

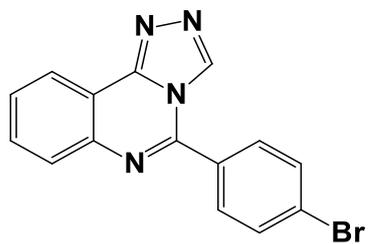
Design, synthesis and photophysical properties of 5-aminobiphenyl substituted [1,2,4]triazolo[4,3-c]- and [1,2,4]triazolo[1,5-c]quinazolines

Tatyana N. Moshkina, Alexandra E. Kopotilova, Marya A. Ivan'kina, Ekaterina S. Starnovskaya, Denis A. Gazizov , Emiliya V. Nosova , Dmitry S. Kopchuk, Oleg S. El'tsov, Pavel A. Slepukhin, and Valery N. Charushin

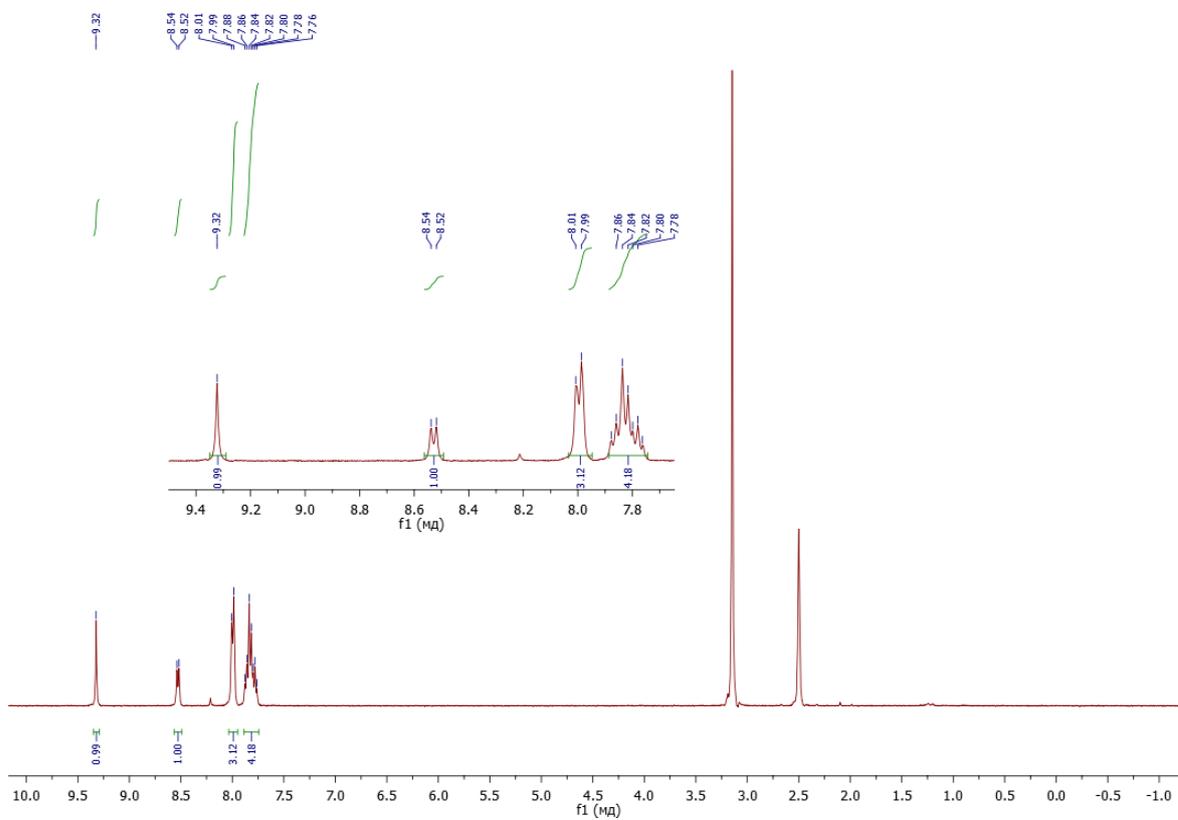
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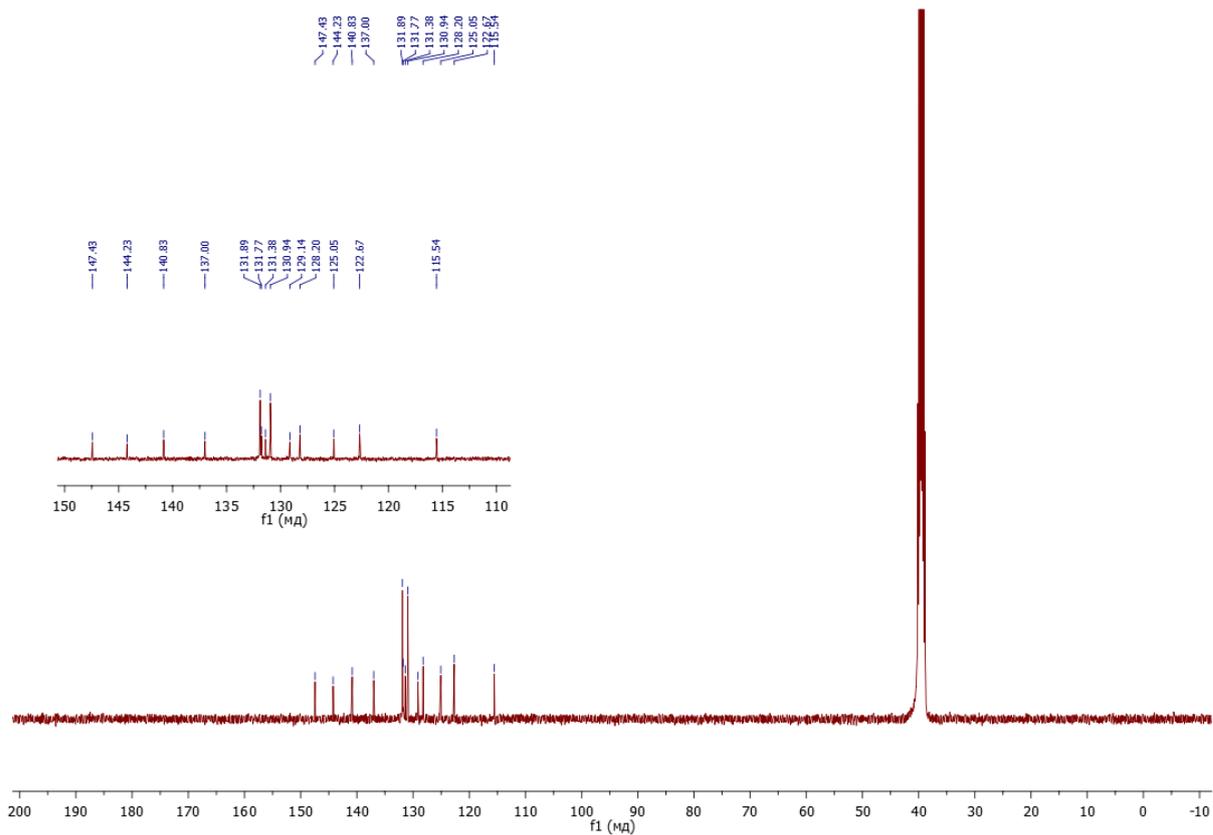
1. NMR and mass spectra of 5-aryl-substituted [1,2,4]triazolo[4,3-c]quinazolines and [1,2,4]triazolo[1,5-c]quinazolines



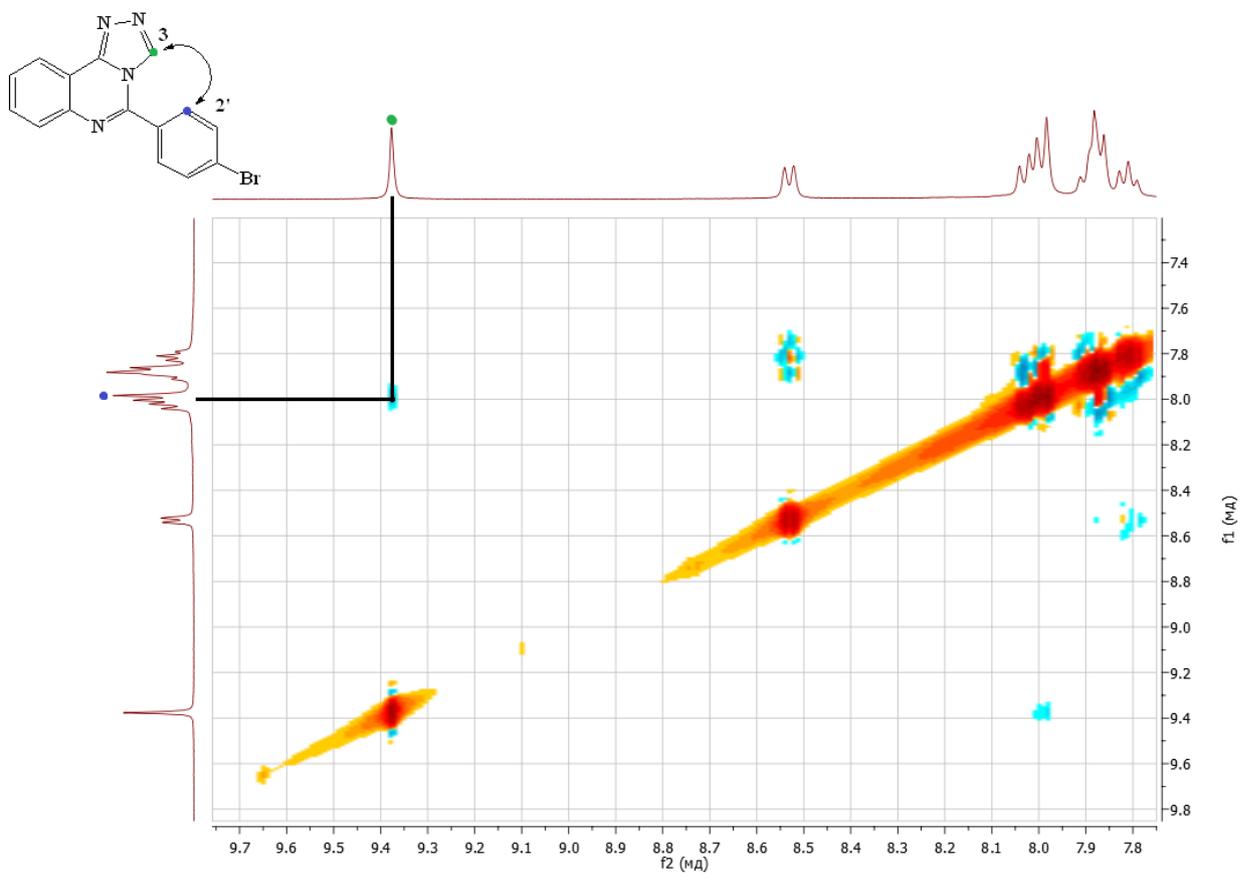
2a



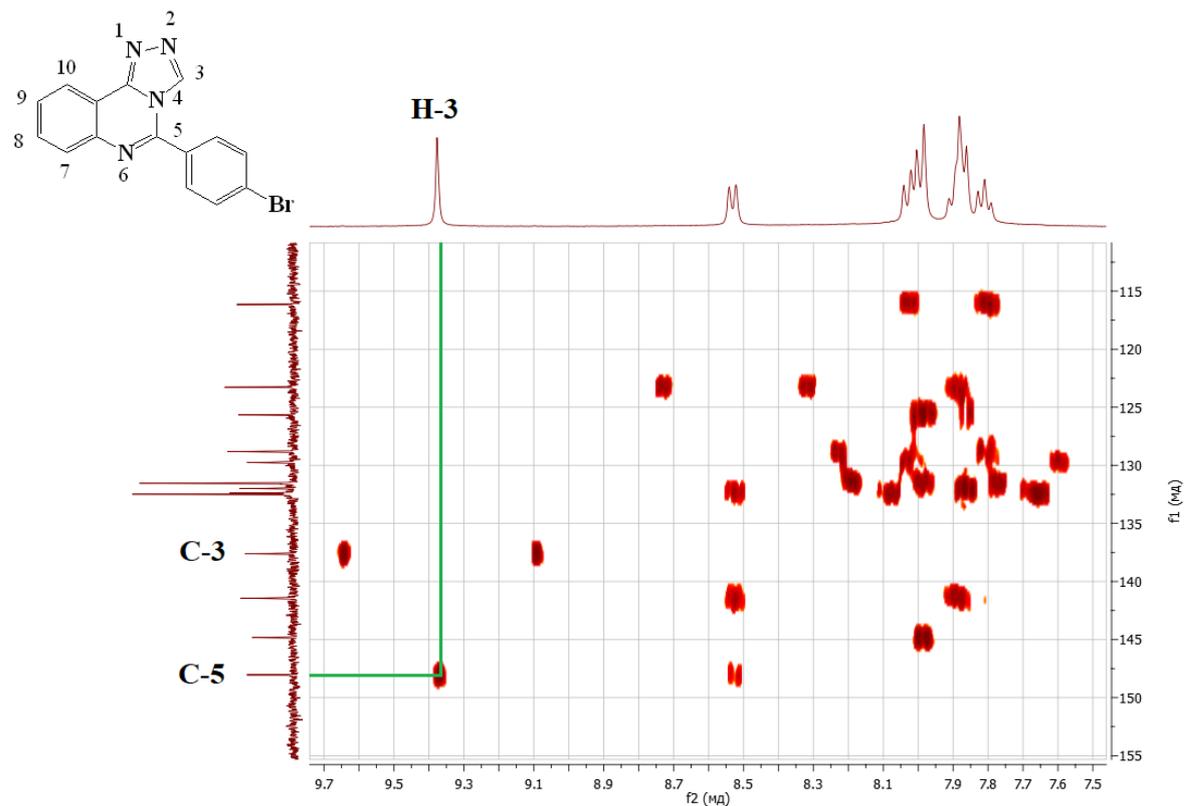
a



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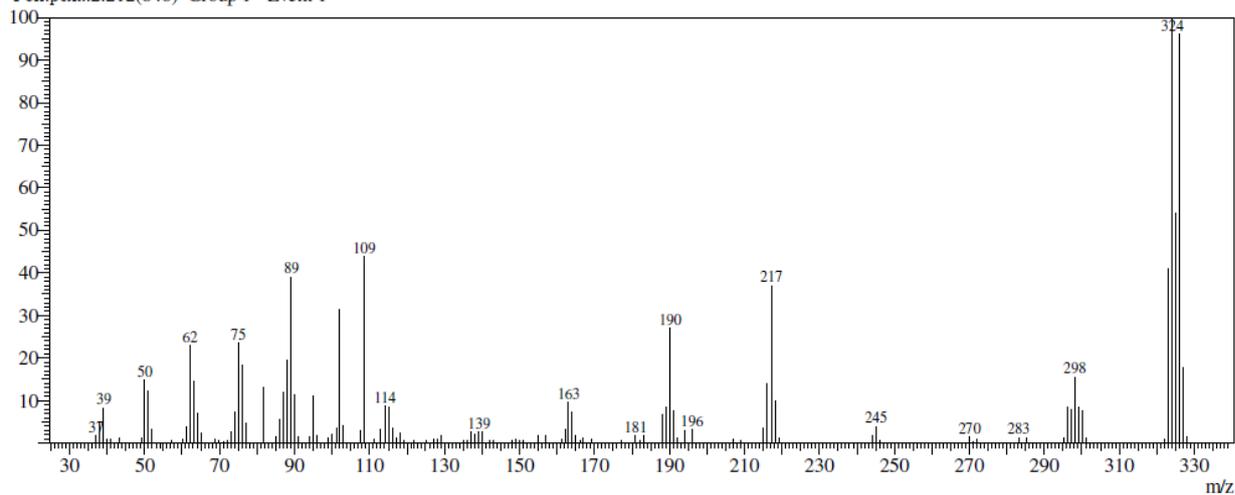


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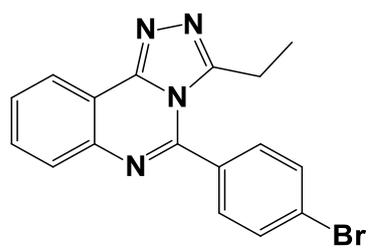
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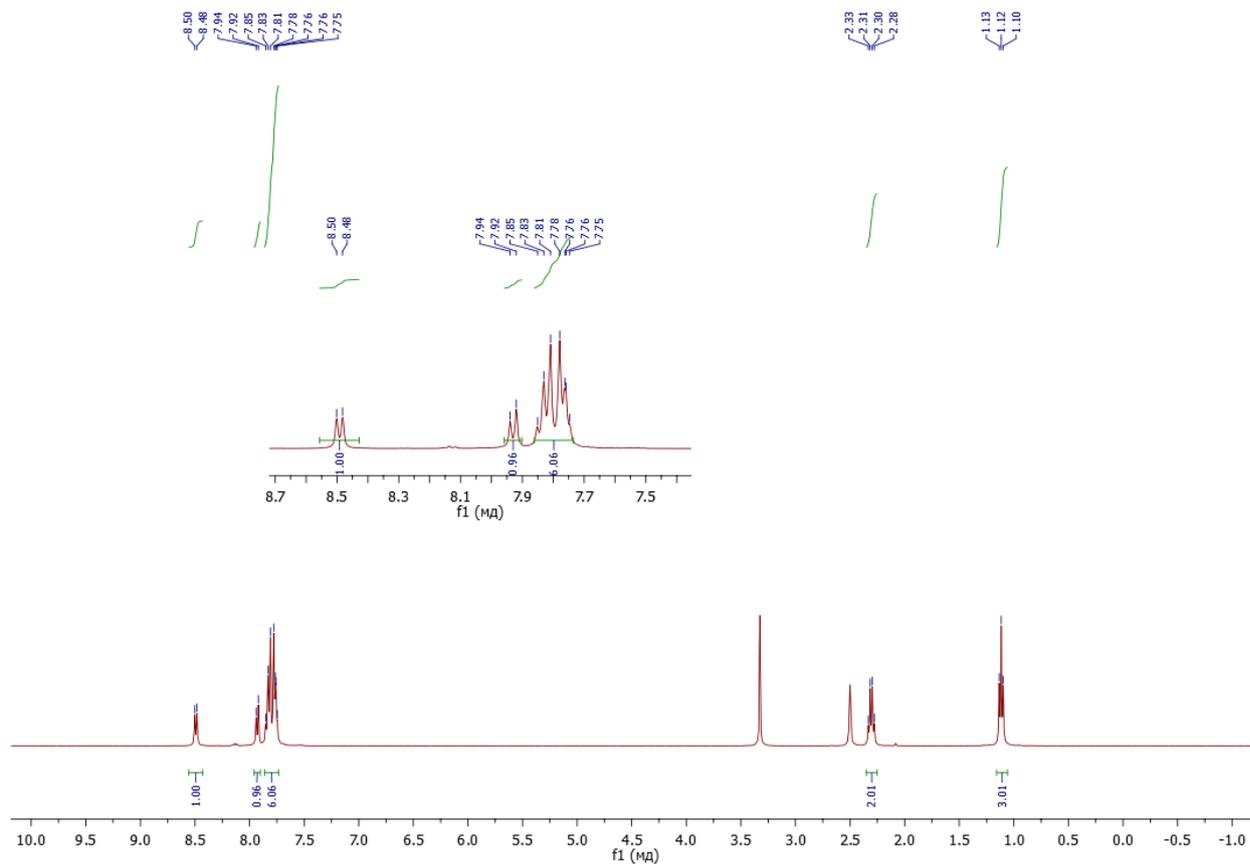


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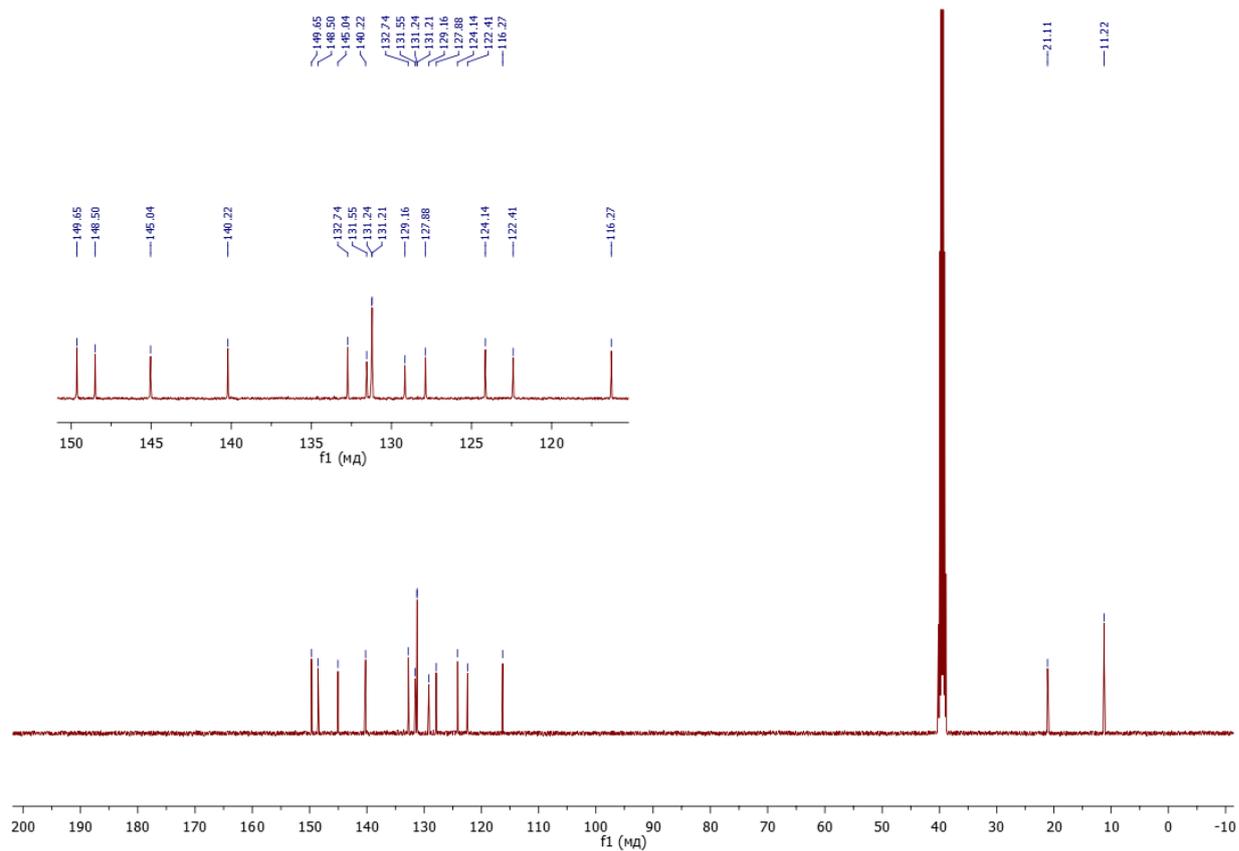
Figure S1. ^1H (a), ^{13}C (b) NMR spectra of **2a** in DMSO-d_6 ; ^1H - ^1H NOESY (c) and ^1H - ^{13}C HMBC (d) spectra of **2a** in DMSO-d_6 ; mass spectrum (e) of **2a**.



2b



a



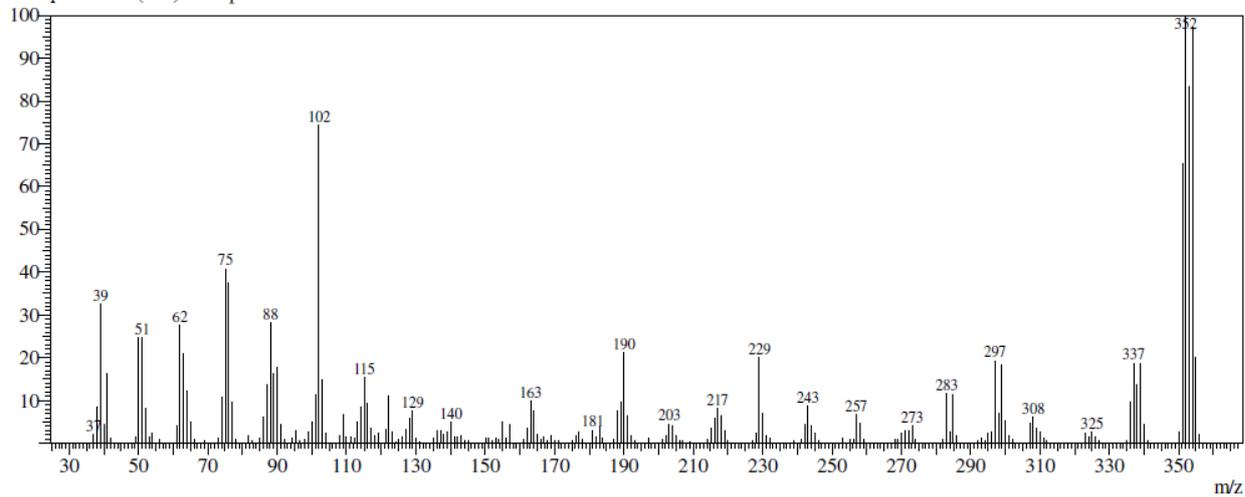
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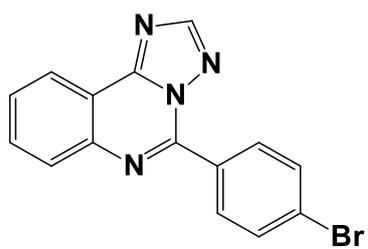
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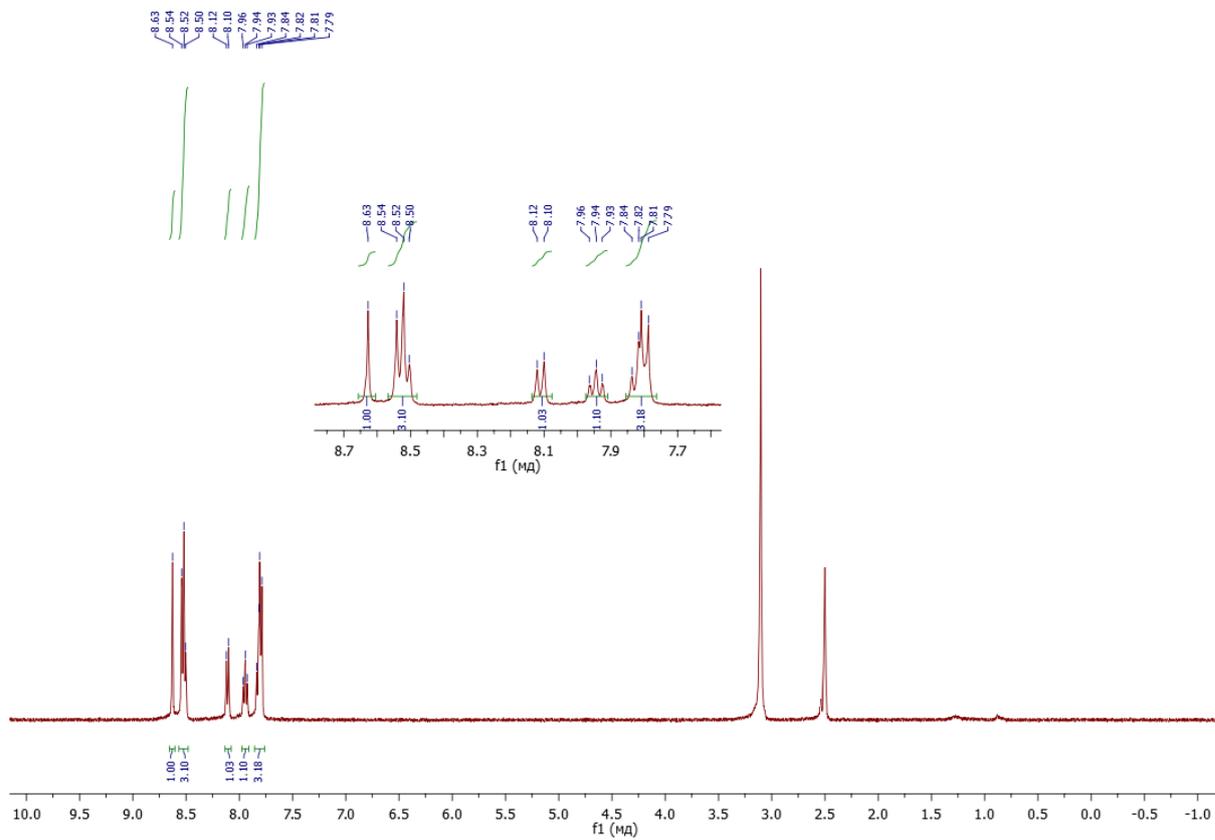


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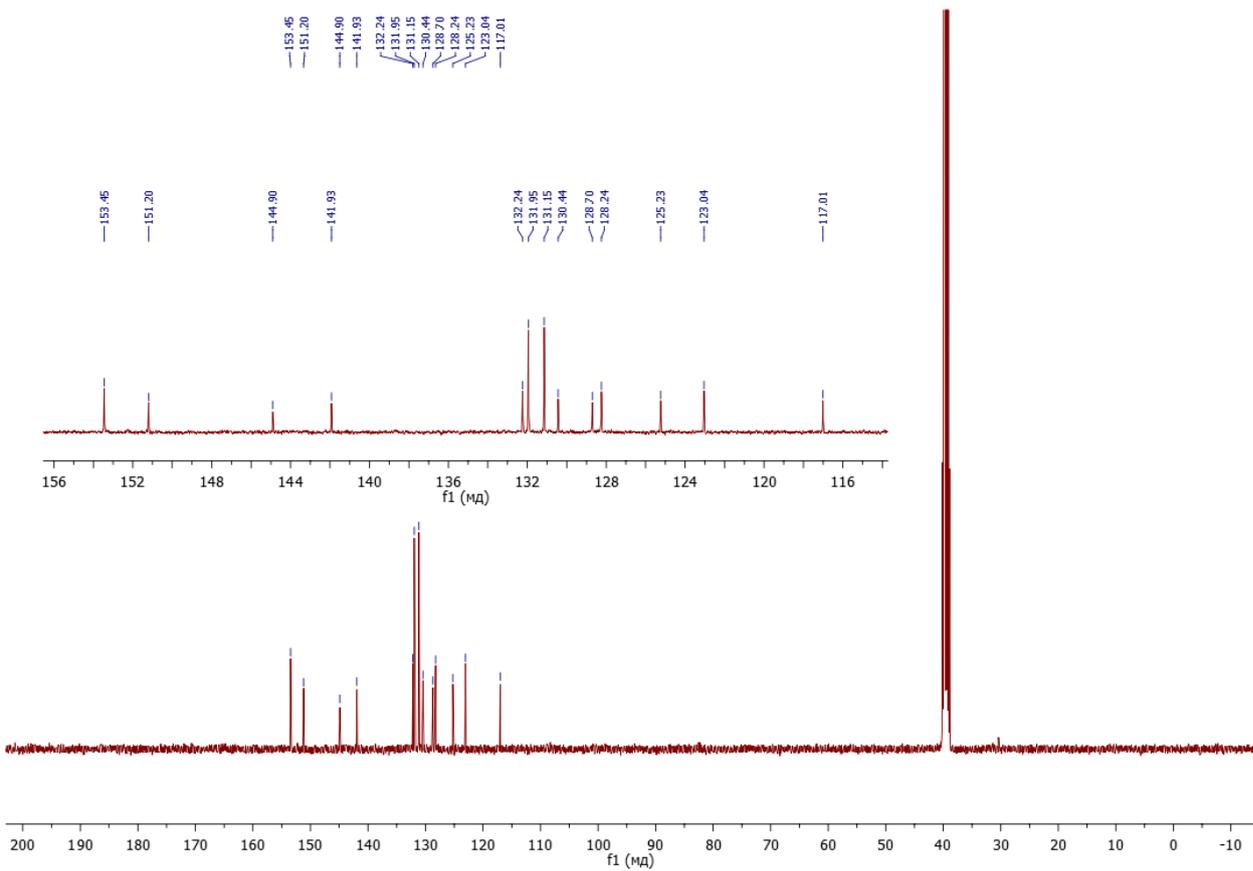
Figure S2. ¹H (a), ¹³C (b) NMR spectra of **2b** in DMSO-d₆; mass spectrum (c) of **2b**.



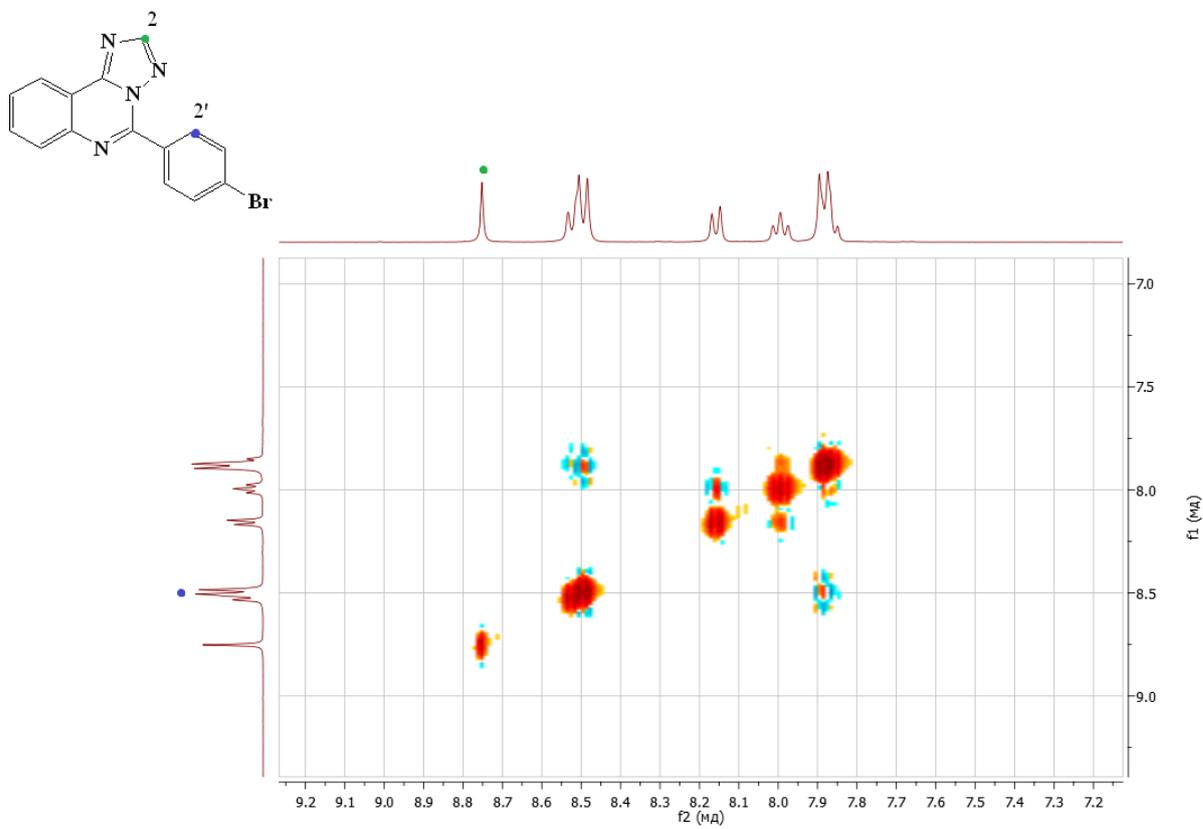
3a



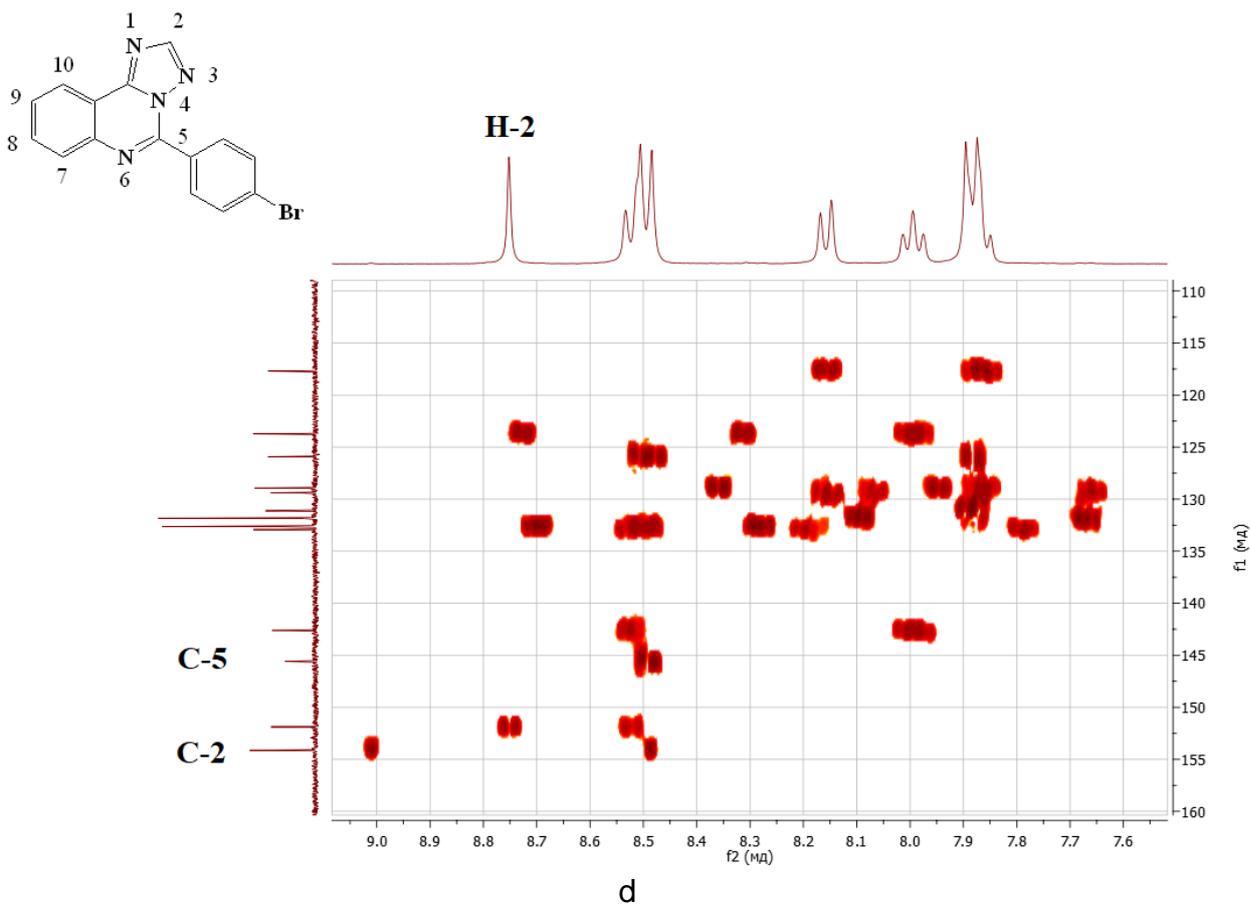
a



b



c



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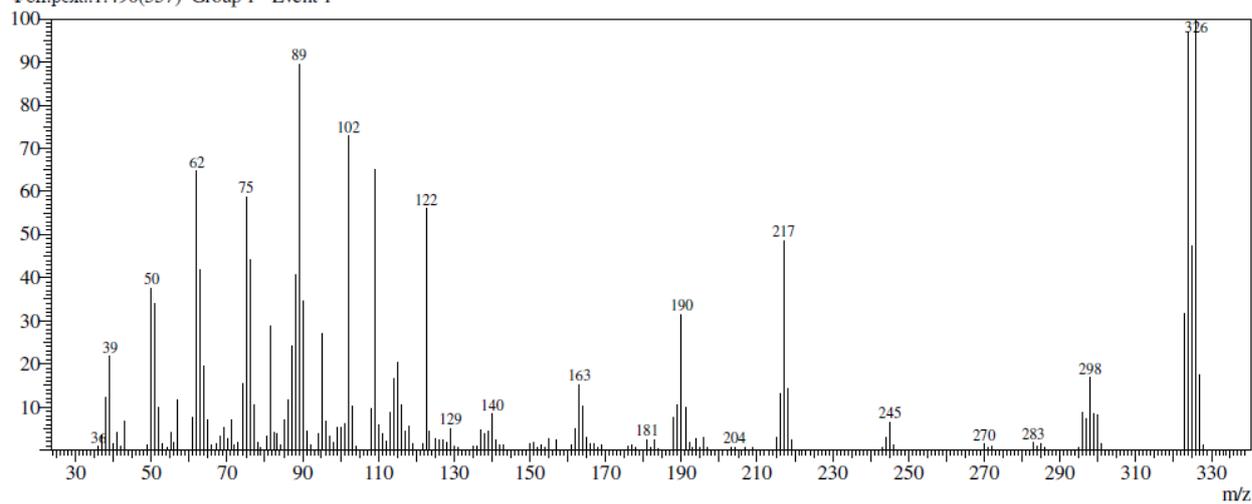
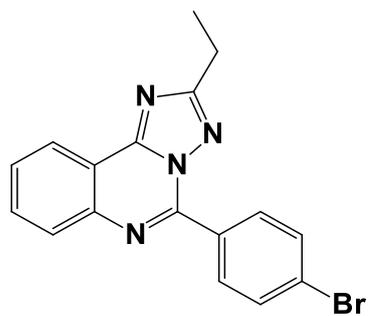
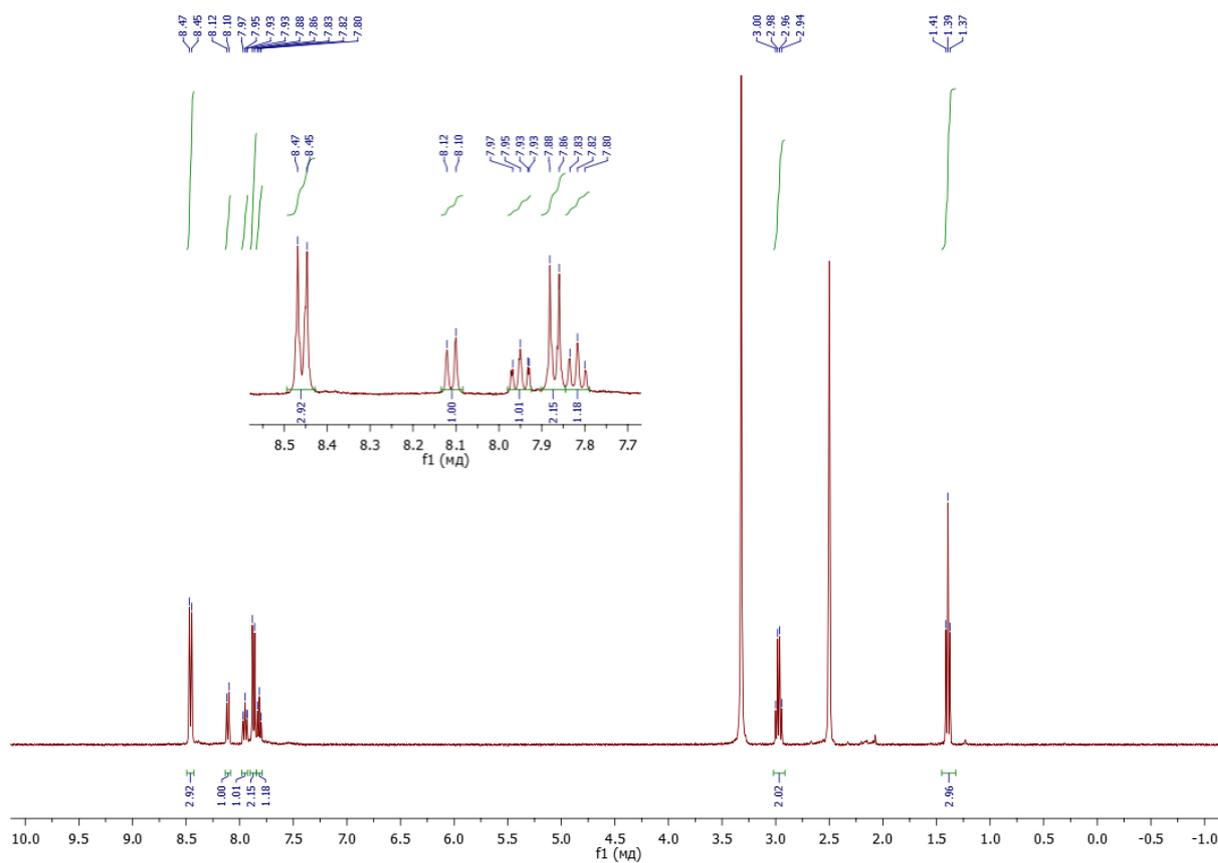


