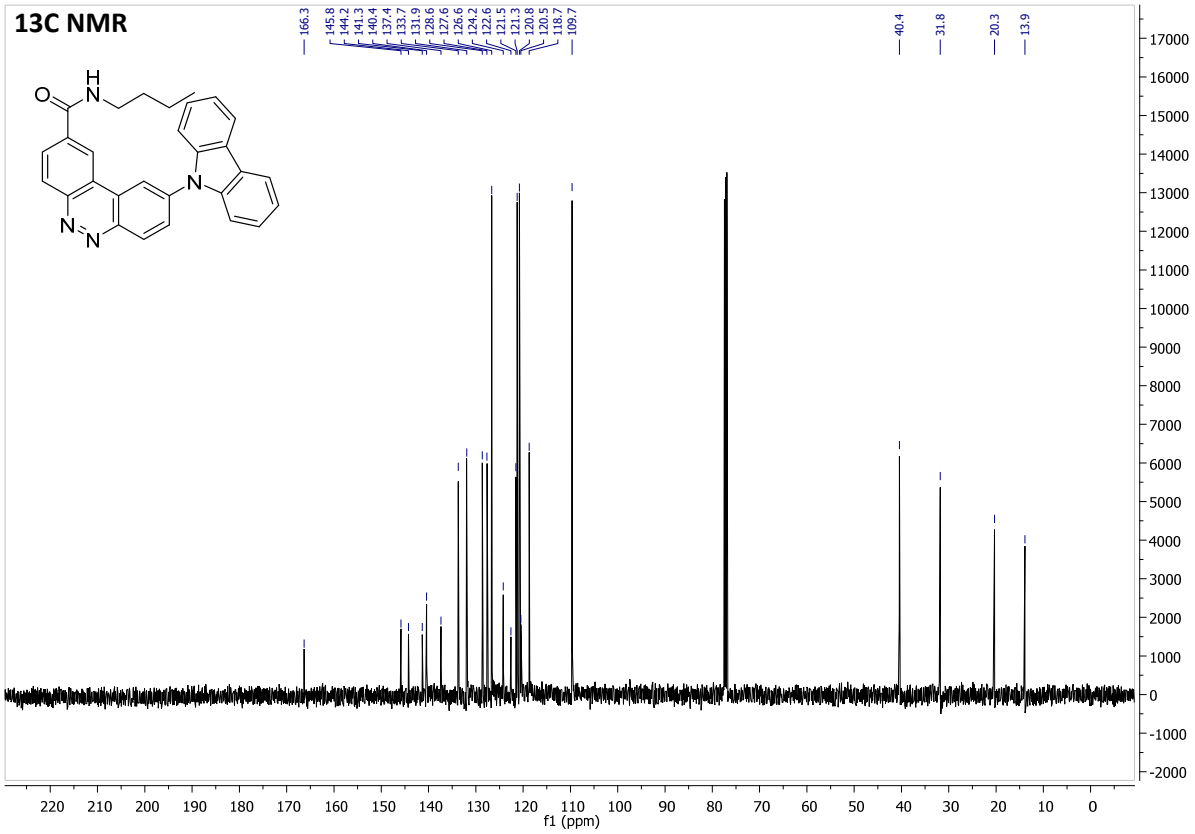
Compound 11d





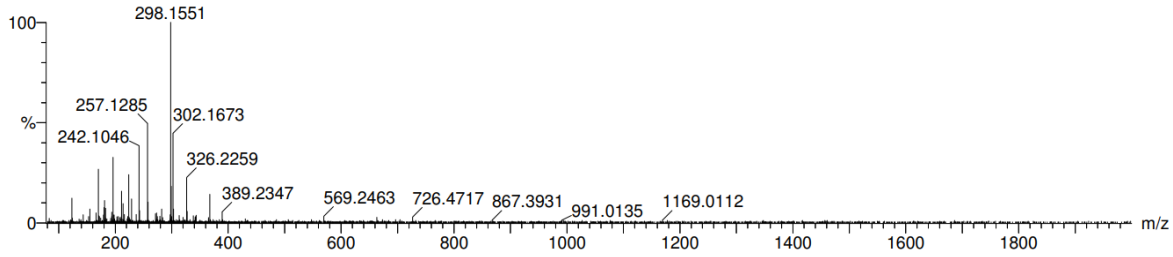
Compound 11e



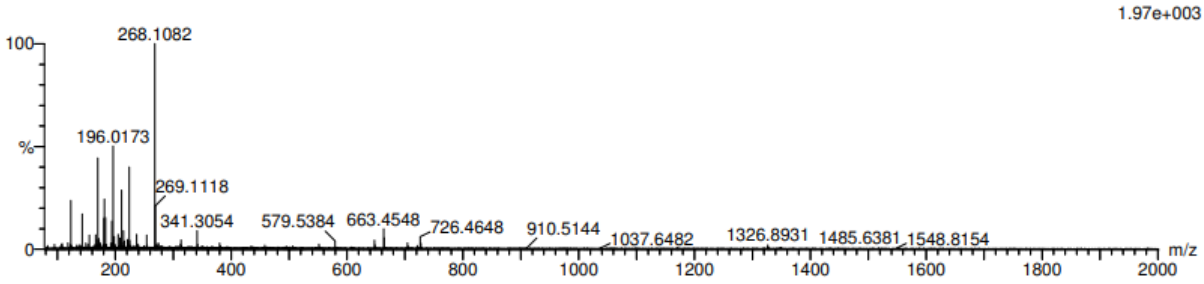


IV. HMRS Spectra

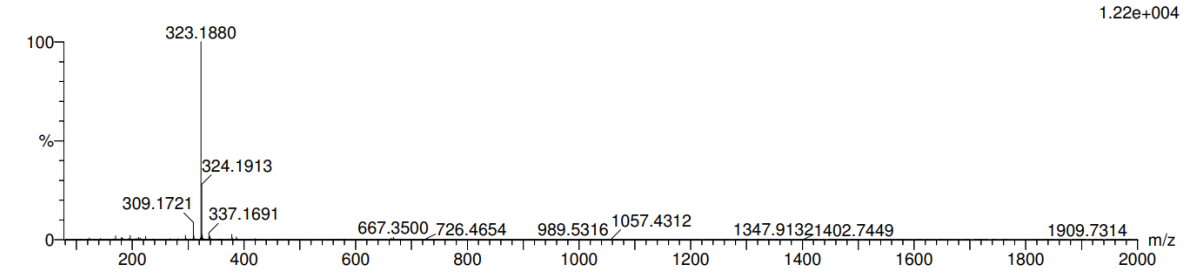
Compound 2



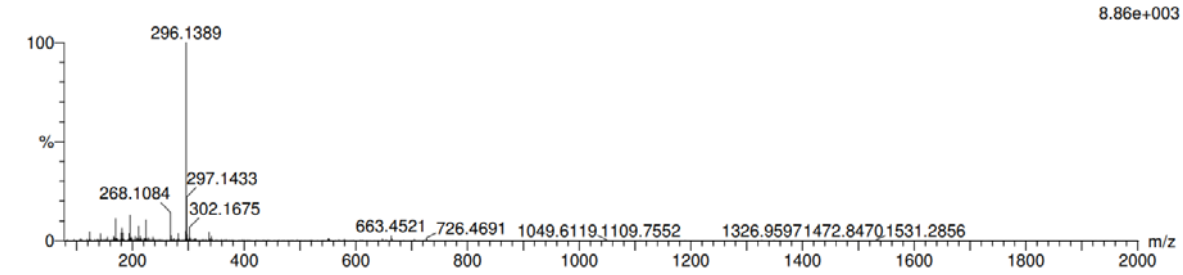
Compound 3



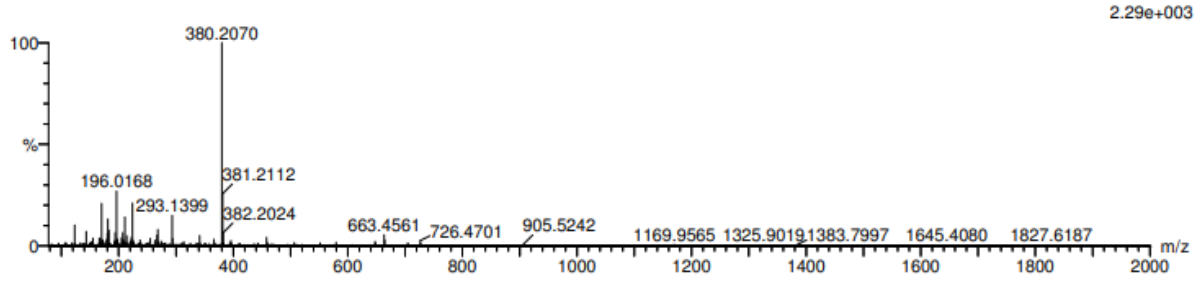
Compound 4a



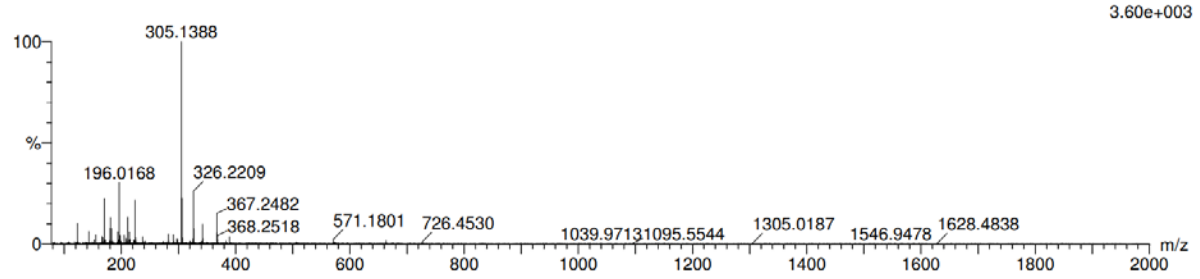
Compound 4b



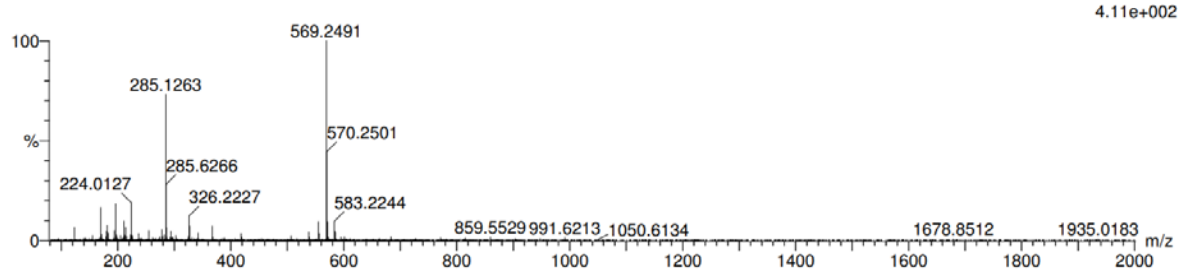
Compound 4c



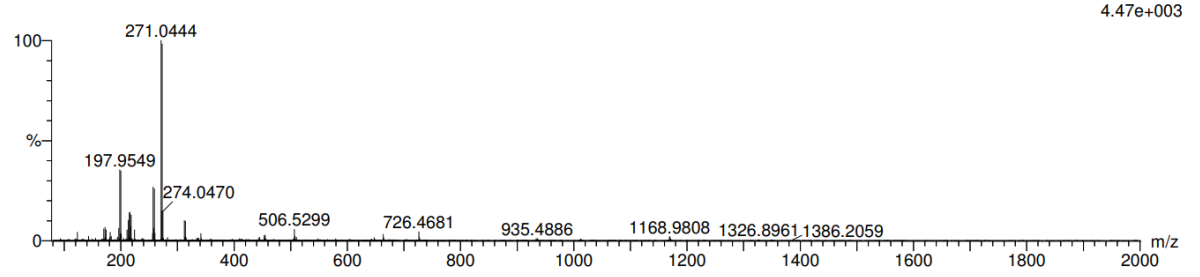
Compound 4d



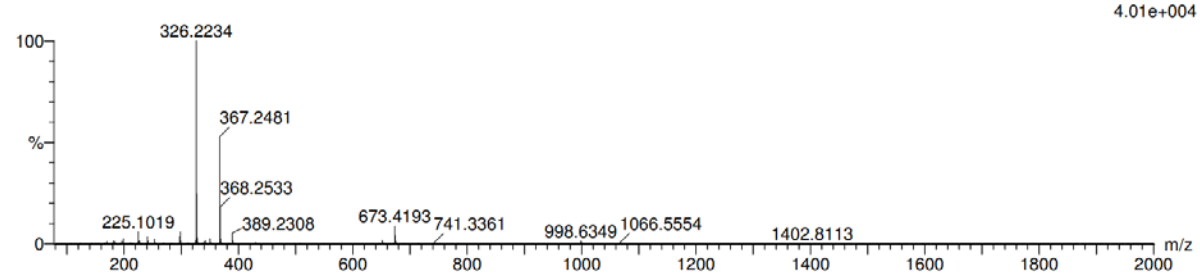
Compound 4e



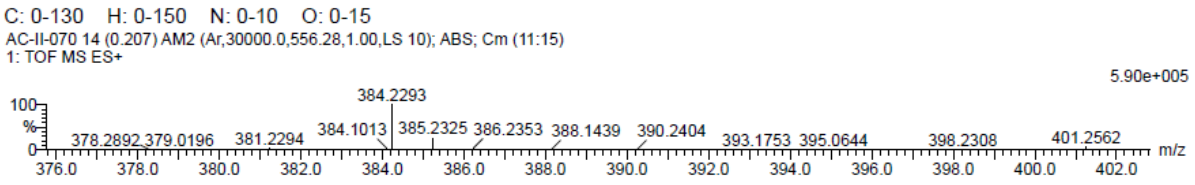
Compound 5



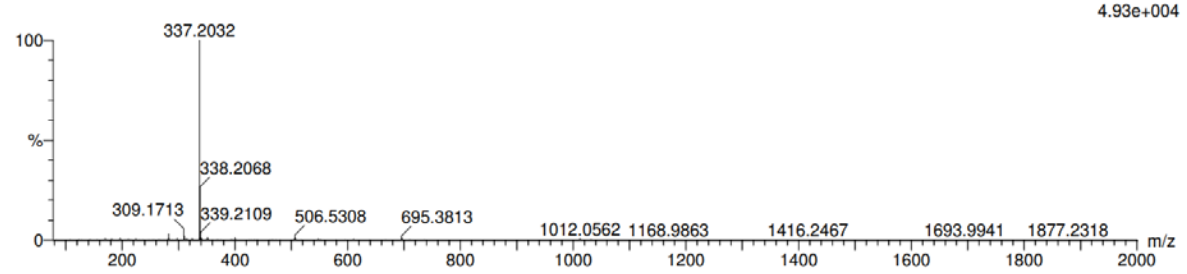
Compound 6a



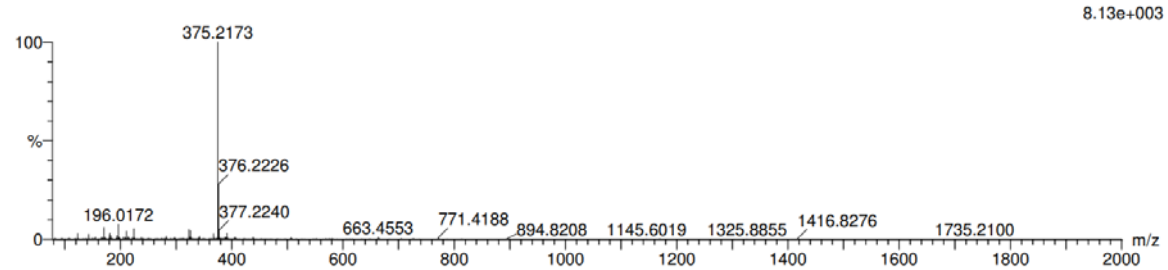
Compound 6c



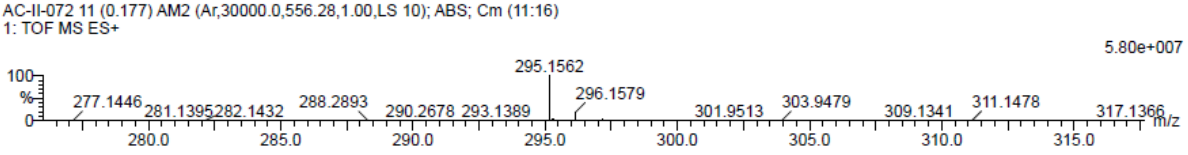
Compound 7a



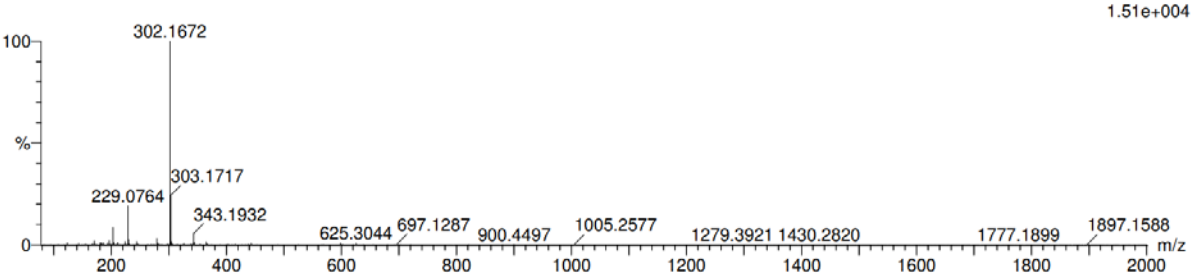
Compound 7b



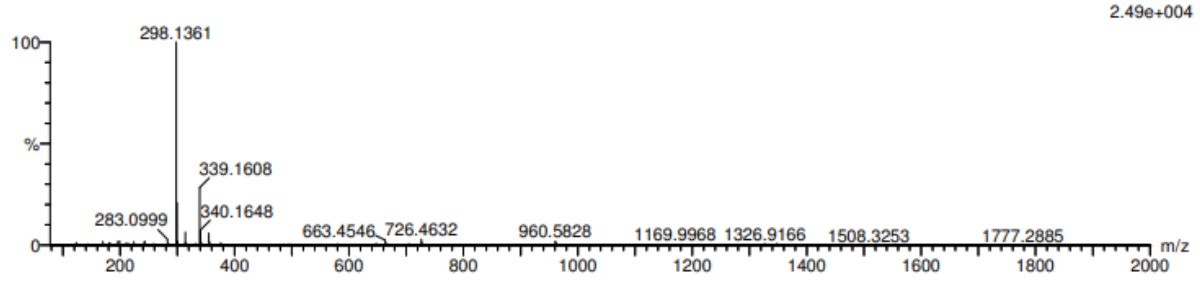
Compound 7d



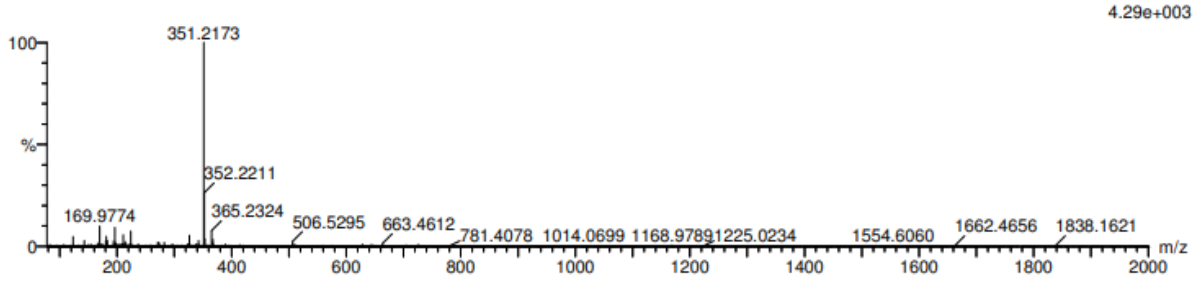
Compound 9



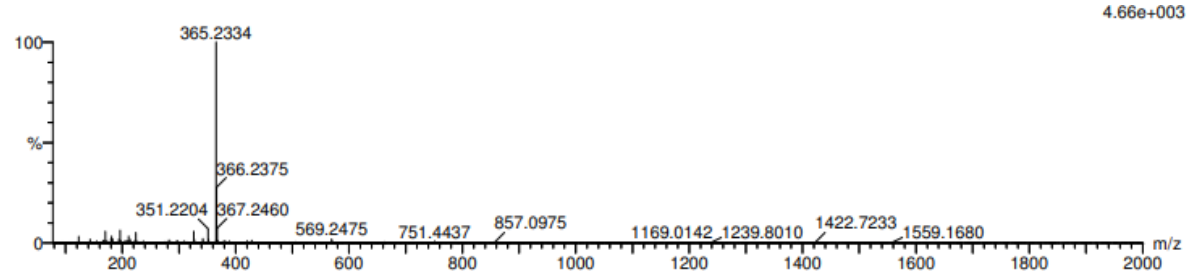
Compound 10



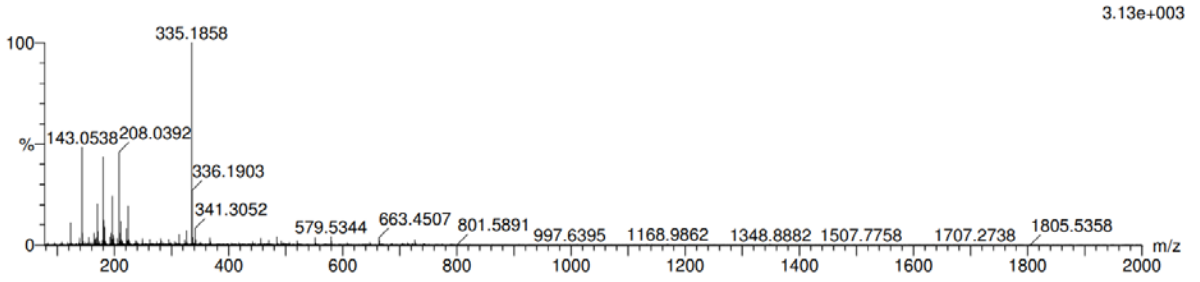
Compound 11a



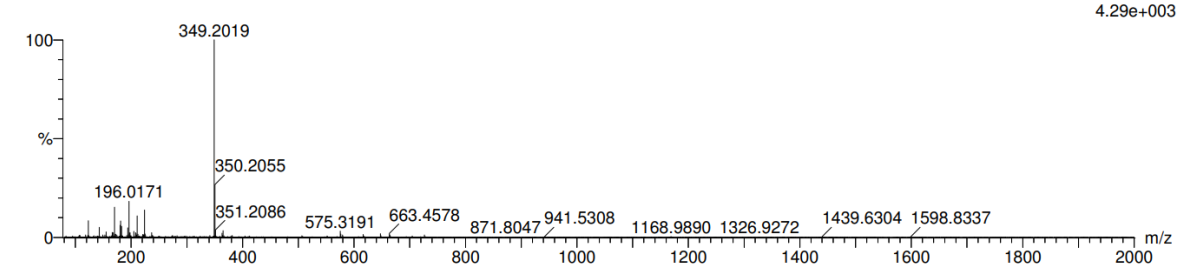
Compound 11b



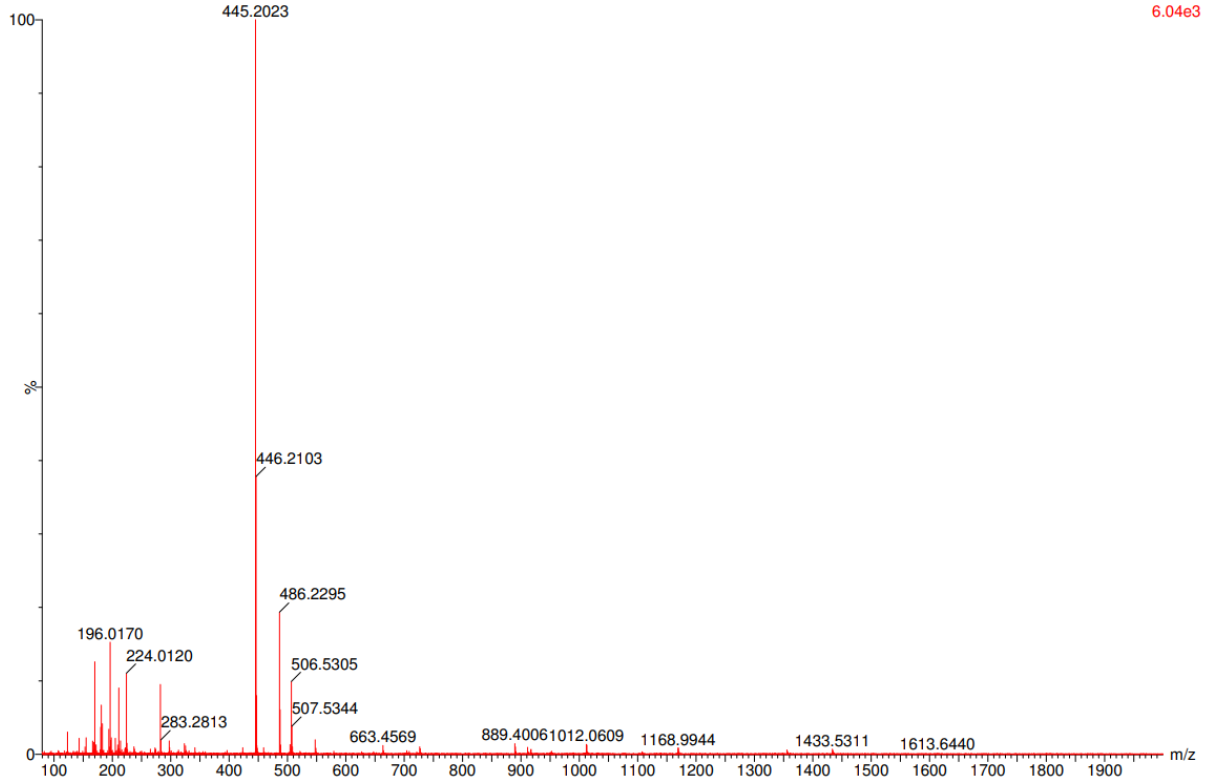
Compound 11c



Compound 11d



Compound 11e



V. TD-DFT

(TD-)DFT calculations were performed using GAUSSIAN 16 with the PBE0, the B3LYP with D3BJ correction and the CAM-B3LYP functional at the 6-31+G(d,p)/PCM level of theory (Figure 3). Solvent effects were included using the PCM solvation model and frequency calculation was performed on all optimized geometries to ensure the absence of imaginaries frequencies. Data were analyzed with Avogadro, GaussSum and MULTIFWN softwares. TD-DFT calculations based on the ground state geometry were performed with 100 excited states and TD DFT calculations based on the S1 excited state geometry were performed with 5 excited states

Optimized geometry at the ground state, PBE0/6-31+G(d,p)

Optimized geometry of 4a in $CHCl_3$

C	-1.9618790000	1.7835010000	-0.9936580000
C	-1.0637780000	2.6940760000	-0.4852430000
C	0.2418760000	2.2898040000	-0.1375140000
C	0.6429230000	0.9472340000	-0.3336410000
C	-0.2846040000	0.0388260000	-0.8759810000
C	-1.5727700000	0.4386010000	-1.1860810000
N	1.0703270000	3.2650840000	0.3835370000
N	2.2727720000	2.9677240000	0.7170870000

C	2.7555950000	1.6954590000	0.5635620000
C	1.9960020000	0.6186440000	0.0396050000
C	4.0926380000	1.4617890000	0.9555350000
C	4.6564640000	0.2195770000	0.8350370000
C	3.9064900000	-0.8795890000	0.3077060000
C	2.5748870000	-0.6482300000	-0.0811980000
C	-2.4883770000	-0.5704750000	-1.8117980000
O	-2.0725840000	-1.3130160000	-2.7064550000
N	-3.7729900000	-0.6260920000	-1.3911060000
C	-4.3781490000	-0.0662870000	-0.1926390000
C	-5.1554920000	-1.1243850000	0.5820040000
C	-5.8332670000	-0.5537230000	1.8238410000
C	-6.6207880000	-1.6032220000	2.5991360000
N	4.4775490000	-2.1106610000	0.1903720000
C	3.7114420000	-3.2123150000	-0.3531820000
C	5.8508000000	-2.3309390000	0.5986250000
H	-2.9624020000	2.1033510000	-1.2690030000
H	-1.3313350000	3.7364460000	-0.3412680000
H	-0.0045360000	-0.9921420000	-1.0656950000
H	4.6626560000	2.2957600000	1.3545360000
H	5.6847620000	0.0758760000	1.1437770000
H	1.9850840000	-1.4614830000	-0.4833880000
H	-4.3287300000	-1.2974320000	-1.9070830000
H	-3.5866660000	0.3459120000	0.4380880000
H	-5.0471280000	0.7630620000	-0.4607930000
H	-5.9163410000	-1.5705020000	-0.0742890000
H	-4.4713720000	-1.9343720000	0.8670010000
H	-5.0732220000	-0.1066210000	2.4783830000
H	-6.5036060000	0.2644010000	1.5280370000
H	-7.0971810000	-1.1699770000	3.4842350000
H	-7.4087970000	-2.0442660000	1.9782180000

H	-5.9689910000	-2.4172200000	2.9358910000
H	2.8279970000	-3.4311640000	0.2606480000
H	3.3767160000	-3.0039950000	-1.3775340000
H	4.3352140000	-4.1050890000	-0.3771840000
H	6.5515480000	-1.7154170000	0.0207310000
H	5.9970680000	-2.1170450000	1.6646180000
H	6.1062320000	-3.3764330000	0.4297770000

Optimized geometry of 4a in toluene

C	-1.9594960000	1.7520700000	-1.0119950000
C	-1.0638400000	2.6737000000	-0.5192850000
C	0.2425490000	2.2789280000	-0.1645720000
C	0.6475240000	0.9350190000	-0.3402500000
C	-0.2779050000	0.0147340000	-0.8651630000
C	-1.5680250000	0.4045210000	-1.1796740000
N	1.0670480000	3.2658640000	0.3418590000
N	2.2693220000	2.9791030000	0.6795650000
C	2.7570790000	1.7052010000	0.5429130000
C	2.0026210000	0.6185650000	0.0350060000
C	4.0948340000	1.4836770000	0.9364560000
C	4.6650750000	0.2424670000	0.8312220000
C	3.9205630000	-0.8660530000	0.3186570000
C	2.5882370000	-0.6473470000	-0.0705110000
C	-2.4793630000	-0.6227790000	-1.7814520000
O	-2.0555910000	-1.4072330000	-2.6319850000
N	-3.7771040000	-0.6470430000	-1.3869150000
C	-4.3946300000	-0.0623300000	-0.2076430000
C	-5.1821380000	-1.1022940000	0.5816540000
C	-5.8742790000	-0.5053330000	1.8030210000
C	-6.6723290000	-1.5371800000	2.5910990000

N	4.4991100000	-2.0974540000	0.2146900000
C	3.7376090000	-3.2085860000	-0.3132590000
C	5.8739490000	-2.3036570000	0.6206200000
H	-2.9599160000	2.0650090000	-1.2956880000
H	-1.3313870000	3.7183720000	-0.3932110000
H	0.0037350000	-1.0182350000	-1.0412620000
H	4.6590820000	2.3269880000	1.3236810000
H	5.6944290000	0.1078640000	1.1407900000
H	2.0018110000	-1.4679120000	-0.4628930000
H	-4.3217810000	-1.3394750000	-1.8861500000
H	-3.6100640000	0.3626580000	0.4234410000
H	-5.0601520000	0.7626580000	-0.4985260000
H	-5.9356880000	-1.5629140000	-0.0734100000
H	-4.5022170000	-1.9067240000	0.8914560000
H	-5.1217120000	-0.0449320000	2.4570270000
H	-6.5399950000	0.3072790000	1.4823740000
H	-7.1585800000	-1.0849480000	3.4611310000
H	-7.4537100000	-1.9906320000	1.9707830000
H	-6.0259900000	-2.3447020000	2.9528730000
H	2.8555710000	-3.4239730000	0.3042960000
H	3.4000410000	-3.0158690000	-1.3400190000
H	4.3649370000	-4.0994290000	-0.3266030000
H	6.5693490000	-1.6885660000	0.0352370000
H	6.0228590000	-2.0790230000	1.6844280000
H	6.1372740000	-3.3488570000	0.4606740000

Optimized geometry of 4a in DMSO

C	-1.9618800000	1.7835000000	-0.9936600000
C	-1.0637800000	2.6940800000	-0.4852400000
C	0.2418800000	2.2898000000	-0.1375100000
C	0.6429200000	0.9472300000	-0.3336400000
C	-0.2846000000	0.0388300000	-0.8759800000

C	-1.5727700000	0.4386000000	-1.1860800000
N	1.0703300000	3.2650800000	0.3835400000
N	2.2727700000	2.9677200000	0.7170900000
C	2.7556000000	1.6954600000	0.5635600000
C	1.9960000000	0.6186400000	0.0396100000
C	4.0926400000	1.4617900000	0.9555400000
C	4.6564600000	0.2195800000	0.8350400000
C	3.9064900000	-0.8795900000	0.3077100000
C	2.5748900000	-0.6482300000	-0.0812000000
C	-2.4883800000	-0.5704700000	-1.8118000000
O	-2.0725800000	-1.3130200000	-2.7064600000
N	-3.7729900000	-0.6260900000	-1.3911100000
C	-4.3781500000	-0.0662900000	-0.1926400000
C	-5.1554900000	-1.1243810000	0.5820000000
C	-5.8332700000	-0.5537210000	1.8238400000
C	-6.6207900000	-1.6032210000	2.5991400000
N	4.4775500000	-2.1106600000	0.1903700000
C	3.7114400000	-3.2123100000	-0.3531800000
C	5.8508000000	-2.3309390000	0.5986200000
H	-2.9624000000	2.1033500000	-1.2690000000
H	-1.3313300000	3.7364500000	-0.3412700000
H	-0.0045400000	-0.9921400000	-1.0657000000
H	4.6626600000	2.2957600000	1.3545400000
H	5.6847600000	0.0758810000	1.1437800000
H	1.9850800000	-1.4614800000	-0.4833900000
H	-4.3287300000	-1.2974300000	-1.9070800000
H	-3.5866700000	0.3459100000	0.4380900000
H	-5.0471300000	0.7630590000	-0.4607900000
H	-5.9163400000	-1.5705010000	-0.0742900000
H	-4.4713700000	-1.9343700000	0.8670000000
H	-5.0732200000	-0.1066210000	2.4783800000

H	-6.5036100000	0.2643990000	1.5280400000
H	-7.0971800000	-1.1699810000	3.4842300000
H	-7.4088000000	-2.0442710000	1.9782200000
H	-5.9689900000	-2.4172210000	2.9358900000
H	2.8280000000	-3.4311600000	0.2606500000
H	3.3767200000	-3.0040000000	-1.3775300000
H	4.3352100000	-4.1050900000	-0.3771800000
H	6.5515500000	-1.7154190000	0.0207300000
H	5.9970700000	-2.1170490000	1.6646200000
H	6.1062300000	-3.3764290000	0.4297800000

Optimized geometry of 4a in MeOH

C	-1.9671220000	1.8531080000	-0.9465580000
C	-1.0628640000	2.7380380000	-0.4049770000
C	0.2407260000	2.3124840000	-0.0736860000
C	0.6317940000	0.9741170000	-0.3159090000
C	-0.3012620000	0.0931990000	-0.8938070000
C	-1.5854920000	0.5145670000	-1.1915610000
N	1.0781010000	3.2618020000	0.4785920000
N	2.2796760000	2.9420660000	0.8014090000
C	2.7509360000	1.6727080000	0.6088310000
C	1.9806930000	0.6195490000	0.0499650000
C	4.0857140000	1.4127930000	0.9955940000
C	4.6363390000	0.1693540000	0.8389850000
C	3.8750790000	-0.9067140000	0.2780620000
C	2.5458540000	-0.6486220000	-0.1073990000
C	-2.5105520000	-0.4561050000	-1.8630810000
O	-2.1106460000	-1.1255060000	-2.8242640000
N	-3.7779760000	-0.5565720000	-1.4129260000
C	-4.3603560000	-0.0627150000	-0.1740900000
C	-5.0891270000	-1.1711080000	0.5769270000

C	-5.7411970000	-0.6674210000	1.8607860000
C	-6.4817390000	-1.7661940000	2.6139080000
N	4.4316410000	-2.1378540000	0.1274710000
C	3.6544230000	-3.2168260000	-0.4476630000
C	5.8015750000	-2.3870250000	0.5349520000
H	-2.9670800000	2.1883990000	-1.2050640000
H	-1.3273000000	3.7750900000	-0.2214910000
H	-0.0269920000	-0.9328100000	-1.1162760000
H	4.6656860000	2.2265490000	1.4212720000
H	5.6622200000	0.0054280000	1.1453910000
H	1.9480690000	-1.4443830000	-0.5319700000
H	-4.3492120000	-1.1891780000	-1.9604990000
H	-3.5598590000	0.3420620000	0.4496370000
H	-5.0550290000	0.7597810000	-0.3908890000
H	-5.8592590000	-1.6075020000	-0.0746070000
H	-4.3778160000	-1.9747130000	0.8082390000
H	-4.9716770000	-0.2302370000	2.5109020000
H	-6.4380500000	0.1460300000	1.6185260000
H	-6.9402700000	-1.3810630000	3.5302580000
H	-7.2784070000	-2.1986550000	1.9979630000
H	-5.8021420000	-2.5782320000	2.8963270000
H	2.7670480000	-3.4410350000	0.1578740000
H	3.3258990000	-2.9766440000	-1.4667600000
H	4.2686160000	-4.1149930000	-0.4933790000
H	6.5111010000	-1.7639620000	-0.0230440000
H	5.9450480000	-2.2047950000	1.6068070000
H	6.0439440000	-3.4303040000	0.3374010000

