Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Rh(III)-Catalyzed C-H/N-H Annulation of 2-Thienyl- and 2-Phenyl-Quinazolin-4(3*H*)-ones with Diphenylacetylene

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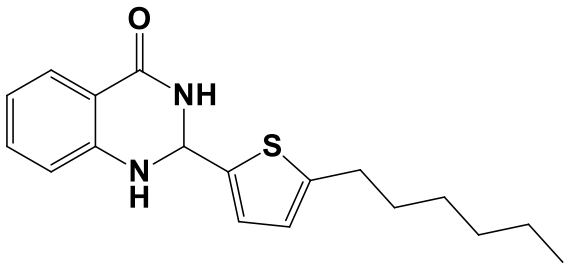
Contents

1. NMR and mass spectra of intermediates



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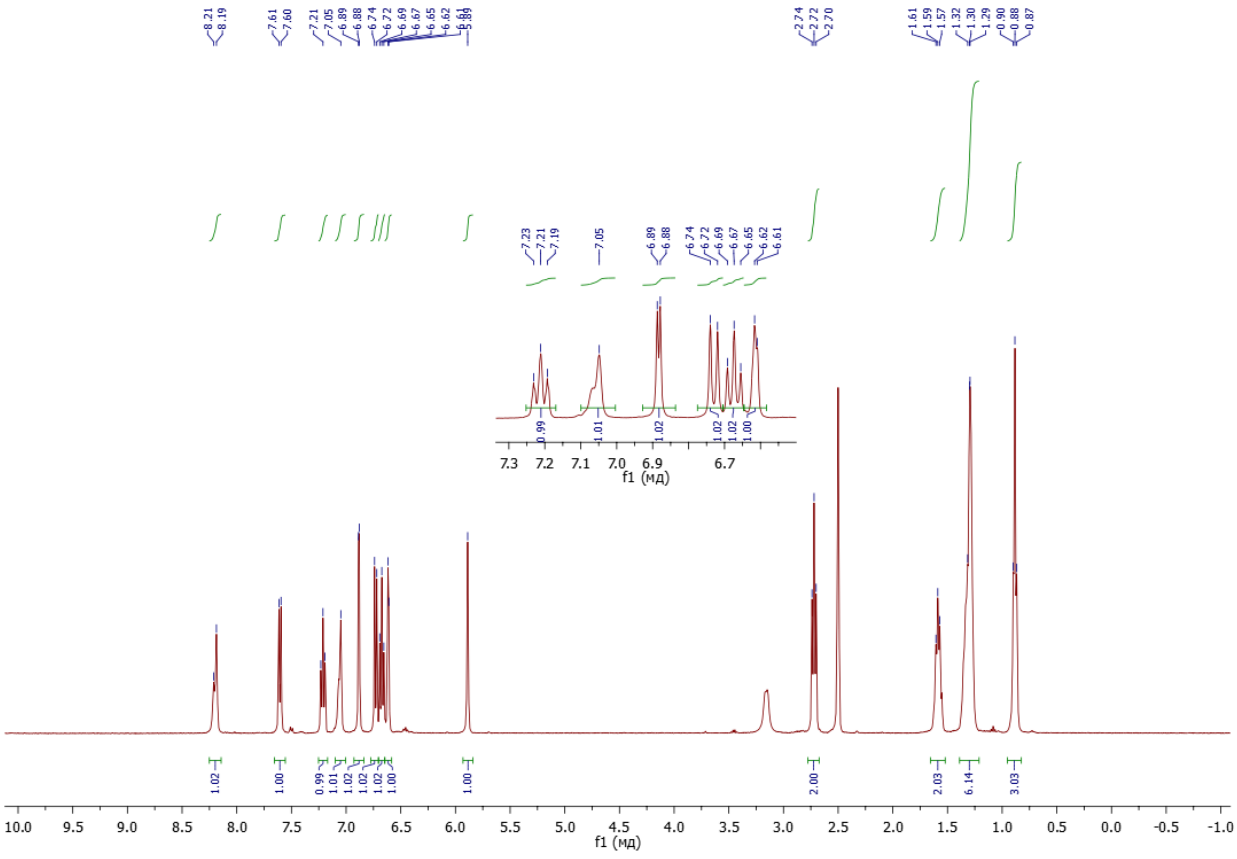

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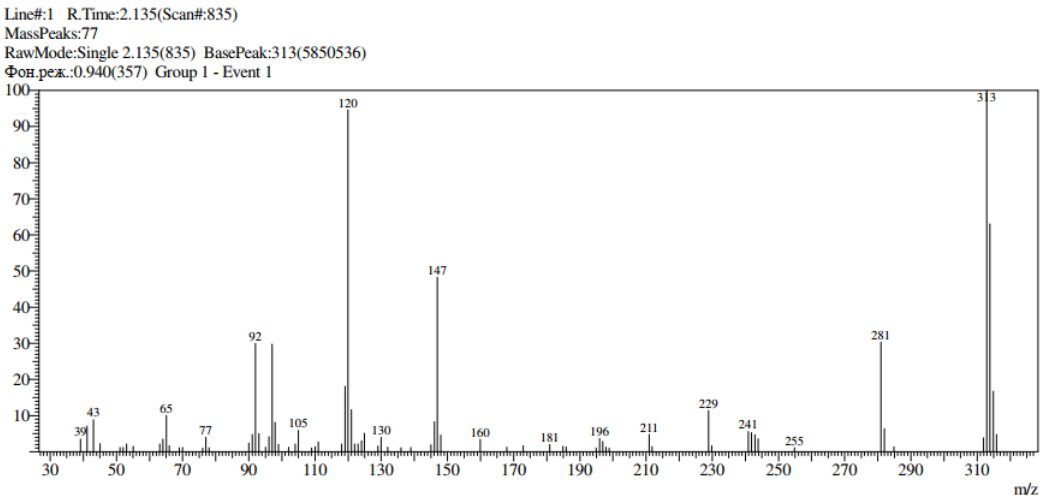

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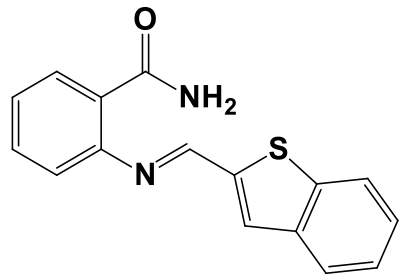
Figure S1. NMR ^{1}H (a) in DMSO-d_6 and mass spectrum (EI) (b) of **3c**.



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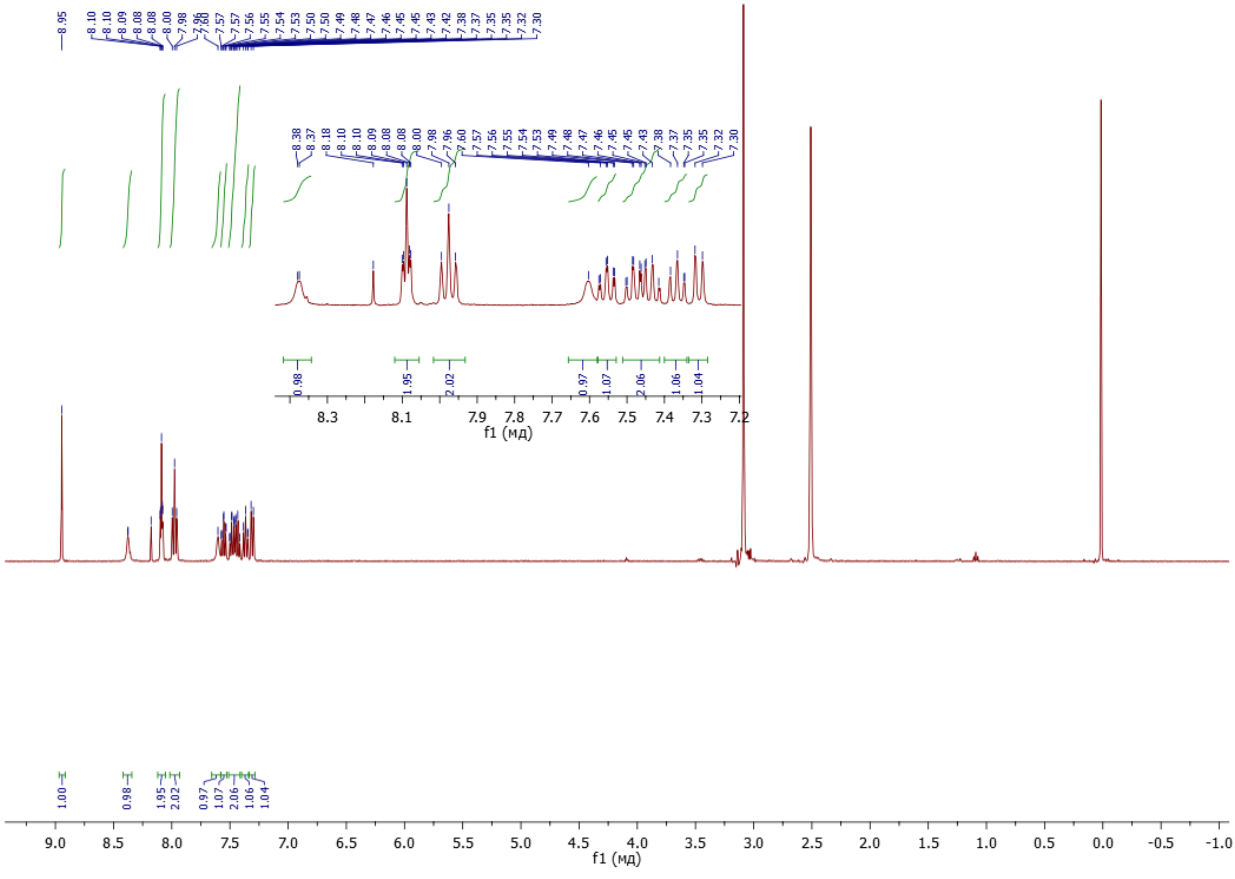

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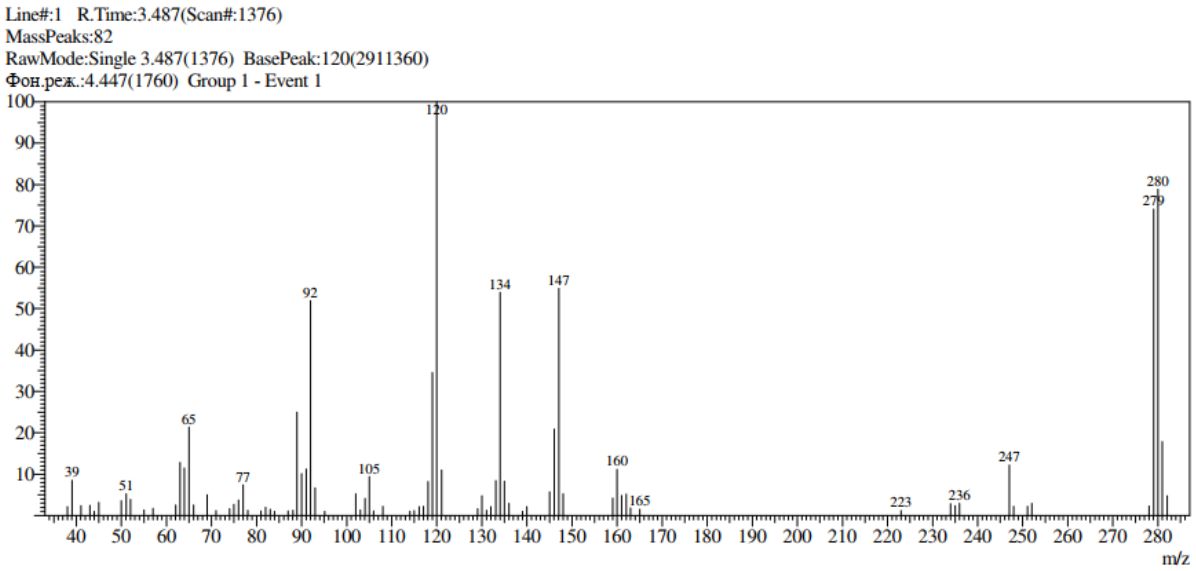

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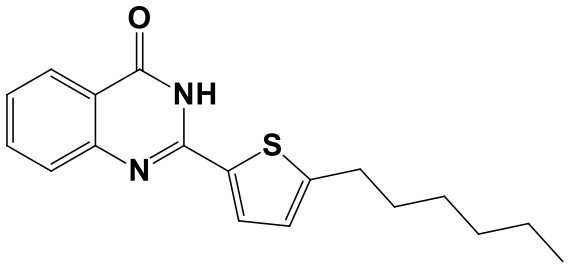

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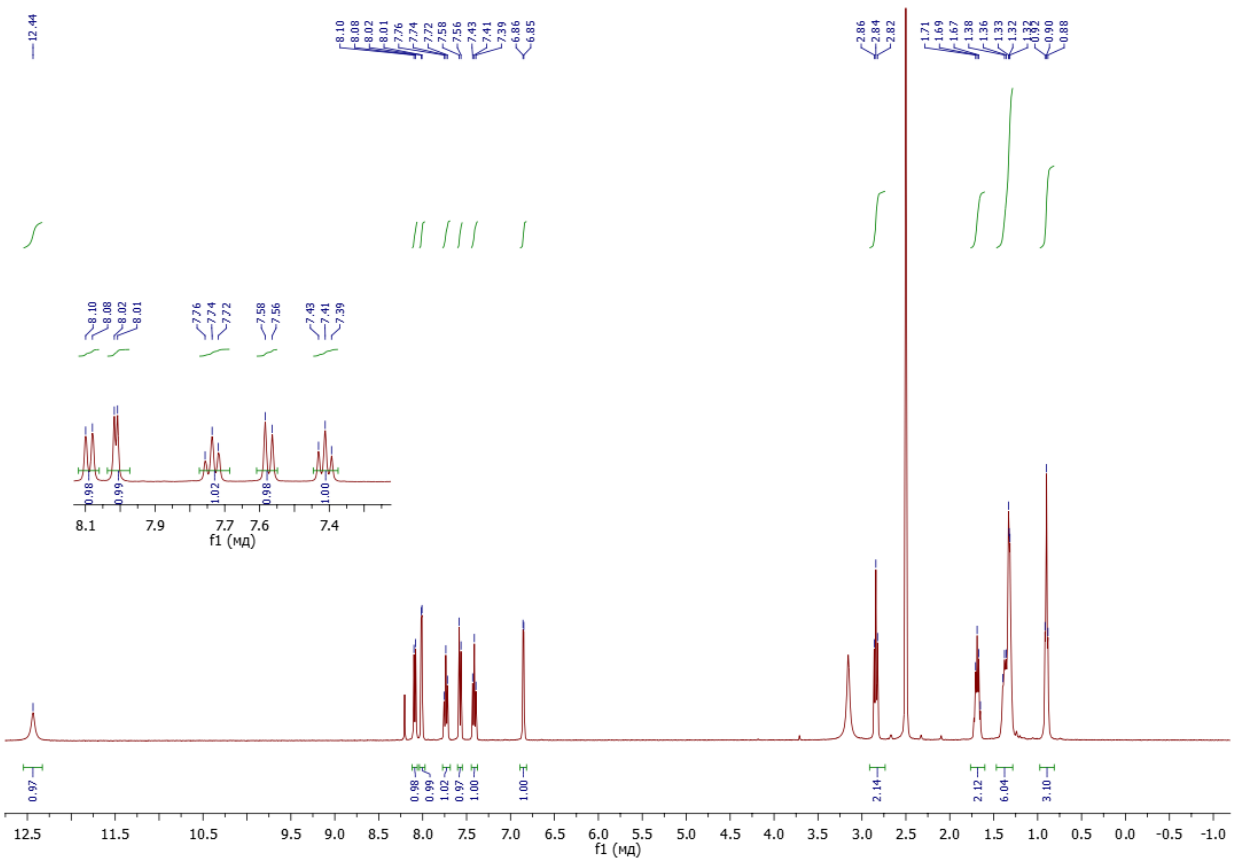

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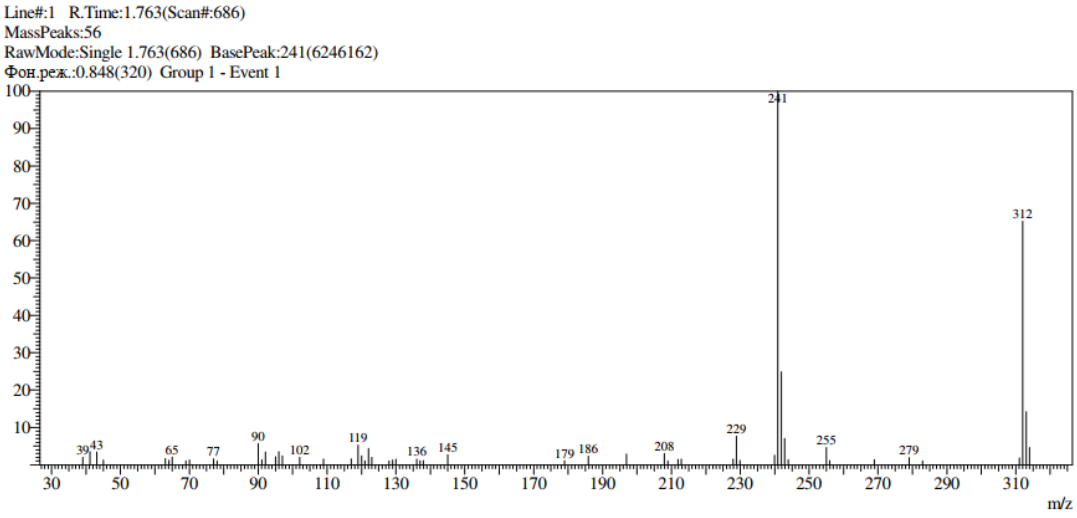