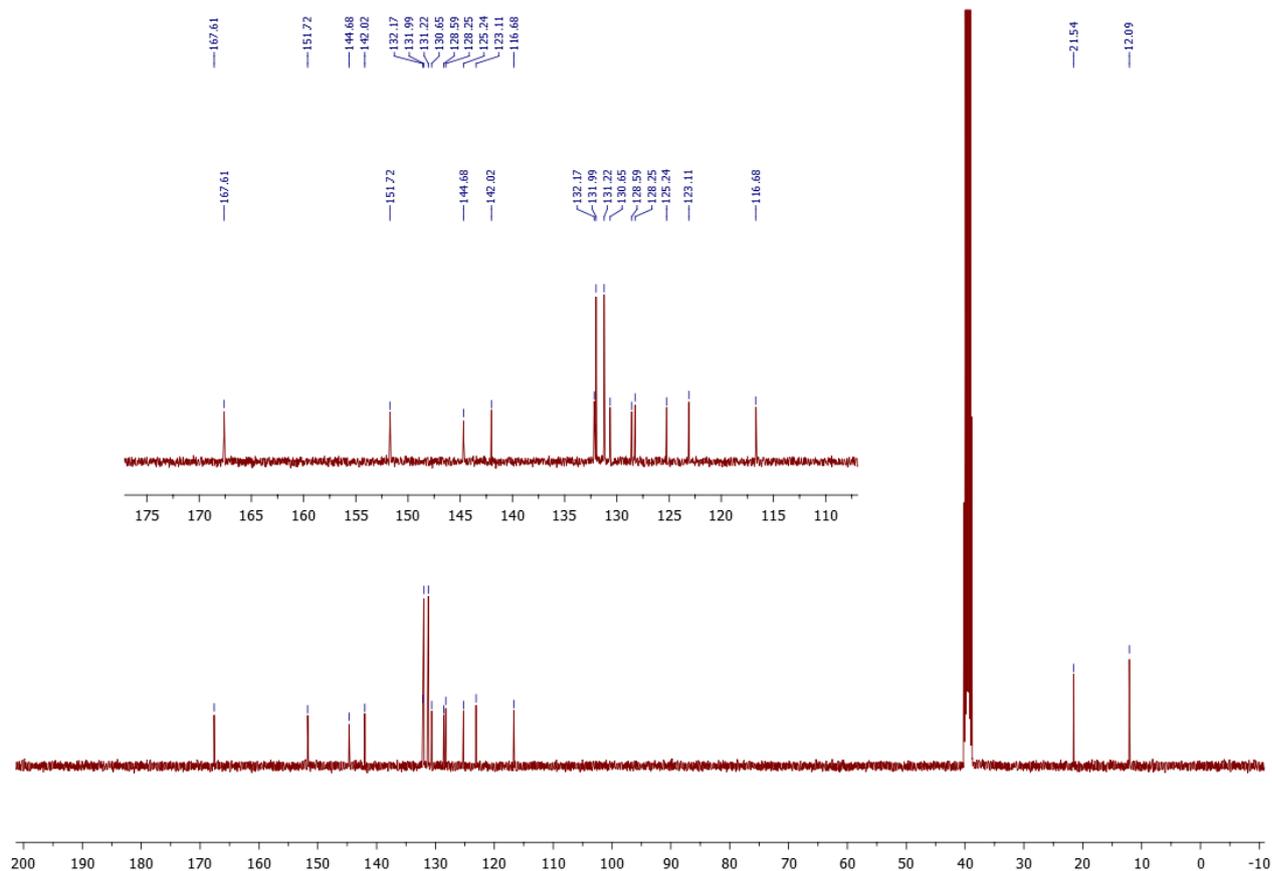
Figure S3. ^1H (a), ^{13}C (b) NMR spectra of **3a** in DMSO-d_6 ; and ^1H - ^1H NOESY (c) ^1H - ^{13}C HMBC (d) spectra of **3a** in DMSO-d_6 ; mass spectrum (d) of **3a**.



3b

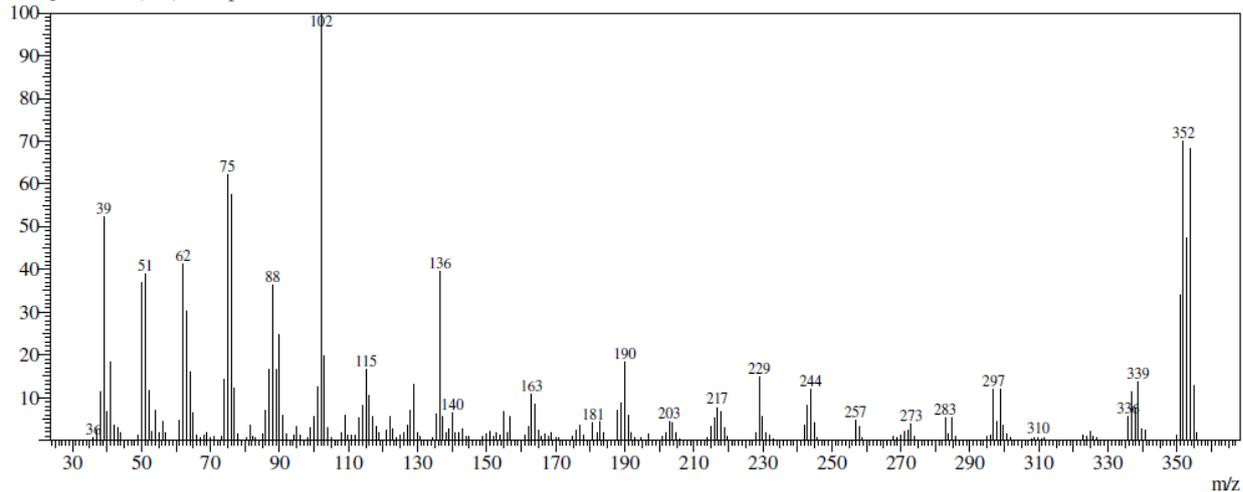


a



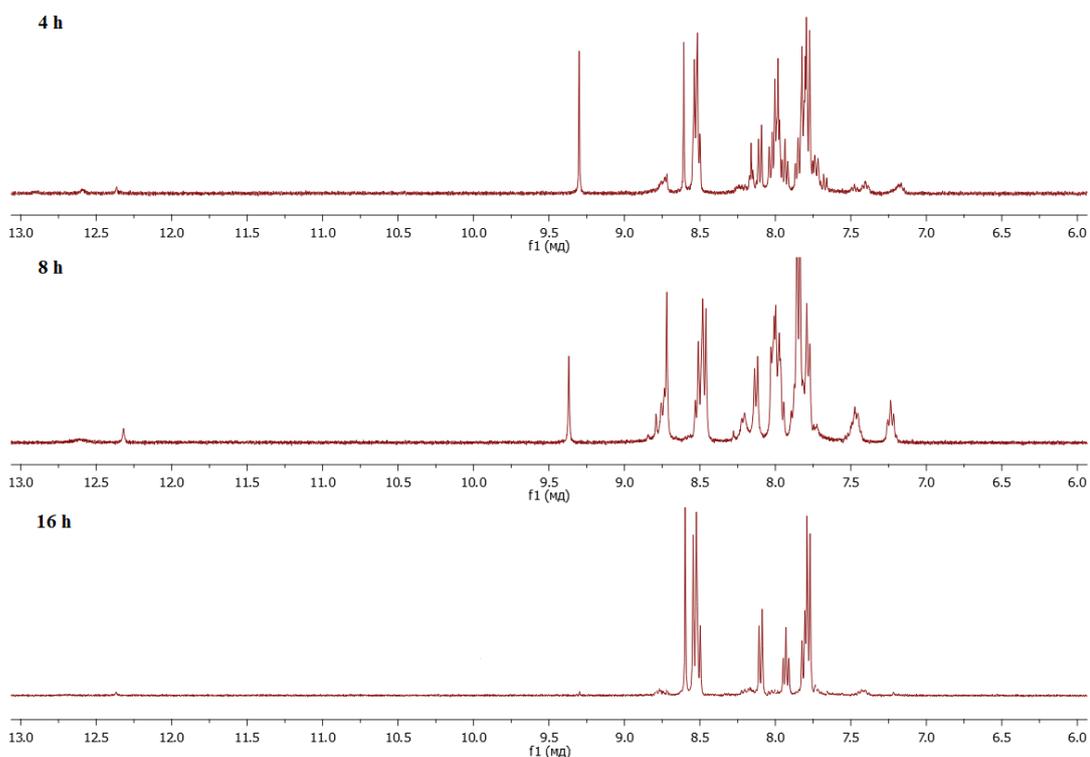
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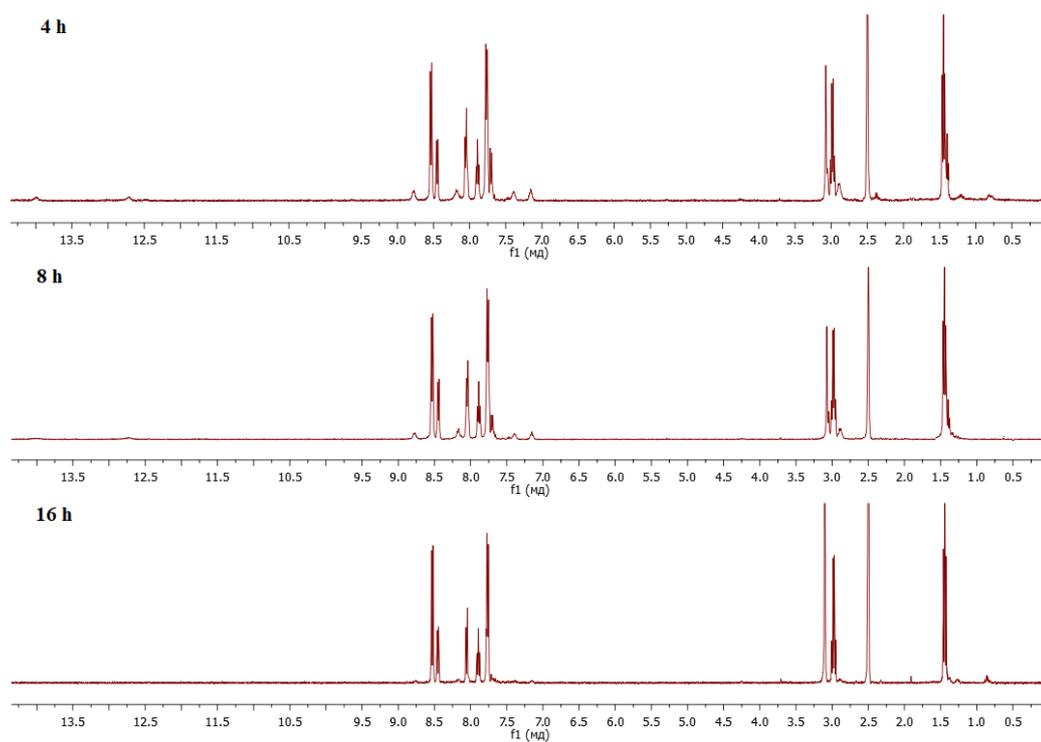


c

Figure S4. ^1H (a), ^{13}C (b) NMR spectra of **3b** in DMSO-d_6 ; mass spectrum (c) of **3b**.

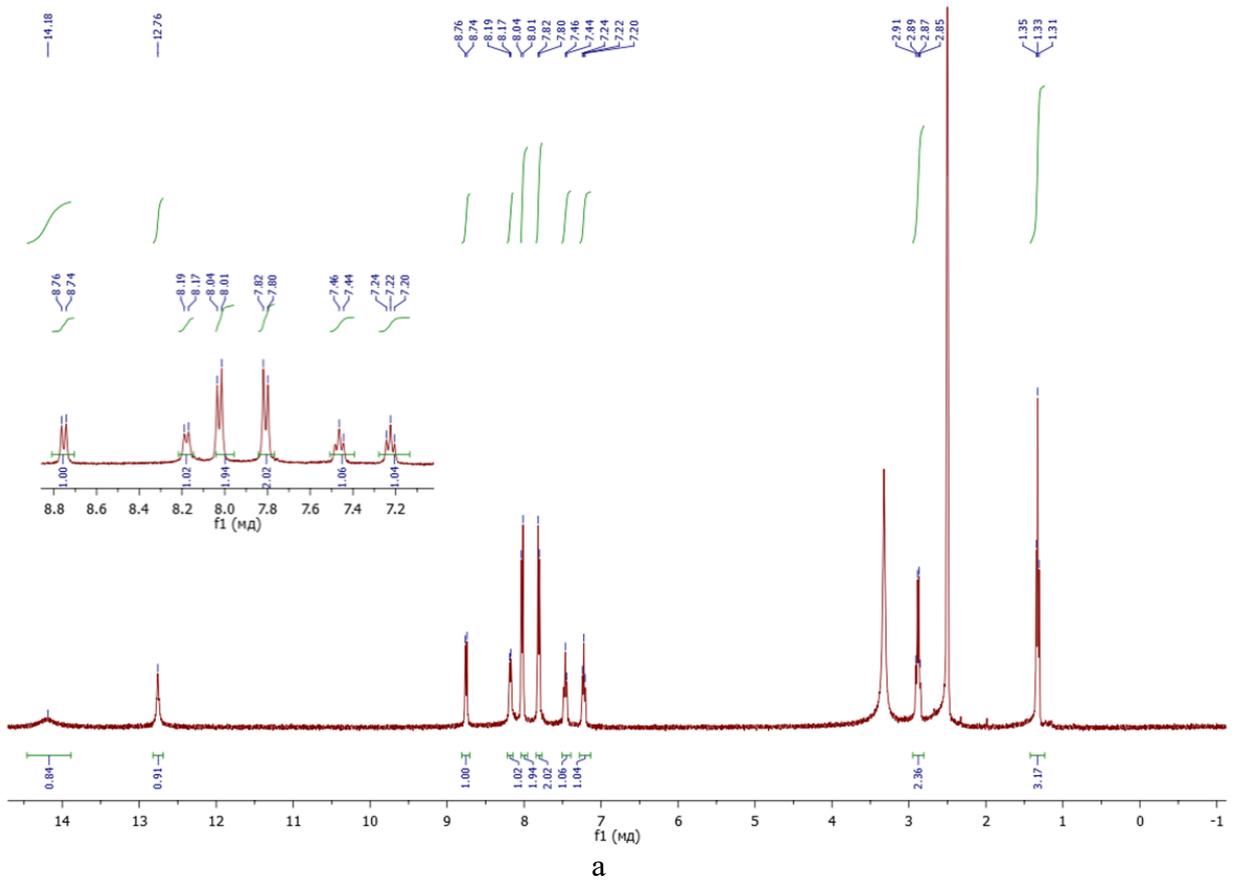
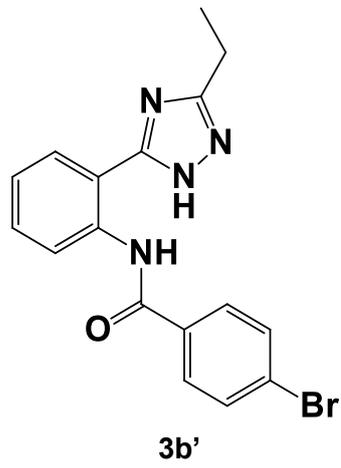


a

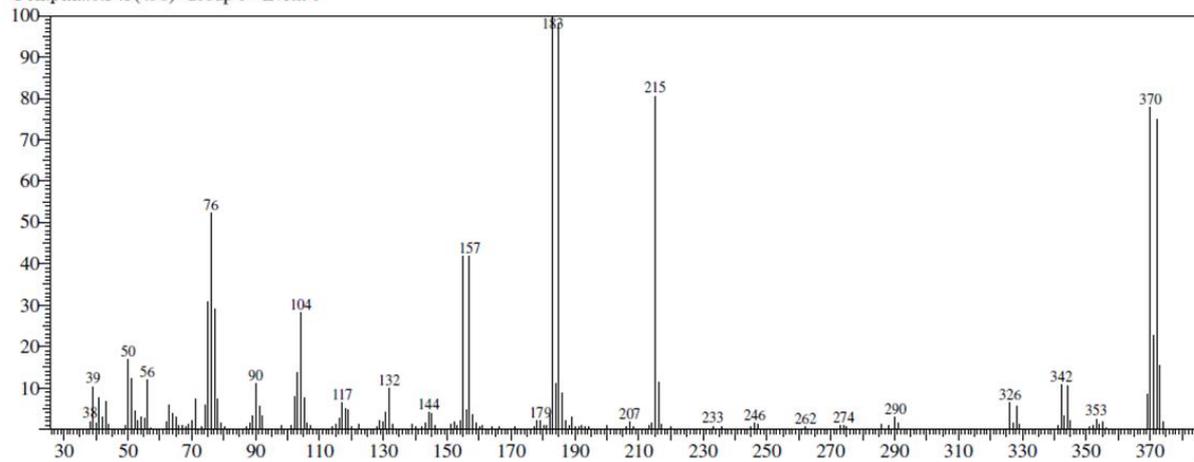


b

Figure S5. ^1H NMR monitoring of the reaction progress of 2-(4-bromophenyl)-4-hydrazinoquinazoline with triethyl orthoformate (a) or triethyl orthopropionate (b) in acetic media after 4 h, 8 h and 16 h. Spectra were recorded in DMSO-d_6 .

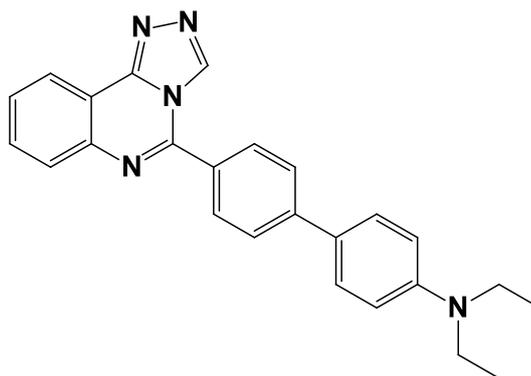


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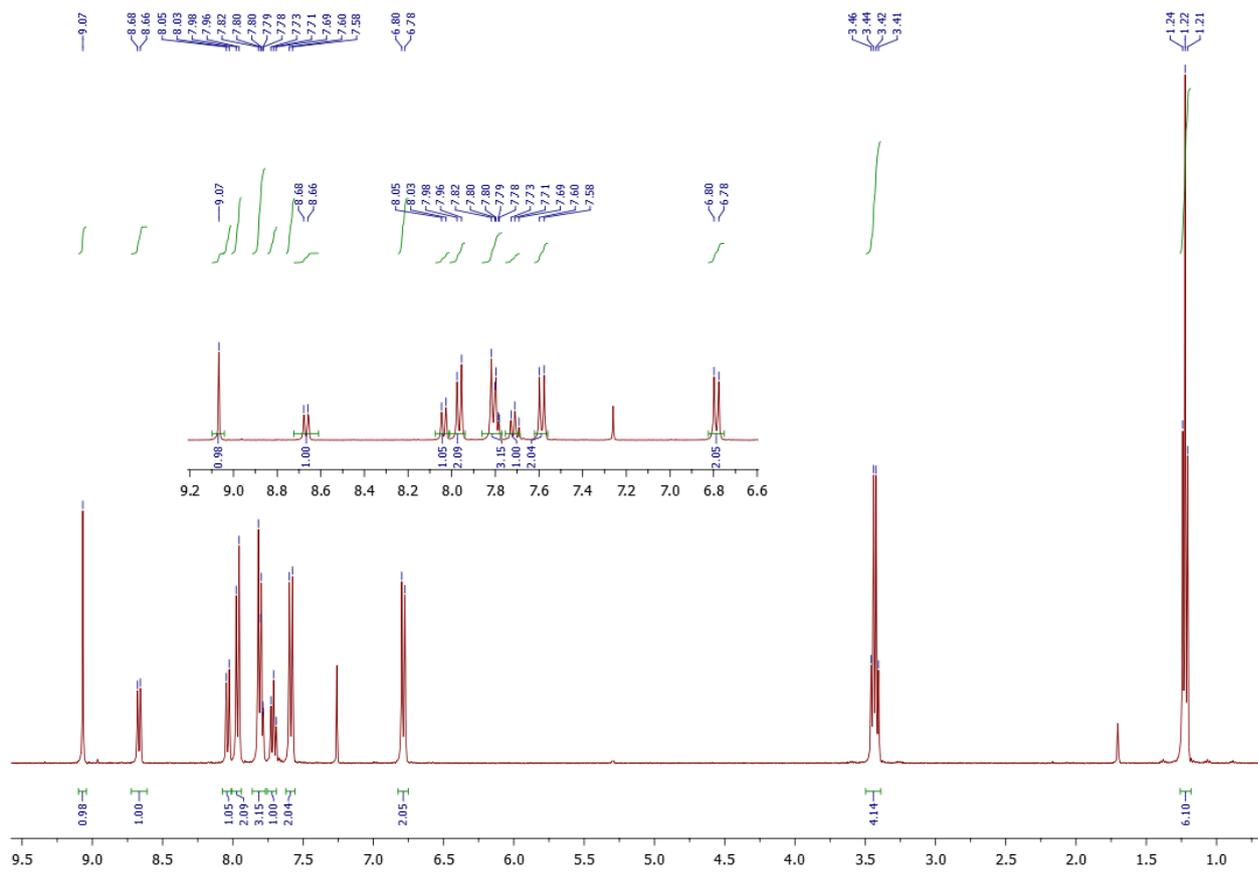


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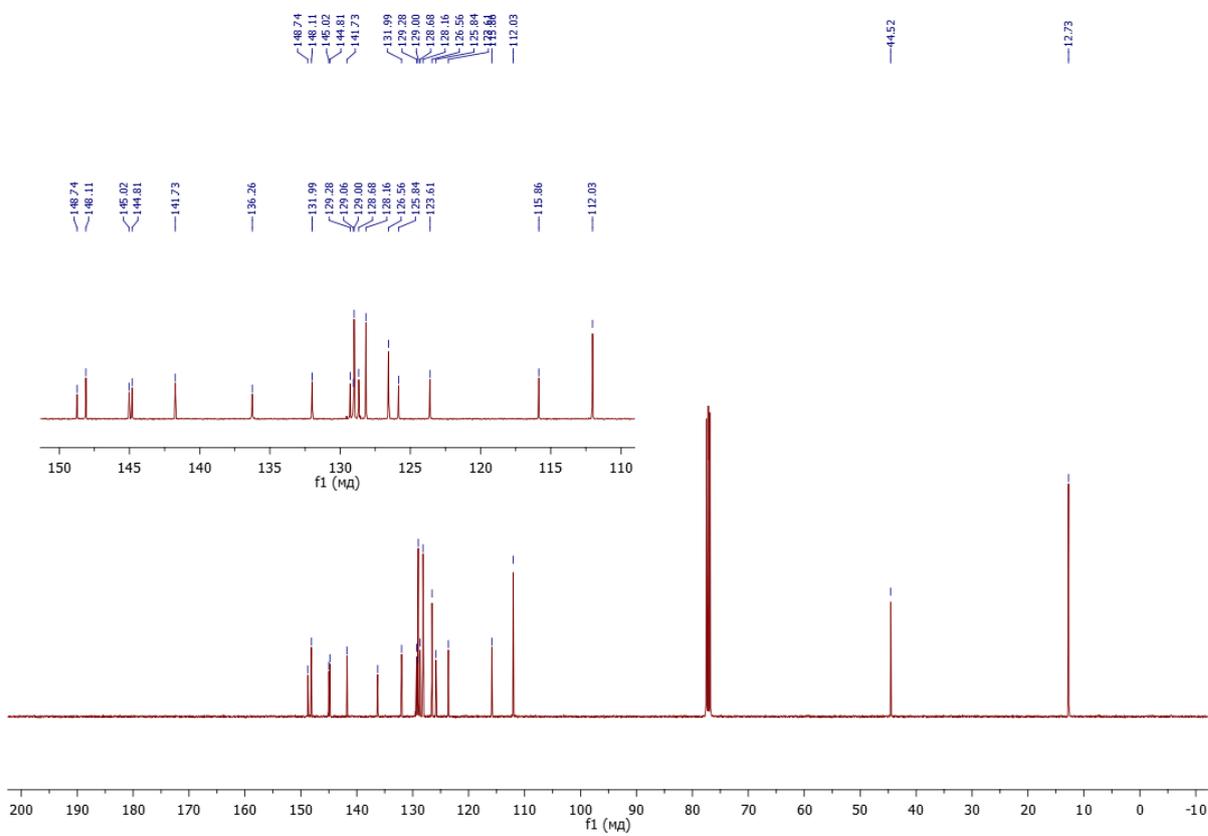
Figure S6. ^1H (a) NMR spectrum of **3b'** in DMSO-d_6 ; mass spectrum (b) of **3b'**.



4a

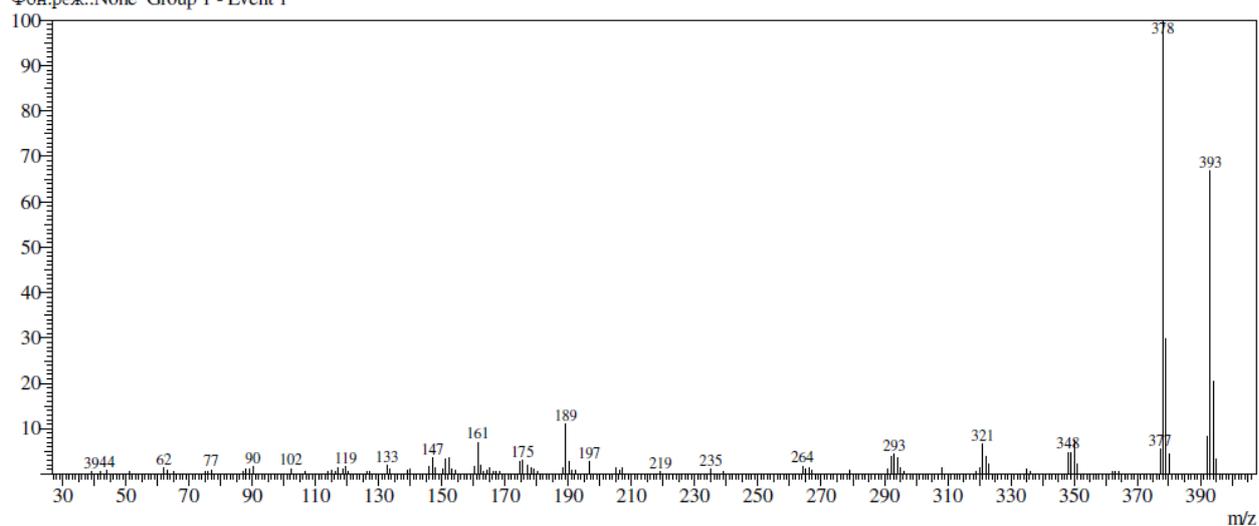


a



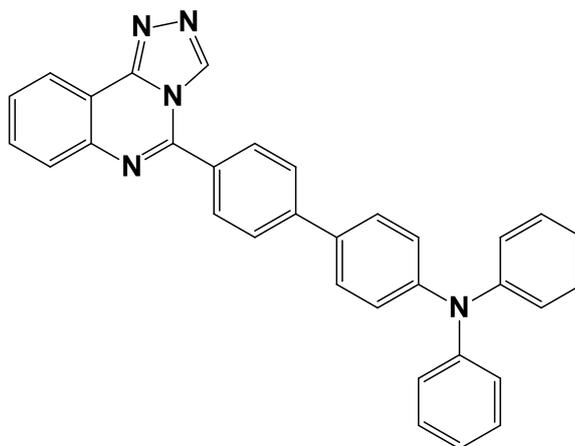
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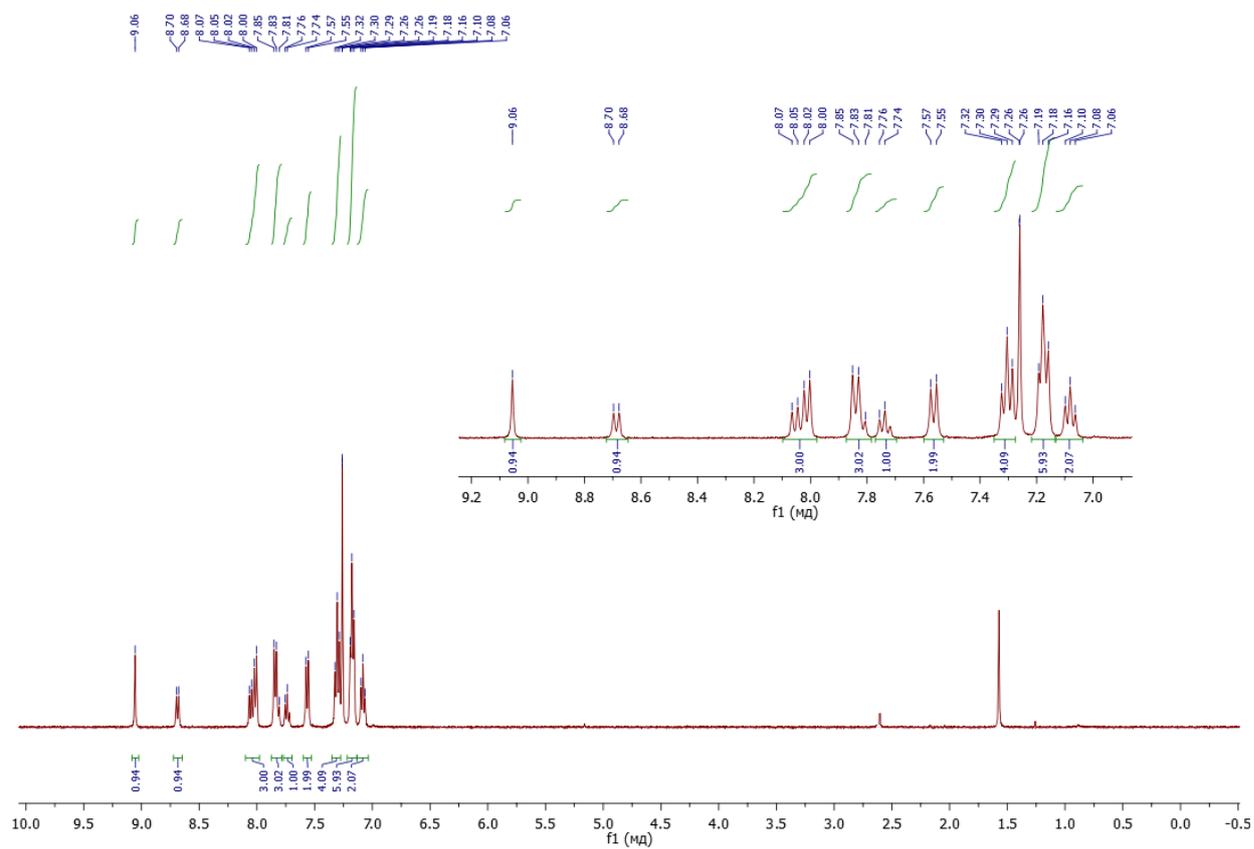


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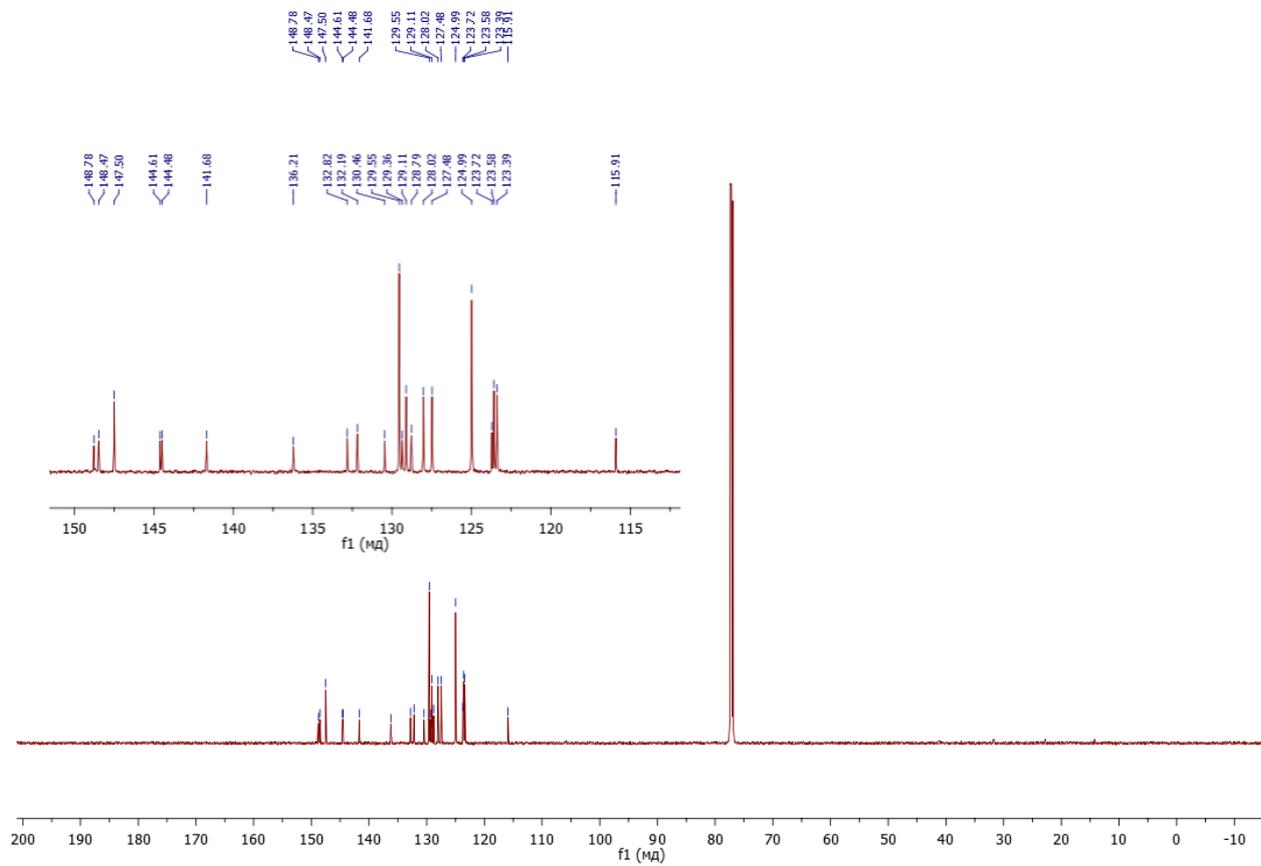
Figure S7. ^1H (a), ^{13}C (b) NMR spectra of **4a** in DCCl_3 ; mass spectrum (c) of **4a**.



4b

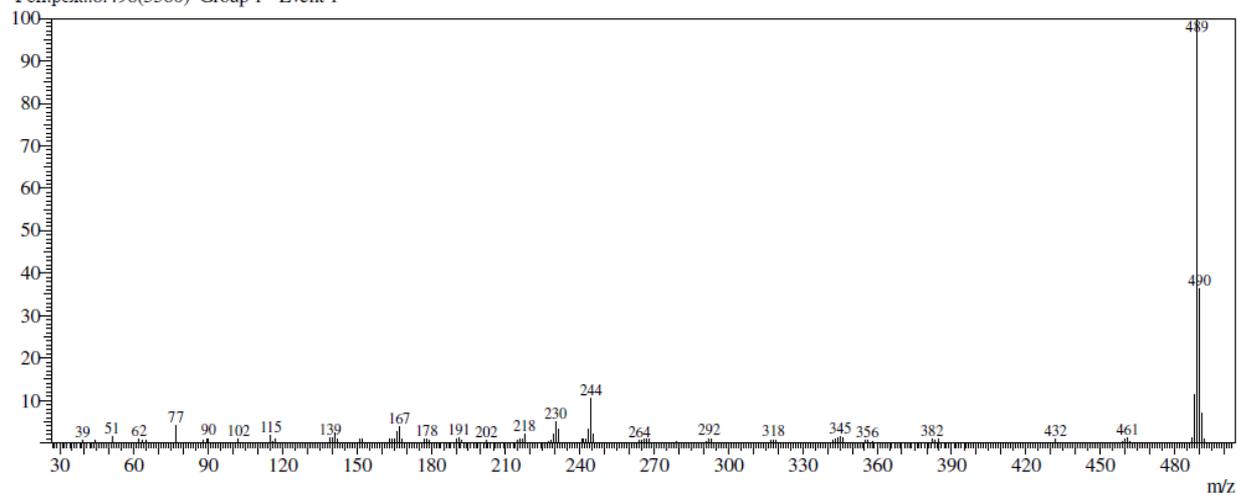


a



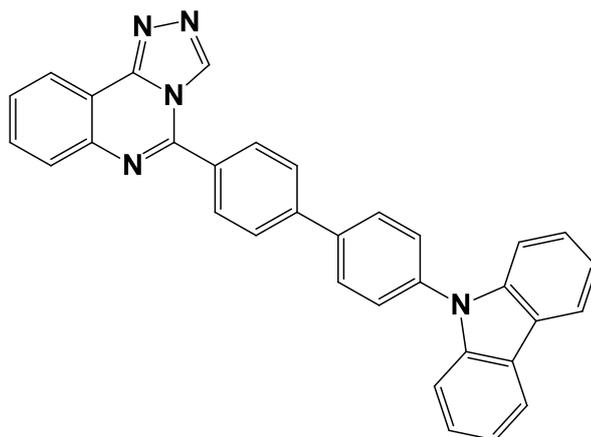
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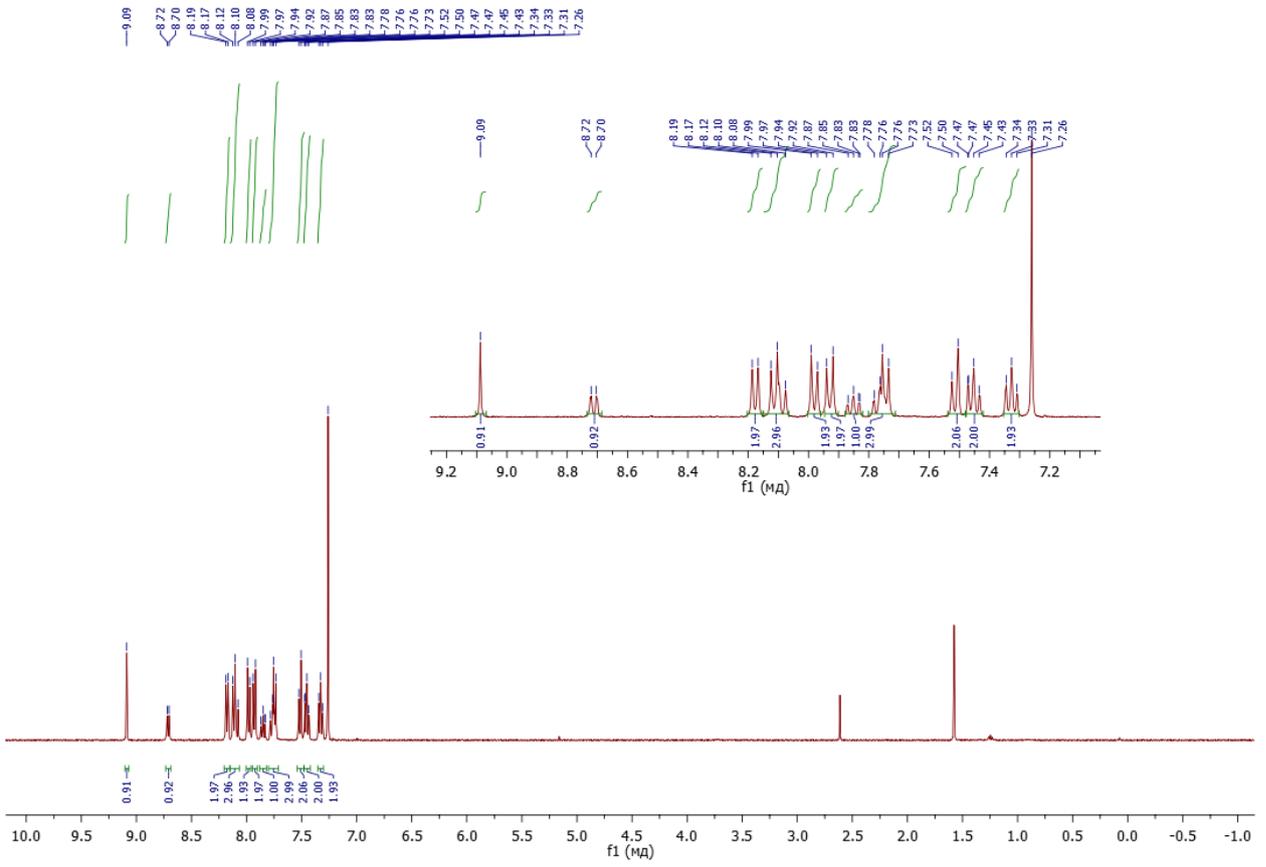


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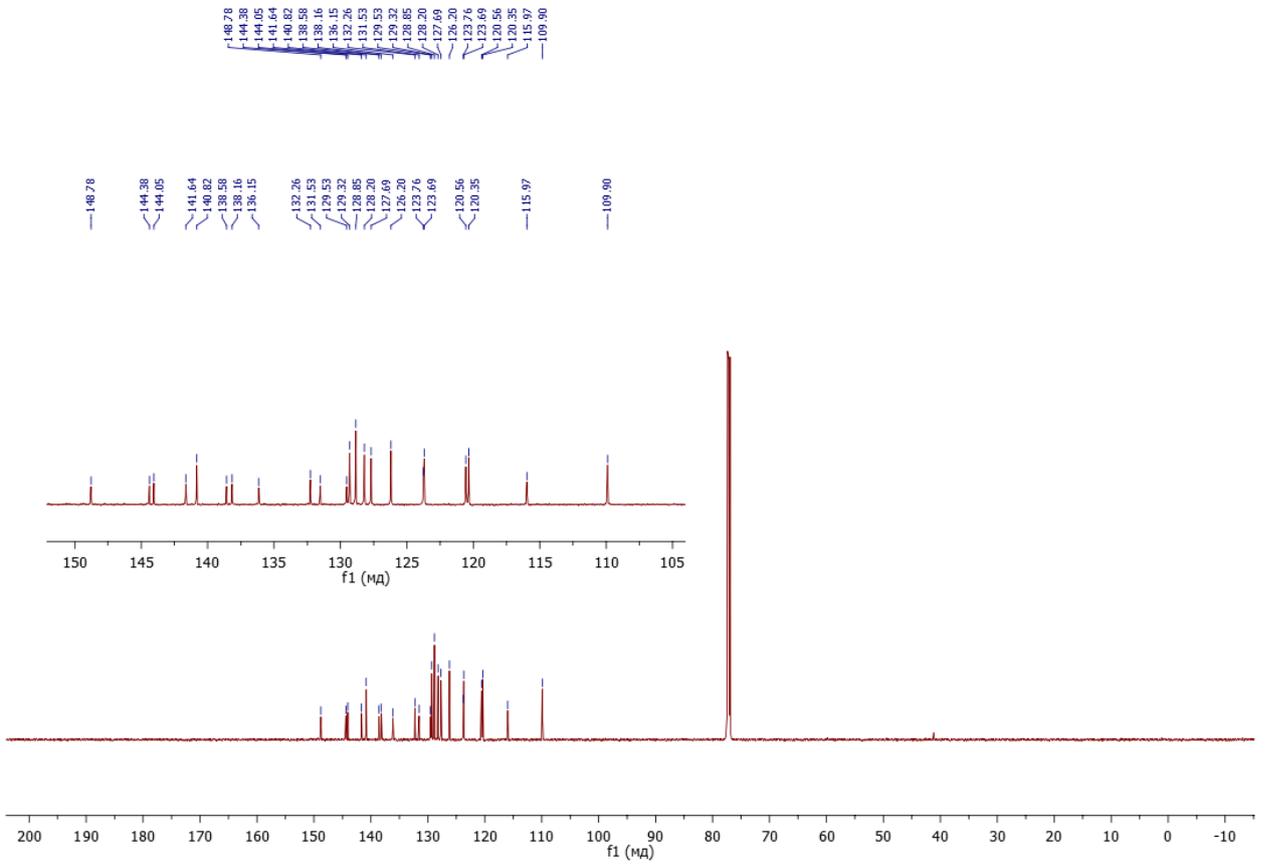
Figure S8. ^1H (a), ^{13}C (b) NMR spectra of **4b** in DCCl_3 ; mass spectrum (c) of **4b**.



