Supporting Information

Octupolar chimeric compounds built from quinoline caged acetate moieties. A novel approach for 2-photon uncaging of biomolecules

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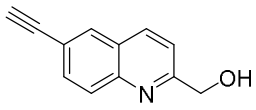
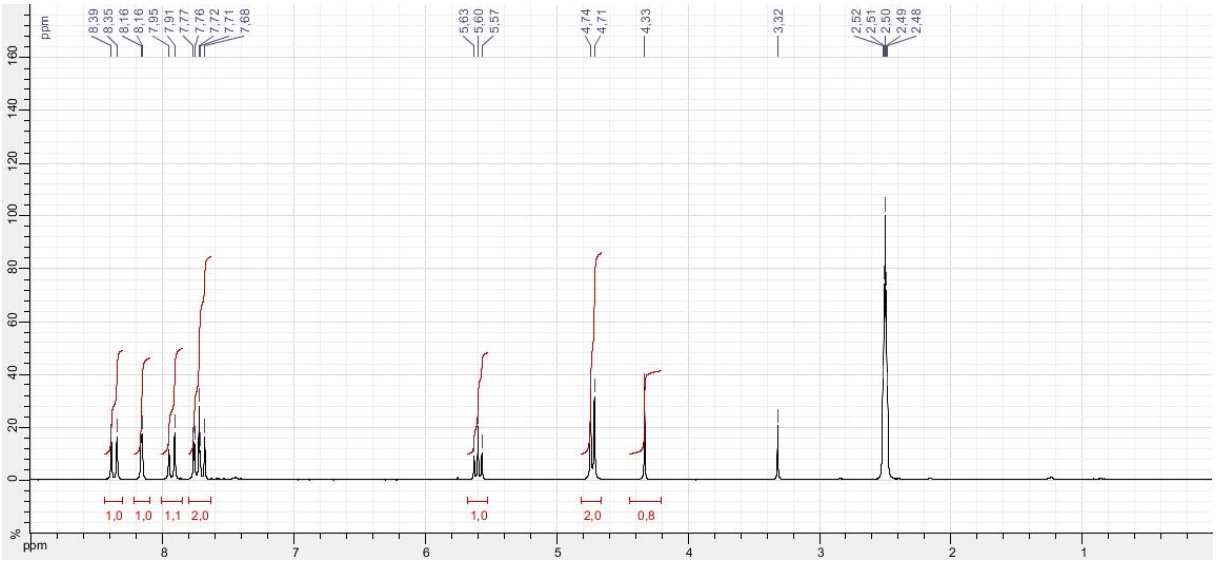
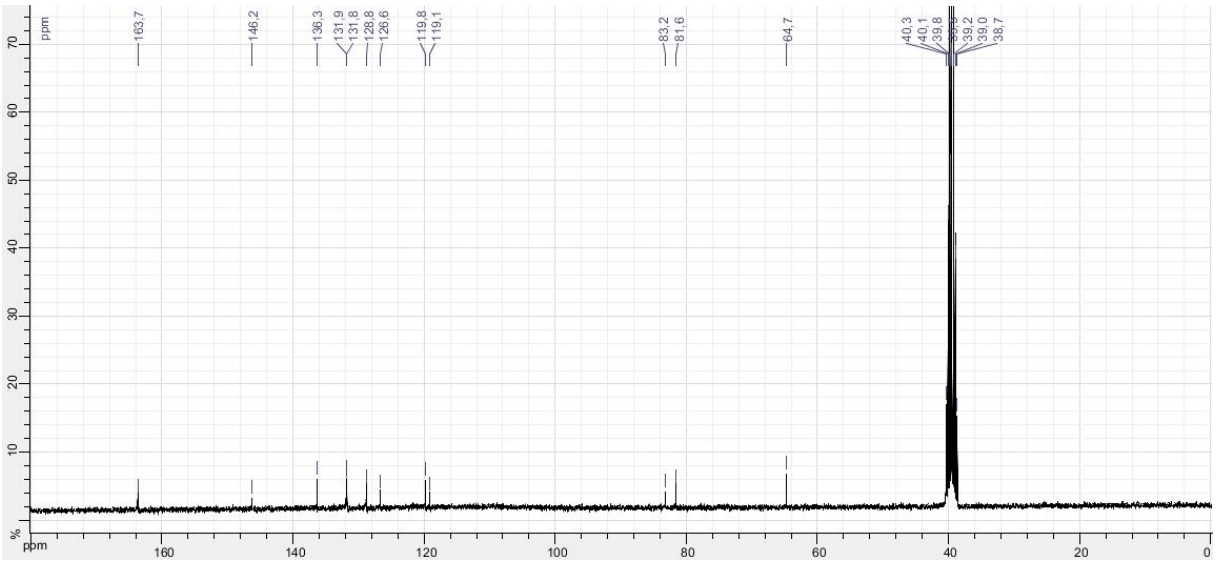


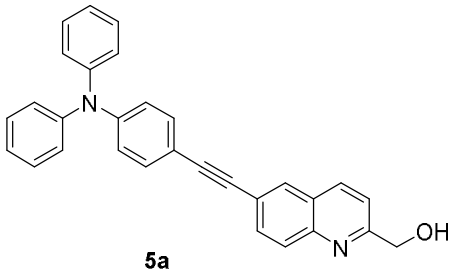
3

-^{1}H NMR (200 MHz, DMSO-d_6)



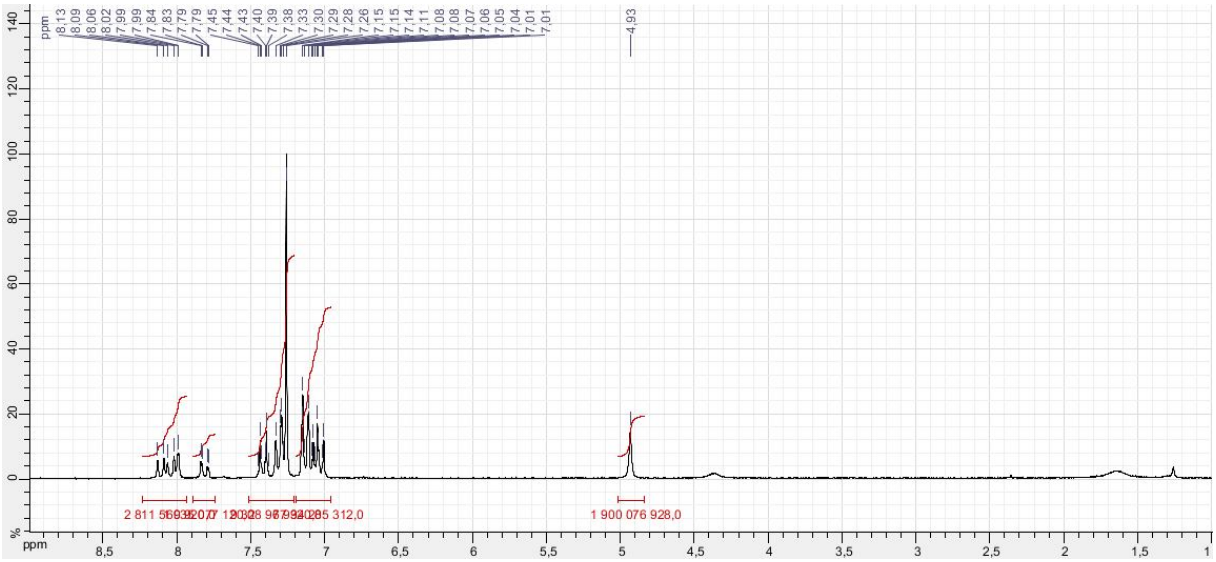
-^{13}C NMR (75 MHz, $CDCl_3$)





5a

-^{1}H NMR (300 MHz, $CDCl_3$)



