

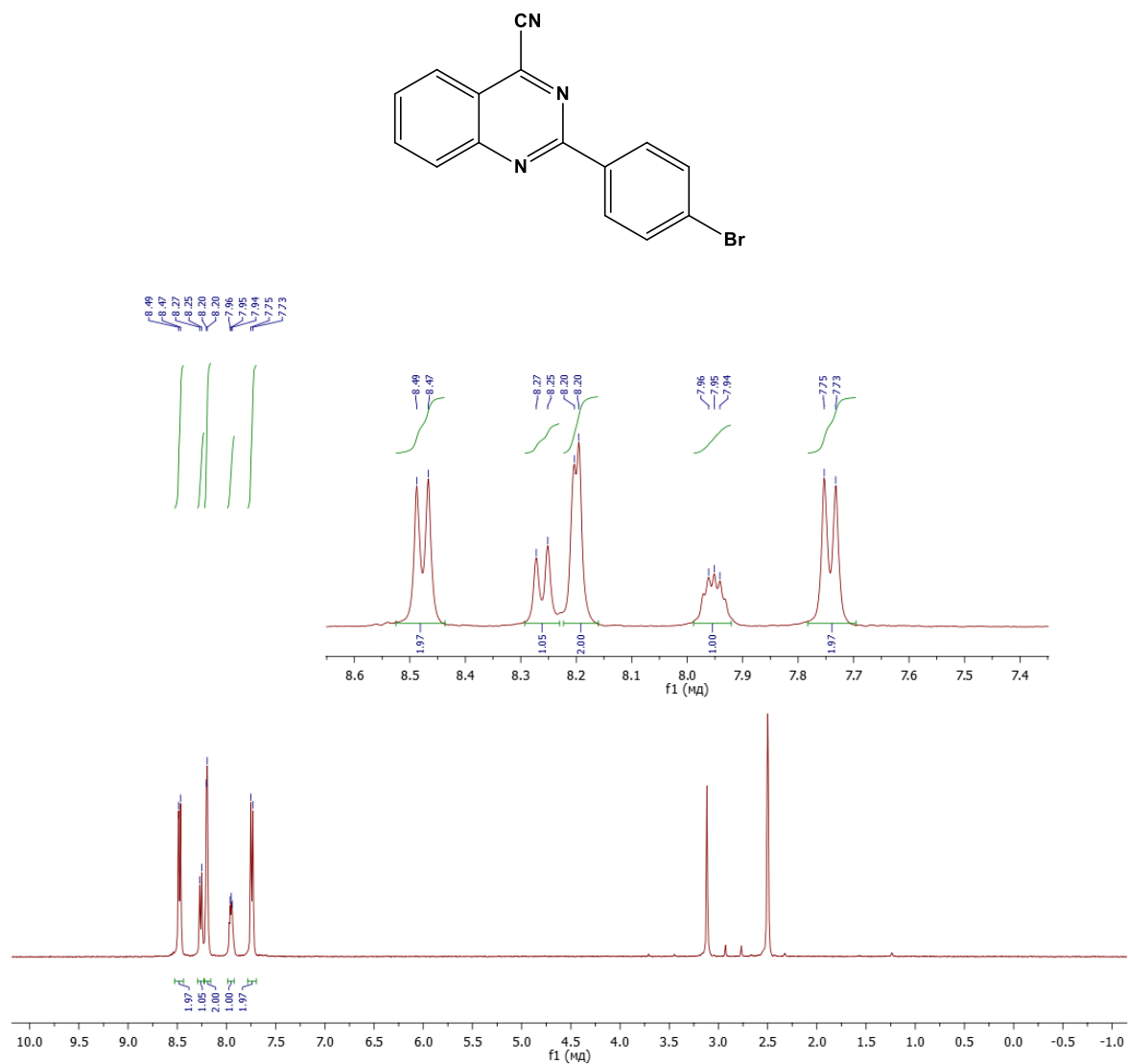
Push-pull structures based on 2-aryl/thienyl substituted quinazolin-4(3*H*)-ones and 4-cyanoquinazolines

Tatyana N. Moshkina, Emiliya V. Nosova, Julia V. Permyakova, Galina N. Lipunova, Ekaterina F. Zhilina, Grigory A. Kim, Pavel A. Slepukhin, Valery N. Charushin

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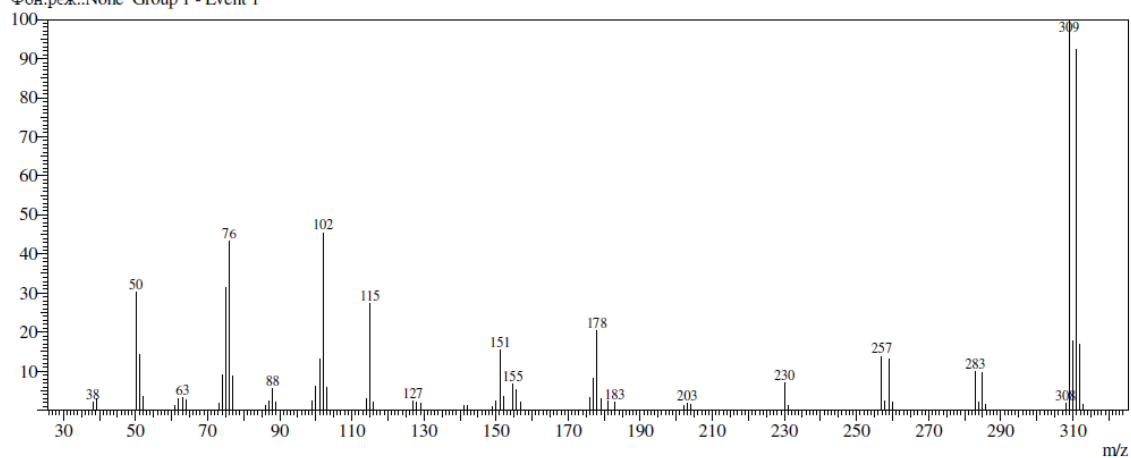
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1. NMR and mass spectra of bromophenyl intermediates.



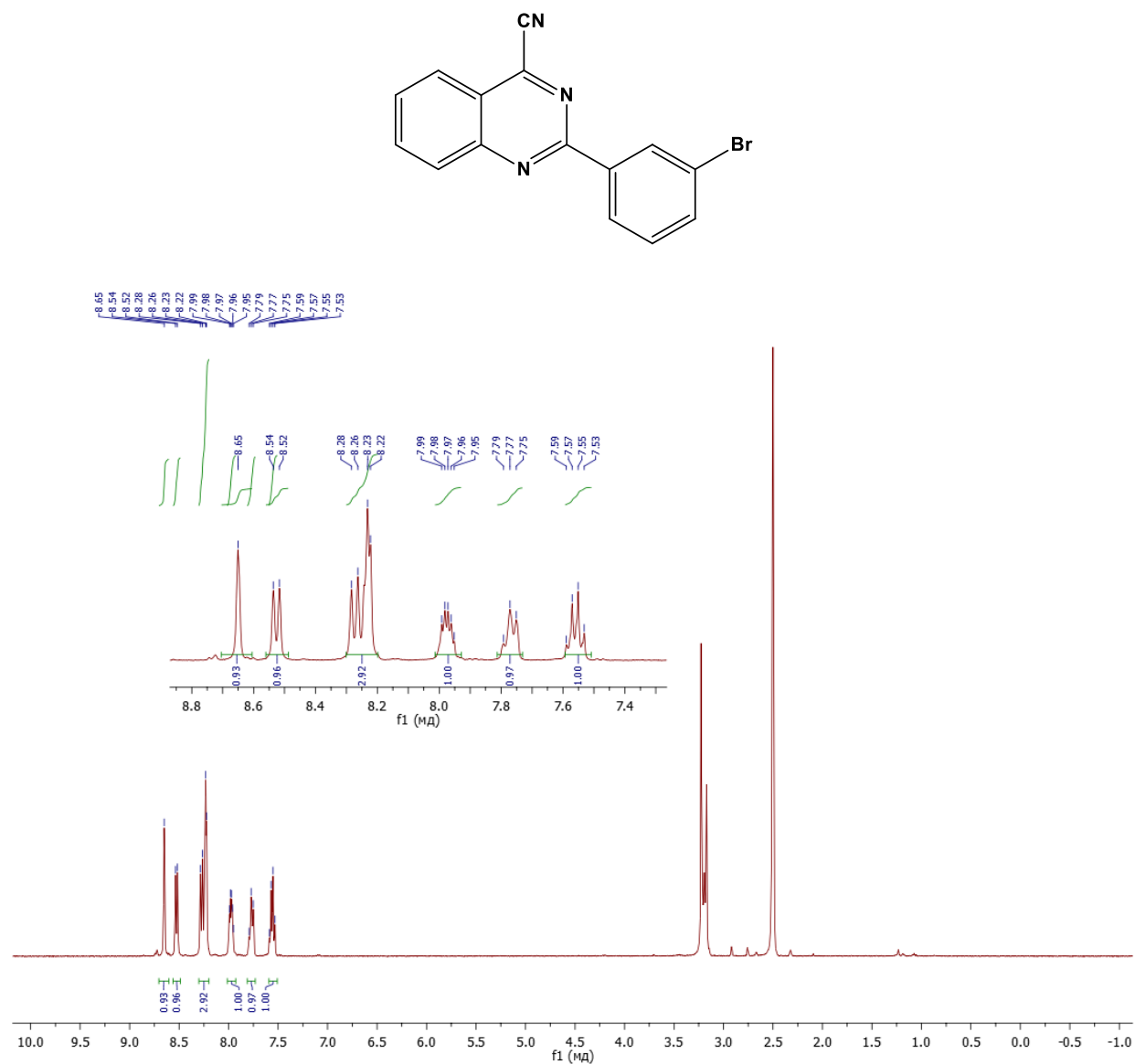
a

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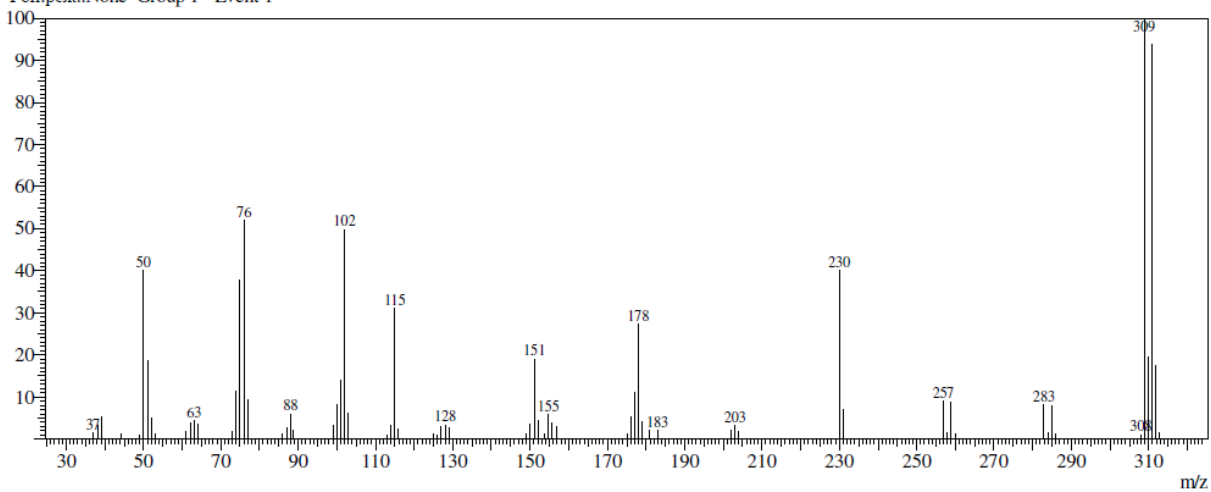
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Figure S1. ¹H NMR spectrum (a) in DMSO-d₆ and mass spectrum (b) of 2-(4-bromophenyl)-4-cyanoquinazoline.



a

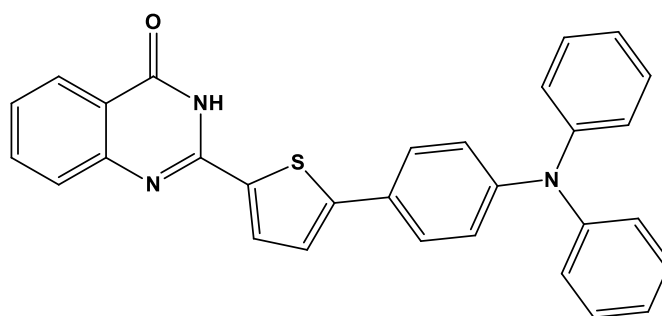
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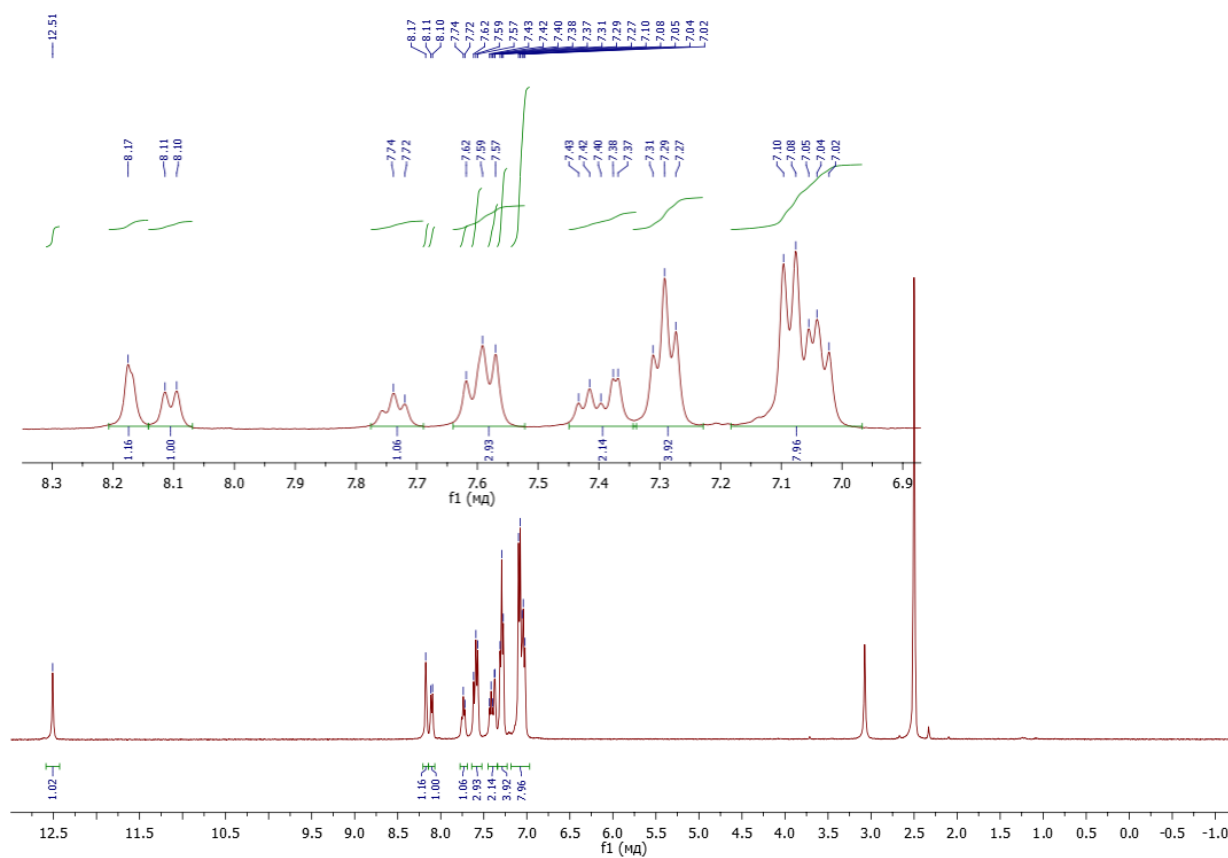
b

Figure S2. ¹H NMR spectrum (a) in DMSO-d₆ and mass spectrum (b) of 2-(3-bromophenyl)-4-cyanoquinazoline.

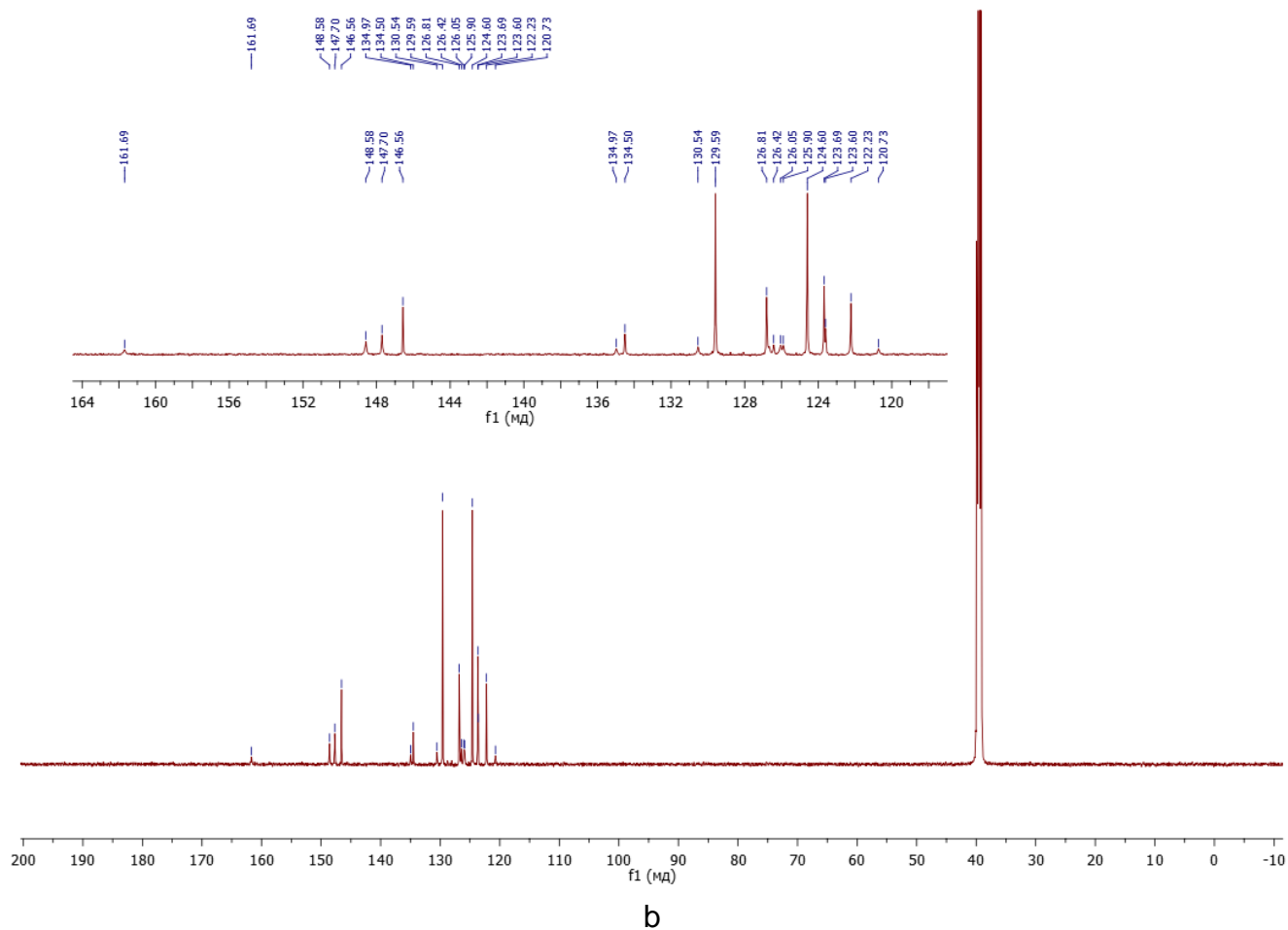
2. NMR and mass spectra of target compounds 4-6, 8, 9, 11.



4b



a



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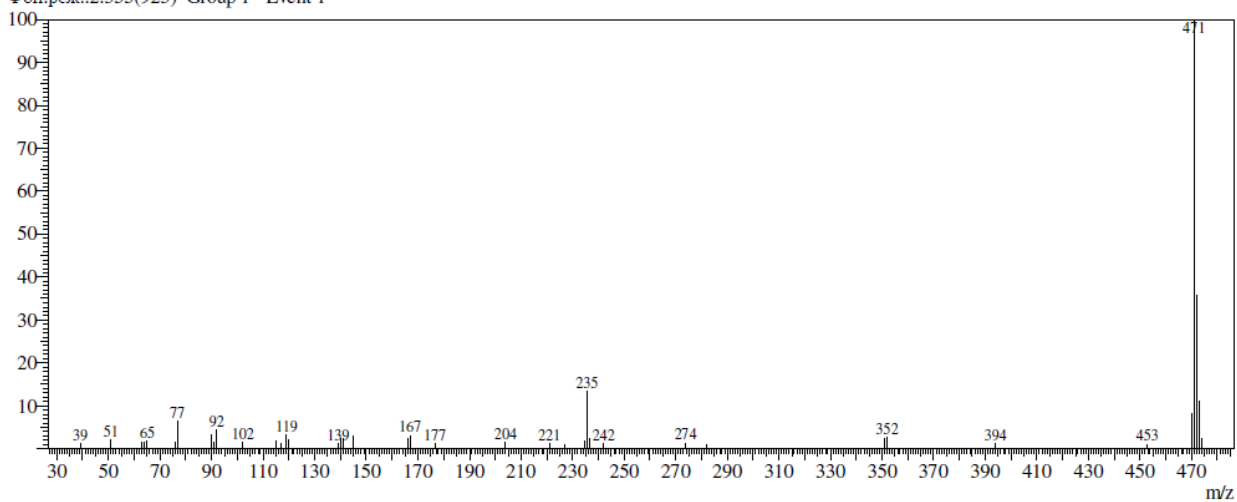
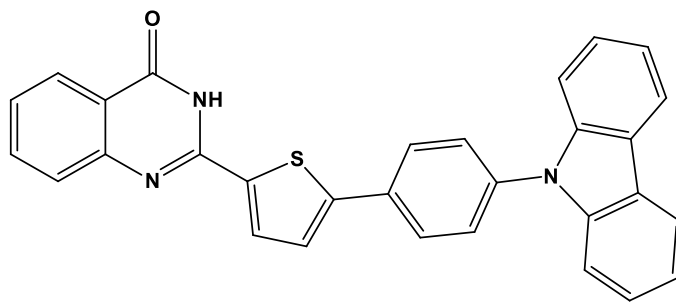
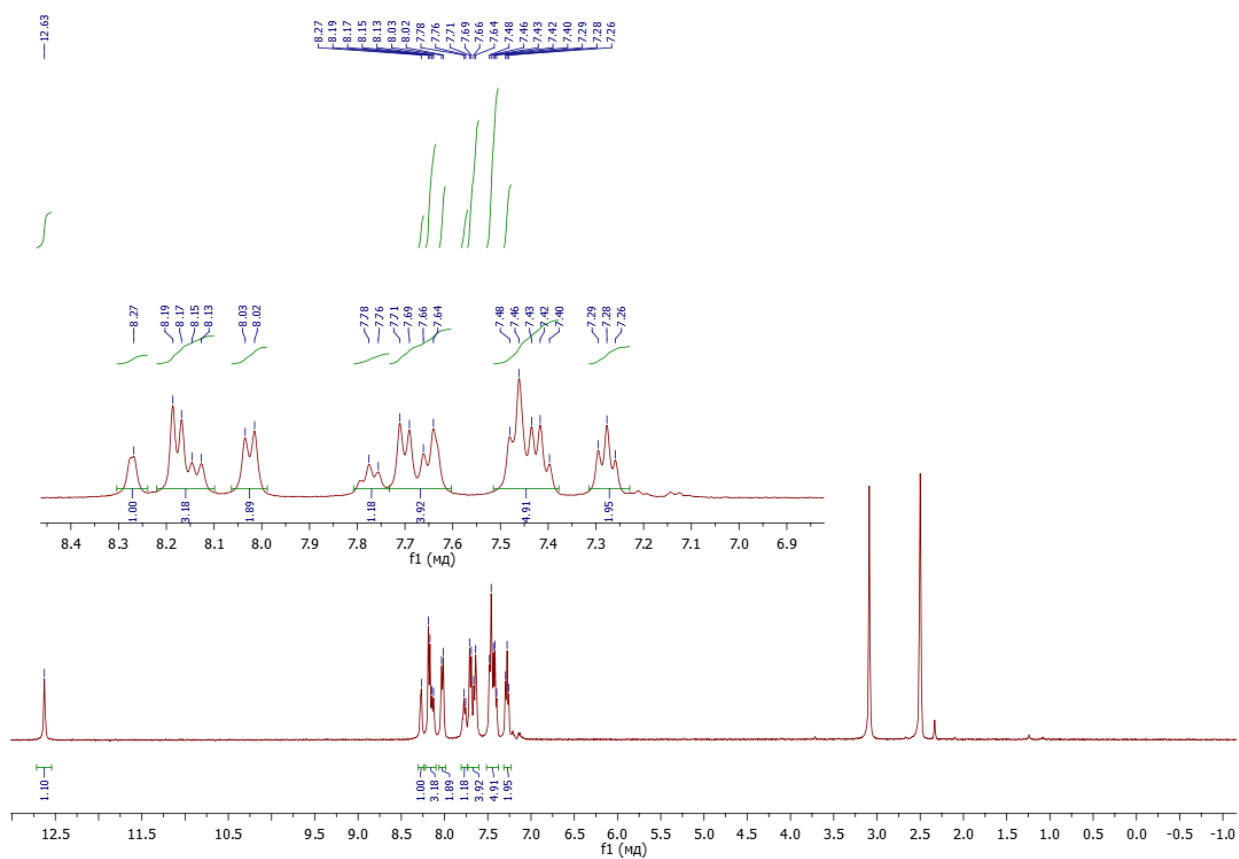


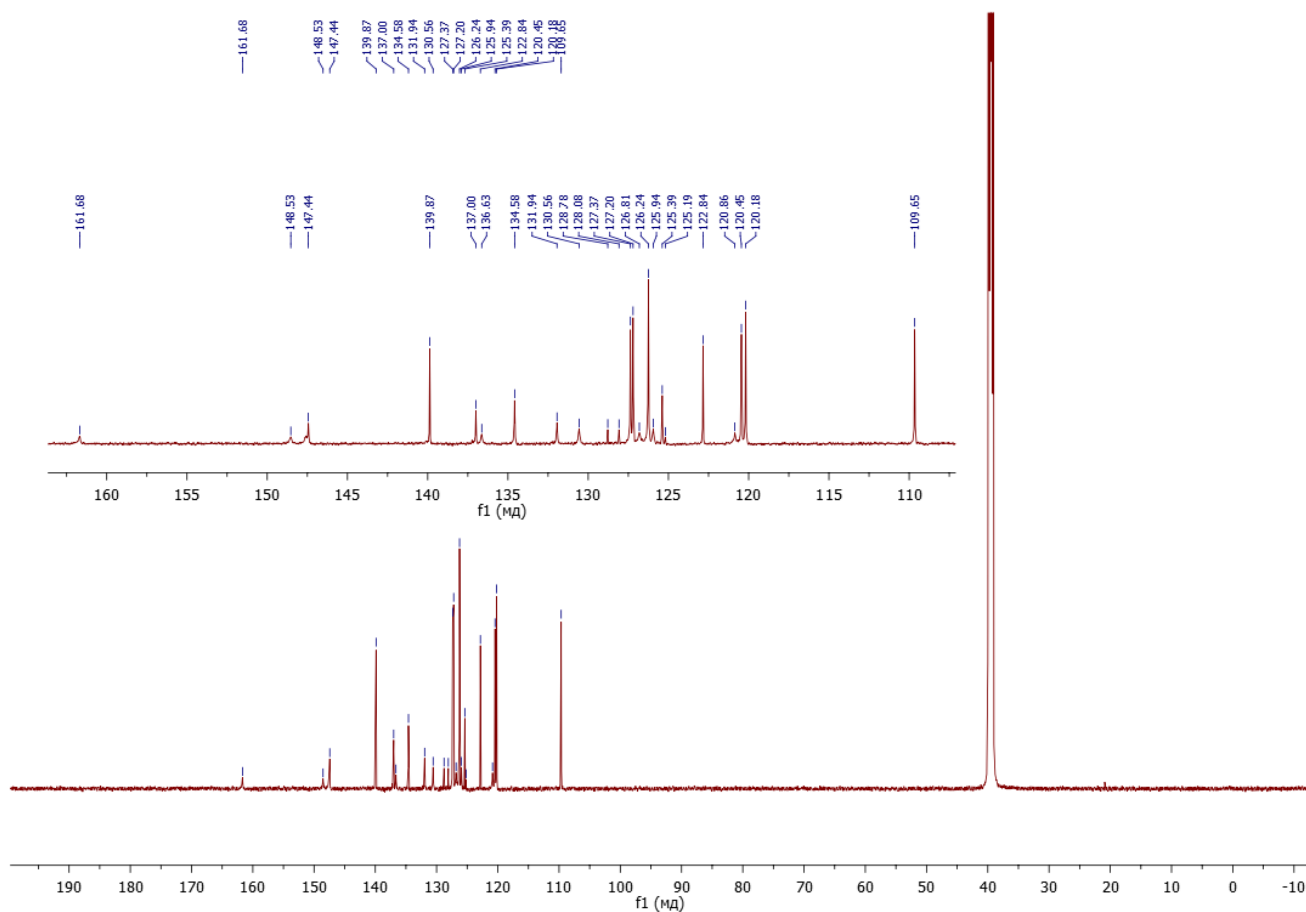
Figure S3. ¹H NMR spectrum (a) and ¹³C NMR spectrum in DMSO-d₆ (b); mass spectrum (c) of **4b**.



4c

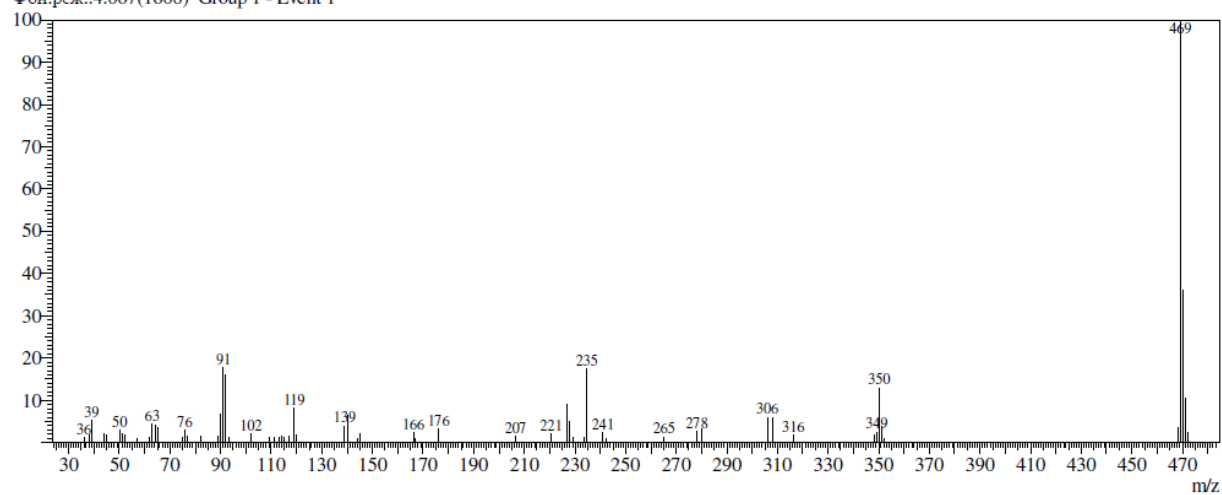


a



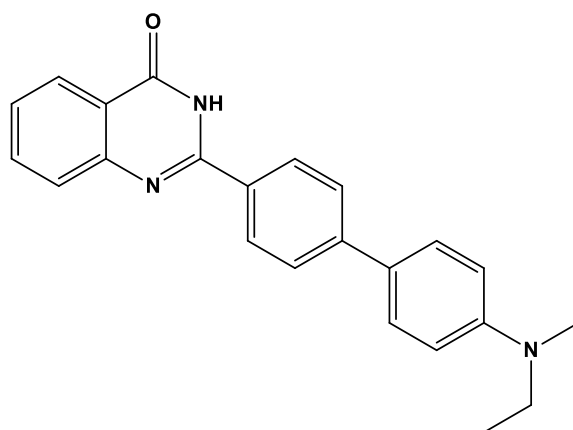
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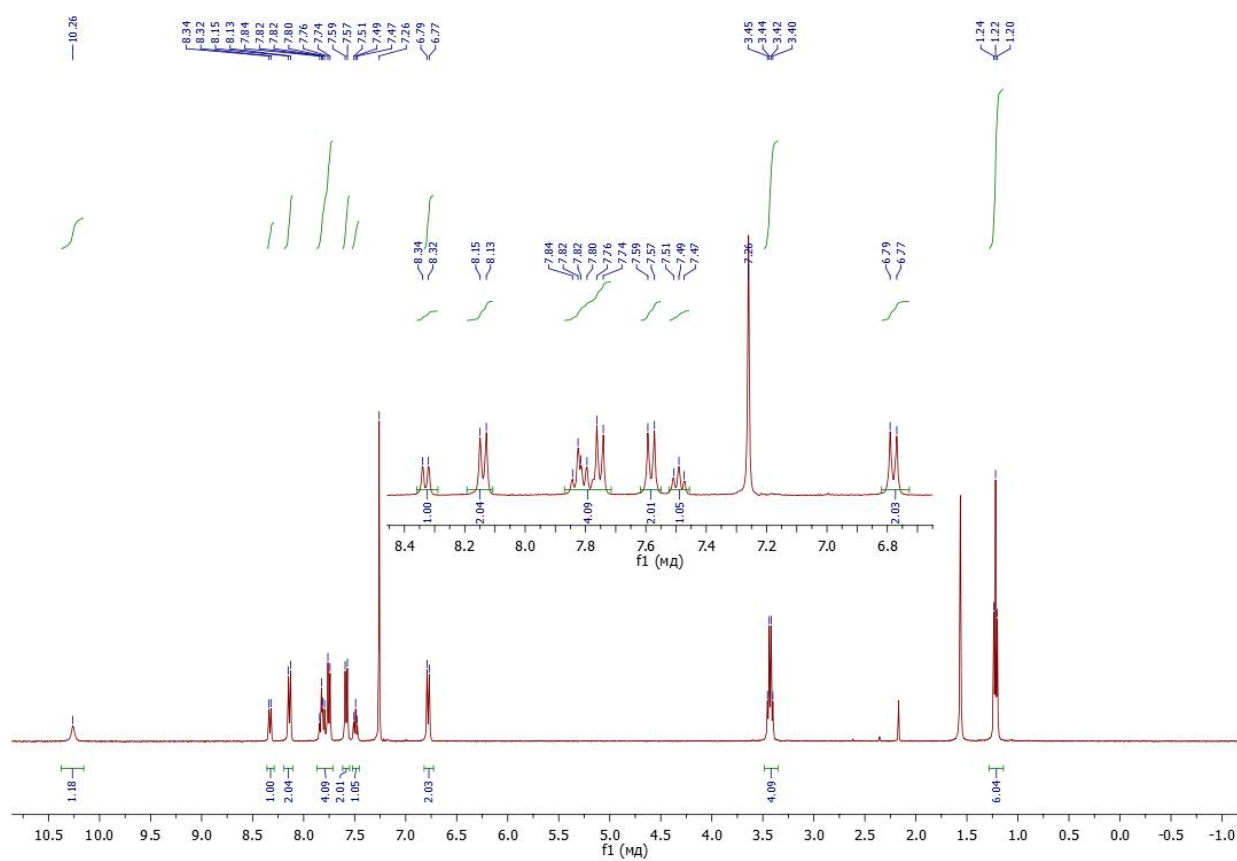


c

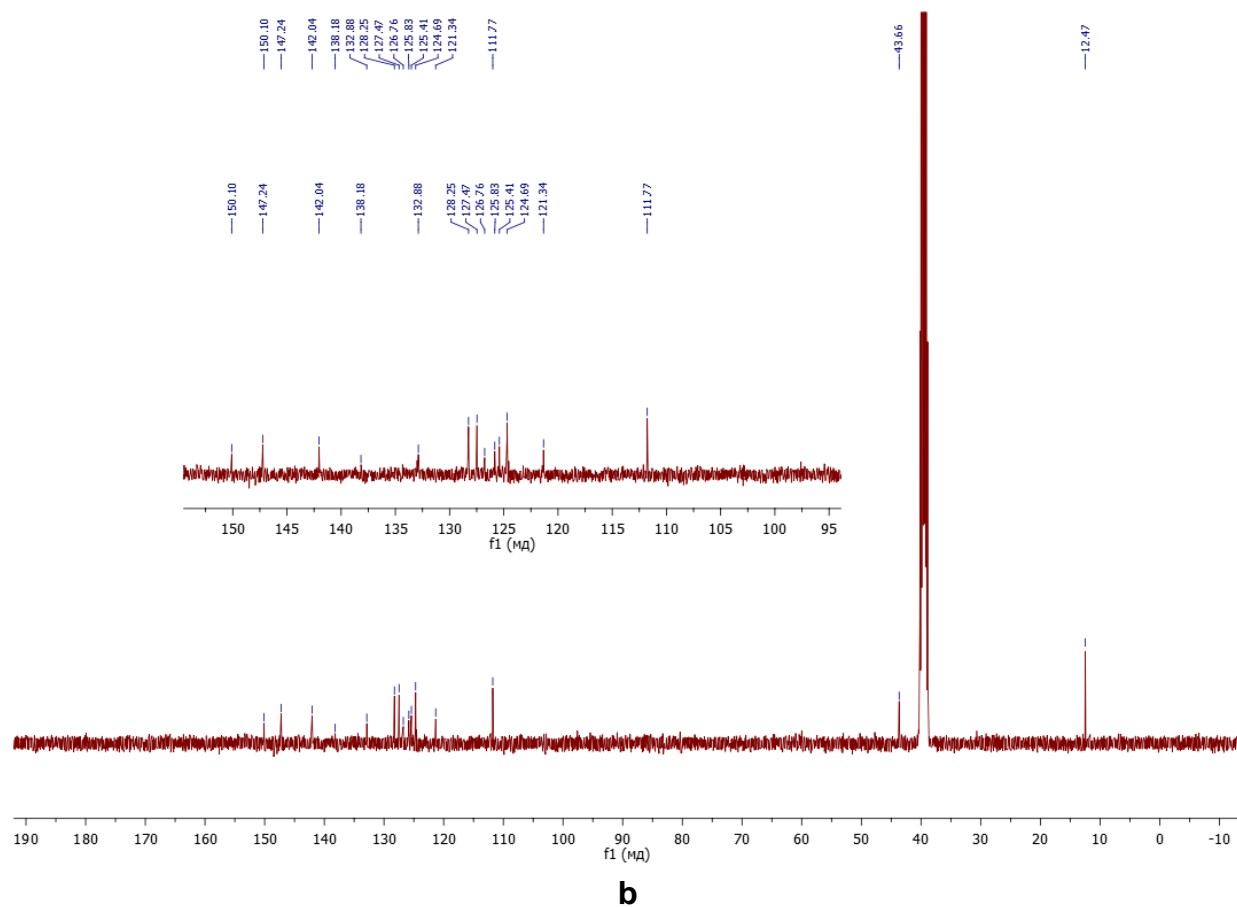
Figure S4. ¹H NMR spectrum (a) and ¹³C NMR spectrum in DMSO-d₆ (b); mass spectrum (c) of **4c**.



