

New flexible molecular probes bearing dansyl and TEMPO moieties for host-guest interactions in solution and gels

Sorin Mocanu,^a Iulia Matei,*^a Anca Leonties,^a Victorita Tecuceanu,^b Ana Maria Hanganu,^{b,c} Zamfirica Minea,^a Alina Stancu,^a Elena Irina Popescu^a and Gabriela Ionita*^a

^a “Ilie Murgulescu” Institute of Physical Chemistry of the Romanian Academy, 202 Splaiul Independentei, Bucharest 060021, Romania. E-mails: ige@icf.ro; iuliamatei@icf.ro.

^b Organic Chemistry Centre of the Romanian Academy, 202B Splaiul Independentei, 78100 Bucharest, Romania.

^c Department of Organic Chemistry, Biochemistry and Catalysis, University of Bucharest, 90-92 Panduri, 050663 Bucharest, Romania

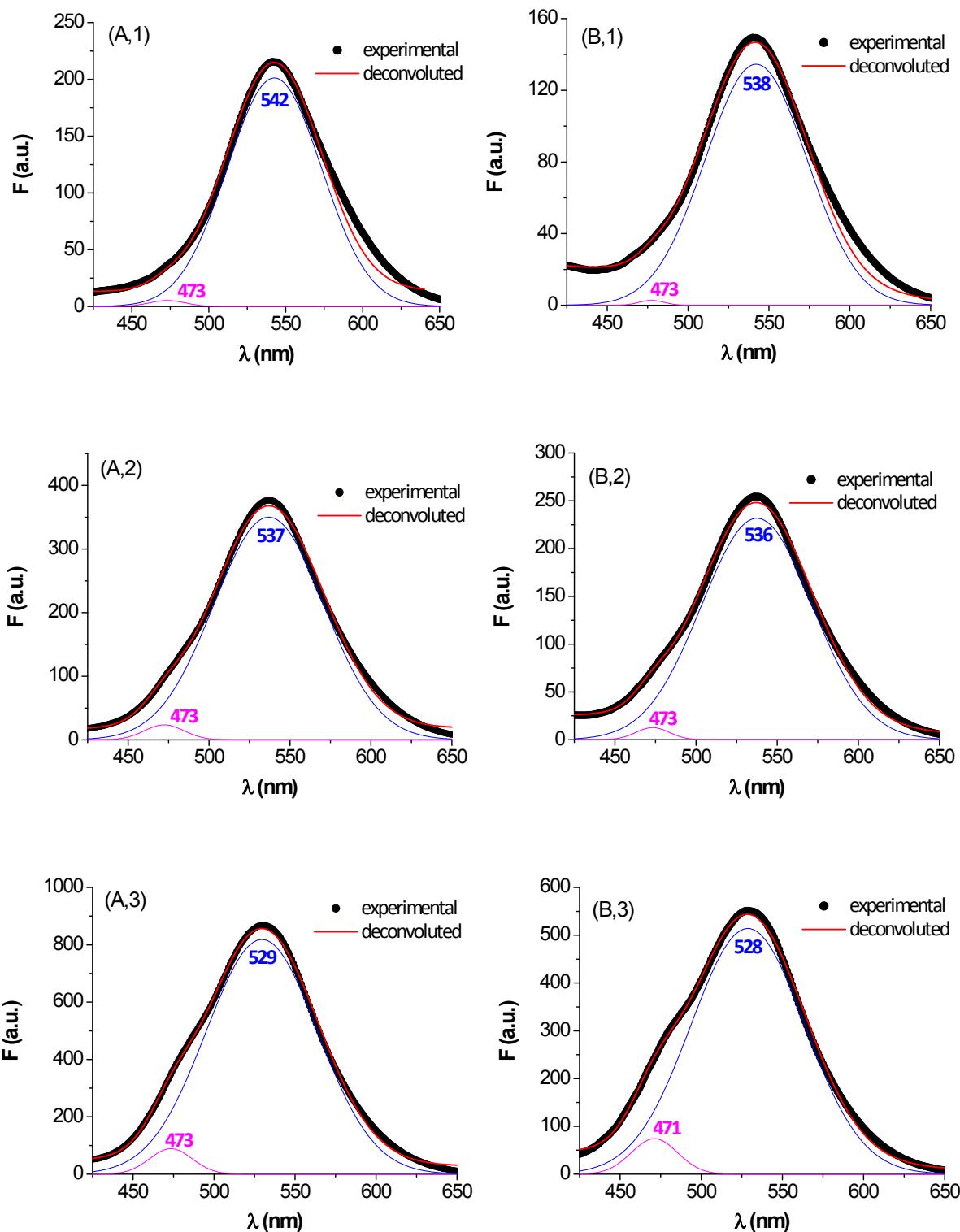


Fig. S1. Deconvolution of the fluorescence spectra of (A) DA_{1.7} and (B) DA_{1.7}T in water in the absence (1) and in the presence of β-CD at 10⁻³ M (2) and 10⁻² M (3) concentrations.

Table S1. Position (λ , in nm) and relative area (A, in %) of the two fluorescence bands obtained by deconvolution of the emission spectra of DA_{1,n} and DA_{1,n}T in the absence and in the presence of β -CD

[β -CD] (M)	DA _{1,n}				DA _{1,n} T			
	λ_1	A ₁	λ_2	A ₂	λ_1	A ₁	λ_2	A ₂
0	473	0.9	542	99.1	473	0.3	538	99.7
10 ⁻³	473	2.4	537	97.6	473	1.7	536	98.3
10 ⁻²	473	4.2	529	95.8	471	5.6	528	94.4

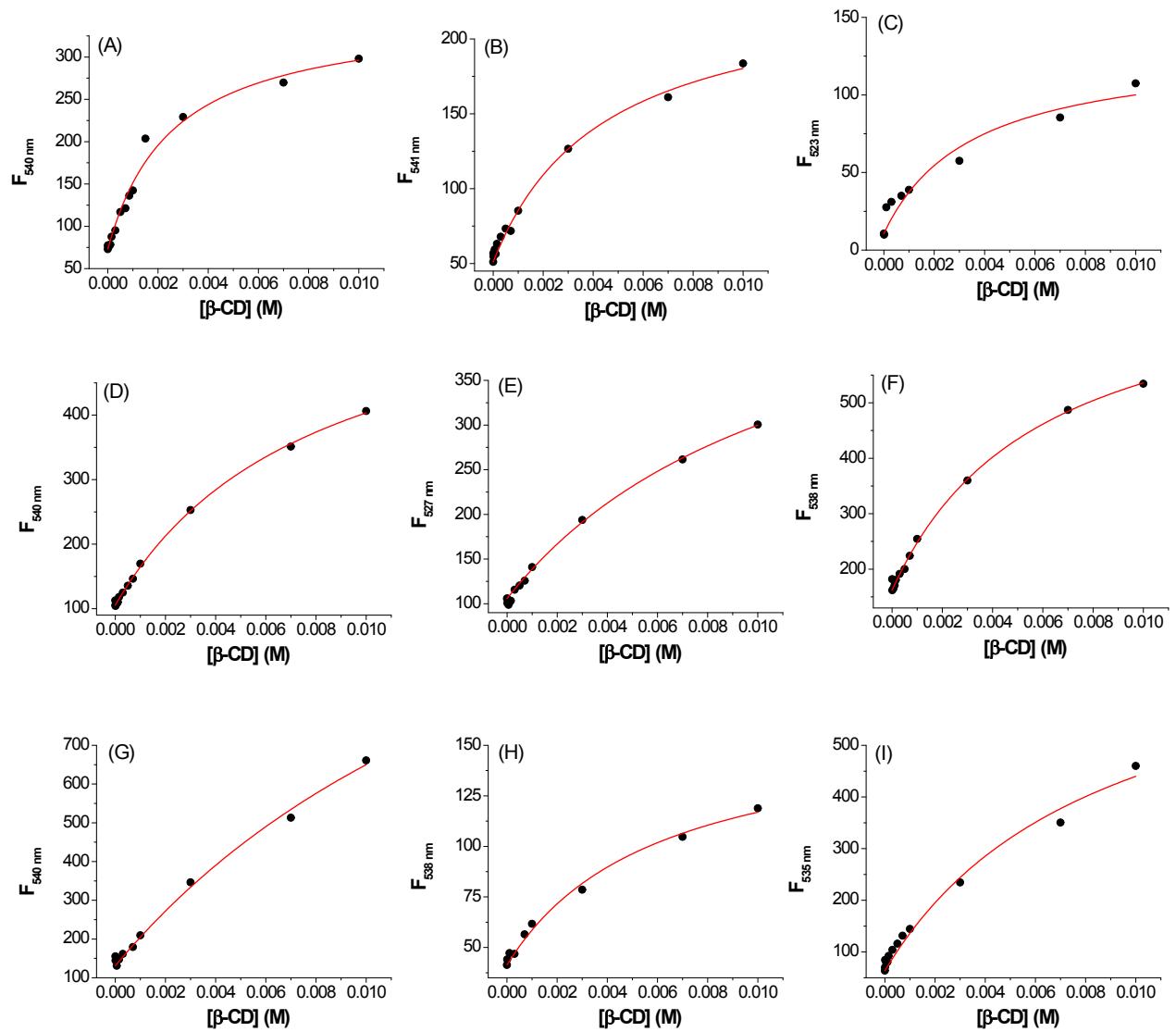
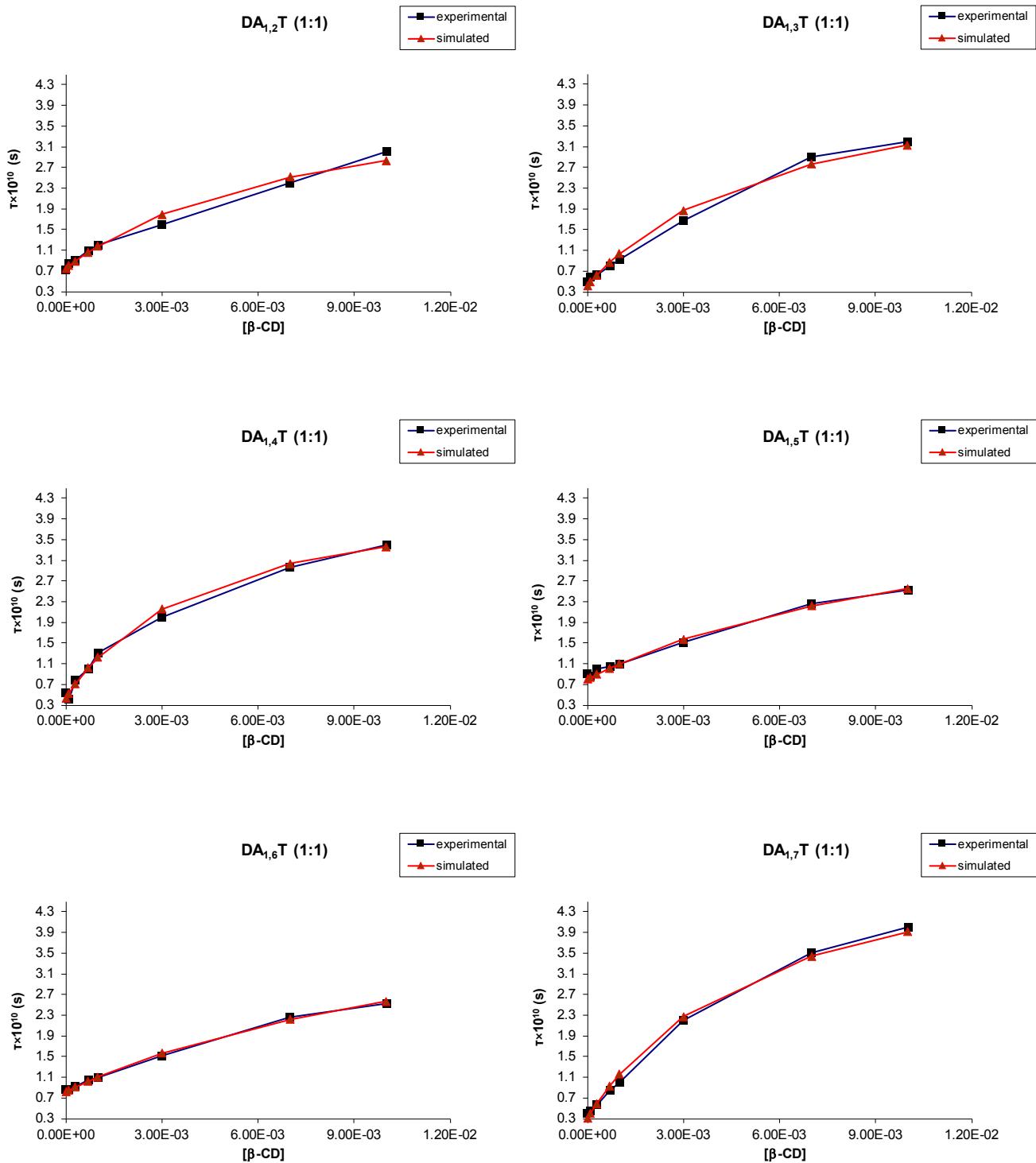


Fig. S2. Dependence of the normalized fluorescence emission of DA_{1,n}T probes on the cyclodextrin concentration. The solid lines represent the best fits according to eq. (3) for (A) DA_{1,2}T, (B) DA_{1,3}T, (C) DA_{1,4}T, (D) DA_{1,5}T, (E) DA_{1,6}T, (F) DA_{1,7}T, (G) DA_{1,8}T, (H) DA_{1,10}T, (I) DA_{1,12}T.



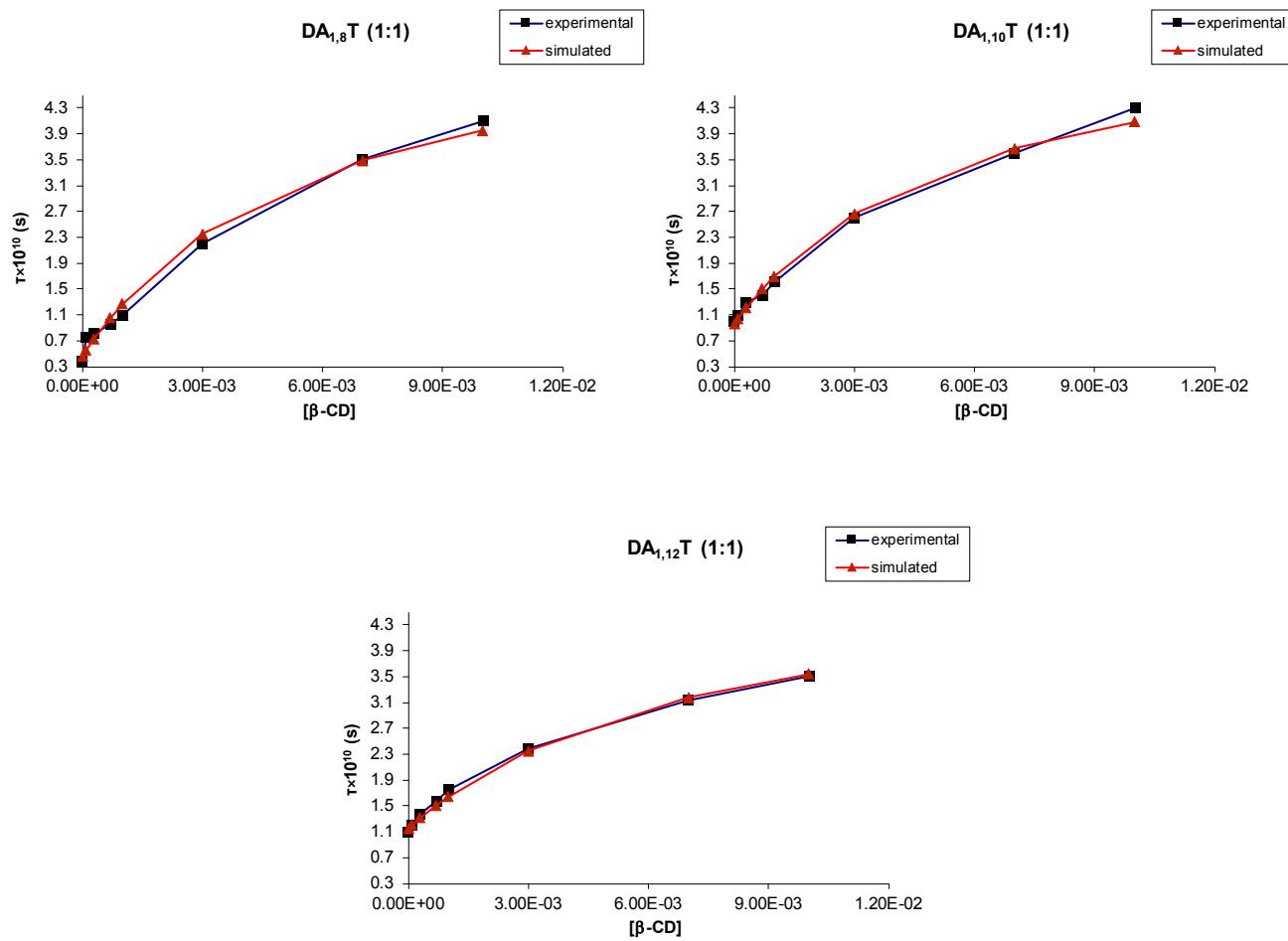


Fig. S3. Dependence of the rotational correlation time of DA_{1,n}T probes on the cyclodextrin concentration.

**NMR spectra of DA_{1.3} and DA_{1.3}T (reduced with hydrazine)
in the absence and in the presence of β-cyclodextrin**

The NMR spectra of DA_{1.3} and DA_{1.3}T (reduced with hydrazine) have been recorded in the absence and in the presence of β-CD in deuterated water and in DMSO. This allowed us to evidence the differences in chemical shifts of the proton signals assigned to the dansyl group. Unfortunately, the corresponding dual probe, DA_{1.3}T, is not soluble in deuterated water at concentrations that would allow us to record NMR spectra. While fluorescence and EPR measurements can be performed at concentrations of ~10⁻⁶–10⁻⁴ M, NMR measurements require higher concentrations of the probes (~10⁻² M). Moreover, while the complex of DA_{1.3} with β-CD is soluble in deuterated water, the solid complex of DA_{1.3}T separated from solution. Therefore, in this case both β-CD and DA_{1.3}T were in too low concentration in solution to record the NMR spectra.

For this reason, we recorded the NMR spectra in another polar solvent that solubilizes both DA_{1.3}T and the mixture DA_{1.3}T/β-CD. As can be noticed from Figs. S4, S5 and Tables S1, S2, chemical shifts in the NMR spectrum of the DA_{1.3}T/β-CD mixture are observed for protons of the dansyl group but not of the TEMPO moiety. This sustain our conclusion, based on fluorescence and EPR data, that the dansyl moiety is involved in the inclusion process.

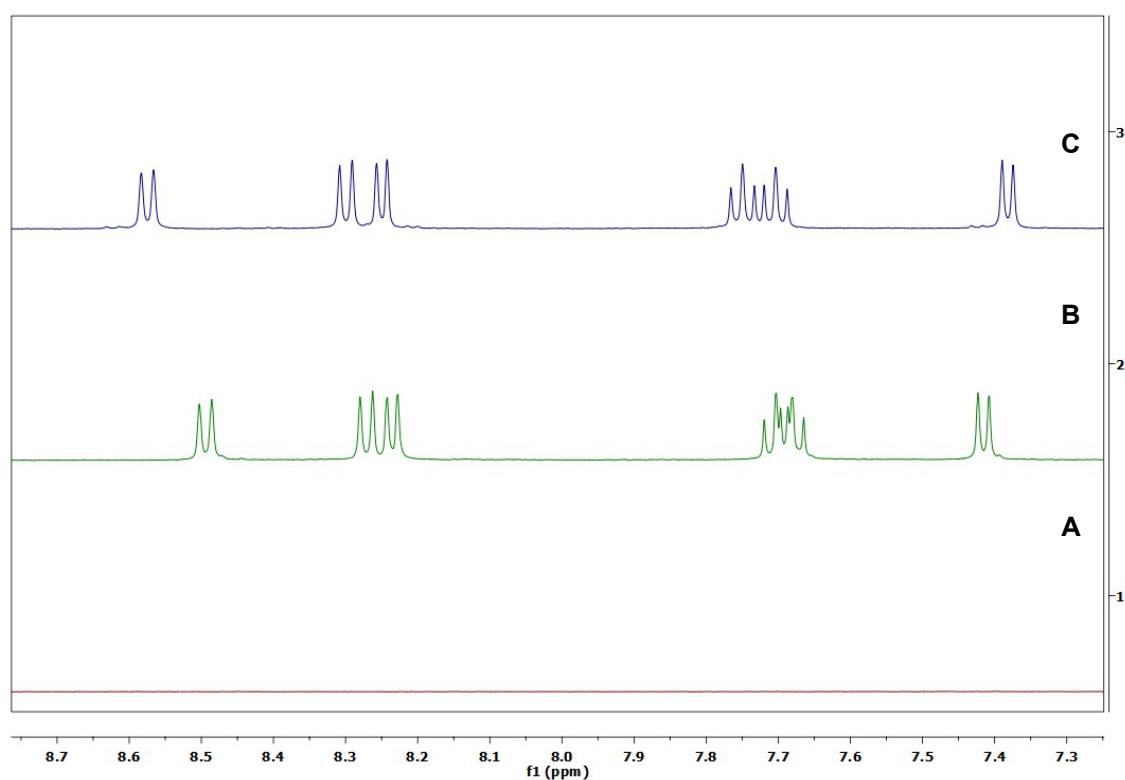
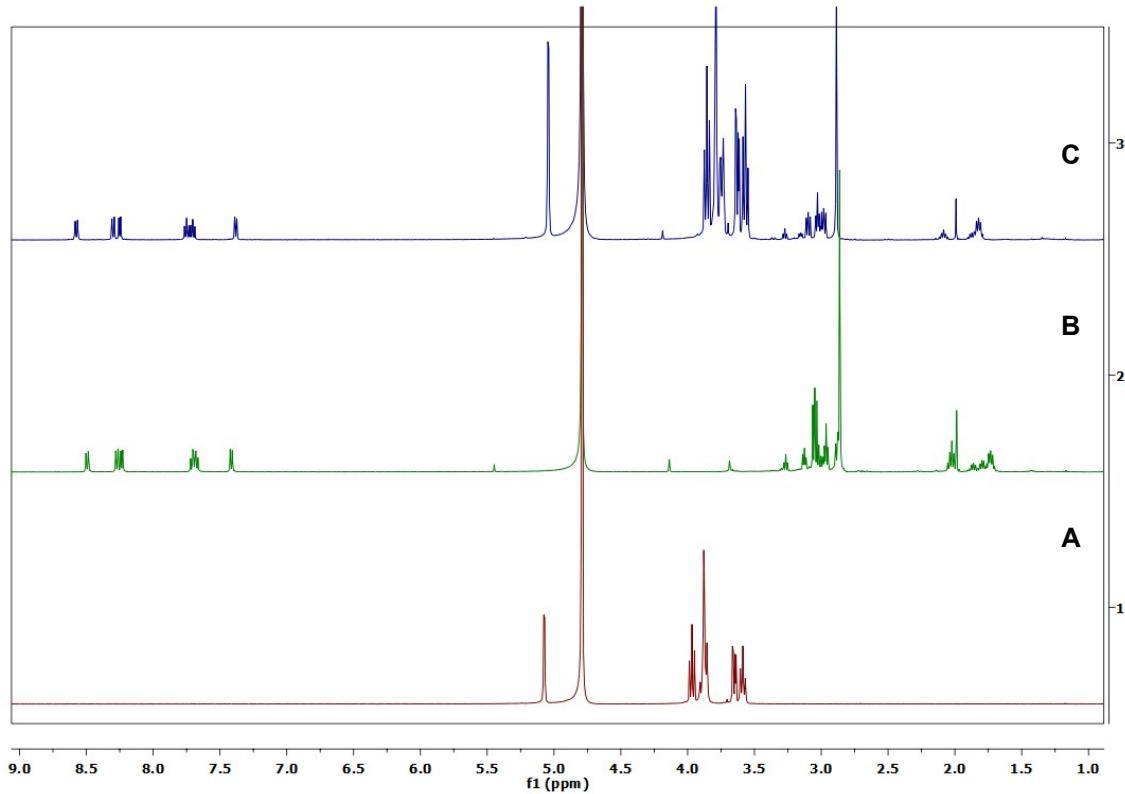
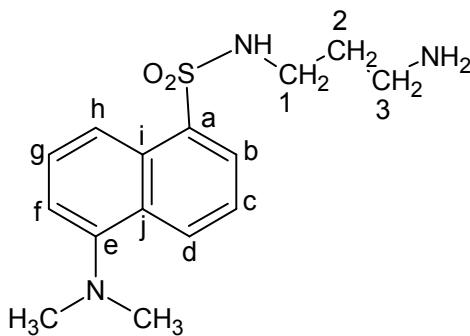
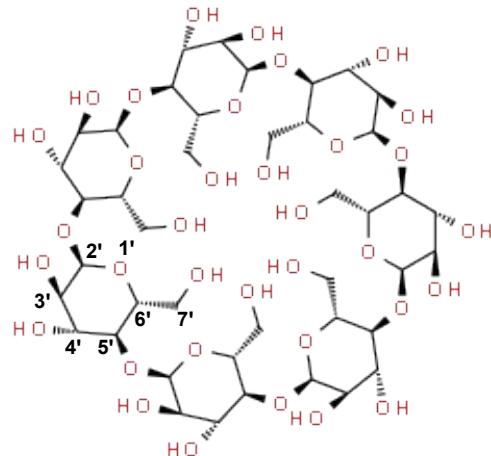


Fig. S4. ^1H -NMR spectra in D_2O of: **A** – β -cyclodextrin, **B** – DA_{1,3}; **C** - β -cyclodextrin + DA_{1,3}.