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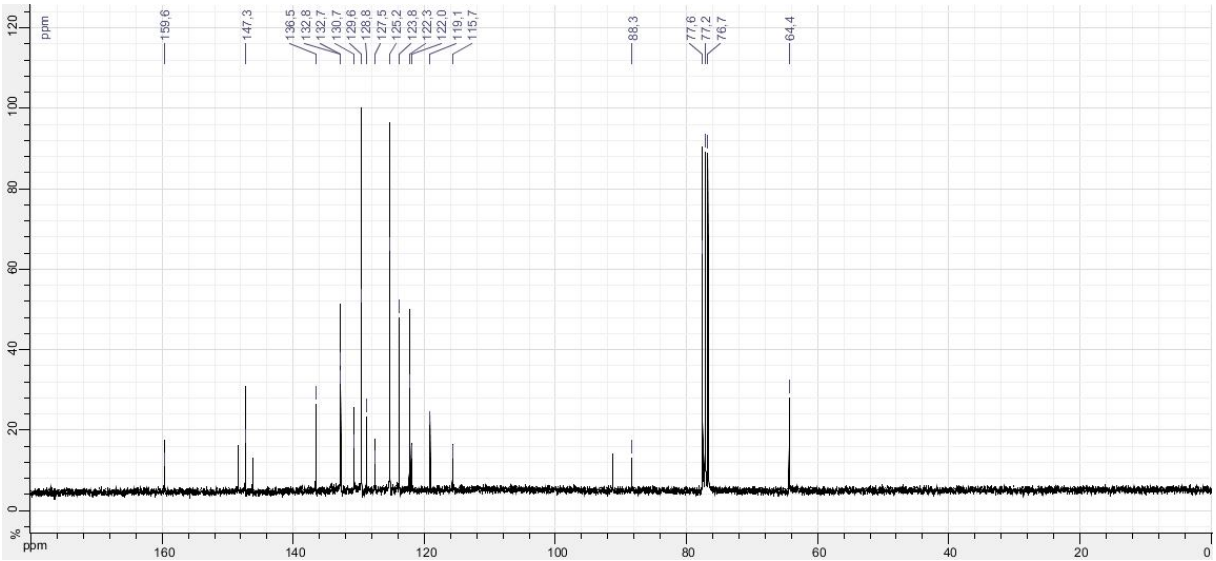
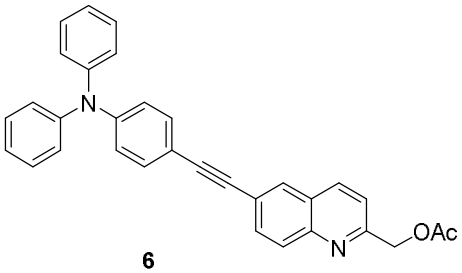
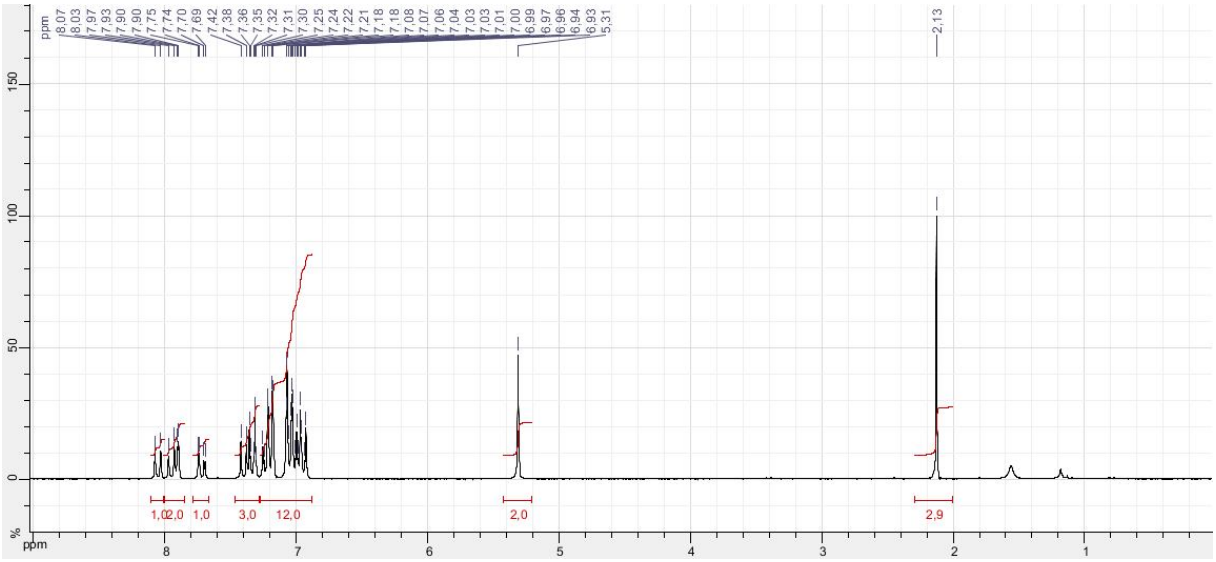


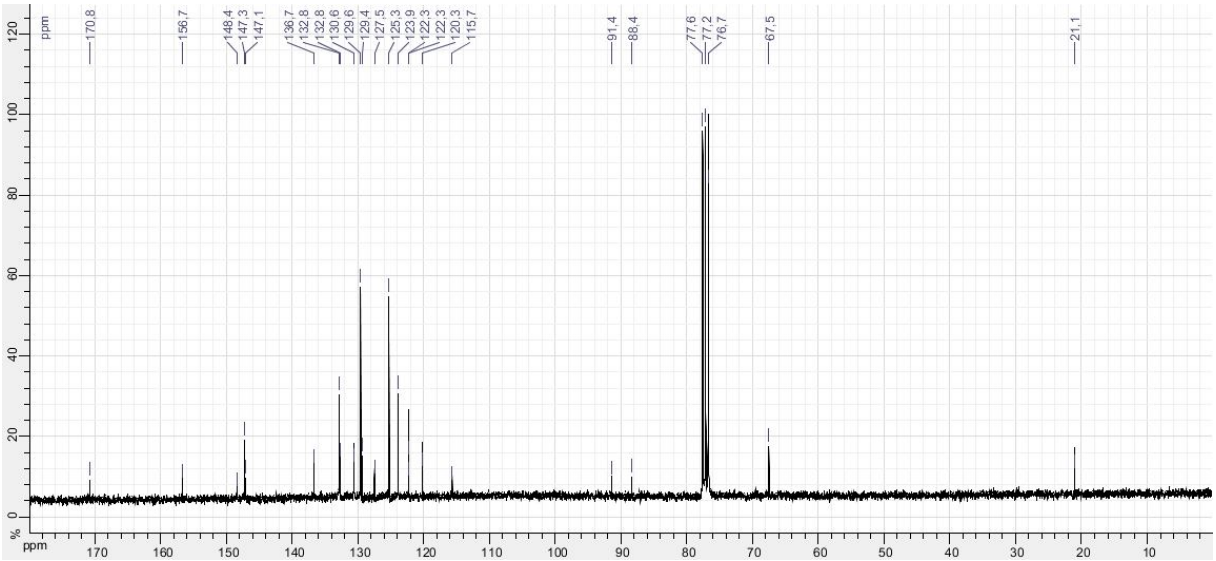


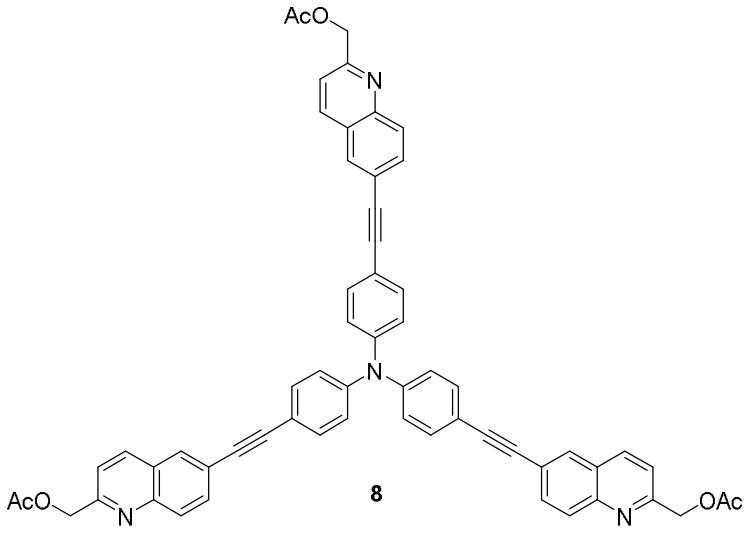
6

-^{1}H NMR (300 MHz, $CDCl_3$)



-^{13}C NMR (75 MHz, $CDCl_3$)