4c



a



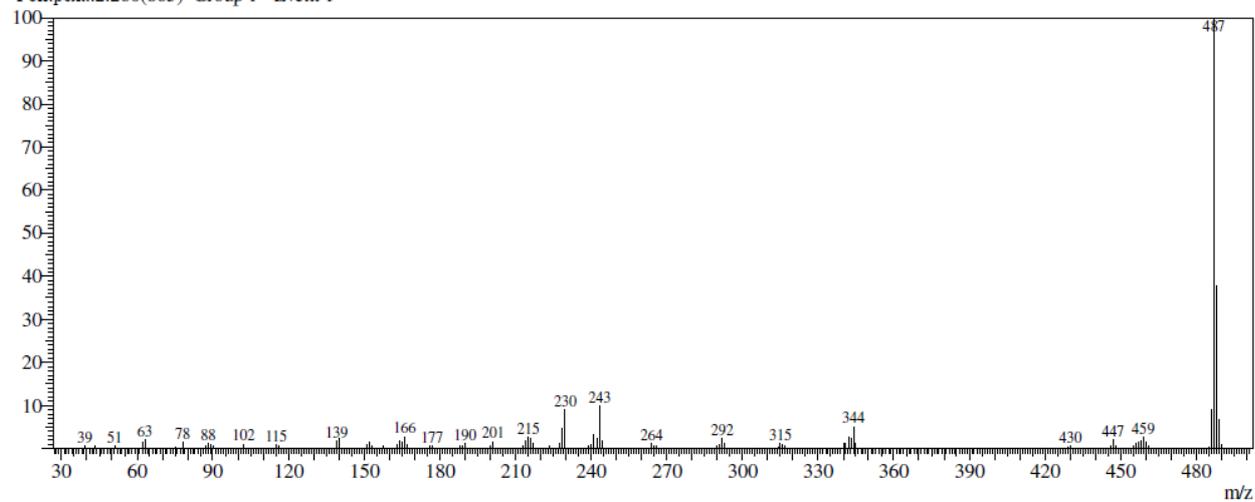
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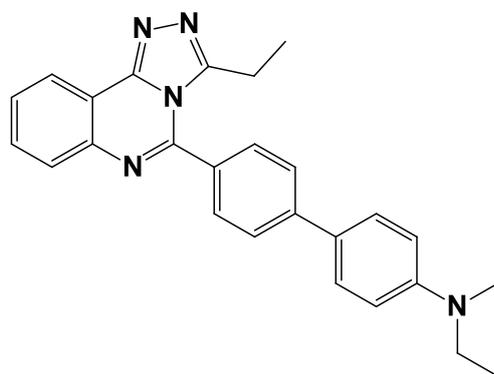
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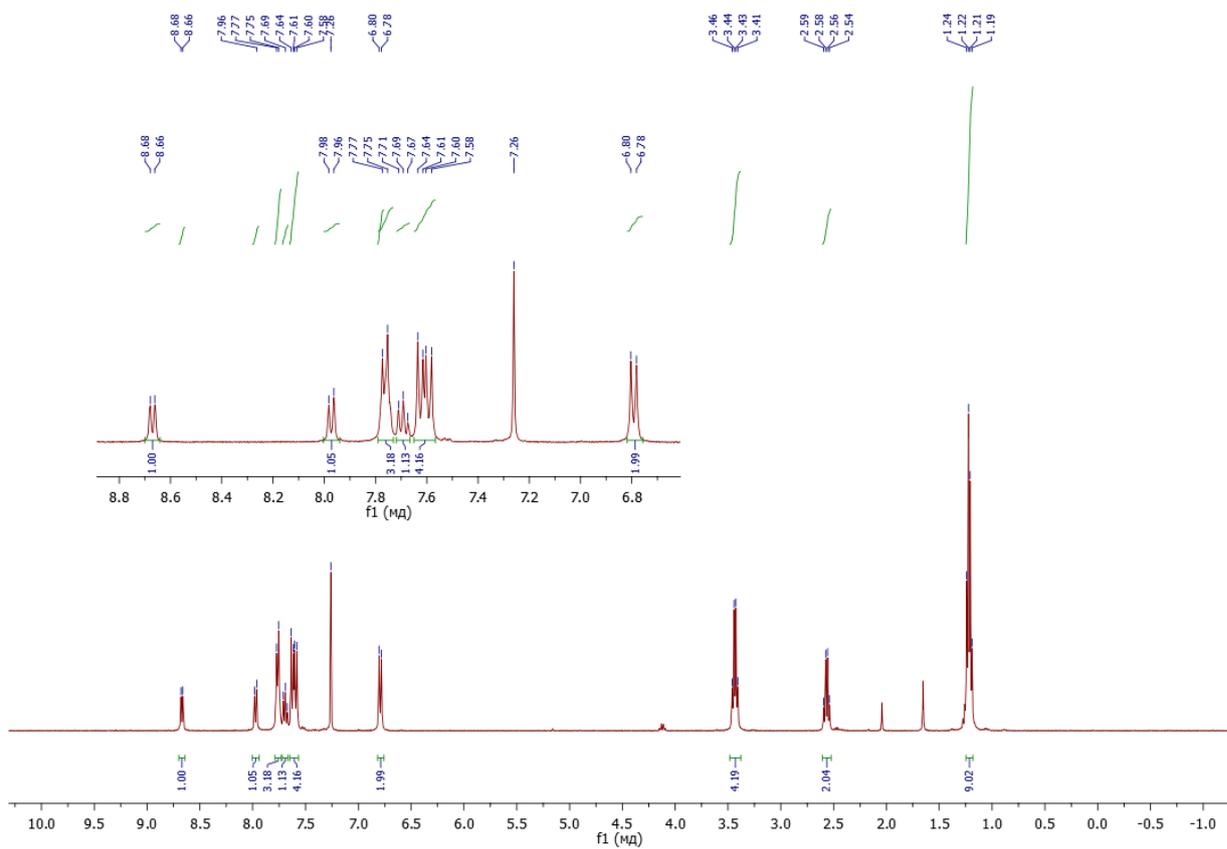


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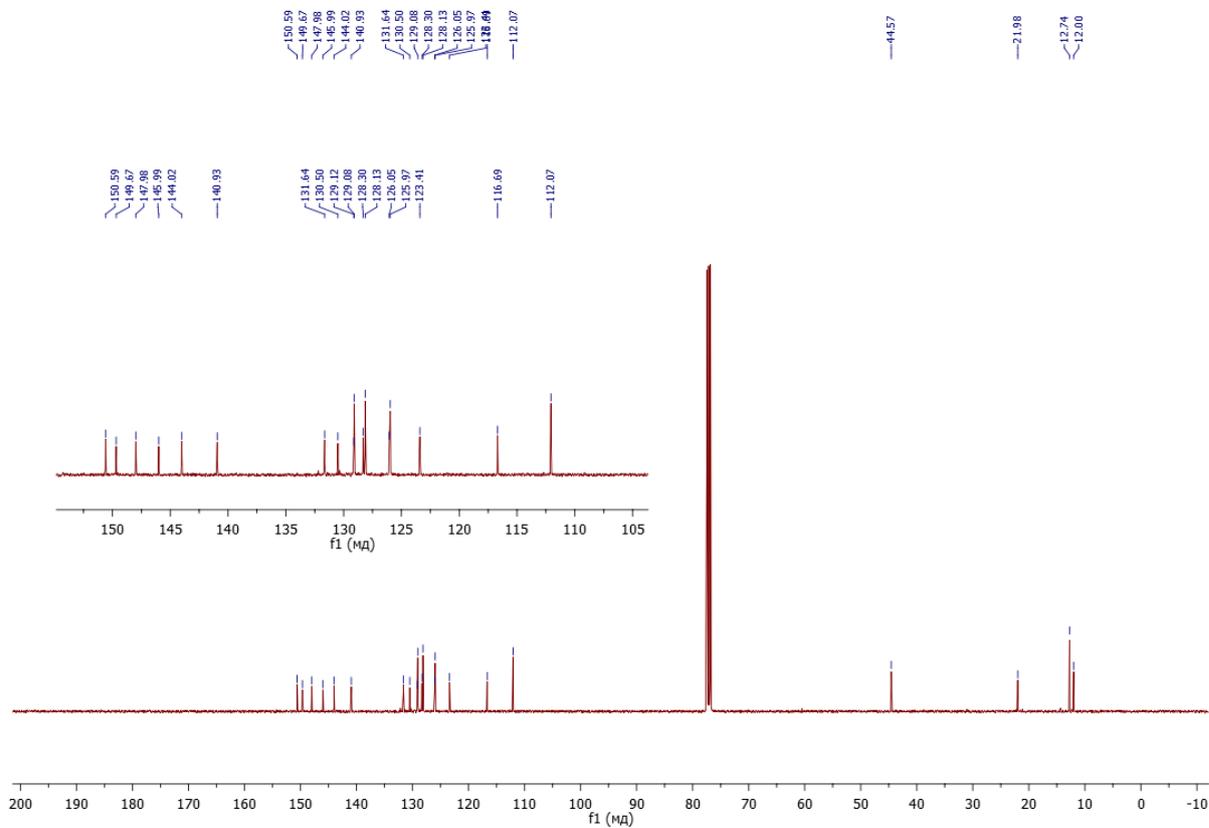
Figure S9. ^1H (a), ^{13}C (b) NMR spectra of **4c** in DCCl_3 ; mass spectrum (c) of **4c**.



4d

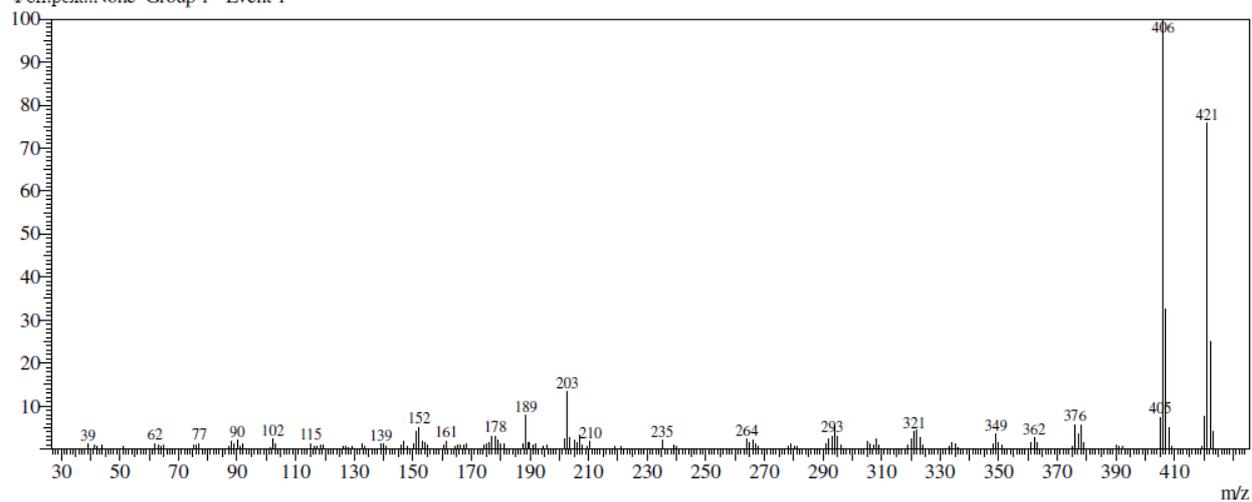


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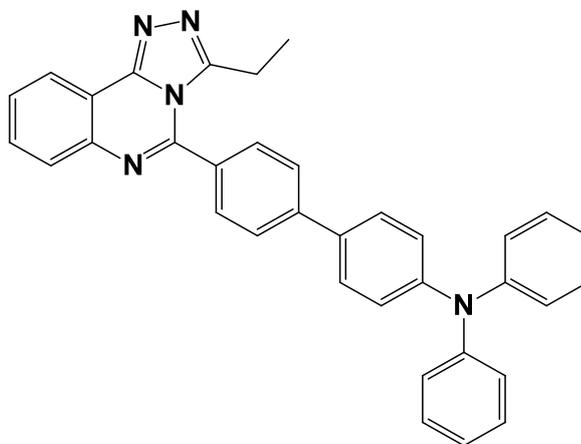
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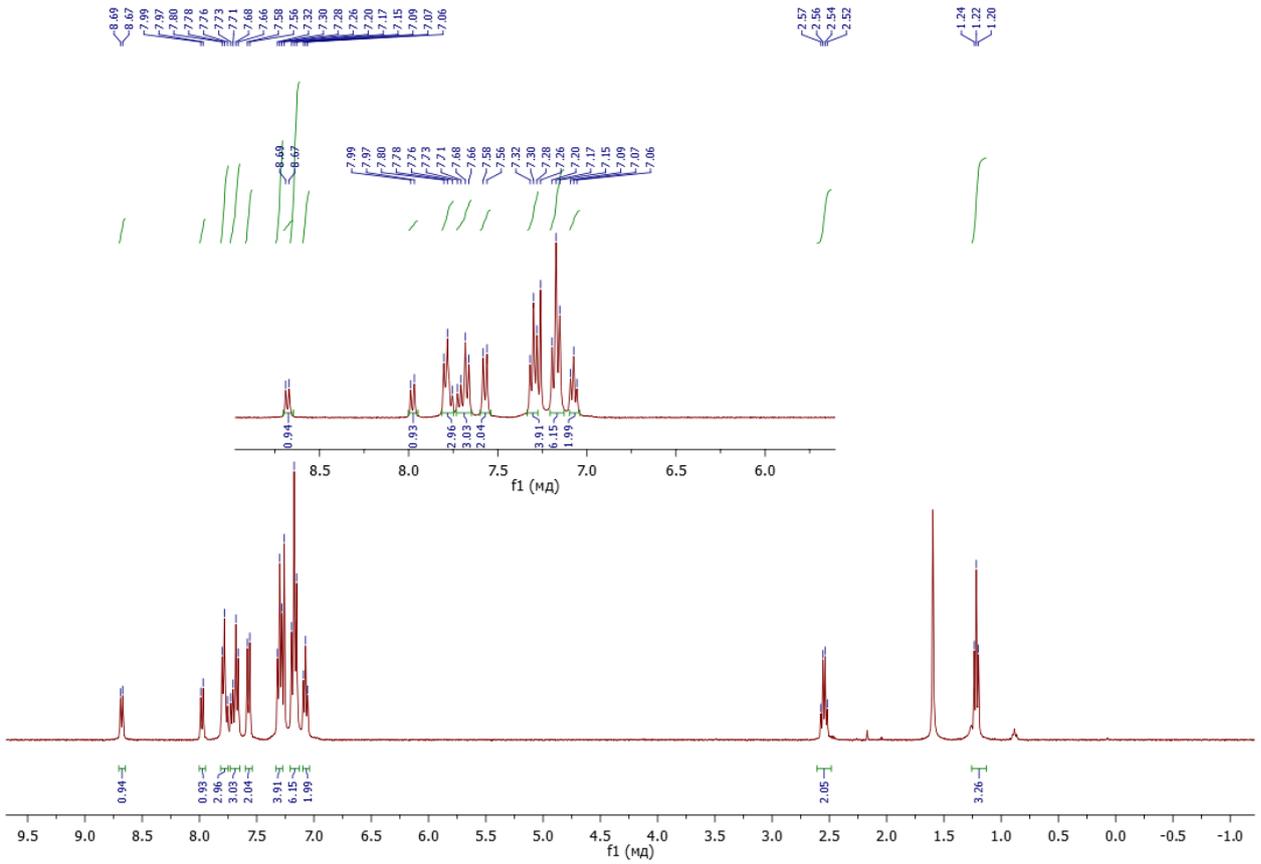


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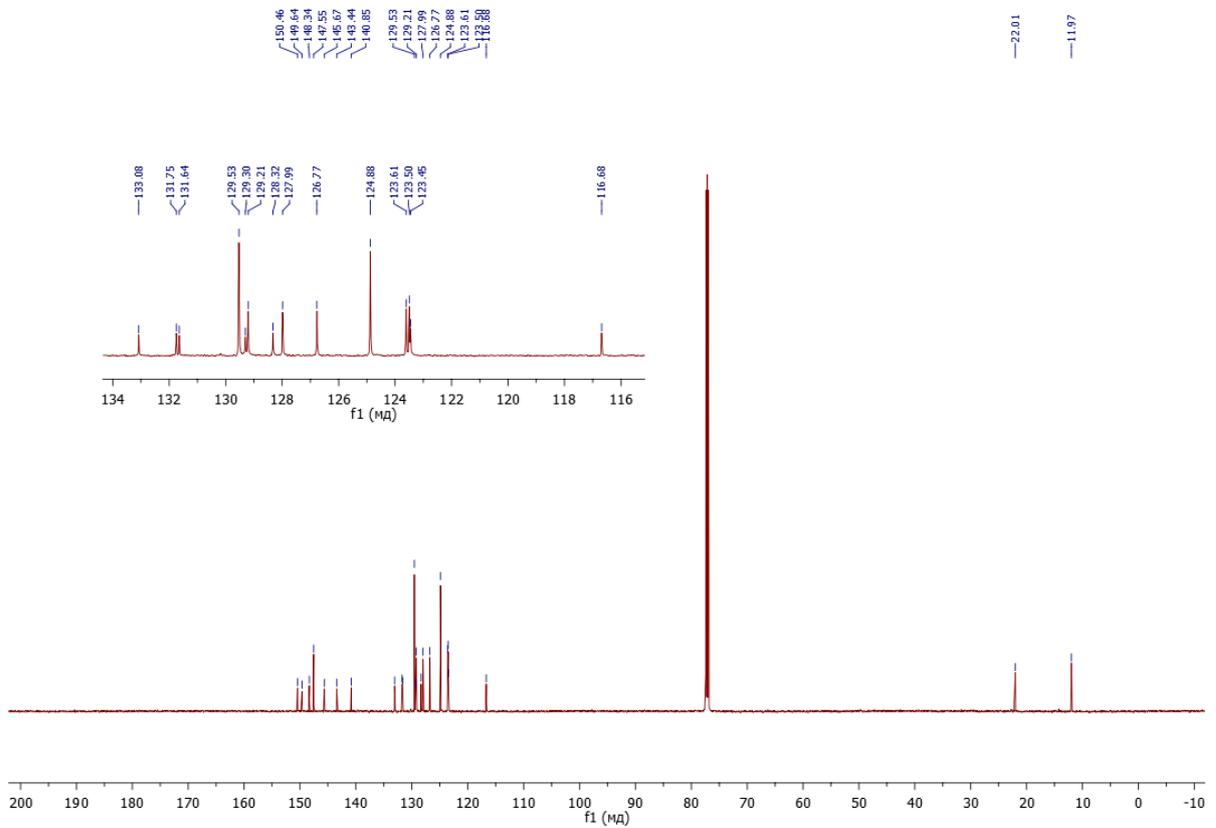
Figure S10. ^1H (a), ^{13}C (b) NMR spectra of **4d** in DCCl_3 ; mass spectrum (c) of **4d**.



4e

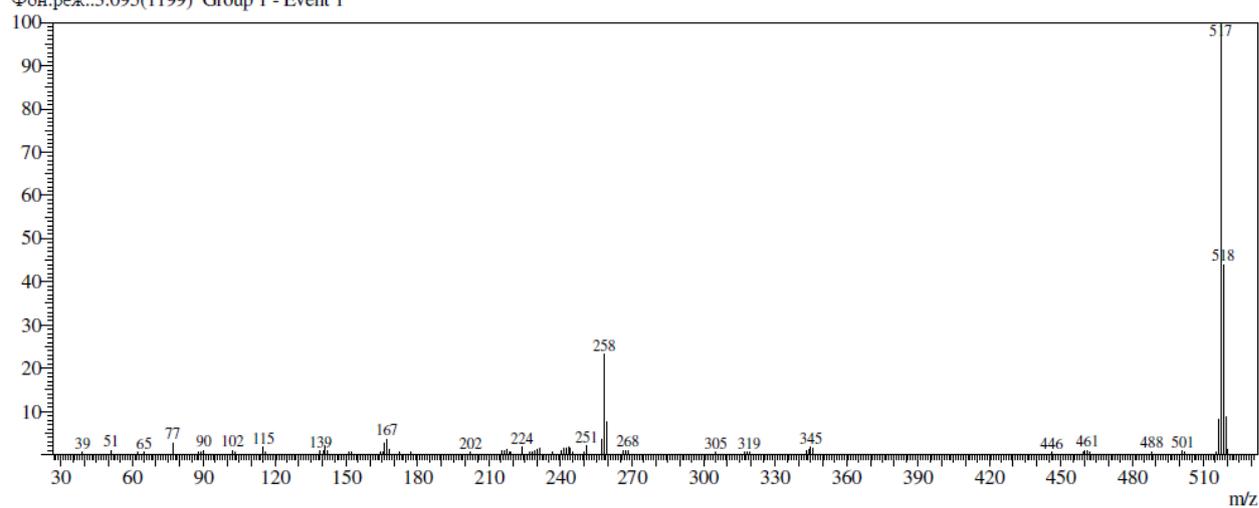


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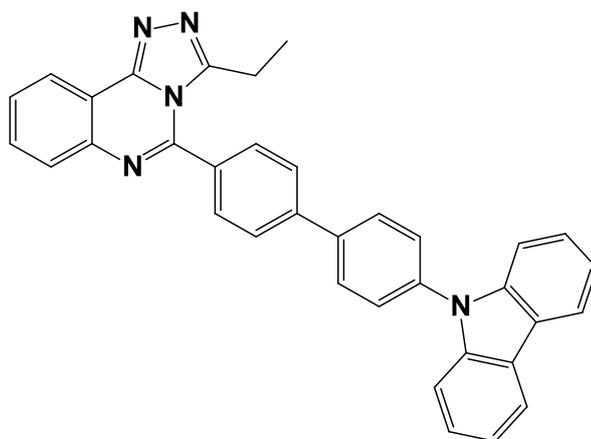
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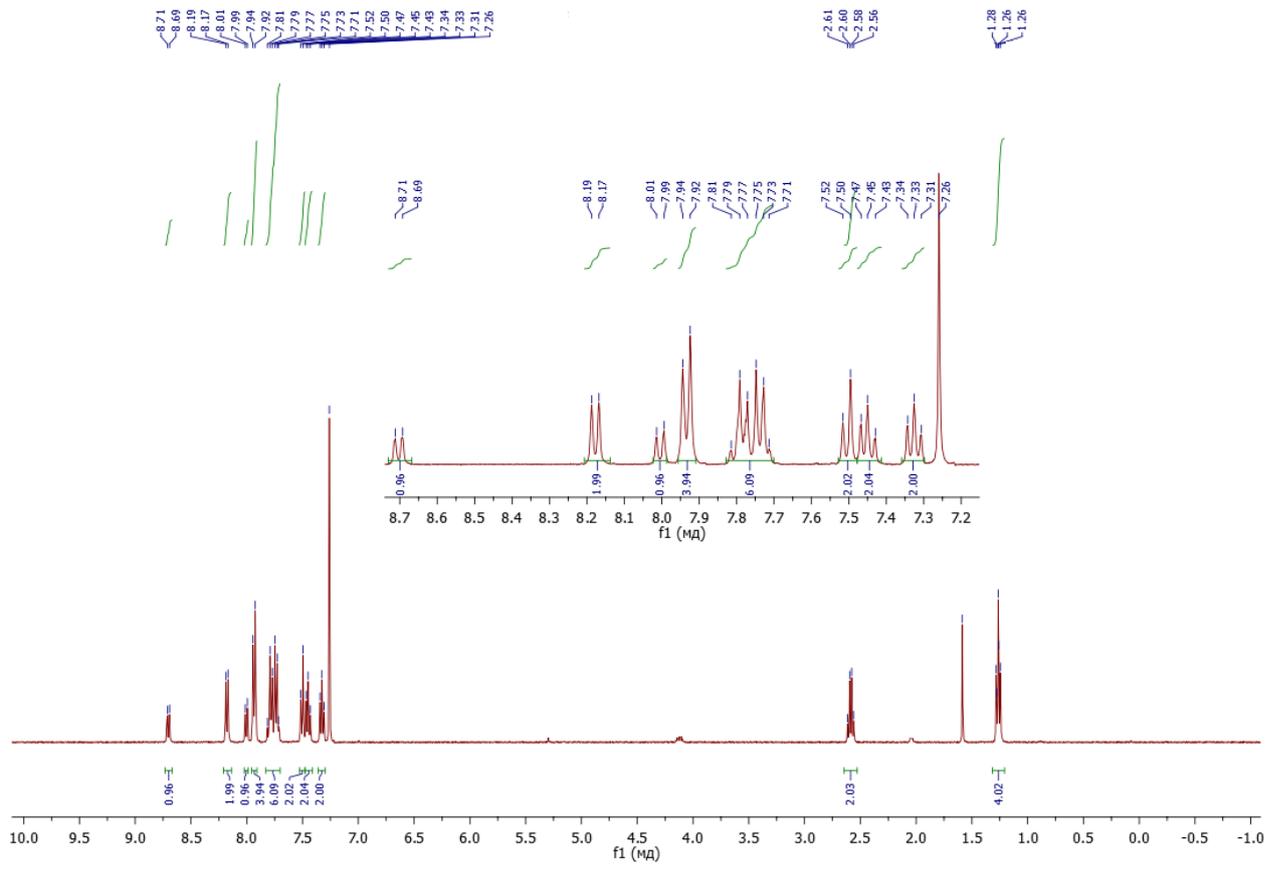


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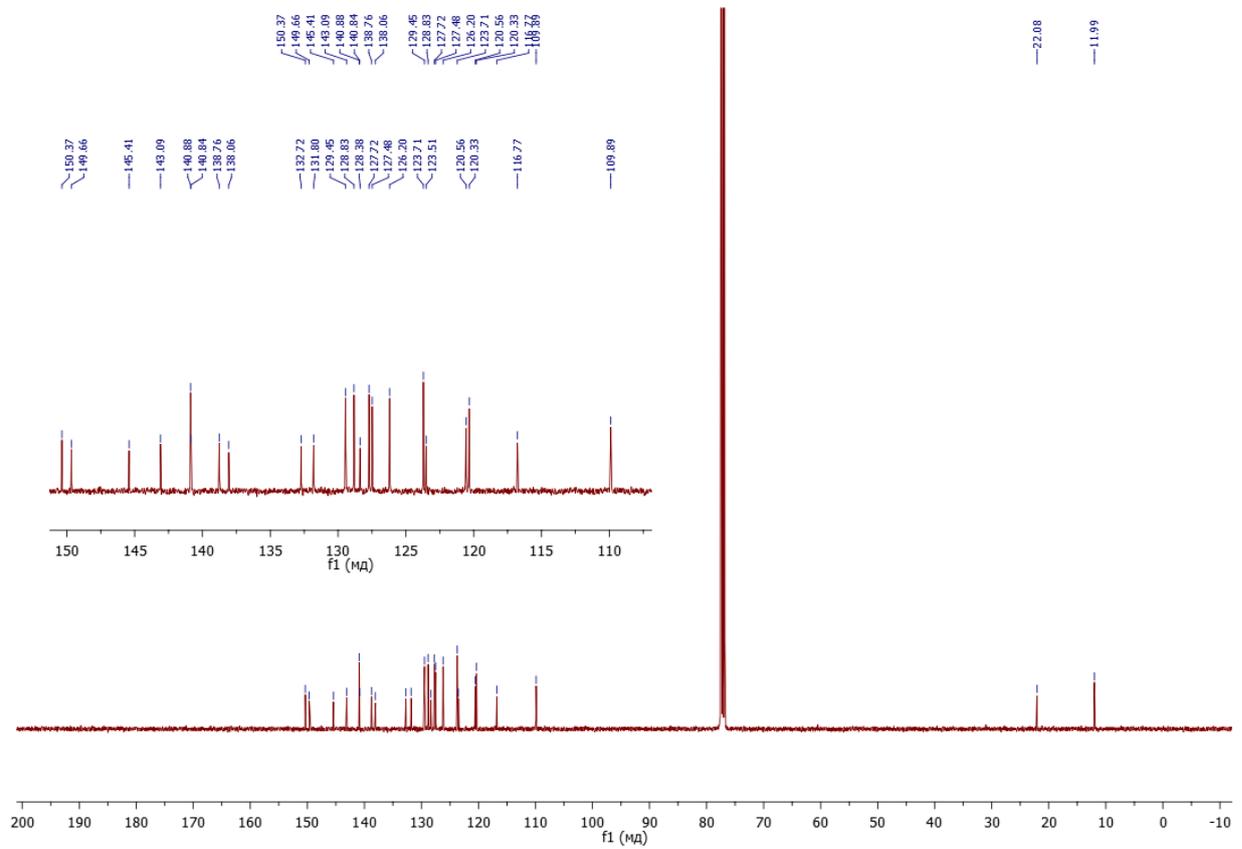
Figure S11. ^1H (a), ^{13}C (b) NMR spectra of **4e** in DCCl_3 ; mass spectrum (c) of **4e**.



4f

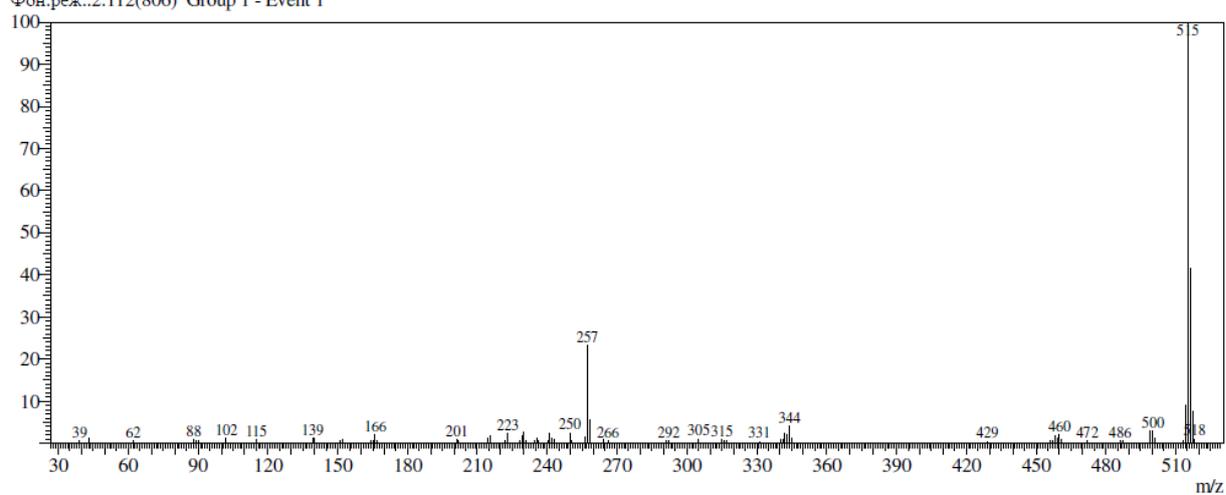


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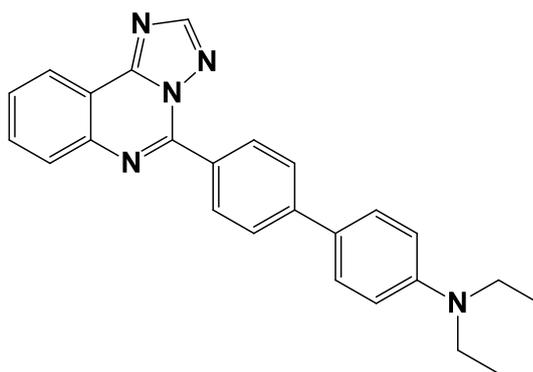
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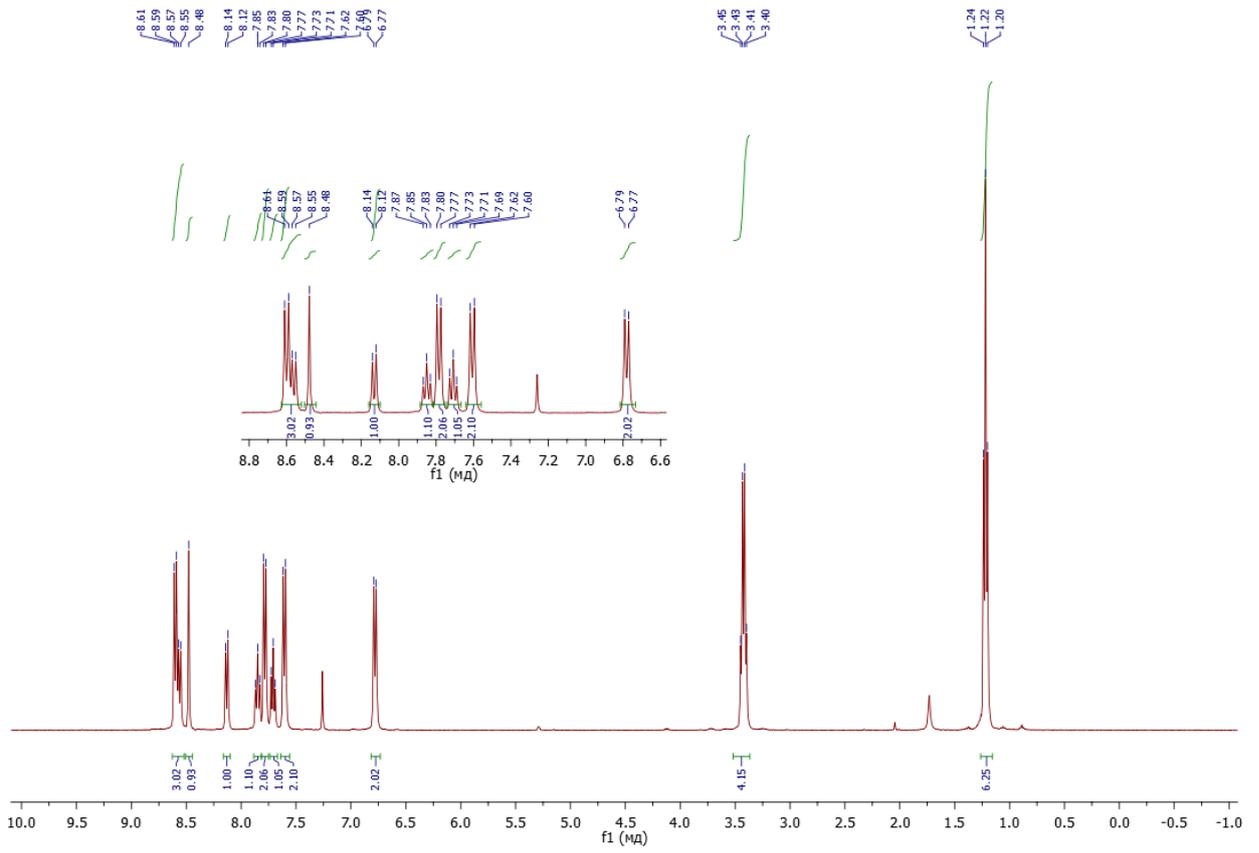


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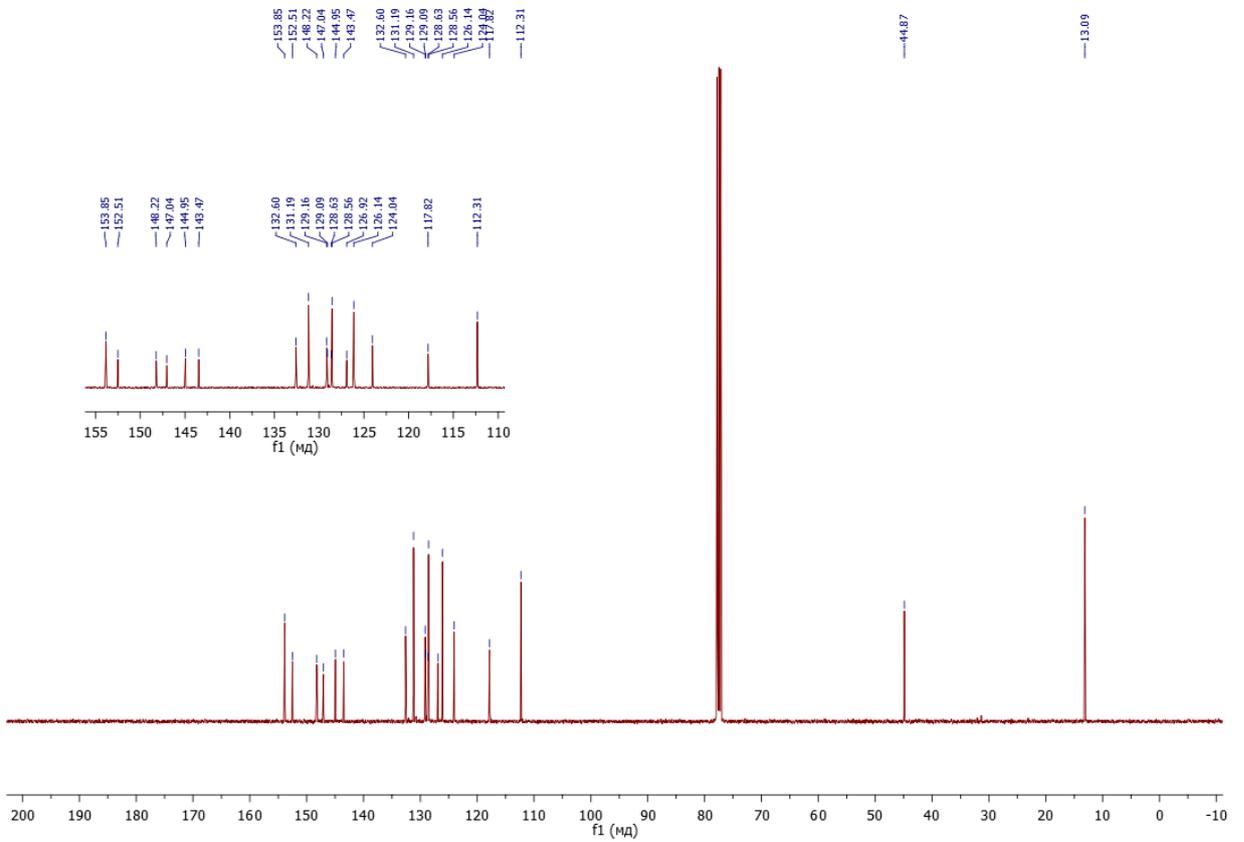
Figure S12. ^1H (a), ^{13}C (b) NMR spectra of **4f** in DCCl_3 ; mass spectrum (c) of **4f**.