DA_{1.3} structure



β-Cyclodextrin structure

Table S1. Chemical shifts of DA_{1.3} and β-CD protons in D₂O

Compounds protons	Chemical shifts of β-CD (ppm)	Chemical shifts of DA _{1.3} (ppm)	Chemical shifts of β-CD + DA _{1.3} (ppm)	$\Delta\delta = \delta_{BCD \text{ or } DA_{1.3}} - \delta_{BCD + DA_{1.3}} $	
				ppm	Hz
H-b	-	8.23	8.25	0.02	11.1
H-c	-	7.68	7.70	0.02	11.2
H-d	-	8.49	8.57	0.08	40.3
H-f	-	7.41	7.38	0.03	17.2
H-g	-	7.70	7.74	0.05	22.8
H-h	-	8.27	8.30	0.03	14.1
H-1	-	2.96	3.02	0.06	32.0
H-2	-	1.73	1.82	0.09	45.70
H-3	-	2.88	2.98	0.11	52.3
-N(CH ₃) ₂	-	2.86	2.88	0.02	11.8
H-2 [¶]	5.07	-	5.04	0.03	15.2
H-3 [¶]	3.58	-	3.56	0.02	10.1
H-4 [¶]	3.97	-	3.85	0.12	55.8
H-5 [¶]	3.90-3.85	-	3.79-3.72	0.11-0.13	57.5-64.8
H-6 [¶]	3.65	-	3.63	0.02	12.0
H-7 [¶]	3.90-3.85	-	3.79-3.72	0.11-0.13	57.5-64.8

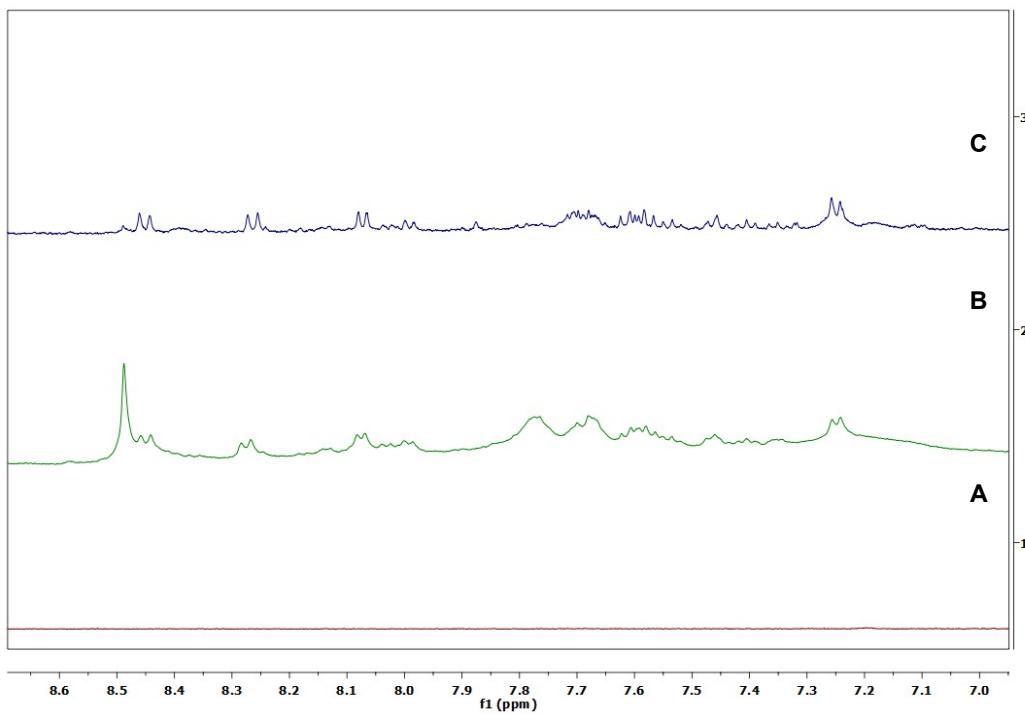
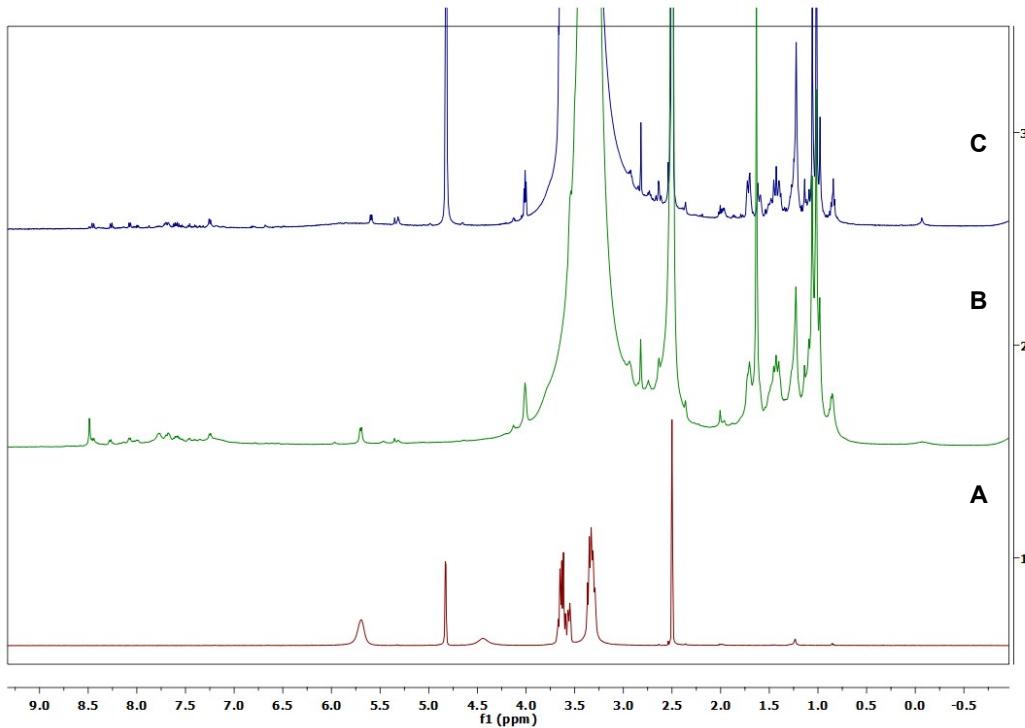


Fig. S5. ^1H -NMR spectra in DMSO of: **A** – β -cyclodextrin, **B** – DA_{1,3}T; **C** - β -cyclodextrin + DA_{1,3}T.

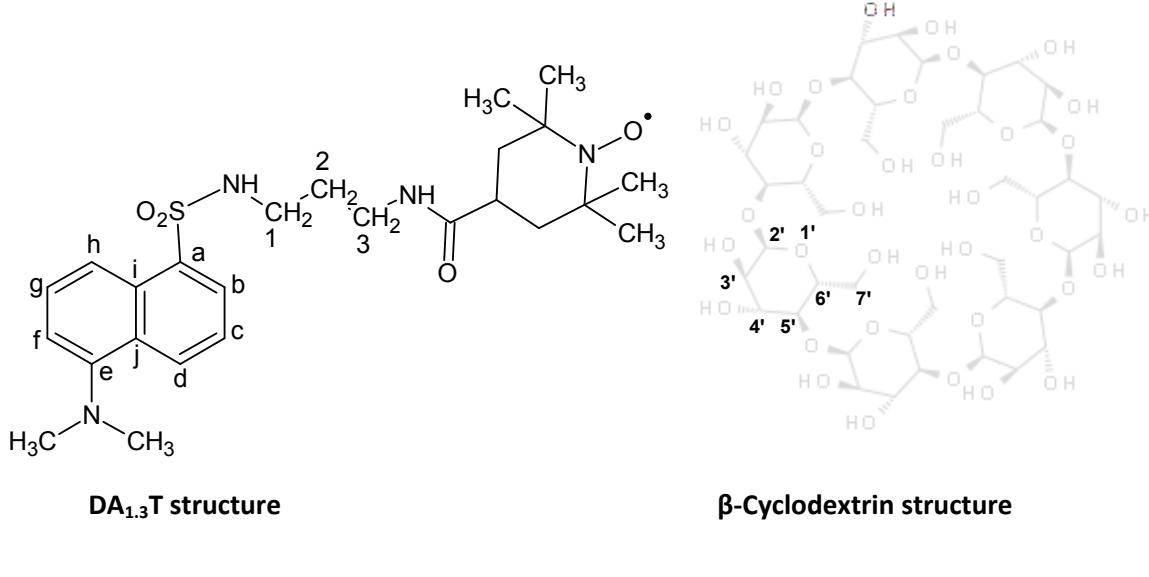
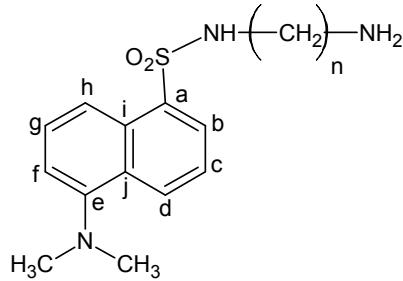


Table S2. Chemical shifts of DA_{1,3}T and β-CD protons in DMSO

Compounds protons	Chemical shifts of β-CD (ppm)	Chemical shifts of DA _{1,3} T (ppm)	Chemical shifts of β-CD + DA _{1,3} T (ppm)	$\Delta\delta = \delta_{BCD \text{ or } DA_{1,3}T} - \delta_{BCD + DA_{1,3}T} $	
				ppm	Hz
H-b	-	8.08	8.06	0.02	9.6
H-c	-	7.62-7.53	7.64-7.55	0.02	9.4
H-d	-	8.45	8.43	0.02	8.98
H-f	-	7.25	7.23	0.02	9.7
H-g	-	7.62-7.53	7.64-7.55	0.02	9.4
H-h	-	8.28	8.26	0.02	10.8
H-1	-	2.93	2.92	0.01	6.7
H-2	-	1.43	1.40	0.03	15.3
H-3	-	2.74	2.72	0.02	9.6
-N(CH ₃) ₂	-	2.82	2.81	0.01	6.2
H-2 [¶]	4.83	-	4.82	0.01	4.5
H-3 [¶]	3.36-3.29	-	Overlapped with water signal from DMSO	-	-
H-4 [¶]	3.67-3.55	-	3.65-3.52	0.02-0.03	11.1-15.6
H-5 [¶]	3.67-3.55	-	3.65-3.52	0.02-0.03	11.1-15.6
H-6 [¶]	3.36-3.29	-	Overlapped with water signal from DMSO	-	-
H-7 [¶]	3.67-3.55	-	3.65-3.52	0.02-0.03	11.1-15.6
-CH (TEMPO)	-	2.63	2.63	0	0.0
-CH ₂ -(TEMPO)	-	1.74	1.74	0	0.0
-CH ₃ (TEMPO)	-	1.06 and 1.02	1.055-1.015	0.005	1.6

Spectral characterization of DA_{1,n}

Notation of H atoms for assignment of NMR ¹H signals



n= 2,3,4,5,6,7,8,10,12

MAD-2, n=2, -NH-¹CH₂-²CH₂-NH₂

MAD-3, n=3, -NH-¹CH₂-²CH₂-³CH₂-NH₂

MAD-4, n=4, -NH-¹CH₂-²CH₂-³CH₂-⁴CH₂-NH₂

MAD-5, n=5, -NH-¹CH₂-²CH₂-³CH₂-⁴CH₂-⁵CH₂-NH₂

MAD-6, n=6, -NH-¹CH₂-²CH₂-³CH₂-⁴CH₂-⁵CH₂-⁶CH₂-NH₂

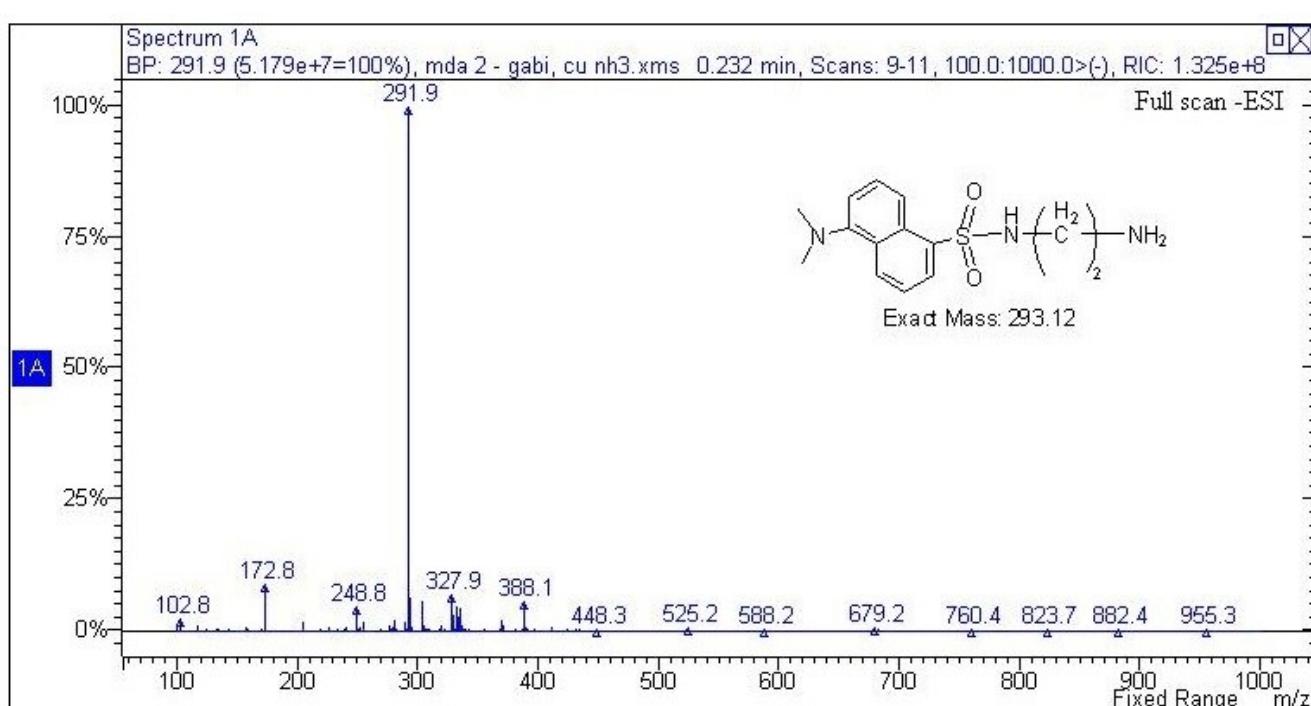
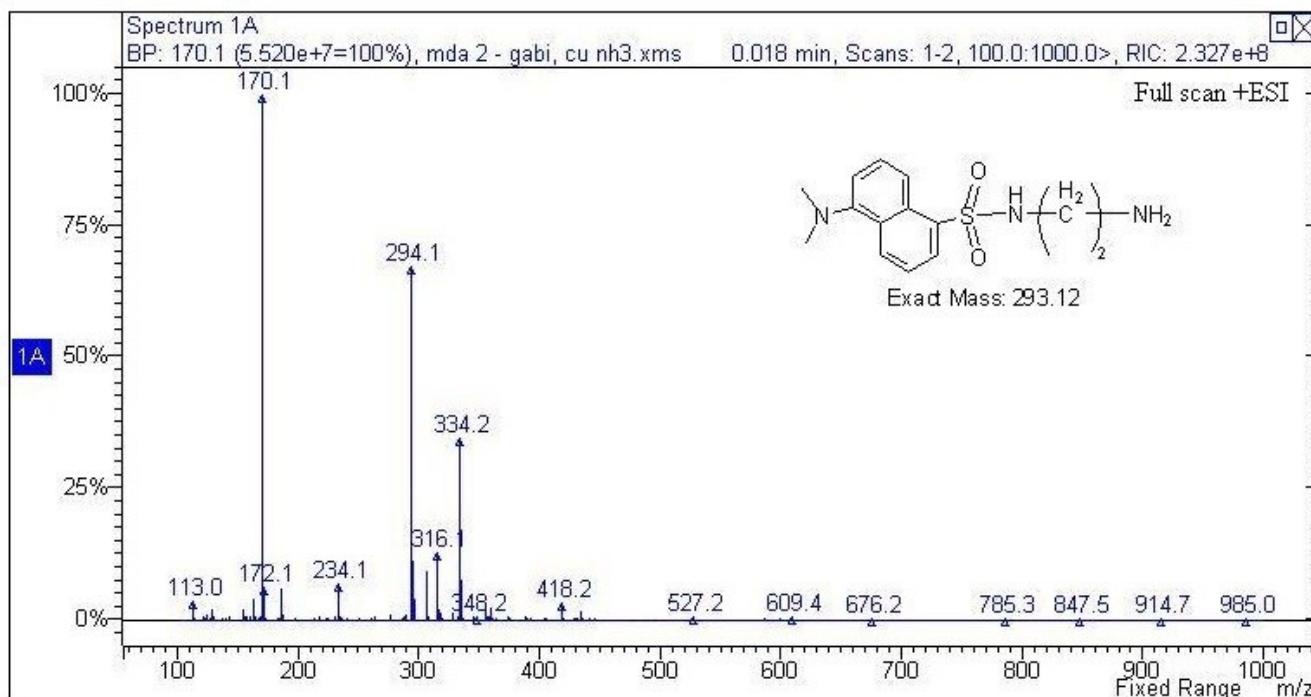
MAD-7, n=7, -NH-¹CH₂-²CH₂-³CH₂-⁴CH₂-⁵CH₂-⁶CH₂-⁷CH₂-NH₂

MAD-8, n=8, -NH-¹CH₂-²CH₂-³CH₂-⁴CH₂-⁵CH₂-⁶CH₂-⁷CH₂-⁸CH₂-NH₂

MAD-10, n=10, -NH-¹CH₂-²CH₂-³CH₂-⁴CH₂-⁵CH₂-⁶CH₂-⁷CH₂-⁸CH₂-⁹CH₂-¹⁰CH₂-NH₂

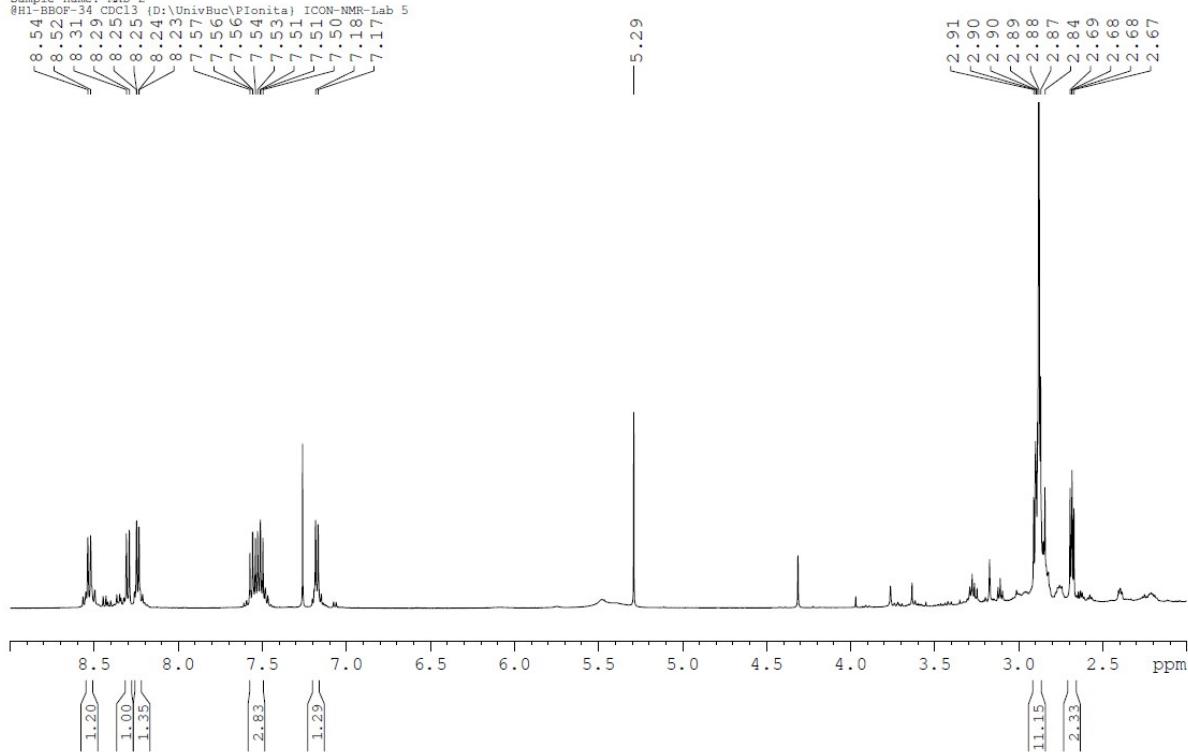
MAD-12, n=12, -NH-¹CH₂-²CH₂-³CH₂-⁴CH₂-⁵CH₂-⁶CH₂-⁷CH₂-⁸CH₂-⁹CH₂-¹⁰CH₂-¹¹CH₂-¹²CH₂-NH₂

DA_{1,2} (dansyl ethylenediamine)



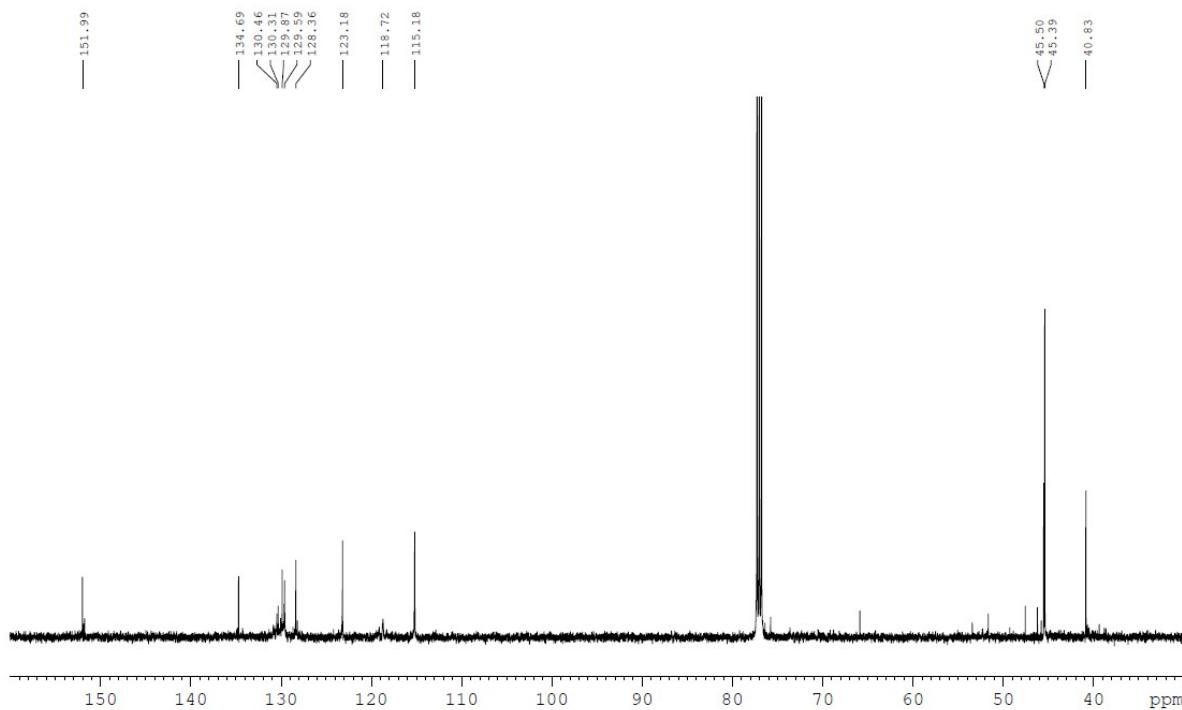
Instrument Bruker AvanceIII 500MHz (UnivBucuresti)
Operator CS
Registry ID: 2185
User Name: Ionita
Sample Changer Position 9
Sample name: MAD1_2
@H1-BBOF-34 CDCl3 (D:\UnivBuc\Plonita) ICON-NMR-Lab 5

8.54 8.52 8.31 8.29 8.25 8.24 8.23 8.21 8.17 7.57 7.56 7.53 7.51 7.50 7.54 7.53 7.51 7.50 7.18 7.17

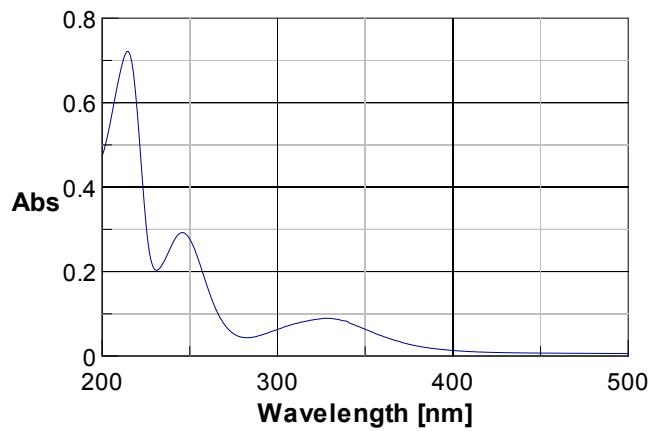


¹H NMR spectrum of compound DA_{1.2}

Instrument Bruker AvanceIII 500MHz (UnivBucuresti)
Operator CS
Registry No. 2185
User G. Ionita
Sample Changer Position 9
Sample name: MAD_2
CDCl₃
a072_0000_0000_2A

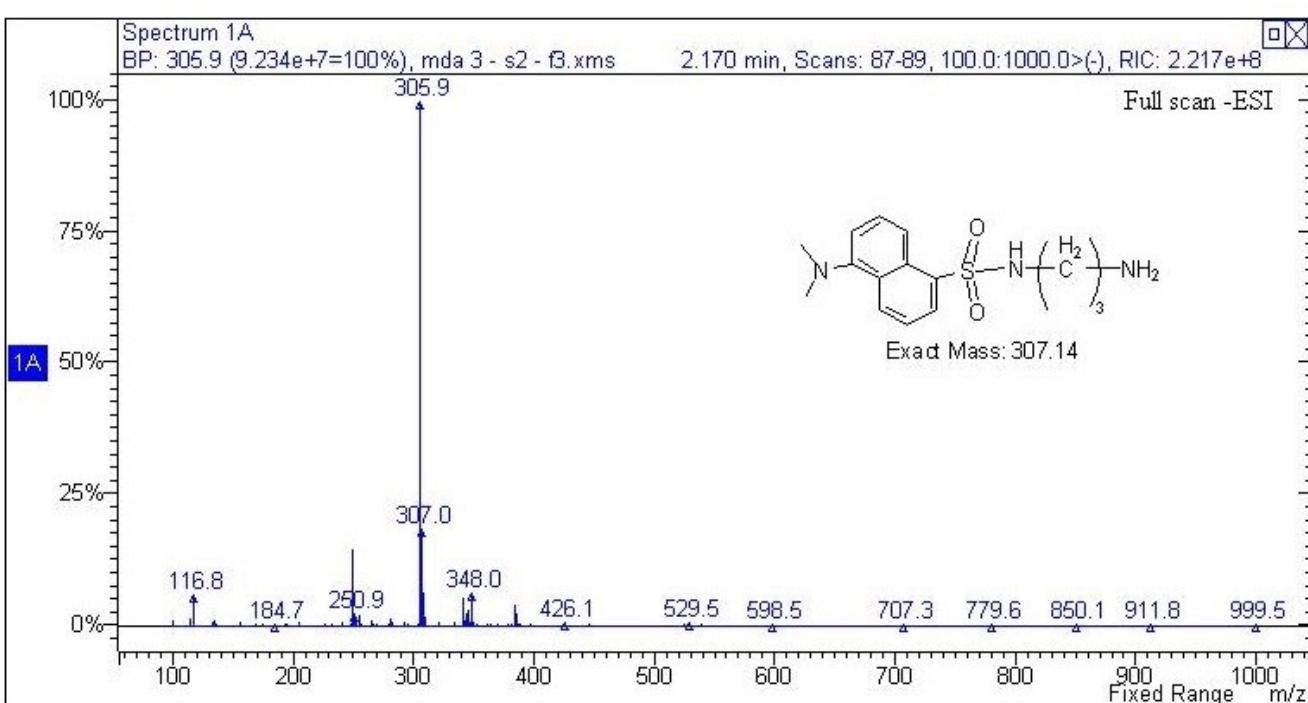
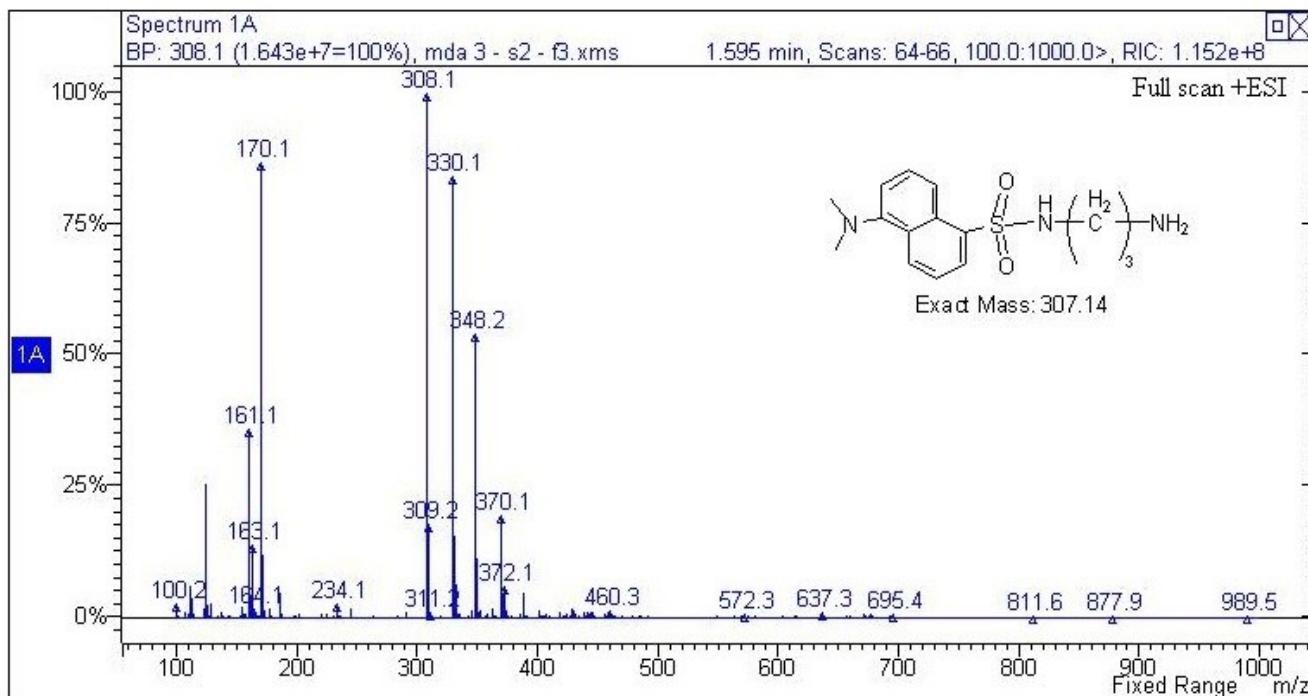