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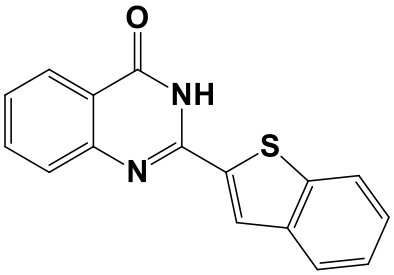

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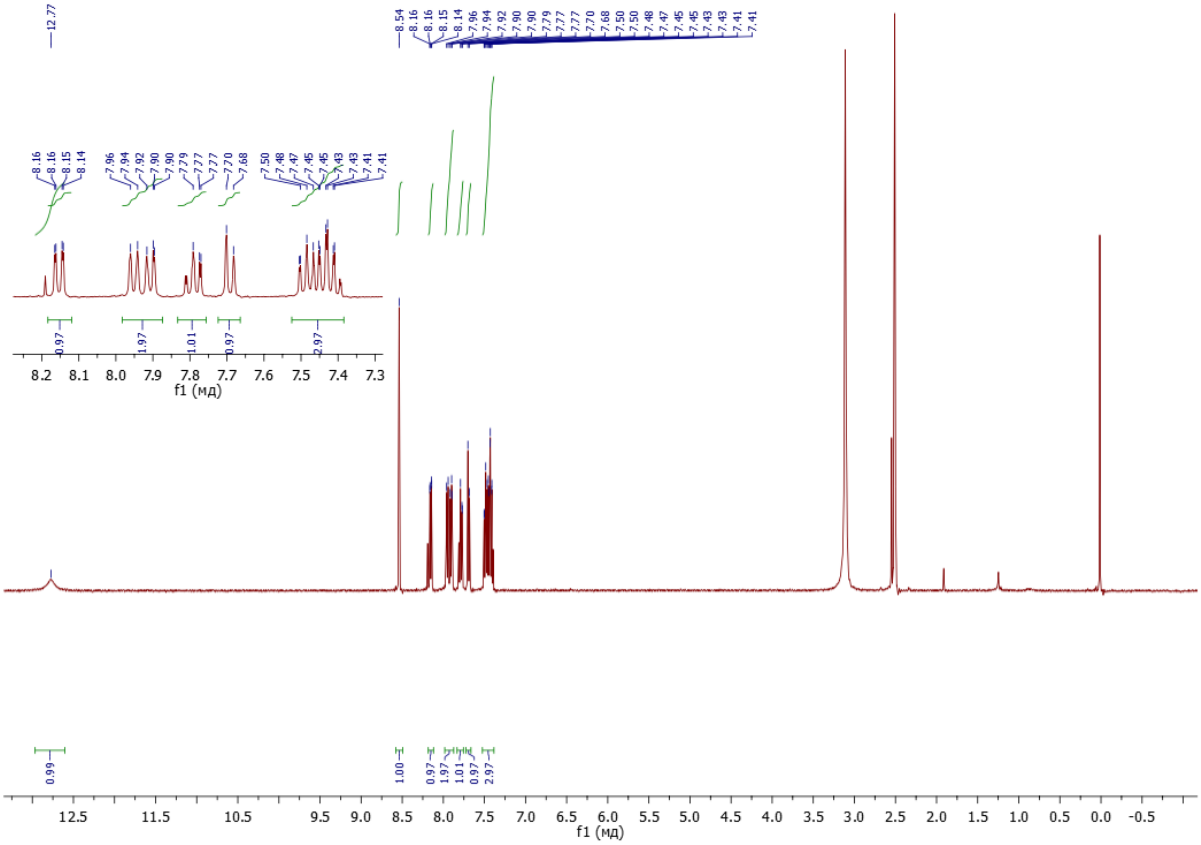

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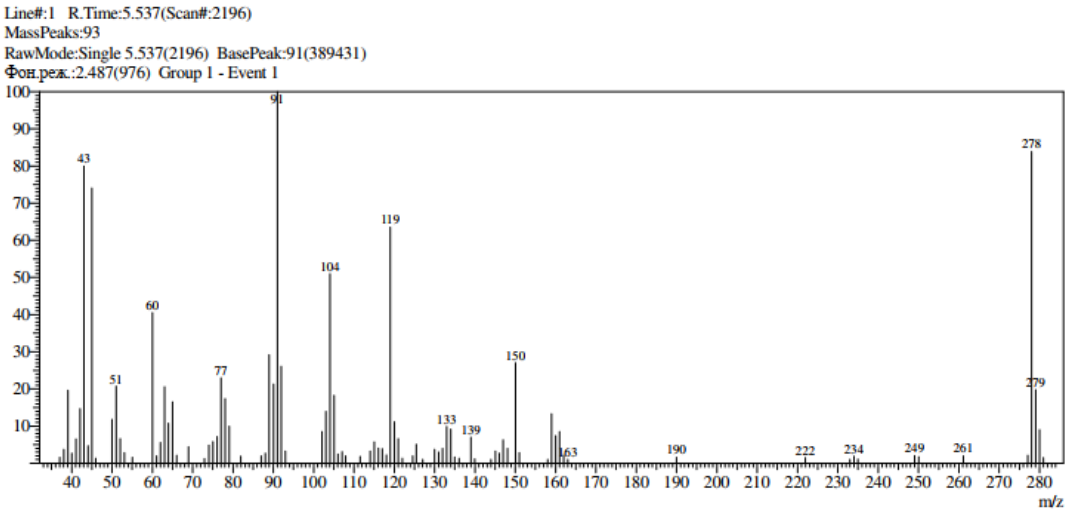

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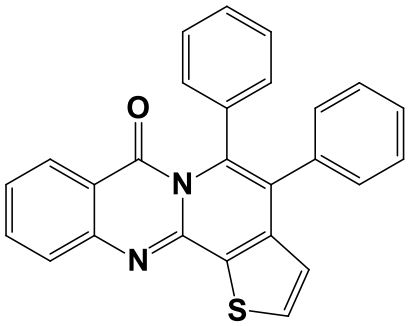
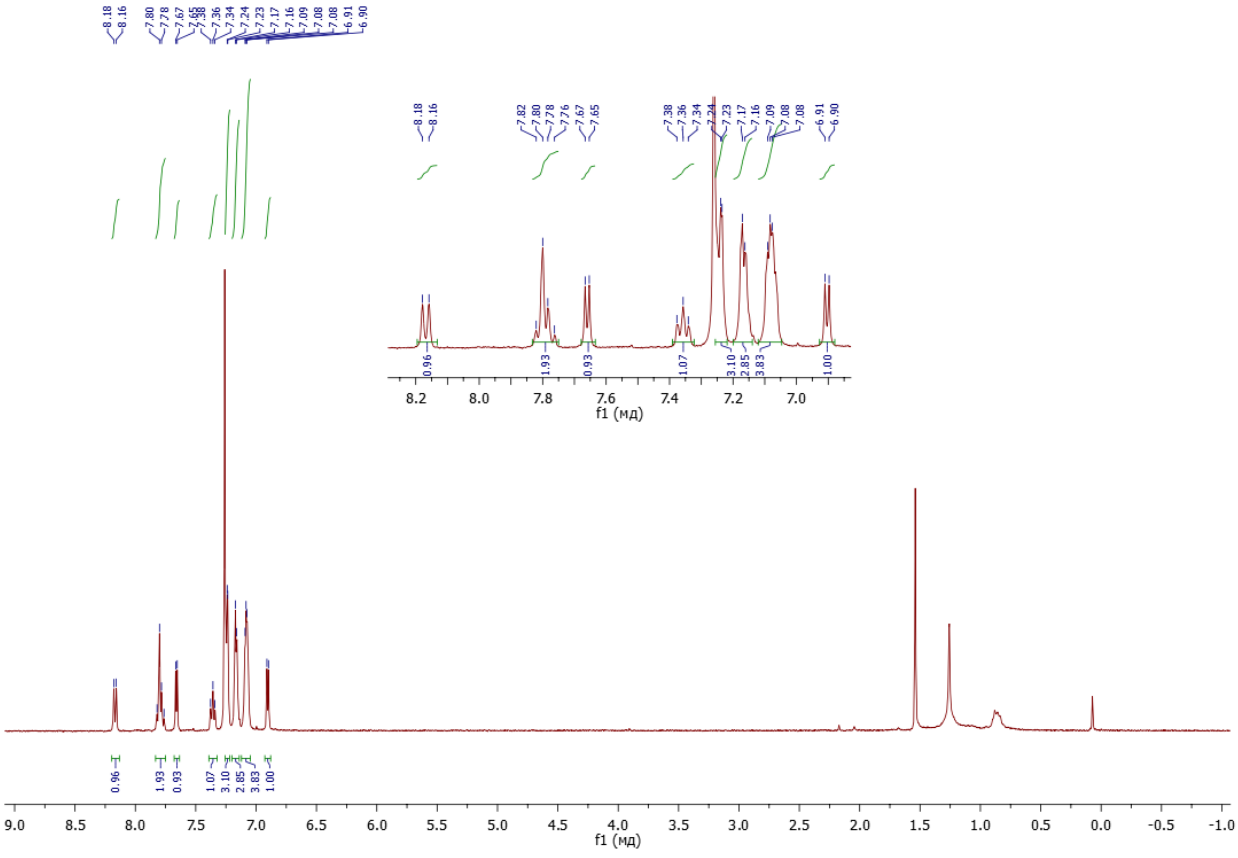
Figure S4. NMR ^{1}H (a) in DMSO-d_6 and mass spectrum (EI) (b) of **4d**.

2. NMR and mass spectra of products 5 and 7



5a



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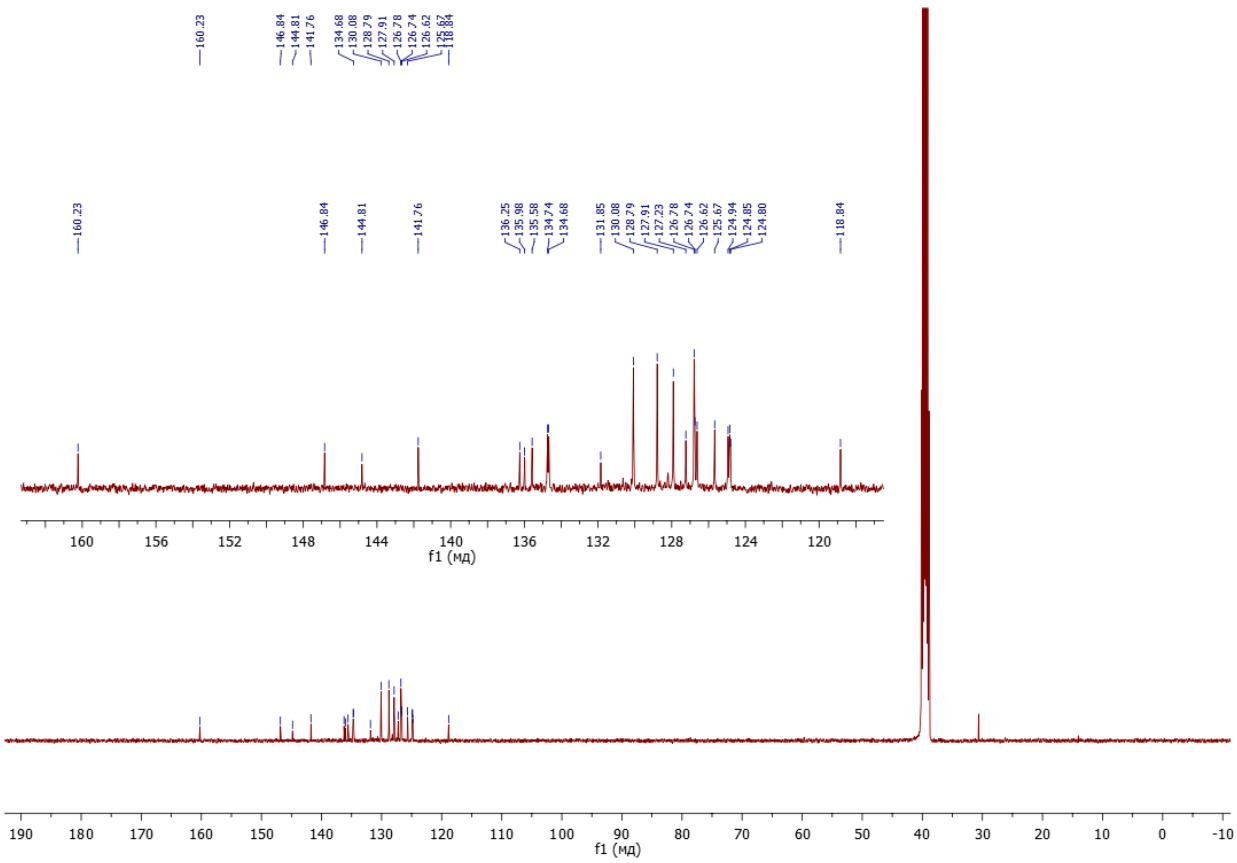

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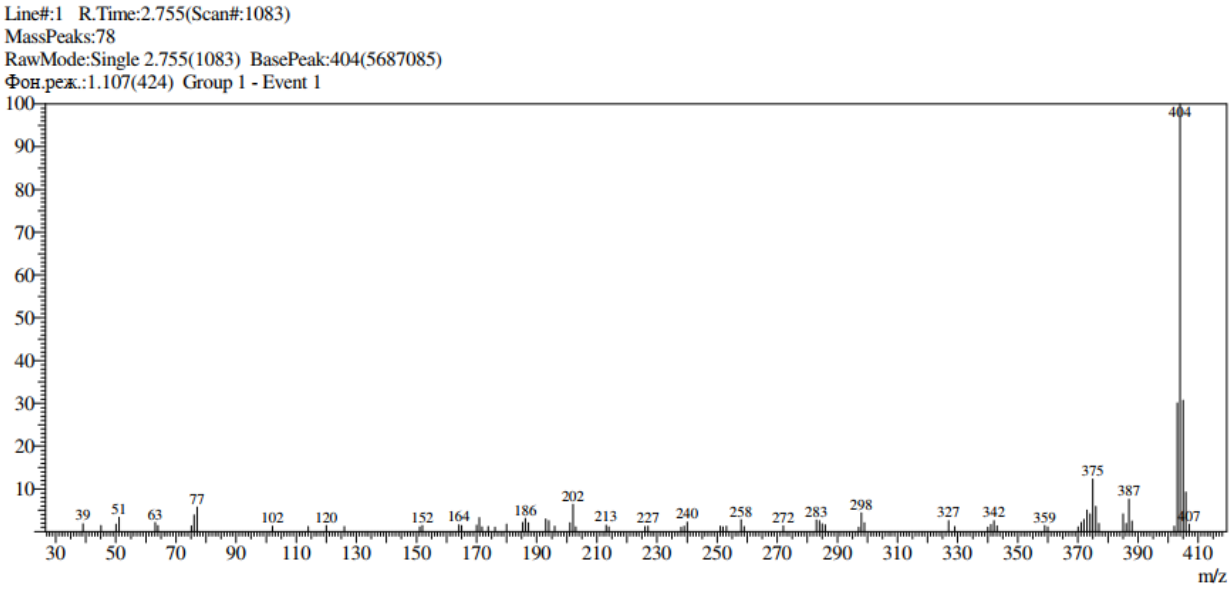
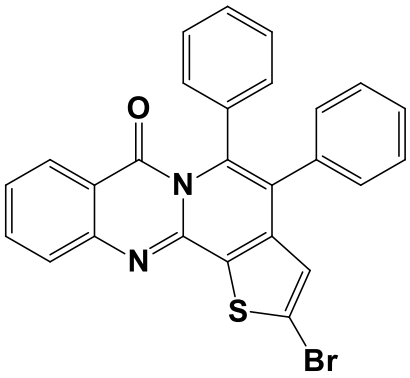


c

Figure S5. NMR ^{1}H (a), ^{13}C (b), in $CDCl_3$ and mass spectrum (EI) (c) of **5a**.



