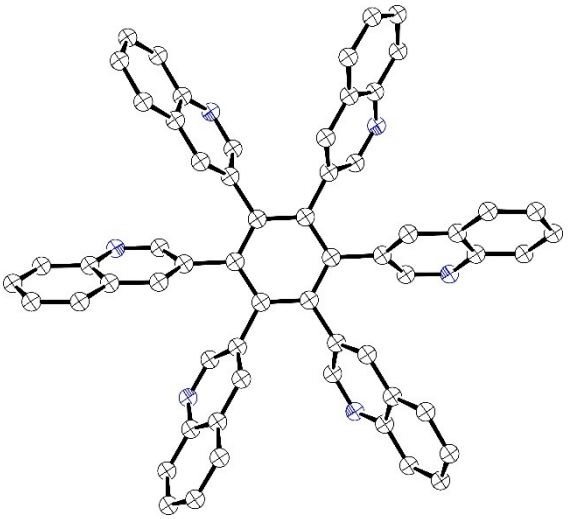
Contents



21 (6,0)

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scf done: -2633.605650

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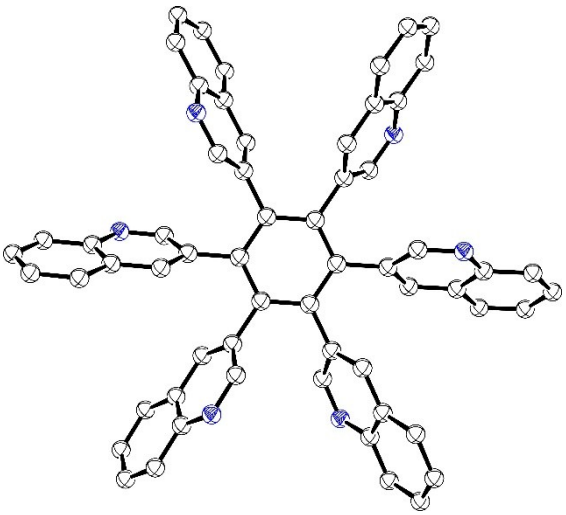

21 (3,3)-1,3,5

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scf done: -2633.607088

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C	4.056047	-0.207177	-5.779170
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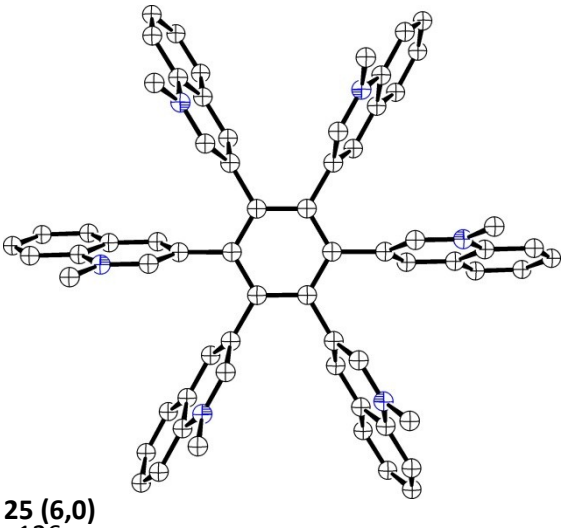

25 (6,0)
126
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H	4.199574	-0.380139	1.875389
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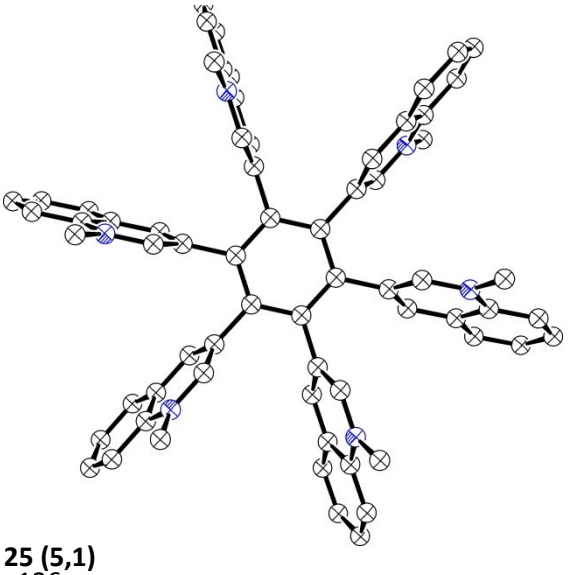

25 (5,1)
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C	-0.022703	-2.914004	-0.054522
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C	-0.012500	2.923559	-0.103802
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C	0.268194	-4.999551	1.178381
C	-0.061435	-5.743096	-0.002785
N	-0.349977	-5.029428	-1.151985
C	-0.337301	-3.692605	-1.175043
C	3.247415	-1.603683	1.060256
C	4.457929	-2.315843	1.076349
C	4.941526	-2.892991	-0.144049
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C	3.025575	-2.041621	-1.265587
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C	-0.234706	3.603516	1.101553
C	-3.343403	1.517870	1.046205
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C	-4.963421	2.947120	-0.101689
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C	-2.992139	-2.086015	1.085885
C	-4.218849	-2.768430	1.132735
C	-5.027744	-2.826805	-0.050118
N	-4.551372	-2.198282	-1.186522
C	-3.385366	-1.544165	-1.195447
C	0.562935	-5.707424	2.371389
C	0.532640	-7.080104	2.388543
C	0.208779	-7.796056	1.212806
C	-0.084802	-7.146961	0.028986
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C	-6.921163	3.721671	1.053060
C	-6.160117	3.681972	-0.099689
C	3.055629	1.934932	1.076973
C	4.277884	2.627528	1.096755
C	4.966499	2.856761	-0.140028
N	4.384804	2.376135	-1.298731
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C	-4.687798	-3.399641	2.313008
C	-5.894540	-4.054872	2.316398
C	-6.675899	-4.105758	1.138812
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C	6.716864	3.997077	1.044051
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H	-0.580584	-3.240161	-2.130403
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H	-4.081676	-3.354303	3.213578
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H	6.730408	3.736694	-1.070900
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H	0.638581	7.907608	-3.069768
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H	-4.827751	-1.721880	-3.216519
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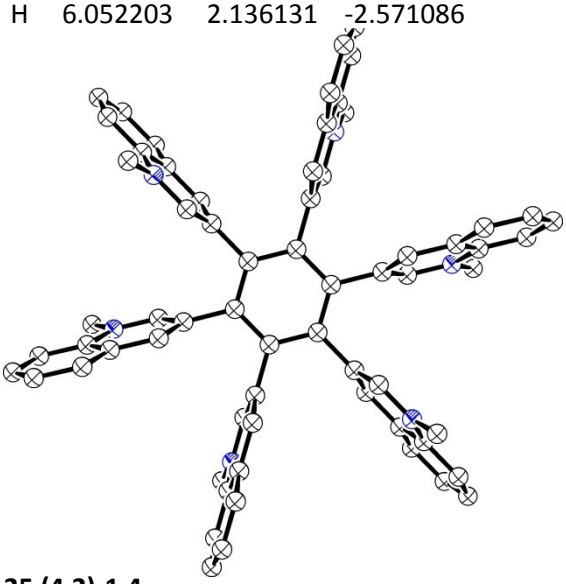

25 (4,2)-1,4

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C	-0.718564	-3.642407	0.240419
C	0.435163	-2.847005	0.249414
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C	0.331011	-1.345655	0.223805
C	0.045595	-0.633940	1.412957
C	-0.057304	0.776849	1.383664
C	0.137657	1.475107	0.168880
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C	0.519377	-0.647801	-0.992318
C	-0.408154	1.535743	2.635853
C	-1.709741	1.930037	2.921197
C	-2.024996	2.635861	4.094485
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N	0.309923	2.558475	4.690634
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C	-1.257293	3.671816	6.190993
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C	-1.444852	-1.587079	3.232397
C	-1.633942	-2.297258	4.430004
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C	-0.646380	-3.522524	6.322446
C	-1.919481	-3.723193	6.820373
C	-3.061947	-3.227686	6.150368
C	-2.921757	-2.526970	4.977660
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C	-0.008016	-2.678010	-4.196800
C	1.346299	-2.835600	-4.641086
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C	2.076127	-1.596191	-2.748174
C	1.625287	-3.541387	-5.823105
C	0.578007	-4.074011	-6.549471
C	-0.764275	-3.925434	-6.129455
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C	1.957388	-3.085537	5.259393
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H	1.925678	-1.783924	3.078202
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H	2.248487	4.163635	-6.087714
H	-4.152685	2.785982	3.715710
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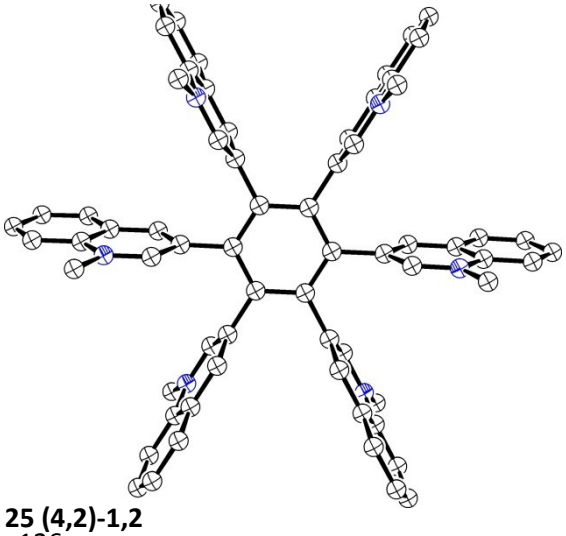

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C	3.097754	-1.776340	-1.163013
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C	-3.121097	-2.037900	1.156276
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N	4.118302	2.689669	-1.199269
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H	-7.729722	-4.632884	1.115729
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H	7.673885	4.386534	1.109526
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H	-0.378917	5.368049	-3.335285
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H	-4.753853	-1.881510	-3.239345
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H	4.689953	4.298566	-2.441097
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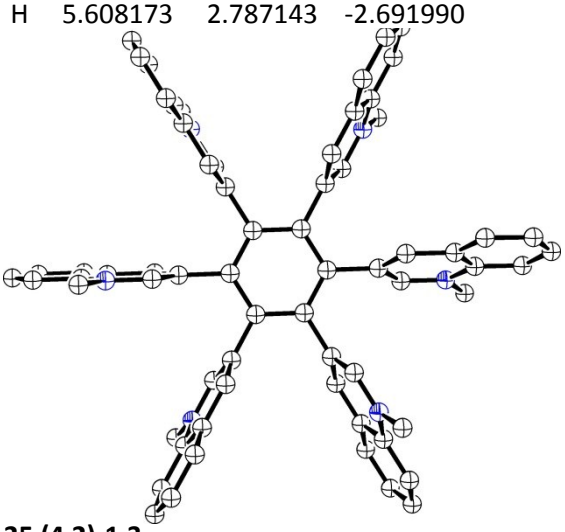

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126

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C	-0.805131	8.614334	2.394902
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C	-0.158058	9.557706	4.549735
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C	1.431803	4.144350	5.133124
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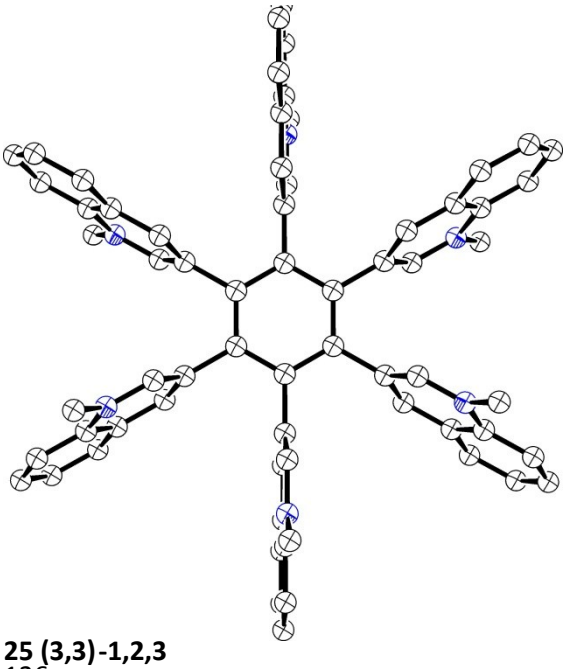

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126
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C	0.078123	7.866917	1.190244
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C	0.030335	5.737705	-0.021517
C	-0.093418	6.436734	-1.245295
C	0.166549	8.627008	2.485994
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C	1.420574	9.513112	4.382244
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C	2.634033	9.700132	5.091744
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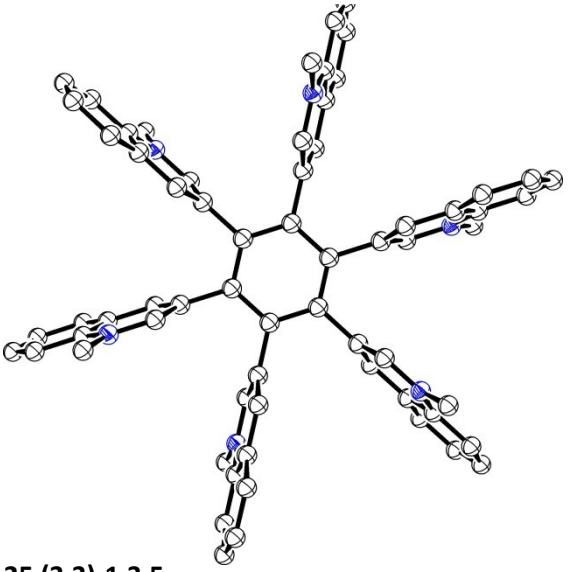

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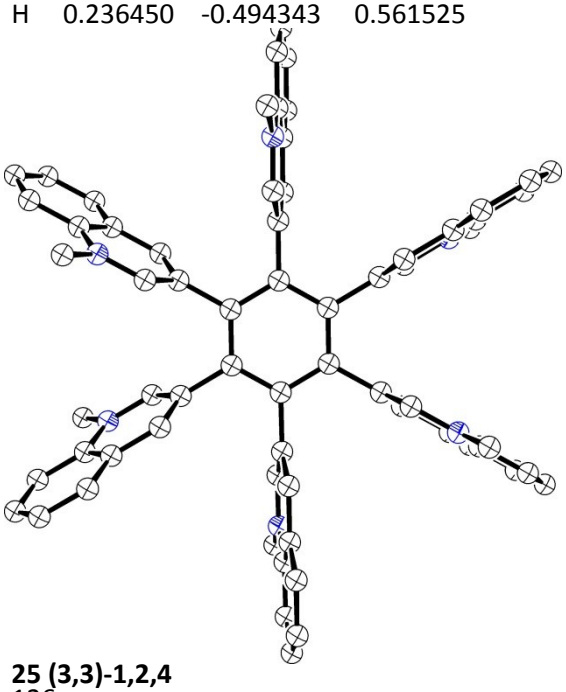

25 (3,3)-1,2,4
126
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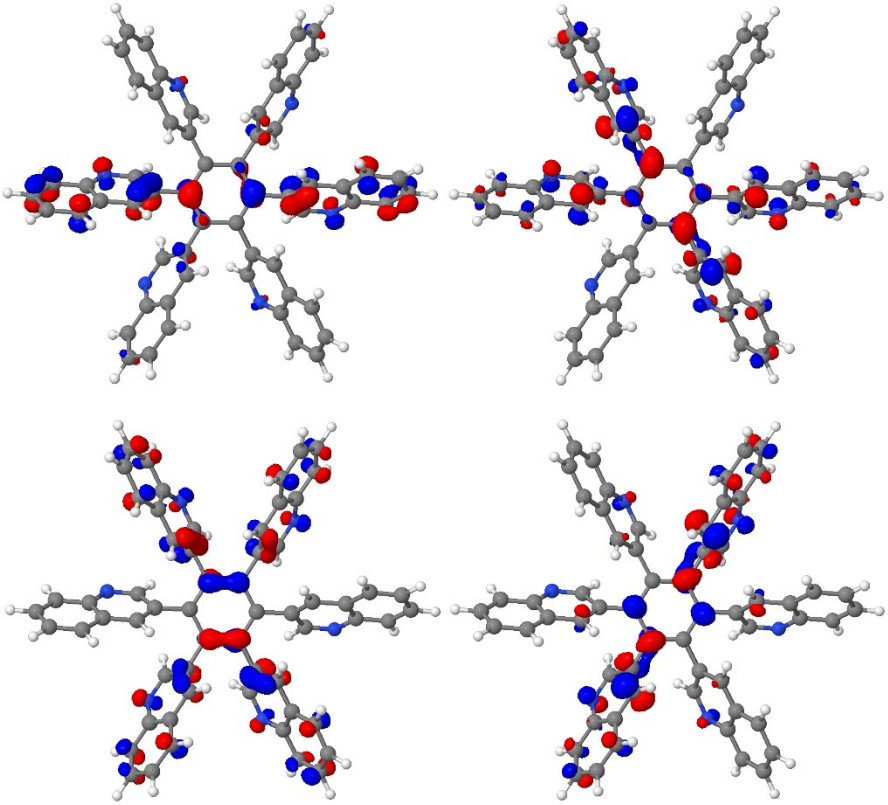
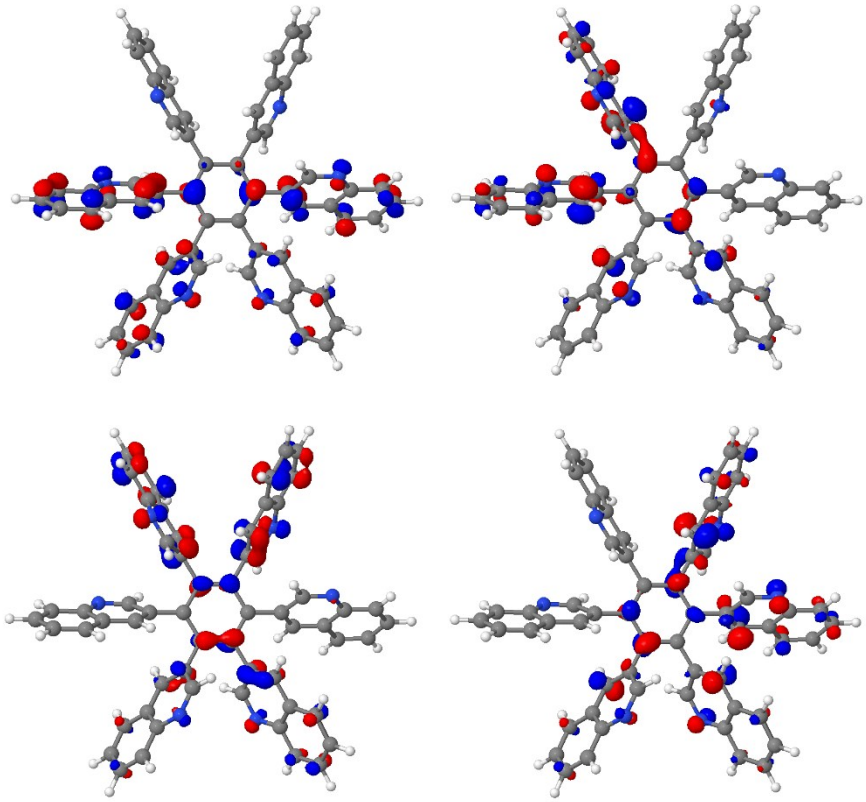
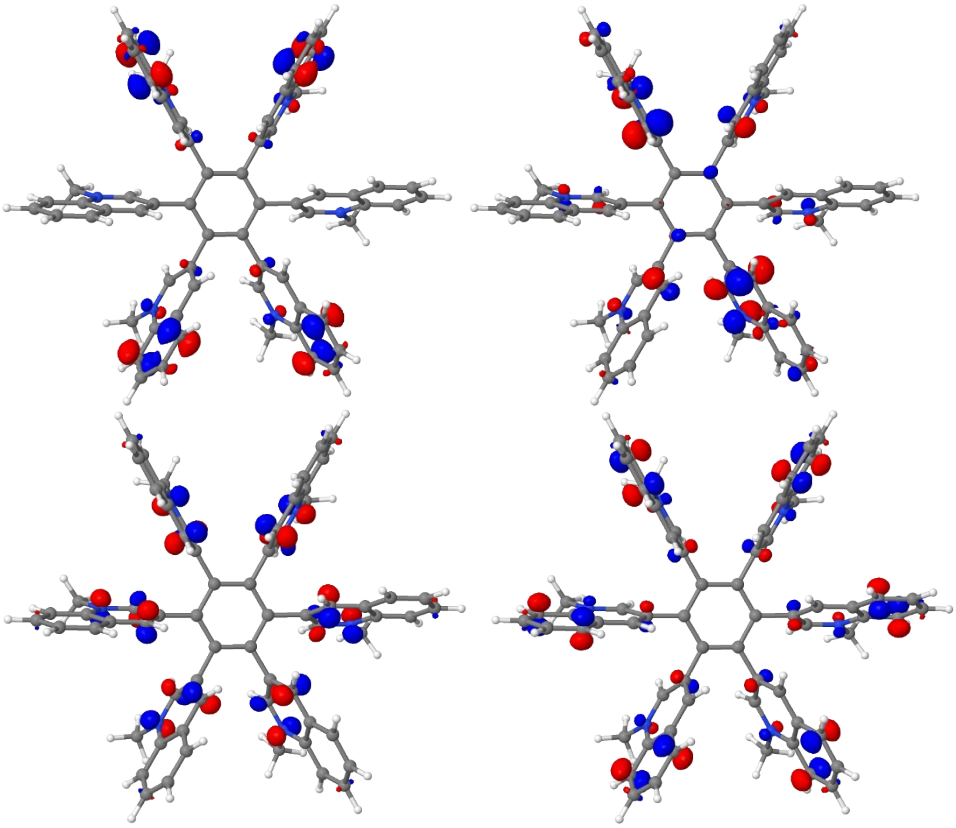
HOMO/LUMO (above) and HOMO-1/LUMO+1 (below) profiles of **21 (6,0)** rotamer



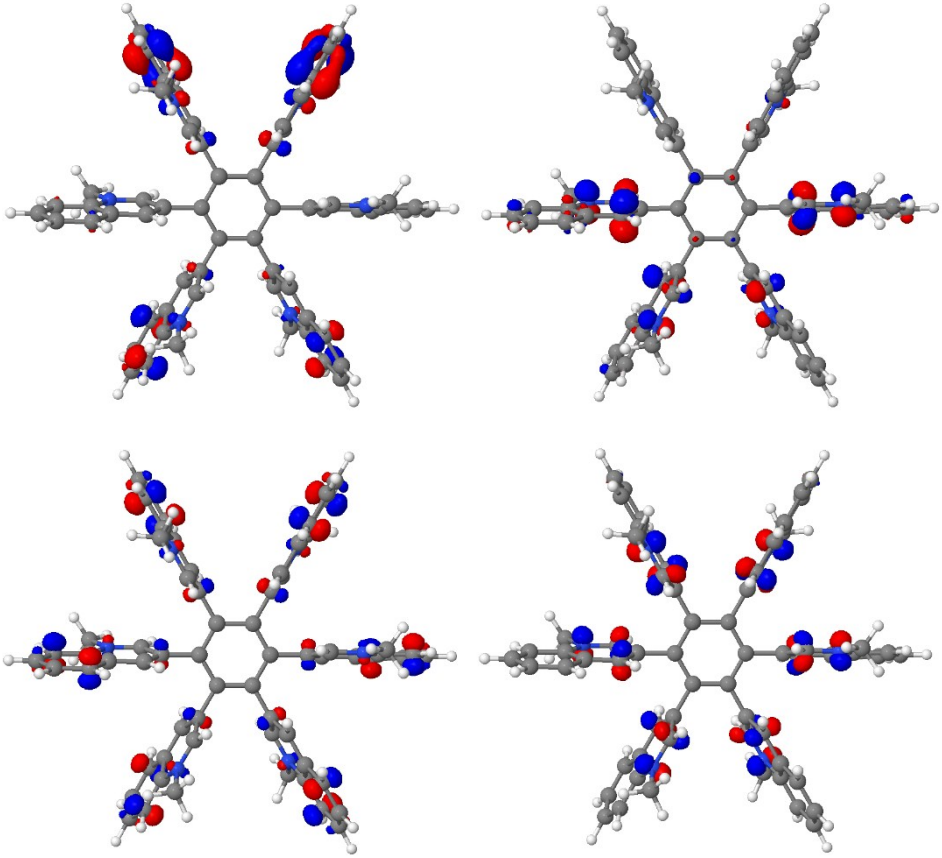
HOMO/LUMO (above) and HOMO-1/LUMO+1 (below) profiles of **21 (3,3)-1,3,5** rotamer