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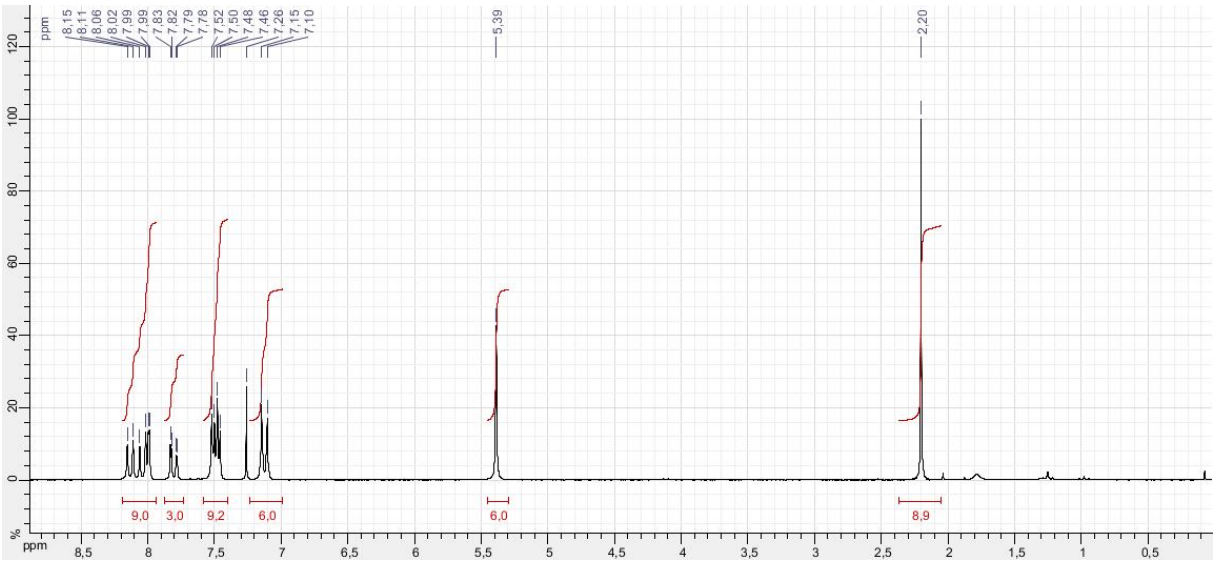
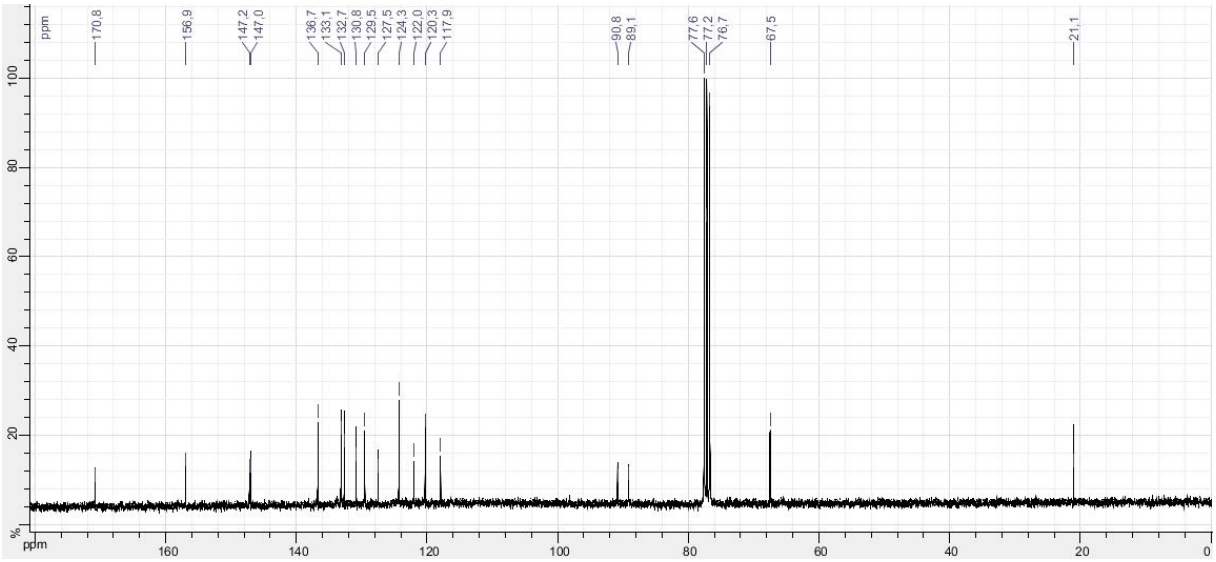
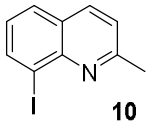
-^{1}H NMR (300 MHz, $CDCl_3$)



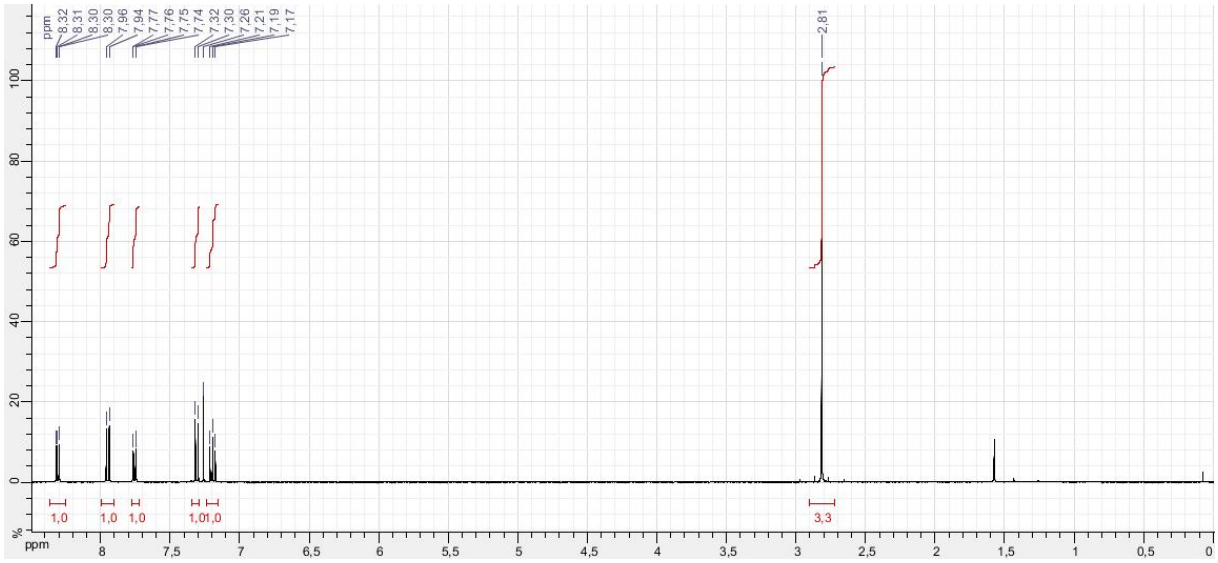
-^{13}C NMR (75 MHz, $CDCl_3$)



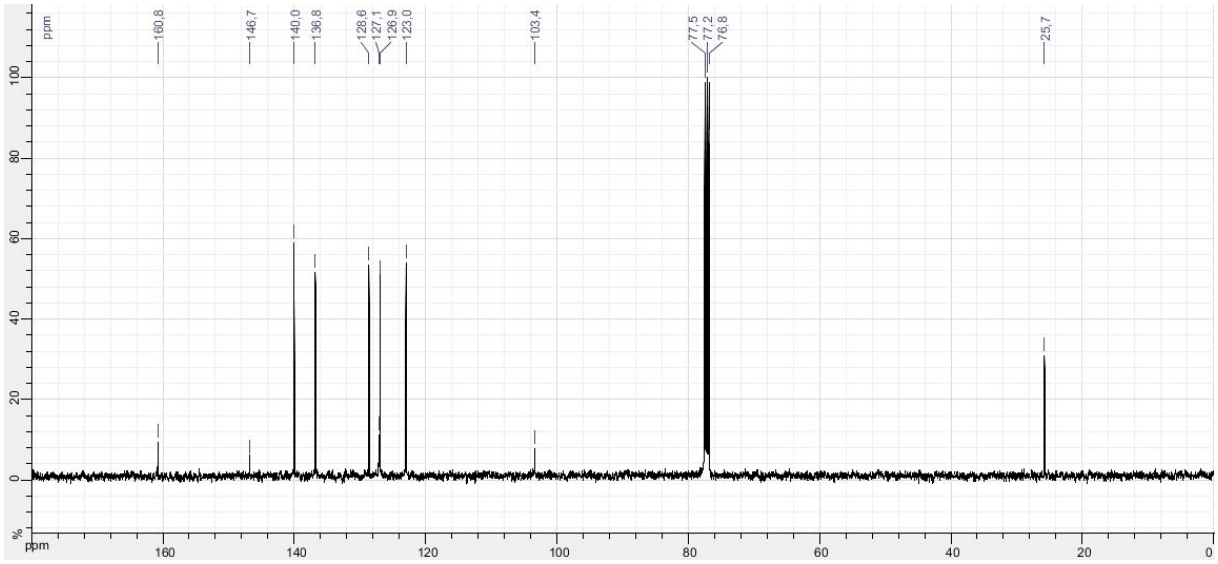


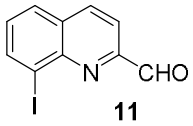
10

-^{1}H NMR (400 MHz, $CDCl_3$)