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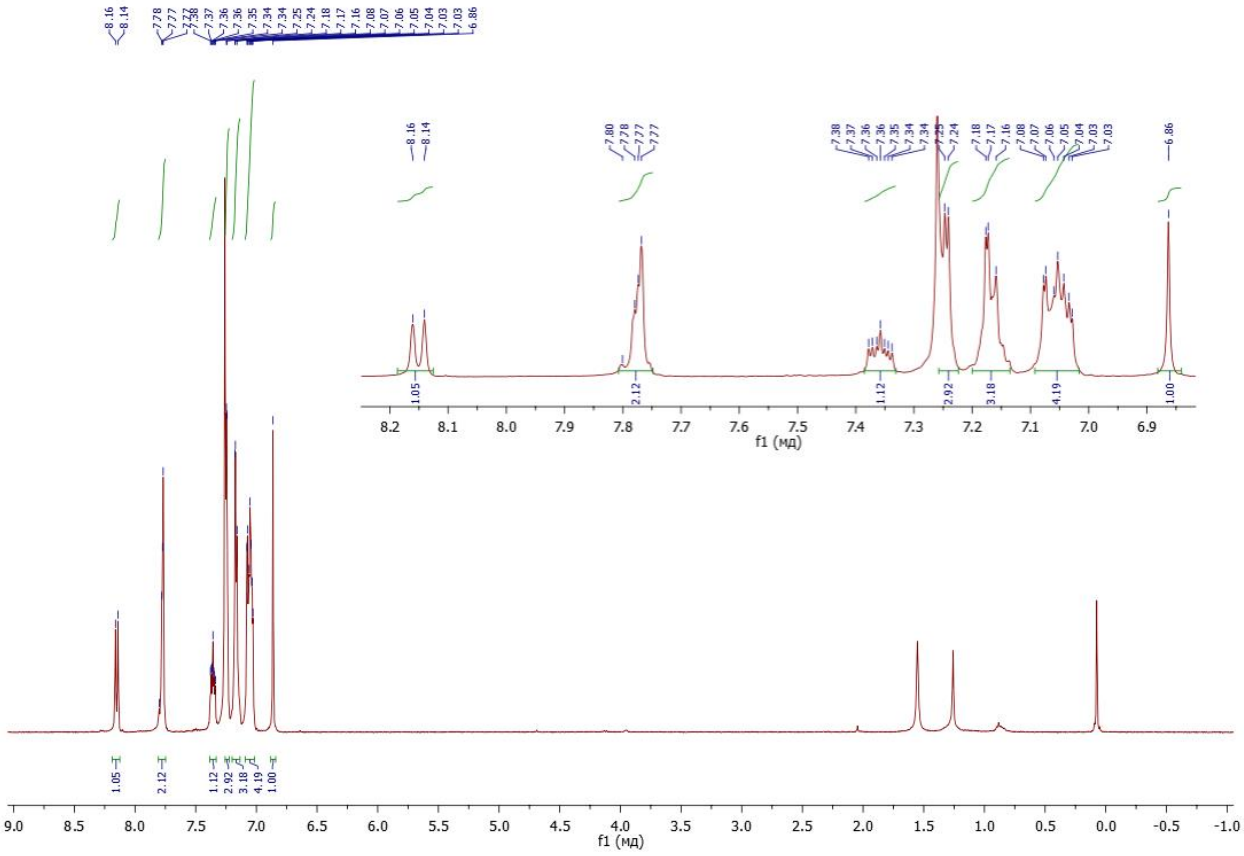
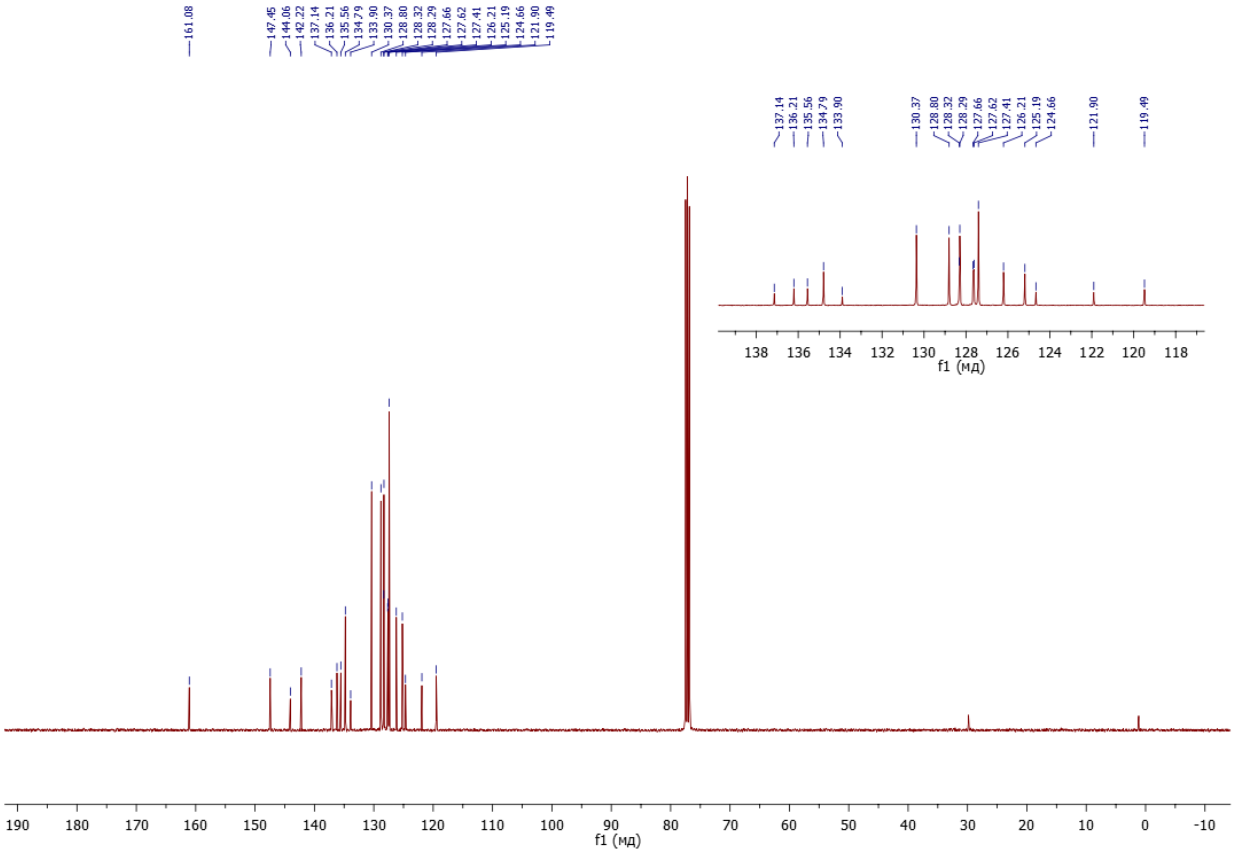


a



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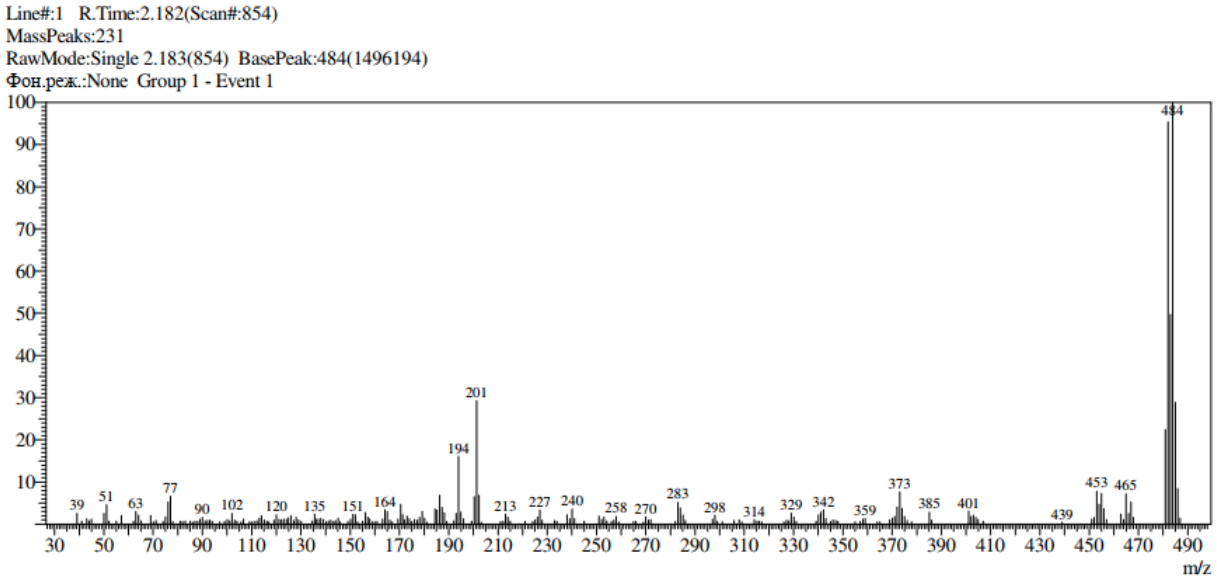

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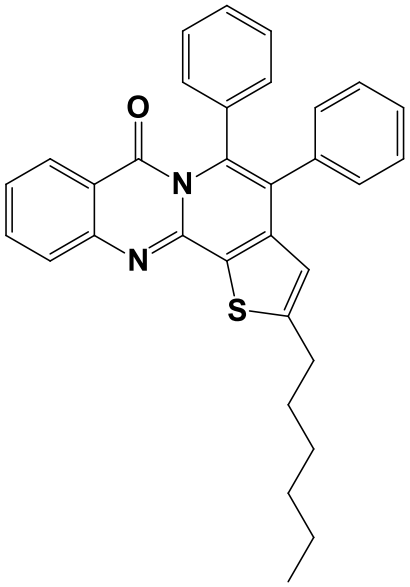
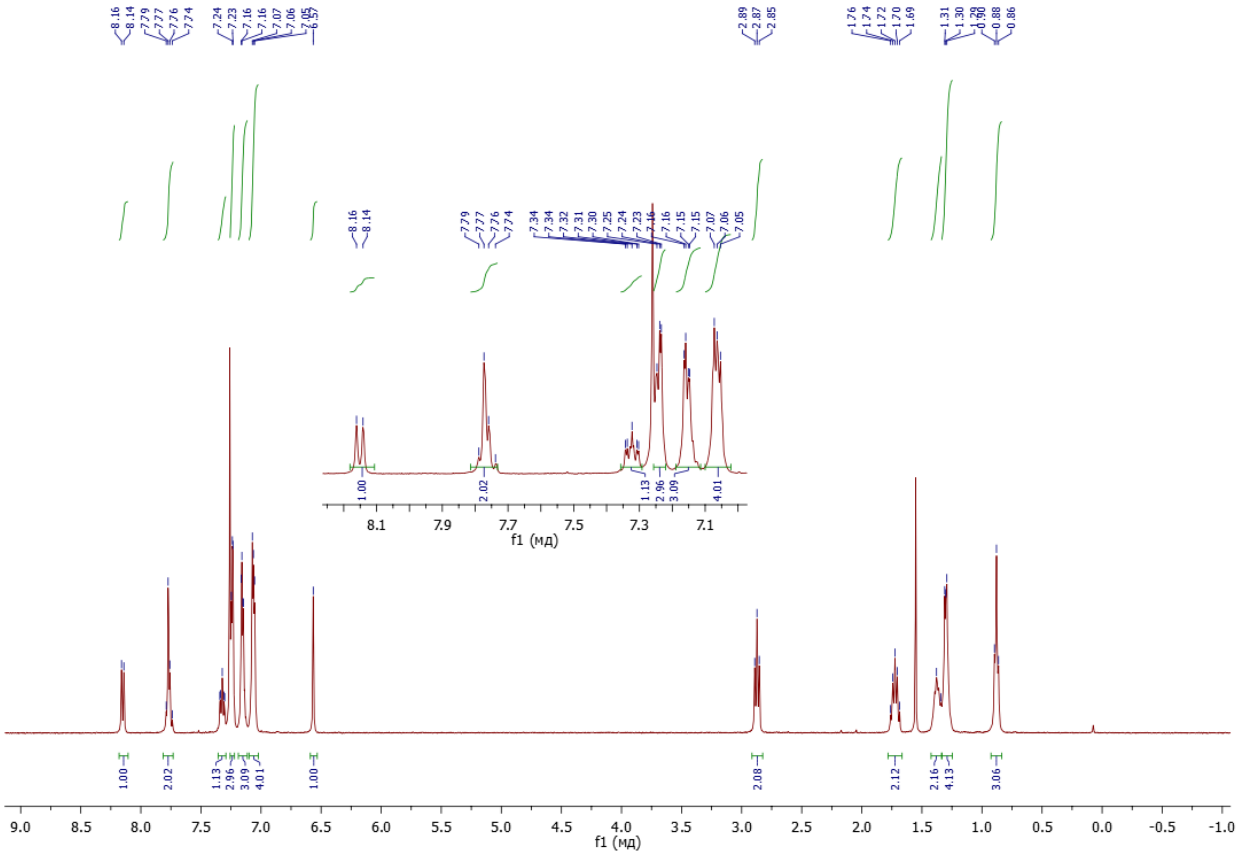
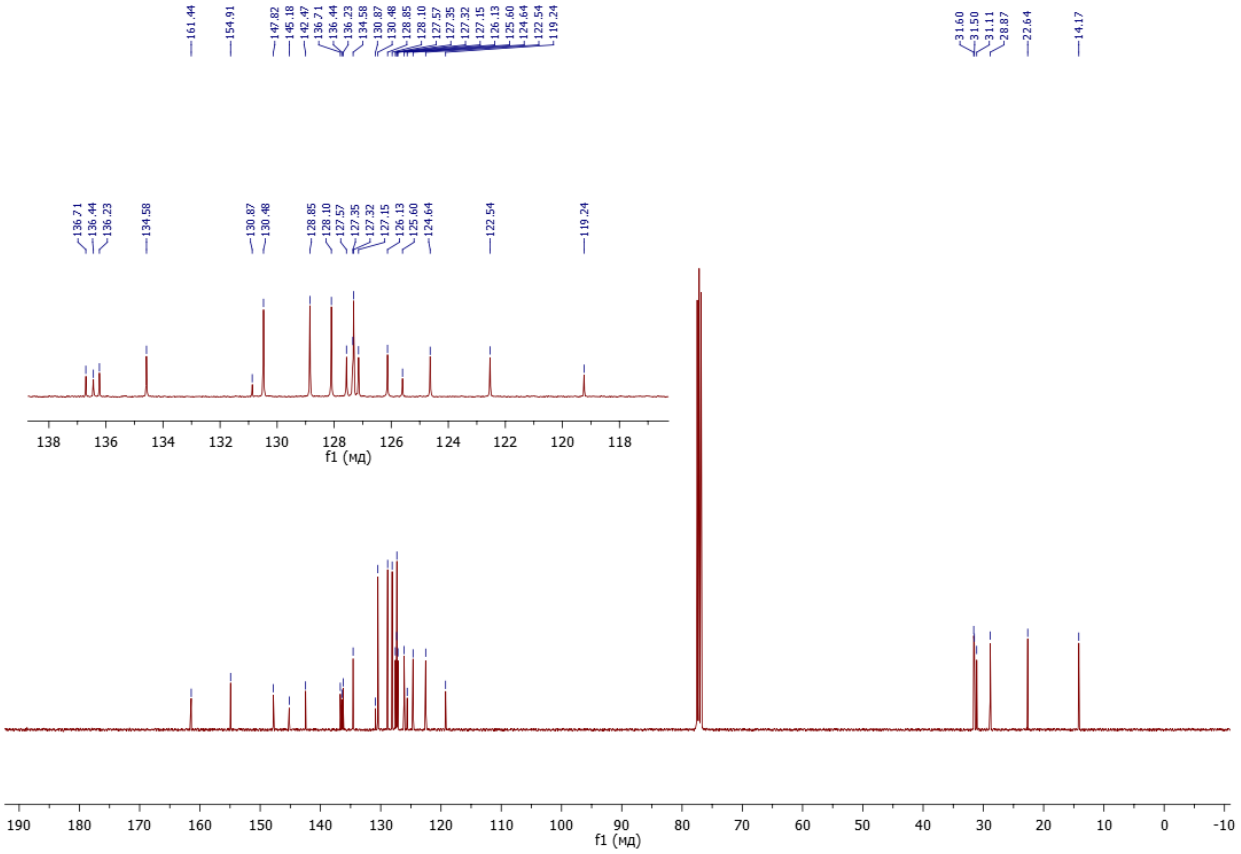
Figure S6. NMR ^{1}H (a), ^{13}C (b), in $CDCl_3$ and mass spectrum (EI) (c) of **5b**.