¹³C NMR spectrum of compound DA_{1.2}

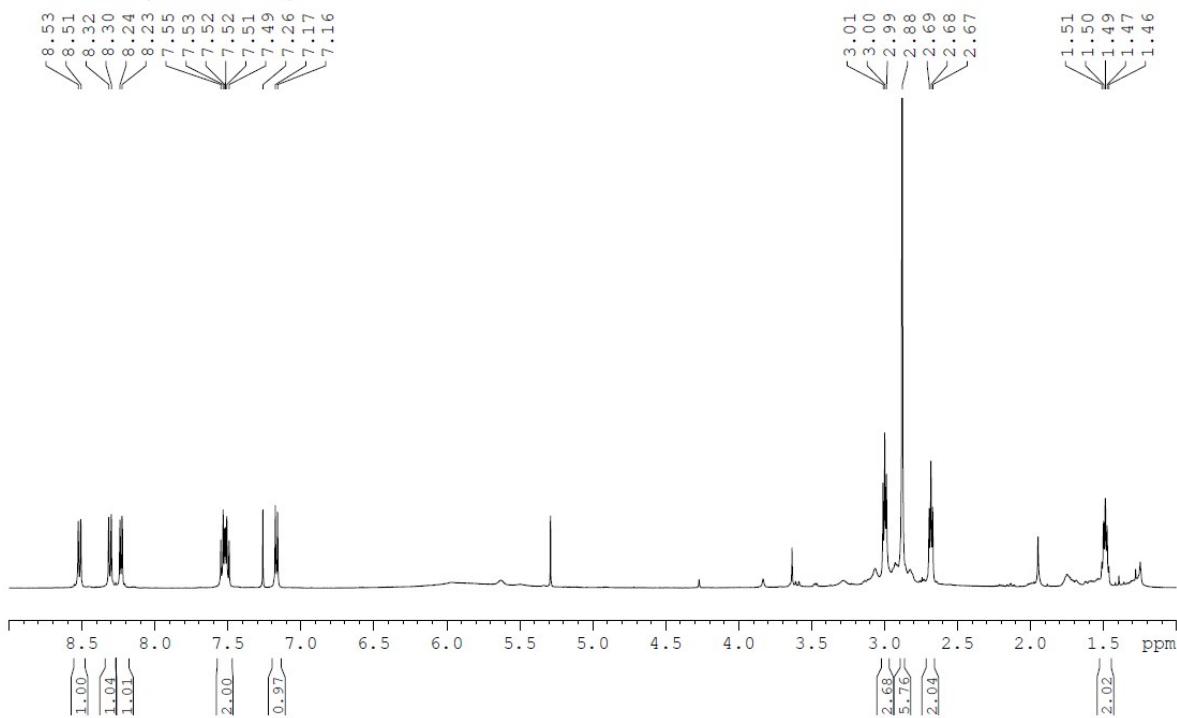


UV-Vis spectrum of compound DA_{1.2}

DA_{1,3} (dansyl 1,3-diaminopropane)

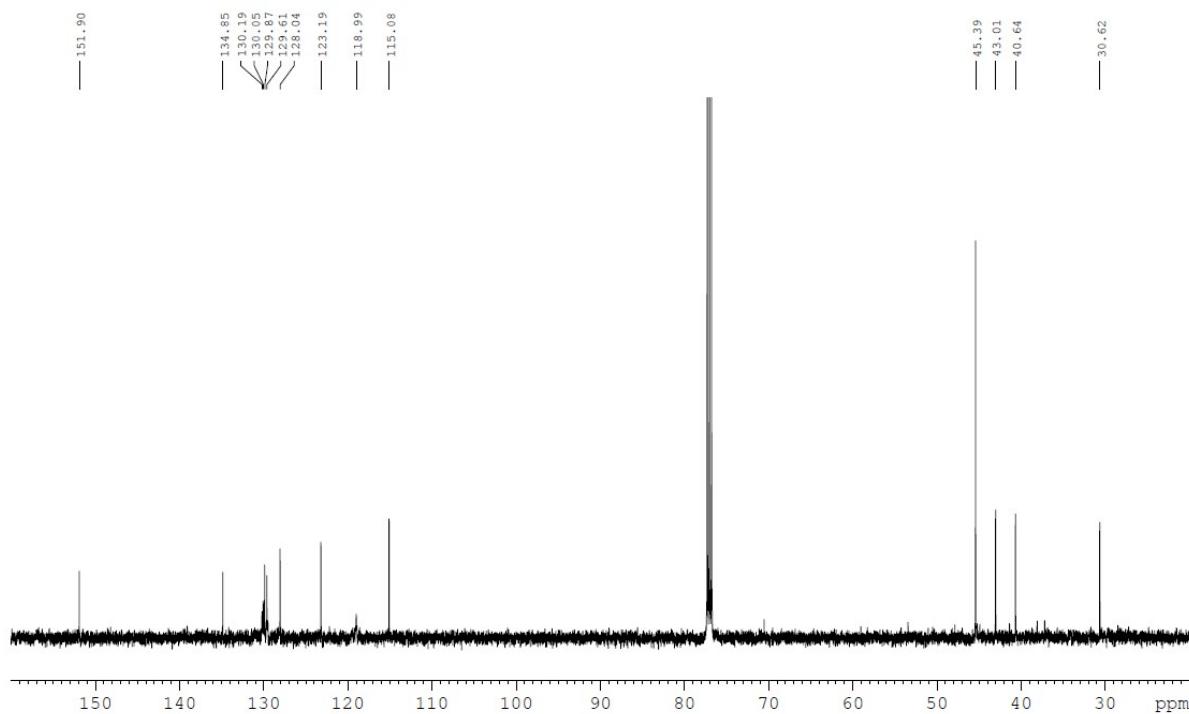


Instrument: Bruker AvanceIII 500MHz (UnivBucuresti)
Operator: Cr
Protocol No.: 2186
User: G. Ionita
Sample Changer Position 4
Sample name: MAD-3
@H1-BBOF-34 CDCl3 (D:\UnivBuc\Plionita) ICON-NMR-Lab 5

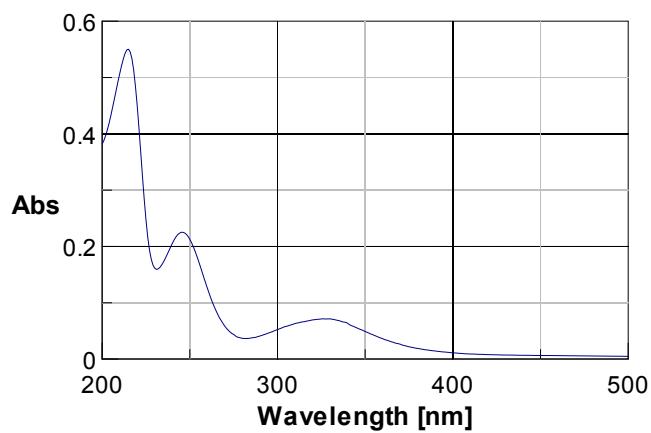


¹H NMR spectrum of compound DA_{1.3}

Instrument Bruker AvanceIII 500MHz (UnivBucuresti)
Operator CS
Registry No. 2186
User G. Ionita
Sample Changer Position 4
Sample name: MDA-3
CDCl₃
a012...000...000...2A

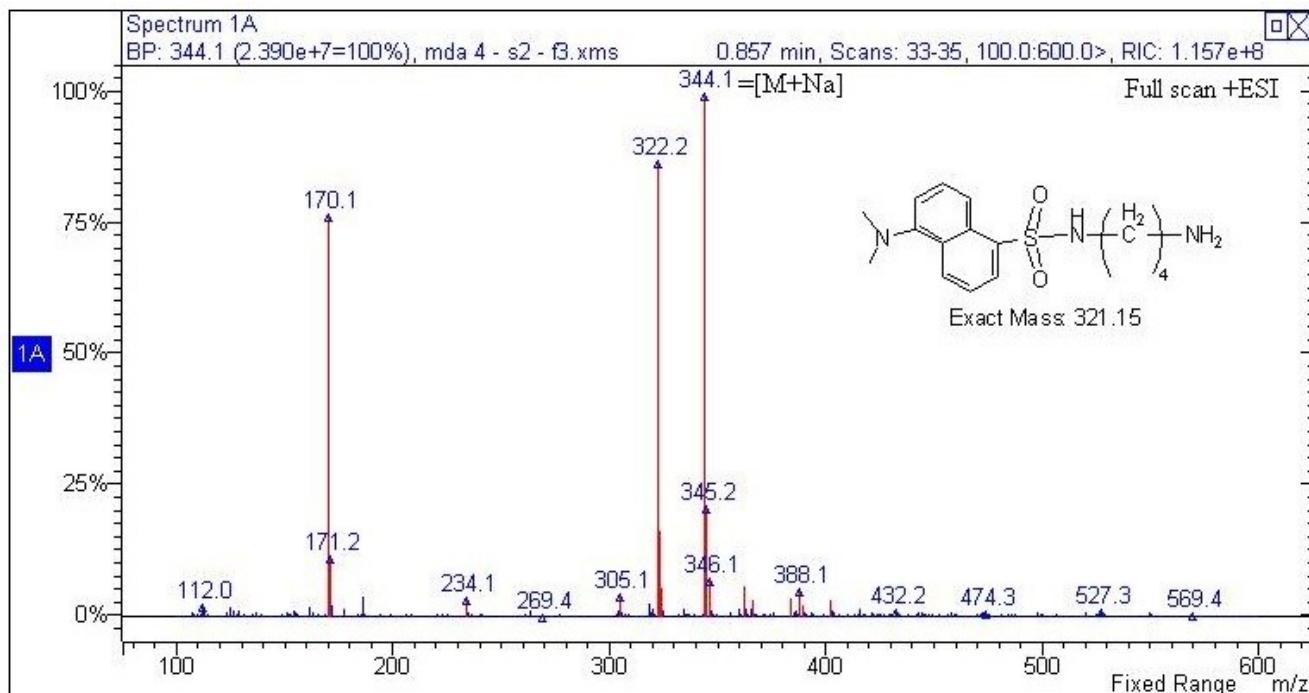


¹³C NMR spectrum of compound DA_{1.3}

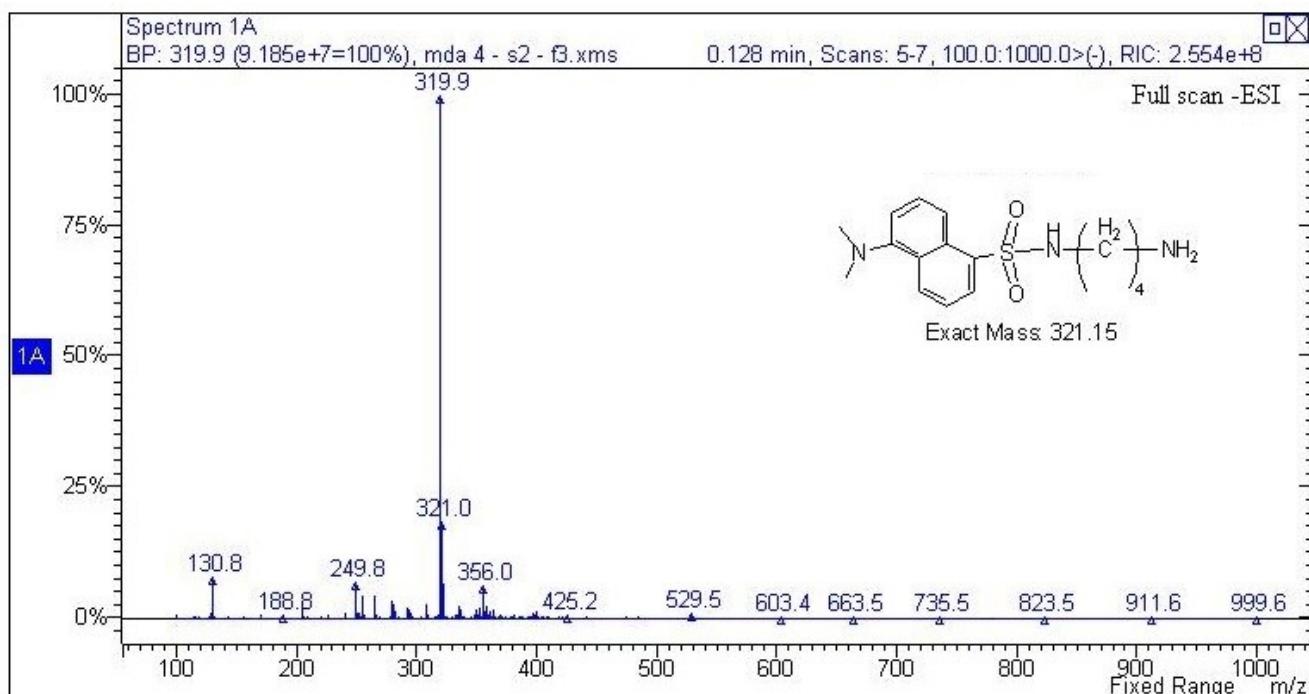


UV-Vis spectrum of compound DA_{1.3}

DA_{1.4} (dansyl 1,4-diaminobutane)



ESI-MS (*m/z*): 321 (DA_{1.4} + H⁺)

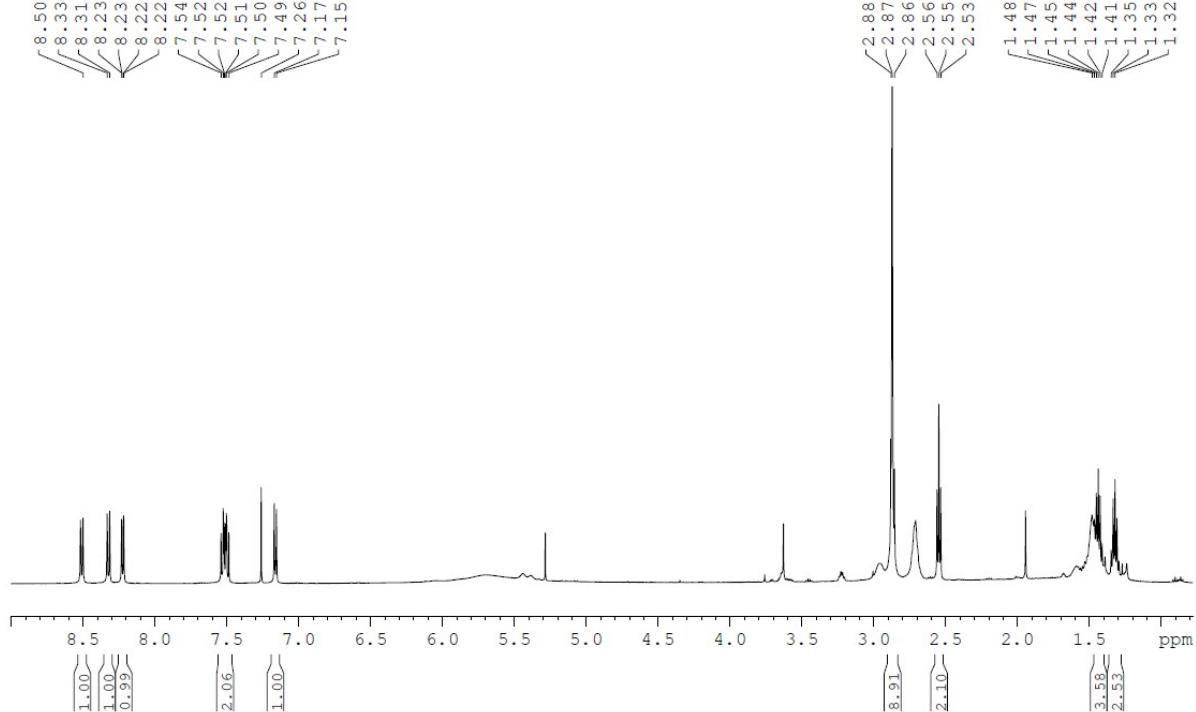


ESI-MS (*m/z*): 320 (DA_{1.4} - H⁺)

Instrument Bruker AvanceIII 500MHz (UnivBucuresti)
Operator CS
Registry No. 2187
User G. Ionita
Sample Changer Position 11
Sample name: MDA_4
@H1-BBOF-34 CDCl3 (D:\UnivBuc\Plionita) ICON-NMR-Lab 5

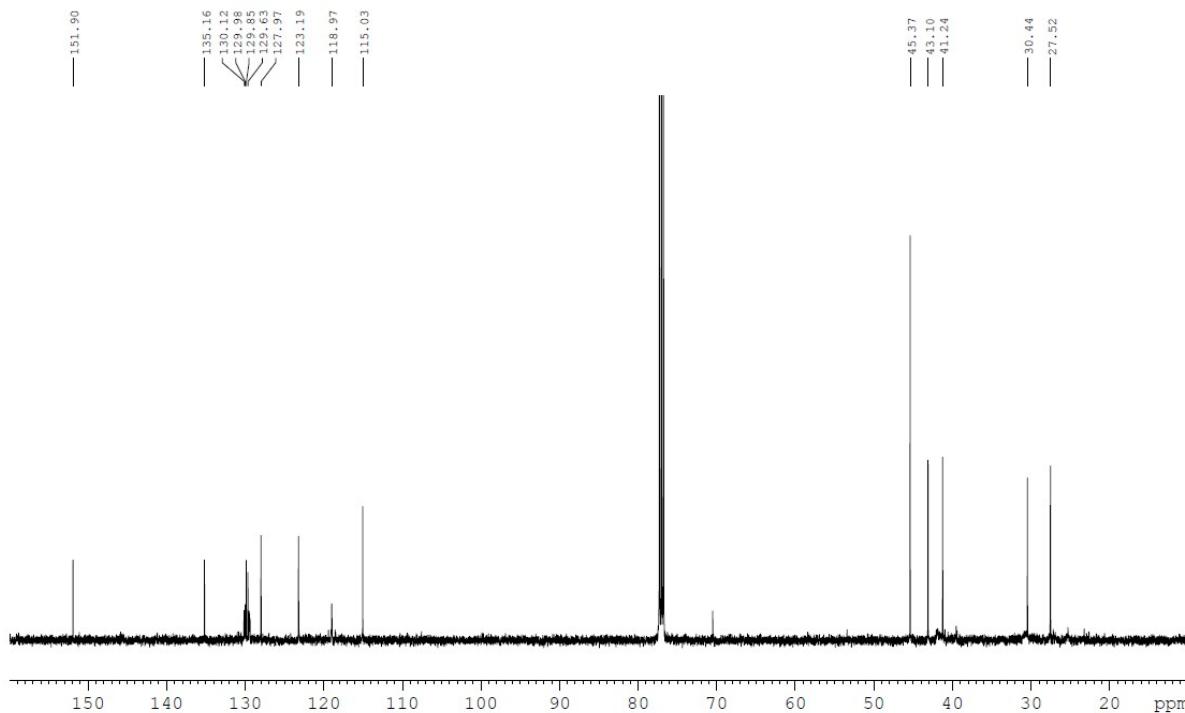
5.0 3.3 3.1 2.3 2.2 2.0 1.8 1.6 1.5 1.4 1.3 1.2 1.1 1.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1 0.0

7.50 7.51 7.52 7.54 7.55 7.56 7.57 7.58 7.59 7.60 7.61 7.62 7.63 7.64 7.65 7.66 7.67 7.68 7.69 7.70 7.71 7.72 7.73 7.74 7.75 7.76 7.77 7.78 7.79 7.80 7.81 7.82 7.83 7.84 7.85 7.86 7.87 7.88 7.89 7.90 7.91 7.92 7.93 7.94 7.95 7.96 7.97 7.98 7.99 7.00 7.01 7.02 7.03 7.04 7.05 7.06 7.07 7.08 7.09 7.10 7.11 7.12 7.13 7.14 7.15 7.16 7.17 7.18 7.19 7.20 7.21 7.22 7.23 7.24 7.25 7.26 7.27 7.28 7.29 7.30 7.31 7.32 7.33

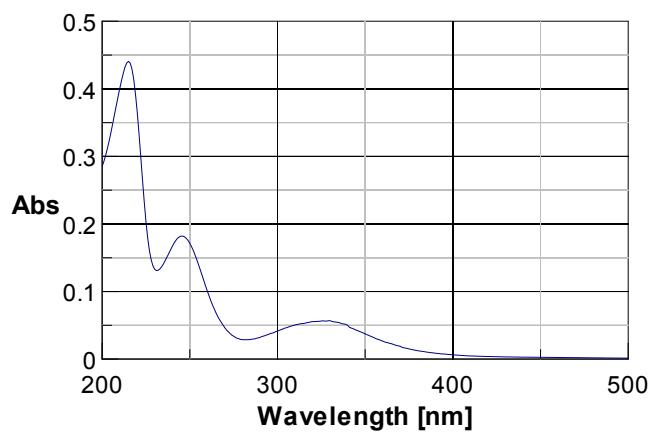


¹H NMR spectrum of compound DA_{1.4}

Instrument Bruker AvanceIII 500MHz (UnivBucuresti)
Operator CS
Registry No. 2187
User G. Ionita
Sample Changer Position 11
Sample name: MAD-4
CDCl₃
δ_{CH} 2-150 ppm - δ_{CH} 2-20 ppm

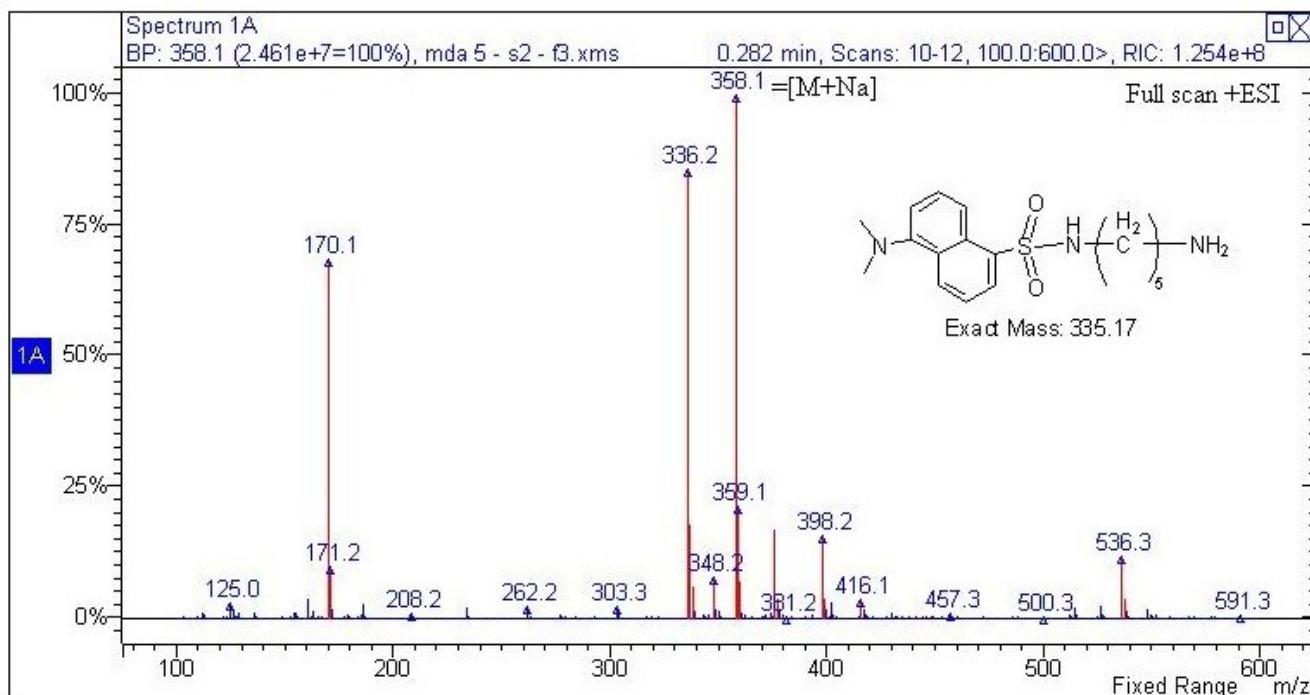


¹³C NMR spectrum of compound DA_{1.4}

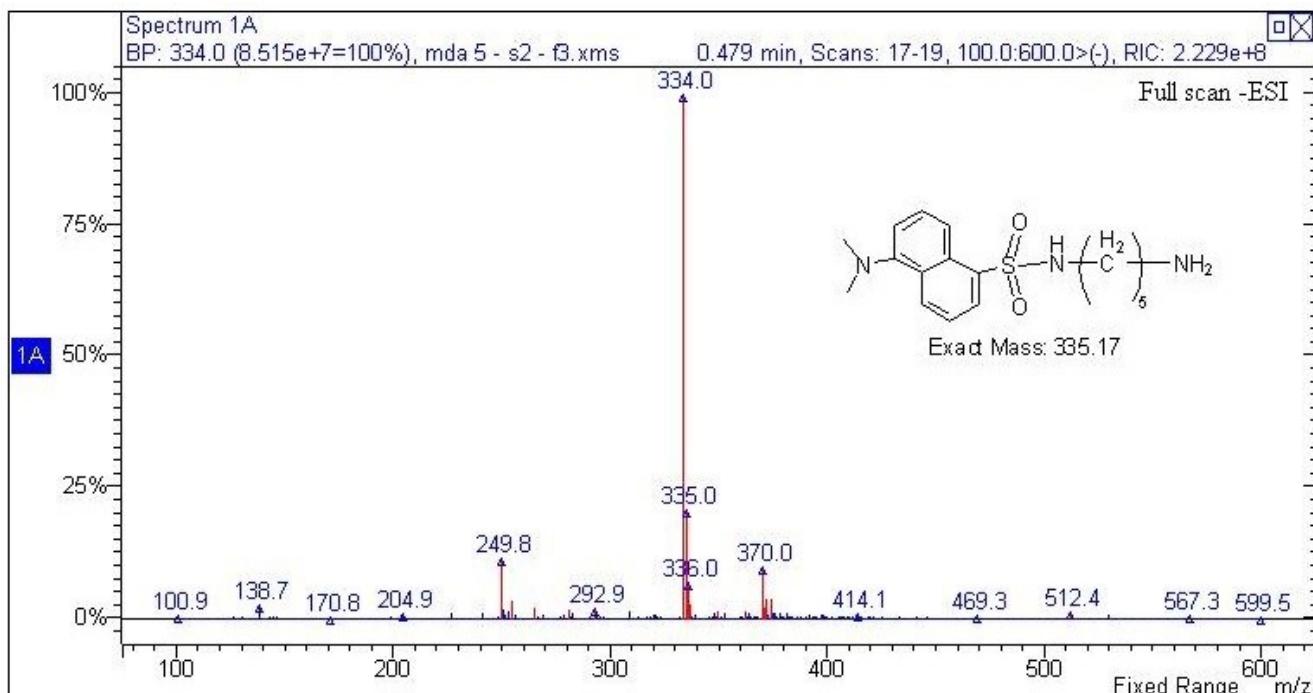


UV-Vis spectrum of compound DA_{1.4}

DA_{1.5} (dansyl 1,5-diaminopentane)

