Supplementary Material

1,3,4-Thiadiazol-2-ylphenyl-1,2,4,5-tetrazines: efficient synthesis via Pinner reaction and their luminescent properties

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^{1}H and ^{13}C NMR Spectra of synthesized compounds 6a-d

Figure S1: ^{1}H NMR 4-(5-Phenyl-1,3,4-thiadiazol-2-yl)benzonitrile (6a)

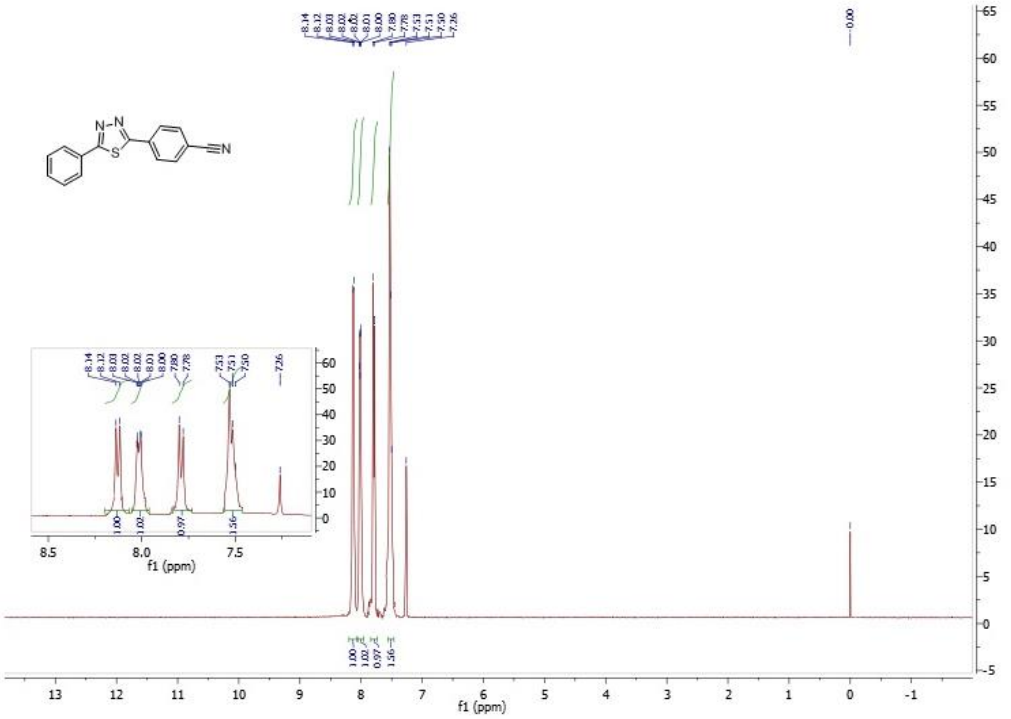


Figure S2: ^{13}C NMR 4-(5-Phenyl-1,3,4-thiadiazol-2-yl)benzonitrile (6a)

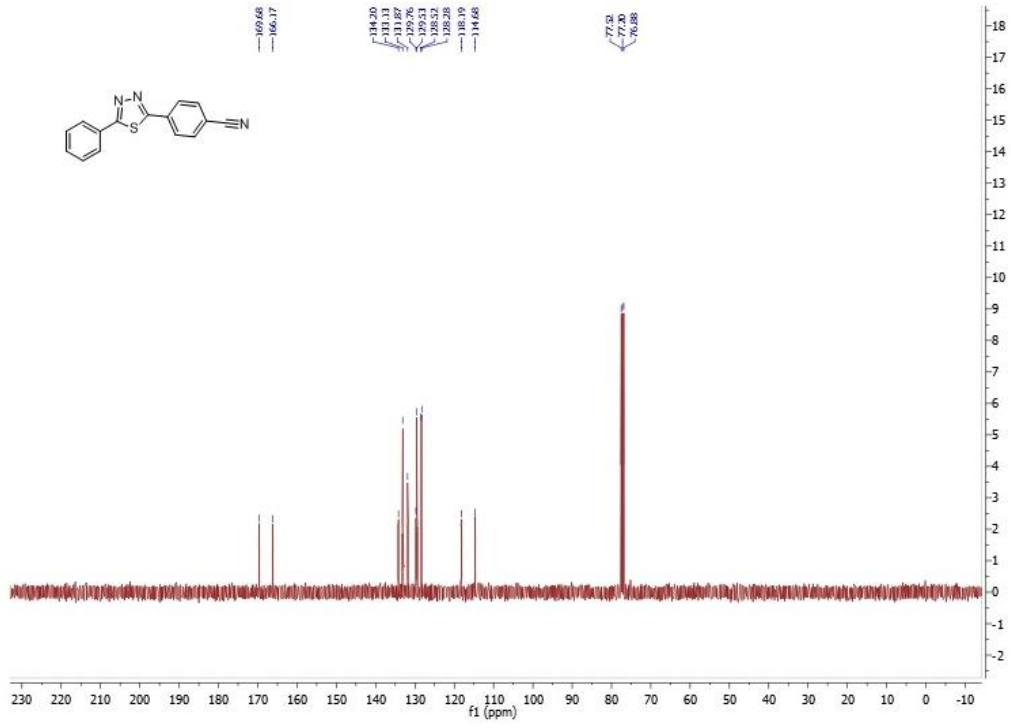


Figure S3: ^{1}H NMR 4-(5-(4-Methoxyphenyl)-1,3,4-thiadiazol-2-yl)benzonitrile (6b)

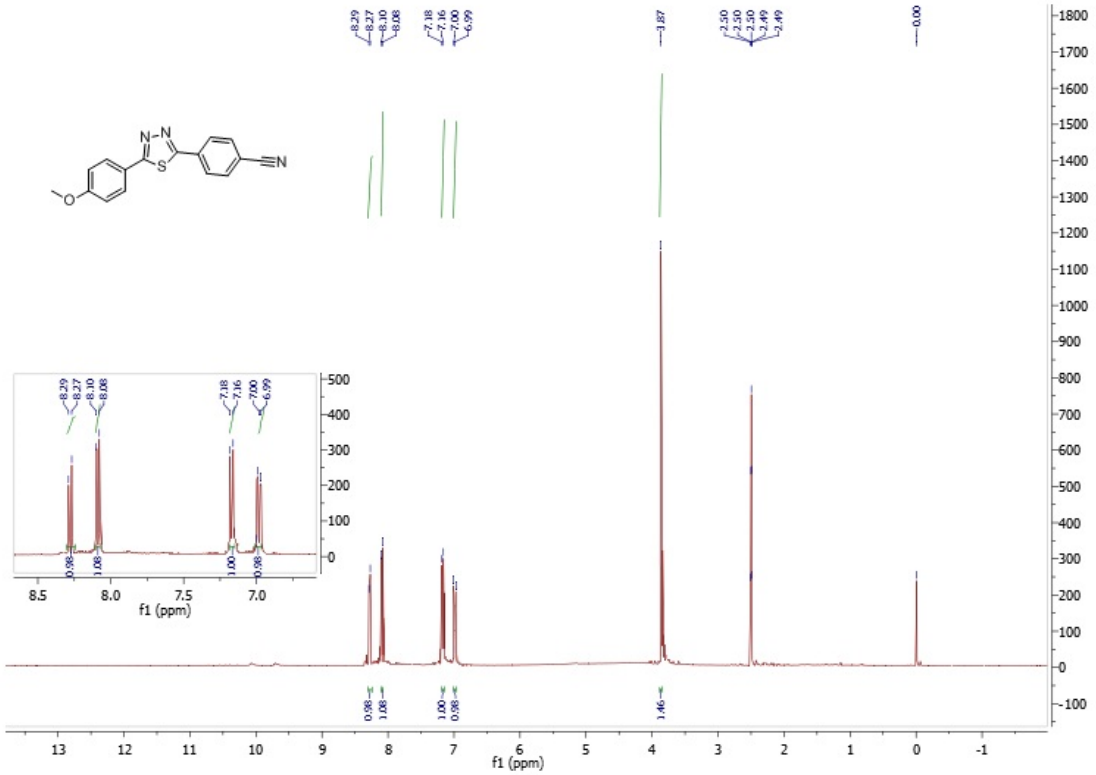


Figure S4: ^{13}C NMR 4-(5-(4-Methoxyphenyl)-1,3,4-thiadiazol-2-yl)benzonitrile (6b)

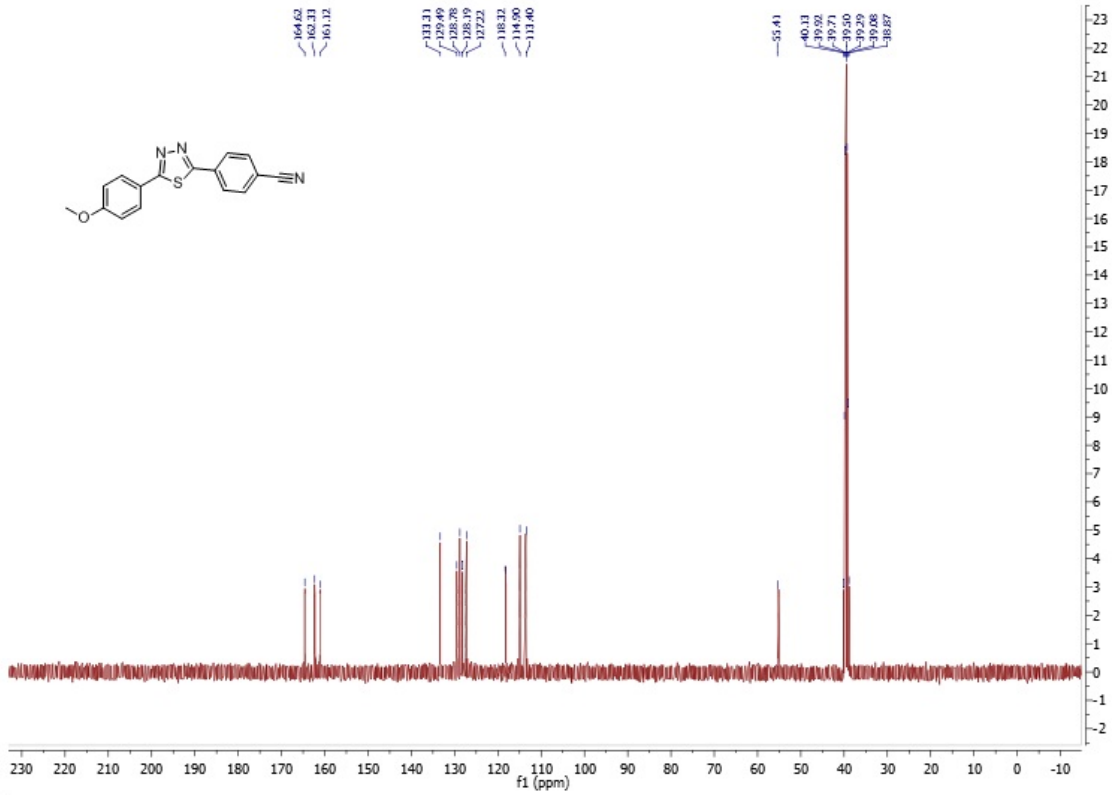


Figure S5: ^{1}H NMR 4-(5-(4-(*tert*-Butyl)phenyl)-1,3,4-thiadiazol-2-yl)benzonitrile (6c)

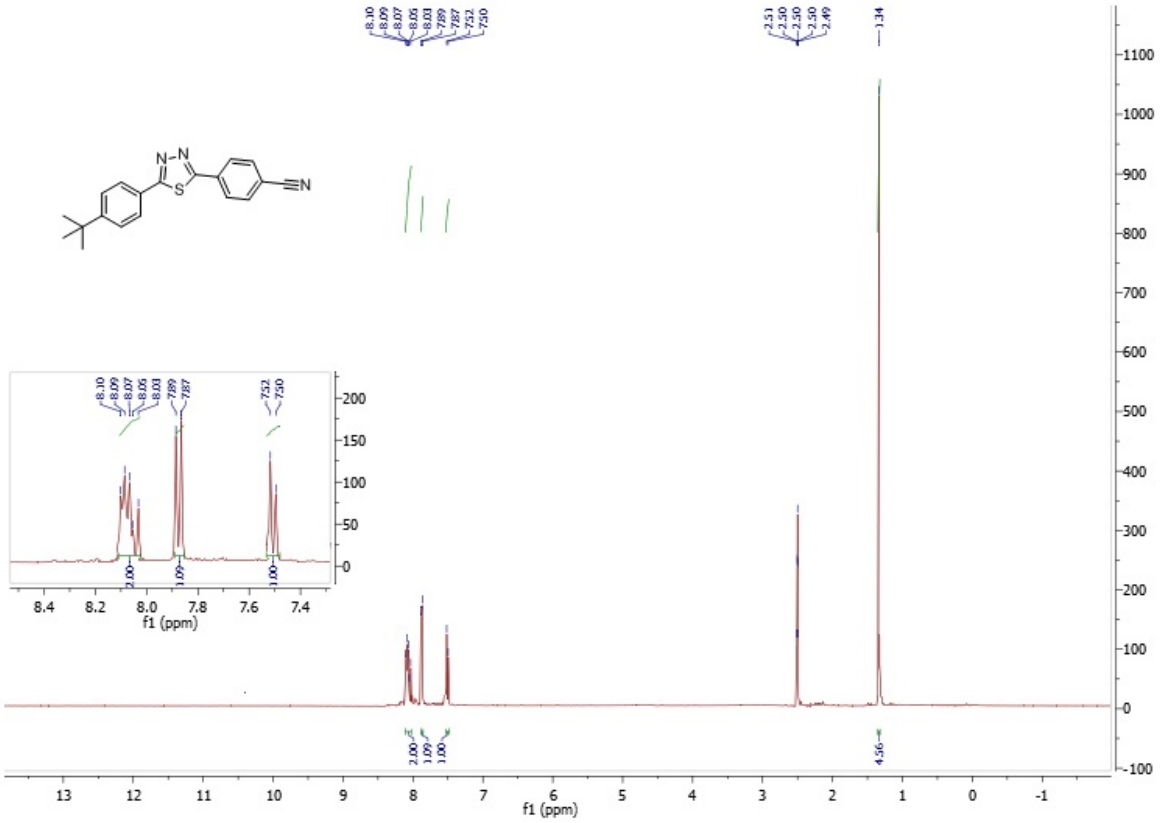


Figure S6: ^{13}C NMR 4-(5-(4-(*tert*-Butyl)phenyl)-1,3,4-thiadiazol-2-yl)benzonitrile (6c)