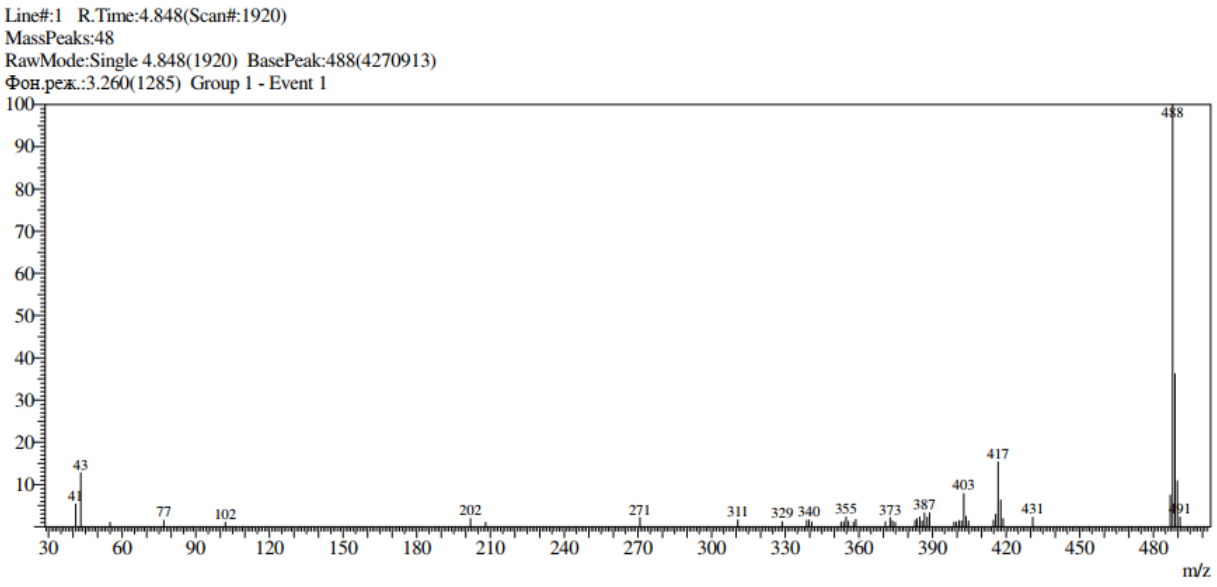
5c



a

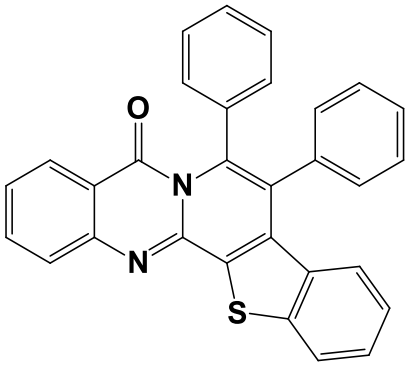


b

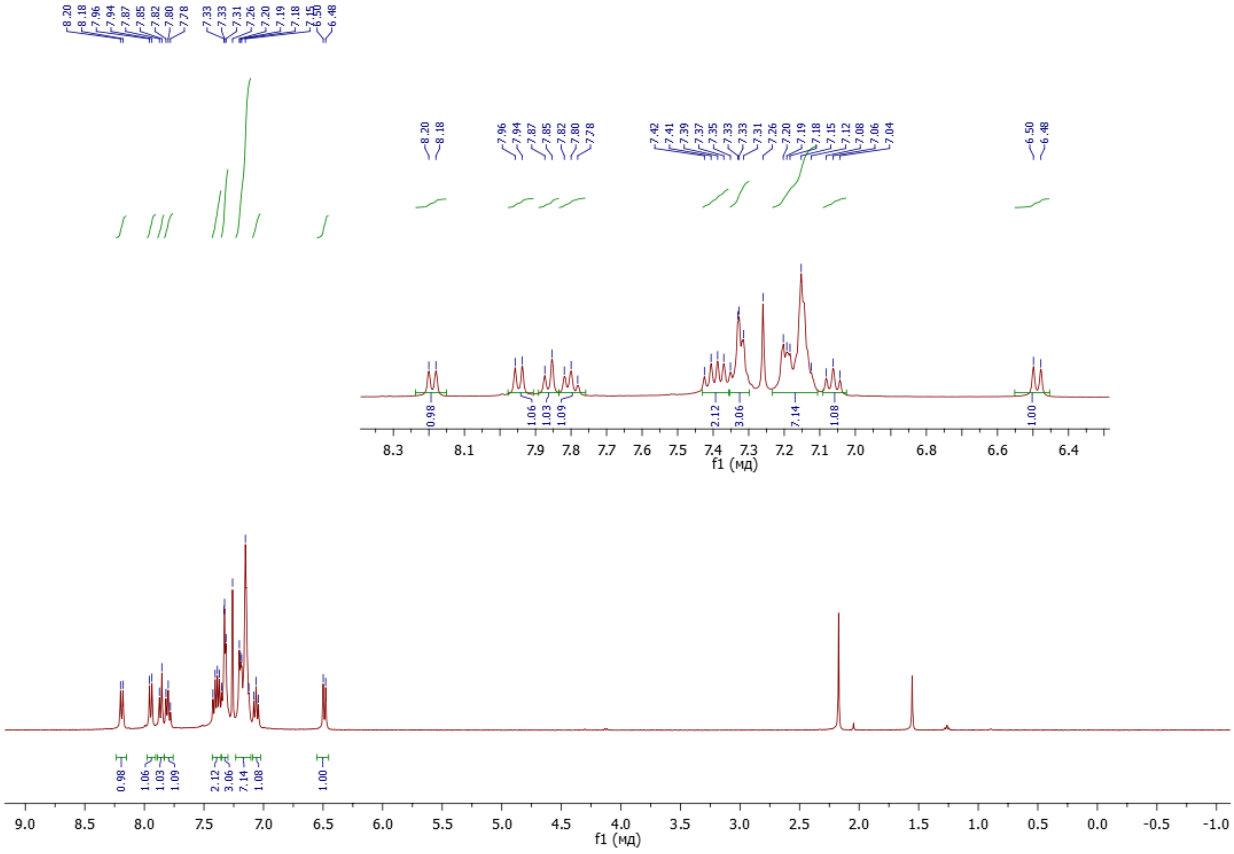


c

Figure S7. NMR ^{1}H (a), ^{13}C (b), in $CDCl_3$ and mass spectrum (EI) (c) of **5c**.


O
N
N
S

5d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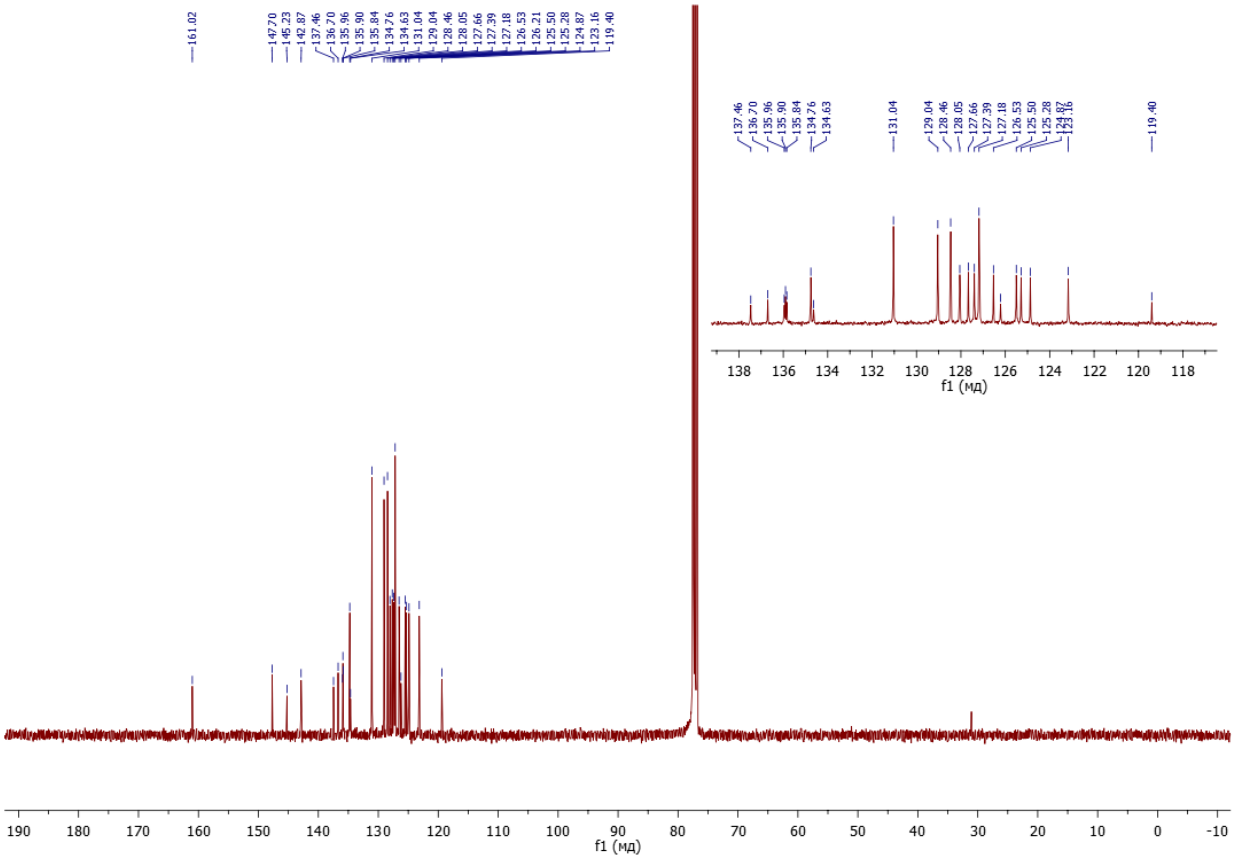
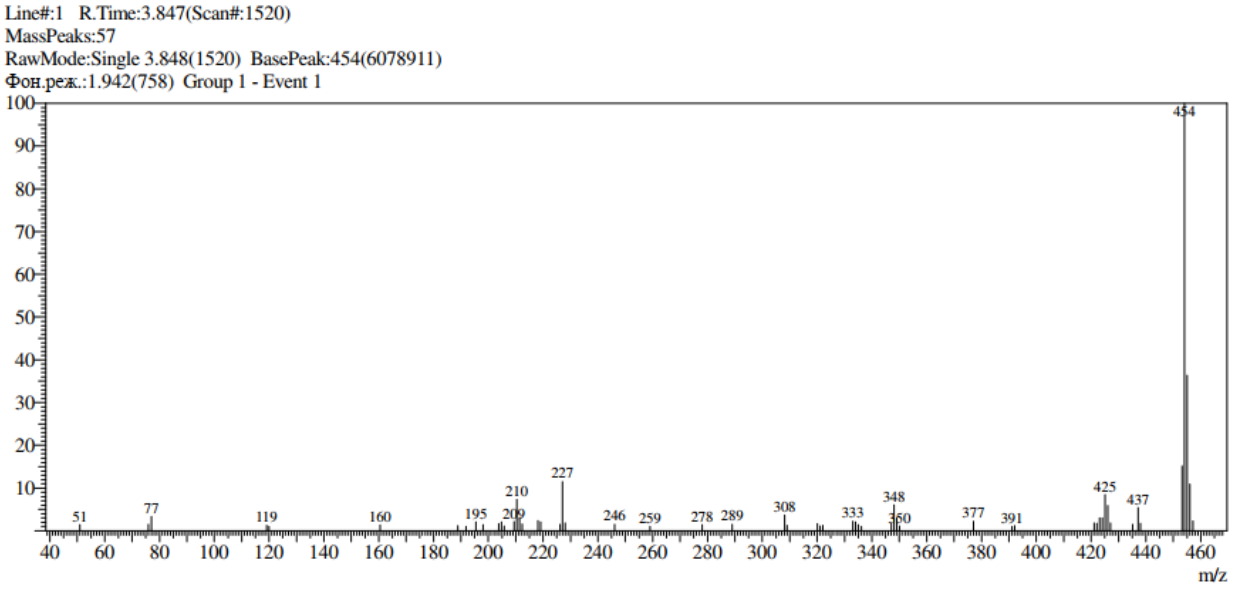
7.94
7.87
7.85
7.82
7.80
7.78
7.33
7.31
7.26
7.20
7.19
7.18
6.50
6.48
0.98
1.06
1.03
1.09
2.12
3.06
7.14
1.08
1.00
f1 (мд)

a

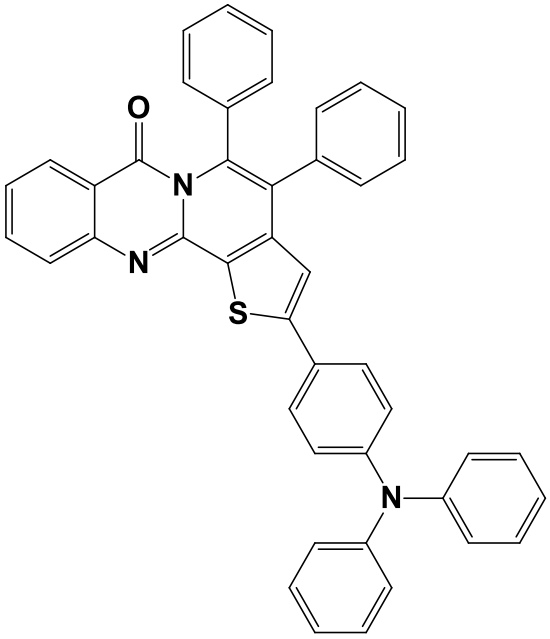


b

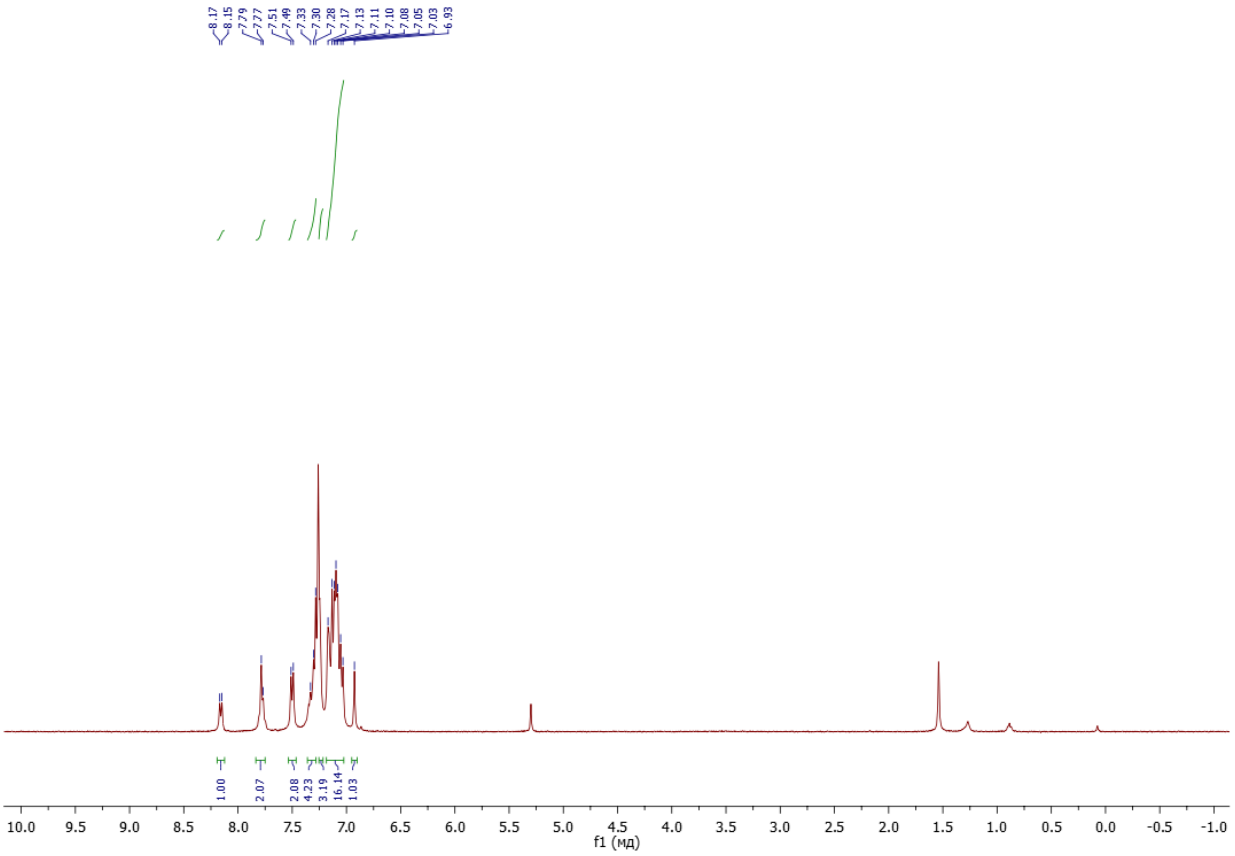


c

Figure S8. NMR ^{1}H (a), ^{13}C (b), in $CDCl_3$ and mass spectrum (EI) (c) of **5d**.


O
N
N
S
N

5e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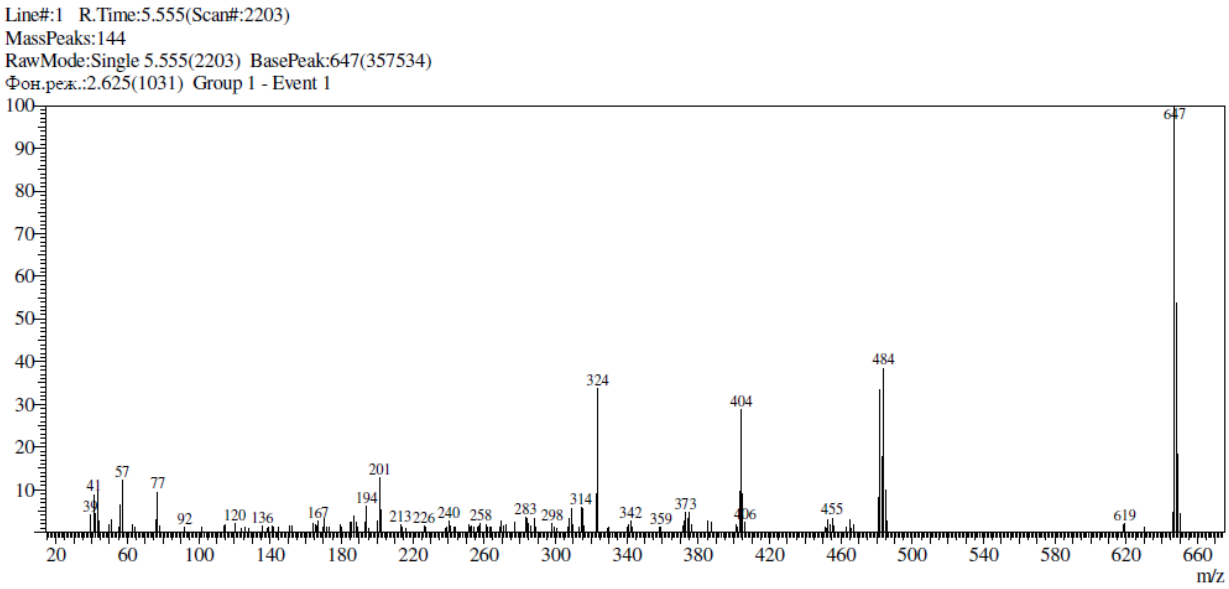
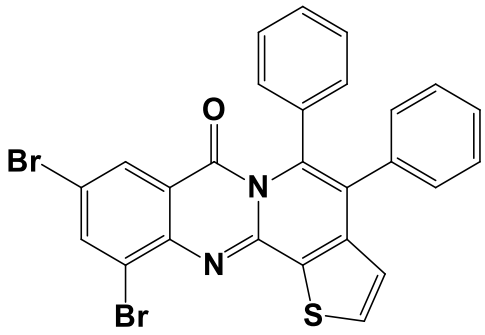
7.77
7.51
7.49
7.33
7.30
7.28
7.17
7.13
7.11
7.10
7.08
7.05
7.03
6.93
1.00
2.07
2.08
4.23
3.19
16.14
1.03
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (мд)