5a



a



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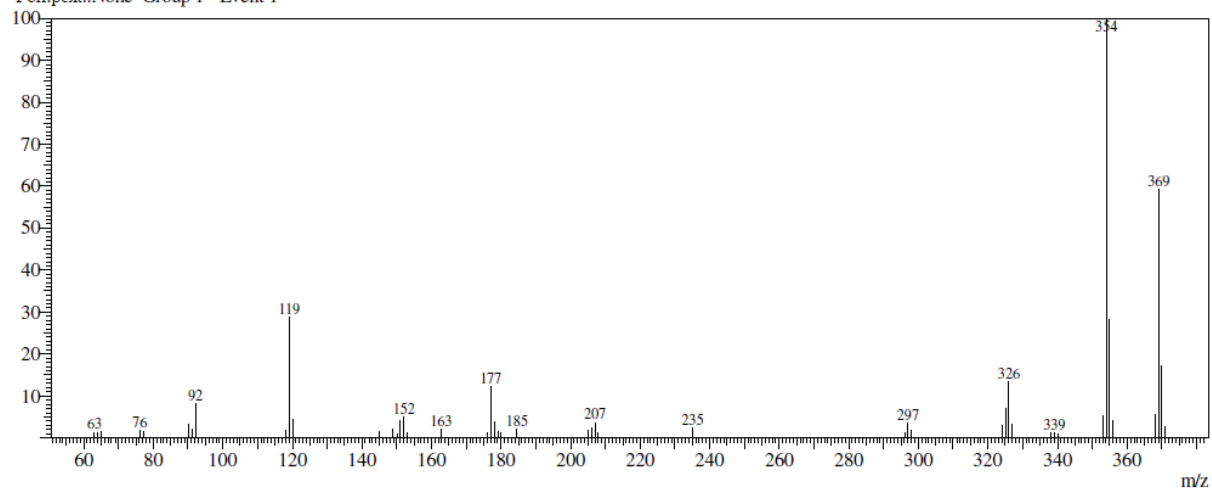
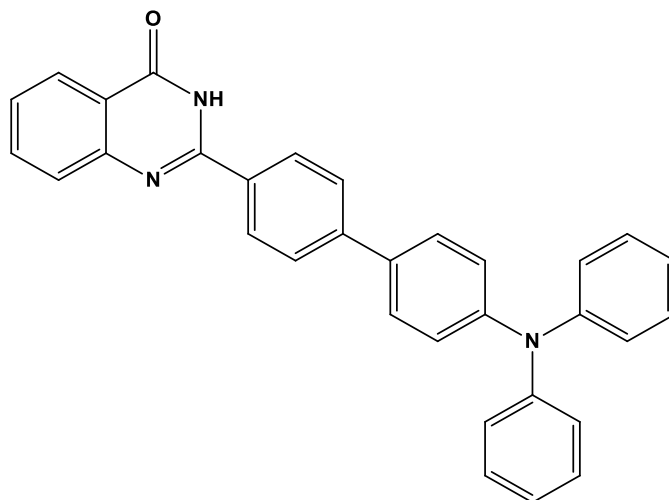
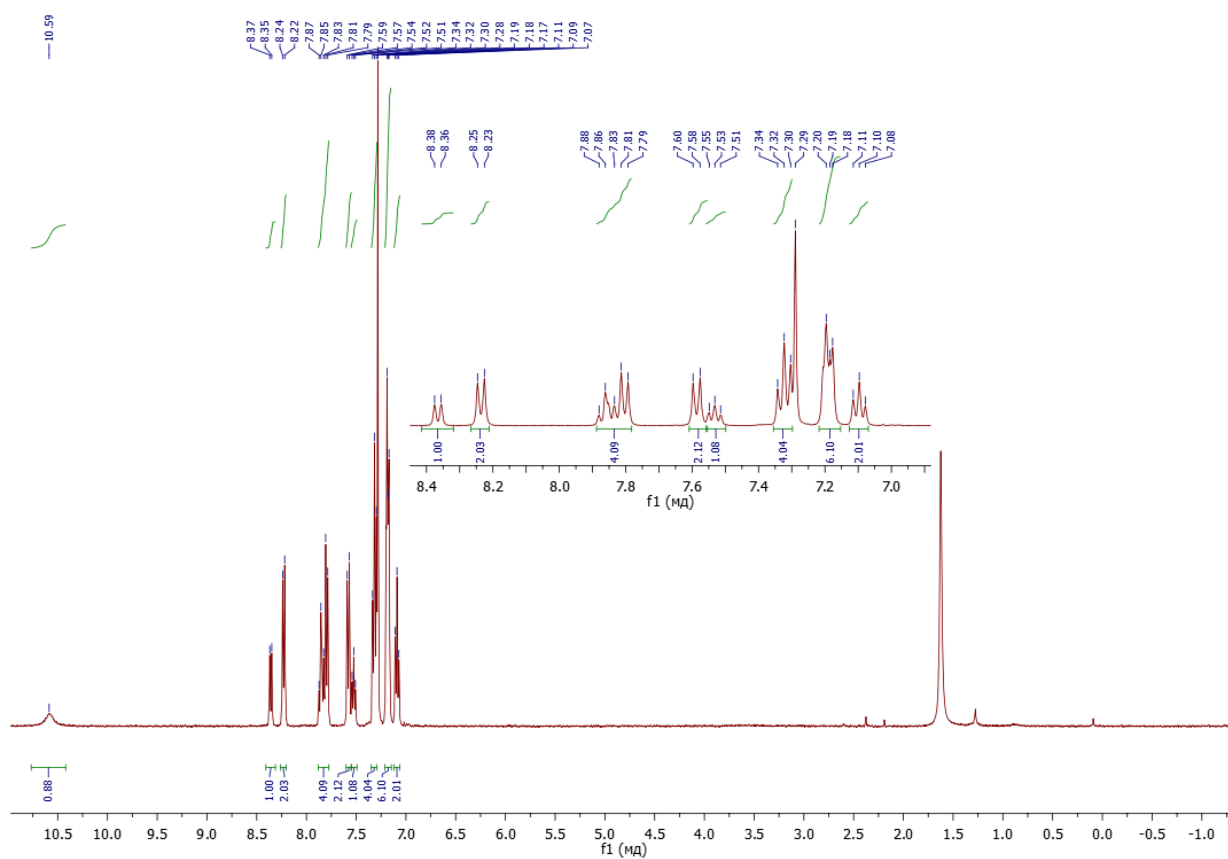


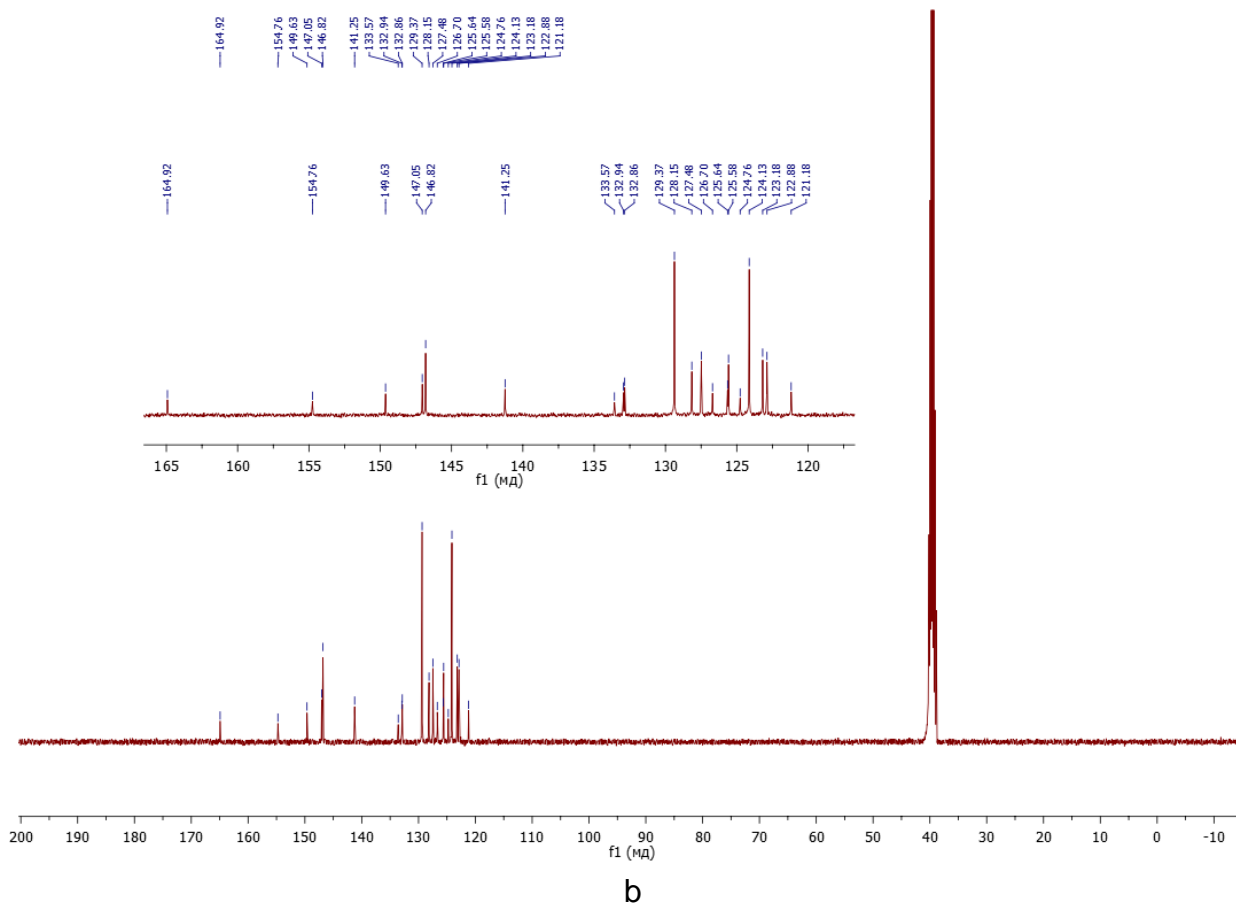
Figure S5. ^1H NMR spectrum in DCCl_3 (a) and ^{13}C NMR spectrum in DMSO-d_6 (b); mass spectrum (c) of **5a**.



5b



a



Line#:1 R.Time:5.685(Scan#:2255)
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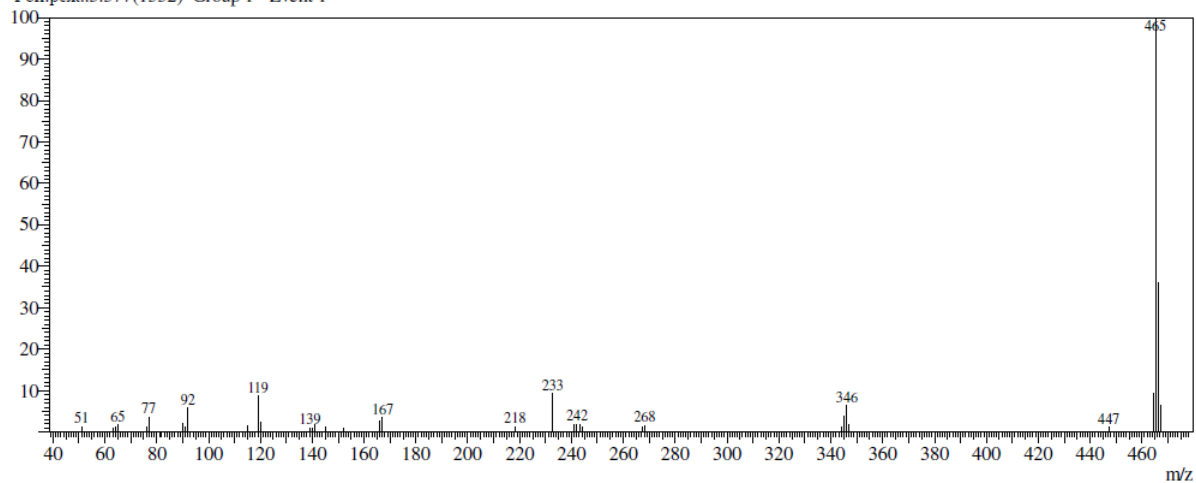
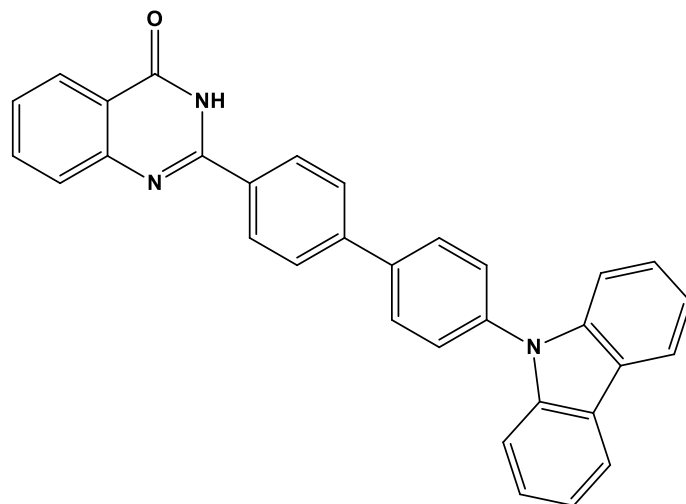
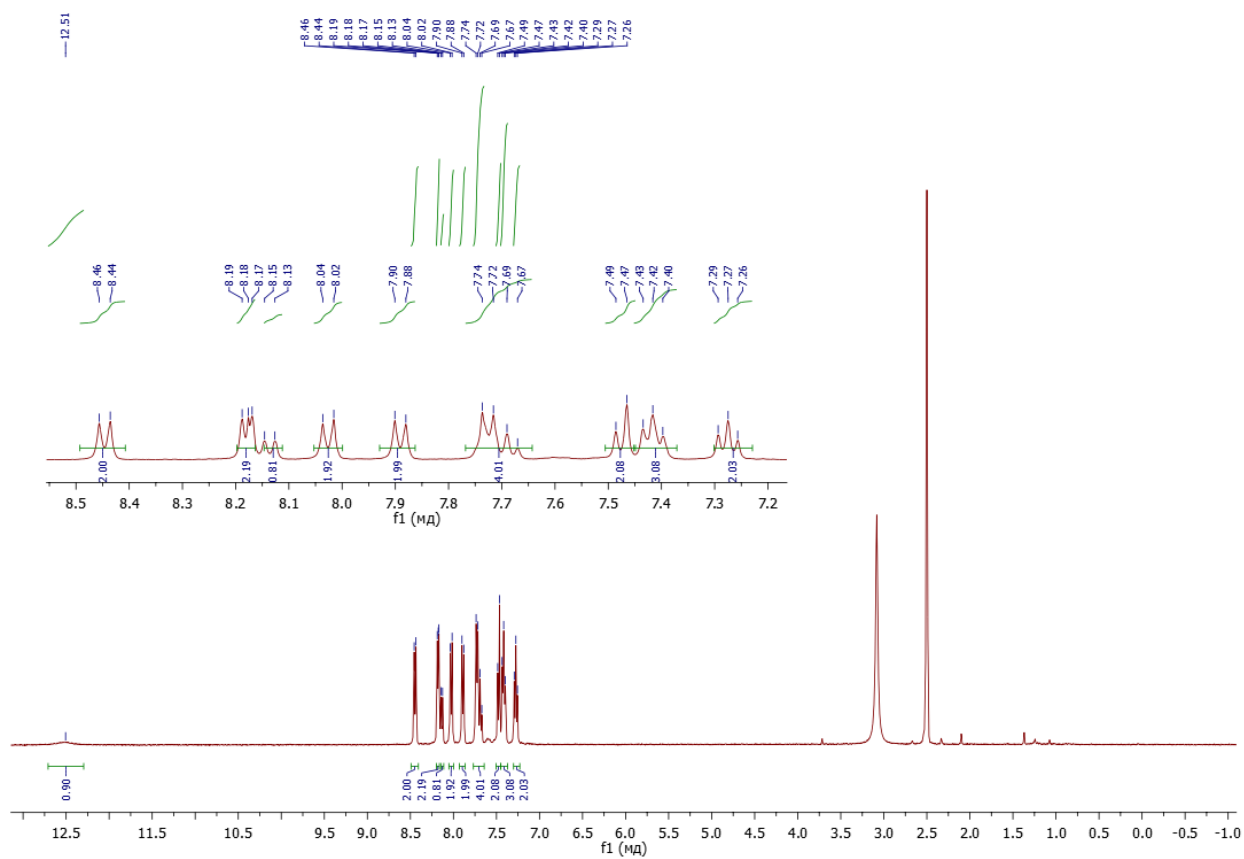


Figure S6. ^1H NMR spectrum in DCCl_3 (a) and ^{13}C NMR spectrum in DMSO-d_6 (b); mass spectrum (c) of **5b**.

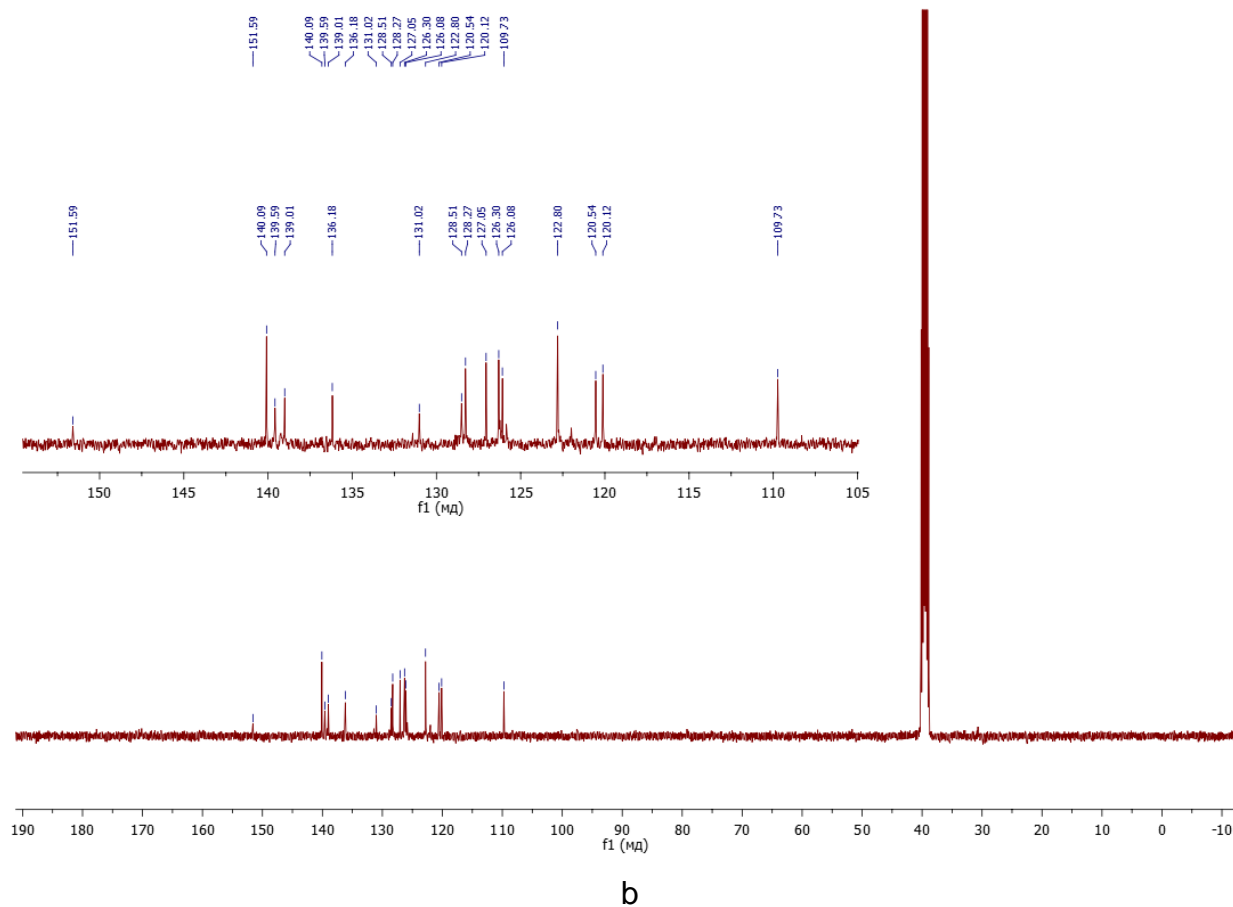


5c

a



b



Line#:1 R.Time:3.930(Scan#:1553)
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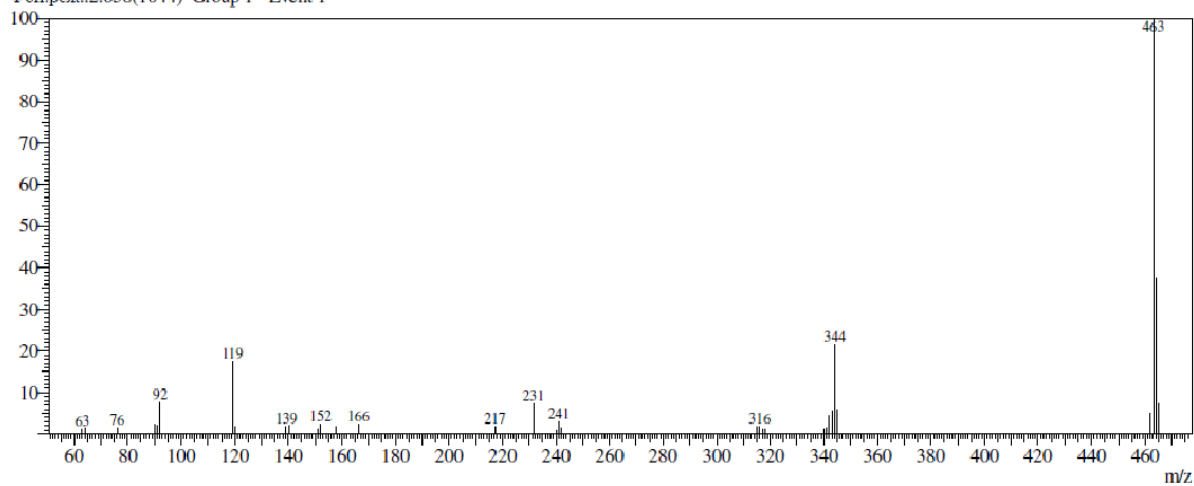
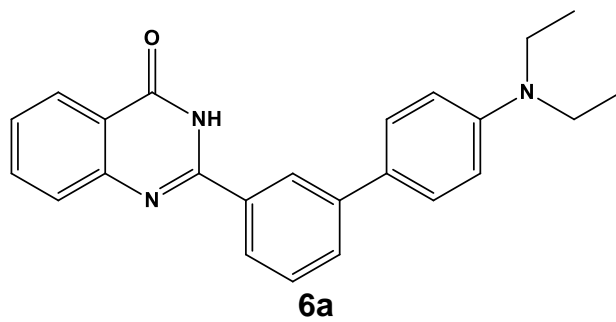
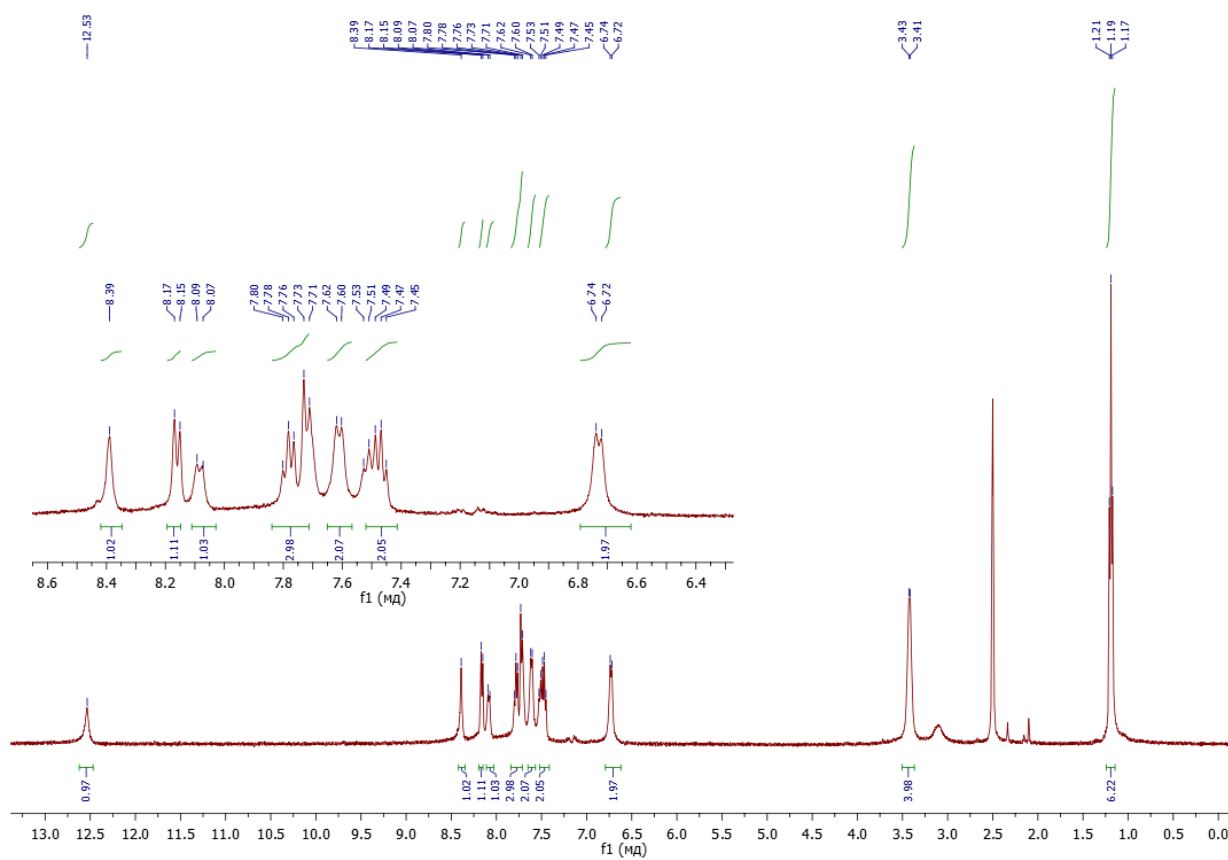


Figure S7. ¹H NMR spectrum (a) and ¹³C NMR spectrum in DMSO-d₆ (b); mass spectrum (c) of **5c**.



a



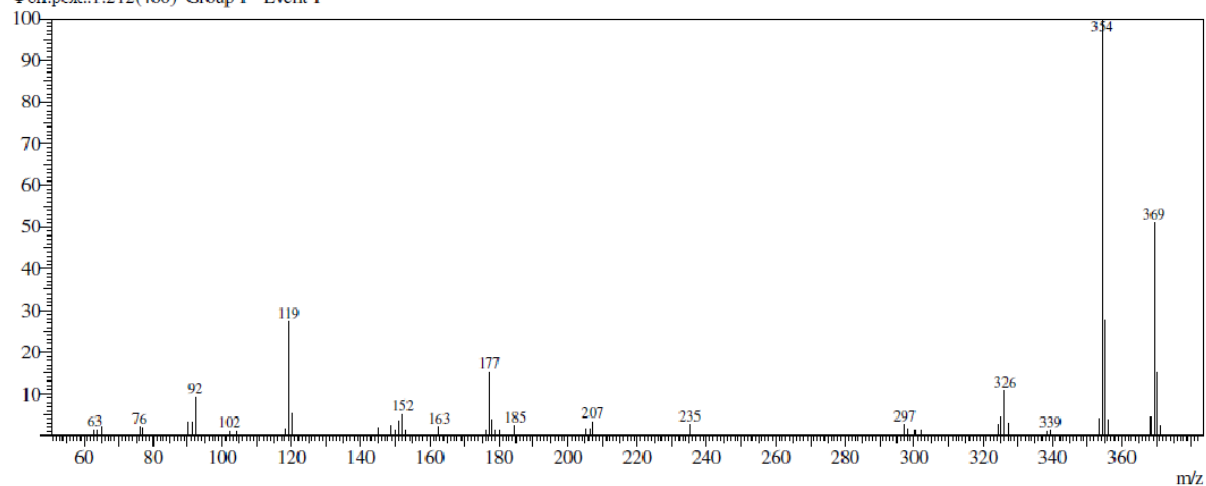
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MassPeaks:48