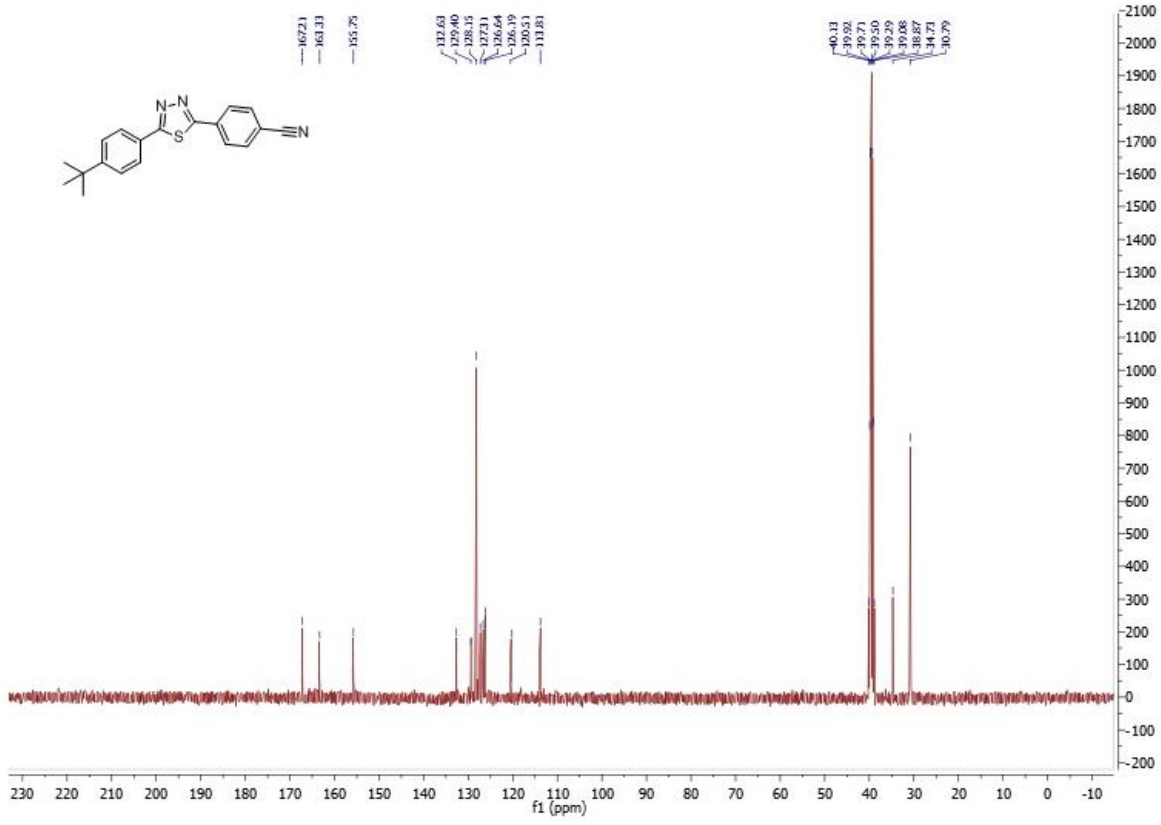


Figure S7: ^{1}H NMR 4-(5-(4-Nitrophenyl)-1,3,4-thiadiazol-2-yl)benzonitrile (6d)

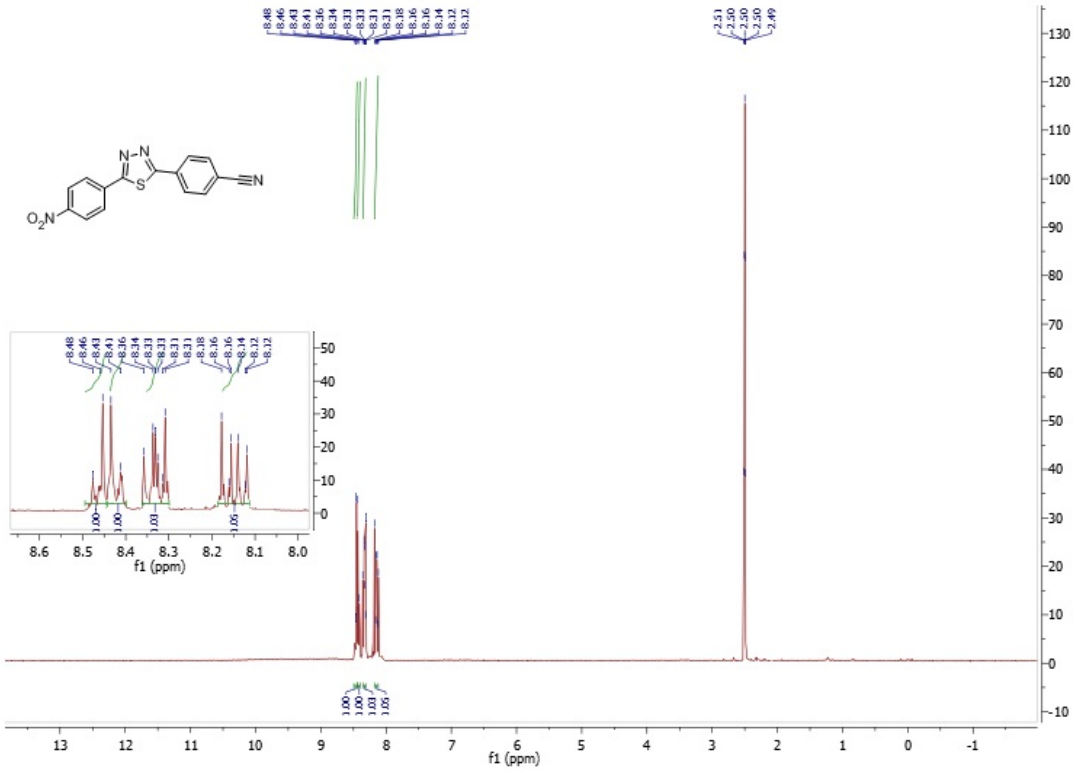
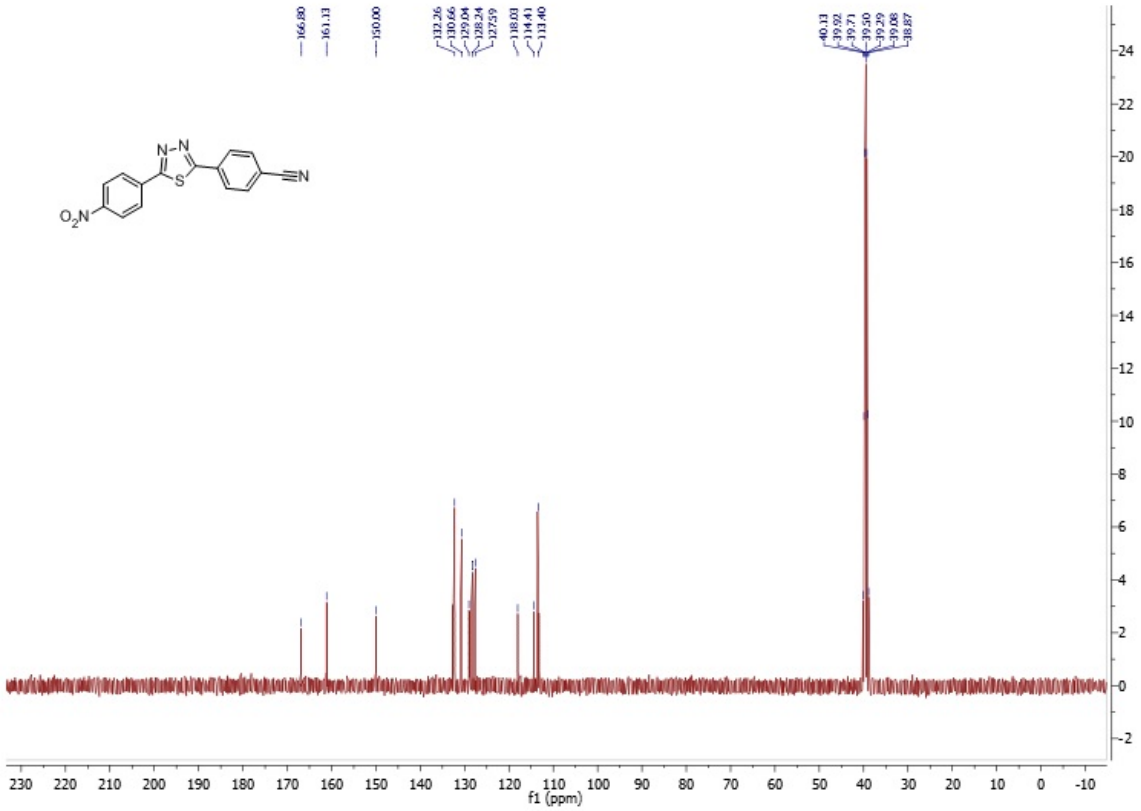


Figure S8: ^{13}C NMR 4-(5-(4-Nitrophenyl)-1,3,4-thiadiazol-2-yl)benzonitrile (6d)



^{1}H and ^{13}C NMR Spectra of synthesized compounds 8a-j

Figure S9: ^{1}H NMR 3,6-Bis(4-(5-phenyl-1,3,4-thiadiazol-2-yl)phenyl)-1,2,4,5-tetrazine (8a)

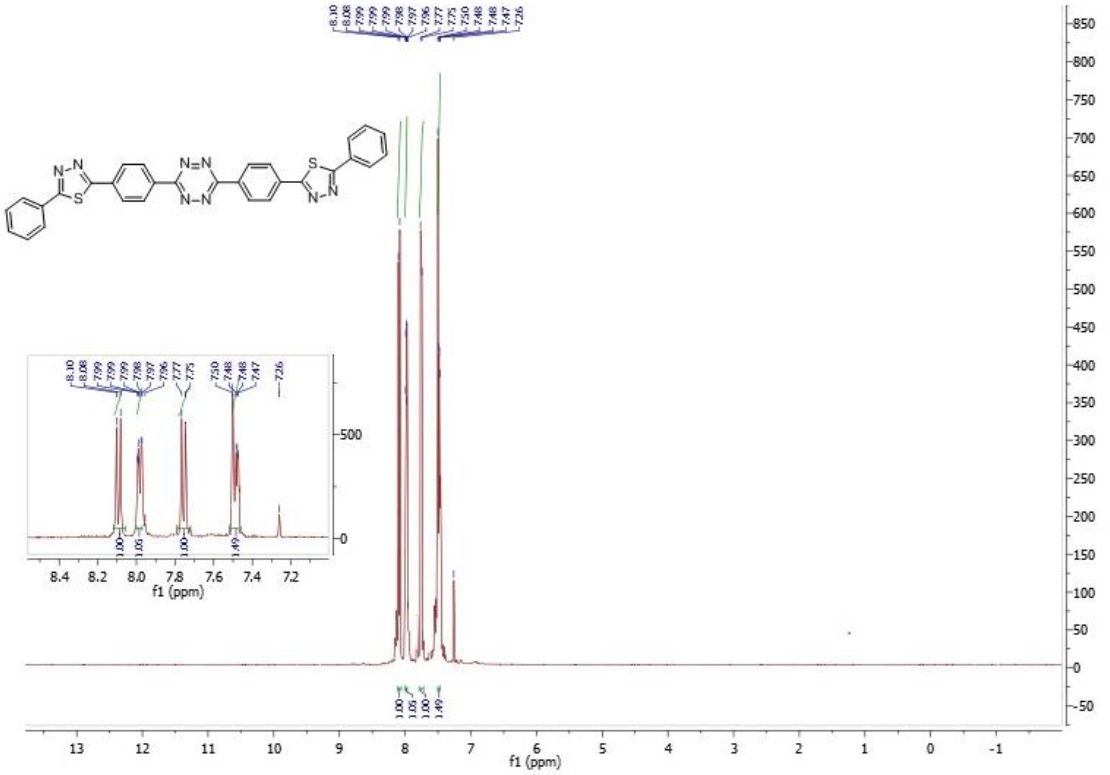


Figure S10: ^{13}C NMR 3,6-Bis(4-(5-phenyl-1,3,4-thiadiazol-2-yl)phenyl)-1,2,4,5-tetrazine (8a)

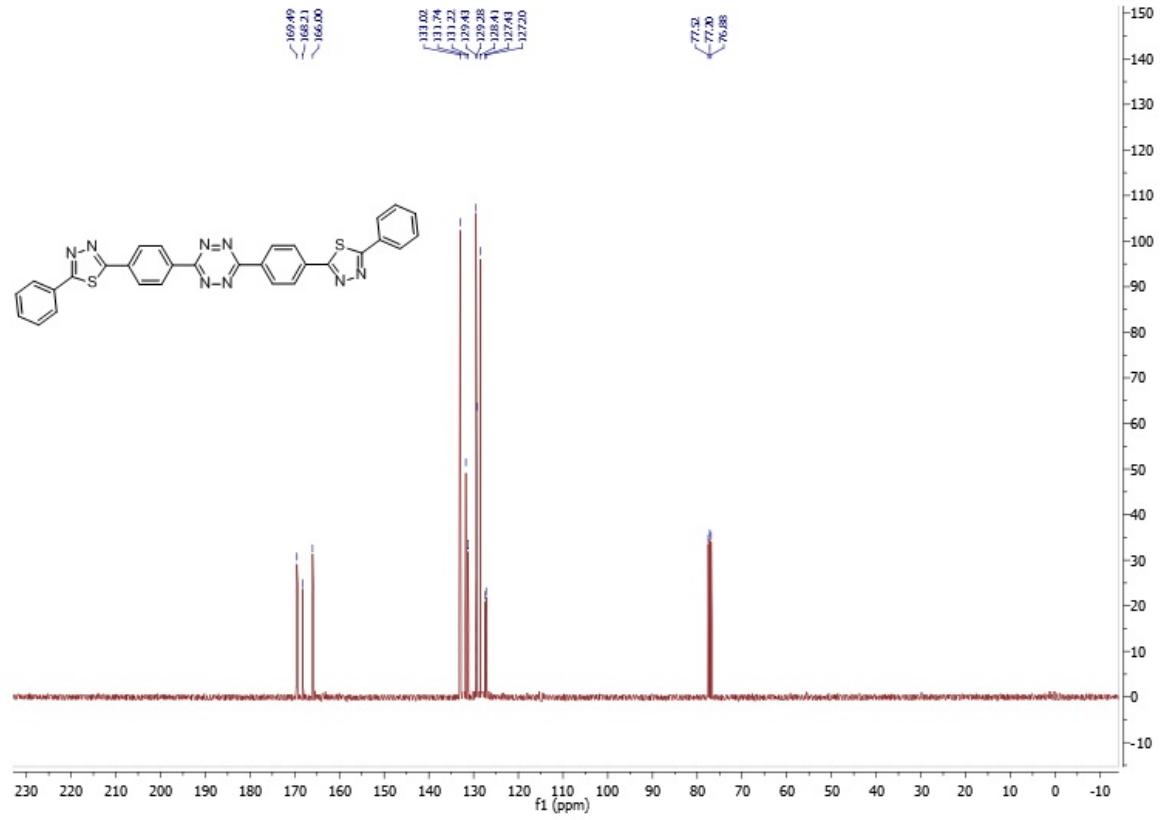


Figure S11: ^{1}H NMR 3,6-Bis(4-(5-(4-methoxyphenyl)-1,3,4-thiadiazol-2-yl)phenyl)-1,2,4,5-tetrazine (8b)