5a

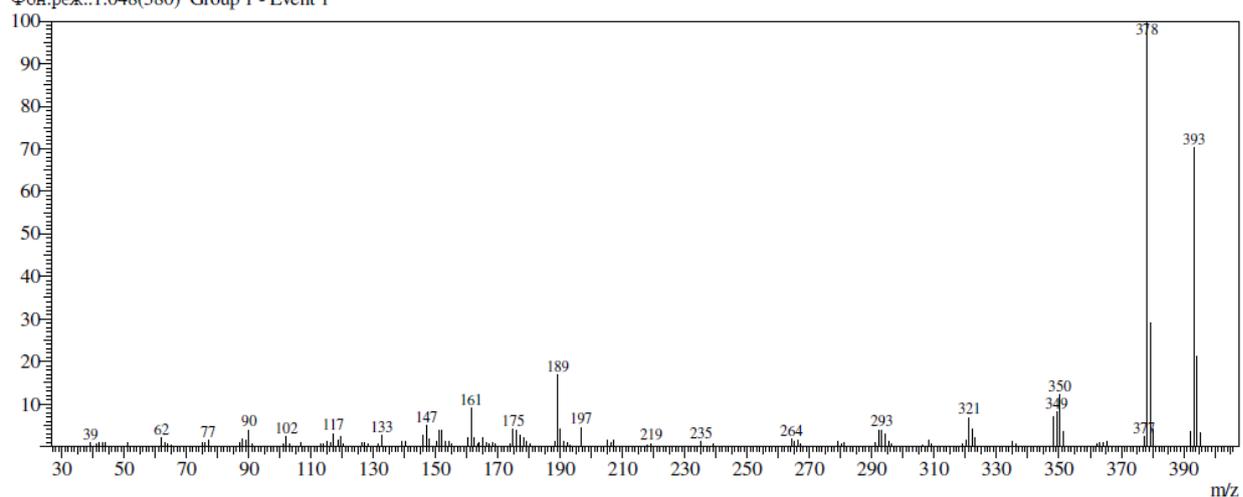


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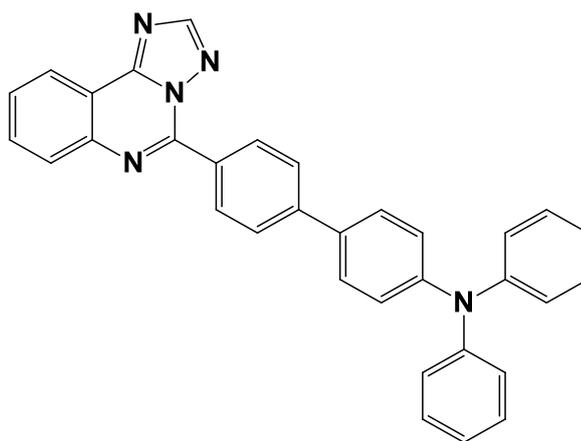
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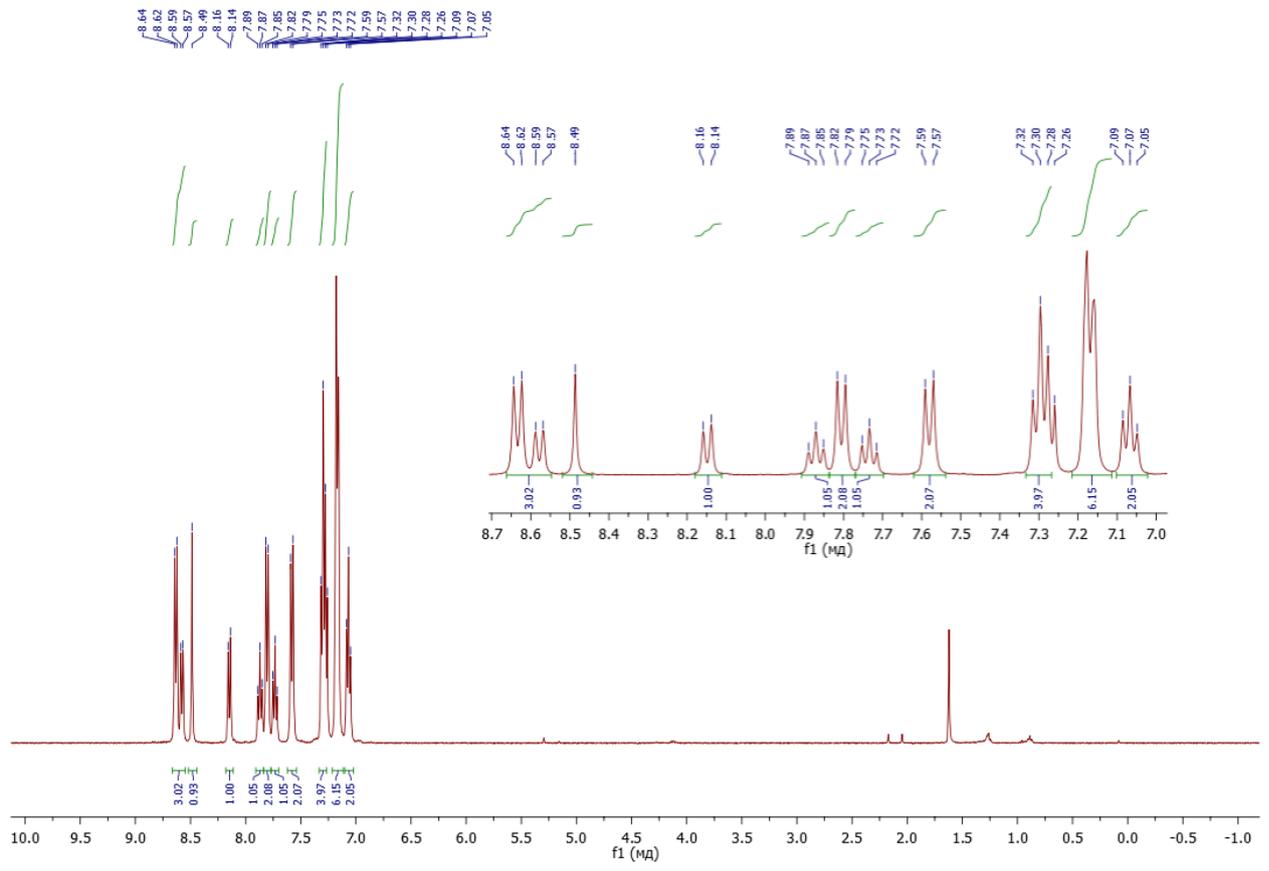


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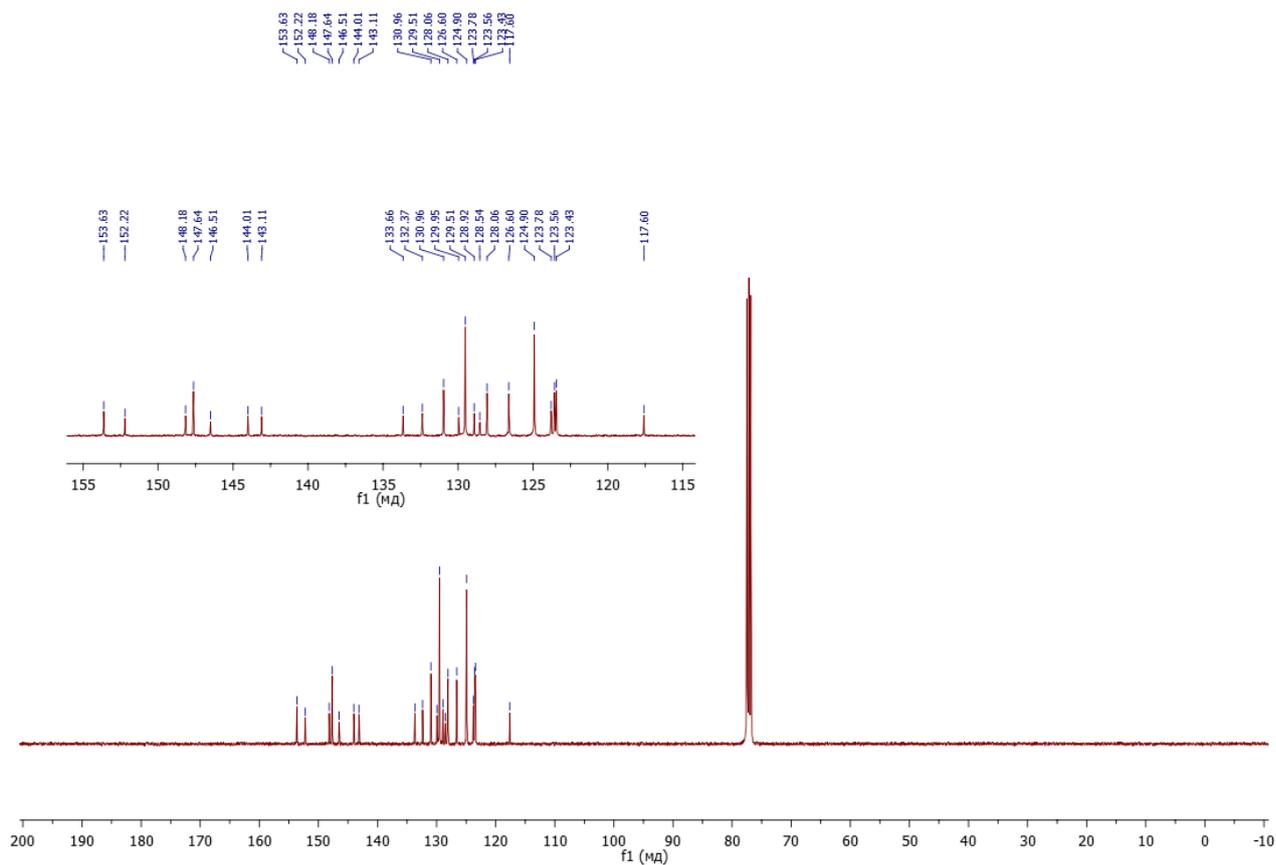
Figure S13. ^1H (a), ^{13}C (b) NMR spectra of **5a** in DCCl_3 ; mass spectrum (c) of **5a**.



5b

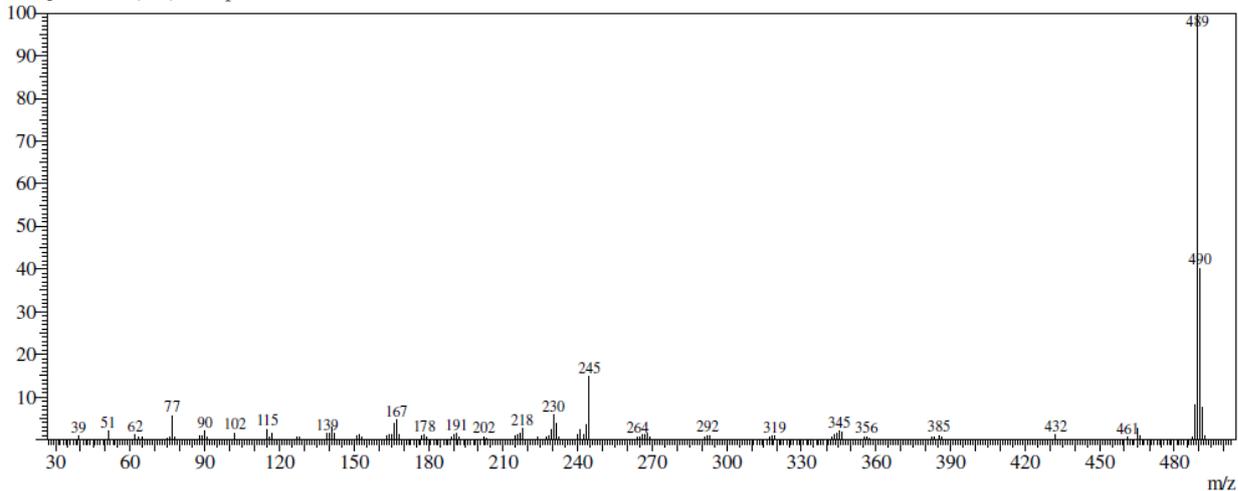


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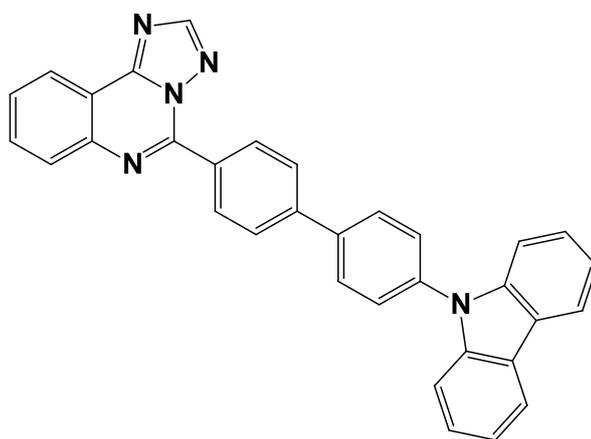
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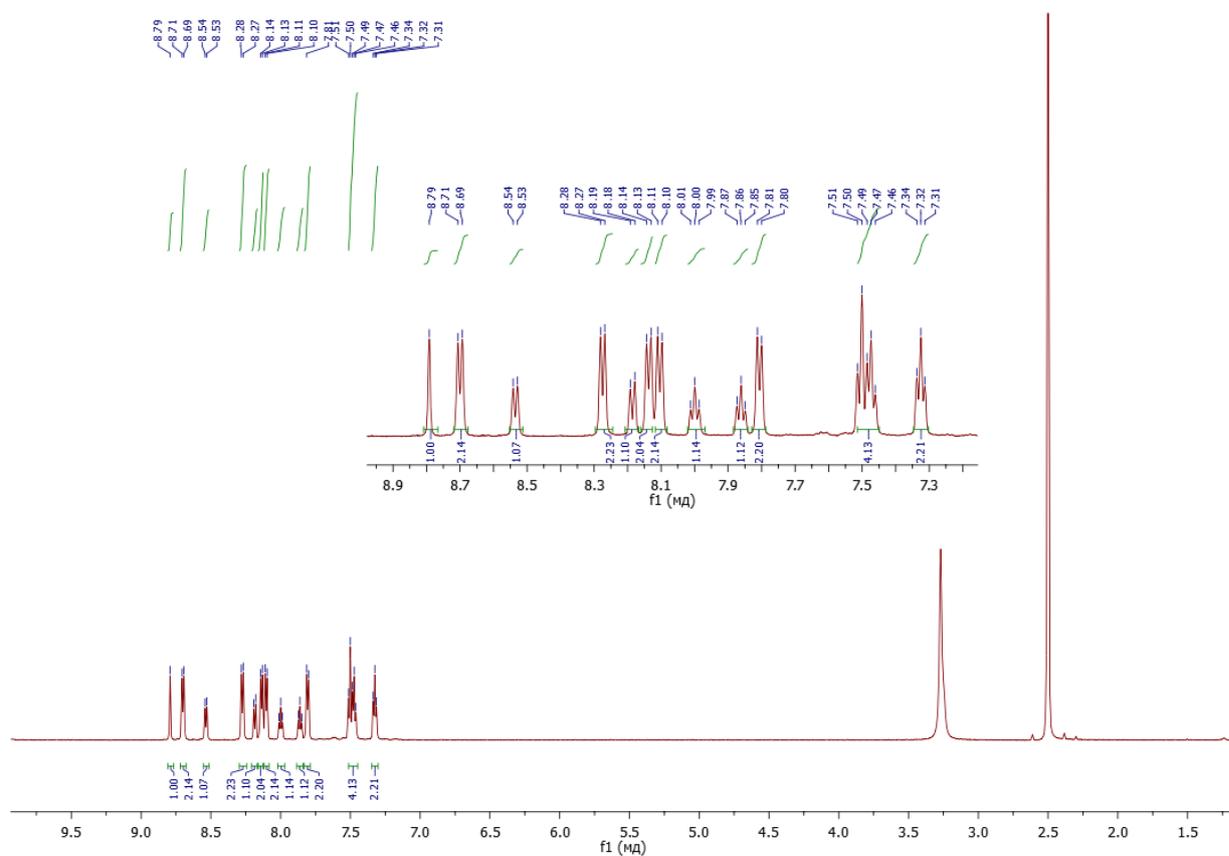


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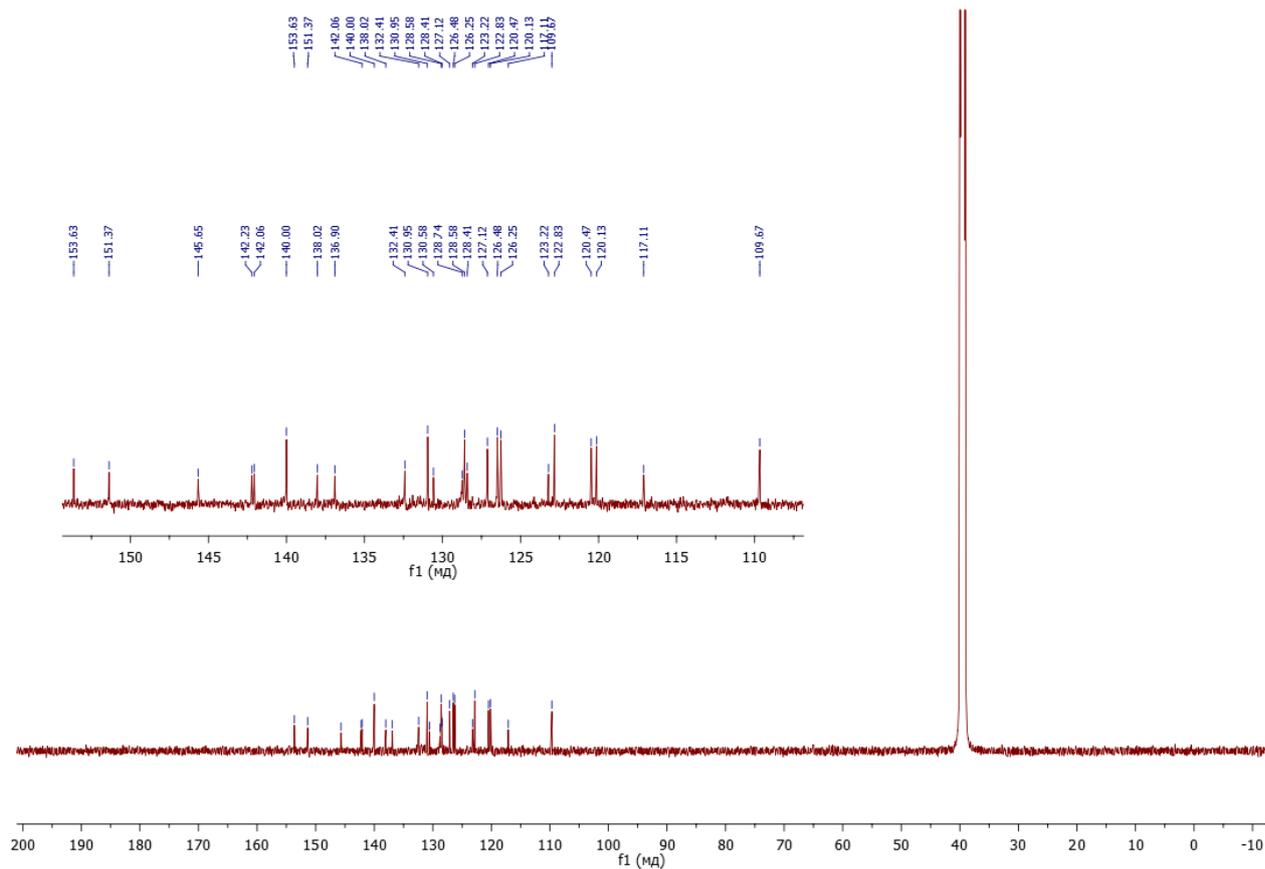
Figure S14. ^1H (a), ^{13}C (b) NMR spectra of **5b** in DCCl_3 ; mass spectrum (c) of **5b**.



5c



a



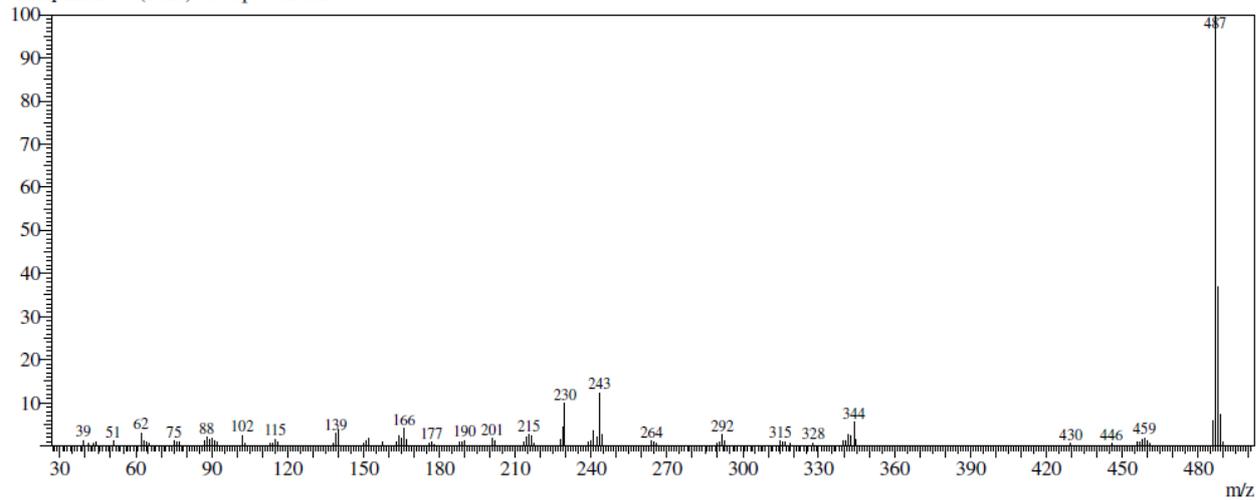
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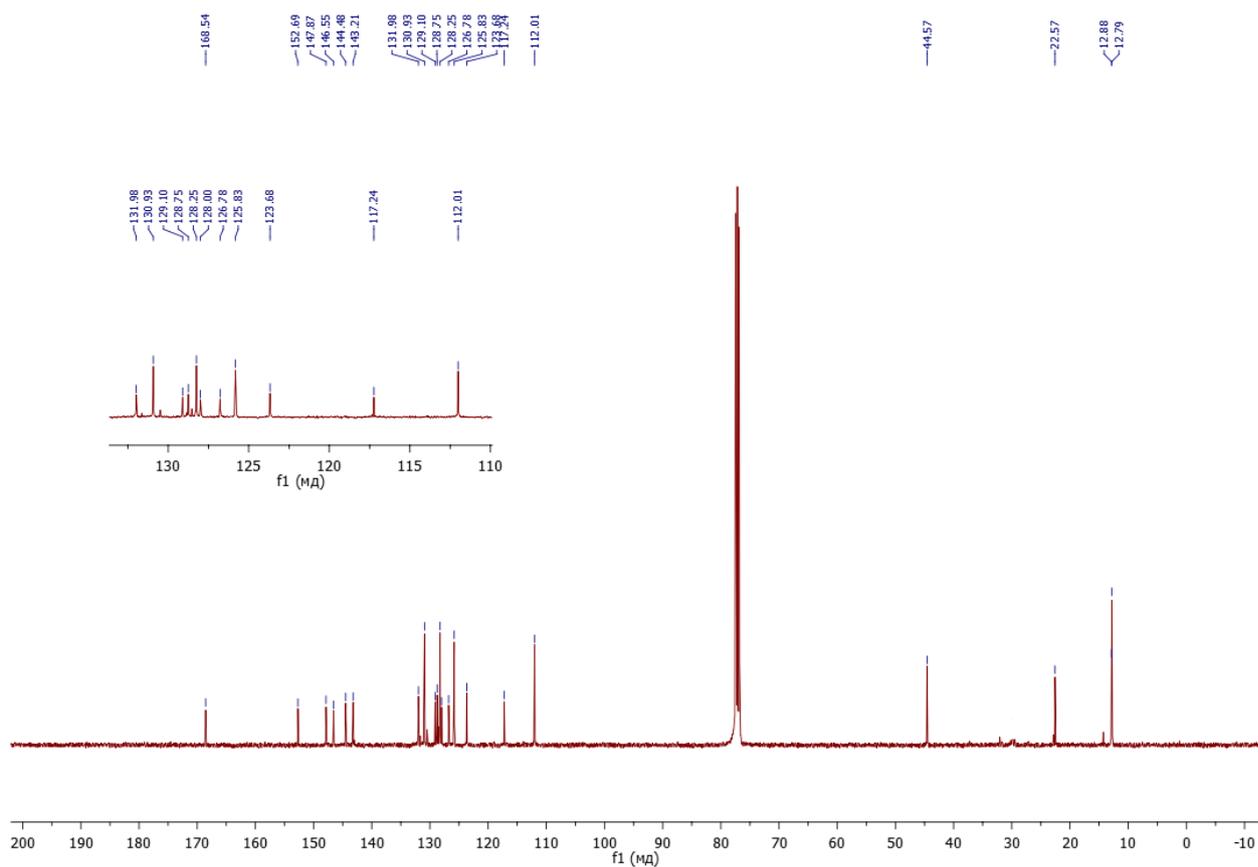
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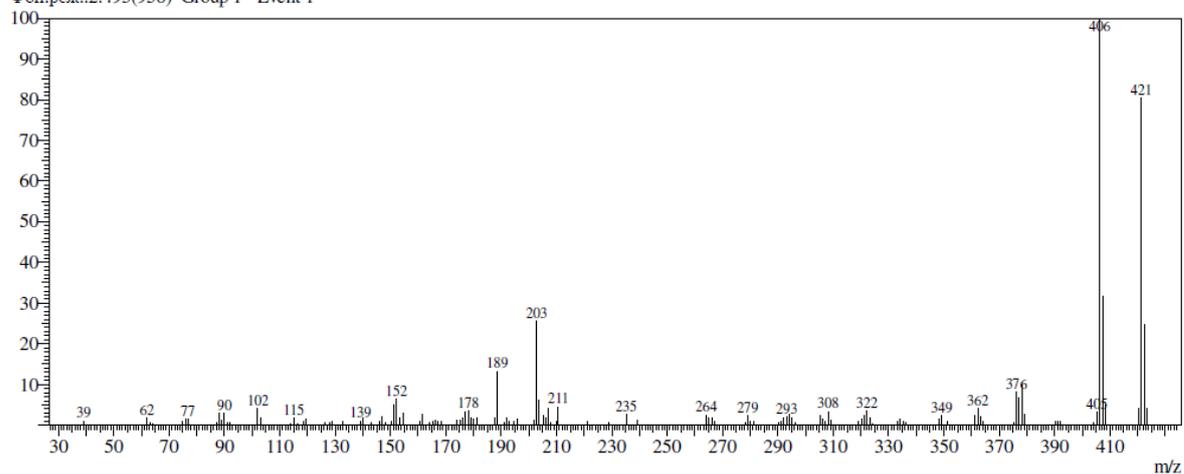
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Figure S15. ^1H (a), ^{13}C (b) NMR spectra of **5c** in DMSO-d_6 ; mass spectrum (c) of **5c**.



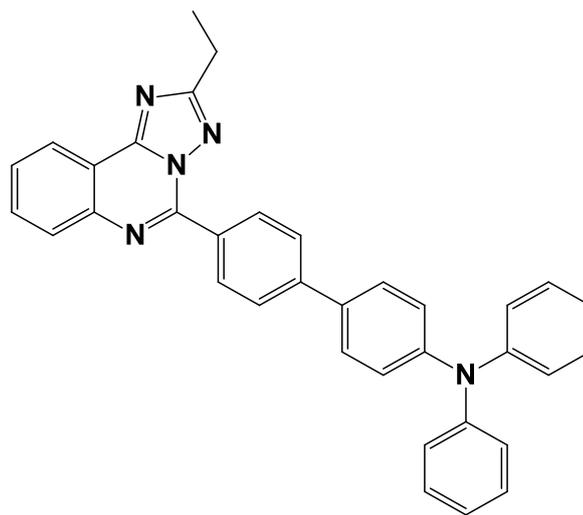
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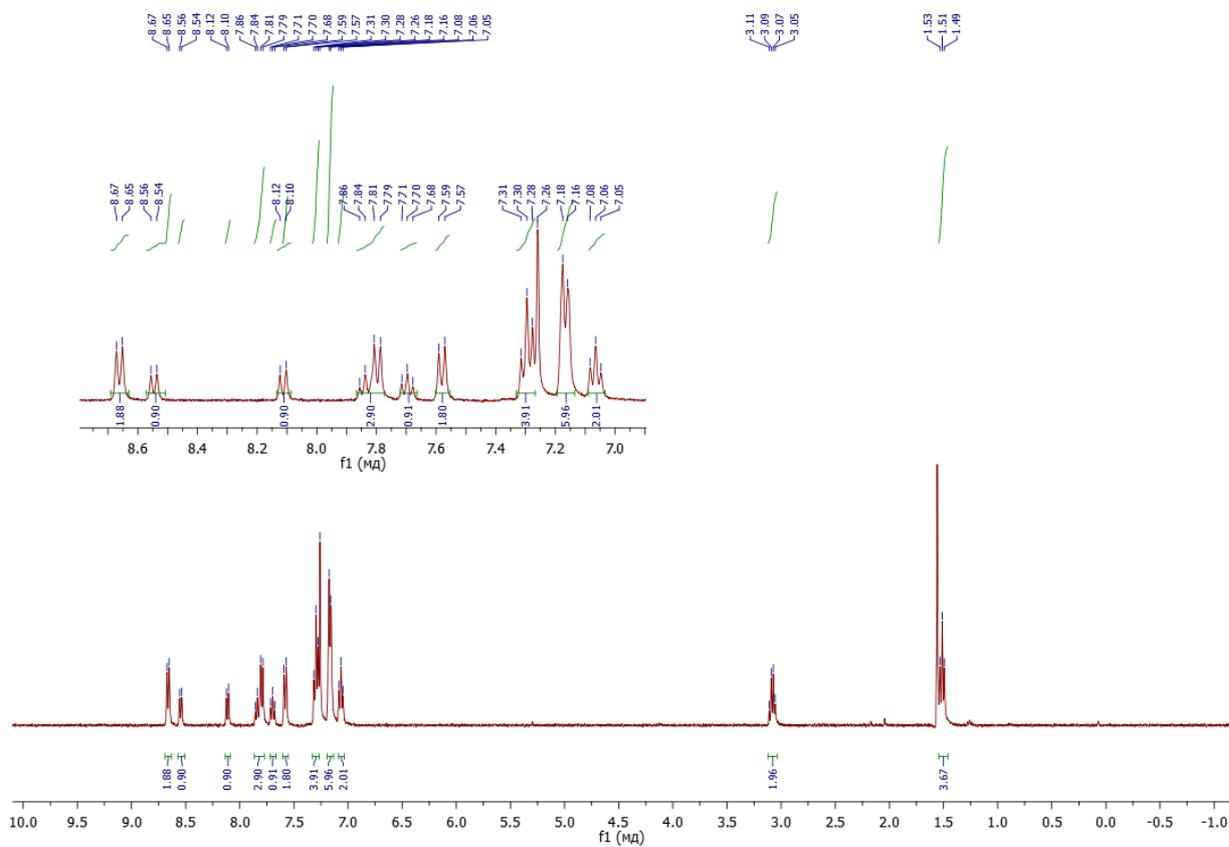


c

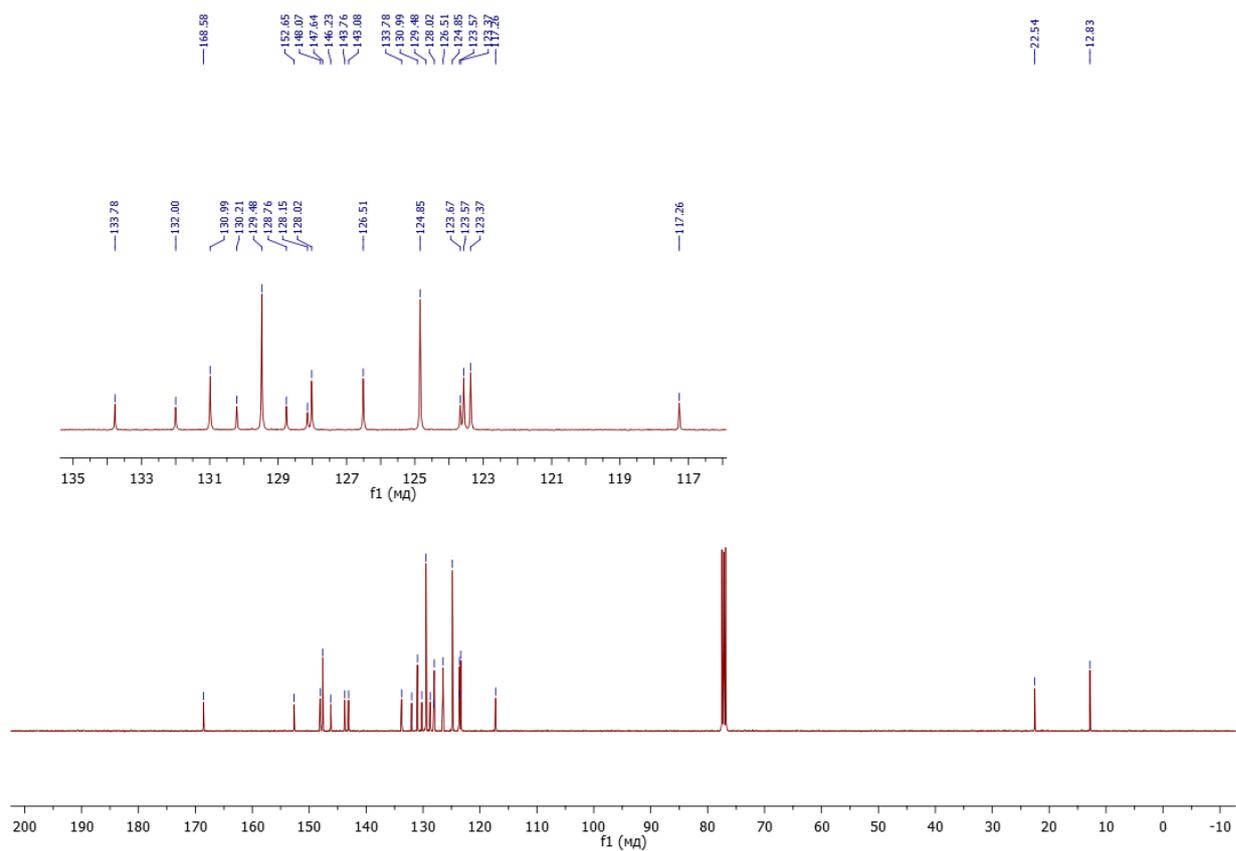
Figure S16. ^1H (a), ^{13}C (b) NMR spectra of **5d** in DCCl_3 ; mass spectrum (c) of **5d**.



5e



a



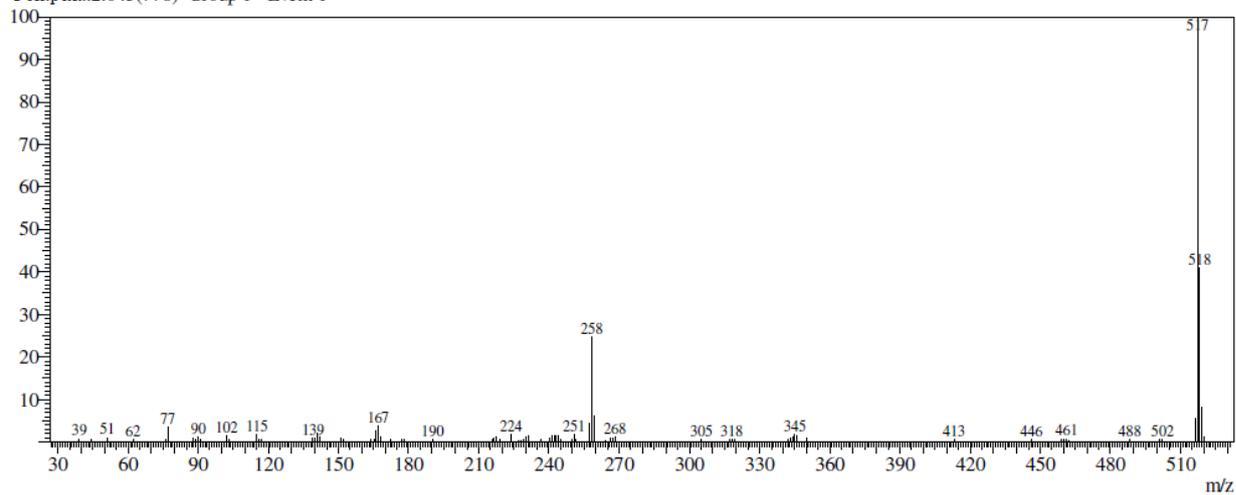
b

Line#:1 R.Time:2.907(Scan#:1124)

MassPeaks:81

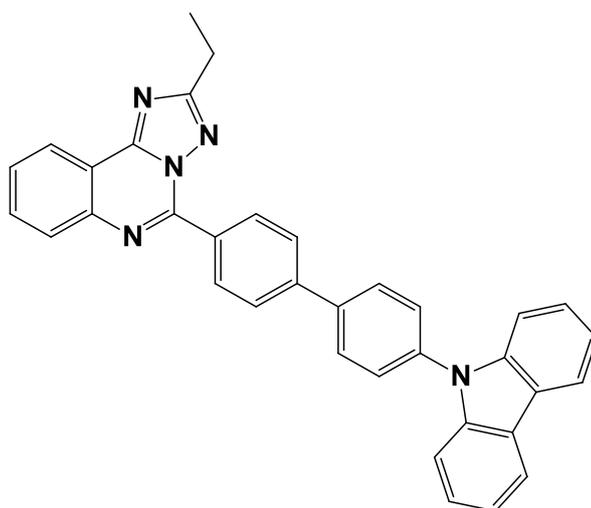
RawMode:Single 2.908(1124) BasePeak:517(5561356)

Фон.реш.:2.043(778) Group 1 - Event 1

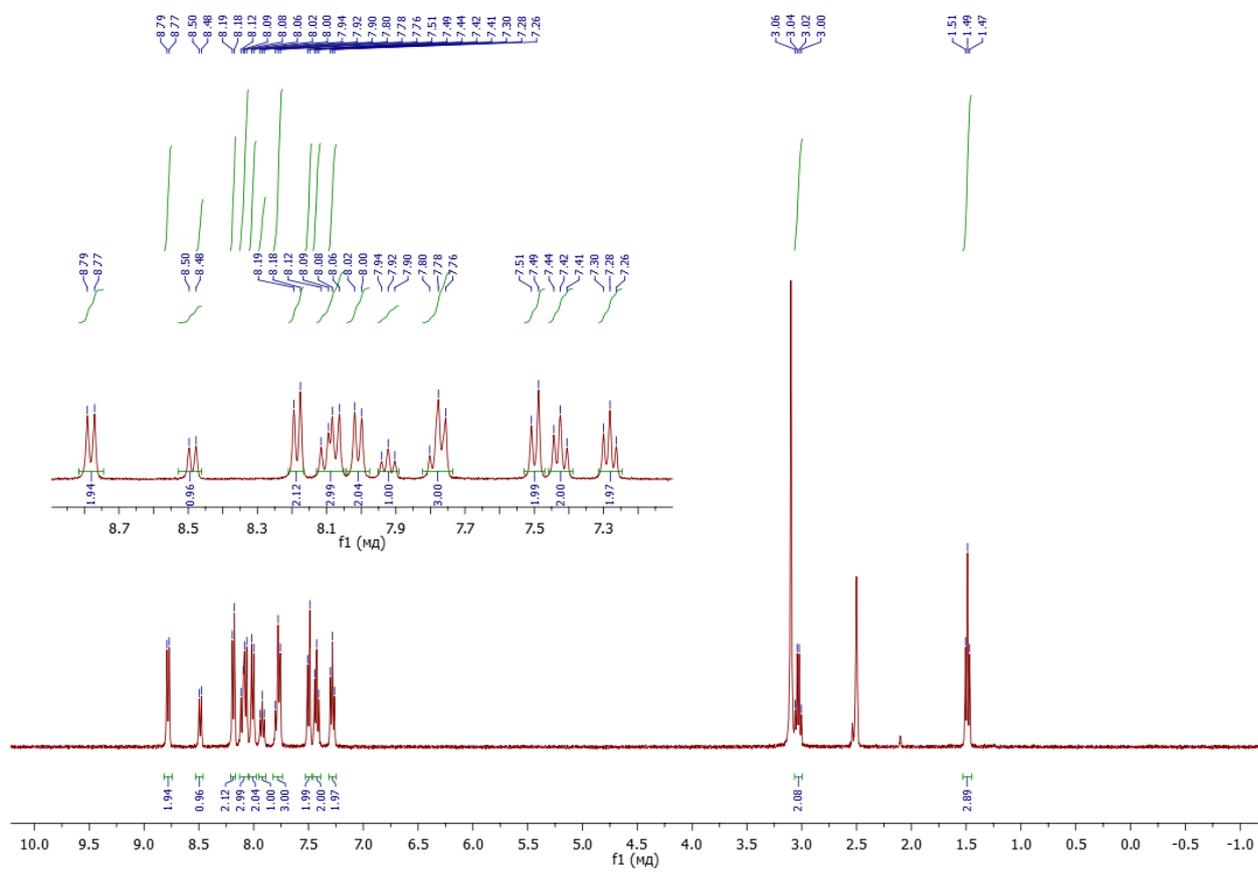


c

Figure S17. ^1H (a), ^{13}C (b) NMR spectra of **5e** in CDCl_3 ; mass spectrum (c) of **5e**.