HOMO-1/LUMO+1 (above) and HOMO/LUMO (below) profiles of **25 (6,0)** rotamer

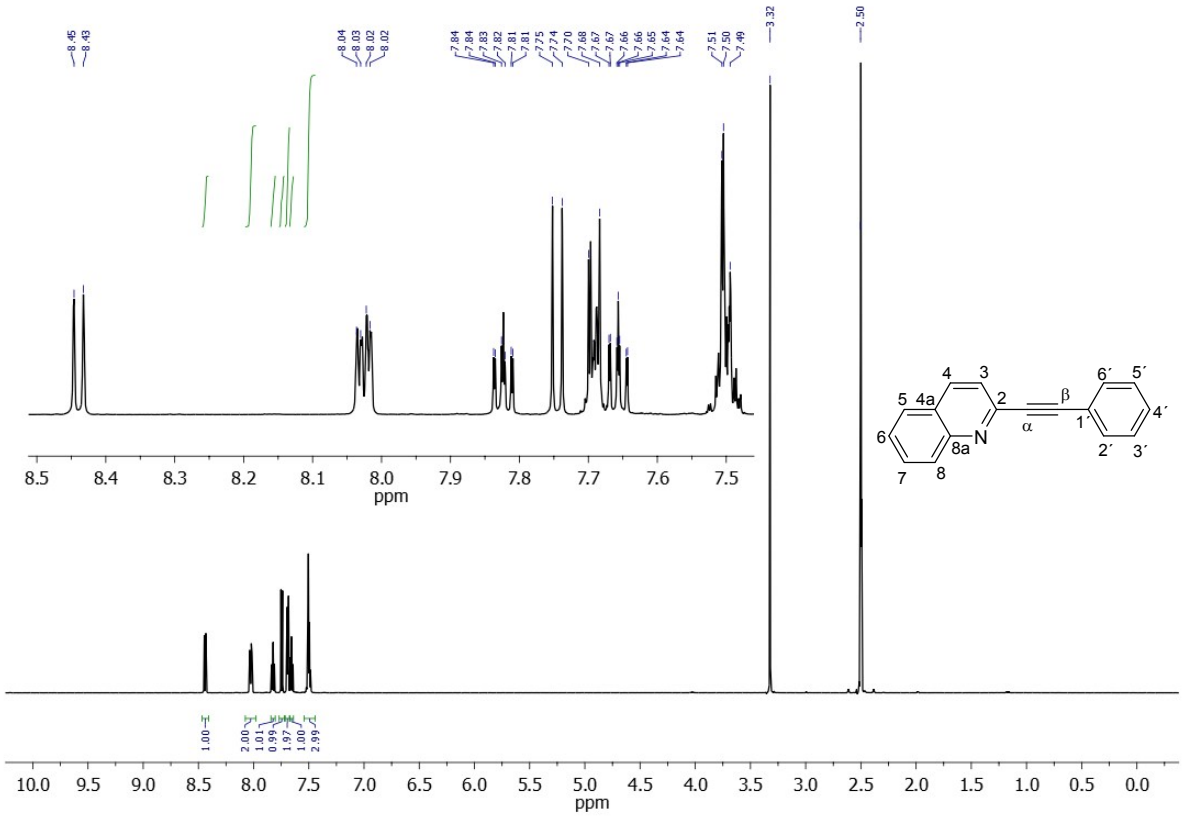


HOMO-1/LUMO+1 (above) **and** HOMO/LUMO (**below**) profiles **of 25 (3,3)-1,3,5** rotamer

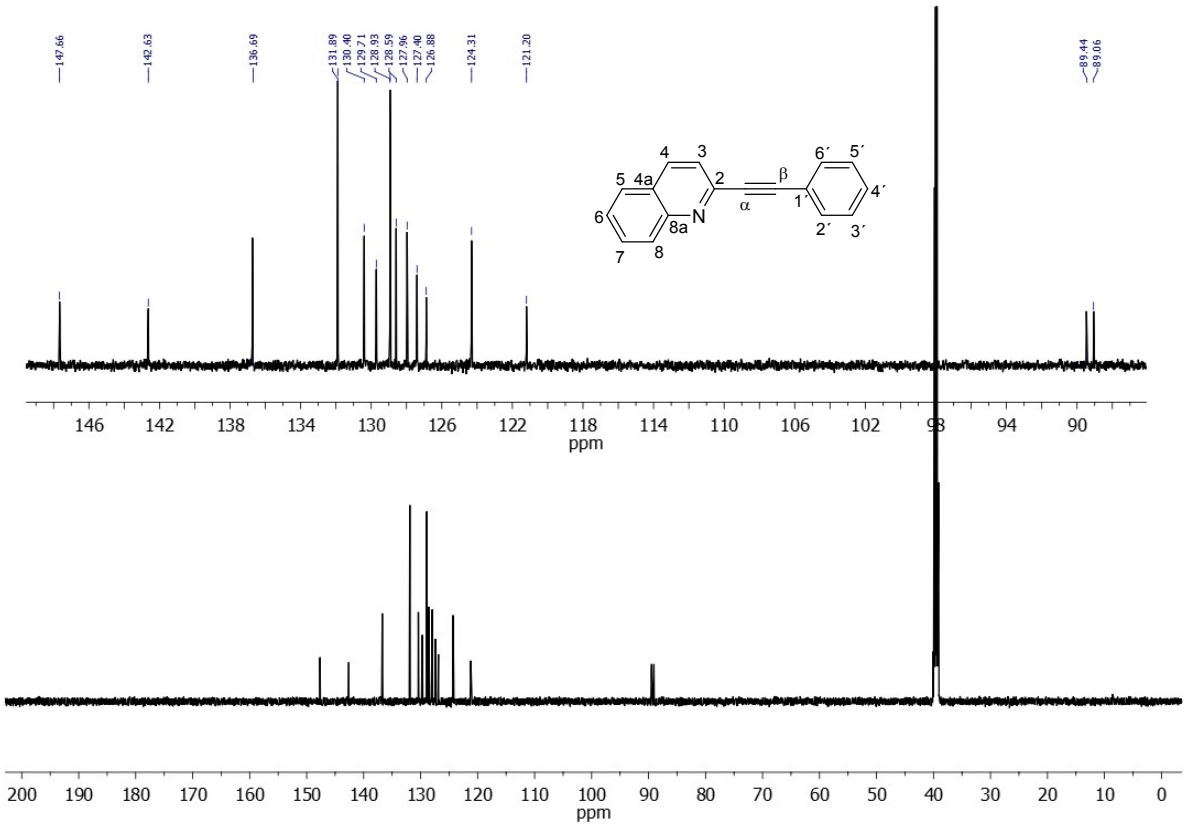


2-(Phenylethynyl)quinoline (8a)

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

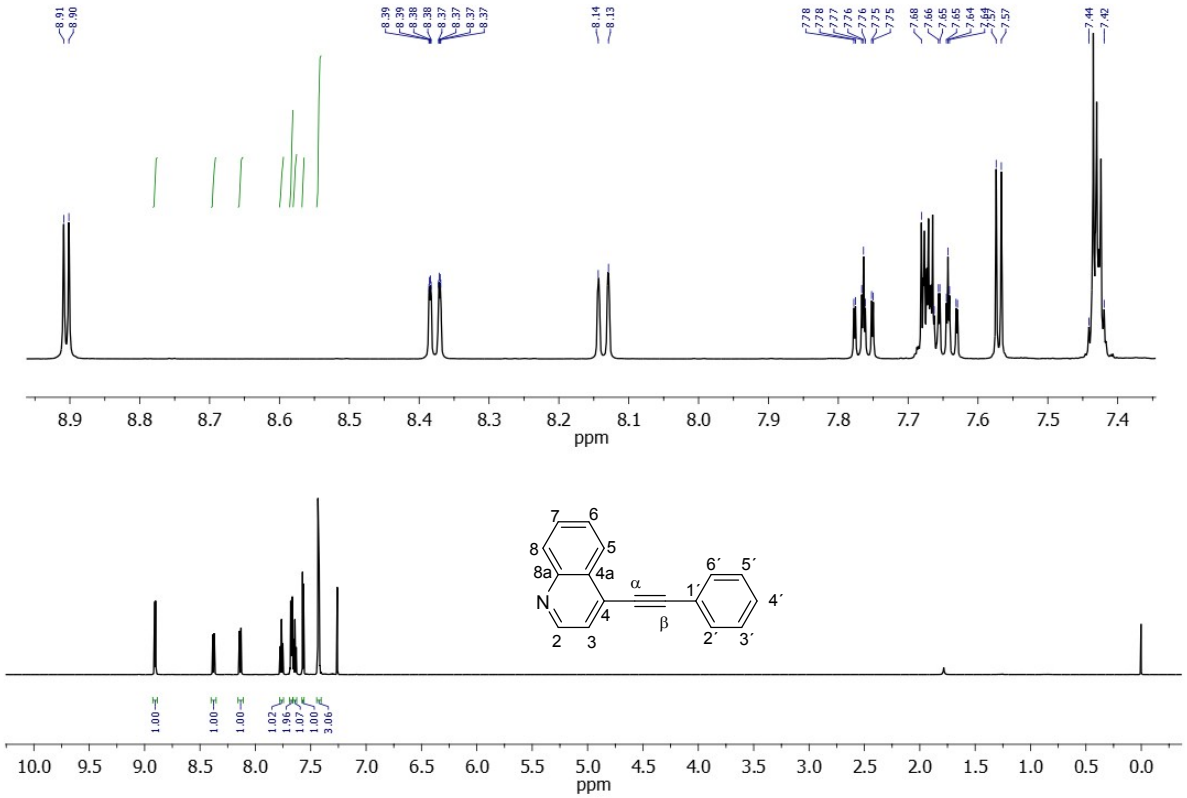


^{13}C NMR (150 MHz, $CDCl_3$)

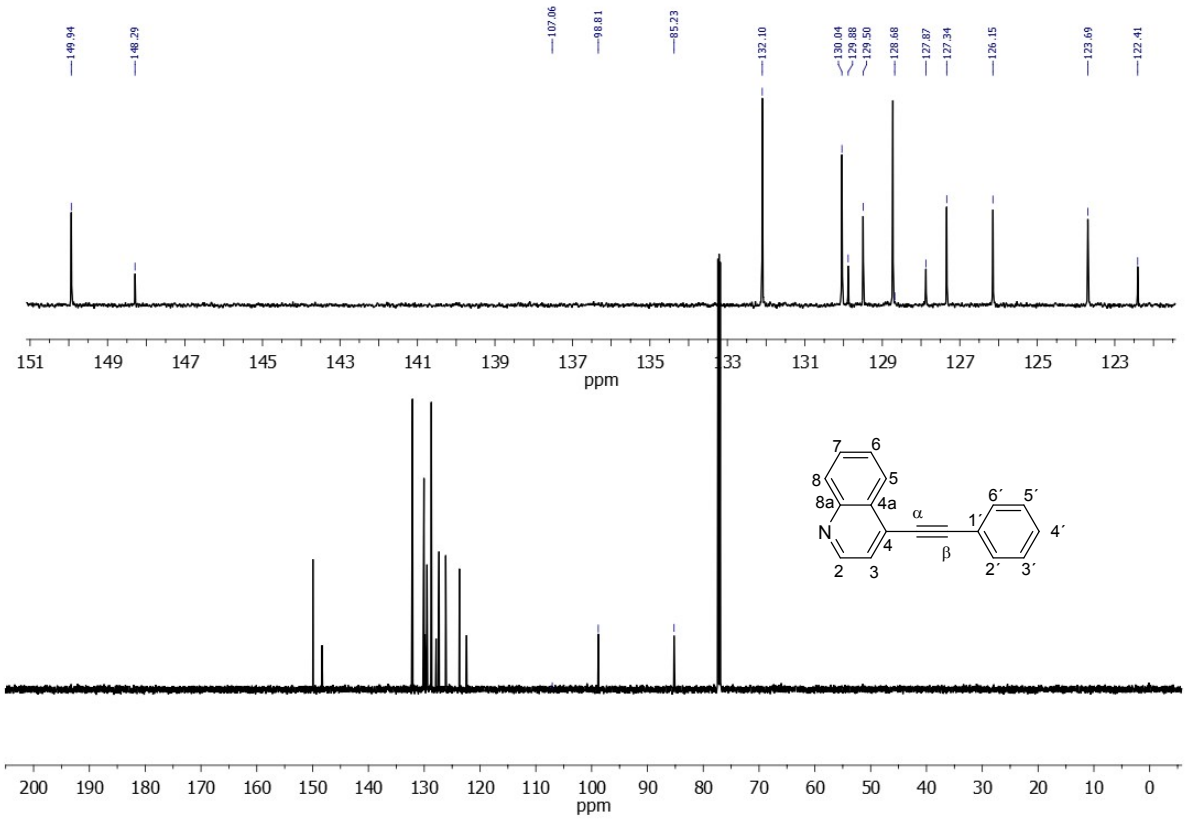


4-(Phenylethynyl)quinoline (8c)

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

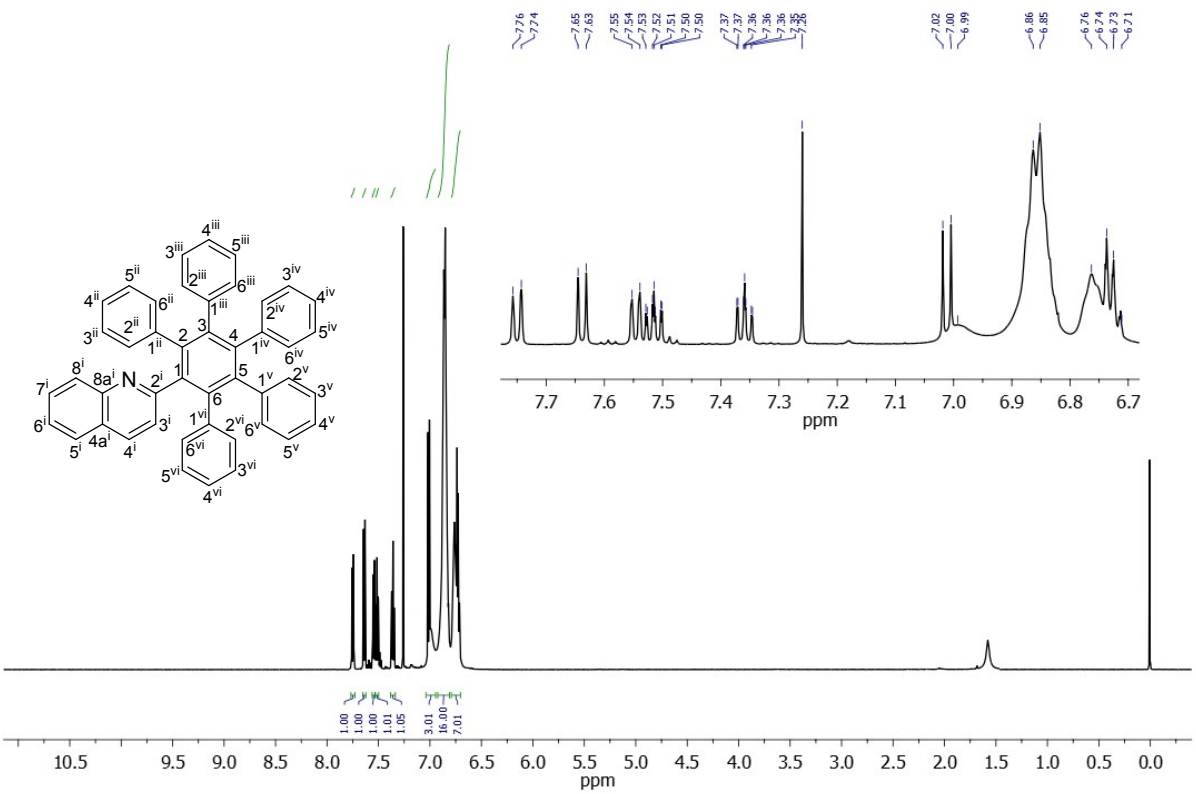


^{13}C NMR (150 MHz, $CDCl_3$)

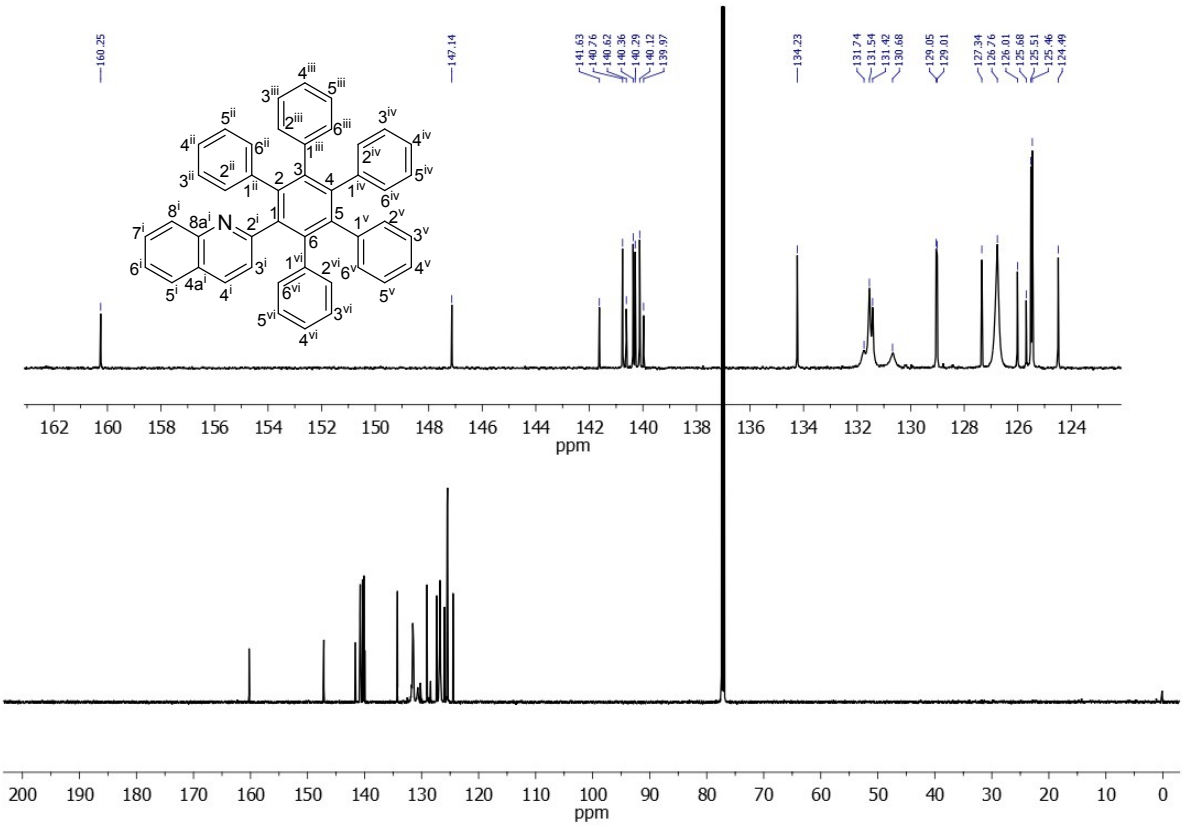


2,3,4,5,6-Pentaphenyl-1-(quinoline-2-yl)benzene (10a)

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

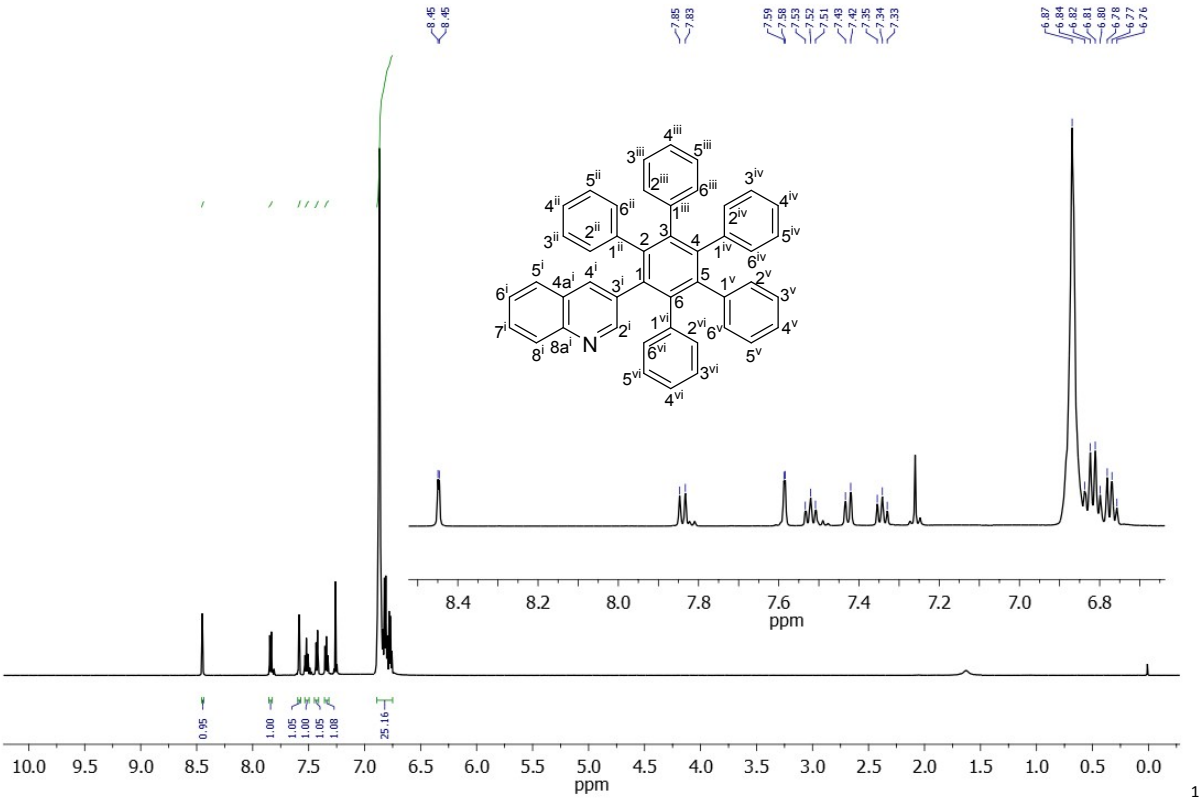


^{13}C NMR (150 MHz, $CDCl_3$)



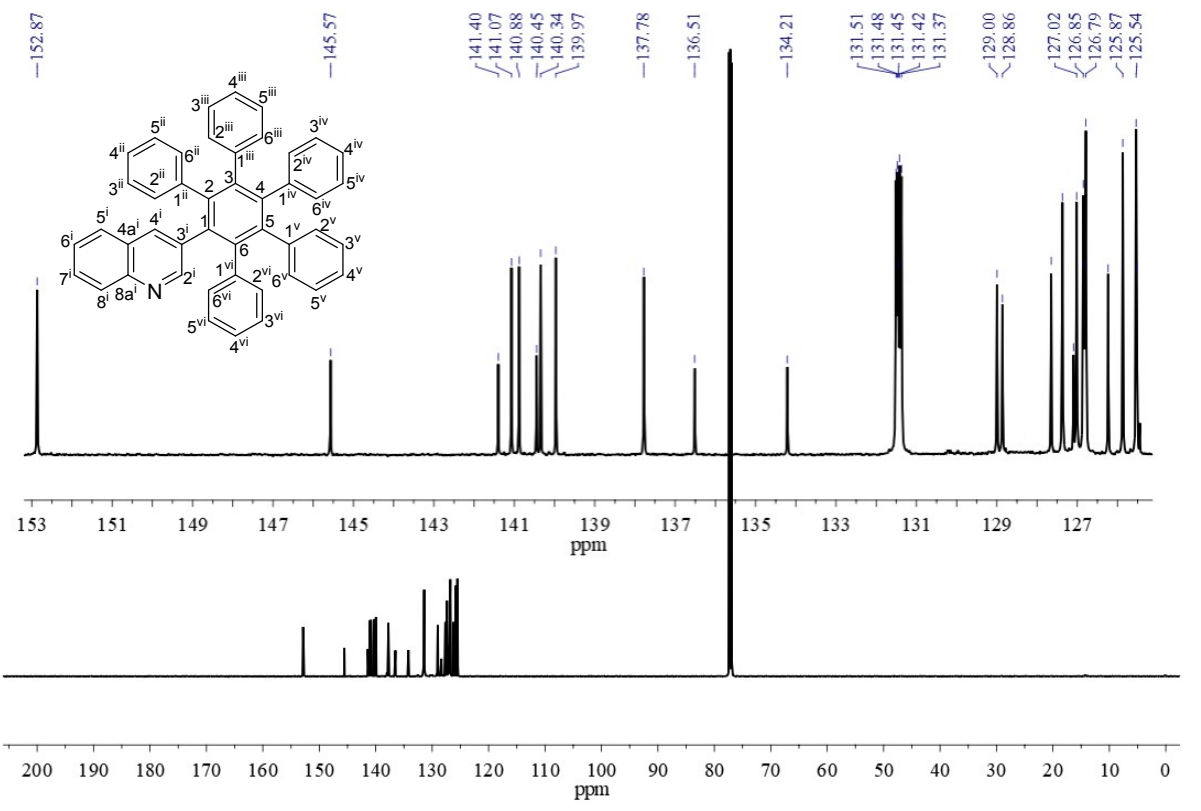
2,3,4,5,6-Pentaphenyl-1-(quinoline-3-yl)benzene (10b)