Optimized geometry of 11e in $CHCl_3$

C	-3.44350	-3.82146	0.14431
C	-4.25556	-2.72259	-0.02306

C -2.04070 -3.66608 0.21364

C -1.46296 -2.37494 0.11695

C -2.31509 -1.26481 -0.06615

C -3.69064 -1.43083 -0.14885

N -1.29850 -4.82707 0.38875

N -0.01840 -4.77155 0.47308

C 0.63898 -3.55327 0.39372

C -0.02554 -2.31250 0.22030

C 2.04738 -3.59026 0.49744

C 2.78345 -2.42833 0.43700

C 2.12732 -1.18510 0.25294

C 0.74377 -1.13420 0.14130

O -5.79871 -0.34931 0.10486

N -4.15561 0.81884 -0.96792

C -4.64866 -0.27862 -0.31893

N 2.88974 0.00456 0.19202

C 2.66518 1.16775 0.94600

C 3.64122 2.13453 0.59775

C 4.48909 1.53529 -0.41221

C 4.00051 0.22439 -0.63793

C 5.59042 1.99725 -1.14146

C 6.17983 1.15874 -2.08275

C 5.67120 -0.13105 -2.30785

C 4.57550 -0.61509 -1.59589

C 1.70901 1.41841 1.93381

C 1.72815 2.66639 2.55352

C 2.67690 3.64238 2.20673

C 3.63767 3.38056 1.23468

C -4.62331 5.76917 -0.09572

C -5.19607 4.52252 -0.77615

C -4.36589 3.26026 -0.51324

C -4.94926 2.01936 -1.19931

H -3.84422 -4.82564 0.23303

H -5.33528 -2.81241 -0.05826

H -1.88941 -0.26737 -0.10433

H 2.51734 -4.55711 0.64272

H 3.86175 -2.44623 0.54767

H 0.26893 -0.17429 -0.02327

H -3.25475 0.74839 -1.41575

H 5.97557 2.99951 -0.97766

H 7.03583 1.50454 -2.65367

H 6.13663 -0.76651 -3.05529

H 4.18260 -1.60674 -1.78960

H 0.98149 0.66764 2.22065

H 0.99430 2.88365 3.32386

H 2.66298 4.60544 2.70734

H 4.38004 4.13031 0.97687

H -5.23667 6.65210 -0.30101

H -4.57775 5.64111 0.99142

H -3.60697 5.98123 -0.44641

H -5.26336 4.69462 -1.85905

H -6.22483 4.35568 -0.43059

H -4.30371 3.07040 0.56565

H -3.33513 3.42212 -0.86031

H -5.03777 2.19321 -2.28010

H -5.94906 1.80005 -0.81792

Optimized geometry at the ground state, B3LYP-D3BJ/6-31+G(d,p)

Optimized geometry of 4a in toluene

C -2.35104 1.93313 -0.82112

C -1.47497 2.77773 -0.17241

C -0.15457 2.35812 0.10876

C 0.28340 1.07320 -0.30335

C -0.62370 0.23447 -0.98288

C -1.92549 0.64379 -1.22415

N 0.65287 3.26059 0.78574

N 1.87108 2.94323 1.06898

C 2.38702 1.72068 0.70555

C 1.64852 0.72471 0.01013

C 3.73431 1.45788 1.05033

C 4.32856 0.26462 0.72198

C 3.60010 -0.75169 0.02008

C 2.25939 -0.49205 -0.32243

C -2.83700 -0.28750 -1.97059

O -2.47283 -0.81717 -3.02572

N -4.08498 -0.49788 -1.45706

C -4.47001 -0.38067 -0.04646

C -3.89441 -1.49361 0.83499

C -4.31338 -1.35231 2.30138

C -3.72769 -2.45128 3.19262

N 4.20239 -1.93919 -0.30319

C 3.45929 -2.95234 -1.03793

C 5.59978 -2.17944 0.03225

H -3.36032 2.26085 -1.04695

H -1.76929 3.77541 0.13573

H -0.31559 -0.74535 -1.32849

H 4.28543 2.22799 1.58003

H 5.36093 0.09762 0.99889

H 1.68745 -1.23744 -0.85564

H -4.61548 -1.16438 -2.00720

H -4.15386 0.59208 0.33397

H -5.56383 -0.39353 -0.01289

H -4.21701 -2.46835 0.44516

H -2.79939 -1.47127 0.76075

H -3.99494 -0.36945 2.67372

H -5.40956 -1.36797 2.36994

H -4.03969 -2.32799 4.23478

H -4.05370 -3.44353 2.85991

H -2.63208 -2.43467 3.16664

H 2.57321 -3.28099 -0.48025

H 3.13107 -2.58098 -2.01748

H 4.09929 -3.81887 -1.19837

H 6.26507 -1.45463 -0.45374

H 5.76851 -2.13370 1.11495

H 5.87825 -3.17541 -0.30950

Optimized geometry of 4a in chloroform

C -1.99957 1.93557 -0.92612

C -1.09622 2.79489 -0.33704

C 0.20272 2.34703 -0.00345

C 0.58931 1.01334 -0.29639

C -0.34445 0.15884 -0.91738

C -1.62430 0.60035 -1.21516

N 1.04232 3.26944 0.60264

N 2.24464 2.92551 0.92805

C 2.71023 1.65645 0.68145

C 1.93441 0.63459 0.06641

C 4.04185 1.36657 1.06670

C 4.58497 0.12437 0.85421

C 3.81834 -0.91889 0.23538

C 2.49288 -0.63191 -0.14756

C -2.55601 -0.34282 -1.92023

O -2.16152 -1.00128 -2.89399

N -3.84026 -0.42286 -1.48435

C -4.39294 -0.03160 -0.18651

C -4.92183 -1.23890 0.59208

C -5.52825 -0.83904 1.94107

C -6.06593 -2.03890 2.72606

N 4.36927 -2.15334 0.02793

C 3.58755 -3.19805 -0.61949

C 5.74908 -2.42735 0.41213

H -2.99258 2.28518 -1.18756

H -1.35458 3.82545 -0.11763

H -0.07410 -0.85835 -1.17466

H 4.62344 2.15469 1.53374

H 5.60592 -0.06219 1.15908

H 1.89318 -1.39732 -0.61799

H -4.40818 -1.05181 -2.04175

H -3.60912 0.46280 0.38824

H -5.19675 0.69928 -0.33948

H -5.68027 -1.75783 -0.01046

H -4.10001 -1.94982 0.74659

H -4.76796 -0.31938 2.53916

H -6.33782 -0.11601 1.77456

H -6.49209 -1.72771 3.68535

H -6.85021 -2.55790 2.16299

H -5.26917 -2.76288 2.93197

H 2.68550 -3.43714 -0.04261

H 3.28169 -2.90238 -1.63110

H 4.19188 -4.10059 -0.69548

H 6.45514 -1.78232 -0.12526

H 5.90203 -2.28963 1.48909

H 5.98334 -3.46242 0.16839

Optimized geometry of 4a in DMSO

C 1.99931 1.98069 0.88256

C 1.09125 2.82063 0.27333

C -0.20762 2.35964 -0.04373

C -0.58750 1.03120 0.28188

C 0.35037 0.19753 0.92539

C 1.62787 0.65359 1.21089

N -1.05449 3.26254 -0.66746

N -2.25766 2.90304 -0.98160

C -2.71454 1.63849 -0.70864

C -1.92985 0.63430 -0.07276

C -4.04511 1.33004 -1.08710

C -4.57794 0.08862 -0.85011

C -3.80209 -0.93730 -0.21118

C -2.47750 -0.63145 0.16567

C 2.56789 -0.25906 1.94507

O 2.19106 -0.84607 2.97438

N 3.82997 -0.39236 1.47504

C 4.36100 -0.04114 0.15615

C 4.89657 -1.27105 -0.58043

C 5.48365 -0.91448 -1.94990

C 6.02806 -2.13697 -2.69432

N -4.34191 -2.16927 0.01928

C -3.54686 -3.20178 0.67264

C -5.71721 -2.46639 -0.36933

H 2.99358 2.33901 1.12659

H 1.34917 3.84465 0.02456

H 0.08363 -0.81494 1.20446

H -4.63485 2.10224 -1.57043

H -5.59695 -0.11256 -1.15179

H -1.87102 -1.38432 0.64729

H 4.41535 -0.98759 2.05138

H 3.56250 0.41981 -0.42599

H 5.15620 0.70502 0.27292

H 5.66826 -1.75591 0.03305

H 4.08204 -1.99692 -0.69948

H 4.71065 -0.42719 -2.55880

H 6.28597 -0.17639 -1.81880

H 6.44110 -1.85732 -3.66906

H 6.82399 -2.62450 -2.11954

H 5.23792 -2.87744 -2.86427

H -2.64830 -3.44081 0.09083

H -3.23563 -2.89052 1.67747

H -4.14486 -4.10663 0.76474

H -6.43126 -1.81234 0.14484

H -5.86157 -2.35950 -1.45071

H -5.94422 -3.49576 -0.09773

Optimized geometry of 4a in Methanol

C -1.99965 1.97660 -0.88523

C -1.09198 2.81819 -0.27766

C 0.20709 2.35848 0.04027

C 0.58766 1.02965 -0.28301

C -0.34981 0.19428 -0.92474

C -1.62765 0.64901 -1.21091

N 1.05344 3.26296 0.66234

N 2.25672 2.90491 0.97696

C 2.71445 1.64008 0.70596

C 1.93039 0.63435 0.07193

C 4.04525 1.33330 1.08466

C 4.57894 0.09183 0.84957

C 3.80376 -0.93564 0.21252

C 2.47892 -0.63146 -0.16448

C -2.56715 -0.26577 -1.94296

O -2.18897 -0.85850 -2.96825

N -3.83123 -0.39392 -1.47587

C -4.36358 -0.03992 -0.15827

C -4.89963 -1.26814 0.58084

C -5.48592 -0.90880 1.94995

C -6.03147 -2.12950 2.69648

N 4.34456 -2.16767 -0.01632

C 3.55078 -3.20101 -0.66972

C 5.71898 -2.46422 0.37556

H -2.99401 2.33403 -1.13024

H -1.35019 3.84264 -0.03097

H -0.08262 -0.81850 -1.20230

H 4.63445 2.10687 1.56643

H 5.59829 -0.10795 1.15104

H 1.87281 -1.38562 -0.64457

H -4.41547 -0.99140 -2.05101

H -3.56578 0.42257 0.42364

H -5.15875 0.70593 -0.27739

H -5.67181 -1.75383 -0.03139

H -4.08545 -1.99424 0.70093

H -4.71213 -0.42146 2.55781

H -6.28744 -0.16999 1.81806

H -6.44375 -1.84788 3.67097

H -6.82824 -2.61699 2.12282

H -5.24217 -2.87068 2.86723

H 2.65358 -3.44309 -0.08694

H 3.23727 -2.88895 -1.67357

H 4.15070 -4.10436 -0.76432

H 6.43454 -1.81311 -0.14036

H 5.86179 -2.35271 1.45667

H 5.94546 -3.49504 0.10898

Optimized geometry at the ground state, CAM-B3LYP/6-31+G(d,p)

Optimized geometry of 4a in toluene

C -1.94430 1.72744 -1.02109

C -1.05302 2.65634 -0.54379

C 0.25452 2.26914 -0.18714

C 0.66256 0.93045 -0.34192

C -0.26153 -0.00133 -0.85118

C -1.54840 0.37951 -1.17027

N 1.08208 3.26714 0.30393

N 2.28203 2.98867 0.64086

C 2.77396 1.70997 0.52182

C 2.02050 0.62155 0.03482

C 4.11285 1.49630 0.91357

C 4.68206 0.25644 0.82499

C 3.93586 -0.85972 0.33233

C 2.60603 -0.64696 -0.05416

C -2.46110 -0.65945 -1.75425

O -2.03806 -1.45270 -2.59660

N -3.75579 -0.69215 -1.35193

C -4.38431 -0.07491 -0.18894

C -5.23884 -1.08272 0.57407

C -5.95322 -0.45451 1.76907

C -6.81820 -1.45469 2.53176

N 4.51627 -2.09500 0.24549

C 3.75210 -3.21720 -0.26550

C 5.89755 -2.29452 0.64750

H -2.94530 2.03305 -1.30506

H -1.32369 3.70038 -0.43121

H 0.02493 -1.03386 -1.01065

H 4.67755 2.34459 1.28552

H 5.71107 0.12724 1.13202

H 2.01817 -1.47054 -0.43202

H -4.29845 -1.39232 -1.84327

H -3.60391 0.31627 0.46575

H -5.00556 0.77416 -0.50072

H -5.98408 -1.51656 -0.10620

H -4.60191 -1.90936 0.91108

H -5.20926 -0.02032 2.44829

H -6.57650 0.37886 1.42192

H -7.31706 -0.98110 3.38192

H -7.59265 -1.87994 1.88492

H -6.21571 -2.28347 2.91765

H 2.87159 -3.42203 0.35550

H 3.41329 -3.04072 -1.29344

H 4.37894 -4.10723 -0.26516

H 6.58829 -1.68909 0.04906

H 6.05252 -2.05268 1.70529

H 6.15974 -3.34114 0.50287

Optimized geometry of 4a in chloroform

C -1.94860 1.77478 -1.00220

C -1.05450 2.68746 -0.50000

C 0.25084 2.28568 -0.15015

C 0.65322 0.94881 -0.33522

C -0.27337 0.03433 -0.87154

C -1.55688 0.42984 -1.18567

N 1.08247 3.26645 0.36629

N 2.28101 2.97259 0.70070

C 2.76619 1.69577 0.55551

C 2.00743 0.62251 0.04068

C 4.10261 1.46415 0.94864

C 4.66357 0.22307 0.83607

C 3.91188 -0.87812 0.31591

C 2.58448 -0.64719 -0.07278

C -2.47558 -0.58507 -1.80158

O -2.06397 -1.32752 -2.69809

N -3.75510 -0.65295 -1.36919

C -4.36487 -0.07506 -0.17540

C -5.18896 -1.11448 0.57805

C -5.88067 -0.52766 1.80692

C -6.71271 -1.55982 2.56363

N 4.48317 -2.11321 0.20630

C 3.71383 -3.22031 -0.33175

C 5.86012 -2.33340 0.61664

H -2.94888 2.09068 -1.27737

H -1.32364 3.72880 -0.36172

H 0.01005 -0.99561 -1.05188

H 4.67313 2.29895 1.34182

H 5.69013 0.08031 1.14505

H 1.99306 -1.45915 -0.46951

H -4.31097 -1.32762 -1.88157

H -3.57414 0.30785 0.47136

H -5.00233 0.77351 -0.45245

H -5.94525 -1.53723 -0.09652

H -4.53452 -1.94210 0.87679

H -5.12522 -0.10182 2.47868

H -6.52342 0.30578 1.49767

H -7.19758 -1.11545 3.43742

H -7.49619 -1.97962 1.92413

H -6.08902 -2.38905 2.91329

H 2.83049 -3.43330 0.28208

H 3.37983 -3.01835 -1.35629

H 4.33605 -4.11308 -0.34936

H 6.56069 -1.72256 0.03598

H 6.00693 -2.11349 1.68004

H 6.11355 -3.37925 0.45371

Optimized geometry of 4a in DMSO

C -1.95153 1.84048 -0.96158

C -1.05181 2.72939 -0.42815

C 0.25135 2.30733 -0.09245

C 0.64419 0.97365 -0.31930

C -0.28765 0.08453 -0.88915

C -1.56696 0.50078 -1.19316

N 1.09137 3.26373 0.45329

N 2.28892 2.94855 0.77883

C 2.76285 1.67428 0.59809

C 1.99397 0.62272 0.05068

C 4.09697 1.41760 0.98746

C 4.64515 0.17501 0.84189

C 3.88273 -0.90488 0.29006

C 2.55773 -0.64860 -0.09626

C -2.49489 -0.47862 -1.85157

O -2.10003 -1.15003 -2.81392

N -3.75533 -0.59217 -1.38843

C -4.34198 -0.07347 -0.15533

C -5.13280 -1.15575 0.57256

C -5.79614 -0.63121 1.84449

C -6.59689 -1.70541 2.57615

N 4.43996 -2.14010 0.15001

C 3.66002 -3.22612 -0.41782

C 5.81350 -2.38794 0.56092

H -2.95107 2.17096 -1.22196

H -1.31809 3.76611 -0.25361

H -0.00998 -0.94151 -1.09864

H 4.67701 2.23351 1.40574

H 5.66920 0.01299 1.14941

H 1.95865 -1.44435 -0.51359

H -4.32750 -1.23032 -1.92947

H -3.53920 0.29230 0.48612

H -4.99613 0.77639 -0.38315

H -5.90285 -1.55699 -0.09915

H -4.46063 -1.98689 0.81715

H -5.02675 -0.22749 2.51401

H -6.45547 0.20754 1.58959

H -7.06159 -1.30585 3.48207

H -7.39355 -2.10427 1.93949

H -5.95539 -2.54254 2.87062

H 2.77277 -3.44372 0.18811

H 3.33218 -2.99436 -1.43779

H 4.27306 -4.12421 -0.45538

H 6.52297 -1.77059 -0.00106

H 5.95700 -2.19699 1.62998

H 6.05423 -3.43211 0.37192

Optimized geometry of 4a in Methanol

C -1.95130 1.83485 -0.96553

C -1.05211 2.72586 -0.43469

C 0.25124 2.30555 -0.09763

C 0.64494 0.97153 -0.32080

C -0.28640 0.08016 -0.88788

C -1.56604 0.49464 -1.19295

N 1.09050 3.26405 0.44566

N 2.28816 2.95066 0.77212

C 2.76308 1.67619 0.59453

C 1.99507 0.62269 0.04985

C 4.09741 1.42163 0.98436

C 4.64667 0.17914 0.84171

C 3.88517 -0.90265 0.29253

C 2.55995 -0.64852 -0.09413

C -2.49318 -0.48784 -1.84785

O -2.09696 -1.16488 -2.80544

N -3.75488 -0.59815 -1.38655

C -4.34340 -0.07396 -0.15673

C -5.13758 -1.15229 0.57336

C -5.80320 -0.62207 1.84174

C -6.60723 -1.69236 2.57552

N 4.44357 -2.13783 0.15515

C 3.66461 -3.22568 -0.41035

C 5.81743 -2.38336 0.56614

H -2.95091 2.16407 -1.22721

H -1.31875 3.76301 -0.26330

H -0.00818 -0.94627 -1.09470

H 4.67668 2.23916 1.40054

H 5.67092 0.01877 1.14944

H 1.96156 -1.44571 -0.50970

H -4.32586 -1.23935 -1.92519

H -3.54150 0.29291 0.48523

H -4.99576 0.77614 -0.38891

H -5.90661 -1.55490 -0.09871

H -4.46728 -1.98355 0.82262

H -5.03482 -0.21694 2.51159

H -6.46071 0.21669 1.58218

H -7.07355 -1.28872 3.47879

H -7.40294 -2.09251 1.93847

H -5.96766 -2.52928 2.87471

H 2.77767 -3.44300 0.19617

H 3.33632 -2.99633 -1.43074

H 4.27849 -4.12329 -0.44626

H 6.52618 -1.76666 0.00250

H 5.96116 -2.18980 1.63471

H 6.05915 -3.42774 0.37951

Optimized geometry at the first excited state, PBE0 /6-31+G(d,p)

Optimized geometry of 4a in the S1 state in toluene

C -1.96019 1.56952 -0.95231

C -1.09756 2.58322 -0.60095

C 0.24193 2.26575 -0.26377

C 0.71574 0.90210 -0.31954

C -0.19311 -0.07176 -0.69642

C -1.53817 0.22336 -0.99310

N 1.14516 3.17515 0.10612

N 2.32838 3.00520 0.40680

C 2.92701 1.77674 0.40168

C 2.11971 0.66080 0.02491

C 4.27352 1.59722 0.74387

C 4.83596 0.33654 0.71625

C 4.07031 -0.79759 0.34277

C 2.71316 -0.59725 0.00561

C -2.39614 -0.89428 -1.43944

O -1.90926 -1.89017 -1.99269

N -3.75091 -0.80846 -1.26763

C -4.49341 -0.07098 -0.25820

C -5.49076 -0.97139 0.46265

C -6.31586 -0.21853 1.50151

C -7.32324 -1.11180 2.21586

N 4.62886 -2.04739 0.30985

C 3.82761 -3.18933 -0.06939

C 6.01682 -2.23218 0.66847

H -2.97539 1.82734 -1.23752

H -1.41545 3.61987 -0.58877

H 0.11590 -1.10902 -0.77893

H 4.86577 2.46056 1.02876

H 5.87967 0.22874 0.98544

H 2.10494 -1.44553 -0.28169

H -4.22507 -1.60845 -1.66676

H -3.78631 0.34555 0.46538

H -5.03069 0.77526 -0.71136

H -6.16720 -1.42769 -0.27478

H -4.94701 -1.79594 0.94242

H -5.64139 0.23722 2.23879

H -6.84312 0.61241 1.01369

H -7.90107 -0.54919 2.95596

H -8.03167 -1.55459 1.50653

H -6.82154 -1.93348 2.73928

H 2.98250 -3.34113 0.61595

H 3.42893 -3.08658 -1.08744

H 4.44704 -4.08565 -0.04146

H 6.68759 -1.66657 0.00784

H 6.21621 -1.92613 1.70453

H 6.27104 -3.28797 0.57692

Optimized geometry of 4a in the S1 state in chloroform

C -1.96318 1.56744 -0.95565

C -1.10077 2.58122 -0.60227

C 0.23874 2.26457 -0.26654

C 0.71431 0.90182 -0.32385

C -0.19358 -0.07212 -0.70452

C -1.53873 0.22249 -1.00152

N 1.14038 3.17566 0.10627

N 2.32523 3.00651 0.40637

C 2.92432 1.77679 0.40165

C 2.11791 0.66055 0.02396

C 4.27055 1.59807 0.74537

C 4.83377 0.33778 0.71952

C 4.06884 -0.79782 0.34647

C 2.71162 -0.59758 0.00648

C -2.39782 -0.89226 -1.45376

O -1.91120 -1.87581 -2.03466

N -3.74616 -0.82195 -1.25691

C -4.48628 -0.07859 -0.24918

C -5.48543 -0.97569 0.47288

C -6.30839 -0.21735 1.50945

C -7.31729 -1.10660 2.22669

N 4.62728 -2.04614 0.31705

C 3.82784 -3.18973 -0.06324

C 6.01696 -2.22963 0.67377

H -2.97913 1.82553 -1.23770

H -1.42057 3.61729 -0.58637

H 0.11880 -1.10858 -0.78535

H 4.86260 2.46151 1.03066

H 5.87716 0.23081 0.99023

H 2.10477 -1.44688 -0.28097

H -4.22801 -1.61287 -1.66511

H -3.77730 0.33730 0.47266

H -5.02084 0.76702 -0.70564

H -6.16275 -1.43176 -0.26363

H -4.94372 -1.79992 0.95546

H -5.63275 0.23921 2.24509

H -6.83414 0.61272 1.01868

H -7.89391 -0.54021 2.96489

H -8.02641 -1.55025 1.51856

H -6.81676 -1.92736 2.75278

H 2.97951 -3.33880 0.61835

H 3.43462 -3.08982 -1.08365

H 4.44717 -4.08565 -0.02895

H 6.68577 -1.66521 0.01059

H 6.21727 -1.92080 1.70848

H 6.27082 -3.28548 0.58439

Optimized geometry of 4a in the S1 state in DMSO

C -1.94518 1.52522 -0.95369

C -1.07004 2.52458 -0.61701

C 0.29039 2.22392 -0.27894

C 0.71764 0.85220 -0.33780

C -0.18530 -0.13682 -0.70221

C -1.53143 0.16555 -0.99138

N 1.09022 3.24456 0.06225

N 2.36728 3.06059 0.38395

C 2.86752 1.78140 0.35716

C 2.10882 0.64197 0.00747

C 4.23718 1.60704 0.70489

C 4.83821 0.37513 0.70838

C 4.08448 -0.78182 0.35501

C 2.71797 -0.61871 0.00817

C -2.40517 -0.93857 -1.42410

O -1.92960 -1.94531 -1.98817

N -3.75309 -0.84628 -1.23904

C -4.48833 -0.07828 -0.24486

C -5.51326 -0.94959 0.47251

C -6.33222 -0.16502 1.49259

C -7.36724 -1.02755 2.20531

N 4.64953 -2.01964 0.34654

C 3.87979 -3.19527 -0.01530

C 6.04495 -2.18372 0.70035

H -2.96126 1.78800 -1.23095

H -1.38048 3.56517 -0.60682

H 0.11817 -1.17656 -0.76937

H 4.80540 2.49300 0.97285

H 5.88262 0.29296 0.98088

H 2.13024 -1.48608 -0.26216

H -4.24797 -1.63275 -1.64064

H -3.77858 0.32840 0.48143

H -5.00032 0.77344 -0.71452

H -6.19076 -1.39747 -0.26858

H -4.99406 -1.77997 0.96922

H -5.65591 0.28419 2.23205

H -6.83513 0.67067 0.98788

H -7.94078 -0.44290 2.93170

H -8.07665 -1.46274 1.49218

H -6.88931 -1.85350 2.74429

H 3.03411 -3.33538 0.66734

H 3.49769 -3.11325 -1.03896

H 4.52164 -4.07095 0.04507

H 6.68794 -1.61511 0.01821

H 6.22955 -1.83518 1.72323

H 6.31029 -3.23612 0.63577

Optimized geometry of 4a in the S1 state in MeOH

C -1.94484 1.52360 -0.95379

C -1.06987 2.52344 -0.61811

C 0.29053 2.22325 -0.27964

C 0.71790 0.85157 -0.33731

C -0.18491 -0.13803 -0.70038

C -1.53110 0.16383 -0.98974

N 1.09018 3.24437 0.06083

N 2.36707 3.06113 0.38233

C 2.86758 1.78187 0.35617

C 2.10915 0.64211 0.00763

C 4.23742 1.60810 0.70336

C 4.83888 0.37635 0.70729

C 4.08538 -0.78096 0.35493

C 2.71876 -0.61851 0.00866

C -2.40443 -0.94112 -1.42092

O -1.92851 -1.94934 -1.98175

N -3.75283 -0.84815 -1.23785

C -4.48915 -0.07865 -0.24580

C -5.51492 -0.94876 0.47186

C -6.33534 -0.16255 1.48951

C -7.37103 -1.02396 2.20258

N 4.65083 -2.01880 0.34689

C 3.88127 -3.19473 -0.01425

C 6.04633 -2.18229 0.70047

H -2.96083 1.78598 -1.23175

H -1.38018 3.56405 -0.60920

H 0.11855 -1.17782 -0.76680

H 4.80532 2.49452 0.97044

H 5.88349 0.29465 0.97925

H 2.13111 -1.48607 -0.26122

H -4.24693 -1.63563 -1.63835

H -3.78028 0.32920 0.48071

H -5.00063 0.77244 -0.71725

H -6.19139 -1.39815 -0.26928

H -4.99623 -1.77821 0.97067

H -5.66005 0.28821 2.22895

H -6.83783 0.67213 0.98268

H -7.94561 -0.43810 2.92716

H -8.07948 -1.46069 1.48944

H -6.89360 -1.84878 2.74371

H 3.03597 -3.33505 0.66885

H 3.49849 -3.11314 -1.03771

H 4.52343 -4.07022 0.04592

H 6.68910 -1.61411 0.01774

H 6.23120 -1.83294 1.72303

H 6.31191 -3.23470 0.63665

Optimized geometry at the first excited state, B3LYP-D3BJ /6-31+G(d,p)

Optimized geometry of 4a in the S1 state in toluene

C -2.21432 1.82426 -0.94062

C -1.36254 2.75812 -0.39358

C -0.03510 2.37349 -0.05744

C 0.43604 1.02752 -0.31983

C -0.46066 0.13573 -0.88886

C -1.79520 0.49262 -1.18523

N 0.85768 3.20443 0.49402

N 2.03161 2.97310 0.81099

C 2.62352 1.74951 0.62820

C 1.82407 0.71640 0.03962

C 3.95860 1.50076 0.98633

C 4.51482 0.25201 0.77523

C 3.75281 -0.80299 0.20095

C 2.41208 -0.53098 -0.16205

C -2.66131 -0.51941 -1.81733

O -2.19355 -1.41725 -2.53867

N -4.03260 -0.42683 -1.62796

C -4.65456 -0.14564 -0.32644

C -4.40211 -1.23597 0.72034

C -5.06871 -0.92714 2.06417

C -4.81200 -2.00927 3.11712

N 4.29981 -2.05170 0.00914

C 3.54746 -3.06626 -0.71430

C 5.71864 -2.26796 0.24948

H -3.21348 2.13009 -1.23046

H -1.67412 3.78279 -0.22869

H -0.15133 -0.87678 -1.12069

H 4.54541 2.30041 1.42413

H 5.54717 0.09205 1.05563

H 1.81326 -1.30902 -0.61297

H -4.49259 -1.17592 -2.13542

H -4.29434 0.81205 0.05228

H -5.72932 -0.03043 -0.50355

H -4.76579 -2.19880 0.33628

H -3.31852 -1.34432 0.86115

H -4.70190 0.03960 2.43490

H -6.15074 -0.80915 1.91498

H -5.29681 -1.76501 4.06816

H -5.19607 -2.98059 2.78452

H -3.73870 -2.12434 3.30742

H 2.60458 -3.29615 -0.20535

H 3.31632 -2.75525 -1.74320

H 4.13574 -3.98234 -0.75584

H 6.35023 -1.65332 -0.40830

H 5.98211 -2.04301 1.28898

H 5.95268 -3.31641 0.06768

Optimized geometry of 4a in the S1 state in chloroform

C -1.94419 1.54901 -0.97717

C -1.07183 2.54763 -0.62418

C 0.28625 2.24181 -0.27109

C 0.71312 0.86750 -0.33488

C -0.18827 -0.12361 -0.70975

C -1.53307 0.18271 -1.01336

N 1.08983 3.26323 0.09012

N 2.36434 3.07670 0.42302

C 2.86496 1.78150 0.38233

C 2.10116 0.65361 0.01555

C 4.23288 1.59796 0.73242

C 4.83056 0.35925 0.72231

C 4.07044 -0.78980 0.35022

C 2.70731 -0.61782 0.00043

C -2.41078 -0.91752 -1.44464

O -1.94317 -1.95581 -1.96513

N -3.77413 -0.78230 -1.31093

C -4.49812 -0.04701 -0.27067

C -5.49034 -0.95300 0.46222

C -6.28487 -0.20193 1.53536

C -7.28668 -1.09977 2.26717

N 4.63213 -2.04100 0.32698

C 3.85156 -3.21115 -0.06274

C 6.03138 -2.22016 0.69080

H -2.95485 1.81163 -1.26825

H -1.37822 3.58817 -0.61314

H 0.11400 -1.16160 -0.77813

H 4.80209 2.47840 1.01231

H 5.87259 0.26851 0.99567

H 2.11480 -1.47405 -0.28594

H -4.26569 -1.57978 -1.69749

H -3.77460 0.35448 0.44257

H -5.03453 0.80661 -0.70676

H -6.18785 -1.39211 -0.26521

H -4.94223 -1.78738 0.91887

H -5.58680 0.23717 2.26043

H -6.81650 0.63885 1.07032

H -7.84014 -0.54059 3.02872

H -8.01566 -1.52662 1.56855

H -6.77734 -1.93222 2.76632

H 2.99987 -3.35383 0.61141

H 3.47587 -3.10571 -1.08621

H 4.48702 -4.09184 -0.01325

H 6.68171 -1.64892 0.01834

H 6.20978 -1.88049 1.71735

H 6.28813 -3.27397 0.61831

Optimized geometry of 4a in the S1 state in DMSO

C -1.95214 1.58376 -0.97372

C -1.07738 2.57190 -0.59724

C 0.28115 2.25577 -0.25266

C 0.70610 0.88137 -0.34520

C -0.19703 -0.09664 -0.75021

C -1.54050 0.22034 -1.04809

N 1.08607 3.26616 0.12854

N 2.36505 3.06534 0.46072

C 2.85892 1.77258 0.40480

C 2.09148 0.65196 0.01385

C 4.22339 1.57537 0.76505

C 4.81258 0.33379 0.74319

C 4.04895 -0.80718 0.35004

C 2.68871 -0.62103 -0.01096

C -2.42491 -0.86194 -1.51487

O -1.96310 -1.86401 -2.11170

N -3.77861 -0.74944 -1.32902

C -4.48337 -0.04239 -0.25570

C -5.44547 -0.97527 0.48313

C -6.21674 -0.25489 1.59365

C -7.19043 -1.17861 2.33115

N 4.60339 -2.05769 0.31716

C 3.81738 -3.22298 -0.07852

C 6.00303 -2.24681 0.67799

H -2.96409 1.85442 -1.25293

H -1.38519 3.61164 -0.55935

H 0.10571 -1.13304 -0.83938

H 4.79767 2.44628 1.06393

H 5.85079 0.23240 1.02659

H 2.09509 -1.47120 -0.31212

H -4.28686 -1.51967 -1.74842

H -3.74484 0.35184 0.44546

H -5.03906 0.81259 -0.66263

H -6.15825 -1.40532 -0.23430

H -4.87634 -1.81283 0.90688

H -5.50298 0.17394 2.30948

H -6.76804 0.59064 1.16149

H -7.72781 -0.64186 3.11992

H -7.93407 -1.59594 1.64231

H -6.66005 -2.01723 2.79699

H 2.95788 -3.35528 0.58701

H 3.45566 -3.11626 -1.10683

H 4.44521 -4.10811 -0.01894

H 6.65291 -1.66053 0.01874

H 6.17990 -1.93088 1.71228

H 6.25787 -3.29870 0.58124

Optimized geometry of 4a in the S1 state in methanol

C -1.95151 1.58020 -0.97447

C -1.07702 2.56939 -0.60020

C 0.28149 2.25433 -0.25483

C 0.70677 0.87995 -0.34469

C -0.19612 -0.09936 -0.74694

C -1.53980 0.21653 -1.04533

N 1.08619 3.26579 0.12458

N 2.36480 3.06633 0.45698

C 2.85945 1.77339 0.40263

C 2.09245 0.65199 0.01378

C 4.22417 1.57763 0.76227

C 4.81419 0.33636 0.74166

C 4.05105 -0.80548 0.35032

C 2.69055 -0.62076 -0.01000

C -2.42374 -0.86736 -1.50870

O -1.96153 -1.87293 -2.09907

N -3.77824 -0.75271 -1.32699

C -4.48456 -0.04282 -0.25656

C -5.44980 -0.97303 0.48156

C -6.22304 -0.24971 1.58880

C -7.19978 -1.17084 2.32549

N 4.60635 -2.05588 0.31852

C 3.82115 -3.22187 -0.07652

C 6.00604 -2.24377 0.67958

H -2.96337 1.85009 -1.25468

H -1.38488 3.60918 -0.56480

H 0.10677 -1.13589 -0.83393

H 4.79794 2.44942 1.05952

H 5.85269 0.23600 1.02439

H 2.09728 -1.47159 -0.30999

H -4.28529 -1.52533 -1.74345

H -3.74724 0.35168 0.44578

H -5.03814 0.81230 -0.66614

H -6.16131 -1.40348 -0.23693

H -4.88290 -1.81062 0.90824

H -5.51060 0.17956 2.30568

H -6.77216 0.59576 1.15374

H -7.73850 -0.63201 3.11192

H -7.94221 -1.58850 1.63553

H -6.67169 -2.00931 2.79420

H 2.96209 -3.35490 0.58948

H 3.45865 -3.11566 -1.10462

H 4.44977 -4.10647 -0.01722

H 6.65574 -1.65869 0.01906

H 6.18297 -1.92560 1.71317

H 6.26124 -3.29580 0.58504

Optimized geometry at the first excited state, CAM-B3LYP/6-31+G(d,p)