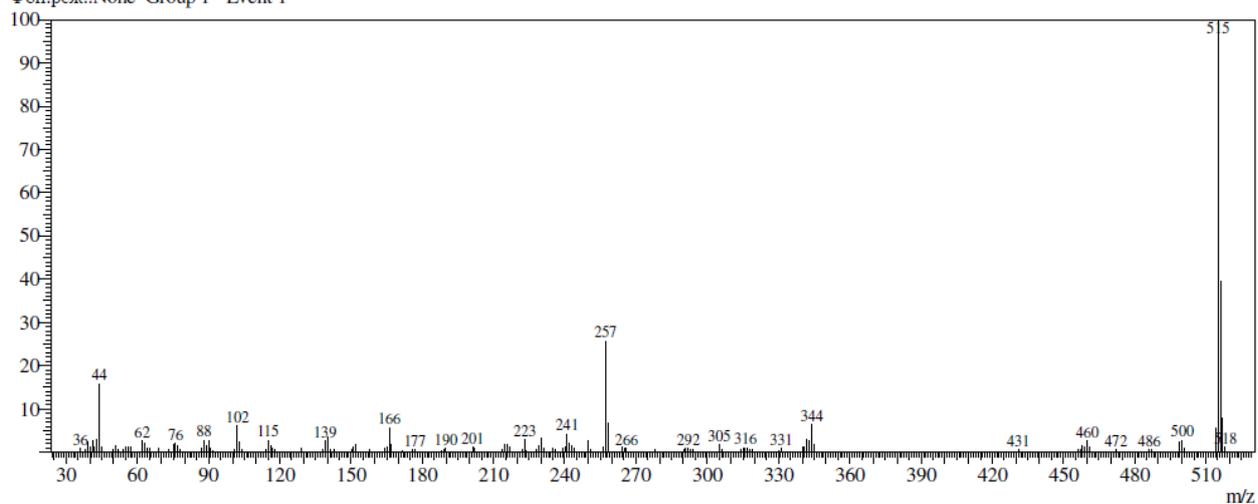


5f



a

Line#:1 R.Time:4.707(Scan#:1844)
MassPeaks:130
RawMode:Single 4.707(1844) BasePeak:515(762196)
Фон.реж.:None Group 1 - Event 1



b

Figure S18. ^1H (a) NMR spectrum of **5f** in DMSO- d_6 ; mass spectrum (b) of **5f**.

2. Crystallographic data of triazoloquinazolines

Table S1. Selected bond lengths of compound **4a**.

Bond	Bond length (Å)	Bond	Bond length (Å)
N(3) – C(2)	1.413(2)	C(23) – C(24)	1.403(3)
N(3) – C(7)	1.380(2)	N(5) – C(4)	1.294(2)
N(3) – C(4)	1.378(2)	C(21) – C(20)	1.392(3)
N(1) – C(2)	1.289(2)	C(21) – C(22)	1.380(3)
N(1) – C(13)	1.397(2)	C(16) – C(15)	1.374(3)
N(2) – C(23)	1.376(2)	C(7) – C(8)	1.435(3)
N(2) – C(26)	1.461(3)	C(20) – C(25)	1.385(3)
N(2) – C(29)	1.462(3)	C(24) – C(25)	1.385(3)
N(6) – N(5)	1.391(2)	C(13) – C(8)	1.403(3)
N(6) – C(7)	1.310(2)	C(13) – C(12)	1.398(3)
C(14) – C(2)	1.474(3)	C(8) – C(9)	1.395(3)
C(14) – C(15)	1.394(2)	C(18) – C(19)	1.379(3)
C(14) – C(19)	1.390(3)	C(12) – C(11)	1.371(3)
C(17) – C(16)	1.387(3)	C(26) – C(28)	1.481(3)
C(17) – C(20)	1.485(3)	C(29) – C(27)	1.508(3)
C(17) – C(18)	1.397(3)	C(9) – C(10)	1.371(3)
C(23) – C(22)	1.403(3)	C(11) – C(10)	1.387(3)

Table S2. Selected bond angles of compound **4a**.

Angle	(°)	Angle	(°)
C(7) – N(3) – C(2)	121.80(16)	N(6) – C(7) – N(3)	110.89(18)
C(4) – N(3) – C(2)	134.49(17)	N(6) – C(7) – C(8)	130.6(2)
C(4) – N(3) – C(7)	103.63(16)	C(21) – C(20) – C(17)	121.8(2)
C(2) – N(1) – C(13)	120.43(17)	C(25) – C(20) – C(17)	121.50(18)
C(23) – N(2) – C(26)	121.86(19)	C(25) – C(20) – C(21)	116.63(19)
C(23) – N(2) – C(29)	121.87(17)	C(21) – C(22) – C(23)	121.54(18)
C(26) – N(2) – C(29)	115.15(18)	C(16) – C(15) – C(14)	120.57(19)
C(7) – N(6) – N(5)	106.58(17)	C(25) – C(24) – C(23)	120.6(2)
C(15) – C(14) – C(2)	123.77(19)	C(24) – C(25) – C(20)	122.66(19)
C(19) – C(14) – C(2)	118.35(17)	N(1) – C(13) – C(8)	122.66(17)
C(19) – C(14) – C(15)	117.82(18)	N(1) – C(13) – C(12)	118.34(19)
N(3) – C(2) – C(14)	119.22(17)	C(12) – C(13) – C(8)	119.00(19)
N(1) – C(2) – N(3)	120.44(17)	C(13) – C(8) – C(7)	116.22(18)
N(1) – C(2) – C(14)	120.33(18)	C(9) – C(8) – C(7)	123.4(2)
C(16) – C(17) – C(20)	121.86(17)	C(9) – C(8) – C(13)	120.32(19)
C(16) – C(17) – C(18)	117.20(18)	C(19) – C(18) – C(17)	121.0(2)
C(18) – C(17) – C(20)	120.91(19)	C(18) – C(19) – C(14)	121.23(18)
N(2) – C(23) – C(22)	121.91(18)	N(5) – C(4) – N(3)	110.74(18)
N(2) – C(23) – C(24)	121.3(2)	C(11) – C(12) – C(13)	119.8(2)
C(22) – C(23) – C(24)	116.75(19)	N(2) – C(26) – C(28)	112.6(2)
C(4) – N(5) – N(6)	108.15(16)	N(2) – C(29) – C(27)	114.9(2)
C(22) – C(21) – C(20)	121.8(2)	C(10) – C(9) – C(8)	119.6(2)
C(15) – C(16) – C(17)	122.06(17)	C(12) – C(11) – C(10)	121.1(2)
N(3) – C(7) – C(8)	118.40(18)	C(9) – C(10) – C(11)	120.2(2)

Table S3. Selected bond lengths of compound **4e**.

Bond	Bond length (Å)	Bond	Bond length (Å)
N(5) – C(5)	1.387(4)	C(24) – C(25)	1.382(4)
N(5) – C(13)	1.401(4)	C(27) – C(32)	1.384(5)
N(5) – C(2)	1.394(4)	C(27) – C(28)	1.378(5)
N(12) – C(13)	1.287(4)	C(17) – C(16)	1.371(4)
N(12) – C(11)	1.400(4)	C(2) – C(1)	1.481(5)
N(2) – C(24)	1.415(4)	C(11) – C(96)	1.395(5)
N(2) – C(27)	1.411(4)	C(11) – C(10)	1.391(5)
N(2) – C(38)	1.416(4)	C(26) – C(25)	1.386(4)
N(3) – N(4)	1.398(4)	C(38) – C(33)	1.386(4)
N(3) – C(2)	1.315(4)	C(38) – C(37)	1.368(5)
N(4) – C(5)	1.307(4)	C(6) – C(7)	1.402(4)
C(21) – C(18)	1.484(4)	C(1) – C(14)	1.493(5)
C(21) – C(22)	1.391(4)	C(32) – C(31)	1.384(5)
C(21) – C(26)	1.376(4)	C(10) – C(9)	1.376(5)
C(18) – C(19)	1.389(4)	C(7) – C(8)	1.356(5)
C(18) – C(17)	1.395(4)	C(8) – C(9)	1.368(6)
C(22) – C(23)	1.383(4)	C(33) – C(34)	1.400(5)
C(15) – C(13)	1.482(4)	C(34) – C(35)	1.349(6)
C(15) – C(20)	1.384(4)	C(28) – C(29)	1.382(5)
C(15) – C(16)	1.373(4)	C(30) – C(31)	1.328(6)
C(5) – C(6)	1.422(5)	C(30) – C(29)	1.354(7)
C(19) – C(20)	1.374(4)	C(37) – C(36)	1.378(5)
C(24) – C(23)	1.384(4)	C(35) – C(36)	1.360(6)

Table S4. Selected bond angles of compound **2e**.

Angle	(°)	Angle	(°)
C(5) – N(5) – C(13)	121.0(3)	C(16) – C(17) – C(18)	121.1(3)
C(5) – N(5) – C(2)	104.6(3)	N(5) – C(2) – C(1)	127.0(3)
C(2) – N(5) – C(13)	134.4(3)	N(3) – C(2) – N(5)	109.0(3)
C(13) – N(12) – C(11)	119.4(3)	N(3) – C(2) – C(1)	123.9(3)
C(24) – N(2) – C(38)	119.7(2)	C(6) – C(11) – N(12)	122.5(3)
C(27) – N(2) – C(24)	119.2(2)	C(10) – C(11) – N(12)	118.0(3)
C(27) – N(2) – C(38)	121.1(3)	C(10) – C(11) – C(6)	119.5(3)
C(2) – N(3) – N(4)	108.6(3)	C(21) – C(26) – C(25)	122.0(3)
C(5) – N(4) – N(3)	107.0(3)	C(33) – C(38) – N(2)	121.1(3)
C(22) – C(21) – C(18)	121.1(3)	C(37) – C(38) – N(2)	120.8(3)
C(26) – C(21) – C(18)	122.3(3)	C(37) – C(38) – C(33)	118.1(3)
C(26) – C(21) – C(22)	116.5(3)	C(22) – C(23) – C(24)	120.0(3)
C(19) – C(18) – C(21)	121.7(3)	C(17) – C(16) – C(15)	121.4(3)
C(19) – C(18) – C(17)	116.8(3)	C(11) – C(6) – C(5)	117.0(3)
C(17) – C(18) – C(21)	121.4(3)	C(11) – C(6) – C(7)	119.4(3)
C(23) – C(22) – C(21)	122.4(3)	C(7) – C(6) – C(5)	123.5(3)
C(20) – C(15) – C(13)	121.8(3)	C(24) – C(25) – C(26)	120.7(3)
C(16) – C(15) – C(13)	119.9(3)	C(2) – C(1) – C(14)	113.1(3)
C(16) – C(15) – C(20)	118.3(3)	C(31) – C(32) – C(27)	119.5(4)
N(5) – C(5) – C(6)	118.1(3)	C(9) – C(10) – C(11)	119.3(4)
N(4) – C(5) – N(5)	110.7(3)	C(8) – C(7) – C(6)	120.0(4)
N(4) – C(5) – C(6)	131.0(3)	C(7) – C(8) – C(9)	120.6(4)

C(20) – C(19) – C(18)	121.8(3)	C(38) – C(33) – C(34)	120.0(3)
N(5) – C(13) – C(15)	117.9(3)	C(35) – C(34) – C(33)	120.6(4)
N(12) – C(13) – N(5)	121.7(3)	C(27) – C(28) – C(29)	119.9(4)
N(12) – C(13) – C(15)	120.4(3)	C(8) – C(9) – C(10)	121.1(4)
C(23) – C(24) – N(2)	120.0(3)	C(31) – C(30) – C(29)	120.4(4)
C(25) – C(24) – N(2)	121.6(3)	C(30) – C(31) – C(32)	121.2(4)
C(25) – C(24) – C(23)	118.3(3)	C(38) – C(37) – C(36)	120.8(4)
C(19) – C(20) – C(15)	120.4(3)	C(34) – C(35) – C(36)	119.3(4)
C(32) – C(27) – N(2)	119.7(3)	C(35) – C(36) – C(37)	121.1(4)
C(28) – C(27) – N(2)	121.6(3)	C(30) – C(29) – C(28)	120.4(4)
C(28) – C(27) – C(32)	118.6(3)		

Table S5. Selected bond lengths of compound **5d**.

Bond	Bond length (Å)	Bond	Bond length (Å)
N(3) – N(4)	1.376(2)	N(2) – C(25)	1.373(3)
N(3) – C(7)	1.374(2)	N(2) – C(1)	1.438(3)
N(3) – C(2)	1.395(2)	N(2) – C(4)	1.607(6)
N(1) – C(2)	1.303(2)	C(17) – C(18)	1.374(3)
N(1) – C(13)	1.387(2)	C(8) – C(13)	1.405(3)
N(6) – C(7)	1.324(2)	C(8) – C(9)	1.397(3)
N(6) – C(5)	1.364(3)	C(13) – C(12)	1.401(3)
N(4) – C(5)	1.321(2)	C(5) – C(14)	1.495(3)
C(16) – C(2)	1.472(3)	C(27) – C(26)	1.374(3)
C(16) – C(21)	1.392(3)	C(9) – C(10)	1.369(3)
C(16) – C(17)	1.397(3)	C(25) – C(24)	1.402(3)
C(19) – C(20)	1.395(2)	C(25) – C(26)	1.402(3)
C(19) – C(22)	1.478(3)	C(24) – C(23)	1.376(3)
C(19) – C(18)	1.403(3)	C(10) – C(11)	1.396(3)
C(20) – C(21)	1.375(2)	C(11) – C(12)	1.365(3)
C(7) – C(8)	1.428(3)	C(14) – C(15)	1.490(4)
C(22) – C(27)	1.391(3)	C(1) – C(3)	1.499(4)
C(22) – C(23)	1.391(3)	C(4) – C(6)	1.508(7)

Table S6. Selected bond angles of compound **5d**.

Angle	(°)	Angle	(°)
N(4) – N(3) – C(2)	127.16(15)	C(18) – C(17) – C(16)	121.48(19)
C(7) – N(3) – N(4)	109.48(15)	C(13) – C(8) – C(7)	115.61(17)
C(7) – N(3) – C(2)	123.20(16)	C(9) – C(8) – C(7)	124.08(18)
C(2) – N(1) – C(13)	120.09(17)	C(9) – C(8) – C(13)	120.24(18)
C(7) – N(6) – C(5)	103.21(16)	C(17) – C(18) – C(19)	121.52(18)
C(5) – N(4) – N(3)	101.93(15)	N(1) – C(13) – C(8)	123.32(18)
C(21) – C(16) – C(2)	124.04(17)	N(1) – C(13) – C(12)	118.26(18)
C(21) – C(16) – C(17)	117.43(17)	C(12) – C(13) – C(8)	118.42(18)
C(17) – C(16) – C(2)	118.50(18)	N(6) – C(5) – C(14)	122.57(19)
C(20) – C(19) – C(22)	121.48(17)	N(4) – C(5) – N(6)	115.84(18)
C(20) – C(19) – C(18)	116.25(17)	N(4) – C(5) – C(14)	121.6(2)
C(18) – C(19) – C(22)	122.27(17)	C(26) – C(27) – C(22)	122.63(18)
C(21) – C(20) – C(19)	122.52(18)	C(10) – C(9) – C(8)	119.8(2)
N(3) – C(7) – C(8)	118.17(17)	N(2) – C(25) – C(24)	121.84(18)
N(6) – C(7) – N(3)	109.54(17)	N(2) – C(25) – C(26)	122.30(19)

N(6) – C(7) – C(8)	132.23(18)	C(24) – C(25) – C(26)	115.86(18)
N(3) – C(2) – C(16)	120.44(17)	C(23) – C(24) – C(25)	121.36(18)
N(1) – C(2) – N(3)	119.49(17)	C(24) – C(23) – C(22)	122.97(18)
N(1) – C(2) – C(16)	120.07(17)	C(9) – C(10) – C(11)	120.4(2)
C(27) – C(22) – C(19)	121.93(17)	C(27) – C(26) – C(25)	121.77(19)
C(27) – C(22) – C(23)	115.40(17)	C(12) – C(11) – C(10)	120.2(2)
C(23) – C(22) – C(19)	122.66(17)	C(15) – C(14) – C(5)	115.4(2)
C(25) – N(2) – C(1)	121.96(19)	C(11) – C(12) – C(13)	120.9(2)
C(25) – N(2) – C(4)	117.6(2)	N(2) – C(1) – C(3)	114.0(2)
C(1) – N(2) – C(4)	116.8(2)	C(6) – C(4) – N(2)	105.8(5)
C(20) – C(21) – C(16)	120.75(17)		

Table S7. Selected bond lengths of compound **5e**.

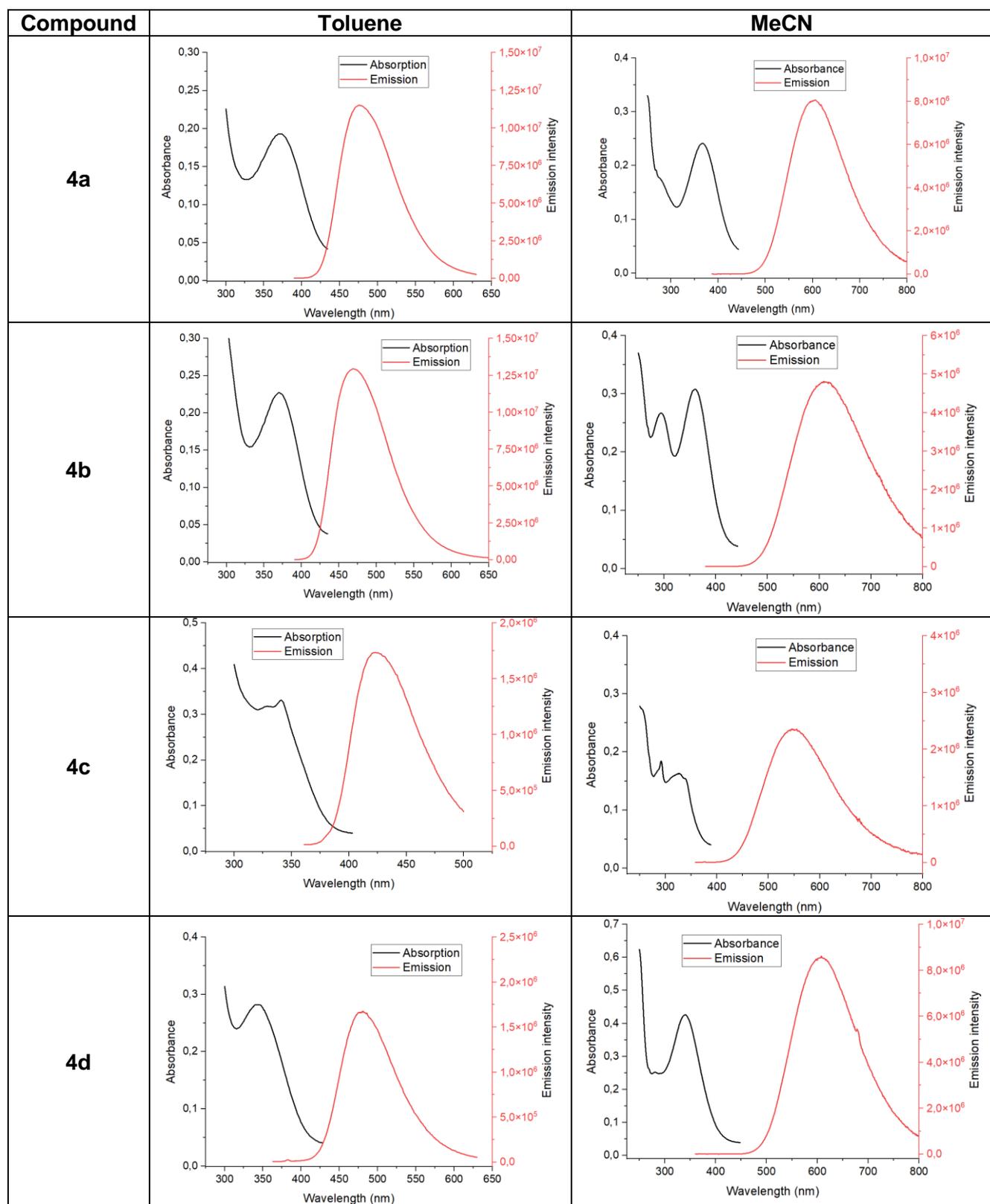
Bond	Bond length (Å)	Bond	Bond length (Å)
C(1) – C(2)	1.480(6)	C(15) – C(16)	1.372(3)
C(1) – C(3)	1.484(3)	C(16) – C(17)	1.395(3)
C(1) – C(4)	1.560(17)	C(17) – C(18)	1.391(3)
N(1) – N(2)	1.371(2)	C(17) – C(20)	1.476(3)
N(1) – C(5)	1.362(3)	C(18) – C(19)	1.384(3)
N(1) – C(13)	1.387(3)	C(20) – C(21)	1.387(3)
N(2) – C(3)	1.322(3)	C(20) – C(25)	1.387(3)
C(3) – N(4)	1.369(3)	C(21) – C(22)	1.375(3)
N(3) – C(23)	1.409(3)	C(22) – C(23)	1.384(3)
N(3) – C(26)	1.419(3)	C(23) – C(24)	1.387(3)
N(3) – C(32)	1.425(3)	C(24) – C(25)	1.374(3)
N(4) – C(5)	1.323(3)	C(26) – C(27)	1.384(4)
C(5) – C(6)	1.418(3)	C(26) – C(31)	1.381(4)
C(6) – C(7)	1.397(3)	C(27) – C(28)	1.376(4)
C(6) – C(11)	1.401(3)	C(28) – C(29)	1.367(5)
C(7) – C(8)	1.366(4)	C(29) – C(30)	1.376(5)
C(8) – C(9)	1.390(4)	C(30) – C(31)	1.369(4)
C(9) – C(10)	1.362(4)	C(32) – C(33)	1.378(3)
C(10) – C(11)	1.404(3)	C(32) – C(37)	1.371(3)
C(11) – N(12)	1.383(3)	C(33) – C(34)	1.379(4)
N(12) – C(13)	1.293(3)	C(34) – C(35)	1.365(4)
C(13) – C(14)	1.469(3)	C(35) – C(36)	1.360(4)
C(14) – C(15)	1.386(3)	C(36) – C(37)	1.374(4)

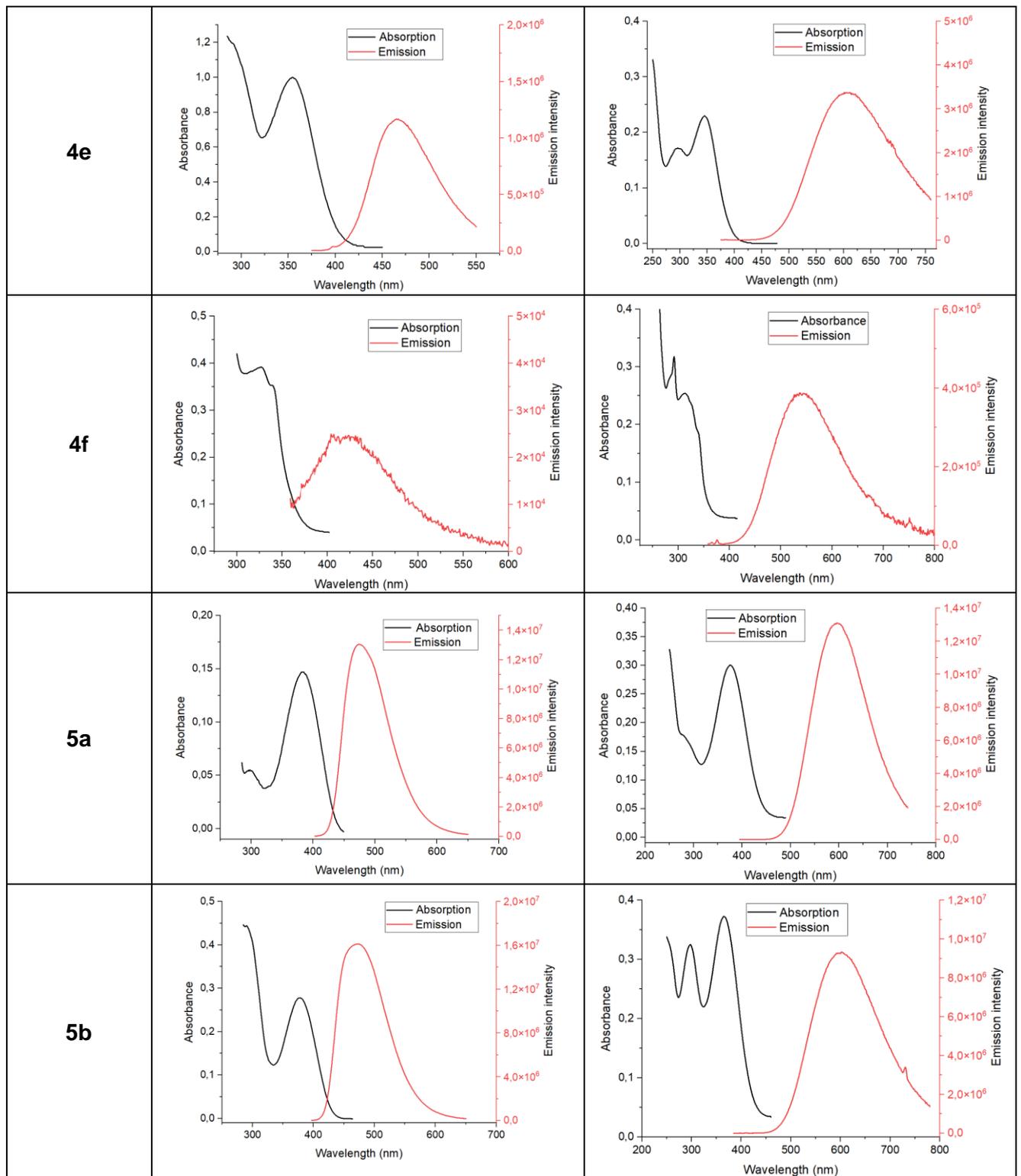
Table S8. Selected bond angles of compound **5d**.

Angle	(°)	Angle	(°)
C(2) – C(1) – C(3)	111.6(3)	C(16) – C(15) – C(14)	121.5(2)
C(3) – C(1) – C(4)	111.4(8)	C(15) – C(16) – C(17)	120.7(2)
N(2) – N(1) – C(13)	127.13(19)	C(16) – C(17) – C(20)	120.6(2)
C(5) – N(1) – N(2)	109.72(18)	C(18) – C(17) – C(16)	117.4(2)
C(5) – N(1) – C(13)	123.07(18)	C(18) – C(17) – C(20)	122.0(2)
C(3) – N(2) – N(1)	101.91(19)	C(19) – C(18) – C(17)	121.8(2)
N(2) – C(3) – C(1)	121.8(2)	C(14) – C(19) – C(18)	120.1(2)
N(2) – C(3) – N(4)	115.6(2)	C(21) – C(20) – C(17)	120.66(19)
N(4) – C(3) – C(1)	122.6(2)	C(21) – C(20) – C(25)	116.9(2)
C(23) – N(3) – C(26)	121.25(19)	C(25) – C(20) – C(17)	122.4(2)

C(23) – N(3) – C(32)	118.4(2)	C(22) – C(21) – C(20)	121.8(2)
C(26) – N(3) – C(32)	118.4(2)	C(21) – C(22) – C(23)	120.8(2)
C(5) – N(4) – C(3)	102.8(2)	C(22) – C(23) – N(3)	121.9(2)
N(1) – C(5) – C(6)	118.4(2)	C(22) – C(23) – C(24)	117.9(2)
N(4) – C(5) – N(1)	109.99(19)	C(24) – C(23) – N(3)	120.2(2)
N(4) – C(5) – C(6)	131.6(2)	C(25) – C(24) – C(23)	120.9(2)
C(7) – C(6) – C(5)	124.1(2)	C(24) – C(25) – C(20)	121.7(2)
C(7) – C(6) – C(11)	120.1(2)	C(27) – C(26) – N(3)	120.5(2)
C(11) – C(6) – C(5)	115.8(2)	C(31) – C(26) – N(3)	120.8(2)
C(8) – C(7) – C(6)	119.6(2)	C(31) – C(26) – C(27)	118.6(3)
C(7) – C(8) – C(9)	120.7(3)	C(28) – C(27) – C(26)	120.1(3)
C(10) – C(9) – C(8)	120.7(2)	C(29) – C(28) – C(27)	121.1(3)
C(9) – C(10) – C(11)	120.0(2)	C(28) – C(29) – C(30)	118.7(3)
C(6) – C(11) – C(10)	118.9(2)	C(31) – C(30) – C(29)	121.0(3)
N(12) – C(11) – C(6)	122.8(2)	C(30) – C(31) – C(26)	120.5(3)
N(12) – C(11) – C(10)	118.3(2)	C(33) – C(32) – N(3)	120.7(2)
C(13) – N(12) – C(11)	120.3(2)	C(37) – C(32) – N(3)	120.5(2)
N(1) – C(13) – C(14)	120.94(19)	C(37) – C(32) – C(33)	118.8(2)
N(12) – C(13) – N(1)	119.6(2)	C(32) – C(33) – C(34)	120.4(3)
N(12) – C(13) – C(14)	119.4(2)	C(35) – C(34) – C(33)	120.1(3)
C(15) – C(14) – C(13)	116.9(2)	C(36) – C(35) – C(34)	119.8(3)
C(19) – C(14) – C(13)	124.6(2)	C(35) – C(36) – C(37)	120.4(3)
C(19) – C(14) – C(15)	118.5(2)	C(32) – C(37) – C(36)	120.5(2)

3. Absorption and emission spectra of fluorophores in toluene and MeCN





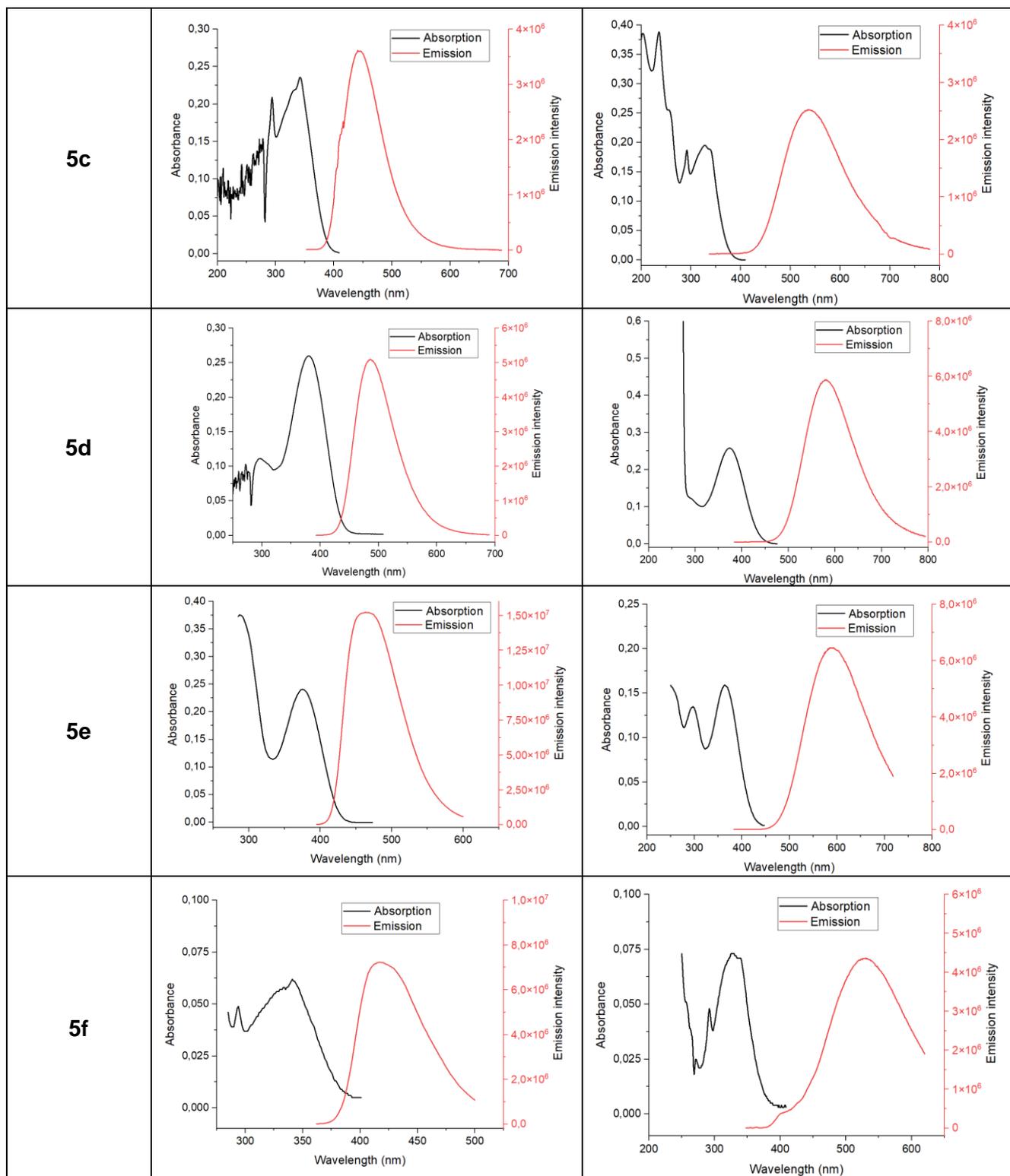


Figure S19. Absorption and emission spectra of compounds **4a-f** and **5a-f** in toluene and in MeCN

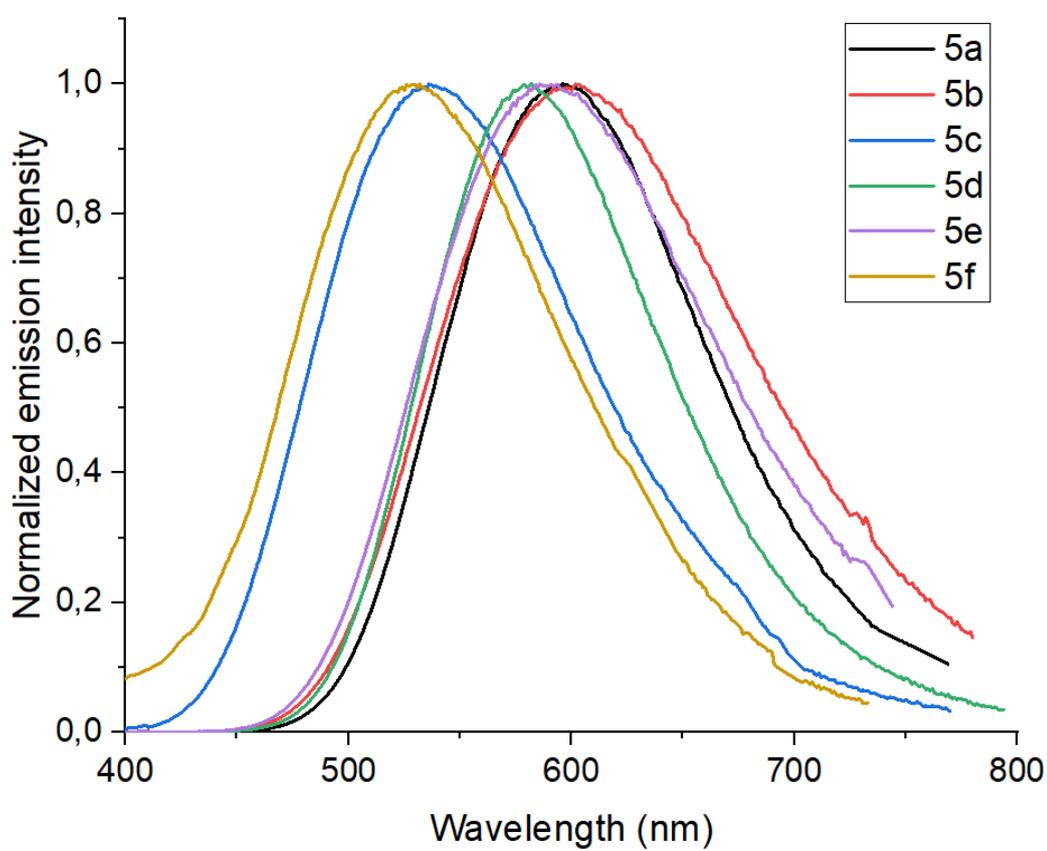
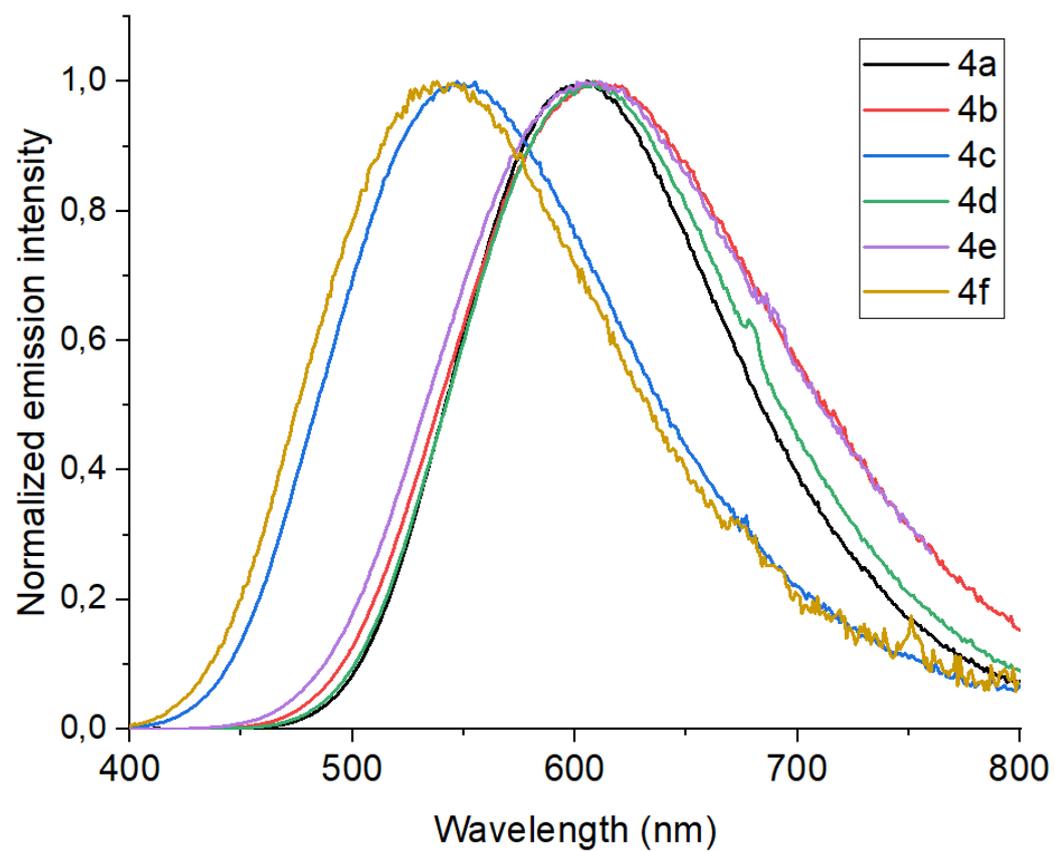


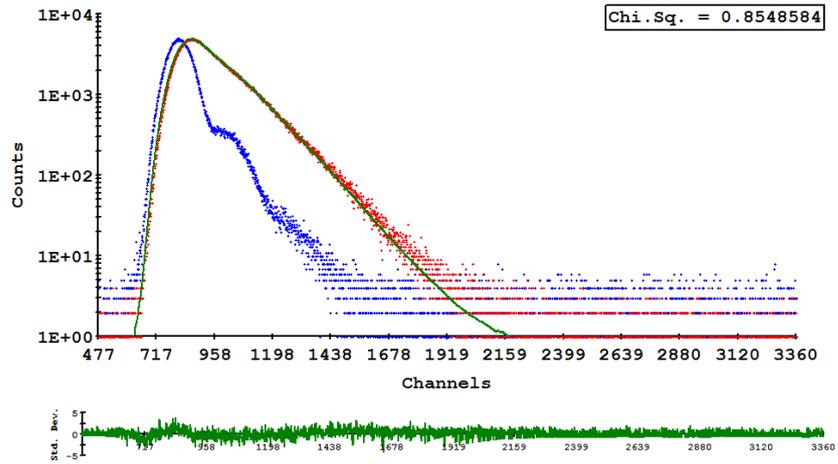
Figure S20. Combined normalized emission spectra of compounds **4a-f** and **5a-f** in MeCN.

Table S9. Detailed data of the fluorescence lifetime measurements of **4a-f** and **5a-f** (C = 2×10^{-6} M) in toluene.