a

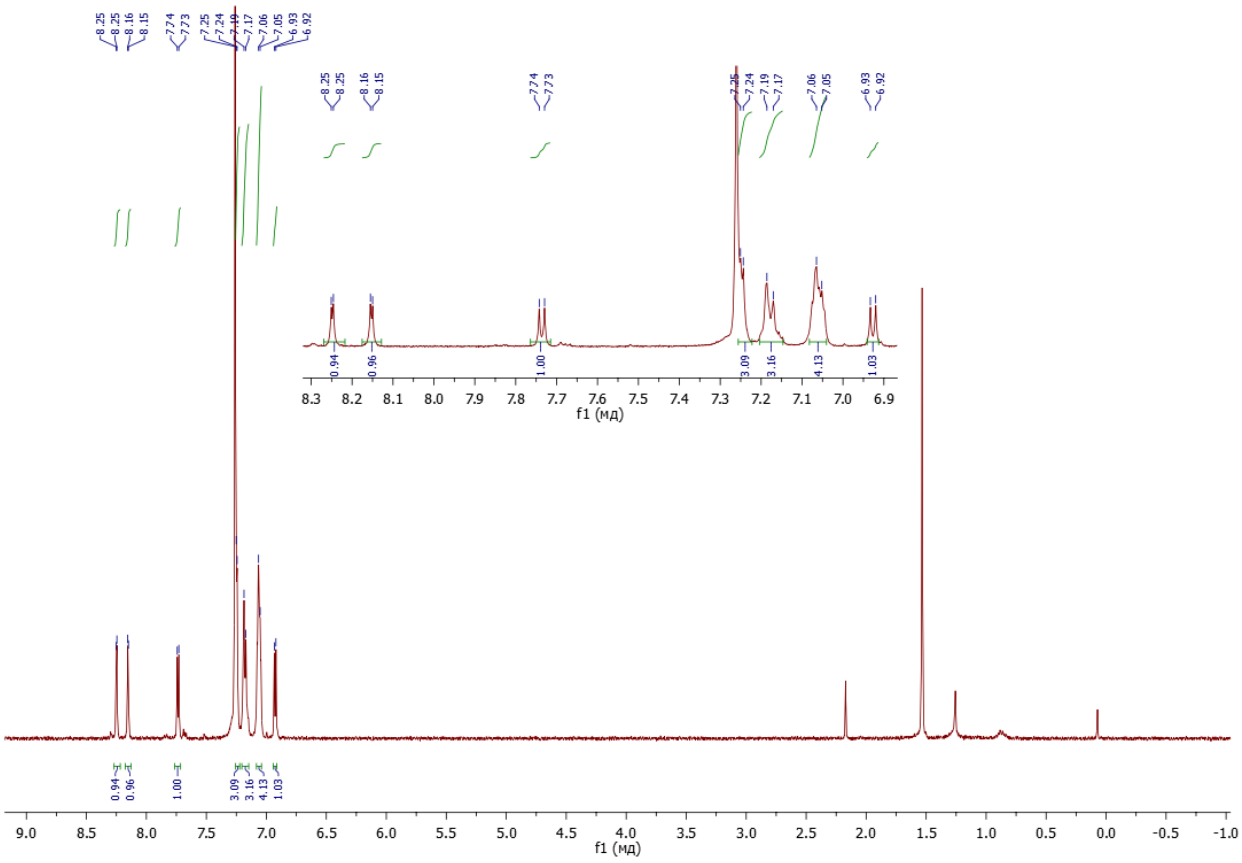


b

Figure S9. NMR ^{1}H (a) in $CDCl_3$ and mass spectrum (EI) (b) of **5e**.


O
Br
N
N
Br
S

5f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7.73
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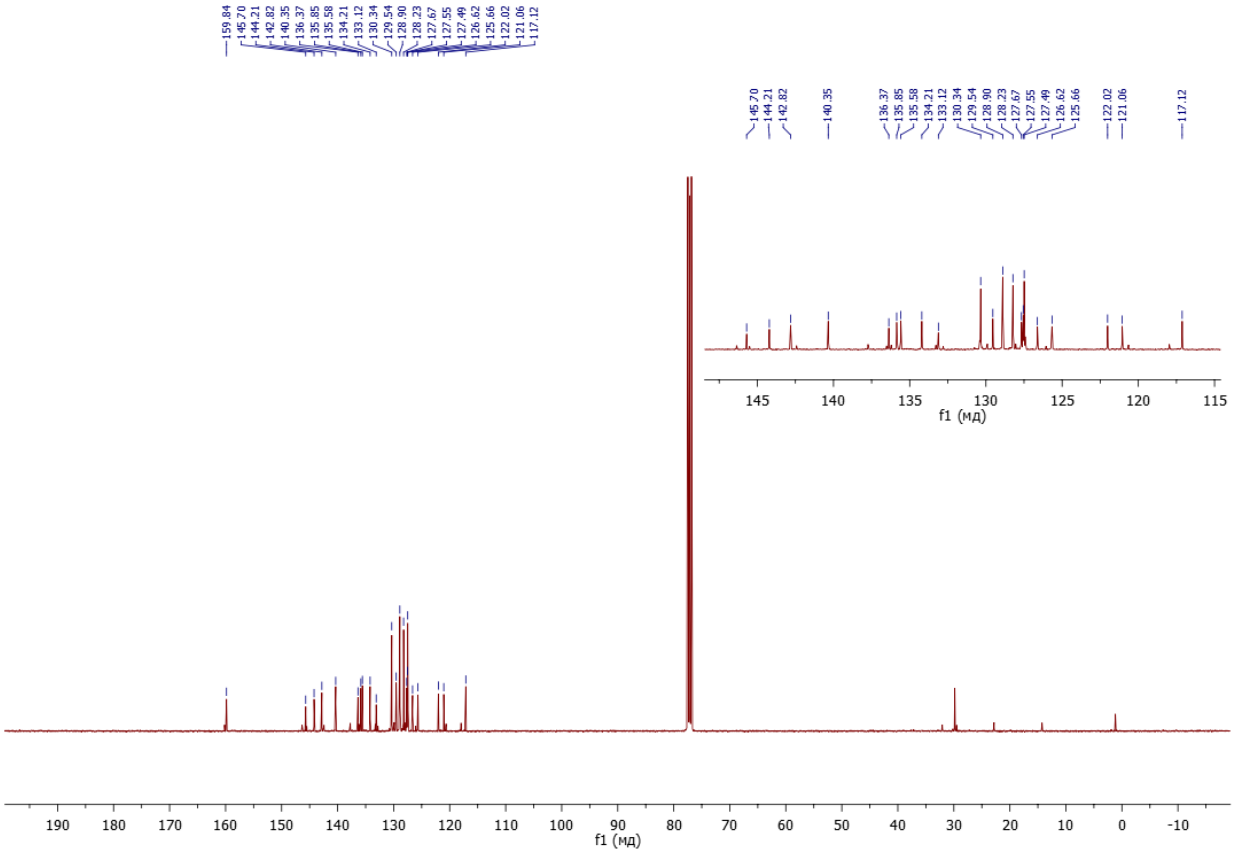
7.19
7.17
7.06
7.05
6.93
6.92
0.94
0.96
1.00
3.09
3.16
4.13
1.03
f1 (мд)

a



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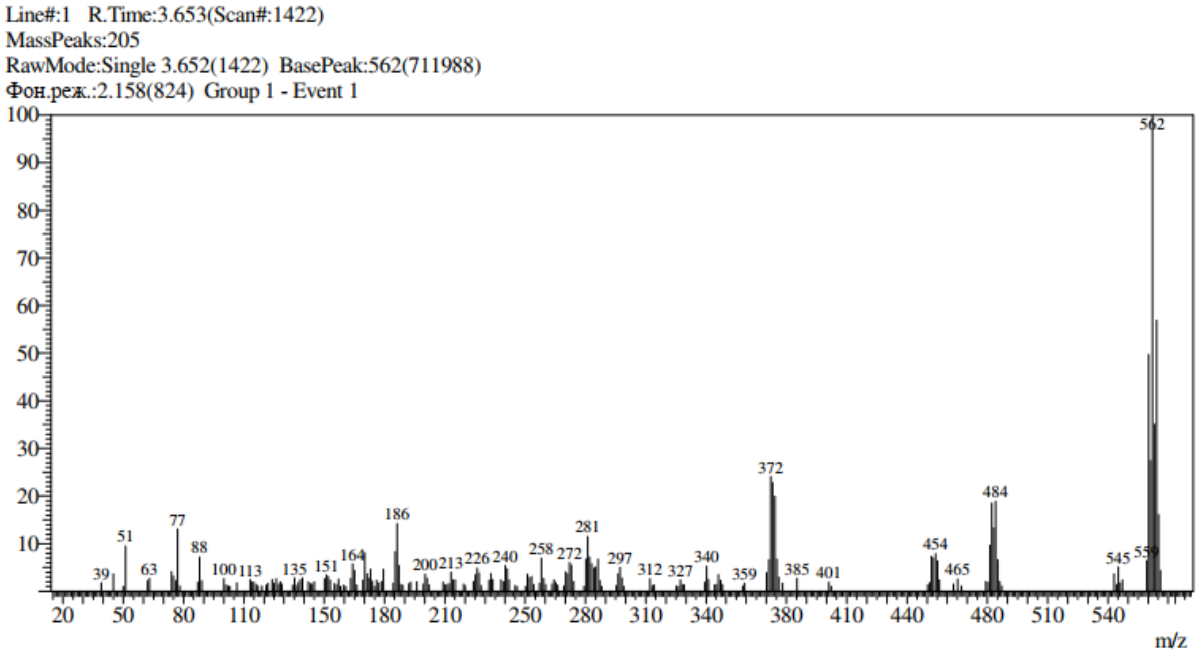
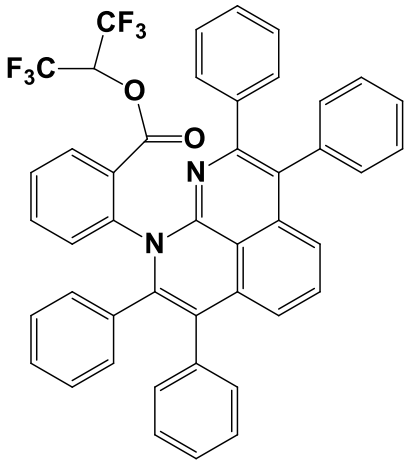
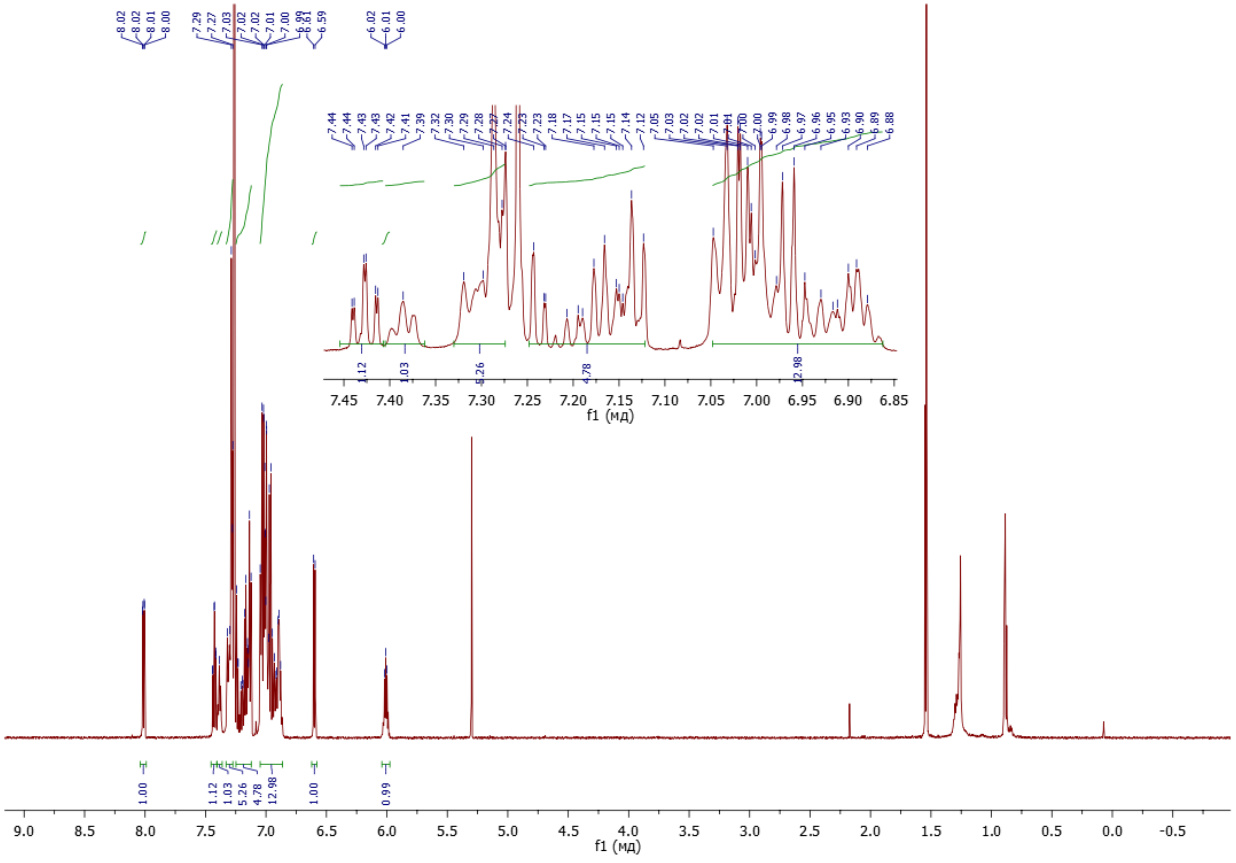


c

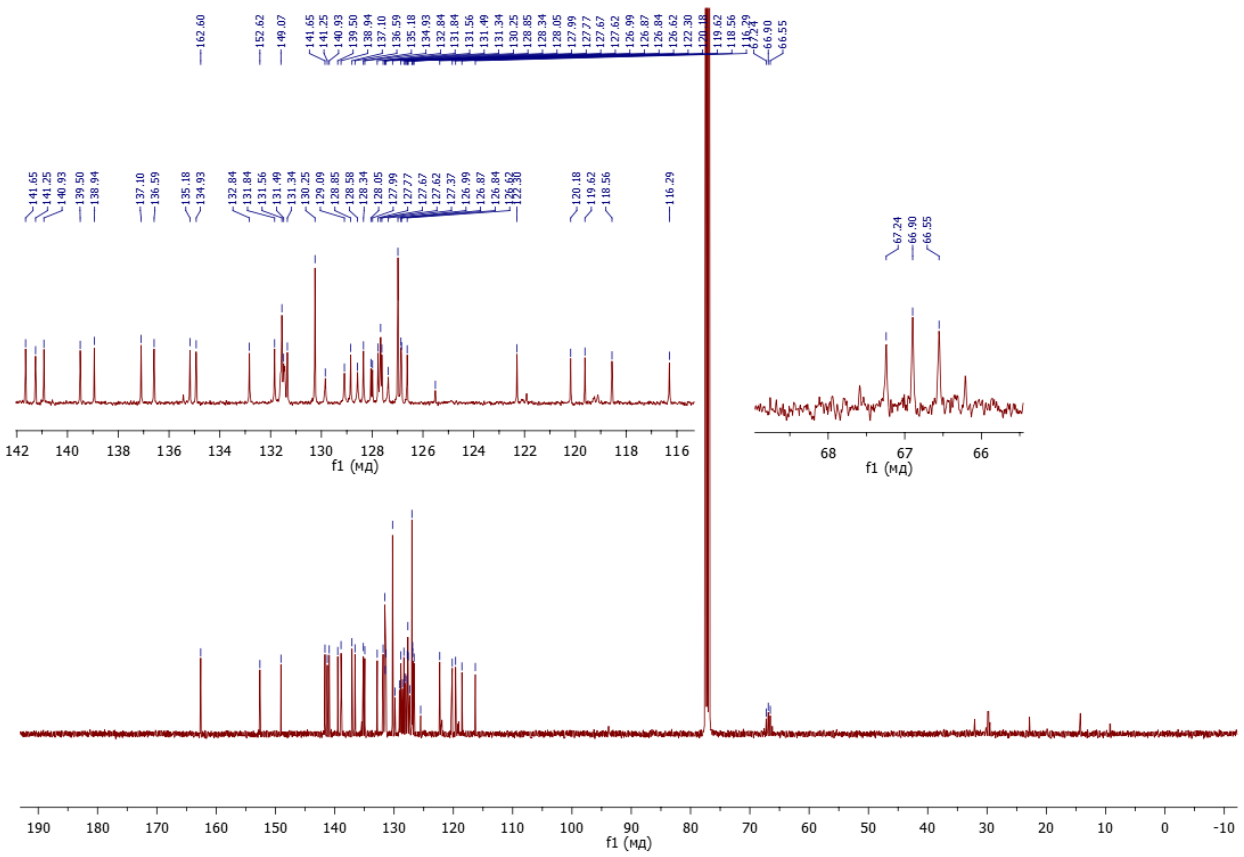
Figure S10. NMR ^{1}H (a), ^{13}C (b), in $CDCl_3$ and mass spectrum (EI) (c) of **5f**.