Optimized geometry of 4a in the S1 state in toluene

C -1.94872 1.47716 -1.09945

C -1.09281 2.51719 -0.79658

C 0.21958 2.23029 -0.37928

C 0.69524 0.87977 -0.32030

C -0.19833 -0.12626 -0.65357

C -1.52293 0.14332 -1.01637

N 1.13717 3.18668 -0.11442

N 2.23679 3.01580 0.45056

C 2.88209 1.79559 0.41297

C 2.11178 0.66876 0.02403

C 4.21170 1.64022 0.80949

C 4.79732 0.38986 0.80978

C 4.06604 -0.75729 0.42093

C 2.72243 -0.58057 0.03329

C -2.37725 -1.01513 -1.40103

O -1.88079 -2.00880 -1.94190

N -3.71837 -0.96339 -1.17080

C -4.46906 -0.12846 -0.23964

C -5.49404 -0.95632 0.52961

C -6.33309 -0.10889 1.48396

C -7.36710 -0.93081 2.24929

N 4.64370 -2.00728 0.43114

C 3.92655 -3.13401 -0.13461

C 6.06738 -2.13863 0.67403

H -2.95521 1.70793 -1.42952

H -1.41180 3.55027 -0.86694

H 0.11889 -1.16251 -0.65543

H 4.77993 2.51553 1.10345

H 5.83270 0.30444 1.11027

H 2.13514 -1.44079 -0.25448

H -4.19590 -1.78308 -1.52494

H -3.77115 0.33620 0.45995

H -4.98284 0.68017 -0.77547

H -6.15872 -1.46345 -0.18281

H -4.97243 -1.74247 1.08875

H -5.67005 0.39945 2.19487

H -6.84052 0.68135 0.91683

H -7.95332 -0.30205 2.92537

H -8.06415 -1.42432 1.56401

H -6.88568 -1.70897 2.85053

H 2.98871 -3.31719 0.40000

H 3.69244 -2.98887 -1.19836

H 4.53905 -4.02938 -0.03877

H 6.67164 -1.62265 -0.08540

H 6.34044 -1.74211 1.65723

H 6.33351 -3.19465 0.66118

Optimized geometry of 4a in the S1 state in chloroform

C -1.95264 1.51173 -1.10037

C -1.09326 2.54227 -0.77297

C 0.21611 2.24335 -0.35903

C 0.68908 0.89287 -0.33196

C -0.20435 -0.10520 -0.69315

C -1.52760 0.17631 -1.04913

N 1.14179 3.19692 -0.08749

N 2.21248 2.99698 0.53878

C 2.87038 1.78722 0.43767

C 2.10940 0.67368 -0.00645

C 4.19369 1.61659 0.85368

C 4.78470 0.37067 0.80754

C 4.06827 -0.75875 0.34047

C 2.72187 -0.57357 -0.03989

C -2.38858 -0.96776 -1.46476

O -1.90017 -1.93179 -2.06877

N -3.71823 -0.93566 -1.19311

C -4.45240 -0.12487 -0.22667

C -5.45067 -0.97707 0.55091

C -6.27013 -0.15472 1.54349

C -7.27732 -0.99989 2.31922

N 4.66261 -1.99362 0.26455

C 3.87751 -3.15471 -0.10953

C 6.00492 -2.18507 0.78104

H -2.95974 1.75143 -1.42220

H -1.41108 3.57727 -0.81774

H 0.11484 -1.14042 -0.72255

H 4.75127 2.47802 1.20418

H 5.81183 0.27222 1.13165

H 2.13662 -1.42739 -0.35019

H -4.20998 -1.73412 -1.57579

H -3.74009 0.33092 0.46367

H -4.98427 0.68891 -0.73543

H -6.12998 -1.47481 -0.15404

H -4.90871 -1.76966 1.08077

H -5.59223 0.34467 2.24662

H -6.79828 0.64207 1.00533

H -7.85007 -0.38893 3.02267

H -7.98835 -1.48532 1.64255

H -6.77406 -1.78567 2.89208

H 3.06807 -3.35589 0.60536

H 3.43457 -3.03234 -1.10349

H 4.52698 -4.02793 -0.14144

H 6.72664 -1.54392 0.26396

H 6.06867 -1.97677 1.85747

H 6.30414 -3.21893 0.61696

Optimized geometry of 4a in the S1 state in chloroform

C -1.95264 1.51173 -1.10037

C -1.09326 2.54227 -0.77297

C 0.21611 2.24335 -0.35903

C 0.68908 0.89287 -0.33196

C -0.20435 -0.10520 -0.69315

C -1.52760 0.17631 -1.04913

N 1.14179 3.19692 -0.08749

N 2.21248 2.99698 0.53878

C 2.87038 1.78722 0.43767

C 2.10940 0.67368 -0.00645

C 4.19369 1.61659 0.85368

C 4.78470 0.37067 0.80754

C 4.06827 -0.75875 0.34047

C 2.72187 -0.57357 -0.03989

C -2.38858 -0.96776 -1.46476

O -1.90017 -1.93179 -2.06877

N -3.71823 -0.93566 -1.19311

C -4.45240 -0.12487 -0.22667

C -5.45067 -0.97707 0.55091

C -6.27013 -0.15472 1.54349

C -7.27732 -0.99989 2.31922

N 4.66261 -1.99362 0.26455

C 3.87751 -3.15471 -0.10953

C 6.00492 -2.18507 0.78104

H -2.95974 1.75143 -1.42220

H -1.41108 3.57727 -0.81774

H 0.11484 -1.14042 -0.72255

H 4.75127 2.47802 1.20418

H 5.81183 0.27222 1.13165

H 2.13662 -1.42739 -0.35019

H -4.20998 -1.73412 -1.57579

H -3.74009 0.33092 0.46367

H -4.98427 0.68891 -0.73543

H -6.12998 -1.47481 -0.15404

H -4.90871 -1.76966 1.08077

H -5.59223 0.34467 2.24662

H -6.79828 0.64207 1.00533

H -7.85007 -0.38893 3.02267

H -7.98835 -1.48532 1.64255

H -6.77406 -1.78567 2.89208

H 3.06807 -3.35589 0.60536

H 3.43457 -3.03234 -1.10349

H 4.52698 -4.02793 -0.14144

H 6.72664 -1.54392 0.26396

H 6.06867 -1.97677 1.85747

H 6.30414 -3.21893 0.61696

Optimized geometry of 4a in the S1 state in DMSO

C -1.94565 1.52730 -0.95961

C -1.07221 2.52554 -0.62328

C 0.29159 2.22948 -0.28349

C 0.71735 0.85573 -0.34070

C -0.18519 -0.12624 -0.70532

C -1.52802 0.17372 -0.99744

N 1.08396 3.24403 0.05499

N 2.38459 3.04073 0.38485

C 2.87468 1.78692 0.35924

C 2.11522 0.63266 0.00673

C 4.25437 1.60314 0.71091

C 4.84673 0.37543 0.71423

C 4.09351 -0.78655 0.36012

C 2.71603 -0.61183 0.00946

C -2.40184 -0.93647 -1.43290

O -1.92243 -1.91844 -2.03231

N -3.74012 -0.87835 -1.20357

C -4.47855 -0.09464 -0.21679

C -5.52751 -0.95452 0.48138

C -6.35421 -0.15940 1.48989

C -7.41275 -1.01149 2.18564

N 4.65076 -2.01442 0.35258

C 3.87579 -3.19600 -0.01234

C 6.05385 -2.18703 0.70789

H -2.96183 1.78827 -1.23177

H -1.38420 3.56426 -0.61022

H 0.11921 -1.16423 -0.77161

H 4.82245 2.48745 0.97906

H 5.88926 0.28984 0.98736

H 2.13117 -1.47922 -0.25963

H -4.23641 -1.66233 -1.60970

H -3.77477 0.29896 0.51952

H -4.96906 0.76173 -0.69551

H -6.19704 -1.39111 -0.27149

H -5.02830 -1.79082 0.98562

H -5.68541 0.27951 2.24041

H -6.83883 0.68116 0.97823

H -7.99006 -0.42035 2.90231

H -8.11461 -1.43662 1.46049

H -6.95335 -1.84260 2.73088

H 3.03031 -3.33539 0.66779

H 3.50020 -3.11690 -1.03680

H 4.51748 -4.07036 0.05259

H 6.69964 -1.62688 0.02445

H 6.24075 -1.84405 1.73016

H 6.30953 -3.24089 0.64250

Optimized geometry of 4a in the S1 state in methanol

C -1.94536 1.52477 -0.96029

C -1.07219 2.52371 -0.62555

C 0.29160 2.22845 -0.28498

C 0.71768 0.85475 -0.34030

C -0.18469 -0.12807 -0.70304

C -1.52761 0.17106 -0.99551

N 1.08363 3.24369 0.05227

N 2.38392 3.04131 0.38284

C 2.87463 1.78756 0.35797

C 2.11571 0.63277 0.00656

C 4.25444 1.60476 0.70938

C 4.84750 0.37731 0.71331

C 4.09485 -0.78517 0.36005

C 2.71729 -0.61149 0.00979

C -2.40101 -0.94036 -1.42845

O -1.92113 -1.92473 -2.02322

N -3.73997 -0.88079 -1.20182

C -4.47952 -0.09500 -0.21761

C -5.52976 -0.95319 0.48073

C -6.35806 -0.15590 1.48620

C -7.41775 -1.00642 2.18209

N 4.65281 -2.01295 0.35301

C 3.87841 -3.19493 -0.01161

C 6.05582 -2.18468 0.70876

H -2.96147 1.78511 -1.23327

H -1.38414 3.56245 -0.61434

H 0.11983 -1.16610 -0.76790

H 4.82199 2.48966 0.97670

H 5.89020 0.29248 0.98610

H 2.13273 -1.47931 -0.25861

H -4.23531 -1.66647 -1.60576

H -3.77673 0.29985 0.51900

H -4.96913 0.76067 -0.69855

H -6.19812 -1.39134 -0.27231

H -5.03150 -1.78852 0.98752

H -5.69046 0.28463 2.23684

H -6.84181 0.68361 0.97198

H -7.99621 -0.41371 2.89654

H -8.11848 -1.43311 1.45676

H -6.95930 -1.83636 2.72988

H 3.03362 -3.33533 0.66923

H 3.50170 -3.11580 -1.03566

H 4.52081 -4.06887 0.05229

H 6.70166 -1.62504 0.02491

H 6.24249 -1.84058 1.73071

H 6.31195 -3.23853 0.64455

Table of 100rst electronic transitions with PBE0/6-31+G(d,p) levels of theory

100 first electronic transitions of 4a in toluene

HOMO is 86					
No.	Energy (cm-1)	Wavelength (nm)	Osc. Strength	Symmetry	Major contribs
1	24943.5022713	400.906011163	0.0025	Singlet-A	H-1->LUMO (97%)
2	25952.5018619	385.319305753	0.4186	Singlet-A	HOMO->LUMO (97%)
3	29682.8160961	336.895258443	0.0122	Singlet-A	H-2->LUMO (22%), HOMO->L+1 (76%)
4	33322.7962341	300.09486388	0.0629	Singlet-A	H-2->LUMO (70%), HOMO->L+1 (20%)
5	33463.9432592	298.829098607	0.0001	Singlet-A	H-1->L+1 (97%)
6	35273.0448435	283.502602182	0.0669	Singlet-A	H-5->LUMO (10%), H-3->LUMO (73%)
7	37294.2702425	268.137704129	0.0873	Singlet-A	H-4->LUMO (48%), HOMO->L+2 (37%)
8	37709.6457735	265.184140421	0.049	Singlet-A	H-5->LUMO (19%), H-4->LUMO (41%), HOMO->L+2 (28%)
9	39288.072791	254.530173908	0.4254	Singlet-A	H-5->LUMO (25%), H-2->L+1 (38%), HOMO->L+2 (23%)
10	39710.7073118	251.821251167	0.0013	Singlet-A	H-1->L+2 (93%)
11	40172.0564452	248.929252941	0.4804	Singlet-A	H-5->LUMO (20%), H-3->L+1 (18%), H-2->L+1 (37%)
12	40756.8084062	245.357779253	0.3247	Singlet-A	H-3->L+1 (43%), H-2->L+1 (16%), H-2->L+2 (11%)
13	41402.0519494	241.533922333	0.0309	Singlet-A	HOMO->L+3 (92%)
14	42525.582269	235.15257091	0.0058	Singlet-A	H-4->L+1 (58%), H-3->L+1 (23%)
15	43698.3124088	228.841789277	0.107	Singlet-A	H-5->L+1 (10%), H-4->L+1 (29%), H-2->L+2 (16%), HOMO->L+4 (15%), HOMO->L+5 (17%)
16	44550.0338858	224.466720399	0.0251	Singlet-A	H-8->LUMO (71%)
17	44721.8299792	223.604445629	0.0387	Singlet-A	H-8->LUMO (12%), H-6->LUMO (31%), H-5->L+1 (27%), HOMO->L+4 (15%)
18	44939.599675	222.520896321	0.1105	Singlet-A	H-2->L+2 (43%), HOMO->L+4 (25%)
19	45503.3812209	219.763888566	0.0069	Singlet-A	HOMO->L+4 (13%), HOMO->L+5 (32%), HOMO->L+6 (12%), HOMO->L+7 (21%)

20	45775.1900635	218.458950932	0.1394	Singlet-A	H-6->LUMO (12%), H-5->L+1 (24%), H-3->L+2 (27%)
21	46144.5919919	216.710118528	0.0893	Singlet-A	H-6->LUMO (15%), H-5->L+1 (17%), H-3->L+2 (13%), HOMO->L+6 (13%)
22	46454.3088927	215.265284069	0.0357	Singlet-A	HOMO->L+5 (14%), HOMO->L+6 (20%), HOMO->L+10 (15%)
23	47619.7800426	209.996770062	0.0034	Singlet-A	H-1->L+4 (26%), H-1->L+5 (56%)
24	47813.3531055	209.146595051	0.0169	Singlet-A	HOMO->L+8 (44%), HOMO->L+9 (16%), HOMO->L+10 (20%)
25	47918.2051813	208.688951562	0.0017	Singlet-A	HOMO->L+6 (21%), HOMO->L+7 (30%), HOMO->L+11 (31%)
26	48176.3025986	207.570931363	0.0011	Singlet-A	HOMO->L+10 (52%)
27	48621.5206434	205.670243704	0.1592	Singlet-A	H-7->LUMO (64%), H-4->L+2 (13%)
28	49343.3868574	202.661402812	0.0224	Singlet-A	H-4->L+2 (43%), HOMO->L+11 (15%)
29	49378.8752522	202.515750894	0.0087	Singlet-A	H-4->L+2 (27%), HOMO->L+6 (14%), HOMO->L+7 (10%), HOMO->L+11 (21%)
30	49531.3140393	201.892483451	0.0044	Singlet-A	H-1->L+3 (61%)
31	49795.0573376	200.823144599	0.0112	Singlet-A	HOMO->L+8 (16%), HOMO->L+9 (40%), HOMO->L+12 (25%), HOMO->L+14 (10%)
32	50233.822947	199.069061707	0.008	Singlet-A	H-5->L+2 (50%), H-3->L+2 (19%)
33	50632.2608349	197.502537613	0.0222	Singlet-A	HOMO->L+8 (10%), HOMO->L+9 (18%), HOMO->L+14 (50%)
34	50805.6700371	196.828424715	0.0309	Singlet-A	H-6->L+1 (18%), H-2->L+3 (60%)
35	50992.7906647	196.106152843	0.0065	Singlet-A	H-6->L+1 (14%), H-2->L+3 (12%), H-1->L+4 (16%), H-1->L+8 (15%), H-1->L+9 (11%)
36	51150.0687783	195.503158429	0.0323	Singlet-A	H-6->L+1 (33%), H-1->L+8 (14%)
37	51325.8976438	194.833416639	0.0111	Singlet-A	HOMO->L+12 (15%), HOMO->L+13 (18%), HOMO->L+15 (26%), HOMO->L+16 (10%)
38	51617.0637927	193.734382881	0.0024	Singlet-A	HOMO->L+12 (26%), HOMO->L+14 (26%), HOMO->L+15 (20%)
39	51644.4866433	193.631511318	0.0094	Singlet-A	H-1->L+4 (23%), H-1->L+5 (17%), H-1->L+6 (10%)
40	52345.3824421	191.038818201	0.0039	Singlet-A	H-8->L+1 (77%)
41	52584.9291075	190.16855532	0.0037	Singlet-A	H-3->L+3 (15%), H-3->L+4 (14%), H-2->L+4 (13%)
42	52635.7420365	189.984972437	0.031	Singlet-A	H-7->L+1 (10%), H-2->L+4 (31%), H-1->L+6 (18%)
43	52831.7347628	189.280174972	0.0157	Singlet-A	H-3->L+4 (12%)
44	53224.5267697	187.883305065	0.0398	Singlet-A	H-7->L+1 (21%), H-2->L+4 (15%), H-2->L+5 (35%)

45	53325.3460733	187.528084417	0.01	Singlet-A	HOMO->L+13 (31%), HOMO->L+15 (23%), HOMO->L+17 (10%)
46	53921.3897964	185.455160517	0.0435	Singlet-A	H-4->L+4 (10%), H-3->L+3 (16%)
47	54035.9205253	185.062082829	0.0325	Singlet-A	HOMO->L+16 (11%)
48	54243.2050135	184.354888276	0.0058	Singlet-A	H-1->L+7 (20%), H-1->L+8 (12%), HOMO->L+16 (16%)
49	54300.470378	184.160467311	0.0347	Singlet-A	H-1->L+7 (13%), HOMO->L+16 (17%), HOMO->L+17 (10%)
50	54698.9082659	182.819005297	0.0021	Singlet-A	H-9->LUMO (57%), H-1->L+6 (10%)
51	54741.6556507	182.676243185	0.0021	Singlet-A	H-9->LUMO (39%), H-1->L+6 (17%), H-1->L+7 (15%), H-1->L+10 (15%)
52	54819.8914303	182.415538212	0.0111	Singlet-A	H-2->L+6 (40%), H-2->L+7 (16%)
53	54969.9105541	181.917705508	0.1679	Singlet-A	H-2->L+8 (29%), H-2->L+9 (10%)
54	55206.2310018	181.138973238	0.0037	Singlet-A	HOMO->L+16 (13%), HOMO->L+17 (36%)
55	55511.9151304	180.141506135	0.0045	Singlet-A	H-12->LUMO (10%), H-3->L+3 (14%), H-3->L+4 (15%)
56	55542.5641987	180.042101842	0.0137	Singlet-A	H-12->LUMO (35%)
57	55635.317958	179.741940318	0.0075	Singlet-A	H-12->LUMO (22%), H-1->L+8 (12%), H-1->L+9 (31%)
58	55892.6088208	178.914532905	0.021	Singlet-A	H-3->L+4 (14%), H-3->L+6 (17%)
59	55962.7790562	178.690196746	0.2196	Singlet-A	HOMO->L+19 (30%)
60	56054.7262611	178.397089184	0.0015	Singlet-A	H-4->L+6 (14%), H-3->L+5 (15%), H-3->L+6 (18%), H-2->L+7 (14%)
61	56140.2210305	178.125411985	0.0147	Singlet-A	H-3->L+5 (20%)
62	56215.2305924	177.887734242	0.1471	Singlet-A	H-7->L+1 (17%), H-2->L+5 (10%), H-2->L+7 (11%)
63	56510.4295135	176.958485117	0.0034	Singlet-A	H-4->L+3 (19%), H-4->L+6 (14%), H-2->L+10 (20%)
64	56645.9306575	176.535187681	0.0163	Singlet-A	HOMO->L+18 (34%), HOMO->L+20 (13%)
65	56747.5565156	176.219041207	0.007	Singlet-A	H-4->L+3 (15%), HOMO->L+18 (11%), HOMO->L+20 (23%)
66	56789.4973459	176.088897901	0.0059	Singlet-A	H-15->LUMO (25%)
67	56807.2415433	176.033895122	0.0094	Singlet-A	H-15->LUMO (10%), H-1->L+11 (25%)
68	56905.6411837	175.729502243	0.003	Singlet-A	H-1->L+11 (22%), HOMO->L+20 (16%)
69	57023.3981303	175.366609635	0.0162	Singlet-A	H-6->L+2 (31%)

70	57183.9024617	174.874388937	0.0017	Singlet-A	H-4->L+6 (15%)
71	57294.4004184	174.537126263	0.0071	Singlet-A	H-10->LUMO (81%)
72	57501.6849067	173.907947501	0.0151	Singlet-A	H-1->L+9 (12%), H-1->L+12 (26%), H-1->L+13 (16%), H-1->L+15 (15%)
73	57575.8879142	173.683817346	0.0176	Singlet-A	HOMO->L+21 (22%), HOMO->L+22 (21%), HOMO->L+25 (14%)
74	57650.8974761	173.457837394	0.0479	Singlet-A	H-4->L+4 (11%), H-4->L+5 (52%)
75	57752.5233341	173.152607413	0.0079	Singlet-A	H-2->L+9 (19%), HOMO->L+21 (16%), HOMO->L+24 (10%)
76	57791.2379467	173.036611696	0.0307	Singlet-A	H-2->L+9 (24%)
77	57938.8374072	172.595800114	0.0087	Singlet-A	H-1->L+12 (42%), H-1->L+13 (17%), H-1->L+14 (13%)
78	58045.3025918	172.279229386	0.0021	Singlet-A	H-3->L+7 (14%), H-2->L+11 (22%)
79	58393.7341052	171.251250725	0.0038	Singlet-A	H-3->L+8 (13%), H-2->L+11 (15%)
80	58542.1401201	170.817123861	0.0065	Singlet-A	H-5->L+3 (24%), H-3->L+7 (10%)
81	58624.4086719	170.577413513	0.0066	Singlet-A	H-1->L+13 (24%), H-1->L+14 (19%)
82	58683.2871452	170.406268743	0.004	Singlet-A	H-4->L+8 (11%), HOMO->L+23 (31%)
83	58758.2967071	170.188731812	0.0016	Singlet-A	H-11->LUMO (33%), H-8->L+2 (31%)
84	58775.2343501	170.139687414	0.0154	Singlet-A	H-5->L+4 (13%), H-4->L+9 (12%)
85	59112.3741014	169.169317795	0.0048	Singlet-A	HOMO->L+22 (17%), HOMO->L+24 (24%), HOMO->L+27 (13%)
86	59168.026357	169.010200537	0.0014	Singlet-A	H-15->LUMO (15%), H-11->LUMO (20%), H-8->L+2 (21%)
87	59201.0950886	168.915794295	0.0306	Singlet-A	H-4->L+8 (24%), H-1->L+14 (20%), H-1->L+15 (16%)
88	59376.9239541	168.415595387	0.0216	Singlet-A	H-4->L+8 (14%), H-1->L+15 (23%)
89	59504.3595539	168.054913539	0.002	Singlet-A	
90	59568.0773538	167.875151327	0.053	Singlet-A	H-2->L+12 (30%)
91	59768.1028522	167.313324713	0.0068	Singlet-A	H-5->L+5 (11%), H-2->L+12 (18%)
92	59896.3450064	166.955095489	0.0108	Singlet-A	H-4->L+9 (12%), H-3->L+10 (13%), H-2->L+12 (12%)
93	60133.4720085	166.296734015	0.0119	Singlet-A	H-1->L+16 (15%), H-1->L+19 (23%)
94	60183.4783831	166.158558273	0.001	Singlet-A	H-5->L+4 (11%), H-4->L+9 (11%)

95	**60259.2944994**	**165.949503443**	**0.0072**	**Singlet-A**	**H-3->L+10 (10%), H-2->L+13 (15%), HOMO->L+25 (12%)**
96	**60352.0482588**	**165.694459236**	**0.0039**	**Singlet-A**	**H-2->L+13 (12%)**
97	**60397.2153068**	**165.570547404**	**0.0097**	**Singlet-A**	**H-9->L+1 (73%)**
98	**60475.4510864**	**165.356352377**	**0.0164**	**Singlet-A**	**H-9->L+1 (13%), H-2->L+14 (13%), HOMO->L+25 (19%)**
99	**60527.8771243**	**165.213129472**	**0.0082**	**Singlet-A**	**H-2->L+14 (34%), HOMO->L+25 (11%)**
100	**60601.2735773**	**165.013033715**	**0.0016**	**Singlet-A**	**H-12->L+1 (46%)**

100 first electronic transitions of 4a in $CHCl_3$

HOMO is 86						
No.	Energy (cm-1)	Wavelength (nm)	Osc. Strength	Symmetry	Major contribs	Minor contribs
1	25437.92 01362	393.1139 00289	0.00 53	Singlet-A	H-1->LUMO (97%)	
2	25580.68 02702	390.9200 18326	0.41 18	Singlet-A	HOMO->LUMO (97%)	
3	29471.49 88357	339.3108 73049	0.01 2	Singlet-A	H-2->LUMO (21%), HOMO->L+1 (77%)	
4	33110.67 24193	302.0174 24272	0.06 38	Singlet-A	H-2->LUMO (72%), HOMO->L+1 (20%)	H-3->LUMO (2%), H-3->L+1 (2%)
5	34196.29 46807	292.4293 43394	0.0	Singlet-A	H-1->L+1 (97%)	H-1->L+2 (2%)
6	35438.38 85014	282.1798 73941	0.06 92	Singlet-A	H-3->LUMO (72%)	H-5->LUMO (8%), H-5->L+2 (3%), H-4->LUMO (3%), HOMO->L+2 (7%)
7	37119.24 79314	269.4020 09935	0.07 74	Singlet-A	H-4->LUMO (61%), HOMO->L+2 (25%)	H-5->LUMO (3%), H-3->LUMO (6%), H-2->L+1 (2%)
8	37545.10 867	266.3462 79296	0.07 82	Singlet-A	H-5->LUMO (19%), H-4->LUMO (29%), HOMO->L+2 (42%)	H-2->L+1 (2%)
9	39238.06 64164	254.8545 56131	0.34 43	Singlet-A	H-5->LUMO (33%), H-2->L+1 (32%), HOMO->L+2 (20%)	H-4->LUMO (2%), H-3->LUMO (6%)
10	40210.77 10578	248.6895 85823	0.49 28	Singlet-A	H-5->LUMO (16%), H-3->L+1 (17%), H-2->L+1 (42%)	H-6->LUMO (5%), H-4->L+1 (2%), H-3->LUMO (5%), HOMO->L+4 (2%)
11	40459.99 63764	247.1577 0874	0.00 92	Singlet-A	H-1->L+2 (92%)	H-1->L+1 (2%)
12	40863.27 35909	244.7185 24025	0.31 86	Singlet-A	H-3->L+1 (39%), H-2->L+1 (17%), H-2->L+2 (12%)	H-6->LUMO (6%), H-5->LUMO (7%), H-4->LUMO (2%), H-4->L+1 (4%), H-3->LUMO (2%), HOMO->L+4 (2%), HOMO->L+5 (2%)

13	41893.2435967	238.701975342	0.0296	Singlet-A	HOMO->L+3 (85%), HOMO->L+4 (10%)	
14	42571.5558715	234.898626449	0.0044	Singlet-A	H-4->L+1 (64%), H-3->L+1 (24%)	H-6->LUMO (2%), H-2->L+2 (3%), HOMO->L+4 (3%)
15	43636.2077178	229.167485513	0.1158	Singlet-A	H-4->L+1 (23%), H-2->L+2 (13%), HOMO->L+4 (30%), HOMO->L+5 (12%)	H-7->LUMO (2%), H-5->L+1 (6%), H-3->L+1 (8%), HOMO->L+3 (2%)
16	44653.2728527	223.947750325	0.0623	Singlet-A	H-8->LUMO (33%), H-6->LUMO (31%), H-5->L+1 (20%)	H-2->L+2 (6%), HOMO->L+4 (3%)
17	44745.2200576	223.48755883	0.0022	Singlet-A	H-8->LUMO (33%), H-6->LUMO (13%), HOMO->L+4 (15%)	H-5->L+1 (8%), H-4->L+1 (2%), H-3->L+1 (2%), H-3->L+2 (6%), H-2->L+2 (7%), HOMO->L+5 (3%)
18	44943.6324472	222.50092962	0.1232	Singlet-A	H-8->LUMO (23%), H-2->L+2 (43%), HOMO->L+4 (11%)	H-6->LUMO (4%), H-6->L+1 (3%), H-5->L+1 (3%), HOMO->L+5 (2%), HOMO->L+7 (3%)
19	45745.3475496	218.601465191	0.0093	Singlet-A	HOMO->L+4 (14%), HOMO->L+5 (40%), HOMO->L+8 (18%)	H-3->L+2 (8%), HOMO->L+3 (3%), HOMO->L+6 (3%), HOMO->L+7 (2%)
20	45928.435405	217.730038305	0.1315	Singlet-A	H-5->L+1 (31%), H-3->L+2 (20%), HOMO->L+5 (11%)	H-6->LUMO (9%), H-5->LUMO (2%), H-5->L+2 (4%), H-5->L+7 (2%), H-3->LUMO (2%), H-3->L+1 (2%), H-2->L+2 (2%), HOMO->L+8 (3%)
21	46189.75904	216.498206699	0.0737	Singlet-A	H-6->LUMO (10%), H-5->L+1 (17%), H-3->L+2 (11%), HOMO->L+6 (22%), HOMO->L+7 (14%)	H-7->LUMO (4%), H-5->LUMO (2%), H-3->L+7 (2%), HOMO->L+8 (5%), HOMO->L+10 (2%)
22	46516.4135837	214.977880485	0.045	Singlet-A	H-3->L+2 (10%), HOMO-	H-7->LUMO (2%), H-6->LUMO (8%), H-5->L+1 (6%), HOMO->L+4 (2%), HOMO->L+5 (9%), HOMO->L+8 (5%)

					>L+6 (34%), HOMO->L+10 (15%)	
23	47526.2197288	210.410170577	0.0202	Singlet-A	HOMO->L+7 (69%)	H-6->LUMO (3%), H-6->L+1 (2%), H-3->L+2 (8%), HOMO->L+6 (2%), HOMO->L+10 (8%)
24	48188.400915	207.518818017	0.005	Singlet-A	HOMO->L+8 (43%), HOMO->L+11 (23%)	H-7->LUMO (3%), HOMO->L+3 (3%), HOMO->L+5 (4%), HOMO->L+6 (8%), HOMO->L+12 (4%), HOMO->L+13 (7%)
25	48309.3840794	206.999120162	0.0038	Singlet-A	H-1->L+4 (44%), H-1->L+5 (36%)	H-1->L+3 (8%), H-1->L+7 (7%)
26	48443.2721146	206.427013773	0.1343	Singlet-A	H-7->LUMO (68%)	H-6->LUMO (2%), H-5->L+1 (2%), H-5->L+2 (5%), H-4->L+2 (7%), H-2->L+2 (2%), HOMO->L+11 (2%)
27	48715.0809572	205.275241332	0.0018	Singlet-A	HOMO->L+10 (63%)	HOMO->L+4 (2%), HOMO->L+5 (6%), HOMO->L+6 (9%), HOMO->L+7 (4%), HOMO->L+11 (3%), HOMO->L+12 (5%), HOMO->L+13 (4%)
28	49311.9312346	202.790678638	0.0446	Singlet-A	H-4->L+2 (84%)	H-7->LUMO (8%)
29	49754.7296162	200.985917864	0.0023	Singlet-A	HOMO->L+6 (17%), HOMO->L+8 (19%), HOMO->L+11 (33%), HOMO->L+13 (10%)	HOMO->L+12 (7%), HOMO->L+14 (4%)
30	50073.3186156	199.707154957	0.0126	Singlet-A	HOMO->L+9 (47%), HOMO->L+12 (29%)	HOMO->L+11 (3%), HOMO->L+14 (5%), HOMO->L+15 (5%)
31	50262.8589064	198.954063051	0.0018	Singlet-A	H-5->L+2 (23%), H-3->L+2 (11%), H-1->L+3 (28%)	H-5->L+7 (2%), H-3->L+7 (2%), H-1->L+5 (5%), H-1->L+6 (8%), H-1->L+7 (2%), H-1->L+10 (4%), H-1->L+11 (2%), HOMO->L+9 (3%)
32	50399.9731594	198.412804078	0.0077	Singlet-A	H-5->L+2 (26%), H-3->L+2 (11%), H-1->L+3 (27%)	H-7->LUMO (3%), H-6->L+1 (5%), H-3->L+7 (2%), H-1->L+5 (3%), H-1->L+6 (6%), H-1->L+7 (2%), H-1->L+10 (4%)

33	**51032.3118317**	**195.954281534**	**0.0834**	**Singlet-A**	**H-6->L+1 (39%), HOMO->L+9 (11%), HOMO->L+14 (15%), HOMO->L+15 (10%)**	**H-2->L+3 (4%), H-2->L+4 (3%), H-2->L+5 (2%), H-1->L+3 (2%), HOMO->L+12 (3%), HOMO->L+16 (2%)**
34	**51118.6131556**	**195.623460471**	**0.0183**	**Singlet-A**	**H-6->L+1 (18%), H-2->L+3 (16%), HOMO->L+9 (24%), HOMO->L+14 (17%)**	**H-2->L+4 (3%), HOMO->L+12 (5%), HOMO->L+15 (5%), HOMO->L+16 (2%)**
35	**51375.097464**	**194.64683268**	**0.0041**	**Singlet-A**	**H-2->L+3 (42%), HOMO->L+15 (13%)**	**H-6->L+1 (8%), H-2->L+4 (2%), H-2->L+5 (3%), H-2->L+10 (2%), HOMO->L+9 (2%), HOMO->L+10 (2%), HOMO->L+11 (6%), HOMO->L+13 (7%), HOMO->L+16 (2%)**
36	**51588.8343877**	**193.840394316**	**0.0098**	**Singlet-A**	**H-2->L+3 (26%), HOMO->L+13 (17%), HOMO->L+15 (17%)**	**HOMO->L+10 (2%), HOMO->L+11 (9%), HOMO->L+12 (3%), HOMO->L+14 (8%), HOMO->L+16 (8%)**
37	**51804.1844202**	**193.034599655**	**0.0019**	**Singlet-A**	**H-8->L+1 (12%), H-1->L+4 (10%), H-1->L+7 (61%)**	**H-1->L+10 (5%), H-1->L+19 (3%)**
38	**51936.4593466**	**192.542967422**	**0.0007**	**Singlet-A**	**HOMO->L+12 (29%), HOMO->L+14 (39%)**	**HOMO->L+8 (2%), HOMO->L+9 (8%), HOMO->L+11 (6%), HOMO->L+13 (5%), HOMO->L+17 (4%)**
39	**52630.90271**	**190.002441248**	**0.0056**	**Singlet-A**	**H-8->L+1 (71%)**	**H-7->L+1 (6%), H-2->L+4 (3%), H-1->L+4 (7%), H-1->L+7 (6%)**
40	**52709.1384896**	**189.720422047**	**0.0351**	**Singlet-A**	**H-7->L+1 (21%), H-2->L+4 (26%), H-1->L+4 (10%)**	**H-8->L+1 (4%), H-2->L+5 (5%), H-2->L+7 (2%), H-1->L+3 (7%), H-1->L+5 (6%), H-1->L+6 (6%)**

41	52979.3342233	188.752843851	0.0138	Singlet-A	H-2->L+4 (10%), H-1->L+3 (14%), H-1->L+4 (10%), H-1->L+5 (12%), H-1->L+6 (17%)	H-8->L+1 (6%), H-7->L+1 (9%), H-2->L+7 (3%), H-1->L+7 (3%), H-1->L+10 (3%), H-1->L+11 (2%)
42	53235.8185317	187.843453446	0.007	Singlet-A	H-4->L+3 (11%), H-3->L+3 (27%), H-3->L+4 (10%)	H-4->L+4 (8%), H-4->L+5 (8%), H-4->L+6 (6%), H-4->L+8 (3%), H-3->L+5 (6%), H-3->L+6 (5%), H-1->L+5 (3%), H-1->L+6 (2%)
43	53550.374759	186.740056349	0.0109	Singlet-A	HOMO->L+13 (19%), HOMO->L+15 (31%)	H-2->L+7 (3%), HOMO->L+9 (2%), HOMO->L+11 (9%), HOMO->L+12 (6%), HOMO->L+14 (2%), HOMO->L+16 (2%), HOMO->L+17 (9%), HOMO->L+18 (2%), HOMO->L+19 (5%)
44	53613.2860045	186.520930636	0.0079	Singlet-A	H-9->LUMO (77%)	H-7->L+1 (2%), H-3->L+3 (2%), H-2->L+4 (2%), H-2->L+5 (3%), H-1->L+5 (3%)
45	53641.5154095	186.422772057	0.0206	Singlet-A	H-9->LUMO (20%), H-2->L+5 (15%), H-1->L+5 (10%)	H-7->L+1 (7%), H-4->L+3 (2%), H-3->L+3 (5%), H-2->L+4 (9%), H-1->L+3 (2%), H-1->L+4 (4%), H-1->L+6 (5%), H-1->L+8 (2%), H-1->L+10 (2%)
46	53737.4953866	186.089804299	0.0191	Singlet-A	H-2->L+5 (15%), H-1->L+5 (13%), H-1->L+6 (12%)	H-4->L+3 (8%), H-4->L+4 (4%), H-4->L+5 (2%), H-2->L+4 (8%), H-1->L+3 (4%), H-1->L+4 (6%), H-1->L+8 (4%), H-1->L+10 (6%)
47	54094.7989986	184.860655463	0.0772	Singlet-A	H-3->L+7 (10%), H-2->L+7 (24%)	H-6->L+1 (2%), H-5->L+2 (8%), H-5->L+7 (2%), H-3->L+2 (2%), H-3->L+4 (5%), H-3->L+5 (3%), H-2->L+4 (6%), H-2->L+5 (6%), HOMO->L+13 (4%), HOMO->L+15 (3%), HOMO->L+17 (2%), HOMO->L+18 (4%), HOMO->L+19 (2%)
48	54263.3688743	184.286383383	0.02	Singlet-A	HOMO->L+13 (10%), HOMO->L+16 (37%)	H-4->L+3 (6%), H-4->L+4 (2%), H-3->L+3 (8%), H-2->L+5 (2%), H-2->L+6 (7%), HOMO->L+12 (2%), HOMO->L+18 (6%)
49	54499.689322	183.487284504	0.0278	Singlet-A	H-3->L+3 (12%), H-2->L+6 (19%), HOMO->L+16 (14%)	H-4->L+3 (8%), H-4->L+4 (3%), H-4->L+5 (2%), H-2->L+4 (2%), H-2->L+5 (5%), H-2->L+7 (9%), HOMO->L+13 (6%), HOMO->L+17 (2%), HOMO->L+18 (3%)

50	55008.6251667	181.789673341	0.1182	Singlet-A	H-3->L+7 (15%), H-2->L+7 (33%)	H-6->L+1 (3%), H-5->L+2 (6%), H-5->L+7 (3%), H-3->L+4 (4%), H-3->L+5 (4%), H-3->L+6 (5%), HOMO->L+17 (3%)
51	55228.0079713	181.067548284	0.0055	Singlet-A	H-2->L+6 (41%), HOMO->L+17 (13%)	H-4->L+3 (2%), H-4->L+4 (2%), H-3->L+3 (5%), H-3->L+4 (2%), H-2->L+3 (2%), H-2->L+7 (2%), H-2->L+8 (8%), H-2->L+10 (3%), HOMO->L+23 (2%)
52	55319.9551763	180.766596215	0.0079	Singlet-A	H-12->LUMO (63%)	H-15->LUMO (2%), H-13->LUMO (8%), H-11->LUMO (7%), H-8->L+2 (5%), H-1->L+7 (2%)
53	55365.9287787	180.616495028	0.0066	Singlet-A	HOMO->L+17 (40%)	H-4->L+3 (2%), H-3->L+3 (4%), H-3->L+7 (3%), H-2->L+6 (7%), HOMO->L+13 (2%), HOMO->L+14 (2%), HOMO->L+15 (2%), HOMO->L+19 (6%), HOMO->L+20 (3%), HOMO->L+22 (2%), HOMO->L+23 (4%)
54	55578.859148	179.924528018	0.0184	Singlet-A	H-1->L+8 (25%), H-1->L+10 (10%), HOMO->L+18 (13%), HOMO->L+19 (12%)	H-1->L+6 (3%), H-1->L+11 (3%), H-1->L+12 (2%), H-1->L+13 (2%), HOMO->L+16 (7%), HOMO->L+20 (4%), HOMO->L+21 (2%)
55	55665.1604719	179.645579304	0.0725	Singlet-A	H-1->L+8 (22%), H-1->L+10 (10%), HOMO->L+18 (14%), HOMO->L+19 (14%)	H-6->L+2 (3%), H-2->L+7 (2%), H-1->L+6 (2%), H-1->L+12 (2%), H-1->L+13 (2%), HOMO->L+16 (6%), HOMO->L+20 (2%)
56	55869.2187424	178.989436851	0.0809	Singlet-A	H-3->L+4 (11%), H-1->L+6 (15%), H-1->L+10 (12%)	H-7->L+1 (4%), H-6->L+2 (4%), H-4->L+4 (4%), H-3->L+5 (5%), H-3->L+7 (5%), H-2->L+4 (3%), H-2->L+5 (4%), H-2->L+8 (2%), H-1->L+4 (2%), H-1->L+5 (2%), H-1->L+8 (8%)
57	56081.3425572	178.312421636	0.0233	Singlet-A	H-10->LUMO (22%), H-3->L+4 (15%)	H-7->L+1 (4%), H-6->L+2 (5%), H-4->L+4 (2%), H-4->L+5 (2%), H-3->L+5 (8%), H-3->L+7 (7%), H-2->L+5 (2%), H-1->L+6 (5%), H-1->L+8 (4%), H-1->L+10 (8%)
58	56205.5519393	177.918366691	0.0725	Singlet-A	H-10->LUMO (51%)	H-7->L+1 (5%), H-6->L+2 (4%), H-5->L+3 (2%), H-3->L+3 (2%), H-3->L+4