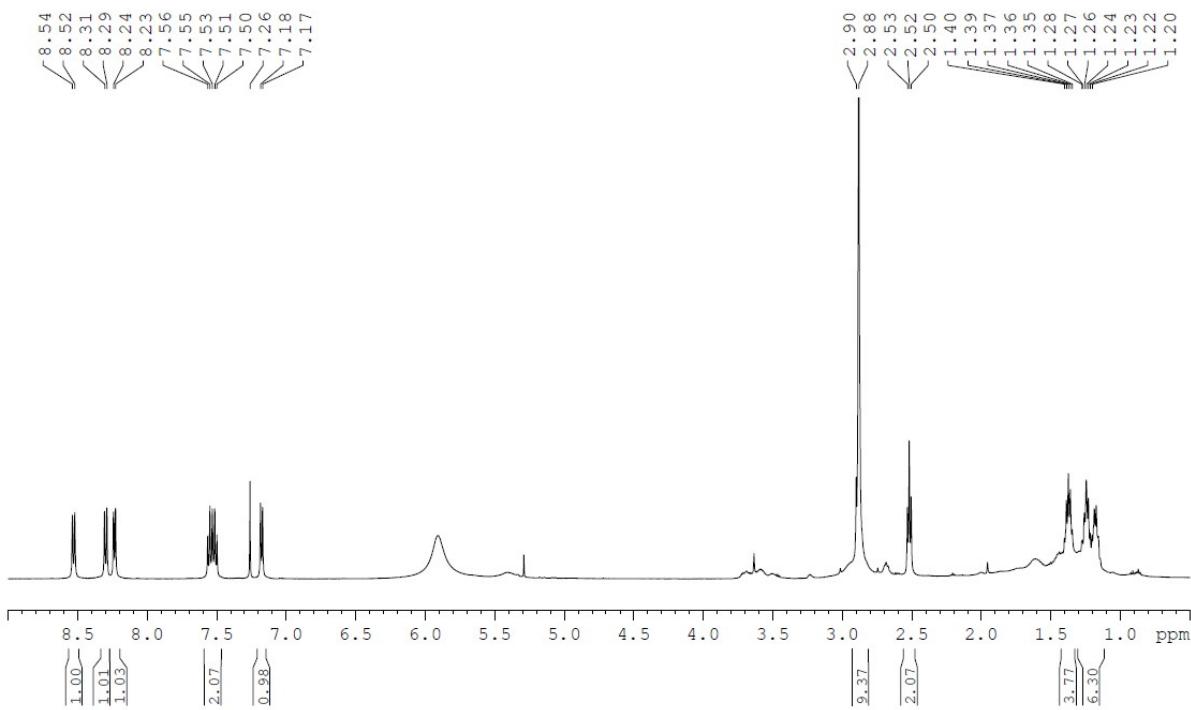


ESI-MS (*m/z*): 335 (DA_{1.5} + H⁺)



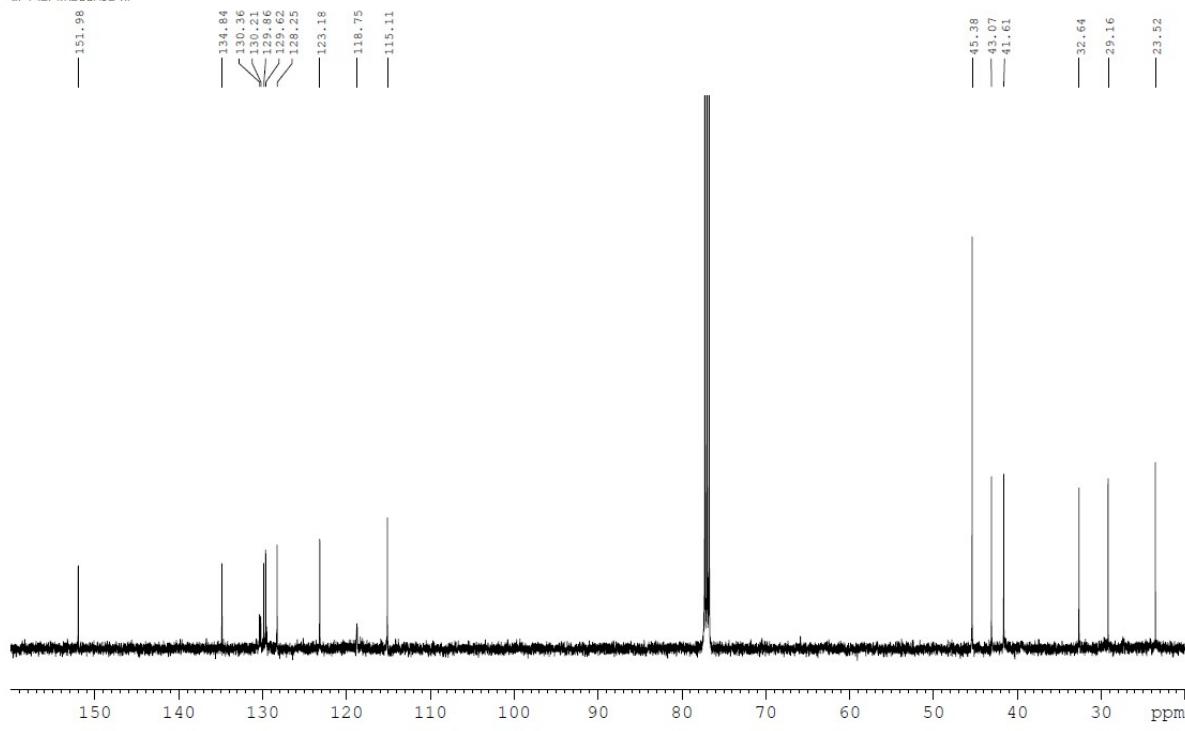
ESI-MS (*m/z*): 334 (DA_{1.5} - H⁺)

Instrument: Bruker AvanceIII 500MHz (UnivBucuresti)
Operator: CS
Report No.: 2188
User: G. Ionita
Sample Changer Position 13
Sample name: MAD_5
@H1-BBOF-34 CDCl3 (D:\UnivBuc\PIonita) ICON-NMR-Lab 5

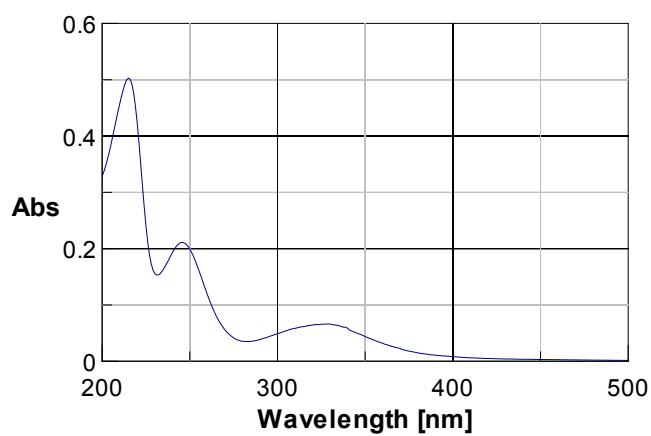


^1H NMR spectrum of compound DA_{1.5}

Instrument Bruker AvanceIII 500MHz (UnivBucuresti)
Operator CS
Registry No. 2188
User G. Ionita
Sample Changer Position 13
Sample name: MAD-5
CDCl₃
g:/12_cnmr_boxe_2A

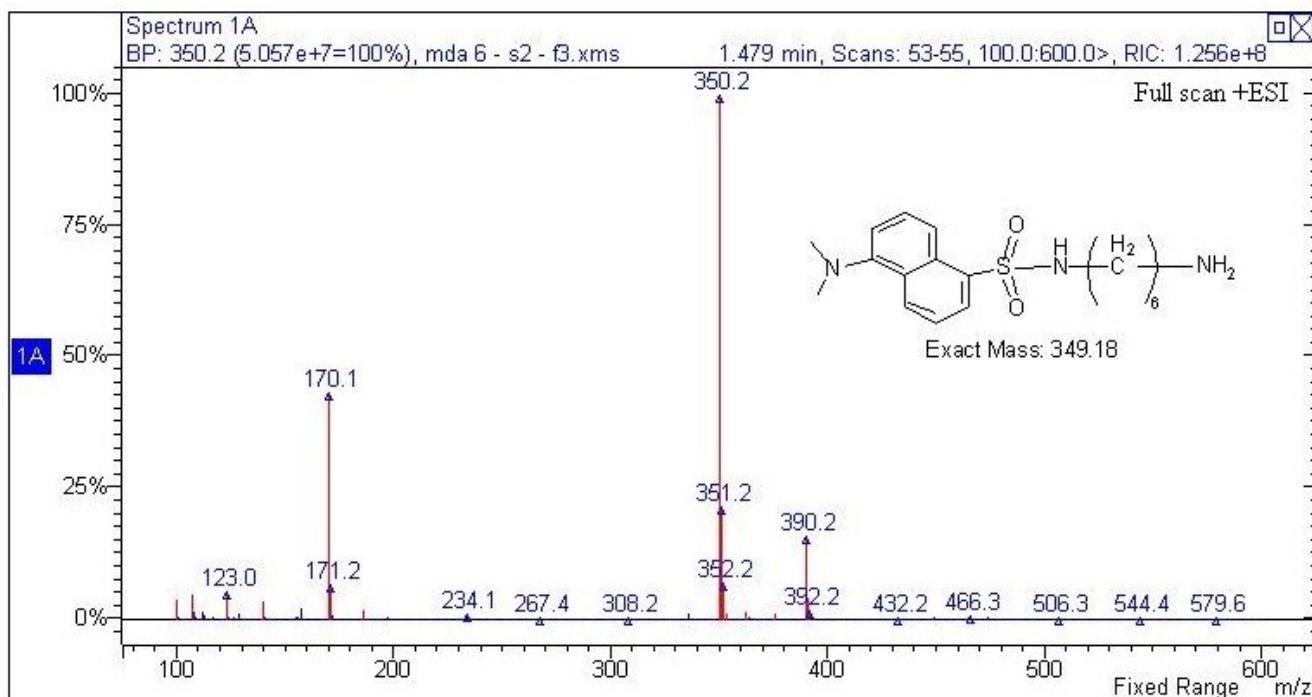


¹³C NMR spectrum of compound DA_{1.5}

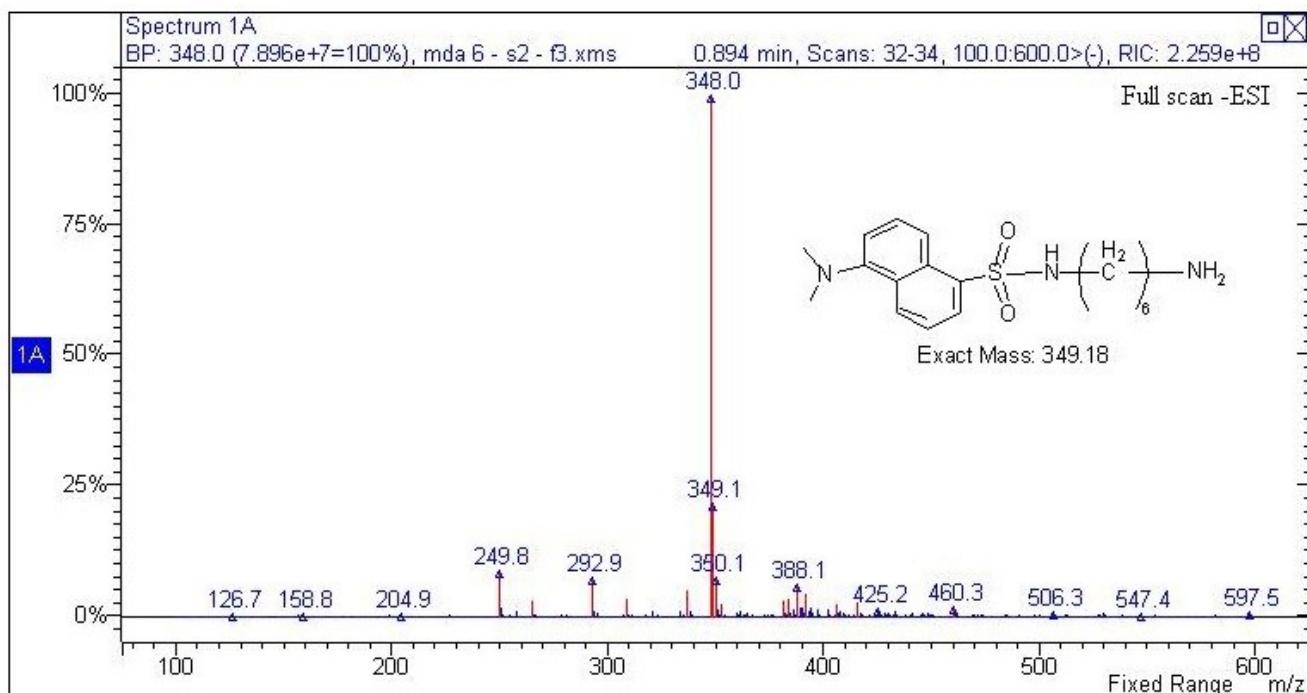


UV-Vis spectrum of compound DA_{1.5}

DA_{1.6} (dansyl 1,6-diaminohexane)

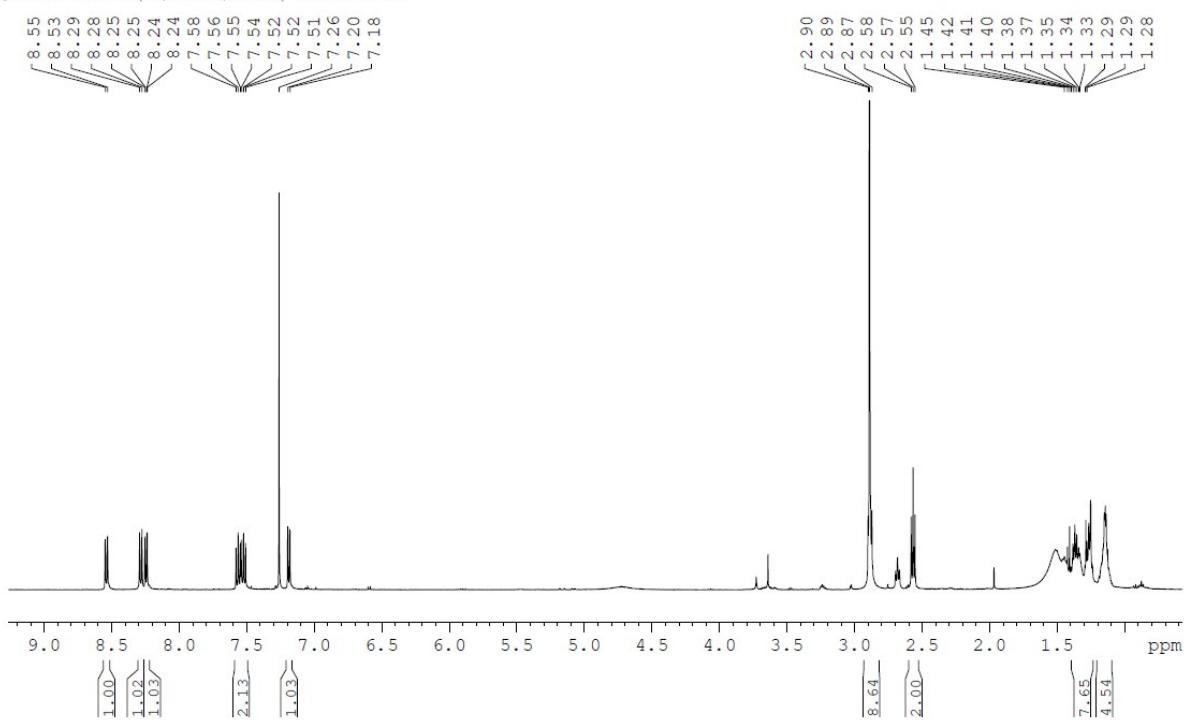


ESI-MS (*m/z*): 350 (DA_{1.6} + H⁺)



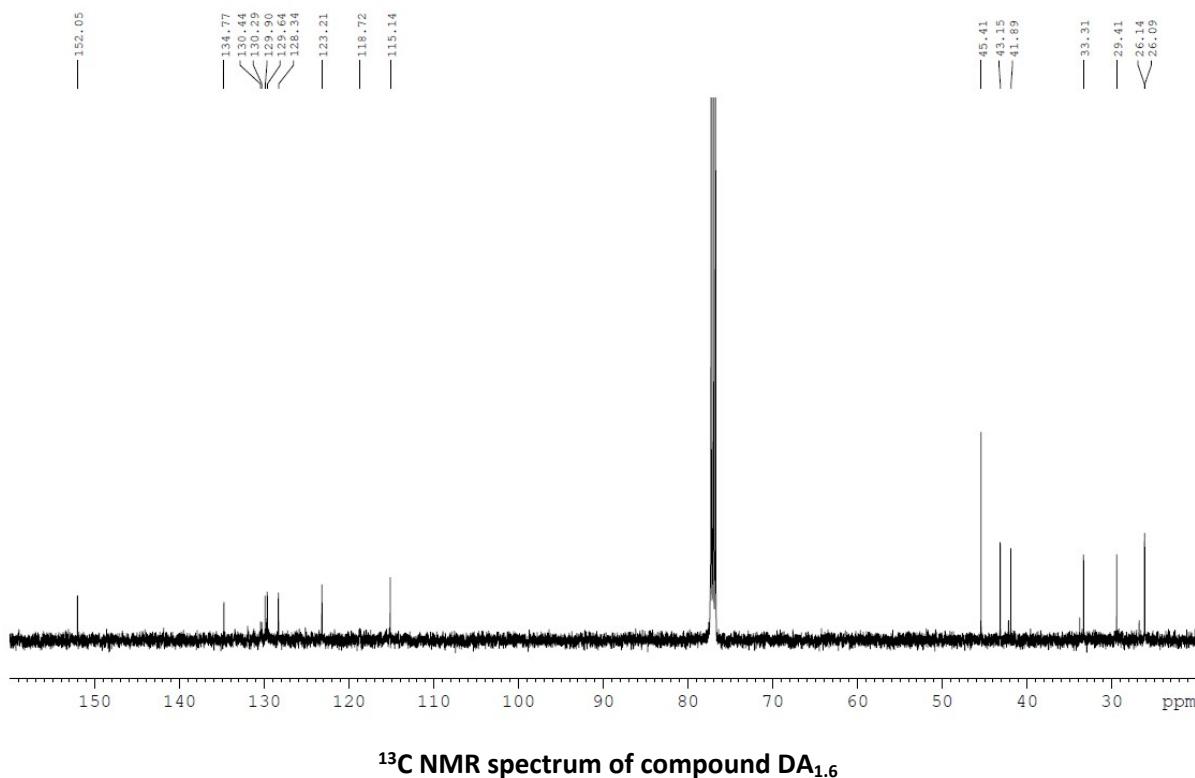
ESI-MS (*m/z*): 348 (DA_{1.6} - H⁺)

Instrument Bruker AvanceIII 500MHz (UnivBucuresti)
Operator CS
Ref ID: 2189
User G. Ionita
Sample Changer Position 6
Sample name: MAD_6
@H1-BBOF-34 CDCl3 (D:\UnivBuc\Plonita) ICON-NMR-Lab 5

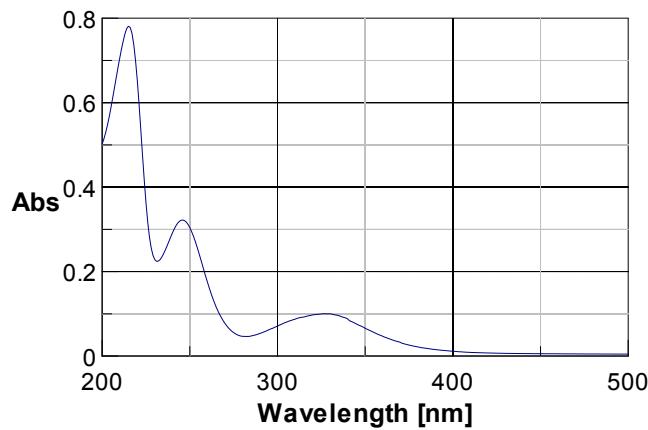


¹H NMR spectrum of compound DA_{1.6}

Instrument Bruker AvanceIII 500MHz (UnivBucuresti)
Operator CS
Registry No. 2189
User G. Ionita
Sample Changer Position 6
Sample name: MAD-6
CDCl₃
5012-0000-0000-2A

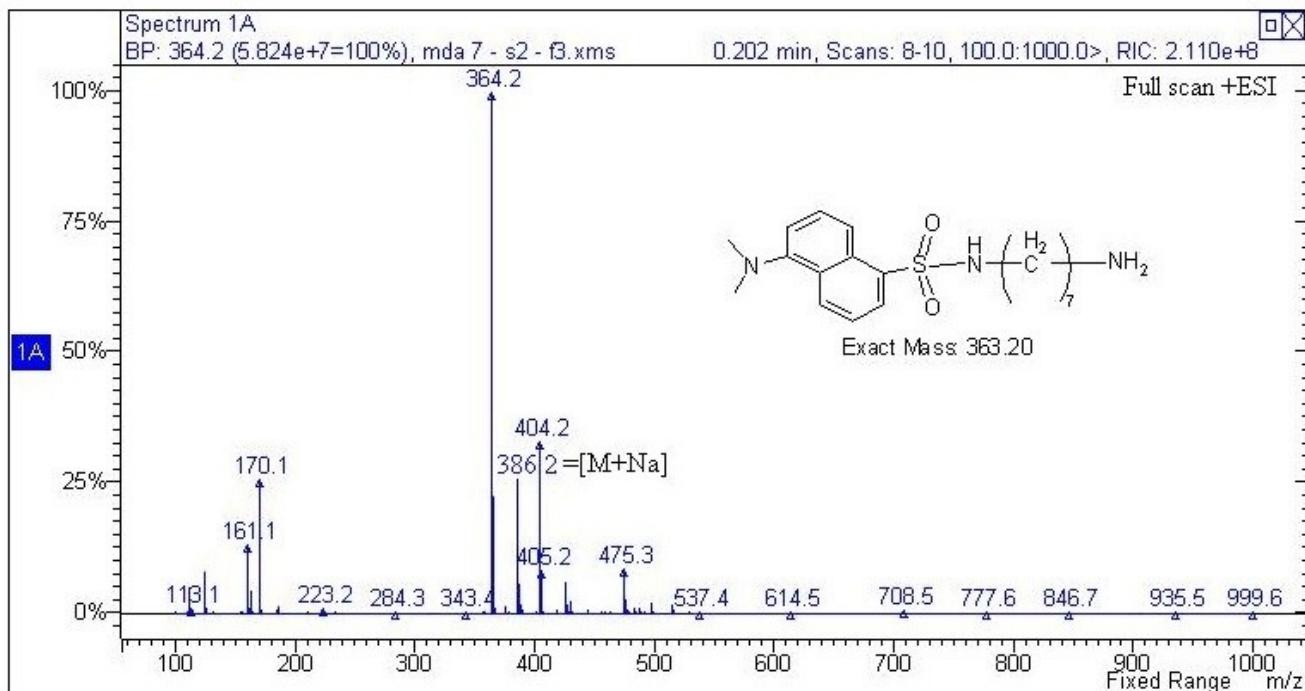


¹³C NMR spectrum of compound DA_{1.6}

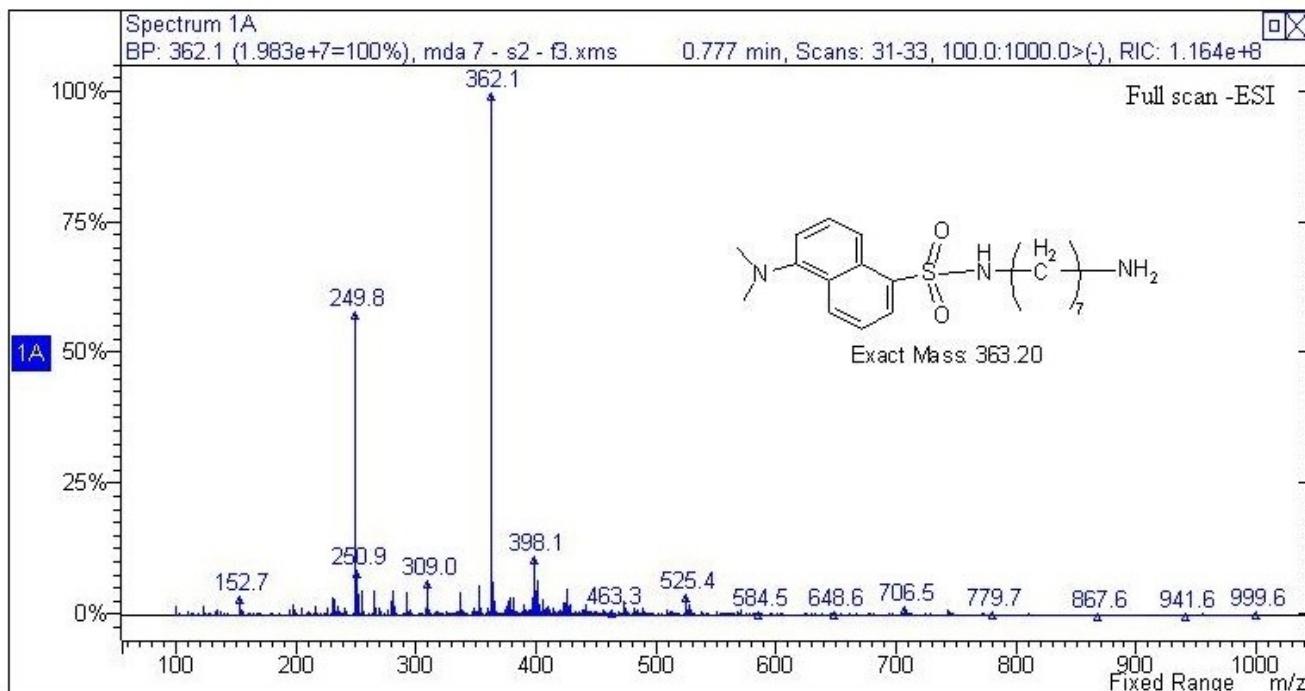


UV-Vis spectrum of compound DA_{1.6}

DA_{1.7} (dansyl 1,7-diaminoheptane)