7



a



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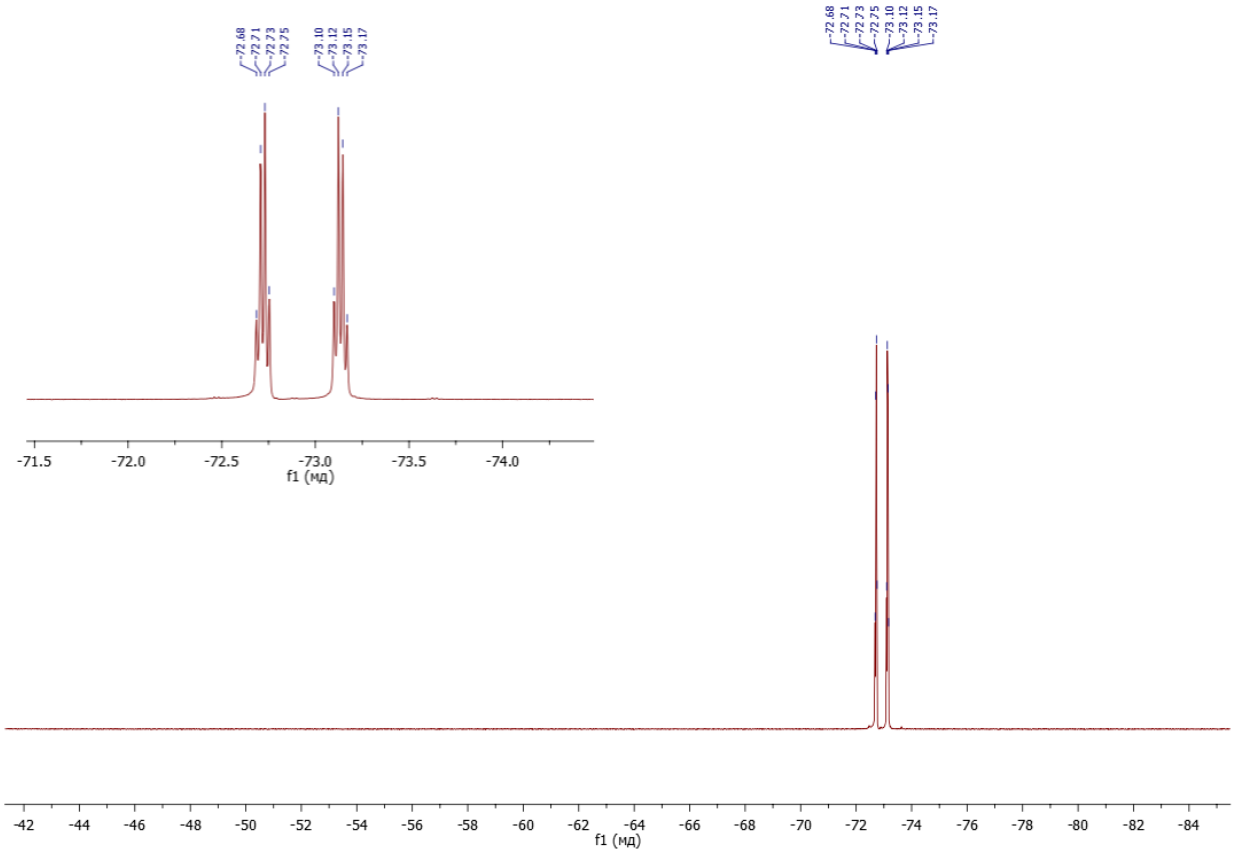

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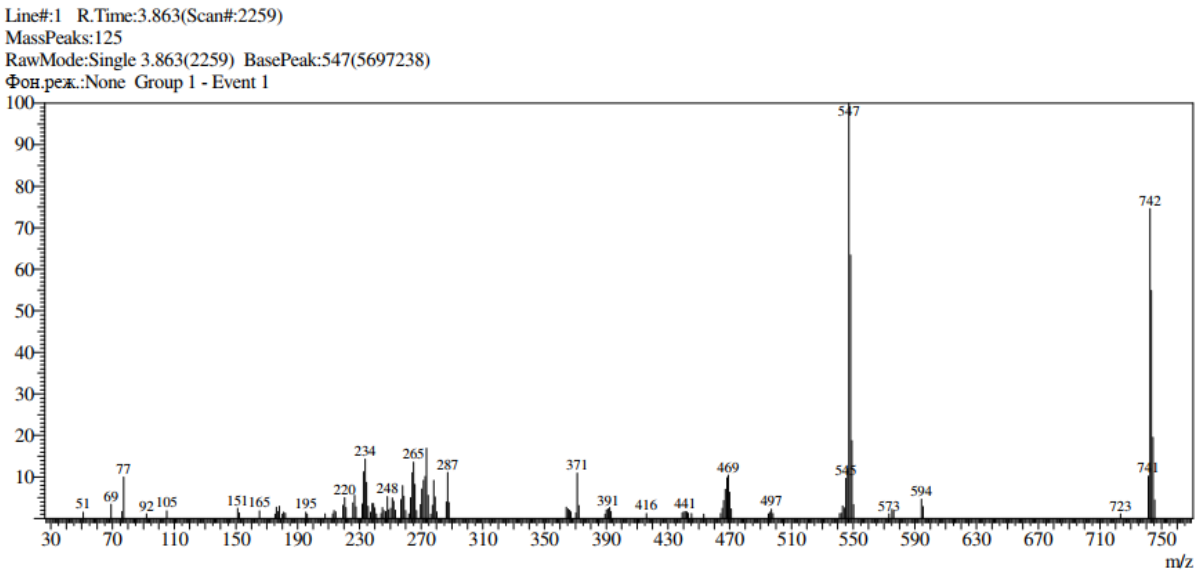
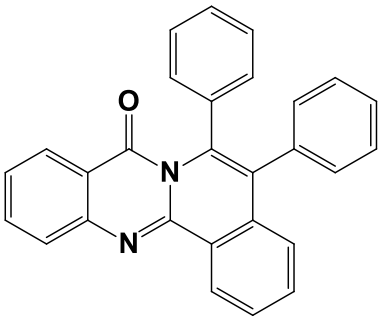
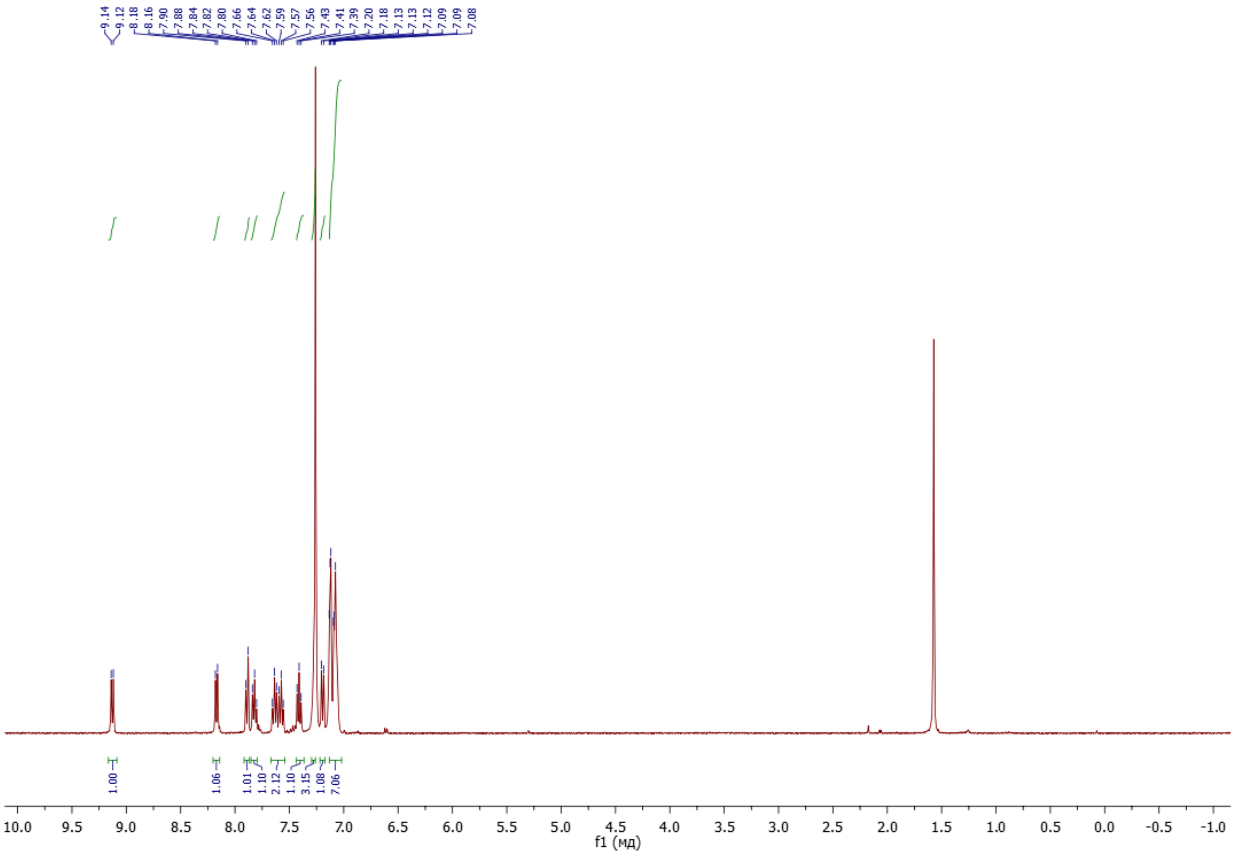


d

Figure S11. NMR ^{1}H (a), ^{13}C (b), ^{19}F (c) in $CDCl_3$ and mass (d) spectra of **7**.


O
N
N

8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7.64
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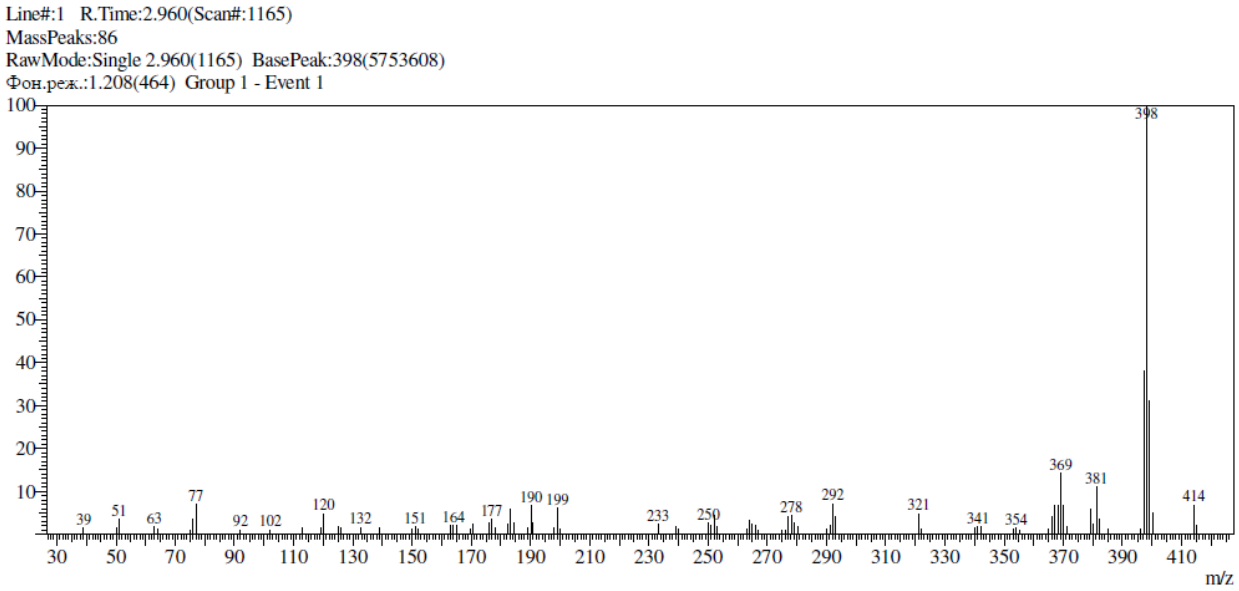
7.59
7.57
7.56
7.43
7.41
7.39
7.20
7.18
7.13
7.12
7.09
7.09
7.08
1.00
1.06
1.01
1.10
2.12
1.10
3.15
1.08
7.06
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (мд)

a



c

Figure S12. NMR ^{1}H (a) in $CDCl_3$ and mass (d) spectra of **8**.

3. UV/Vis, fluorescence excitation and fluorescence emission spectra of compounds 5a-e, 7

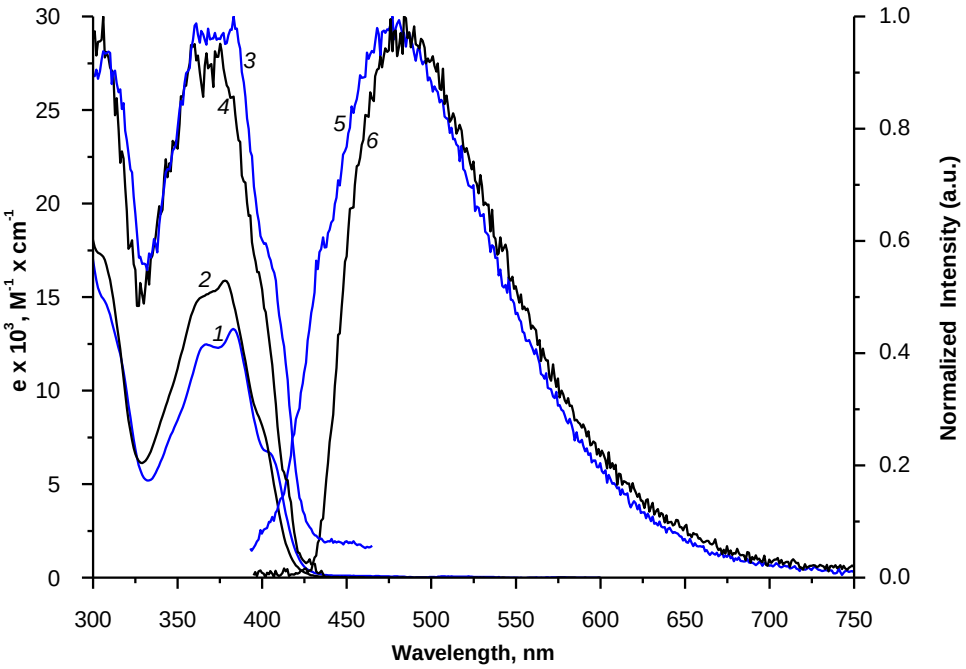


Figure S13. UV/Vis (1, 2), fluorescence excitation (3,4) and fluorescence emission (5, 6) spectra of **5a** in toluene (1, 3, 5) and MeCN (2, 4, 6) at room temperature.

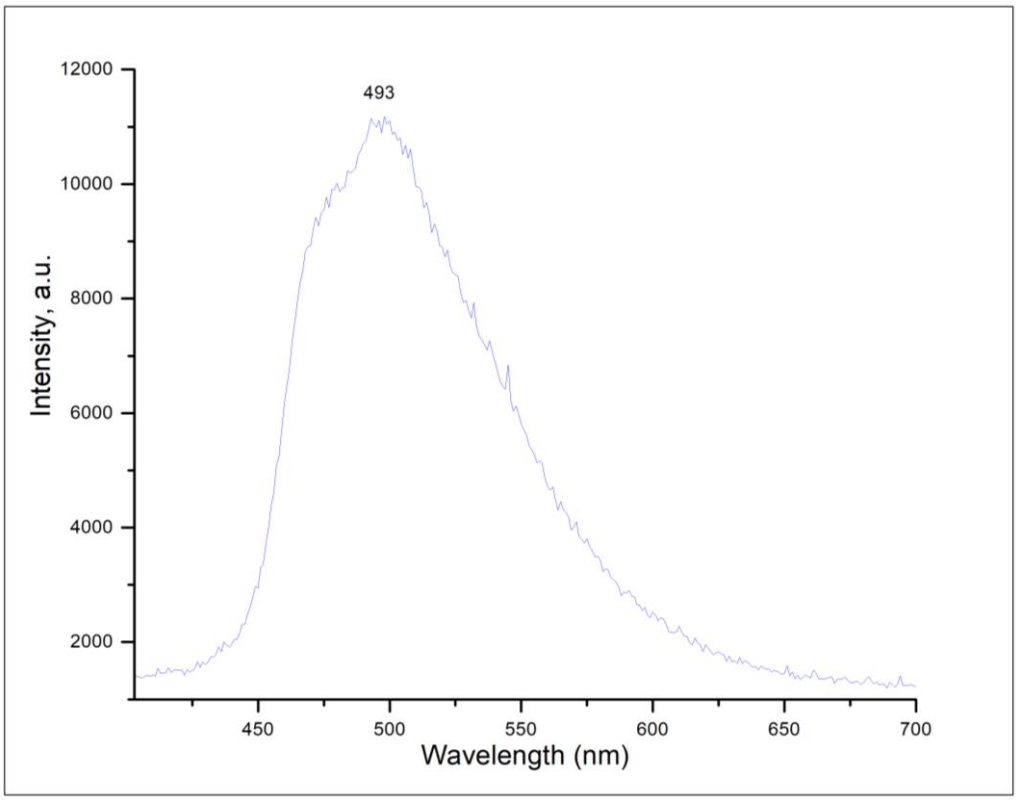


Figure S14. Fluorescence emission spectrum of **5a** in solid state at room temperature.