						(3%), H-3->L+6 (4%), H-2->L+5 (6%), H-2->L+8 (6%)
59	56232.1682355	177.834152831	0.136	Singlet-A	H-10->LUMO (12%), H-7->L+1 (14%), H-2->L+5 (11%), H-1->L+8 (11%)	H-6->L+1 (2%), H-5->L+7 (3%), H-3->L+7 (2%), H-2->L+4 (4%), H-1->L+6 (7%), H-1->L+9 (3%), H-1->L+10 (7%), HOMO->L+21 (2%)
60	56323.3088859	177.546387061	0.014	Singlet-A	H-3->L+5 (14%), H-2->L+8 (21%)	H-10->LUMO (9%), H-7->L+1 (5%), H-5->L+3 (6%), H-4->L+7 (2%), H-3->L+3 (6%), H-3->L+6 (6%), H-3->L+7 (4%), H-2->L+4 (3%)
61	56598.3439462	176.683614798	0.0059	Singlet-A	H-3->L+6 (20%), H-2->L+8 (14%)	H-5->L+3 (2%), H-4->L+4 (3%), H-4->L+6 (5%), H-3->L+3 (2%), H-3->L+7 (2%), H-2->L+10 (9%), HOMO->L+18 (5%), HOMO->L+19 (8%), HOMO->L+24 (3%)
62	56681.4190524	176.424658507	0.0045	Singlet-A	H-15->LUMO (35%), H-13->LUMO (12%), H-11->LUMO (15%)	H-12->LUMO (3%), H-10->LUMO (2%), H-8->L+2 (4%), H-6->L+2 (6%)
63	56816.9201965	176.003908086	0.0258	Singlet-A	HOMO->L+18 (17%), HOMO->L+19 (13%)	H-15->LUMO (2%), H-6->L+2 (9%), H-4->L+3 (3%), H-4->L+4 (3%), H-4->L+6 (9%), H-4->L+8 (2%), H-3->L+3 (2%), H-3->L+4 (3%), H-3->L+8 (2%), H-2->L+8 (3%), H-1->L+9 (3%), HOMO->L+15 (2%), HOMO->L+17 (4%), HOMO->L+24 (7%)
64	56870.9593432	175.836668055	0.0122	Singlet-A	H-4->L+6 (13%), H-3->L+4 (14%)	H-15->LUMO (2%), H-6->L+2 (5%), H-5->L+3 (2%), H-3->L+3 (2%), H-3->L+5 (8%), H-3->L+6 (6%), H-2->L+8 (5%), H-2->L+10 (3%), H-1->L+9 (2%), HOMO->L+18 (2%), HOMO->L+19 (4%), HOMO->L+21 (6%)
65	56950.0016773	175.592619938	0.0019	Singlet-A	H-2->L+10 (11%), H-1->L+9 (19%), HOMO->L+19 (10%)	H-6->L+2 (4%), H-5->L+3 (2%), H-4->L+6 (8%), H-3->L+5 (2%), H-2->L+8 (2%), H-1->L+8 (2%), H-1->L+11 (5%), HOMO->L+18 (3%), HOMO->L+21 (2%), HOMO->L+22 (2%), HOMO->L+24 (6%)
66	57062.1127429	175.247629632	0.0009	Singlet-A	H-1->L+9 (32%)	H-6->L+2 (3%), H-4->L+3 (4%), H-4->L+6 (8%), H-4->L+8 (2%), H-3->L+6 (2%), H-2->L+4 (2%), H-2->L+10 (8%), H-1->L+8 (3%), H-1->L+10 (2%), H-1->L+11 (7%), H-1->L+12 (3%), HOMO->L+18 (2%), HOMO->L+20 (2%), HOMO->L+21 (2%)

67	57164.5451554	174.933605661	0.0334	Singlet-A	H-6->L+2 (23%), HOMO->L+20 (14%), HOMO->L+21 (12%), HOMO->L+22 (12%)	H-4->L+6 (2%), H-3->L+4 (2%), H-3->L+5 (5%), H-2->L+7 (2%), H-1->L+9 (3%), HOMO->L+27 (2%)
68	57255.6858059	174.65514314	0.0076	Singlet-A	H-4->L+3 (15%), H-3->L+5 (10%), HOMO->L+21 (18%)	H-6->L+2 (5%), H-4->L+4 (3%), H-4->L+8 (6%), H-4->L+10 (3%), H-3->L+3 (3%), H-3->L+4 (3%), H-3->L+6 (4%), H-3->L+8 (5%), H-2->L+10 (2%), HOMO->L+20 (4%), HOMO->L+22 (3%), HOMO->L+25 (2%)
69	57480.7144915	173.971393509	0.0081	Singlet-A	H-4->L+3 (12%), H-4->L+4 (14%), H-2->L+10 (15%), HOMO->L+21 (13%)	H-4->L+8 (6%), H-3->L+5 (3%), H-2->L+6 (2%), H-2->L+8 (9%), HOMO->L+22 (3%), HOMO->L+24 (3%), HOMO->L+25 (3%)
70	57513.7832231	173.871365081	0.0263	Singlet-A	H-2->L+10 (12%), HOMO->L+20 (16%), HOMO->L+21 (14%), HOMO->L+22 (11%)	H-6->L+2 (5%), H-2->L+6 (2%), H-2->L+8 (5%), HOMO->L+19 (5%), HOMO->L+24 (4%), HOMO->L+25 (9%)
71	57721.8742658	173.244547707	0.0191	Singlet-A	H-4->L+5 (47%), H-4->L+6 (13%)	H-4->L+3 (3%), H-4->L+7 (8%), H-4->L+10 (2%), H-3->L+4 (6%), H-2->L+10 (3%)
72	57764.6216506	173.116342049	0.0201	Singlet-A	H-4->L+4 (24%), H-4->L+5 (11%), H-3->L+5 (12%), H-2->L+10 (12%)	H-6->L+2 (2%), H-5->L+3 (4%), H-4->L+6 (4%), H-3->L+6 (9%), H-2->L+6 (4%), H-2->L+8 (2%), HOMO->L+22 (2%)
73	57967.0668122	172.511747617	0.0298	Singlet-A	HOMO->L+20 (28%), HOMO->L+22	HOMO->L+16 (8%), HOMO->L+17 (5%), HOMO->L+18 (8%), HOMO->L+19 (3%), HOMO->L+25 (3%), HOMO->L+26 (8%)

					(14%), HOMO->L+24 (10%)	
74	58159.0267663	171.942354541	0.0162	Singlet-A	H-11->LUMO (46%)	H-15->LUMO (9%), H-12->LUMO (2%), H-8->L+2 (6%), H-1->L+8 (3%), H-1->L+11 (7%), H-1->L+12 (3%), H-1->L+13 (6%), H-1->L+14 (5%)
75	58203.3872599	171.811306365	0.0029	Singlet-A	H-11->LUMO (17%), H-1->L+11 (26%)	H-15->LUMO (3%), H-8->L+2 (2%), H-2->L+9 (5%), H-2->L+11 (2%), H-1->L+8 (6%), H-1->L+9 (2%), H-1->L+10 (5%), H-1->L+12 (8%), H-1->L+13 (7%), H-1->L+14 (6%)
76	58342.9211761	171.400399541	0.001	Singlet-A	H-2->L+9 (46%), H-2->L+11 (23%)	H-3->L+8 (2%), H-2->L+12 (2%), H-1->L+9 (2%), H-1->L+11 (5%)
77	58559.8843175	170.765364661	0.0083	Singlet-A	H-1->L+9 (19%), H-1->L+11 (19%), H-1->L+13 (17%), H-1->L+14 (11%)	H-11->LUMO (2%), H-4->L+7 (2%), H-1->L+6 (3%), H-1->L+10 (4%), H-1->L+12 (3%), H-1->L+15 (6%)
78	58772.8146868	170.146692026	0.0185	Singlet-A	H-3->L+8 (12%), H-2->L+9 (17%), H-2->L+12 (13%)	H-5->L+4 (3%), H-4->L+6 (2%), H-4->L+7 (9%), H-4->L+8 (2%), H-3->L+6 (4%), H-2->L+8 (6%), H-2->L+11 (8%), H-2->L+13 (4%)
79	58830.8866057	169.978740369	0.053	Singlet-A	H-4->L+7 (22%), HOMO->L+23 (20%), HOMO->L+24 (17%)	H-5->L+3 (3%), H-2->L+9 (2%), HOMO->L+17 (3%), HOMO->L+21 (2%), HOMO->L+22 (2%), HOMO->L+28 (5%)
80	59006.7154712	169.472235832	0.0097	Singlet-A	HOMO->L+23 (31%)	H-5->L+3 (8%), H-4->L+5 (2%), H-4->L+7 (5%), H-2->L+11 (4%), H-2->L+12 (2%), H-1->L+12 (8%), H-1->L+13 (3%), HOMO->L+17 (2%), HOMO->L+22 (2%), HOMO->L+26 (3%), HOMO->L+28 (2%), HOMO->L+29 (2%)
81	59022.8465598	169.425918655	0.0002	Singlet-A	H-8->L+2 (18%), H-1->L+12 (23%)	H-15->LUMO (2%), H-12->LUMO (4%), H-12->L+1 (2%), H-5->L+7 (2%), H-3->L+7 (3%), H-2->L+11 (2%), H-1->L+9 (3%), H-1->L+13 (3%), H-1->L+14 (3%), H-1->L+18 (2%), H-1->L+19 (2%), HOMO->L+22 (2%),

						HOMO->L+23 (6%), HOMO->L+24 (2%), HOMO->L+26 (2%)
82	59173.672238	168.994074929	0.0099	Singlet-A	H-5->L+3 (19%), HOMO->L+24 (15%)	H-8->L+2 (4%), H-5->L+4 (5%), H-4->L+7 (4%), H-4->L+9 (3%), H-3->L+6 (6%), H-3->L+9 (2%), H-3->L+10 (2%), H-1->L+12 (2%), HOMO->L+18 (2%), HOMO->L+22 (5%), HOMO->L+26 (4%), HOMO->L+29 (2%)
83	59194.6426532	168.934206742	0.0304	Singlet-A	H-4->L+7 (10%), H-2->L+11 (11%), HOMO->L+24 (14%)	H-8->L+2 (2%), H-5->L+3 (6%), H-5->L+4 (4%), H-4->L+6 (2%), H-3->L+6 (6%), H-3->L+7 (2%), H-2->L+10 (2%), H-2->L+12 (5%), H-2->L+13 (3%), HOMO->L+21 (2%), HOMO->L+22 (3%), HOMO->L+26 (3%), HOMO->L+29 (2%)
84	59237.3900379	168.812299016	0.0027	Singlet-A	H-8->L+2 (30%), H-1->L+12 (25%)	H-15->LUMO (4%), H-12->LUMO (3%), H-12->L+1 (5%), H-4->L+7 (2%), H-1->L+9 (3%), H-1->L+14 (6%), HOMO->L+23 (2%), HOMO->L+24 (2%)
85	59388.2157161	168.383573735	0.0088	Singlet-A	H-4->L+9 (18%), H-3->L+9 (19%)	H-5->L+3 (9%), H-4->L+3 (4%), H-4->L+4 (5%), H-4->L+5 (3%), H-4->L+6 (3%), H-4->L+12 (2%), H-3->L+8 (9%), H-3->L+10 (6%), H-3->L+12 (3%)
86	59493.0677919	168.086810298	0.0028	Singlet-A	H-9->L+1 (93%)	
87	59618.8902828	167.732072042	0.0053	Singlet-A	H-3->L+8 (16%)	H-9->L+1 (3%), H-5->L+3 (4%), H-5->L+4 (7%), H-5->L+7 (3%), H-4->L+7 (7%), H-4->L+8 (8%), H-4->L+9 (9%), H-4->L+10 (2%), H-2->L+11 (2%), H-1->L+13 (4%), H-1->L+14 (5%), HOMO->L+23 (2%)
88	59738.2603383	167.396906829	0.0158	Singlet-A	H-1->L+13 (11%), H-1->L+14 (23%)	H-13->LUMO (2%), H-7->L+2 (5%), H-5->L+5 (3%), H-5->L+7 (6%), H-4->L+7 (5%), H-4->L+8 (2%), H-4->L+9 (3%), H-3->L+7 (5%), H-3->L+8 (6%), H-1->L+10 (2%), H-1->L+20 (2%)
89	59978.6135582	166.726094632	0.0047	Singlet-A	H-1->L+13 (18%), H-1->L+14 (13%)	H-15->LUMO (2%), H-14->LUMO (4%), H-13->LUMO (6%), H-12->L+1 (3%), H-5->L+3 (2%), H-5->L+4 (5%), H-5->L+5 (6%), H-5->L+6 (3%), H-5->L+7 (5%), H-3->L+7 (6%), HOMO->L+25 (2%)
90	60170.5735123	166.194194542	0.0138	Singlet-A	H-3->L+10 (28%), H-2->L+12 (18%)	H-5->L+6 (3%), H-5->L+7 (2%), H-4->L+9 (2%), H-4->L+10 (3%), H-2->L+9 (6%), H-2->L+11 (4%), H-2->L+13 (4%), H-1->L+15 (2%)
91	60224.612659	166.04506959	0.0295	Singlet-A	H-7->L+2 (12%), H-5->L+4 (13%),	H-16->LUMO (2%), H-14->LUMO (5%), H-13->LUMO (8%), H-12->LUMO (2%), H-4->L+9 (2%), H-3->L+8 (3%), H-3->L+9 (2%), H-3->L+10

					H-5->L+5 (10%)	(4%), H-2->L+9 (5%), H-2->L+12 (7%), H-2->L+14 (4%)
92	60348.8220411	165.703317178	0.0128	Singlet-A	H-12->L+1 (19%), H-1->L+15 (17%), H-1->L+19 (11%)	H-13->LUMO (8%), H-13->L+1 (3%), H-12->LUMO (2%), H-11->L+1 (2%), H-7->L+2 (7%), H-3->L+10 (2%), H-1->L+14 (3%), H-1->L+18 (3%), HOMO->L+25 (2%)
93	60387.5366537	165.597084335	0.0108	Singlet-A	H-4->L+8 (15%), H-4->L+10 (10%), H-3->L+9 (15%)	H-7->L+2 (3%), H-5->L+5 (4%), H-4->L+3 (7%), H-4->L+4 (6%), H-4->L+5 (4%), H-4->L+6 (3%), H-4->L+9 (2%), H-4->L+13 (2%), H-3->L+8 (4%), H-3->L+12 (2%), H-2->L+14 (2%)
94	60507.7132636	165.268185833	0.0013	Singlet-A	H-13->LUMO (11%), H-1->L+15 (18%), H-1->L+19 (12%)	H-12->L+1 (4%), H-5->L+4 (2%), H-5->L+5 (3%), H-4->L+8 (2%), H-2->L+12 (4%), H-1->L+13 (3%), H-1->L+18 (5%), HOMO->L+21 (2%), HOMO->L+25 (8%), HOMO->L+26 (2%), HOMO->L+27 (3%)
95	60542.395104	165.1735116	0.0298	Singlet-A	H-14->LUMO (10%), H-12->L+1 (10%), H-2->L+12 (15%)	H-15->LUMO (4%), H-13->LUMO (5%), H-7->L+2 (2%), H-3->L+7 (2%), H-3->L+8 (2%), H-3->L+10 (8%), H-2->L+9 (2%), H-2->L+11 (2%), H-2->L+14 (3%), H-2->L+15 (2%), HOMO->L+25 (3%), HOMO->L+26 (2%)
96	60650.4733975	164.879174717	0.0159	Singlet-A	H-12->L+1 (19%)	H-15->LUMO (6%), H-13->LUMO (4%), H-13->L+1 (2%), H-11->L+1 (2%), H-8->L+2 (6%), H-7->L+2 (7%), H-3->L+10 (2%), H-2->L+11 (2%), H-2->L+12 (4%), H-2->L+14 (2%), H-1->L+15 (3%), HOMO->L+21 (3%), HOMO->L+25 (8%), HOMO->L+26 (4%), HOMO->L+27 (4%)
97	60687.5749012	164.778375413	0.0142	Singlet-A	H-7->L+2 (15%), HOMO->L+25 (11%)	H-13->LUMO (3%), H-4->L+9 (7%), H-3->L+9 (4%), H-2->L+11 (2%), H-2->L+12 (2%), H-2->L+15 (2%), H-1->L+13 (3%), H-1->L+16 (2%), H-1->L+18 (6%), H-1->L+19 (5%), HOMO->L+21 (3%), HOMO->L+26 (3%), HOMO->L+27 (7%)
98	60786.781096	164.509451228	0.0069	Singlet-A	H-2->L+11 (12%), H-2->L+13 (32%), H-2->L+14 (20%)	H-12->L+1 (2%), H-7->L+2 (4%), H-5->L+7 (2%), H-2->L+12 (2%), H-1->L+15 (2%), HOMO->L+26 (3%)
99	60902.1183794	164.197900929	0.0021	Singlet-A	H-5->L+4 (12%), H-4->L+9 (13%),	H-5->L+6 (2%), H-5->L+7 (8%), H-3->L+10 (2%), H-3->L+11 (2%), H-3->L+12 (2%), H-2->L+9 (2%), H-2-

					H-3->L+9 (14%)	**>L+12 (3%), H-1->L+15 (2%), H-1->L+16 (3%), H-1->L+18 (5%), H-1->L+19 (3%)**
100	**60931.9608932**	**164.11748208**	**0.0177**	**Singlet-A**	**H-4->L+9 (10%), H-2->L+13 (15%)**	**H-8->L+2 (2%), H-7->L+2 (9%), H-5->L+5 (3%), H-5->L+7 (7%), H-3->L+9 (7%), H-3->L+10 (3%), H-3->L+12 (3%), H-2->L+11 (2%), H-2->L+12 (2%), H-2->L+14 (9%), H-2->L+15 (6%)**

100 first electronic transitions of 4a in DMSO

HOMO is 86						
No.	Energy (cm-1)	Wavelength (nm)	Osc. Strength	Symmetry	Major contribs	Minor contribs
1	25145.9474329	397.678394368	0.4162	Singlet-A	HOMO->LUMO (97%)	
2	26056.5473833	383.780700217	0.0027	Singlet-A	H-1->LUMO (97%)	
3	29220.6604082	342.223613713	0.0119	Singlet-A	H-2->LUMO (19%), HOMO->L+1 (79%)	
4	32853.3815565	304.382670101	0.0649	Singlet-A	H-2->LUMO (74%), HOMO->L+1 (18%)	H-3->L+1 (2%)
5	35094.7963146	284.942528526	0.0001	Singlet-A	H-1->L+1 (97%)	H-1->L+2 (2%)
6	35558.5651113	281.226195958	0.0758	Singlet-A	H-3->LUMO (69%), HOMO->L+2 (13%)	H-5->LUMO (5%), H-5->L+2 (2%), H-4->LUMO (6%), H-2->L+1 (2%)
7	36856.3111876	271.323951795	0.0463	Singlet-A	H-4->LUMO (76%), H-3->LUMO (12%)	HOMO->L+2 (8%)
8	37415.2534069	267.270674109	0.1329	Singlet-A	H-5->LUMO (19%), H-4->LUMO (12%), HOMO->L+2 (58%)	H-5->L+2 (2%)
9	39186.446933	255.190270685	0.2752	Singlet-A	H-5->LUMO (43%), H-2->L+1 (28%), HOMO->L+2 (15%)	H-3->LUMO (6%)
10	40239.0004628	248.515119287	0.4975	Singlet-A	H-5->LUMO (13%), H-3->L+1 (16%), H-2->L+1 (47%)	H-6->LUMO (6%), H-4->L+1 (3%), H-3->LUMO (4%), HOMO->L+4 (3%)
11	40955.2207958	244.169114601	0.3175	Singlet-A	H-3->L+1 (34%), H-2->L+1 (18%), H-2->L+2 (13%)	H-6->LUMO (6%), H-5->LUMO (8%), H-4->L+1 (4%), H-3->LUMO (2%), HOMO->L+3 (2%), HOMO->L+4 (5%)

12	41407.6978304	241.500989525	0.0015	Singlet-A	H-1->L+2 (92%)	H-1->L+1 (2%)
13	42316.6846719	236.313408707	0.0281	Singlet-A	HOMO->L+3 (74%), HOMO->L+4 (14%)	HOMO->L+5 (7%)
14	42553.0051196	235.001029231	0.0016	Singlet-A	H-4->L+1 (69%), H-3->L+1 (23%)	HOMO->L+4 (3%)
15	43506.3524547	229.851491467	0.1138	Singlet-A	H-4->L+1 (15%), H-3->L+1 (11%), HOMO->L+4 (50%)	H-7->LUMO (2%), H-5->L+1 (3%), H-2->L+2 (7%), HOMO->L+3 (5%), HOMO->L+5 (2%)
16	44666.984278	223.879005078	0.0519	Singlet-A	H-6->LUMO (50%), H-5->L+1 (22%)	H-9->LUMO (3%), H-4->L+1 (4%), H-3->L+1 (4%), H-3->L+2 (2%), HOMO->L+3 (2%), HOMO->L+4 (8%)
17	44792.8067689	223.250131468	0.0963	Singlet-A	H-9->LUMO (25%), H-2->L+2 (41%)	H-6->L+1 (2%), H-3->L+1 (2%), H-3->L+2 (4%), HOMO->L+4 (8%), HOMO->L+6 (2%), HOMO->L+7 (4%)
18	45025.9009989	222.094389632	0.0675	Singlet-A	H-9->LUMO (59%), H-2->L+2 (20%)	H-6->LUMO (4%), H-5->L+1 (3%), HOMO->L+4 (2%)
19	45910.6912075	217.814189614	0.0203	Singlet-A	H-3->L+2 (14%), HOMO->L+5 (39%), HOMO->L+6 (10%)	H-9->LUMO (2%), H-5->LUMO (2%), H-5->L+2 (2%), H-2->L+2 (2%), HOMO->L+3 (6%), HOMO->L+4 (2%), HOMO->L+7 (5%), HOMO->L+10 (3%)
20	46113.9429236	216.854152258	0.1374	Singlet-A	H-5->L+1 (48%), H-3->L+2 (10%)	H-6->LUMO (9%), H-5->L+2 (3%), H-3->L+1 (2%), HOMO->L+5 (9%), HOMO->L+6 (3%)
21	46228.4736526	216.316897572	0.0072	Singlet-A	HOMO->L+5 (21%), HOMO->L+6 (46%), HOMO->L+8 (13%)	H-5->L+1 (2%), H-3->L+2 (4%), HOMO->L+3 (2%), HOMO->L+9 (4%)
22	46432.5319231	215.366244007	0.0737	Singlet-A	H-5->L+1 (12%), H-3->L+2 (10%), HOMO->L+6 (17%), HOMO->L+7 (21%)	H-7->LUMO (5%), H-6->LUMO (7%), H-5->LUMO (2%), HOMO->L+5 (6%), HOMO->L+8 (3%), HOMO->L+10 (8%)
23	47227.7945901	211.739719942	0.032	Singlet-A	H-3->L+2 (16%), HOMO->L+7 (57%)	H-7->LUMO (3%), H-6->LUMO (5%), H-5->LUMO (2%), HOMO->L+6 (3%), HOMO->L+10 (3%)

24	48200.4992315	207.466730832	0.1209	Singlet-A	H-7->LUMO (71%)	H-6->LUMO (3%), H-5->L+1 (3%), H-5->L+2 (4%), H-4->L+2 (4%), H-2->L+2 (2%)
25	48612.6485447	205.707779752	0.0018	Singlet-A	HOMO->L+8 (44%), HOMO->L+11 (16%)	HOMO->L+3 (3%), HOMO->L+5 (4%), HOMO->L+6 (5%), HOMO->L+9 (8%), HOMO->L+12 (9%), HOMO->L+13 (4%)
26	49139.3285868	203.502984017	0.0026	Singlet-A	H-1->L+3 (18%), H-1->L+4 (62%), H-1->L+5 (10%)	H-9->L+1 (2%), H-1->L+7 (5%)
27	49224.8233563	203.149535502	0.0541	Singlet-A	H-4->L+2 (85%)	H-7->LUMO (4%), H-3->L+2 (2%), HOMO->L+10 (2%)
28	49313.5443435	202.784045096	0.0009	Singlet-A	HOMO->L+10 (66%)	H-4->L+2 (2%), HOMO->L+5 (5%), HOMO->L+6 (3%), HOMO->L+7 (6%), HOMO->L+11 (4%), HOMO->L+12 (3%), HOMO->L+13 (4%)
29	50133.8101978	199.466187799	0.0126	Singlet-A	HOMO->L+8 (26%), HOMO->L+11 (35%), HOMO->L+13 (15%)	HOMO->L+6 (4%), HOMO->L+9 (5%), HOMO->L+14 (2%), HOMO->L+16 (3%)
30	50399.9731594	198.412804078	0.0087	Singlet-A	H-5->L+2 (12%), HOMO->L+9 (22%), HOMO->L+12 (35%)	H-3->L+2 (5%), HOMO->L+6 (5%), HOMO->L+15 (5%)
31	50481.4351567	198.092624922	0.007	Singlet-A	H-5->L+2 (34%), H-3->L+2 (18%), HOMO->L+9 (11%), HOMO->L+12 (10%)	H-6->L+1 (2%), H-5->L+7 (2%), H-3->L+7 (3%)
32	50884.7123712	196.522679092	0.009	Singlet-A	H-6->L+1 (21%), H-1->L+3 (34%), H-1->L+6 (17%)	H-1->L+4 (7%), H-1->L+5 (4%), H-1->L+10 (6%)
33	51248.4684187	195.127782518	0.0988	Singlet-A	H-6->L+1 (47%), H-1->L+3 (12%)	H-7->LUMO (2%), H-2->L+2 (2%), H-2->L+3 (5%), H-2->L+4 (8%), H-2->L+5 (2%), H-2->L+7 (2%), H-1->L+4 (2%), H-1->L+6 (5%), H-1->L+10 (2%)
34	51482.3692031	194.241254915	0.0063	Singlet-A	H-2->L+3 (10%), HOMO->L+9 (12%),	HOMO->L+8 (6%), HOMO->L+11 (3%), HOMO->L+12 (7%), HOMO->L+15 (2%)

					HOMO->L+13 (30%), HOMO->L+14 (13%), HOMO->L+16 (12%)	
35	51729.9814128	193.311494164	0.0025	Singlet-A	H-2->L+3 (21%), HOMO->L+9 (17%), HOMO->L+11 (13%), HOMO->L+15 (23%)	H-2->L+4 (4%), HOMO->L+8 (4%), HOMO->L+10 (4%), HOMO->L+12 (2%), HOMO->L+13 (3%)
36	51838.0597063	192.908454843	0.0059	Singlet-A	H-2->L+3 (48%), HOMO->L+11 (10%), HOMO->L+13 (11%)	H-2->L+4 (3%), H-2->L+6 (2%), HOMO->L+9 (5%), HOMO->L+14 (3%), HOMO->L+15 (6%)
37	52264.7269992	191.333631192	0.0012	Singlet-A	H-8->LUMO (96%)	H-9->LUMO (2%)
38	52361.5135307	190.979964591	0.0028	Singlet-A	HOMO->L+12 (13%), HOMO->L+14 (49%)	HOMO->L+9 (8%), HOMO->L+11 (2%), HOMO->L+13 (3%), HOMO->L+15 (9%), HOMO->L+16 (3%), HOMO->L+18 (3%), HOMO->L+19 (2%)
39	52536.5358418	190.343726319	0.0015	Singlet-A	H-9->L+1 (40%), H-1->L+7 (37%)	H-1->L+4 (3%), H-1->L+5 (2%), H-1->L+6 (5%), H-1->L+17 (2%)
40	52829.3150995	189.288844293	0.0455	Singlet-A	H-7->L+1 (39%), H-2->L+4 (37%)	H-2->L+2 (2%), H-2->L+7 (5%), H-1->L+7 (4%)
41	53088.2190712	188.365708531	0.0031	Singlet-A	H-9->L+1 (51%), H-1->L+7 (23%)	H-13->LUMO (3%), H-1->L+4 (9%), H-1->L+6 (3%)
42	53628.6105386	186.467631728	0.0504	Singlet-A	H-2->L+7 (10%), HOMO->L+15 (12%), HOMO->L+17 (17%)	H-5->L+2 (5%), H-3->L+3 (7%), H-3->L+4 (4%), H-3->L+7 (4%), H-2->L+5 (2%), H-2->L+6 (3%), HOMO->L+11 (5%), HOMO->L+12 (3%), HOMO->L+14 (7%), HOMO->L+16 (3%), HOMO->L+18 (5%), HOMO->L+19 (2%)
43	53802.0197409	185.866628208	0.0029	Singlet-A	H-4->L+3 (21%), H-4->L+5 (12%),	H-4->L+6 (9%), H-4->L+8 (3%), H-3->L+5 (8%), H-3->L+6 (5%), H-1->L+6 (3%), HOMO->L+15 (2%)

					H-3->L+3 (25%)	
44	54014.1435557	185.136694608	0.0587	Singlet-A	HOMO->L+15 (21%)	H-7->L+1 (3%), H-5->L+2 (4%), H-4->L+3 (2%), H-3->L+6 (2%), H-3->L+7 (2%), H-2->L+5 (8%), H-2->L+6 (3%), H-2->L+7 (4%), H-1->L+3 (2%), HOMO->L+11 (6%), HOMO->L+12 (5%), HOMO->L+13 (4%), HOMO->L+14 (7%), HOMO->L+17 (3%), HOMO->L+18 (7%)
45	54302.8900413	184.152261369	0.0254	Singlet-A	HOMO->L+13 (13%), HOMO->L+16 (31%), HOMO->L+17 (10%)	H-7->L+1 (2%), H-4->L+3 (9%), H-3->L+3 (7%), H-2->L+5 (6%), H-2->L+6 (2%), HOMO->L+14 (2%)
46	54326.2801197	184.072974957	0.0086	Singlet-A	H-1->L+3 (19%), H-1->L+6 (21%)	H-4->L+3 (3%), H-2->L+5 (3%), H-1->L+4 (8%), H-1->L+5 (9%), H-1->L+7 (7%), H-1->L+10 (2%), H-1->L+13 (3%), HOMO->L+13 (2%), HOMO->L+16 (7%)
47	54452.9091651	183.644917293	0.0502	Singlet-A	H-2->L+5 (17%), H-2->L+7 (12%)	H-6->L+1 (2%), H-5->L+2 (2%), H-4->L+3 (4%), H-3->L+3 (8%), H-3->L+6 (2%), H-3->L+7 (3%), H-2->L+4 (5%), H-2->L+6 (9%), H-1->L+3 (3%), H-1->L+5 (2%), H-1->L+6 (4%), HOMO->L+16 (9%)
48	54748.1080861	182.654713552	0.0257	Singlet-A	H-2->L+5 (22%), H-2->L+6 (23%)	H-13->LUMO (3%), H-7->L+1 (2%), H-5->L+2 (3%), H-4->L+3 (4%), H-3->L+3 (5%), H-3->L+4 (2%), H-3->L+7 (5%), H-1->L+5 (4%), HOMO->L+17 (2%)
49	54844.8946176	182.332376965	0.0051	Singlet-A	H-10->LUMO (76%)	H-13->LUMO (3%), H-1->L+5 (7%), H-1->L+6 (2%)
50	54902.9665365	182.139520519	0.0155	Singlet-A	H-13->LUMO (10%), H-1->L+5 (32%)	H-12->LUMO (4%), H-11->LUMO (2%), H-10->LUMO (7%), H-3->L+4 (2%), H-2->L+5 (6%), H-2->L+6 (3%), H-1->L+3 (3%), H-1->L+6 (6%), H-1->L+8 (4%), H-1->L+10 (4%)
51	55013.4644932	181.773681991	0.0003	Singlet-A	H-13->LUMO (29%), H-12->LUMO (12%), H-10->LUMO (13%)	H-11->LUMO (5%), H-9->L+2 (2%), H-5->L+2 (2%), H-2->L+6 (2%), H-1->L+5 (2%), H-1->L+6 (2%), H-1->L+7 (2%), HOMO->L+16 (2%), HOMO->L+17 (8%)
52	55114.2837969	181.441167536	0.0204	Singlet-A	H-2->L+7 (14%),	H-13->LUMO (8%), H-12->LUMO (3%), H-5->L+2 (5%), H-3->L+4 (3%), H-3->L+6 (9%), H-3->L+7 (7%), H-2-

					HOMO->L+17 (14%)	>L+6 (2%), H-1->L+5 (7%), H-1->L+7 (3%)
53	55179.6147056	181.2263 46964	0.1229	Singlet-A	H-2->L+7 (25%), HOMO->L+16 (10%), HOMO->L+17 (23%)	H-6->L+1 (3%), H-6->L+2 (3%), H-4->L+3 (2%), H-3->L+3 (3%), H-2->L+4 (3%), H-1->L+5 (2%), HOMO->L+13 (2%), HOMO->L+19 (5%)
54	55582.0853657	179.9140 84443	0.0053	Singlet-A	H-2->L+6 (27%), HOMO->L+18 (18%)	H-7->L+1 (2%), H-4->L+3 (5%), H-4->L+5 (2%), H-3->L+3 (7%), H-2->L+3 (3%), H-2->L+5 (2%), H-2->L+7 (8%), H-2->L+8 (4%), HOMO->L+14 (2%), HOMO->L+20 (3%), HOMO->L+23 (3%)
55	55686.130887	179.5779 27946	0.0042	Singlet-A	HOMO->L+18 (39%)	H-4->L+3 (4%), H-3->L+3 (8%), H-2->L+5 (3%), H-2->L+6 (7%), HOMO->L+14 (6%), HOMO->L+20 (7%), HOMO->L+23 (4%)
56	56064.4049142	178.3662 91684	0.1269	Singlet-A	H-4->L+4 (10%), H-3->L+4 (26%)	H-7->L+1 (7%), H-6->L+2 (5%), H-3->L+5 (4%), H-3->L+6 (2%), H-3->L+7 (6%), H-2->L+4 (8%), H-2->L+5 (3%), H-1->L+5 (3%), H-1->L+6 (2%)
57	56205.5519393	177.9183 66691	0.1432	Singlet-A	H-7->L+1 (23%), H-3->L+4 (13%)	H-11->LUMO (3%), H-6->L+1 (3%), H-6->L+2 (7%), H-5->L+7 (2%), H-4->L+7 (2%), H-3->L+5 (4%), H-3->L+7 (2%), H-2->L+4 (9%), H-2->L+5 (7%), H-2->L+6 (2%), H-2->L+17 (2%), H-1->L+5 (2%)
58	56374.9283694	177.3838 17403	0.01	Singlet-A	H-15->LUMO (18%), H-13->LUMO (11%), H-11->LUMO (41%)	H-17->LUMO (2%), H-16->LUMO (5%), H-14->LUMO (3%), H-9->L+2 (2%), H-6->L+2 (5%)
59	56740.2975257	176.2415 85541	0.0631	Singlet-A	H-3->L+6 (11%), HOMO->L+19 (28%)	H-6->L+2 (2%), H-5->L+3 (7%), H-4->L+4 (2%), H-4->L+7 (2%), H-3->L+3 (5%), H-3->L+5 (2%), H-3->L+7 (6%), H-2->L+5 (2%), H-2->L+8 (2%), HOMO->L+15 (3%), HOMO->L+16 (3%), HOMO->L+17 (2%), HOMO->L+20 (2%), HOMO->L+22 (2%), HOMO->L+23 (2%), HOMO->L+24 (5%)
60	56871.7658976	175.8341 74342	0.0108	Singlet-A	H-2->L+8 (13%), HOMO->L+19 (20%)	H-5->L+3 (4%), H-4->L+4 (2%), H-3->L+3 (4%), H-3->L+5 (3%), H-3->L+6 (8%), H-3->L+7 (3%), HOMO->L+17 (2%), HOMO->L+21 (5%), HOMO->L+22 (2%), HOMO->L+23 (4%), HOMO->L+24 (6%)

