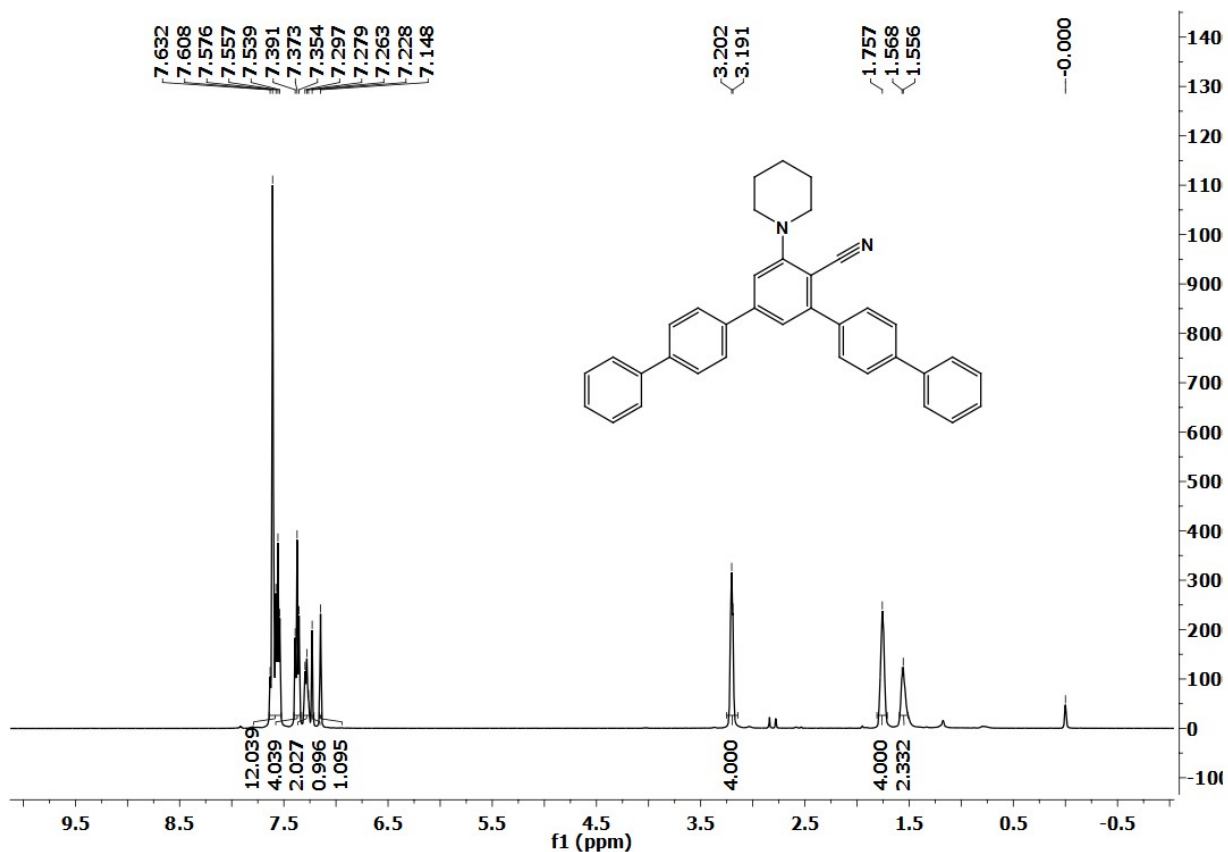
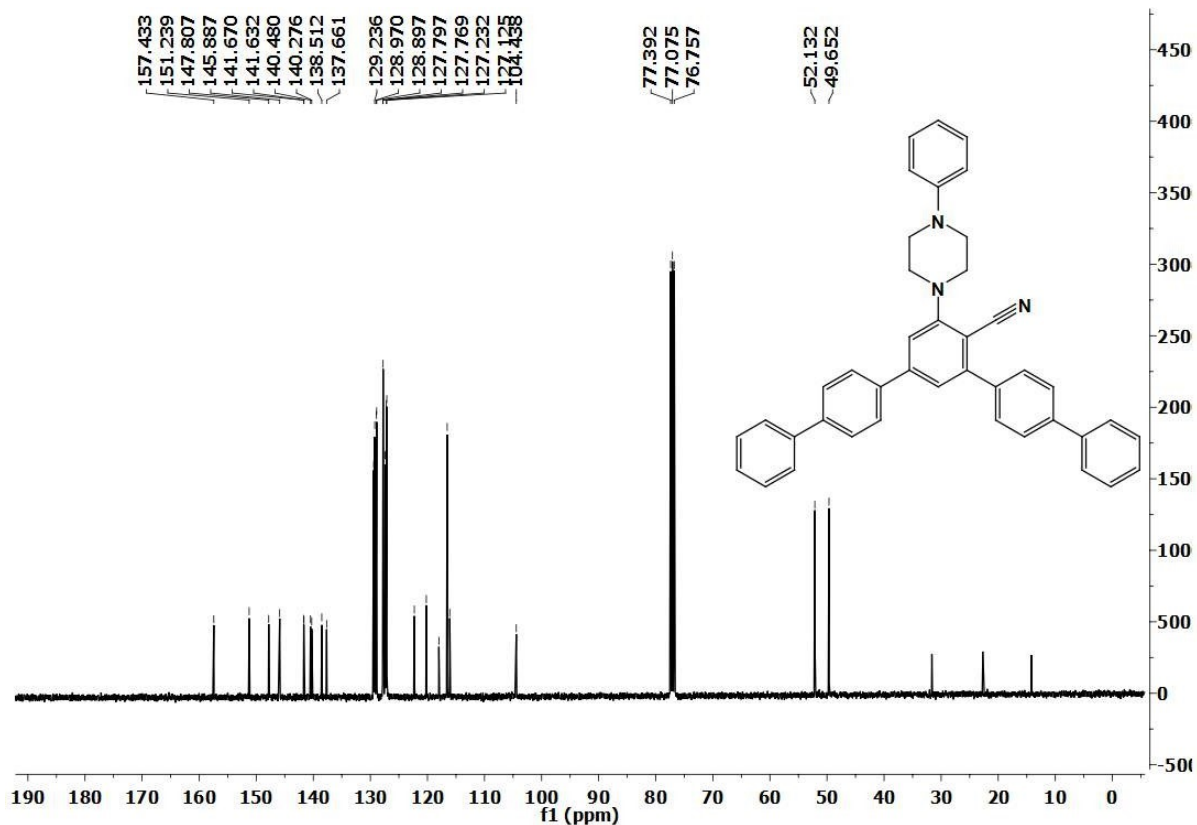


Supporting Information

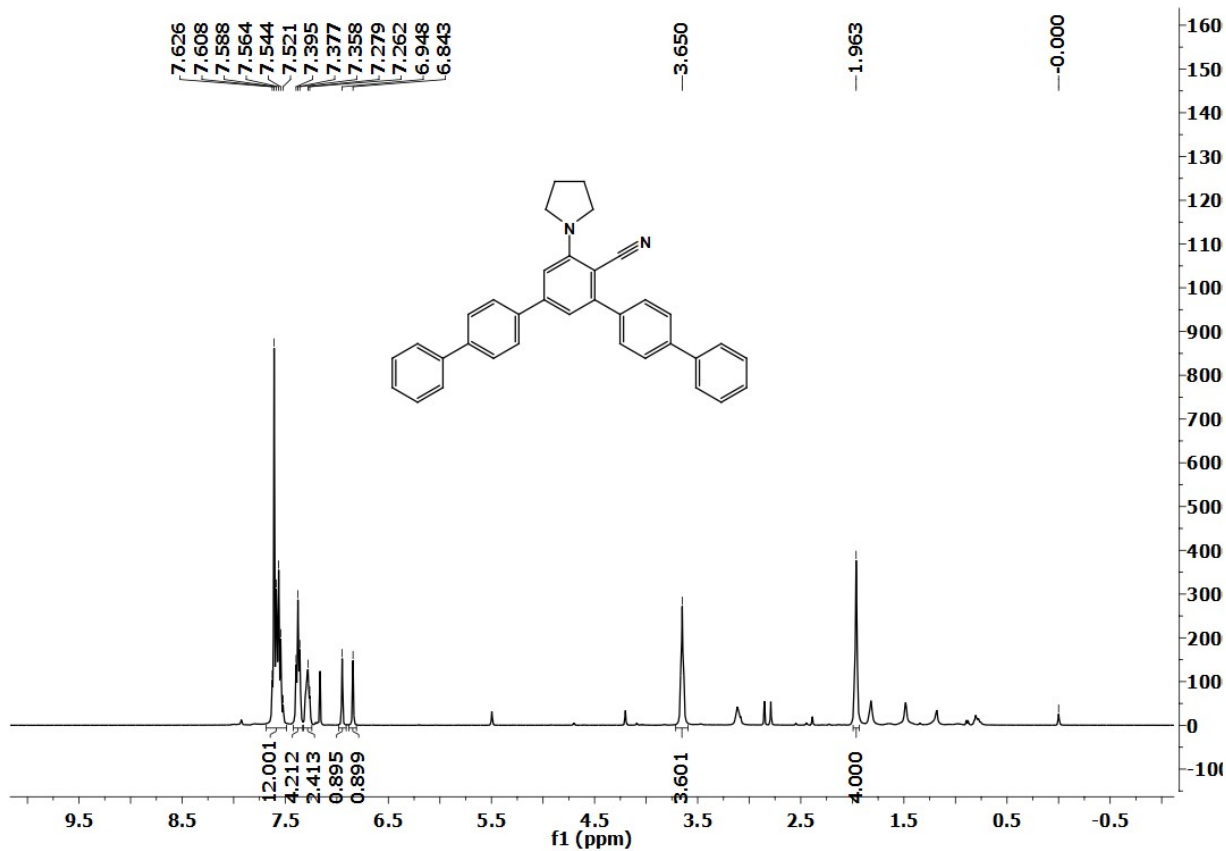
Metal Free Synthesis of Thermally Stable Blue Fluorescent *m*-Terphenyls by Ring Transformation of 2*H*-pyran-2-ones: Chemical Synthesis, Spectroscopy and Computational Studies