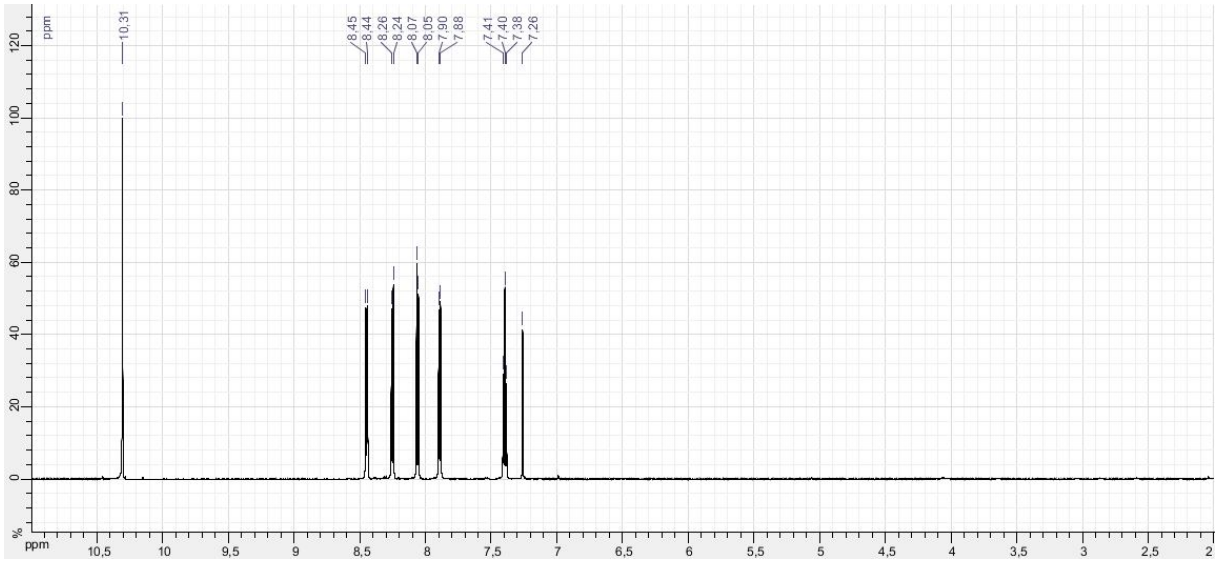
-^{13}C NMR (100 MHz, $CDCl_3$)





11

-^{1}H NMR (600 MHz, $CDCl_3$)



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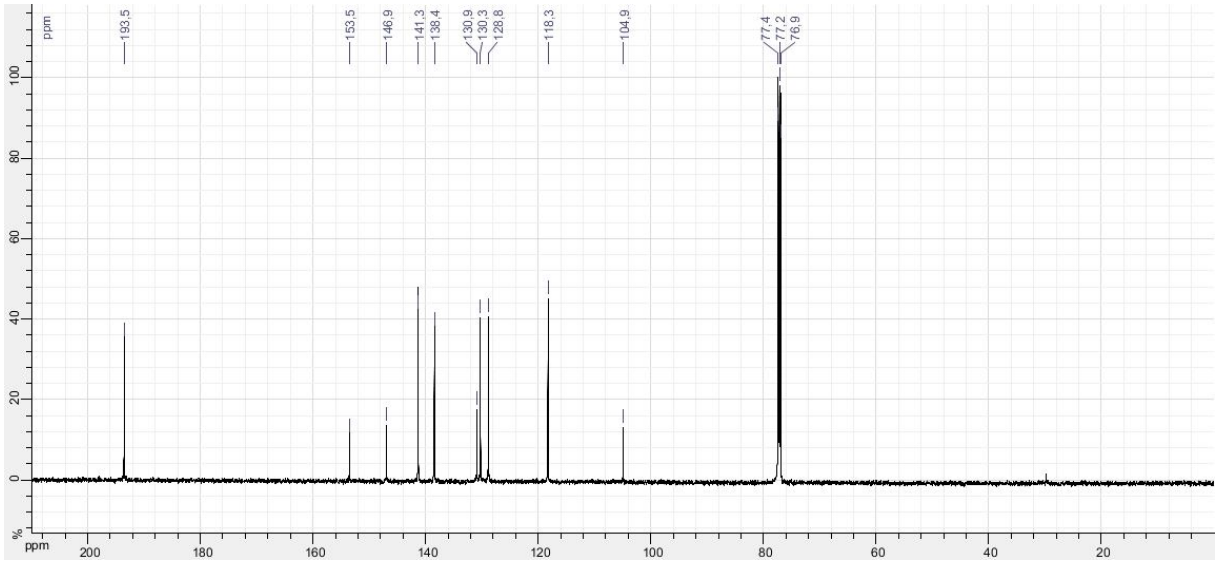
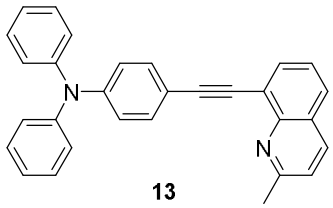
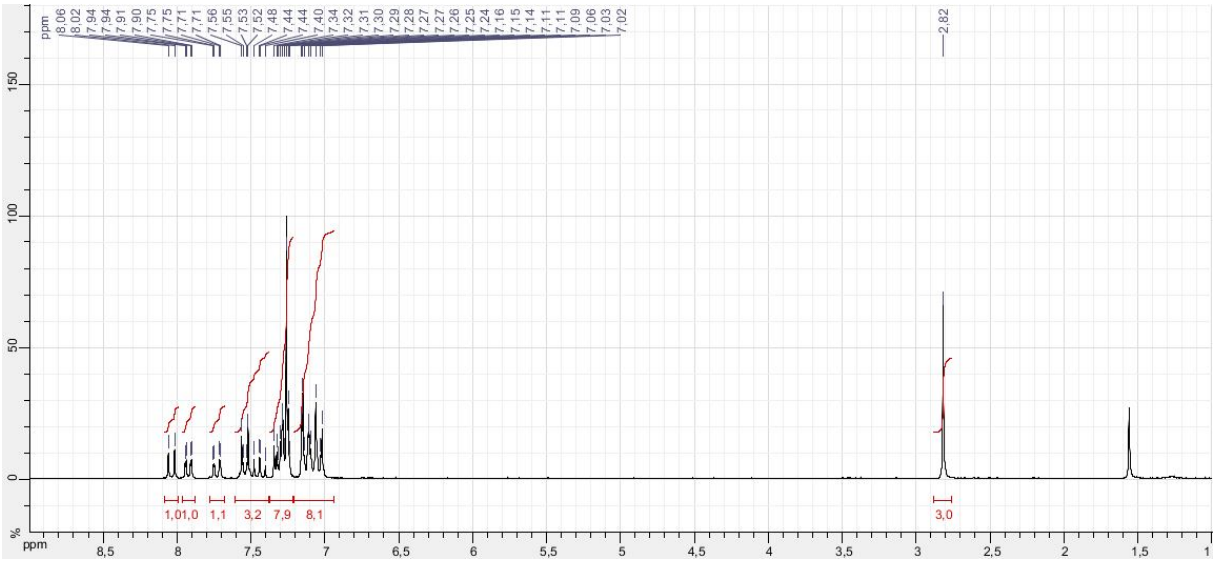


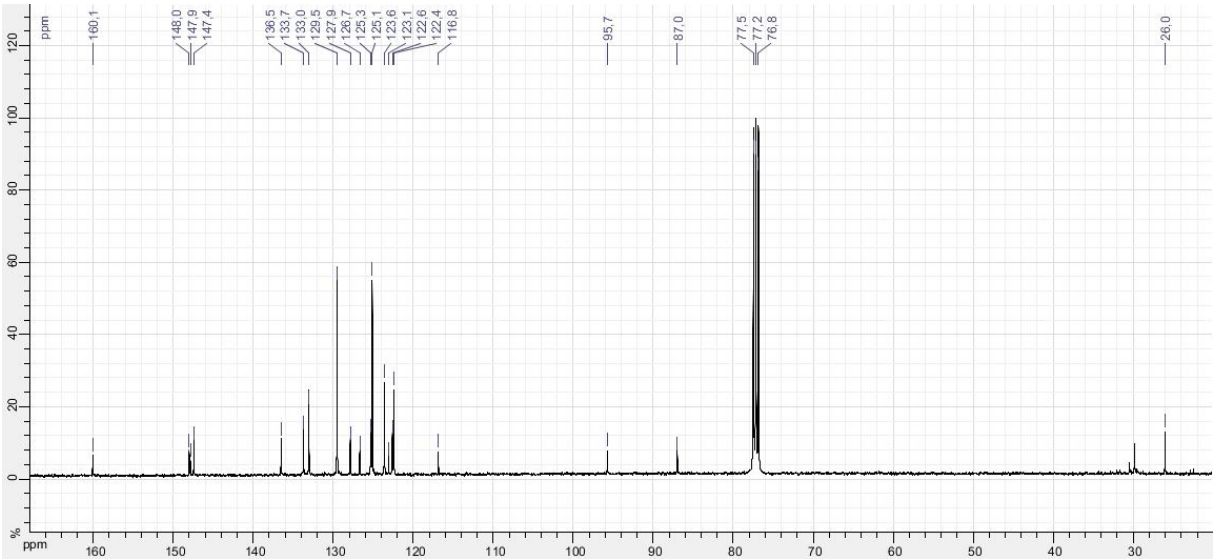


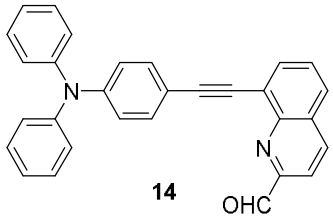
13

-^{1}H NMR (400 MHz, $CDCl_3$)