61	57033.0767834	175.336849491	0.0463	Singlet-A	H-6->L+2 (39%), H-4->L+4 (10%)	H-16->LUMO (4%), H-7->L+1 (2%), H-4->L+6 (7%), H-4->L+7 (2%), H-3->L+4 (5%), HOMO->L+21 (2%)
62	57198.4204414	174.830002696	0.0089	Singlet-A	H-1->L+8 (31%), H-1->L+10 (14%)	H-4->L+4 (4%), H-4->L+6 (6%), H-3->L+4 (2%), H-2->L+8 (8%), H-2->L+10 (2%), H-1->L+9 (2%), H-1->L+12 (7%), H-1->L+13 (4%)
63	57214.55153	174.780711071	0.0311	Singlet-A	H-2->L+8 (14%), H-1->L+8 (18%), HOMO->L+21 (12%)	H-4->L+3 (4%), H-4->L+4 (2%), H-4->L+6 (5%), H-3->L+4 (3%), H-3->L+5 (2%), H-3->L+7 (2%), H-2->L+9 (2%), H-2->L+10 (6%), H-1->L+10 (2%), H-1->L+12 (3%), H-1->L+13 (2%), HOMO->L+20 (2%)
64	57379.8951879	174.277069821	0.0059	Singlet-A	H-11->LUMO (13%), HOMO->L+21 (23%)	H-16->LUMO (4%), H-15->LUMO (8%), H-12->LUMO (3%), H-9->L+2 (2%), H-4->L+3 (2%), H-4->L+6 (4%), H-4->L+7 (2%), H-1->L+6 (2%), H-1->L+8 (5%), HOMO->L+19 (3%), HOMO->L+20 (4%), HOMO->L+25 (3%)
65	57440.3867701	174.093535269	0.0238	Singlet-A	H-11->LUMO (22%)	H-16->LUMO (4%), H-15->LUMO (9%), H-12->LUMO (5%), H-9->L+2 (3%), H-6->L+2 (7%), H-2->L+10 (3%), H-1->L+8 (2%), HOMO->L+19 (4%), HOMO->L+20 (6%), HOMO->L+21 (9%), HOMO->L+25 (3%)
66	57483.9407093	173.961629572	0.0006	Singlet-A	H-4->L+6 (14%), H-2->L+10 (17%)	H-15->LUMO (2%), H-11->LUMO (5%), H-5->L+3 (4%), H-4->L+3 (5%), H-4->L+7 (6%), H-4->L+8 (3%), H-3->L+4 (3%), H-3->L+6 (4%), H-2->L+8 (4%), H-1->L+10 (2%), HOMO->L+19 (4%), HOMO->L+20 (4%)
67	57546.0454003	173.773887162	0.0278	Singlet-A	H-1->L+6 (15%), H-1->L+10 (36%)	H-6->L+2 (8%), H-4->L+4 (4%), H-4->L+6 (2%), H-3->L+4 (2%), H-1->L+5 (2%), H-1->L+7 (3%), H-1->L+8 (6%), H-1->L+9 (2%), H-1->L+11 (2%), HOMO->L+21 (4%)
68	57711.3890582	173.276023384	0.0031	Singlet-A	HOMO->L+20 (21%), HOMO->L+22 (30%)	H-5->L+3 (2%), H-3->L+4 (2%), H-3->L+5 (7%), H-2->L+8 (3%), H-2->L+10 (2%), HOMO->L+19 (2%), HOMO->L+21 (6%), HOMO->L+23 (2%), HOMO->L+26 (3%), HOMO->L+27 (4%)
69	57822.6935694	172.942479547	0.0117	Singlet-A	H-4->L+4 (38%), H-4->L+8 (10%), H-3->L+4 (11%)	H-4->L+3 (6%), H-4->L+5 (4%), H-4->L+6 (4%), H-4->L+7 (5%), H-3->L+6 (3%), H-3->L+8 (4%), H-1->L+8 (2%), H-1->L+10 (2%)
70	58024.3321767	172.341492351	0.0081	Singlet-A	H-3->L+5 (29%),	H-4->L+3 (2%), H-4->L+5 (4%), H-4->L+10 (4%), H-3->L+3 (2%), H-3->L+6 (8%), H-3->L+7 (4%), H-3->L+8 (3%),

					HOMO->L+20 (13%)	H-3->L+10 (2%), H-2->L+8 (2%), HOMO->L+16 (2%), HOMO->L+21 (8%), HOMO->L+25 (2%)
71	58150.1546676	171.968588169	0.0064	Singlet-A	H-4->L+5 (20%), H-2->L+10 (11%)	H-4->L+3 (8%), H-4->L+6 (4%), H-4->L+8 (6%), H-4->L+10 (4%), H-2->L+8 (5%), HOMO->L+16 (2%), HOMO->L+18 (2%), HOMO->L+20 (6%), HOMO->L+21 (3%), HOMO->L+22 (5%), HOMO->L+25 (4%), HOMO->L+26 (3%)
72	58307.4327813	171.504721148	0.0226	Singlet-A	H-2->L+8 (19%), H-2->L+10 (20%), HOMO->L+22 (11%)	H-8->L+1 (4%), H-5->L+3 (3%), H-3->L+5 (3%), H-2->L+7 (2%), HOMO->L+16 (2%), HOMO->L+18 (2%), HOMO->L+19 (3%), HOMO->L+20 (5%), HOMO->L+21 (2%), HOMO->L+25 (3%), HOMO->L+26 (5%)
73	58358.2457103	171.355390798	0.0016	Singlet-A	H-8->L+1 (89%)	H-9->L+1 (2%)
74	58452.6125785	171.078751811	0.0012	Singlet-A	H-4->L+5 (16%), H-2->L+10 (14%)	H-8->L+1 (2%), H-4->L+3 (3%), H-4->L+4 (3%), H-4->L+6 (6%), H-4->L+7 (6%), H-4->L+10 (3%), H-3->L+5 (9%), H-3->L+6 (3%), H-3->L+7 (2%), H-2->L+6 (2%), HOMO->L+19 (2%), HOMO->L+22 (5%), HOMO->L+23 (4%)
75	58566.336753	170.74655091	0.014	Singlet-A	H-1->L+9 (46%), H-1->L+11 (24%)	H-4->L+7 (5%), H-1->L+5 (2%), H-1->L+10 (5%), H-1->L+12 (2%), H-1->L+14 (2%)
76	58692.1592439	170.380509574	0.0789	Singlet-A	H-4->L+7 (34%)	H-5->L+4 (2%), H-4->L+4 (6%), H-4->L+6 (9%), H-3->L+6 (3%), H-3->L+7 (4%), H-2->L+8 (3%), H-2->L+9 (3%), H-2->L+11 (3%), H-1->L+9 (5%), HOMO->L+24 (2%)
77	58995.4237092	169.504672927	0.0104	Singlet-A	H-2->L+9 (30%), H-2->L+11 (24%), HOMO->L+24 (10%)	H-7->L+2 (2%), H-6->L+2 (2%), H-5->L+3 (2%), H-4->L+7 (3%), H-2->L+8 (4%), H-2->L+10 (3%), H-2->L+13 (2%), HOMO->L+28 (2%)
78	59143.0231697	169.081650955	0.0118	Singlet-A	HOMO->L+23 (50%)	H-4->L+7 (2%), H-3->L+5 (2%), HOMO->L+18 (2%), HOMO->L+19 (5%), HOMO->L+22 (9%), HOMO->L+24 (2%), HOMO->L+26 (7%), HOMO->L+29 (7%)
79	59145.442833	169.074733758	0.0046	Singlet-A	H-12->LUMO (28%), H-9->L+2 (30%)	H-13->LUMO (4%), H-13->L+1 (2%), H-5->L+7 (3%), H-3->L+7 (4%), H-2->L+9 (2%), H-1->L+13 (4%), HOMO->L+24 (2%)
80	59318.0454808	168.582762951	0.026	Singlet-A	HOMO->L+24 (44%)	H-12->LUMO (2%), H-9->L+2 (3%), H-4->L+7 (3%), H-2->L+9 (5%), H-1->L+8 (2%), H-1->L+13 (3%), HOMO->L+18

						(4%), HOMO->L+19 (2%), HOMO->L+21 (3%), HOMO->L+23 (4%), HOMO->L+28 (6%)
81	59370.4715187	168.433898943	0.0276	Singlet-A	H-1->L+13 (42%)	H-14->LUMO (3%), H-12->LUMO (2%), H-9->L+2 (4%), H-4->L+7 (2%), H-2->L+9 (2%), H-1->L+8 (9%), H-1->L+12 (5%), H-1->L+14 (6%), H-1->L+23 (2%), HOMO->L+24 (4%)
82	59597.1133132	167.79336186	0.0024	Singlet-A	H-13->L+1 (11%), H-9->L+2 (14%), H-5->L+3 (14%)	H-16->LUMO (5%), H-15->LUMO (4%), H-13->LUMO (7%), H-12->LUMO (6%), H-12->L+1 (3%), H-4->L+7 (2%), H-3->L+5 (2%), H-3->L+6 (2%), H-3->L+7 (2%), H-2->L+9 (3%), H-1->L+9 (3%), H-1->L+13 (2%)
83	59639.860698	167.673094 52	0.0014	Singlet-A	H-12->LUMO (11%), H-2->L+9 (16%), H-2->L+12 (13%)	H-16->LUMO (3%), H-15->LUMO (3%), H-13->LUMO (6%), H-13->L+1 (3%), H-9->L+2 (2%), H-5->L+3 (7%), H-5->L+4 (2%), H-3->L+5 (3%), H-3->L+6 (2%), H-3->L+7 (2%), H-3->L+8 (5%), H-2->L+11 (3%), H-2->L+13 (3%)
84	59821.3354445	167.164439337	0.0109	Singlet-A	H-5->L+3 (11%), H-2->L+11 (11%), H-2->L+12 (18%)	H-13->LUMO (3%), H-12->LUMO (8%), H-5->L+4 (4%), H-5->L+7 (2%), H-4->L+6 (2%), H-3->L+7 (7%), H-2->L+9 (4%), H-2->L+10 (2%), H-2->L+13 (7%)
85	59977.8070037	166.728336689	0.0163	Singlet-A	H-7->L+2 (10%), H-5->L+3 (11%), H-1->L+9 (16%), H-1->L+11 (16%)	H-14->LUMO (2%), H-5->L+6 (4%), H-5->L+7 (5%), H-3->L+5 (2%), H-3->L+6 (6%), H-2->L+12 (3%), H-1->L+12 (4%)
86	60131.0523452	166.303425767	0.0097	Singlet-A	H-1->L+11 (25%)	H-13->L+1 (3%), H-5->L+4 (3%), H-5->L+6 (4%), H-5->L+7 (5%), H-4->L+8 (4%), H-4->L+9 (6%), H-3->L+5 (2%), H-3->L+6 (3%), H-3->L+7 (2%), H-3->L+9 (3%), H-1->L+8 (2%), H-1->L+9 (9%), H-1->L+10 (2%), H-1->L+17 (2%)
87	60281.071469	165.889552994	0.0076	Singlet-A	H-4->L+9 (15%), H-3->L+8 (23%)	H-13->L+1 (2%), H-5->L+3 (6%), H-5->L+4 (8%), H-4->L+5 (3%), H-4->L+12 (2%), H-3->L+9 (2%), H-3->L+10 (5%), H-3->L+11 (3%), H-2->L+13 (3%)
88	60367.3727929	165.652396938	0.0319	Singlet-A	H-7->L+2 (28%)	H-16->LUMO (4%), H-14->LUMO (4%), H-13->L+1 (4%), H-12->L+1 (2%), H-6->L+2 (2%), H-5->L+4 (7%), H-4->L+8 (5%), H-4->L+9 (4%), H-3->L+9 (2%), H-1->L+8 (2%), H-1->L+9 (3%), H-1->L+11 (6%), H-1->L+12 (2%)

89	60477.8707497	165.349736623	0.0249	Singlet-A	H-4->L+8 (12%), H-3->L+8 (12%)	H-13->L+1 (4%), H-12->L+1 (2%), H-7->L+2 (3%), H-5->L+5 (5%), H-4->L+7 (3%), H-4->L+9 (3%), H-4->L+10 (5%), H-3->L+9 (5%), H-2->L+13 (8%), H-2->L+14 (3%), H-1->L+12 (4%), H-1->L+17 (2%)
90	60512.5525902	165.25496896	0.0149	Singlet-A	H-13->L+1 (13%), H-1->L+12 (20%)	H-15->LUMO (2%), H-12->L+1 (6%), H-11->L+1 (2%), H-9->L+2 (4%), H-5->L+4 (6%), H-5->L+5 (2%), H-2->L+13 (2%), H-1->L+8 (2%), H-1->L+13 (3%), H-1->L+17 (5%), HOMO->L+25 (2%), HOMO->L+26 (2%)
91	60572.2376179	165.092134504	0.0054	Singlet-A	H-13->L+1 (10%), H-1->L+12 (28%)	H-15->LUMO (2%), H-14->LUMO (4%), H-12->L+1 (5%), H-11->L+1 (2%), H-9->L+2 (9%), H-7->L+2 (2%), H-5->L+4 (5%), H-1->L+8 (3%), H-1->L+9 (2%), H-1->L+13 (5%), H-1->L+14 (2%), H-1->L+15 (2%), H-1->L+20 (2%)
92	60781.9417694	164.522549114	0.0115	Singlet-A	H-14->LUMO (11%), HOMO->L+25 (11%), HOMO->L+26 (13%)	H-10->L+1 (6%), H-9->L+2 (2%), H-5->L+7 (7%), H-4->L+10 (2%), H-2->L+9 (2%), H-1->L+10 (2%), H-1->L+12 (2%), H-1->L+14 (3%), HOMO->L+21 (3%), HOMO->L+23 (2%), HOMO->L+27 (5%)
93	60826.302263	164.402563167	0.0108	Singlet-A	H-14->LUMO (10%), H-3->L+10 (24%)	H-10->L+1 (4%), H-7->L+2 (4%), H-5->L+3 (2%), H-5->L+4 (2%), H-5->L+6 (2%), H-5->L+7 (5%), H-4->L+10 (3%), H-3->L+8 (2%), H-2->L+11 (2%), H-2->L+14 (6%), H-1->L+14 (3%), H-1->L+17 (3%), HOMO->L+26 (2%)
94	60891.6331718	164.226174913	0.0188	Singlet-A	H-14->LUMO (21%), H-3->L+10 (12%)	H-10->L+1 (4%), H-7->L+2 (6%), H-5->L+4 (2%), H-5->L+6 (3%), H-2->L+9 (2%), H-2->L+11 (3%), H-2->L+12 (2%), H-2->L+14 (2%), HOMO->L+25 (8%), HOMO->L+26 (3%), HOMO->L+27 (2%)
95	60948.8985362	164.071873982	0.0066	Singlet-A	H-10->L+1 (55%)	H-14->LUMO (6%), H-7->L+2 (2%), H-2->L+13 (2%), H-2->L+14 (3%), HOMO->L+25 (6%), HOMO->L+26 (4%), HOMO->L+27 (4%)
96	61018.2622171	163.88536213	0.01	Singlet-A	H-10->L+1 (21%), H-2->L+13 (21%)	H-7->L+2 (3%), H-5->L+4 (6%), H-5->L+7 (4%), H-4->L+10 (2%), H-3->L+8 (2%), H-2->L+11 (3%), H-2->L+12 (5%), H-2->L+14 (8%), H-2->L+15 (2%)
97	61081.1734626	163.716566548	0.0043	Singlet-A	H-1->L+14 (10%), H-1->L+15	H-9->L+2 (2%), H-7->L+2 (3%), H-3->L+10 (2%), H-1->L+7 (2%), H-1->L+19 (9%), H-1->L+20 (2%)

					(12%), H-1->L+17 (32%)	
98	61105.3700955	163.651737718	0.0143	Singlet-A	H-2->L+11 (21%), H-2->L+13 (12%)	H-10->L+1 (2%), H-7->L+2 (4%), H-5->L+4 (6%), H-5->L+5 (2%), H-5->L+6 (2%), H-4->L+5 (2%), H-4->L+9 (6%), H-3->L+4 (2%), H-3->L+10 (9%), H-2->L+9 (5%), H-2->L+12 (3%), H-2->L+15 (4%)
99	61170.7010042	163.476956056	0.0062	Singlet-A	HOMO->L+25 (12%), HOMO->L+26 (15%)	H-14->LUMO (2%), H-4->L+3 (2%), H-4->L+4 (2%), H-4->L+5 (4%), H-4->L+8 (4%), H-4->L+9 (2%), H-4->L+10 (2%), H-3->L+9 (7%), H-3->L+12 (2%), H-2->L+11 (3%), H-2->L+12 (4%), H-2->L+14 (2%), H-2->L+15 (2%), HOMO->L+20 (3%), HOMO->L+22 (8%), HOMO->L+31 (2%)
100	61232.8056953	163.311151375	0.0024	Singlet-A	H-4->L+9 (11%), HOMO->L+25 (10%)	H-5->L+5 (2%), H-4->L+3 (3%), H-4->L+4 (3%), H-4->L+5 (8%), H-4->L+6 (3%), H-4->L+8 (4%), H-4->L+10 (4%), H-4->L+11 (2%), H-4->L+14 (3%), H-3->L+8 (2%), H-3->L+9 (6%), H-2->L+13 (4%), HOMO->L+20 (2%), HOMO->L+22 (7%), HOMO->L+26 (7%)

100 first electronic transitions of 4a in MeOH

HOMO is 86						
No.	Energy (cm-1)	Wavelength (nm)	Osc. Strength	Symmetry	Major contribs	Minor contribs
1	25248.3798454	396.065017289	0.3982	Singlet-A	HOMO->LUMO (97%)	
2	26031.544196	384.149319945	0.0026	Singlet-A	H-1->LUMO (97%)	
3	29248.8898133	341.893318476	0.011	Singlet-A	H-2->LUMO (20%), HOMO->L+1 (78%)	
4	32900.1617133	303.949873777	0.0606	Singlet-A	H-2->LUMO (74%), HOMO->L+1 (18%)	H-3->L+1 (2%)
5	35043.1768312	285.362256058	0.0001	Singlet-A	H-1->L+1 (97%)	H-1->L+2 (2%)
6	35567.43721	281.156045653	0.0706	Singlet-A	H-3->LUMO (68%), HOMO->L+2 (13%)	H-5->LUMO (5%), H-5->L+2 (2%), H-4->LUMO (5%), H-2->L+1 (2%)
7	36882.9274837	271.12815284	0.0445	Singlet-A	H-4->LUMO (76%), H-3->LUMO (11%)	HOMO->L+2 (8%)
8	37453.9680195	266.994407503	0.1193	Singlet-A	H-5->LUMO (20%), H-4->LUMO (12%), HOMO->L+2 (56%)	H-5->L+2 (2%), H-2->L+1 (2%)
9	39246.1319607	254.802180506	0.2633	Singlet-A	H-5->LUMO (42%), H-2->L+1 (26%), HOMO->L+2 (16%)	H-3->LUMO (6%)

10	40309.9772526	248.077540142	0.4392	Singlet-A	H-5->LUMO (11%), H-3->L+1 (20%), H-2->L+1 (43%)	H-6->LUMO (7%), H-4->L+1 (3%), H-3->LUMO (4%), H-2->L+2 (2%), HOMO->L+4 (3%)
11	41001.1943982	243.895333948	0.3642	Singlet-A	H-3->L+1 (30%), H-2->L+1 (23%), H-2->L+2 (13%)	H-6->LUMO (5%), H-5->LUMO (8%), H-4->L+1 (4%), H-3->LUMO (2%), HOMO->L+3 (2%), HOMO->L+4 (4%)
12	41352.8521293	241.821288862	0.0017	Singlet-A	H-1->L+2 (92%)	H-1->L+1 (2%)
13	42316.6846719	236.313408707	0.0275	Singlet-A	HOMO->L+3 (75%), HOMO->L+4 (13%)	HOMO->L+5 (7%)
14	42557.0378918	234.978760163	0.0016	Singlet-A	H-4->L+1 (69%), H-3->L+1 (23%)	HOMO->L+4 (3%)
15	43536.1949686	229.693936441	0.1134	Singlet-A	H-4->L+1 (15%), H-3->L+1 (10%), HOMO->L+4 (49%)	H-7->LUMO (2%), H-5->L+1 (4%), H-2->L+2 (7%), HOMO->L+3 (5%), HOMO->L+5 (2%)
16	44686.3415843	223.782024786	0.0508	Singlet-A	H-6->LUMO (49%), H-5->L+1 (24%)	H-9->LUMO (4%), H-4->L+1 (3%), H-3->L+1 (4%), H-3->L+2 (2%), HOMO->L+3 (2%), HOMO->L+4 (8%)
17	44810.5509664	223.161728306	0.0807	Singlet-A	H-9->LUMO (30%), H-2->L+2 (37%)	H-6->L+1 (2%), H-3->L+1 (2%), H-3->L+2 (4%), HOMO->L+4 (8%), HOMO->L+7 (3%)
18	45033.1599888	222.05858977	0.078	Singlet-A	H-9->LUMO (52%), H-2->L+2 (24%)	H-8->LUMO (2%), H-6->LUMO (4%), H-6->L+1 (2%), H-5->L+1 (3%), HOMO->L+4 (3%)
19	45921.9829695	217.760631257	0.0194	Singlet-A	H-3->L+2 (14%), HOMO-	H-9->LUMO (2%), H-5->LUMO (2%), H-5->L+2 (2%), H-2->L+2 (2%), HOMO->L+3 (6%), HOMO->L+4 (3%), HOMO-

					>L+5 (41%)	>L+6 (7%), HOMO->L+7 (6%), HOMO->L+10 (3%)
20	46137.3330021	216.744214486	0.1258	Singlet-A	H-5->L+1 (43%), H-3->L+2 (13%), HOMO->L+5 (11%)	H-6->LUMO (8%), H-5->L+2 (3%), H-3->L+1 (2%), HOMO->L+6 (2%), HOMO->L+10 (2%)
21	46230.8933159	216.305575834	0.0118	Singlet-A	HOMO->L+5 (16%), HOMO->L+6 (48%), HOMO->L+8 (13%)	H-6->LUMO (2%), H-5->L+1 (3%), H-3->L+2 (3%), HOMO->L+9 (4%)
22	46459.1482193	215.24286138	0.0799	Singlet-A	H-5->L+1 (13%), H-3->L+2 (10%), HOMO->L+6 (18%), HOMO->L+7 (18%)	H-7->LUMO (5%), H-6->LUMO (9%), H-5->LUMO (2%), HOMO->L+5 (6%), HOMO->L+8 (3%), HOMO->L+10 (8%)
23	47258.4436584	211.602397918	0.0319	Singlet-A	H-3->L+2 (15%), HOMO->L+7 (59%)	H-7->LUMO (3%), H-6->LUMO (6%), H-5->LUMO (2%), HOMO->L+6 (2%), HOMO->L+10 (3%)
24	48235.9876263	207.314092488	0.122	Singlet-A	H-7->LUMO (71%)	H-6->LUMO (3%), H-5->L+1 (3%), H-5->L+2 (5%), H-4->L+2 (4%), H-2->L+2 (2%)
25	48597.3240105	205.772647025	0.0022	Singlet-A	HOMO->L+8 (45%), HOMO->L+11 (17%)	HOMO->L+3 (3%), HOMO->L+5 (4%), HOMO->L+6 (5%), HOMO->L+9 (7%), HOMO->L+12 (9%), HOMO->L+13 (4%)
26	49097.3877565	203.676823899	0.003	Singlet-A	H-1->L+3 (17%), H-1->L+4 (62%), H-1->L+5 (11%)	H-9->L+1 (2%), H-1->L+7 (6%)
27	49249.0199892	203.049725704	0.0463	Singlet-A	H-4->L+2 (75%), HOMO-	H-7->LUMO (4%), H-3->L+2 (2%)

					>L+10 (10%)	
28	49287.7346018	202.890233864	0.0054	Singlet-A	H-4->L+2 (12%), HOMO->L+10 (58%)	HOMO->L+5 (5%), HOMO->L+6 (3%), HOMO->L+7 (5%), HOMO->L+11 (3%), HOMO->L+12 (3%), HOMO->L+13 (3%)
29	50126.5512079	199.49507315	0.011	Singlet-A	HOMO->L+8 (25%), HOMO->L+11 (35%), HOMO->L+13 (15%)	HOMO->L+6 (5%), HOMO->L+9 (5%), HOMO->L+14 (2%), HOMO->L+16 (2%)
30	50389.4879518	198.454090456	0.0084	Singlet-A	HOMO->L+9 (28%), HOMO->L+12 (39%)	H-5->L+2 (7%), H-3->L+2 (2%), HOMO->L+6 (5%), HOMO->L+10 (2%), HOMO->L+15 (6%)
31	50487.8875921	198.067308357	0.0076	Singlet-A	H-5->L+2 (39%), H-3->L+2 (21%)	H-7->LUMO (2%), H-6->L+1 (2%), H-5->L+7 (3%), H-3->L+7 (3%), HOMO->L+9 (6%), HOMO->L+12 (5%)
32	50876.6468269	196.5538341	0.0065	Singlet-A	H-6->L+1 (18%), H-1->L+3 (36%), H-1->L+6 (18%)	H-1->L+4 (6%), H-1->L+5 (4%), H-1->L+10 (6%)
33	51265.4060617	195.063314001	0.0985	Singlet-A	H-6->L+1 (49%), H-1->L+3 (11%)	H-7->LUMO (2%), H-2->L+2 (2%), H-2->L+3 (5%), H-2->L+4 (8%), H-2->L+5 (2%), H-2->L+7 (2%), H-1->L+4 (2%), H-1->L+6 (4%), H-1->L+10 (2%)
34	51474.3036588	194.271690712	0.0063	Singlet-A	HOMO->L+9 (15%), HOMO->L+13 (27%), HOMO->L+14 (15%), HOMO->L+16 (11%)	H-2->L+3 (9%), HOMO->L+8 (5%), HOMO->L+11 (2%), HOMO->L+12 (7%), HOMO->L+15 (2%)
35	51713.0437698	193.374809739	0.0026	Singlet-A	H-2->L+3 (19%), HOMO-	H-2->L+4 (4%), HOMO->L+8 (3%), HOMO->L+10 (4%), HOMO->L+12 (2%), HOMO->L+13 (5%)

					>L+9 (17%), HOMO->L+11 (14%), HOMO->L+15 (24%)	
36	51836.4465974	192.914458	0.0054	Singlet-A	H-2->L+3 (50%), HOMO->L+13 (11%)	H-2->L+4 (3%), H-2->L+6 (2%), HOMO->L+9 (4%), HOMO->L+11 (8%), HOMO->L+14 (3%), HOMO->L+15 (5%)
37	52341.34967	191.053537271	0.0022	Singlet-A	H-8->LUMO (48%), HOMO->L+14 (23%)	H-9->LUMO (2%), HOMO->L+9 (4%), HOMO->L+12 (7%), HOMO->L+13 (2%), HOMO->L+15 (4%), HOMO->L+18 (2%)
38	52343.7693332	191.044705557	0.0016	Singlet-A	H-8->LUMO (46%), HOMO->L+14 (25%)	H-9->LUMO (2%), HOMO->L+9 (4%), HOMO->L+12 (7%), HOMO->L+13 (2%), HOMO->L+15 (4%), HOMO->L+18 (2%)
39	52505.080219	190.457760626	0.0012	Singlet-A	H-9->L+1 (37%), H-1->L+7 (40%)	H-1->L+4 (3%), H-1->L+5 (2%), H-1->L+6 (5%), H-1->L+17 (2%)
40	52838.1871982	189.257060665	0.0422	Singlet-A	H-7->L+1 (39%), H-2->L+4 (36%)	H-2->L+2 (2%), H-2->L+7 (5%), H-1->L+7 (4%)
41	53064.8289928	188.448736947	0.0035	Singlet-A	H-9->L+1 (52%), H-1->L+7 (21%)	H-13->LUMO (3%), H-8->L+1 (2%), H-2->L+4 (2%), H-1->L+4 (8%), H-1->L+6 (2%)
42	53645.5481816	186.408757837	0.0459	Singlet-A	HOMO->L+15 (13%), HOMO->L+17 (15%)	H-5->L+2 (5%), H-3->L+3 (7%), H-3->L+4 (4%), H-3->L+7 (4%), H-2->L+5 (2%), H-2->L+6 (2%), H-2->L+7 (9%), HOMO->L+11 (5%), HOMO->L+12 (4%), HOMO->L+14 (8%), HOMO->L+16 (3%), HOMO->L+18 (6%), HOMO->L+19 (3%)
43	53785.0820979	185.925160099	0.0025	Singlet-A	H-4->L+3 (21%), H-4->L+5 (12%), H-3->L+3 (25%)	H-4->L+6 (9%), H-4->L+8 (3%), H-3->L+5 (8%), H-3->L+6 (5%), H-1->L+3 (2%), H-1->L+6 (3%), HOMO->L+15 (2%)

44	54010.1107836	185.150518207	0.0534	Singlet-A	HOMO->L+15 (20%)	H-7->L+1 (3%), H-5->L+2 (4%), H-4->L+3 (2%), H-3->L+6 (2%), H-3->L+7 (2%), H-2->L+5 (8%), H-2->L+6 (3%), H-2->L+7 (4%), H-1->L+3 (3%), H-1->L+6 (2%), HOMO->L+11 (6%), HOMO->L+12 (4%), HOMO->L+13 (5%), HOMO->L+14 (6%), HOMO->L+17 (4%), HOMO->L+18 (6%)
45	54272.240973	184.256257356	0.0174	Singlet-A	H-1->L+3 (19%), H-1->L+5 (11%), H-1->L+6 (22%)	H-7->L+1 (2%), H-4->L+3 (6%), H-4->L+5 (2%), H-2->L+5 (5%), H-1->L+4 (9%), H-1->L+7 (7%), H-1->L+10 (2%), H-1->L+11 (2%), H-1->L+13 (3%)
46	54310.1490311	184.127647933	0.0166	Singlet-A	HOMO->L+13 (14%), HOMO->L+16 (34%), HOMO->L+17 (10%)	H-4->L+3 (7%), H-3->L+3 (8%), H-2->L+5 (5%), H-2->L+6 (2%), HOMO->L+14 (2%)
47	54444.8436208	183.672122739	0.0512	Singlet-A	H-2->L+5 (19%), H-2->L+7 (13%), HOMO->L+16 (13%)	H-6->L+1 (2%), H-5->L+2 (2%), H-4->L+3 (3%), H-3->L+3 (6%), H-3->L+4 (2%), H-3->L+6 (2%), H-3->L+7 (3%), H-2->L+4 (5%), H-2->L+6 (7%), H-1->L+3 (2%), H-1->L+6 (3%), HOMO->L+13 (2%)
48	54745.6884228	182.662778657	0.0199	Singlet-A	H-2->L+5 (17%), H-2->L+6 (22%)	H-13->LUMO (2%), H-7->L+1 (3%), H-5->L+2 (3%), H-4->L+3 (5%), H-4->L+5 (2%), H-3->L+3 (5%), H-3->L+7 (4%), H-2->L+4 (2%), H-1->L+5 (9%), H-1->L+8 (2%), HOMO->L+17 (2%)
49	54844.0880631	182.335058402	0.021	Singlet-A	H-1->L+5 (37%)	H-10->LUMO (7%), H-3->L+3 (2%), H-3->L+4 (2%), H-2->L+5 (6%), H-2->L+6 (6%), H-1->L+3 (3%), H-1->L+6 (9%), H-1->L+8 (5%), H-1->L+10 (4%), H-1->L+14 (2%), HOMO->L+16 (2%)
50	54921.5172883	182.077999548	0.001	Singlet-A	H-13->LUMO (15%), H-10->LUMO (63%)	H-12->LUMO (7%), H-2->L+5 (2%), H-1->L+5 (2%)
51	55040.0807894	181.685779828	0.0002	Singlet-A	H-13->LUMO (26%), H-12->LUMO (12%), H-	H-11->LUMO (6%), H-9->L+2 (2%), H-5->L+2 (2%), H-2->L+6 (2%), H-1->L+6 (2%), H-1->L+7 (2%), HOMO->L+17 (5%)

					10->LUMO (26%)	
52	55120.7362323	181.419928026	0.0295	Singlet-A	H-2->L+7 (17%), HOMO->L+17 (13%)	H-13->LUMO (8%), H-12->LUMO (3%), H-5->L+2 (6%), H-5->L+7 (2%), H-3->L+4 (4%), H-3->L+6 (9%), H-3->L+7 (9%), H-2->L+6 (2%), H-1->L+5 (3%), H-1->L+7 (2%)
53	55219.1358726	181.096640539	0.1135	Singlet-A	H-2->L+7 (21%), HOMO->L+16 (11%), HOMO->L+17 (30%)	H-6->L+1 (3%), H-6->L+2 (3%), H-4->L+3 (2%), H-3->L+3 (3%), H-2->L+4 (3%), H-1->L+5 (2%), HOMO->L+19 (7%)
54	55571.6001581	179.948030497	0.0041	Singlet-A	H-2->L+6 (27%), HOMO->L+18 (20%)	H-4->L+3 (4%), H-4->L+5 (2%), H-3->L+3 (6%), H-2->L+3 (3%), H-2->L+5 (2%), H-2->L+7 (8%), H-2->L+8 (4%), HOMO->L+14 (2%), HOMO->L+20 (3%), HOMO->L+23 (3%)
55	55674.0325706	179.616951356	0.0037	Singlet-A	HOMO->L+18 (37%)	H-4->L+3 (4%), H-3->L+3 (8%), H-2->L+5 (4%), H-2->L+6 (8%), HOMO->L+14 (5%), HOMO->L+20 (7%), HOMO->L+23 (4%)
56	56098.2802002	178.258584119	0.0696	Singlet-A	H-4->L+4 (10%), H-3->L+4 (33%)	H-7->L+1 (2%), H-6->L+2 (8%), H-3->L+5 (6%), H-3->L+6 (2%), H-3->L+7 (8%), H-2->L+4 (5%), H-1->L+5 (2%), H-1->L+6 (2%)
57	56259.591086	177.747470377	0.1949	Singlet-A	H-7->L+1 (26%), H-2->L+4 (12%)	H-15->LUMO (2%), H-11->LUMO (2%), H-6->L+1 (4%), H-6->L+2 (4%), H-5->L+7 (3%), H-4->L+7 (2%), H-3->L+4 (6%), H-3->L+5 (3%), H-2->L+5 (9%), H-2->L+17 (2%), H-1->L+5 (2%)
58	56403.1577744	177.295037983	0.0142	Singlet-A	H-15->LUMO (19%), H-13->LUMO (11%), H-11->LUMO (39%)	H-17->LUMO (2%), H-16->LUMO (4%), H-14->LUMO (3%), H-9->L+2 (2%), H-6->L+2 (5%)
59	56749.9761789	176.21152771	0.0633	Singlet-A	H-3->L+6 (13%), HOMO->L+19 (26%)	H-5->L+3 (7%), H-4->L+4 (2%), H-4->L+7 (2%), H-3->L+3 (5%), H-3->L+5 (2%), H-3->L+7 (6%), H-2->L+5 (2%), H-2->L+8 (3%), HOMO->L+15 (3%), HOMO->L+16 (2%), HOMO->L+17 (2%), HOMO->L+22 (2%), HOMO->L+23 (2%), HOMO->L+24 (5%)

60	56870.9593432	175.836668055	0.009	Singlet-A	H-2->L+8 (15%), HOMO->L+19 (22%)	H-5->L+3 (4%), H-4->L+4 (2%), H-3->L+3 (3%), H-3->L+5 (4%), H-3->L+6 (7%), H-3->L+7 (2%), HOMO->L+17 (3%), HOMO->L+21 (5%), HOMO->L+22 (3%), HOMO->L+23 (3%), HOMO->L+24 (7%)
61	57047.5947632	175.292228209	0.0438	Singlet-A	H-6->L+2 (38%)	H-16->LUMO (4%), H-15->LUMO (2%), H-7->L+1 (3%), H-4->L+4 (8%), H-4->L+6 (6%), H-4->L+7 (2%), H-3->L+4 (5%), H-1->L+8 (2%), H-1->L+10 (3%), HOMO->L+21 (3%)
62	57133.8960871	175.027447538	0.0194	Singlet-A	H-1->L+8 (46%), H-1->L+10 (16%)	H-4->L+4 (2%), H-4->L+6 (3%), H-1->L+3 (2%), H-1->L+9 (2%), H-1->L+12 (9%), H-1->L+13 (5%)
63	57193.5811148	174.844795606	0.0166	Singlet-A	H-4->L+6 (10%), H-2->L+8 (22%), HOMO->L+21 (10%)	H-4->L+3 (5%), H-4->L+4 (4%), H-3->L+4 (4%), H-3->L+5 (3%), H-3->L+6 (2%), H-3->L+7 (3%), H-2->L+9 (2%), H-2->L+10 (9%), H-2->L+12 (2%), H-1->L+8 (3%)
64	57377.4755246	174.284419253	0.0075	Singlet-A	HOMO->L+21 (24%)	H-15->LUMO (4%), H-11->LUMO (5%), H-4->L+3 (2%), H-4->L+6 (4%), H-4->L+7 (3%), H-2->L+10 (2%), H-1->L+6 (6%), H-1->L+8 (8%), H-1->L+10 (8%), HOMO->L+19 (3%), HOMO->L+20 (4%), HOMO->L+25 (3%)
65	57453.291641	174.05443125	0.0134	Singlet-A	H-11->LUMO (12%), H-2->L+10 (13%)	H-16->LUMO (2%), H-15->LUMO (5%), H-12->LUMO (3%), H-9->L+2 (2%), H-6->L+2 (2%), H-5->L+3 (3%), H-4->L+4 (2%), H-4->L+6 (8%), H-3->L+6 (3%), H-2->L+8 (3%), HOMO->L+19 (5%), HOMO->L+20 (9%), HOMO->L+21 (6%), HOMO->L+25 (3%)
66	57473.4555017	173.993366376	0.0036	Singlet-A	H-11->LUMO (18%), H-1->L+10 (16%)	H-16->LUMO (4%), H-15->LUMO (7%), H-12->LUMO (4%), H-9->L+2 (2%), H-4->L+7 (3%), H-2->L+8 (2%), H-2->L+10 (4%), H-1->L+6 (7%), H-1->L+8 (3%), HOMO->L+19 (2%), HOMO->L+21 (4%)
67	57502.4914611	173.905508195	0.0352	Singlet-A	H-6->L+2 (14%), H-1->L+10 (14%)	H-15->LUMO (4%), H-11->LUMO (7%), H-4->L+3 (3%), H-4->L+4 (2%), H-4->L+6 (8%), H-4->L+7 (3%), H-3->L+4 (6%), H-2->L+10 (3%), H-1->L+6 (6%), H-1->L+7 (2%), H-1->L+8 (2%), HOMO->L+21 (6%)
68	57682.3530988	173.363246518	0.0034	Singlet-A	HOMO->L+20 (22%), HOMO->L+22 (30%)	H-3->L+4 (2%), H-3->L+5 (7%), H-2->L+8 (3%), HOMO->L+19 (2%), HOMO->L+21 (5%), HOMO->L+23 (2%), HOMO->L+26 (3%), HOMO->L+27 (4%)