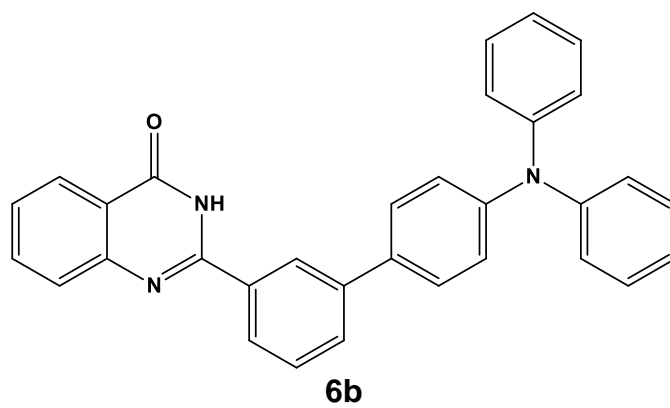
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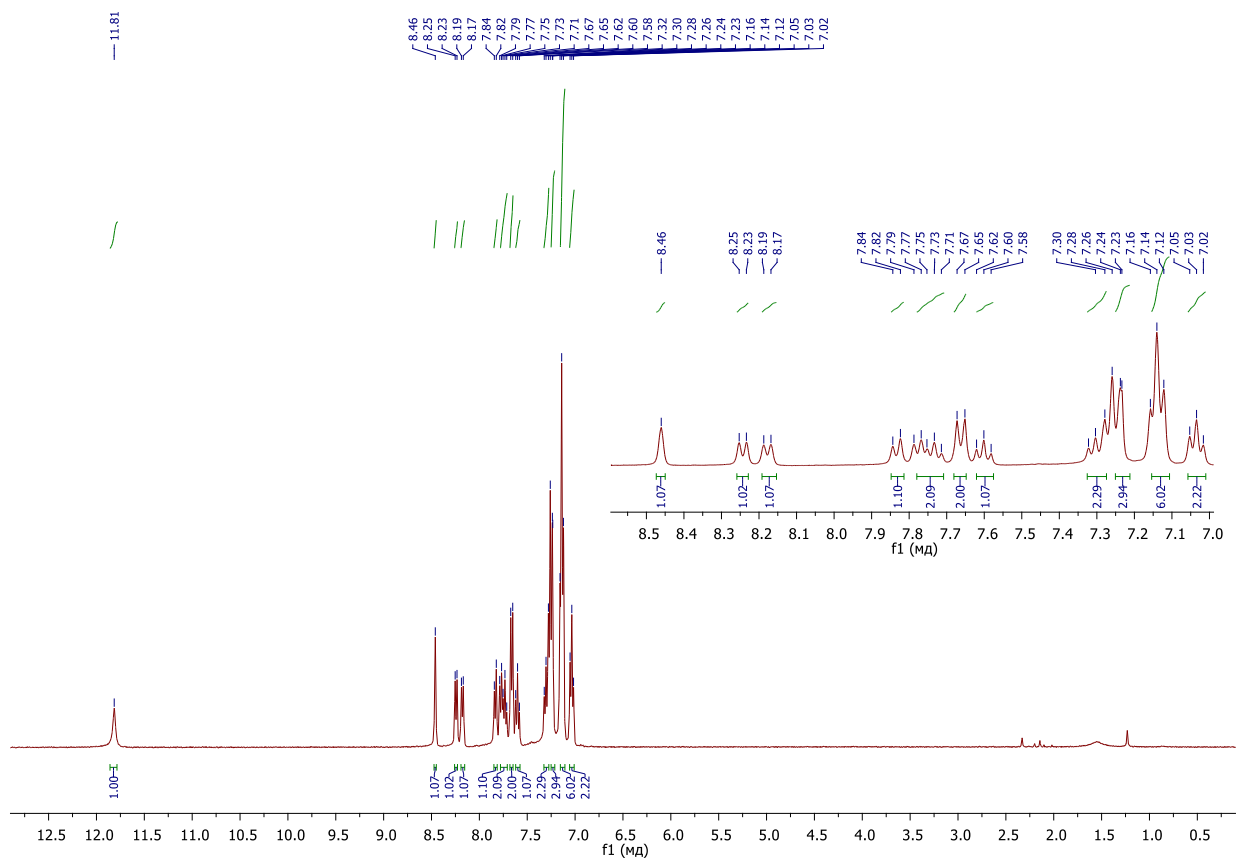
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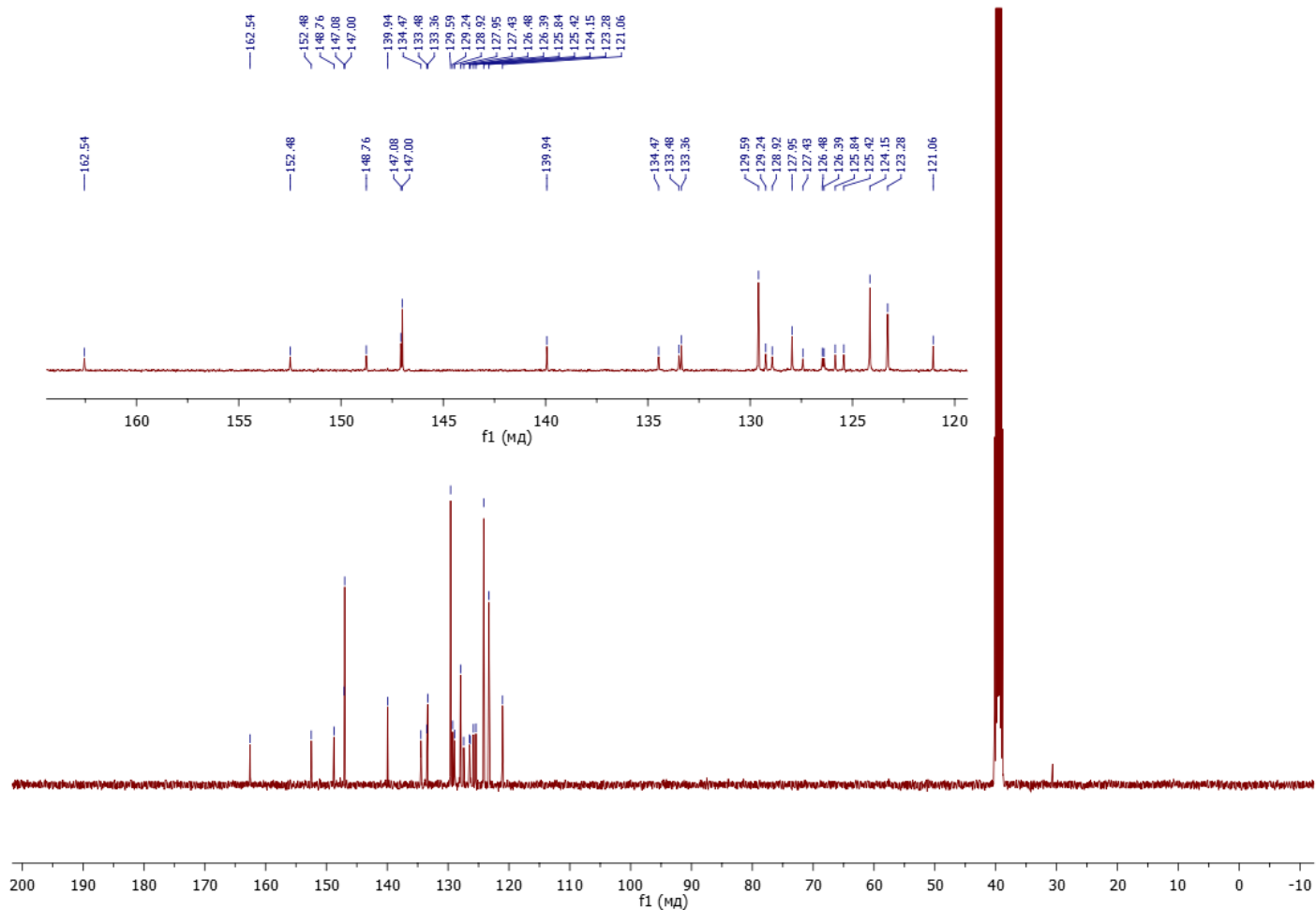
b

Figure S8. ^1H NMR spectrum (a) in DMSO-d_6 ; mass spectrum (b) of **6a**.





a



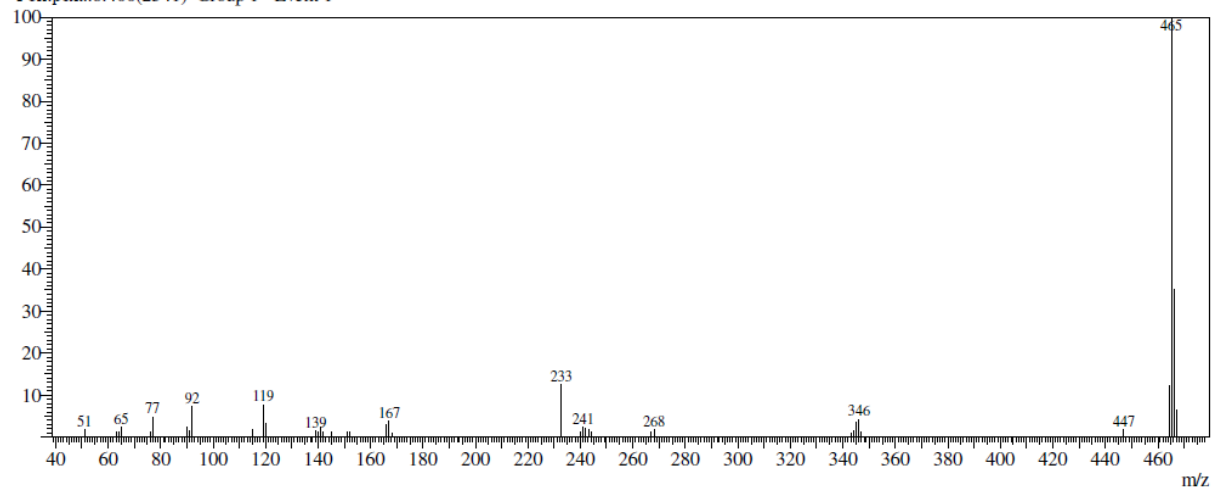
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MassPeaks:40

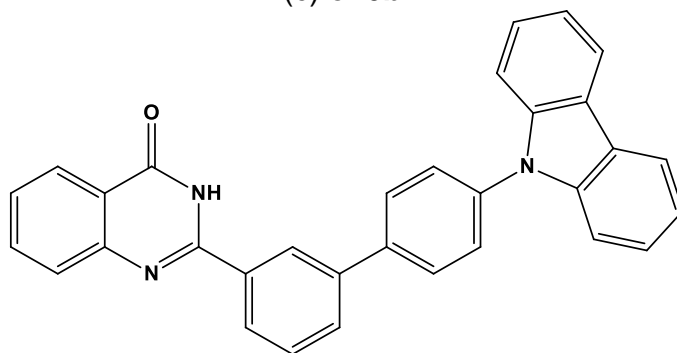
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Фон.реж.:6.400(2541) Group 1 - Event 1

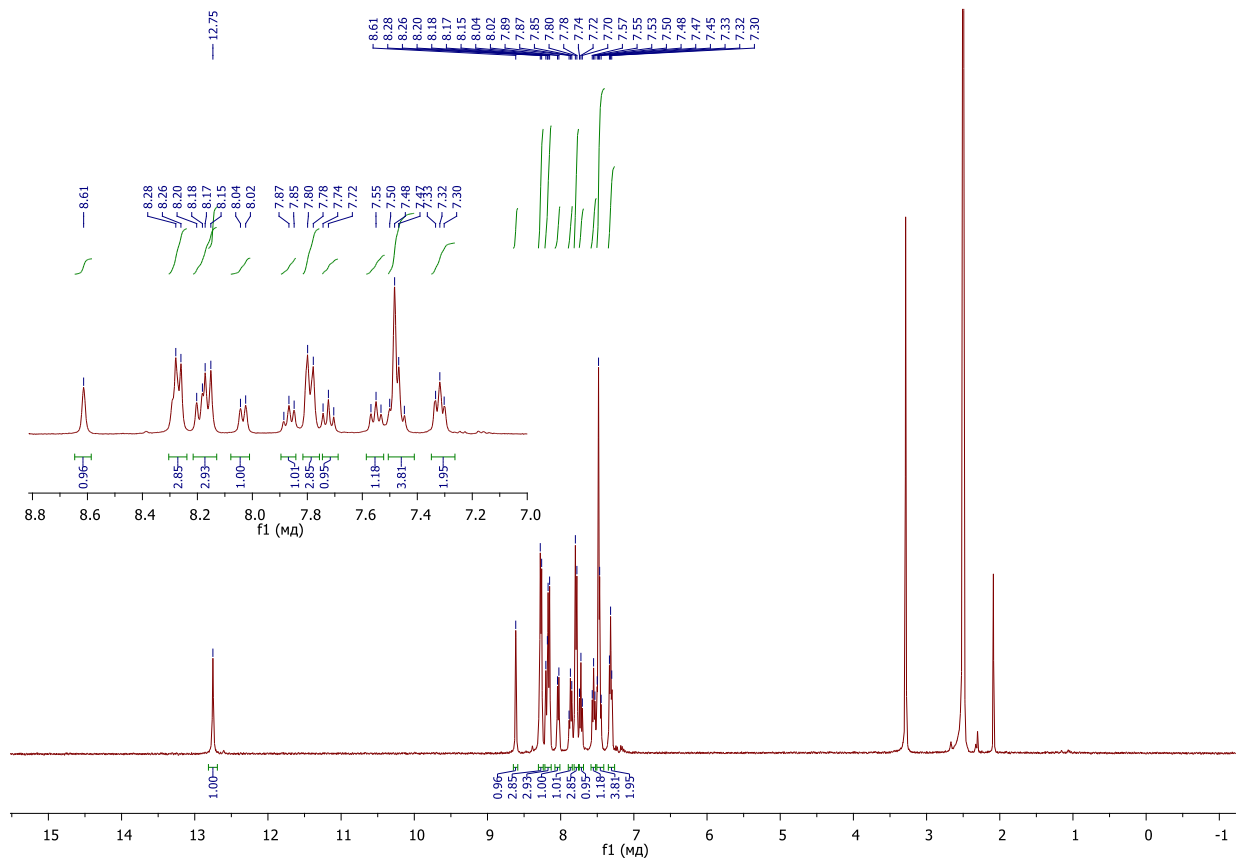


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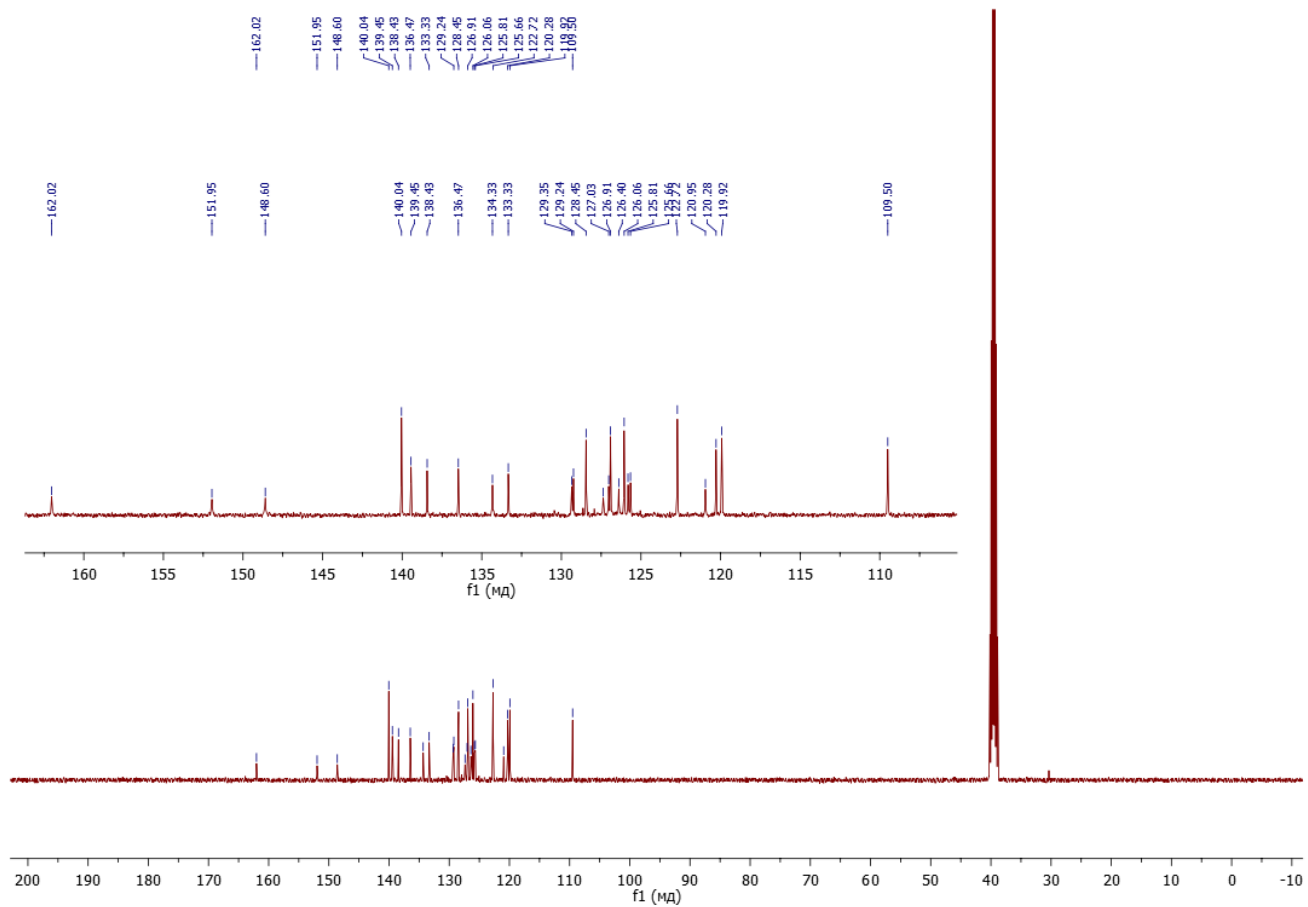
Figure S9. ^1H NMR spectrum in DCCl_3 (a), ^{13}C NMR spectrum in DMSO-d_6 (b) and mass spectrum (c) of **6b**.



6c

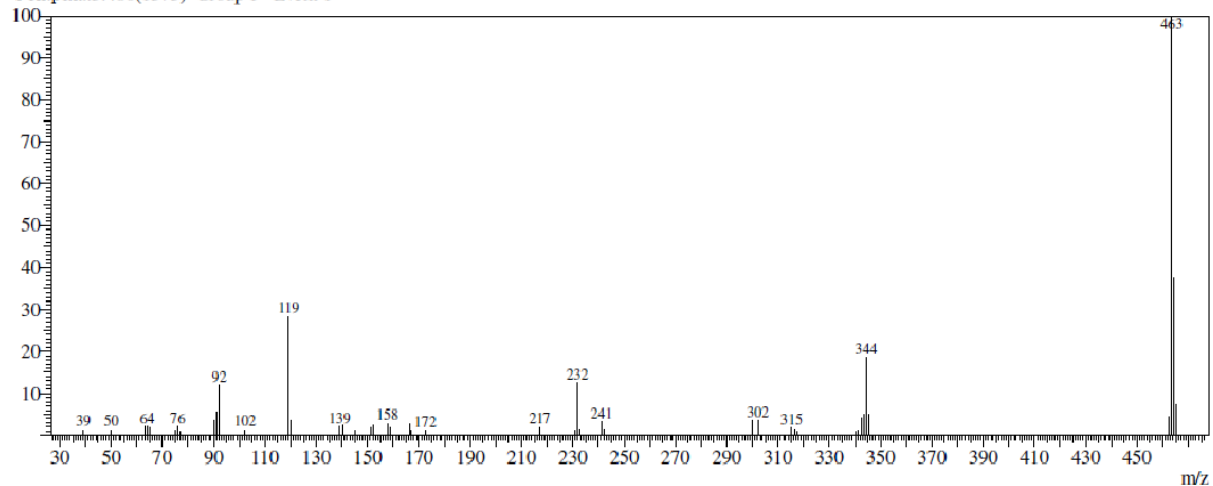


a



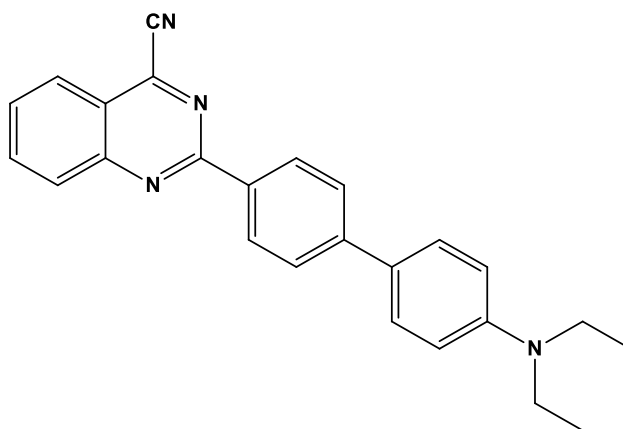
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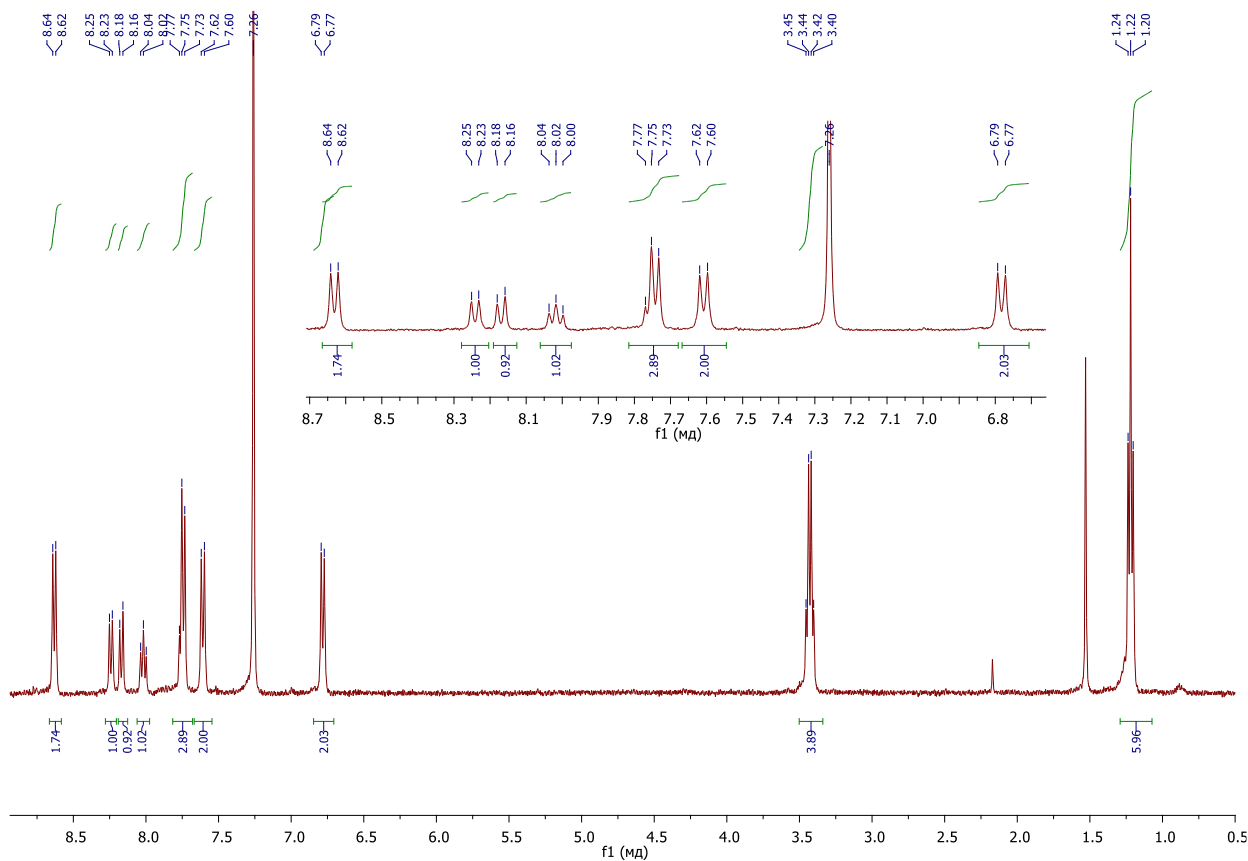


C

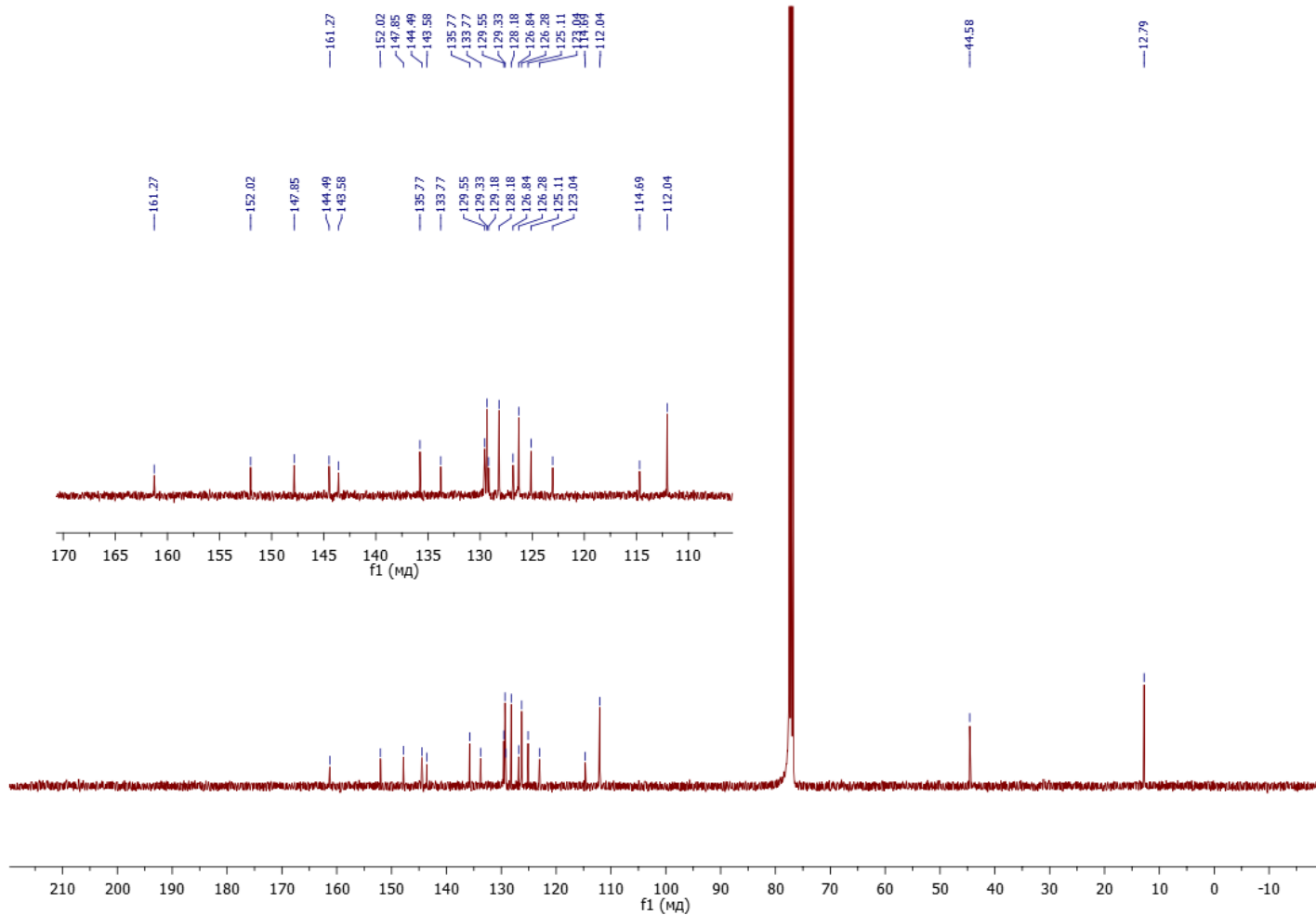
Figure S10. ^1H NMR spectrum (a) and ^{13}C NMR spectrum in DMSO-d_6 (b); mass spectrum (c) of **6c**.



8a

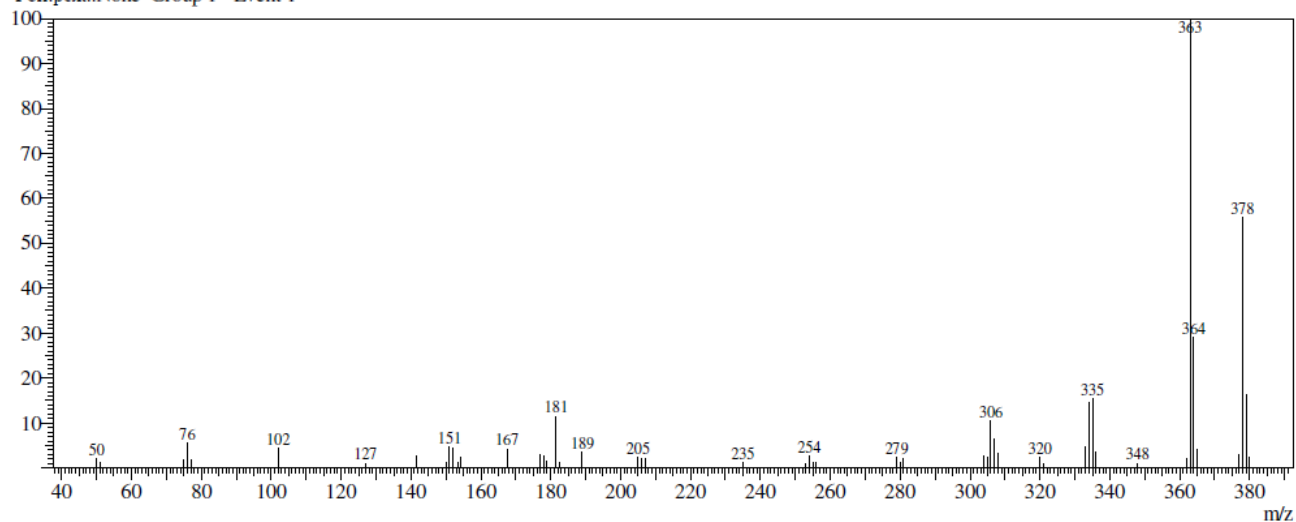


a



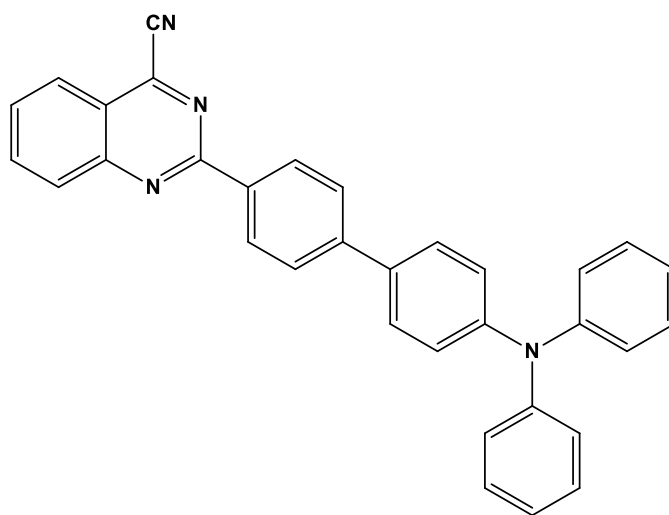
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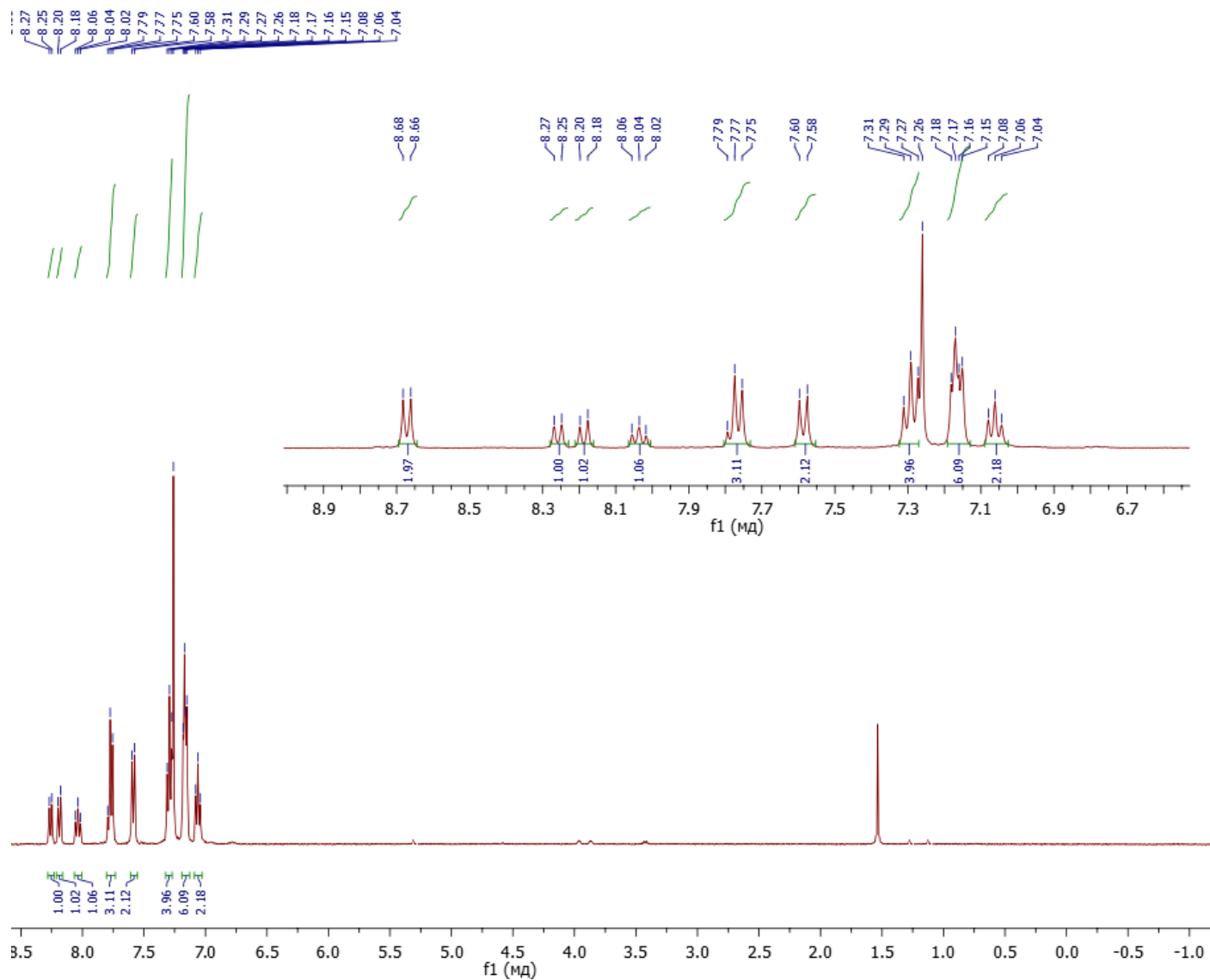


C

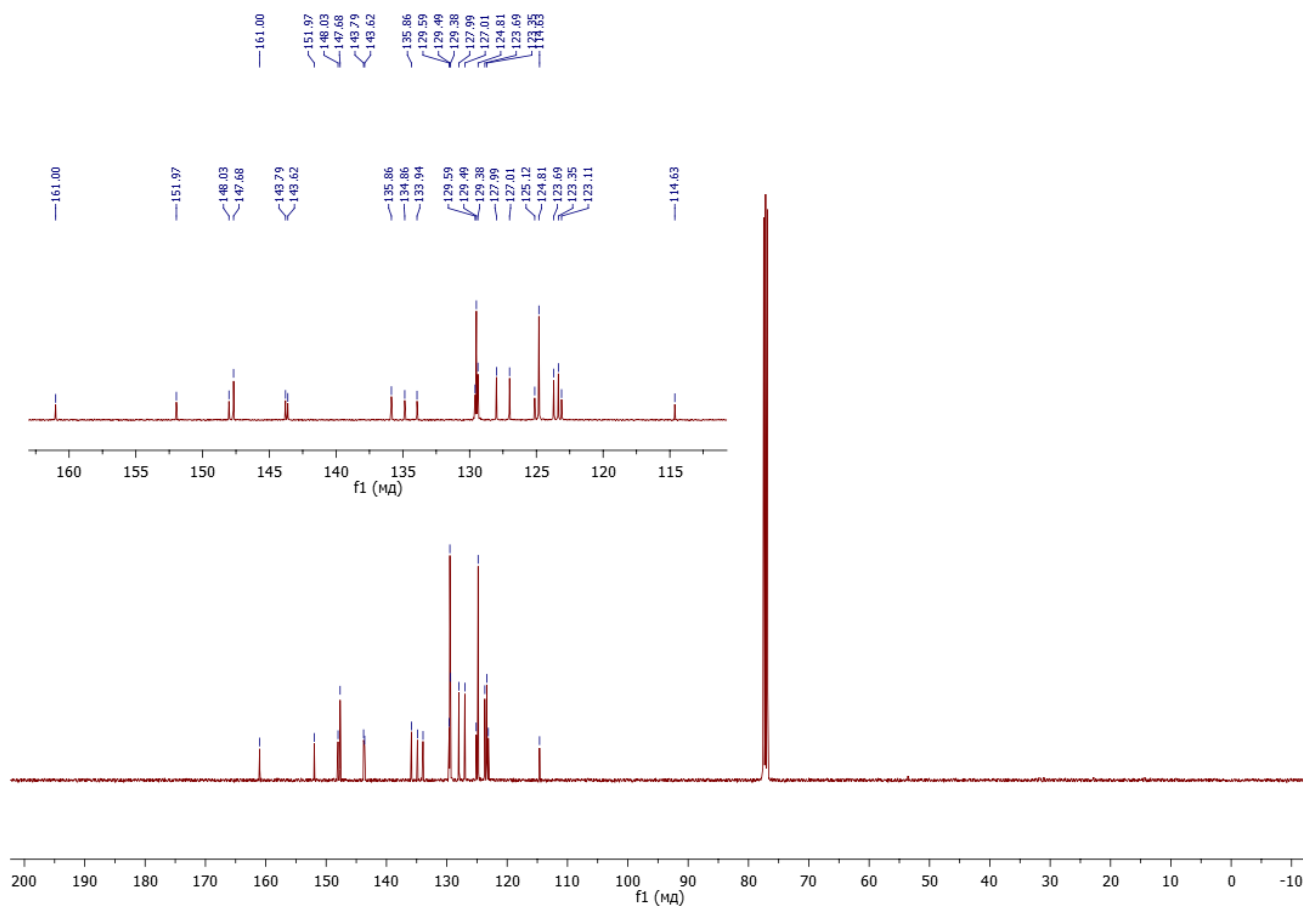
Figure S11. ^1H NMR spectrum (a) and ^{13}C NMR spectrum in DCCl_3 (b); mass spectrum (c) of **8a**.