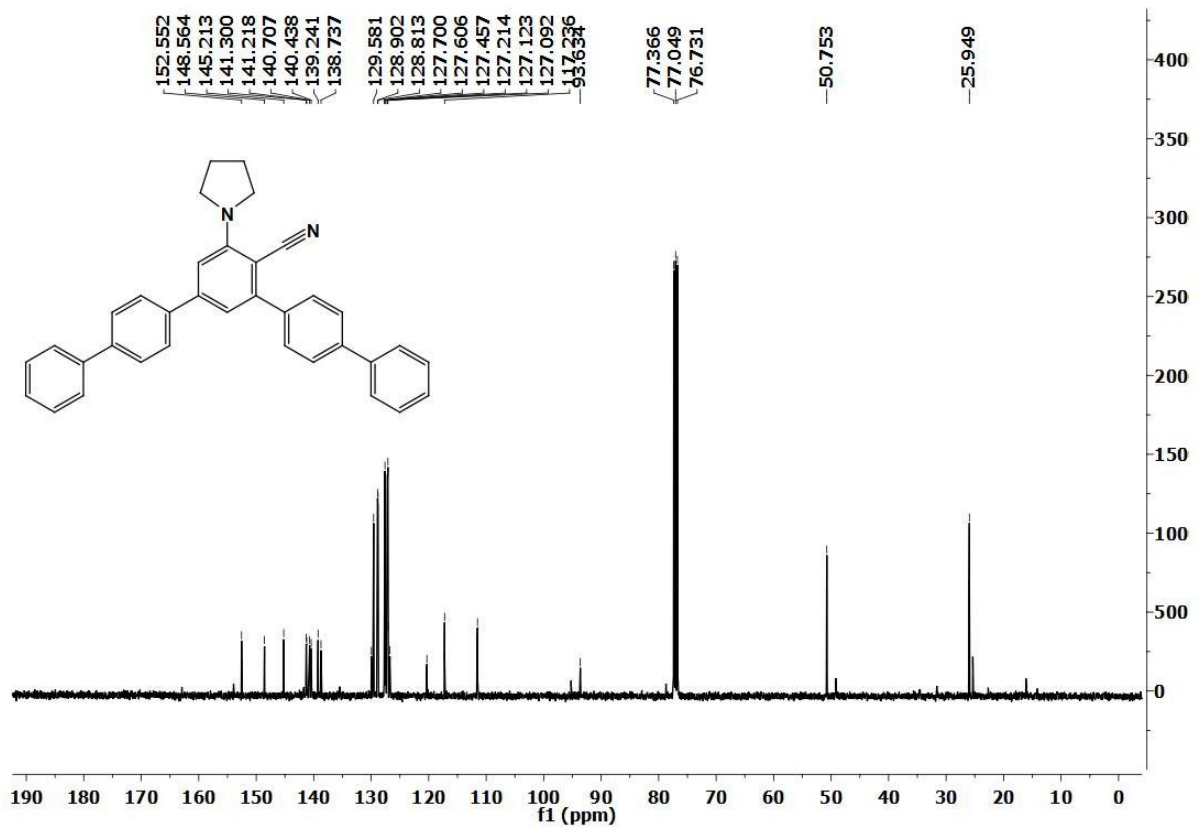
5''-(Piperidin-1-yl)-[1,1':4',1'':3'',1''':4''',1''''-quinquephenyl]-4''-carbonitrile 11a:



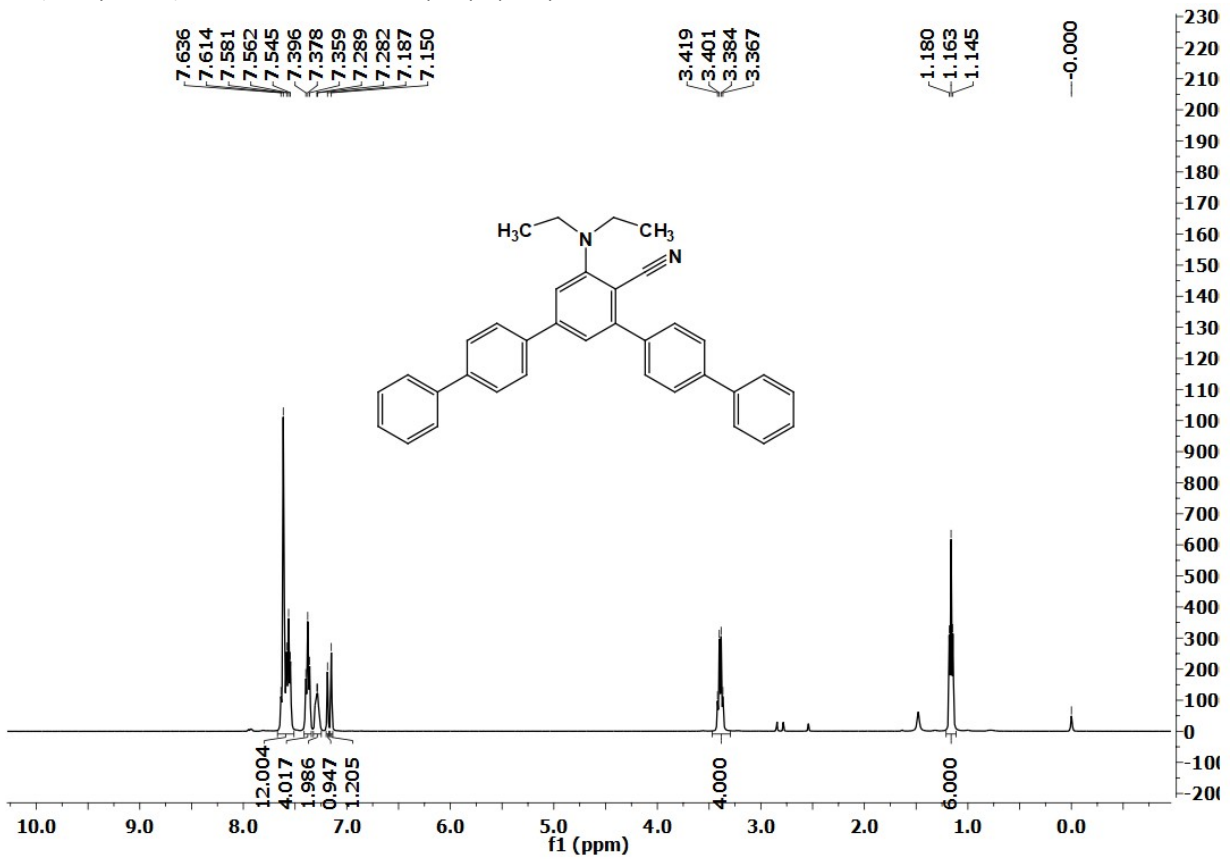


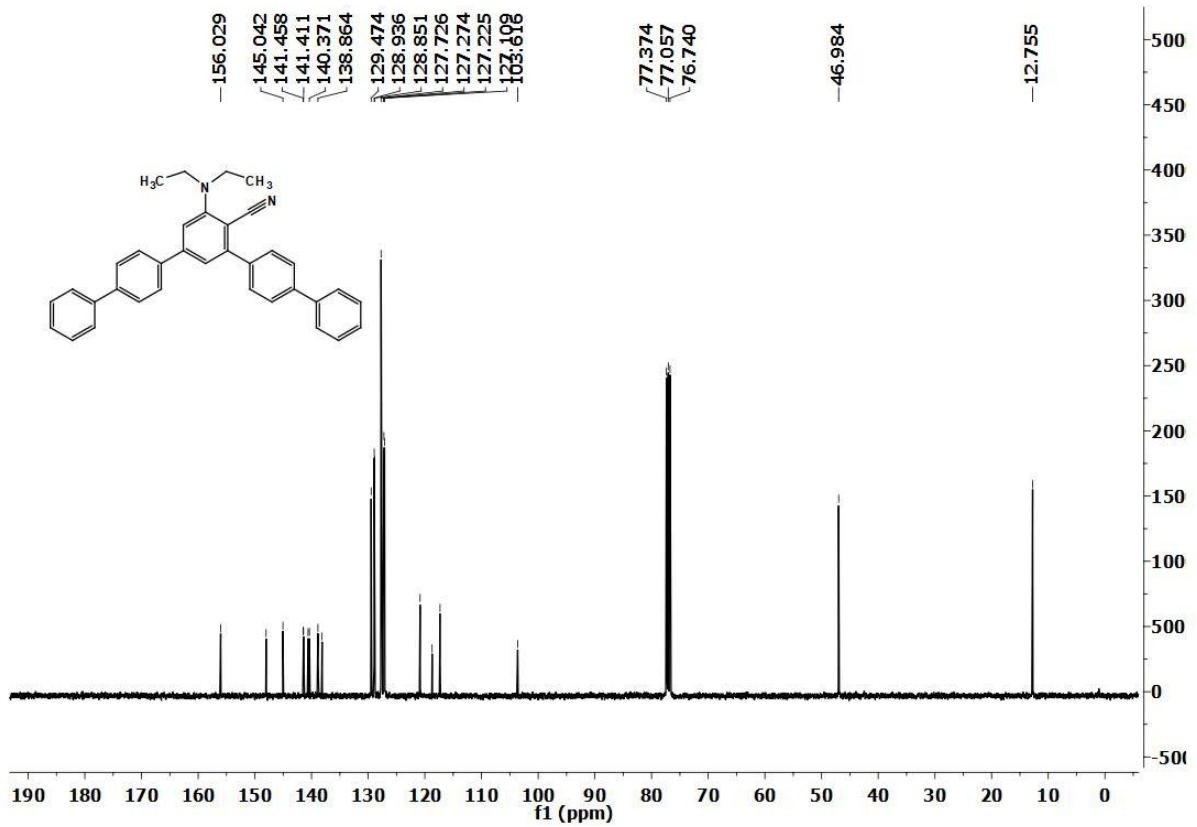
5''-(Pyrrolidin-1-yl)-[1,1':4',1'':3'',1''':4''',1''''-quinquephenyl]-4''-carbonitrile 11c:



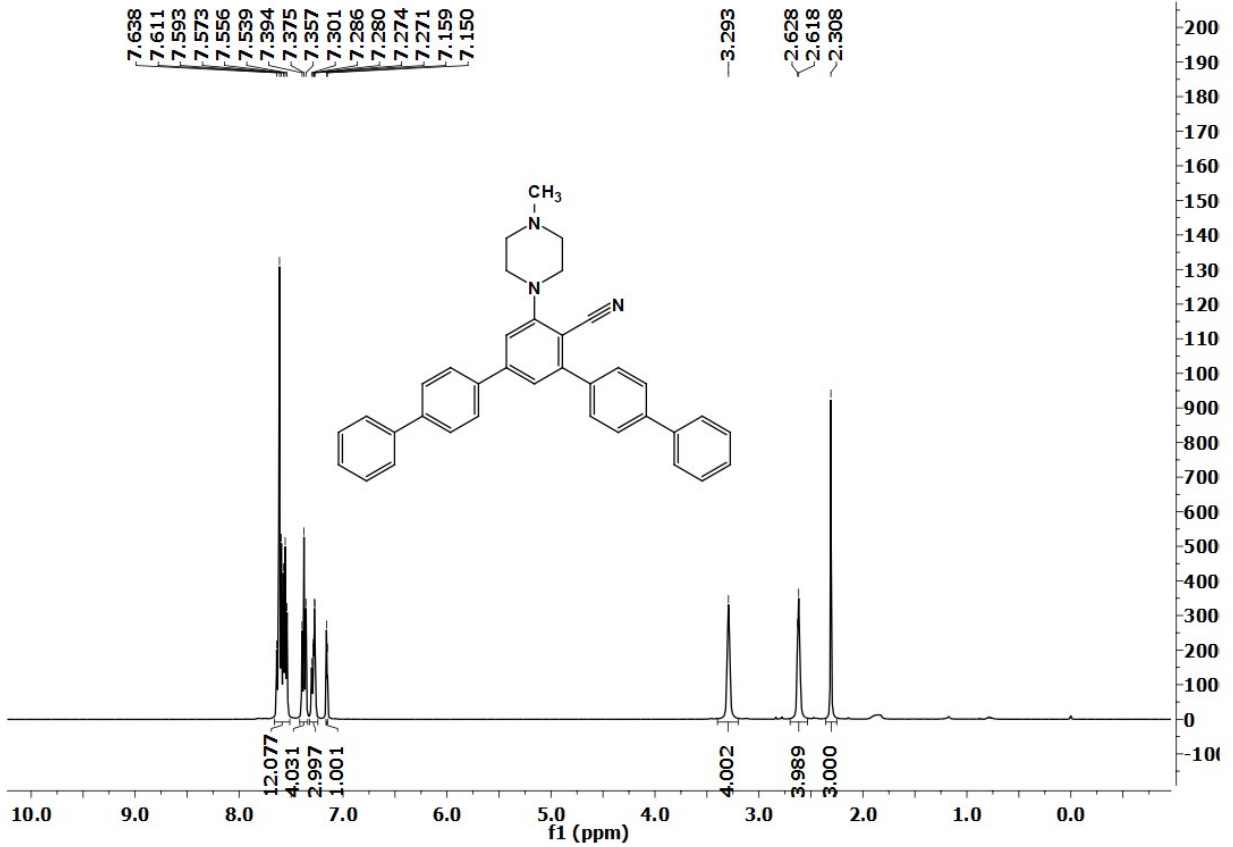


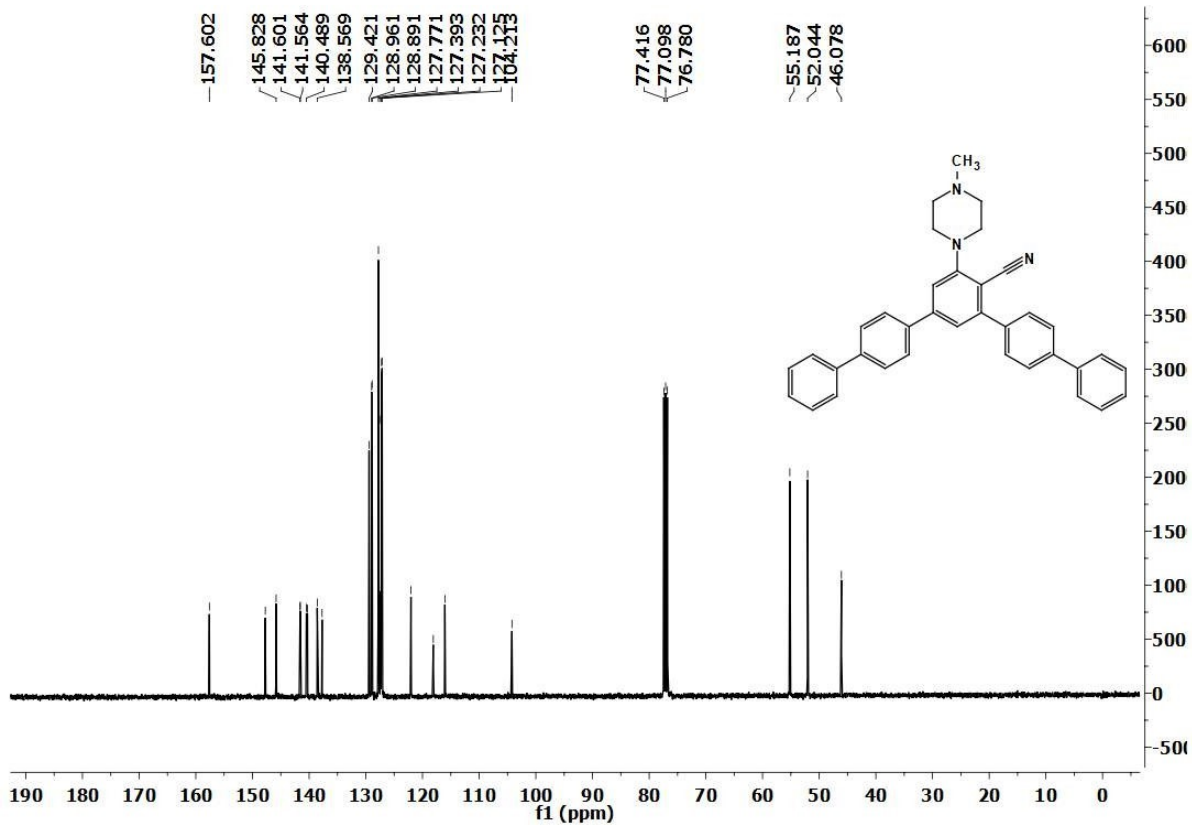
5''-(Diethylamino)-[1,1':4',1'':3'',1''':4''',1''''-quinquephenyl]-4''-carbonitrile 11d:



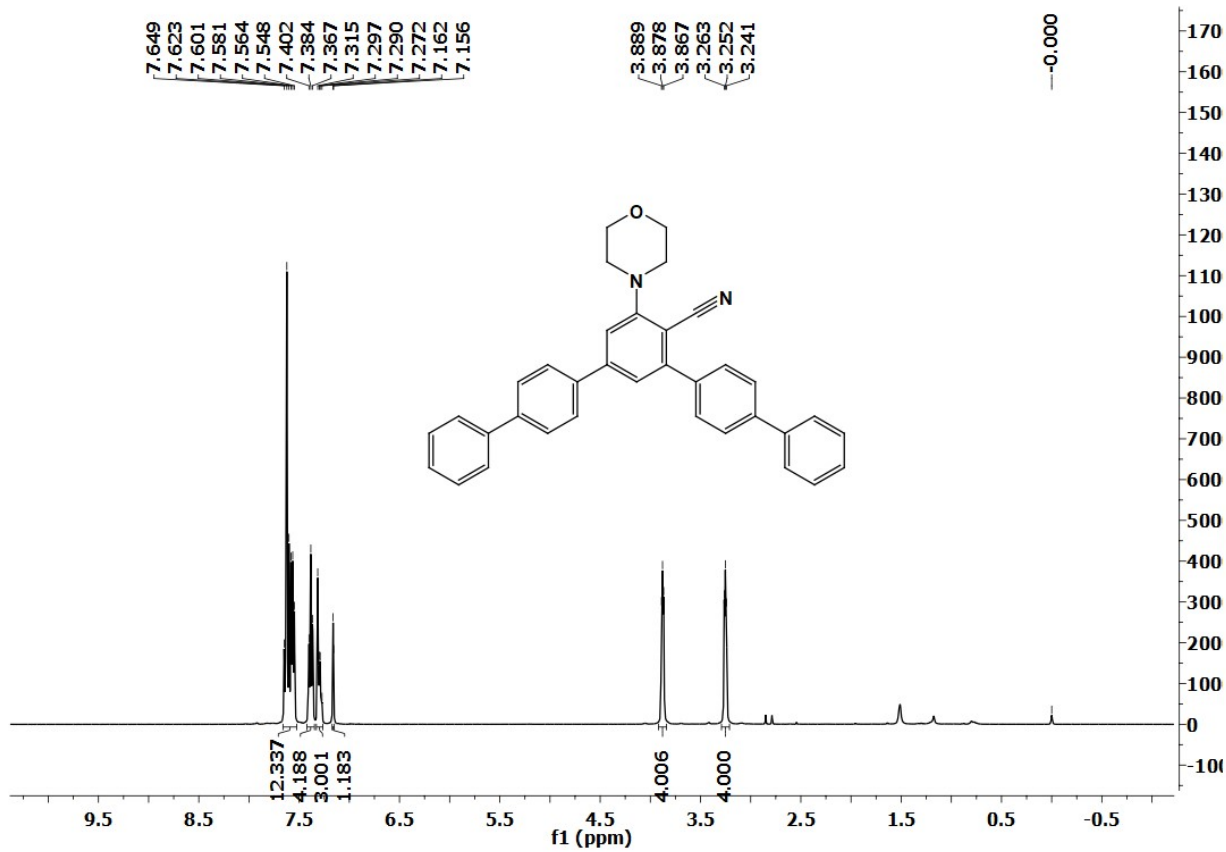


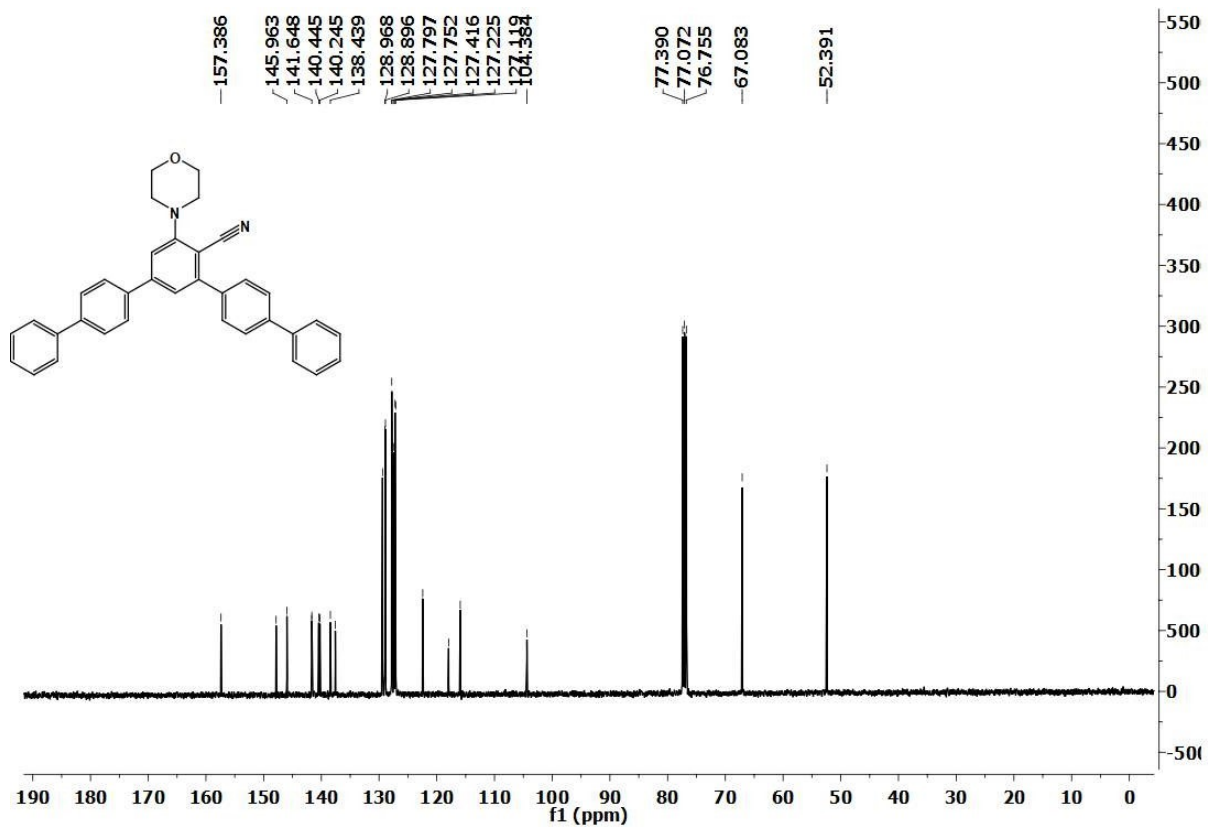
5'-((4-Methylpiperazin-1-yl)-[1,1':4',1'':3'',1'''':4''',1''''-quinquephenyl]-4''-carbonitrile 11e:



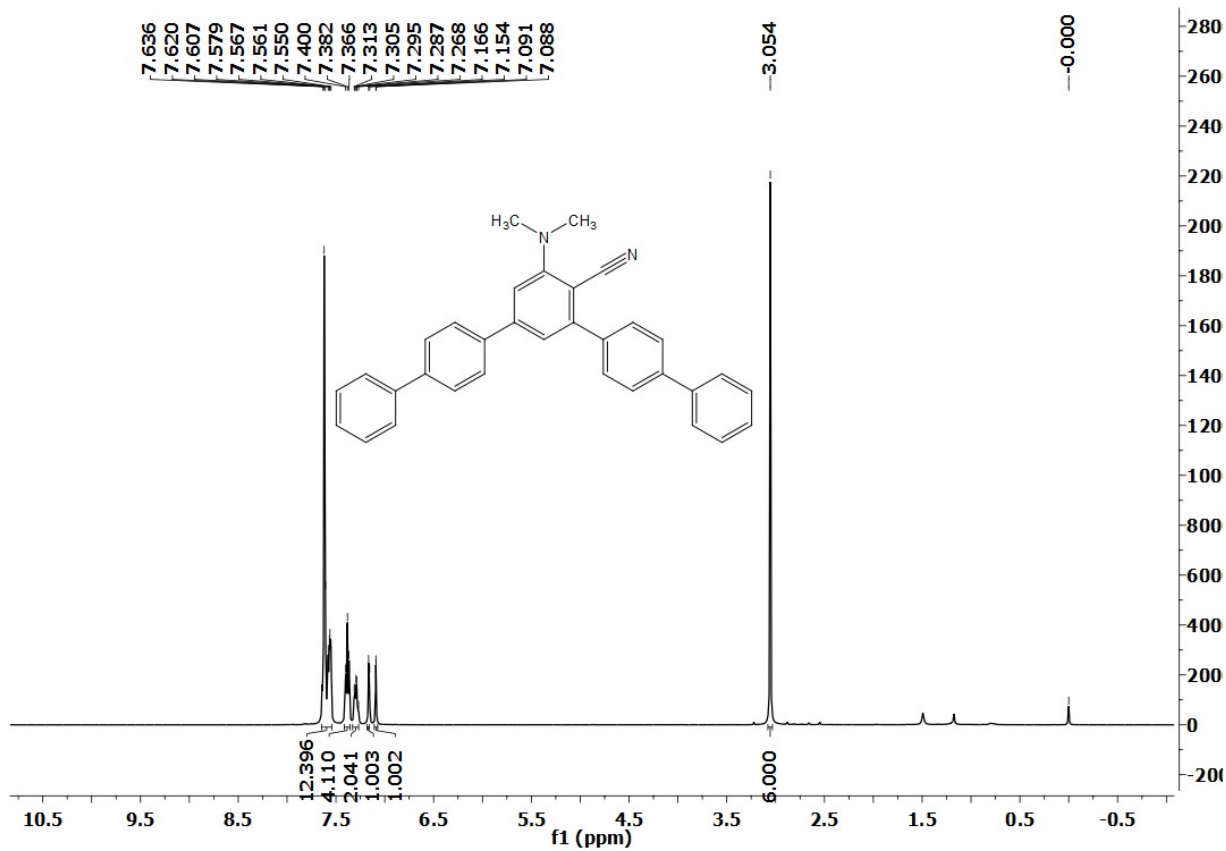


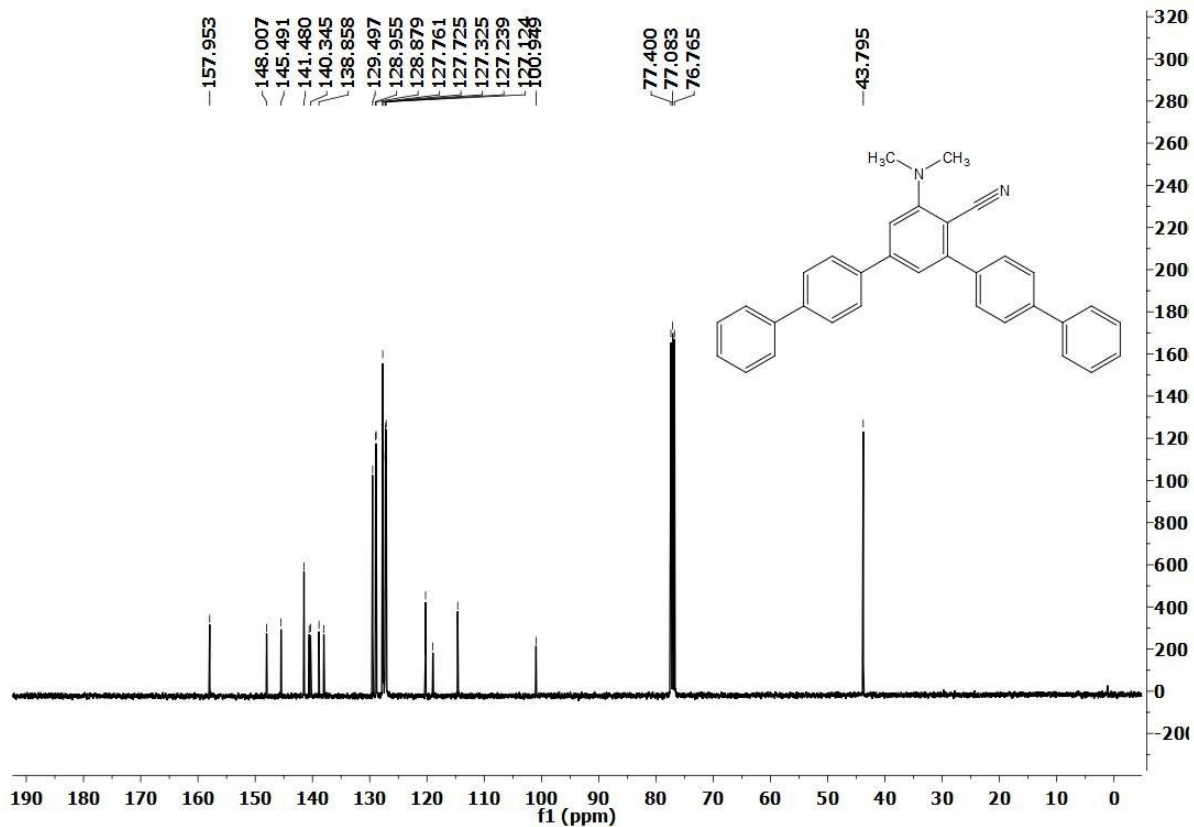
5''-Morpholino-[1,1':4',1'':3'':1'''-quinquephenyl]-4''-carbonitrile 11f:



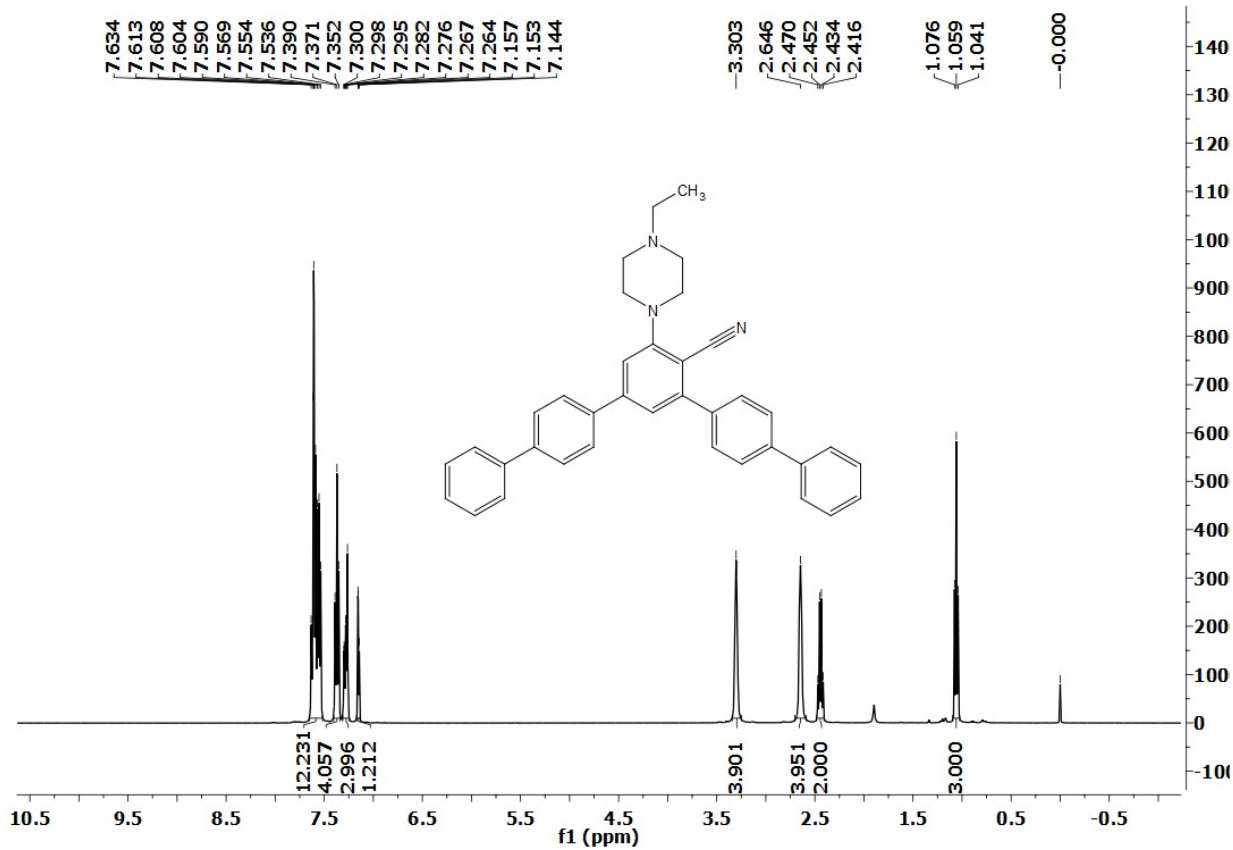


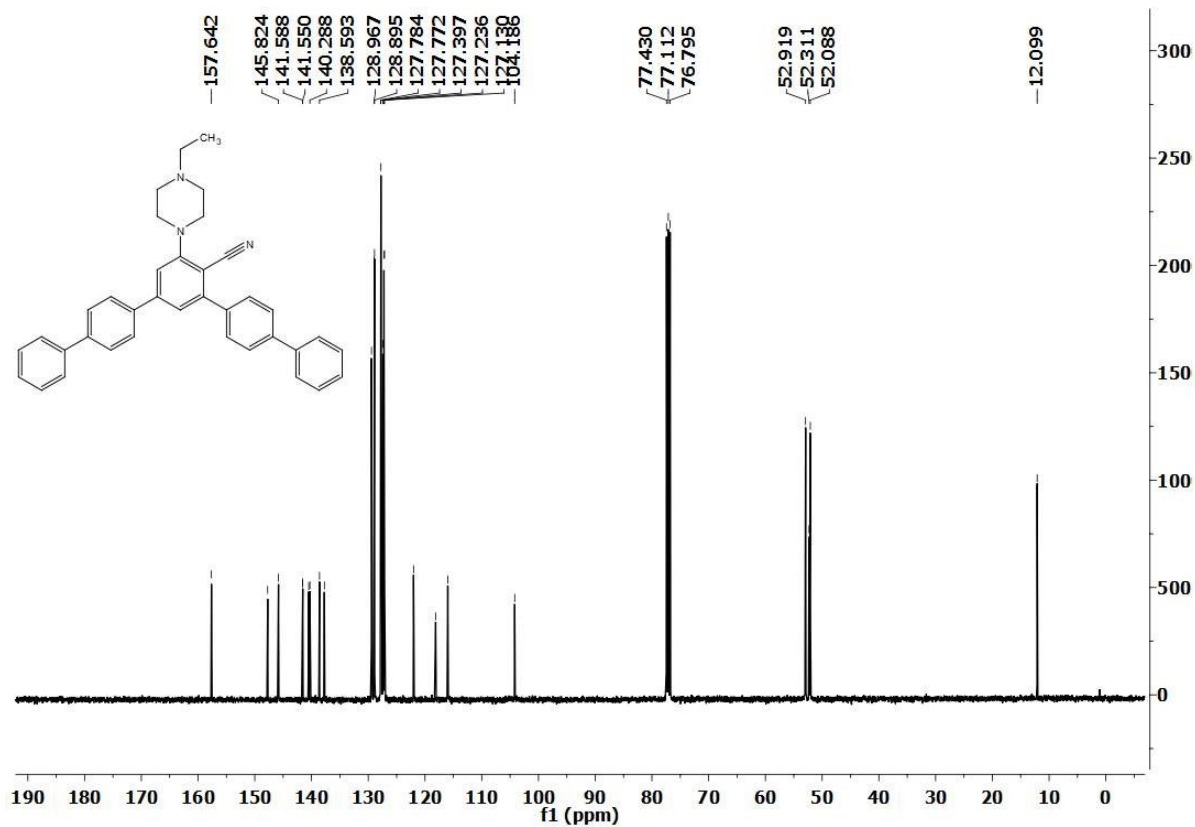
5'-((Dimethylamino)-[1,1':4',1'':3'':1''':4''',1''''-quinquephenyl]-4''-carbonitrile 11g:



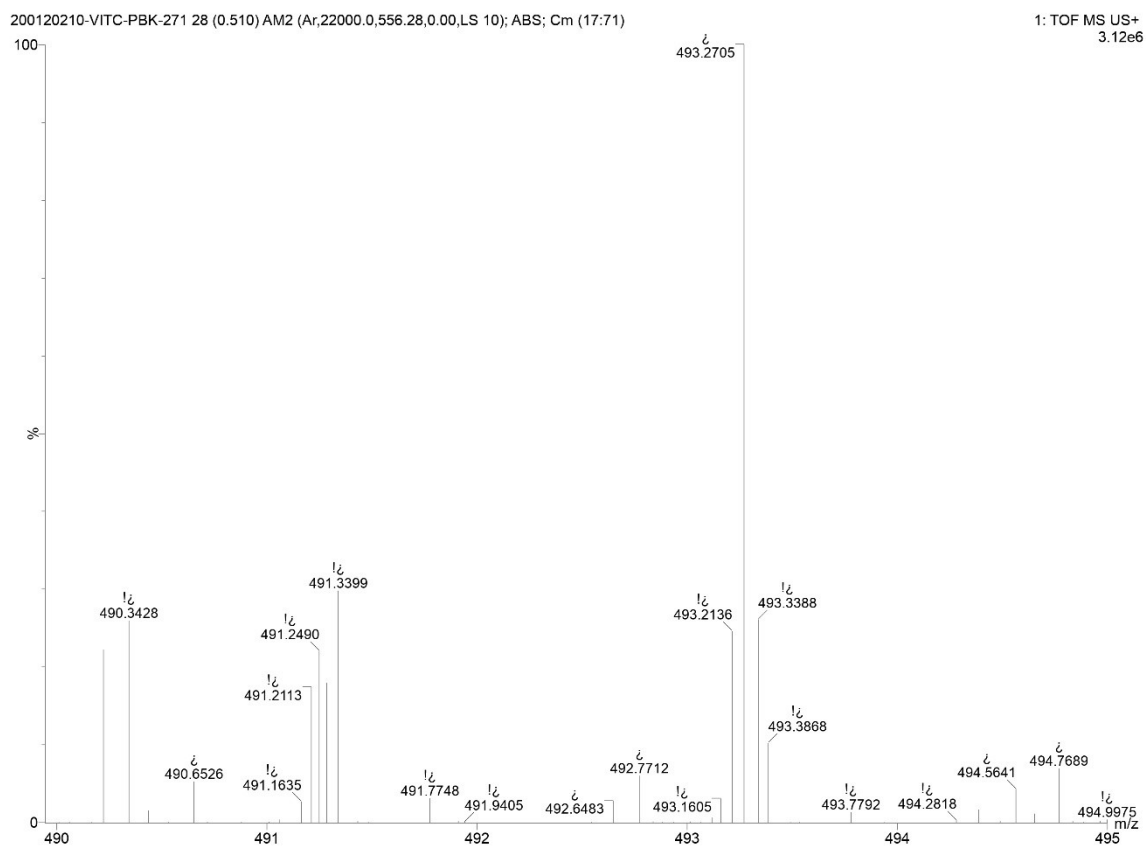


5'-((4-Ethylpiperazin-1-yl)-[1,1':4',1'':3'',1''':4''',1''':4''']-quinquephenyl)-4'-carbonitrile 11h:

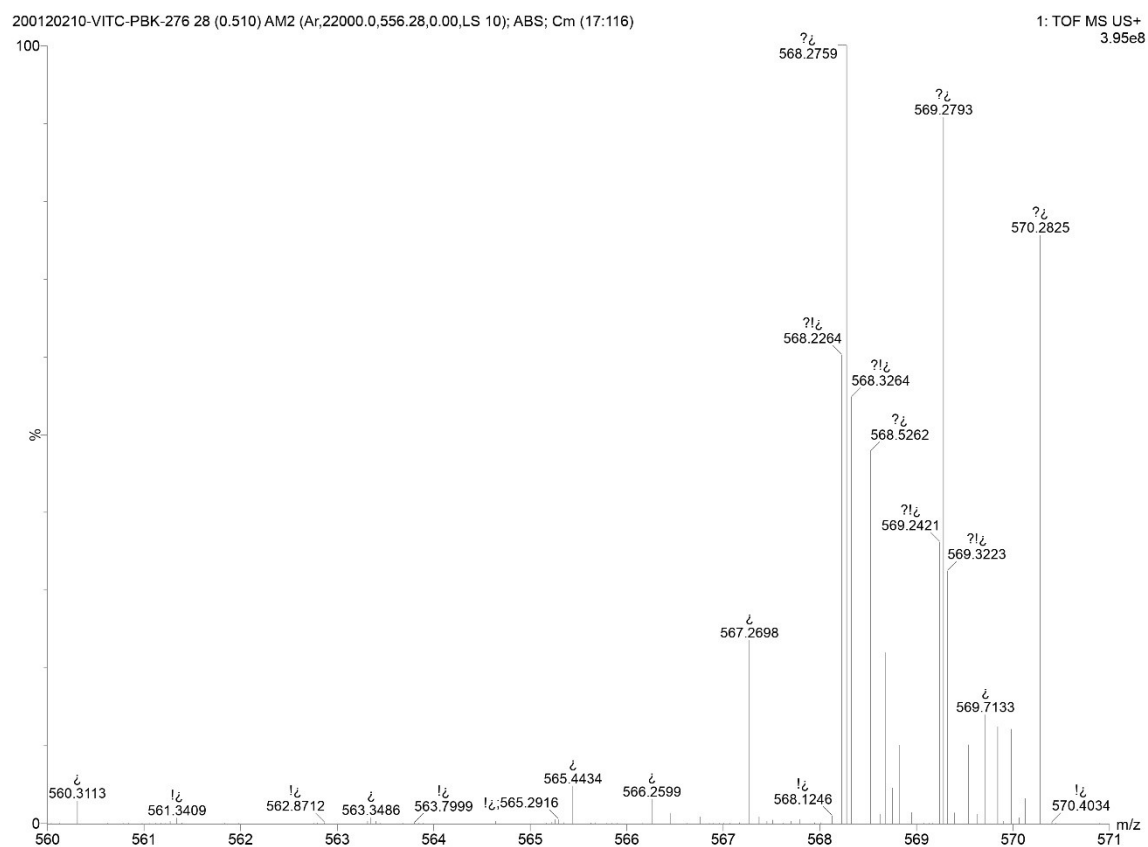




5''-(Piperidin-1-yl)-[1,1':4',1'':3'',1''':4''',1''''-quinquephenyl]-4''-carbonitrile 11a:



5''-(4-Phenylpiperazin-1-yl)-[1,1':4',1'':3'',1''':4''',1''''-quinquephenyl]-4''-carbonitrile 11b:



5''-Morpholino-[1,1':4',1'':3'',1''':4''',1''''-quinquephenyl]-4''-carbonitrile 11f:

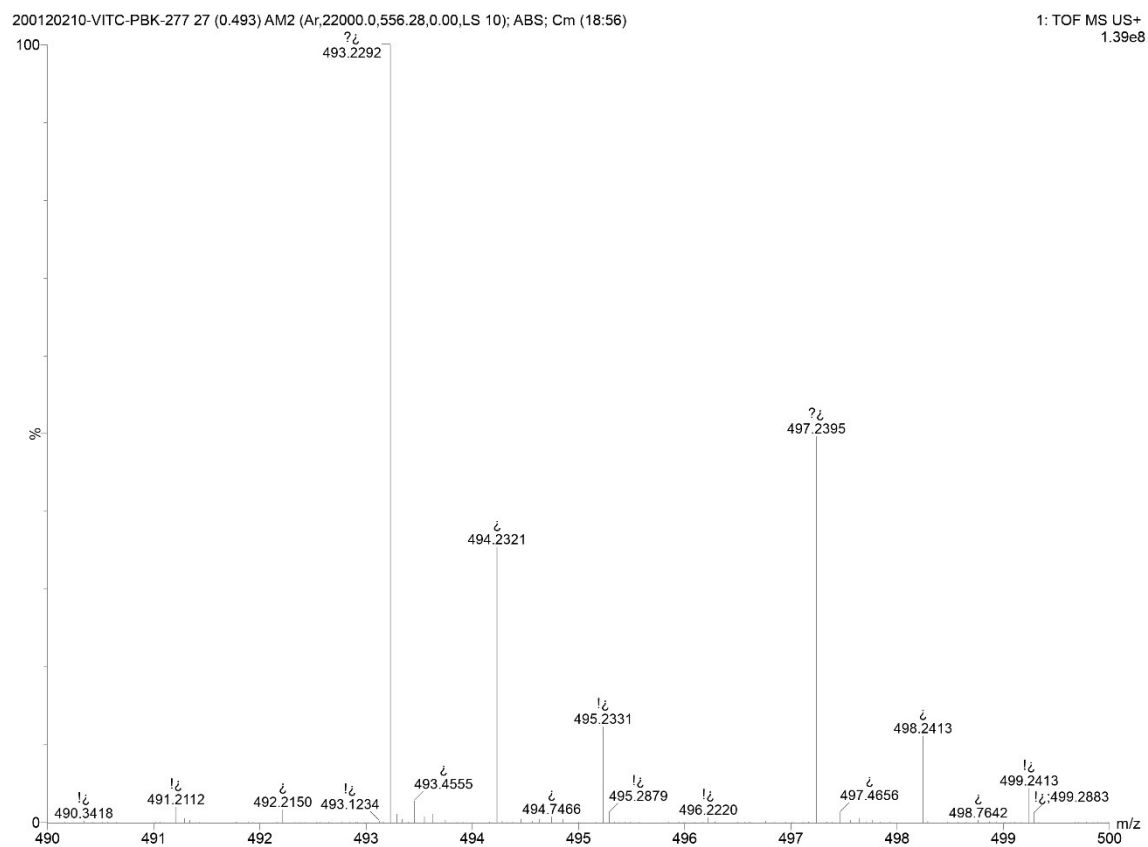


Figure S1: ¹H-NMR, ¹³C-NMR and mass spectra of the synthesized molecules.

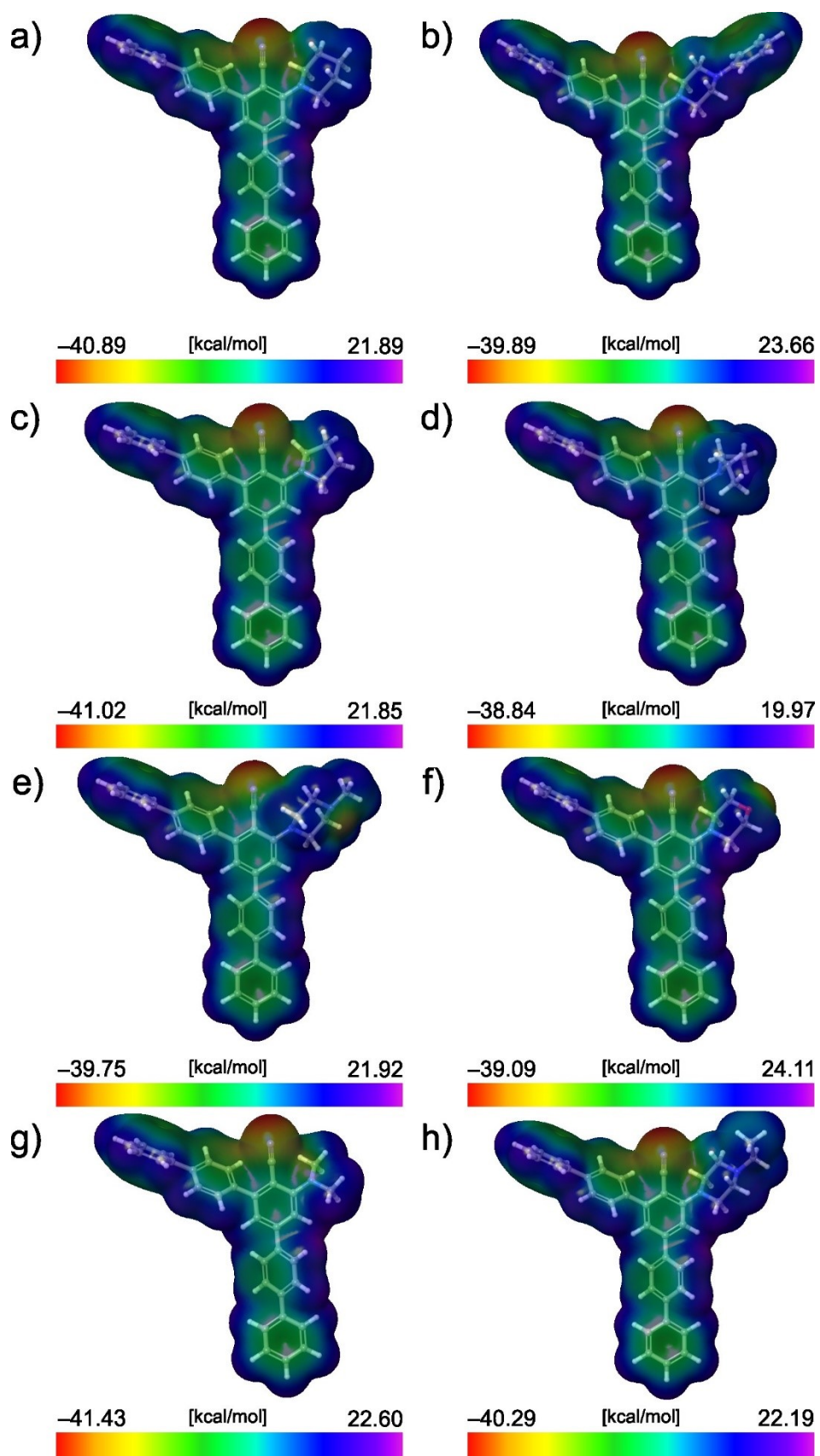


Figure S2: MEP surfaces of 11a-h molecules.

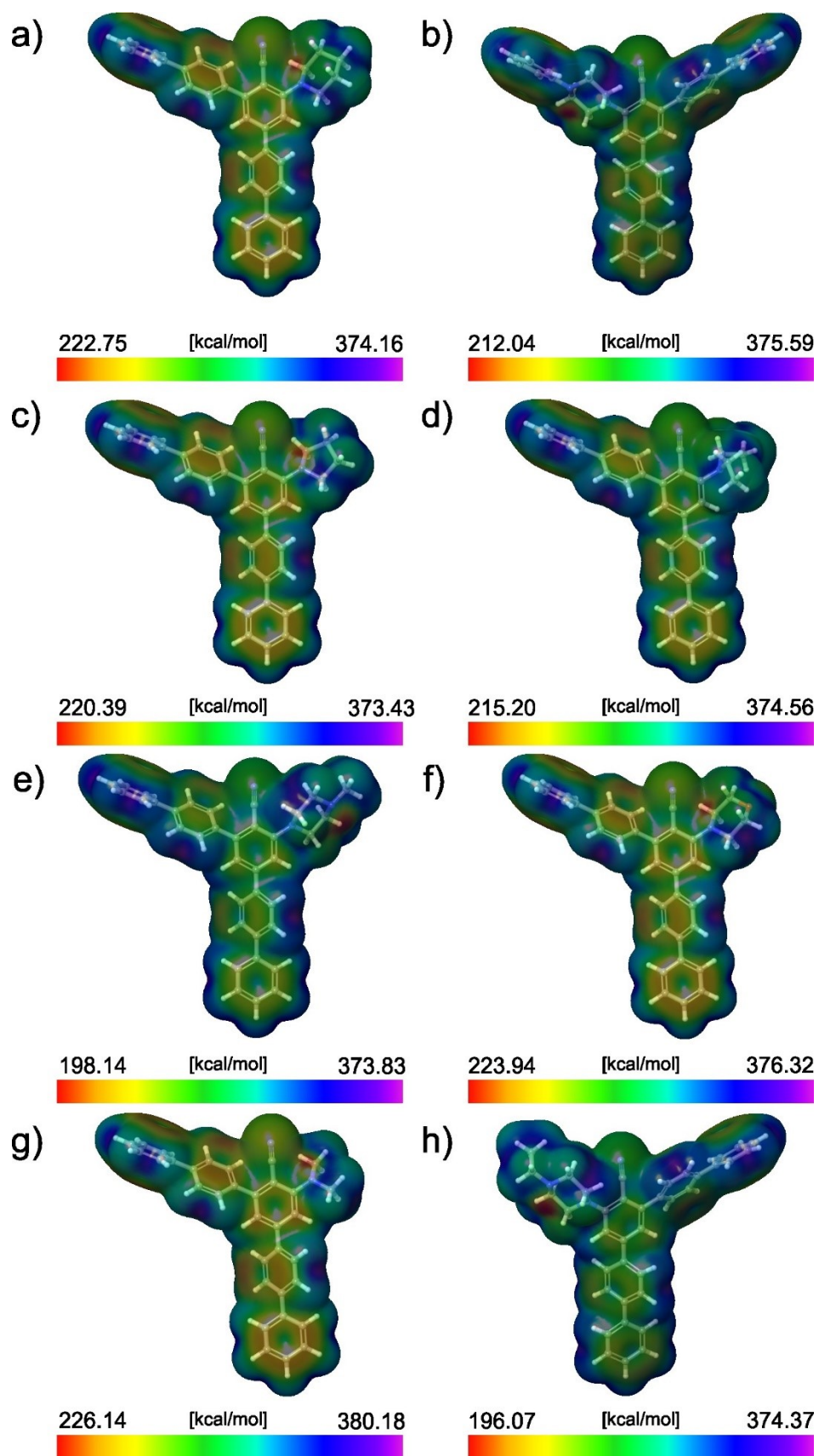


Figure S3: ALIE values of 11a-h molecules.