69	57810.595253	172.978672097	0.0125	Singlet-A	H-4->L+4 (40%), H-4->L+8 (10%), H-3->L+4 (12%)	H-4->L+3 (6%), H-4->L+5 (4%), H-4->L+6 (3%), H-4->L+7 (4%), H-3->L+6 (3%), H-3->L+8 (4%)
70	57994.4896628	172.430174972	0.0102	Singlet-A	H-3->L+5 (30%), HOMO->L+20 (12%)	H-4->L+3 (2%), H-4->L+4 (2%), H-4->L+5 (4%), H-4->L+10 (4%), H-3->L+3 (2%), H-3->L+6 (9%), H-3->L+7 (4%), H-3->L+8 (4%), H-3->L+10 (2%), H-2->L+8 (2%), HOMO->L+16 (2%), HOMO->L+21 (7%)
71	58131.6039157	172.023466177	0.0049	Singlet-A	H-4->L+5 (19%), H-2->L+10 (14%)	H-4->L+3 (7%), H-4->L+6 (4%), H-4->L+8 (6%), H-4->L+10 (4%), H-2->L+8 (6%), HOMO->L+16 (2%), HOMO->L+18 (2%), HOMO->L+20 (7%), HOMO->L+21 (3%), HOMO->L+22 (5%), HOMO->L+25 (3%), HOMO->L+26 (3%)
72	58286.4623661	171.566425445	0.0249	Singlet-A	H-2->L+8 (18%), H-2->L+10 (19%), HOMO->L+22 (12%)	H-5->L+3 (3%), H-3->L+5 (2%), H-2->L+7 (2%), HOMO->L+16 (2%), HOMO->L+18 (3%), HOMO->L+19 (3%), HOMO->L+20 (7%), HOMO->L+21 (2%), HOMO->L+25 (4%), HOMO->L+26 (6%)
73	58407.4455305	171.21104868	0.0014	Singlet-A	H-8->L+1 (31%), H-4->L+5 (11%)	H-4->L+3 (2%), H-4->L+6 (4%), H-4->L+7 (2%), H-4->L+10 (2%), H-3->L+5 (7%), H-3->L+6 (3%), H-2->L+6 (2%), H-2->L+10 (9%), HOMO->L+22 (4%), HOMO->L+23 (3%)
74	58434.0618266	171.133063275	0.0002	Singlet-A	H-8->L+1 (61%)	H-9->L+1 (2%), H-4->L+4 (2%), H-4->L+5 (5%), H-4->L+6 (2%), H-4->L+7 (4%), H-3->L+5 (2%), H-2->L+10 (5%), H-1->L+9 (2%)
75	58492.1337455	170.963159653	0.0066	Singlet-A	H-1->L+9 (49%), H-1->L+11 (24%)	H-4->L+7 (3%), H-1->L+5 (2%), H-1->L+10 (5%), H-1->L+12 (2%), H-1->L+14 (2%)
76	58724.4214211	170.286905482	0.0759	Singlet-A	H-4->L+7 (36%)	H-5->L+4 (2%), H-4->L+4 (5%), H-4->L+6 (9%), H-3->L+6 (3%), H-3->L+7 (3%), H-3->L+8 (2%), H-2->L+8 (3%), H-2->L+9 (4%), H-2->L+11 (4%), HOMO->L+24 (2%)
77	58972.0336308	169.571903567	0.0128	Singlet-A	H-2->L+9 (31%), H-2->L+11 (23%), HOMO->L+24 (11%)	H-7->L+2 (2%), H-6->L+2 (2%), H-5->L+3 (2%), H-4->L+7 (4%), H-2->L+8 (3%), H-2->L+10 (2%), H-2->L+13 (2%), HOMO->L+28 (2%)

78	59144.6362786	169.077039428	0.0129	Singlet-A	HOMO->L+23 (46%)	H-12->LUMO (2%), H-9->L+2 (5%), H-4->L+7 (3%), HOMO->L+18 (2%), HOMO->L+19 (4%), HOMO->L+22 (8%), HOMO->L+26 (6%), HOMO->L+29 (7%)
79	59154.3149317	169.049375545	0.0052	Singlet-A	H-12->LUMO (21%), H-9->L+2 (25%)	H-13->LUMO (3%), H-13->L+1 (2%), H-5->L+7 (3%), H-3->L+7 (4%), H-1->L+13 (6%), HOMO->L+23 (4%), HOMO->L+24 (4%)
80	59302.7209467	168.626326758	0.0259	Singlet-A	H-1->L+13 (10%), HOMO->L+24 (32%)	H-12->LUMO (4%), H-9->L+2 (7%), H-4->L+7 (2%), H-2->L+9 (3%), H-1->L+8 (4%), H-1->L+12 (3%), H-1->L+14 (2%), HOMO->L+18 (3%), HOMO->L+19 (2%), HOMO->L+21 (2%), HOMO->L+23 (4%), HOMO->L+28 (5%)
81	59346.2748858	168.502572727	0.0277	Singlet-A	H-1->L+13 (32%), HOMO->L+24 (14%)	H-9->L+2 (3%), H-4->L+7 (3%), H-2->L+9 (5%), H-1->L+8 (6%), H-1->L+12 (3%), H-1->L+14 (5%), HOMO->L+28 (2%)
82	59583.4018879	167.831974 73	0.0024	Singlet-A	H-5->L+3 (20%), H-2->L+9 (10%)	H-13->LUMO (2%), H-13->L+1 (5%), H-12->L+1 (2%), H-9->L+2 (8%), H-5->L+4 (3%), H-5->L+5 (2%), H-5->L+7 (2%), H-4->L+7 (2%), H-3->L+5 (3%), H-3->L+6 (3%), H-3->L+7 (3%), H-3->L+8 (2%), H-2->L+12 (6%), H-1->L+9 (3%)
83	59636.6344803	167.682165286	0.0016	Singlet-A	H-13->LUMO (10%), H-12->LUMO (14%), H-2->L+12 (12%)	H-16->LUMO (5%), H-15->LUMO (6%), H-13->L+1 (7%), H-12->L+1 (2%), H-9->L+2 (6%), H-3->L+8 (4%), H-2->L+9 (9%), H-2->L+11 (4%), H-2->L+13 (3%)
84	59814.8830091	167.182471936	0.0095	Singlet-A	H-12->LUMO (11%), H-5->L+3 (13%), H-2->L+12 (14%)	H-13->LUMO (6%), H-5->L+4 (4%), H-4->L+6 (2%), H-3->L+6 (2%), H-3->L+7 (6%), H-2->L+9 (2%), H-2->L+10 (2%), H-2->L+11 (9%), H-2->L+13 (6%)
85	59932.6399557	166.853988201	0.0122	Singlet-A	H-1->L+9 (21%), H-1->L+11 (27%)	H-14->LUMO (2%), H-7->L+2 (7%), H-5->L+3 (9%), H-5->L+6 (2%), H-5->L+7 (3%), H-3->L+6 (4%), H-2->L+12 (2%), H-1->L+12 (4%), H-1->L+13 (2%)
86	60098.7901681	166.392700619	0.0136	Singlet-A	H-1->L+11 (16%)	H-13->L+1 (2%), H-7->L+2 (2%), H-5->L+3 (2%), H-5->L+4 (3%), H-5->L+6 (5%), H-5->L+7 (7%), H-4->L+8 (4%), H-4->L+9 (8%), H-3->L+5 (2%), H-3->L+6 (4%), H-3->L+7 (3%), H-3->L+8 (2%), H-

						3->L+9 (3%), H-1->L+8 (2%), H-1->L+9 (4%), HOMO->L+26 (2%)
87	60247.196183	165.982827975	0.0048	Singlet-A	H-4->L+9 (15%), H-3->L+8 (23%)	H-13->L+1 (2%), H-5->L+3 (6%), H-5->L+4 (8%), H-4->L+5 (3%), H-4->L+12 (2%), H-3->L+9 (3%), H-3->L+10 (6%), H-3->L+11 (2%), H-2->L+13 (3%)
88	60355.2744765	165.68560224	0.021	Singlet-A	H-7->L+2 (22%)	H-16->LUMO (3%), H-14->LUMO (3%), H-13->L+1 (3%), H-12->L+1 (2%), H-6->L+2 (2%), H-5->L+4 (7%), H-4->L+8 (7%), H-4->L+9 (4%), H-4->L+10 (2%), H-3->L+9 (2%), H-1->L+8 (3%), H-1->L+9 (3%), H-1->L+11 (4%), H-1->L+12 (9%), H-1->L+17 (2%)
89	60458.5134434	165.40267748	0.0186	Singlet-A	H-13->L+1 (10%), H-1->L+12 (23%)	H-16->LUMO (3%), H-12->L+1 (5%), H-11->L+1 (2%), H-7->L+2 (6%), H-5->L+5 (2%), H-4->L+8 (2%), H-3->L+8 (3%), H-2->L+13 (2%), H-1->L+8 (2%), H-1->L+13 (4%), H-1->L+17 (4%), HOMO->L+26 (2%)
90	60479.4838586	165.345326415	0.0267	Singlet-A	H-3->L+8 (10%), H-1->L+12 (17%)	H-7->L+2 (2%), H-5->L+4 (4%), H-5->L+5 (6%), H-5->L+6 (2%), H-4->L+7 (2%), H-4->L+8 (8%), H-4->L+9 (2%), H-4->L+10 (4%), H-3->L+9 (3%), H-2->L+13 (7%), H-2->L+14 (3%), H-1->L+13 (3%), H-1->L+17 (2%), HOMO->L+25 (2%), HOMO->L+27 (2%)
91	60556.9130837	165.133912724	0.0129	Singlet-A	H-13->L+1 (18%), H-12->L+1 (10%), H-9->L+2 (12%), H-5->L+4 (10%)	H-15->LUMO (4%), H-14->LUMO (2%), H-11->L+1 (3%), H-7->L+2 (5%), H-2->L+9 (2%), H-1->L+12 (8%)
92	60778.7155517	164.531282197	0.0092	Singlet-A	H-14->LUMO (11%), HOMO->L+25 (11%), HOMO->L+26 (12%)	H-10->L+1 (3%), H-9->L+2 (2%), H-5->L+7 (8%), H-4->L+10 (3%), H-3->L+10 (3%), H-2->L+9 (3%), H-2->L+11 (2%), H-2->L+12 (2%), H-1->L+10 (2%), H-1->L+14 (3%), HOMO->L+21 (3%), HOMO->L+23 (2%), HOMO->L+27 (5%)
93	60805.3318479	164.459261978	0.0129	Singlet-A	H-3->L+10 (29%)	H-14->LUMO (7%), H-7->L+2 (2%), H-5->L+3 (2%), H-5->L+6 (4%), H-5->L+7 (4%), H-4->L+10 (3%), H-3->L+8 (2%), H-2->L+9 (2%), H-2->L+11 (3%), H-2->L+12 (2%), H-2->L+14 (5%), H-1->L+14 (4%), H-1->L+17 (3%), HOMO->L+26 (4%)

94	60892.4397262	164.223999645	0.0176	Singlet-A	H-14->LUMO (25%), HOMO->L+25 (11%)	H-10->L+1 (2%), H-7->L+2 (6%), H-5->L+4 (3%), H-5->L+6 (2%), H-5->L+7 (3%), H-3->L+10 (7%), H-2->L+11 (2%), H-1->L+14 (2%), HOMO->L+20 (2%), HOMO->L+26 (3%), HOMO->L+27 (2%)
95	60974.708278	164.002424651	0.0178	Singlet-A	H-10->L+1 (26%)	H-14->LUMO (7%), H-7->L+2 (5%), H-5->L+4 (4%), H-3->L+8 (3%), H-2->L+11 (2%), H-2->L+12 (2%), H-2->L+13 (8%), H-2->L+14 (7%), H-2->L+15 (3%), H-1->L+17 (2%), HOMO->L+25 (3%), HOMO->L+26 (4%), HOMO->L+27 (3%)
96	61037.6195234	163.833387968	0.002	Singlet-A	H-10->L+1 (44%), H-2->L+13 (18%)	H-5->L+4 (2%), H-5->L+7 (2%), H-3->L+10 (2%), H-2->L+11 (5%), H-2->L+12 (2%), H-2->L+14 (5%)
97	61058.5899386	163.777119813	0.0034	Singlet-A	H-1->L+14 (10%), H-1->L+15 (11%), H-1->L+17 (26%)	H-14->LUMO (2%), H-10->L+1 (9%), H-7->L+2 (3%), H-2->L+12 (2%), H-1->L+7 (2%), H-1->L+19 (9%), H-1->L+20 (2%)
98	61087.625898	163.699273838	0.0164	Singlet-A	H-2->L+11 (18%)	H-10->L+1 (7%), H-7->L+2 (6%), H-5->L+4 (5%), H-4->L+5 (2%), H-4->L+9 (6%), H-3->L+4 (2%), H-3->L+10 (7%), H-2->L+9 (5%), H-2->L+12 (5%), H-2->L+13 (7%), H-2->L+15 (4%)
99	61149.7305891	163.533018113	0.005	Singlet-A	H-3->L+9 (11%)	H-4->L+3 (3%), H-4->L+4 (3%), H-4->L+5 (6%), H-4->L+8 (6%), H-4->L+9 (5%), H-4->L+10 (4%), H-4->L+14 (2%), H-3->L+12 (3%), H-3->L+14 (2%), H-2->L+11 (4%), H-2->L+12 (4%), H-2->L+14 (2%), H-2->L+15 (2%), HOMO->L+20 (2%), HOMO->L+22 (3%), HOMO->L+25 (6%), HOMO->L+26 (9%)
100	61215.8680522	163.356337469	0.0028	Singlet-A	HOMO->L+25 (13%), HOMO->L+26 (12%)	H-5->L+4 (2%), H-5->L+5 (2%), H-4->L+3 (2%), H-4->L+4 (2%), H-4->L+5 (4%), H-4->L+6 (2%), H-4->L+8 (3%), H-4->L+9 (7%), H-4->L+10 (2%), H-4->L+14 (2%), H-3->L+8 (2%), H-3->L+9 (3%), H-2->L+12 (2%), H-2->L+13 (6%), HOMO->L+20 (3%), HOMO->L+22 (9%), HOMO->L+31 (2%)

Table of 100rst electronic transitions with B3LYP-D3BJ/6-31+G(d,p) levels of theory

First 100 electronic transition in toluene for 4a

HOMO is 86					
No.	Energy (cm-1)	Wavelength (nm)	Osc. Strength	Symmetry	Major contribs
1	24659.5951122	405.521662237	0.0026	Singlet-A	H-1->LUMO (98%)
2	25062.8723267	398.996566301	0.3766	Singlet-A	HOMO->LUMO (97%)
3	28693.1738117	348.514948734	0.0131	Singlet-A	H-2->LUMO (21%), HOMO->L+1 (77%)
4	32134.7415602	311.189681774	0.0032	Singlet-A	H-1->L+1 (94%)
5	32162.1644108	310.924348009	0.0573	Singlet-A	H-2->LUMO (68%), HOMO->L+1 (19%)
6	34126.9309998	293.023711978	0.0511	Singlet-A	H-3->LUMO (80%)
7	35772.302035	279.545889728	0.0826	Singlet-A	H-4->LUMO (49%), HOMO->L+2 (42%)
8	36773.2360814	271.936904815	0.0867	Singlet-A	H-5->LUMO (19%), H-4->LUMO (43%), HOMO->L+2 (31%)
9	38083.8870285	262.578239257	0.3238	Singlet-A	H-5->LUMO (35%), H-2->L+1 (37%), HOMO->L+2 (14%)
10	38301.6567244	261.085312105	0.0011	Singlet-A	H-1->L+2 (94%)
11	38829.1433209	257.538517328	0.343	Singlet-A	H-5->LUMO (19%), H-3->L+1 (28%), H-2->L+1 (32%)
12	39167.8961811	255.311134245	0.035	Singlet-A	HOMO->L+3 (94%)
13	39432.4460338	253.598267564	0.3639	Singlet-A	H-3->L+1 (44%), H-2->L+1 (22%)
14	40760.8411784	245.333504189	0.0101	Singlet-A	H-4->L+1 (67%), H-3->L+1 (11%)
15	42132.7902621	237.344831372	0.1194	Singlet-A	H-4->L+1 (22%), H-2->L+2 (18%), HOMO->L+5 (37%)
16	42868.3679014	233.272235206	0.0117	Singlet-A	HOMO->L+4 (57%), HOMO->L+6 (17%)
17	43074.8458352	232.154052002	0.0878	Singlet-A	H-6->LUMO (41%), H-5->L+1 (35%)
18	43295.0351943	230.973365771	0.022	Singlet-A	H-8->LUMO (10%), H-3->L+2 (27%), H-2->L+2 (14%), HOMO->L+5 (14%), HOMO->L+8 (10%)
19	43556.3588293	229.587602563	0.0662	Singlet-A	H-8->LUMO (20%), H-3->L+2 (14%), H-2->L+2 (30%), HOMO->L+5 (17%)

20	43809.61692	228.260384433	0.015	Singlet-A	H-8->LUMO (61%), H-3->L+2 (14%)
21	43979.7999045	227.377114532	0.0196	Singlet-A	HOMO->L+4 (12%), HOMO->L+6 (45%), HOMO->L+10 (10%)
22	44276.6119344	225.852872727	0.0742	Singlet-A	H-5->L+1 (33%), HOMO->L+8 (38%)
23	44909.7571611	222.668761359	0.0073	Singlet-A	HOMO->L+4 (16%), HOMO->L+7 (51%)
24	45123.4940848	221.614043921	0.1198	Singlet-A	H-6->LUMO (23%), HOMO->L+6 (12%), HOMO->L+8 (20%)
25	45782.4490533	218.424313395	0.0025	Singlet-A	H-1->L+5 (10%), HOMO->L+9 (24%), HOMO->L+10 (31%), HOMO->L+11 (10%)
26	45814.7112305	218.27050158	0.0047	Singlet-A	H-1->L+5 (54%), H-1->L+8 (14%)
27	46455.9220015	215.25780932	0.0038	Singlet-A	HOMO->L+9 (52%), HOMO->L+10 (23%)
28	46589.0034823	214.642925423	0.0564	Singlet-A	H-7->LUMO (11%), H-1->L+3 (63%)
29	46697.0817758	214.146144035	0.1105	Singlet-A	H-7->LUMO (30%), H-4->L+2 (32%), H-1->L+3 (20%)
30	47264.0895394	211.577121181	0.0031	Singlet-A	HOMO->L+7 (12%), HOMO->L+11 (59%), HOMO->L+15 (13%)
31	47437.4987416	210.803694657	0.0173	Singlet-A	H-7->LUMO (36%), H-4->L+2 (49%)
32	48048.0604444	208.124946304	0.0012	Singlet-A	H-1->L+5 (26%), H-1->L+6 (25%), H-1->L+8 (34%)
33	48158.5584012	207.647411633	0.005	Singlet-A	H-2->L+3 (88%)
34	48563.4487245	205.916183311	0.0128	Singlet-A	HOMO->L+12 (27%), HOMO->L+13 (42%), HOMO->L+14 (10%)
35	48611.0354358	205.714605596	0.0053	Singlet-A	H-5->L+2 (13%), H-1->L+4 (45%), H-1->L+7 (12%)
36	48763.4742229	205.071524524	0.0054	Singlet-A	H-5->L+2 (31%), H-3->L+2 (15%), H-1->L+4 (14%)
37	49086.0959945	203.723677701	0.0093	Singlet-A	HOMO->L+12 (32%), HOMO->L+13 (10%), HOMO->L+14 (14%), HOMO->L+15 (29%)
38	49176.4300906	203.349449758	0.0529	Singlet-A	H-6->L+1 (53%)
39	49318.3836701	202.764147075	0.0078	Singlet-A	HOMO->L+14 (49%), HOMO->L+15 (25%)
40	49699.883915	201.207713425	0.0036	Singlet-A	H-1->L+4 (23%), H-1->L+6 (20%), H-1->L+7 (19%), H-1->L+8 (16%)
41	50184.6231268	199.264224317	0.0581	Singlet-A	H-7->L+1 (19%), H-2->L+5 (48%)
42	50230.5967293	199.081847542	0.0028	Singlet-A	HOMO->L+11 (10%), HOMO->L+12 (21%), HOMO->L+13 (27%), HOMO->L+14 (18%), HOMO->L+15 (15%)
43	50340.2881316	198.648048534	0.0033	Singlet-A	H-3->L+3 (19%), H-3->L+4 (19%), H-2->L+4 (31%)
44	50654.8443589	197.414484766	0.0054	Singlet-A	H-1->L+6 (28%), H-1->L+7 (39%), H-1->L+8 (18%)

45	50825.8338979	196.750338029	0.0066	Singlet-A	H-8->L+1 (57%), H-2->L+4 (11%)
46	50842.7715409	196.684793077	0.0102	Singlet-A	H-8->L+1 (32%), H-3->L+4 (10%), H-2->L+4 (26%)
47	51123.4524822	195.604942829	0.0422	Singlet-A	H-5->L+2 (15%), H-3->L+3 (10%), H-3->L+5 (26%)
48	51496.0806284	194.189535941	0.0153	Singlet-A	H-4->L+3 (10%), H-4->L+4 (11%), H-3->L+3 (25%), H-2->L+6 (23%)
49	51692.0733546	193.453257938	0.0006	Singlet-A	H-1->L+9 (46%), HOMO->L+17 (12%)
50	51741.2731748	193.269306811	0.0118	Singlet-A	H-1->L+9 (19%), HOMO->L+17 (34%)
51	51987.2722756	192.354773818	0.0656	Singlet-A	H-2->L+6 (34%), HOMO->L+17 (15%)
52	52155.0355969	191.736040165	0.0101	Singlet-A	H-2->L+8 (14%), H-1->L+9 (13%), H-1->L+10 (36%)
53	52273.5990979	191.30115723	0.0564	Singlet-A	H-9->LUMO (39%), H-2->L+8 (21%), H-1->L+10 (14%)
54	52307.4743839	191.177267069	0.0725	Singlet-A	H-9->LUMO (57%), H-2->L+8 (15%)
55	52500.2408925	190.475316494	0.0025	Singlet-A	H-2->L+7 (15%), HOMO->L+16 (51%)
56	52648.6469074	189.938404639	0.0385	Singlet-A	H-2->L+7 (46%), HOMO->L+16 (16%)
57	52999.498084	188.681032114	0.0064	Singlet-A	H-4->L+4 (15%), H-3->L+3 (11%), H-3->L+4 (41%)
58	53235.8185317	187.843453446	0.0044	Singlet-A	HOMO->L+18 (57%), HOMO->L+19 (14%)
59	53475.3651971	187.001995463	0.0127	Singlet-A	H-4->L+3 (32%), H-3->L+6 (16%), H-2->L+9 (15%)
60	53510.0470376	186.880792554	0.0057	Singlet-A	HOMO->L+18 (11%), HOMO->L+20 (50%)
61	53689.1021208	186.257538401	0.0107	Singlet-A	H-4->L+3 (15%), H-2->L+9 (39%)
62	53717.3315258	186.15965678	0.0193	Singlet-A	H-1->L+11 (67%)
63	53813.3115029	185.827627416	0.0596	Singlet-A	H-4->L+5 (13%), H-3->L+5 (19%), H-3->L+6 (11%), H-3->L+8 (19%)
64	54014.9501101	185.133930136	0.1067	Singlet-A	H-4->L+5 (26%), H-3->L+8 (11%)
65	54215.782163	184.448136706	0.0119	Singlet-A	H-10->LUMO (59%)
66	54230.3001427	184.398758142	0.0657	Singlet-A	H-10->LUMO (28%), H-3->L+7 (18%), H-2->L+9 (11%)
67	54340.7980994	184.023797032	0.0182	Singlet-A	H-2->L+10 (17%), HOMO->L+19 (28%), HOMO->L+21 (10%)
68	54394.0306918	183.843702569	0.059	Singlet-A	H-7->L+1 (12%), H-2->L+10 (23%), HOMO->L+19 (19%)
69	54604.5413977	183.134950757	0.012	Singlet-A	H-6->L+2 (17%), H-2->L+10 (12%), H-1->L+12 (15%)

70	54643.2560103	183.005200095	0.0123	Singlet-A	H-13->LUMO (16%), H-12->LUMO (29%), H-11->LUMO (11%)
71	54883.6092302	182.203760654	0.0073	Singlet-A	H-6->L+2 (13%), HOMO->L+21 (53%)
72	54923.9369516	182.069978137	0.0181	Singlet-A	H-6->L+2 (12%), H-3->L+6 (12%), H-1->L+12 (30%)
73	54961.0384553	181.947071617	0.0323	Singlet-A	H-4->L+5 (12%), H-1->L+13 (14%)
74	55010.2382755	181.784342578	0.0227	Singlet-A	H-1->L+12 (33%), H-1->L+13 (18%)
75	55169.129498	181.260790065	0.0027	Singlet-A	H-3->L+6 (10%), H-3->L+7 (17%), H-3->L+8 (11%)
76	55227.2014169	181.070192649	0.0114	Singlet-A	H-4->L+5 (10%), H-4->L+6 (31%), H-4->L+7 (13%)
77	55490.9447152	180.209582867	0.0215	Singlet-A	H-11->LUMO (10%), H-1->L+13 (20%), H-1->L+14 (19%), H-1->L+15 (10%)
78	55522.4003379	180.107487053	0.0181	Singlet-A	HOMO->L+22 (60%)
79	55607.088553	179.833187822	0.0142	Singlet-A	H-15->LUMO (23%), H-13->LUMO (17%), H-11->LUMO (14%)
80	55705.4881933	179.515525747	0.0024	Singlet-A	H-3->L+7 (10%), H-2->L+11 (47%)
81	55860.3466437	179.017865102	0.0164	Singlet-A	H-5->L+3 (17%), H-4->L+7 (24%), H-3->L+9 (17%)
82	56022.4640839	178.499824374	0.0244	Singlet-A	H-5->L+3 (34%), H-4->L+6 (10%), H-2->L+11 (11%)
83	56157.1586736	178.071687318	0.0511	Singlet-A	H-3->L+9 (14%), H-1->L+15 (17%)
84	56208.778157	177.908154703	0.0156	Singlet-A	H-1->L+14 (20%), H-1->L+15 (44%)
85	56329.7613214	177.526049559	0.0051	Singlet-A	H-1->L+14 (11%), H-1->L+17 (26%), H-1->L+18 (13%)
86	56586.2456298	176.721390308	0.0103	Singlet-A	H-4->L+8 (18%), H-2->L+12 (12%), HOMO->L+23 (19%)
87	56618.5078069	176.62069149	0.006	Singlet-A	HOMO->L+23 (32%)
88	56778.2055839	176.123917569	0.0099	Singlet-A	H-4->L+9 (11%), H-3->L+9 (10%), H-3->L+10 (15%), H-2->L+12 (11%), HOMO->L+23 (15%)
89	56870.1527888	175.839161838	0.0209	Singlet-A	H-11->LUMO (26%), H-8->L+2 (14%), H-4->L+8 (13%)
90	56977.4245278	175.508108393	0.017	Singlet-A	H-4->L+8 (19%), H-2->L+12 (45%)
91	57235.5219451	174.716673495	0.0219	Singlet-A	H-5->L+5 (26%), HOMO->L+24 (10%)
92	57404.8983752	174.201161975	0.0041	Singlet-A	H-5->L+4 (28%), H-3->L+10 (22%)
93	57484.7472637	173.959188759	0.0049	Singlet-A	HOMO->L+24 (31%)
94	57583.9534585	173.659490177	0.0034	Singlet-A	H-9->L+1 (34%), H-5->L+5 (10%), H-4->L+9 (14%)

95	57650.0909216	173.460264158	0.0011	Singlet-A	H-2->L+13 (57%)
96	57689.6120887	173.341432503	0.0043	Singlet-A	H-15->LUMO (17%), H-9->L+1 (25%), H-8->L+2 (29%)
97	57787.2051746	173.048687331	0.0188	Singlet-A	H-9->L+1 (24%), H-4->L+9 (15%)
98	57837.2115492	172.899068474	0.0327	Singlet-A	H-5->L+5 (10%), H-1->L+16 (49%)
99	57947.7095059	172.569374791	0.0013	Singlet-A	H-2->L+14 (43%), H-2->L+15 (28%)
100	58005.7814248	172.396608655	0.0111	Singlet-A	HOMO->L+26 (48%)

First 100 electronic transition in chlorform for 4a

HOMO is 86					
No.	Energy (cm-1)	Wavelength (nm)	Osc. Strength	Symmetry	Major contribs
1	24532.9660669	407.614797686	0.3807	Singlet-A	HOMO->LUMO (97%)
2	25098.3607216	398.43239608	0.0024	Singlet-A	H-1->LUMO (98%)
3	28490.72865	350.991374171	0.0116	Singlet-A	H-2->LUMO (22%), HOMO->L+1 (77%)
4	31820.9918873	314.257960135	0.0591	Singlet-A	H-2->LUMO (72%), HOMO->L+1 (20%)
5	32987.2695917	303.147248129	0.0	Singlet-A	H-1->L+1 (98%)
6	33951.1021343	294.541248188	0.0605	Singlet-A	H-3->LUMO (78%)
7	35476.2965596	281.878351739	0.0703	Singlet-A	H-4->LUMO (71%), HOMO->L+2 (21%)
8	36215.1004165	276.127910319	0.0942	Singlet-A	H-5->LUMO (23%), H-4->LUMO (22%), HOMO->L+2 (46%)
9	37944.3531123	263.54382615	0.2276	Singlet-A	H-5->LUMO (44%), H-2->L+1 (21%), HOMO->L+2 (18%)
10	38855.7596171	257.3621027776	0.424	Singlet-A	H-3->L+1 (24%), H-2->L+1 (46%)
11	39004.165632	256.38287188	0.0185	Singlet-A	H-1->L+2 (92%)
12	39493.7441704	253.204658359	0.3628	Singlet-A	H-3->L+1 (42%), H-2->L+1 (23%), H-2->L+2 (11%)
13	39817.9790509	251.142831414	0.0317	Singlet-A	HOMO->L+3 (90%)
14	40761.6477328	245.328649753	0.001	Singlet-A	H-4->L+1 (70%), H-3->L+1 (13%)
15	41967.4466042	238.279924302	0.1206	Singlet-A	H-4->L+1 (19%), H-2->L+2 (12%), HOMO->L+4 (34%), HOMO->L+5 (16%)
16	42881.2727722	233.202033277	0.053	Singlet-A	H-6->LUMO (44%), H-5->L+1 (27%), HOMO->L+4 (15%)
17	43187.7634552	231.547067964	0.1465	Singlet-A	H-2->L+2 (48%), HOMO->L+4 (20%)
18	43504.7393458	229.860014113	0.0095	Singlet-A	HOMO->L+4 (10%), HOMO->L+5 (48%)
19	43727.3483682	228.689833095	0.0182	Singlet-A	H-8->LUMO (73%)
20	44076.586436	226.877823547	0.0108	Singlet-A	H-3->L+2 (15%), HOMO->L+6 (46%)
21	44149.982889	226.500654035	0.0757	Singlet-A	H-5->L+1 (29%), H-3->L+2 (21%), HOMO->L+6 (16%)

22	44501.6406201	224.710816515	0.102	Singlet-A	H-6->LUMO (16%), H-5->L+1 (25%), HOMO->L+7 (16%)
23	45261.4148922	220.93874051	0.0678	Singlet-A	H-6->LUMO (10%), HOMO->L+7 (62%)
24	45757.445866	218.543666735	0.001	Singlet-A	HOMO->L+6 (10%), HOMO->L+8 (21%), HOMO->L+9 (41%)
25	46279.2865816	216.079389693	0.0003	Singlet-A	HOMO->L+6 (10%), HOMO->L+10 (70%)
26	46518.833247	214.966698475	0.1419	Singlet-A	H-7->LUMO (66%), H-4->L+2 (12%)
27	46594.6493633	214.616917106	0.0049	Singlet-A	H-1->L+4 (37%), H-1->L+5 (43%)
28	47205.2110661	211.841018696	0.0053	Singlet-A	HOMO->L+8 (65%), HOMO->L+9 (23%)
29	47410.8824455	210.92203908	0.0341	Singlet-A	H-7->LUMO (11%), H-4->L+2 (81%)
30	47575.419549	210.192576225	0.0006	Singlet-A	HOMO->L+11 (36%), HOMO->L+12 (30%)
31	47894.8151029	208.790867624	0.0016	Singlet-A	H-1->L+3 (68%), H-1->L+6 (12%)
32	48621.5206434	205.670243704	0.011	Singlet-A	H-5->L+2 (46%), H-3->L+2 (15%), H-2->L+3 (10%)
33	48801.3822811	204.91222856	0.0144	Singlet-A	HOMO->L+12 (24%), HOMO->L+13 (11%), HOMO->L+14 (12%), HOMO->L+15 (17%)
34	48897.3622581	204.5100009092	0.0169	Singlet-A	H-2->L+3 (64%)
35	49197.4005057	203.26277196	0.043	Singlet-A	H-6->L+1 (37%), HOMO->L+14 (14%)
36	49268.3772955	202.969948453	0.0184	Singlet-A	H-6->L+1 (11%), H-2->L+3 (11%), HOMO->L+11 (11%), HOMO->L+13 (17%), HOMO->L+15 (17%)
37	49413.5570927	202.37361138	0.0175	Singlet-A	H-1->L+4 (15%), H-1->L+7 (51%)
38	49465.1765761	202.162423996	0.0007	Singlet-A	HOMO->L+13 (26%), HOMO->L+14 (47%)
39	50091.062813	199.636410937	0.0083	Singlet-A	H-1->L+3 (10%), H-1->L+4 (18%), H-1->L+5 (20%), H-1->L+6 (13%), H-1->L+7 (21%)
40	50548.3791743	197.830279889	0.0158	Singlet-A	H-7->L+1 (16%), H-2->L+4 (37%)
41	50648.3919235	197.43963471	0.0179	Singlet-A	H-2->L+4 (10%), HOMO->L+11 (12%), HOMO->L+12 (14%), HOMO->L+13 (14%), HOMO->L+15 (26%)
42	50882.2927079	196.532024557	0.0034	Singlet-A	H-1->L+4 (13%), H-1->L+5 (18%), H-1->L+6 (34%)
43	51126.6786999	195.592599682	0.0178	Singlet-A	H-8->L+1 (16%), H-7->L+1 (10%), H-3->L+3 (26%), H-3->L+4 (12%), H-2->L+5 (10%)
44	51277.5043781	195.017291135	0.0022	Singlet-A	H-8->L+1 (75%)
45	51367.8384742	194.674338984	0.009	Singlet-A	H-2->L+4 (15%), H-2->L+5 (34%)

46	51711.430 6609	193.38084 1957	0.062 1	Singlet-A	H-2->L+7 (10%), HOMO->L+16 (17%), HOMO->L+17 (22%)
47	51896.938 1796	192.68959 5008	0.000 5	Singlet-A	H-9->LUMO (98%)
48	51948.557 663	192.49812 6028	0.036 1	Singlet-A	H-4->L+3 (13%), HOMO->L+16 (18%)
49	52128.419 3007	191.83393 8841	0.049 5	Singlet-A	H-2->L+6 (31%), HOMO->L+16 (13%)
50	52566.378 3556	190.23566 6082	0.080 1	Singlet-A	H-2->L+7 (31%)
51	52663.971 4416	189.88313 5021	0.001 7	Singlet-A	H-2->L+6 (36%)
52	52714.784 3706	189.70010 2531	0.021 7	Singlet-A	H-1->L+8 (29%), H-1->L+9 (23%)
53	52777.695 616	189.47397 9174	0.008 3	Singlet-A	HOMO->L+16 (16%), HOMO->L+17 (22%), HOMO->L+18 (24%)
54	53065.635 5472	188.44587 268	0.001	Singlet-A	H-1->L+6 (17%), H-1->L+10 (48%)
55	53143.871 3268	188.16845 1984	0.082 7	Singlet-A	H-2->L+7 (13%), HOMO->L+18 (33%)
56	53505.207 711	186.89769 5155	0.029 9	Singlet-A	H-3->L+4 (26%), H-2->L+9 (14%)
57	53647.161 2905	186.40315 2738	0.006 4	Singlet-A	H-1->L+8 (40%), H-1->L+9 (45%)
58	53786.695 2067	185.91958 4045	0.007 5	Singlet-A	H-3->L+4 (14%), H-3->L+5 (14%), H-3->L+7 (11%), H-2->L+8 (20%), H-2->L+9 (10%)
59	53921.389 7964	185.45516 0517	0.003 1	Singlet-A	H-10->LUMO (81%)
60	54059.310 6037	184.98201 1208	0.001 8	Singlet-A	H-3->L+5 (27%), H-3->L+7 (11%)
61	54189.165 8668	184.53873 279	0.035 4	Singlet-A	H-12->LUMO (48%), H-11->LUMO (10%)
62	54224.654 2617	184.41795 7775	0.021	Singlet-A	H-12->LUMO (14%), H-3->L+6 (10%), HOMO->L+19 (24%)
63	54351.283 307	183.98829 598	0.017 6	Singlet-A	H-3->L+6 (13%), H-2->L+10 (16%), HOMO->L+19 (32%)
64	54446.456 7296	183.66668 1005	0.235 7	Singlet-A	H-7->L+1 (20%), H-2->L+5 (11%)
65	54539.210 489	183.35432 2704	0.014 8	Singlet-A	H-4->L+3 (20%), H-4->L+6 (17%), H-2->L+10 (11%)
66	54639.223 2382	183.01870 721	0.001 1	Singlet-A	H-4->L+3 (20%), H-4->L+4 (17%), H-2->L+10 (23%)
67	54775.530 9367	182.56326 9201	0.038 9	Singlet-A	H-6->L+2 (50%)
68	54839.248 7366	182.35114 8683	0.017 3	Singlet-A	HOMO->L+20 (14%), HOMO->L+21 (57%)
69	55052.179 1058	181.64585 2397	0.000 4	Singlet-A	HOMO->L+20 (37%), HOMO->L+21 (14%)
70	55118.316 569	181.42789 2259	0.004 7	Singlet-A	H-15->LUMO (13%), H-12->LUMO (11%), H-11->LUMO (39%)