8b



a



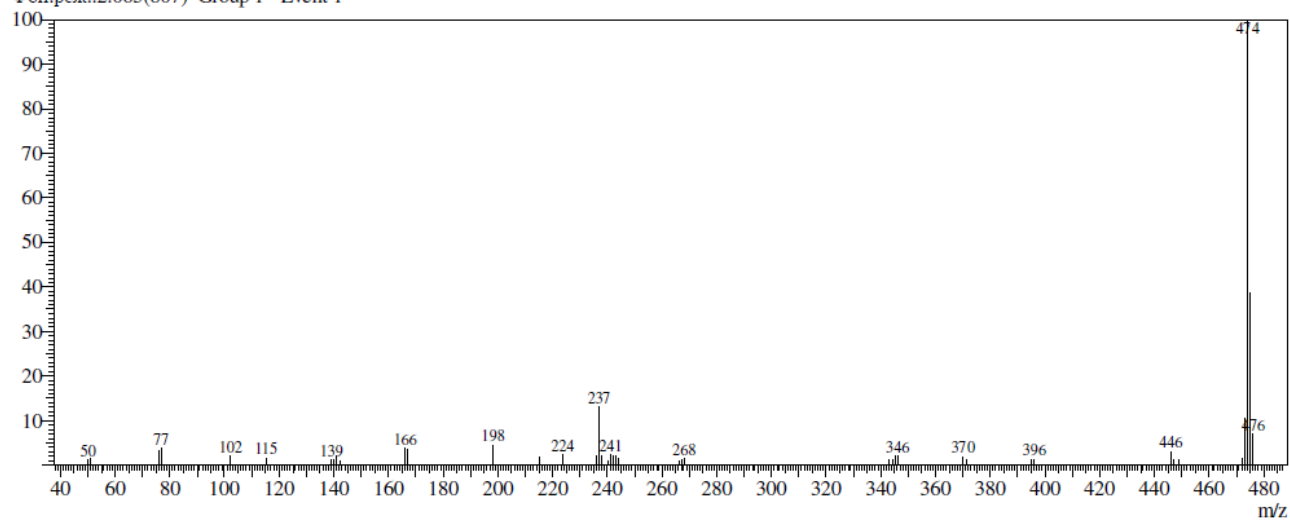
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MassPeaks:42

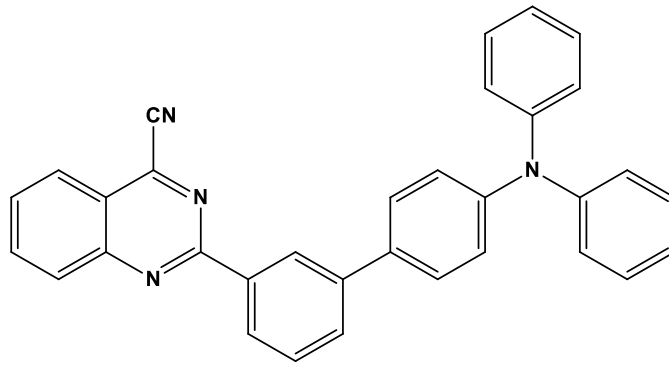
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Фон.реж.:2.065(807) Group 1 - Event 1

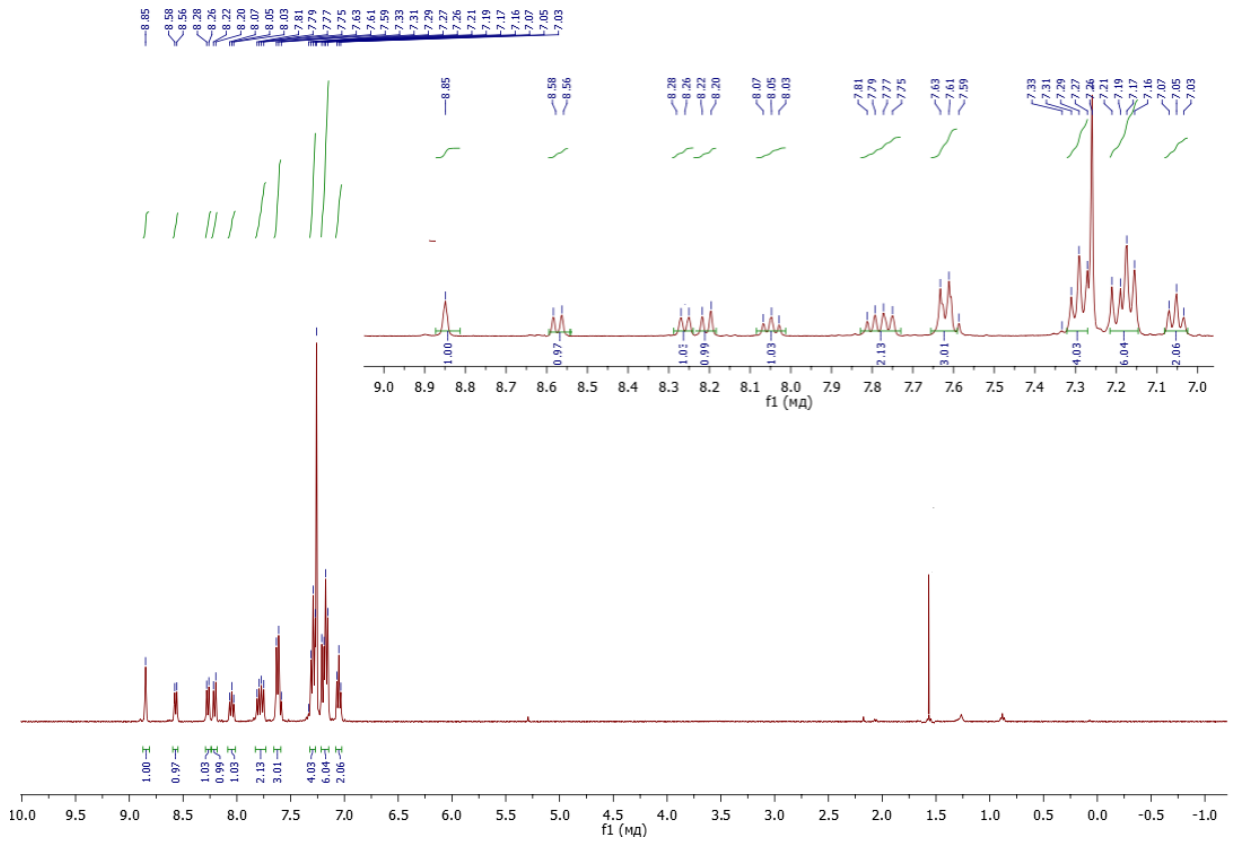


c

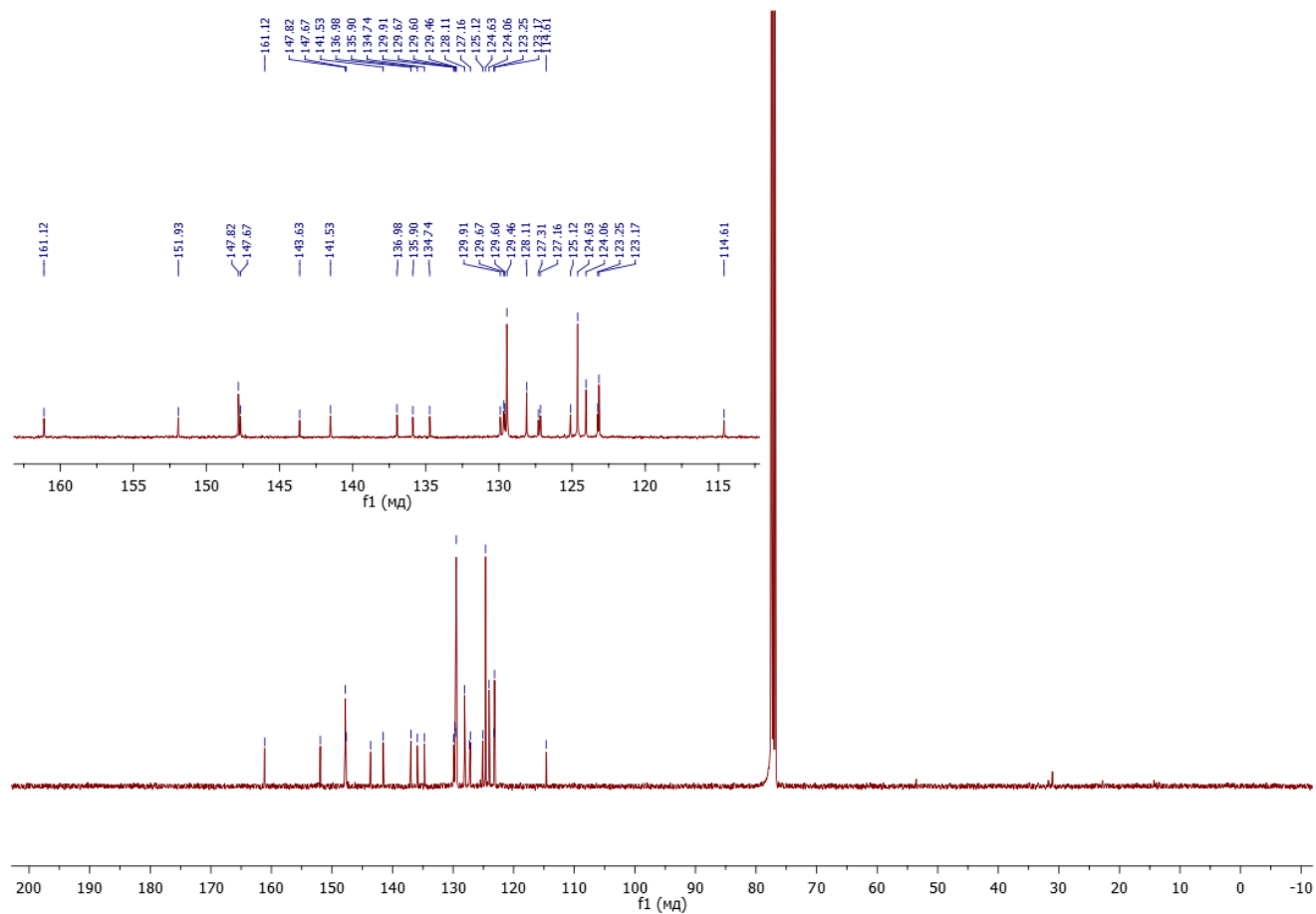
Figure S12. ^1H NMR spectrum (a) and ^{13}C NMR spectrum (b) in DCCl_3 ; mass spectrum (c) of **8b**.



9



a



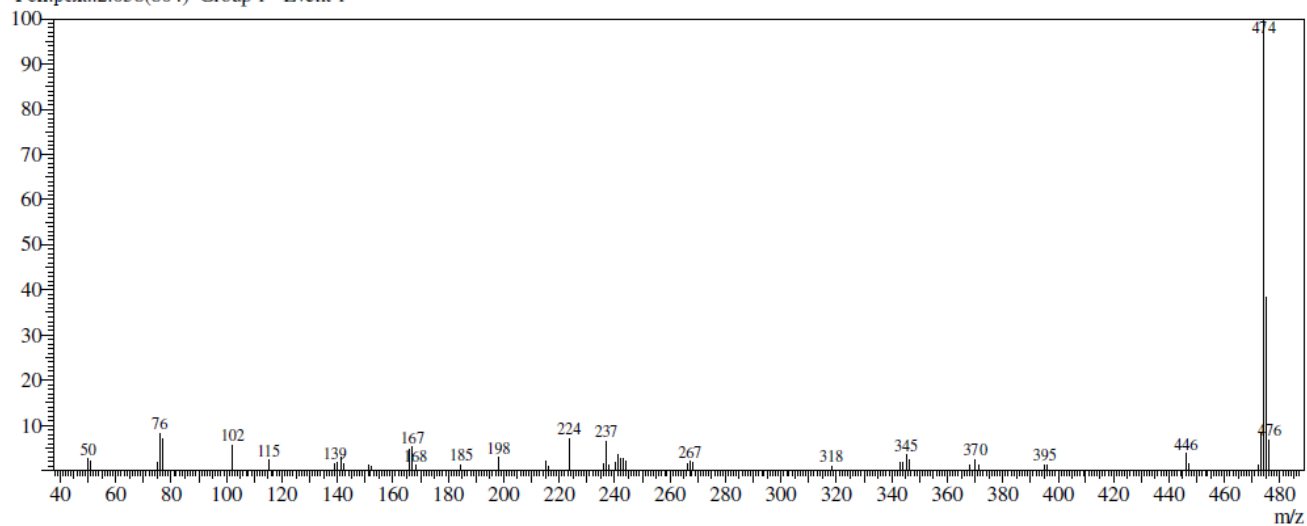
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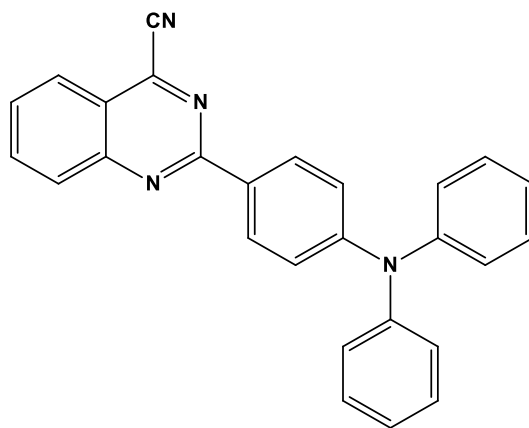
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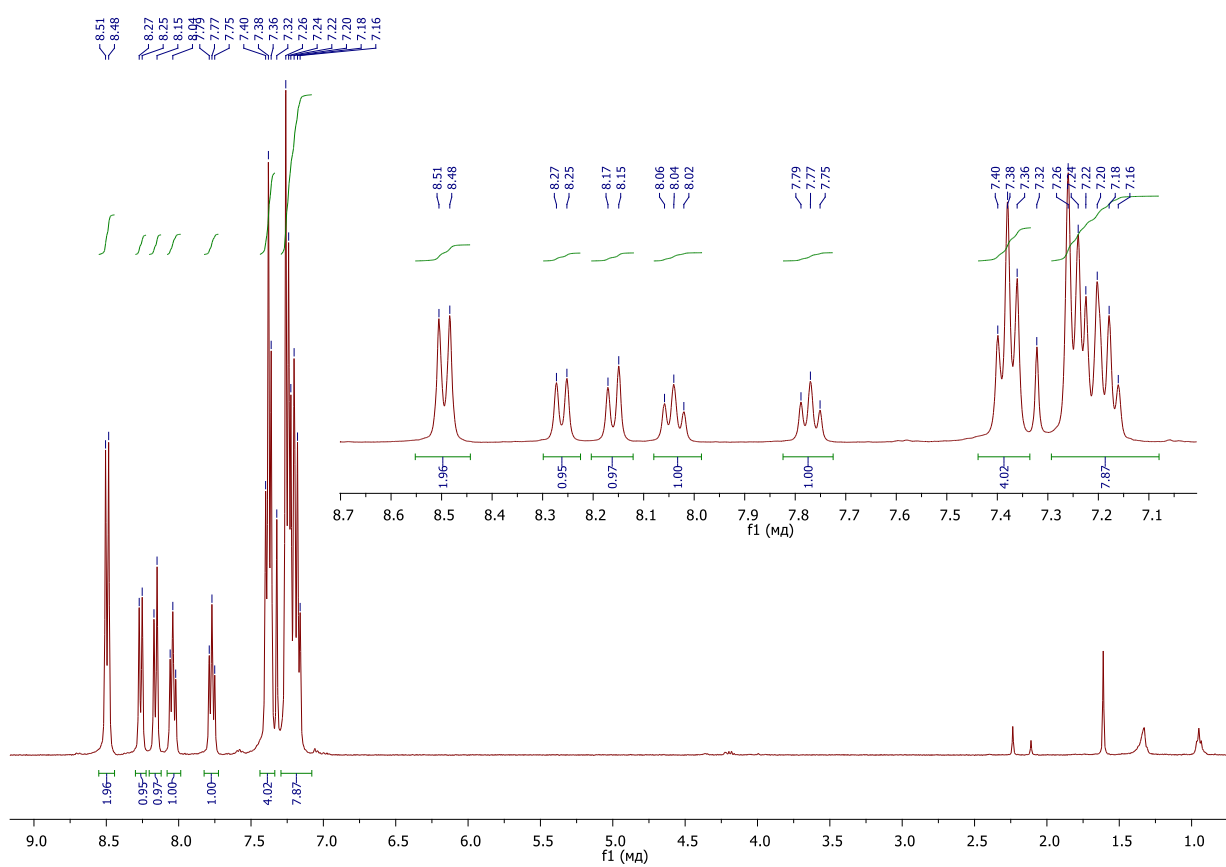


c

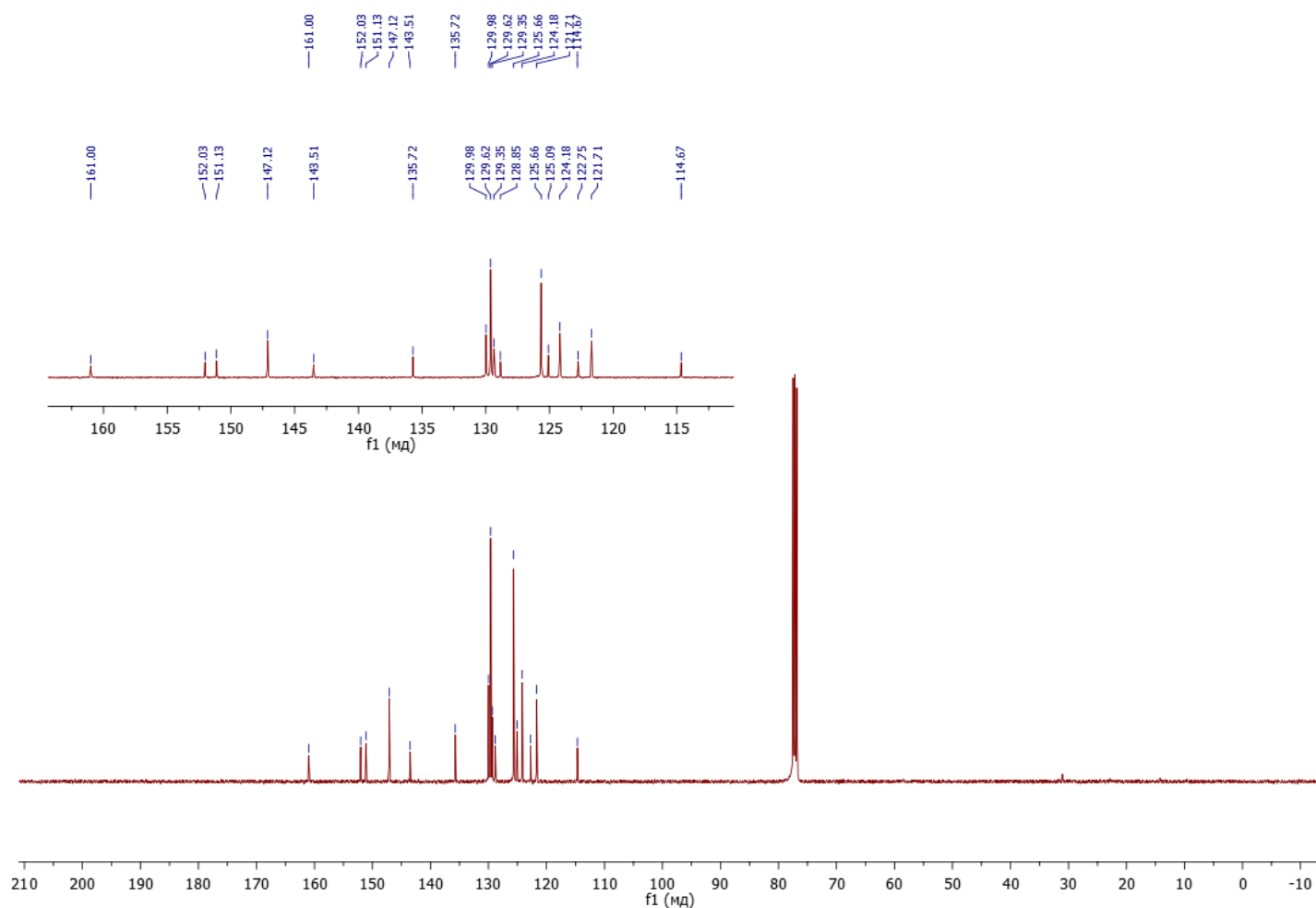
Figure S13. ^1H NMR spectrum (a) and ^{13}C NMR spectrum (b) in DCCl_3 ; mass spectrum (c) of **9**.



11



a



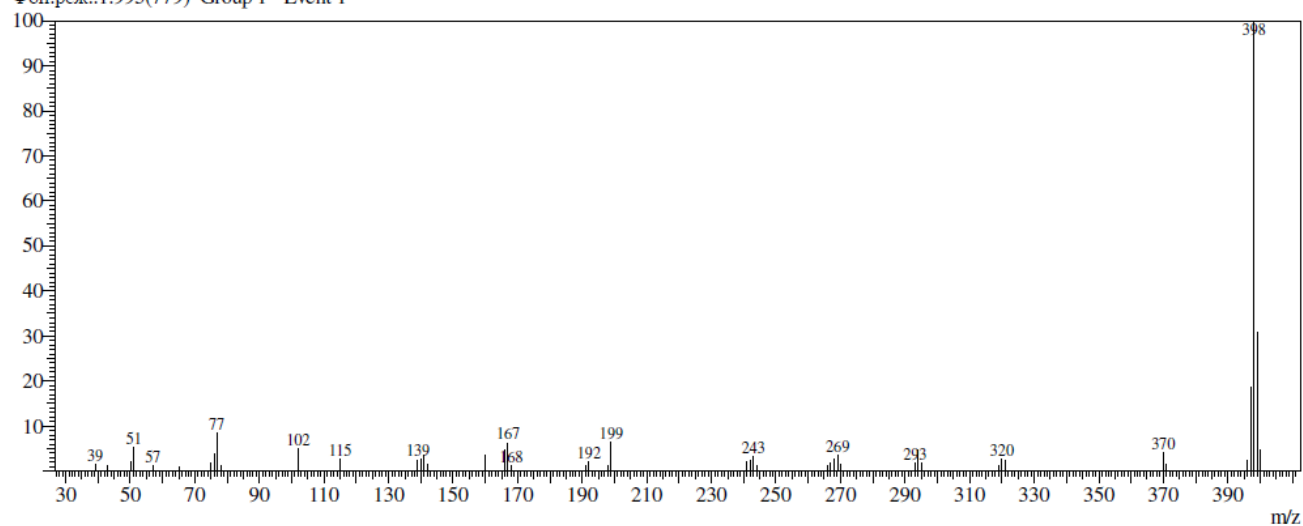
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MassPeaks:46

RawMode:Single 3.228(1272) BasePeak:398(6868237)

Фон.реж.:1.995(779) Group 1 - Event 1



c

Figure S14. ^1H NMR spectrum (a) and ^{13}C NMR spectrum in DCCl_3 (b); mass spectrum (c) of **11**.

3. Crystallographic data of compounds 11

Table S1. Selected bond lengths of compound 11.

Bond	Bond length (Å)	Bond	Bond length (Å)
N(3) – C(2)	1.374(2)	C(1) – C(5)	1.418(3)
N(3) – C(4)	1.314(3)	C(23) – C(24)	1.385(3)
N(1) – C(2)	1.325(3)	C(23) – C(28)	1.373(3)
N(1) – C(9)	1.368(3)	C(24) – C(25)	1.454(3)
N(4) – C(14)	1.402(3)	C(4) – C(10)	1.385(3)
N(4) – C(13)	1.433(3)	C(18) – C(19)	1.405(3)
N(4) – C(23)	1.430(2)	C(9) – C(8)	1.141(3)
C(12) – C(11)	1.391(3)	N(2) – C(10)	1.381(3)
C(12) – C(17)	1.376(3)	C(28) – C(27)	1.357(4)
C(11) – C(2)	1.469(3)	C(5) – C(6)	1.372(4)
C(11) – C(16)	1.396(3)	C(27) – C(26)	1.371(4)
C(14) – C(17)	1.401(3)	C(19) – C(20)	1.375(4)
C(14) – C(15)	1.398(3)	C(25) – C(26)	1.384(3)
C(13) – C(18)	1.382(3)	C(22) – C(21)	1.372(4)
C(13) – C(22)	1.371(3)	C(20) – C(21)	1.366(4)
C(15) – C(16)	1.381(3)	C(8) – C(7)	1.403(4)
C(1) – C(4)	1.415(3)	C(6) – C(7)	1.373(3)
C(1) – C(9)	1.409(3)		

Table S2. Selected bond angles of compound 11.

Angle	(°)	Angle	(°)
C(4) – N(3) – C(2)	116.46(19)	N(1) – C(2) – N(3)	125.0(2)
C(2) – N(1) – C(9)	117.92(18)	N(1) – C(2) – C(11)	118.09(18)
C(14) – N(4) – C(13)	121.14(15)	C(15) – C(16) – C(11)	121.27(19)
C(14) – N(4) – C(23)	120.89(17)	C(25) – C(24) – C(23)	120.4(2)
C(23) – N(4) – C(13)	117.54(16)	N(3) – C(4) – C(1)	124.25(19)
C(17) – C(12) – C(11)	121.41(19)	N(3) – C(4) – C(10)	116.2(2)
C(12) – C(11) – C(2)	120.88(19)	C(1) – C(4) – C(10)	119.6(2)
C(12) – C(11) – C(16)	117.56(19)	C(13) – C(18) – C(19)	120.3(2)
C(16) – C(11) – C(2)	121.53(18)	N(1) – C(9) – C(1)	121.4(2)
C(17) – C(14) – N(4)	120.45(17)	N(1) – C(9) – C(8)	119.3(2)
C(15) – C(14) – N(4)	122.05(18)	C(8) – C(9) – C(1)	119.2(2)
C(15) – C(14) – C(17)	117.49(19)	C(27) – C(28) – C(23)	120.0(2)

C(12) – C(17) – C(14)	121.00(18)	N(2) – C(10) – C(4)	179.1(3)
C(18) – C(13) – N(4)	119.4(2)	C(6) – C(5) – C(1)	119.6(2)
C(22) – C(13) – N(4)	120.6(2)	C(26) – C(27) – C(28)	120.6(2)
C(22) – C(13) – C(18)	119.9(2)	C(20) – C(19) – C(18)	119.5(3)
C(16) – C(15) – C(14)	120.89(19)	C(24) – C(25) – C(26)	120.5(3)
C(4) – C(1) – C(5)	125.3(2)	C(13) – C(22) – C(21)	119.6(2)
C(9) – C(1) – C(4)	114.9(2)	C(19) – C(20) – C(21)	120.1(2)
C(9) – C(1) – C(5)	119.8(2)	C(27) – C(26) – C(25)	119.4(2)
C(24) – C(23) – N(4)	121.8(2)	C(20) – C(21) – C(22)	120.6(2)
C(24) – C(23) – C(28)	118.92(19)	C(7) – C(8) – C(9)	119.8(3)
C(28) – C(23) – N(4)	119.2(2)	C(5) – C(6) – C(7)	120.6(3)
N(3) – C(2) – C(11)	116.89(19)	C(8) – C(7) – C(6)	121.1(3)

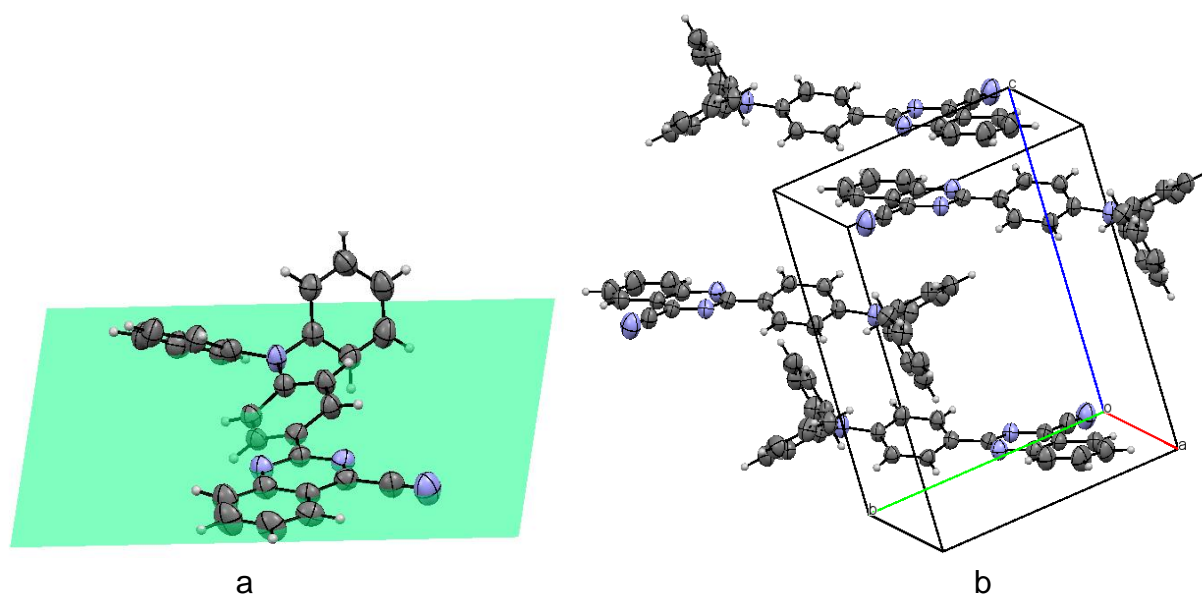


Figure S15. Planarity (a) and packing (b) of compounds **11**.

4. Absorption, excitation and emission spectra of chromophores in toluene and MeCN

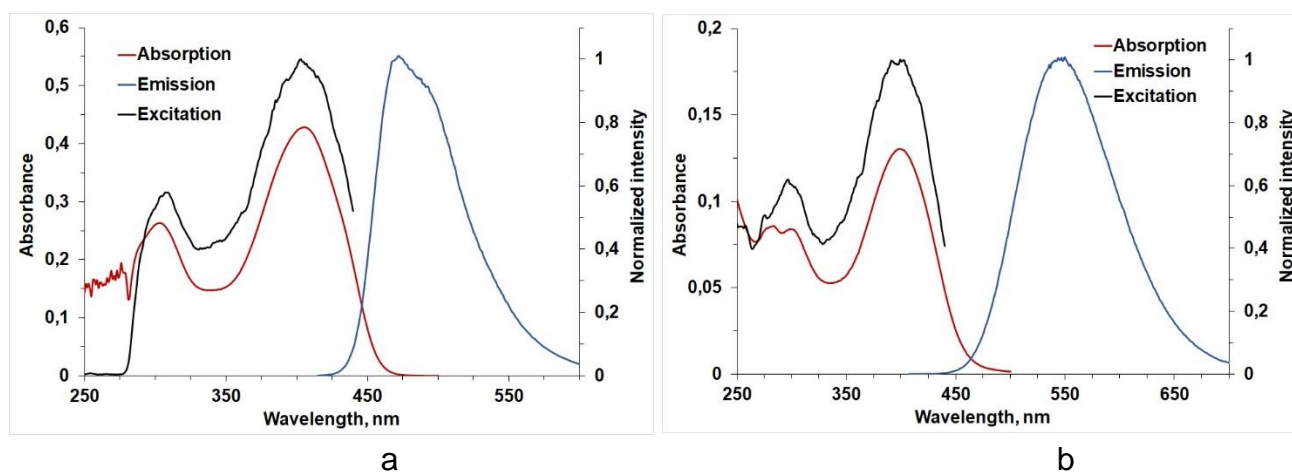


Figure S16. Absorption, excitation and emission spectra of chromophore **4b** in toluene (a) and MeCN (b).

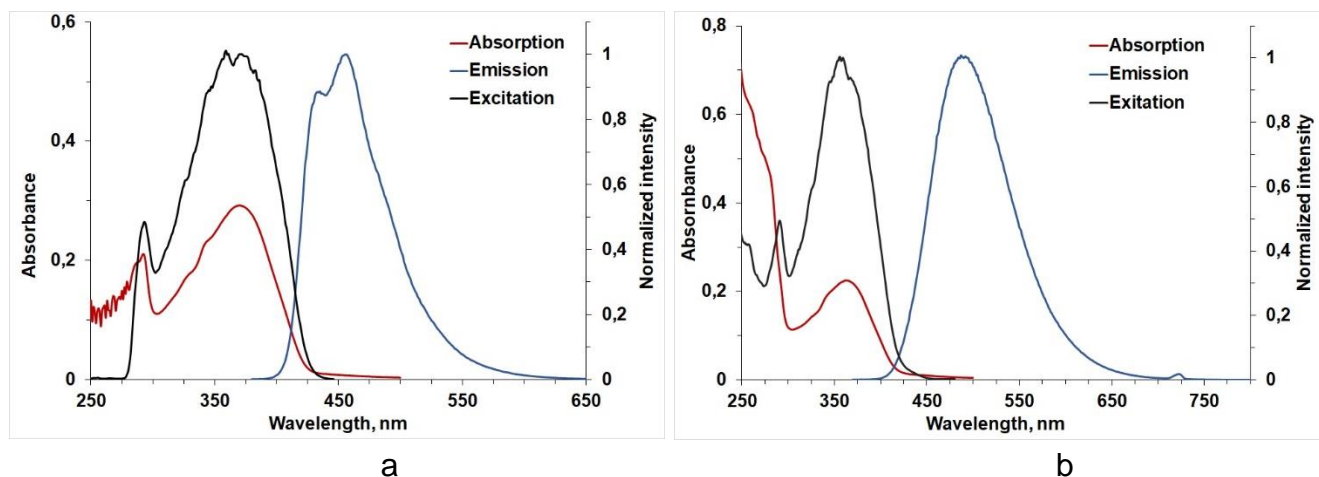


Figure S17. Absorption, excitation and emission spectra of chromophore **4c** in toluene (a) and MeCN (b).