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



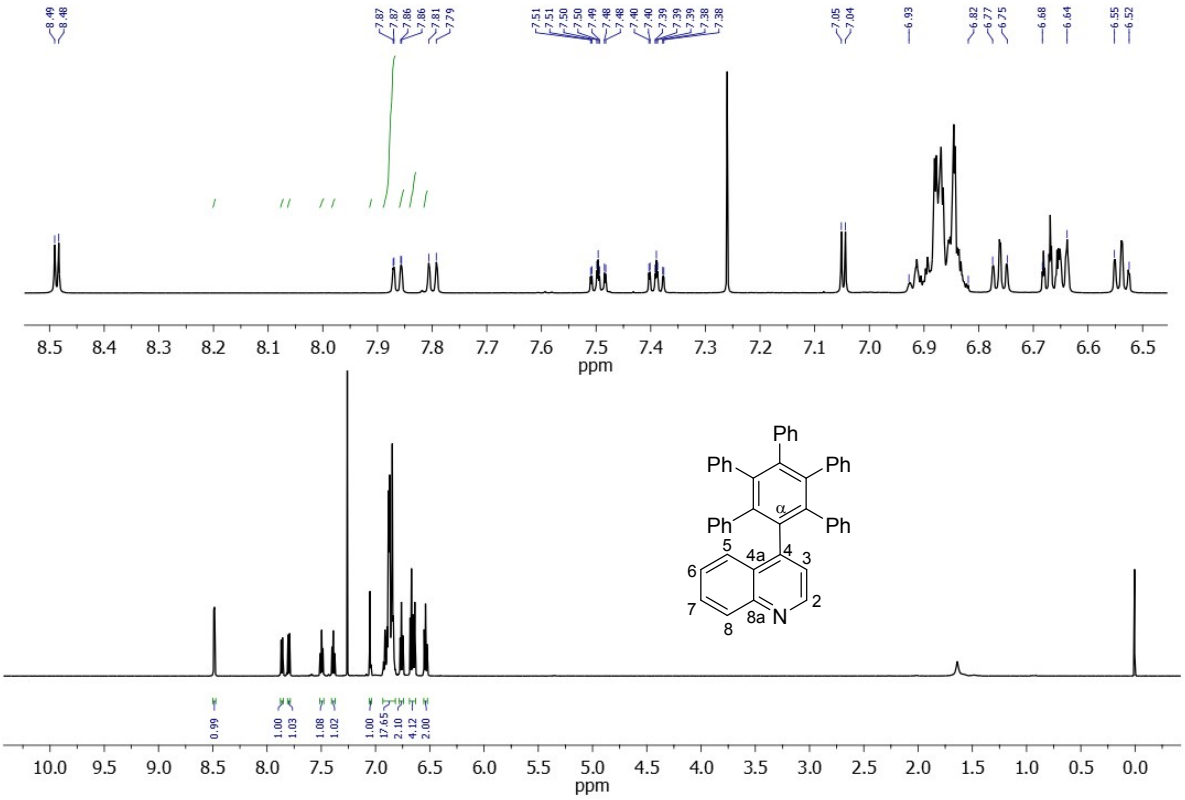
1

^{3}C MNR (150 MHz, $CDCl_3$)

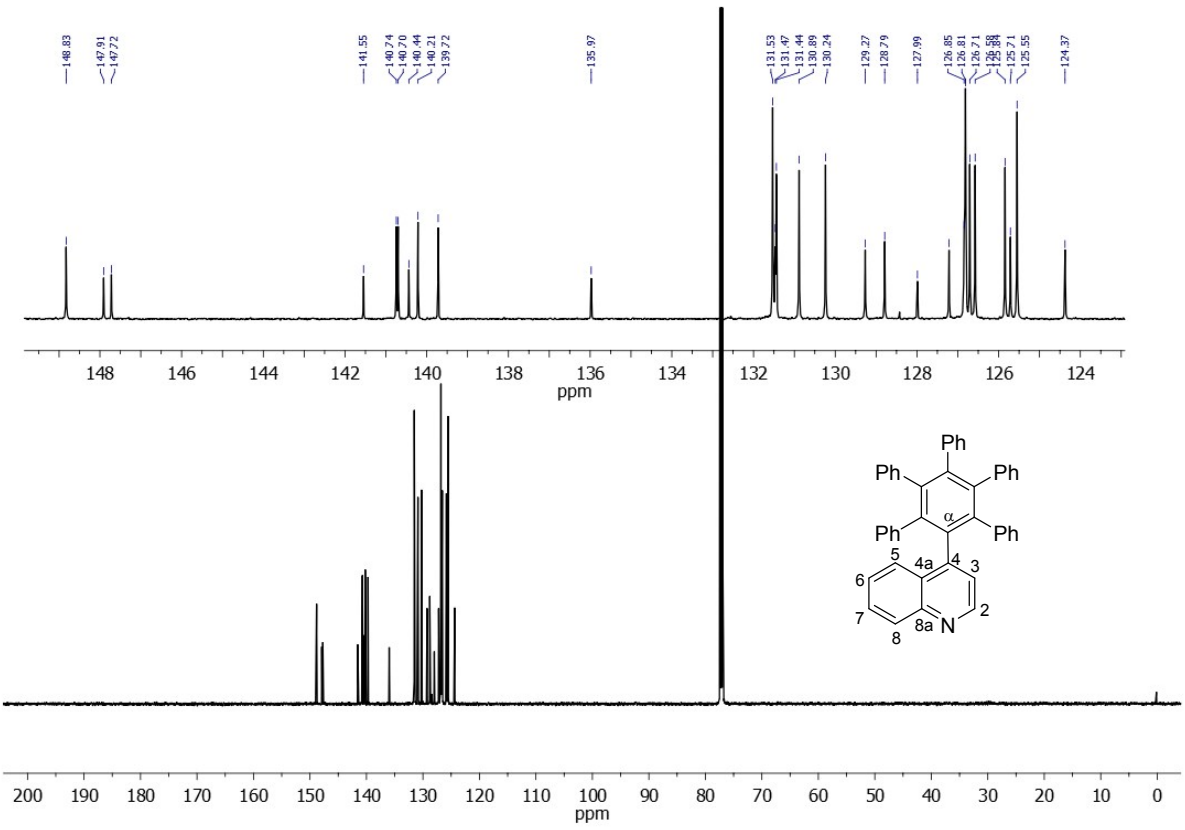


2,3,4,5,6-Pentaphenyl-1-(quinoline-4-yl)benzene (10c)

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

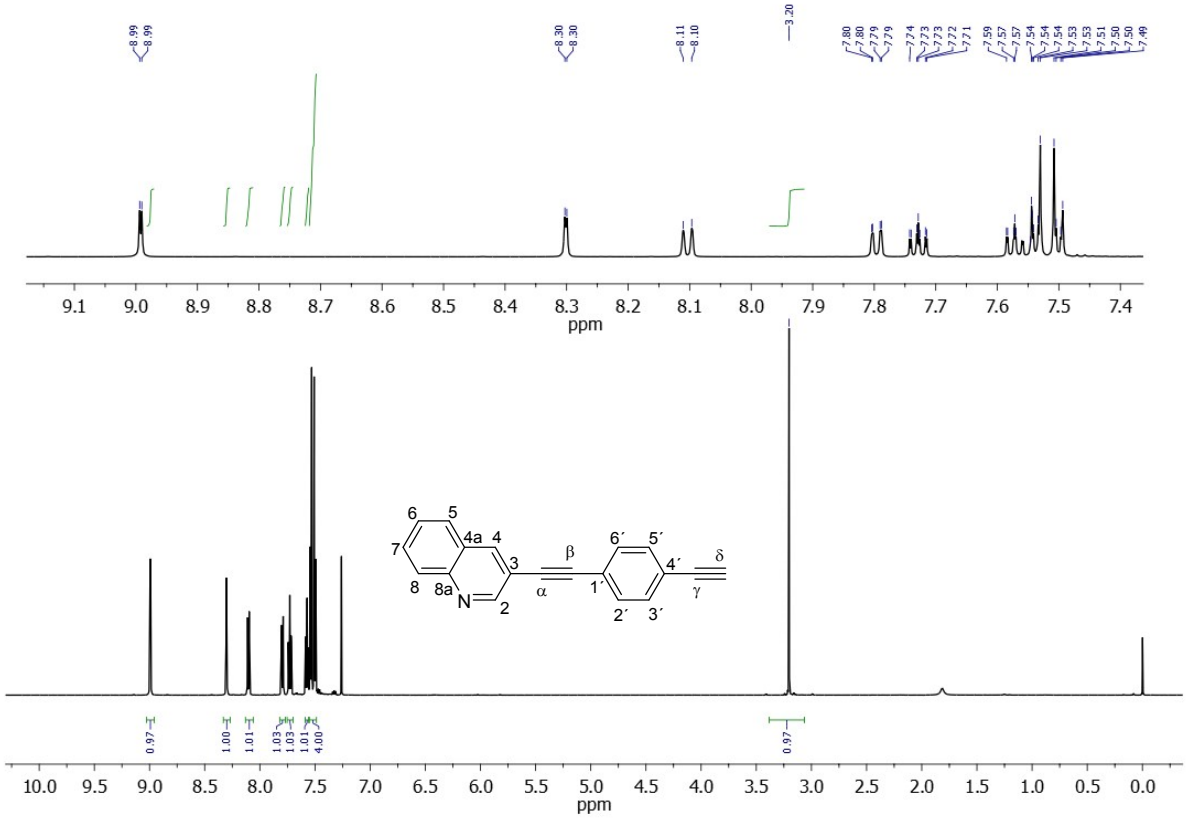


^{13}C NMR (150 MHz, $CDCl_3$)

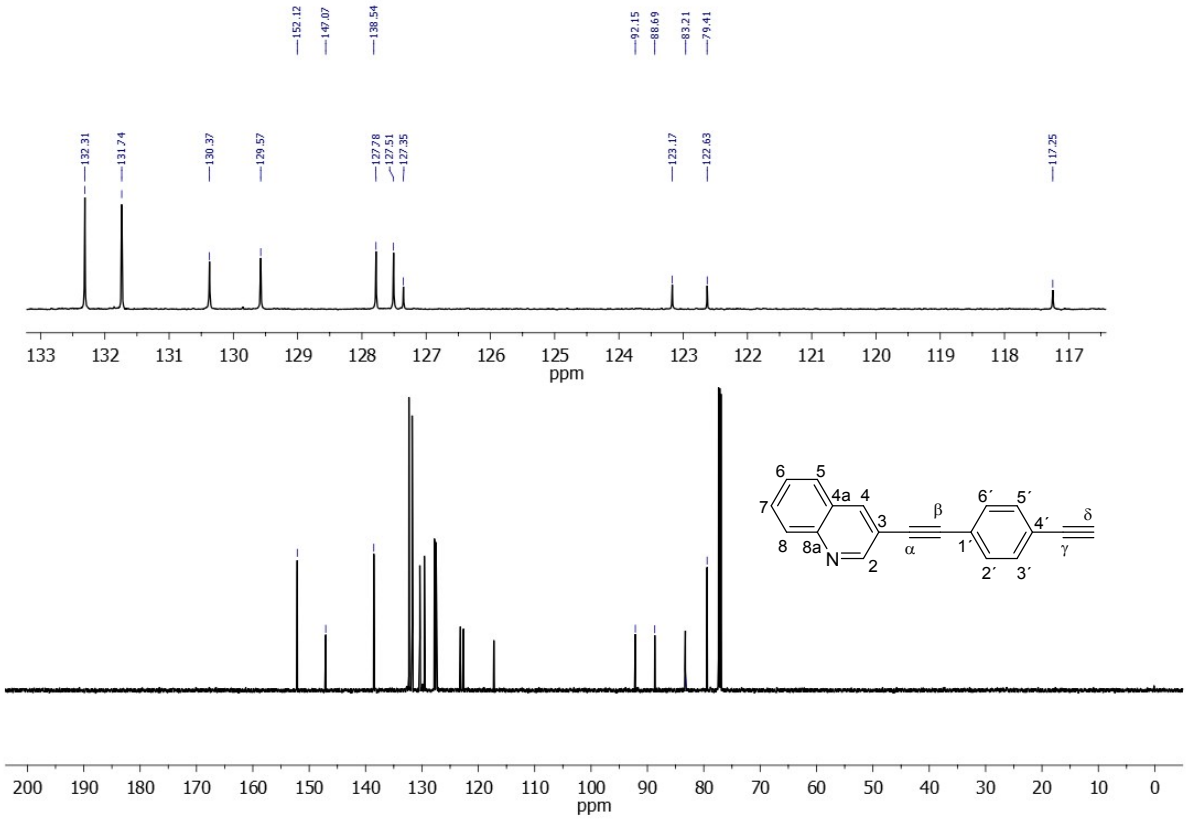


3-((4-Ethynylphenyl)ethynyl)quinoline (14)

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

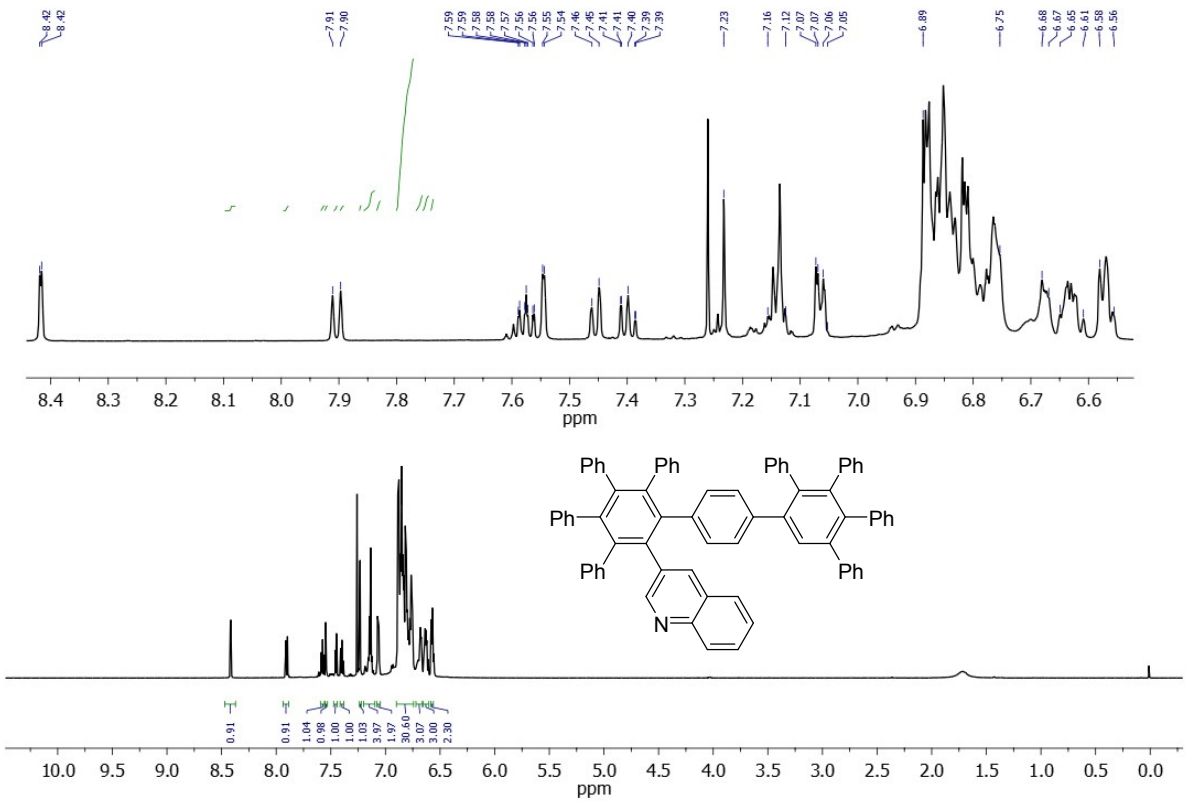


^{13}C NMR (150 MHz, $CDCl_3$)

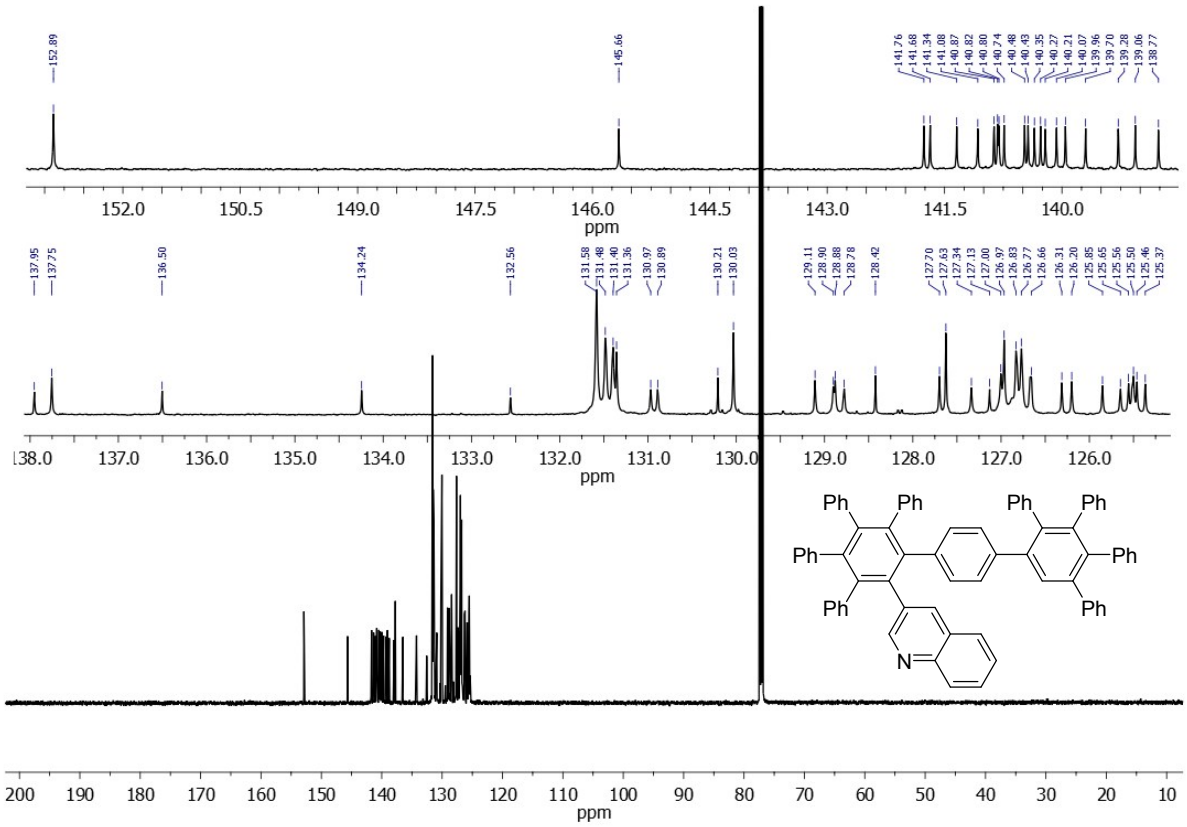


1-(Quinolin-3-yl)-2,3,4,5,-tetraphenyl-6-(4-(1,2,3,4-tetraphenyl)phenyl)-benzene (15)

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

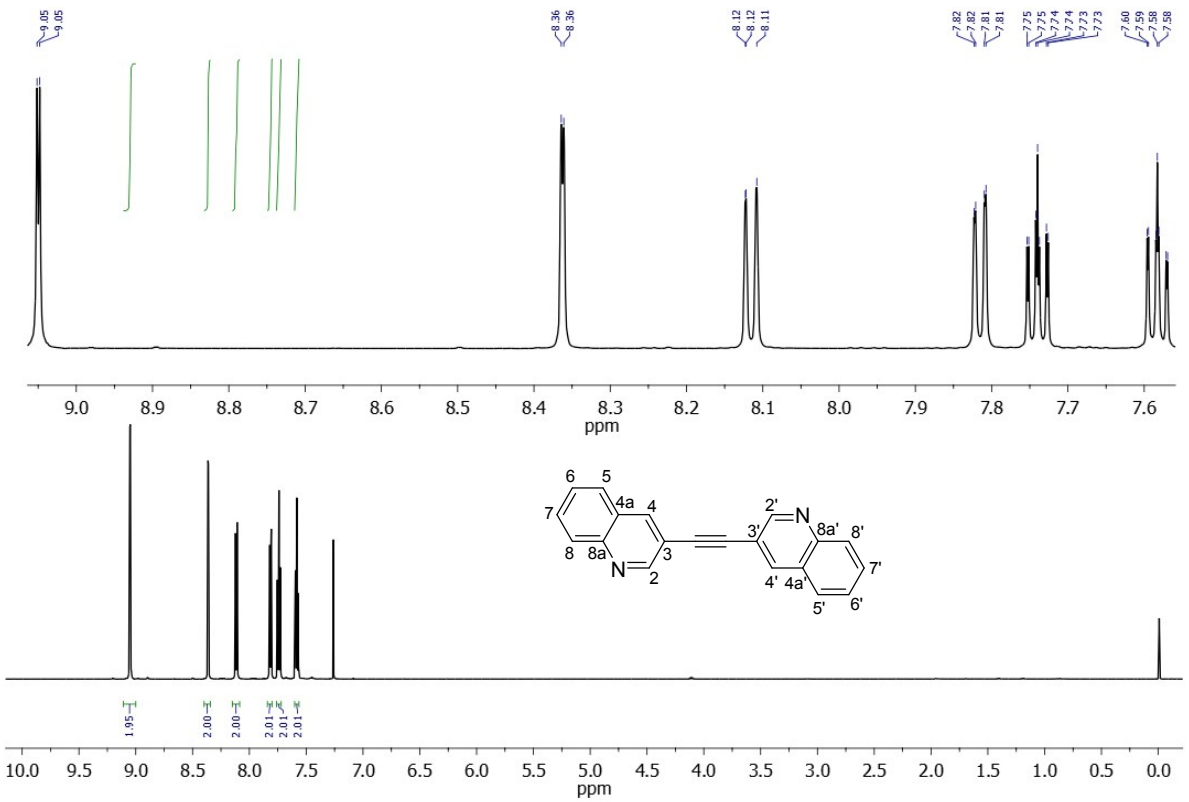


^{13}C NMR (150 MHz, $CDCl_3$)