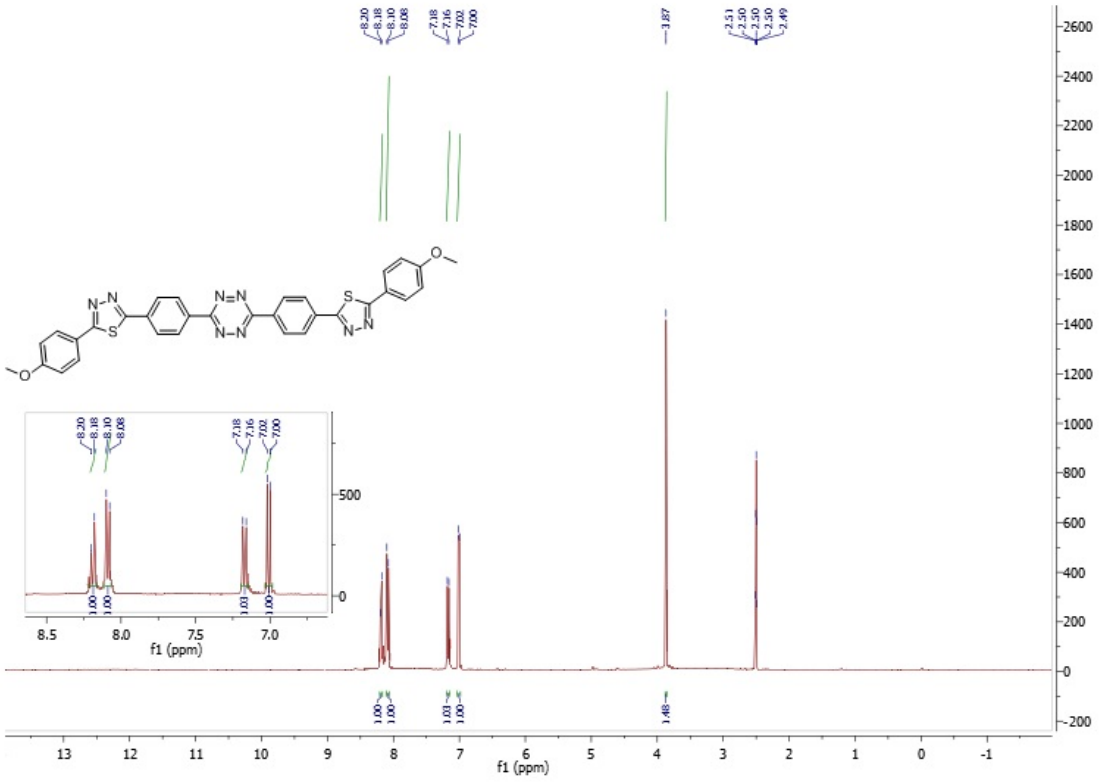


Figure S12: ^{13}C NMR 3,6-Bis(4-(5-(4-methoxyphenyl)-1,3,4-thiadiazol-2-yl)phenyl)-1,2,4,5-tetrazine (8b)

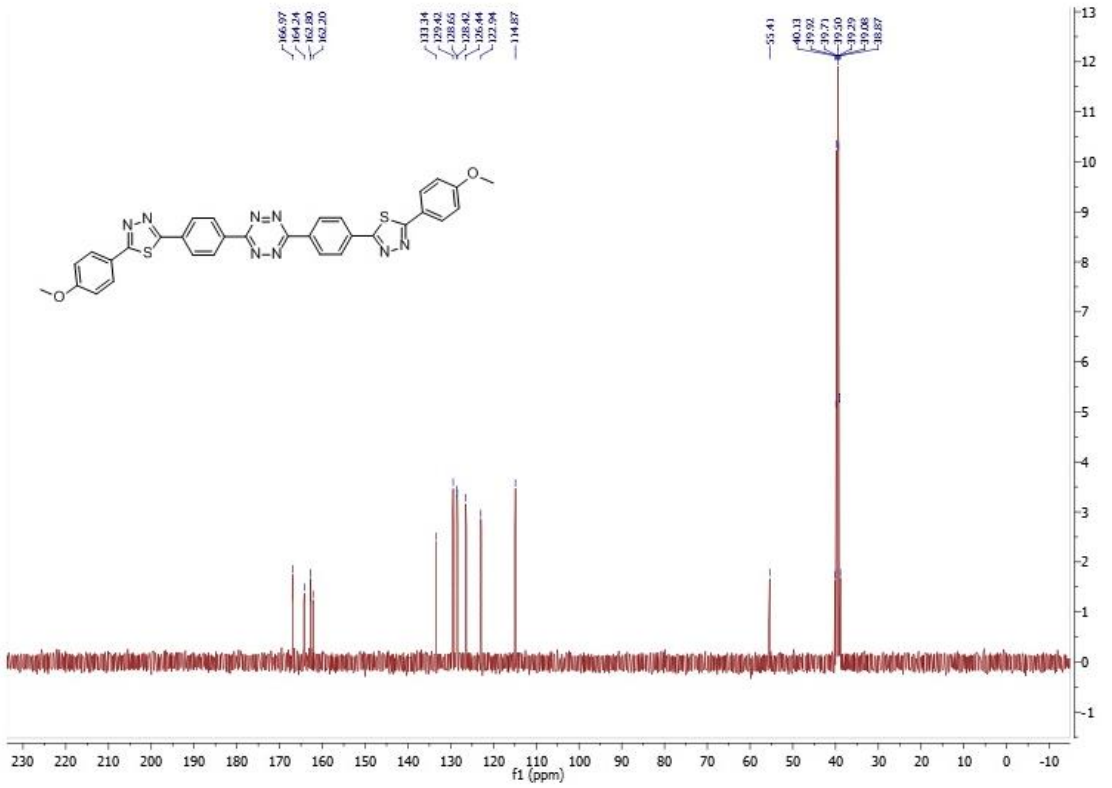


Figure S13: ^{1}H NMR 3,6-Bis(4-(5-(4-(*tert*-butyl)phenyl)-1,3,4-thiadiazol-2-yl)phenyl)-1,2,4,5-tetrazine (8c)

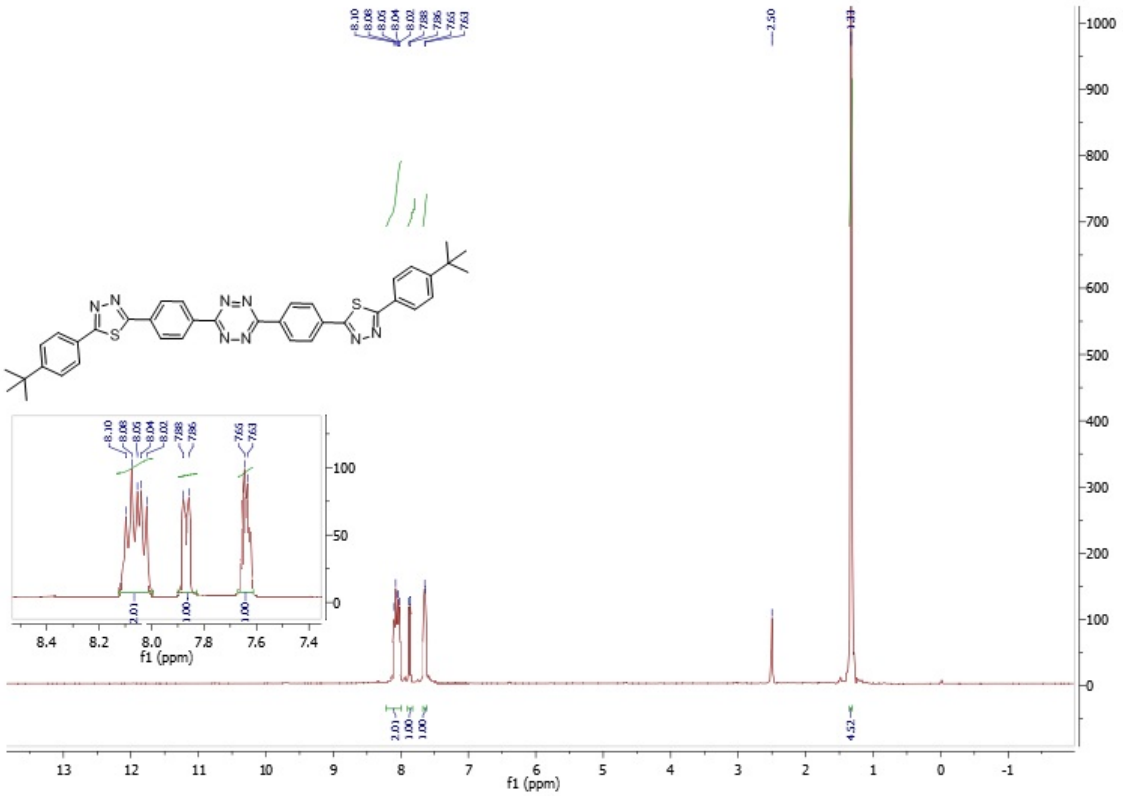


Figure S14: ^{13}C NMR 3,6-Bis(4-(5-(4-(*tert*-butyl)phenyl)-1,3,4-thiadiazol-2-yl)phenyl)-1,2,4,5-tetrazine (8c)

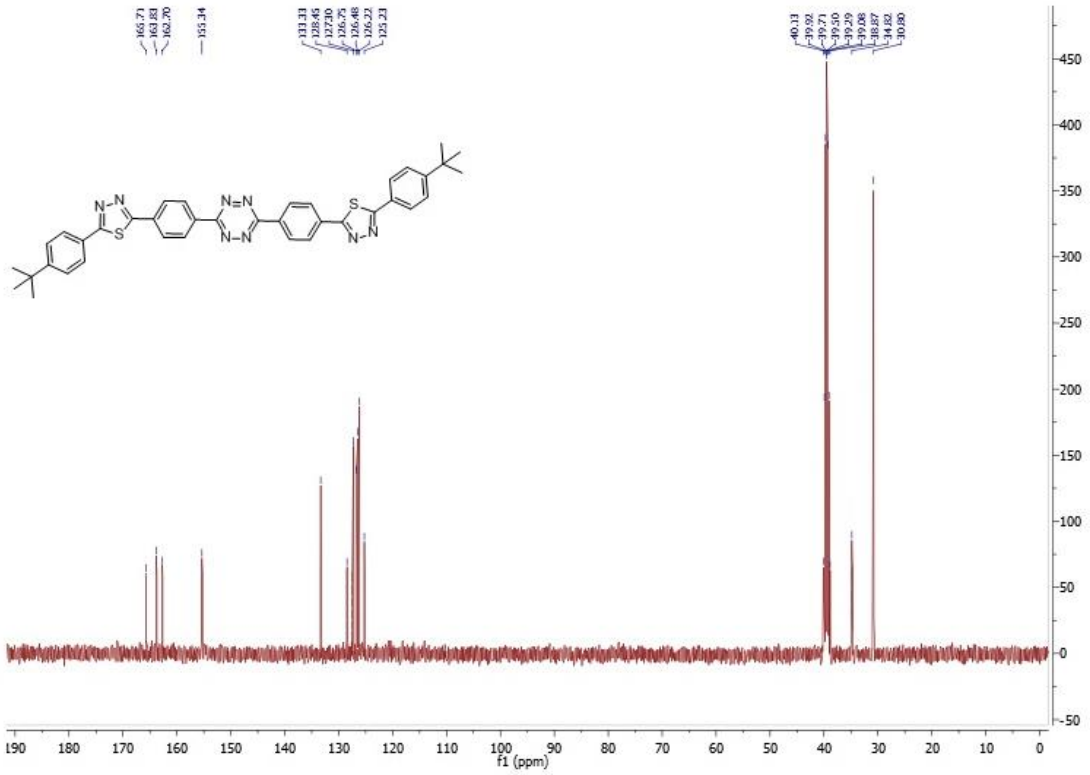


Figure S15: ^{1}H NMR 3,6-Bis(4-(5-(4-nitrophenyl)-1,3,4-thiadiazol-2-yl)phenyl)-1,2,4,5-tetrazine (8d)

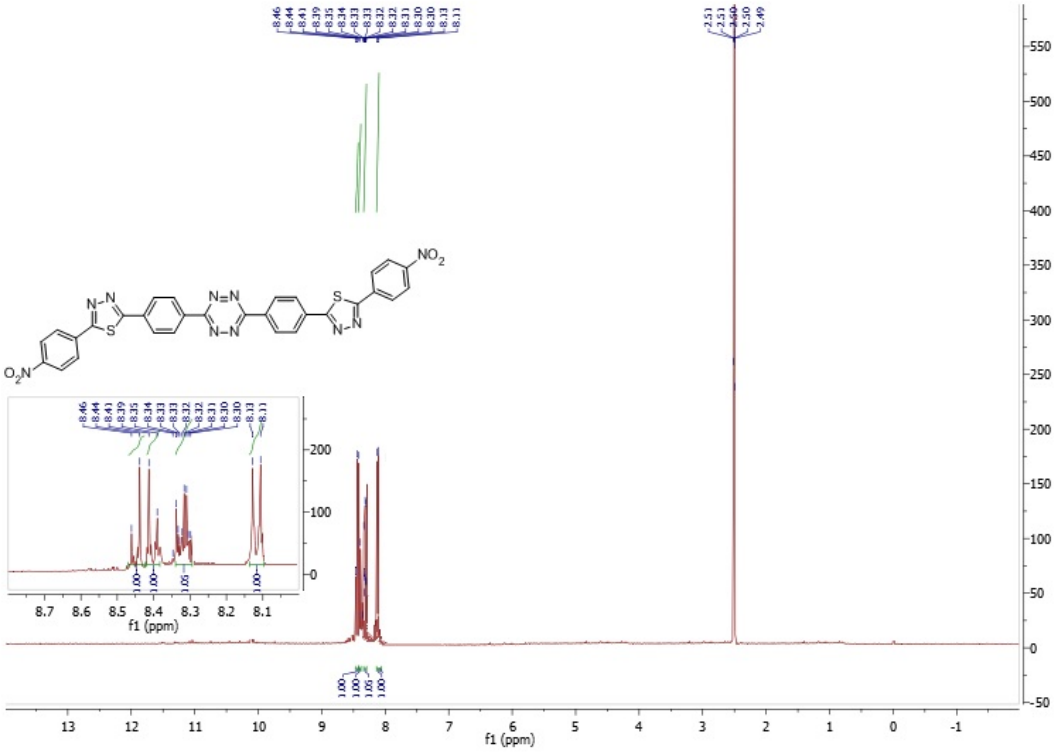


Figure S16: ^{13}C NMR 3,6-Bis(4-(5-(4-nitrophenyl)-1,3,4-thiadiazol-2-yl)phenyl)-1,2,4,5-tetrazine (8d)

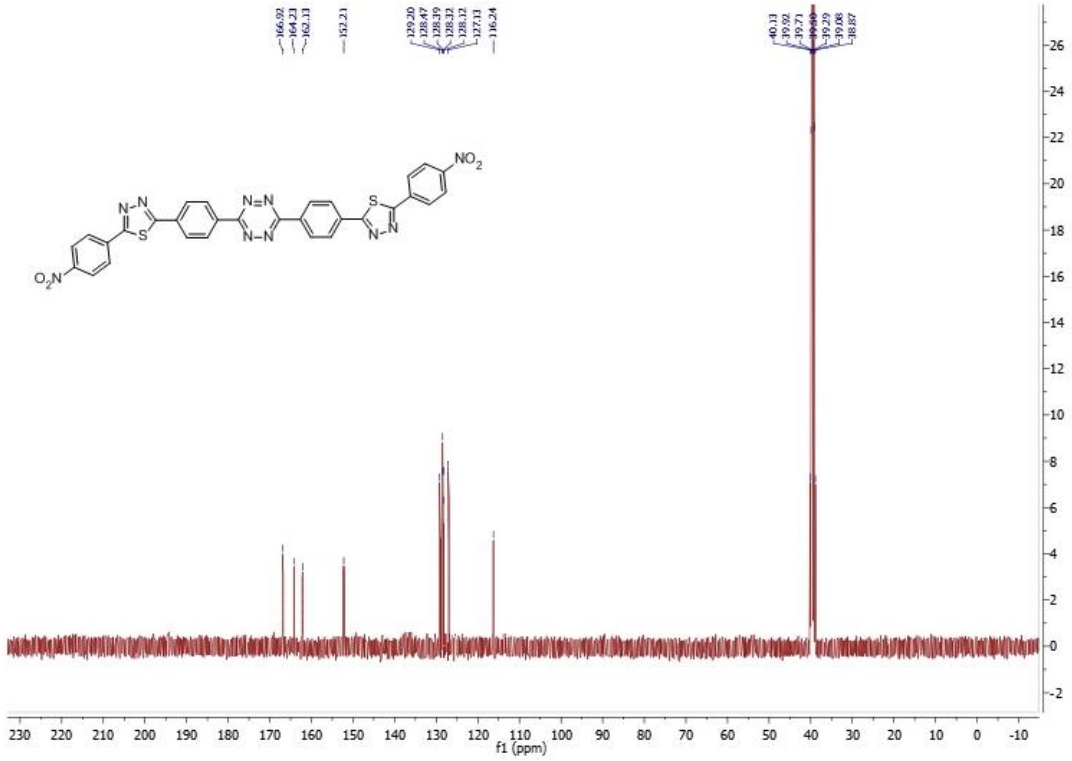


Figure S17: ^{1}H NMR 2-(4-Methoxyphenyl)-5-(4-(6-(4-(5-phenyl-1,3,4-thiadiazol-2-yl)phenyl)-1,2,4,5-tetrazin-3-yl)phenyl)-1,3,4-thiadiazole (8e)