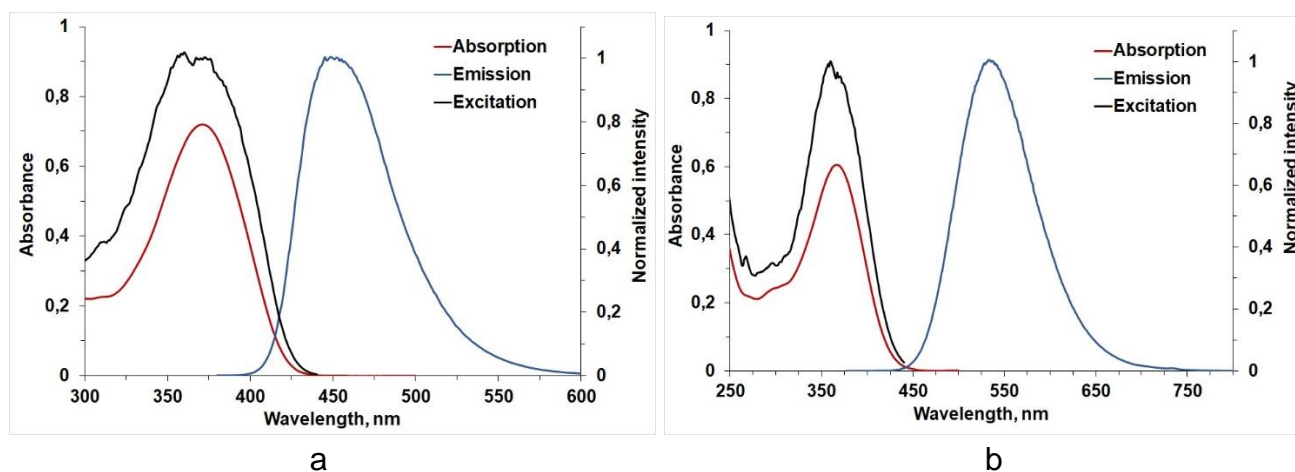


Figure S18. Absorption, excitation and emission spectra of chromophore **5a** in toluene (a) and MeCN (b).

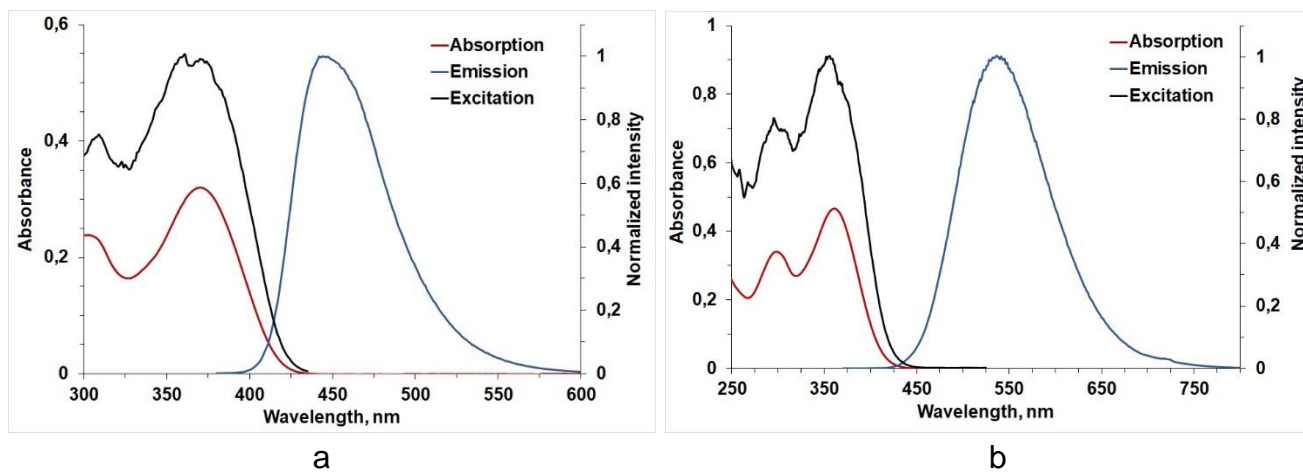


Figure S19. Absorption, excitation and emission spectra of chromophore **5b** in toluene (a) and MeCN (b).

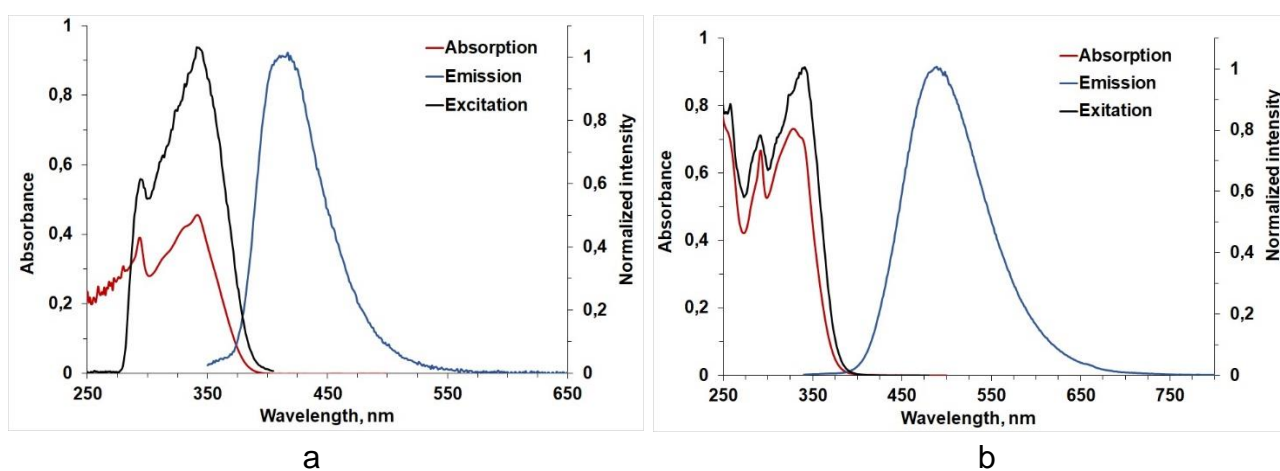


Figure S20. Absorption, excitation and emission spectra of chromophore **5c** in toluene (a) and MeCN (b).

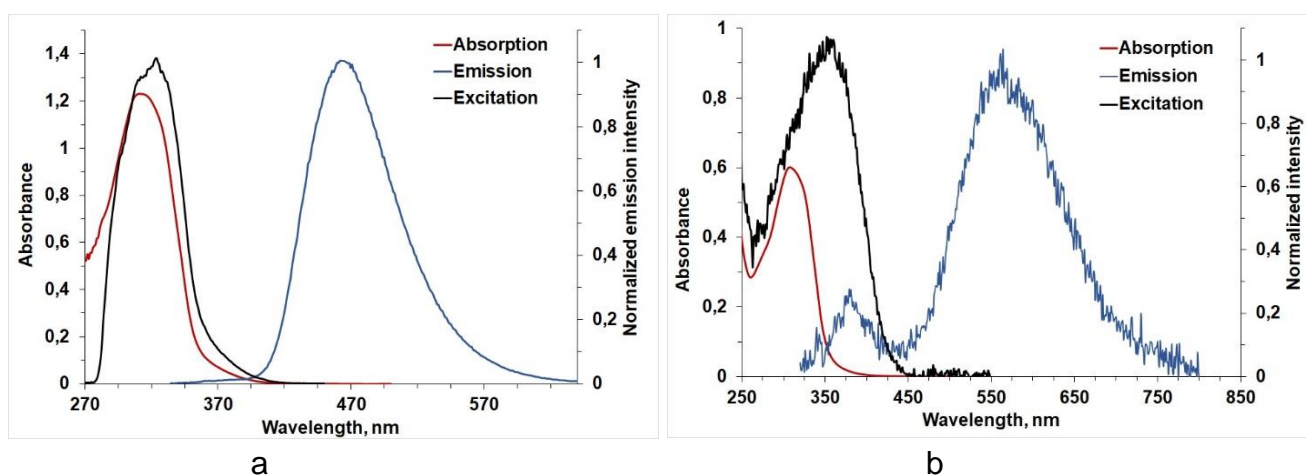


Figure S21. Absorption, excitation and emission spectra of chromophore **6a** in toluene (a) and MeCN (b).

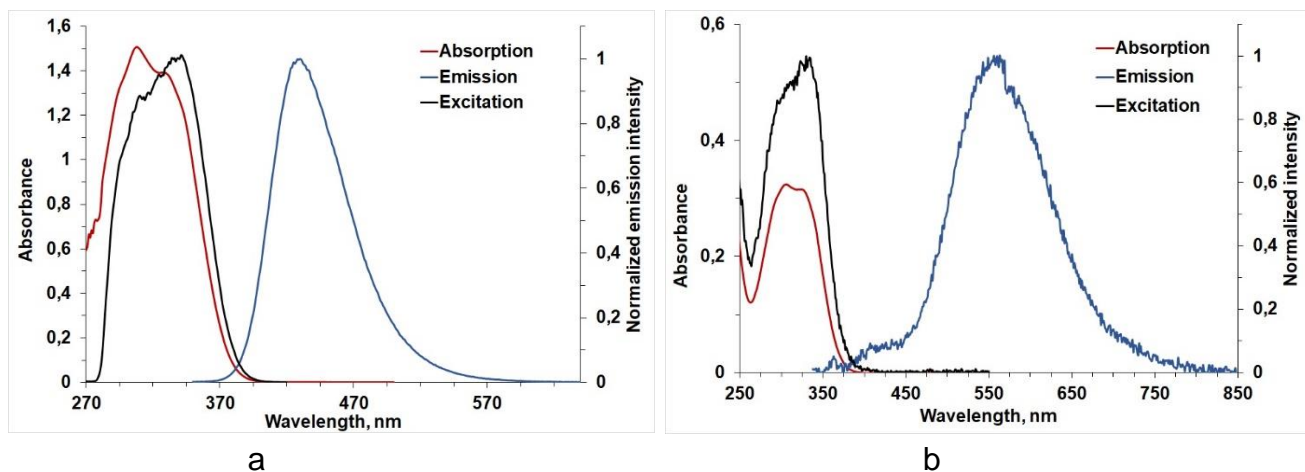


Figure S22. Absorption, excitation and emission spectra of chromophore **6b** in toluene (a) and MeCN (b).

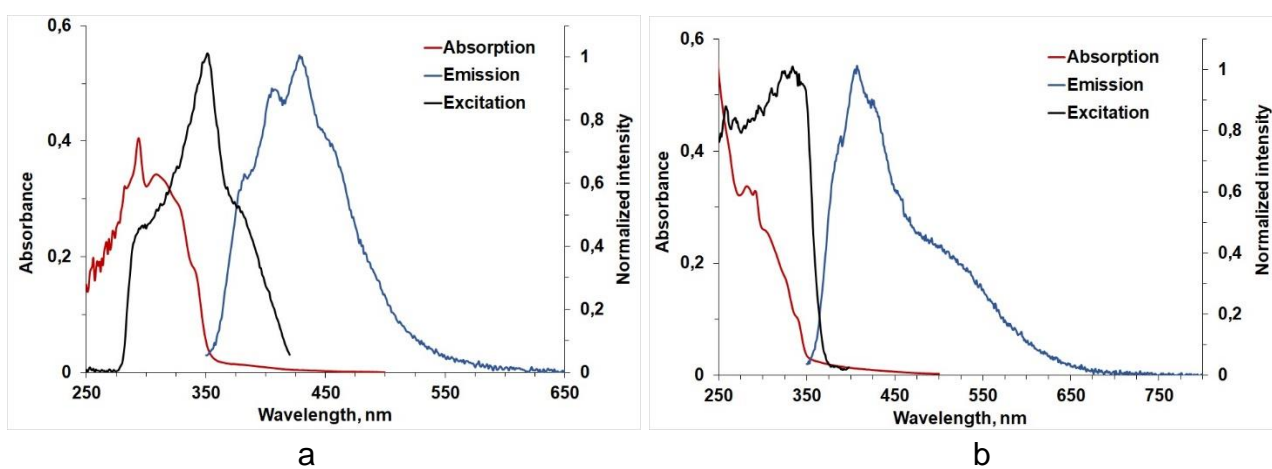


Figure S23. Absorption, excitation and emission spectra of chromophore **6c** in toluene (a) and MeCN (b).

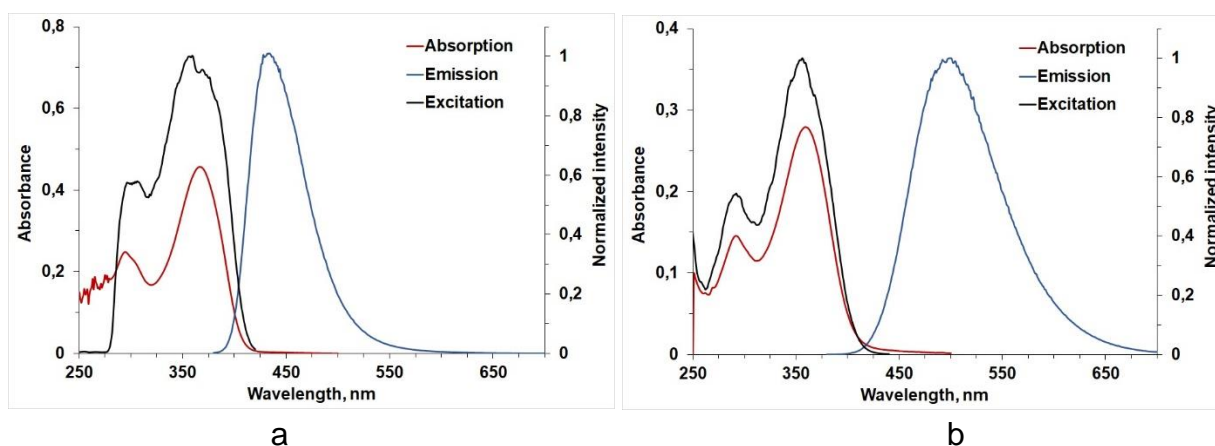


Figure S24. Absorption, excitation and emission spectra of chromophore **10** in toluene (a) and MeCN (b).

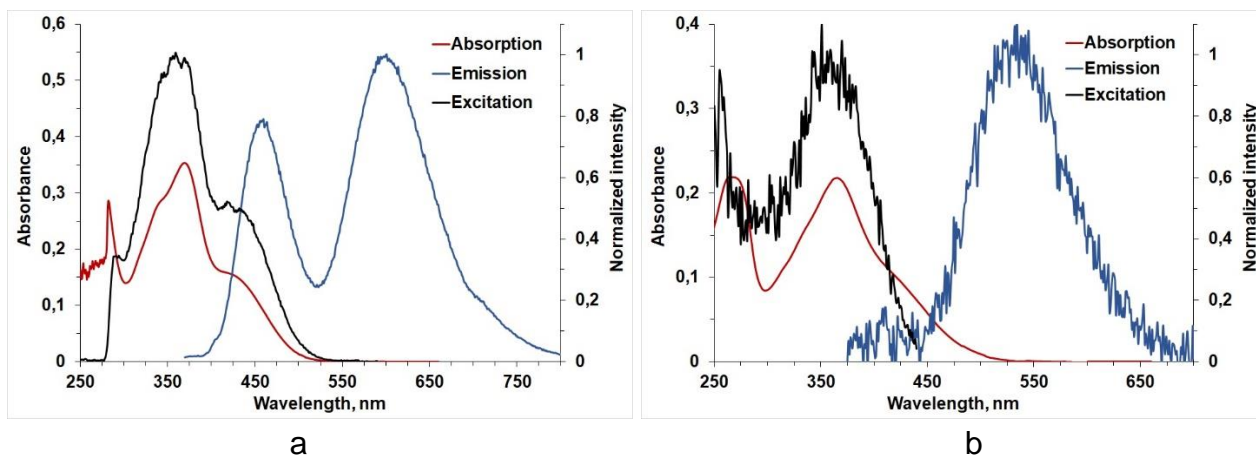


Figure S25. Absorption, excitation and emission spectra of chromophore **8a** in toluene (a) and MeCN (b).

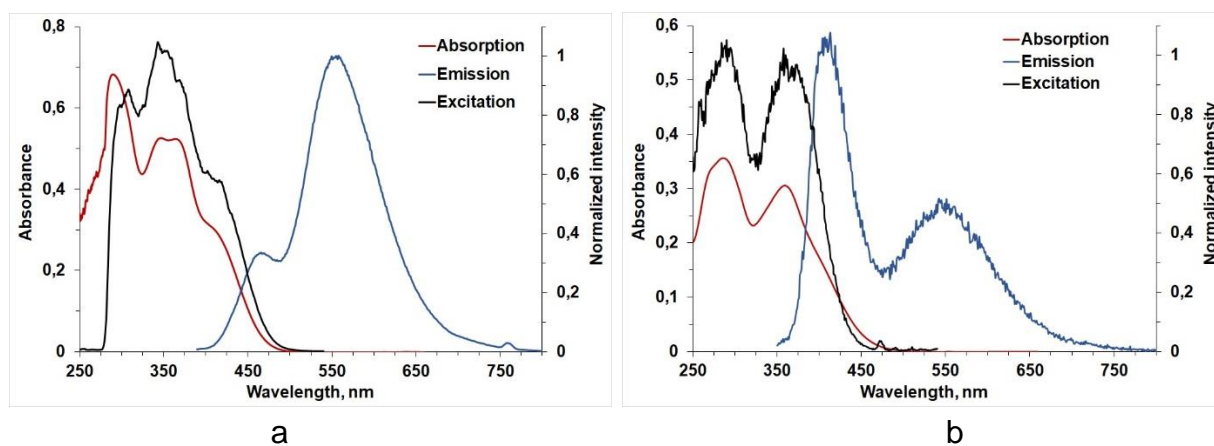


Figure S26. Absorption, excitation and emission spectra of chromophore **8b** in toluene (a) and MeCN (b).

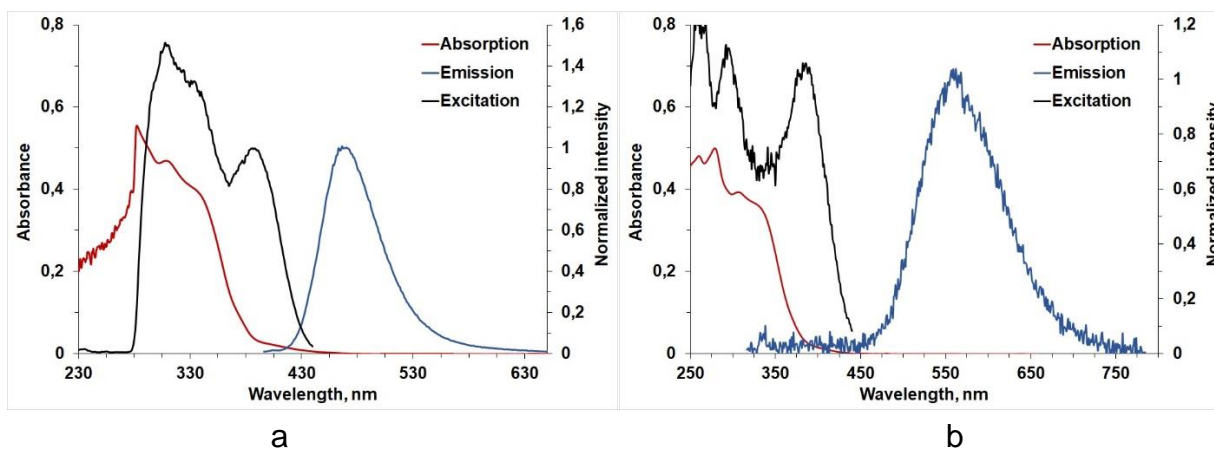


Figure S27. Absorption, excitation and emission spectra of chromophore **9** in toluene (a) and MeCN (b).

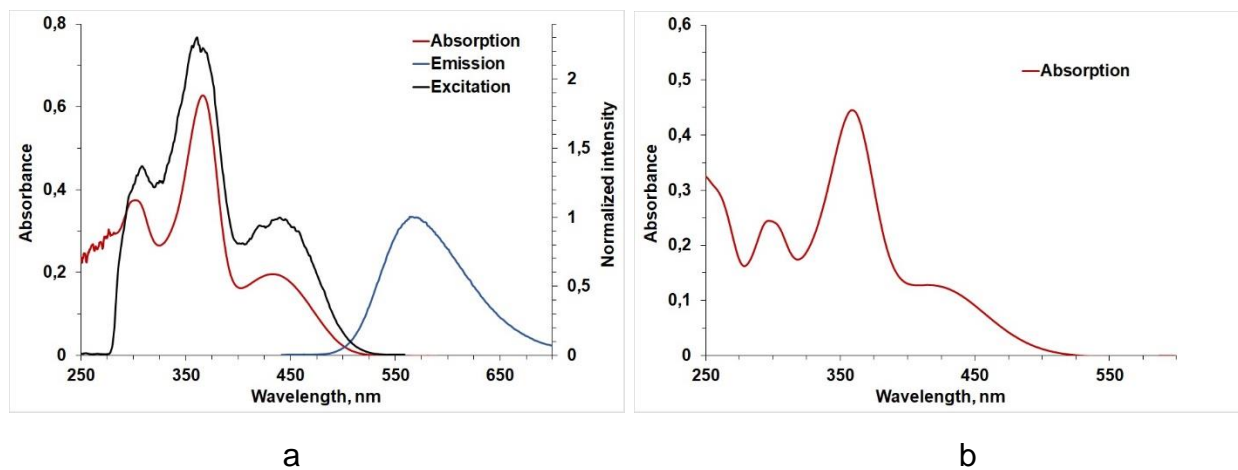
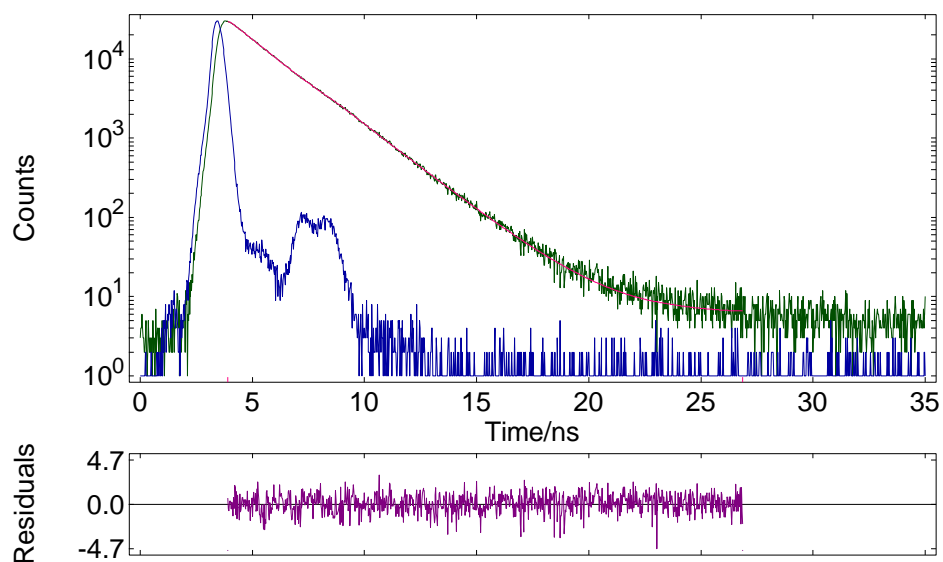


Figure S28. Absorption, excitation and emission spectra of chromophore **11** in toluene (a) and absorption spectrum in MeCN (b).

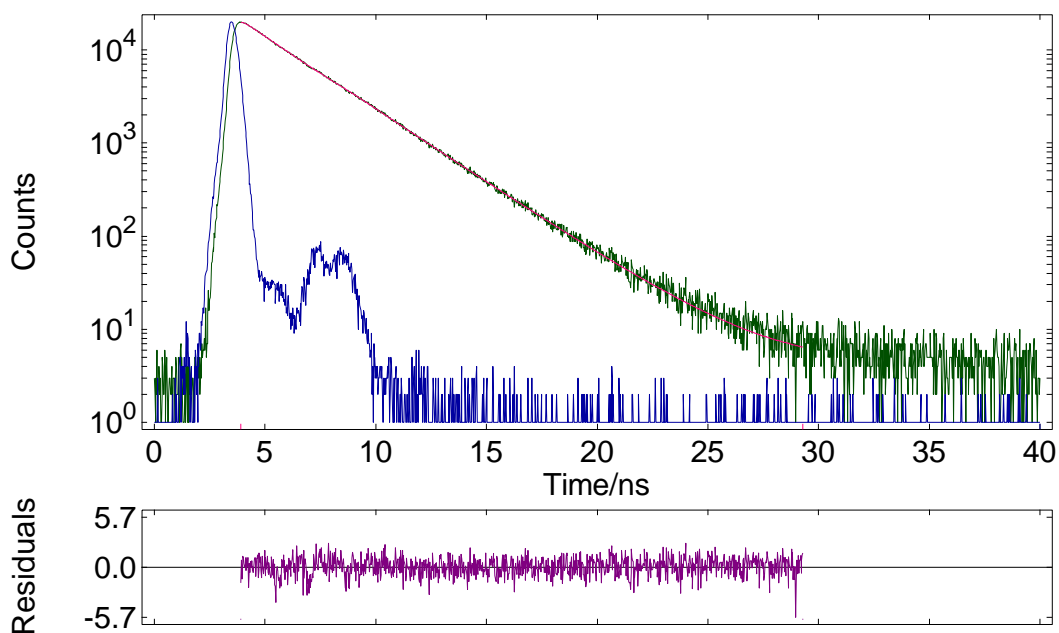
5. Time-resolved fluorescence emission measurements

Table S3. Detailed data of the fluorescence lifetime measurements of **4a-c**, **5a-c**, **6a-c**, **10**, **7a-c**, **8a,b**, **9**, **11**: τ – lifetime, f - fractional contribution, τ_{avg} – average lifetime, χ^2 - chi-squared distribution.

[illegible]

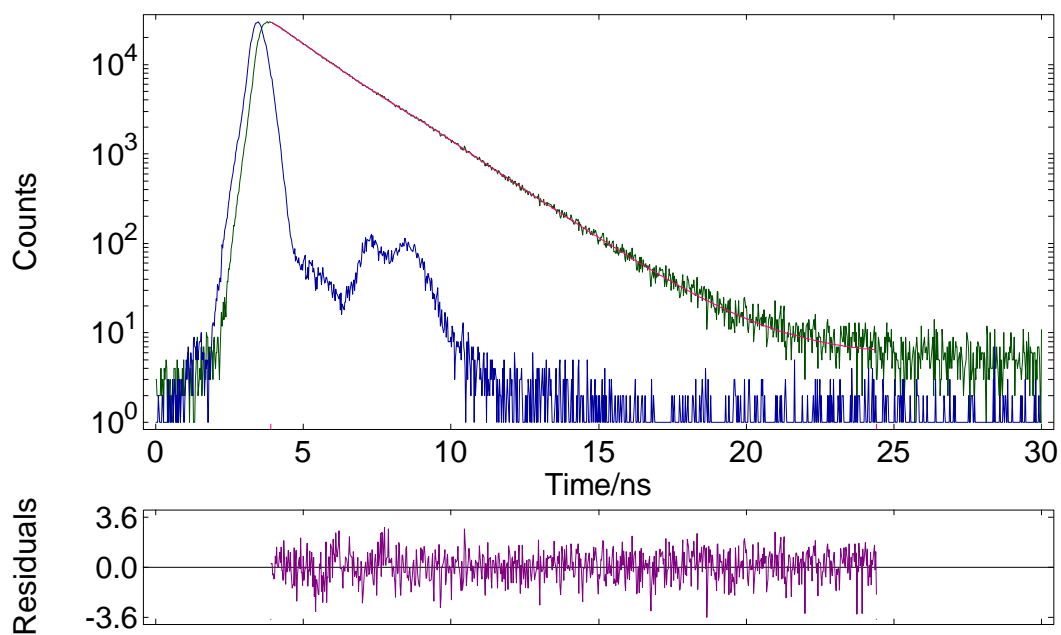


a

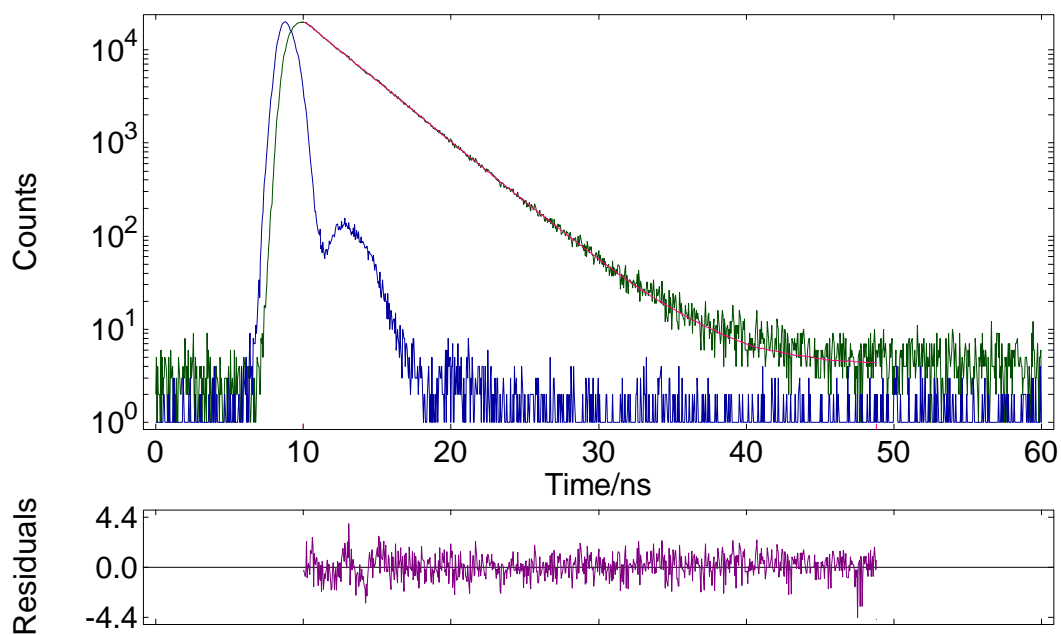


b

Figure S29. Time-resolved fluorescence lifetime decay profile of **4a** (a) in toluene, instrumental response function (IRF, blue). $\lambda_{\text{ex}} = 375$ nm, $\lambda_{\text{em}} = 490$ nm; (b) in MeCN, IRF (blue). $\lambda_{\text{ex}} = 375$ nm, $\lambda_{\text{em}} = 541$ nm.