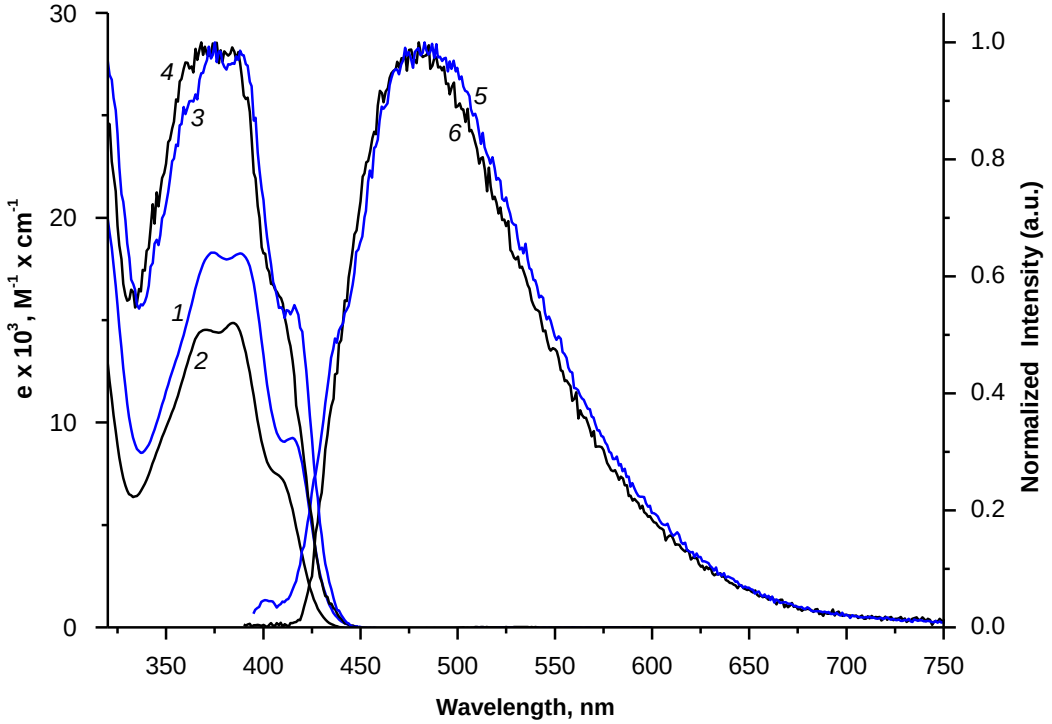


Figure S15. UV/Vis (1, 2), fluorescence excitation (3, 4) and fluorescence emission (5, 6) spectra of **5b** in toluene (1, 3, 5) and MeCN (2, 4, 6) at room temperature.

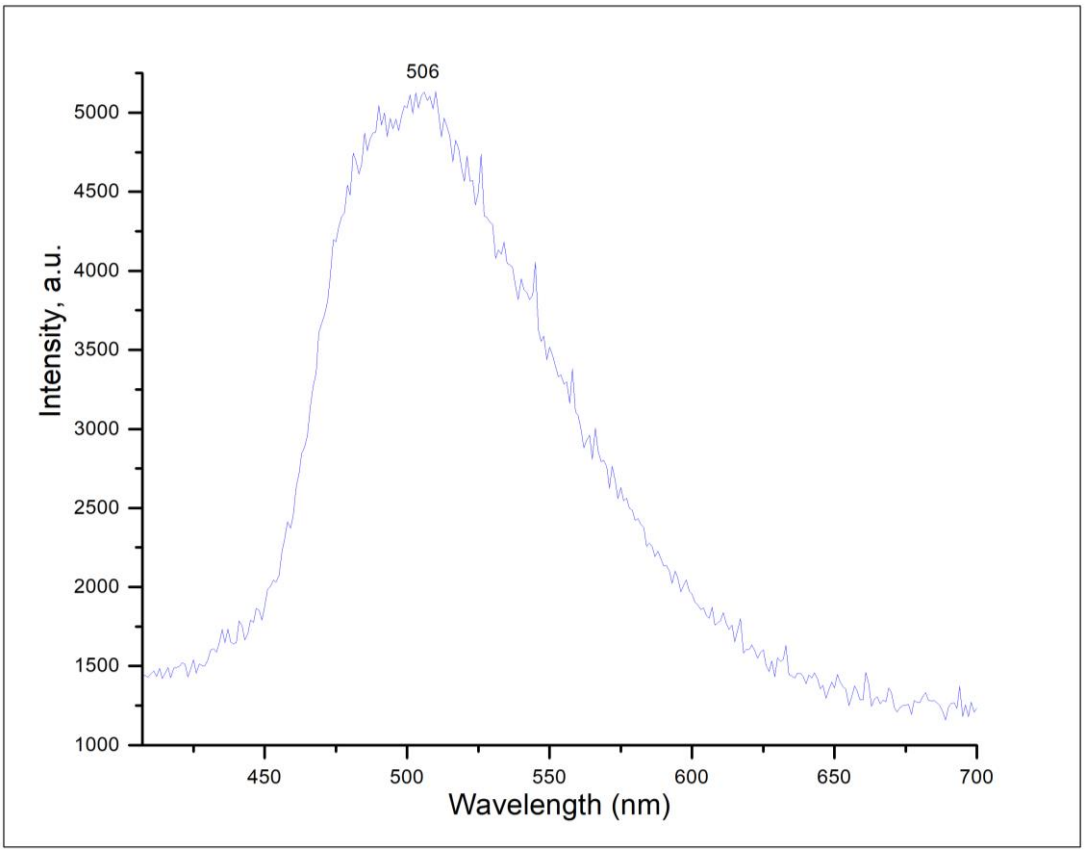


Figure S16. Fluorescence emission spectrum of **5b** in solid state at room temperature.

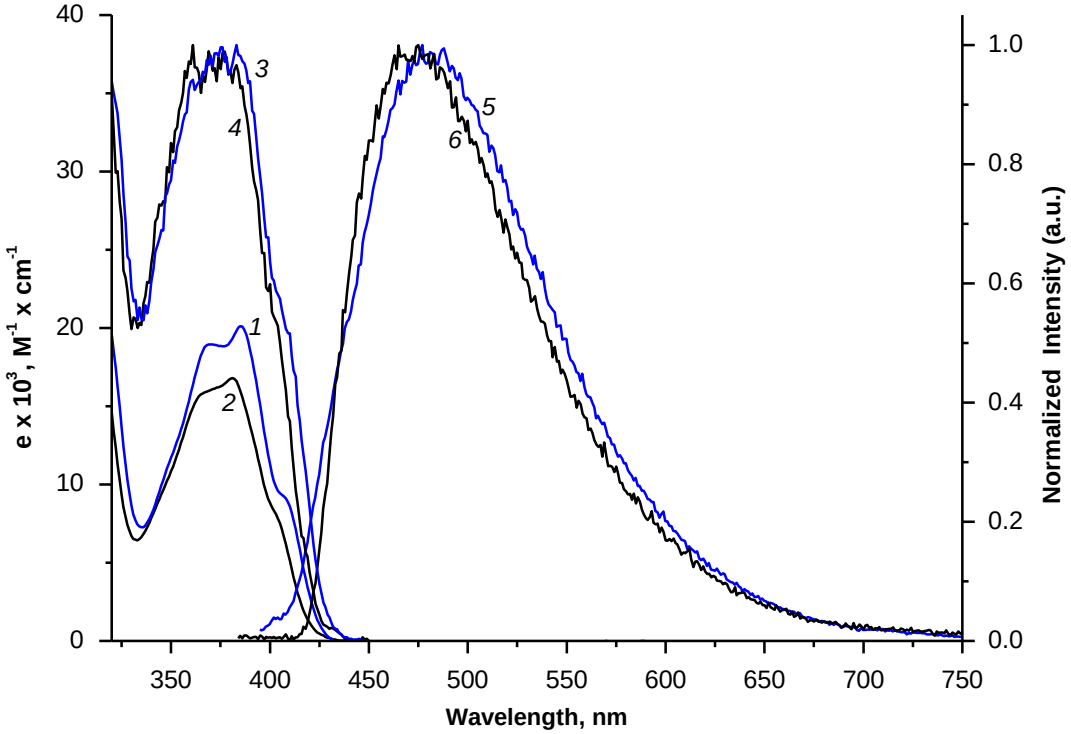


Figure S17. UV/Vis (1, 2), fluorescence excitation (3, 4) and fluorescence emission (5, 6) spectra of **5c** in toluene (1, 3, 5) and MeCN (2, 4, 6) at room temperature.

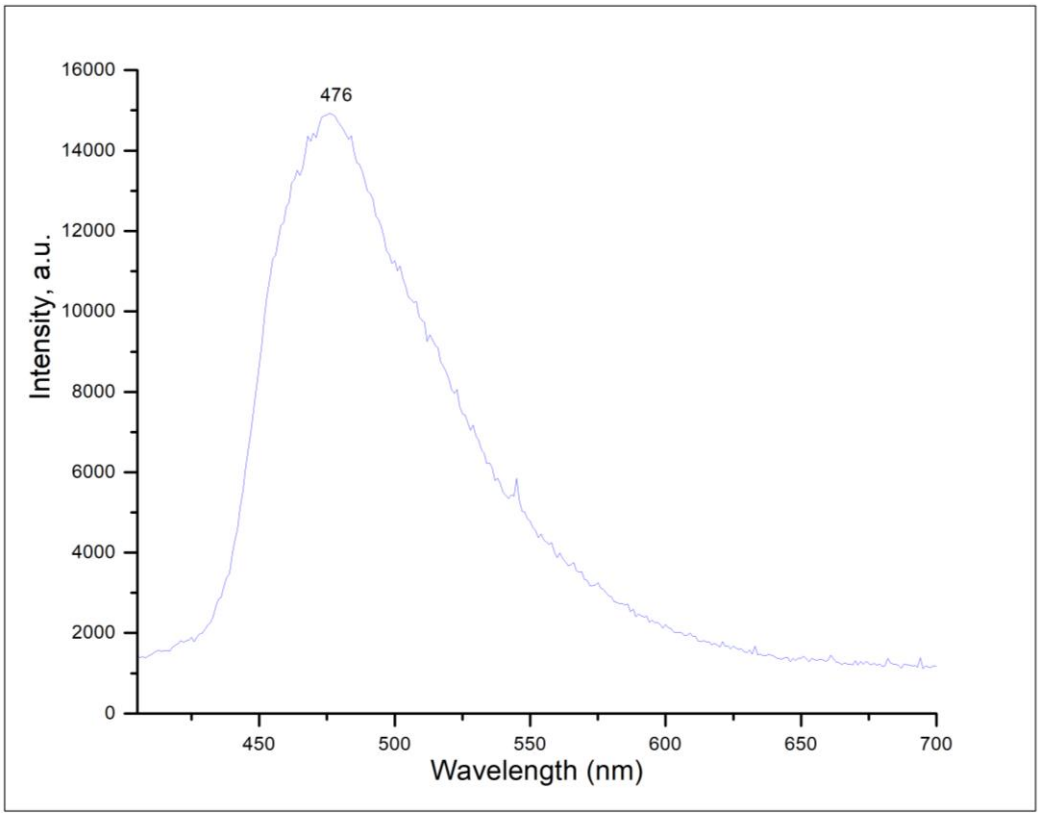


Figure S18. Fluorescence emission spectrum of **5c** in solid state at room temperature.

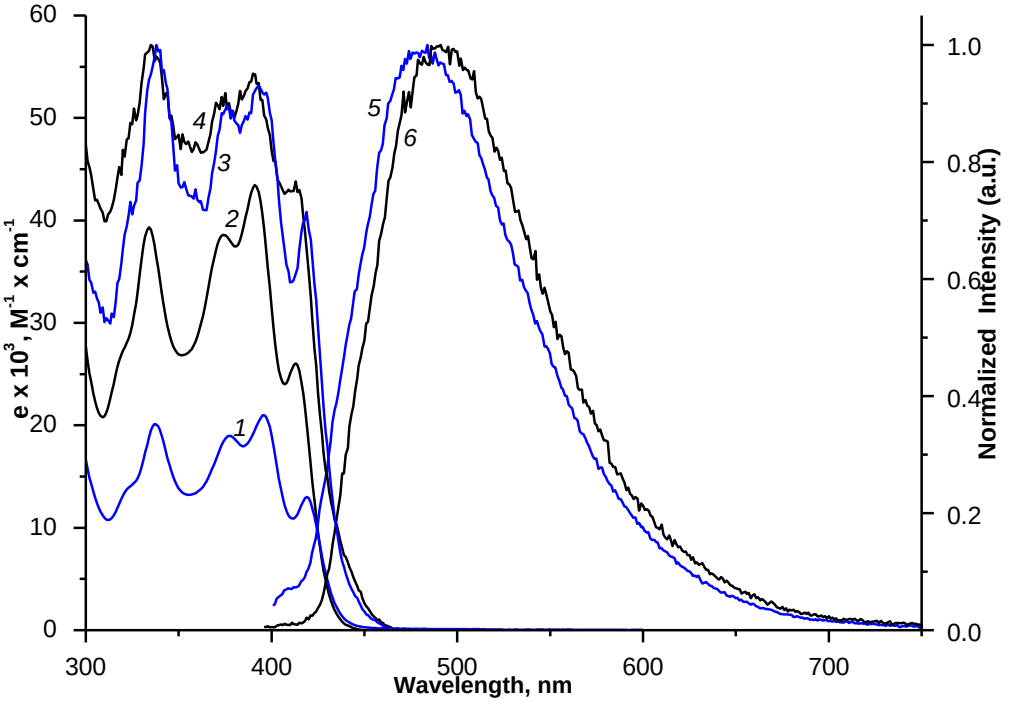


Figure S19. UV/Vis (1, 2), fluorescence excitation (3, 4) and fluorescence emission (5, 6) spectra of **5d** in toluene (1, 3, 5) and MeCN (2, 4, 6) at room temperature.

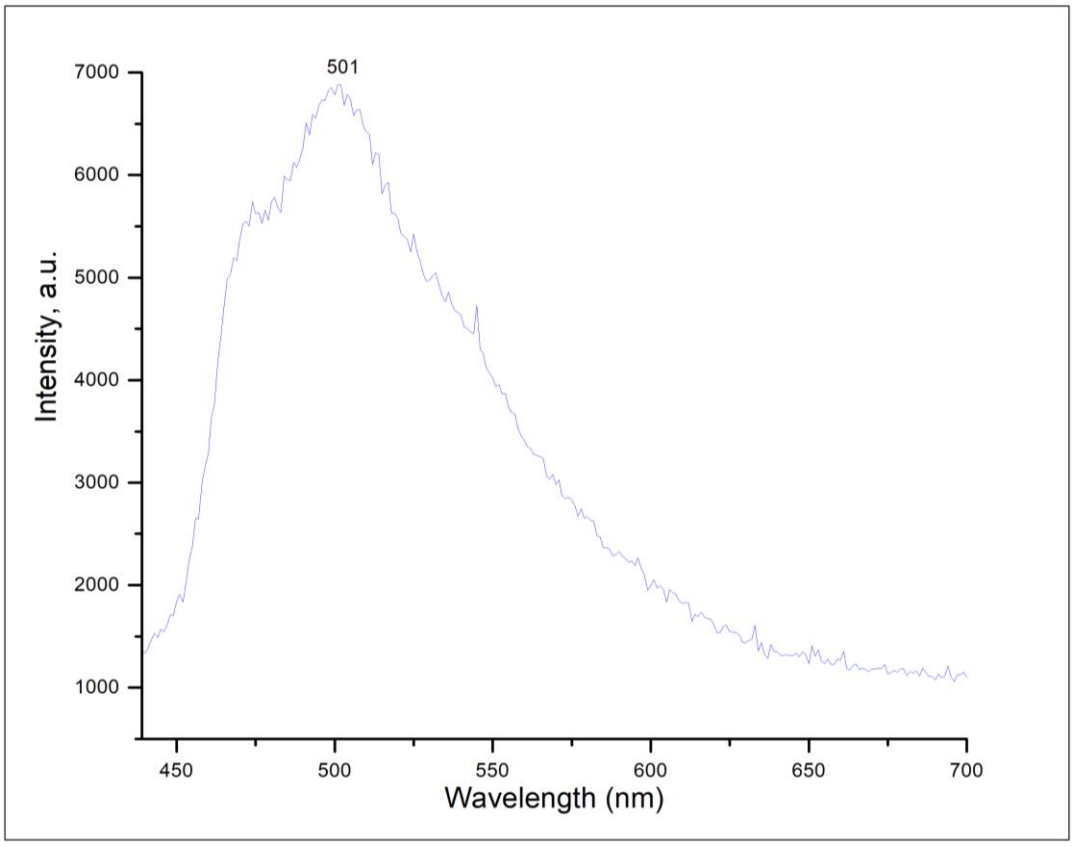


Figure S20. Fluorescence emission spectrum of **5d** in solid state at room temperature.

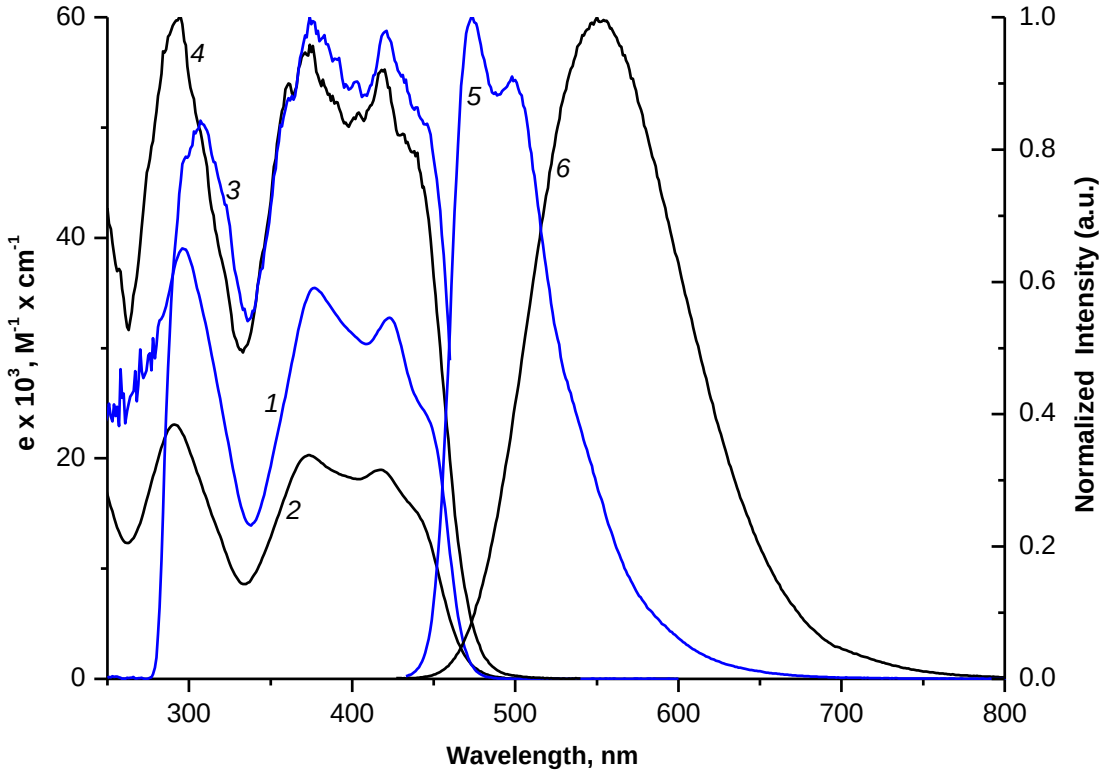


Figure S21. UV/Vis (1, 2), fluorescence excitation (3, 4) and fluorescence emission (5, 6) spectra of **5e** in toluene (1, 3, 5) and MeCN (2, 4, 6) at room temperature.