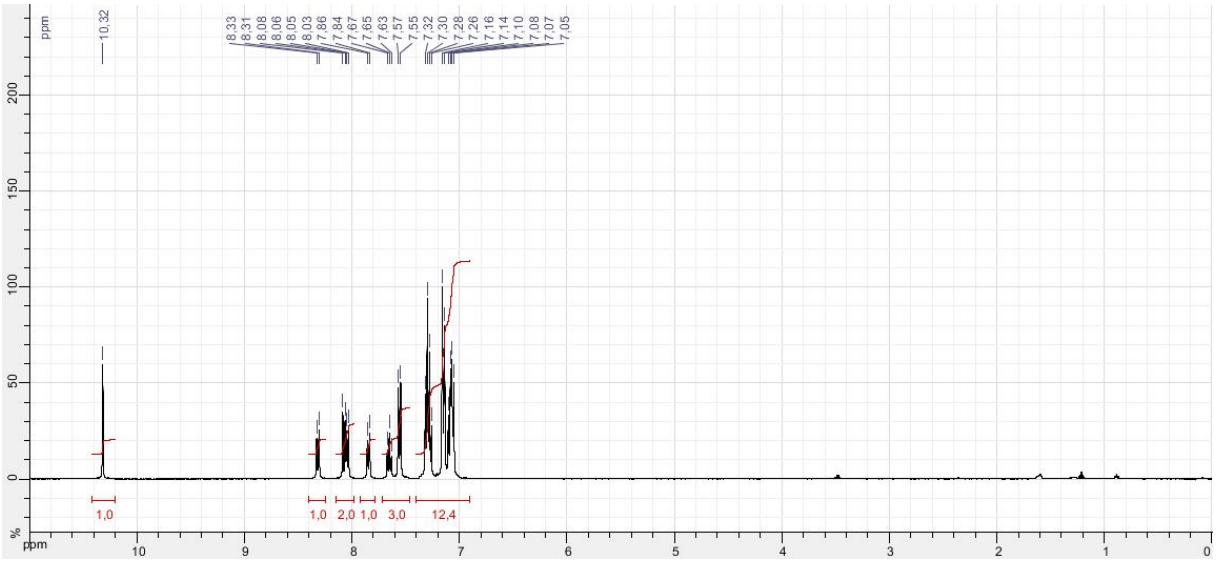
-^{13}C NMR (100 MHz, $CDCl_3$)



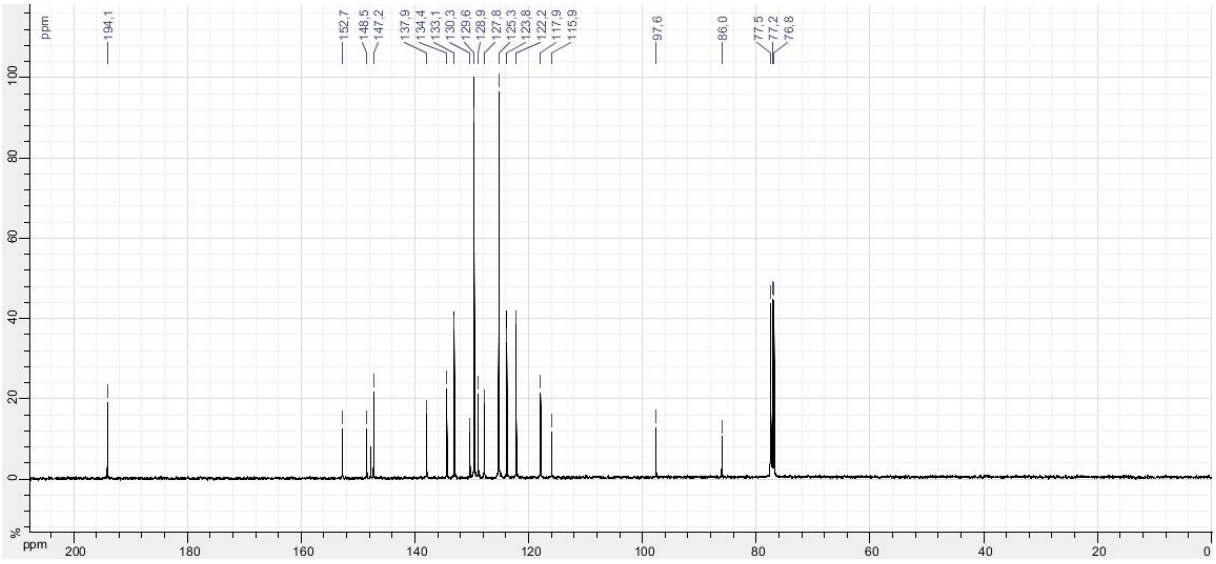


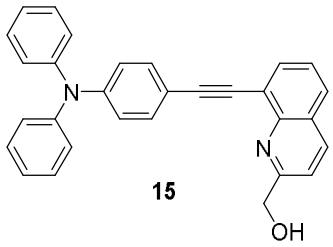
14

-^{1}H NMR (400 MHz, $CDCl_3$)



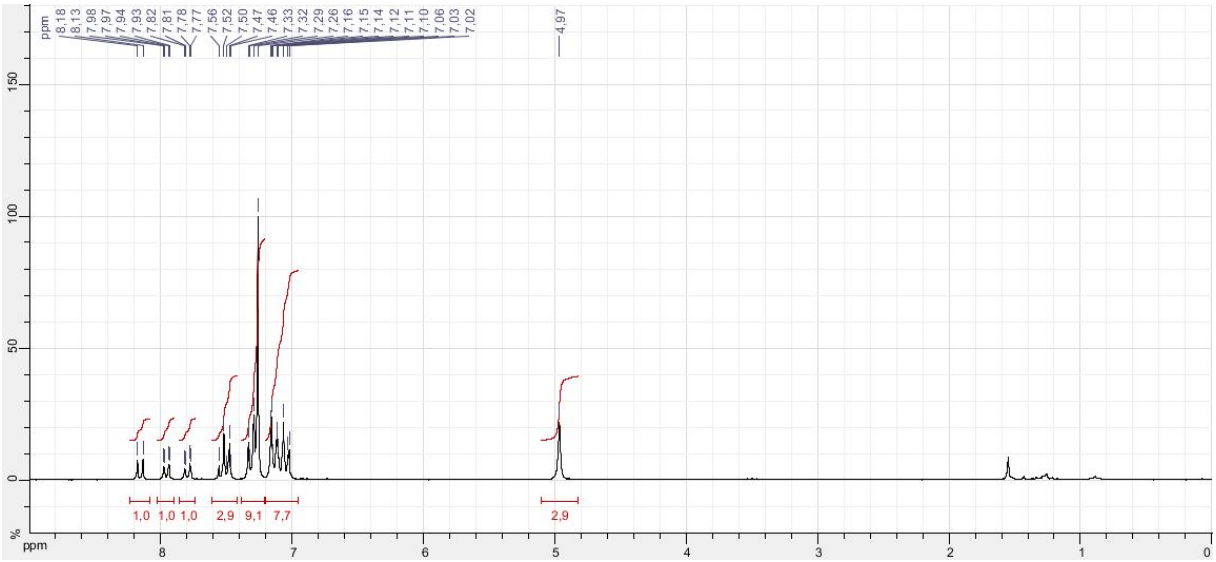
-^{13}C NMR (100 MHz, $CDCl_3$)



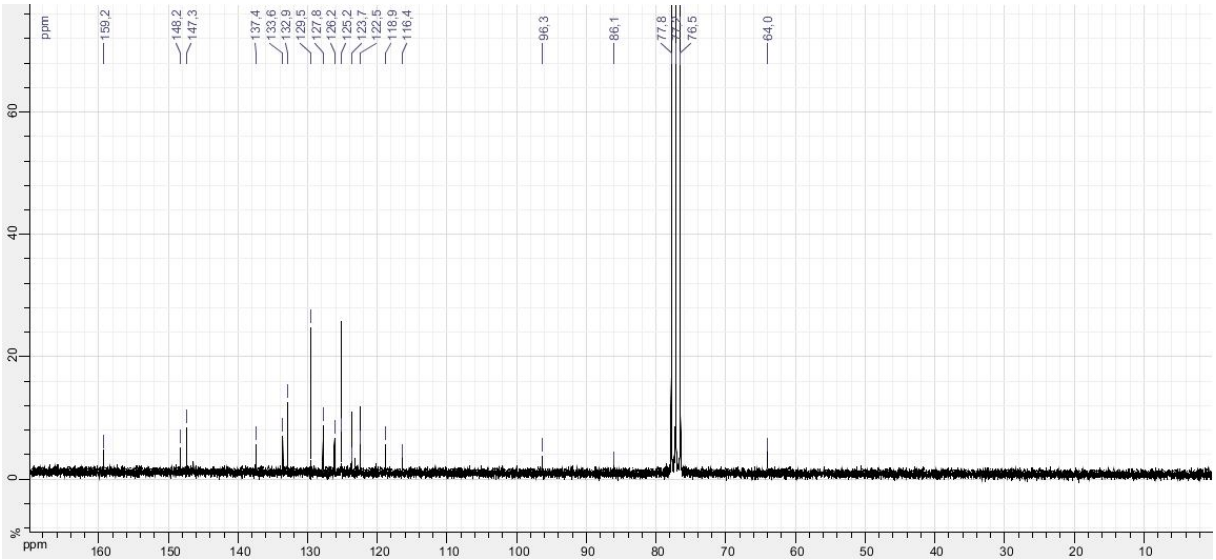


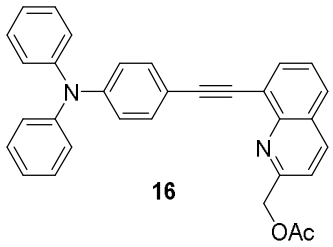
15

-^{1}H NMR (400 MHz, $CDCl_3$)