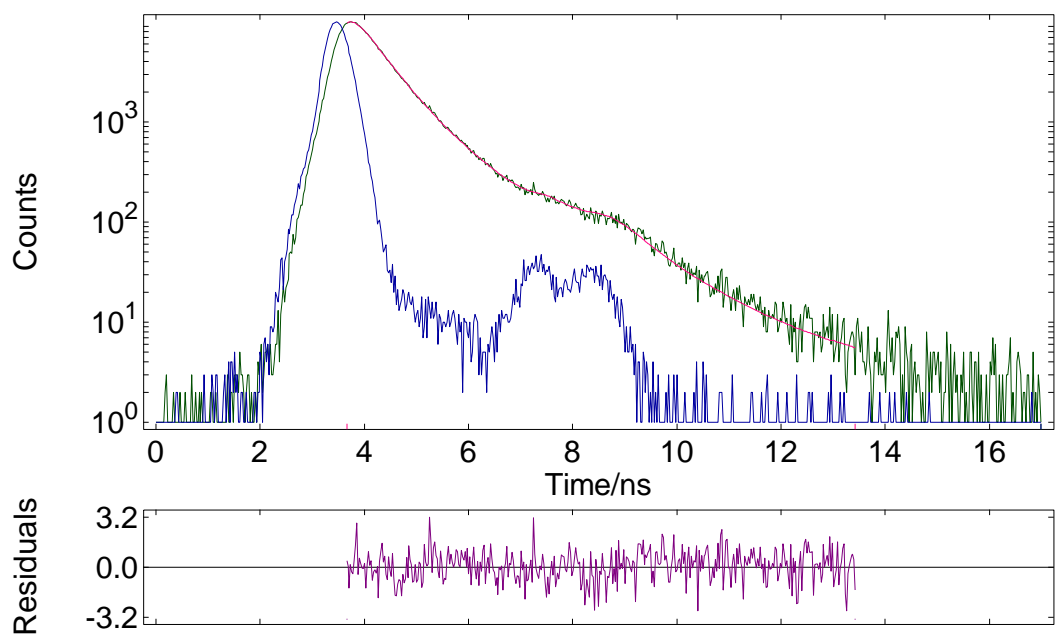


a

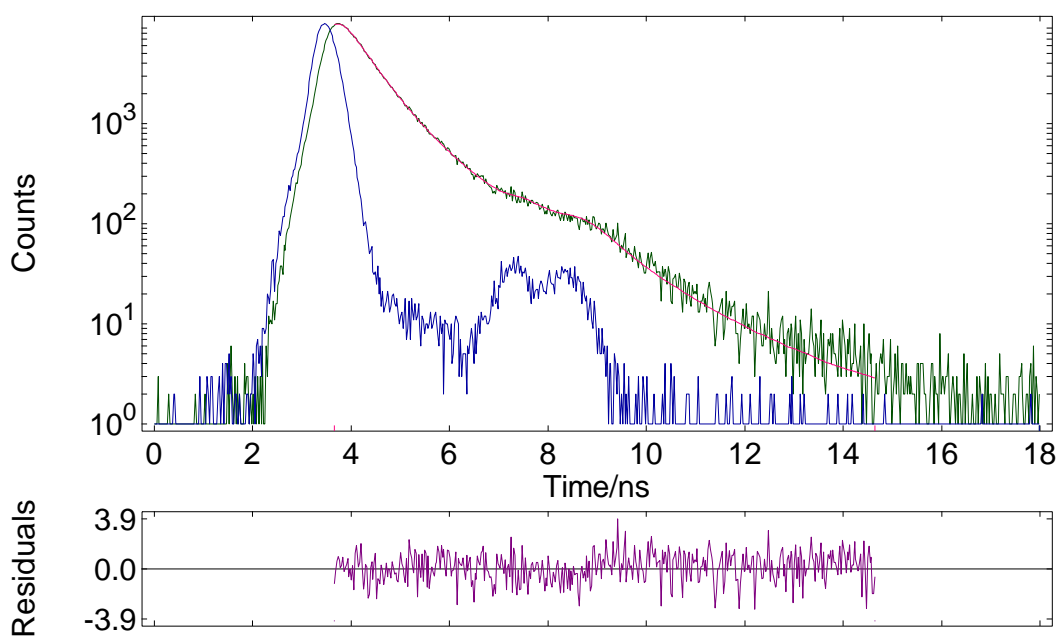


b

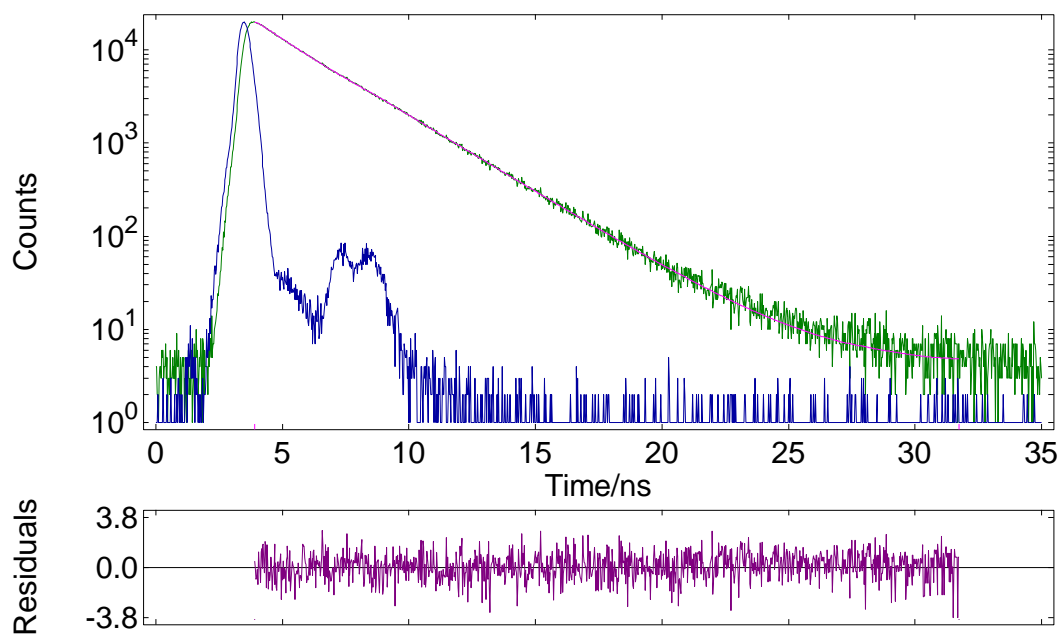
Figure S30. Time-resolved fluorescence lifetime decay profile of **4b** (a) in toluene, IRF (blue). $\lambda_{\text{ex}} = 375 \text{ nm}$, $\lambda_{\text{em}} = 470 \text{ nm}$; (b) in MeCN, IRF (blue). $\lambda_{\text{ex}} = 375 \text{ nm}$, $\lambda_{\text{em}} = 545 \text{ nm}$.



a

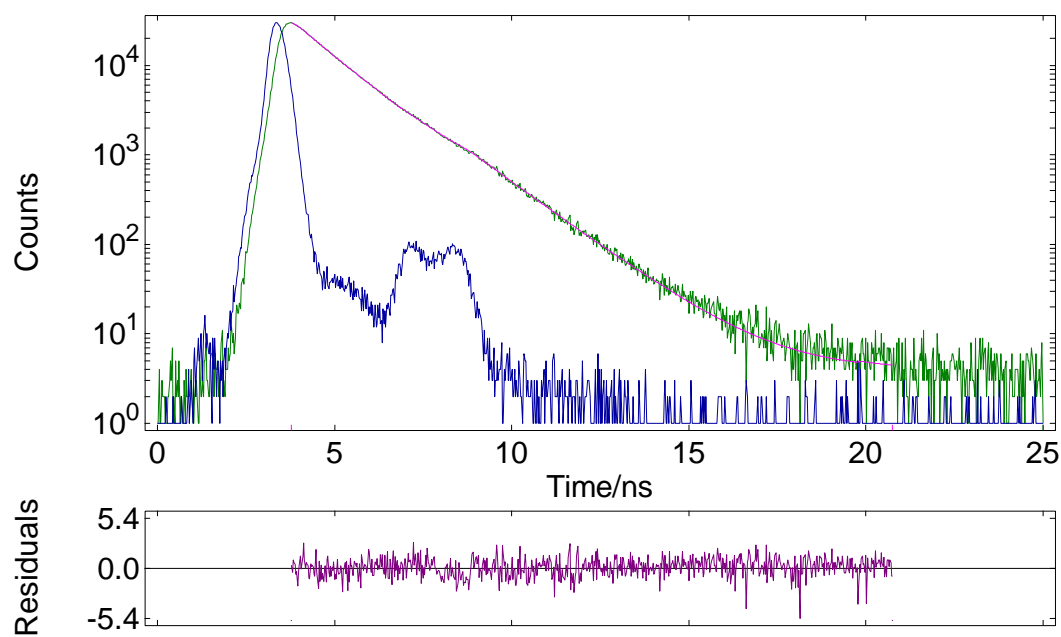


b

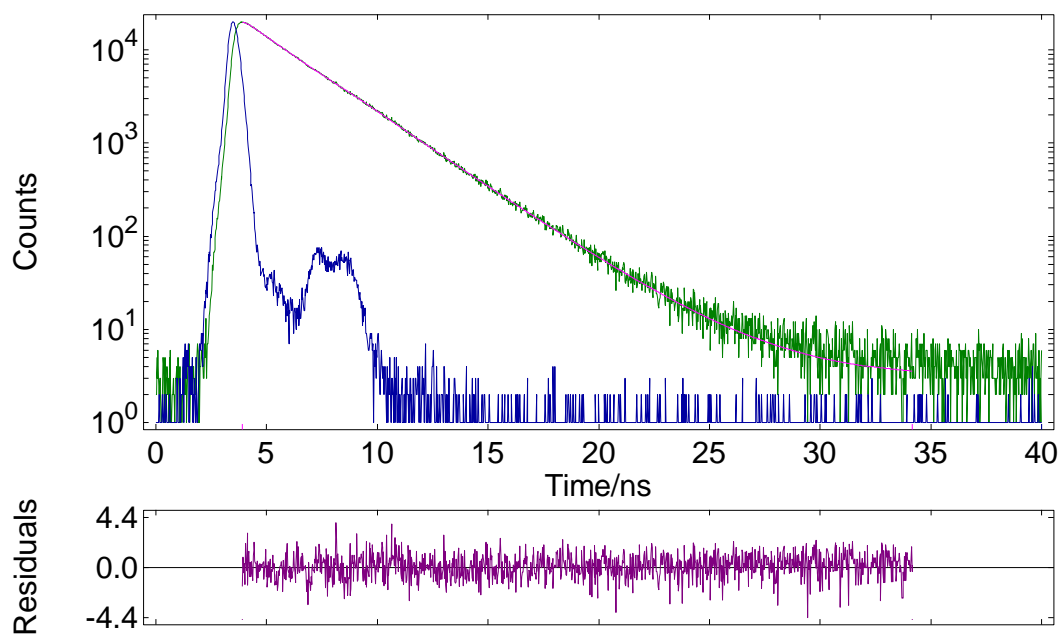


c

Figure 31. Time-resolved fluorescence lifetime decay profile of **4c** (a) in toluene, IRF (blue). $\lambda_{\text{ex}} = 375 \text{ nm}$, $\lambda_{\text{em}} = 430 \text{ nm}$; (b) in toluene, IRF (blue). $\lambda_{\text{ex}} = 375 \text{ nm}$, $\lambda_{\text{em}} = 456 \text{ nm}$; (c) in MeCN, IRF (blue). $\lambda_{\text{ex}} = 375 \text{ nm}$, $\lambda_{\text{em}} = 490 \text{ nm}$.

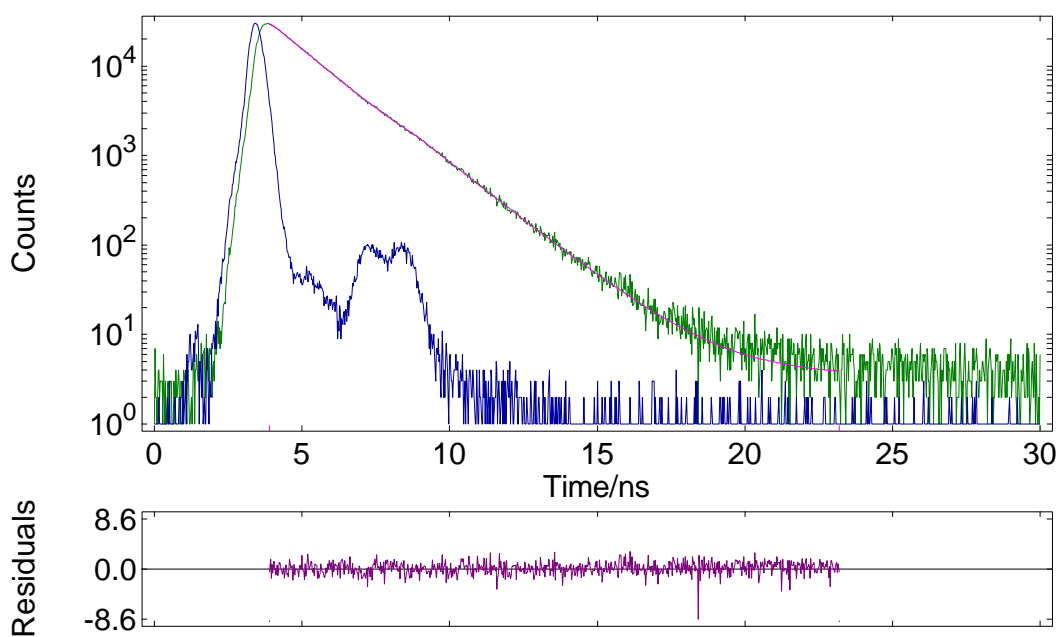


a

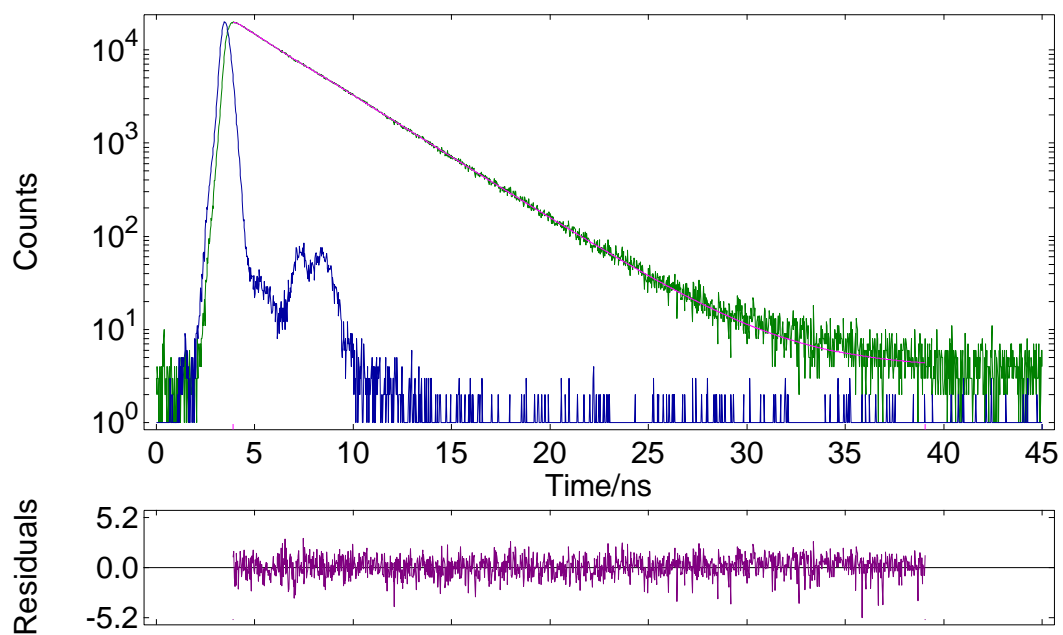


b

Figure 32. Time-resolved fluorescence lifetime decay profile of **5a** (a) in toluene, IRF (blue). $\lambda_{\text{ex}} = 375 \text{ nm}$, $\lambda_{\text{em}} = 450 \text{ nm}$; (b) in MeCN, IRF (blue). $\lambda_{\text{ex}} = 375 \text{ nm}$, $\lambda_{\text{em}} = 535 \text{ nm}$.

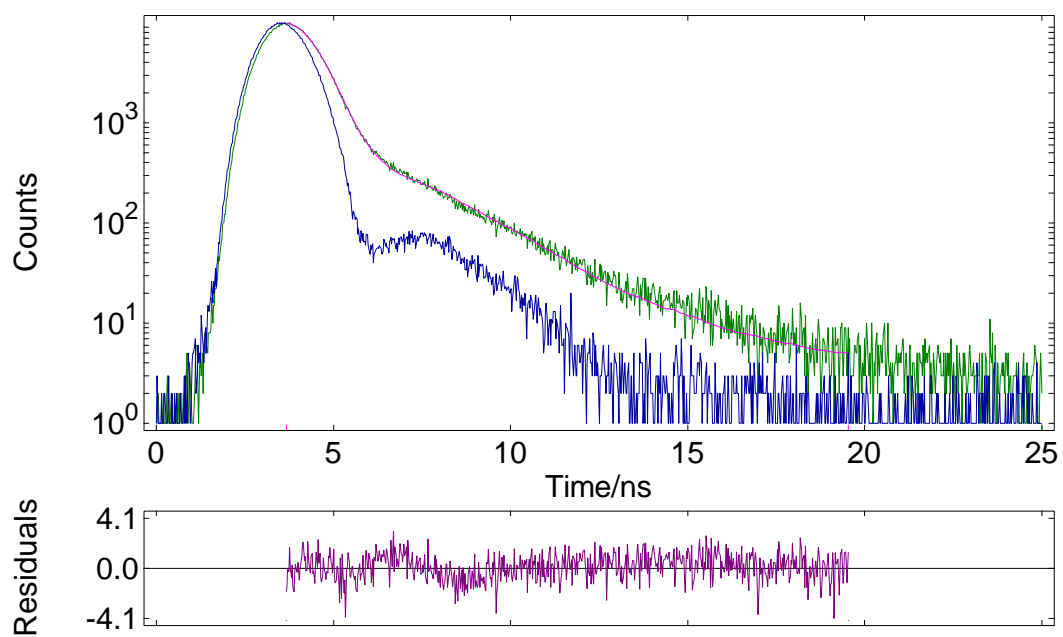


a

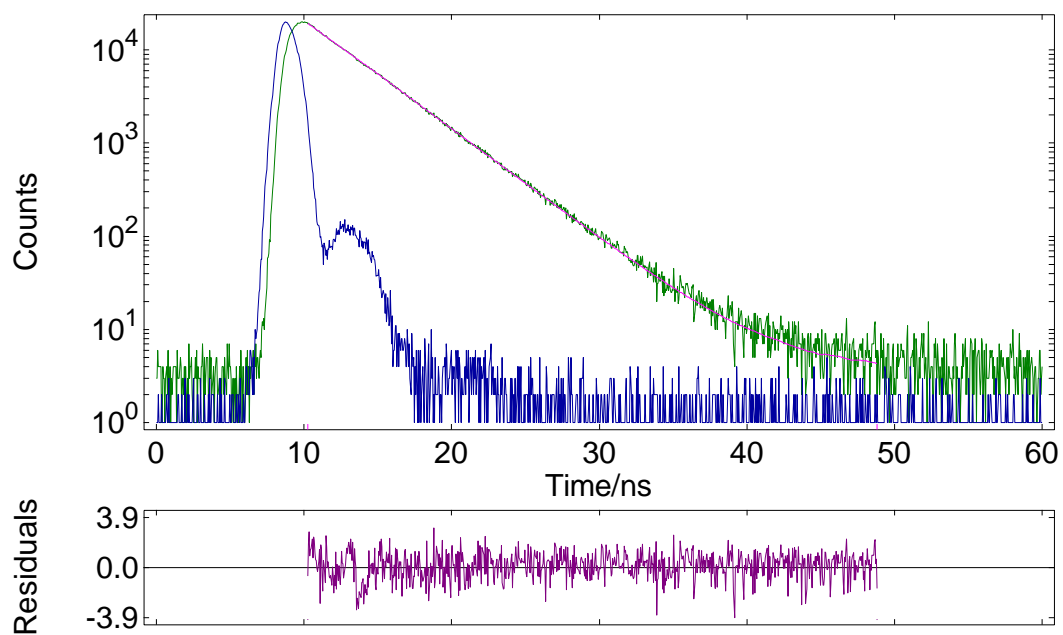


b

Figure S33. Time-resolved fluorescence lifetime decay profile of **5b** (a) in toluene, IRF (blue). $\lambda_{\text{ex}} = 375 \text{ nm}$, $\lambda_{\text{em}} = 445 \text{ nm}$; (b) in MeCN, IRF (blue). $\lambda_{\text{ex}} = 375 \text{ nm}$, $\lambda_{\text{em}} = 535 \text{ nm}$.



a



b

Figure S34. Time-resolved fluorescence lifetime decay profile of **5c** (a) in toluene, IRF (blue). $\lambda_{\text{ex}} = 300 \text{ nm}$, $\lambda_{\text{em}} = 415 \text{ nm}$; (b) in MeCN, IRF (blue). $\lambda_{\text{ex}} = 300 \text{ nm}$, $\lambda_{\text{em}} = 490 \text{ nm}$.

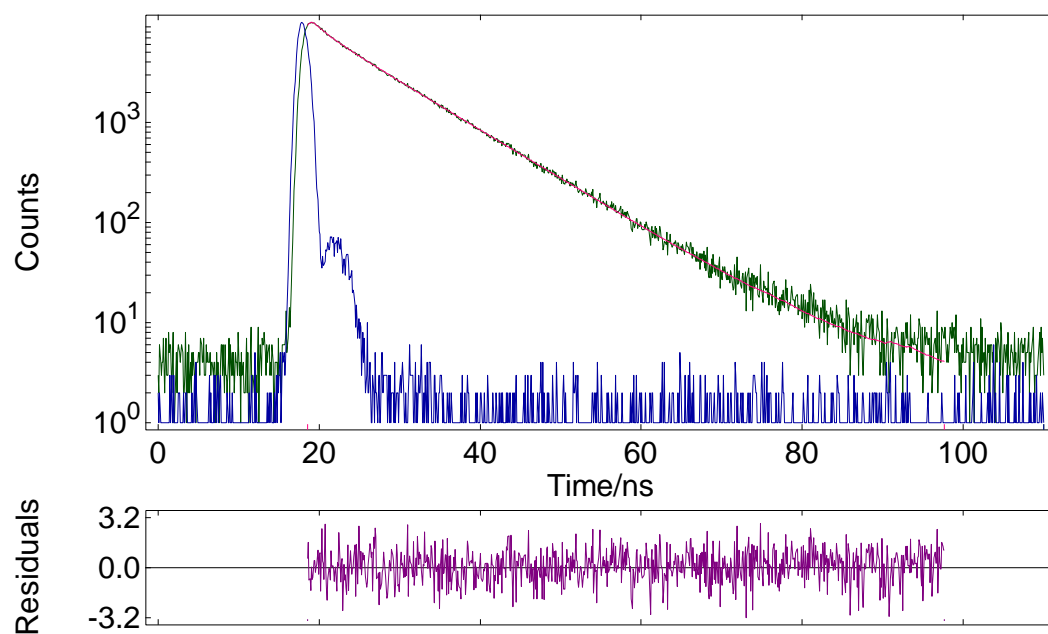
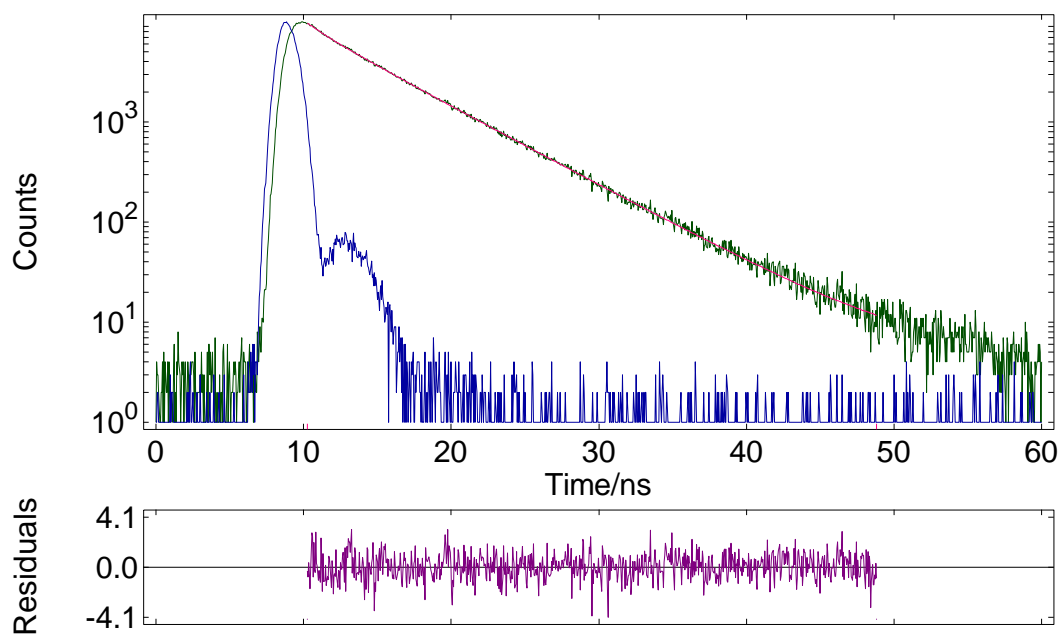
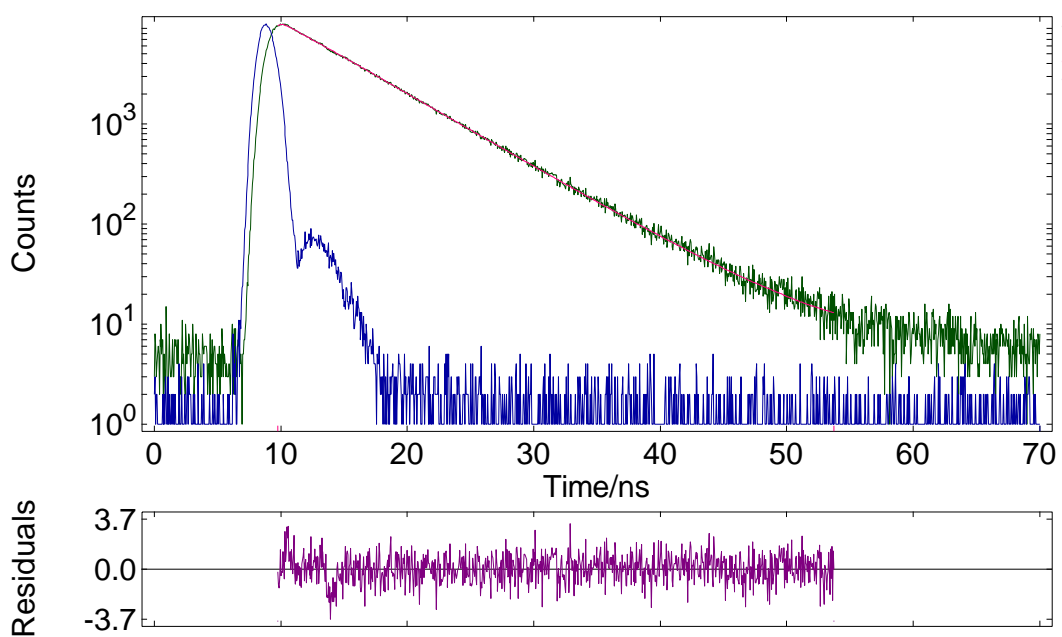


Figure S35. Time-resolved fluorescence lifetime decay profile of **6a** in toluene, IRF (blue). $\lambda_{\text{ex}} = 300 \text{ nm}$, $\lambda_{\text{em}} = 460 \text{ nm}$.

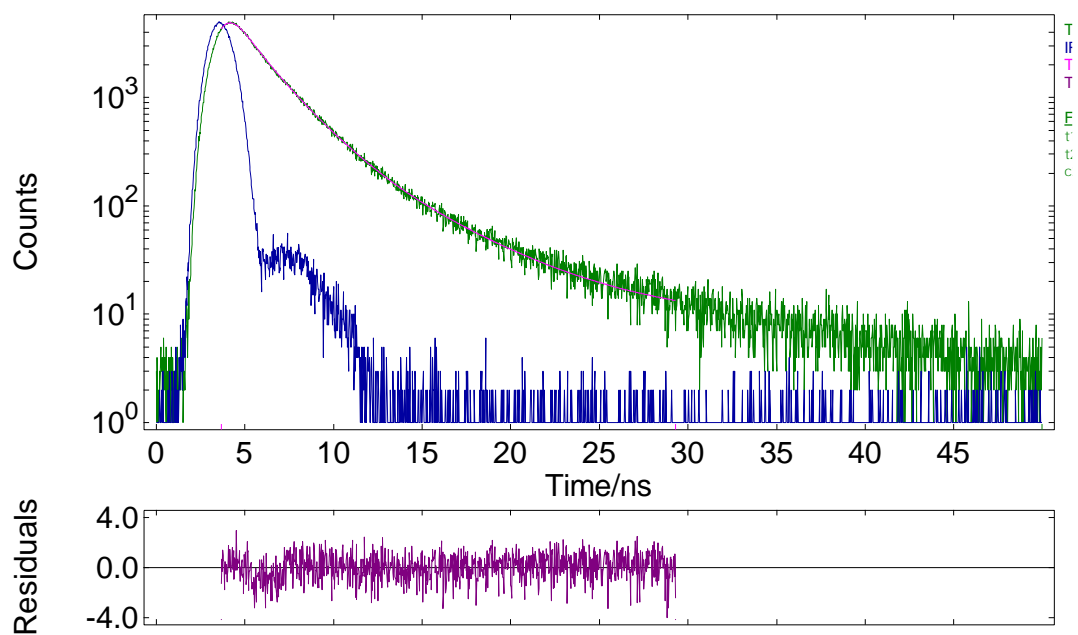


a

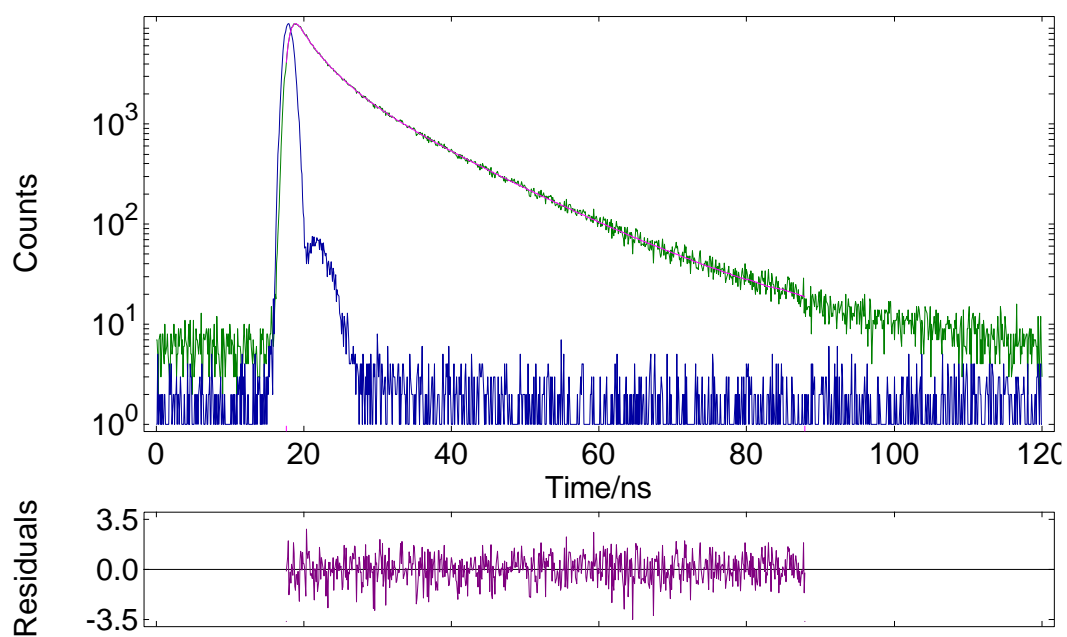


b

Figure S36. Time-resolved fluorescence lifetime decay profile of **6b** (a) in toluene, IRF (blue). $\lambda_{\text{ex}} = 300 \text{ nm}$, $\lambda_{\text{em}} = 430 \text{ nm}$; (b) in MeCN, IRF (blue). $\lambda_{\text{ex}} = 300 \text{ nm}$, $\lambda_{\text{em}} = 565 \text{ nm}$.

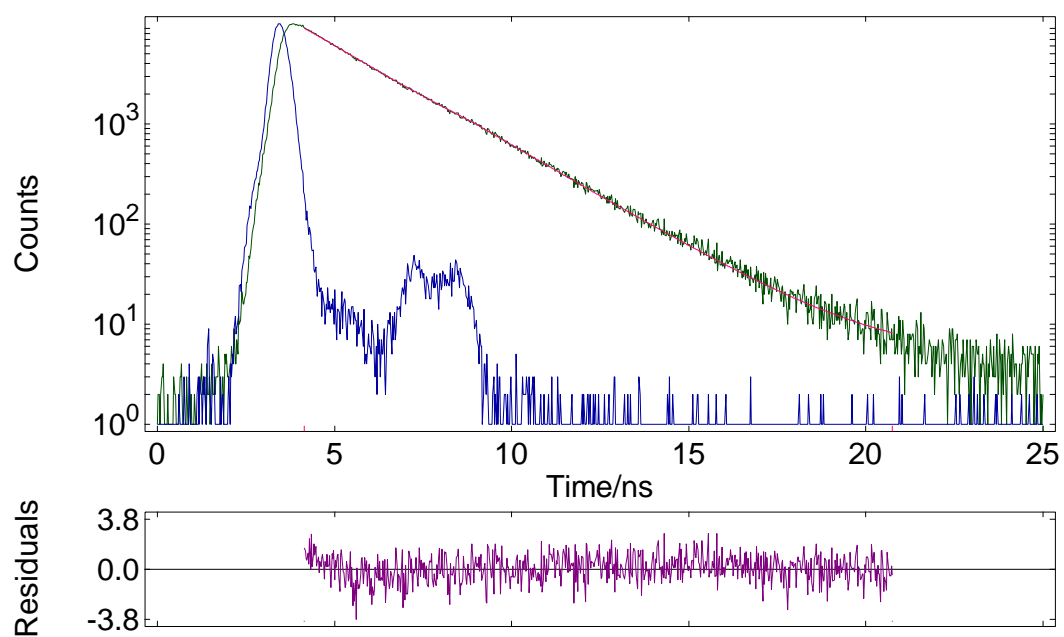


a

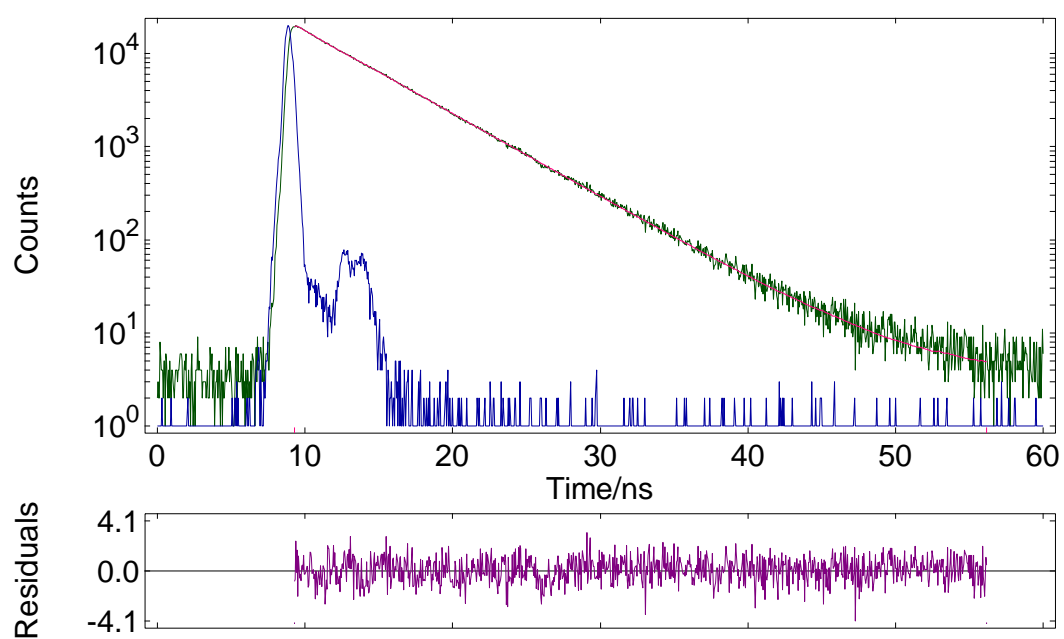


b

Figure S37. Time-resolved fluorescence lifetime decay profile of **6c** (a) in toluene, IRF (blue). $\lambda_{\text{ex}} = 300 \text{ nm}$, $\lambda_{\text{em}} = 430 \text{ nm}$; (b) in MeCN, IRF (blue). $\lambda_{\text{ex}} = 300 \text{ nm}$, $\lambda_{\text{em}} = 408 \text{ nm}$.