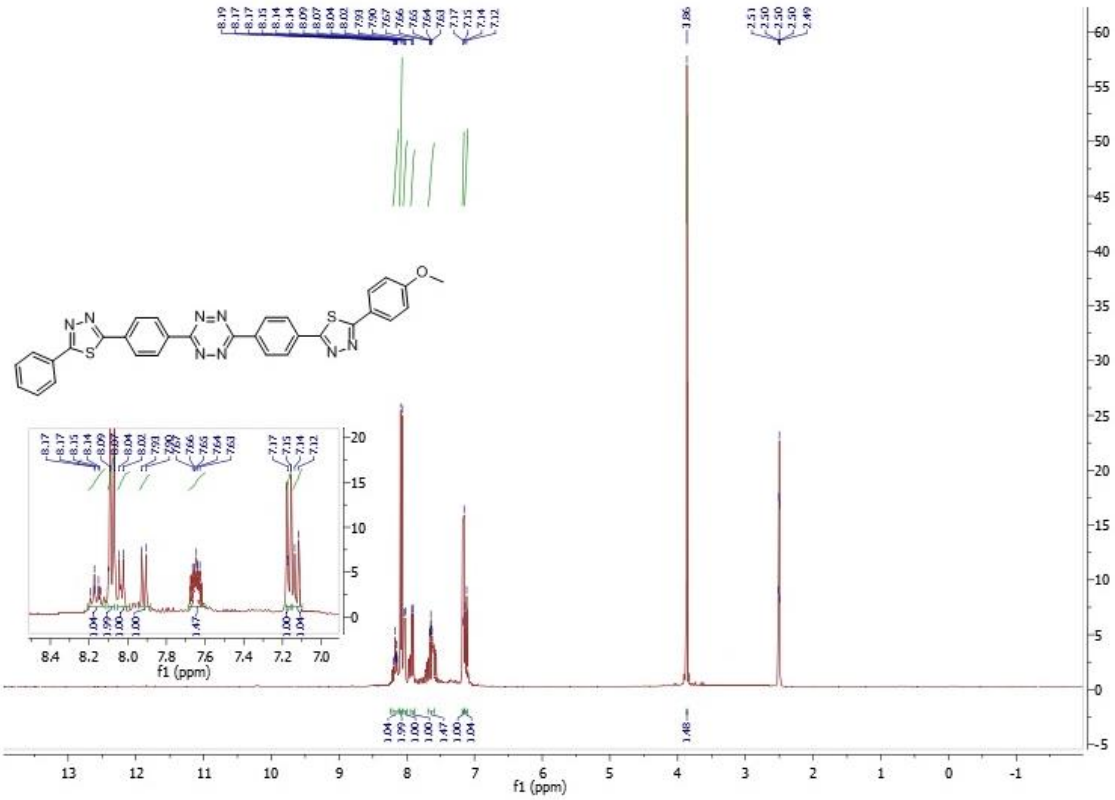


Figure S18: ^{13}C NMR 2-(4-Methoxyphenyl)-5-(4-(6-(4-(5-phenyl-1,3,4-thiadiazol-2-yl)phenyl)-1,2,4,5-tetrazin-3-yl)phenyl)-1,3,4-thiadiazole (8e)

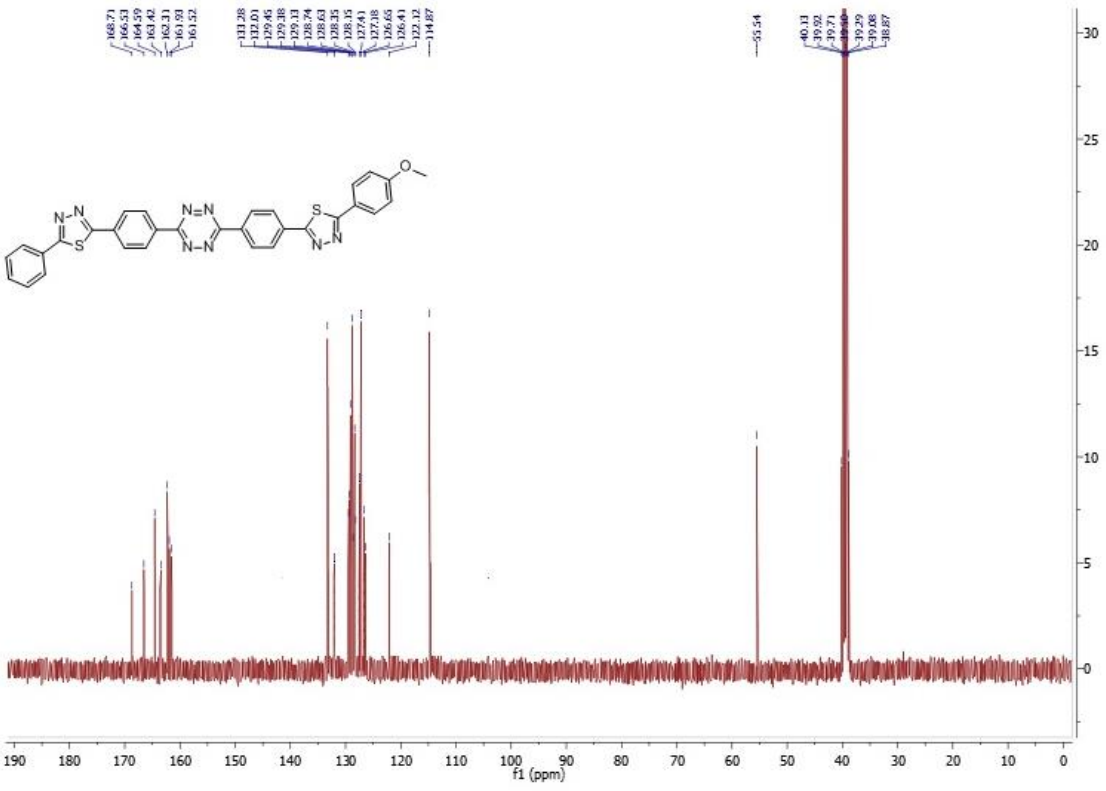


Figure S19: ^{1}H NMR 2-(4-(*tert*-Butyl)phenyl)-5-(4-(6-(4-(5-phenyl-1,3,4-thiadiazol-2-yl)phenyl)-1,2,4,5-tetrazin-3-yl)phenyl)-1,3,4-thiadiazole (8f)

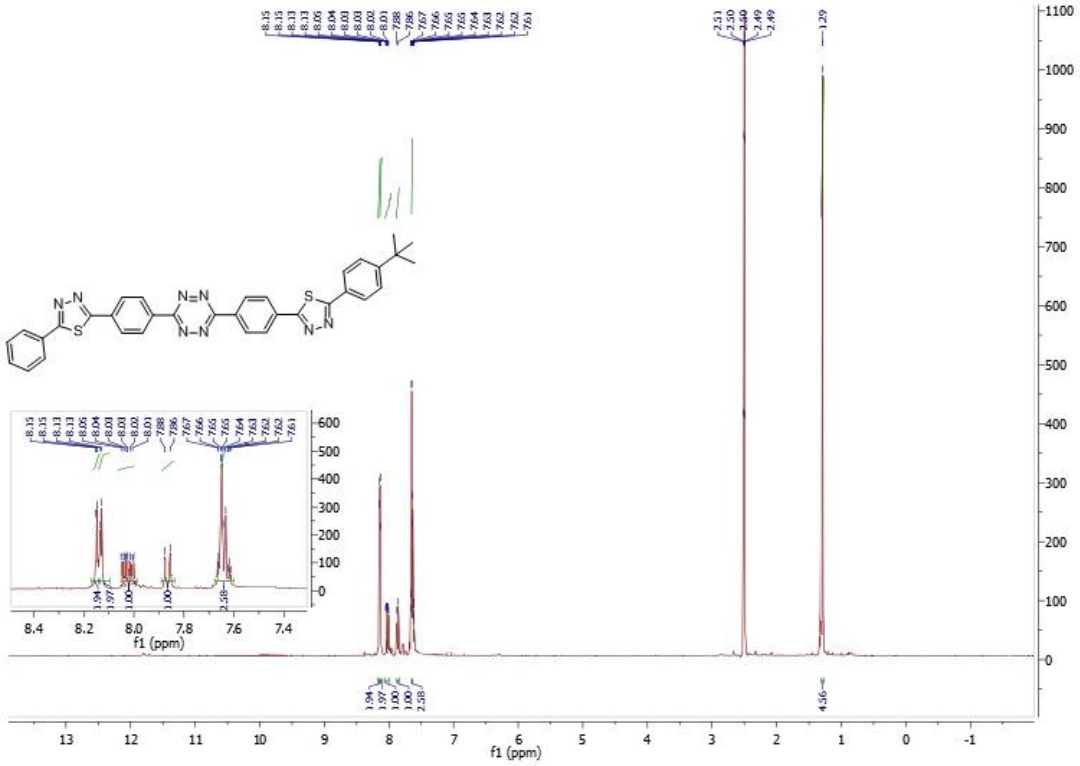


Figure S20: ^{13}C NMR 2-(4-(*tert*-Butyl)phenyl)-5-(4-(6-(4-(5-phenyl-1,3,4-thiadiazol-2-yl)phenyl)-1,2,4,5-tetrazin-3-yl)phenyl)-1,3,4-thiadiazole (8f)

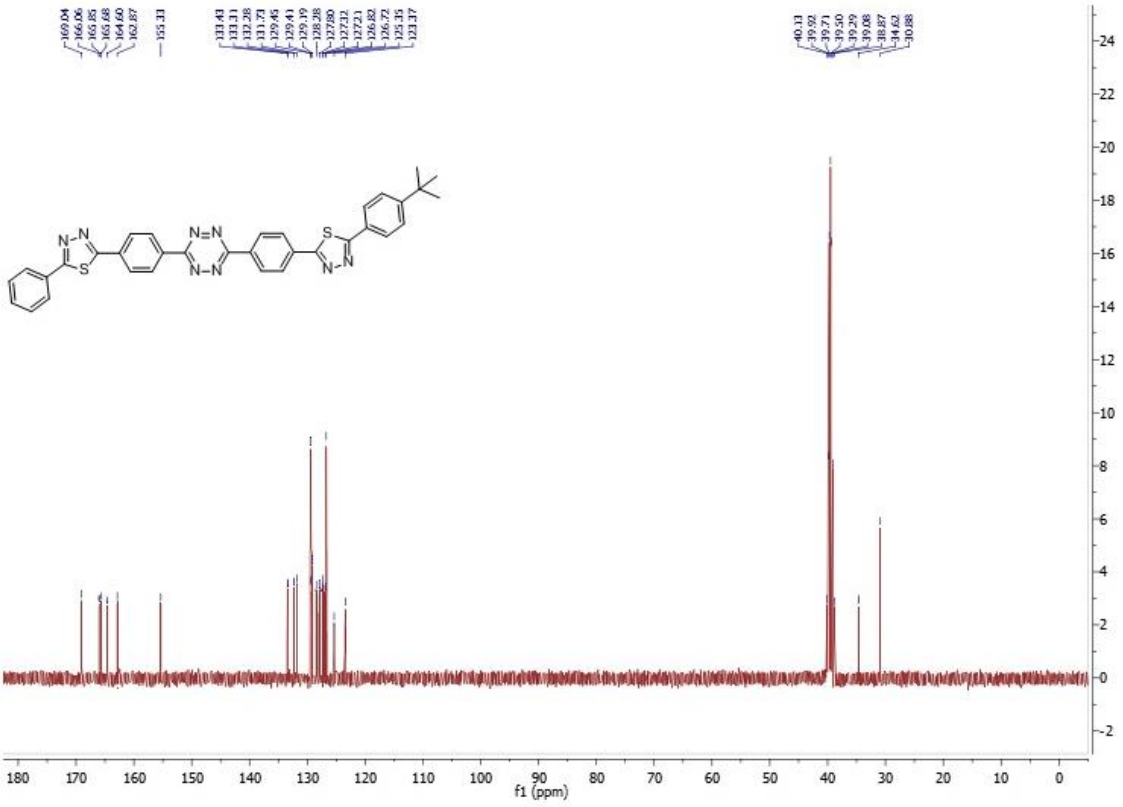


Figure S21: ^{1}H NMR 2-(4-Nitrophenyl)-5-(4-(6-(4-(5-phenyl-1,3,4-thiadiazol-2-yl)phenyl)-1,2,4,5-tetrazin-3-yl)phenyl)-1,3,4-thiadiazole (8g)

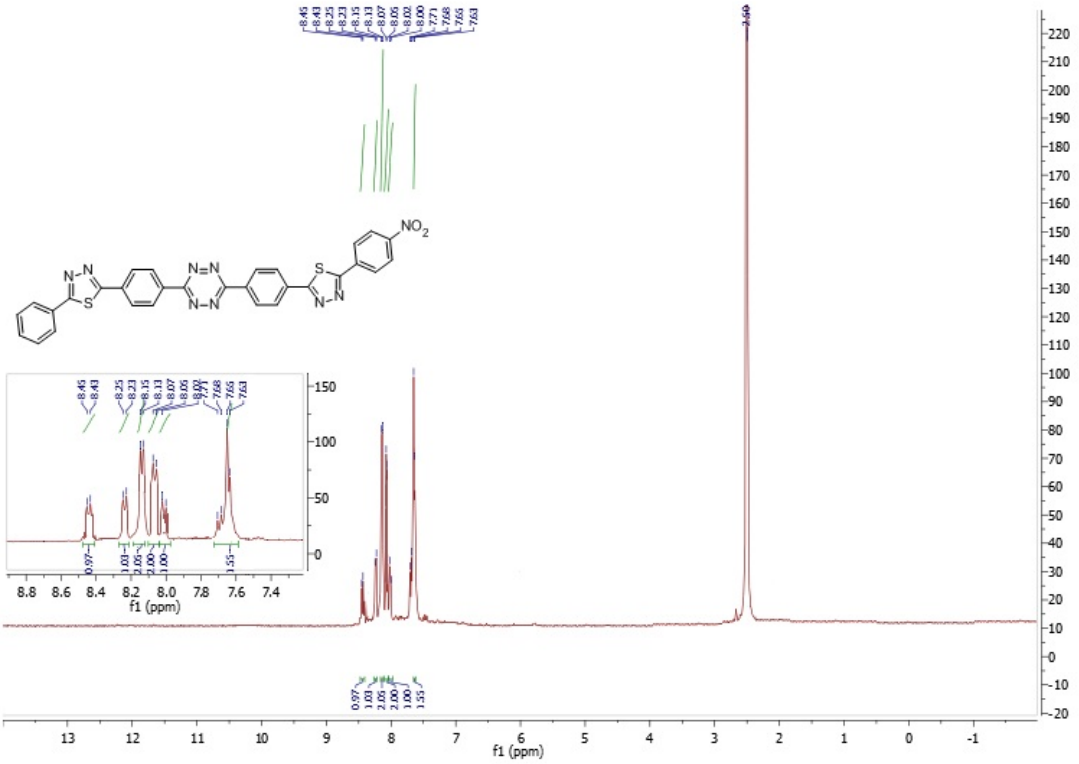


Figure S22: ^{13}C NMR 2-(4-Nitrophenyl)-5-(4-(6-(4-(5-phenyl-1,3,4-thiadiazol-2-yl)phenyl)-1,2,4,5-tetrazin-3-yl)phenyl)-1,3,4-thiadiazole (8g)