71	55209.4572195	181.128388208	0.0434	Singlet-A	H-2->L+8 (24%), H-2->L+9 (21%)
72	55259.4635941	180.964478292	0.0062	Singlet-A	H-4->L+4 (12%), H-4->L+6 (16%), H-2->L+8 (13%), H-2->L+10 (10%)
73	55337.6993737	180.70863287	0.0141	Singlet-A	H-1->L+11 (54%)
74	55394.1581837	180.524451095	0.0171	Singlet-A	H-4->L+5 (50%), H-4->L+6 (13%)
75	55486.9119431	180.222680445	0.0469	Singlet-A	HOMO->L+22 (42%), HOMO->L+24 (15%)
76	55640.1572846	179.726307186	0.021	Singlet-A	H-1->L+12 (43%), H-1->L+14 (15%)
77	56053.1131522	178.402223135	0.0023	Singlet-A	H-3->L+8 (16%), H-3->L+9 (15%), H-2->L+11 (14%), H-2->L+12 (10%)
78	56256.3648683	177.757663927	0.0162	Singlet-A	H-1->L+13 (20%)
79	56374.9283694	177.383817403	0.0125	Singlet-A	H-15->LUMO (11%), H-11->LUMO (23%), H-1->L+13 (16%)
80	56395.0922301	177.320394463	0.0101	Singlet-A	H-5->L+3 (13%), H-1->L+12 (12%), H-1->L+13 (15%), H-1->L+14 (13%)
81	56495.9115337	177.003958845	0.0077	Singlet-A	H-5->L+3 (11%), H-3->L+8 (10%), HOMO->L+23 (35%)
82	56510.4295135	176.958485117	0.0062	Singlet-A	H-3->L+8 (21%), HOMO->L+23 (25%)
83	56567.6948779	176.779344139	0.0185	Singlet-A	H-5->L+3 (14%), H-2->L+11 (11%), H-2->L+12 (10%)
84	56724.9729916	176.289198084	0.0123	Singlet-A	H-1->L+13 (16%), H-1->L+14 (27%)
85	56904.8346292	175.731992987	0.0054	Singlet-A	HOMO->L+22 (13%), HOMO->L+24 (40%)
86	57087.1159302	175.170874147	0.0256	Singlet-A	H-4->L+7 (19%)
87	57237.9416084	174.709287563	0.0032	Singlet-A	H-5->L+4 (10%), H-4->L+9 (12%), H-3->L+9 (18%)
88	57376.6689702	174.286869201	0.0158	Singlet-A	H-3->L+10 (19%), H-2->L+12 (10%), H-2->L+13 (10%)
89	57392.8000588	174.237883319	0.0034	Singlet-A	H-8->L+2 (18%)
90	57504.9111244	173.898190684	0.0095	Singlet-A	H-2->L+11 (16%), H-2->L+12 (16%)
91	57608.1500913	173.586549545	0.0202	Singlet-A	H-8->L+2 (12%), H-1->L+15 (36%)
92	57677.5137722	173.377792245	0.0218	Singlet-A	HOMO->L+25 (10%)
93	57735.5856911	173.203404457	0.0028	Singlet-A	H-9->L+1 (94%)
94	57772.6871948	173.092173578	0.0006	Singlet-A	H-4->L+8 (16%), H-4->L+9 (21%), H-3->L+8 (11%), H-2->L+13 (16%)
95	57864.6343997	172.817129214	0.0047	Singlet-A	H-1->L+15 (11%), H-1->L+17 (18%), H-1->L+18 (10%), HOMO->L+25 (13%)

96	57883.991706	172.759336481	0.0	Singlet-A	H-2->L+13 (21%), HOMO->L+25 (10%)
97	57971.9061388	172.497346837	0.0071	Singlet-A	H-2->L+14 (12%), HOMO->L+25 (28%)
98	58150.961222	171.966202963	0.0174	Singlet-A	H-14->LUMO (11%), H-5->L+7 (11%), H-2->L+13 (11%)
99	58343.7277306	171.398030071	0.0126	Singlet-A	H-13->LUMO (11%), H-2->L+14 (18%), HOMO->L+26 (16%)
100	58370.3440267	171.319874274	0.0072	Singlet-A	H-2->L+14 (36%), HOMO->L+26 (21%)

First 100 electronic transitions in DMSO for 4a

HOMO is 86					
No.	Energy (cm-1)	Wavelength (nm)	Osc. Strength	Symmetry	Major contribs
1	24115.1708727	414.67672167	0.3838	Singlet-A	HOMO->LUMO (97%)
2	25766.9943433	388.093382829	0.0025	Singlet-A	H-1->LUMO (98%)
3	28254.4082023	353.927073199	0.0112	Singlet-A	H-2->LUMO (20%), HOMO->L+1 (78%)
4	31552.4092625	316.933008722	0.0604	Singlet-A	H-2->LUMO (74%), HOMO->L+1 (19%)
5	33955.1349065	294.506266211	0.0011	Singlet-A	H-1->L+1 (97%)
6	34080.9573974	293.418987131	0.0695	Singlet-A	H-3->LUMO (73%), HOMO->L+2 (15%)
7	35206.9073803	284.035172189	0.043	Singlet-A	H-4->LUMO (84%)
8	36086.8582623	277.109188262	0.133	Singlet-A	H-5->LUMO (21%), H-4->LUMO (11%), HOMO->L+2 (56%)
9	37866.9238871	264.082713183	0.1734	Singlet-A	H-5->LUMO (53%), H-2->L+1 (17%), HOMO->L+2 (14%)
10	38931.5757334	256.860910755	0.4882	Singlet-A	H-3->L+1 (19%), H-2->L+1 (55%)
11	39634.8911955	252.302950718	0.3086	Singlet-A	H-3->L+1 (41%), H-2->L+1 (21%), H-2->L+2 (13%)
12	40020.4242126	249.872413818	0.0015	Singlet-A	H-1->L+2 (95%)
13	40304.3313716	248.112291153	0.0267	Singlet-A	HOMO->L+3 (82%), HOMO->L+4 (10%)
14	40799.555791	245.100707744	0.0009	Singlet-A	H-4->L+1 (77%), H-3->L+1 (13%)
15	41830.3323512	239.060974128	0.118	Singlet-A	H-4->L+1 (13%), HOMO->L+4 (54%)
16	42891.7579798	233.145025315	0.0786	Singlet-A	H-6->LUMO (52%), H-5->L+1 (24%)
17	43218.4125235	231.382862444	0.1634	Singlet-A	H-2->L+2 (56%), HOMO->L+6 (11%)
18	43623.3028469	229.235279023	0.0057	Singlet-A	HOMO->L+5 (65%)
19	43936.2459653	227.602513148	0.0054	Singlet-A	H-8->LUMO (81%)
20	44033.8390513	227.098073106	0.0007	Singlet-A	HOMO->L+6 (52%), HOMO->L+7 (17%), HOMO->L+9 (12%)
21	44307.2610027	225.696641447	0.0246	Singlet-A	H-3->L+2 (23%), HOMO->L+7 (35%)

22	44425.0179493	225.098389637	0.1137	Singlet-A	H-5->L+1 (51%), HOMO->L+7 (13%)
23	45090.4253532	221.776572779	0.1086	Singlet-A	H-6->LUMO (15%), H-3->L+2 (22%), HOMO->L+6 (16%), HOMO->L+7 (17%)
24	46136.5264477	216.748003588	0.0069	Singlet-A	HOMO->L+8 (10%), HOMO->L+9 (58%)
25	46330.906065	215.838645287	0.1197	Singlet-A	H-7->LUMO (68%)
26	46786.6093174	213.736369143	0.0007	Singlet-A	HOMO->L+10 (78%)
27	47376.200605	211.076444972	0.0417	Singlet-A	H-4->L+2 (88%)
28	47494.7641061	210.549524526	0.0053	Singlet-A	H-1->L+3 (14%), H-1->L+4 (60%), H-1->L+5 (18%)
29	47597.1965186	210.096407592	0.0081	Singlet-A	HOMO->L+8 (76%)
30	48031.9293558	208.194843183	0.0011	Singlet-A	HOMO->L+11 (17%), HOMO->L+12 (51%)
31	48708.6285217	205.302434158	0.0023	Singlet-A	H-5->L+2 (27%), H-3->L+2 (11%), H-1->L+3 (27%)
32	48834.4510127	204.773470217	0.0039	Singlet-A	H-6->L+1 (10%), H-5->L+2 (22%), H-1->L+3 (26%)
33	49149.00724	203.462909254	0.0112	Singlet-A	HOMO->L+11 (37%), HOMO->L+12 (14%), HOMO->L+15 (21%)
34	49215.1447032	203.189486901	0.0078	Singlet-A	H-2->L+3 (20%), HOMO->L+13 (26%), HOMO->L+14 (22%)
35	49339.3540852	202.677967424	0.0913	Singlet-A	H-6->L+1 (39%), H-2->L+3 (21%)
36	49485.3404369	202.080048591	0.0104	Singlet-A	H-6->L+1 (15%), H-2->L+3 (45%)
37	49869.2603451	200.524329633	0.0034	Singlet-A	HOMO->L+13 (28%), HOMO->L+14 (38%), HOMO->L+15 (21%)
38	50324.157043	198.711723903	0.0017	Singlet-A	H-1->L+4 (14%), H-1->L+6 (41%), H-1->L+7 (30%)
39	50633.0673893	197.499391516	0.0053	Singlet-A	H-9->LUMO (90%)
40	50666.1361209	197.370487778	0.025	Singlet-A	H-7->L+1 (28%), H-2->L+4 (37%), H-2->L+6 (10%)
41	50987.1447837	196.127867964	0.01	Singlet-A	HOMO->L+11 (14%), HOMO->L+12 (16%), HOMO->L+14 (10%), HOMO->L+15 (41%)
42	51407.3596412	194.524676424	0.0282	Singlet-A	H-1->L+3 (13%), H-1->L+7 (19%), HOMO->L+17 (18%)
43	51583.9950611	193.858579355	0.0442	Singlet-A	H-8->L+1 (27%), H-3->L+3 (13%)
44	51638.8407623	193.652681826	0.0107	Singlet-A	H-8->L+1 (64%)
45	51750.1452735	193.23617252	0.0083	Singlet-A	H-3->L+3 (24%), HOMO->L+16 (19%)
46	51902.5840606	192.668634539	0.0084	Singlet-A	H-4->L+3 (14%), H-2->L+5 (42%)

47	52068.734273	192.053833066	0.0885	Singlet-A	HOMO->L+16 (33%)
48	52204.235417	191.55533876	0.0033	Singlet-A	H-1->L+5 (39%), H-1->L+6 (22%)
49	52329.2513535	191.097708095	0.0266	Singlet-A	H-4->L+3 (14%), H-2->L+6 (25%)
50	52478.4639229	190.554357969	0.0038	Singlet-A	H-3->L+6 (15%), HOMO->L+17 (33%)
51	52711.5581529	189.71171315	0.0006	Singlet-A	H-10->LUMO (97%)
52	52793.8267046	189.416085633	0.116	Singlet-A	H-2->L+7 (40%), HOMO->L+17 (13%)
53	53009.9832916	188.6437116	0.007	Singlet-A	H-3->L+3 (13%), H-2->L+6 (15%), H-2->L+7 (11%), HOMO->L+18 (21%)
54	53082.5731902	188.385743174	0.0032	Singlet-A	HOMO->L+18 (49%)
55	53756.8526928	186.022795217	0.0039	Singlet-A	H-13->LUMO (51%), H-12->LUMO (16%), H-11->LUMO (22%)
56	53916.5504698	185.471806205	0.0183	Singlet-A	H-3->L+4 (41%), H-3->L+6 (12%)
57	54182.7134314	184.560708881	0.0099	Singlet-A	HOMO->L+19 (46%)
58	54277.0802996	184.239829129	0.0307	Singlet-A	H-2->L+9 (16%), HOMO->L+19 (22%)
59	54290.7917248	184.19329839	0.188	Singlet-A	H-1->L+9 (14%)
60	54402.9027905	183.81372109	0.0164	Singlet-A	H-13->LUMO (10%), H-11->LUMO (25%), H-1->L+9 (14%), H-1->L+10 (17%)
61	54487.5910055	183.528025656	0.1145	Singlet-A	H-11->LUMO (21%), H-1->L+9 (13%)
62	54640.0297926	183.016005627	0.0084	Singlet-A	H-1->L+10 (46%)
63	54707.7803646	182.789357078	0.0142	Singlet-A	H-3->L+7 (16%), H-2->L+9 (17%), H-2->L+10 (17%)
64	54849.7339441	182.316289997	0.0154	Singlet-A	H-6->L+2 (41%)
65	55044.920116	181.669806749	0.0087	Singlet-A	H-4->L+4 (11%), H-2->L+10 (15%), HOMO->L+20 (17%)
66	55114.2837969	181.441167536	0.0038	Singlet-A	H-3->L+5 (24%), HOMO->L+20 (12%), HOMO->L+22 (11%)
67	55144.1263107	181.34297647	0.0839	Singlet-A	H-6->L+2 (18%), HOMO->L+20 (10%), HOMO->L+21 (25%)
68	55273.9815738	180.916947093	0.004	Singlet-A	H-4->L+4 (21%), HOMO->L+21 (26%)
69	55360.2828977	180.634915079	0.0106	Singlet-A	H-4->L+3 (12%), H-4->L+4 (14%), H-2->L+10 (10%)
70	55395.7712926	180.519194275	0.001	Singlet-A	H-1->L+8 (46%), H-1->L+9 (29%)
71	55474.0070722	180.264605493	0.0027	Singlet-A	H-4->L+5 (16%), H-3->L+7 (11%), H-2->L+10 (23%)

72	55612.734434	179.814930911	0.0335	Singlet-A	HOMO->L+22 (41%)
73	55819.2123678	179.149786889	0.0005	Singlet-A	H-4->L+5 (31%), H-4->L+6 (10%), H-4->L+7 (20%)
74	55916.8054537	178.837112007	0.0043	Singlet-A	H-16->LUMO (34%), H-15->LUMO (17%), H-12->LUMO (16%), H-11->LUMO (11%)
75	55969.2314916	178.669596375	0.0025	Singlet-A	H-2->L+8 (59%), H-2->L+9 (17%)
76	56437.0330604	177.188619914	0.0824	Singlet-A	H-4->L+6 (25%), H-4->L+7 (22%)
77	56708.0353486	176.341852412	0.0314	Singlet-A	H-9->L+1 (15%), H-1->L+12 (18%), H-1->L+13 (11%), H-1->L+14 (16%)
78	56712.8746751	176.326805109	0.0035	Singlet-A	H-9->L+1 (69%)
79	56794.3366725	176.073893735	0.0149	Singlet-A	HOMO->L+23 (60%)
80	56809.6612066	176.026397405	0.003	Singlet-A	H-9->L+1 (10%), H-5->L+3 (12%), HOMO->L+24 (20%)
81	56908.8674014	175.71953997	0.0138	Singlet-A	H-1->L+11 (42%), HOMO->L+24 (14%)
82	57022.5915759	175.369090103	0.0132	Singlet-A	H-5->L+3 (15%), H-1->L+11 (16%), HOMO->L+24 (28%)
83	57170.9975908	174.913862297	0.0228	Singlet-A	H-2->L+11 (11%), H-2->L+12 (28%)
84	57262.9447957	174.63300282	0.0053	Singlet-A	H-12->LUMO (30%), H-8->L+2 (12%), H-5->L+3 (13%)
85	57491.1996991	173.93966472	0.0136	Singlet-A	H-4->L+8 (24%), H-3->L+8 (25%)
86	57561.3699344	173.727623429	0.0055	Singlet-A	H-5->L+4 (12%), H-3->L+9 (14%)
87	57686.3858709	173.351126943	0.0019	Singlet-A	H-1->L+12 (36%), H-1->L+13 (21%)
88	57890.4441415	172.740080825	0.0054	Singlet-A	H-4->L+8 (11%)
89	57946.0963971	172.574178793	0.0122	Singlet-A	H-5->L+4 (11%), H-2->L+11 (30%), H-2->L+12 (11%)
90	57971.9061388	172.497346837	0.0122	Singlet-A	H-16->LUMO (11%), H-8->L+2 (24%), H-3->L+10 (19%)
91	58035.6239387	172.307960548	0.0059	Singlet-A	H-8->L+2 (10%), H-3->L+10 (14%), HOMO->L+25 (22%)
92	58112.2466094	172.08076754	0.0062	Singlet-A	H-1->L+14 (14%), HOMO->L+25 (25%)
93	58159.8333208	171.939970062	0.0205	Singlet-A	H-3->L+10 (12%), H-2->L+13 (14%)
94	58186.4496169	171.861319359	0.0123	Singlet-A	H-14->LUMO (22%), H-1->L+13 (12%)
95	58237.2625459	171.711367651	0.001	Singlet-A	H-4->L+9 (21%), H-4->L+10 (10%), H-3->L+9 (12%)
96	58384.8620065	171.277273874	0.0131	Singlet-A	H-1->L+15 (11%), H-1->L+17 (38%)

97	58466.3240038	171.038630706	0.0296	Singlet-A	HOMO->L+26 (36%)
98	58494.5534088	170.956087657	0.0059	Singlet-A	H-5->L+4 (14%), H-4->L+8 (10%), H-3->L+8 (23%)
99	58560.690872	170.763012716	0.0274	Singlet-A	H-2->L+13 (23%)
100	58661.5101756	170.469528828	0.045	Singlet-A	H-7->L+2 (27%)

First 100 electronic transitions in methanol for 4a

HOMO is 86					
No.	Energy (cm-1)	Wavelength (nm)	Osc. Strength	Symmetry	Major contribs
1	24211.150849768	413.03282368	0.3667	Singlet-A	HOMO->LUMO (97%)
2	25735.538720502	388.56773540	0.0024	Singlet-A	H-1->LUMO (98%)
3	28280.217944	353.60406414	0.0104	Singlet-A	H-2->LUMO (21%), HOMO->L+1 (78%)
4	31596.769756102	316.48804853	0.0563	Singlet-A	H-2->LUMO (73%), HOMO->L+1 (19%)
5	33897.869542	295.00379035	0.0004	Singlet-A	H-1->L+1 (98%)
6	34085.796724	293.37732900	0.0649	Singlet-A	H-3->LUMO (74%), HOMO->L+2 (15%)
7	35229.490904304	283.85309419	0.0426	Singlet-A	H-4->LUMO (83%)
8	36123.959766102	276.82458027	0.1202	Singlet-A	H-5->LUMO (22%), H-4->LUMO (11%), HOMO->L+2 (54%)
9	37912.897489602	263.76248353	0.167	Singlet-A	H-5->LUMO (52%), H-2->L+1 (15%), HOMO->L+2 (15%)
10	38997.713196602	256.42529216	0.4241	Singlet-A	H-3->L+1 (24%), H-2->L+1 (50%)
11	39676.025471402	252.04137463	0.3522	Singlet-A	H-3->L+1 (37%), H-2->L+1 (26%), H-2->L+2 (13%)
12	39956.706412702	250.27087810	0.0018	Singlet-A	H-1->L+2 (95%)
13	40300.298599402	248.13711926	0.0266	Singlet-A	HOMO->L+3 (83%), HOMO->L+4 (10%)
14	40797.942682102	245.11039877	0.0008	Singlet-A	H-4->L+1 (76%), H-3->L+1 (13%)
15	41860.981419502	238.88594249	0.119	Singlet-A	H-4->L+1 (13%), HOMO->L+4 (53%)
16	42908.695622802	233.05299438	0.0729	Singlet-A	H-6->LUMO (50%), H-5->L+1 (25%)
17	43244.222265302	231.24476464	0.1638	Singlet-A	H-2->L+2 (55%), HOMO->L+6 (11%)
18	43625.722510202	229.22256468	0.005	Singlet-A	HOMO->L+5 (65%)
19	43929.793529902	227.63594354	0.0057	Singlet-A	H-8->LUMO (82%)
20	44048.357031	227.02322343	0.0007	Singlet-A	HOMO->L+6 (54%), HOMO->L+7 (16%), HOMO->L+9 (12%)
21	44328.231417802	225.58987083	0.0281	Singlet-A	H-3->L+2 (27%), HOMO->L+7 (30%)

22	44448.4080278	224.979936149	0.105	Singlet-A	H-5->L+1 (48%), HOMO->L+7 (18%)
23	45121.0744215	221.625928199	0.1109	Singlet-A	H-6->LUMO (15%), H-3->L+2 (20%), HOMO->L+6 (16%), HOMO->L+7 (18%)
24	46122.8150224	216.812438598	0.0048	Singlet-A	HOMO->L+8 (10%), HOMO->L+9 (59%)
25	46362.3616878	215.692204537	0.1239	Singlet-A	H-7->LUMO (69%)
26	46763.219239	213.843276035	0.0007	Singlet-A	HOMO->L+10 (78%)
27	47395.5579113	210.990237075	0.0363	Singlet-A	H-4->L+2 (85%)
28	47448.7905036	210.753528043	0.008	Singlet-A	H-1->L+3 (13%), H-1->L+4 (57%), H-1->L+5 (19%)
29	47578.6457667	210.178323465	0.0078	Singlet-A	HOMO->L+8 (76%)
30	48012.5720495	208.278781434	0.0011	Singlet-A	HOMO->L+11 (19%), HOMO->L+12 (50%)
31	48697.3367597	205.350038942	0.0013	Singlet-A	H-5->L+2 (19%), H-1->L+3 (36%)
32	48823.9658051	204.817446414	0.0054	Singlet-A	H-5->L+2 (30%), H-3->L+2 (11%), H-1->L+3 (18%)
33	49139.3285868	203.502984017	0.0115	Singlet-A	HOMO->L+11 (33%), HOMO->L+12 (16%), HOMO->L+15 (21%)
34	49215.1447032	203.189486901	0.007	Singlet-A	H-2->L+3 (23%), HOMO->L+11 (11%), HOMO->L+13 (21%), HOMO->L+14 (24%)
35	49349.0327384	202.638216903	0.0841	Singlet-A	H-6->L+1 (36%), H-2->L+3 (23%)
36	49486.9535457	202.073461458	0.0141	Singlet-A	H-6->L+1 (19%), H-2->L+3 (40%), H-2->L+4 (10%)
37	49852.3227021	200.592459047	0.0035	Singlet-A	HOMO->L+13 (31%), HOMO->L+14 (35%), HOMO->L+15 (21%)
38	50270.1178963	198.925334144	0.0017	Singlet-A	H-1->L+4 (14%), H-1->L+6 (40%), H-1->L+7 (31%)
39	50665.3295665	197.373629769	0.0281	Singlet-A	H-7->L+1 (29%), H-2->L+4 (38%), H-2->L+6 (10%)
40	50705.6572879	197.216652635	0.0008	Singlet-A	H-9->LUMO (93%)
41	50973.4333584	196.180624713	0.0089	Singlet-A	HOMO->L+11 (14%), HOMO->L+12 (17%), HOMO->L+15 (41%)
42	51371.0646919	194.662113	0.0128	Singlet-A	H-1->L+3 (16%), H-1->L+5 (10%), H-1->L+7 (26%), HOMO->L+17 (11%)
43	51568.670527	193.916187829	0.0481	Singlet-A	H-8->L+1 (32%), H-3->L+3 (14%)
44	51620.2900104	193.722274671	0.0146	Singlet-A	H-8->L+1 (58%)
45	51736.4338482	193.28738485	0.0111	Singlet-A	H-3->L+3 (21%), HOMO->L+16 (20%), HOMO->L+17 (11%)
46	51883.2267543	192.740517997	0.0082	Singlet-A	H-4->L+3 (12%), H-2->L+5 (42%)

47	52076.7998172	192.024088175	0.0778	Singlet-A	HOMO->L+16 (28%)
48	52148.5831614	191.759764001	0.0103	Singlet-A	H-1->L+5 (32%), H-1->L+6 (20%)
49	52333.2841257	191.082982218	0.0269	Singlet-A	H-4->L+3 (14%), H-2->L+6 (27%)
50	52502.6605558	190.466538155	0.004	Singlet-A	H-3->L+6 (15%), H-2->L+7 (10%), HOMO->L+17 (31%)
51	52773.6628439	189.488458089	0.0002	Singlet-A	H-10->LUMO (96%)
52	52833.3478716	189.274395866	0.1137	Singlet-A	H-2->L+7 (37%), HOMO->L+17 (14%)
53	53002.7243017	188.669547306	0.0089	Singlet-A	H-3->L+3 (13%), H-2->L+6 (16%), HOMO->L+18 (22%)
54	53074.5076459	188.414371485	0.0047	Singlet-A	HOMO->L+18 (47%)
55	53781.8558801	185.936313211	0.0038	Singlet-A	H-13->LUMO (50%), H-12->LUMO (18%), H-11->LUMO (21%)
56	53924.6160141	185.444065052	0.0145	Singlet-A	H-6->L+2 (10%), H-3->L+4 (39%), H-3->L+6 (12%)
57	54192.3920845	184.527746707	0.0084	Singlet-A	H-3->L+5 (10%), HOMO->L+19 (40%)
58	54261.7557654	184.291861901	0.0298	Singlet-A	H-2->L+9 (12%), H-1->L+9 (16%), HOMO->L+19 (25%)
59	54270.6278641	184.261734083	0.0851	Singlet-A	H-2->L+9 (13%), H-1->L+8 (11%), H-1->L+9 (23%)
60	54381.1258209	183.887329456	0.0601	Singlet-A	H-11->LUMO (15%), H-1->L+10 (29%)
61	54523.0794004	183.408569545	0.1538	Singlet-A	H-11->LUMO (23%), H-7->L+1 (11%)
62	54598.0889623	183.156593757	0.0121	Singlet-A	H-11->LUMO (18%), H-1->L+10 (36%)
63	54689.2296128	182.85135978	0.0153	Singlet-A	H-3->L+7 (17%), H-2->L+9 (16%), H-2->L+10 (18%)
64	54849.7339441	182.316289997	0.0123	Singlet-A	H-6->L+2 (39%)
65	55041.6938982	181.680455156	0.0078	Singlet-A	H-2->L+10 (17%), HOMO->L+20 (15%)
66	55090.8937184	181.518202466	0.0095	Singlet-A	H-3->L+5 (26%), HOMO->L+22 (10%)
67	55144.9328652	181.340324132	0.0823	Singlet-A	H-6->L+2 (18%), HOMO->L+20 (15%), HOMO->L+21 (22%)
68	55245.7521688	181.009391807	0.0053	Singlet-A	H-4->L+4 (15%), H-1->L+8 (15%), HOMO->L+21 (23%)
69	55314.3092952	180.785046897	0.0016	Singlet-A	H-4->L+4 (13%), H-1->L+8 (32%), H-1->L+9 (23%)
70	55339.3124825	180.703365318	0.0119	Singlet-A	H-4->L+3 (10%), H-2->L+10 (12%), HOMO->L+20 (10%), HOMO->L+21 (14%)
71	55455.4563203	180.324906935	0.0033	Singlet-A	H-4->L+4 (12%), H-4->L+5 (18%), H-3->L+7 (11%), H-2->L+10 (20%)

72	55607.8951074	179.830579465	0.0353	Singlet-A	HOMO->L+22 (41%)
73	55799.8550615	179.211935031	0.0002	Singlet-A	H-4->L+5 (30%), H-4->L+6 (10%), H-4->L+7 (21%)
74	55932.1299879	178.788113418	0.0064	Singlet-A	H-2->L+8 (53%), H-2->L+9 (15%)
75	55940.1955322	178.76233547	0.0019	Singlet-A	H-16->LUMO (31%), H-15->LUMO (17%), H-12->LUMO (13%), H-11->LUMO (11%)
76	56463.6493566	177.105095295	0.073	Singlet-A	H-4->L+6 (23%), H-4->L+7 (20%)
77	56671.7403993	176.454789099	0.0343	Singlet-A	H-1->L+11 (10%), H-1->L+12 (21%), H-1->L+13 (11%), H-1->L+14 (21%)
78	56745.1368523	176.226555344	0.0009	Singlet-A	H-9->L+1 (44%)
79	56783.8514649	176.106405994	0.0132	Singlet-A	HOMO->L+23 (58%)
80	56808.0480978	176.031395812	0.005	Singlet-A	H-9->L+1 (49%), HOMO->L+24 (14%)
81	56842.7299382	175.923992582	0.0101	Singlet-A	H-1->L+11 (51%)
82	57010.4932594	175.406305546	0.0146	Singlet-A	H-5->L+3 (18%), HOMO->L+24 (33%)
83	57155.6730567	174.960760065	0.0265	Singlet-A	H-2->L+11 (13%), H-2->L+12 (28%)
84	57271.01034	174.608409047	0.0061	Singlet-A	H-12->LUMO (30%), H-8->L+2 (15%), H-5->L+3 (10%)
85	57450.0654232	174.064205608	0.0083	Singlet-A	H-4->L+8 (19%), H-3->L+8 (29%)
86	57553.3043902	173.751969691	0.0055	Singlet-A	H-12->LUMO (13%), H-5->L+4 (10%), H-3->L+9 (12%)
87	57621.8615166	173.545243711	0.0026	Singlet-A	H-1->L+12 (35%), H-1->L+13 (19%), H-1->L+14 (10%)
88	57875.9261618	172.783412088	0.005	Singlet-A	
89	57925.9325364	172.634251399	0.0098	Singlet-A	H-2->L+11 (32%), H-2->L+12 (13%)
90	57956.5816047	172.542957558	0.0124	Singlet-A	H-16->LUMO (10%), H-8->L+2 (22%), H-3->L+10 (21%)
91	58021.105959	172.351075263	0.006	Singlet-A	H-8->L+2 (10%), H-3->L+10 (11%), HOMO->L+25 (17%)
92	58077.564769	172.183528007	0.0034	Singlet-A	H-1->L+13 (14%), H-1->L+14 (18%), HOMO->L+25 (19%)
93	58142.8956778	171.990058002	0.016	Singlet-A	HOMO->L+25 (17%)
94	58180.8037359	171.877996828	0.0186	Singlet-A	H-14->LUMO (13%), H-2->L+14 (12%)
95	58200.1610422	171.820830405	0.0008	Singlet-A	H-4->L+9 (15%), H-3->L+9 (11%)
96	58354.2129381	171.367232913	0.0088	Singlet-A	H-8->L+2 (10%), H-1->L+15 (11%), H-1->L+17 (42%)

97	58458.2584595	171.062229076	0.0168	Singlet-A	H-4->L+8 (10%), H-3->L+8 (11%), HOMO->L+26 (22%)
98	58475.1961025	171.012680017	0.022	Singlet-A	H-3->L+8 (14%), HOMO->L+26 (17%)
99	58548.5925555	170.798298704	0.0162	Singlet-A	H-14->LUMO (12%), H-2->L+13 (24%)
100	58659.8970667	170.474216629	0.0615	Singlet-A	H-7->L+2 (33%)

Table of 100rst electronic transitions with CAM-B3LYP/6-31+G(d,p) levels of theory

First 100 electronic transitions for 4a in toluene

HOMO is 86					
No.	Energy (cm-1)	Wavelength (nm)	Osc. Strength	Symmetry	Major contribs
1	26668.7221949	374.971096362	0.0035	Singlet-A	H-2->LUMO (91%)
2	29362.6139877	340.569133394	0.55	Singlet-A	HOMO->LUMO (92%)
3	32166.1971829	310.885366496	0.0104	Singlet-A	H-1->LUMO (31%), HOMO->L+1 (61%)
4	36828.0817826	271.531926616	0.1067	Singlet-A	H-1->LUMO (57%), HOMO->L+1 (28%)
5	38900.1201107	257.068614995	0.0001	Singlet-A	H-2->L+1 (89%)
6	39599.4028006	252.529060864	0.1199	Singlet-A	H-5->LUMO (15%), H-5->L+2 (10%), H-3->LUMO (48%)
7	41234.2886282	242.516612574	0.2439	Singlet-A	H-1->L+1 (59%), HOMO->L+2 (15%)
8	42265.8717429	236.597509708	0.4989	Singlet-A	H-1->L+1 (11%), HOMO->L+2 (70%)
9	42688.5062637	234.255092887	0.0423	Singlet-A	HOMO->L+3 (79%)
10	43206.3142071	231.447652583	0.2137	Singlet-A	H-3->L+1 (29%), H-1->L+2 (17%)
11	43615.2373026	229.277670338	0.6368	Singlet-A	H-5->LUMO (17%), H-3->LUMO (26%), H-1->L+1 (18%)
12	45040.4189786	222.022801447	0.0572	Singlet-A	H-4->LUMO (69%), H-4->L+2 (11%)
13	45951.8254834	217.619210876	0.001	Singlet-A	H-8->LUMO (18%), H-2->L+2 (60%)
14	47982.7295356	208.408318926	0.0024	Singlet-A	HOMO->L+4 (24%), HOMO->L+5 (14%), HOMO->L+6 (43%)
15	48002.0868419	208.324276253	0.0005	Singlet-A	H-8->LUMO (63%), H-2->L+2 (16%)
16	48180.3353707	207.553557339	0.1553	Singlet-A	H-3->L+1 (30%), H-1->L+2 (44%)
17	48665.0745826	205.486174341	0.0029	Singlet-A	HOMO->L+4 (13%), HOMO->L+5 (13%), HOMO->L+8 (45%)
18	49618.4219177	201.538050053	0.1042	Singlet-A	H-6->LUMO (13%), H-3->L+1 (15%), HOMO->L+9 (18%), HOMO->L+11 (10%)
19	50110.4201193	199.559292782	0.0256	Singlet-A	H-6->LUMO (16%), HOMO->L+10 (19%), HOMO->L+12 (13%)
20	50525.7956503	197.918704125	0.0282	Singlet-A	H-6->LUMO (34%), HOMO->L+9 (23%), HOMO->L+11 (13%)

21	51165.3933125	195.444603326	0.0508	Singlet-A	H-5->L+1 (10%), H-4->L+1 (45%), HOMO->L+11 (12%), HOMO->L+13 (13%)
22	51262.9863984	195.072521181	0.0016	Singlet-A	H-4->L+1 (19%), HOMO->L+11 (12%), HOMO->L+13 (33%)
23	51962.2690883	192.447331024	0.0187	Singlet-A	HOMO->L+4 (11%), HOMO->L+10 (13%)
24	52207.4616347	191.543501386	0.0502	Singlet-A	H-5->L+1 (29%), H-4->L+1 (10%)
25	52517.1785355	190.413885111	0.0029	Singlet-A	H-5->L+1 (14%), H-2->L+8 (13%)
26	52863.9969399	189.16465986	0.0445	Singlet-A	H-5->L+1 (13%), H-3->L+2 (20%), H-2->L+8 (10%)
27	53356.8016961	187.417530327	0.0048	Singlet-A	H-1->L+3 (49%), H-1->L+8 (15%)
28	53689.9086752	186.254740355	0.0076	Singlet-A	H-2->L+9 (41%), H-2->L+11 (26%)
29	53806.8590674	185.849911578	0.0087	Singlet-A	HOMO->L+11 (10%), HOMO->L+14 (30%)
30	53917.3570242	185.469031717	0.1702	Singlet-A	H-7->LUMO (42%), H-6->L+1 (12%)
31	54308.5359223	184.133117017	0.001	Singlet-A	H-4->L+4 (30%), H-4->L+5 (15%)
32	54562.6005674	183.275721758	0.0578	Singlet-A	H-7->LUMO (10%), H-6->L+1 (13%), H-3->L+2 (14%), HOMO->L+15 (13%)
33	54845.701172	182.329695606	0.0031	Singlet-A	HOMO->L+13 (12%)
34	55157.837736	181.297897279	0.0795	Singlet-A	
35	55544.9838619	180.034258806	0.0499	Singlet-A	HOMO->L+5 (15%)
36	55720.006173	179.468752551	0.0316	Singlet-A	H-6->L+1 (26%), HOMO->L+16 (13%)
37	56016.8182029	178.517815199	0.016	Singlet-A	H-1->L+4 (46%)
38	56660.4486373	176.489954466	0.0141	Singlet-A	HOMO->L+7 (11%)
39	56995.9752797	175.450984932	0.0204	Singlet-A	H-8->L+1 (39%)
40	57180.676244	174.884255606	0.0214	Singlet-A	H-8->L+1 (31%)
41	57357.3116639	174.34568863	0.1812	Singlet-A	H-1->L+9 (14%), H-1->L+11 (16%)
42	57773.4937493	173.089757102	0.0596	Singlet-A	H-4->L+2 (22%), H-1->L+5 (11%)
43	58130.7973613	172.025852972	0.0185	Singlet-A	H-1->L+5 (14%), H-1->L+6 (14%)
44	58413.8979659	171.192136601	0.042	Singlet-A	H-7->L+1 (10%), H-2->L+4 (20%)
45	58560.690872	170.763012716	0.0812	Singlet-A	HOMO->L+21 (11%), HOMO->L+22 (23%), HOMO->L+23 (23%)

46	58667.962611	170.450780203	0.0374	Singlet-A	
47	58820.4013981	170.00904044	0.046	Singlet-A	
48	58909.1223853	169.752995718	0.0133	Singlet-A	H-1->L+8 (12%)
49	59036.5579851	169.386568955	0.0068	Singlet-A	H-12->LUMO (13%)
50	59062.3677268	169.312548495	0.0224	Singlet-A	HOMO->L+7 (32%), HOMO->L+19 (10%)
51	59349.5011035	168.493412987	0.0106	Singlet-A	
52	59372.891182	168.427034644	0.025	Singlet-A	
53	59622.1165005	167.722995877	0.0018	Singlet-A	H-4->L+5 (12%), HOMO->L+7 (14%)
54	59652.7655688	167.636821271	0.0529	Singlet-A	H-7->L+1 (11%), H-4->L+4 (15%), H-4->L+5 (21%)
55	59705.1916067	167.489622441	0.0558	Singlet-A	
56	60318.1729728	165.787514892	0.0093	Singlet-A	H-3->L+3 (14%), HOMO->L+19 (13%)
57	60476.2576408	165.354147067	0.0031	Singlet-A	H-15->LUMO (43%)
58	60755.3254733	164.594624786	0.0053	Singlet-A	
59	60767.4237897	164.56185529	0.0198	Singlet-A	H-2->L+3 (26%)
60	60881.9545186	164.252282619	0.0202	Singlet-A	H-4->L+8 (12%)
61	60969.062397	164.017611668	0.0102	Singlet-A	H-1->L+8 (14%), H-1->L+11 (10%)
62	61494.1293302	162.617149131	0.001	Singlet-A	H-12->LUMO (23%), H-2->L+15 (16%)
63	61600.5945149	162.336095597	0.006	Singlet-A	H-1->L+7 (11%), H-1->L+11 (17%)
64	61688.5089476	162.104744799	0.0	Singlet-A	H-3->L+3 (10%)
65	61782.8758158	161.857146789	0.0079	Singlet-A	HOMO->L+27 (16%)
66	62300.6837592	160.511881999	0.0073	Singlet-A	H-3->L+4 (14%)
67	62376.4998756	160.316786289	0.0003	Singlet-A	H-2->L+11 (17%), H-2->L+20 (17%)
68	62648.3087181	159.621228483	0.0292	Singlet-A	H-3->L+9 (10%)
69	62761.2263382	159.334044018	0.0122	Singlet-A	H-5->L+2 (17%)
70	62896.7274823	158.990783786	0.0029	Singlet-A	