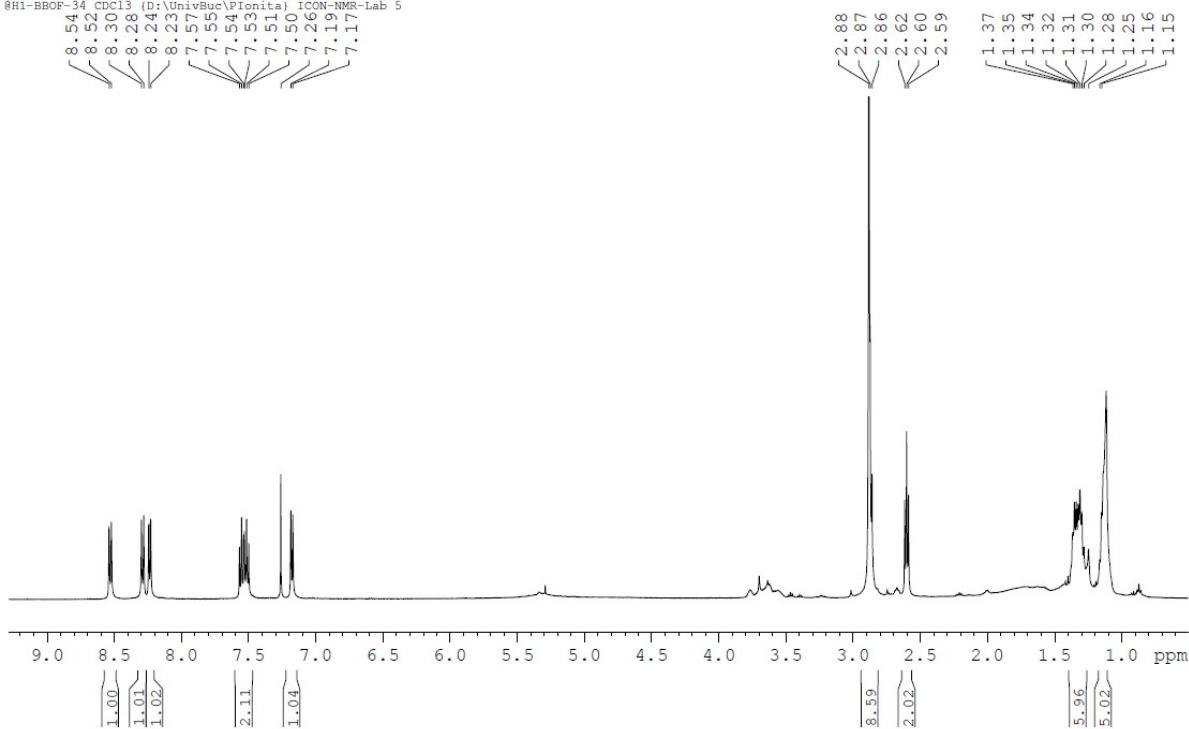
ESI-MS (*m/z*): 364 (DA_{1.7} + H⁺)



ESI-MS (*m/z*): 362 (DA_{1.7} - H⁺)

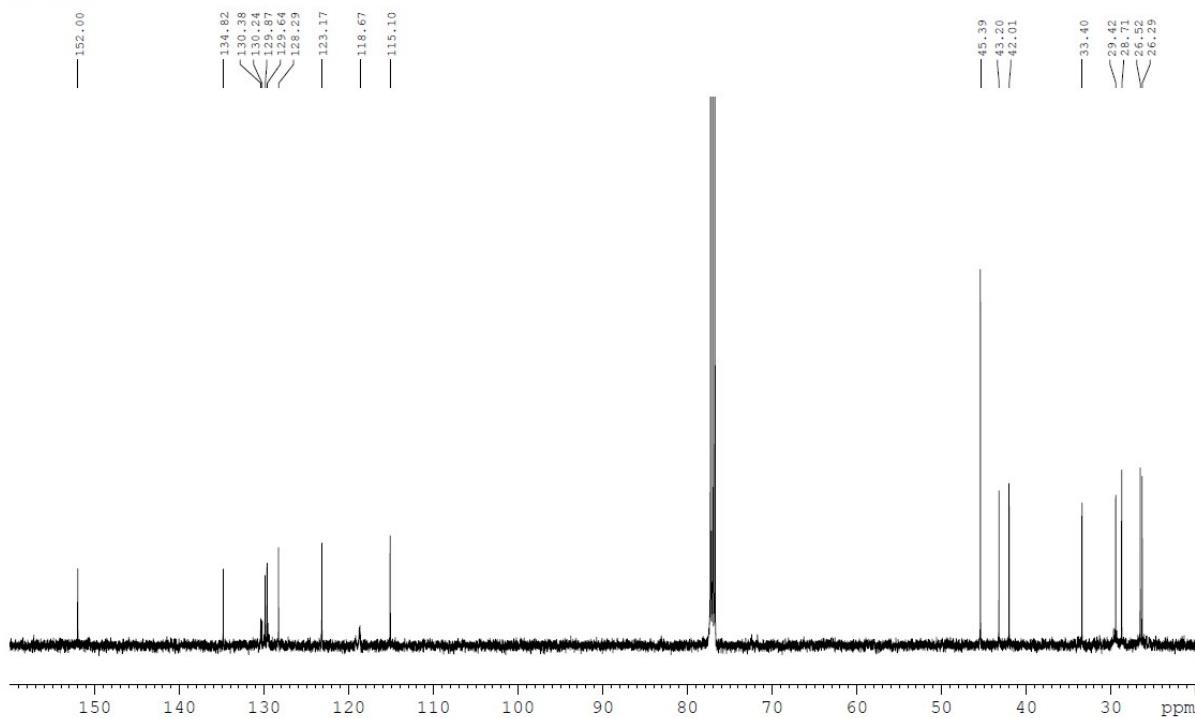
Instrument Bruker AvanceIII 500MHz (UnivBucuresti)
Operator CS
Registry No. 2190
User G. Ionita
Sample Changer Position 11
Sample name: MAD-7

@H1-BBOF-34 CDC13 (D:\UnivBuc\Plionita) ICON-NMR-Lab 5
54 5.2 8.24 8.28 8.30 8.57 8.55 8.54 8.53 8.51 8.50 8.49 8.48 8.47 8.46 8.45 8.44 8.43 8.42 8.41 8.40 8.39 8.38 8.37 8.36 8.35 8.34 8.33 8.32 8.31 8.30 8.29 8.28 8.27 8.26 8.25 8.24 8.23 8.22 8.21 8.20 8.19 8.18 8.17 8.16 8.15 8.14 8.13 8.12 8.11 8.10 8.09 8.08 8.07 8.06 8.05 8.04 8.03 8.02 8.01 8.00 7.99 7.98 7.97 7.96 7.95 7.94 7.93 7.92 7.91 7.90 7.89 7.88 7.87 7.86 7.85 7.84 7.83 7.82 7.81 7.80 7.79 7.78 7.77 7.76 7.75 7.74 7.73 7.72 7.71 7.70 7.69 7.68 7.67 7.66 7.65 7.64 7.63 7.62 7.61 7.60 7.59 7.58 7.57 7.56 7.55 7.54 7.53 7.52 7.51 7.50 7.49 7.48 7.47 7.46 7.45 7.44 7.43 7.42 7.41 7.40 7.39 7.38 7.37 7.36 7.35 7.34 7.33 7.32 7.31 7.30 7.29 7.28 7.27 7.26 7.25 7.24 7.23 7.22 7.21 7.20 7.19 7.18 7.17 7.16 7.15 7.14 7.13 7.12 7.11 7.10 7.09 7.08 7.07 7.06 7.05 7.04 7.03 7.02 7.01 7.00 6.99 6.98 6.97 6.96 6.95 6.94 6.93 6.92 6.91 6.90 6.89 6.88 6.87 6.86 6.85 6.84 6.83 6.82 6.81 6.80 6.79 6.78 6.77 6.76 6.75 6.74 6.73 6.72 6.71 6.70 6.69 6.68 6.67 6.66 6.65 6.64 6.63 6.62 6.61 6.60 6.59 6.58 6.57 6.56 6.55 6.54 6.53 6.52 6.51 6.50 6.49 6.48 6.47 6.46 6.45 6.44 6.43 6.42 6.41 6.40 6.39 6.38 6.37 6.36 6.35 6.34 6.33 6.32 6.31 6.30 6.29 6.28 6.27 6.26 6.25 6.24 6.23 6.22 6.21 6.20 6.19 6.18 6.17 6.16 6.15 6.14 6.13 6.12 6.11 6.10 6.09 6.08 6.07 6.06 6.05 6.04 6.03 6.02 6.01 6.00 5.99 5.98 5.97 5.96 5.95 5.94 5.93 5.92 5.91 5.90 5.89 5.88 5.87 5.86 5.85 5.84 5.83 5.82 5.81 5.80 5.79 5.78 5.77 5.76 5.75 5.74 5.73 5.72 5.71 5.70 5.69 5.68 5.67 5.66 5.65 5.64 5.63 5.62 5.61 5.60 5.59 5.58 5.57 5.56 5.55 5.54 5.53 5.52 5.51 5.50 5.49 5.48 5.47 5.46 5.45 5.44 5.43 5.42 5.41 5.40 5.39 5.38 5.37 5.36 5.35 5.34 5.33 5.32 5.31 5.30 5.29 5.28 5.27 5.26 5.25 5.24 5.23 5.22 5.21 5.20 5.19 5.18 5.17 5.16 5.15 5.14 5.13 5.12 5.11 5.10 5.09 5.08 5.07 5.06 5.05 5.04 5.03 5.02 5.01 5.00 4.99 4.98 4.97 4.96 4.95 4.94 4.93 4.92 4.91 4.90 4.89 4.88 4.87 4.86 4.85 4.84 4.83 4.82 4.81 4.80 4.79 4.78 4.77 4.76 4.75 4.74 4.73 4.72 4.71 4.70 4.69 4.68 4.67 4.66 4.65 4.64 4.63 4.62 4.61 4.60 4.59 4.58 4.57 4.56 4.55 4.54 4.53 4.52 4.51 4.50 4.49 4.48 4.47 4.46 4.45 4.44 4.43 4.42 4.41 4.40 4.39 4.38 4.37 4.36 4.35 4.34 4.33 4.32 4.31 4.30 4.29 4.28 4.27 4.26 4.25 4.24 4.23 4.22 4.21 4.20 4.19 4.18 4.17 4.16 4.15 4.14 4.13 4.12 4.11 4.10 4.09 4.08 4.07 4.06 4.05 4.04 4.03 4.02 4.01 4.00 3.99 3.98 3.97 3.96 3.95 3.94 3.93 3.92 3.91 3.90 3.89 3.88 3.87 3.86 3.85 3.84 3.83 3.82 3.81 3.80 3.79 3.78 3.77 3.76 3.75 3.74 3.73 3.72 3.71 3.70 3.69 3.68 3.67 3.66 3.65 3.64 3.63 3.62 3.61 3.60 3.59 3.58 3.57 3.56 3.55 3.54 3.53 3.52 3.51 3.50 3.49 3.48 3.47 3.46 3.45 3.44 3.43 3.42 3.41 3.40 3.39 3.38 3.37 3.36 3.35 3.34 3.33 3.32 3.31 3.30 3.29 3.28 3.27 3.26 3.25 3.24 3.23 3.22 3.21 3.20 3.19 3.18 3.17 3.16 3.15 3.14 3.13 3.12 3.11 3.10 3.09 3.08 3.07 3.06 3.05 3.04 3.03 3.02 3.01 3.00 2.99 2.98 2.97 2.96 2.95 2.94 2.93 2.92 2.91 2.90 2.89 2.88 2.87 2.86 2.85 2.84 2.83 2.82 2.81 2.80 2.79 2.78 2.77 2.76 2.75 2.74 2.73 2.72 2.71 2.70 2.69 2.68 2.67 2.66 2.65 2.64 2.63 2.62 2.61 2.60 2.59 2.58 2.57 2.56 2.55 2.54 2.53 2.52 2.51 2.50 2.49 2.48 2.47 2.46 2.45 2.44 2.43 2.42 2.41 2.40 2.39 2.38 2.37 2.36 2.35 2.34 2.33 2.32 2.31 2.30 2.29 2.28 2.27 2.26 2.25 2.24 2.23 2.22 2.21 2.20 2.19 2.18 2.17 2.16 2.15 2.14 2.13 2.12 2.11 2.10 2.09 2.08 2.07 2.06 2.05 2.04 2.03 2.02 2.01 2.00 1.99 1.98 1.97 1.96 1.95 1.94 1.93 1.92 1.91 1.90 1.89 1.88 1.87 1.86 1.85 1.84 1.83 1.82 1.81 1.80 1.79 1.78 1.77 1.76 1.75 1.74 1.73 1.72 1.71 1.70 1.69 1.68 1.67 1.66 1.65 1.64 1.63 1.62 1.61 1.60 1.59 1.58 1.57 1.56 1.55 1.54 1.53 1.52 1.51 1.50 1.49 1.48 1.47 1.46 1.45 1.44 1.43 1.42 1.41 1.40 1.39 1.38 1.37 1.36 1.35 1.34 1.33 1.32 1.31 1.30 1.29 1.28 1.27 1.26 1.25 1.24 1.23 1.22 1.21 1.20 1.19 1.18 1.17 1.16 1.15 1.14 1.13 1.12 1.11 1.10 1.09 1.08 1.07 1.06 1.05 1.04 1.03 1.02 1.01 1.00 0.99 0.98 0.97 0.96 0.95 0.94 0.93 0.92 0.91 0.90 0.89 0.88 0.87 0.86 0.85 0.84 0.83 0.82 0.81 0.80 0.79 0.78 0.77 0.76 0.75 0.74 0.73 0.72 0.71 0.70 0.69 0.68 0.67 0.66 0.65 0.64 0.63 0.62 0.61 0.60 0.59 0.58 0.57 0.56 0.55 0.54 0.53 0.52 0.51 0.50 0.49 0.48 0.47 0.46 0.45 0.44 0.43 0.42 0.41 0.40 0.39 0.38 0.37 0.36 0.35 0.34 0.33 0.32 0.31 0.30 0.29 0.28 0.27 0.26 0.25 0.24 0.23 0.22 0.21 0.20 0.19 0.18 0.17 0.16 0.15 0.14 0.13 0.12 0.11 0.10 0.09 0.08 0.07 0.06 0.05 0.04 0.03 0.02 0.01 0.00

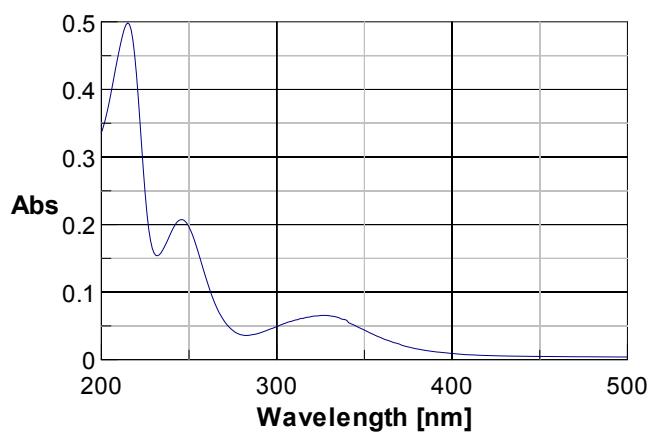


¹H NMR spectrum of compound DA_{1.7}

Instrument Bruker AvanceIII 500MHz (UnivBucuresti)
Operator CS
Registration No. 2190
User G. Ionita
Sample Changer Position 11
Sample name: MAD-7
CDCl₃
0.123_mml_bone_2A

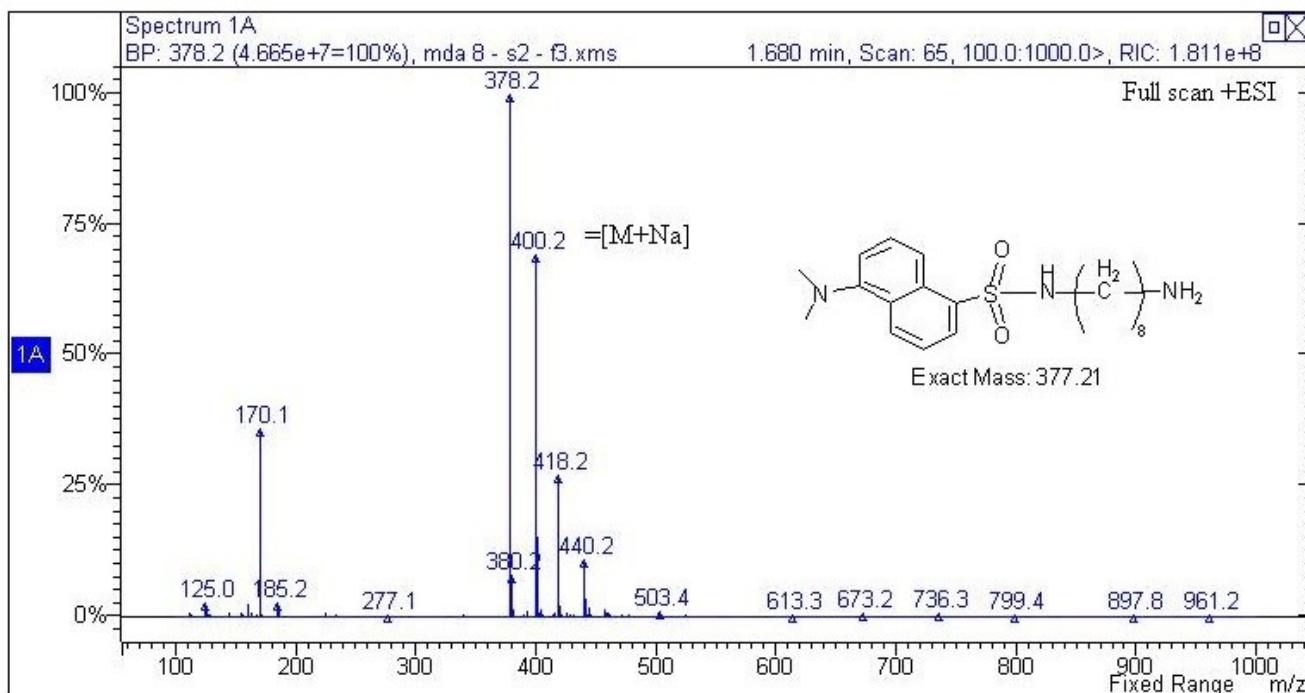


¹³C NMR spectrum of compound DA_{1.7}

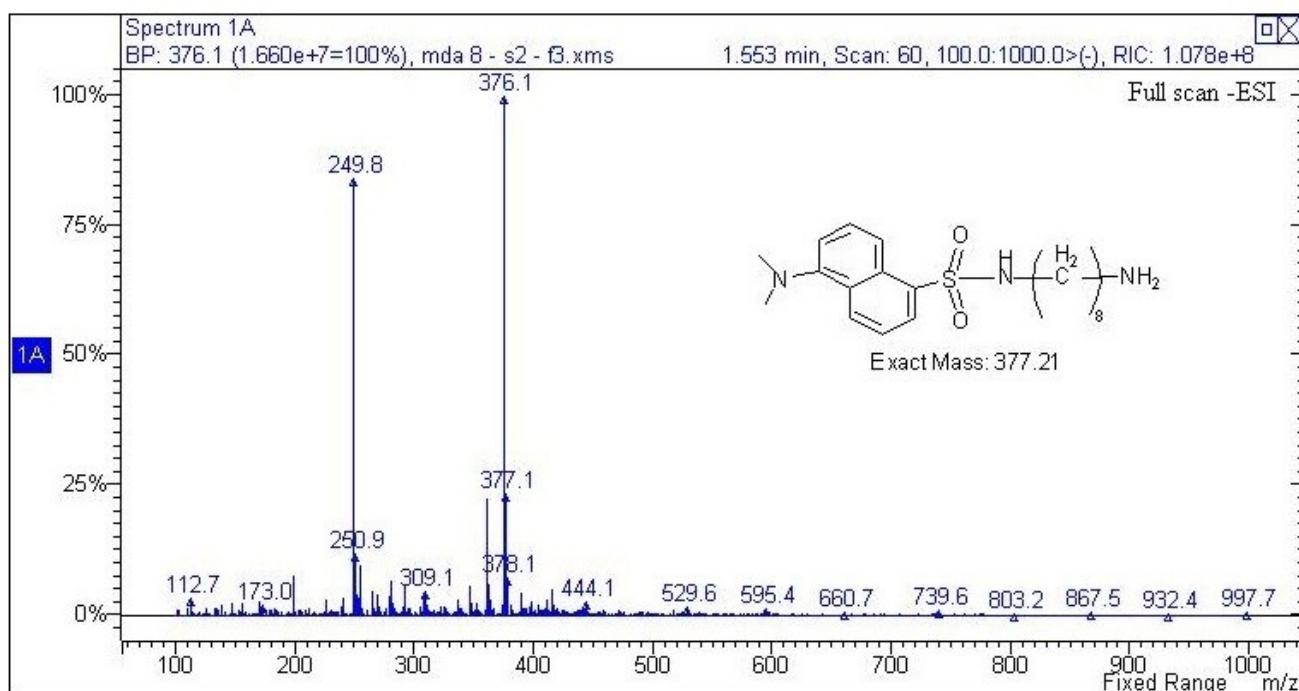


UV-Vis spectrum of compound DA_{1.7}

DA_{1.8} (dansyl 1,8-diaminoctane)

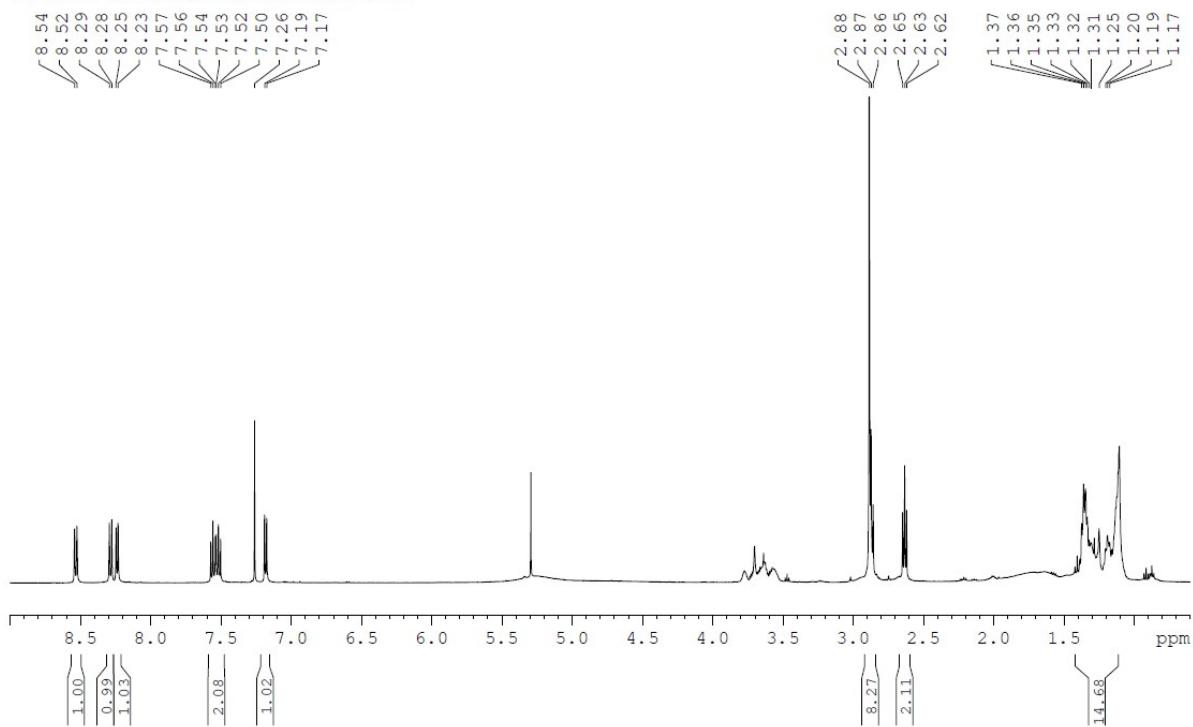


ESI-MS (*m/z*): 378 (DA_{1.8} + H⁺)



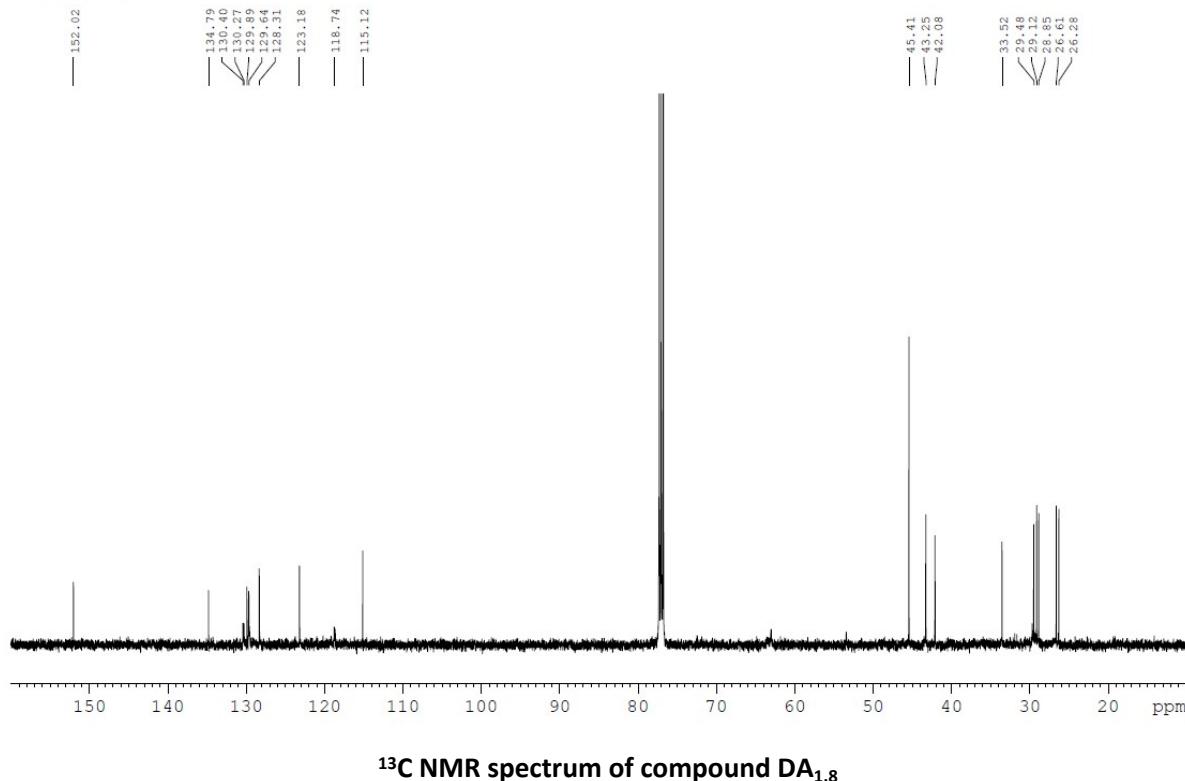
ESI-MS (*m/z*): 376 (DA_{1.8} - H⁺)

Instrument Bruker AvanceIII 500MHz (UnivBucuresti)
Operator CS
Registry No. 2191
User G. Ionita
Sample Changer Position 4
Sample name: MA1.8
@H1-BBOF-34 CDCl₃ (D:\UnivBuc\PIonita) ICON-NMR-Lab 5

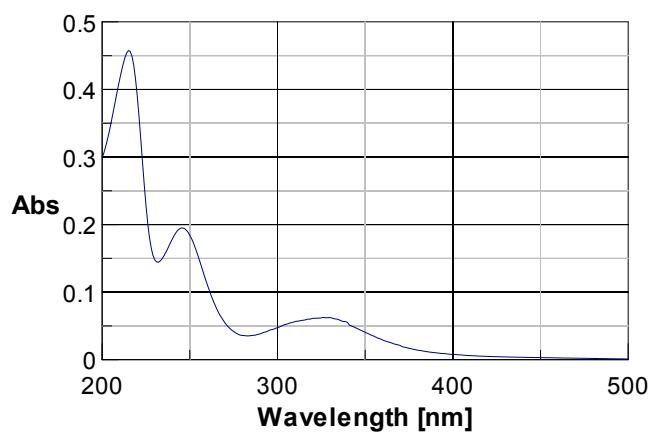


¹H NMR spectrum of compound DA_{1.8}

Instrument Bruker AvanceIII 500MHz (UnivBucuresti)
Operator CS
Registry No. 2191
User G. Ionita
Sample Changer Position 4
Sample name: MAD-8
CDCl₃
smt2_rnmn_ddone-2A