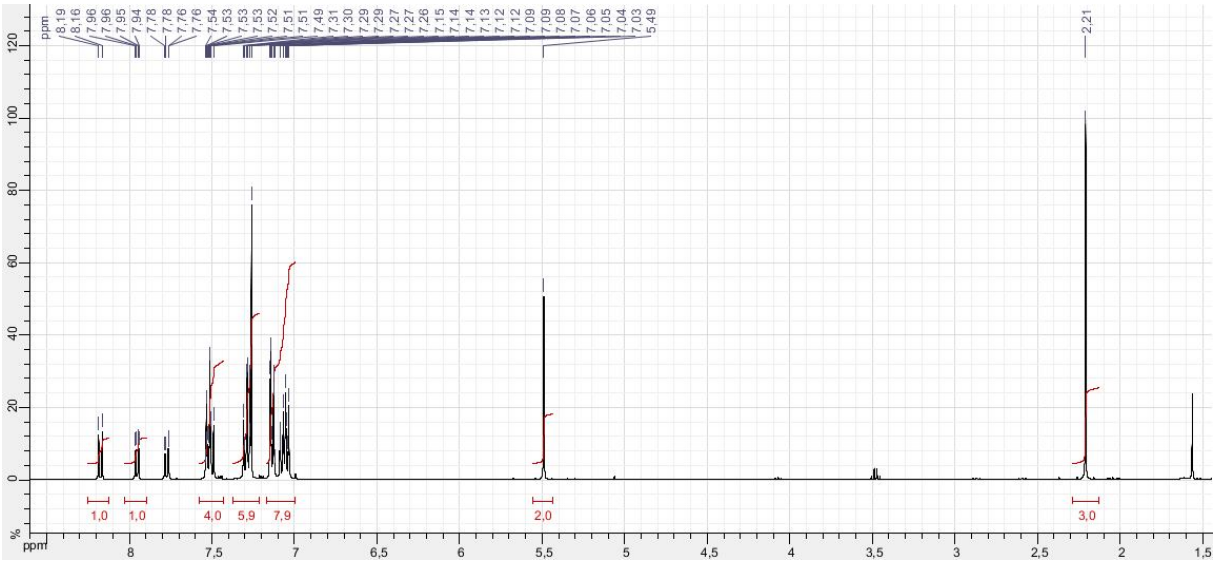
-^{13}C NMR (50 MHz, $CDCl_3$)



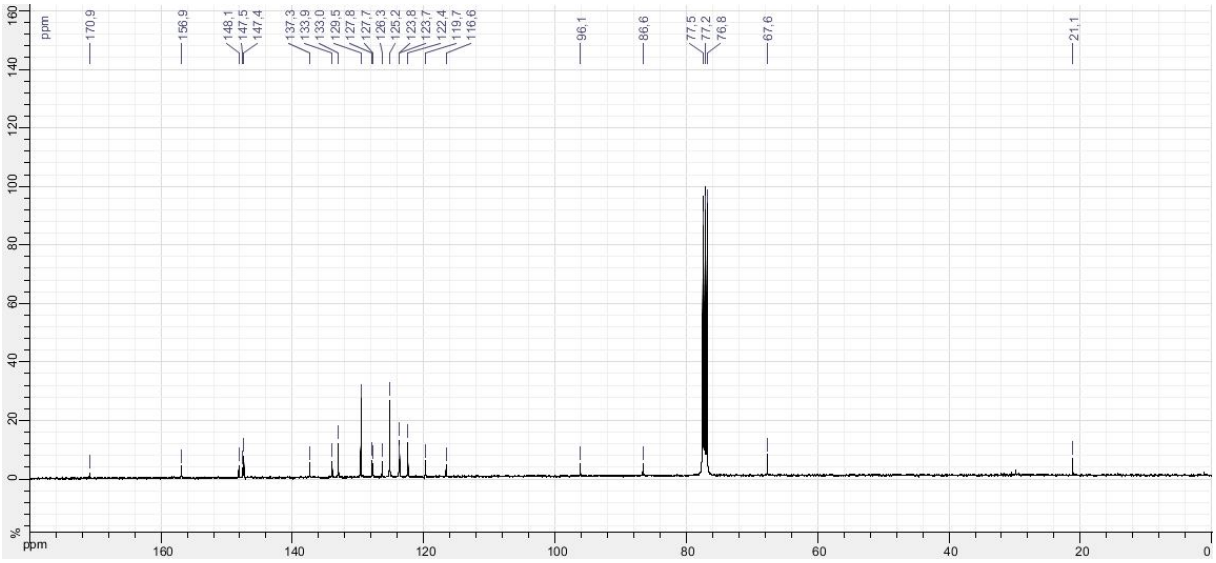


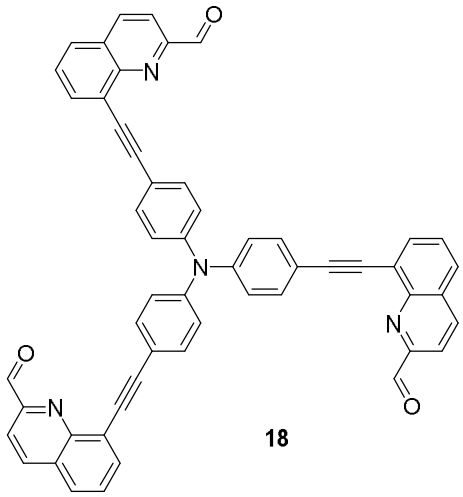
16

-^{1}H NMR (400 MHz, $CDCl_3$)



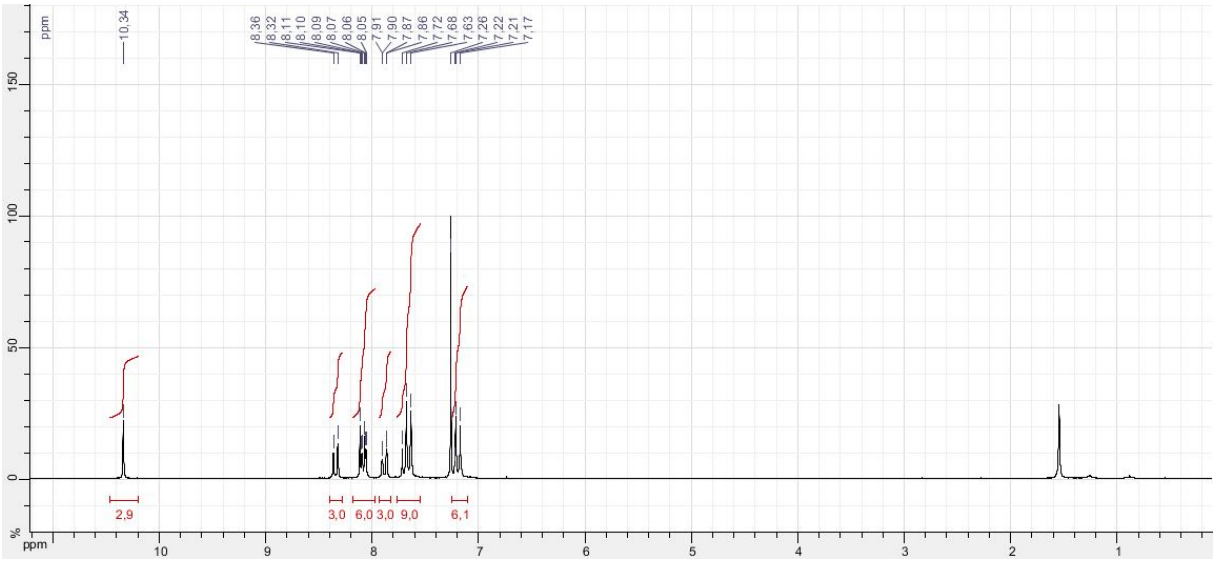
-^{13}C NMR (100 MHz, $CDCl_3$)