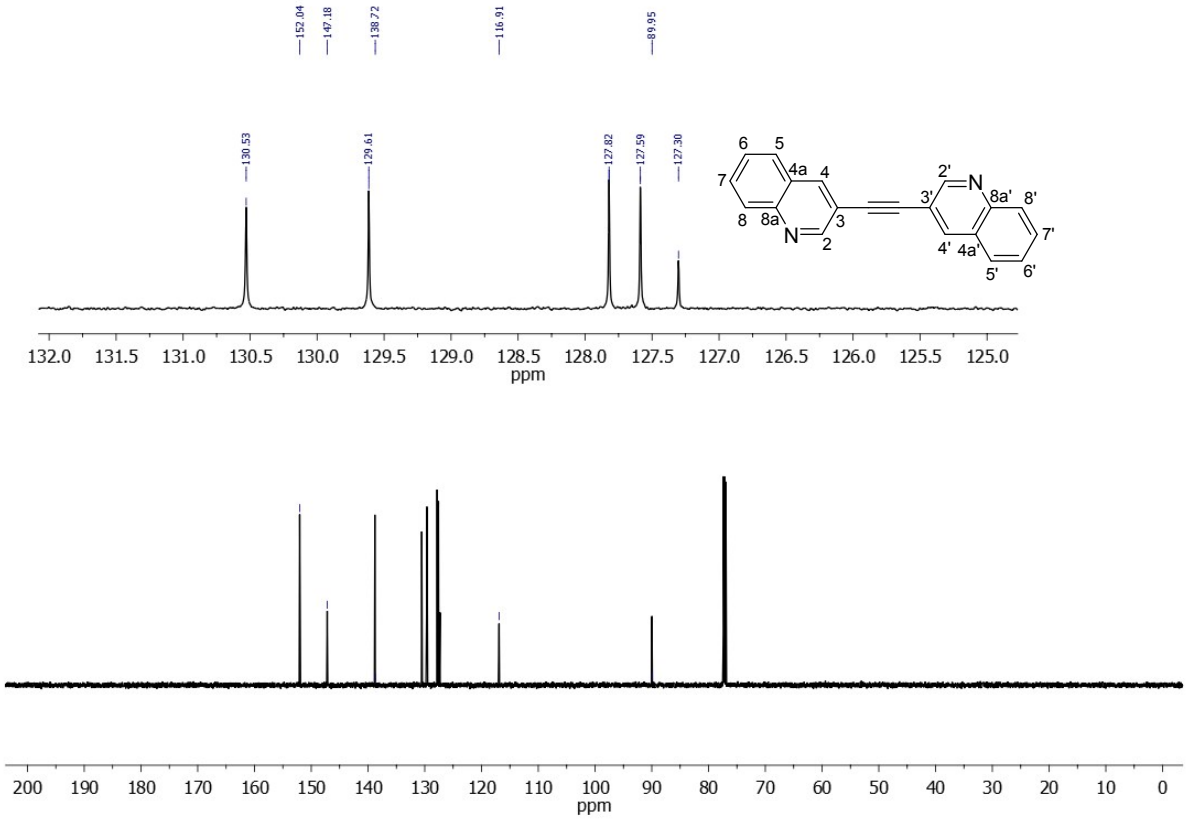


3,3'-Ethyne-1,2-diyldiquinoline (18a)

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

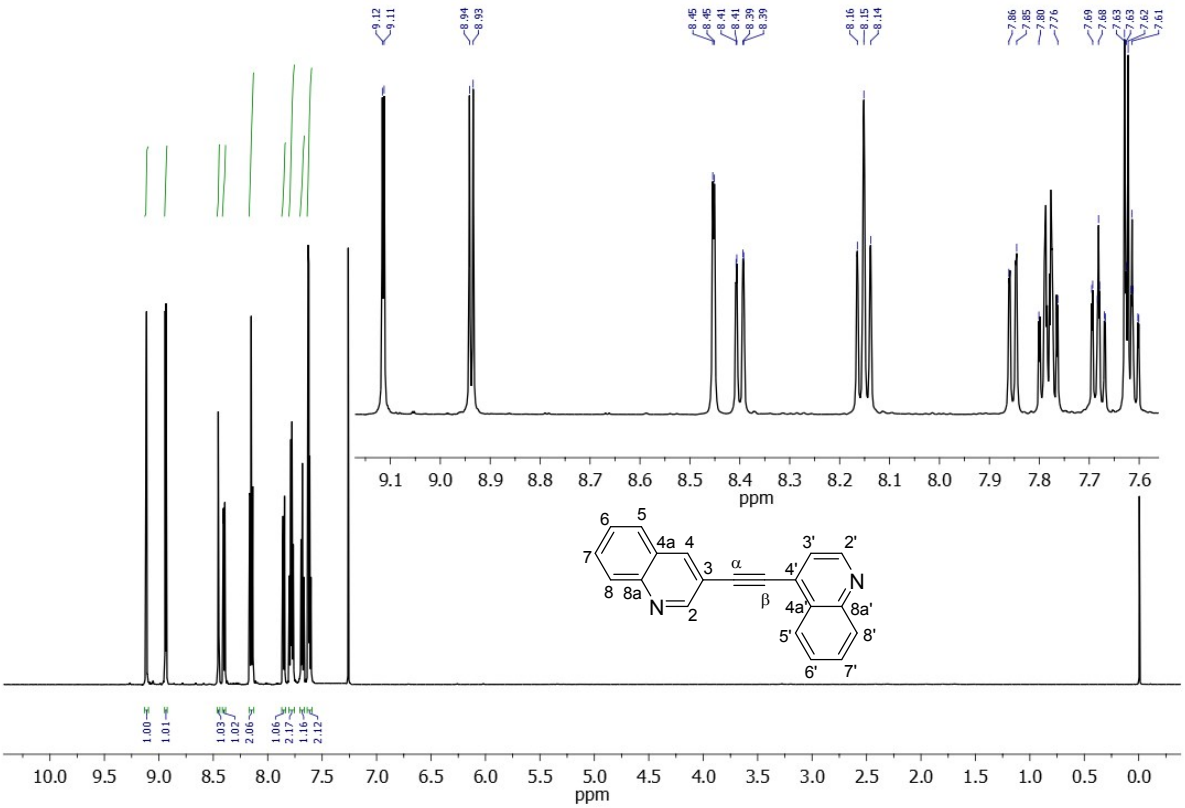


^{13}C NMR (150 MHz, $CDCl_3$)

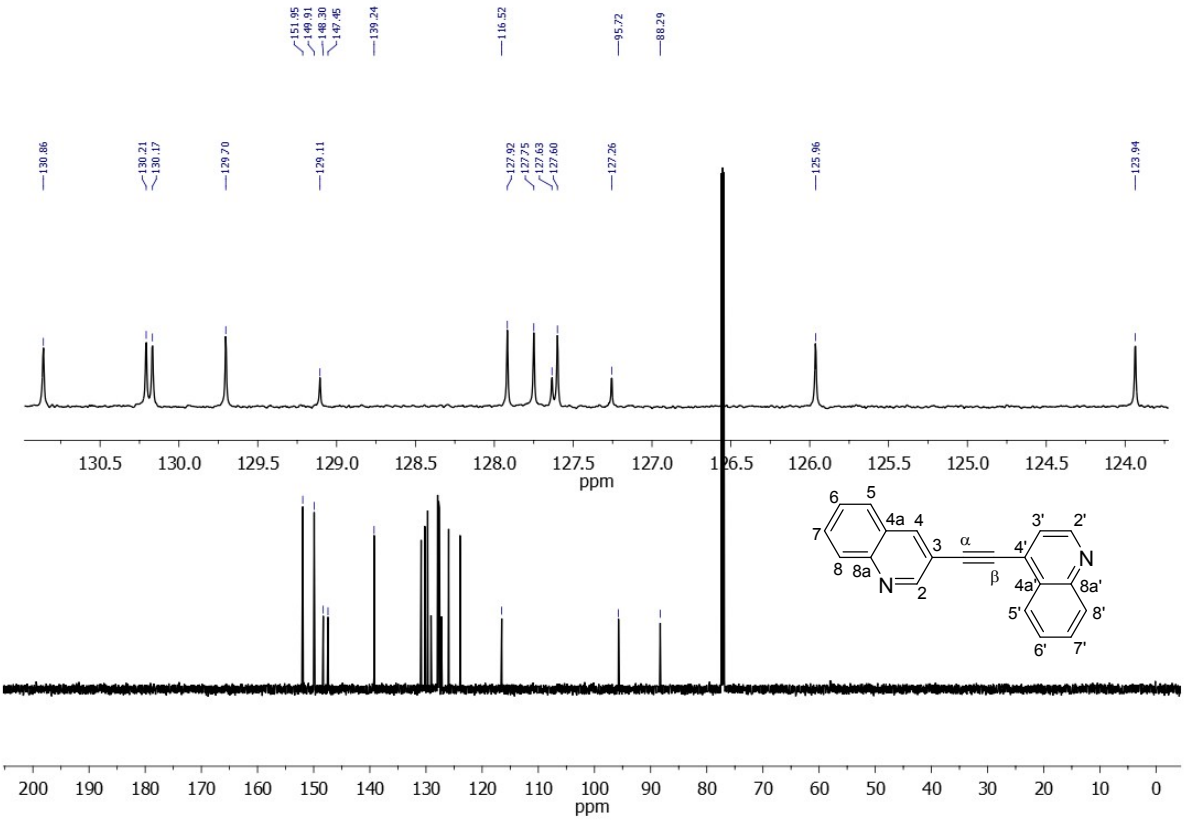


3-(Quinolin-4-ylethynyl)quinoline (18b)

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

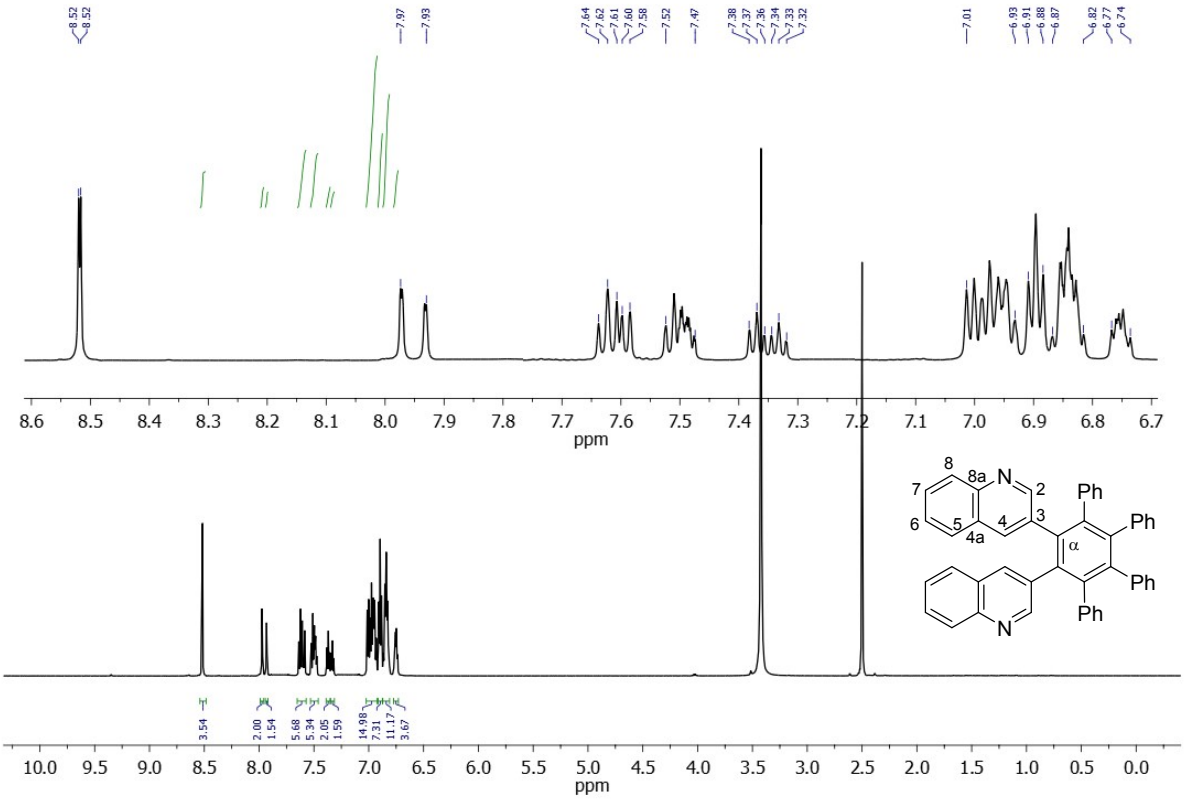


^{13}C NMR (150 MHz, $CDCl_3$)

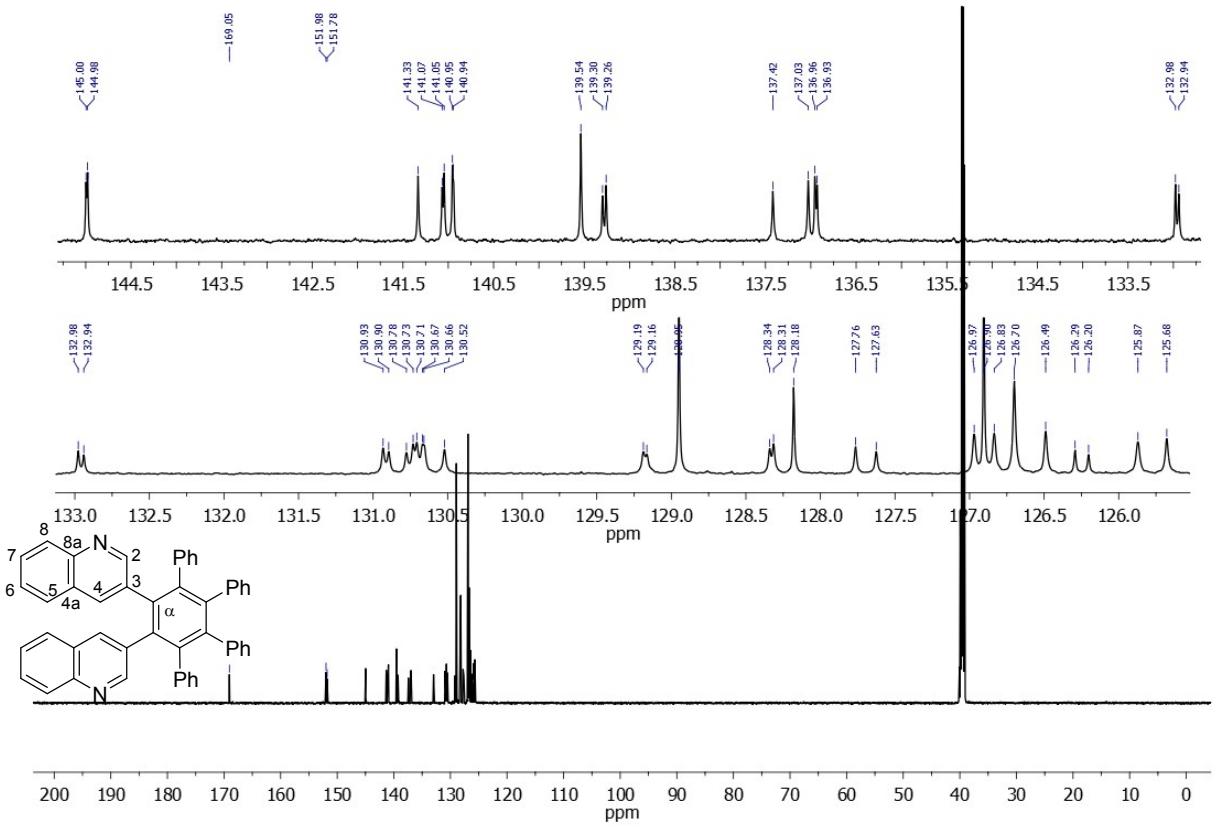


1,2-Di(quinoline-3-yl)-3,4,5,6-tetraphenylbenzene (19a)

^{1}H NMR (600 MHz, DMSO-d_6)

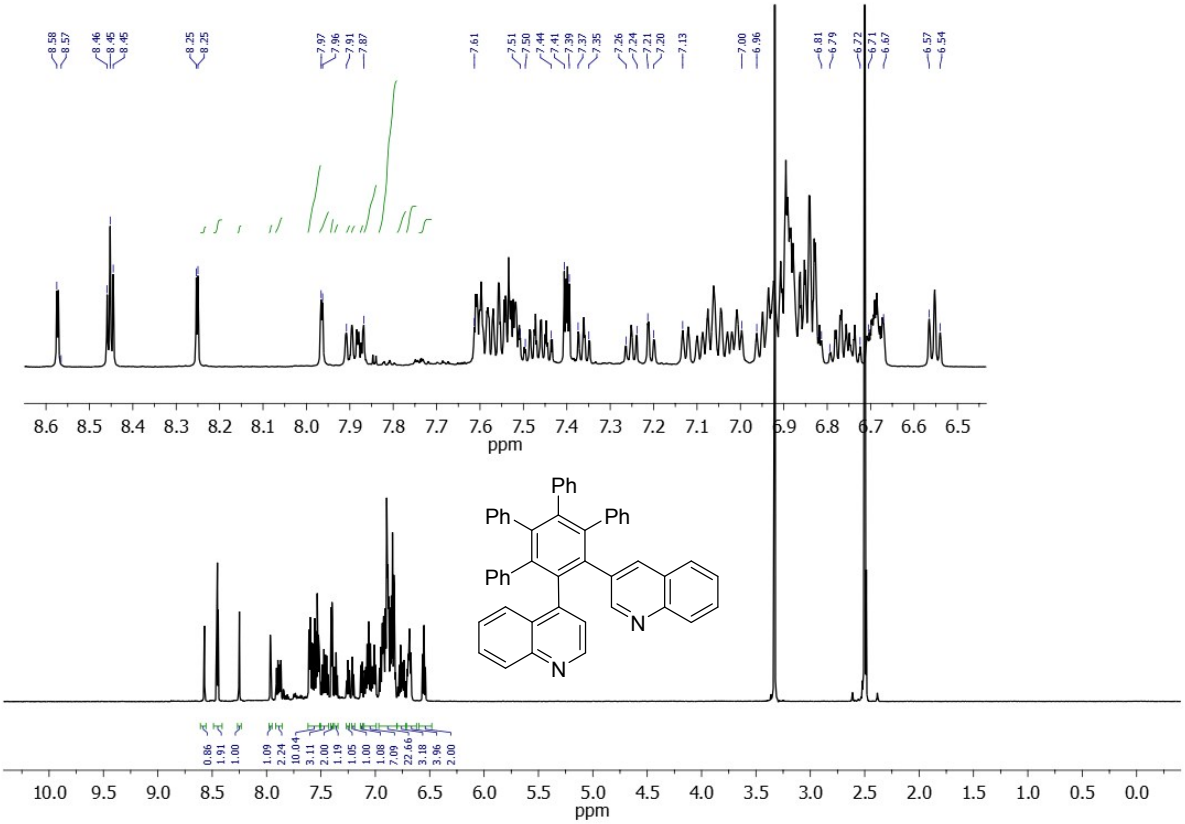


^{13}C NMR (150 MHz, DMSO-d_6)

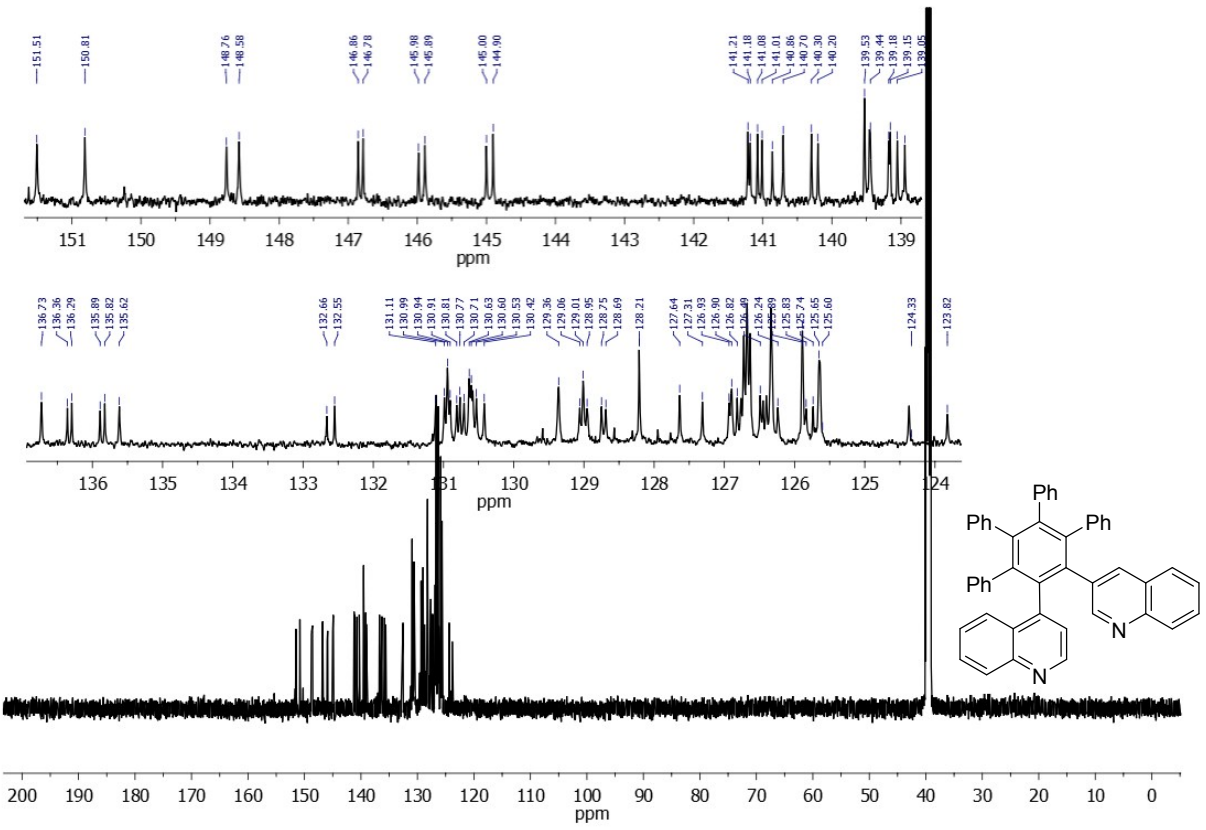


1-(Quinoline-3-yl)-2-(quinoline-4-yl)-3,4,5,6-tetraphenylbenzene (19b)

^{1}H NMR (600 MHz, DMSO-d_6)

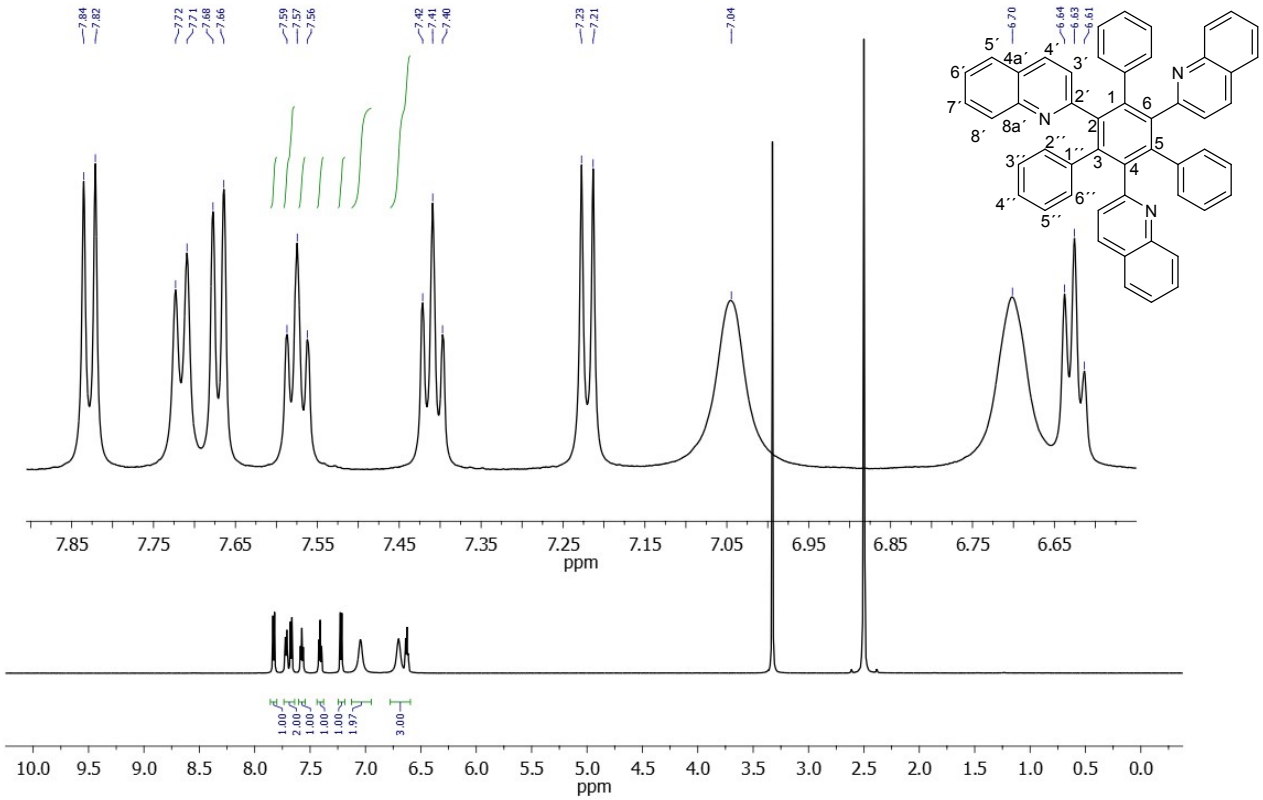


^{13}C NMR (150 MHz, DMSO-d_6)