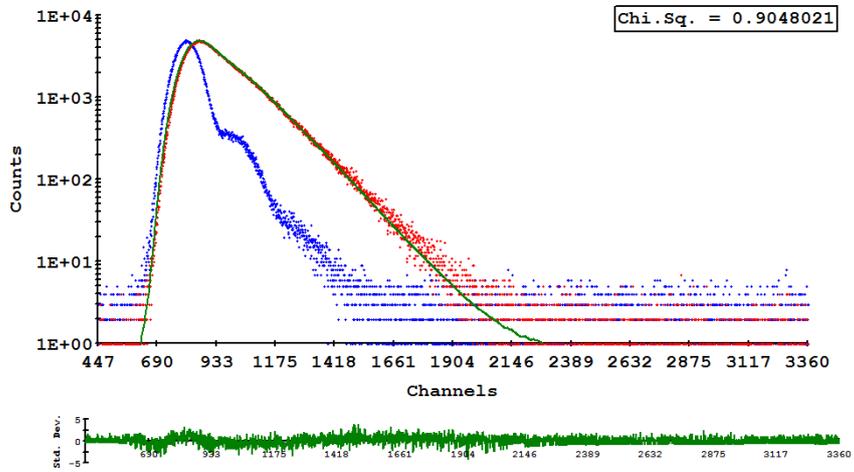
Compound	τ_1 , ns ^a	α_1 ^b	τ_2 , ns ^a	α_2 ^b	τ , ns ^a	χ^2 ^d
4a	1.737249	100			1.73	0.8548584
4b	1.852698	100			1.85	0.9048021
4c	0.136076	73.45	1.492942	26.55	0.49	1.246706
4d	0.220293	100			0.22	1.251333
4e	0.422897	17.77	1.696579	82.23	1.47	1.037248
5a	1.682252	100			1.68	0.9323888
5b	1.746369	100			1.74	0.9317798
5c	1.261517	100			1.26	0.990872
5d	1.604809	100			1.60	0.9300374
5e	1.663215	100			1.66	0.8256598
5f	1.112374	100			1.11	0.7840446

^a Decay time, ^b Fractional contribution, ^c Weighted average decay time $\tau_{av} = \sum (\tau_i \times \alpha_i)$, ^d Quality of fitting

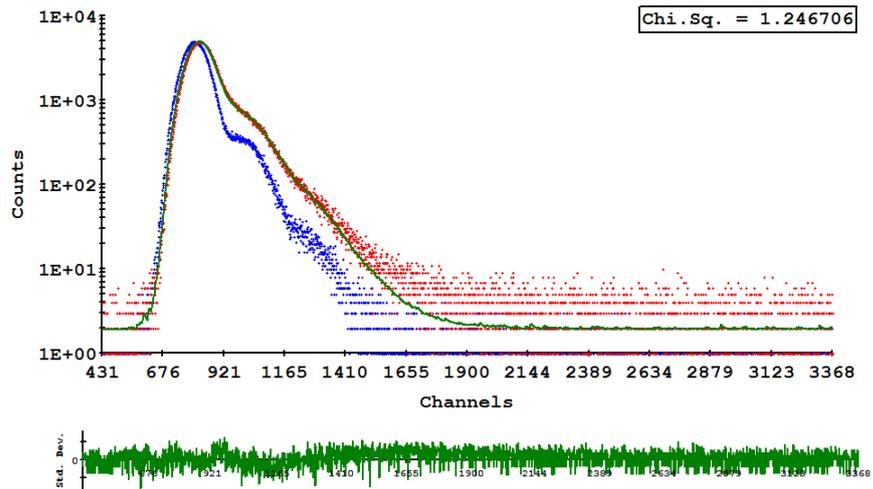
4a



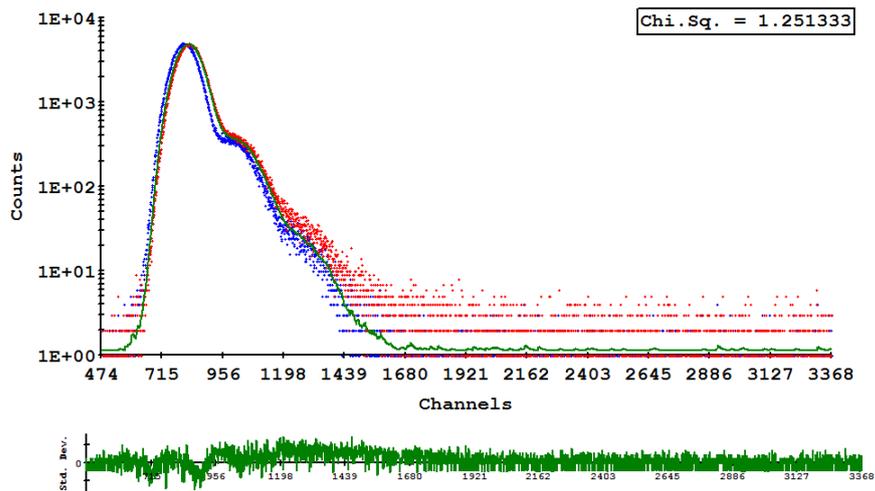
4b



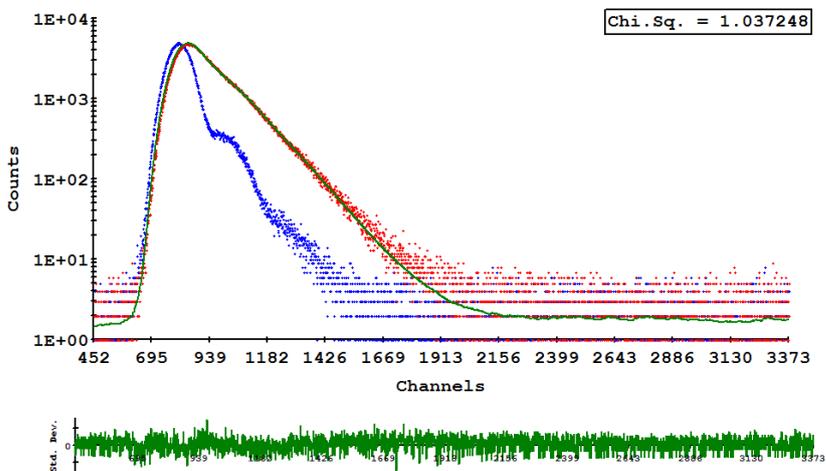
4c



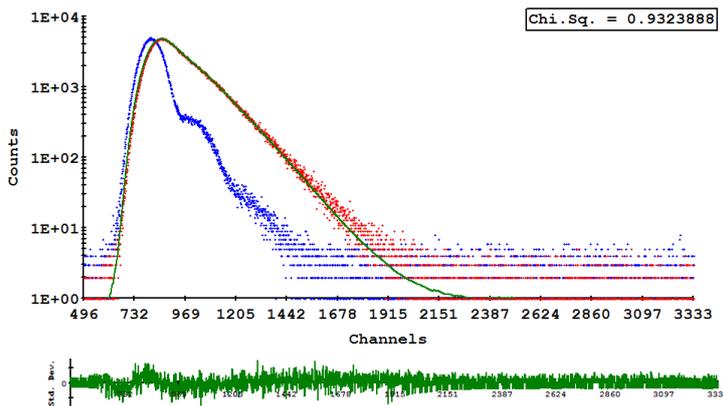
4d



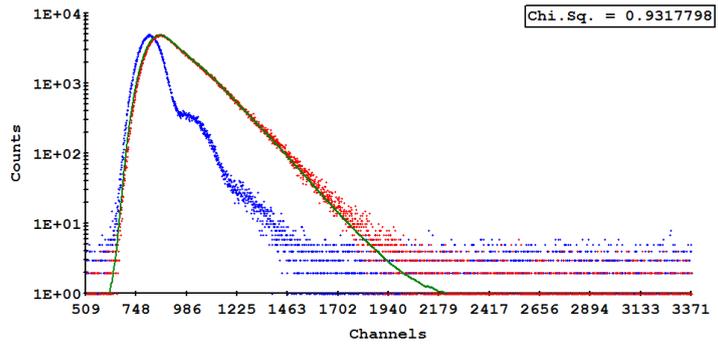
4e



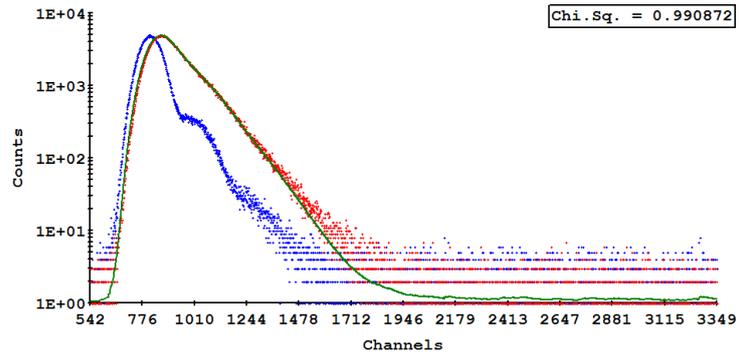
5a



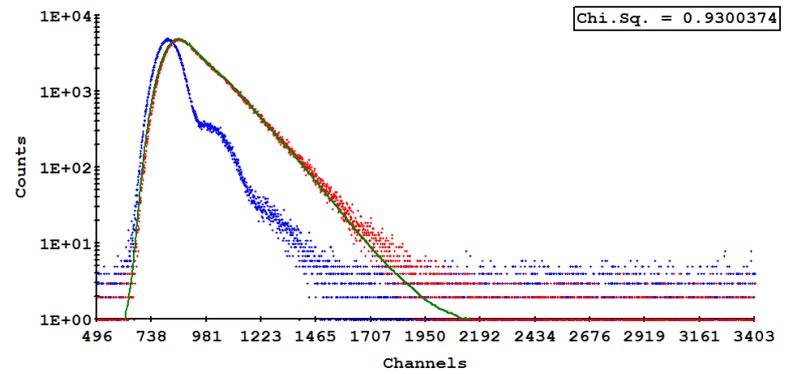
5b



5c



5d



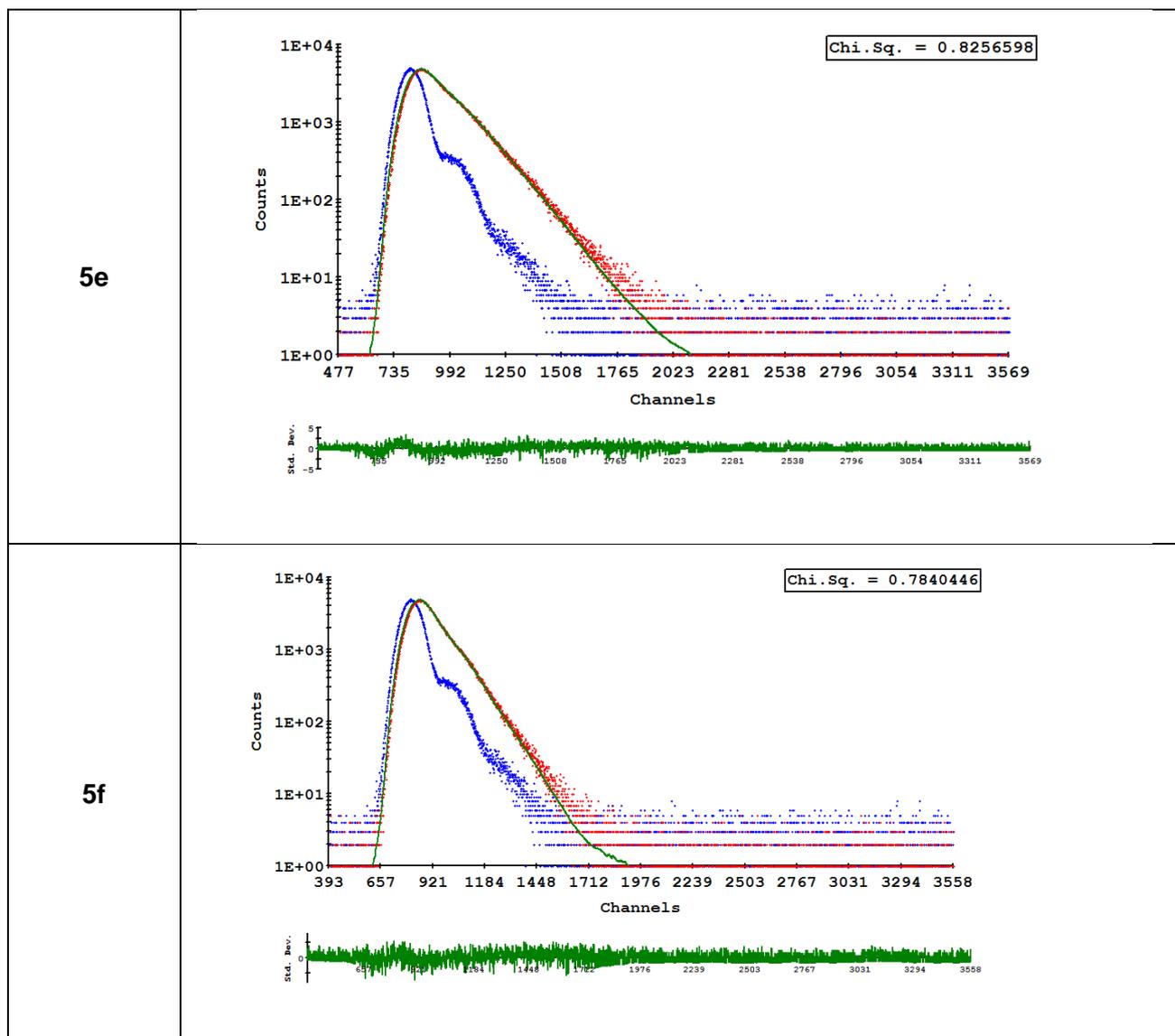
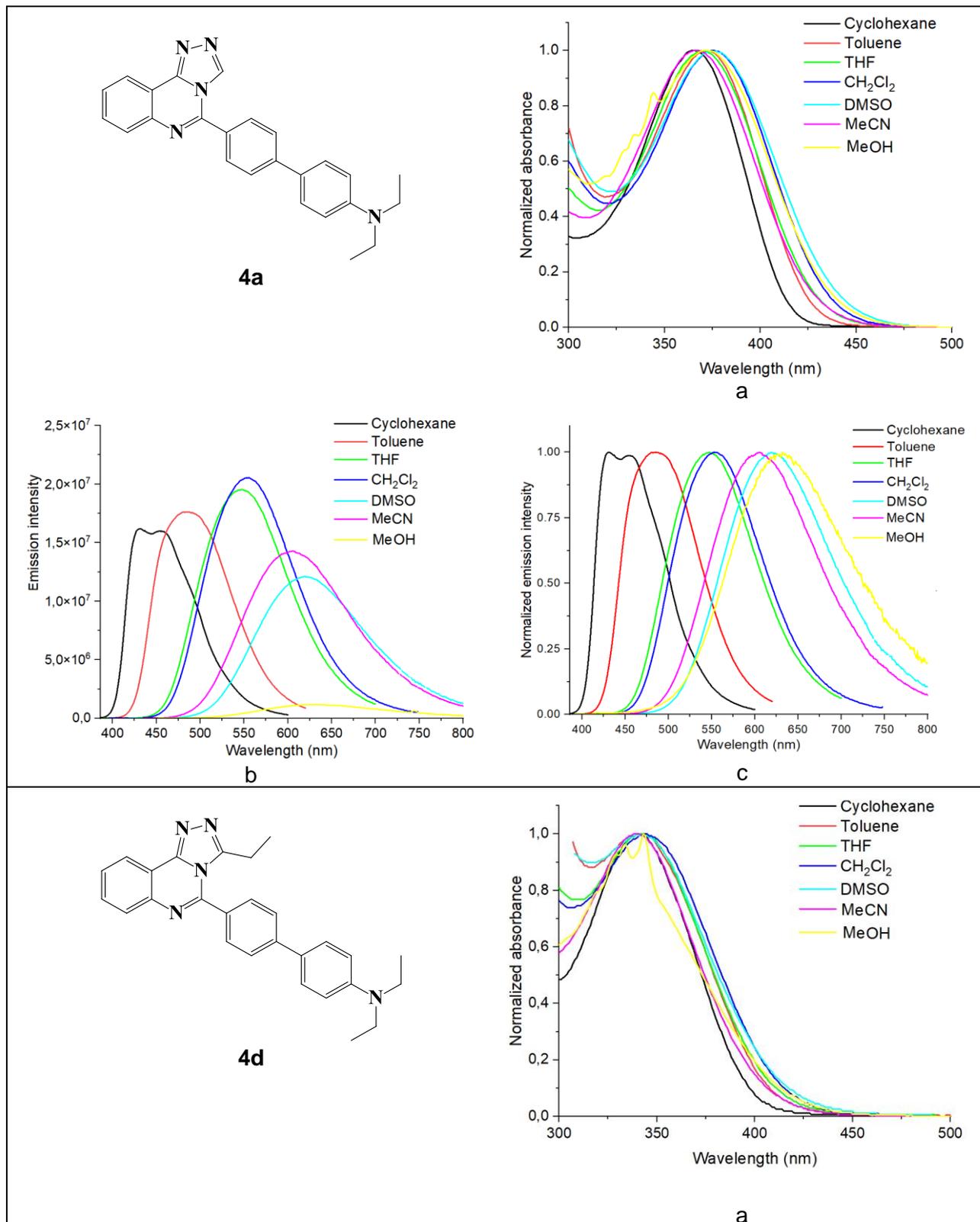
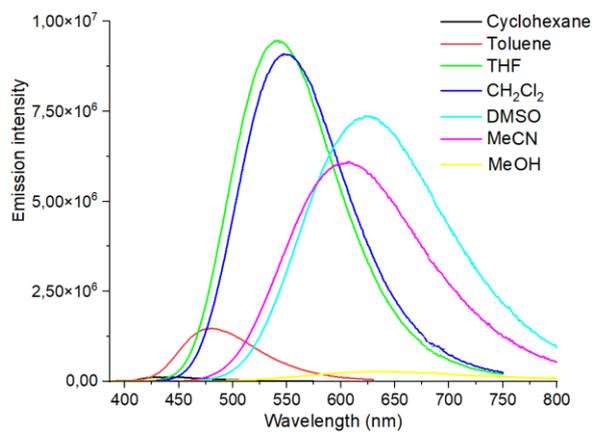


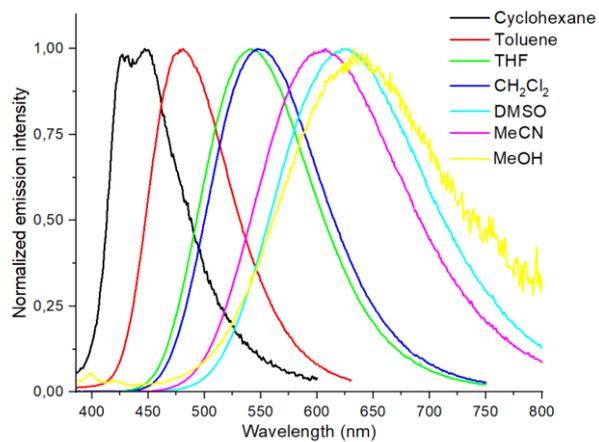
Figure S21. Time-resolved fluorescence lifetime decay profiles of **4a-f** and **5a-f** in toluene, instrumental response function (IRF, blue).

4. Solvatochromic study for compounds 4 and 5

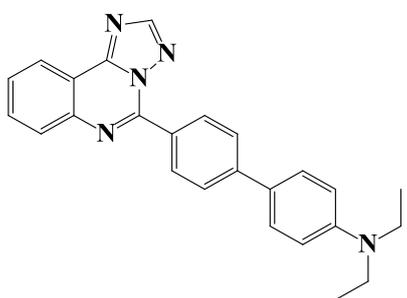




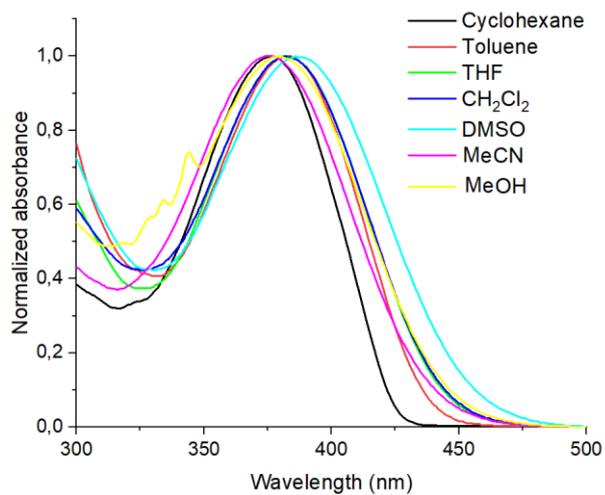
b



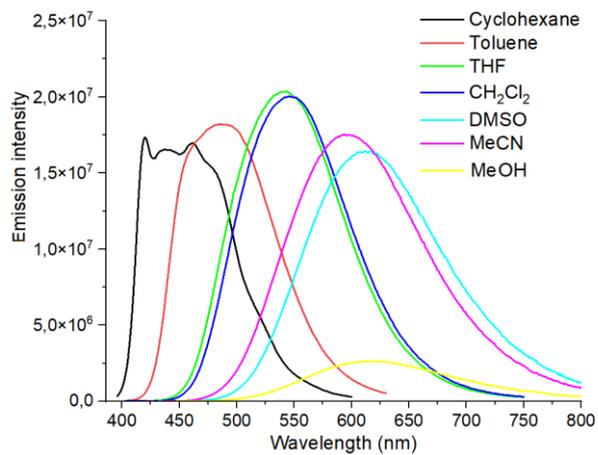
c



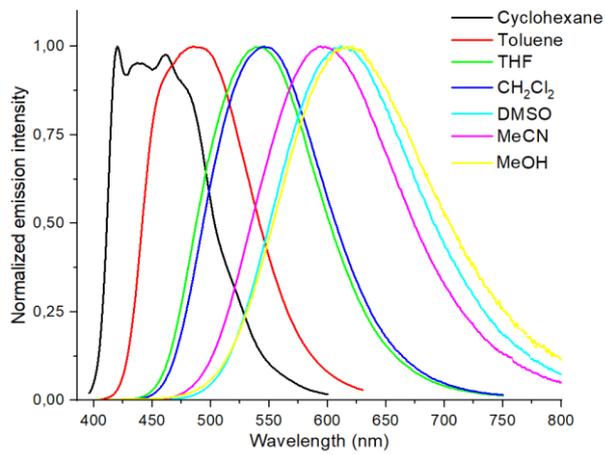
5a



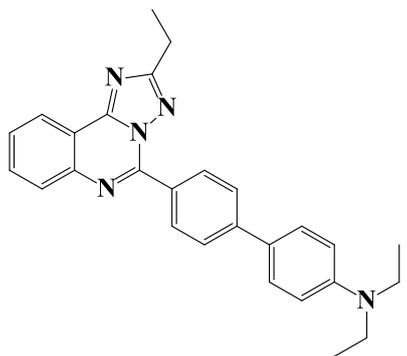
a



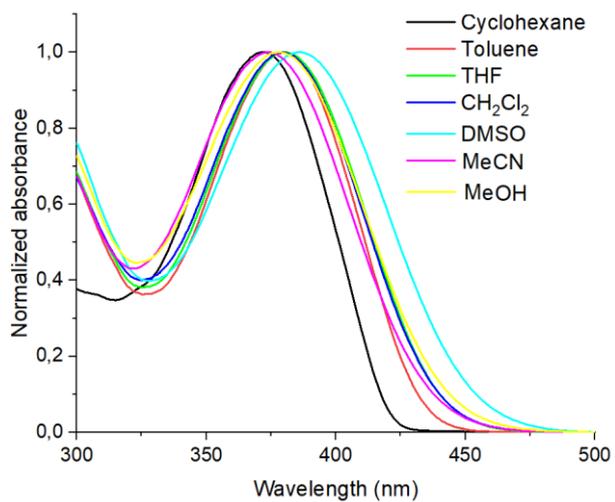
b



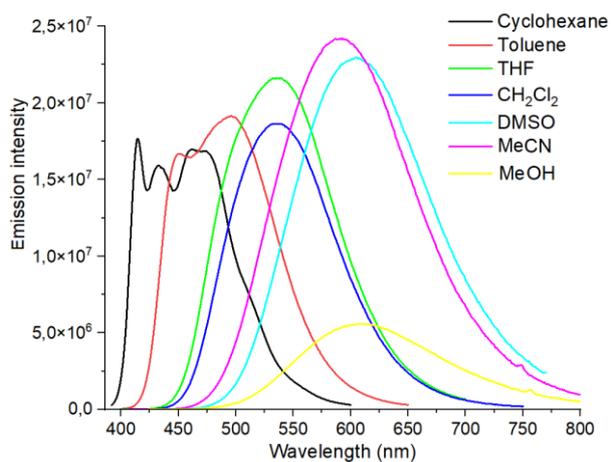
c



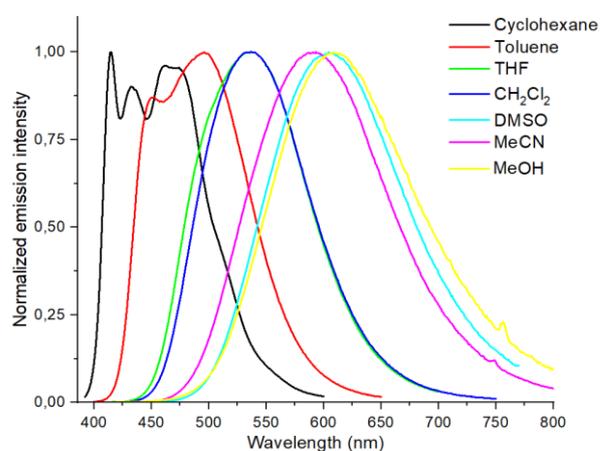
5d



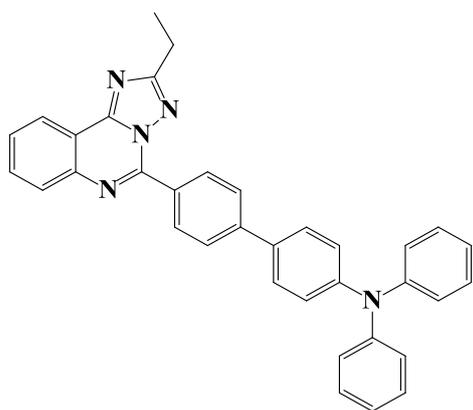
a



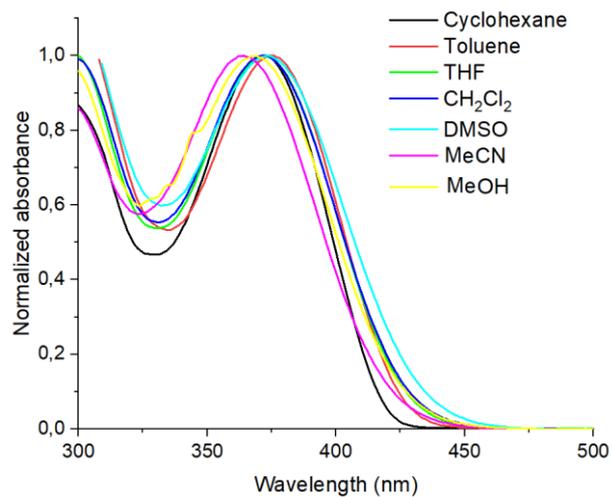
b



c



5e



a

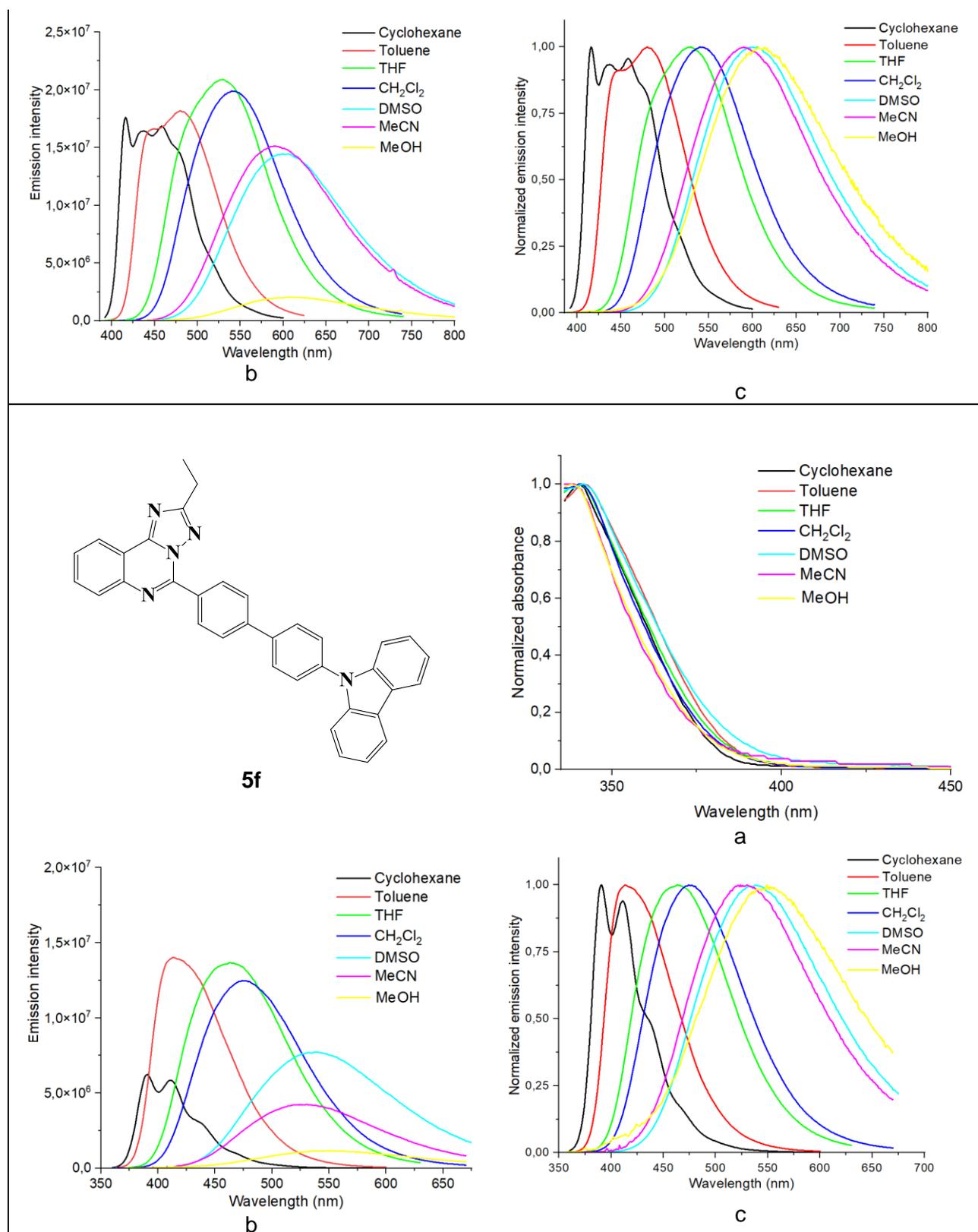


Figure S22. Normalized absorption (a), emission (b) and normalized emission (c) spectra of compounds **4a**, **4d**, **5a**, **5d-f** in different solvents.

Table S10. Orientation polarizability for solvents (Δf), absorption and emission maxima (λ_{abs} , λ_{em} , nm) and Stokes shift (nm, cm^{-1}) of **4a** in different solvents.

Solvent	Δf	λ_{abs} , nm	λ_{em} , nm	Stokes shift, nm	Stokes shift, cm^{-1}
Cyclohexane	-0,003	366	432, 455	89	5344
Toluene	0,013	371	476	105	5946
THF	0,208	369	548	179	8852
CH_2Cl_2	0,219	376	555	179	8578
DMSO	0,263	374	623	249	10687
MeCN	0,307	366	605	239	10793
MeOH	0,308	372	635	263	11134

Table S11. Orientation polarizability for solvents (Δf), absorption and emission maxima (λ_{abs} , λ_{em} , nm) and Stokes shift (nm, cm^{-1}) of **4d** in different solvents.

Solvent	Δf	λ_{abs} , nm	λ_{em} , nm	Stokes shift, nm	Stokes shift, cm^{-1}
Cyclohexane	-0,003	340	420, 447	107	7040
Toluene	0,013	343	481	138	8364
THF	0,208	343	541	198	10670
CH_2Cl_2	0,219	344	550	206	10888
DMSO	0,263	340	626	286	13437
MeCN	0,307	340	608	268	12964
MeOH	0,308	343	640	297	13530

Table S12. Orientation polarizability for solvents (Δf), absorption and emission maxima (λ_{abs} , λ_{em} , nm) and Stokes shift (nm, cm^{-1}) of **5a** in different solvents.

Solvent	Δf	λ_{abs} , nm	λ_{em} , nm	Stokes shift, nm	Stokes shift, cm^{-1}
Cyclohexane	-0,003	376	420, 440, 462	86	4951
Toluene	0,013	383	479	96	5233
THF	0,208	382	543	161	7762
CH_2Cl_2	0,219	382	547	165	7896
DMSO	0,263	386	614	228	9620
MeCN	0,307	375	598	223	9944
MeOH	0,308	379	620	241	10256

Table S13. Orientation polarizability for solvents (Δf), absorption and emission maxima (λ_{abs} , λ_{em} , nm) and Stokes shift (nm, cm^{-1}) of **5d** in different solvents.

Solvent	Δf	λ_{abs} , nm	λ_{em} , nm	Stokes shift, nm	Stokes shift, cm^{-1}
Cyclohexane	-0,003	372	415, 434, 469	97	5560
Toluene	0,013	380	486	106	5740
THF	0,208	380	537	157	7694
CH_2Cl_2	0,219	380	537	157	7694
DMSO	0,263	386	606	220	9405
MeCN	0,307	374	579	205	9467
MeOH	0,308	378	612	234	10115

Table S14. Orientation polarizability for solvents (Δf), absorption and emission maxima (λ_{abs} , λ_{em} , nm) and Stokes shift (nm, cm^{-1}) of **5e** in different solvents.

Solvent	Δf	λ_{abs} , nm	λ_{em} , nm	Stokes shift, nm	Stokes shift, cm^{-1}
Cyclohexane	-0,003	372	416, 437, 459	87	5095
Toluene	0,013	375	465	190	5161
THF	0,208	372	529	157	7978
CH_2Cl_2	0,219	372	543	171	8466
DMSO	0,263	374	604	230	10182
MeCN	0,307	363	593	230	10685
MeOH	0,308	369	613	244	10787

Table S15. Orientation polarizability for solvents (Δf), absorption and emission maxima (λ_{abs} , λ_{em} , nm) and Stokes shift (nm, cm^{-1}) of **5f** in different solvents.

Solvent	Δf	λ_{abs} , nm	λ_{em} , nm	Stokes shift, nm	Stokes shift, cm^{-1}
Cyclohexane	-0,003	340	391, 411	71	5081
Toluene	0,013	342	420	78	5430
THF	0,208	341	464	123	7774
CH_2Cl_2	0,219	340	477	137	8447
DMSO	0,263	341	540	199	10807
MeCN	0,307	339	530	191	10631
MeOH	0,308	338	553	215	11503

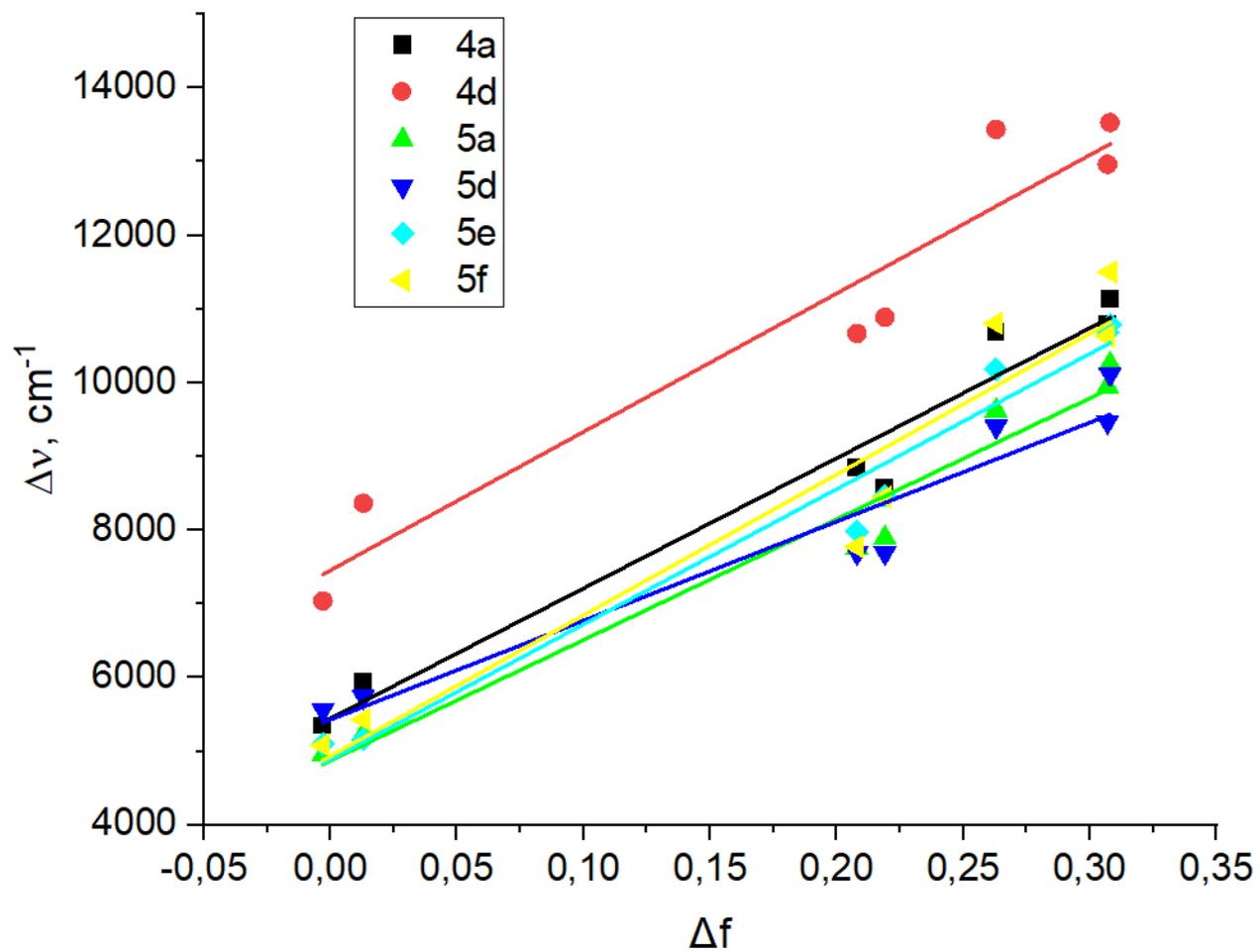


Figure S23. Lippert-Mataga plot of fluorophores **4a**, **4d**, **5a**, **5d**, **5e** and **5f** in cyclohexane, toluene, THF, CH_2Cl_2 , DMSO, MeCN and MeOH.

5. Cyclic voltammograms for compounds 4a-f and 5a-f

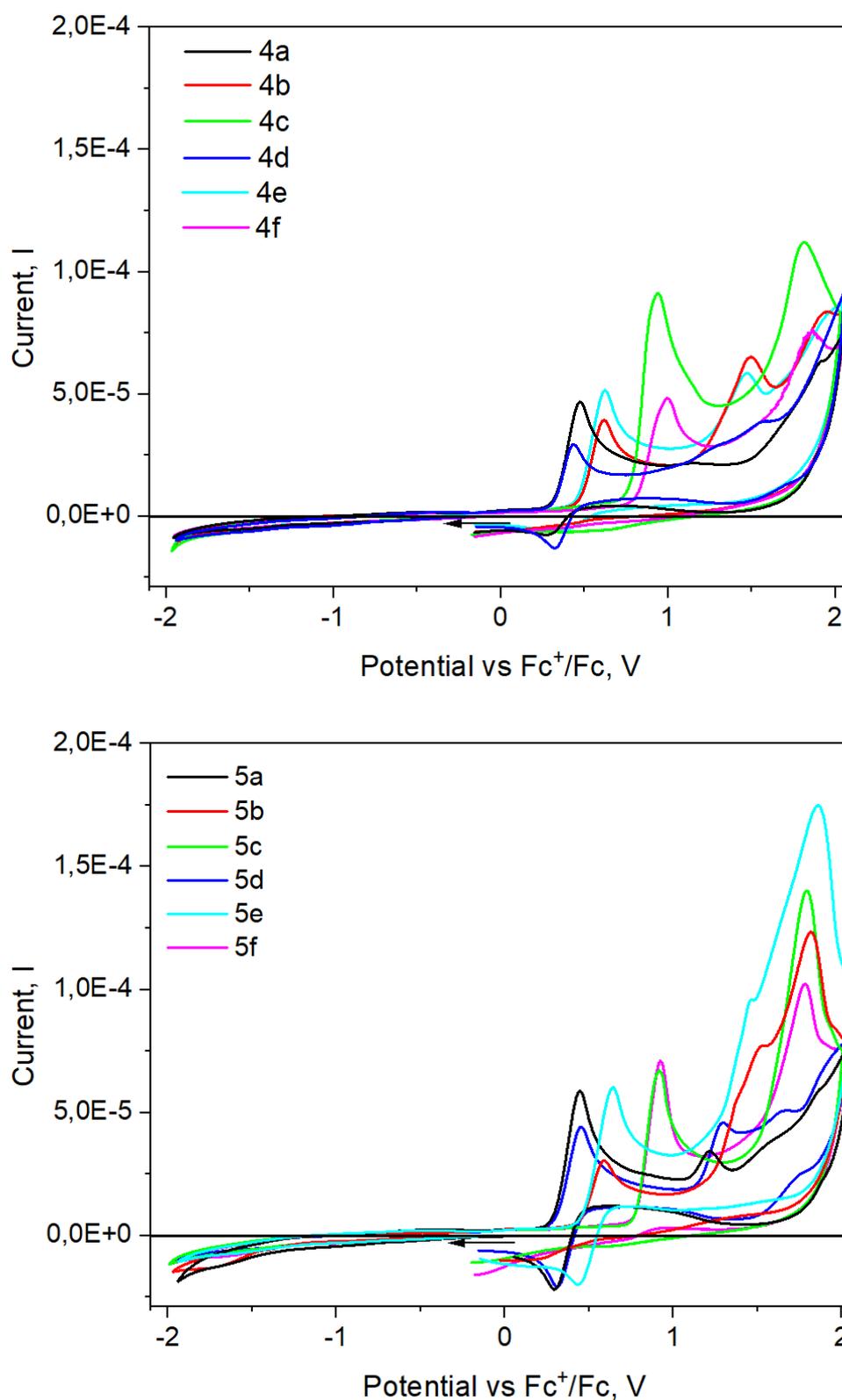


Figure S24. General view of voltammograms for **4a-f** and **5a-f** (0.1 M Bu₄NPF₆ in CH₂Cl₂ as supporting electrolyte, scan rate 100 mV/s, platinum disk working electrode, glassy carbon disk counter electrode, Ag/AgNO₃ pseudoreference electrode, Fc⁺/Fc couple as an internal standard).