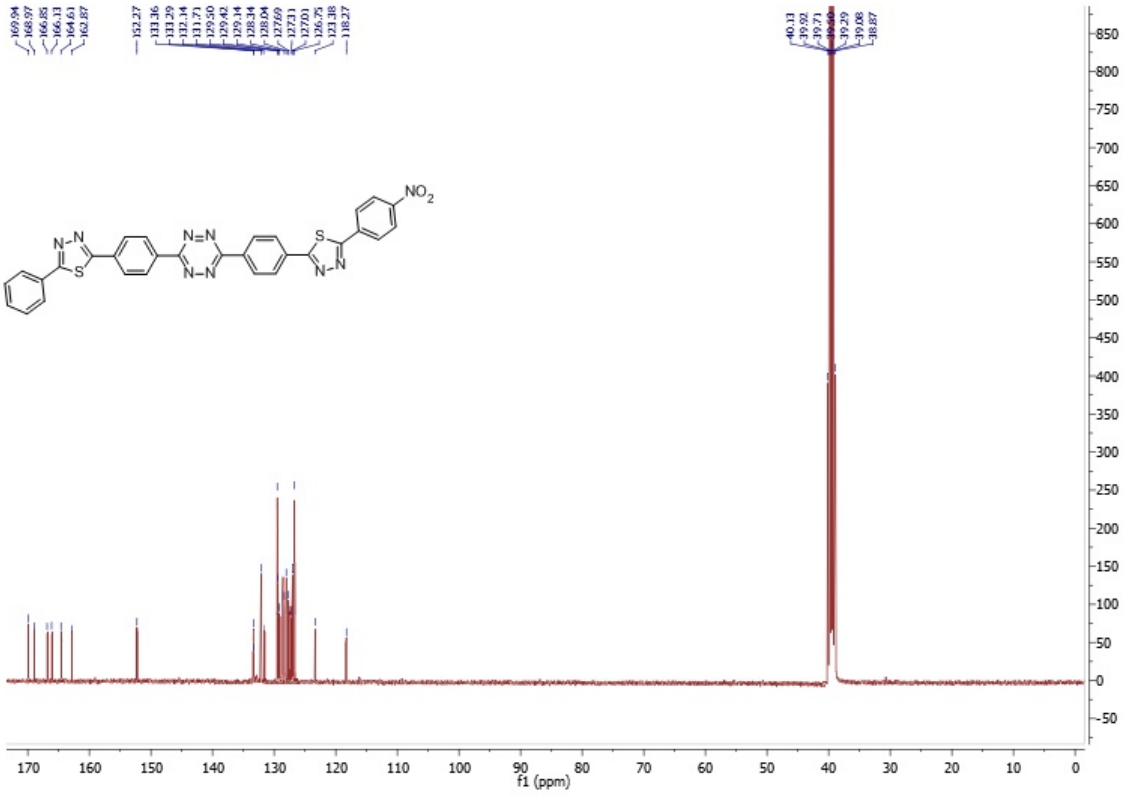


Figure S23: ^{1}H NMR 2-(4-(*tert*-Butyl)phenyl)-5-(4-(6-(4-(5-(4-methoxyphenyl)-1,3,4-thiadiazol-2-yl)phenyl)-1,2,4,5-tetrazin-3-yl)phenyl)-1,3,4-thiadiazole (8h)

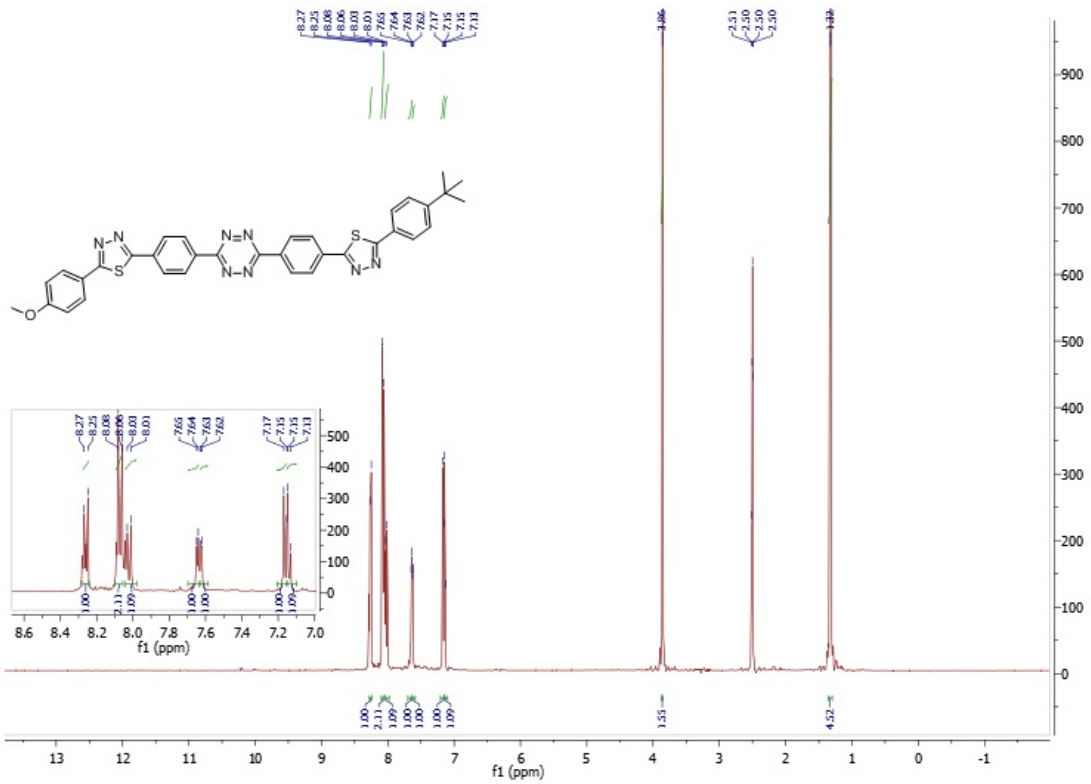


Figure S24: ^{13}C NMR 2-(4-(*tert*-Butyl)phenyl)-5-(4-(6-(4-(5-(4-methoxyphenyl)-1,3,4-thiadiazol-2-yl)phenyl)-1,2,4,5-tetrazin-3-yl)phenyl)-1,3,4-thiadiazole (8h)

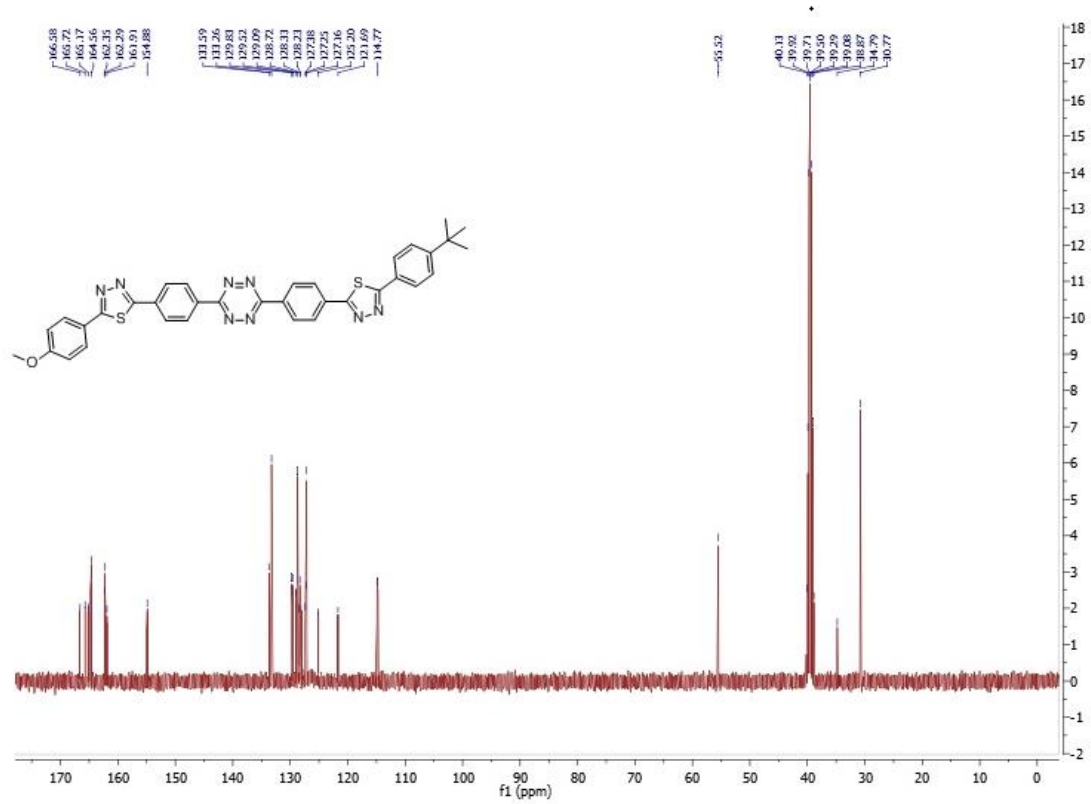


Figure S25: ^{1}H NMR 2-(4-Methoxyphenyl)-5-(4-(6-(4-(5-(4-nitrophenyl)-1,3,4-thiadiazol-2-yl)phenyl)-1,2,4,5-tetrazin-3-yl)phenyl)-1,3,4-thiadiazole (8i)

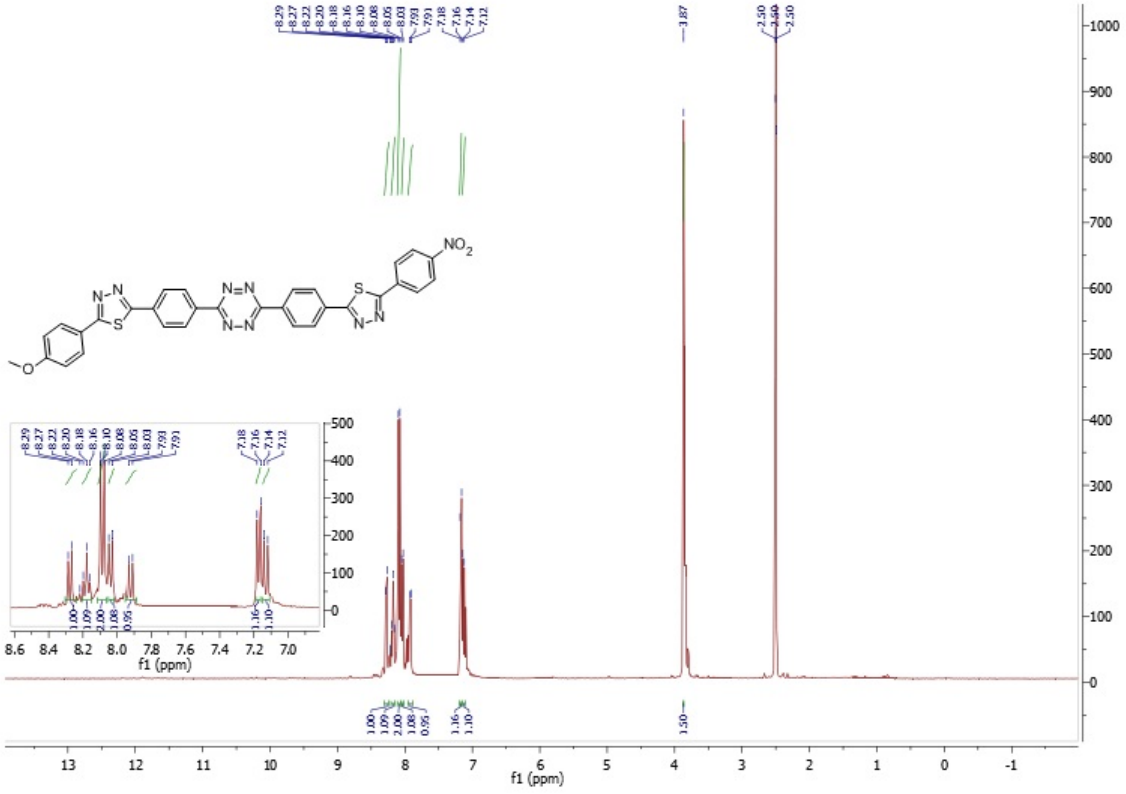


Figure S26: ^{13}C NMR 2-(4-Methoxyphenyl)-5-(4-(6-(4-(5-(4-nitrophenyl)-1,3,4-thiadiazol-2-yl)phenyl)-1,2,4,5-tetrazin-3-yl)phenyl)-1,3,4-thiadiazole (8i)

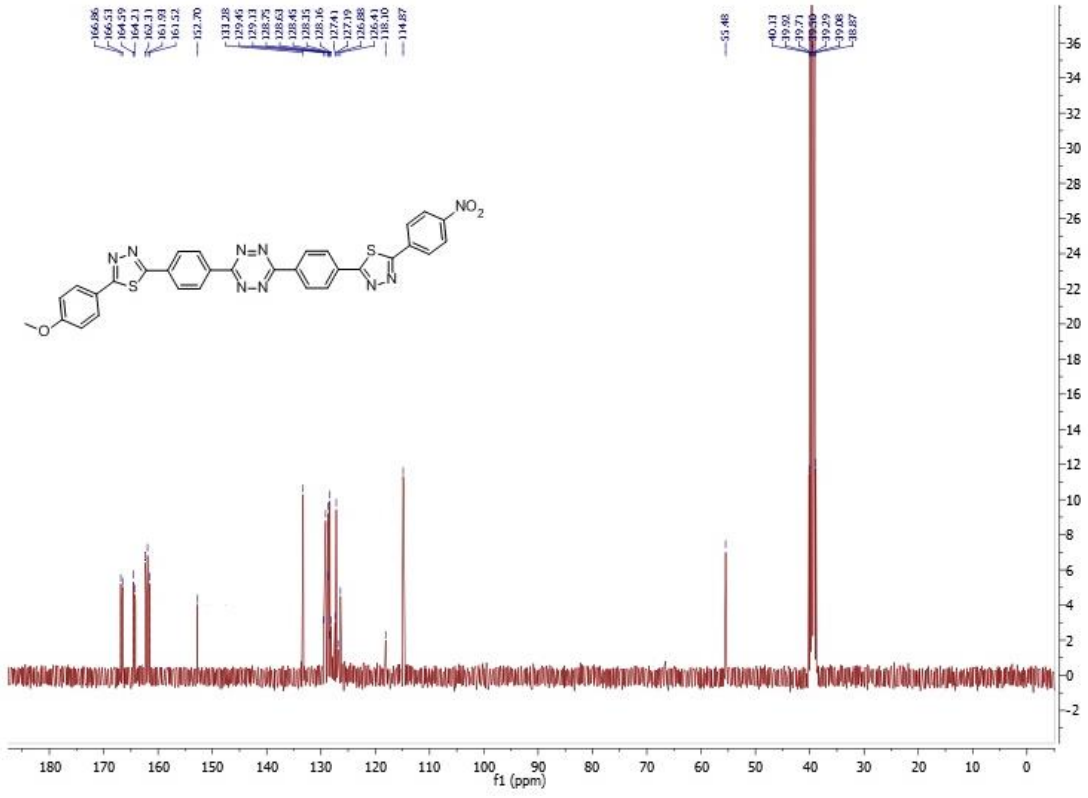


Figure S27: ^{1}H NMR 2-(4-(*tert*-Butyl)phenyl)-5-(4-(6-(4-(5-(4-nitrophenyl)-1,3,4-thiadiazol-2-yl)phenyl)-1,2,4,5-tetrazin-3-yl)phenyl)-1,3,4-thiadiazole (8j)