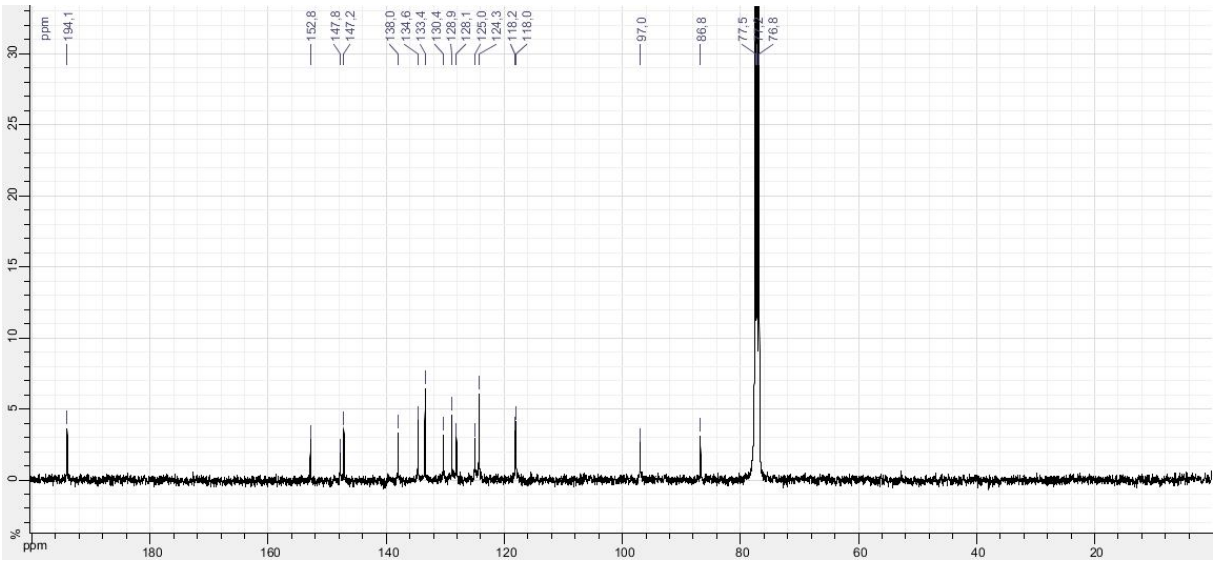


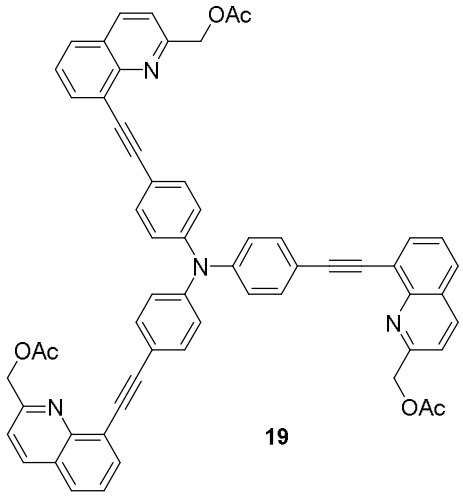
18

-^{1}H NMR (400 MHz, $CDCl_3$)



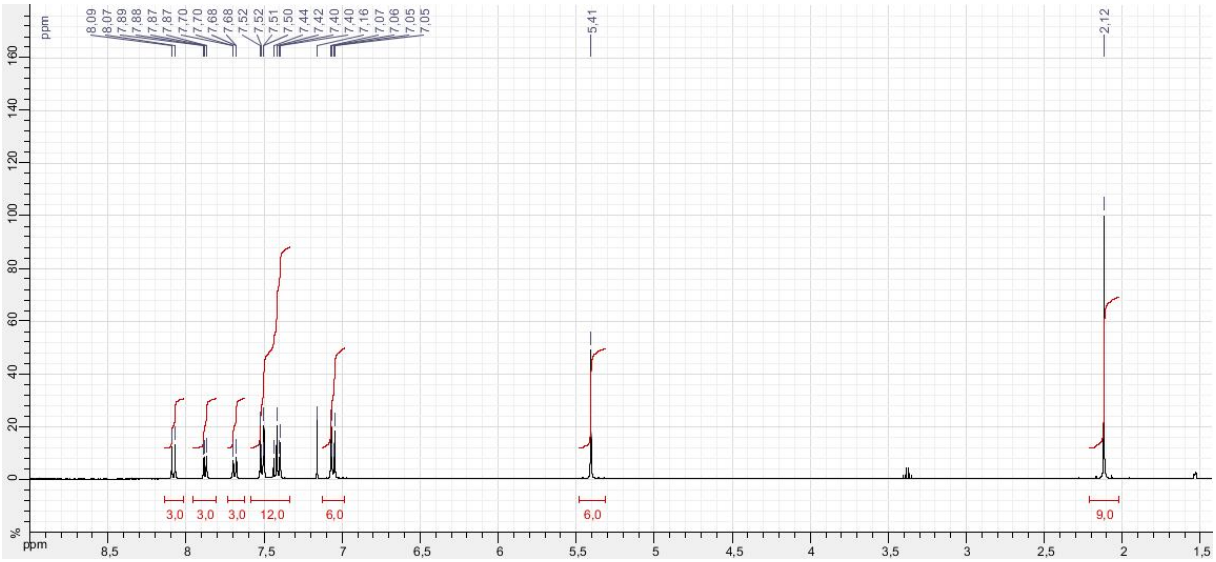
-^{13}C NMR (100 MHz, $CDCl_3$)



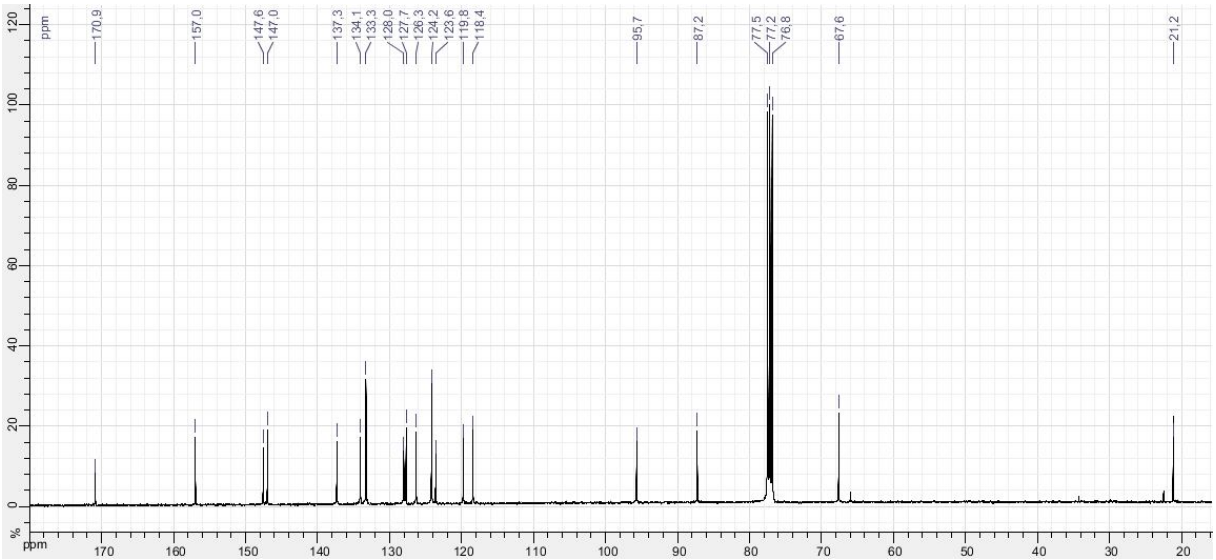


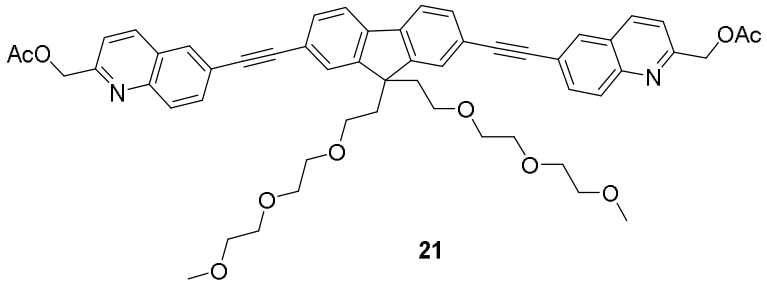
19

-^{1}H NMR (400 MHz, $CDCl_3$)