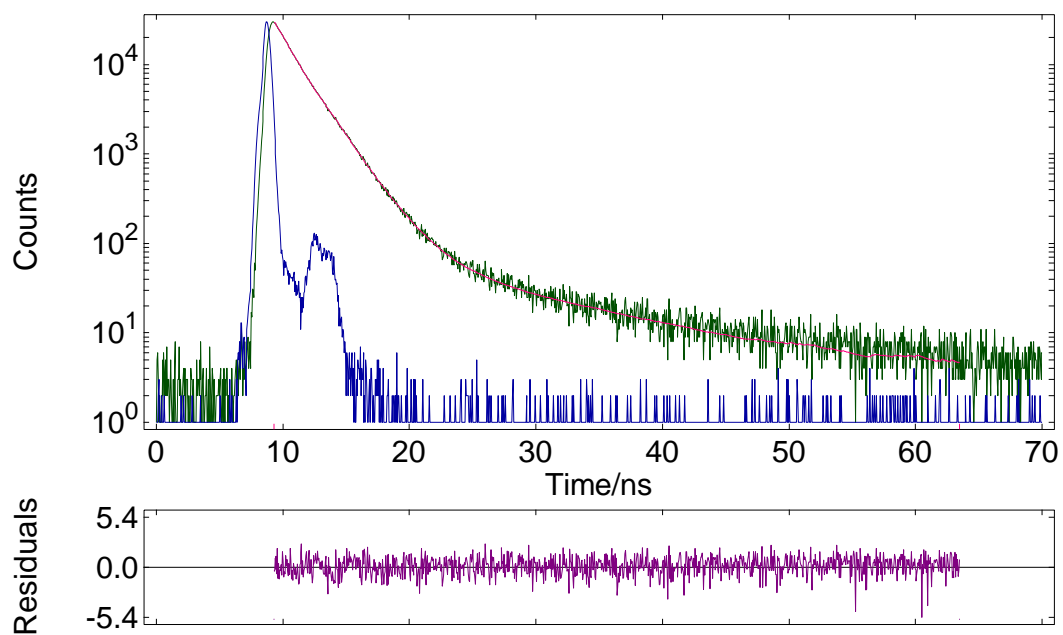


a

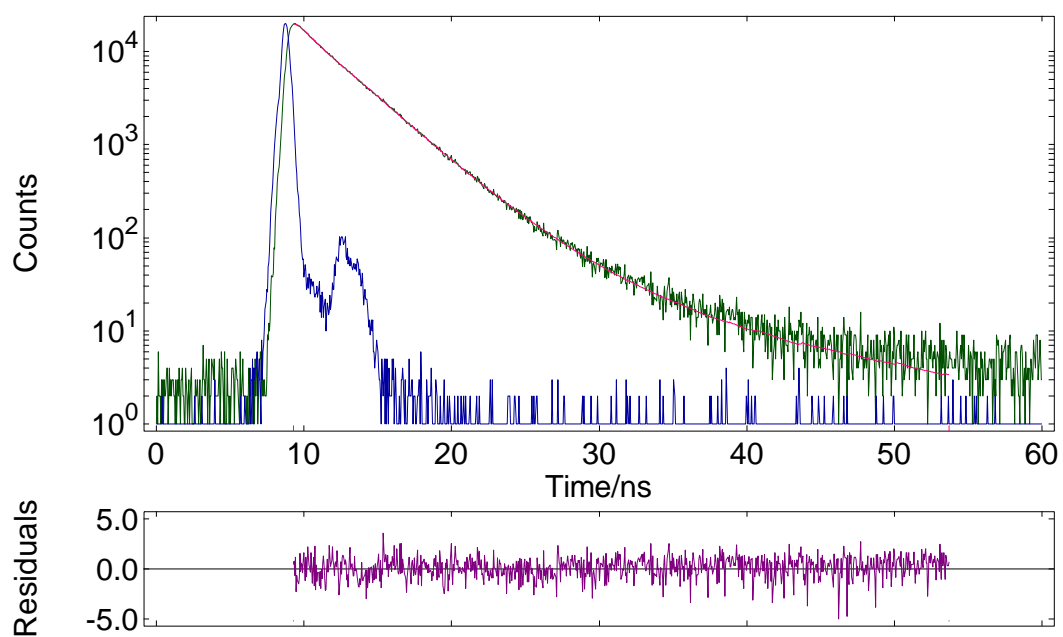


b

Figure S38. Time-resolved fluorescence lifetime decay profile of **10** (a) in toluene, IRF (blue). $\lambda_{\text{ex}} = 375 \text{ nm}$, $\lambda_{\text{em}} = 430 \text{ nm}$; (b) in MeCN, IRF (blue). $\lambda_{\text{ex}} = 375 \text{ nm}$, $\lambda_{\text{em}} = 500 \text{ nm}$.

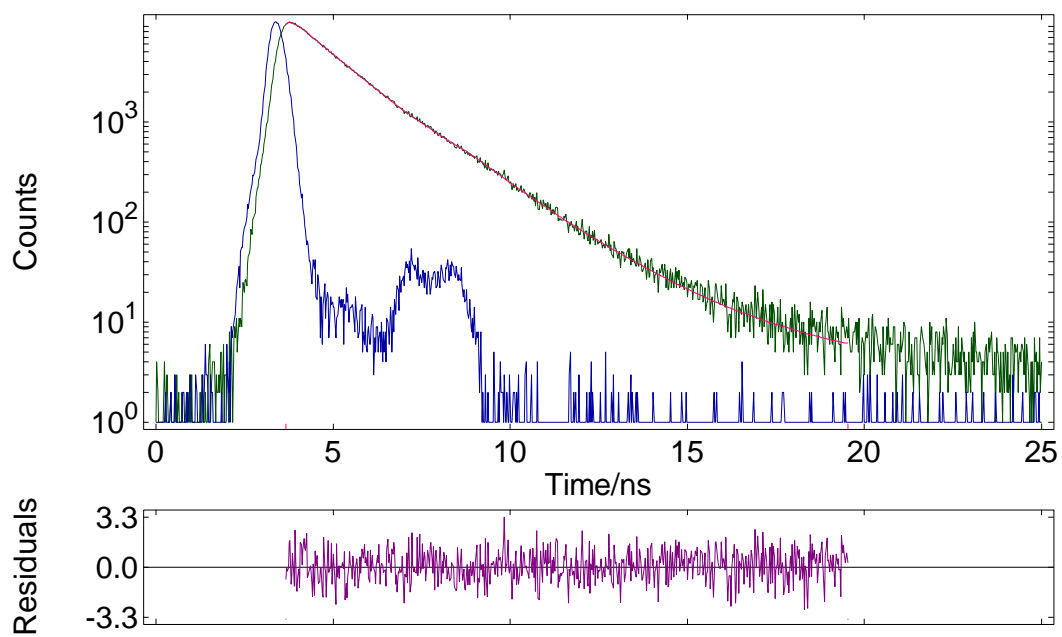


a

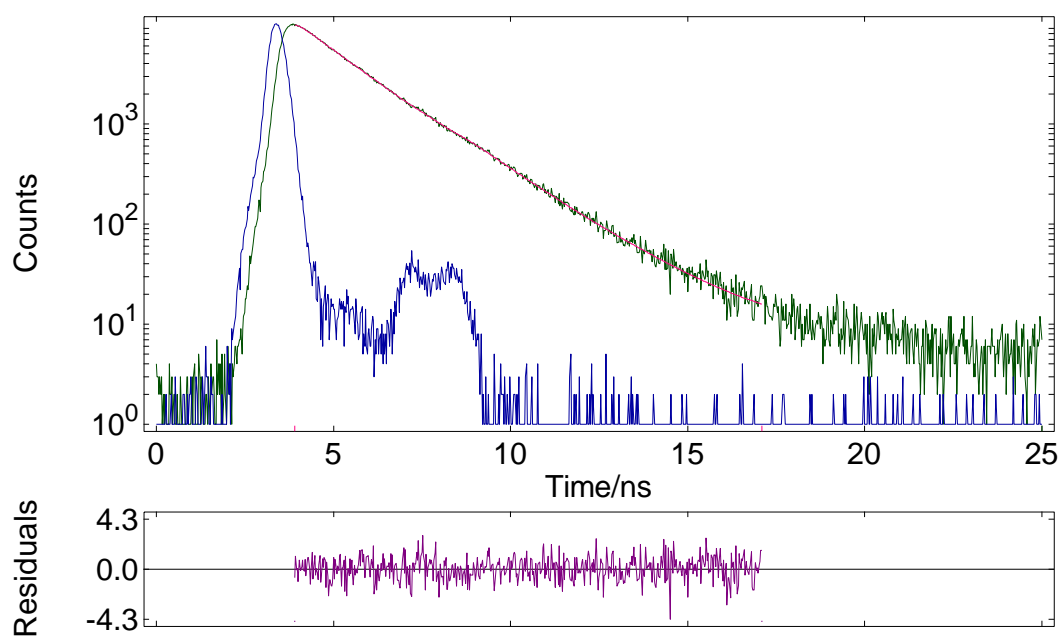


b

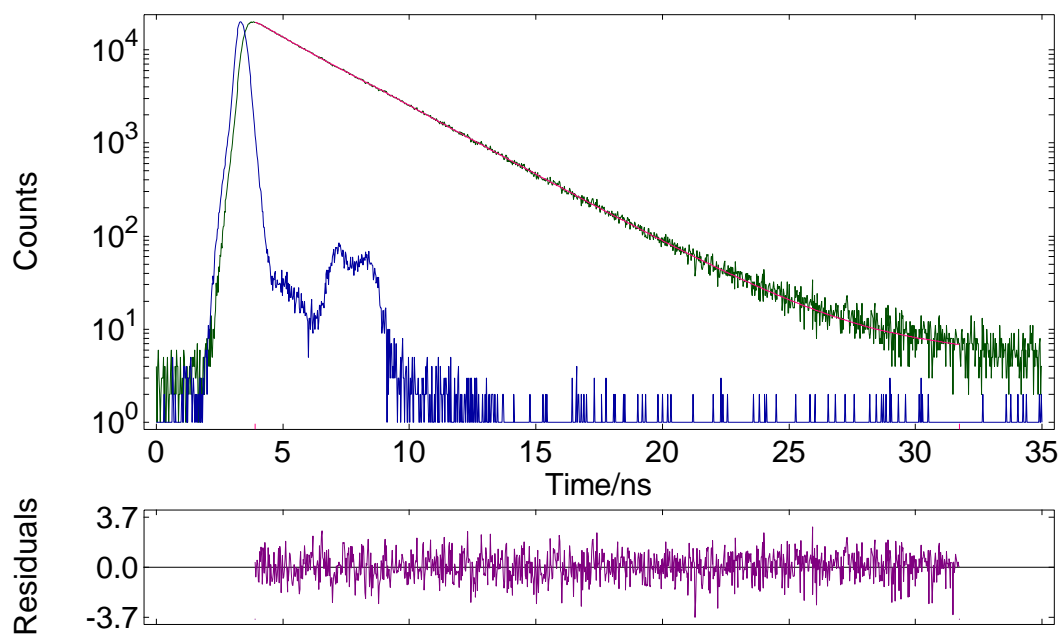
Figure S39. Time-resolved fluorescence lifetime decay profile of **7a** (a) in toluene, IRF (blue). $\lambda_{\text{ex}} = 375$ nm, $\lambda_{\text{em}} = 471$ nm; (b) in MeCN, IRF (blue). $\lambda_{\text{ex}} = 375$ nm, $\lambda_{\text{em}} = 539$ nm.



a

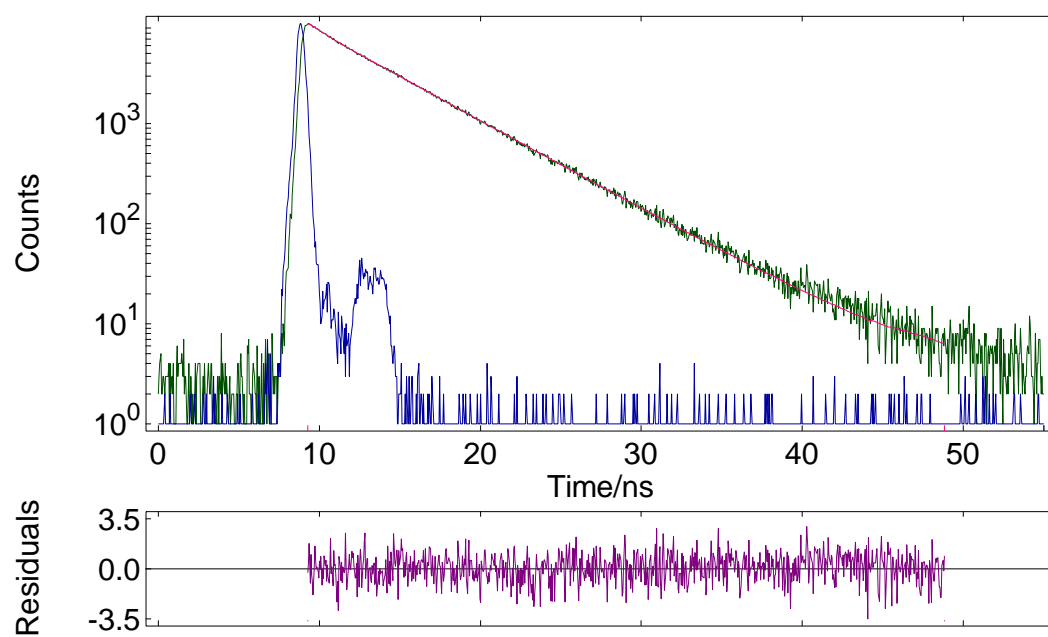


b

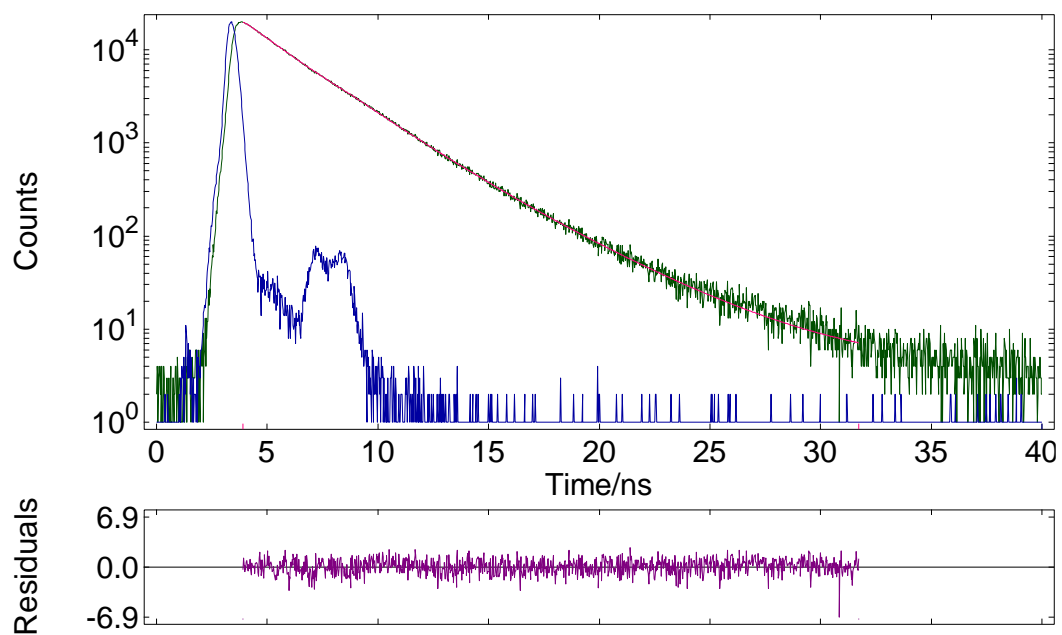


c

Figure S40. Time-resolved fluorescence lifetime decay profile of **7b** (a) in toluene, IRF (blue). $\lambda_{\text{ex}} = 375$ nm, $\lambda_{\text{em}} = 480$ nm; (b) in toluene, IRF (blue). $\lambda_{\text{ex}} = 375$ nm, $\lambda_{\text{em}} = 621$ nm; (c) in MeCN, IRF (blue). $\lambda_{\text{ex}} = 375$ nm, $\lambda_{\text{em}} = 525$ nm.

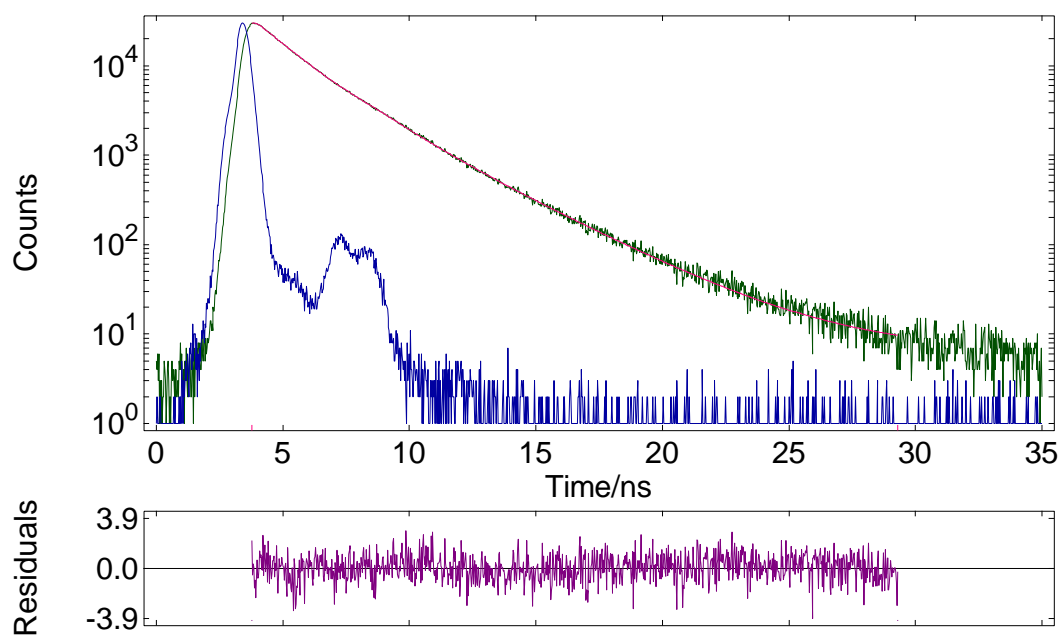


a

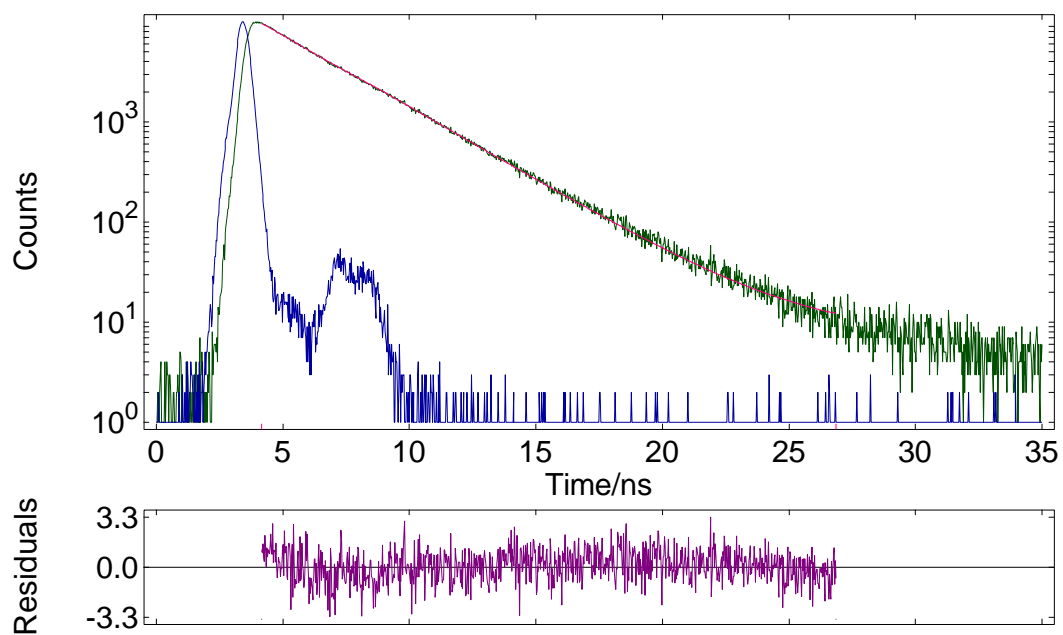


b

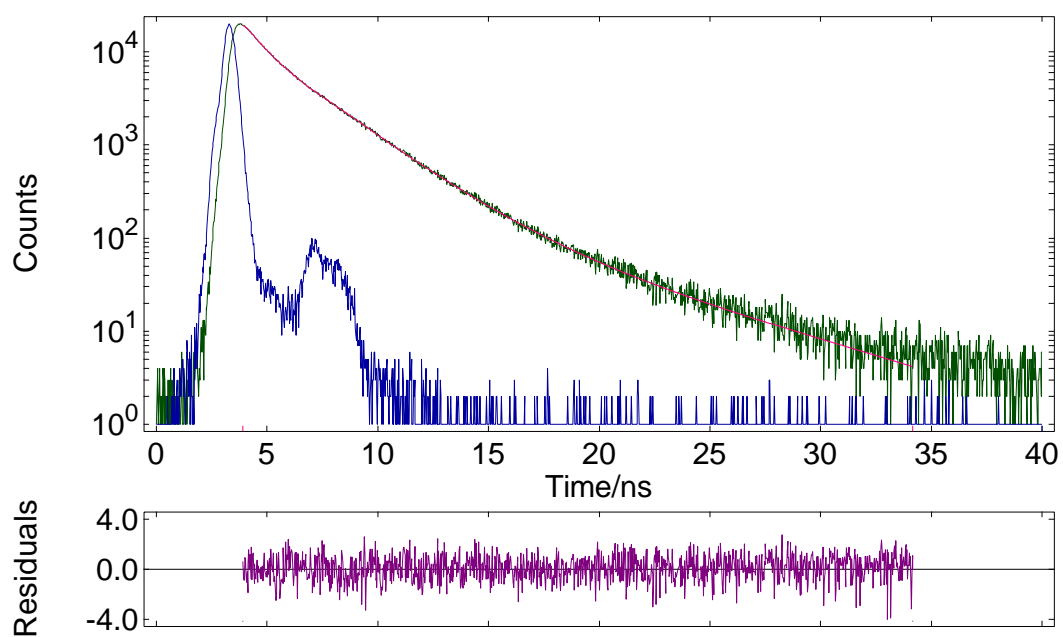
Figure S41. Time-resolved fluorescence lifetime decay profile of **7c** (a) in toluene, IRF (blue). $\lambda_{\text{ex}} = 375$ nm, $\lambda_{\text{em}} = 541$ nm; (b) in MeCN, IRF (blue). $\lambda_{\text{ex}} = 375$ nm, $\lambda_{\text{em}} = 491$ nm.



a



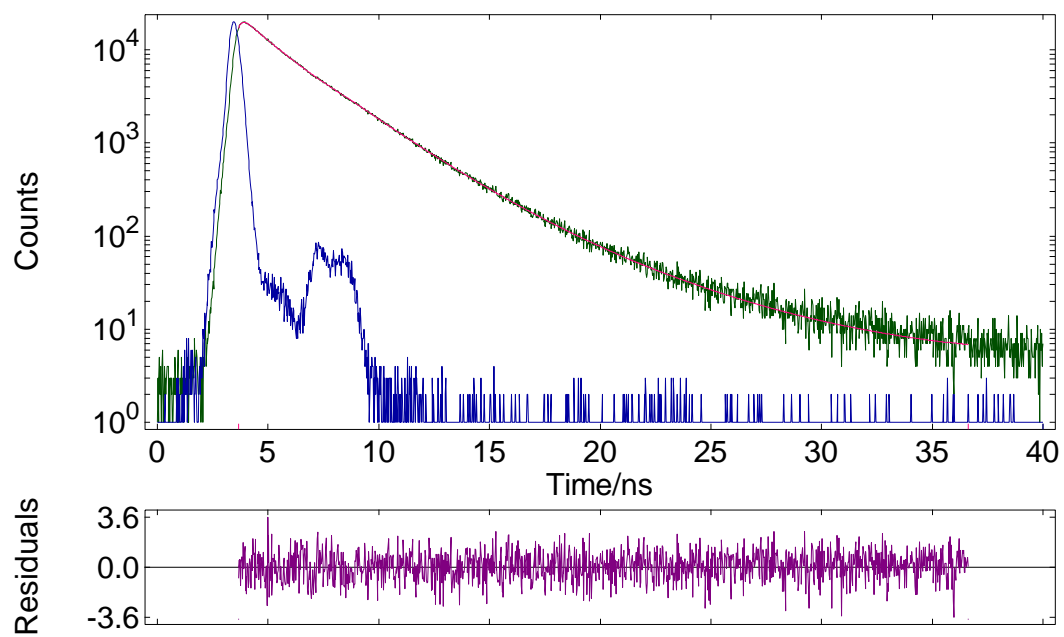
b



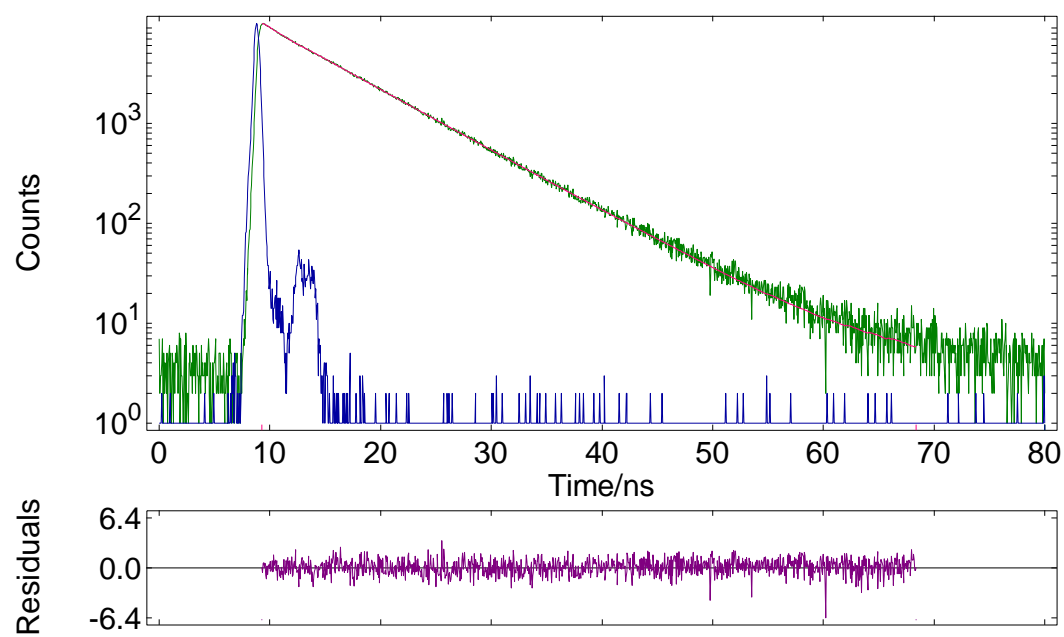
c

Figure S42. Time-resolved fluorescence lifetime decay profile of **8a** (a) in toluene, IRF (blue).

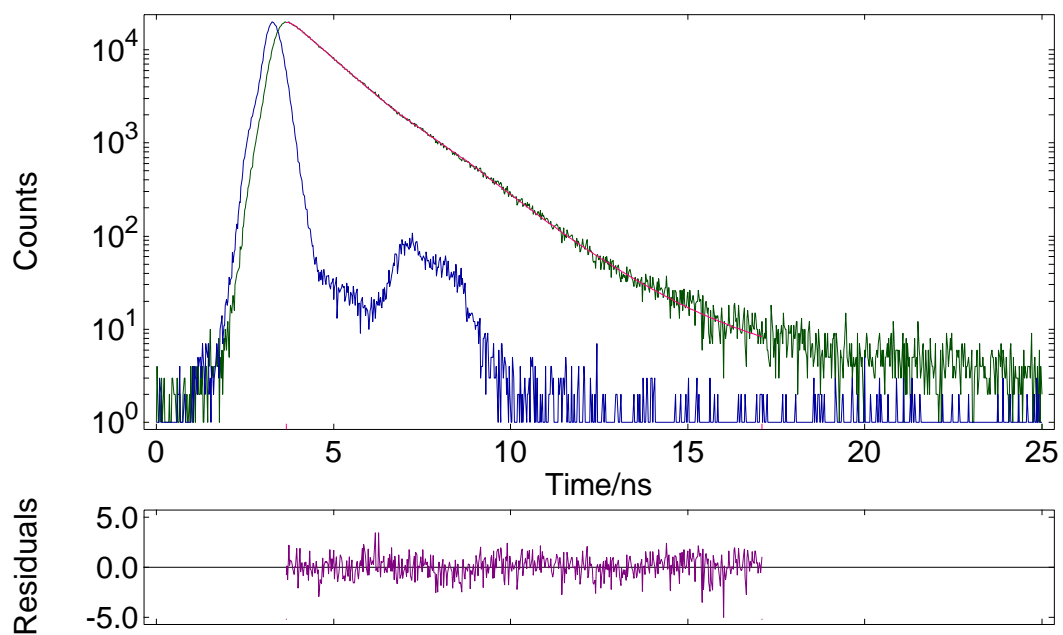
$\lambda_{\text{ex}} = 375$ nm, $\lambda_{\text{em}} = 460$ nm; (b) in toluene, IRF (blue). $\lambda_{\text{ex}} = 375$ nm, $\lambda_{\text{em}} = 600$ nm; (c) in MeCN, IRF (blue). $\lambda_{\text{ex}} = 375$ nm, $\lambda_{\text{em}} = 530$ nm.



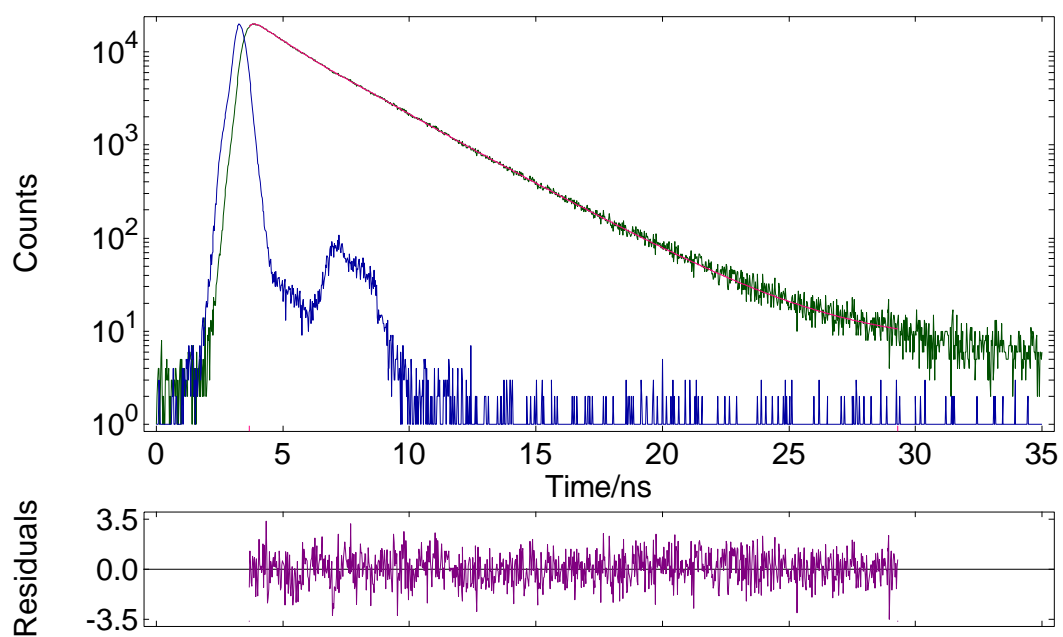
a



b

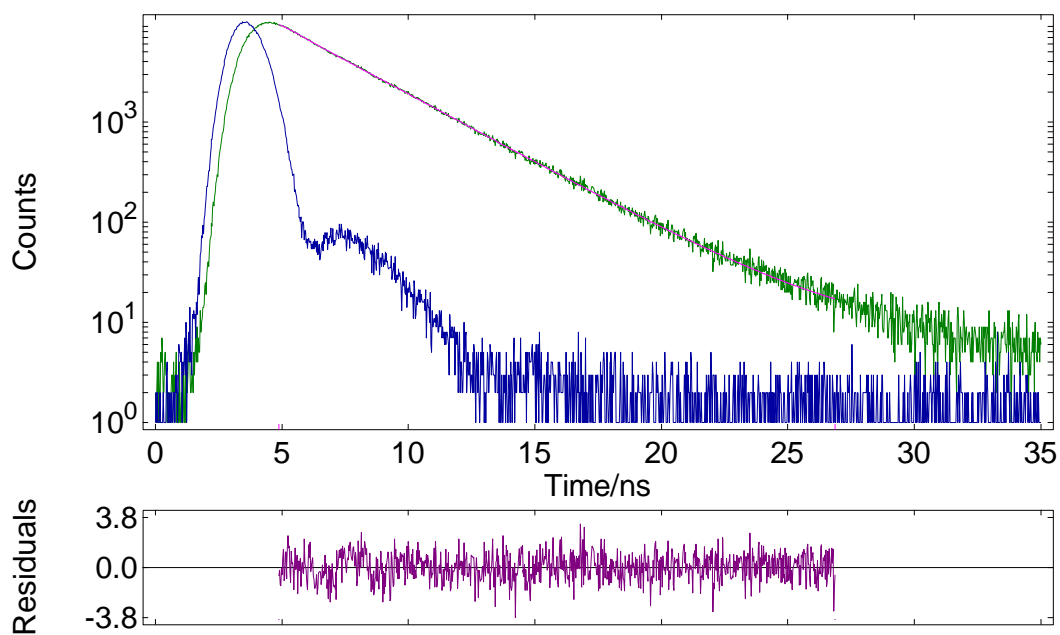


c

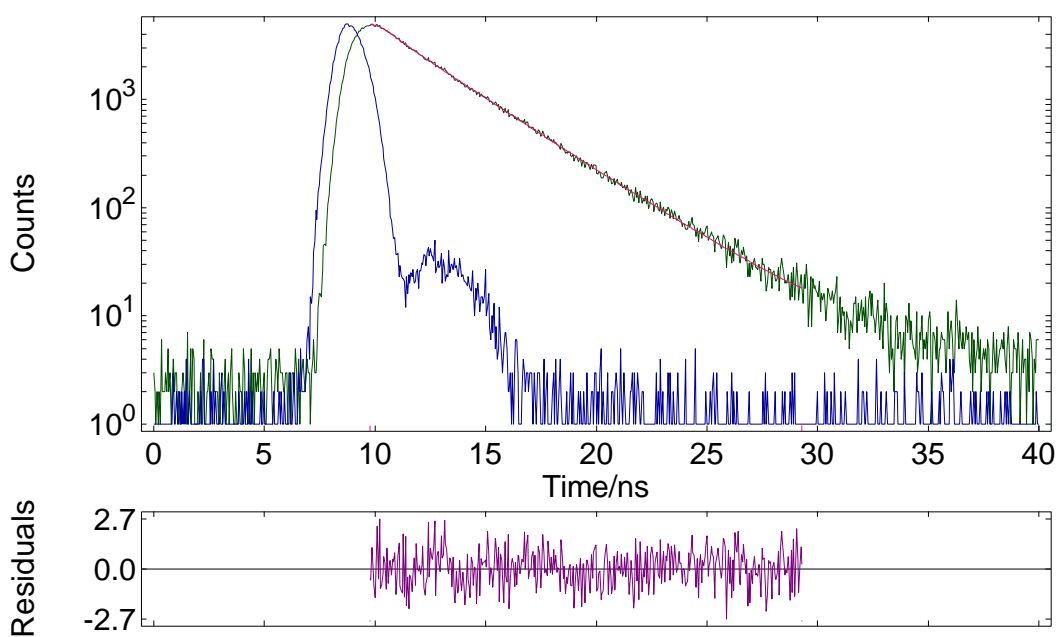


d

Figure S43. Time-resolved fluorescence lifetime decay profile of **8b** (a) in toluene, IRF (blue). $\lambda_{\text{ex}} = 375 \text{ nm}$, $\lambda_{\text{em}} = 465 \text{ nm}$; (b) in toluene, IRF (blue). $\lambda_{\text{ex}} = 375 \text{ nm}$, $\lambda_{\text{em}} = 555 \text{ nm}$; (c) in MeCN, IRF (blue). $\lambda_{\text{ex}} = 375 \text{ nm}$, $\lambda_{\text{em}} = 400 \text{ nm}$; (d) in MeCN, IRF (blue). $\lambda_{\text{ex}} = 375 \text{ nm}$, $\lambda_{\text{em}} = 540 \text{ nm}$.



a



b

Figure S44. Time-resolved fluorescence lifetime decay profile of **9** (a) in toluene, IRF (blue). $\lambda_{\text{ex}} = 300 \text{ nm}$, $\lambda_{\text{em}} = 468 \text{ nm}$; (b) in MeCN, IRF (blue). $\lambda_{\text{ex}} = 300 \text{ nm}$, $\lambda_{\text{em}} = 560 \text{ nm}$.