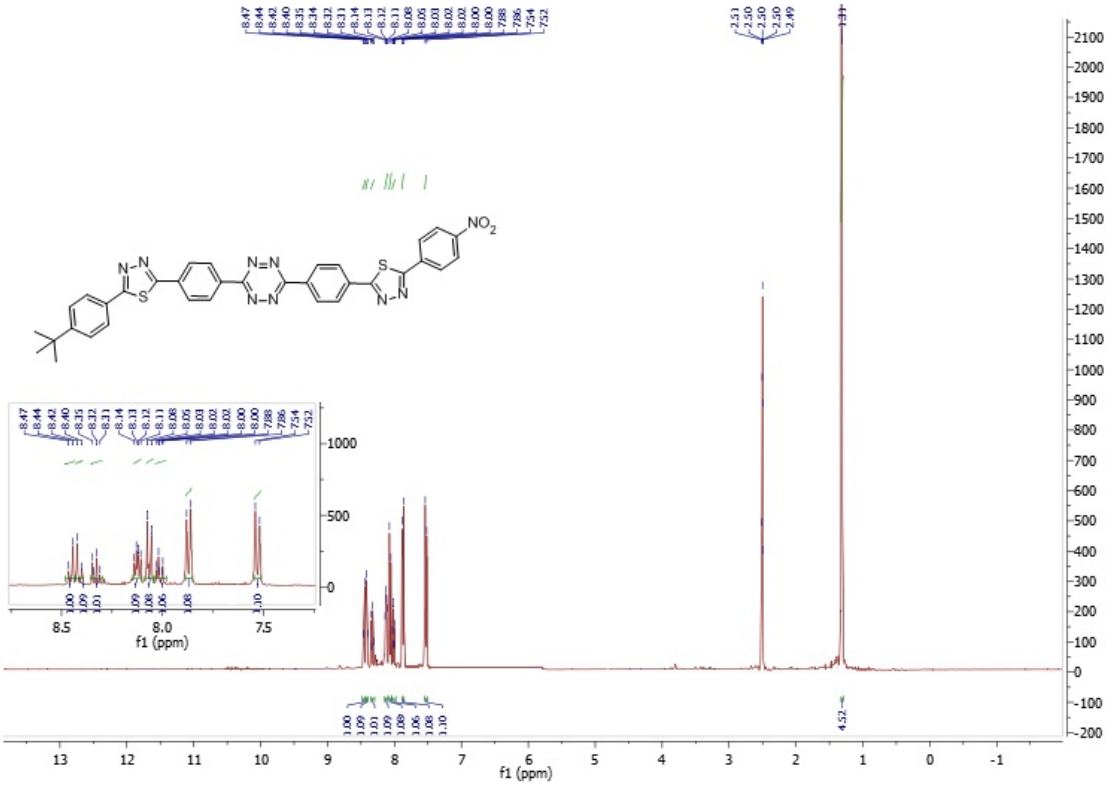
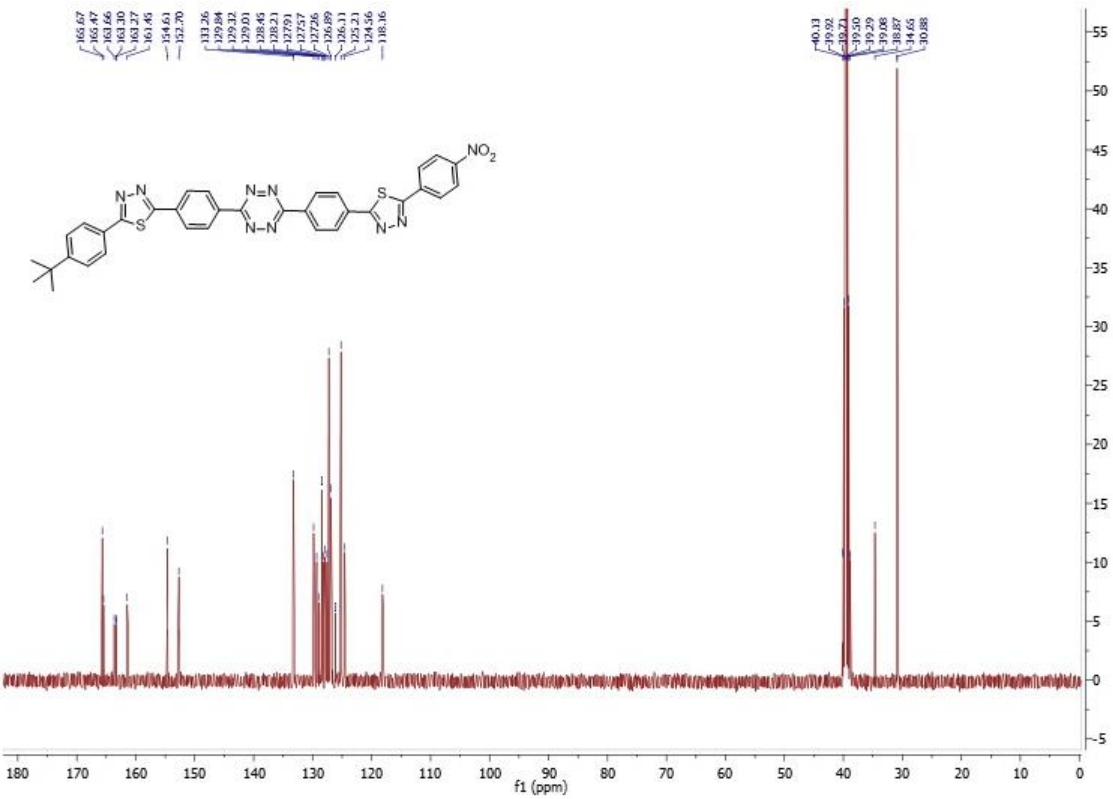
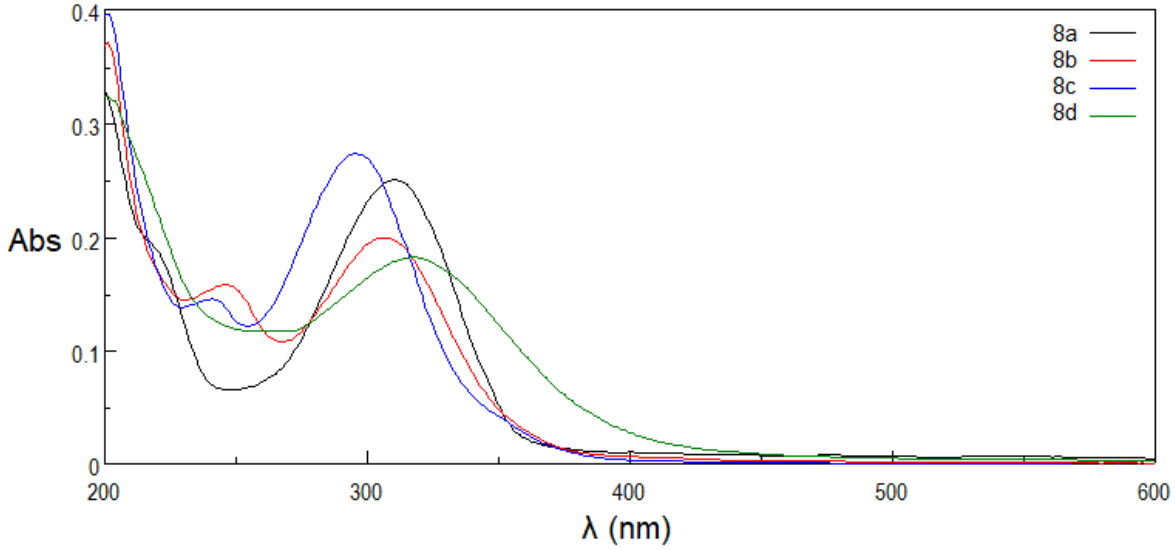


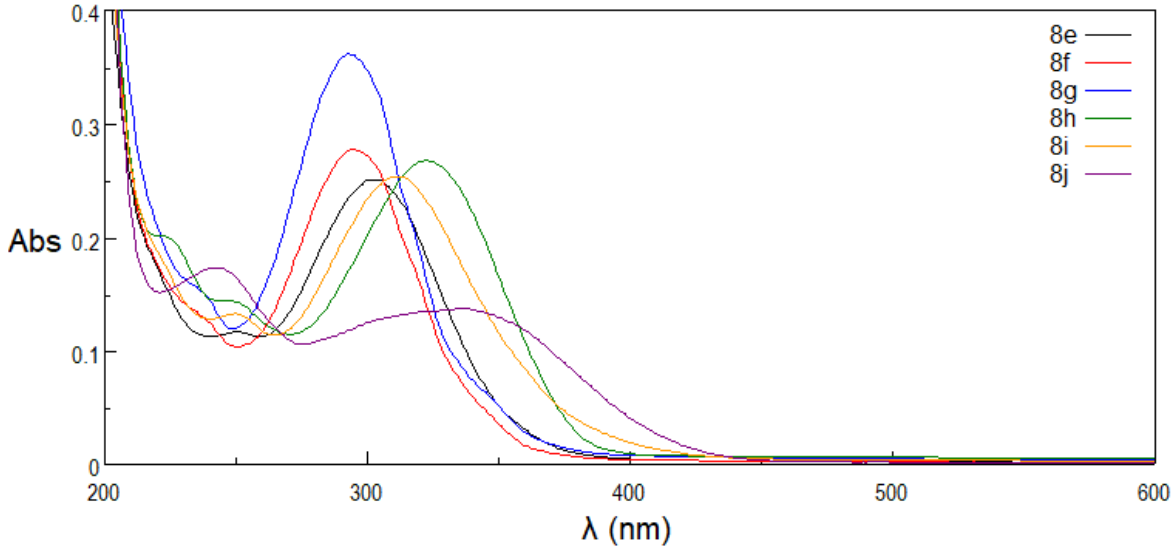
Figure S28: ^{13}C NMR 2-(4-(*tert*-Butyl)phenyl)-5-(4-(6-(4-(5-(4-nitrophenyl)-1,3,4-thiadiazol-2-yl)phenyl)-1,2,4,5-tetrazin-3-yl)phenyl)-1,3,4-thiadiazole (8j)