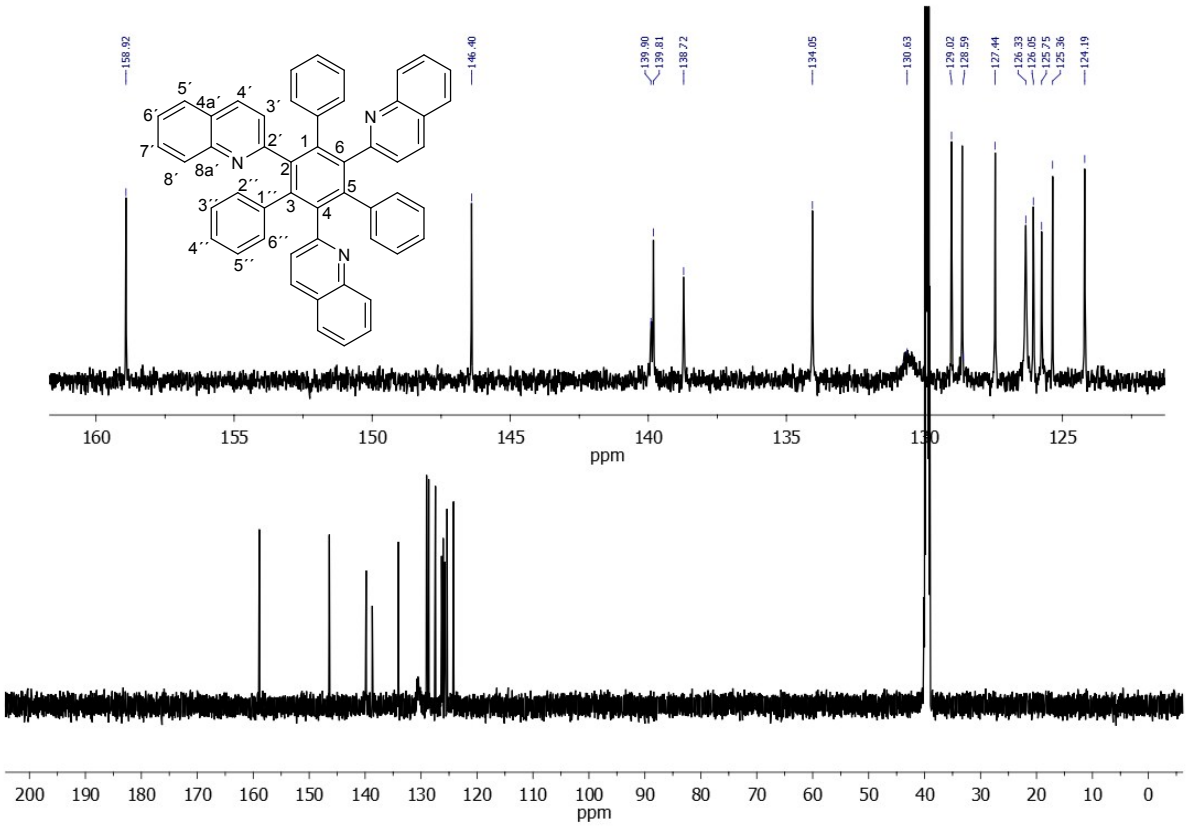


1,3,5-Triphenyl-2,4,6-tri(quinoline-2-yl)benzene (20a)

^{1}H NMR (600 MHz, DMSO-d_6)

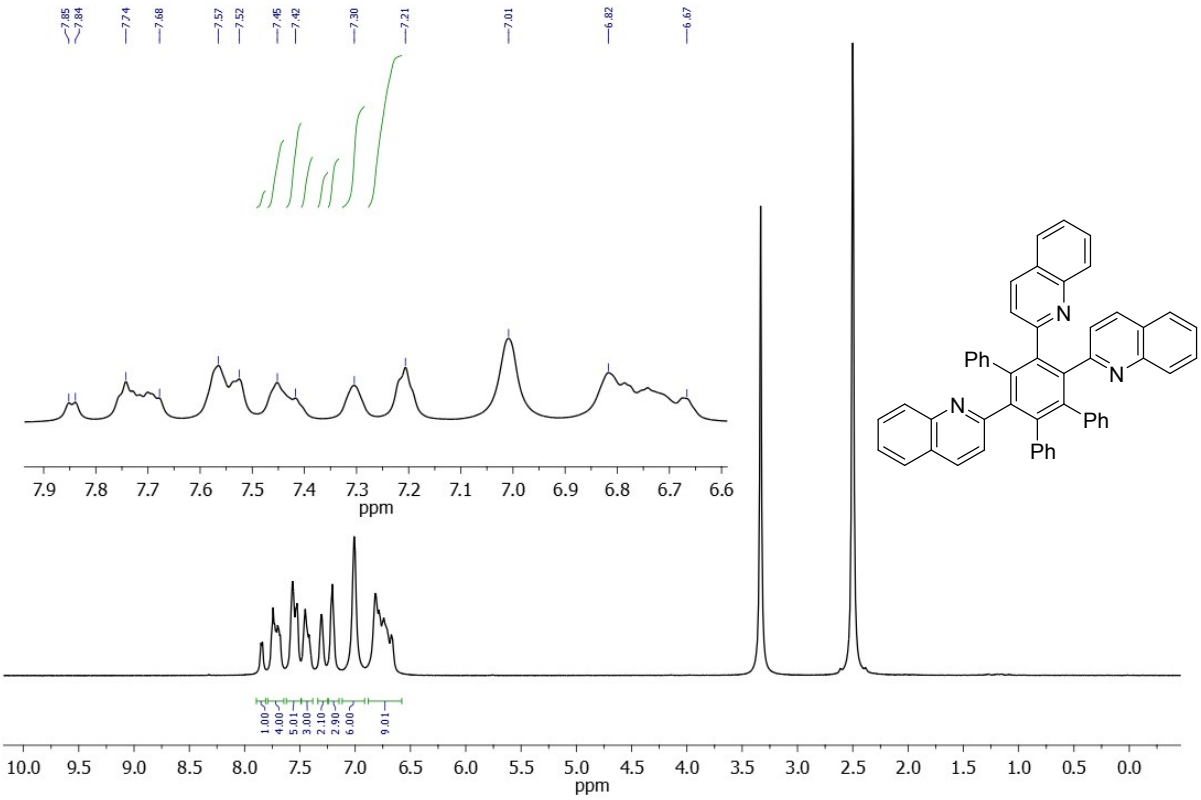


^{13}C NMR (150 MHz, DMSO-d_6)

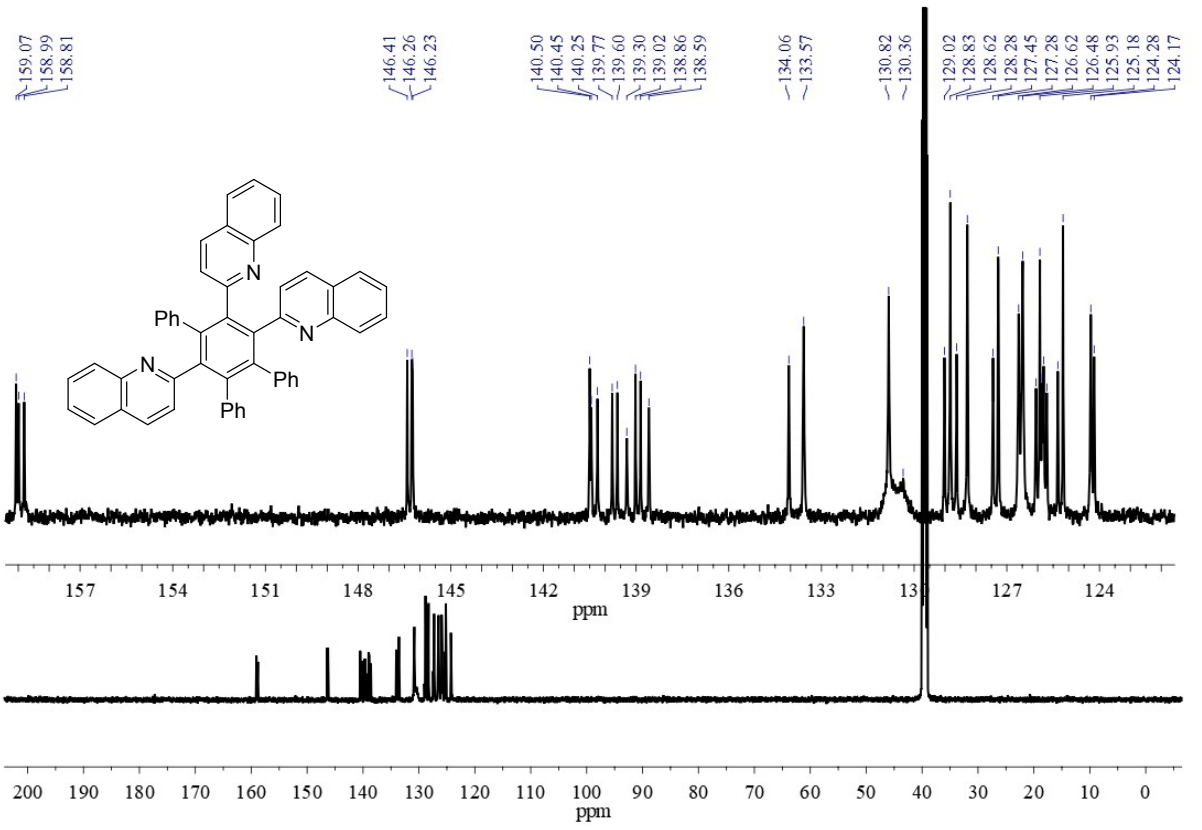


1,2,4-Triphenyl-3,5,6-tri(quinoline-2-yl)benzene (20b)

^{1}H NMR (600 MHz, DMSO-d_6)

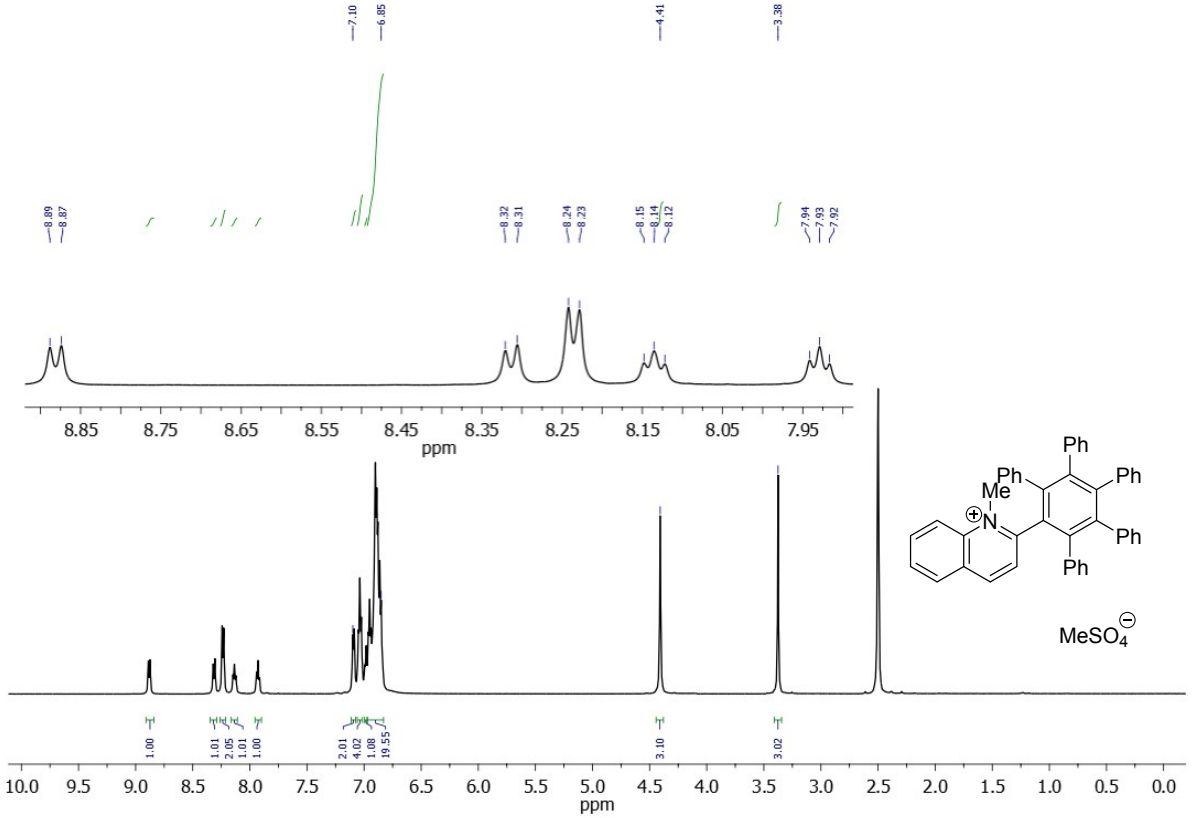


^{13}C NMR (150 MHz, DMSO-d_6)

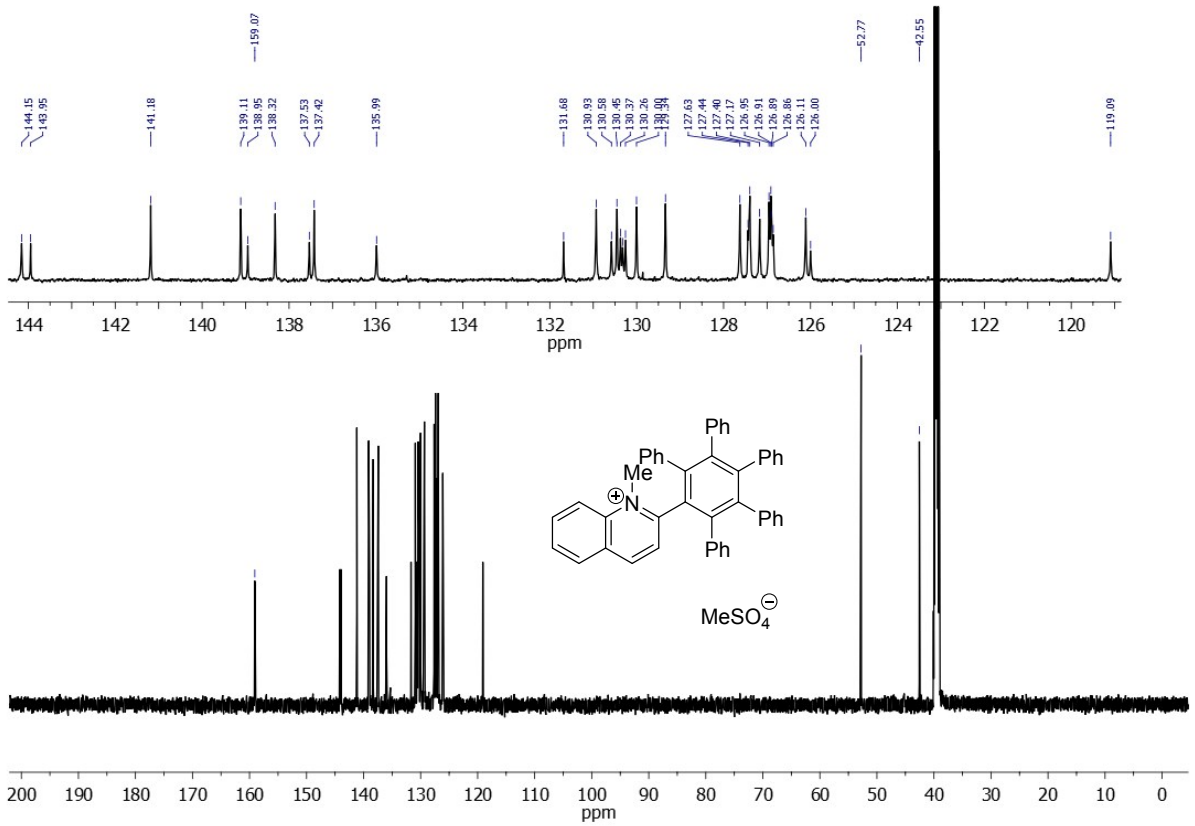


2,3,4,5,6-Pentaphenyl-1-(1-methylquinolinium-2-yl)benzene methylsulfate (22a)

^{1}H NMR (600 MHz, DMSO-d_6)

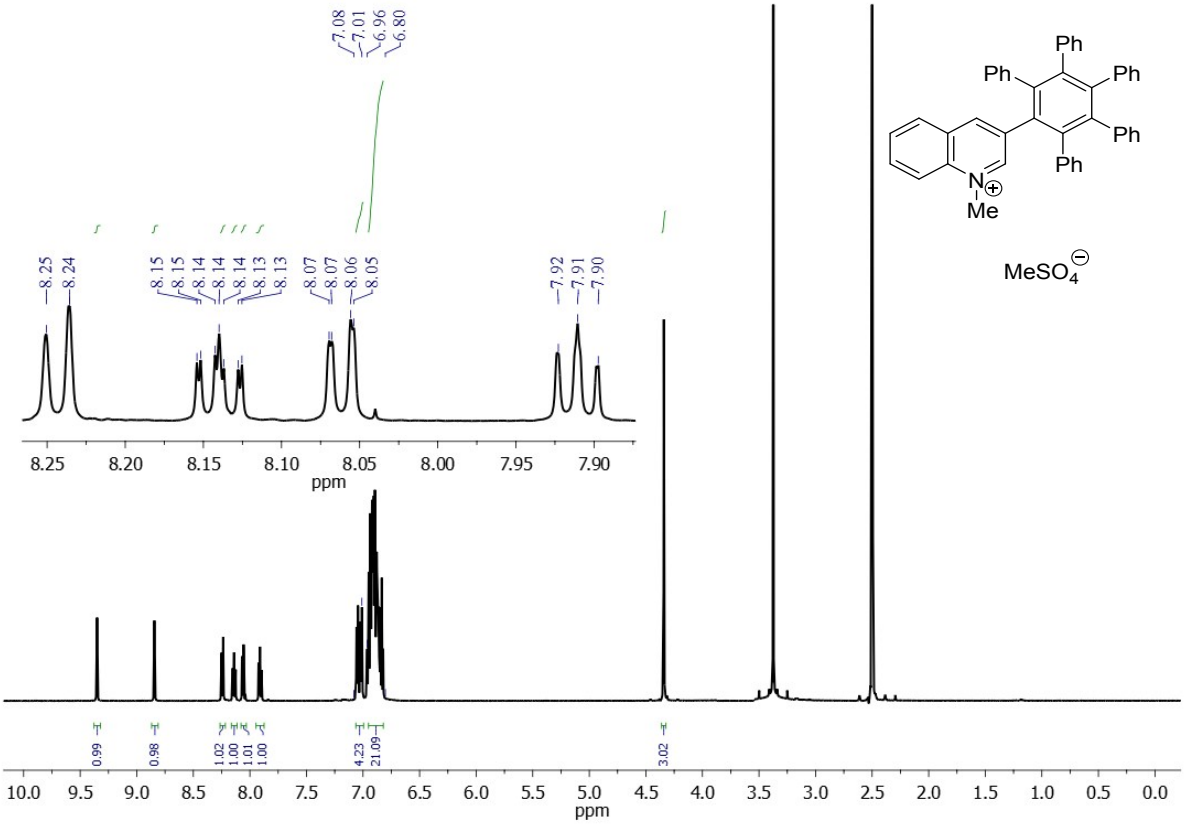


^{13}C NMR (150 MHz, DMSO-d_6)

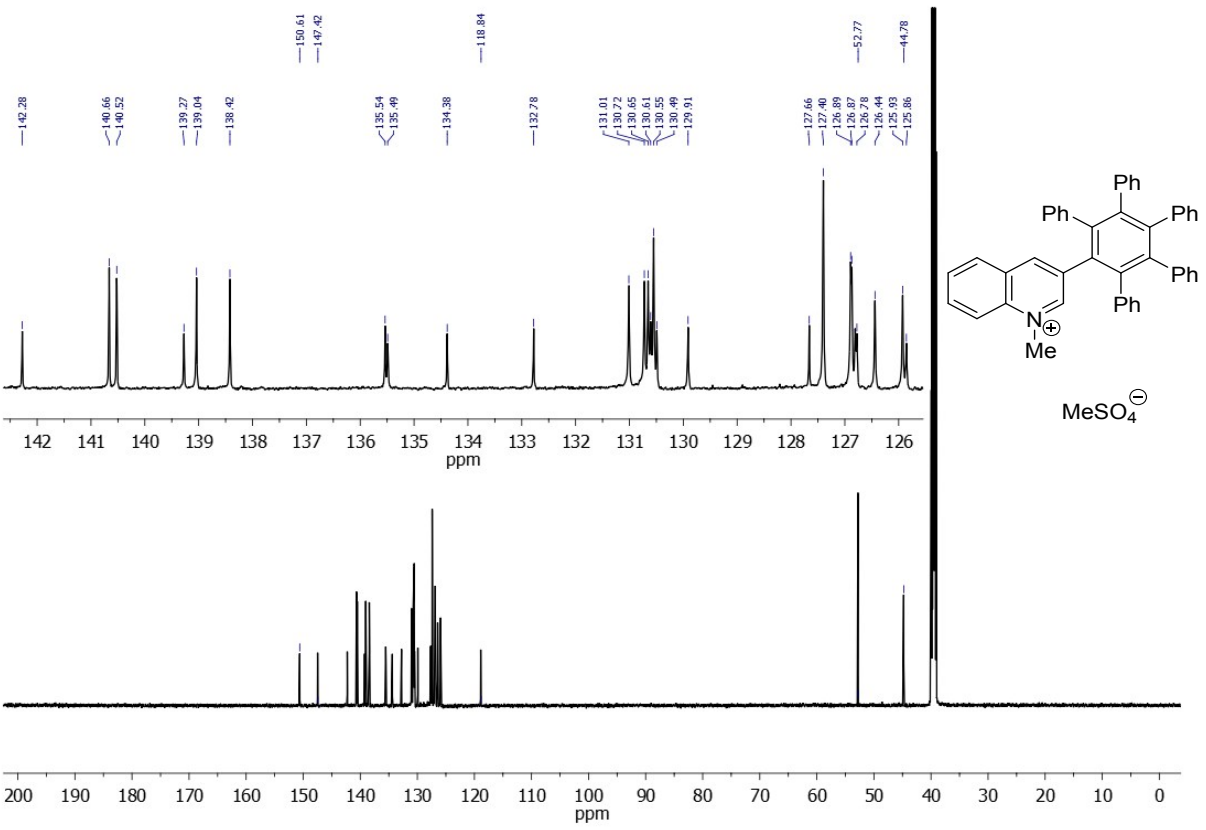


2,3,4,5,6-Phenyl-1-(1-methylquinolinium-3-yl)benzene methylsulfate (22b)

^{1}H NMR (600 MHz, DMSO-d_6)