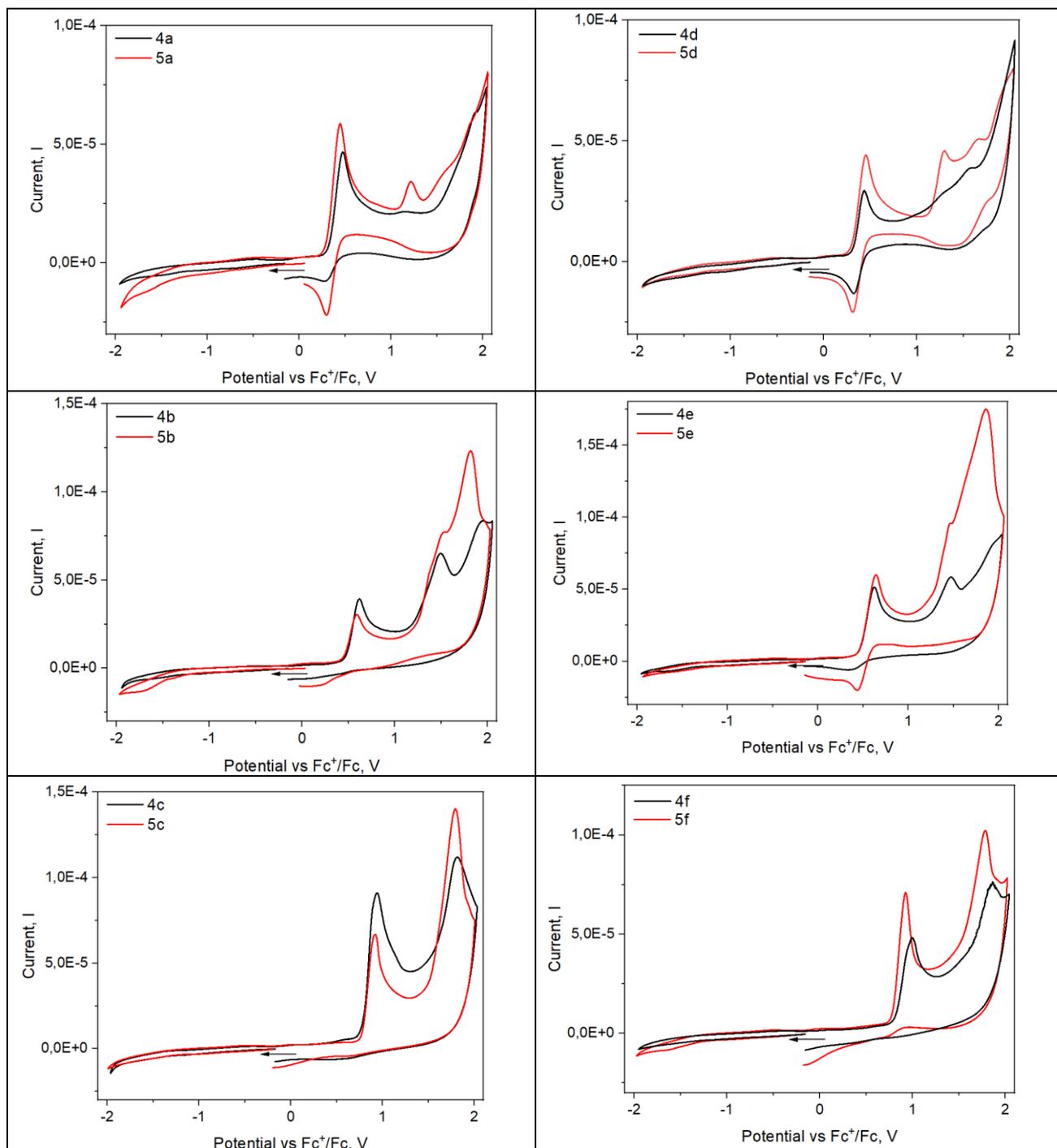
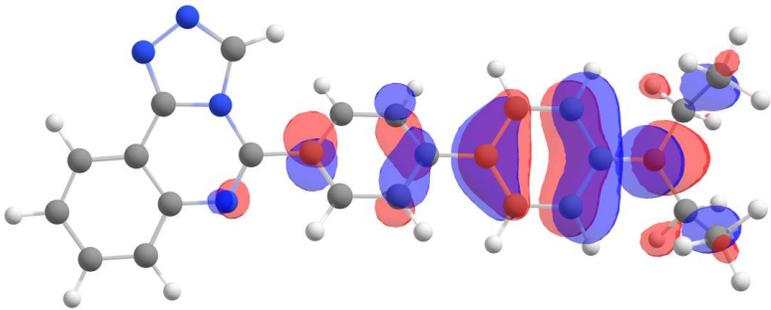
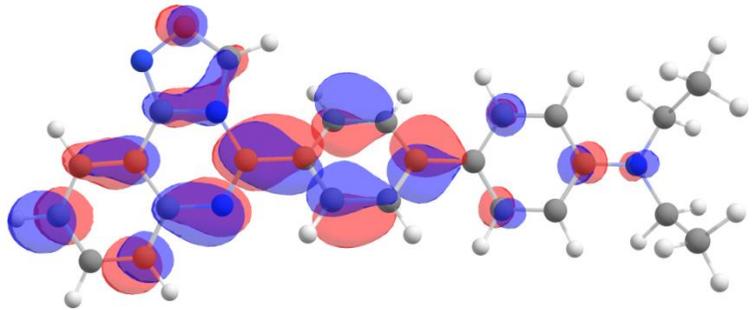
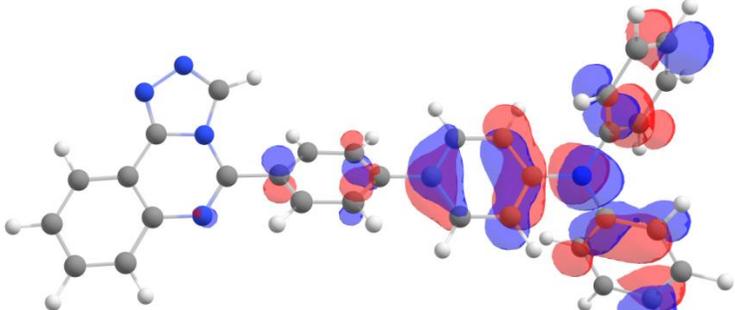
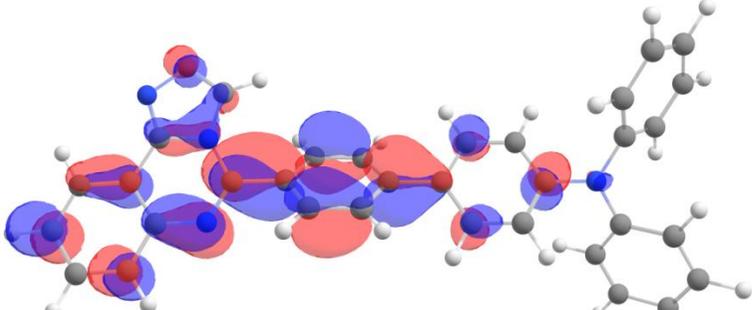
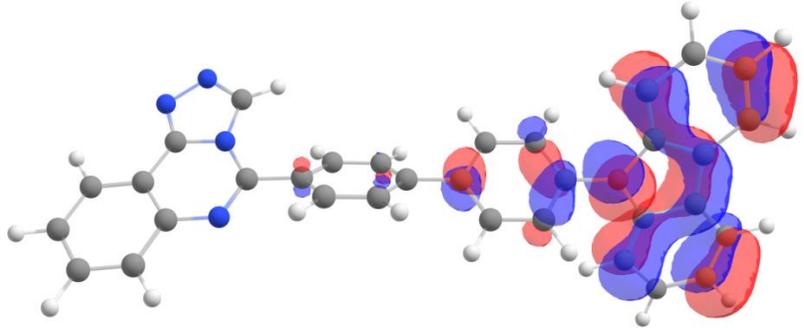
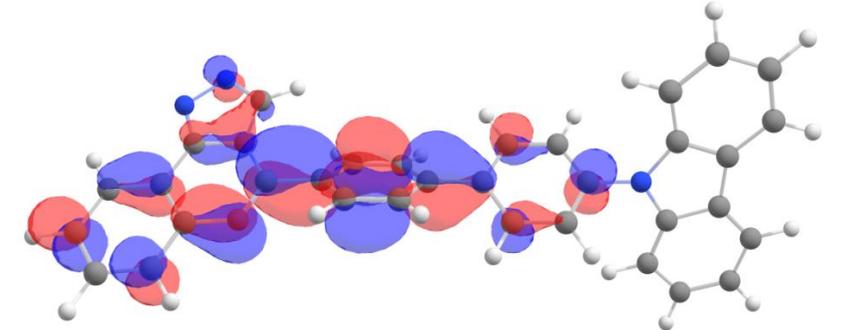
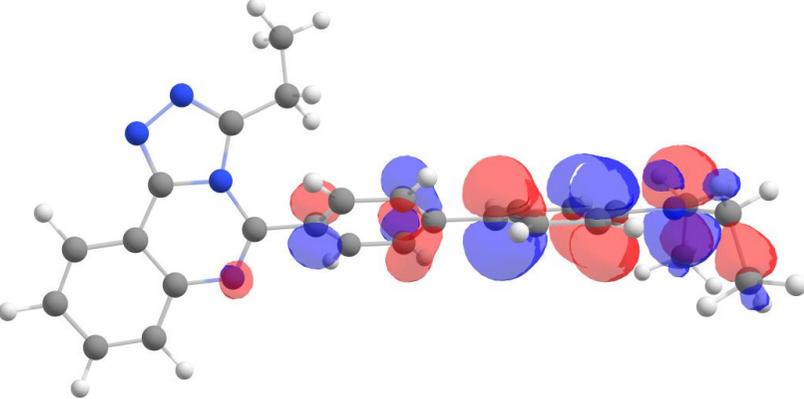
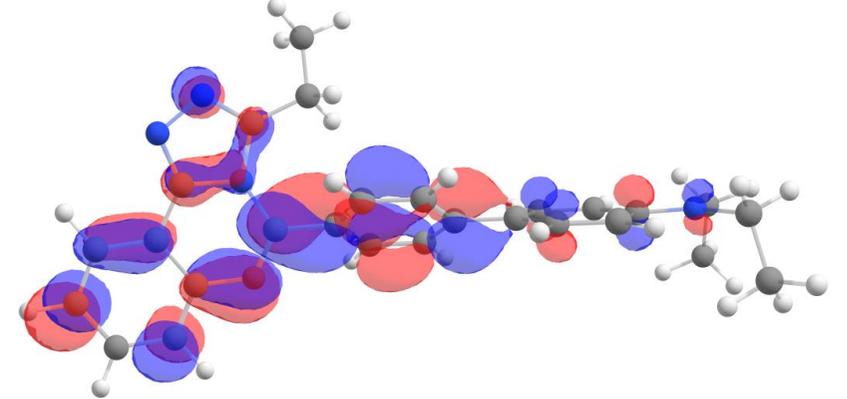
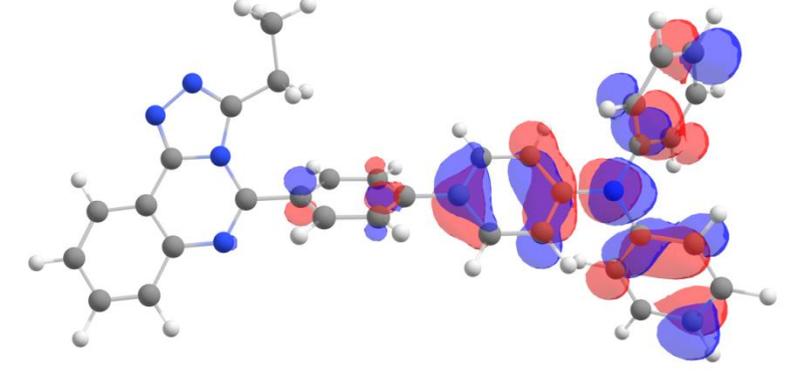
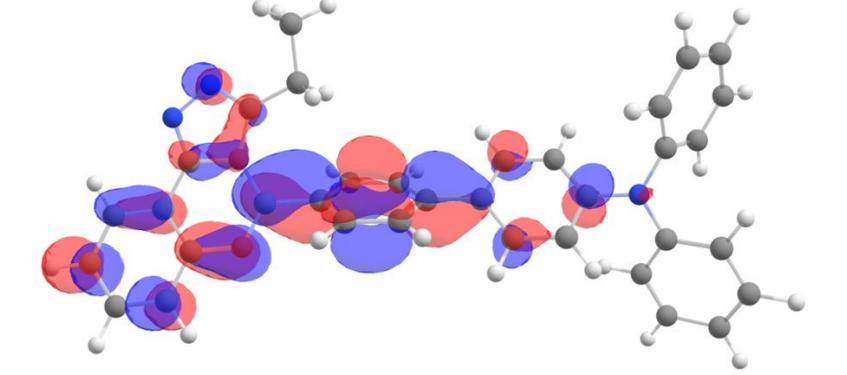


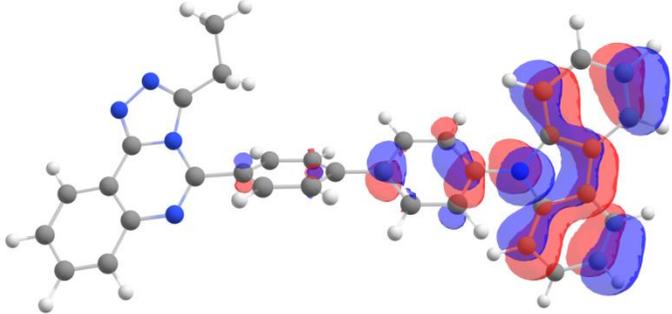
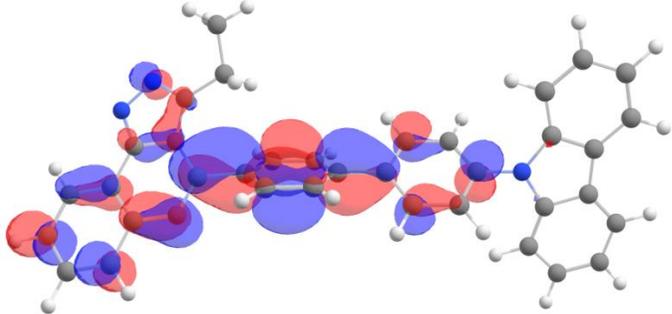
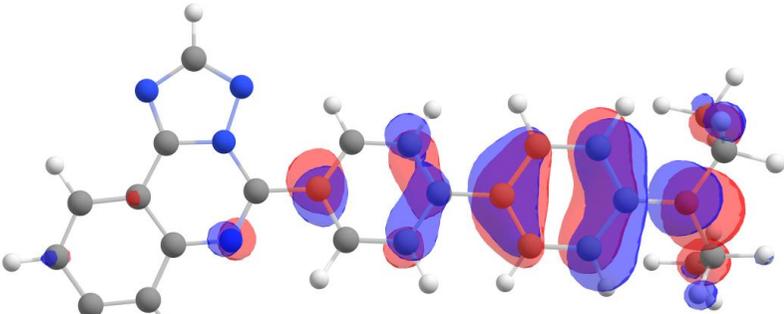
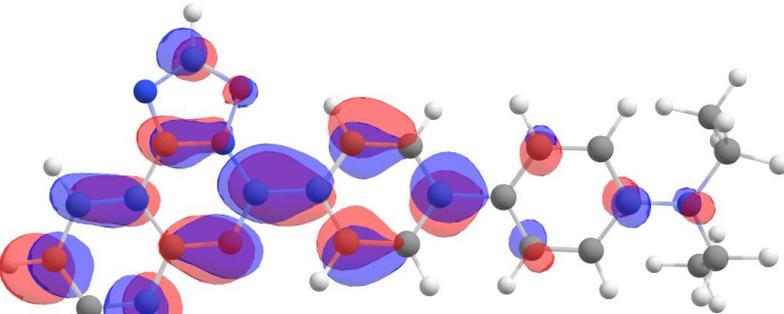
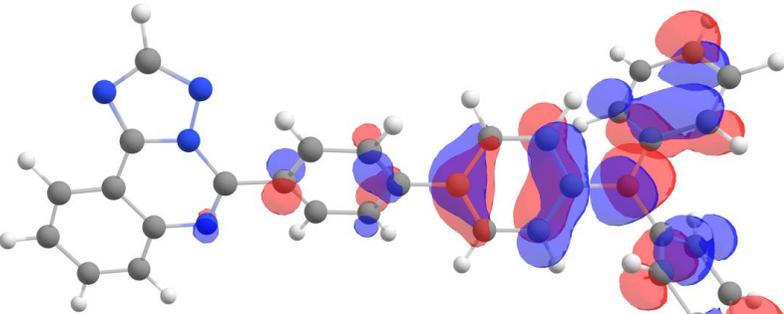
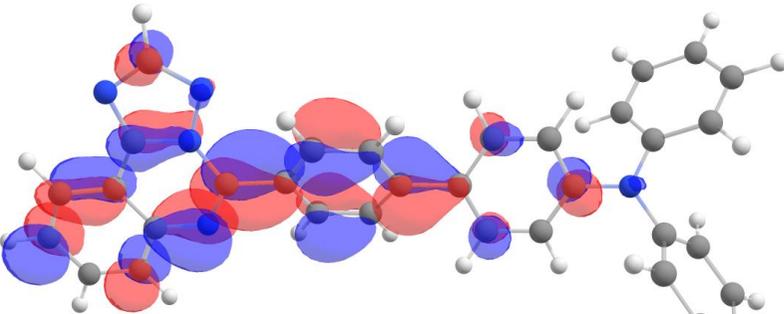
Figure S25. Comparison of voltammograms for each pair of isomers.

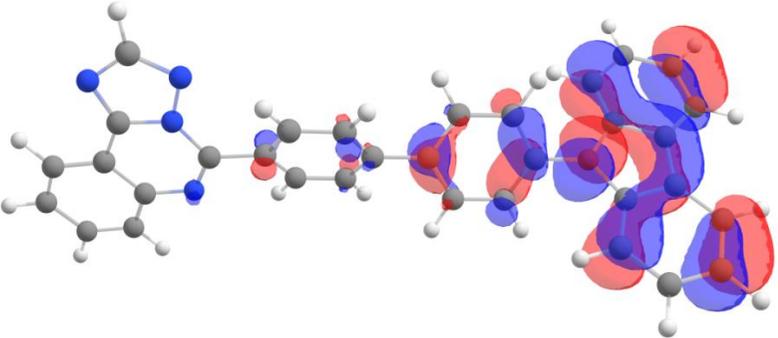
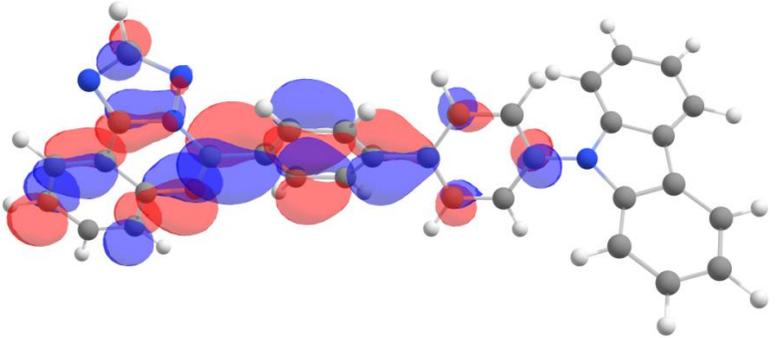
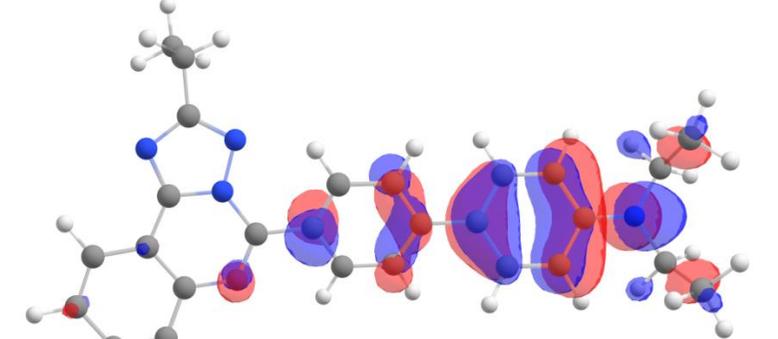
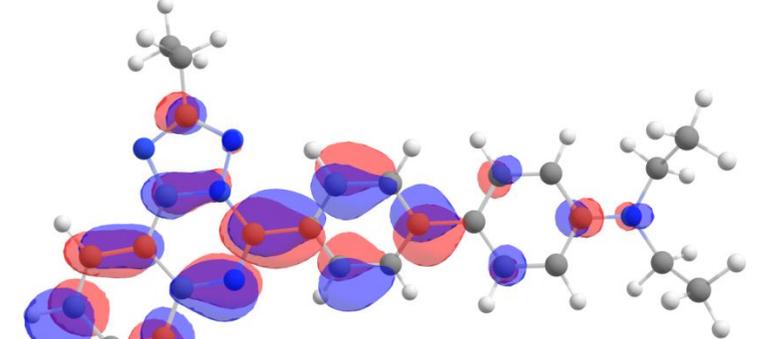
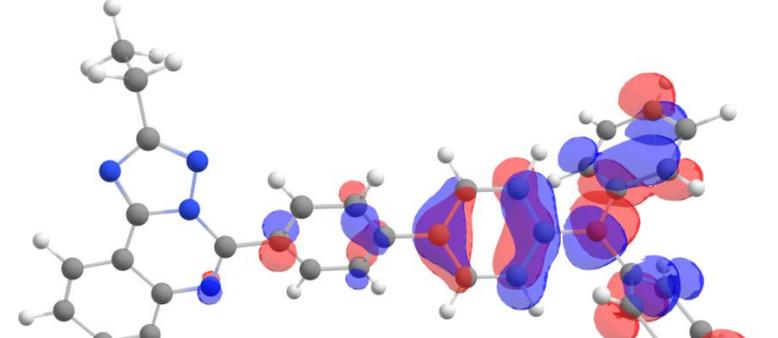
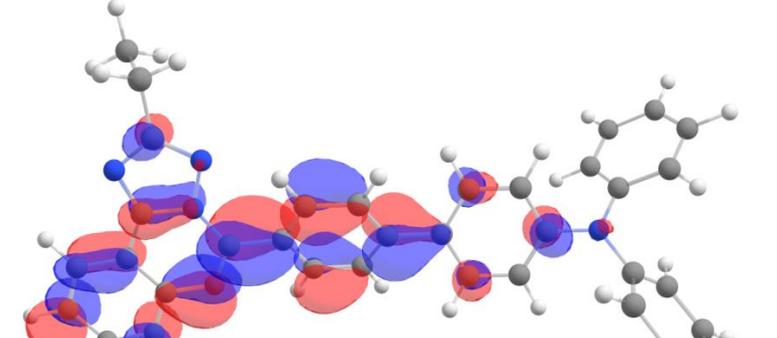
6. Theoretical calculations

Table S16. The electronic distribution in HOMO/LUMO of **4a-f** and **5a-f** calculated for gas phase.

Compound	HOMO, eV	LUMO, eV	E _g
4a	 -5.61	 -1.87	-3.74
4b	 -5.60	 -2.02	-3.58

4c	 <p>-5.98</p>	 <p>-2.21</p>	-3.77
4d	 <p>-5.58</p>	 <p>-1.64</p>	-3.94
4e	 <p>-5.58</p>	 <p>-1.82</p>	-3.76

4f	 <p style="text-align: center;">-5.96</p>	 <p style="text-align: center;">-2.01</p>	-3.95
5a	 <p style="text-align: center;">-5.44</p>	 <p style="text-align: center;">-1.84</p>	-3.6
5b	 <p style="text-align: center;">-5.47</p>	 <p style="text-align: center;">-2.00</p>	-3.47

5c	 <p>-5.86</p>	 <p>-2.15</p>	-3.71
5d	 <p>-5.41</p>	 <p>-1.75</p>	-3.66
5e			-3.53

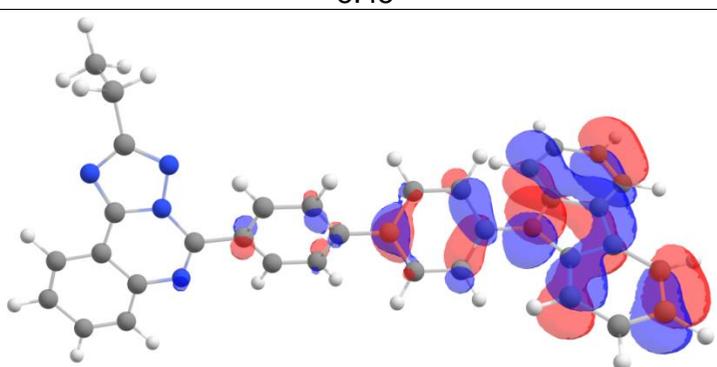
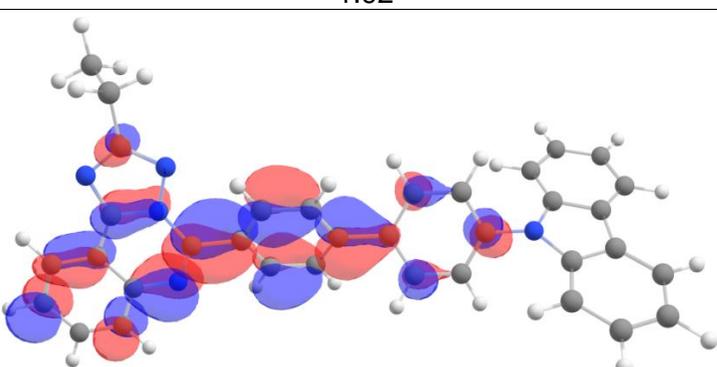
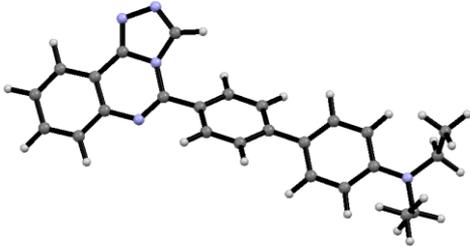
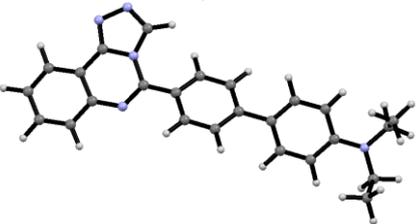
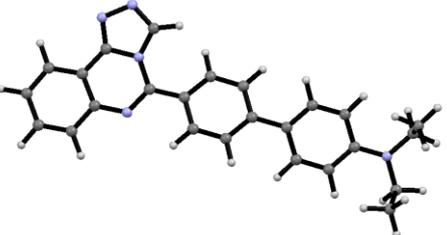
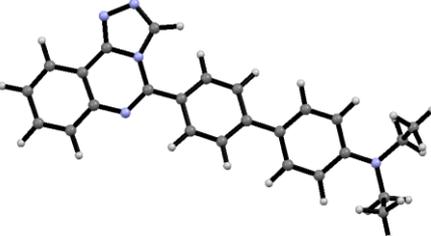
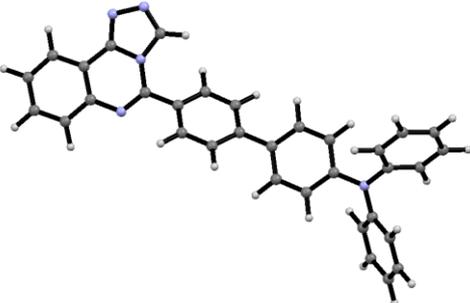
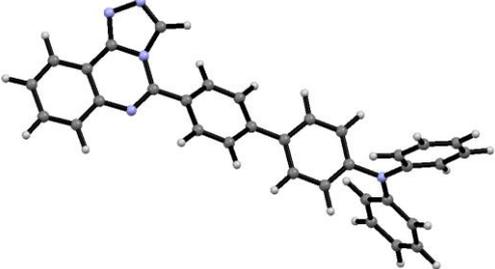
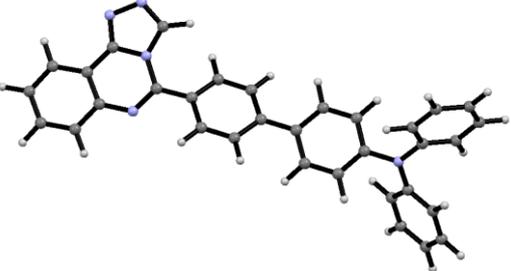
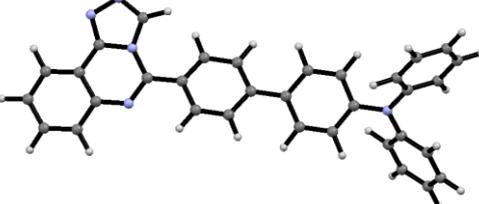
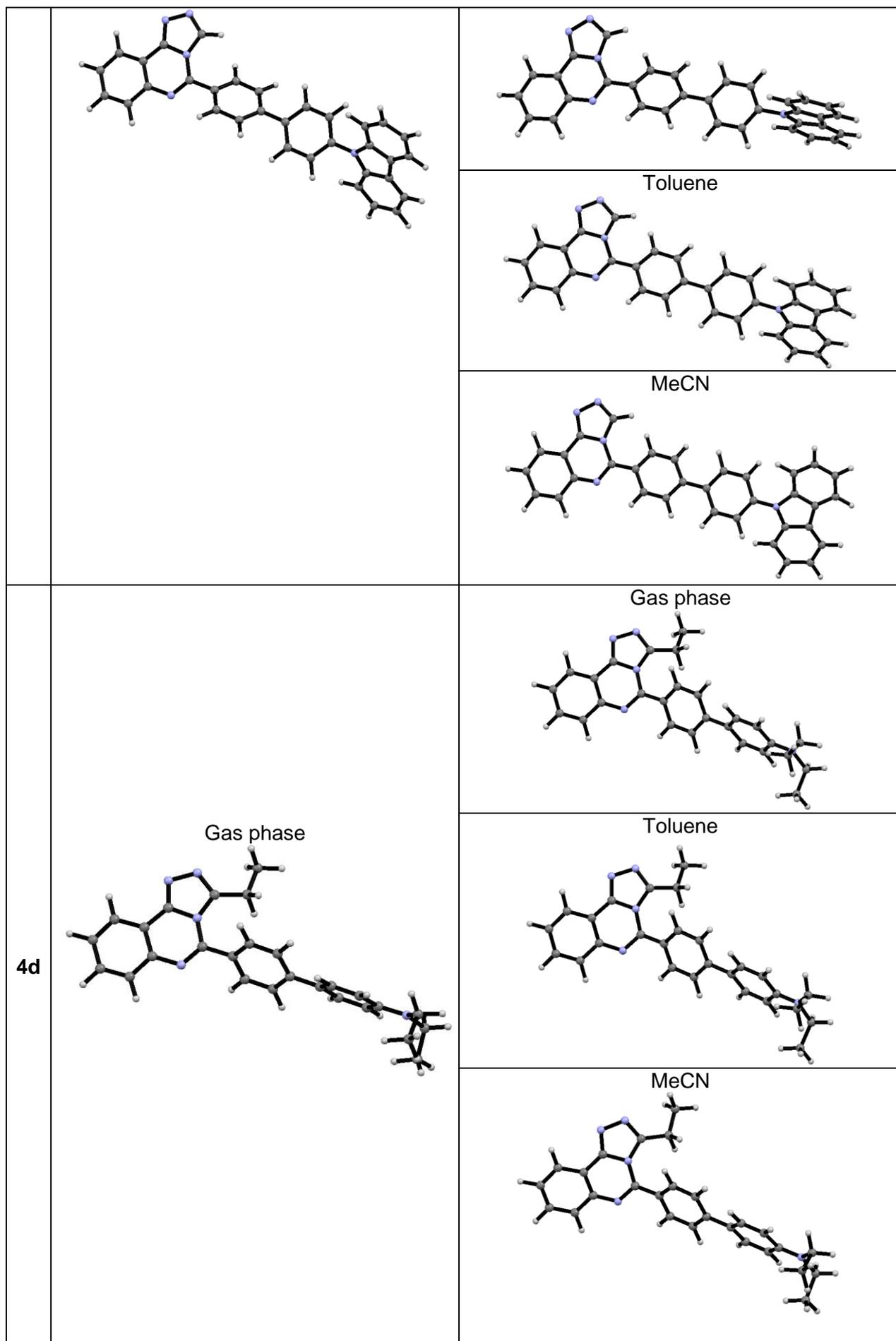
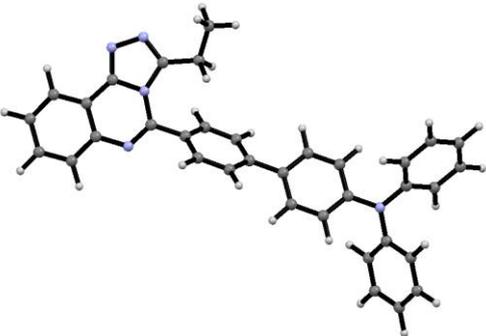
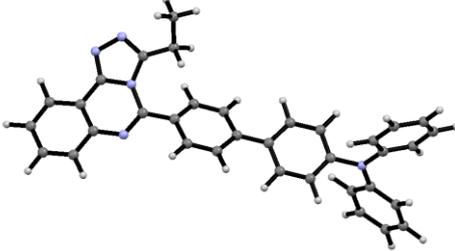
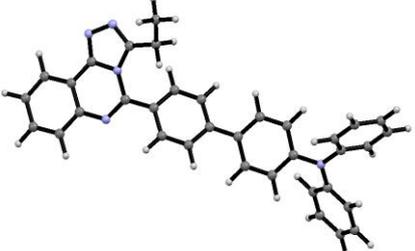
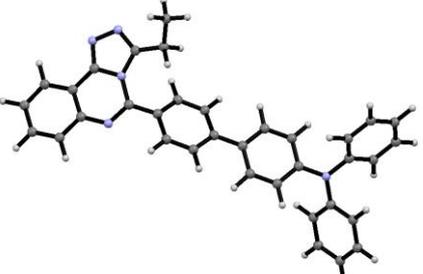
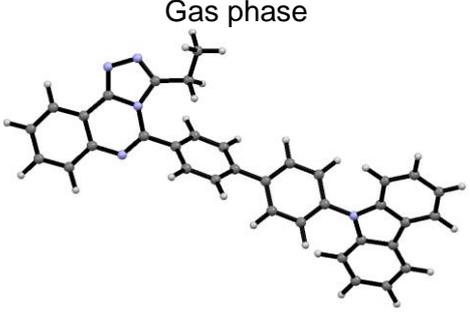
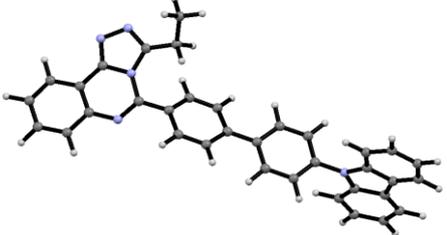
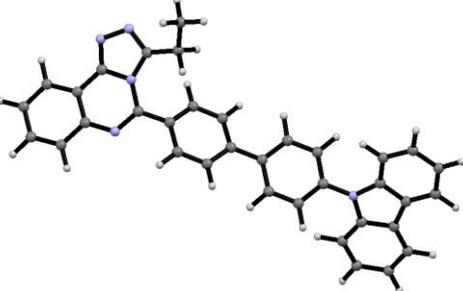
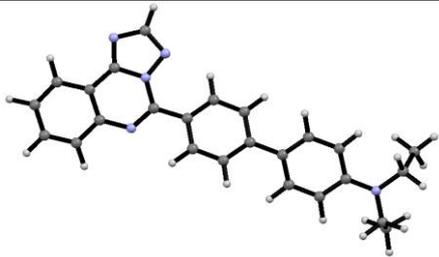
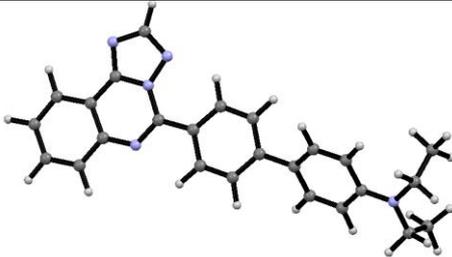
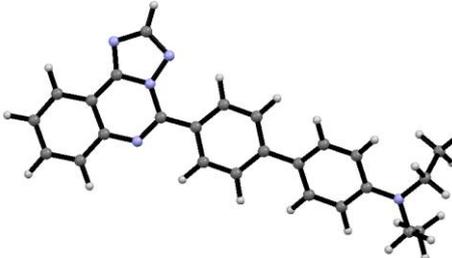
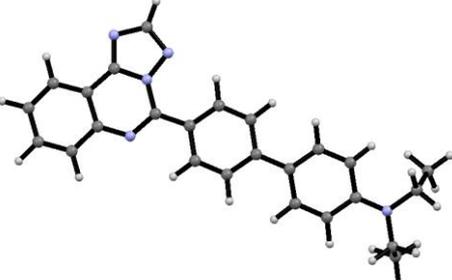
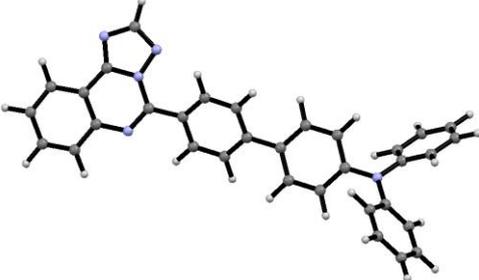
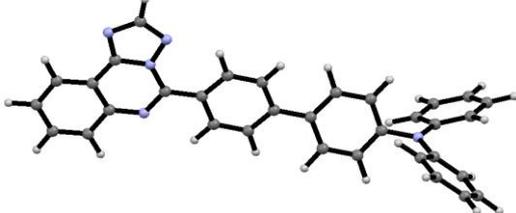
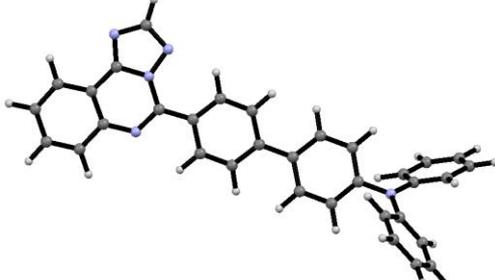
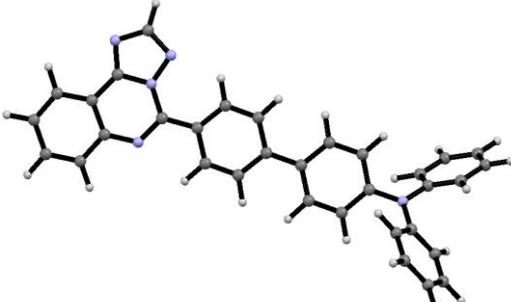
	-5.45	-1.92	
5f	 <p style="text-align: center;">-5.85</p>	 <p style="text-align: center;">-2.07</p>	-3.78

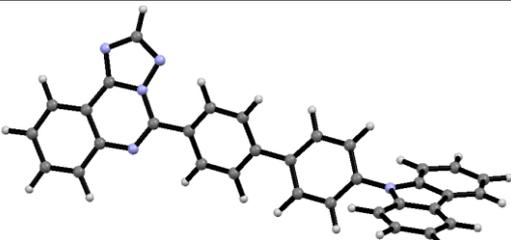
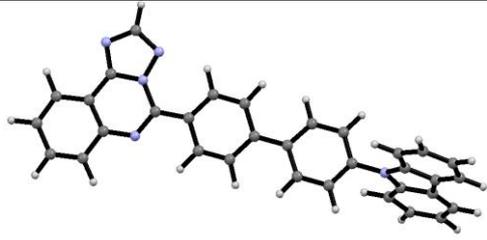
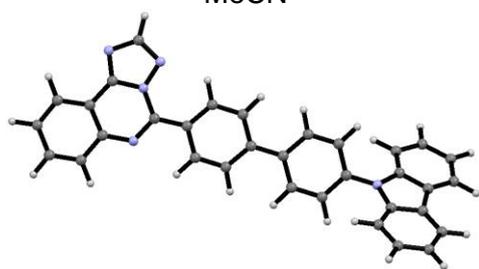
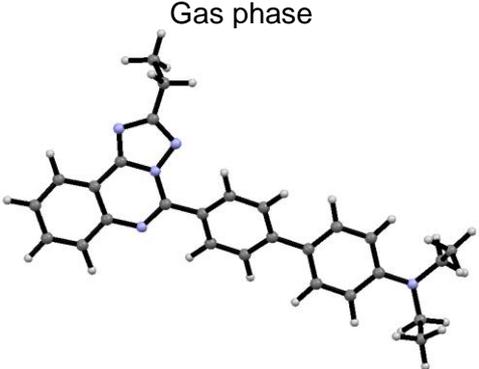
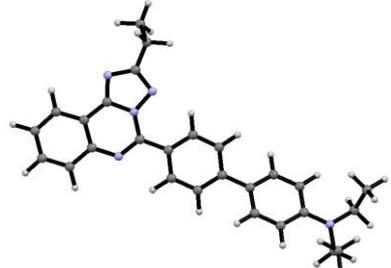
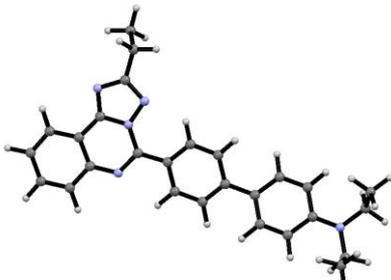
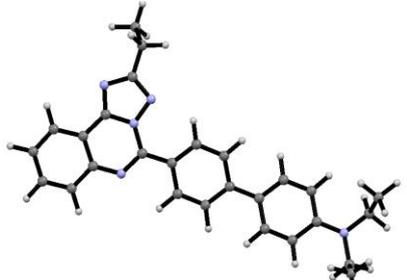
Table S17. The optimized geometries of 4a-f and 5a-f in gas phase, toluene and MeCN