UV-Vis spectra

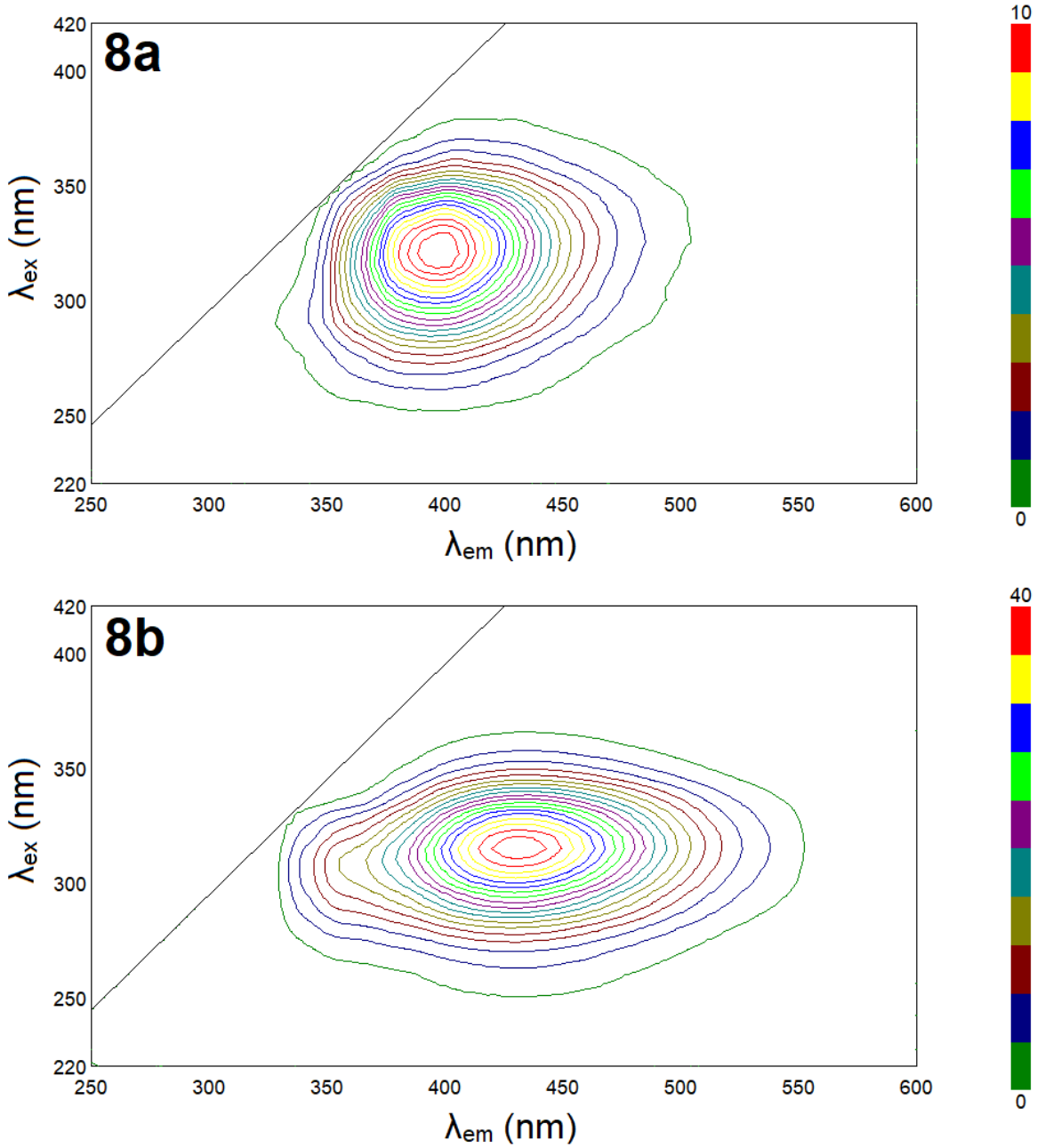
Figure S29: UV-Vis spectra of 8a-j

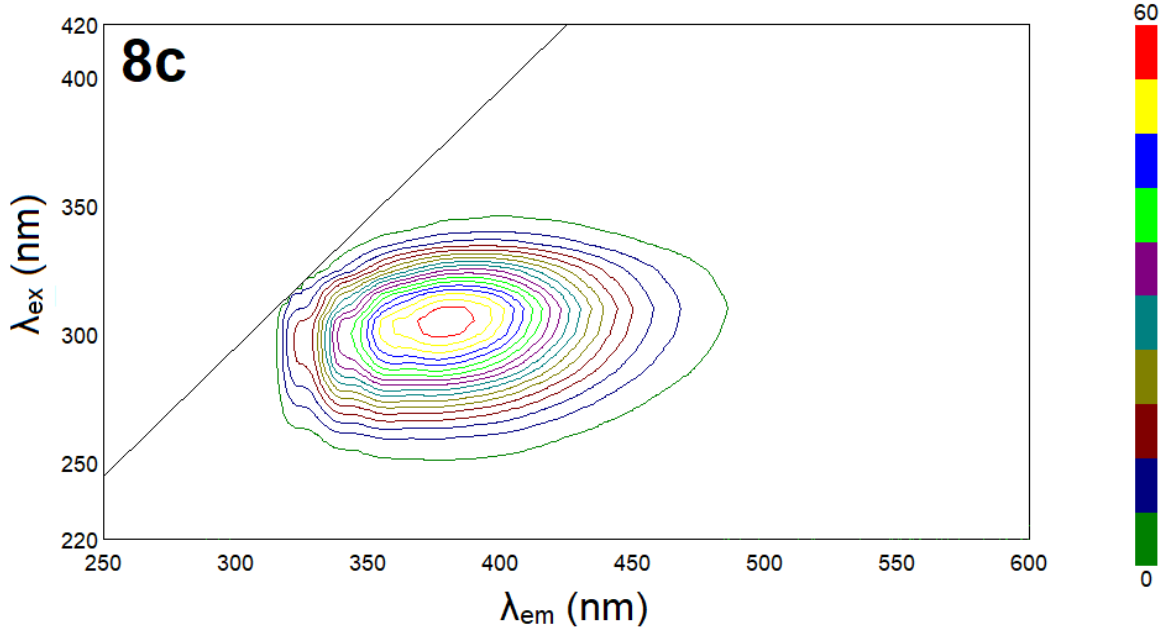


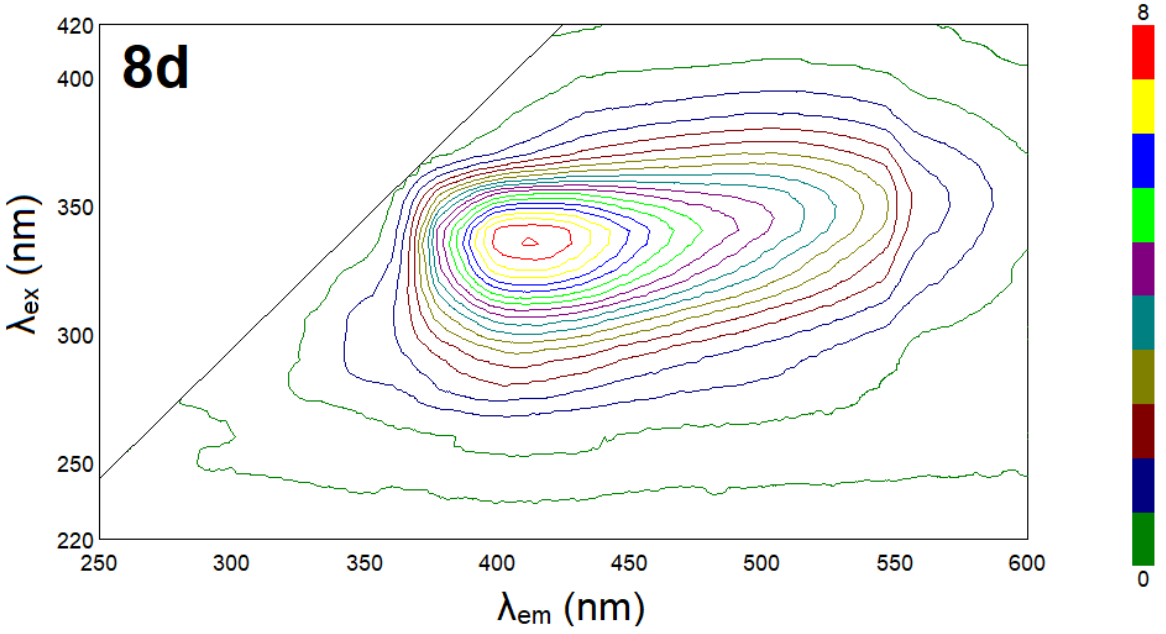


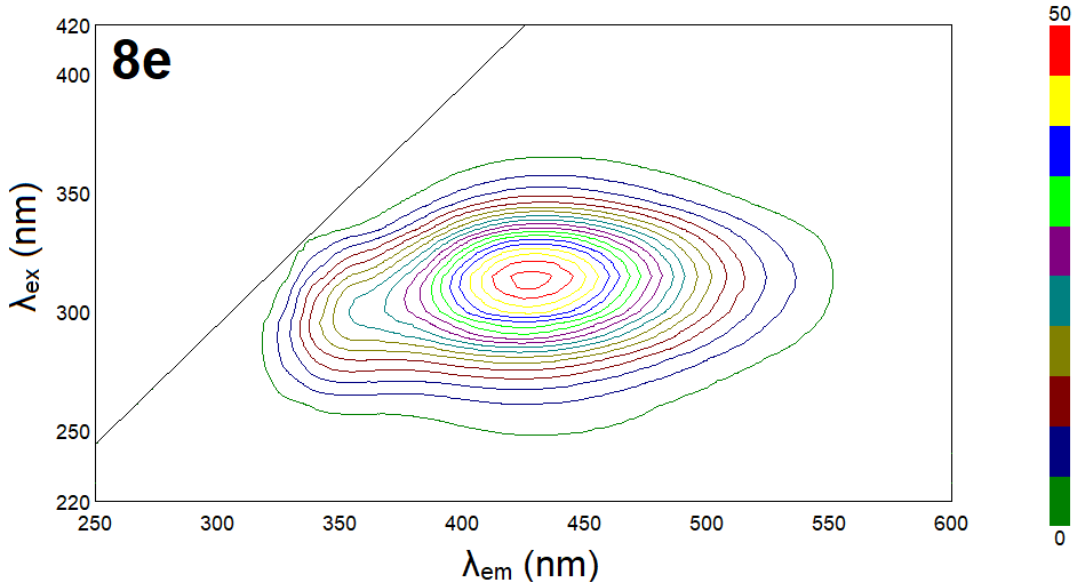
3D fluorescence spectra

Figure S30: 3D fluorescence spectra of compounds 8a-j. The color scale represents a flux of emitted photons. The number above color scales indicates the maximum relative value of emission intensity represented by color scale (and indicated in a respective figure). The unit of measurement in each spectrum represents the same number of emitted photons per second, i.e. fluorescence intensity values in all spectra can be directly compared.




8c
420
400
350
300
250
220
250
300
350
400
450
500
550
600
λex (nm)
λem (nm)
60
0


8d
420
400
350
300
250
220
250
300
350
400
450
500
550
600
λex (nm)
λem (nm)
8
0


8e
λex (nm)
λem (nm)
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400
350
300
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250
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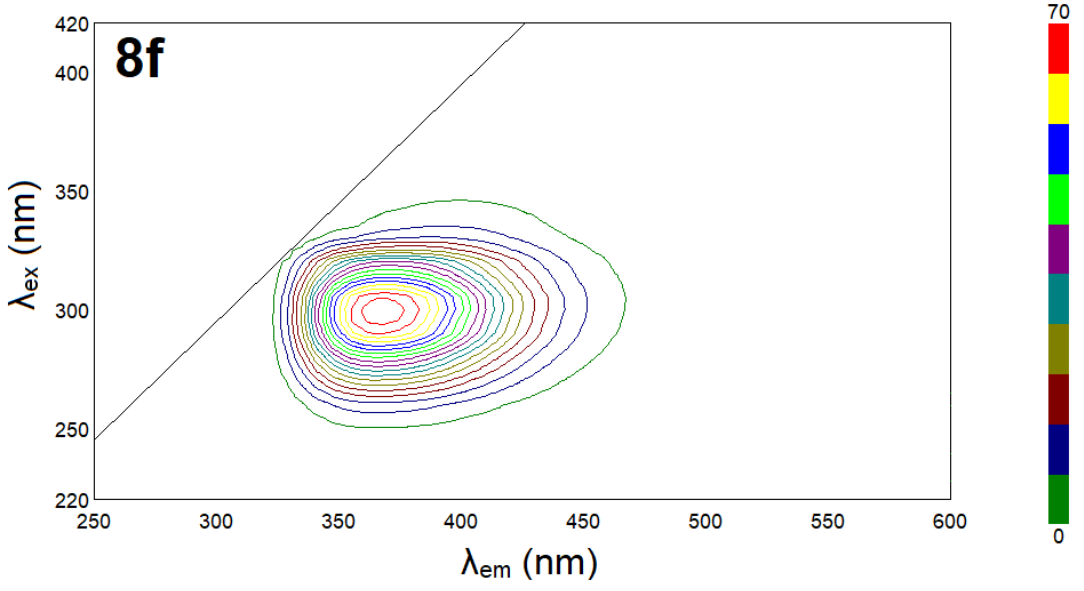
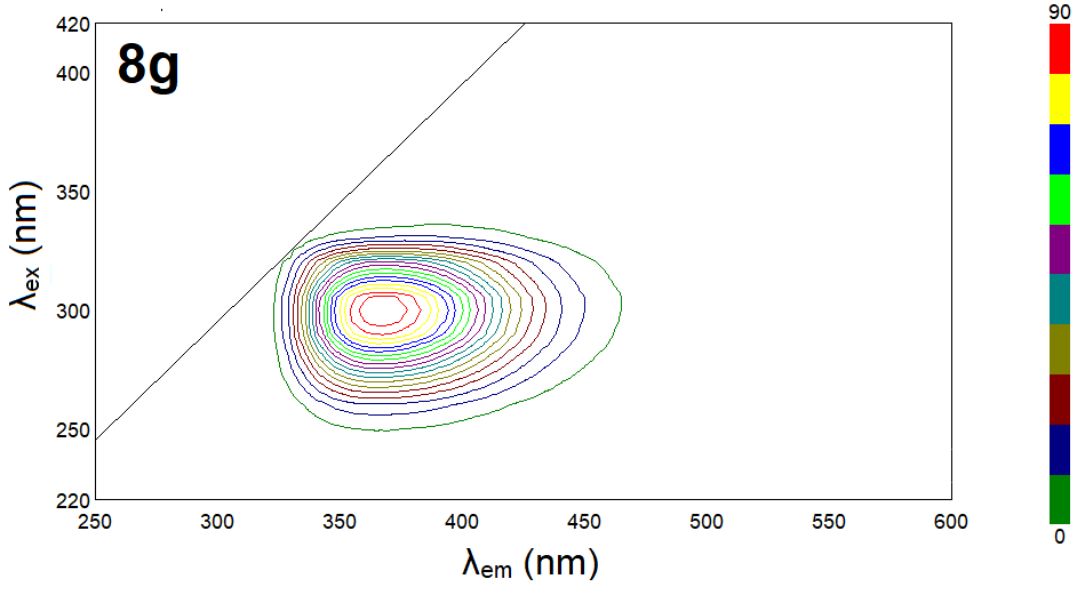
350
400
450
500
550
600
50
0


8f
λex (nm)
λem (nm)
420
400
350
300
250
220
250
300
350
400
450
500
550
600
70
0


8g
λex (nm)
λem (nm)
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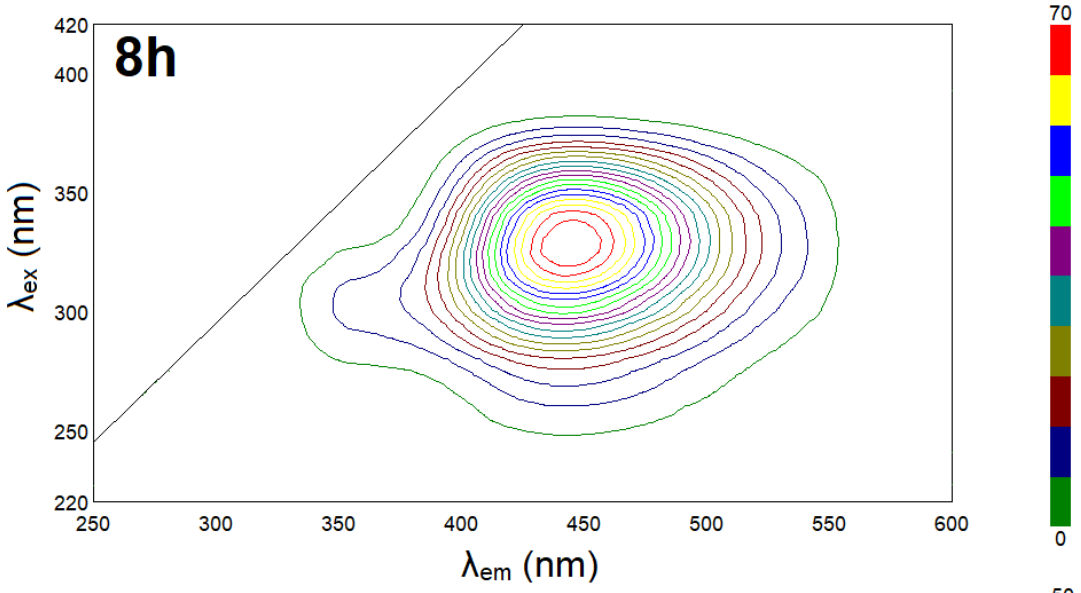
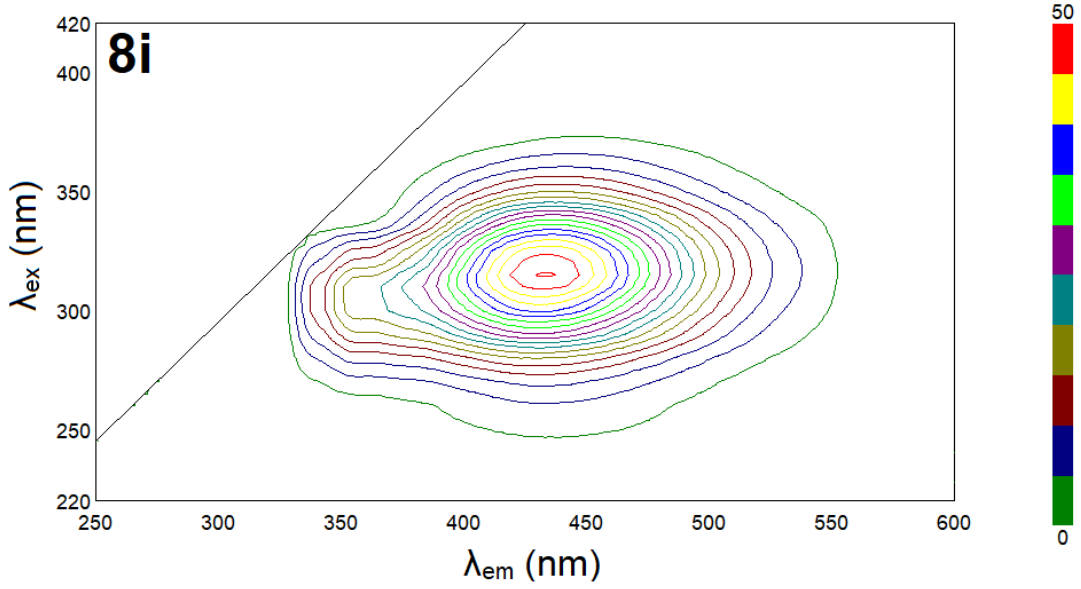
400
350
300
250
220
250
300
350
400
450
500
550
600
90
0