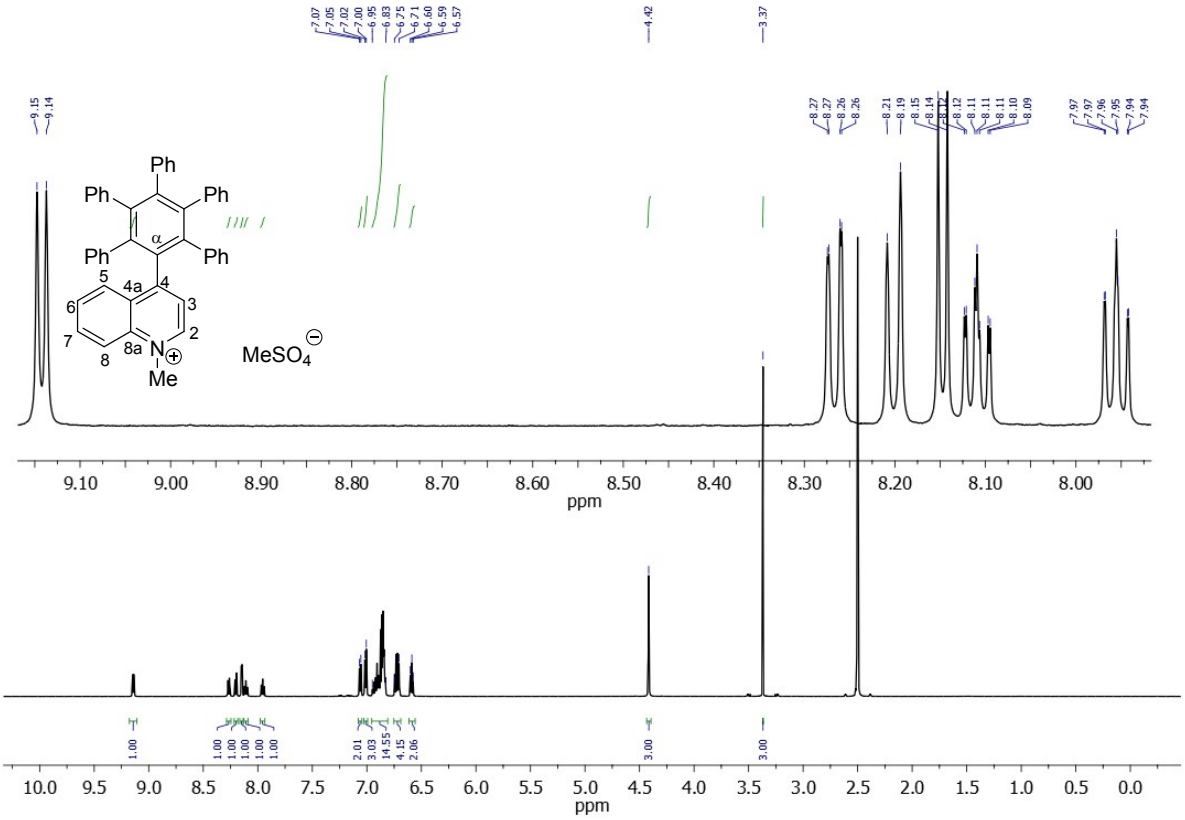


^{13}C NMR (150 MHz, DMSO-d_6)

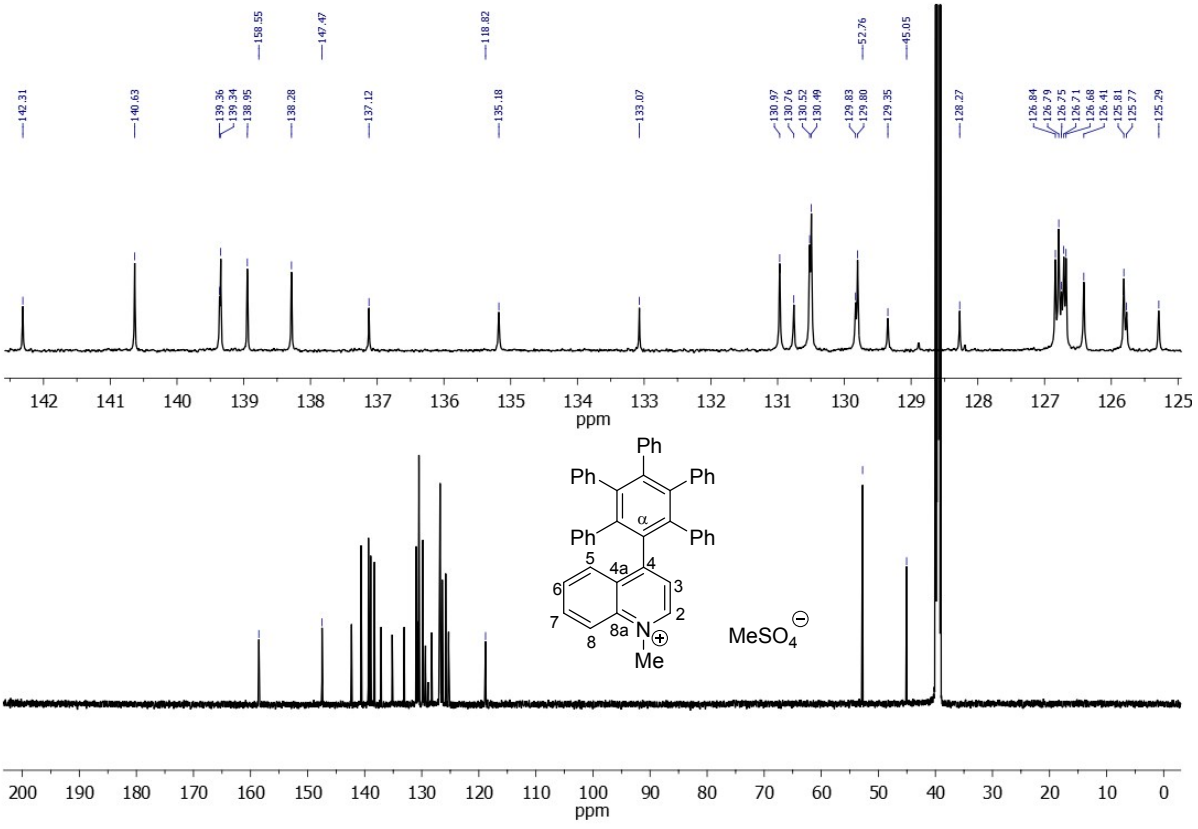


2,3,4,5,6-Pentaphenyl-1-(1-methylquinolinium-4-yl)benzene methylsulfate (22c)

^{1}H NMR (600 MHz, DMSO-d_6)

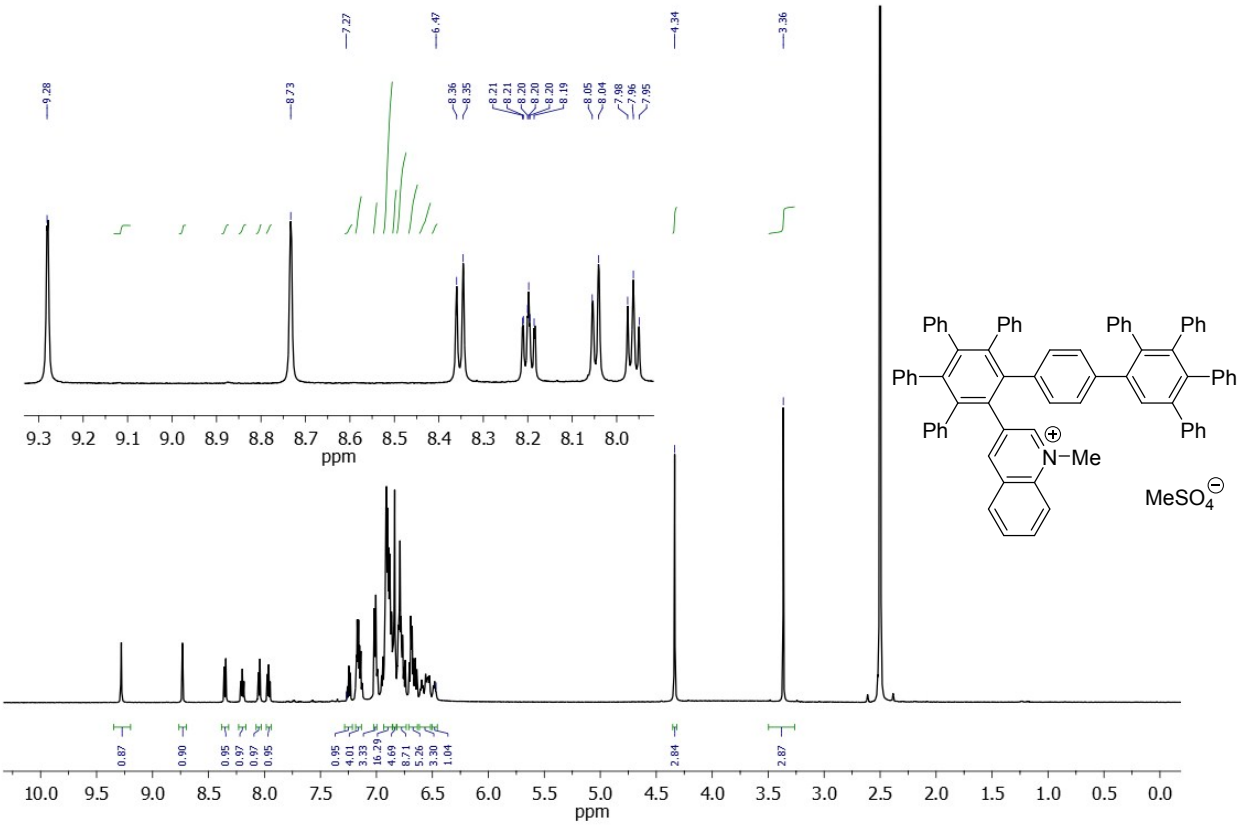


^{13}C NMR (150 MHz, DMSO-d_6)

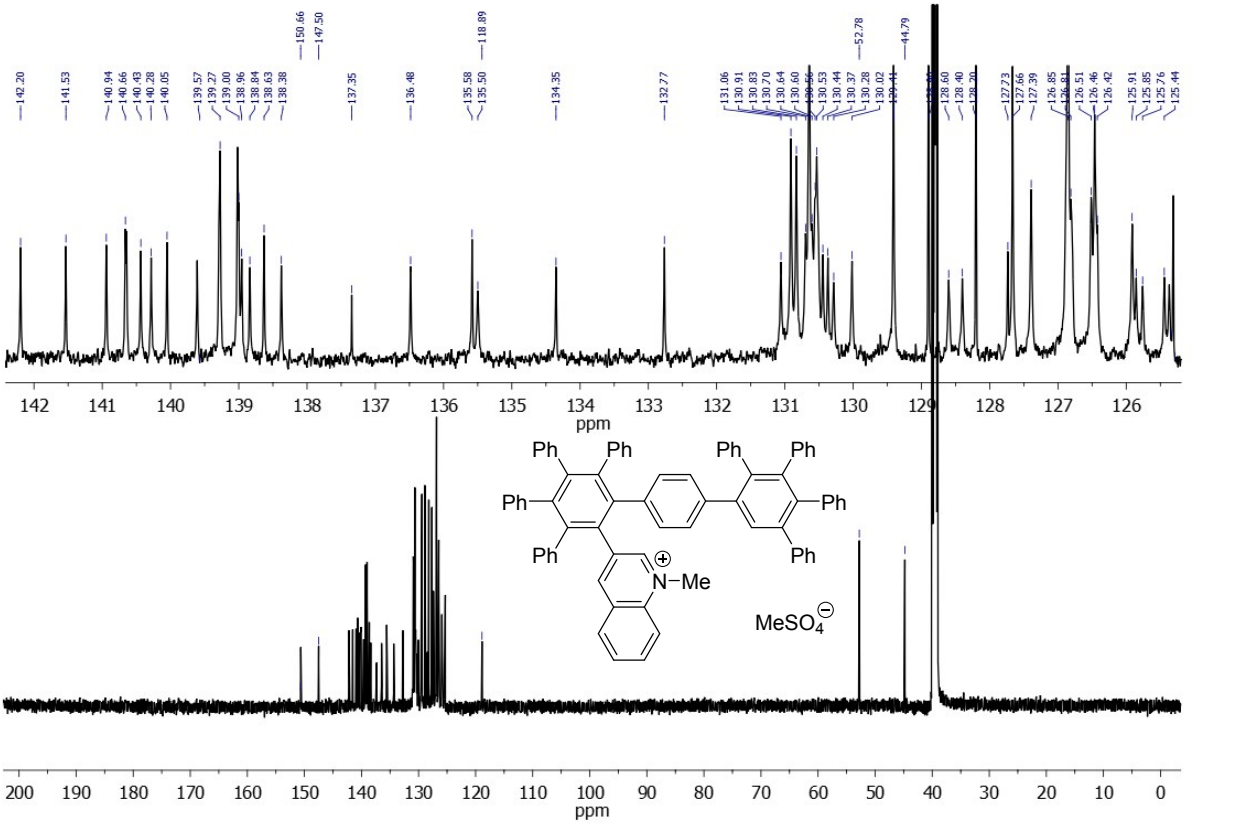


1-(1-Methylquinolinium-3-yl)-2,3,4,5,-tetraphenyl-6-(4-(1,2,3,4-tetraphenyl)-phenyl)benzene methylsulfate (23)

^{1}H NMR (600 MHz, DMSO-d_6)

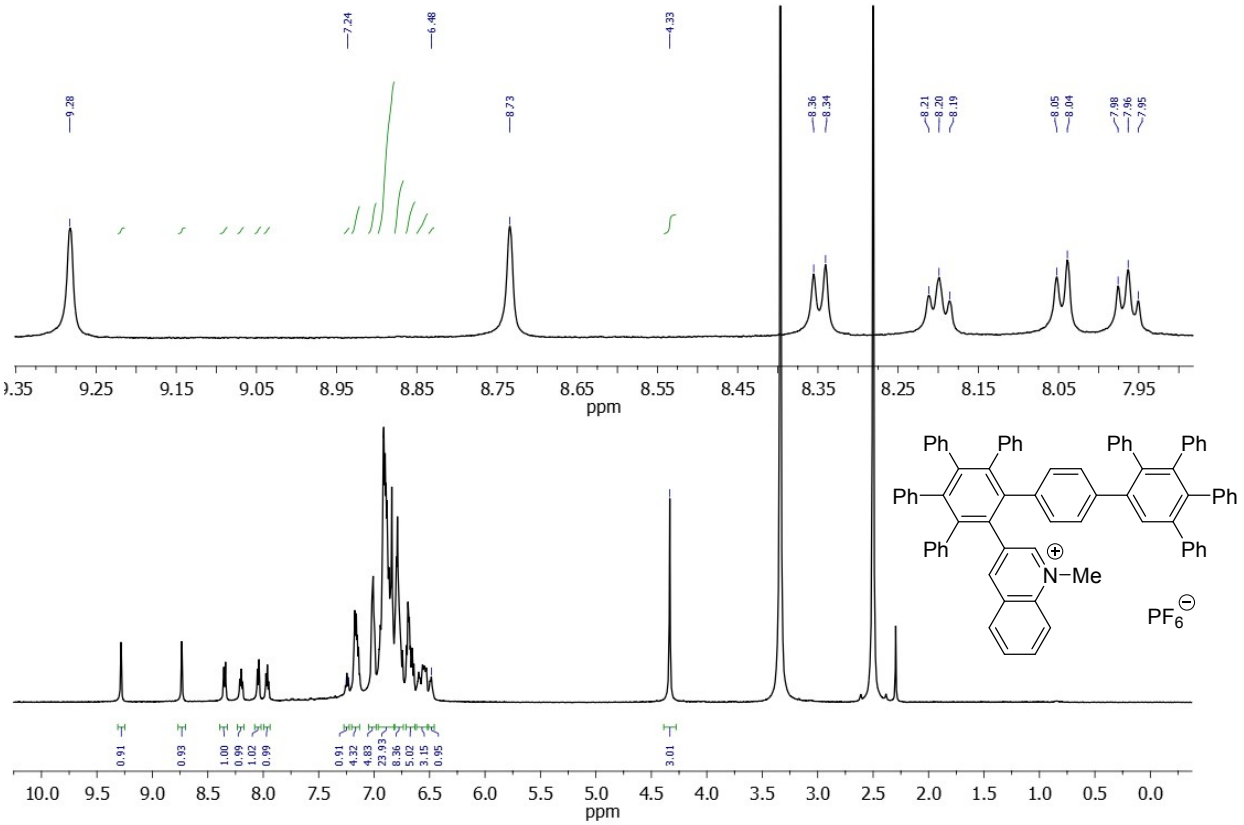


^{13}C NMR (150 MHz, DMSO-d_6)

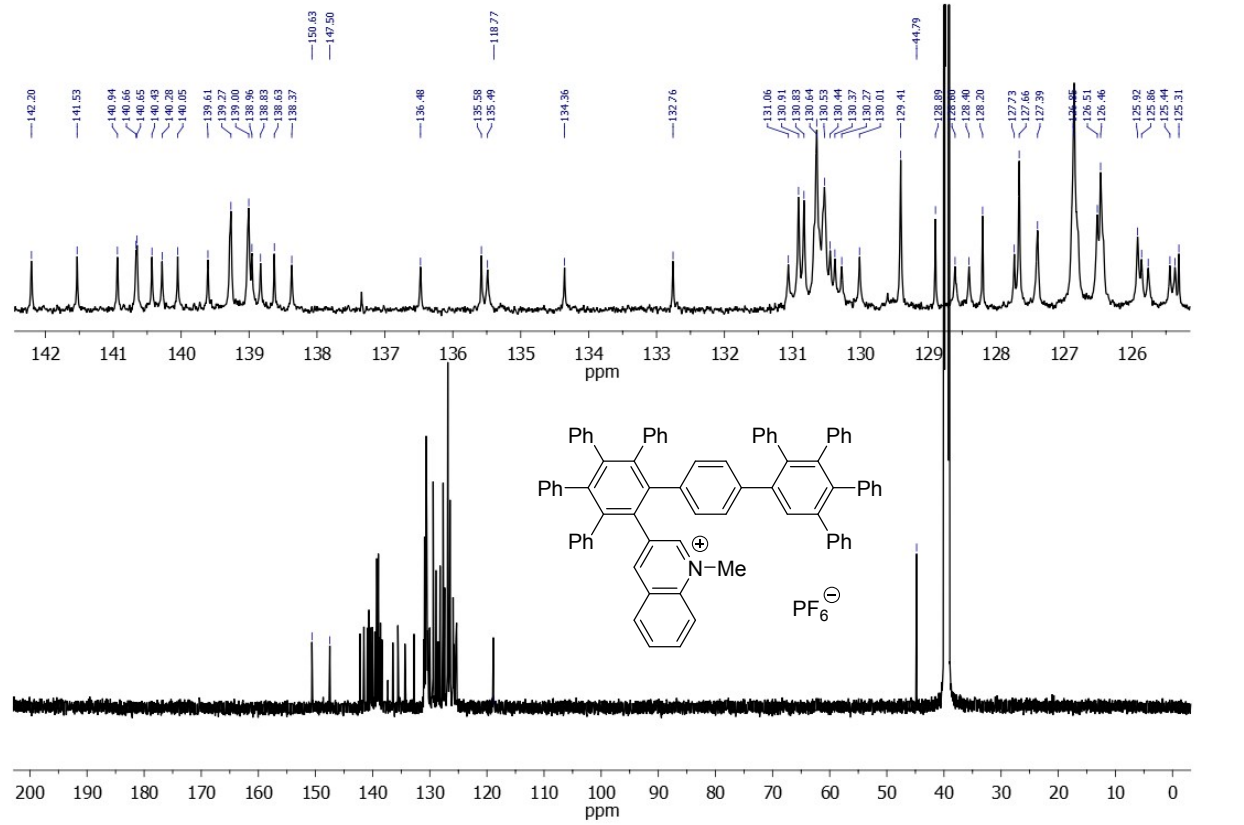


1-(1-Methylquinolinium-3-yl)-2,3,4,5,-tetraphenyl-6-(4-(1,2,3,4-tetraphenyl)phenyl)benzene hexafluorophosphate (23PF_6)

^{1}H NMR (600 MHz, DMSO-d_6)

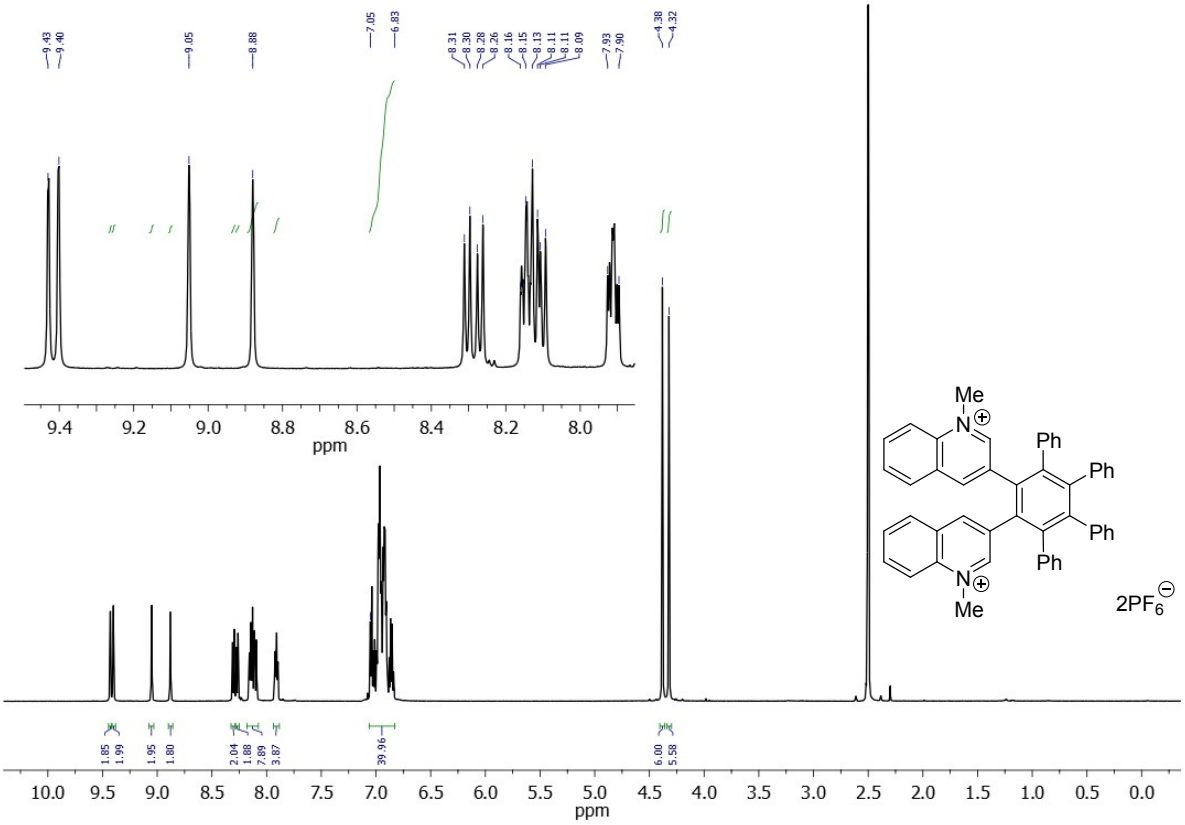


^{13}C NMR (150 MHz, DMSO-d_6)

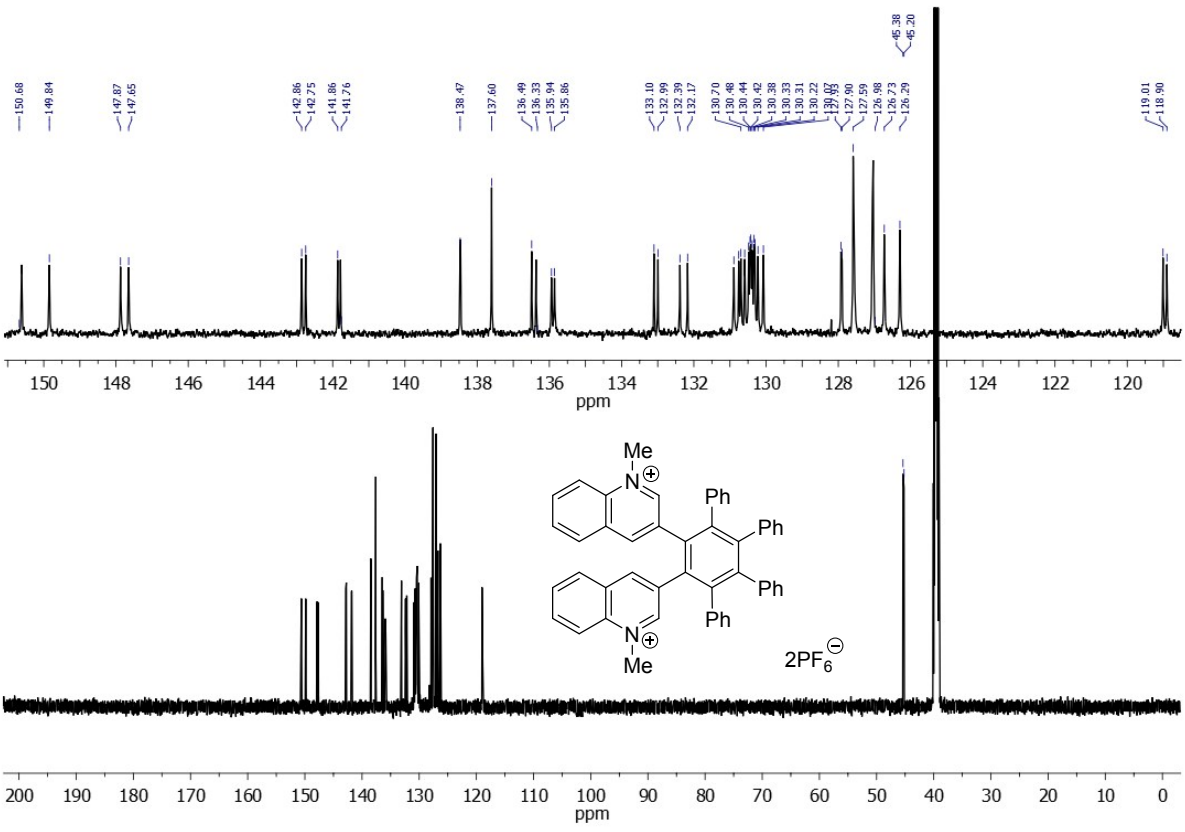


1,2-Di(1-methylquinolinium-3-yl)-3,4,5,6-tetraphenylbenzene dihexafluorophosphate (24a)