#	S_0	S_1
4a	<p data-bbox="454 638 598 672">Gas phase</p> 	<p data-bbox="1061 302 1204 336">Gas phase</p> 
		<p data-bbox="1077 571 1189 604">Toluene</p> 
		<p data-bbox="1093 855 1173 889">MeCN</p> 
4b	<p data-bbox="454 1489 598 1523">Gas phase</p> 	<p data-bbox="1061 1135 1204 1169">Gas phase</p> 
		<p data-bbox="1077 1460 1189 1494">Toluene</p> 
		<p data-bbox="1093 1785 1173 1818">MeCN</p> 
4c	Gas phase	Gas phase



4e	<p>Gas phase</p> 	<p>Gas phase</p> 
		<p>Toluene</p> 
		<p>MeCN</p> 
4f	<p>Gas phase</p> 	<p>Gas phase</p> 
		<p>Toluene</p> 
		<p>MeCN</p> 
5a	Gas phase	Gas phase

		
		<p>Toluene</p> 
		<p>MeCN</p> 
<p>5b</p>	<p>Gas phase</p> 	<p>Gas phase</p> 
		<p>Toluene</p> 
		<p>MeCN</p> 
<p>5c</p>	<p>Gas phase</p>	<p>Gas phase</p>

		 <p>Toluene</p>
		 <p>MeCN</p>
		
5d	<p>Gas phase</p> 	<p>Gas phase</p> 
		<p>Toluene</p> 
		<p>MeCN</p> 
5e	<p>Gas phase</p>	<p>Gas phase</p>

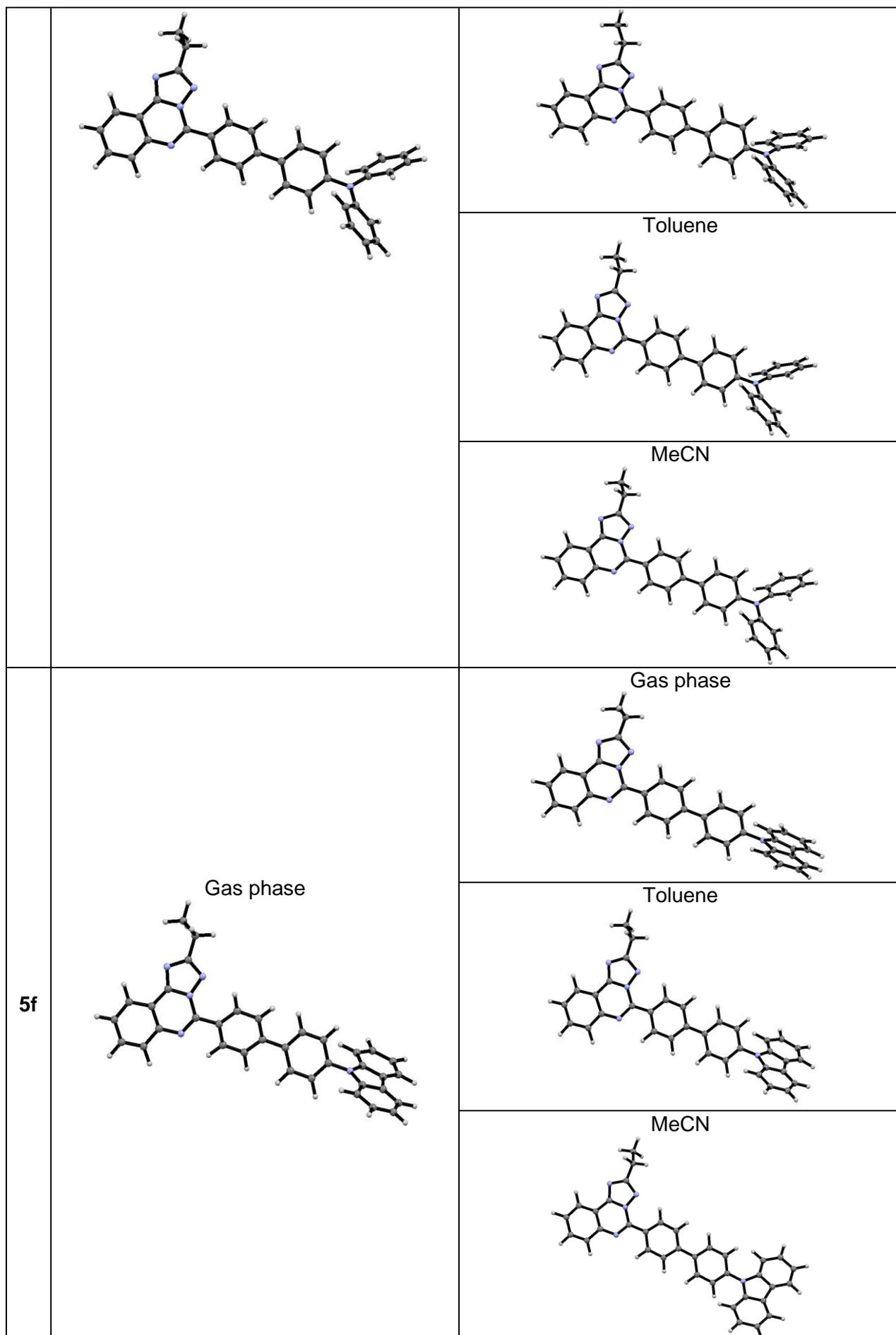
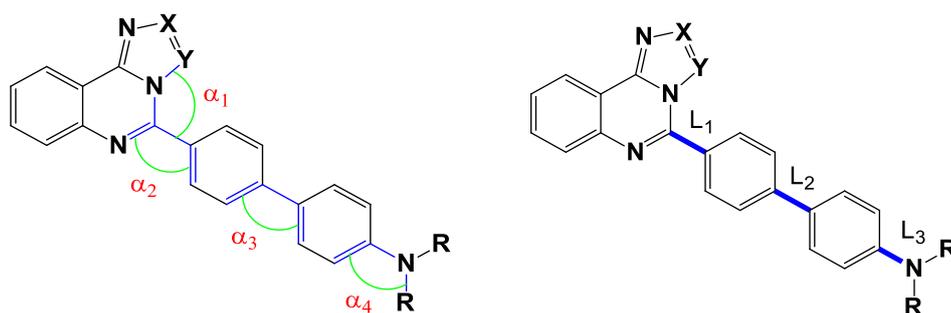


Table S18. Selected dihedral angles (α) and bond lengths (L) in the ground and excited states of **4a-f** and **5a-f** in toluene and MeCN.



	Phase/Solvent	S	$\alpha_1, ^\circ$	$\alpha_2, ^\circ$	$\alpha_3, ^\circ$	$\alpha_4, ^\circ$	$L_1, \text{\AA}$	$L_2, \text{\AA}$	$L_3, \text{\AA}$
4a	Gas	S ₀	-6.9	-38.4	31.2	-6.5	1.467	1.466	1.371
		S ₁	-13.1	-19.0	44.5	-5.7	1.439	1.470	1.361
	Toluene	S ₁	-13.4	-20.4	29.0	-4.8	1.436	1.459	1.356
	MeCN	S ₁	-14.0	-19.8	20.6	-3.8	1.430	1.450	1.349
4b	Gas	S ₀	-6.1	-38.8	31.4	33.0	1.468	1.470	1.399
		S ₁	-12.3	-19.6	19.6	71.9	1.432	1.447	1.440
	Toluene	S ₁	-12.6	-19.9	20.8	45.8	1.431	1.451	1.410
	MeCN	S ₁	-13.3	-18.8	18.7	38.5	1.427	1.445	1.392
4c	Gas	S ₀	-6.9	-36.1	36.9	54.1	1.470	1.472	1.405
		S ₁	-12.1	-19.4	15.3	-87.0	1.431	1.440	1.433
	Toluene	S ₁	-13.4	-19.4	16.8	50.8	1.428	1.443	1.404
	MeCN	S ₁	-14.2	-18.4	10.1	43.3	1.423	1.436	1.387
4d	Gas	S ₀	10.0	54.8	32.8	-5.7	1.472	1.469	1.372
		S ₁	31.3	28.9	33.1	-3.9	1.439	1.463	1.363
	Toluene	S ₁	31.1	30.2	25.8	-5.0	1.436	1.457	1.356
	MeCN	S ₁	31.7	30.2	19.2	-4.6	1.430	1.450	1.349
4e	Gas	S ₀	-11.8	-55.2	34.4	35.1	1.473	1.470	1.401
		S ₁	-26.5	-27.9	19.3	68.8	1.433	1.446	1.437
	Toluene	S ₁	-28.16	-27.9	19.0	44.5	1.431	1.449	1.407
	MeCN	S ₁	-29.8	-27.2	14.5	36.6	1.426	1.444	1.389
4f	Gas	S ₀	-14.0	-52.7	34.7	53.0	1.473	1.472	1.405
		S ₁	-25.5	-28.3	13.2	86.4	1.433	1.438	1.432
	Toluene	S ₁	-29.2	-26.0	16.3	48.9	1.426	1.442	1.399
	MeCN	S ₁	-30.8	-25.3	12.6	43.9	1.420	1.436	1.388
5a	Gas	S ₀	-1.4	-16.5	32.9	0.7	1.468	1.466	1.372
		S ₁	0.5	-1.1	39.7	-1.0	1.448	1.468	1.361
	Toluene	S ₁	-1.1	-2.4	28.2	-0.5	1.441	1.458	1.356
	MeCN	S ₁	-1.4	-4.3	20.7	-0.6	1.433	1.450	1.349
5b	Gas	S ₀	1.7	21.7	-32.1	-36.0	1.468	1.469	1.402
		S ₁	-0.1	0.8	-20.8	-66.7	1.435	1.450	1.437
	Toluene	S ₁	1.4	2.8	-19.1	-44.8	1.434	1.450	1.407
	MeCN	S ₁	2.1	5.3	-12.7	-37.0	1.430	1.444	1.390
5c	Gas	S ₀	1.6	19.3	-36.3	-53.1	1.470	1.471	1.405
		S ₁	0.2	0.1	-15.8	86.9	1.432	1.441	1.433
	Toluene	S ₁	0.7	1.8	-14.5	-49.3	1.432	1.442	1.401
	MeCN	S ₁	0.4	2.0	-6.8	-44.0	1.426	1.436	1.387
5d	Gas	S ₀	2.1	19.6	-30.7	-2.1	1.468	1.467	1.373
		S ₁	0.4	2.4	-37.8	-1.5	1.446	1.466	1.362
	Toluene	S ₁	1.0	4.4	-26.3	-1.1	1.439	1.457	1.356
	MeCN	S ₁	0.7	3.2	-20.4	-0.4	1.432	1.449	1.349
5e	Gas	S ₀	2.0	19.2	-32.5	-35.3	1.469	1.469	1.401
		S ₁	-0.1	1.2	-19.7	-65.7	1.435	1.448	1.436
	Toluene	S ₁	0.0	-0.5	-10.5	-45.4	1.434	1.448	1.408
	MeCN	S ₁	1.0	2.6	-11.8	-37.1	1.430	1.443	1.390

5f	Gas	S ₀	2.2	19.7	-34.9	-52.5	1.471	1.471	1.405
		S ₁	0.1	0.7	-14.2	-87.8	1.433	1.439	1.432
	Toluene	S ₁	-0.9	-0.1	-15.3	-49.5	1.431	1.441	1.400
	MeCN	S ₁	-0.2	0.8	1.5	-43.3	1.427	1.434	1.387

Table S19. The electronic S₀→S_n transition properties of compounds 4a-f and 5a-f.

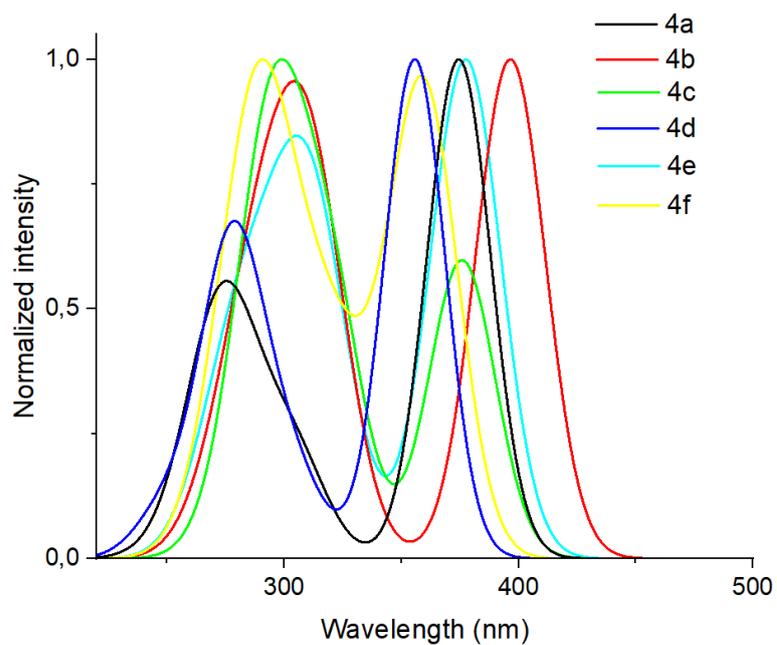
#	State/ Energy(cm ⁻¹)/ Wavelength(nm)/ f _{osc}	
4a	1 26700.4 374.5 0.885420282	STATE 1: E= 0.121656 au 3.310 eV 26700.4 cm ^{**} -1 <S ^{**2} > = 0.000000
	2 32365.1 309.0 0.051737291	103a -> 104a : 0.978340 (c= 0.98911072)
	3 33122.3 301.9 0.134253142	STATE 2: E= 0.147466 au 4.013 eV 32365.1 cm ^{**} -1 <S ^{**2} > = 0.000000 101a -> 104a : 0.135764 (c= 0.36846201) 101a -> 105a : 0.035003 (c= -0.18709090) 101a -> 107a : 0.010457 (c= -0.10225798) 102a -> 104a : 0.637255 (c= 0.79828236) 102a -> 105a : 0.017330 (c= 0.13164379) 103a -> 105a : 0.137650 (c= -0.37101192)
4b	1 25220.2 396.5 0.803416720	STATE 3: E= 0.150916 au 4.107 eV 33122.3 cm ^{**} -1 <S ^{**2} > = 0.000000 102a -> 104a : 0.178986 (c= -0.42306754) 102a -> 105a : 0.010585 (c= 0.10288155) 103a -> 105a : 0.764584 (c= -0.87440508) 103a -> 106a : 0.021318 (c= -0.14600542)
	2 30580.7 327.0 0.014881890	STATE 1: E= 0.114912 au 3.127 eV 25220.2 cm ^{**} -1 <S ^{**2} > = 0.000000 127a -> 128a : 0.968726 (c= 0.98423883) 127a -> 130a : 0.010074 (c= -0.10037013)
	3 31880.4 313.7 0.356740104	STATE 2: E= 0.139336 au 3.792 eV 30580.7 cm ^{**} -1 <S ^{**2} > = 0.000000 127a -> 131a : 0.913650 (c= 0.95585060) 127a -> 132a : 0.014716 (c= -0.12130776) 127a -> 133a : 0.017828 (c= 0.13351977)
4c	1 26600.0 375.9 0.416519327	STATE 3: E= 0.145258 au 3.953 eV 31880.4 cm ^{**} -1 <S ^{**2} > = 0.000000 125a -> 128a : 0.093294 (c= 0.30544074) 125a -> 130a : 0.014512 (c= 0.12046712) 126a -> 128a : 0.734613 (c= 0.85709550) 127a -> 130a : 0.098188 (c= 0.31335007)
	2 30390.1 329.1 0.000009486	STATE 1: E= 0.121198 au 3.298 eV 26600.0 cm ^{**} -1 <S ^{**2} > = 0.000000 126a -> 127a : 0.958550 (c= -0.97905572) 126a -> 129a : 0.020325 (c= -0.14256414)
	3 31316.4 319.3 0.353213004	

		<p>STATE 2: E= 0.138468 au 3.768 eV 30390.1 cm⁻¹ <S²> = 0.000000 125a -> 127a : 0.972326 (c= -0.98606570) 125a -> 129a : 0.019537 (c= -0.13977309)</p> <p>STATE 3: E= 0.142688 au 3.883 eV 31316.4 cm⁻¹ <S²> = 0.000000 123a -> 127a : 0.106187 (c= -0.32586339) 123a -> 129a : 0.016953 (c= 0.13020313) 124a -> 127a : 0.826608 (c= -0.90917960)</p>
4d	<p>1 28114.0 355.7 0.758649112 2 32351.5 309.1 0.046029421 3 33518.7 298.3 0.105717891</p>	<p>STATE 1: E= 0.128097 au 3.486 eV 28114.0 cm⁻¹ <S²> = 0.000000 111a -> 112a : 0.971124 (c= -0.98545601)</p> <p>STATE 2: E= 0.147404 au 4.011 eV 32351.5 cm⁻¹ <S²> = 0.000000 109a -> 112a : 0.047261 (c= -0.21739689) 109a -> 113a : 0.043346 (c= -0.20819722) 109a -> 114a : 0.011932 (c= 0.10923302) 110a -> 112a : 0.810595 (c= -0.90033048) 111a -> 113a : 0.041884 (c= -0.20465666)</p> <p>STATE 3: E= 0.152722 au 4.156 eV 33518.7 cm⁻¹ <S²> = 0.000000 109a -> 112a : 0.010431 (c= 0.10213395) 110a -> 112a : 0.055189 (c= -0.23492372) 111a -> 113a : 0.809555 (c= 0.89975297) 111a -> 115a : 0.083501 (c= 0.28896486)</p>
4e	<p>1 26500.2 377.4 0.707712188 2 30574.0 327.1 0.014845948 3 31816.2 314.3 0.244345473</p>	<p>STATE 1: E= 0.120744 au 3.286 eV 26500.2 cm⁻¹ <S²> = 0.000000 135a -> 136a : 0.952880 (c= -0.97615571) 135a -> 138a : 0.014714 (c= -0.12130176)</p> <p>STATE 2: E= 0.139306 au 3.791 eV 30574.0 cm⁻¹ <S²> = 0.000000 135a -> 139a : 0.926021 (c= 0.96230006) 135a -> 140a : 0.010780 (c= 0.10382794) 135a -> 141a : 0.011292 (c= 0.10626289)</p> <p>STATE 3: E= 0.144965 au 3.945 eV 31816.2 cm⁻¹ <S²> = 0.000000 133a -> 136a : 0.034409 (c= 0.18549636) 133a -> 138a : 0.023264 (c= -0.15252491) 134a -> 136a : 0.789767 (c= 0.88868851) 135a -> 136a : 0.013327 (c= 0.11544249)</p>

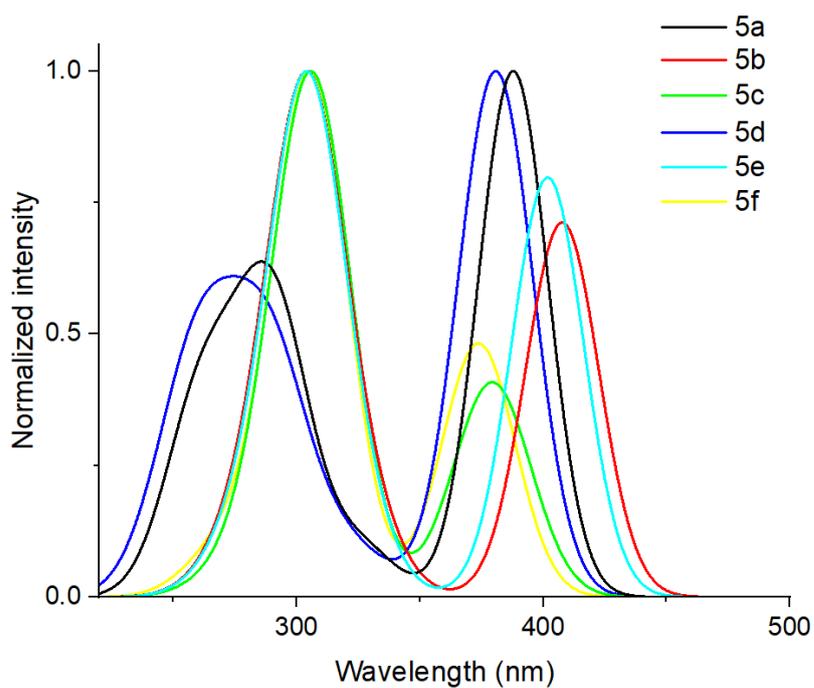
				135a -> 137a : 0.020598 (c= 0.14351845) 135a -> 138a : 0.068068 (c= -0.26089876)
4f	1 27847.0 359.1 0.477044445 2 31191.7 320.6 0.188438477 3 31801.3 314.5 0.000007003			STATE 1: E= 0.126880 au 3.453 eV 27847.0 cm ⁻¹ <S ² > = 0.000000 134a -> 135a : 0.935698 (c= 0.96731475) 134a -> 136a : 0.021599 (c= -0.14696519) 134a -> 137a : 0.018211 (c= 0.13494968) STATE 2: E= 0.142120 au 3.867 eV 31191.7 cm ⁻¹ <S ² > = 0.000000 131a -> 135a : 0.036993 (c= 0.19233585) 131a -> 137a : 0.028225 (c= -0.16800268) 132a -> 135a : 0.879045 (c= 0.93757414) 132a -> 136a : 0.012680 (c= 0.11260730) STATE 3: E= 0.144897 au 3.943 eV 31801.3 cm ⁻¹ <S ² > = 0.000000 133a -> 135a : 0.952008 (c= -0.97570880) 133a -> 136a : 0.022349 (c= 0.14949546) 133a -> 137a : 0.020078 (c= -0.14169529)
5a	1 25784.3 387.8 0.925073934 2 30712.9 325.6 0.088284344 3 34106.1 293.2 0.333398738			STATE 1: E= 0.117482 au 3.197 eV 25784.3 cm ⁻¹ <S ² > = 0.000000 103a -> 104a : 0.982155 (c= 0.99103754) STATE 2: E= 0.139938 au 3.808 eV 30712.9 cm ⁻¹ <S ² > = 0.000000 101a -> 104a : 0.027726 (c= -0.16651031) 102a -> 105a : 0.023762 (c= -0.15414900) 103a -> 105a : 0.938808 (c= 0.96892086) STATE 3: E= 0.155399 au 4.229 eV 34106.1 cm ⁻¹ <S ² > = 0.000000 101a -> 104a : 0.256735 (c= -0.50668999) 101a -> 105a : 0.043712 (c= -0.20907325) 102a -> 104a : 0.546752 (c= 0.73942683) 102a -> 105a : 0.060121 (c= -0.24519633) 103a -> 105a : 0.015764 (c= -0.12555671) 103a -> 107a : 0.022849 (c= -0.15115759)
5b	1 24528.2 407.7 0.790599243 2 30493.6 327.9 0.087947143 3 30565.1 327.2 0.042070589 4 32668.7 306.1 0.704585824			STATE 1: E= 0.111759 au 3.041 eV 24528.2 cm ⁻¹ <S ² > = 0.000000 127a -> 128a : 0.972238 (c= 0.98602136) STATE 2: E= 0.138939 au 3.781 eV 30493.6 cm ⁻¹ <S ² > = 0.000000 126a -> 129a : 0.012839 (c= -0.11330900)

		<p>127a -> 129a : 0.686052 (c= 0.82828273) 127a -> 130a : 0.225419 (c= 0.47478273) 127a -> 131a : 0.041551 (c= 0.20384137)</p> <p>STATE 3: E= 0.139265 au 3.790 eV 30565.1 cm⁻¹ <S²> = 0.000000 127a -> 129a : 0.241908 (c= 0.49184108) 127a -> 130a : 0.704401 (c= -0.83928571)</p> <p>STATE 4: E= 0.148850 au 4.050 eV 32668.7 cm⁻¹ <S²> = 0.000000 125a -> 128a : 0.050437 (c= 0.22458200) 126a -> 128a : 0.412347 (c= -0.64214241) 127a -> 129a : 0.014647 (c= 0.12102642) 127a -> 131a : 0.445252 (c= -0.66727181)</p>
5c	<p>1 26367.6 379.3 0.483467416 2 30393.1 329.0 0.000000727 3 32569.2 307.0 0.929865279</p>	<p>STATE 1: E= 0.120139 au 3.269 eV 26367.6 cm⁻¹ <S²> = 0.000000 126a -> 127a : 0.965679 (c= 0.98268951) 126a -> 130a : 0.016847 (c= -0.12979607)</p> <p>STATE 2: E= 0.138481 au 3.768 eV 30393.1 cm⁻¹ <S²> = 0.000000 125a -> 127a : 0.977074 (c= 0.98847078) 125a -> 130a : 0.015066 (c= -0.12274525)</p> <p>STATE 3: E= 0.148396 au 4.038 eV 32569.2 cm⁻¹ <S²> = 0.000000 123a -> 127a : 0.070011 (c= -0.26459549) 123a -> 128a : 0.020835 (c= -0.14434439) 124a -> 127a : 0.768614 (c= 0.87670651) 126a -> 128a : 0.012922 (c= -0.11367703) 126a -> 129a : 0.069868 (c= -0.26432480)</p>
5d	<p>1 26267.4 380.7 0.976773127 2 31025.3 322.3 0.083638581 3 34178.6 292.6 0.235254227</p>	<p>STATE 1: E= 0.119683 au 3.257 eV 26267.4 cm⁻¹ <S²> = 0.000000 111a -> 112a : 0.980408 (c= -0.99015576)</p> <p>STATE 2: E= 0.141362 au 3.847 eV 31025.3 cm⁻¹ <S²> = 0.000000 109a -> 112a : 0.038052 (c= -0.19506998) 110a -> 113a : 0.028844 (c= 0.16983573) 111a -> 113a : 0.922615 (c= -0.96052875)</p> <p>STATE 3: E= 0.155729 au 4.238 eV 34178.6 cm⁻¹ <S²> = 0.000000 109a -> 112a : 0.367505 (c= -0.60622151)</p>

		109a -> 113a : 0.038445 (c= 0.19607512) 110a -> 112a : 0.402840 (c= 0.63469680) 110a -> 113a : 0.085665 (c= 0.29268636) 111a -> 113a : 0.027844 (c= 0.16686426) 111a -> 115a : 0.030037 (c= -0.17331191)
5e	1 24890.5 401.8 0.844724557 2 30534.0 327.5 0.016394603 3 30942.4 323.2 0.115123211	STATE 1: E= 0.113409 au 3.086 eV 24890.5 cm ⁻¹ <S ² > = 0.000000 135a -> 136a : 0.970602 (c= 0.98519128) STATE 2: E= 0.139123 au 3.786 eV 30534.0 cm ⁻¹ <S ² > = 0.000000 135a -> 138a : 0.938965 (c= -0.96900201) STATE 3: E= 0.140984 au 3.836 eV 30942.4 cm ⁻¹ <S ² > = 0.000000 133a -> 136a : 0.020948 (c= -0.14473298) 134a -> 137a : 0.024037 (c= -0.15503896) 135a -> 137a : 0.902843 (c= -0.95018052) 135a -> 139a : 0.023746 (c= -0.15409703)
5f	1 26754.5 373.8 0.530879882 2 30843.4 324.2 0.000005202 3 32596.7 306.8 0.829471138	STATE 1: E= 0.121902 au 3.317 eV 26754.5 cm ⁻¹ <S ² > = 0.000000 134a -> 135a : 0.962479 (c= -0.98106036) 134a -> 138a : 0.018462 (c= 0.13587420) STATE 2: E= 0.140533 au 3.824 eV 30843.4 cm ⁻¹ <S ² > = 0.000000 133a -> 135a : 0.974352 (c= 0.98709288) 133a -> 138a : 0.017249 (c= -0.13133551) STATE 3: E= 0.148522 au 4.041 eV 32596.7 cm ⁻¹ <S ² > = 0.000000 131a -> 135a : 0.104886 (c= -0.32386105) 131a -> 136a : 0.022135 (c= -0.14877842) 132a -> 135a : 0.704476 (c= 0.83933045) 132a -> 136a : 0.012422 (c= -0.11145288) 134a -> 136a : 0.013011 (c= -0.11406696) 134a -> 137a : 0.094205 (c= -0.30692844)



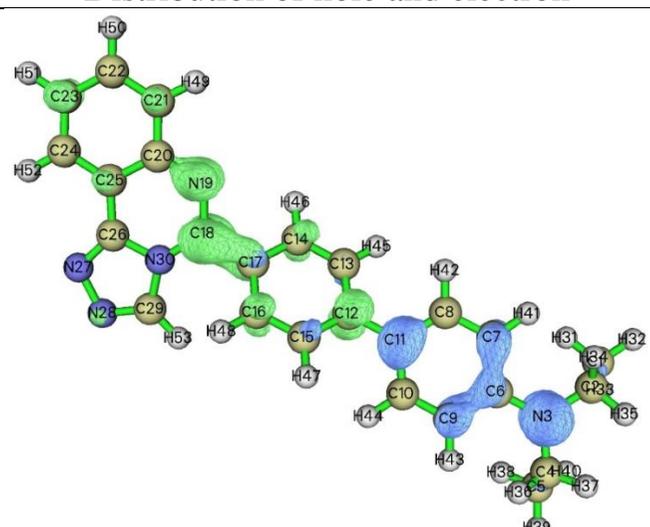
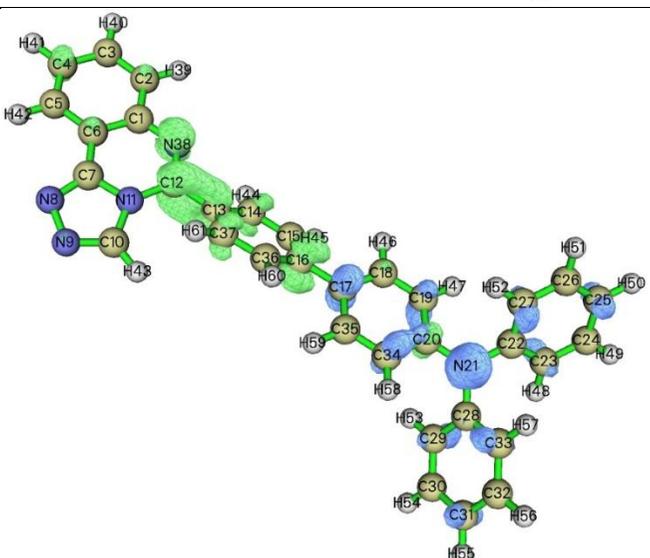
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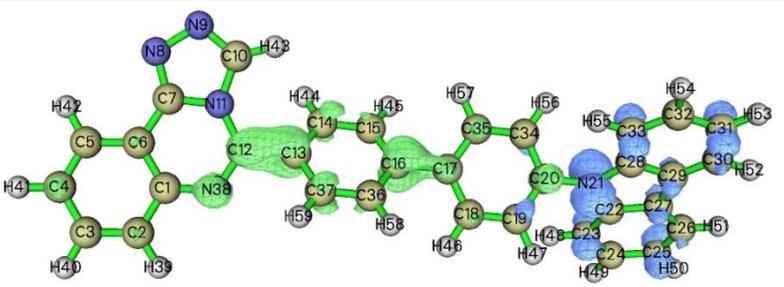
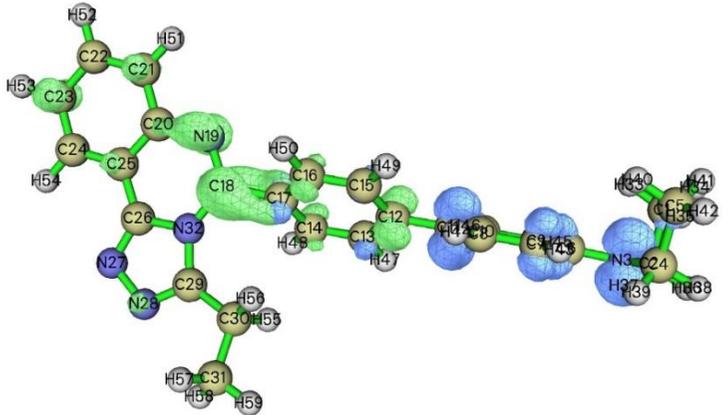
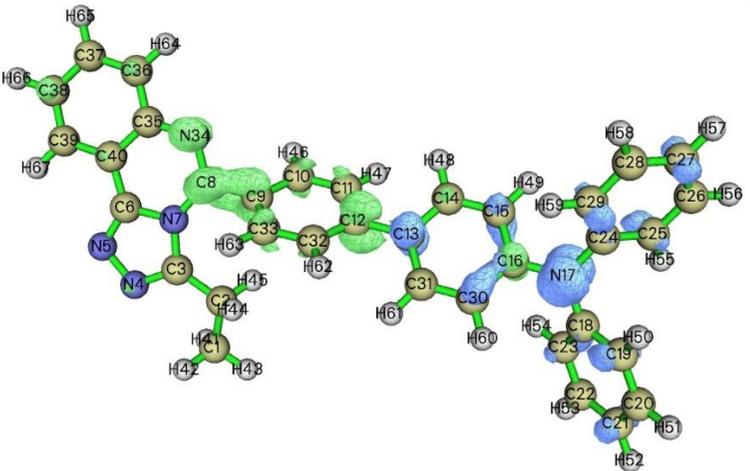


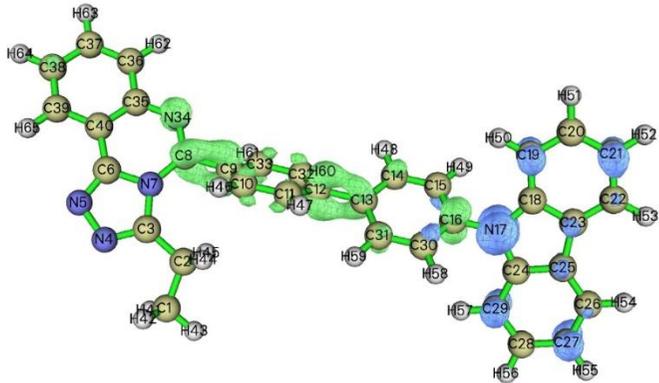
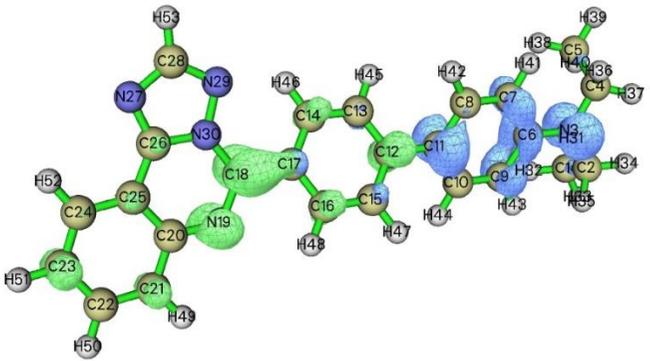
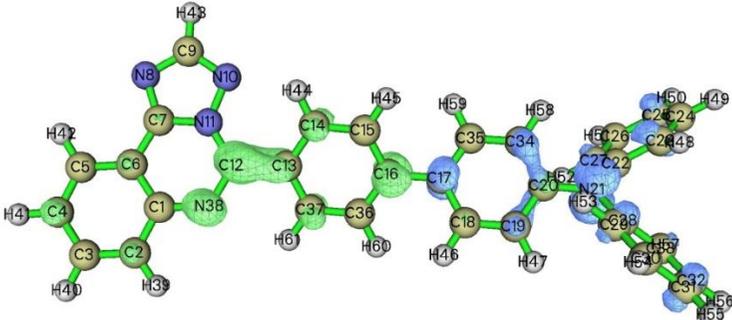
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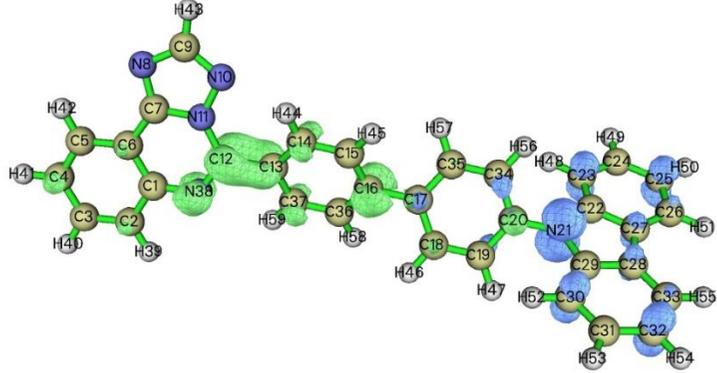
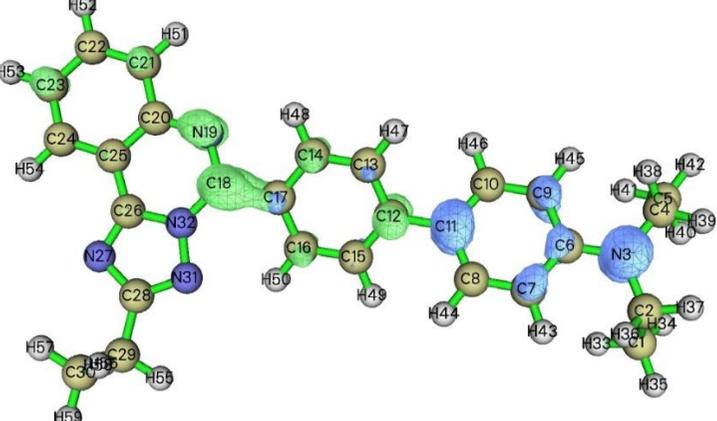
Figure S26. Computed absorption spectra for compounds **4a-f** (a) and **5a-f** (b).

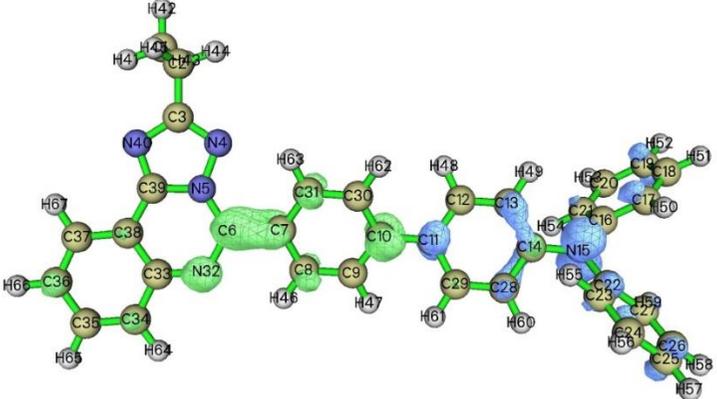
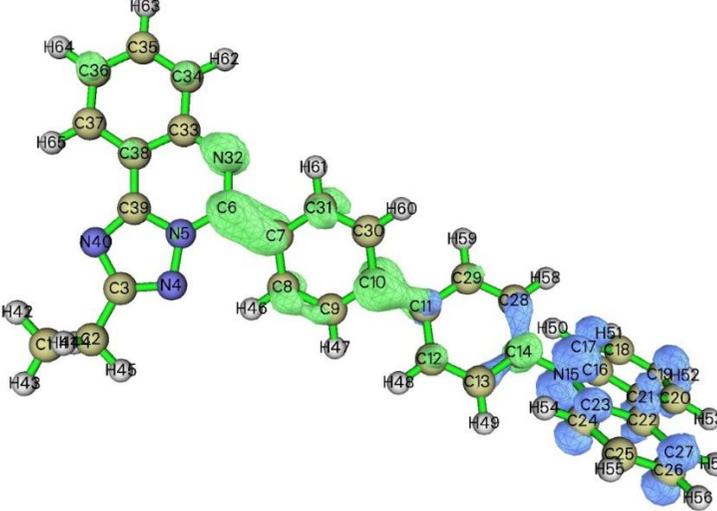
Table S20. Hole-electron interaction analysis result for compounds **4**, **5**.

Comp	Sr(a.u.)	D index (Å)	H index (Å)	t index (Å)	Ec	HDI/EDI	Distribution of hole and electron
4a	0.50544	6.310	3.719	2.895	3.08	8.81/ 6.80	
4b	0.50926	6.850	4.106	3.163	2.76	8.09/ 5.97	

4c	0.39654	7.830	3.934	4.350	2.42	7.99/5.85	
4d	0.50724	6.356	3.755	2.951	2.98	8.44/ 6.79	
4e	0.52832	6.586	4.149	2.880	2.79	8.19/ 5.64	

4f	0.45366	6.982	4.116	3.333	2.66	7.79/5.61	
5a	0.49229	6.546	3.698	3.176	2.94	8.67/ 6.77	
5b	0.48785	7.272	4.074	3.620	2.63	8.07/6.11	

5c	0.40714	8.170	3.994	4.616	2.34	7.74/ 5.98	 <p>ORTEP diagram of compound 5c, showing the molecular structure with atoms labeled C1 through C33, N8 through N11, and H4 through H59. The structure is a complex polycyclic system with multiple nitrogen atoms and a central ring system.</p>
5d	0.51262	6.317	3.748	3.026	2.85	8.48/ 6.65	 <p>ORTEP diagram of compound 5d, showing the molecular structure with atoms labeled C1 through C30, N3 through N7, and H1 through H59. The structure is a complex polycyclic system with multiple nitrogen atoms and a central ring system.</p>

5e	0.50296	7.018	4.104	3.406	2.61	8.06/6.03	 <p>ORTEP diagram of compound 5e, showing the molecular structure with atoms labeled C1 through C39, N1 through N5, and H1 through H65. The structure is a complex polycyclic system with multiple rings and substituents.</p>
5f	0.42992	7.809	4.068	4.233	2.38	7.82/5.83	 <p>ORTEP diagram of compound 5f, showing the molecular structure with atoms labeled C1 through C39, N1 through N5, and H1 through H65. The structure is a complex polycyclic system with multiple rings and substituents, similar to 5e but with a different conformation.</p>