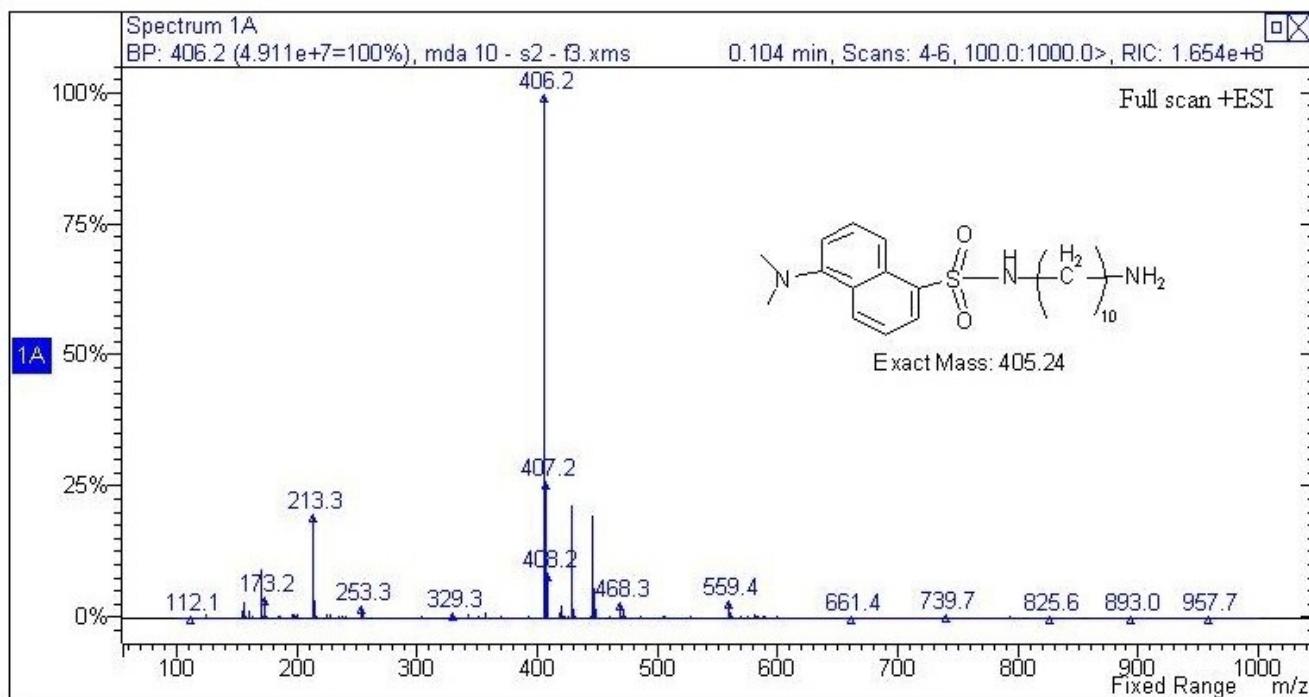


¹³C NMR spectrum of compound DA_{1.8}

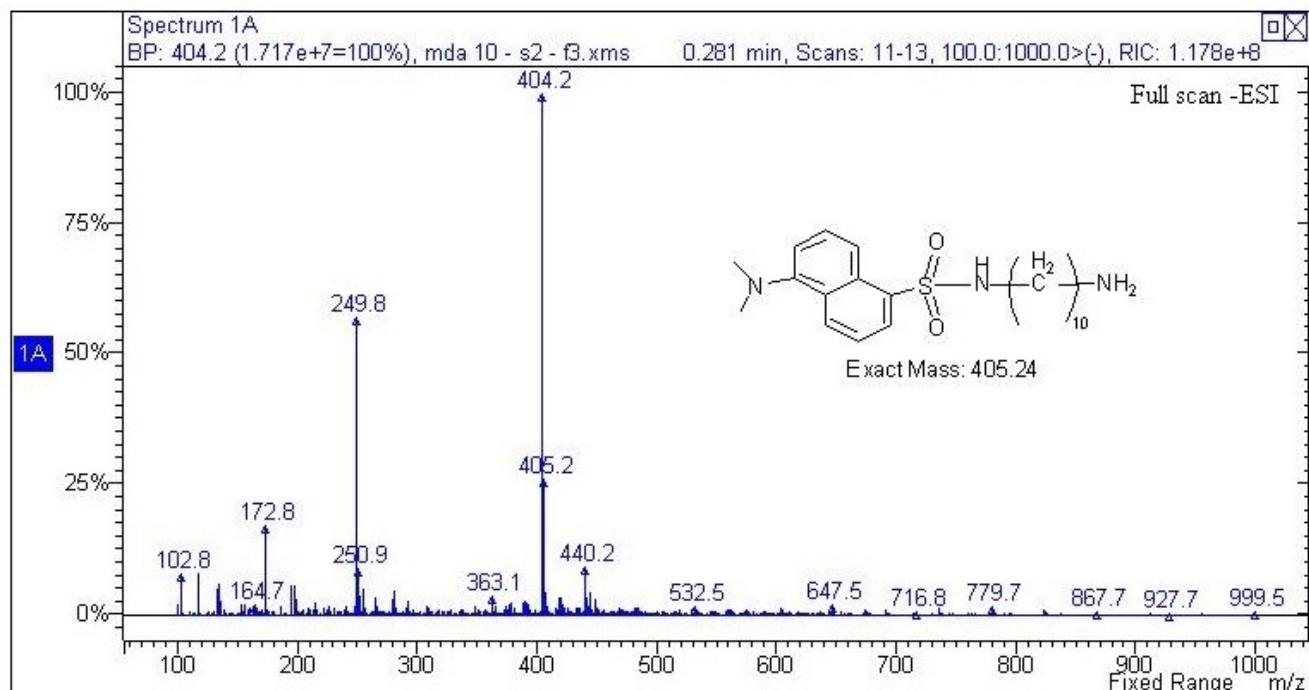


UV-Vis spectrum of compound DA_{1.8}

DA_{1.10} (dansyl 1,10-diaminodecane)

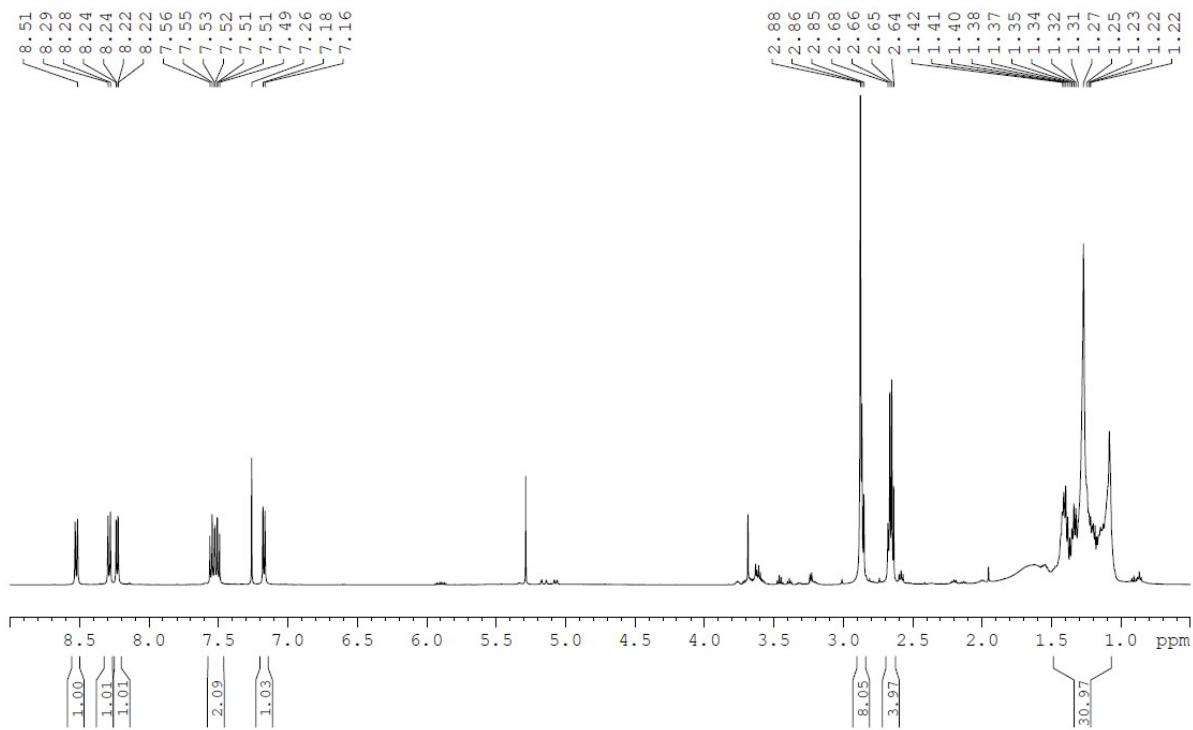


ESI-MS (*m/z*): 406 (DA_{1.10} + H⁺)



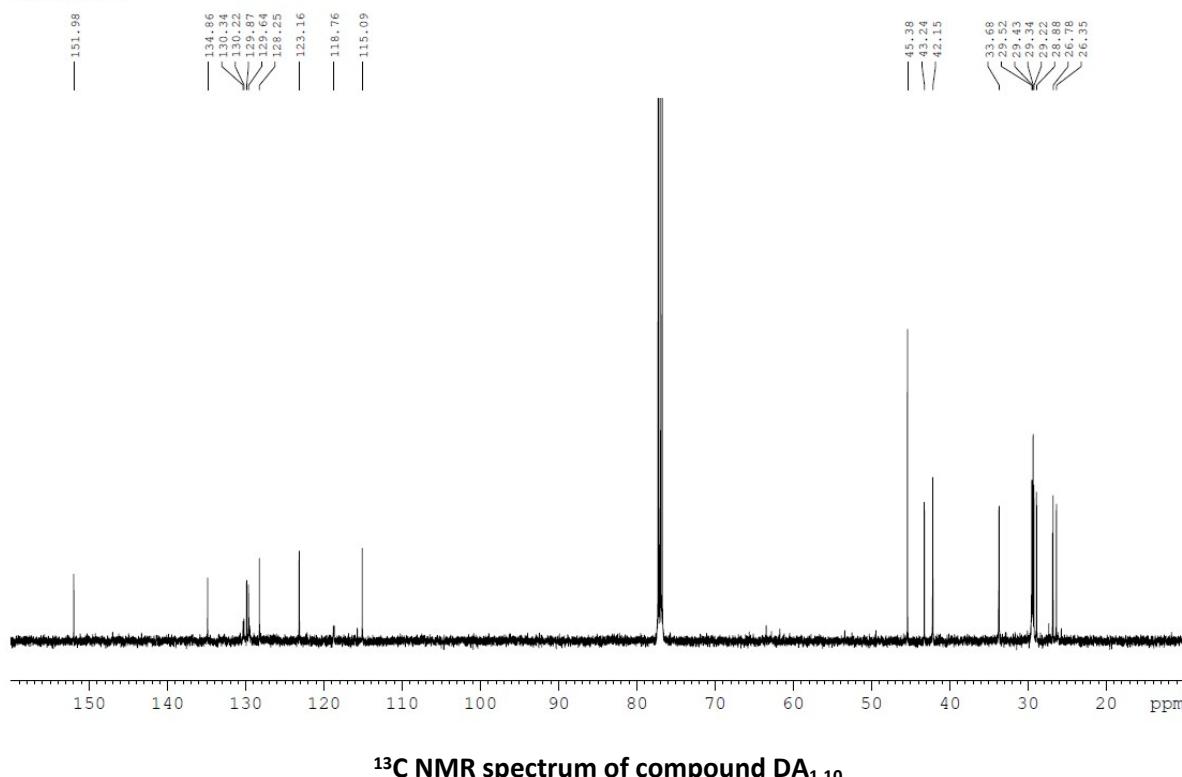
ESI-MS (*m/z*): 404 (DA_{1.10} - H⁺)

Instrument Bruker AvanceIII 500MHz (UnivBucuresti)
Operator CS
Registry No. 2192
User G. Ionita
Sample Changer Position 9
Sample name: MAD-10
@H1-RBOF-34 CDCl3 (D:\UnivBuc\Plionita) ICON-NMR-Lab 5

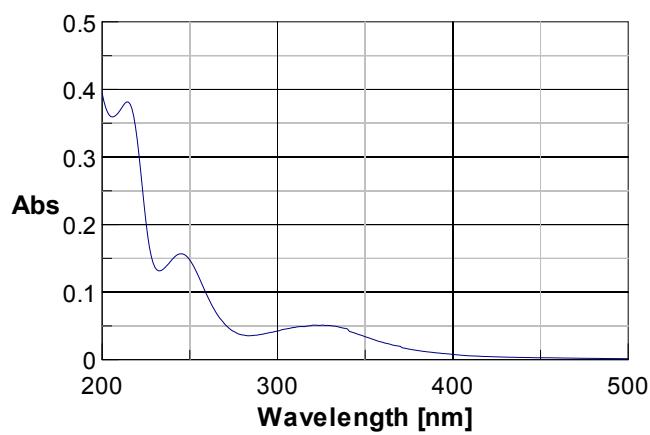


¹H NMR spectrum of compound DA_{1.10}

Instrument Bruker AvanceIII 500MHz (UnivBucuresti)
Operator CS
Registration 2192
User G. Ionita
Sample Changer Position 9
Sample name: MAD-10
CDCl₃
@C13-CPD-BBOF-34

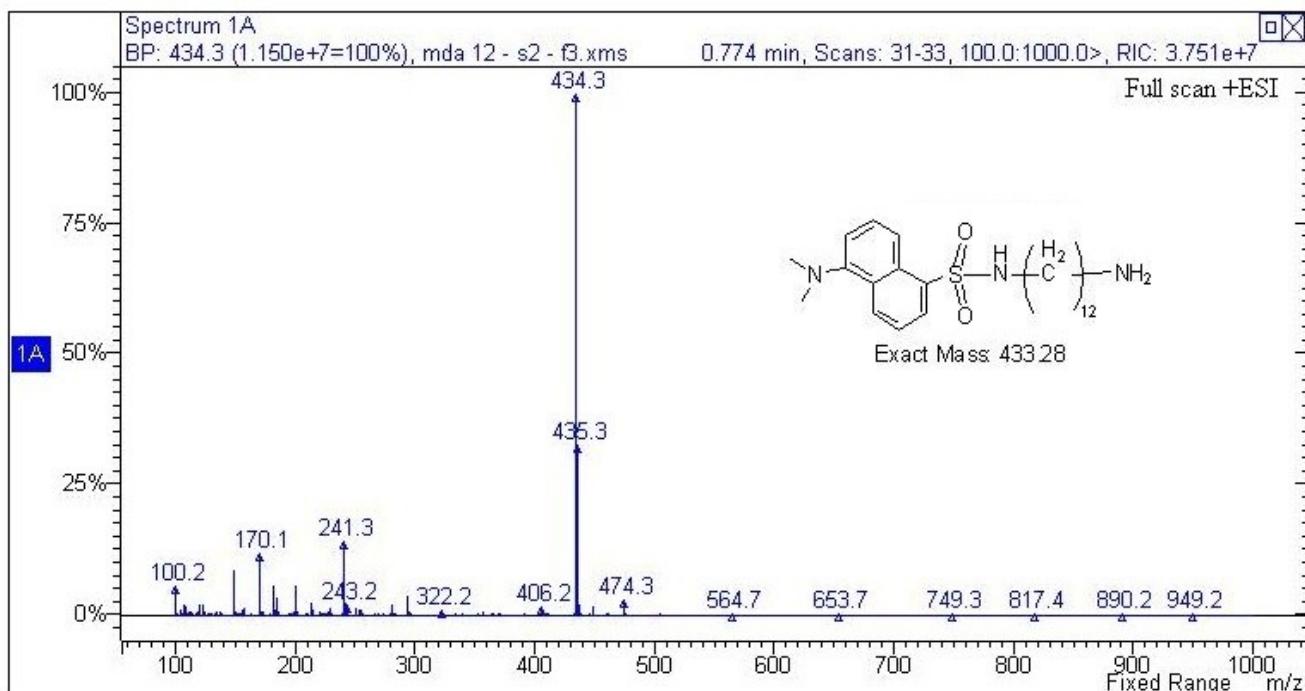


¹³C NMR spectrum of compound DA_{1.10}

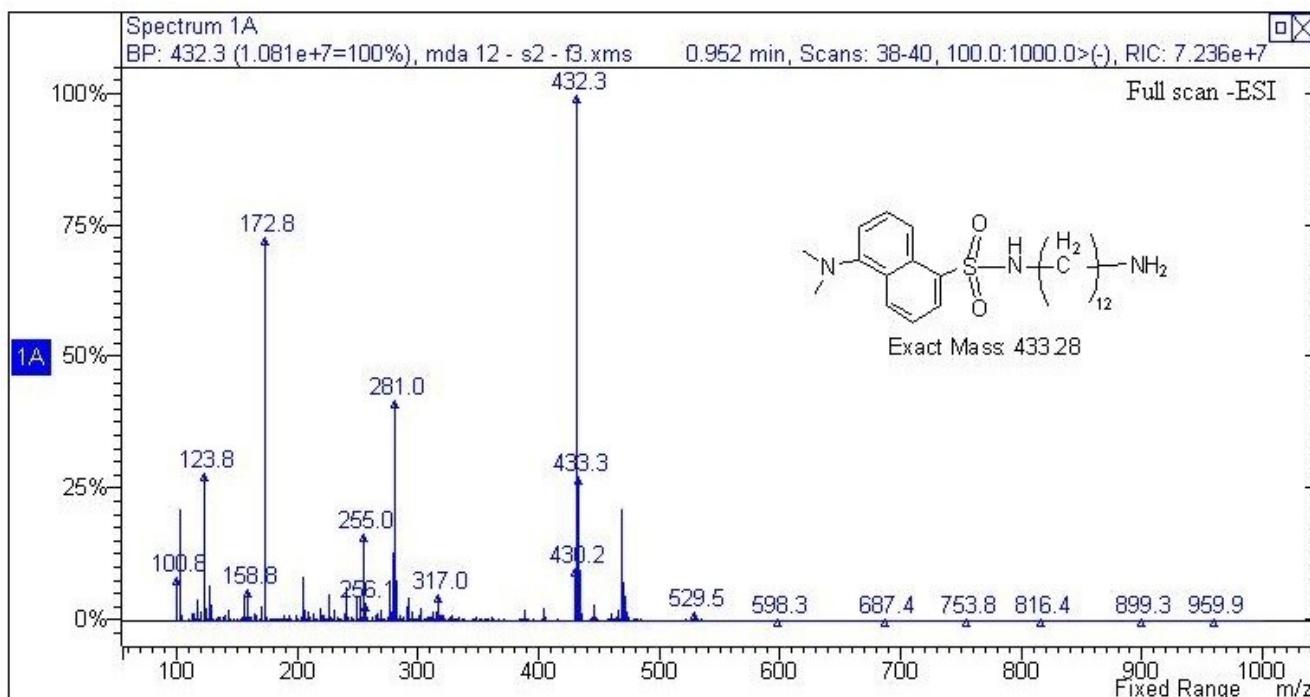


UV-Vis spectrum of compound DA_{1.10}

DA_{1.12} (dansyl 1,12-diaminododecane)

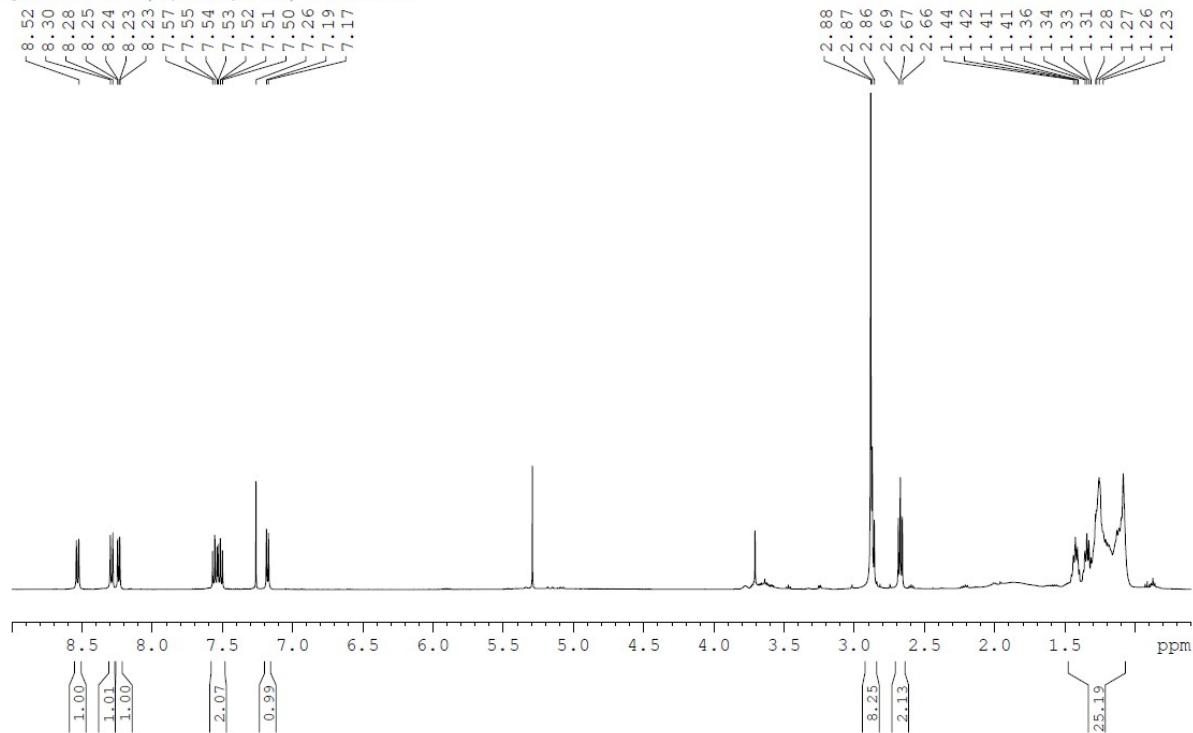


ESI-MS (*m/z*): 434 (DA_{1.12} +H⁺)



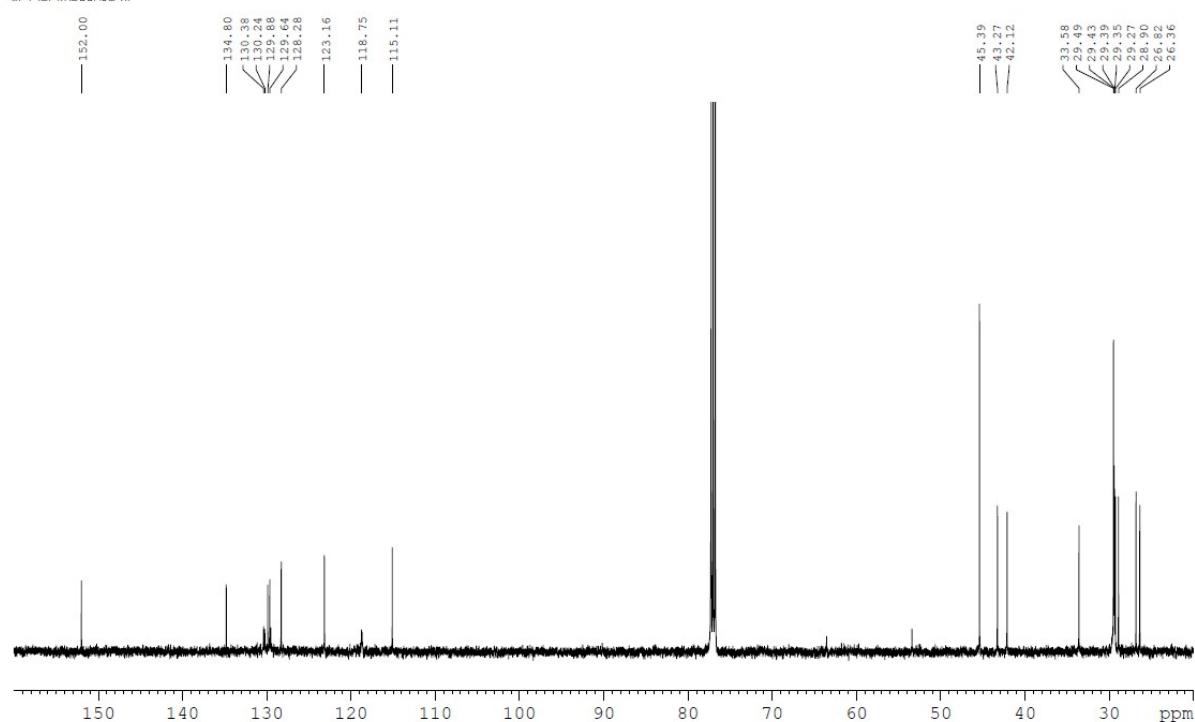
ESI-MS (*m/z*): 432 (DA_{1.12} - H⁺)

Instrument Bruker AvanceIII 500MHz (UnivBucuresti)
Operator CS
Registry No. 2193
User G. Ionita
Sample Changer Position 13
Sample name: MDA-12
@H1-BBOF-34 CDCl3 (D:\UnivBuc\Plionita) ICON-NMR-Lab 5

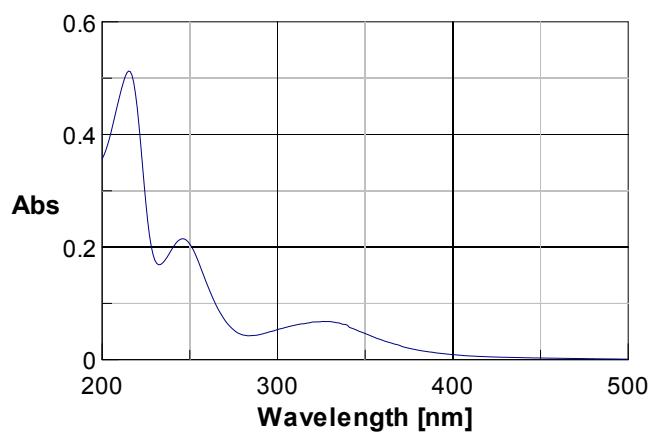


¹H NMR spectrum of compound DA_{1.12}

Instrument Bruker AvanceIII 500MHz (UnivBucuresti)
Operator CS
Registry No. 2193
User G. Ionita
Sample Changer Position 9
Sample name: MAD-12
CDCl₃
alpha-2,6-nona-2A