^{1}H NMR (600 MHz, DMSO-d_6)

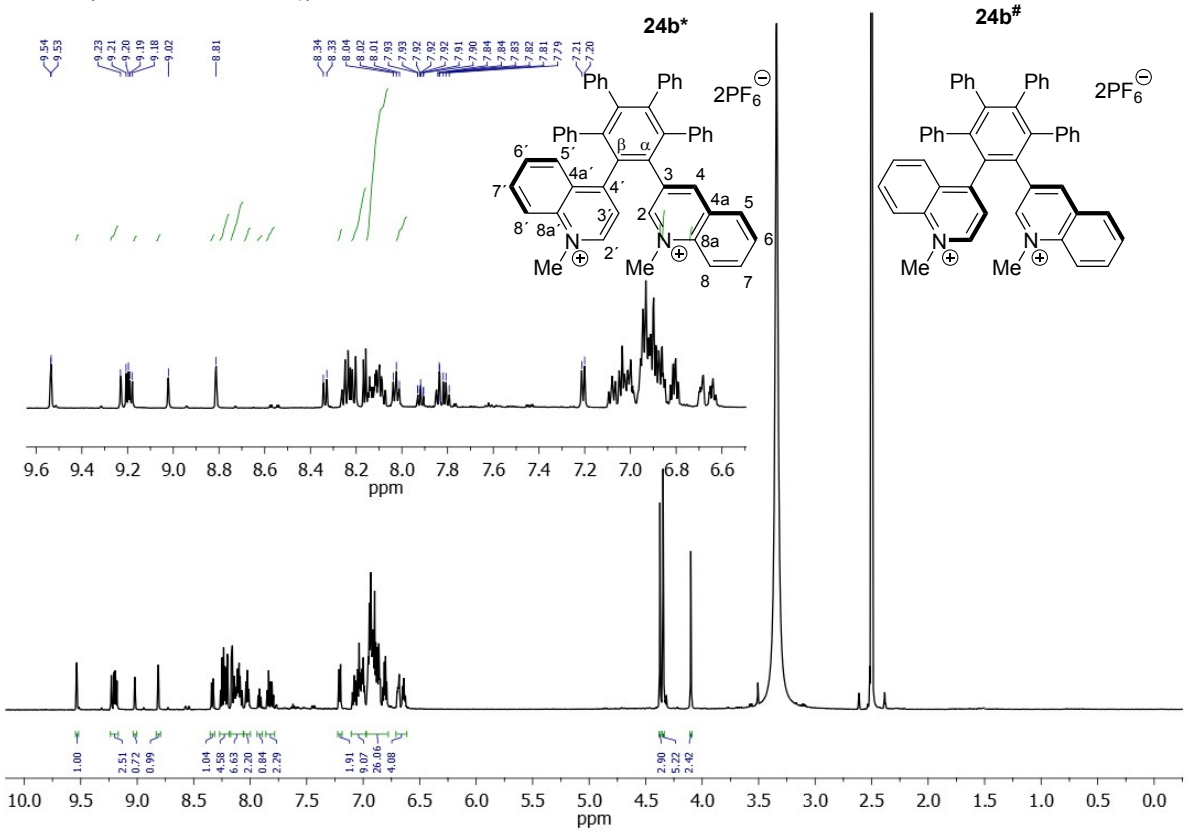


^{13}C NMR (150 MHz, DMSO-d_6)

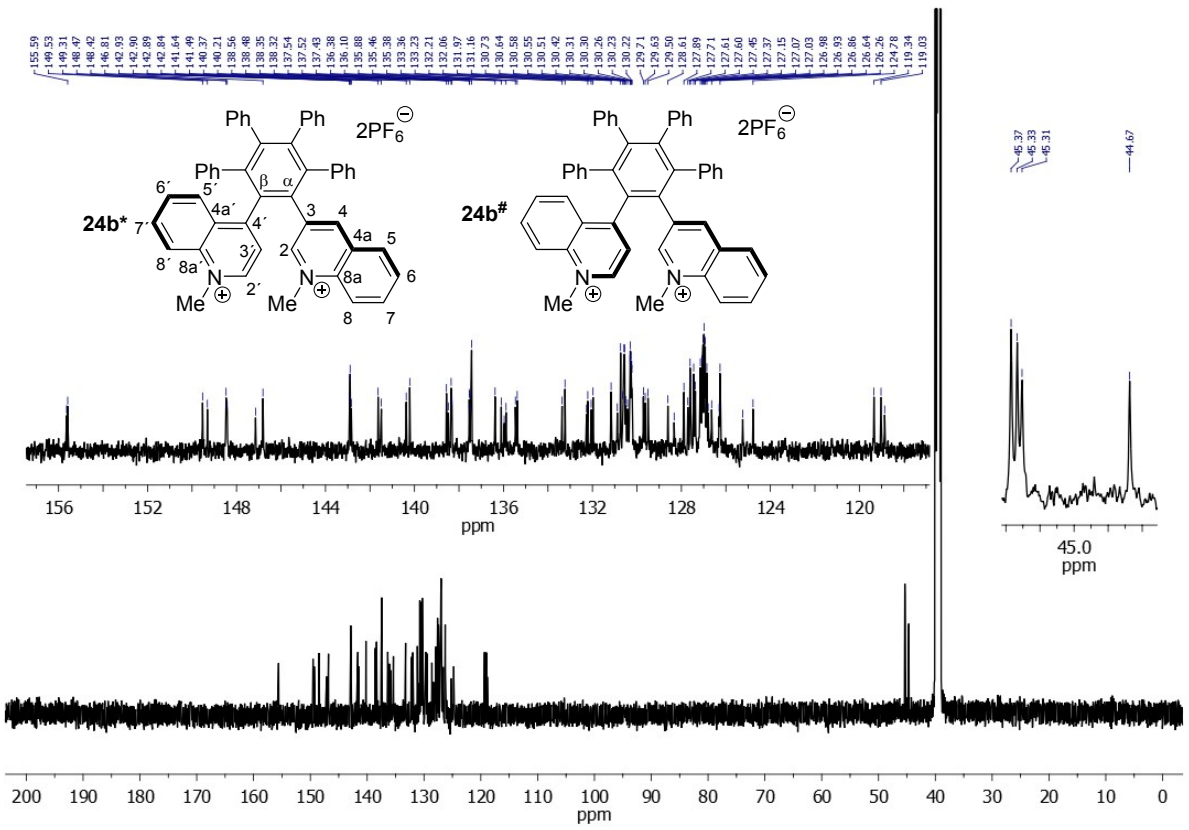


1-(1-Methylquinolinium-3-yl)-2-(1-methylquinolinium -4-yl)-3,4,5,6-tetraphenylbenzene dihexafluorophosphate (24b)

^{1}H NMR (600 MHz, DMSO-d_6)

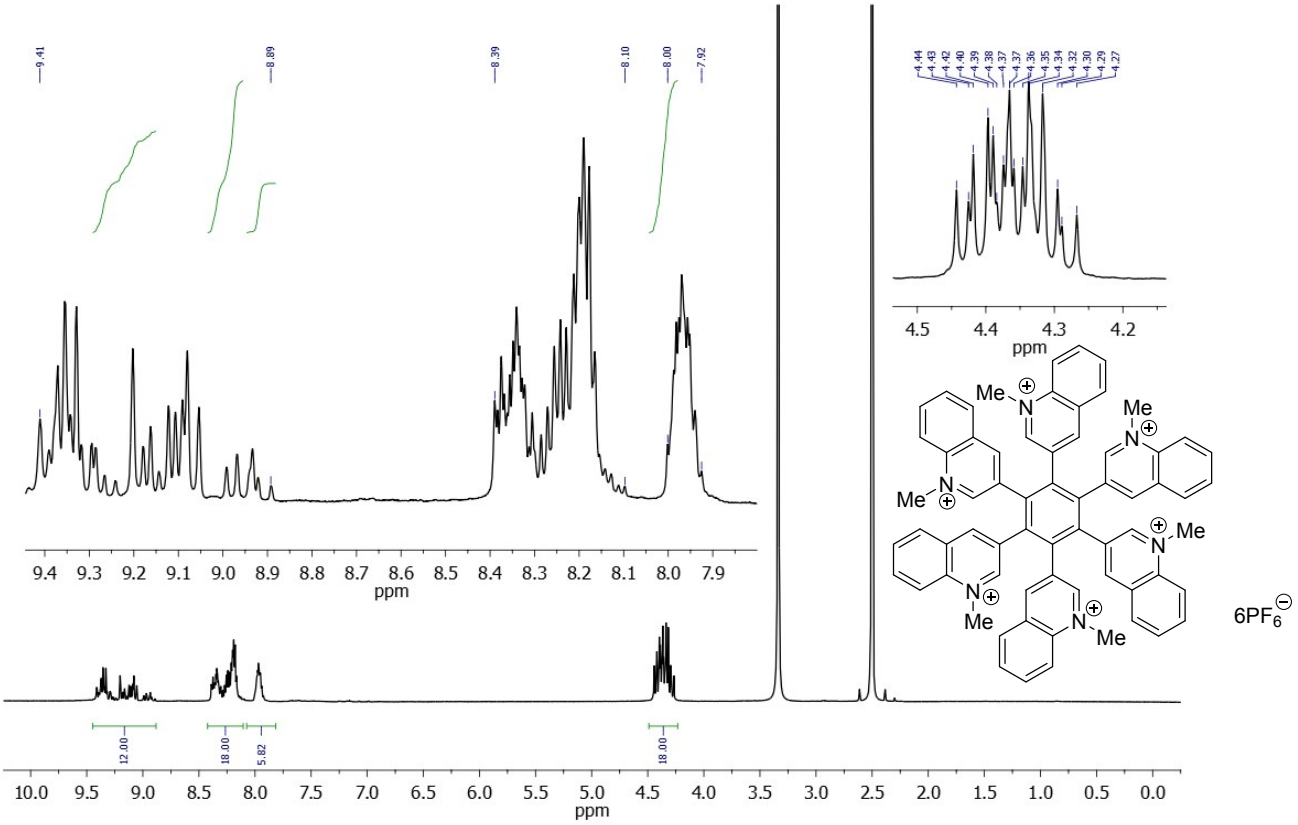


^{13}C NMR (150 MHz, DMSO-d_6)



***Hexakis*(1-methylquinolinium-3-yl)benzene *hexakis* hexafluorophosphate (25)**

^{1}H NMR (600 MHz, DMSO-d_6)



^{13}C NMR (150 MHz, DMSO-d_6)

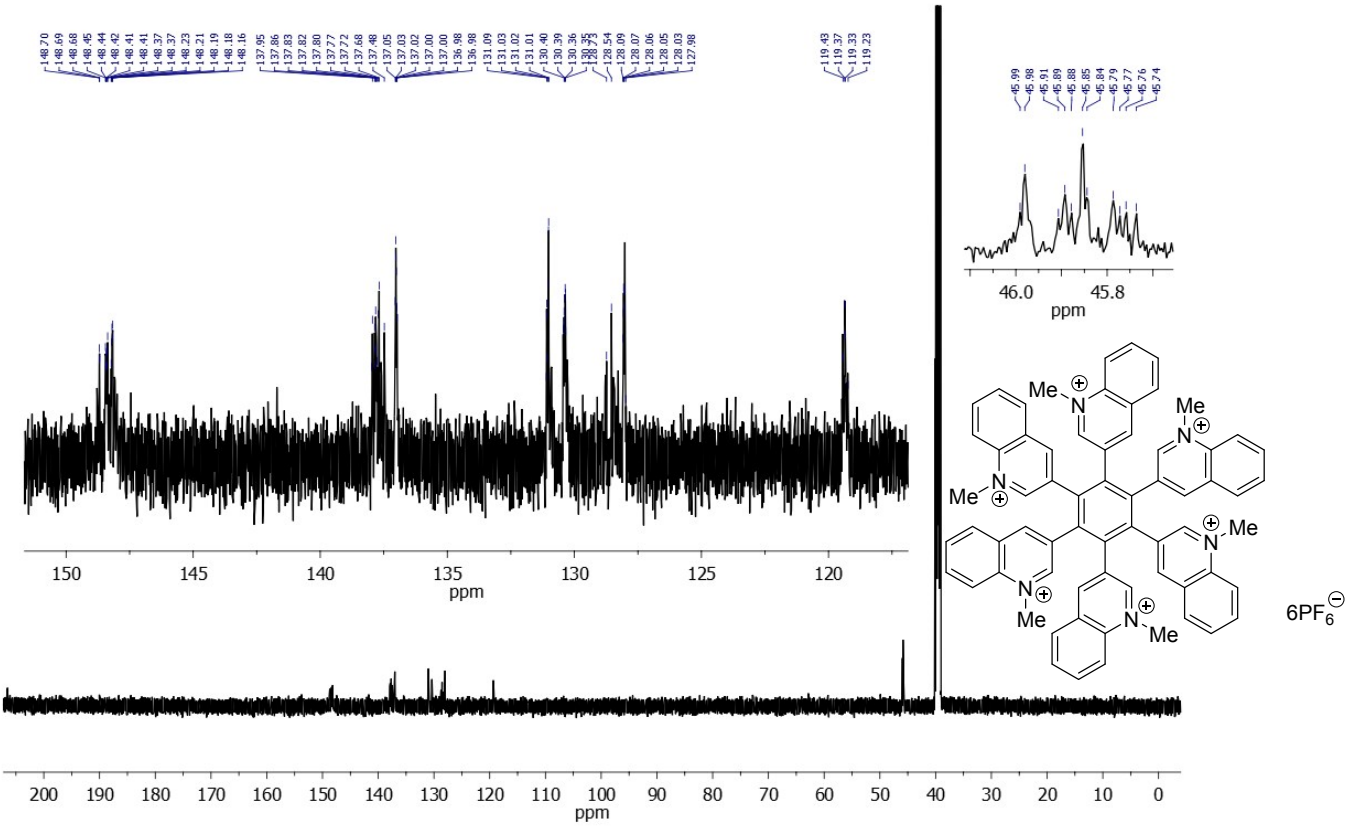
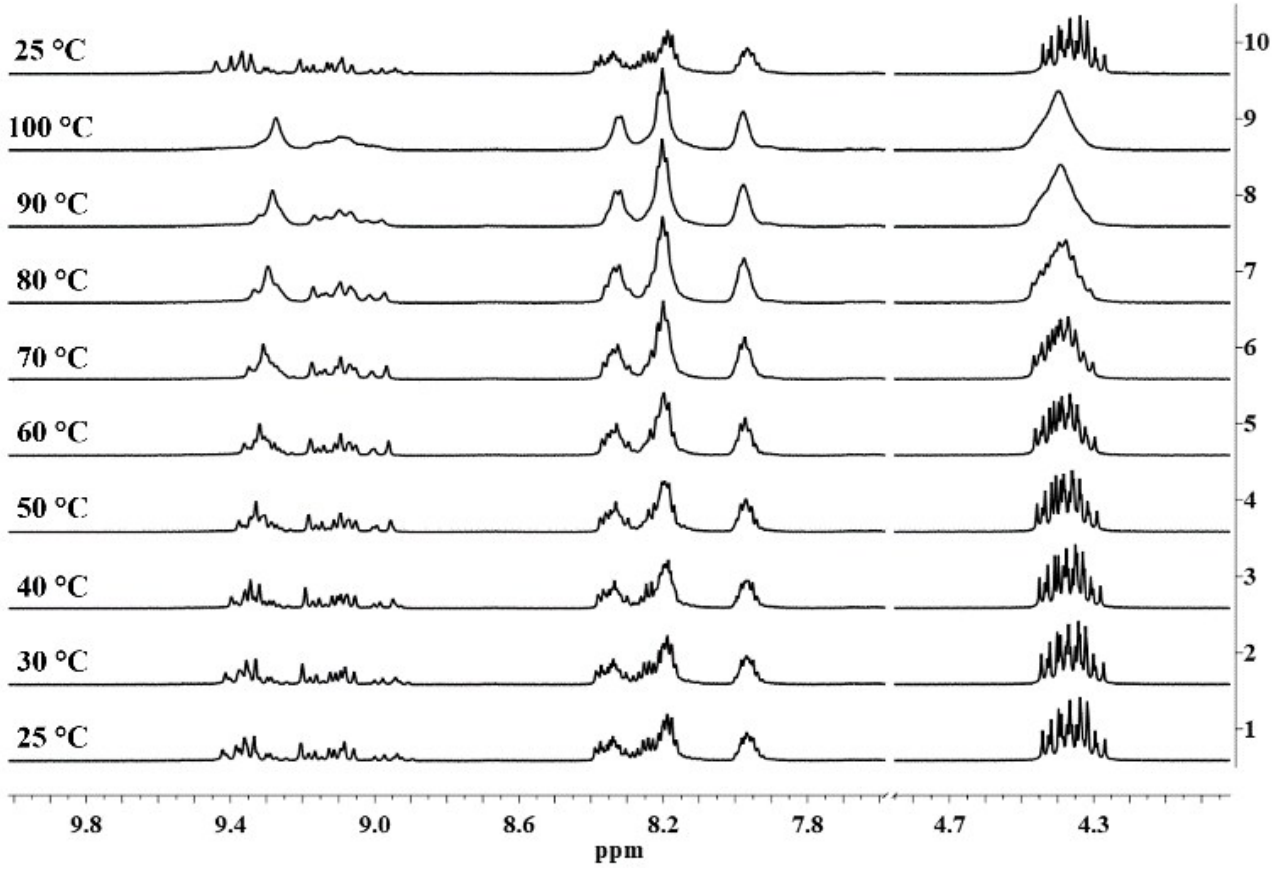
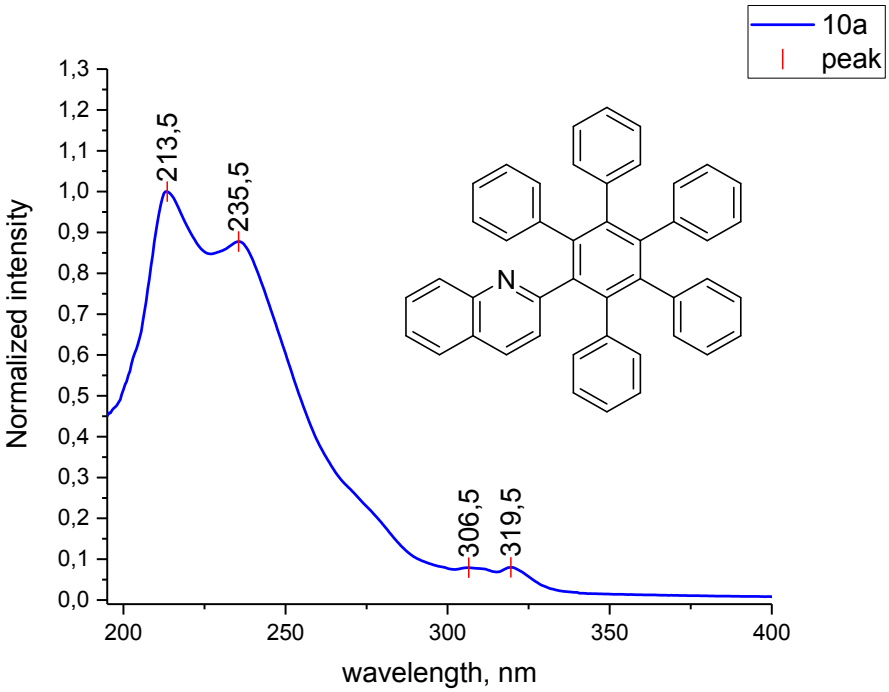


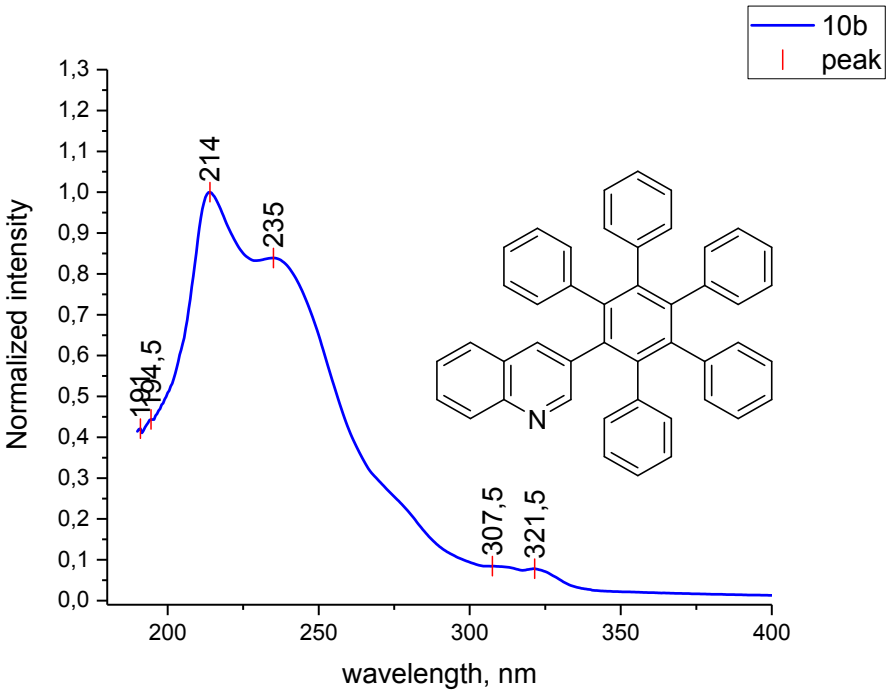
Figure 1: ^{1}H NMR spectra (600 MHz) of **25** in DMSO-d_6 with increasing temperature and final cooling to 25°C again.