71	63112.0775148	158.448277949	0.0088	Singlet-A	H-1->L+13 (10%), H-1->L+15 (12%)
72	63255.6442032	158.088659533	0.0251	Singlet-A	H-1->L+13 (21%)
73	63455.6697016	157.590331125	0.0119	Singlet-A	HOMO->L+18 (14%), HOMO->L+29 (12%)
74	63566.1676583	157.316389652	0.0037	Singlet-A	
75	63640.3706658	157.132962856	0.0058	Singlet-A	H-4->L+7 (10%)
76	63682.3114961	157.029475926	0.0043	Singlet-A	H-2->L+5 (36%)
77	63942.0220223	156.391676142	0.0093	Singlet-A	H-12->L+1 (23%)
78	63997.6742779	156.255678239	0.0217	Singlet-A	H-12->L+1 (14%), H-2->L+4 (19%)
79	64119.4639966	155.958883258	0.0033	Singlet-A	
80	64372.7220873	155.345302727	0.0329	Singlet-A	
81	64521.9346567	154.986053242	0.0067	Singlet-A	
82	64575.167249	154.858290362	0.0048	Singlet-A	H-1->L+13 (12%)
83	64767.1272031	154.399313847	0.0149	Singlet-A	HOMO->L+29 (16%)
84	64890.5300308	154.105691466	0.0153	Singlet-A	HOMO->L+29 (13%)
85	65021.1918483	153.796011973	0.0437	Singlet-A	H-4->L+15 (10%)
86	65186.5355062	153.405913082	0.0046	Singlet-A	H-1->L+14 (18%)
87	65551.0981081	152.552745699	0.0104	Singlet-A	H-8->L+2 (12%)
88	65685.7926978	152.239922657	0.0004	Singlet-A	H-2->L+8 (11%), H-2->L+12 (17%), H-2->L+22 (10%)
89	65722.8942015	152.153981067	0.0158	Singlet-A	H-5->L+5 (11%)
90	65793.8709912	151.989841141	0.0273	Singlet-A	
91	65976.1522922	151.569918108	0.0068	Singlet-A	H-5->L+4 (11%)
92	66198.7613146	151.06022834	0.0198	Singlet-A	H-2->L+6 (19%)
93	66341.5214485	150.735162258	0.0078	Singlet-A	
94	66431.8555446	150.530192451	0.012	Singlet-A	H-14->LUMO (22%)
95	66649.6252404	150.038353013	0.0016	Singlet-A	HOMO->L+21 (10%), HOMO->L+32 (12%)

96	**66838.3589768**	**149.614684637**	**0.012**	**Singlet-A**	**H-2->L+7 (12%)**
97	**66861.7490552**	**149.562345307**	**0.0055**	**Singlet-A**	
98	**67029.5123765**	**149.188016524**	**0.0024**	**Singlet-A**	**H-3->L+6 (11%)**
99	**67078.7121966**	**149.078592485**	**0.0009**	**Singlet-A**	**H-4->L+3 (18%)**
100	**67247.2820723**	**148.704894709**	**0.0033**	**Singlet-A**	**HOMO->L+21 (12%)**

First 100 electronic transitions for 4a in chloroform

HOMO is 86					
No.	Energy (cm-1)	Wavelength (nm)	Osc. Strength	Symmetry	Major contribs
1	27134.9106548	368.528945136	0.0036	Singlet-A	H-2->LUMO (91%)
2	28959.3367732	345.311775553	0.5442	Singlet-A	HOMO->LUMO (93%)
3	31977.4634466	312.720238637	0.0091	Singlet-A	H-1->LUMO (31%), HOMO->L+1 (61%)
4	36631.2825019	272.990714957	0.1087	Singlet-A	H-1->LUMO (59%), HOMO->L+1 (28%)
5	39640.5370765	252.267015977	0.0005	Singlet-A	H-2->L+1 (89%)
6	39900.2476026	250.625011143	0.128	Singlet-A	H-5->LUMO (11%), H-3->LUMO (54%)
7	41296.3933192	242.151897448	0.1766	Singlet-A	H-5->LUMO (10%), H-1->L+1 (46%), HOMO->L+2 (27%)
8	42166.6655481	237.154156489	0.5716	Singlet-A	H-1->L+1 (20%), HOMO->L+2 (59%)
9	42994.1903923	232.589564049	0.0463	Singlet-A	HOMO->L+3 (67%)
10	43170.0192578	231.642240887	0.1569	Singlet-A	H-3->L+1 (26%), H-1->L+2 (15%)
11	43724.9287049	228.702488402	0.6284	Singlet-A	H-5->LUMO (17%), H-3->LUMO (24%), H-1->L+1 (19%)
12	45033.1599888	222.05858977	0.0505	Singlet-A	H-4->LUMO (73%), H-4->L+2 (11%)
13	46560.7740773	214.77306162	0.0005	Singlet-A	H-8->LUMO (29%), H-2->L+2 (52%)
14	48199.692677	207.470202497	0.1167	Singlet-A	H-3->L+1 (22%), H-1->L+2 (41%)
15	48309.3840794	206.999120162	0.0005	Singlet-A	H-8->LUMO (53%), H-2->L+2 (26%)
16	48380.3608691	206.695440471	0.0332	Singlet-A	HOMO->L+4 (21%), HOMO->L+5 (15%), HOMO->L+6 (36%)
17	48648.943494	205.554309751	0.0053	Singlet-A	HOMO->L+4 (16%), HOMO->L+5 (20%), HOMO->L+8 (38%)
18	49519.2157229	201.941808933	0.1231	Singlet-A	H-6->LUMO (12%), H-3->L+1 (19%), HOMO->L+9 (29%)
19	50178.1706914	199.289847801	0.0487	Singlet-A	H-6->LUMO (46%), HOMO->L+9 (17%)
20	50550.7988376	197.82081055	0.0047	Singlet-A	HOMO->L+10 (24%), HOMO->L+12 (14%), HOMO->L+14 (10%)
21	51328.3173071	194.824232015	0.0399	Singlet-A	H-5->L+1 (10%), H-4->L+1 (63%)

22	51460.5922335	194.323453462	0.0094	Singlet-A	HOMO->L+11 (26%), HOMO->L+13 (29%), HOMO->L+15 (11%)
23	52096.963678	191.949766244	0.0455	Singlet-A	H-5->LUMO (10%), H-5->L+1 (13%), H-4->L+1 (10%)
24	52364.7397484	190.96819822	0.0229	Singlet-A	H-5->L+1 (10%)
25	52620.4175024	190.040301363	0.0009	Singlet-A	H-5->L+1 (20%), H-2->L+8 (11%)
26	52976.1080056	188.764338802	0.0651	Singlet-A	H-5->L+1 (17%), H-3->L+2 (16%), H-2->L+8 (10%)
27	53535.0502249	186.79351113	0.0075	Singlet-A	H-1->L+3 (52%), H-1->L+8 (11%)
28	53822.1836016	185.796995418	0.1255	Singlet-A	H-7->LUMO (44%)
29	53924.6160141	185.444065052	0.0148	Singlet-A	HOMO->L+13 (26%)
30	54344.0243172	184.012872172	0.011	Singlet-A	H-2->L+9 (52%), H-2->L+11 (10%)
31	54505.335203	183.468278156	0.0646	Singlet-A	H-6->L+1 (16%), H-3->L+2 (17%), HOMO->L+14 (18%)
32	54752.1408582	182.641260109	0.0128	Singlet-A	H-4->L+3 (14%), H-4->L+4 (27%), H-4->L+5 (19%)
33	55137.6738753	181.364197964	0.0194	Singlet-A	
34	55199.7785663	181.16014701	0.0518	Singlet-A	
35	55620.7999783	179.788856038	0.0368	Singlet-A	HOMO->L+5 (17%), HOMO->L+16 (13%)
36	55764.3666666	179.325985352	0.0389	Singlet-A	H-6->L+1 (38%)
37	56426.5478528	177.221545186	0.0159	Singlet-A	H-1->L+4 (47%)
38	56740.2975257	176.241585541	0.0219	Singlet-A	HOMO->L+15 (16%), HOMO->L+16 (11%), HOMO->L+17 (10%)
39	57191.968006	174.849727132	0.0882	Singlet-A	H-8->L+1 (16%)
40	57370.2165348	174.306471267	0.1567	Singlet-A	H-8->L+1 (14%), H-1->L+9 (18%), H-1->L+11 (13%)
41	57450.0654232	174.064205608	0.0083	Singlet-A	H-8->L+1 (39%)
42	57710.5825038	173.278445064	0.0797	Singlet-A	H-4->L+2 (25%)
43	58442.9339253	171.107083925	0.0117	Singlet-A	H-1->L+5 (19%), H-1->L+6 (15%), HOMO->L+22 (12%)
44	58544.5597834	170.810063941	0.0137	Singlet-A	HOMO->L+21 (13%)
45	58630.8611073	170.558641151	0.1295	Singlet-A	H-7->L+1 (13%), HOMO->L+22 (16%)
46	58867.181555	169.873938854	0.0792	Singlet-A	H-7->L+1 (15%)

47	59028.4924408	169.409713623	0.0027	Singlet-A	H-12->LUMO (30%)
48	59255.1342353	168.761747468	0.0081	Singlet-A	H-1->L+8 (17%)
49	59389.0222706	168.38128694	0.0074	Singlet-A	HOMO->L+7 (16%), HOMO->L+23 (17%)
50	59445.4810806	168.221365497	0.0504	Singlet-A	H-7->L+1 (12%), HOMO->L+7 (10%)
51	59549.5266019	167.927447465	0.0063	Singlet-A	H-2->L+4 (15%)
52	59724.548913	167.435337428	0.0122	Singlet-A	H-7->L+1 (10%), H-2->L+3 (10%), HOMO->L+7 (15%)
53	59830.2075432	167.139650866	0.0009	Singlet-A	HOMO->L+7 (12%)
54	59997.16431	166.674543956	0.039	Singlet-A	H-2->L+6 (11%)
55	60391.5694258	165.586026246	0.021	Singlet-A	H-4->L+4 (22%), H-4->L+5 (36%)
56	60472.2248687	165.365174205	0.0001	Singlet-A	H-15->LUMO (43%)
57	60625.4702102	164.947174271	0.0113	Singlet-A	H-3->L+3 (15%), HOMO->L+19 (17%)
58	60873.0824199	164.276221976	0.0015	Singlet-A	HOMO->L+24 (14%)
59	61312.6545837	163.098467484	0.01	Singlet-A	H-4->L+8 (16%)
60	61395.7296899	162.877777502	0.0148	Singlet-A	H-1->L+8 (12%), H-1->L+10 (14%)
61	61710.2859172	162.047539585	0.0107	Singlet-A	HOMO->L+27 (12%)
62	61834.4952993	161.722028321	0.0136	Singlet-A	H-2->L+3 (13%), H-2->L+14 (18%)
63	61841.7542891	161.703045377	0.0004	Singlet-A	HOMO->L+15 (10%)
64	61979.6750965	161.343214278	0.0047	Singlet-A	
65	62023.2290357	161.22991588	0.0096	Singlet-A	H-2->L+3 (17%)
66	62670.0856877	159.565762361	0.0111	Singlet-A	H-3->L+4 (19%)
67	62716.8658446	159.446743158	0.0359	Singlet-A	H-3->L+9 (13%)
68	62909.6323531	158.958169456	0.0072	Singlet-A	H-2->L+20 (10%)
69	62930.6027683	158.905199698	0.0119	Singlet-A	H-2->L+20 (11%)
70	63041.9072795	158.624642425	0.0065	Singlet-A	H-5->L+2 (14%)
71	63401.6305548	157.724650178	0.0165	Singlet-A	H-1->L+13 (19%), H-1->L+14 (11%)

72	63511.3219572	157.452241456	0.0281	Singlet-A	
73	63581.4921925	157.278472951	0.0034	Singlet-A	H-1->L+13 (10%), HOMO->L+29 (12%)
74	63906.5336274	156.478523124	0.0049	Singlet-A	H-4->L+7 (24%), H-4->L+15 (16%), H-4->L+16 (10%)
75	63971.0579817	156.320691192	0.0022	Singlet-A	H-12->L+1 (40%)
76	64090.4280372	156.029539921	0.0106	Singlet-A	
77	64317.0698317	155.479719865	0.0079	Singlet-A	
78	64462.249629	155.12955346	0.0039	Singlet-A	H-2->L+5 (25%)
79	64546.937844	154.926017159	0.003	Singlet-A	H-3->L+5 (10%)
80	64604.2032085	154.788690261	0.0475	Singlet-A	
81	64702.6028488	154.553287808	0.0577	Singlet-A	H-2->L+5 (11%)
82	64990.54278	153.868541056	0.0017	Singlet-A	HOMO->L+29 (10%)
83	65020.3852938	153.797919757	0.0072	Singlet-A	
84	65194.6010505	153.386934483	0.0138	Singlet-A	
85	65259.9319592	153.233380725	0.0038	Singlet-A	H-2->L+4 (19%)
86	65554.3243258	152.545237905	0.0007	Singlet-A	H-1->L+15 (15%)
87	65693.858242	152.221231445	0.0206	Singlet-A	H-8->L+2 (15%)
88	65823.7135051	151.920933468	0.0119	Singlet-A	H-7->L+2 (10%)
89	66022.9324491	151.462524142	0.0072	Singlet-A	
90	66239.0890361	150.968259762	0.0205	Singlet-A	H-14->LUMO (11%), H-9->LUMO (57%)
91	66387.495051	150.630777563	0.0023	Singlet-A	H-5->L+4 (10%)
92	66600.4254202	150.149191043	0.0195	Singlet-A	H-14->LUMO (20%), H-9->LUMO (19%)
93	66612.5237367	150.12192061	0.0108	Singlet-A	HOMO->L+32 (10%)
94	66806.9033541	149.685129799	0.004	Singlet-A	H-2->L+8 (10%), H-2->L+12 (13%), H-2->L+14 (10%)
95	66948.0503791	149.369547632	0.003	Singlet-A	
96	66985.1518829	149.286815345	0.0182	Singlet-A	

97	**67238.4099736**	**148.724516298**	**0.0011**	**Singlet-A**	**HOMO->L+34 (15%)**
98	**67461.018996**	**148.2337526**	**0.0055**	**Singlet-A**	**H-2->L+6 (15%)**
99	**67530.3826769**	**148.081494634**	**0.0009**	**Singlet-A**	**H-2->L+6 (11%)**
100	**67774.7686689**	**147.547534229**	**0.0003**	**Singlet-A**	

First 100 electronic transitions for 4a in DMSO

HOMO is 86					
No.	Energy (cm-1)	Wavelength (nm)	Osc. Strength	Symmetry	Major contribs
1	27697.0790919	361.048902191	0.0041	Singlet-A	H-2->LUMO (92%)
2	28390.7159008	352.227821057	0.5571	Singlet-A	HOMO->LUMO (93%)
3	31743.5626622	315.02450139	0.0084	Singlet-A	H-1->LUMO (30%), HOMO->L+1 (62%)
4	36335.2770264	275.214634877	0.1177	Singlet-A	H-1->LUMO (61%), HOMO->L+1 (28%)
5	40108.3386453	249.32471246	0.1403	Singlet-A	H-3->LUMO (61%), H-1->L+1 (12%)
6	40551.1370268	246.602209782	0.0004	Singlet-A	H-2->L+1 (89%)
7	41314.9440711	242.043169241	0.1446	Singlet-A	H-1->L+1 (24%), HOMO->L+2 (52%)
8	42069.0724622	237.704313756	0.6766	Singlet-A	H-5->LUMO (11%), H-1->L+1 (38%), HOMO->L+2 (35%)
9	43045.0033213	232.315001241	0.1343	Singlet-A	H-3->L+1 (29%), H-1->L+2 (16%)
10	43290.1958677	230.999185833	0.0358	Singlet-A	HOMO->L+3 (62%), HOMO->L+4 (18%)
11	43808.0038111	228.268789491	0.5525	Singlet-A	H-5->LUMO (19%), H-3->LUMO (21%), H-1->L+1 (18%)
12	44944.4390016	222.49693671	0.046	Singlet-A	H-4->LUMO (76%), H-4->L+2 (11%)
13	47173.7554434	211.982275017	0.0005	Singlet-A	H-9->LUMO (47%), H-2->L+2 (35%)
14	48189.2074695	207.515344724	0.12	Singlet-A	H-3->L+1 (21%), H-1->L+2 (44%)
15	48463.4359753	206.341127053	0.0091	Singlet-A	HOMO->L+5 (42%), HOMO->L+6 (19%), HOMO->L+8 (12%)
16	48742.5038078	205.159752142	0.0337	Singlet-A	HOMO->L+4 (32%), HOMO->L+6 (13%), HOMO->L+8 (14%)
17	48789.2839646	204.963040803	0.0013	Singlet-A	H-9->LUMO (32%), H-2->L+2 (41%)
18	49370.8097079	202.548835216	0.1256	Singlet-A	H-3->L+1 (20%), HOMO->L+9 (32%)
19	49965.2403221	200.139135438	0.0655	Singlet-A	H-6->LUMO (54%), HOMO->L+9 (16%)
20	50844.3846497	196.678552979	0.0008	Singlet-A	HOMO->L+3 (10%), HOMO->L+6 (10%), HOMO->L+11 (19%), HOMO->L+12 (11%), HOMO->L+13 (27%)
21	51441.2349272	194.396577262	0.0277	Singlet-A	H-4->L+1 (71%)

22	51608.998 2484	193.76466 0028	0.019 7	Singlet-A	HOMO->L+10 (30%), HOMO->L+12 (18%), HOMO->L+15 (17%)
23	52073.573 5995	192.03598 5026	0.058	Singlet-A	H-5->LUMO (12%), H-5->L+1 (11%), H-4->L+1 (13%), H-3->L+2 (11%)
24	52629.289 6011	190.00826 49	0.009 3	Singlet-A	H-5->L+1 (14%), HOMO->L+11 (17%)
25	52672.036 9858	189.85405 8667	0.005 9	Singlet-A	H-2->L+3 (13%), H-2->L+5 (13%)
26	53020.468 4992	188.60640 5848	0.101	Singlet-A	H-7->LUMO (13%), H-5->L+1 (26%), H-3->L+2 (13%)
27	53591.509 0349	186.59672 3624	0.034 4	Singlet-A	H-7->LUMO (16%), H-1->L+3 (34%)
28	53705.233 2094	186.20159 3446	0.052 2	Singlet-A	H-7->LUMO (25%), H-1->L+3 (19%)
29	53959.297 8545	185.32487 2591	0.012 7	Singlet-A	HOMO->L+10 (14%), HOMO->L+14 (20%)
30	54460.974 7094	183.61771 9906	0.091 1	Singlet-A	H-6->L+1 (14%), H-3->L+2 (22%), HOMO->L+14 (16%)
31	54994.107 1869	181.83766 4279	0.031 5	Singlet-A	H-2->L+9 (20%)
32	55153.804 9639	181.31115 3538	0.004 9	Singlet-A	H-4->L+3 (24%), H-4->L+4 (23%), H-4->L+5 (20%)
33	55208.650 665	181.13103 4349	0.025	Singlet-A	H-2->L+9 (34%)
34	55491.751 2696	180.20696 3579	0.018 5	Singlet-A	HOMO->L+8 (10%), HOMO->L+15 (11%)
35	55690.163 6592	179.56492 391	0.023 7	Singlet-A	HOMO->L+5 (14%), HOMO->L+16 (16%)
36	55895.835 0386	178.90420 6245	0.055 8	Singlet-A	H-6->L+1 (34%)
37	56712.874 6751	176.32680 5109	0.026 5	Singlet-A	H-3->L+3 (12%), H-1->L+4 (22%)
38	56866.120 0166	175.85163 1817	0.020 4	Singlet-A	H-1->L+4 (17%)
39	57207.292 5401	174.80288 8862	0.193 6	Singlet-A	H-4->L+2 (11%), H-1->L+9 (12%), H-1->L+10 (10%)
40	57383.927 9601	174.26482 2146	0.158 4	Singlet-A	H-4->L+2 (13%), H-1->L+9 (13%)
41	57626.700 8432	173.53066 9875	0.013 7	Singlet-A	H-1->L+5 (13%)
42	57775.913 4126	173.08250 8079	0.010 1	Singlet-A	H-9->L+1 (64%)
43	58409.865 1938	171.20395 6161	0.007 4	Singlet-A	HOMO->L+17 (14%), HOMO->L+19 (14%)
44	58559.077 7631	170.76771 6672	0.079 7	Singlet-A	HOMO->L+20 (16%), HOMO->L+21 (36%), HOMO->L+22 (16%)
45	58767.975 3602	170.16070 298	0.075 3	Singlet-A	H-7->L+1 (21%), H-1->L+5 (22%)
46	58855.889 793	169.90652 9919	0.067 5	Singlet-A	H-1->L+5 (13%)

47	59105.921666	169.187785557	0.0159	Singlet-A	H-12->LUMO (30%)
48	59501.939 8906	168.061747539	0.0276	Singlet-A	H-7->L+1 (19%), H-1->L+9 (10%)
49	59584.208 4424	167.829702893	0.0197	Singlet-A	HOMO->L+23 (16%)
50	59705.998 1612	167.487359863	0.0135	Singlet-A	H-1->L+8 (19%)
51	59935.866 1734	166.845006812	0.0015	Singlet-A	HOMO->L+7 (15%), HOMO->L+20 (11%)
52	60057.655 8922	166.506665161	0.0017	Singlet-A	HOMO->L+7 (26%)
53	60231.871 6489	166.025058266	0.0074	Singlet-A	
54	60386.730 0992	165.59929613	0.0004	Singlet-A	H-17->LUMO (11%), H-16->LUMO (20%), H-15->LUMO (23%)
55	60436.736 4738	165.46227648	0.027	Singlet-A	H-2->L+3 (20%), H-2->L+12 (16%)
56	60848.079 2326	164.343724997	0.0069	Singlet-A	H-3->L+3 (12%), HOMO->L+19 (19%)
57	61100.530 7689	163.664699376	0.0075	Singlet-A	H-2->L+4 (18%)
58	61242.484 3484	163.285341971	0.0047	Singlet-A	H-4->L+5 (19%), H-4->L+6 (10%)
59	61712.705 5805	162.041185943	0.0039	Singlet-A	HOMO->L+27 (12%)
60	61807.879 0031	161.791670597	0.0062	Singlet-A	H-3->L+5 (10%), H-1->L+8 (11%)
61	61883.695 1195	161.593453343	0.0233	Singlet-A	H-4->L+8 (23%)
62	62031.294 58	161.208952154	0.0049	Singlet-A	
63	62244.224 9492	160.65747478	0.0005	Singlet-A	H-1->L+10 (14%), H-1->L+12 (10%)
64	62531.358 3259	159.919762943	0.012	Singlet-A	H-2->L+9 (10%), H-2->L+10 (16%), H-2->L+14 (14%)
65	62679.764 3409	159.541123123	0.0241	Singlet-A	H-3->L+9 (24%)
66	62930.602 7683	158.905199698	0.0084	Singlet-A	
67	63014.484 4289	158.693673219	0.0055	Singlet-A	HOMO->L+25 (10%)
68	63198.378 8387	158.231906953	0.0582	Singlet-A	H-5->L+2 (13%)
69	63360.496 279	157.827046619	0.025	Singlet-A	H-2->L+3 (24%), H-2->L+8 (14%), H-2->L+13 (10%)
70	63516.967 8382	157.438245879	0.0158	Singlet-A	H-2->L+12 (12%), H-2->L+20 (14%)
71	63585.524 9646	157.268497 91	0.0108	Singlet-A	H-2->L+12 (12%)

72	63695.216367	156.997661212	0.0015	Singlet-A	HOMO->L+29 (10%)
73	63964.6055463	156.336460056	0.0096	Singlet-A	H-1->L+6 (13%), H-1->L+13 (17%)
74	63982.3497437	156.293103333	0.0072	Singlet-A	H-13->L+1 (13%), H-12->L+1 (36%)
75	64163.8244902	155.851059058	0.026	Singlet-A	H-4->L+12 (12%)
76	64239.6406066	155.667122443	0.0111	Singlet-A	
77	64301.7452976	155.516774136	0.0197	Singlet-A	H-1->L+14 (11%), HOMO->L+29 (19%)
78	64524.35432	154.980241265	0.0314	Singlet-A	HOMO->L+29 (15%)
79	64692.1176412	154.578337588	0.0202	Singlet-A	H-3->L+4 (12%)
80	65011.5131951	153.818908506	0.0021	Singlet-A	H-8->LUMO (24%)
81	65092.9751924	153.62640854	0.0037	Singlet-A	H-8->LUMO (10%)
82	65106.6866177	153.59405492	0.0306	Singlet-A	H-8->LUMO (35%)
83	65330.1021946	153.068794692	0.006	Singlet-A	
84	65529.3211385	152.603442646	0.0096	Singlet-A	H-2->L+5 (11%), H-1->L+11 (10%)
85	65564.002979	152.522718956	0.0051	Singlet-A	
86	65813.2282975	151.945137151	0.0027	Singlet-A	H-2->L+5 (16%)
87	65861.6215633	151.833492141	0.0095	Singlet-A	
88	66225.3776108	150.999516511	0.0043	Singlet-A	
89	66306.0330537	150.815838913	0.0051	Singlet-A	H-1->L+11 (14%), H-1->L+15 (12%)
90	66548.8059368	150.265656299	0.0031	Singlet-A	H-2->L+4 (22%), H-2->L+6 (10%)
91	66567.3566887	150.223780806	0.0477	Singlet-A	H-2->L+4 (10%)
92	66723.8282479	149.871496624	0.0015	Singlet-A	H-1->L+15 (10%)
93	66841.5851945	149.607463242	0.0079	Singlet-A	
94	67049.6762372	149.143151186	0.0192	Singlet-A	
95	67279.5442495	148.633587096	0.005	Singlet-A	
96	67497.3139453	148.154043702	0.003	Singlet-A	H-10->LUMO (19%)

97	**67533.6088946**	**148.07442048**	**0.0022**	**Singlet-A**	**H-10->LUMO (10%)**
98	**67829.61437**	**147.428230175**	**0.0045**	**Singlet-A**	**HOMO->L+23 (17%)**
99	**68165.1410125**	**146.702549888**	**0.0011**	**Singlet-A**	**H-2->L+8 (11%), H-2->L+13 (21%), H-2->L+15 (11%)**
100	**68223.2129314**	**146.577675989**	**0.004**	**Singlet-A**	**H-1->L+7 (10%), H-1->L+21 (10%)**

First 100 electronic transitions for 4a in methanol

HOMO is 86					
No.	**Energy (cm-1)**	**Wavelength (nm)**	**Osc. Strength**	**Symmetry**	**Major contribs**
1	27687.4004387	361.175113645	0.0037	Singlet-A	H-2->LUMO (92%)
2	28571.3840929	350.000544863	0.5214	Singlet-A	HOMO->LUMO (93%)
3	31780.6641659	314.65673429	0.0076	Singlet-A	H-1->LUMO (31%), HOMO->L+1 (62%)
4	36435.2897756	274.459186727	0.1045	Singlet-A	H-1->LUMO (60%), HOMO->L+1 (28%)
5	40161.5712376	248.994242303	0.1184	Singlet-A	H-3->LUMO (60%), H-1->L+1 (11%)
6	40501.1306522	246.906687269	0.0004	Singlet-A	H-2->L+1 (89%)
7	41381.8880887	241.651612864	0.1239	Singlet-A	H-1->L+1 (23%), HOMO->L+2 (51%)
8	42215.0588139	236.882294636	0.6302	Singlet-A	H-5->LUMO (12%), H-1->L+1 (36%), HOMO->L+2 (36%)
9	43094.2031415	232.049771687	0.1101	Singlet-A	H-3->L+1 (30%), H-1->L+2 (17%), HOMO->L+9 (10%)
10	43317.6187183	230.852948428	0.0335	Singlet-A	HOMO->L+3 (61%), HOMO->L+4 (18%)
11	43933.0197476	227.619227 12	0.6067	Singlet-A	H-5->LUMO (18%), H-3->LUMO (22%), H-1->L+1 (21%)
12	44992.0257129	222.261608397	0.0425	Singlet-A	H-4->LUMO (76%), H-4->L+2 (11%)
13	47146.3325928	212.105575345	0.0005	Singlet-A	H-9->LUMO (45%), H-2->L+2 (36%)
14	48275.5087934	207.144372995	0.1121	Singlet-A	H-3->L+1 (20%), H-1->L+2 (44%)
15	48494.0850436	206.210716029	0.0084	Singlet-A	HOMO->L+5 (41%), HOMO->L+6 (19%), HOMO->L+8 (13%)
16	48749.7627976	205.129203223	0.0303	Singlet-A	HOMO->L+4 (30%), HOMO->L+6 (12%), HOMO->L+8 (13%)
17	48770.7332128	205.041001872	0.0018	Singlet-A	H-9->LUMO (31%), H-2->L+2 (37%)
18	49427.268518	202.317471708	0.1157	Singlet-A	H-3->L+1 (21%), HOMO->L+9 (34%)
19	50022.5056866	199.910017756	0.0707	Singlet-A	H-6->LUMO (57%), HOMO->L+9 (15%)
20	50837.1256599	196.706636542	0.0008	Singlet-A	HOMO->L+3 (10%), HOMO->L+6 (10%), HOMO->L+11 (20%), HOMO->L+12 (12%), HOMO->L+13 (23%)
21	51454.9463525	194.344775554	0.025	Singlet-A	H-4->L+1 (72%)

22	51619.483456	193.725301582	0.0193	Singlet-A	HOMO->L+10 (30%), HOMO->L+12 (18%), HOMO->L+15 (17%)
23	52108.25544	191.908171087	0.0535	Singlet-A	H-5->LUMO (13%), H-5->L+1 (12%), H-4->L+1 (12%), H-3->L+2 (11%)
24	52634.1289277	189.990795017	0.0083	Singlet-A	H-5->L+1 (10%), HOMO->L+11 (20%)
25	52709.945044	189.717518993	0.003	Singlet-A	H-5->L+1 (13%), H-2->L+3 (15%), H-2->L+5 (15%)
26	53041.438 9143	188.53183859	0.0965	Singlet-A	H-7->LUMO (12%), H-5->L+1 (24%), H-3->L+2 (13%)
27	53630.2236475	186.462023088	0.0227	Singlet-A	H-7->LUMO (11%), H-1->L+3 (42%)
28	53755.239584	186.028377464	0.065	Singlet-A	H-7->LUMO (33%), H-1->L+3 (10%)
29	53980.2682697	185.252877034	0.0127	Singlet-A	HOMO->L+10 (13%), HOMO->L+14 (19%)
30	54506.9483118	183.462848494	0.0858	Singlet-A	H-6->L+1 (14%), H-3->L+2 (23%), HOMO->L+14 (17%)
31	54993.3006325	181.840331186	0.0269	Singlet-A	H-2->L+9 (27%)
32	55152.9984094	181.313805022	0.0061	Singlet-A	H-4->L+3 (23%), H-4->L+4 (22%), H-4->L+5 (20%)
33	55207.0375562	181.136326865	0.0293	Singlet-A	H-2->L+9 (26%)
34	55495.7840418	180.193868285	0.0118	Singlet-A	HOMO->L+4 (10%), HOMO->L+8 (11%), HOMO->L+15 (12%), HOMO->L+18 (10%)
35	55704.6816389	179.518124972	0.023	Singlet-A	HOMO->L+5 (15%), HOMO->L+16 (17%)
36	55932.9365423	178.785535289	0.0554	Singlet-A	H-6->L+1 (38%)
37	56748.36307	176.216536637	0.0204	Singlet-A	H-3->L+3 (13%), H-1->L+4 (24%)
38	56869.3462344	175.841655692	0.0186	Singlet-A	H-1->L+4 (15%), HOMO->L+15 (10%)
39	57276.656221	174.591197528	0.1755	Singlet-A	H-4->L+2 (11%), H-1->L+9 (10%)
40	57445.2260967	174.078869203	0.1573	Singlet-A	H-4->L+2 (11%), H-1->L+9 (15%)
41	57642.8319318	173.482108093	0.0185	Singlet-A	H-3->L+3 (10%), H-1->L+5 (13%)
42	57770.2675316	173.099423411	0.013	Singlet-A	H-9->L+1 (61%)
43	58442.1273709	171.109445358	0.0042	Singlet-A	HOMO->L+17 (15%), HOMO->L+19 (14%)
44	58583.274396	170.697184531	0.0704	Singlet-A	HOMO->L+20 (15%), HOMO->L+21 (34%), HOMO->L+22 (18%)
45	58807.4965272	170.046347669	0.0458	Singlet-A	H-7->L+1 (10%), H-1->L+5 (32%), H-1->L+6 (10%)
46	58907.5092764	169.757644192	0.0997	Singlet-A	H-7->L+1 (12%), H-1->L+9 (14%)

47	59124.4724178	169.134701606	0.0292	Singlet-A	H-12->LUMO (28%)
48	59510.8119893	168.036692253	0.0307	Singlet-A	H-7->L+1 (21%), H-1->L+9 (10%)
49	59599.5329765	167.786549669	0.0175	Singlet-A	HOMO->L+23 (17%)
50	59711.6440422	167.471523526	0.0181	Singlet-A	H-1->L+8 (19%)
51	59945.5448266	166.818068447	0.0019	Singlet-A	HOMO->L+7 (18%), HOMO->L+20 (11%)
52	60042.331358	166.549162463	0.0019	Singlet-A	HOMO->L+7 (24%)
53	60239.9371932	166.002829119	0.0064	Singlet-A	
54	60398.0218612	165.568336377	0.0003	Singlet-A	H-17->LUMO (10%), H-16->LUMO (17%), H-15->LUMO (26%)
55	60437.5430283	165.460068344	0.0282	Singlet-A	H-2->L+3 (20%), H-2->L+12 (16%)
56	60845.6595693	164.350260492	0.0071	Singlet-A	H-3->L+3 (13%), HOMO->L+19 (19%)
57	61096.4979967	163.675502326	0.0067	Singlet-A	H-4->L+5 (12%), H-2->L+4 (14%)
58	61223.1270421	163.336968939	0.0041	Singlet-A	H-4->L+5 (16%), H-2->L+4 (10%)
59	61728.8366691	161.998841054	0.0033	Singlet-A	HOMO->L+27 (12%)
60	61797.3937956	161.819121905	0.0055	Singlet-A	H-1->L+8 (11%)
61	61880.4689017	161.601878226	0.0231	Singlet-A	H-4->L+8 (23%)
62	62030.4880255	161.211048281	0.0043	Singlet-A	
63	62245.8380581	160.653311321	0.0003	Singlet-A	H-1->L+10 (15%)
64	62499.0961488	160.002313893	0.01	Singlet-A	H-2->L+9 (10%), H-2->L+10 (15%), H-2->L+14 (17%)
65	62693.4757662	159.506230557	0.0231	Singlet-A	H-3->L+9 (23%)
66	62937.8617582	158.886872236	0.0067	Singlet-A	H-5->L+2 (10%)
67	63014.4844289	158.693673219	0.0052	Singlet-A	HOMO->L+25 (10%)
68	63207.2509374	158.209696699	0.058	Singlet-A	H-5->L+2 (11%)
69	63319.3620031	157.929576099	0.0222	Singlet-A	H-2->L+3 (21%), H-2->L+8 (12%)
70	63500.8367496	157.478239845	0.0136	Singlet-A	H-2->L+12 (18%), H-2->L+20 (22%)
71	63582.2987469	157.276477842	0.0141	Singlet-A	

72	63703.2819113	156.977783561	0.0016	Singlet-A	HOMO->L+29 (10%)
73	63953.3137843	156.364063225	0.0085	Singlet-A	H-1->L+6 (13%), H-1->L+13 (16%)
74	63991.2218424	156.271433989	0.0057	Singlet-A	H-13->L+1 (11%), H-12->L+1 (38%)
75	64180.7621332	155.809929138	0.0178	Singlet-A	H-4->L+7 (14%), H-4->L+12 (13%), H-4->L+13 (10%)
76	64255.7716951	155.628042994	0.0151	Singlet-A	
77	64321.1026039	155.469971676	0.0196	Singlet-A	H-1->L+14 (10%), HOMO->L+29 (20%)
78	64541.291963	154.939569628	0.0287	Singlet-A	HOMO->L+29 (14%)
79	64709.8618387	154.535950408	0.0273	Singlet-A	H-3->L+4 (12%)
80	65008.2869774	153.826542199	0.0001	Singlet-A	H-5->L+3 (10%)
81	65107.4931722	153.59215219	0.002	Singlet-A	
82	65160.7257645	153.466676172	0.0319	Singlet-A	H-8->LUMO (60%)
83	65337.3611844	153.051788727	0.0063	Singlet-A	
84	65513.9966044	152.639138479	0.0115	Singlet-A	H-2->L+5 (16%)
85	65555.9374347	152.541484285	0.0022	Singlet-A	
86	65797.9037634	151.98052564	0.0038	Singlet-A	H-2->L+5 (13%)
87	65860.8150089	151.835351546	0.009	Singlet-A	
88	66214.0858488	151.025267084	0.005	Singlet-A	
89	66293.9347372	150.843362061	0.0044	Singlet-A	H-1->L+11 (14%), H-1->L+15 (13%)
90	66500.412671	150.375006686	0.0139	Singlet-A	H-2->L+4 (31%), H-2->L+6 (14%), H-2->L+11 (13%), H-2->L+17 (11%)
91	66581.8746684	150.191024957	0.0334	Singlet-A	H-14->LUMO (16%)
92	66727.86102	149.862438974	0.0024	Singlet-A	H-14->LUMO (12%)
93	66836.7458679	149.618295597	0.0075	Singlet-A	
94	67058.5483359	149.123418985	0.0201	Singlet-A	
95	67281.1573583	148.630023511	0.0051	Singlet-A	
96	67498.9270542	148.150503074	0.0016	Singlet-A	

97	**67550.5465376**	**148.037292258**	**0.0026**	**Singlet-A**	**H-10->LUMO (21%)**
98	**67824.7750435**	**147.438749242**	**0.0043**	**Singlet-A**	**HOMO->L+23 (17%)**
99	**68094.1642228**	**146.855462787**	**0.0017**	**Singlet-A**	**H-2->L+8 (12%), H-2->L+13 (22%), H-2->L+15 (11%)**
100	**68221.5998225**	**146.581141838**	**0.003**	**Singlet-A**	**H-1->L+7 (10%)**