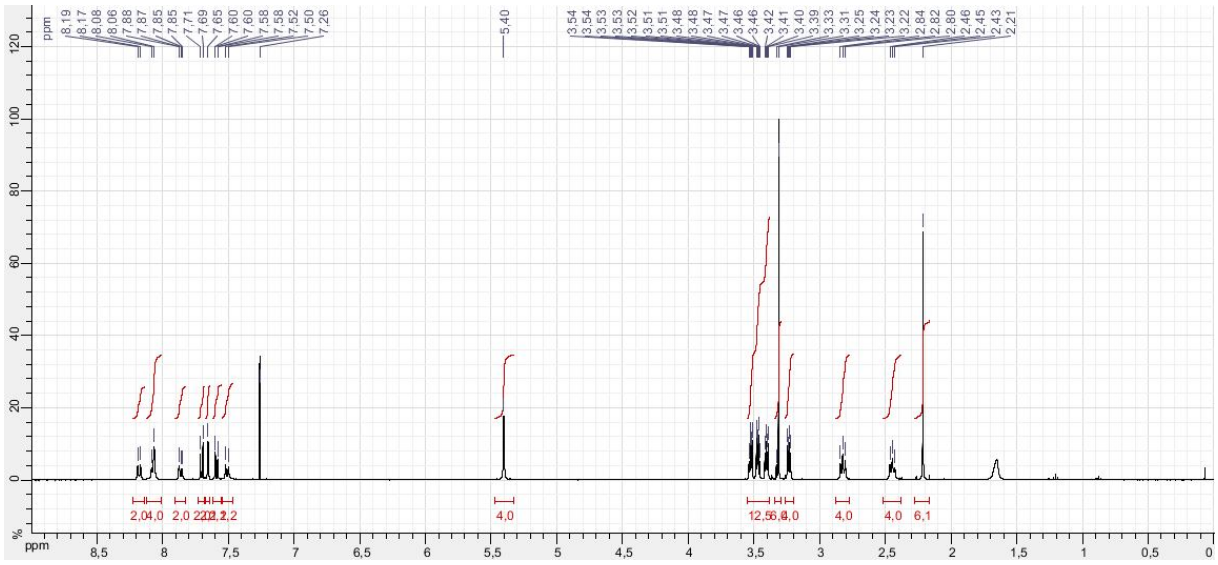
-^{13}C NMR (100 MHz, $CDCl_3$)





21

-^{1}H NMR (400 MHz, $CDCl_3$)



-^{13}C NMR (100 MHz, $CDCl_3$)

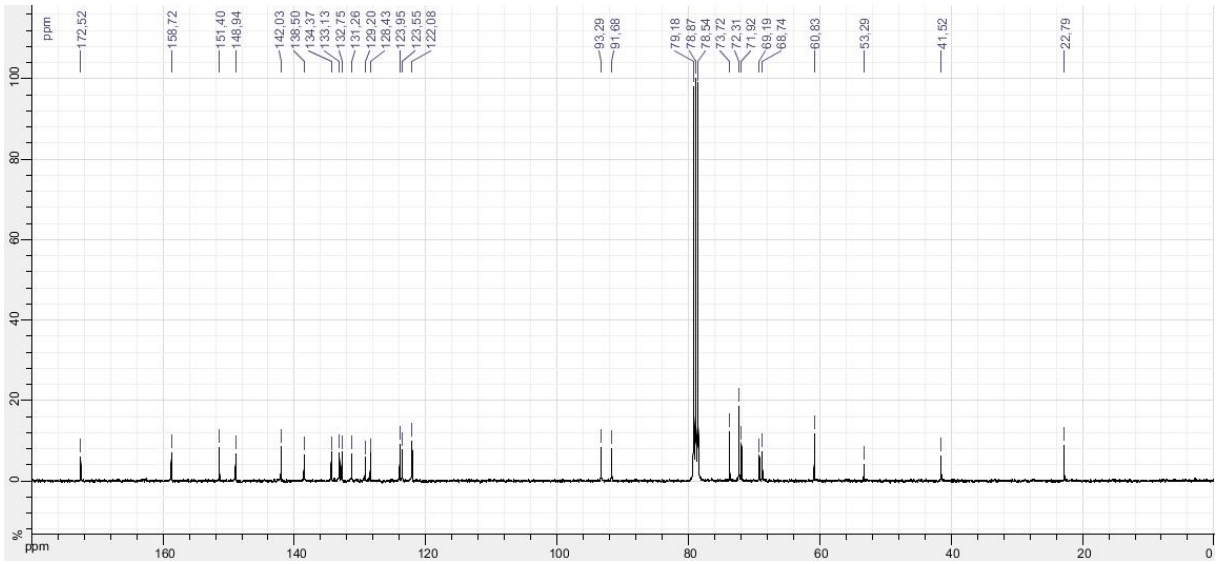


Table S1. Solvatochromic data of the 6-substituted quinoline dipolar, quadrupolar and octupolar compounds in different solvents

	solvent	λ_{abs}^{max} [nm]	ε^{max} [$M^{-1}.cm^{-1}$]	$\lambda_{\varepsilon m}^{max}$ [nm]	Stokes shift [$10^3 cm^{-1}$]
5a	Toluene	372	-	417	2.9
5a	$CHCl_3$	374	$2.9\ 10^4$	463	5.1
5a	AcOEt	365	-	457	5.5
5a	THF	368	$3.8\ 10^4$	465	5.7
5a	CH_2Cl_2	372	-	487	6.3
5a	acetone	366	$3.2\ 10^4$	507	7.6
5a	acetonitrile	365	-	537	8.8
5a	DMSO	370	$1.8\ 10^4$	529	8.1
6	$CHCl_3$	378	$3.2\ 10^4$	475	5.4
6	THF	371	$3.4\ 10^4$	473	5.8
6	acetone	368	$3.4\ 10^4$	527	8.2
6	DMSO	373	$2.1\ 10^4$	555	8.8
8	$CHCl_3$	390	$8.8\ 10^4$	453	3.6
8	THF	385	$9.3\ 10^4$	457	4.1
8	acetone	382	$9.1\ 10^4$	504	6.3
8	DMSO	387	$5.9\ 10^4$	544	7.5
21	Toluene	368	-	393	1.7
21	$CHCl_3$	369	$8.92\ 10^4$	395	1.8
21	THF	366	-	392	1.8
21	DMSO	369	-	398	2.0

Table S2. Solvatochromic data of the 8-substituted quinoline dipolar and octupolar compounds

	solvent	λ_{abs}^{max} [nm]	$\lambda_{\varepsilon m}^{max}$ [nm]	Stokes shift [$10^3 cm^{-1}$])
15	Toluene	382	445	3.7
15	$CHCl_3$	381	480	5.4
15	THF	373	486	6.2
15	acetone	370	523	7.9
15	Acetonitrile	370	552	8.9
15	DMSO	375	541	8.2
16	Toluene	380	450	4.1
16	$CHCl_3$	381	491	5.9
16	THF	375	488	6.2
16	acetone	372	530	8.0
16	Acetonitrile	372	563	9.1
16	DMSO	377	563	8.8
19	Toluene	399	444	2.5
19	$CHCl_3$	397	483	4.5
19	THF	392	481	4.7
19	acetone	388	524	6.7
19	Acetonitrile	386	555	7.9
19	DMSO	392	553	7.4

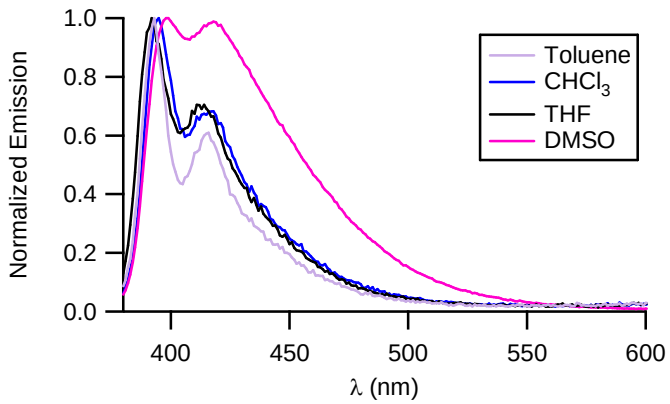


Figure S1. Emission spectra of 6-quinoline quadrupolar derivative **21** in solvents of various polarity.

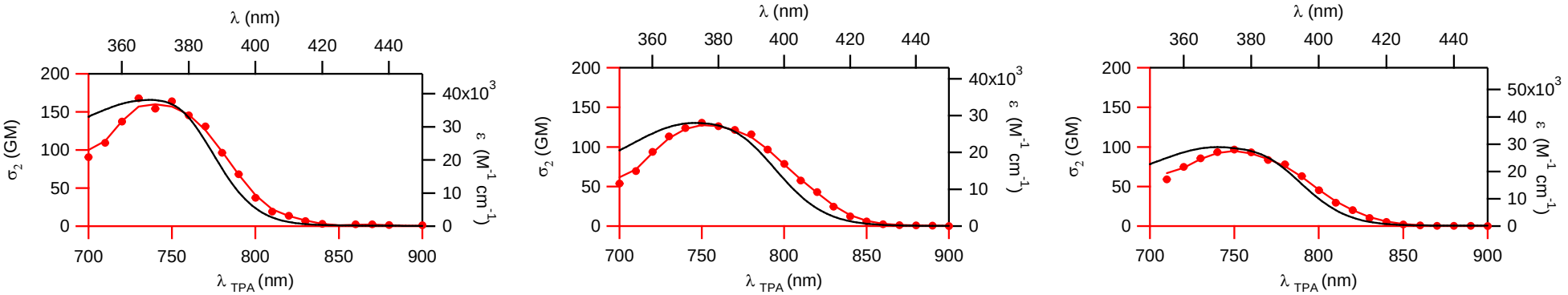


Figure S2. Compared one-photon absorption and two-photon absorption spectra of compounds **5a** (left), **15** (middle) and **13** (right) in THF.