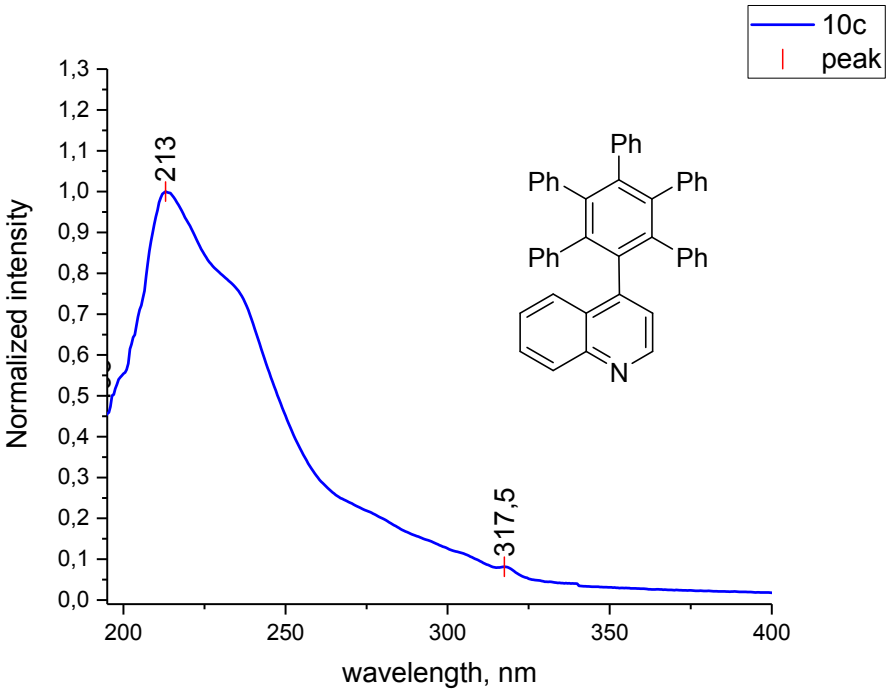
UV/vis absorption spectrum of **10a** in acetonitrile



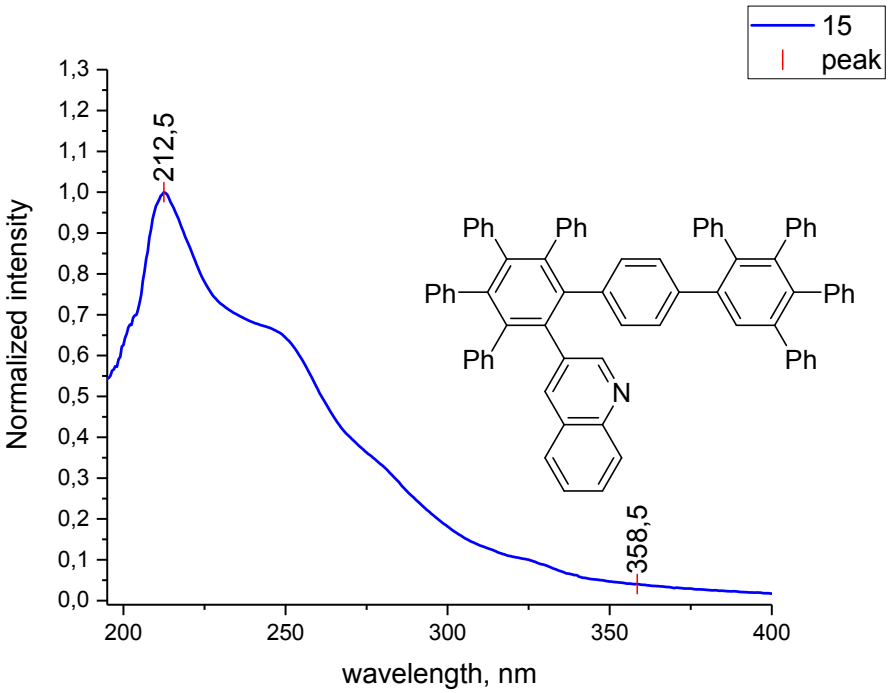
UV/vis absorption spectrum of **10b** in acetonitrile



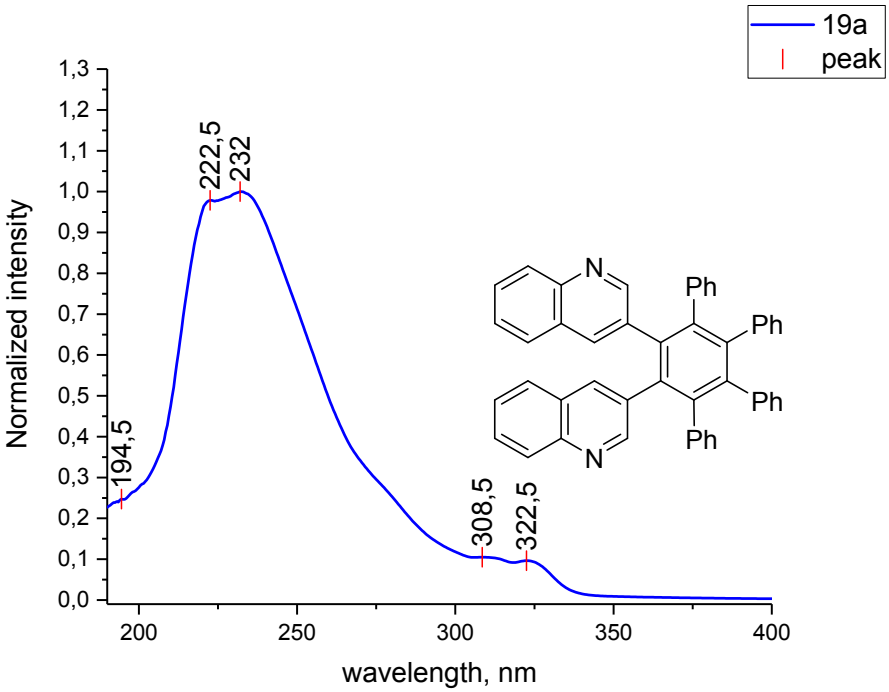
UV/vis absorption spectrum of **10c** in acetonitrile



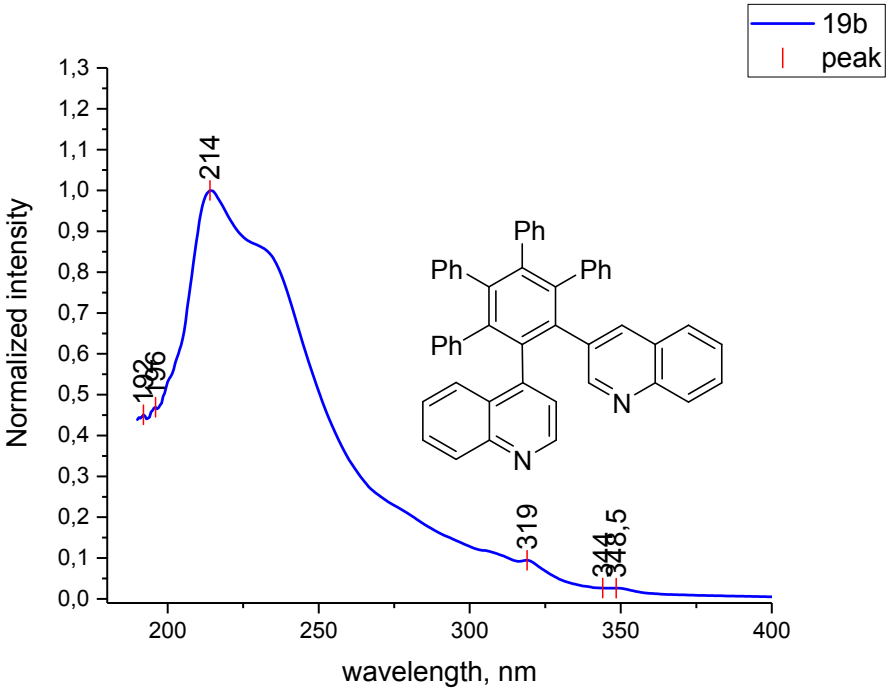
UV/vis absorption spectrum of **15** in acetonitrile



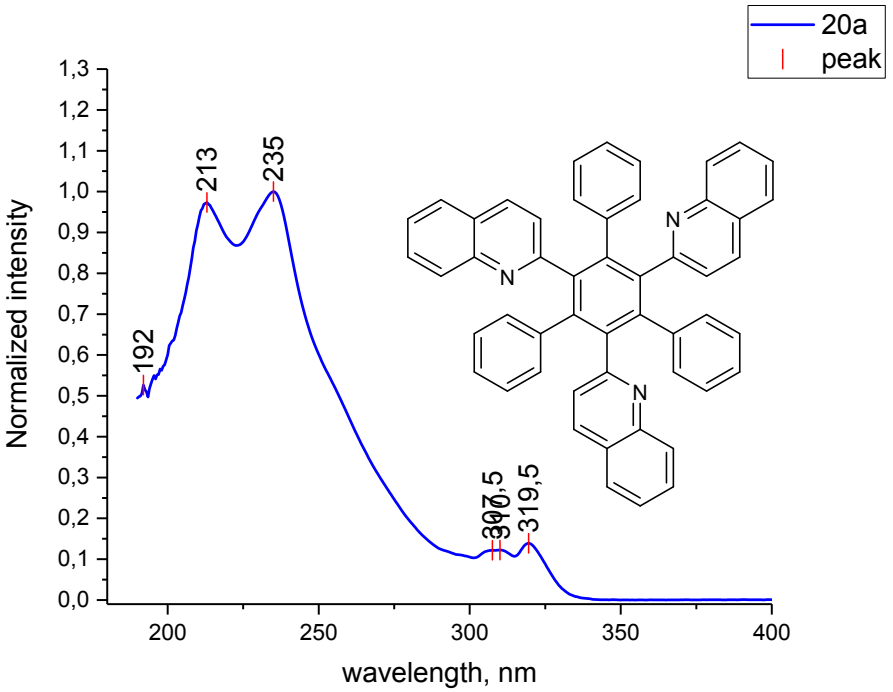
UV/vis absorption spectrum of **19a** in acetonitrile



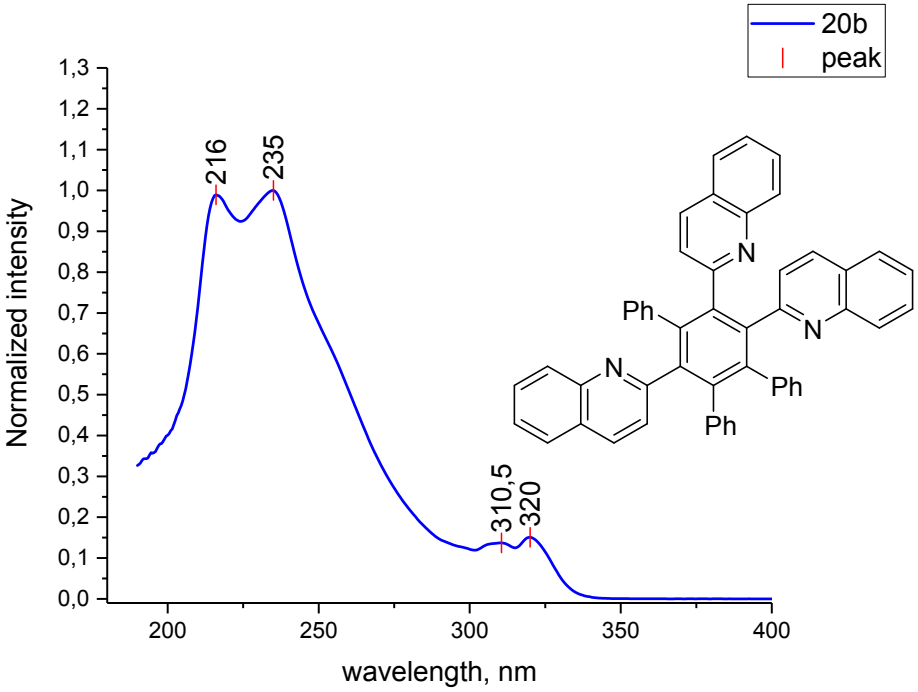
UV/vis absorption spectrum of **19b** in acetonitrile



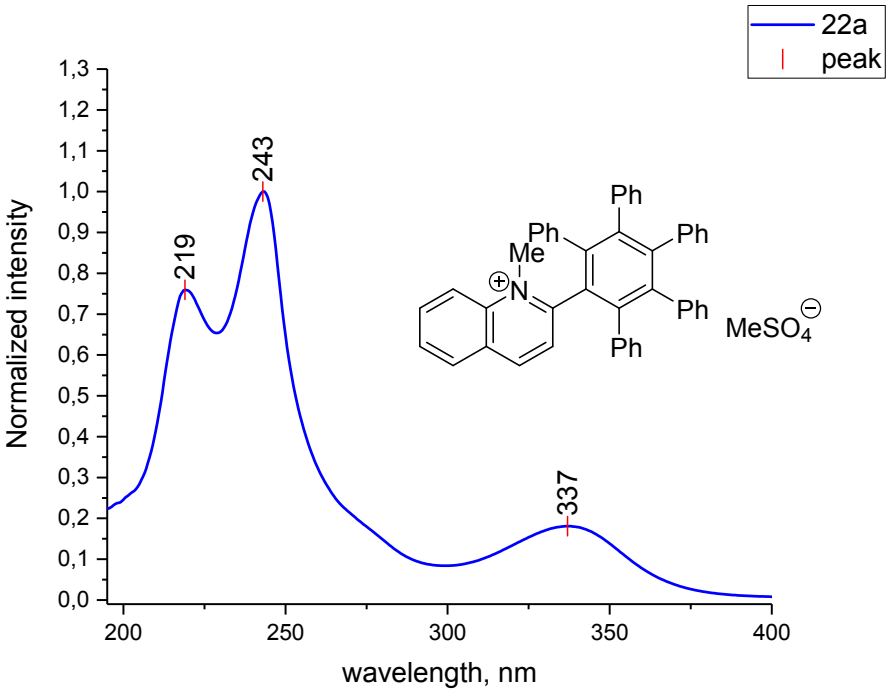
UV/vis absorption spectrum of **20a** in acetonitrile



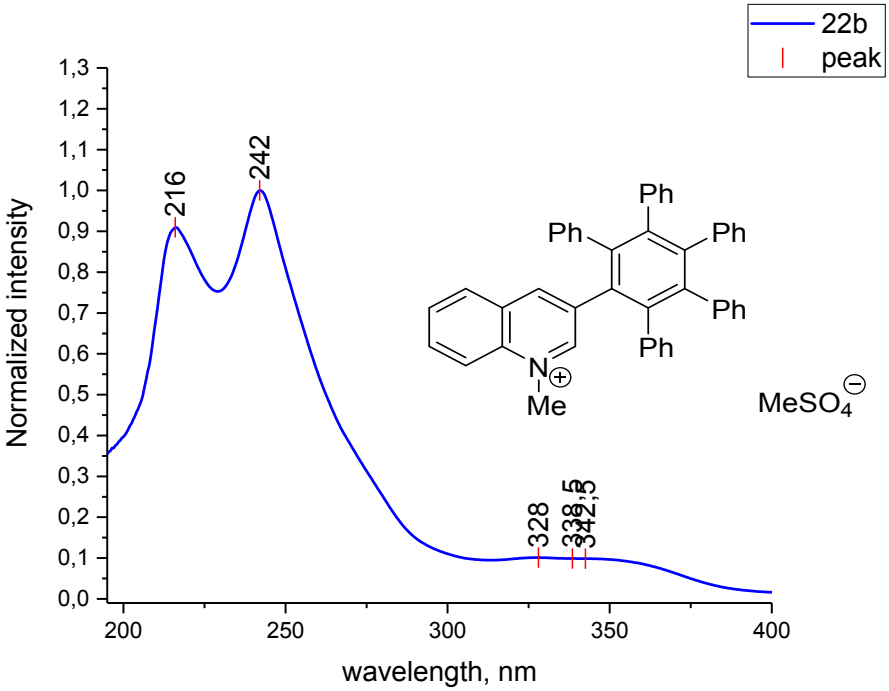
UV/vis absorption spectrum of **20b** in acetonitrile



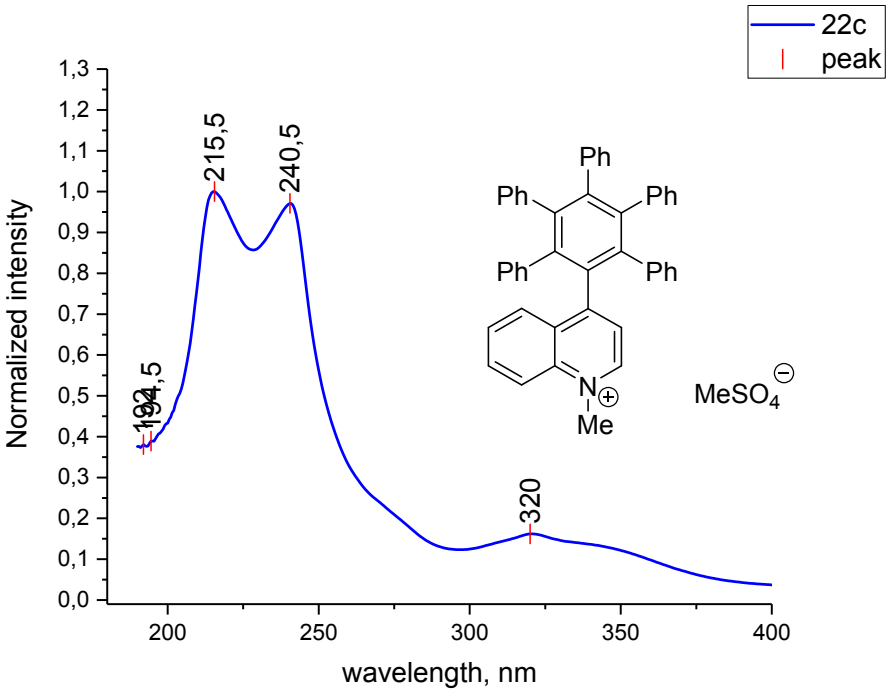
UV/vis absorption spectrum of **22a** in acetonitrile



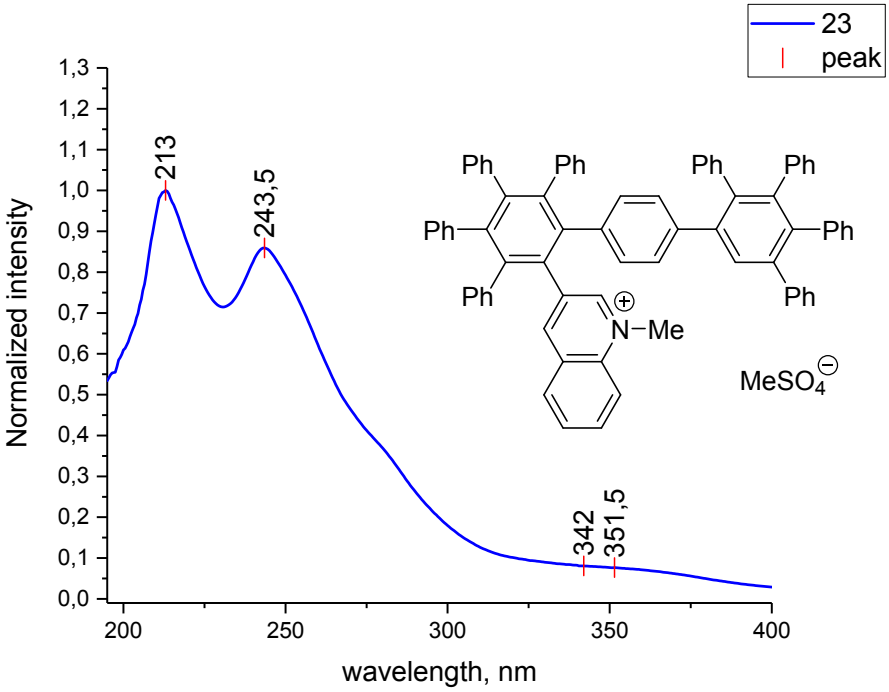
UV/vis absorption spectrum of **22b** in acetonitrile



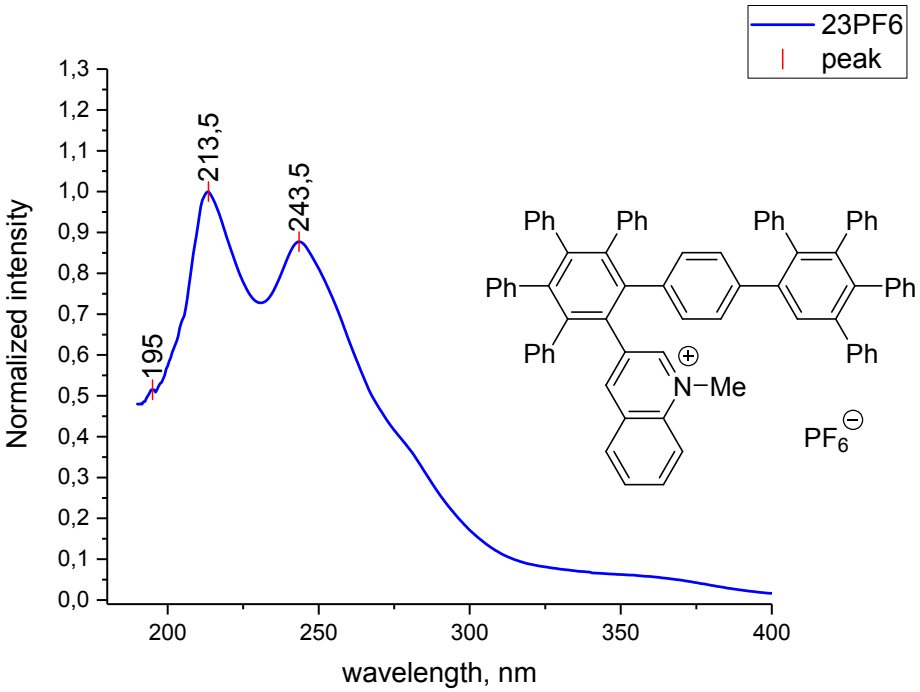
UV/vis absorption spectrum of **22c** in acetonitrile



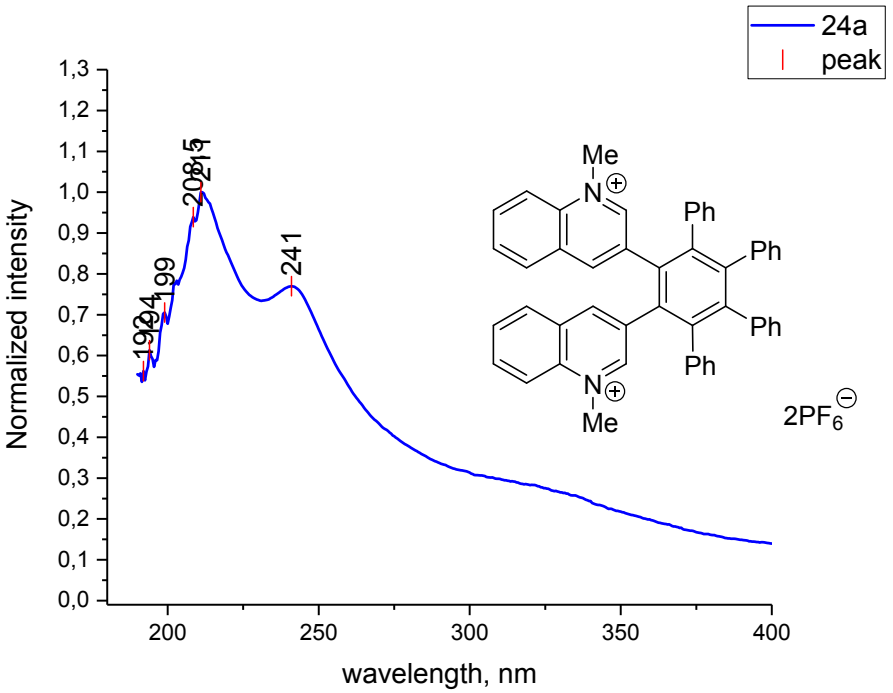
UV/vis absorption spectrum of **23** in acetonitrile



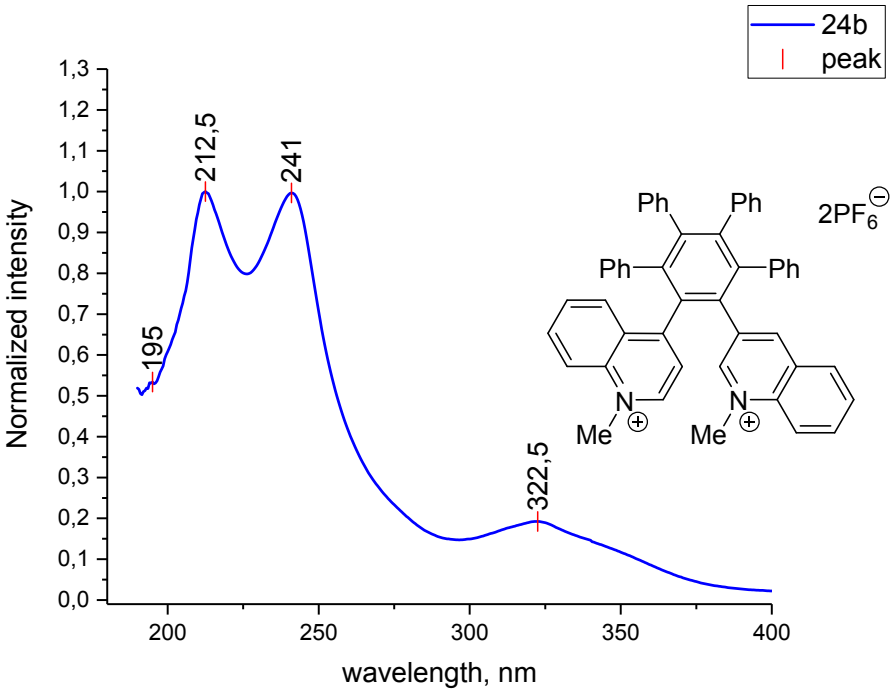
UV/vis absorption spectrum of **23PF6** in acetonitrile



UV/vis absorption spectrum of **24a** in acetonitrile



UV/vis absorption spectrum of **24b** in acetonitrile



UV/vis absorption spectrum of **25** in acetonitrile