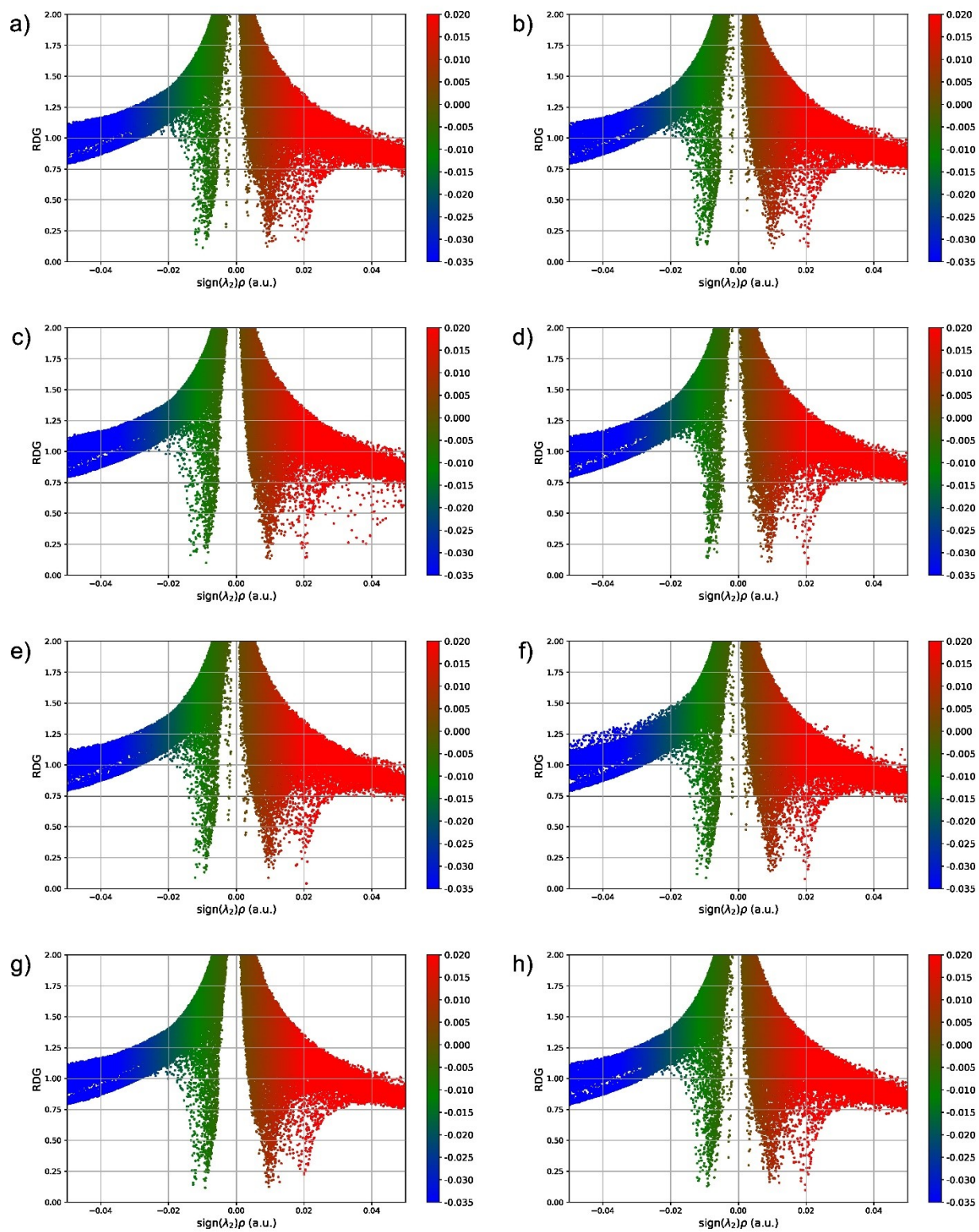


Figure S4. RDG scatter plots of 11a-h molecules.

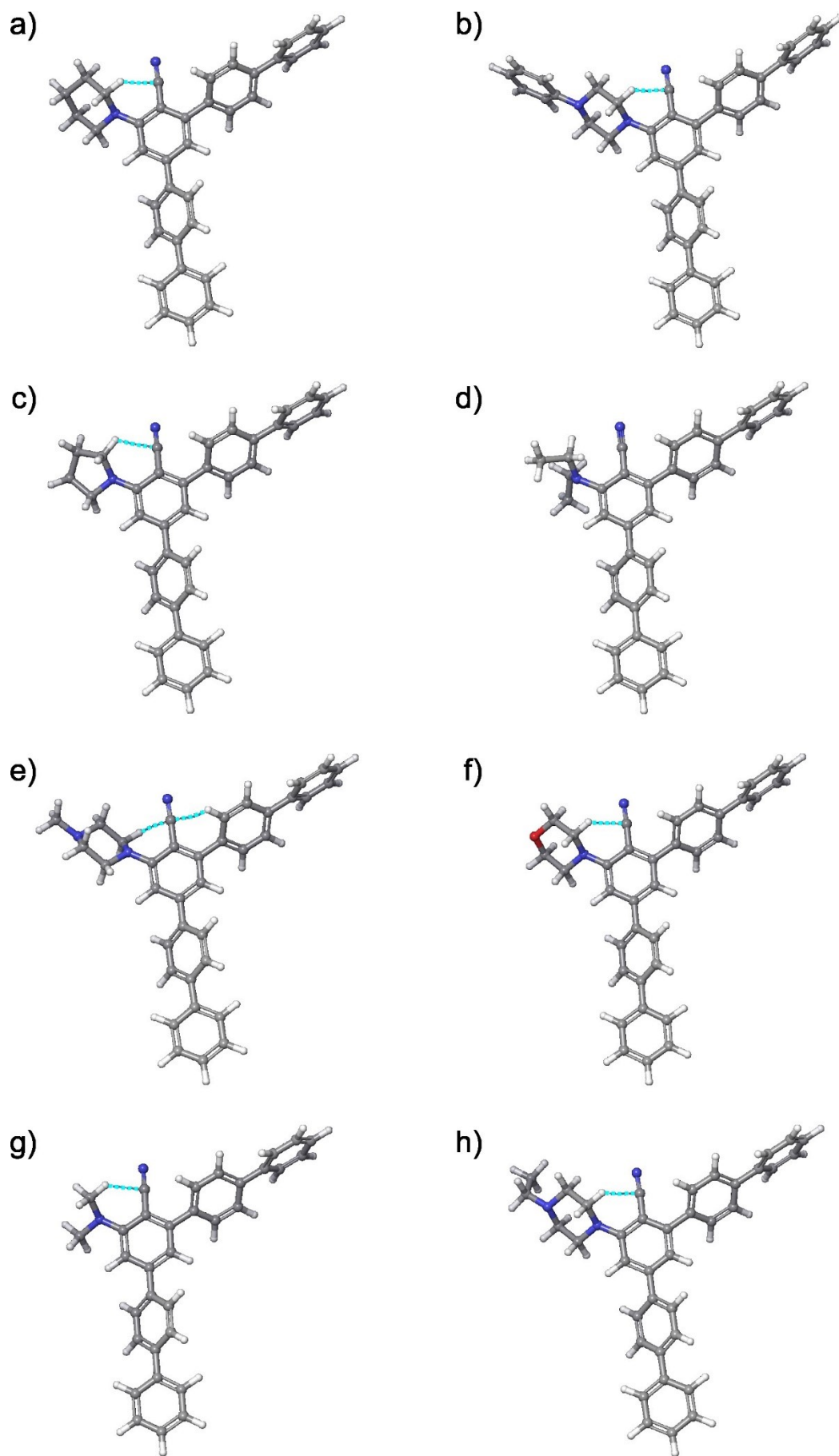


Figure S5. RDG surfaces and non-covalent interactions with numerated non-covalent interactions. Orange lines indicate non-covalent interactions identified by critical points.