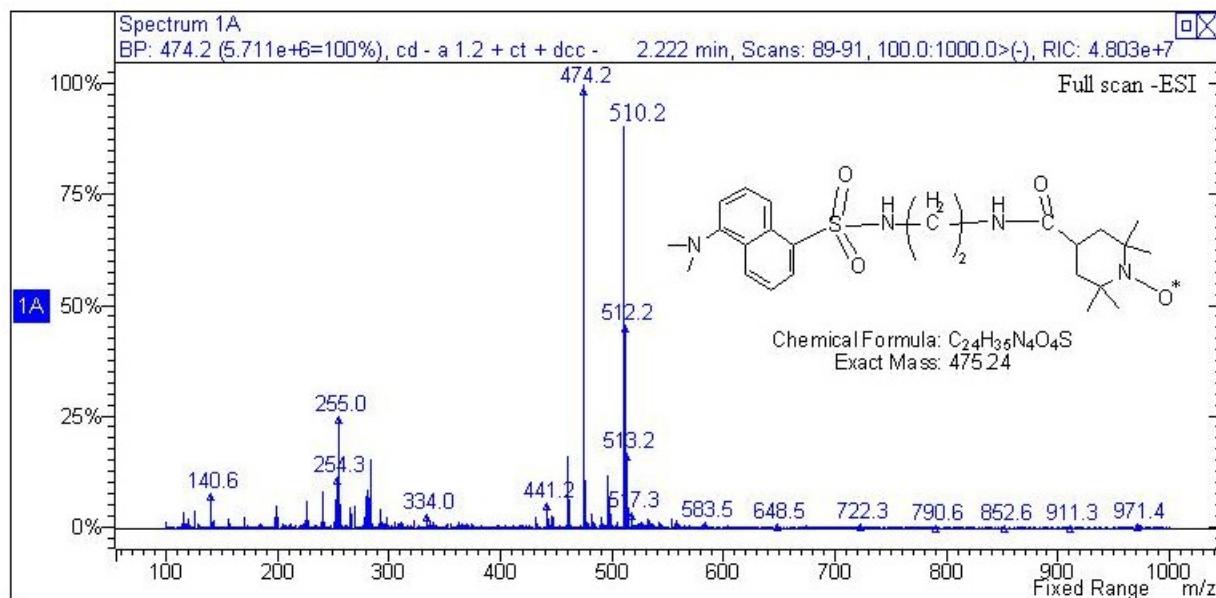
¹³C NMR spectrum of compound DA_{1.12}



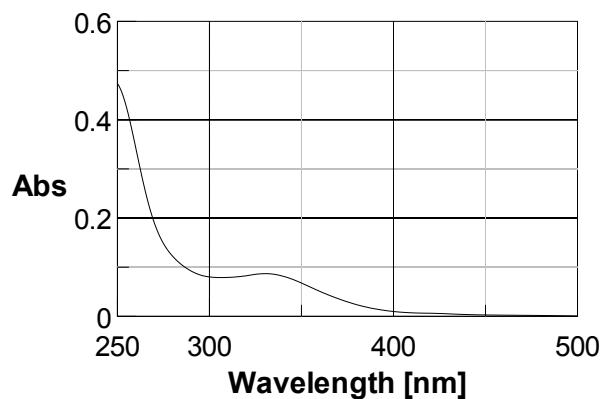
UV-Vis spectrum of compound DA_{1.12}

Spectral characterization of DA_{1,n}T

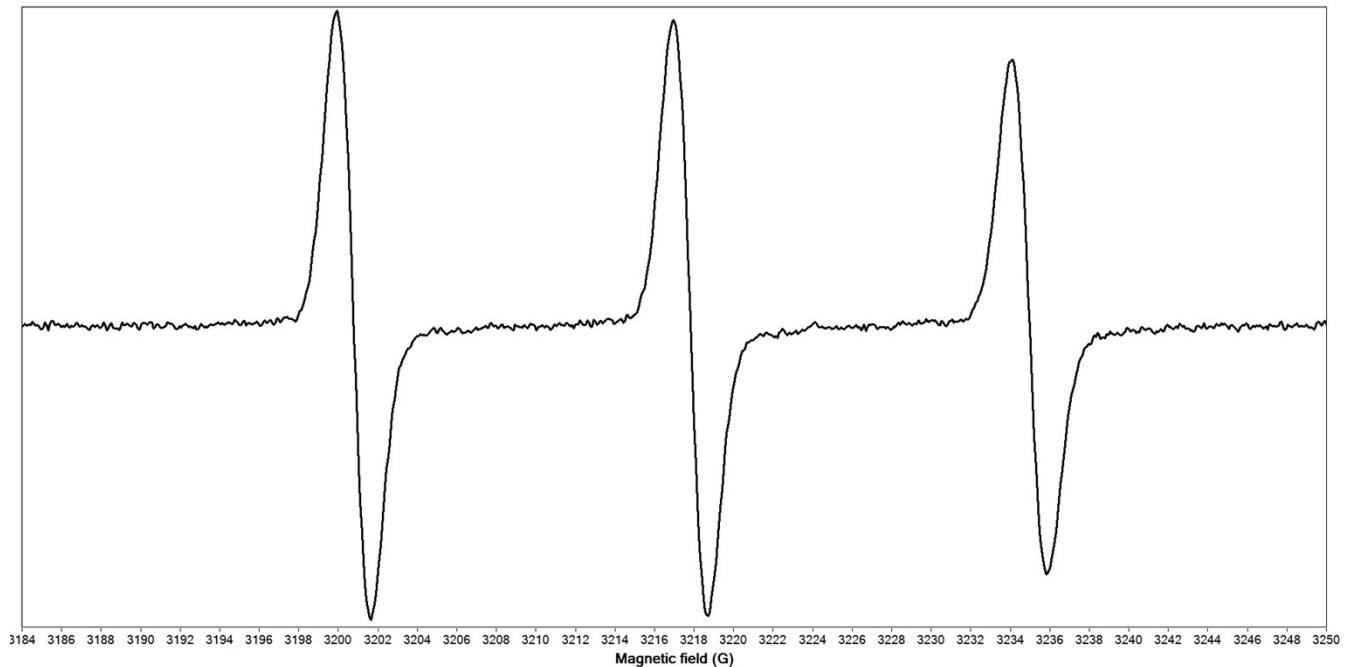
DA_{1,2}T



ESI-MS (*m/z*): 474 (DA_{1,2}T - H⁺)

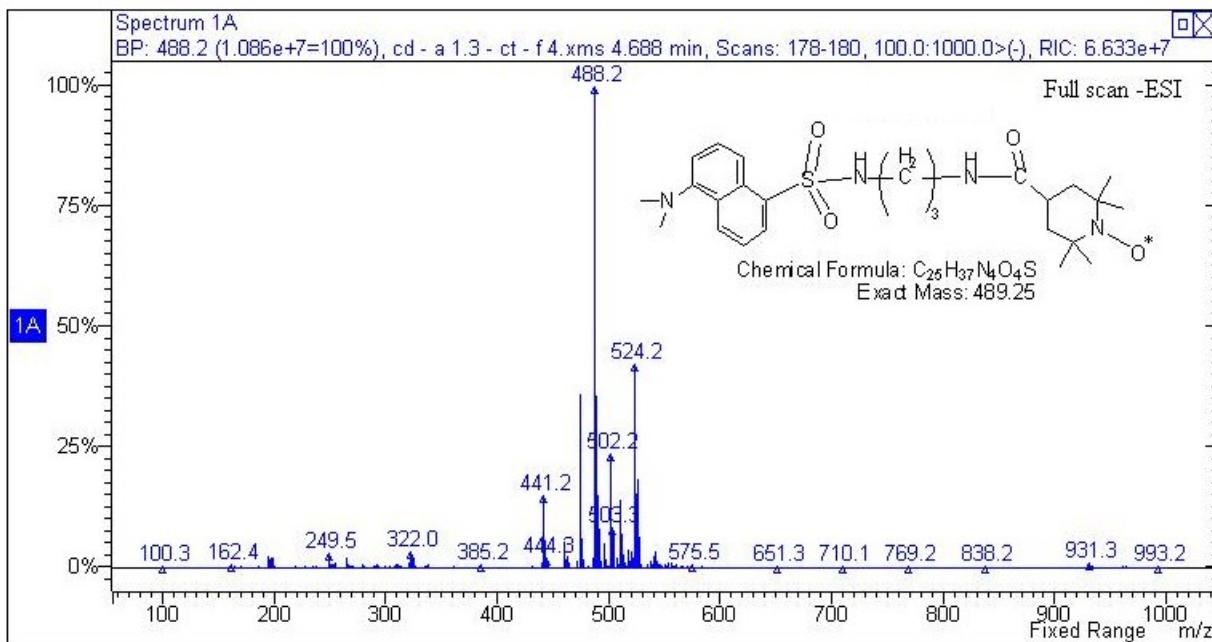


UV-Vis spectrum of compound DA_{1,2}T

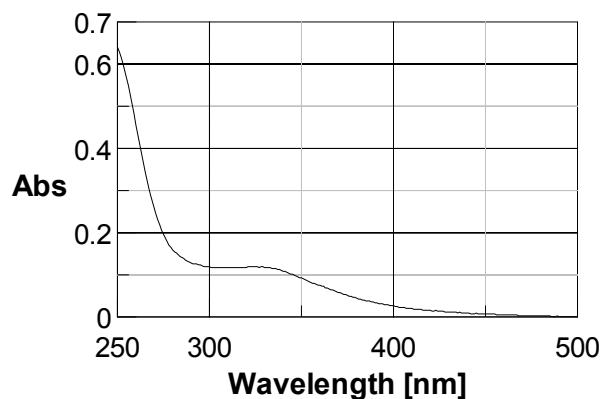


EPR spectrum of DA_{1.2}T

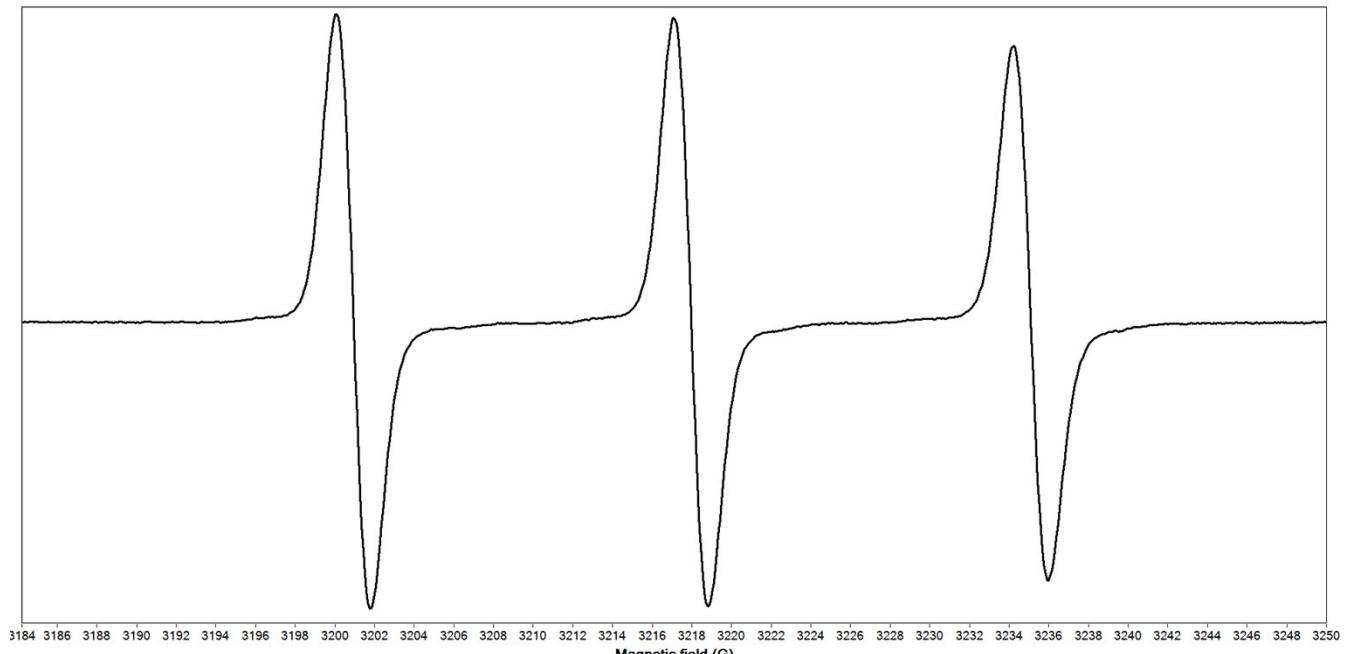
DA_{1.3}T



ESI-MS (*m/z*): 488 (DA_{1.3}T - H⁺)

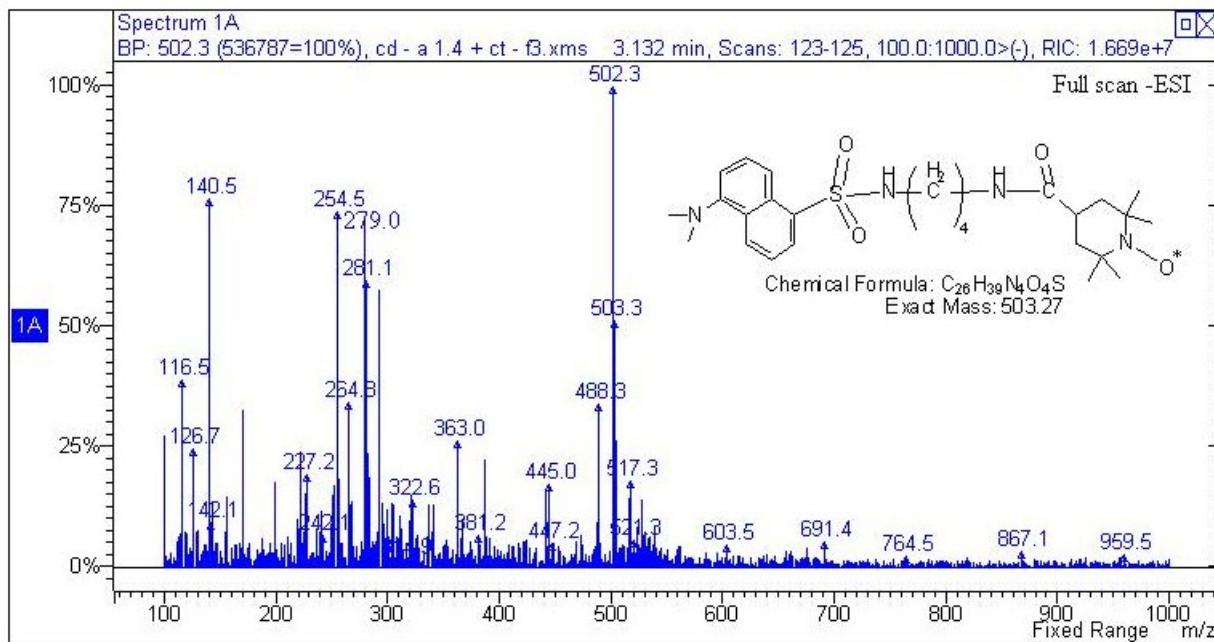


UV-Vis spectrum of compound DA_{1.3}T

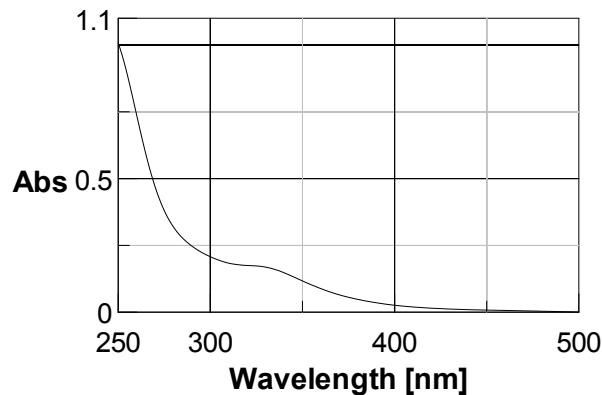


EPR spectrum of DA_{1.3}T

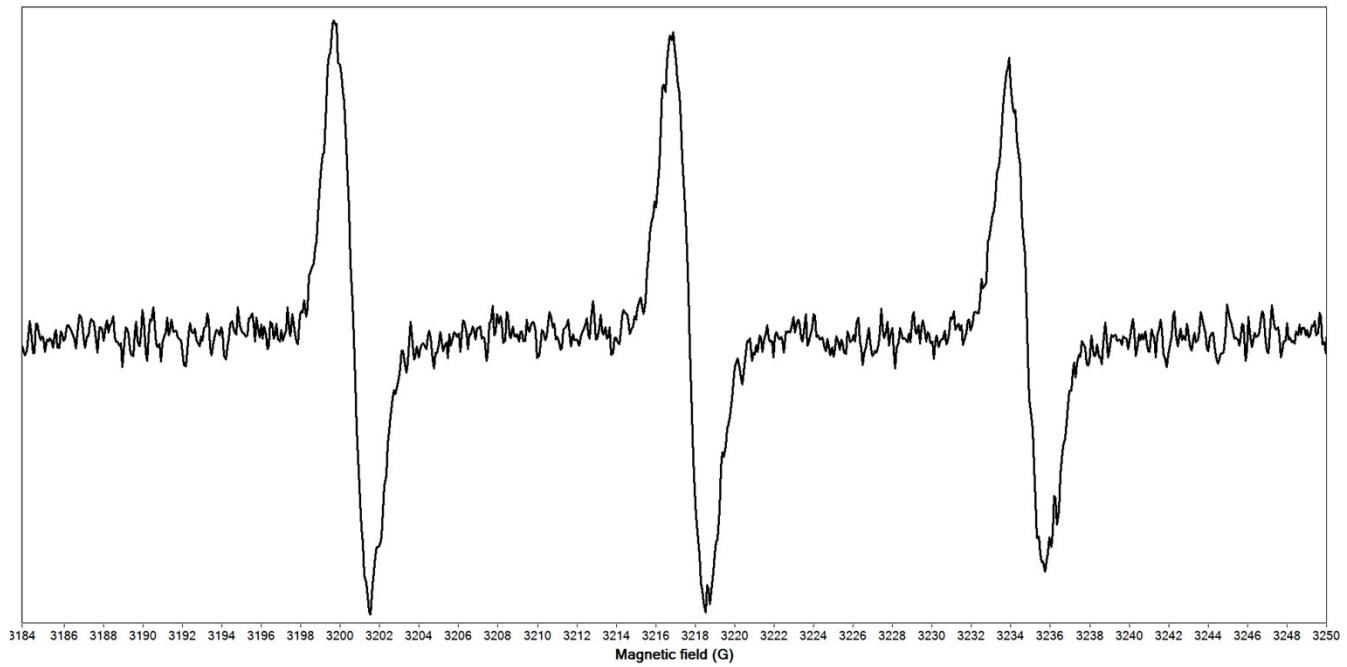
DA_{1.4}T



ESI-MS (*m/z*): 502 (DA_{1.4}T - H⁺)

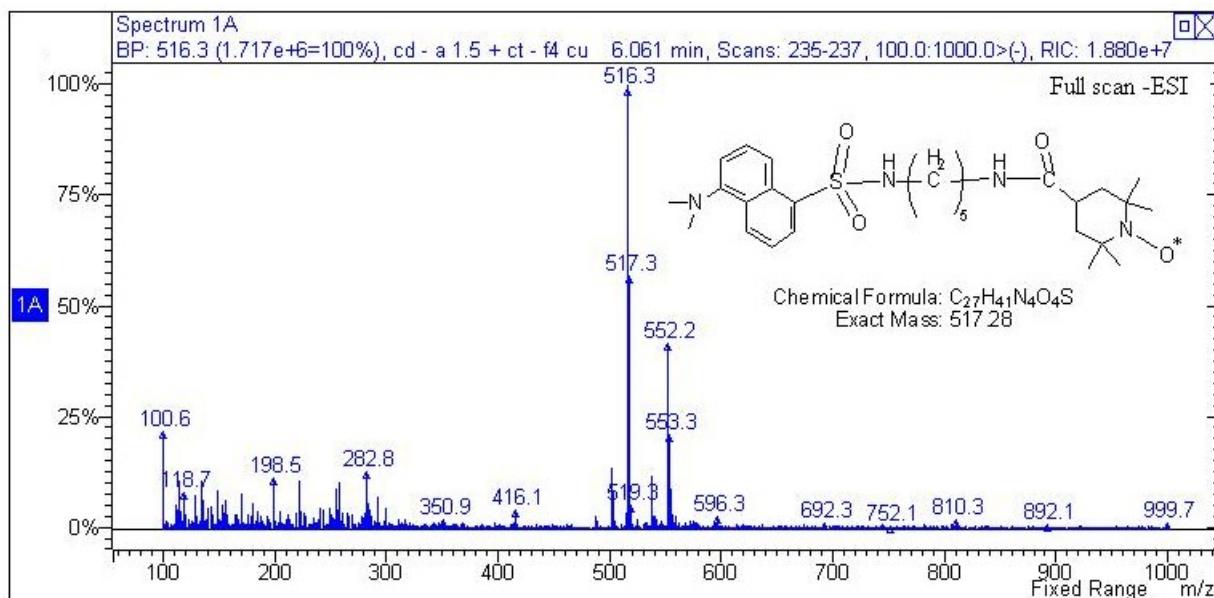


UV-Vis spectrum of compound DA_{1.4}T

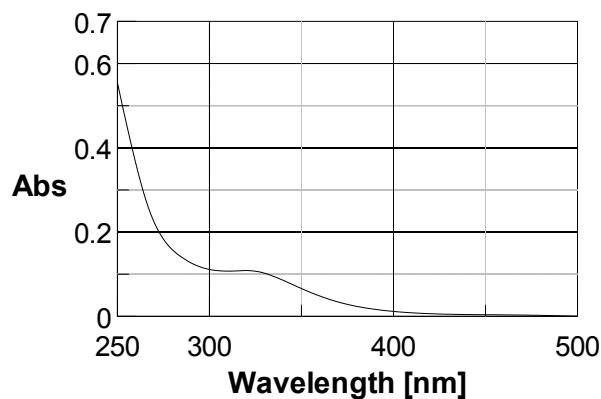


EPR spectrum of DA_{1.4}T

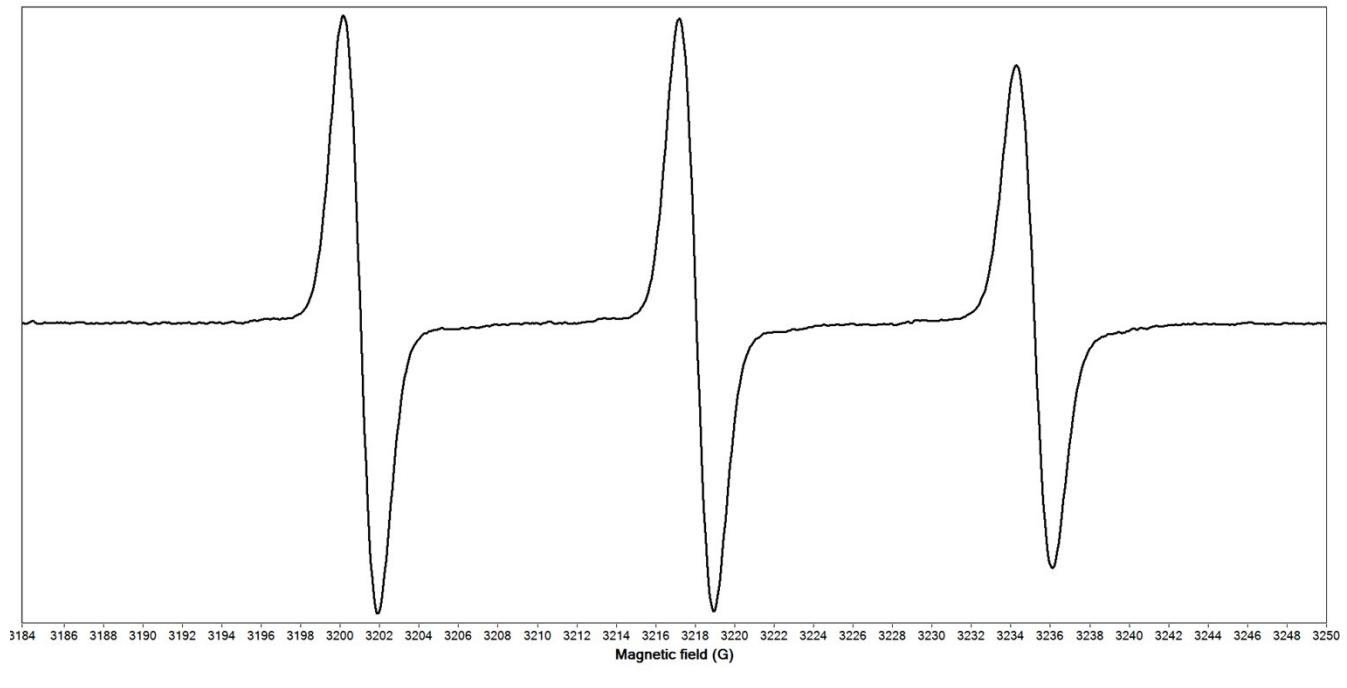
DA_{1.5}T



ESI-MS (*m/z*): 516 (DA_{1.5}T - H⁺)

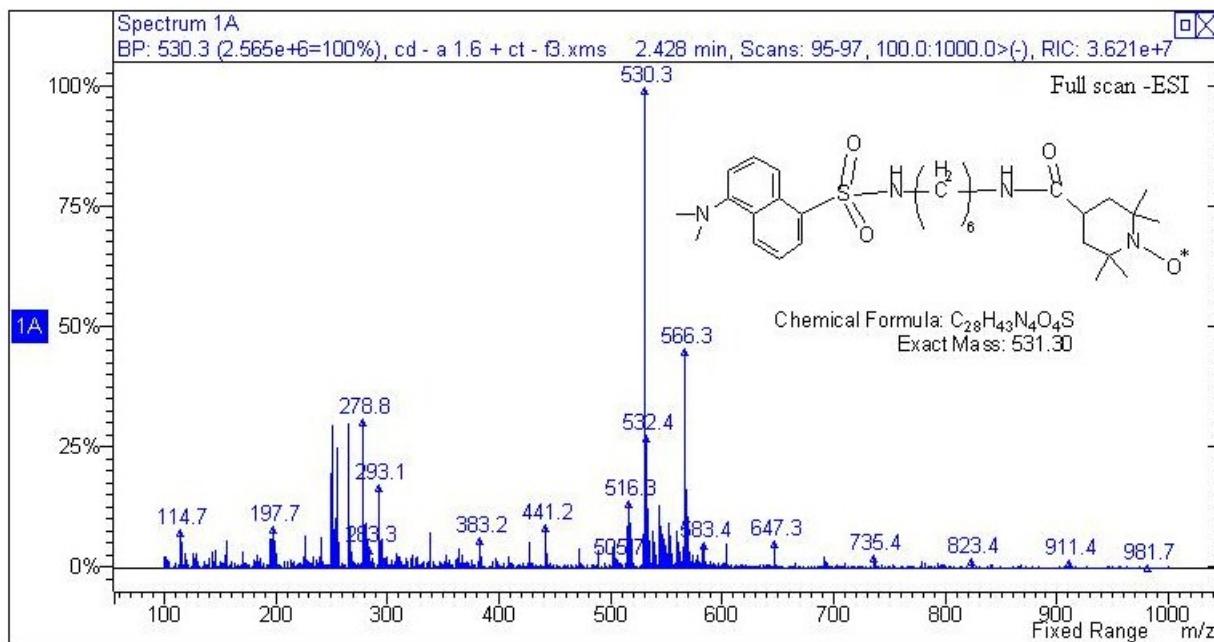


UV-Vis spectrum of compound DA_{1.5}T

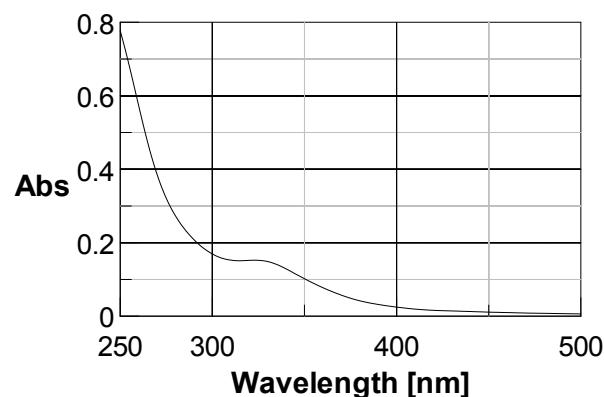


EPR spectrum of DA_{1.5}T

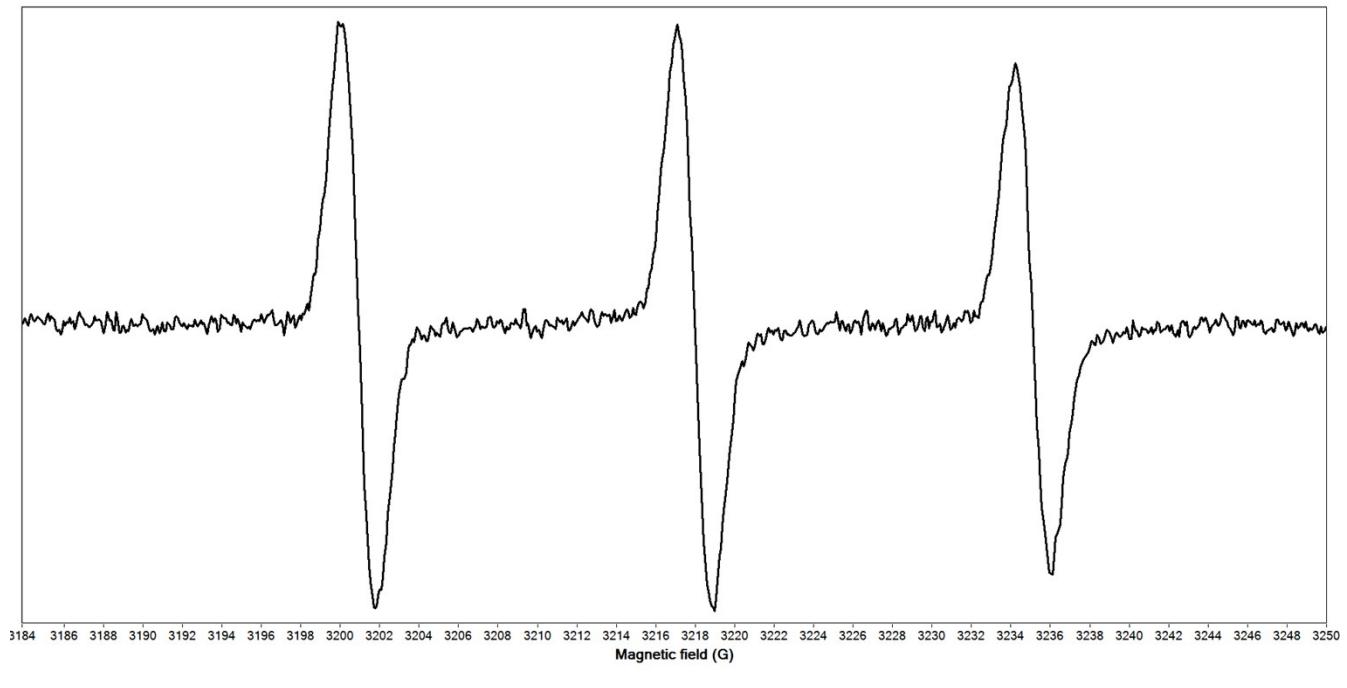
DA_{1.6}T



ESI-MS (*m/z*): 530 (DA_{1.6}T - H⁺)