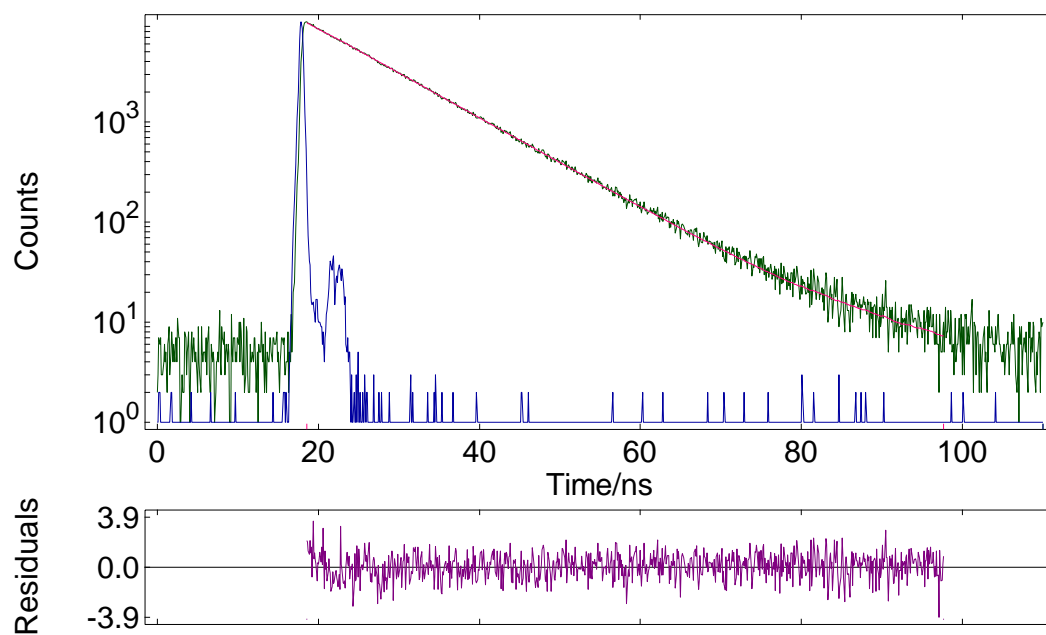
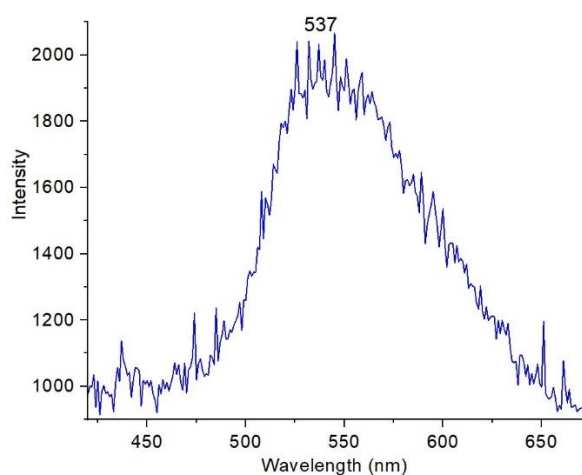
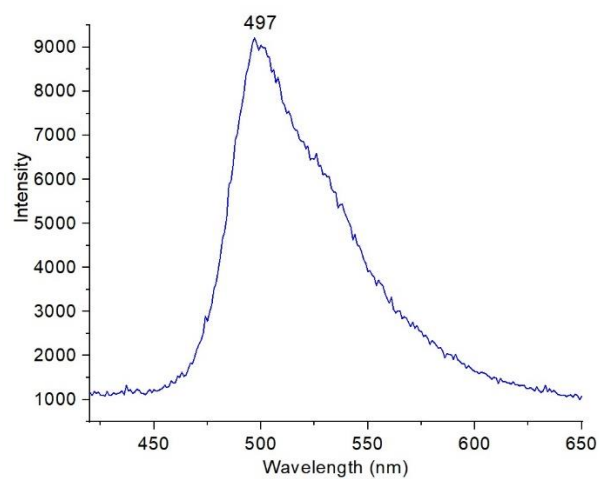


Figure S45. Time-resolved fluorescence lifetime decay profile of **11** in toluene, IRF (blue).
 $\lambda_{\text{ex}} = 375 \text{ nm}$, $\lambda_{\text{em}} = 570 \text{ nm}$.

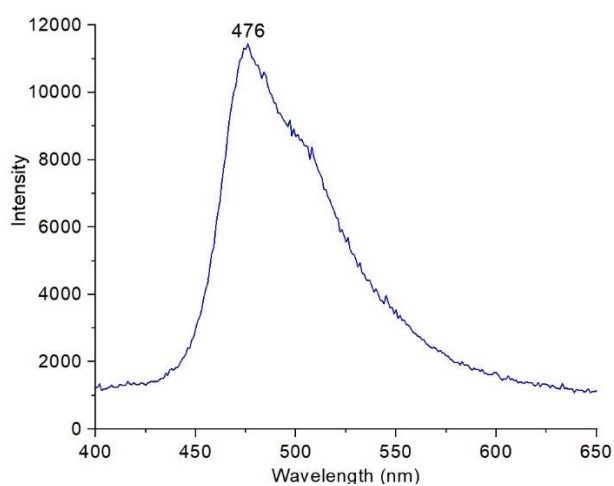
6. Emission spectra of chromophores in solid state



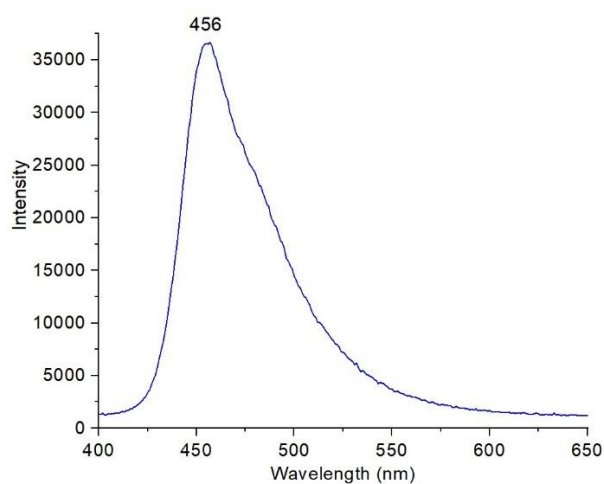
4a



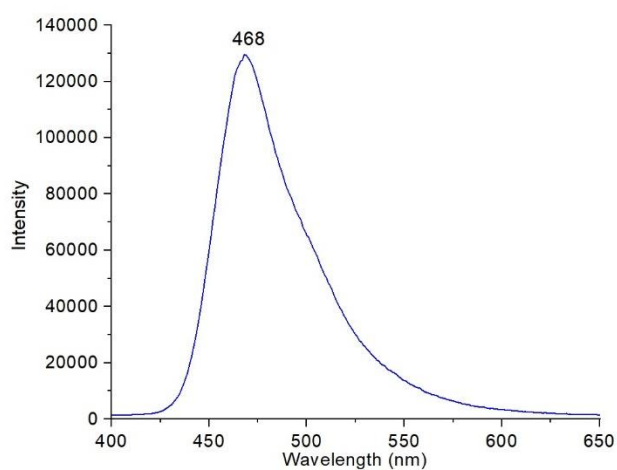
4b



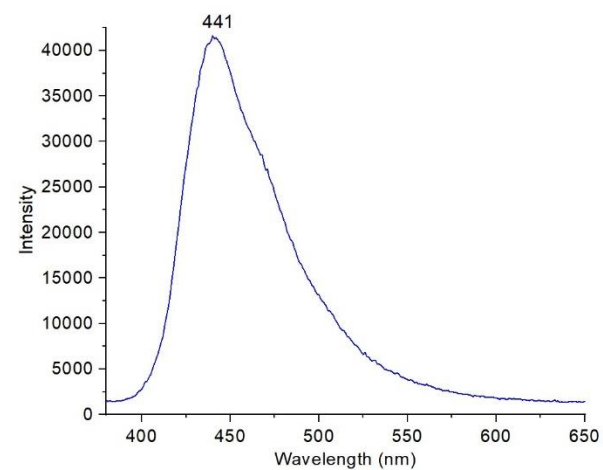
4c



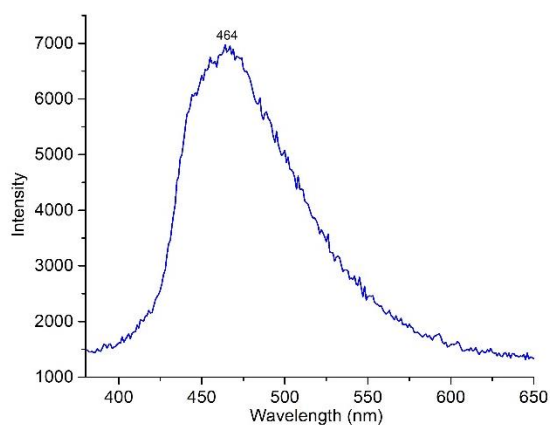
5a



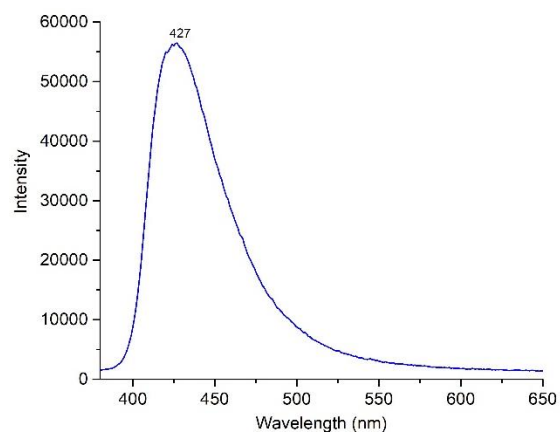
5b



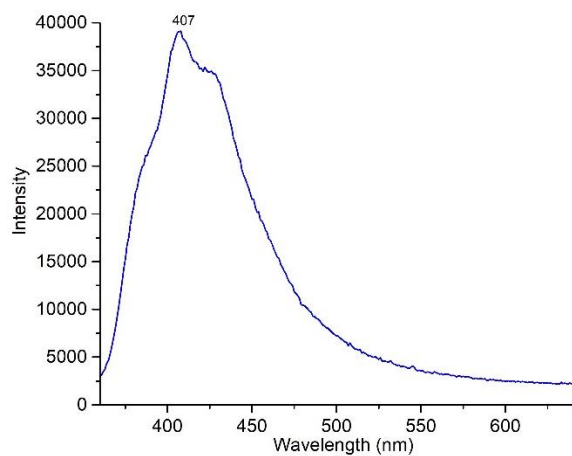
5c



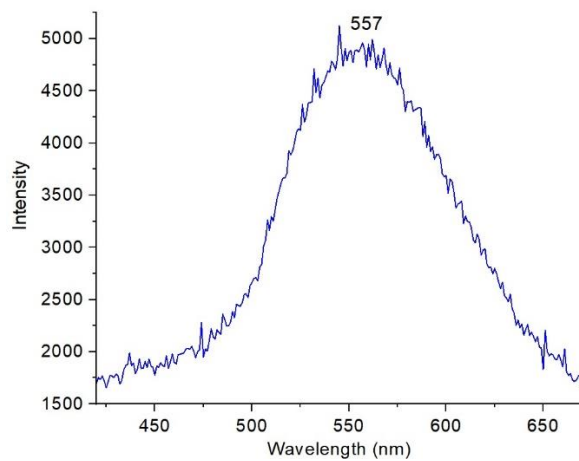
6a



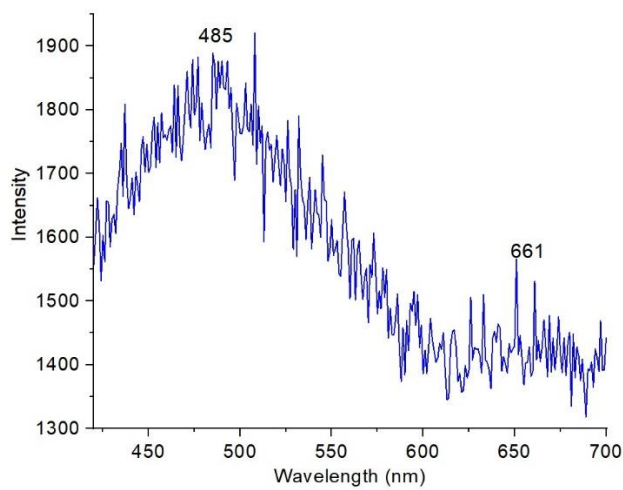
6b



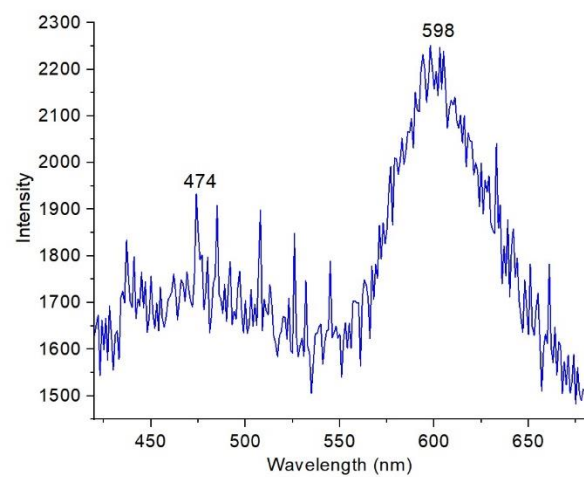
6c



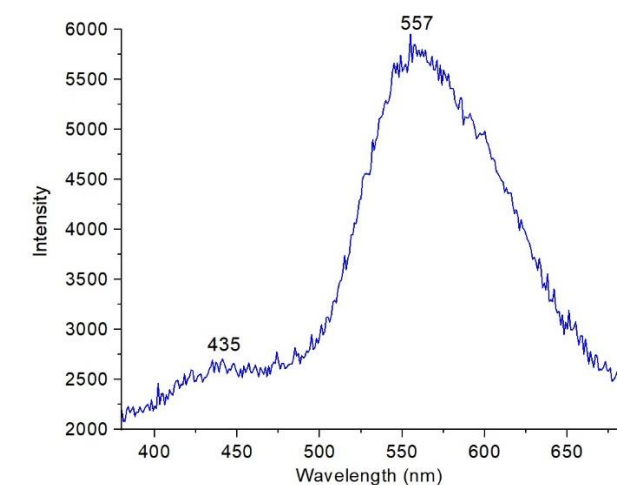
10



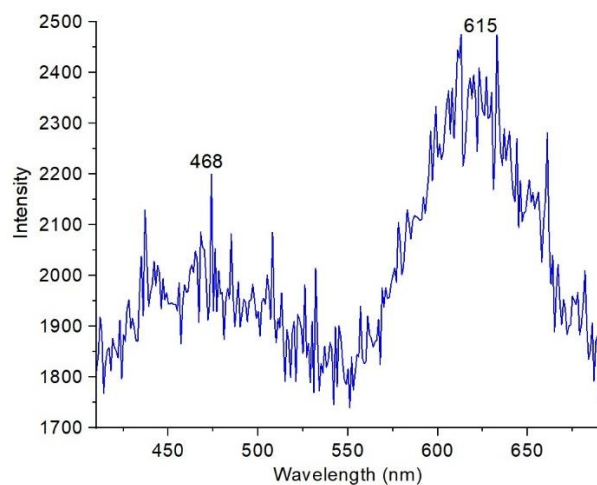
7a



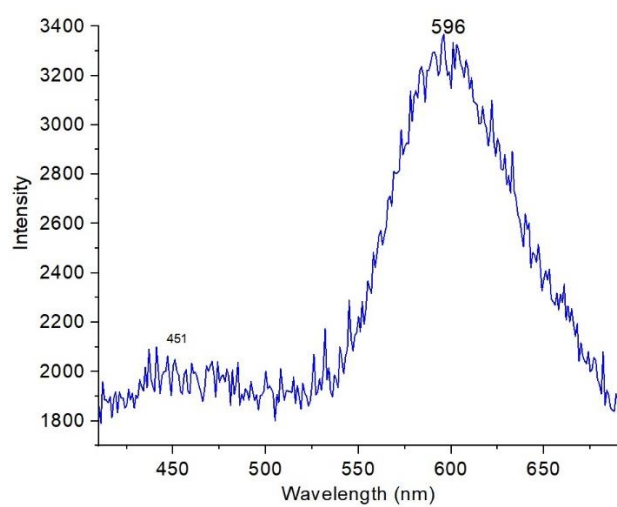
7b



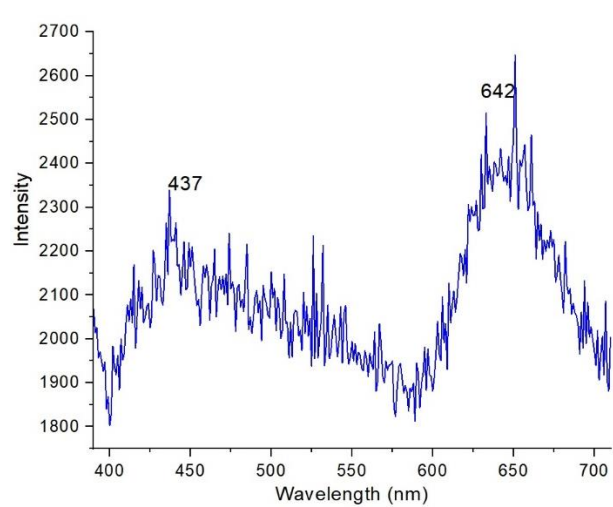
7c



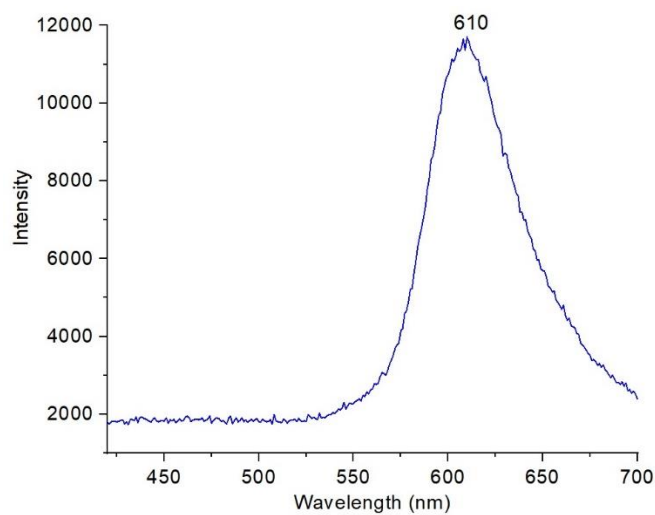
8a



8b



9



11

Figure S46. The emission spectra of compounds **4–11** in solid state.

Behavior of chromophores in MeCN/water mixture

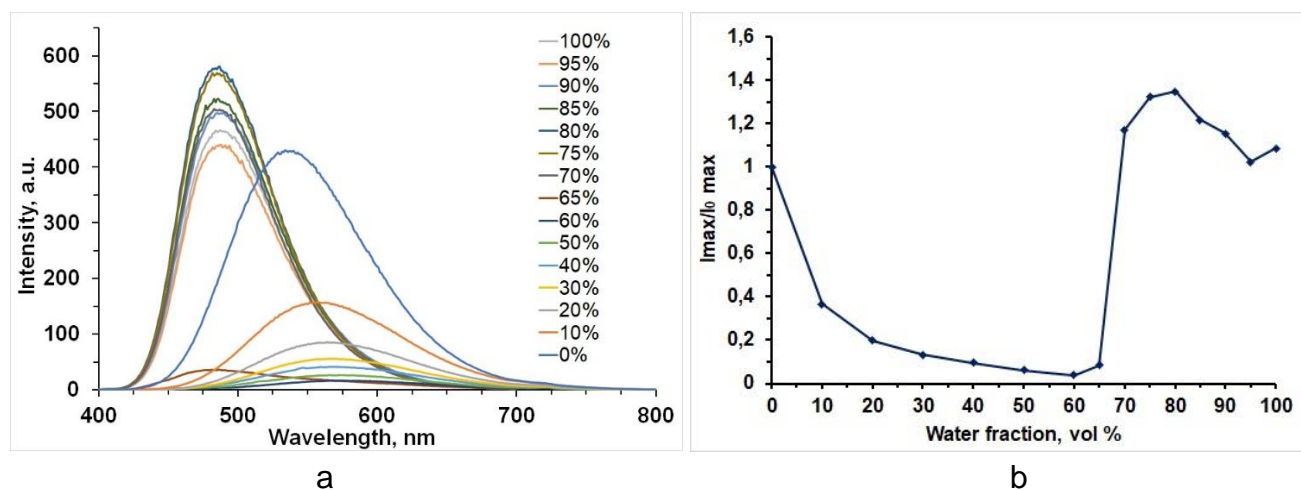


Figure S47. (a) The fluorescence spectra of 10 mM **5b** in MeCN/H₂O mixtures with different water fractions (f_w). (b) A plot of I/I_0 versus the composition of the MeCN/H₂O mixture for **5b**.

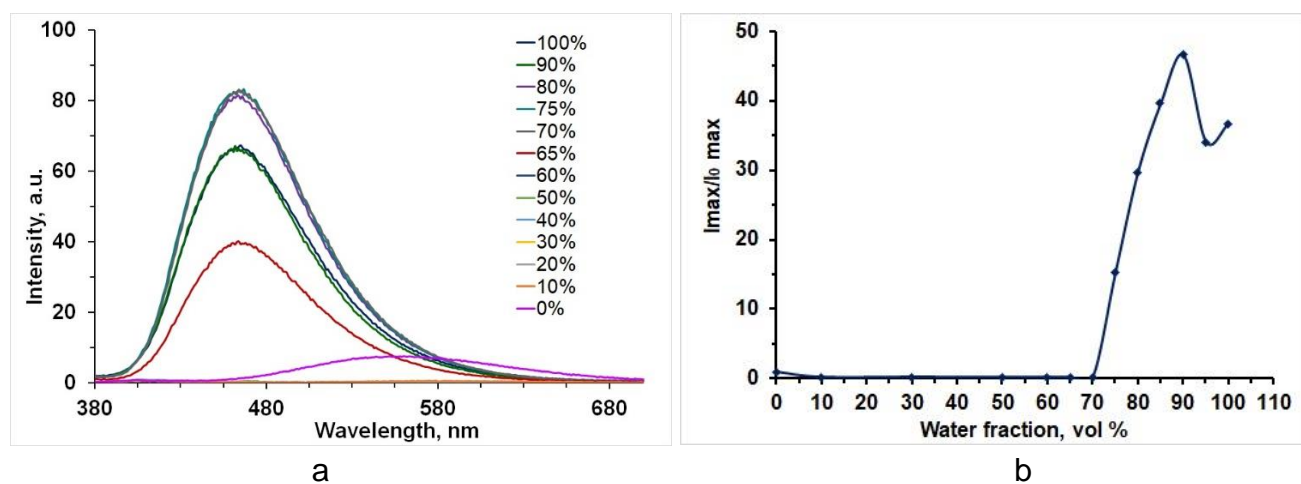


Figure S48. (a) The fluorescence spectra of 10 mM **6b** in MeCN/H₂O mixtures with different water fractions (f_w). (b) A plot of I/I_0 versus the composition of the MeCN/H₂O mixture for **6b**.

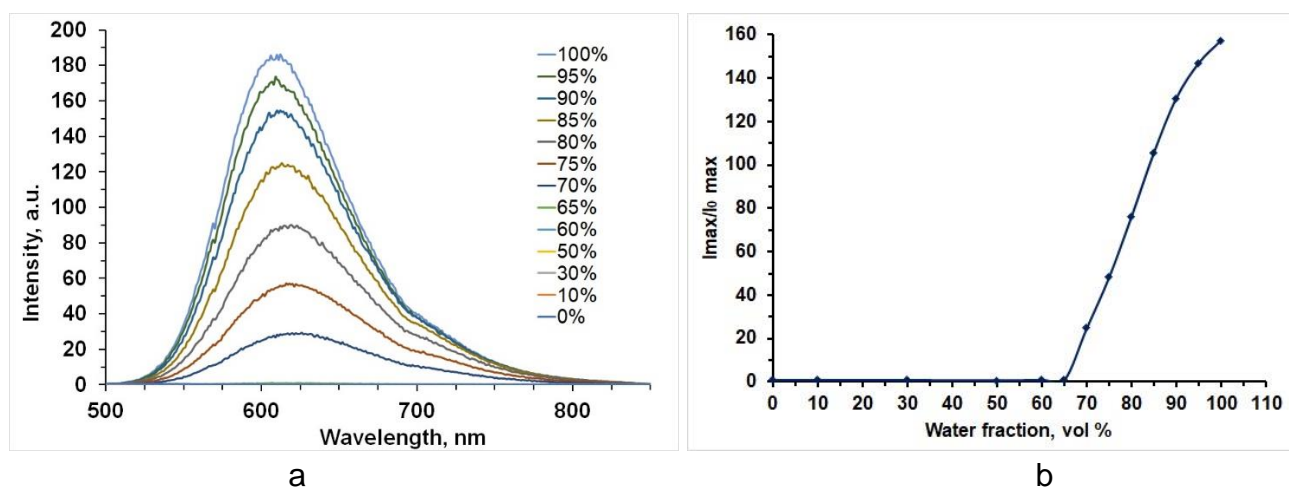
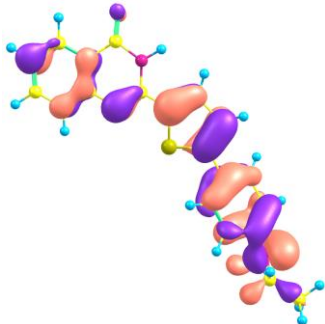
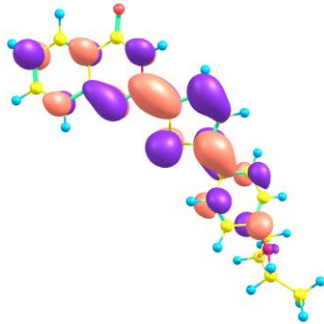
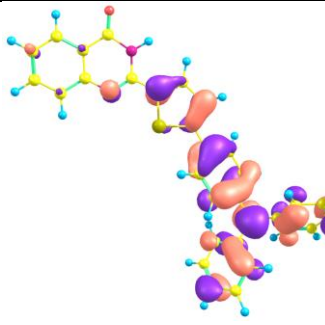
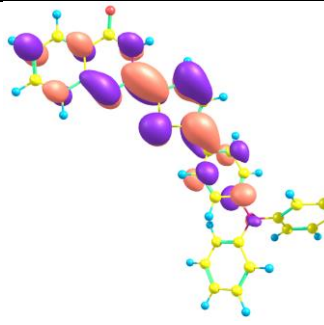
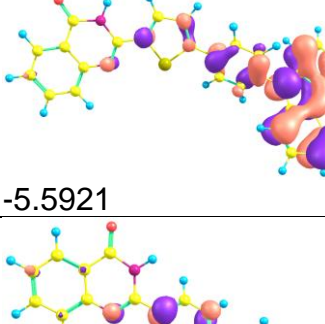
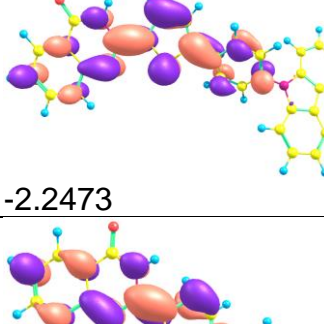
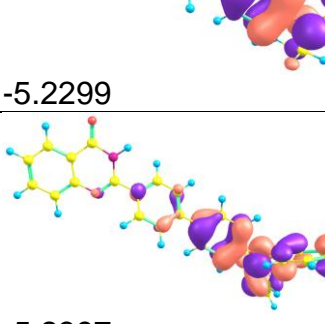
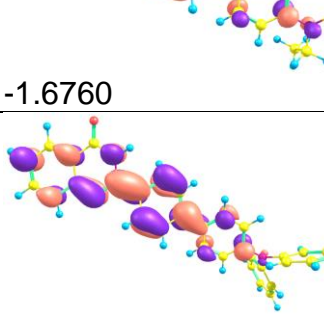
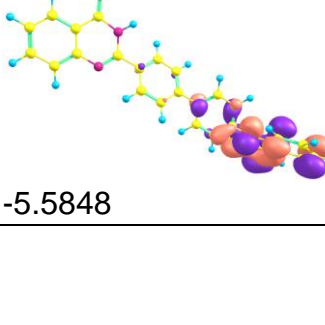
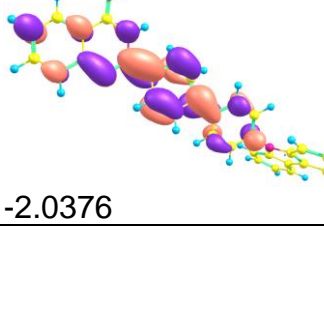


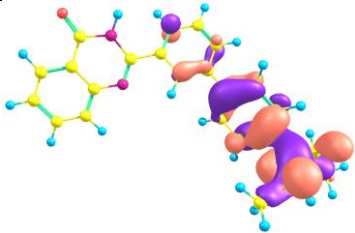
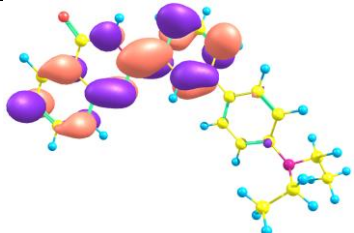
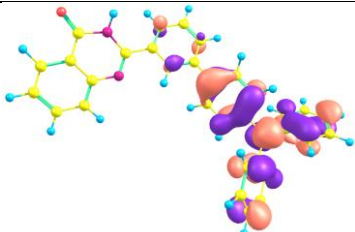
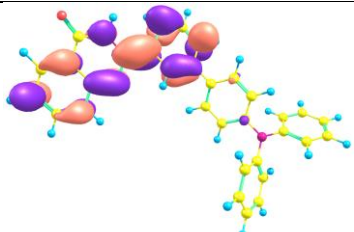
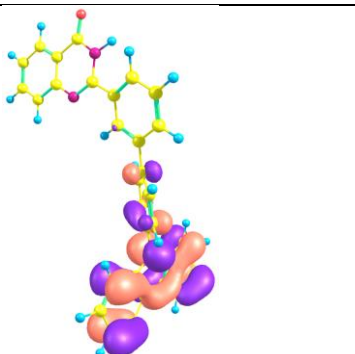
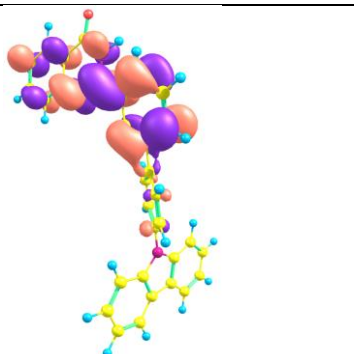
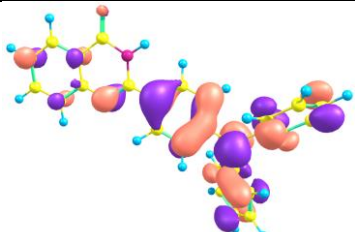
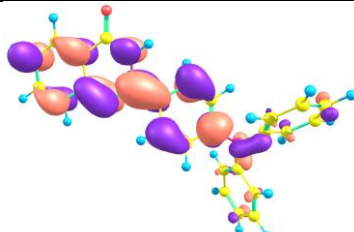
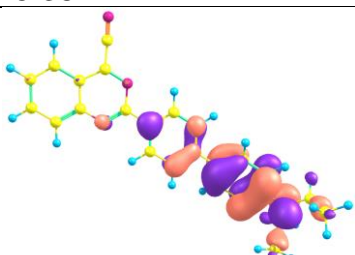
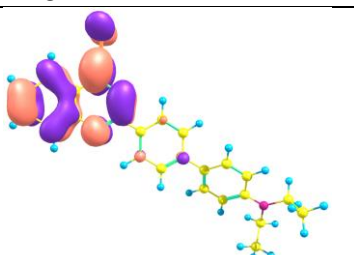
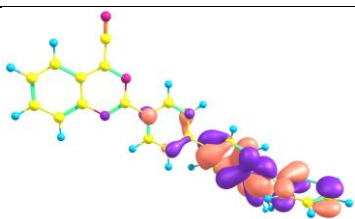
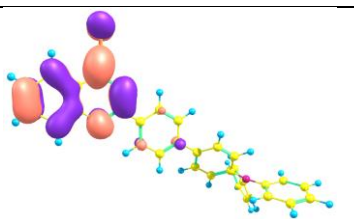


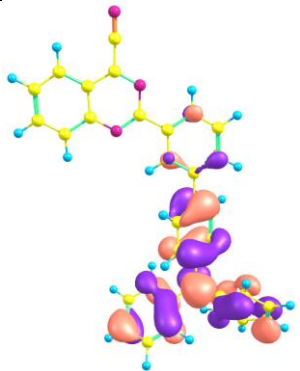
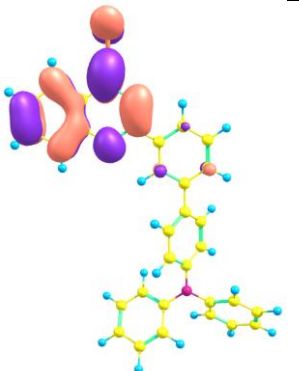
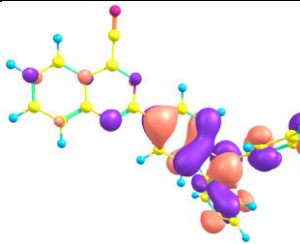
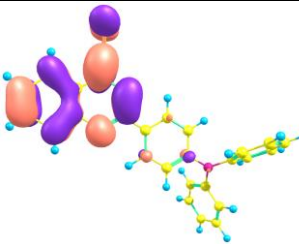
Figure S49. (a) The fluorescence spectra of 10 mM **11** in MeCN/H₂O mixtures with different water fractions (f_w). (b) A plot of I/I_0 versus the composition of the MeCN/H₂O mixture for **11**.

7. Quantum-chemical calculations

Table S4. Calculated frontier molecular orbitals (HOMO, LUMO) of quinazolin-4(3*H*)-ones **4a-c**, **5a-c**, **6a-c**, **10** and 4-cyanoquinazolines **8a,b**, **9**, **11**.

Comp.	HOMO	LUMO	Energy band gap (ΔE)
4a	 -5.6894	 -2.0522	3.6372
4b	 -5.2293	 -2.0303	3.1990
4c	 -5.5921	 -2.2473	3.3448
5a	 -5.2299	 -1.6760	3.5539
5b	 -5.2397	 -1.8526	3.3871
5c	 -5.5848	 -2.0376	3.5472

6a	 -5.8023	 -1.7431	4.0592
6b	 -5.1998	 -1.7321	3.4677
6c	 -5.5502	 -1.8947	3.6555
10	 -5.3822	 -1.6474	3.7348
8a	 -5.1232	 -2.6490	2.4742
8b	 -5.1513	 -2.7618	2.3895

<p>9</p>	 <p>-5.1345</p>	 <p>-2.8046</p>	<p>2.3299</p>
<p>11</p>	 <p>-5.2712</p>	 <p>-2.6591</p>	<p>2.6121</p>