8h
420
400
350
300
250
220
λex (nm)
250
300
350
400
450
500
550
600
λem (nm)
70
0


8i
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400
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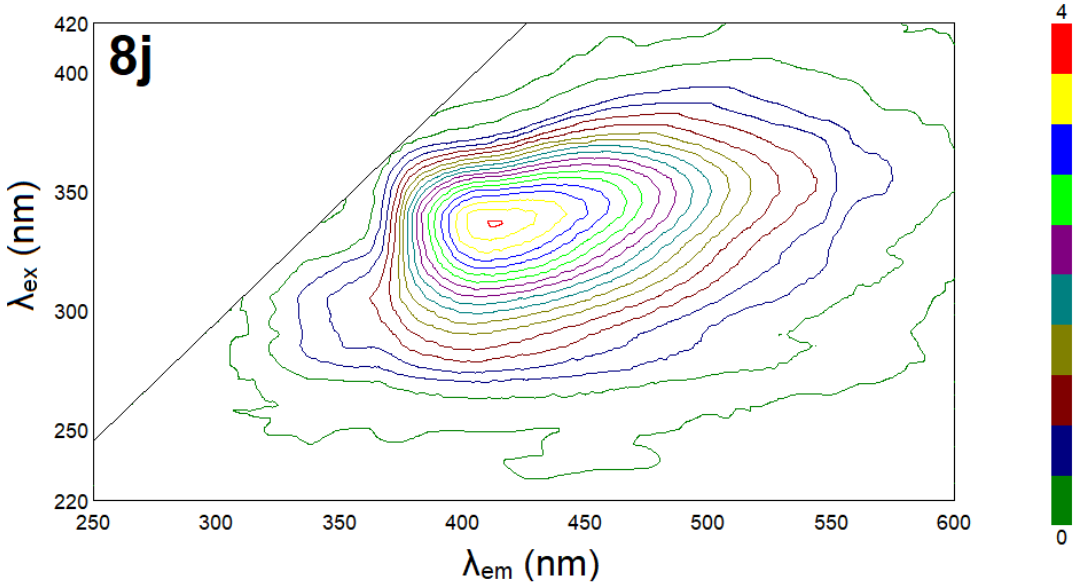
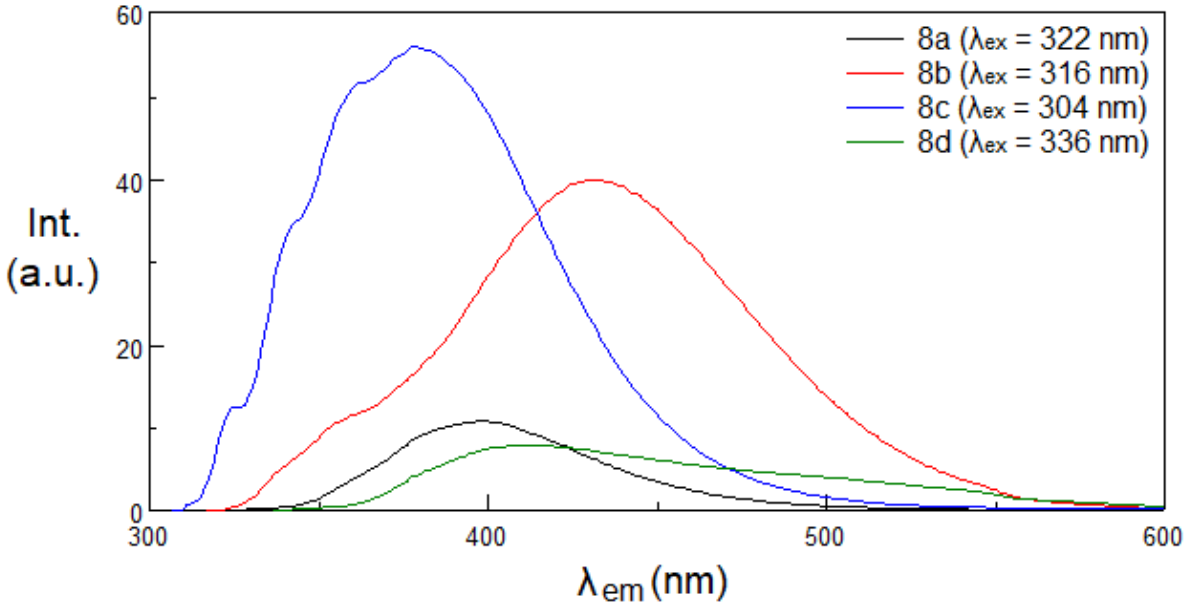
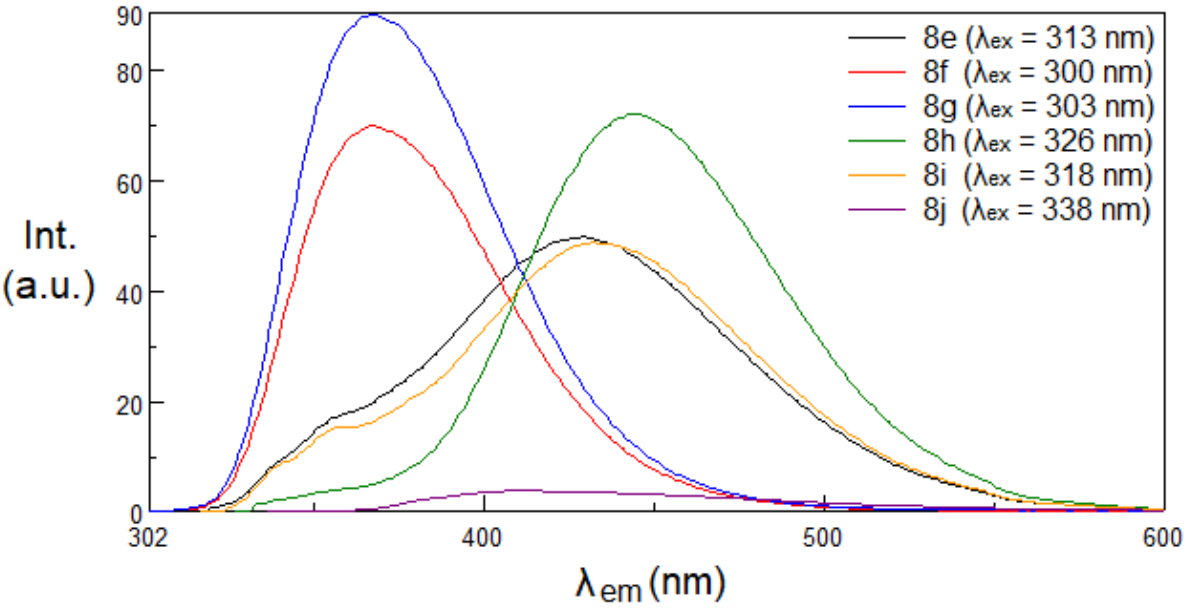
220
λex (nm)
250
300
350
400
450
500
550
600
λem (nm)
50
0


8j
420
400
350
300
250
220
λex (nm)
250
300
350
400
450
500
550
600
λem (nm)
4
0

2D fluorescence spectra

Figure S31: 2D fluorescence spectra (extracted from 3D fluorescence spectra) presenting the global emission maximum for each compound. The unit of measurement in each spectrum represents the same number of emitted photons per second, i.e. fluorescence intensity values in all spectra can be directly compared.





The scatter plots presenting relationships between absorption-emission properties

Figure S32: Quantum yields of studied compounds as a function of fluorescence intensity at global maximum

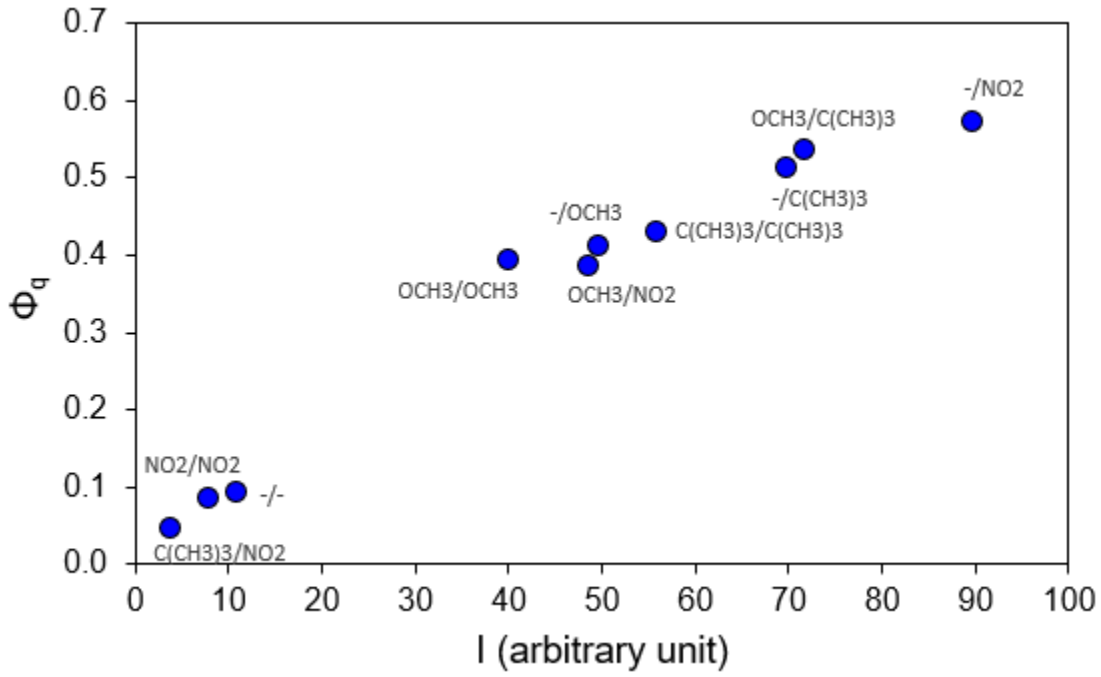


Figure S33: Quantum yields of studied compounds in relation to absorption wavelength at global maximum of fluorescence

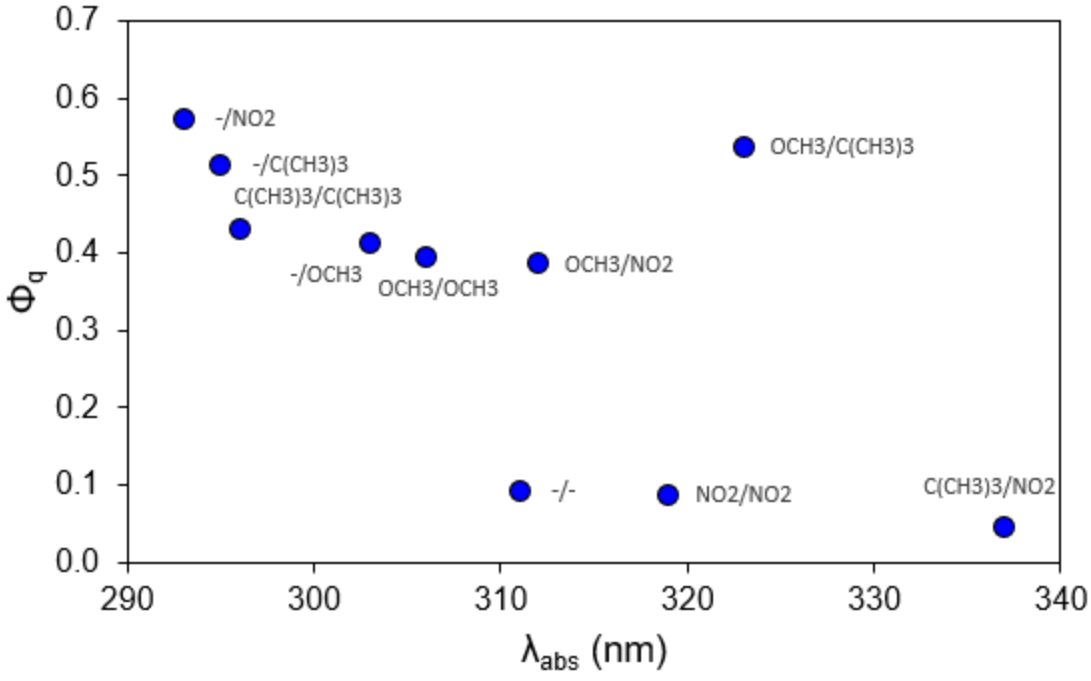
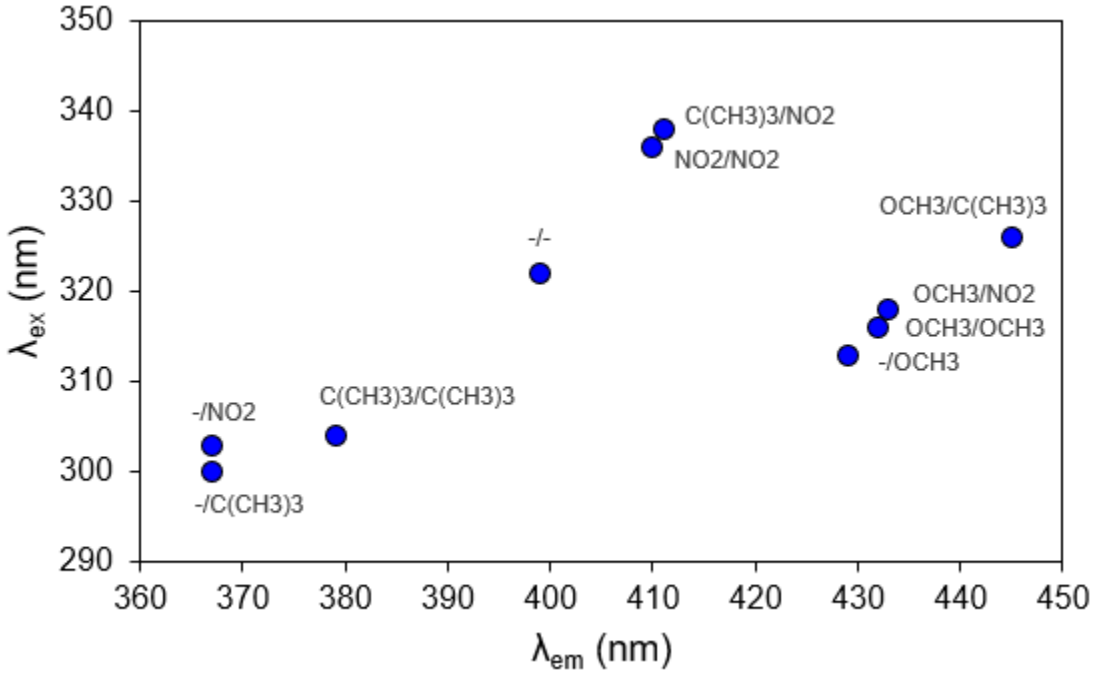


Figure S34: Positions of global maxima for studied compounds.



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