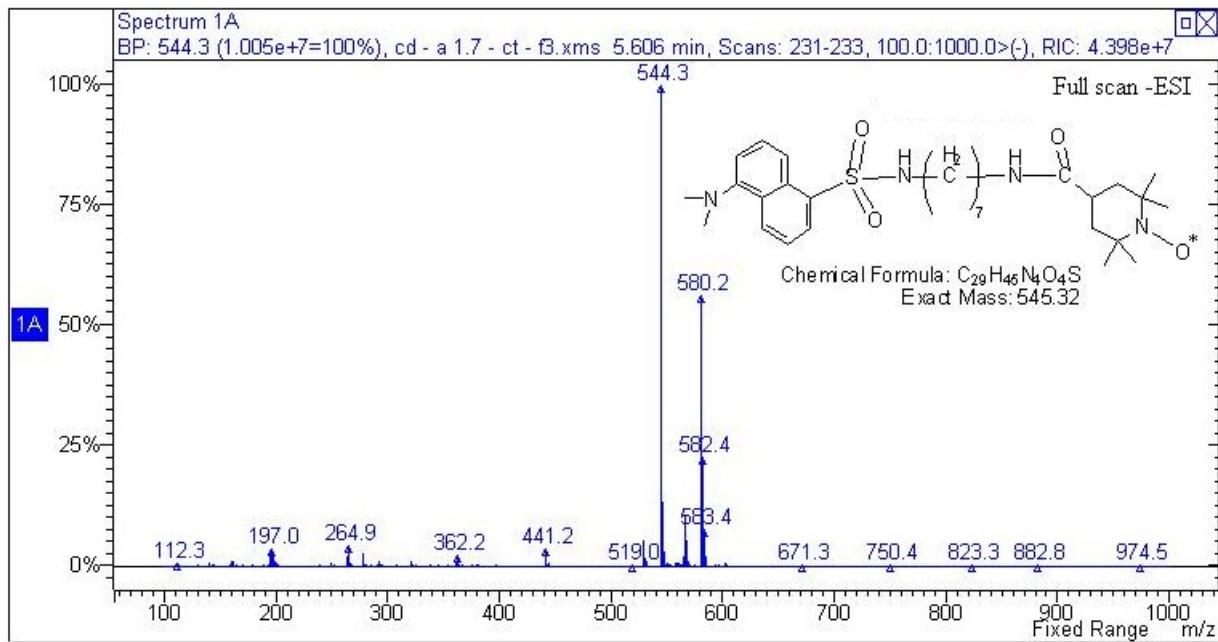


UV-Vis spectrum of compound DA_{1.6}T

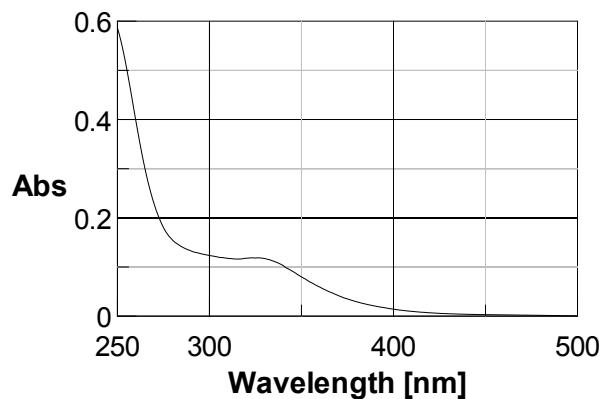


EPR spectrum of DA_{1.6}T

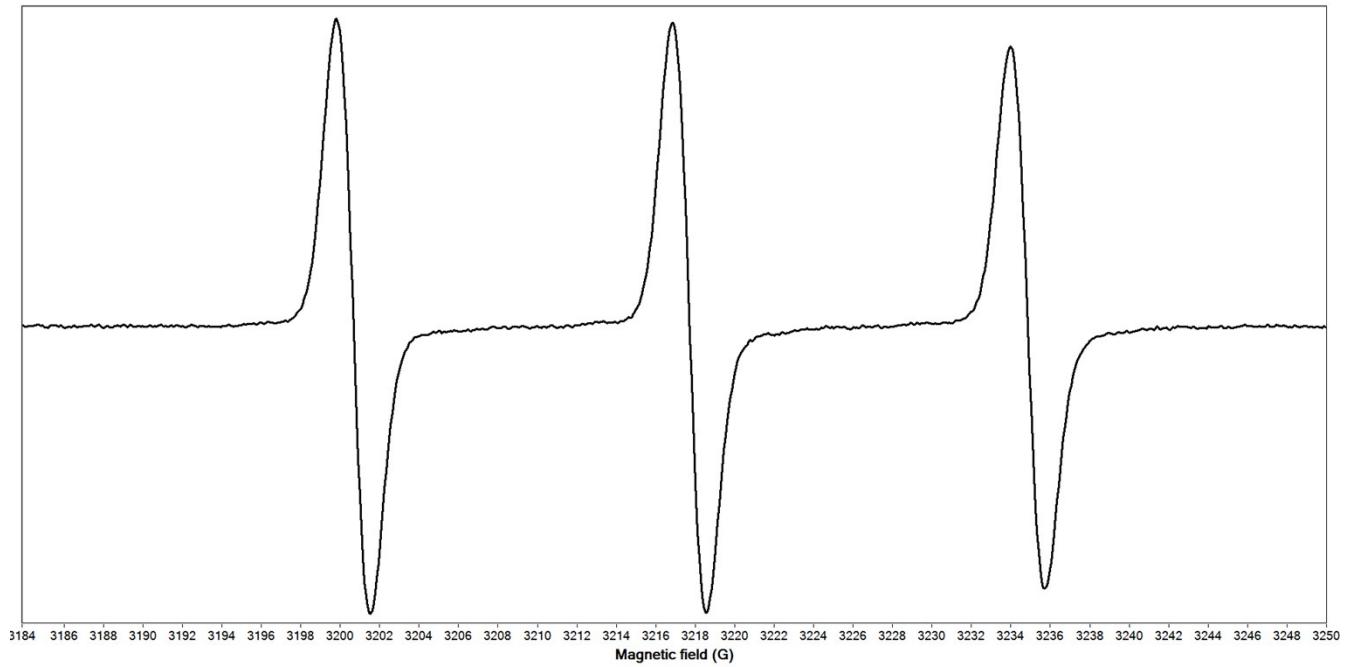
DA_{1.7}T



ESI-MS (*m/z*): 544 (DA_{1.7}T - H⁺)

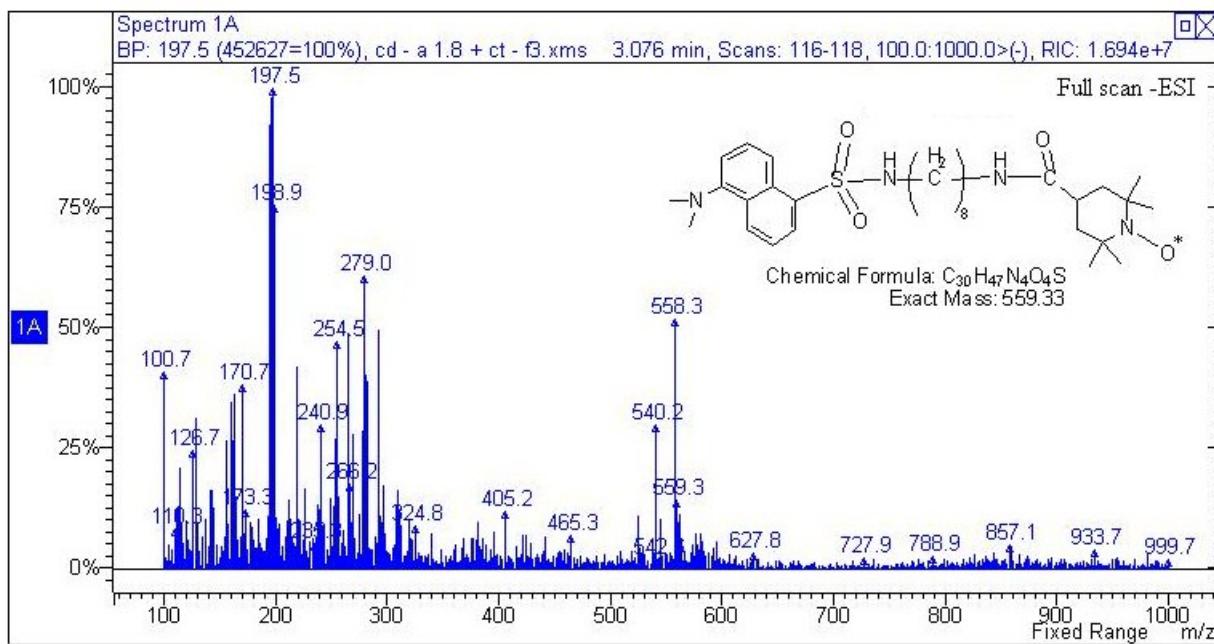


UV-Vis spectrum of compound DA_{1.7}T

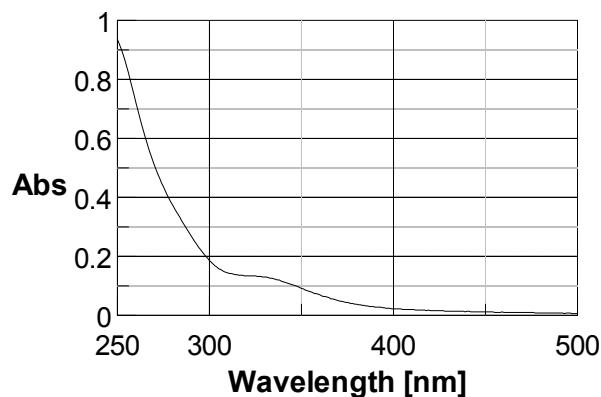


EPR spectrum of DA_{1.7}T

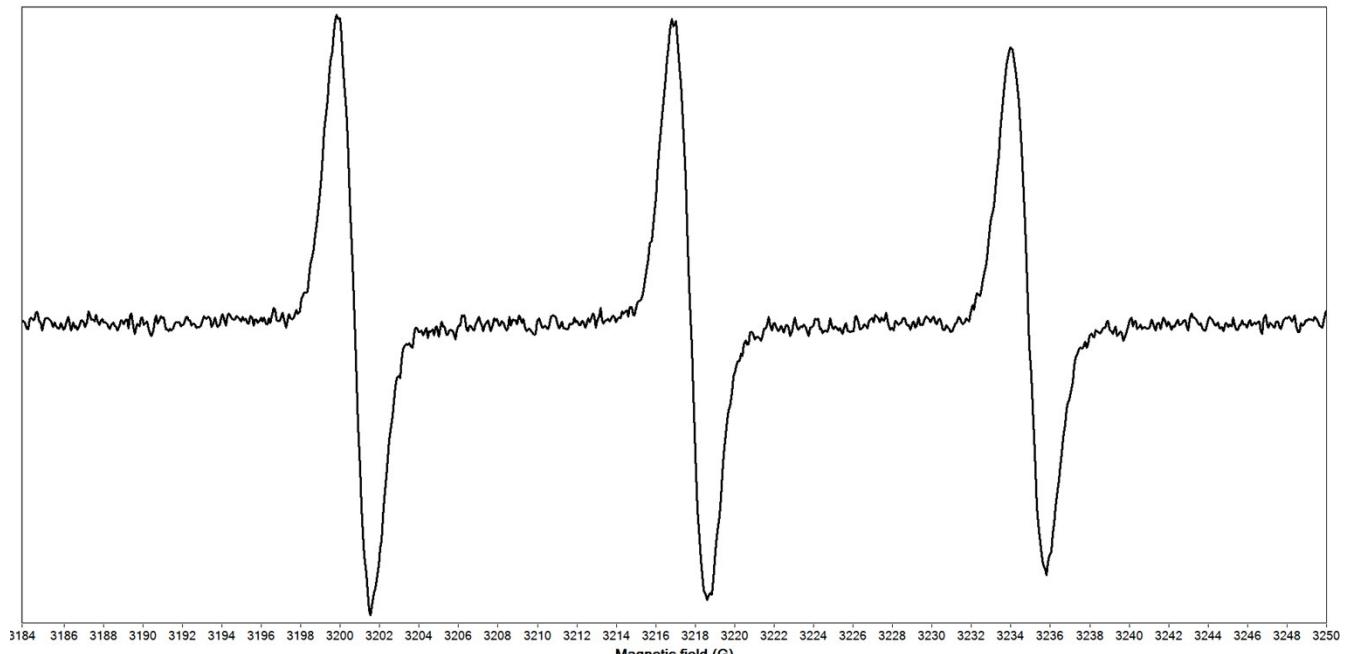
DA_{1.8}T



ESI-MS (*m/z*): 558 (DA_{1.8}T - H⁺)

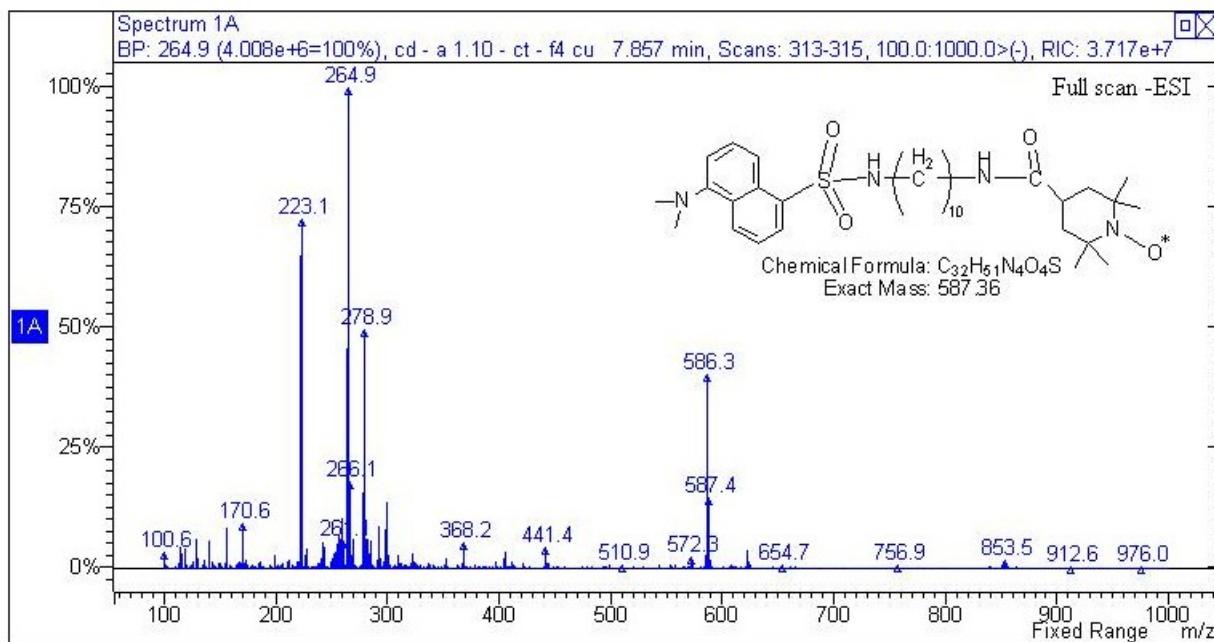


UV-Vis spectrum of compound DA_{1.8}T

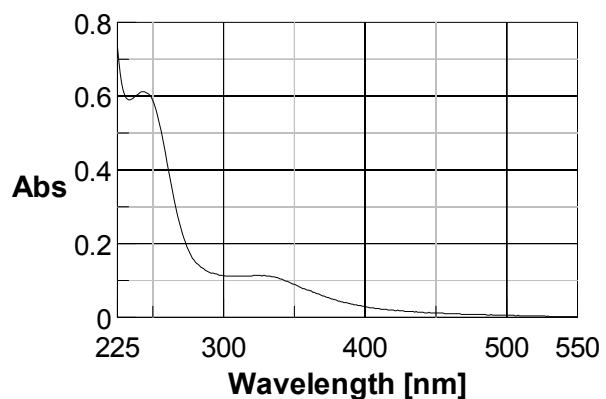


EPR spectrum of DA_{1.8}T

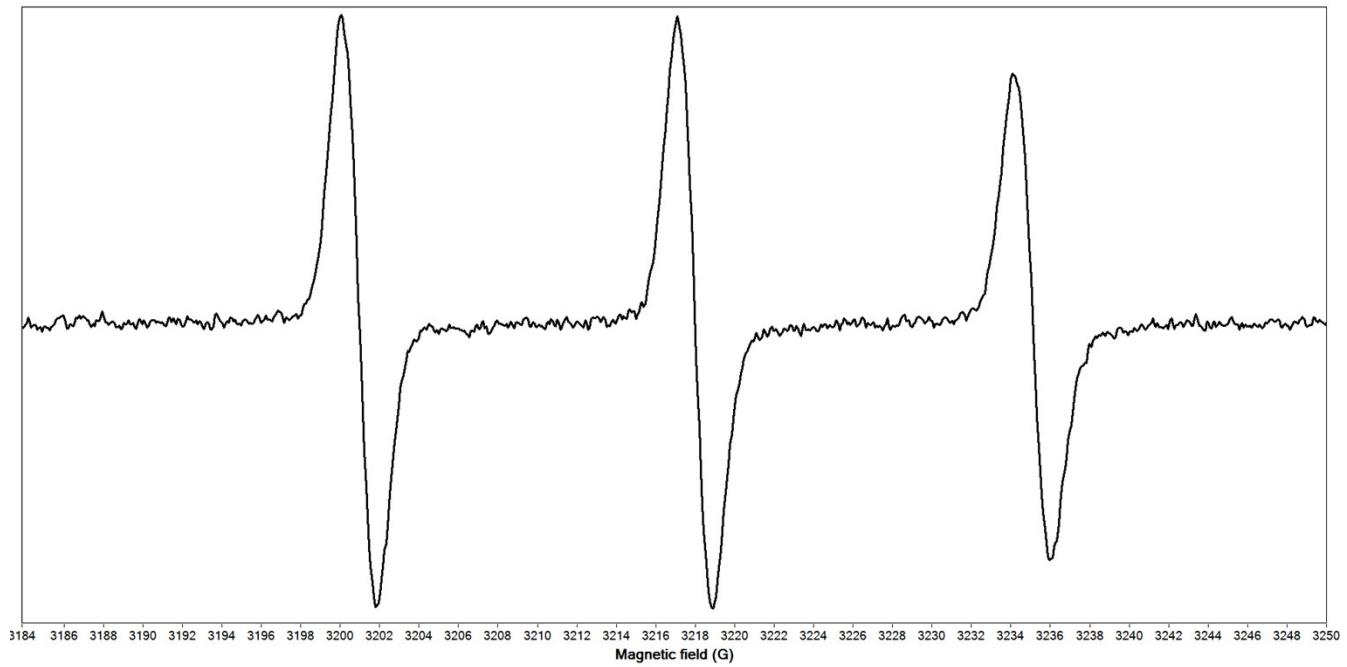
DA_{1.10}T



ESI-MS (*m/z*): 586 (DA_{1.10}T - H⁺)

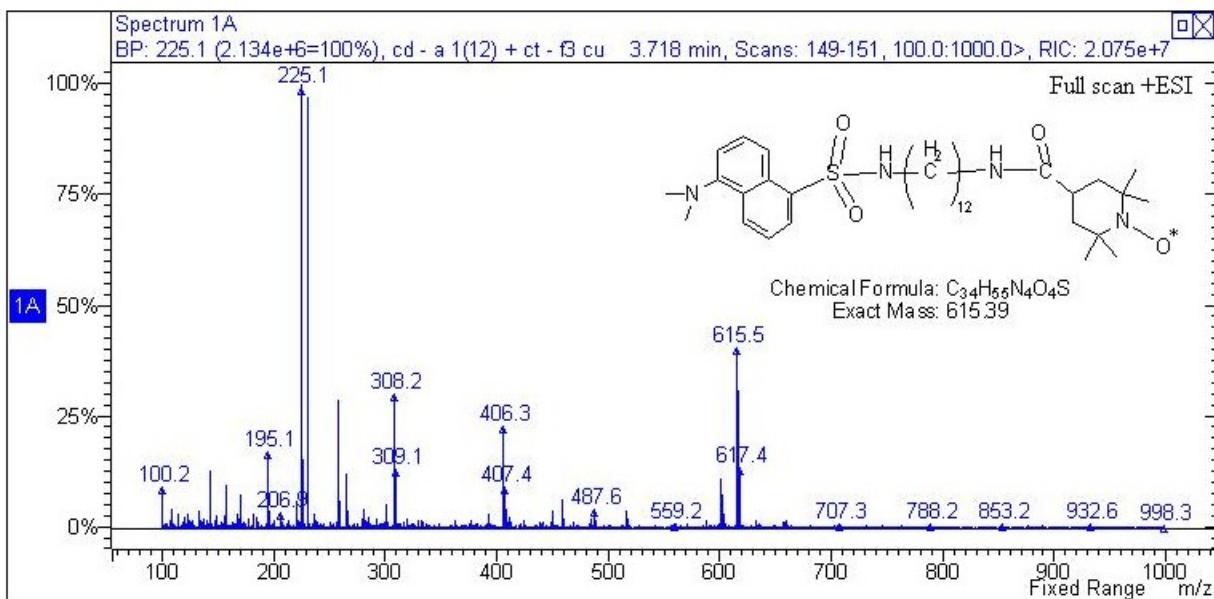


UV-Vis spectrum of compound DA_{1.10}T

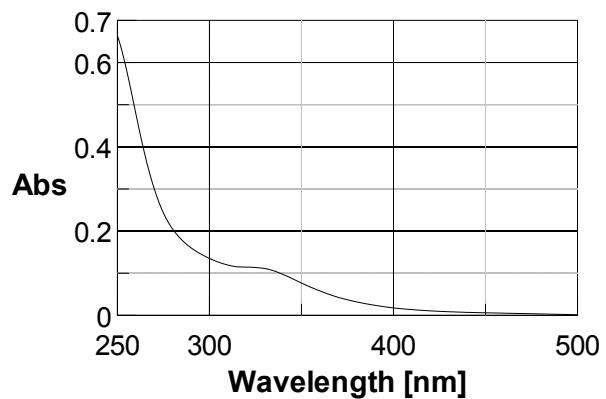


EPR spectrum of DA_{1.10}T

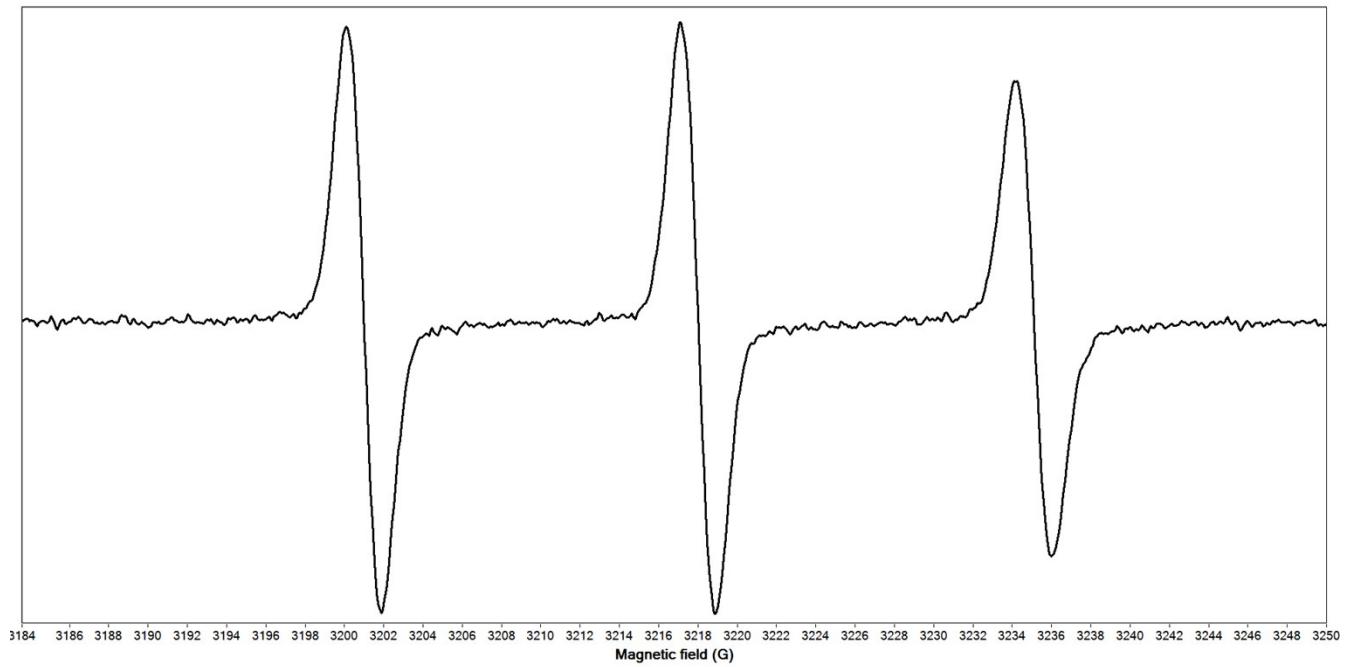
DA_{1.12}T



ESI-MS (*m/z*): 615 (DA_{1.12}T)



UV-Vis spectrum of compound DA_{1.12}T



EPR spectrum of DA_{1.12}T