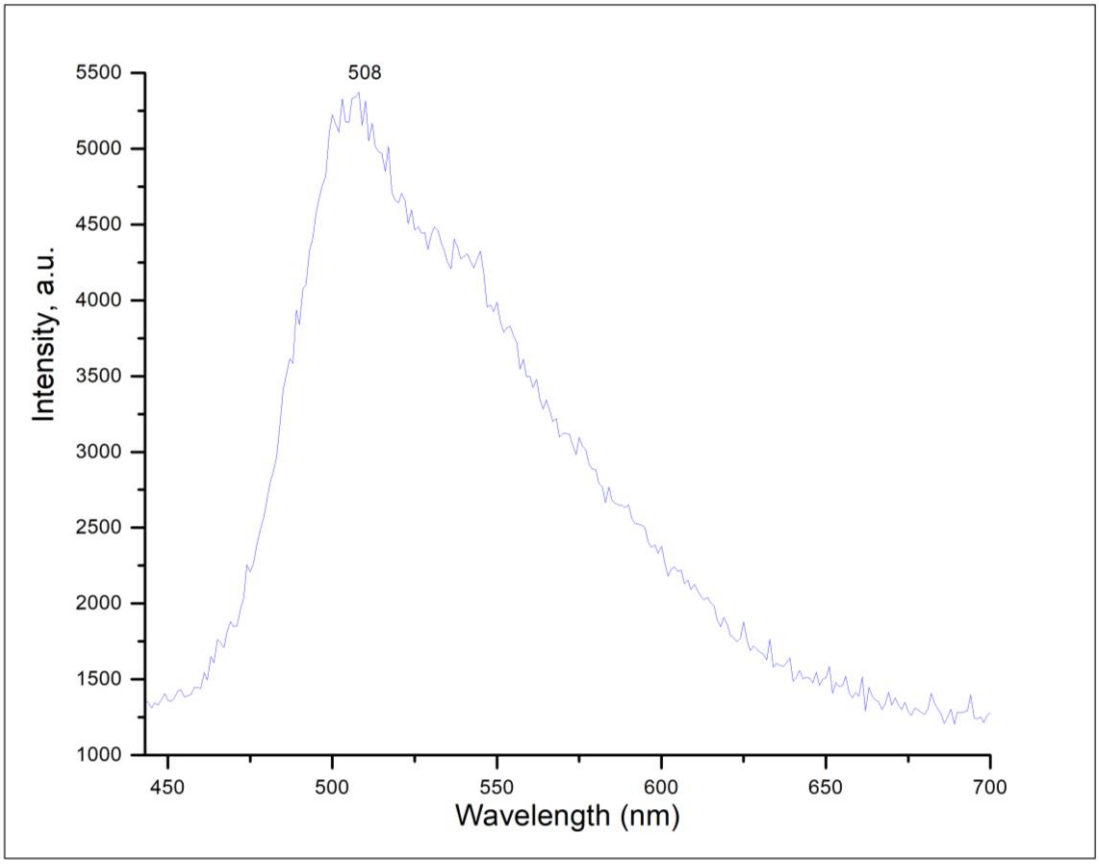


Figure S22. Fluorescence emission spectrum of **5e** in solid state at room temperature.

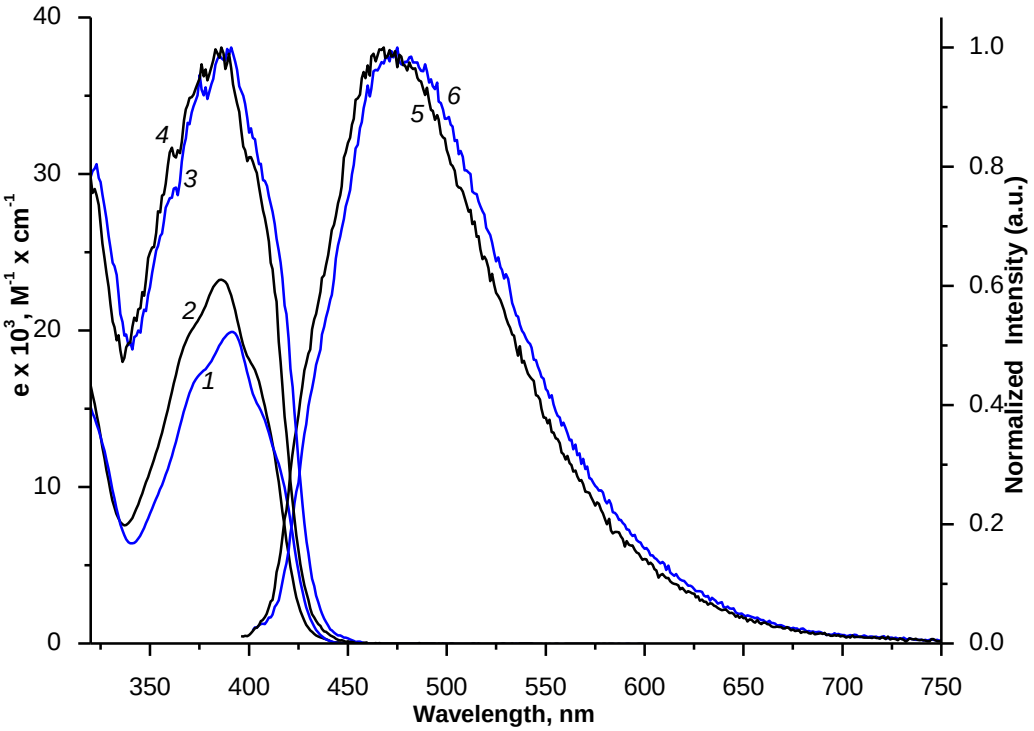


Figure S23. UV/Vis (1, 2), fluorescence excitation (3, 4) and fluorescence emission (5, 6) spectra of **5f** in toluene (1, 3, 5) and MeCN (2, 4, 6) at room temperature.

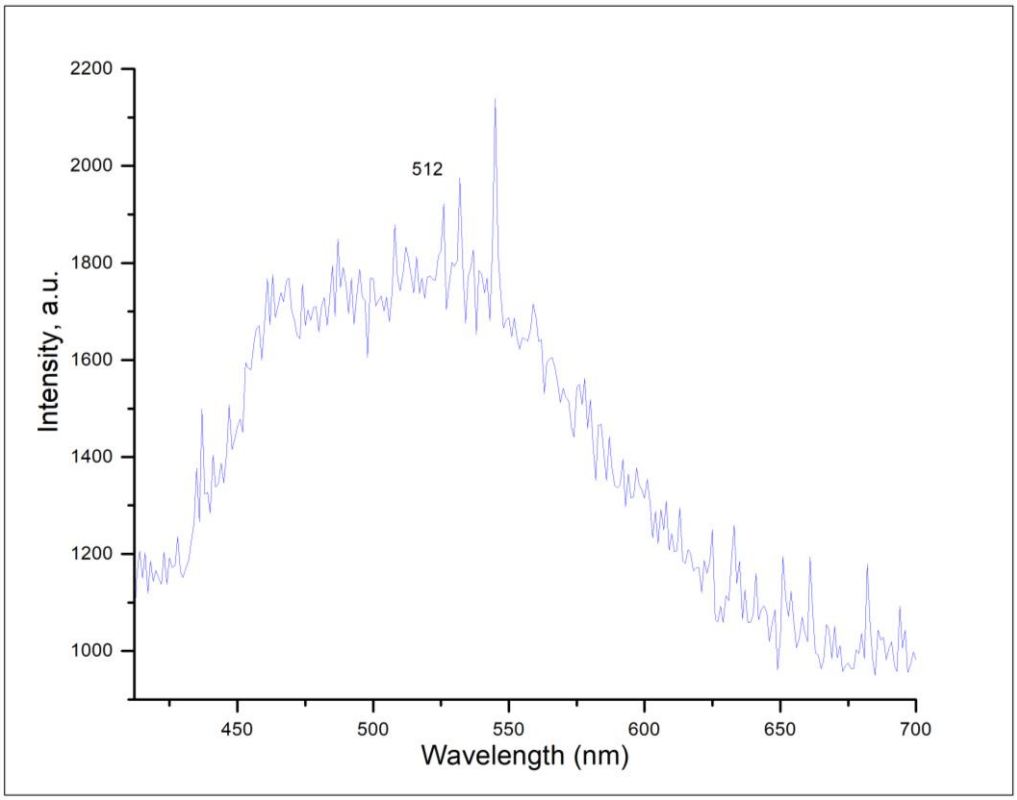


Figure S24. Fluorescence emission spectrum of **5f** in solid state at room temperature.

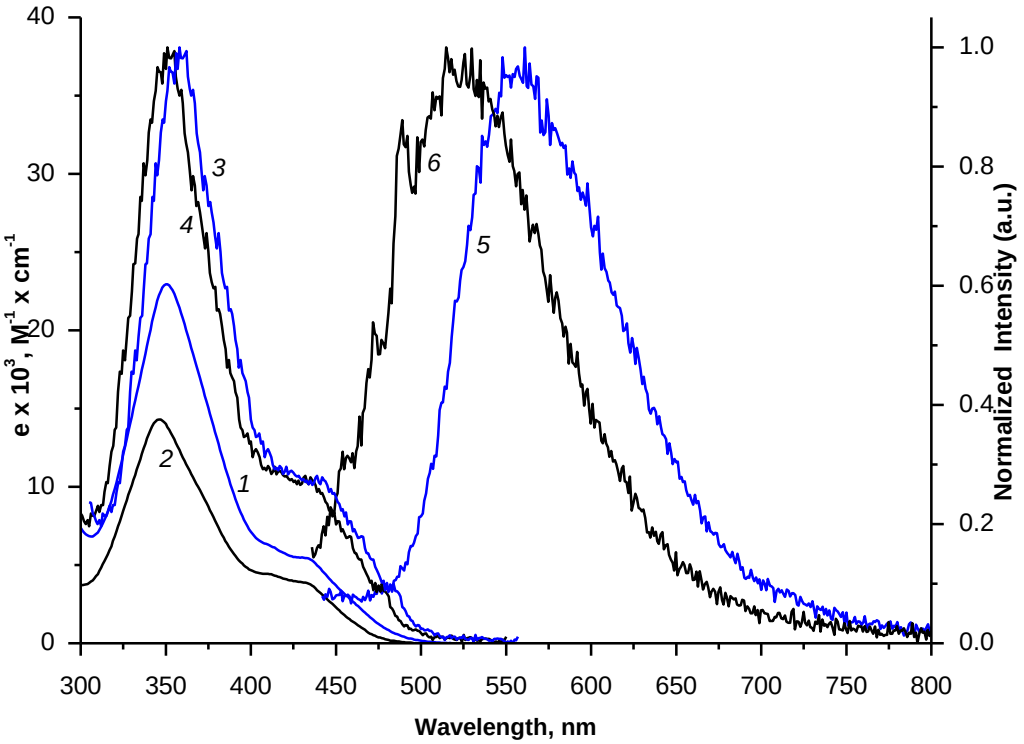


Figure S25. UV/Vis (1, 2), fluorescence excitation (3, 4) and fluorescence emission (5, 6) spectra of **7** in toluene (1, 3, 5) and MeCN (2, 4, 6) at room temperature.

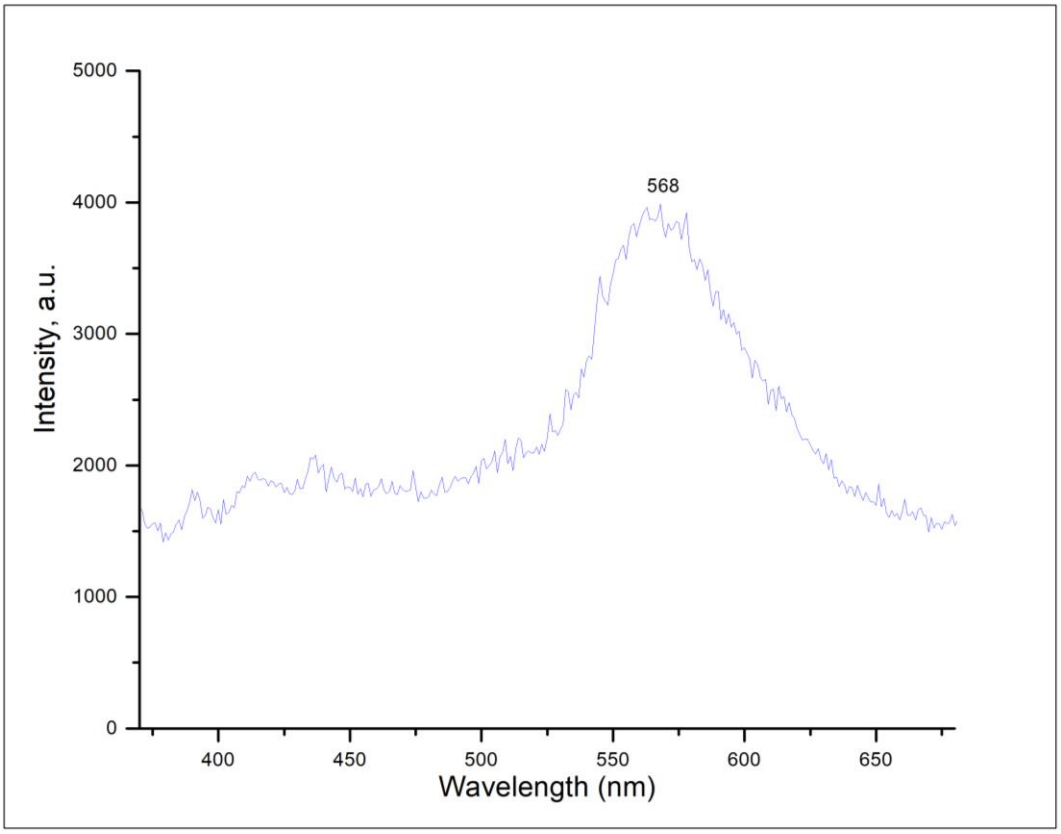


Figure S26. Fluorescence emission spectrum of **7** in solid state at room temperature.

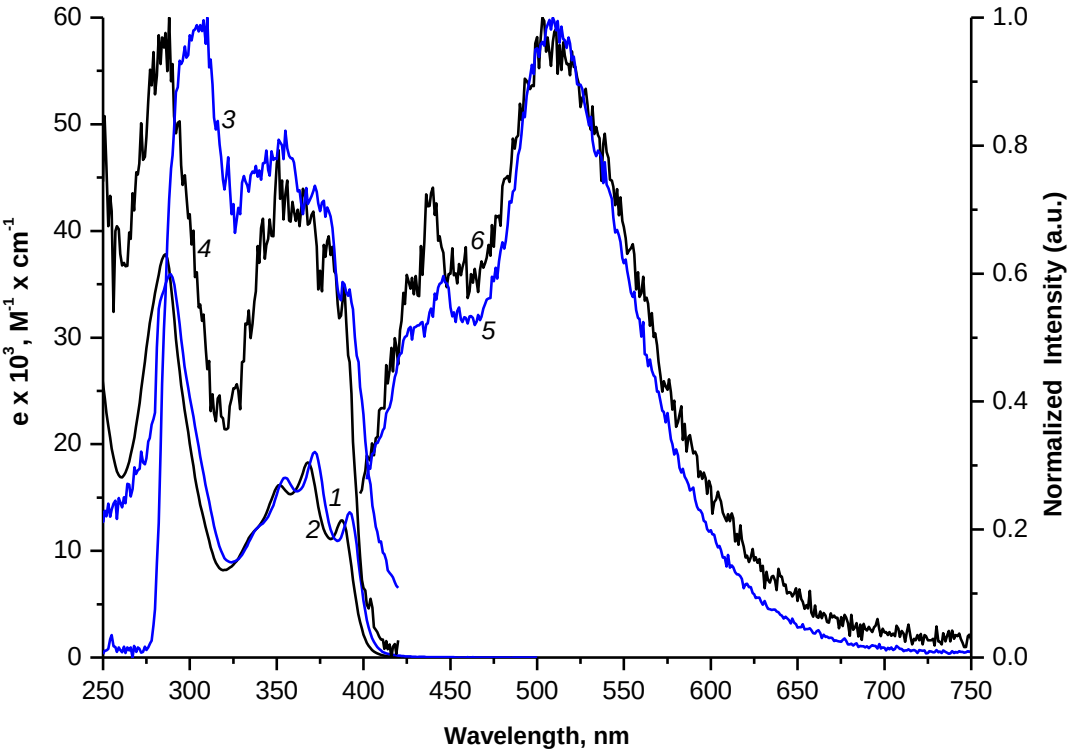


Figure S27. UV/Vis (1, 2), fluorescence excitation (3, 4) and fluorescence emission (5, 6) spectra of **8** in toluene (1, 3, 5) and MeCN (2, 4, 6) at room temperature.

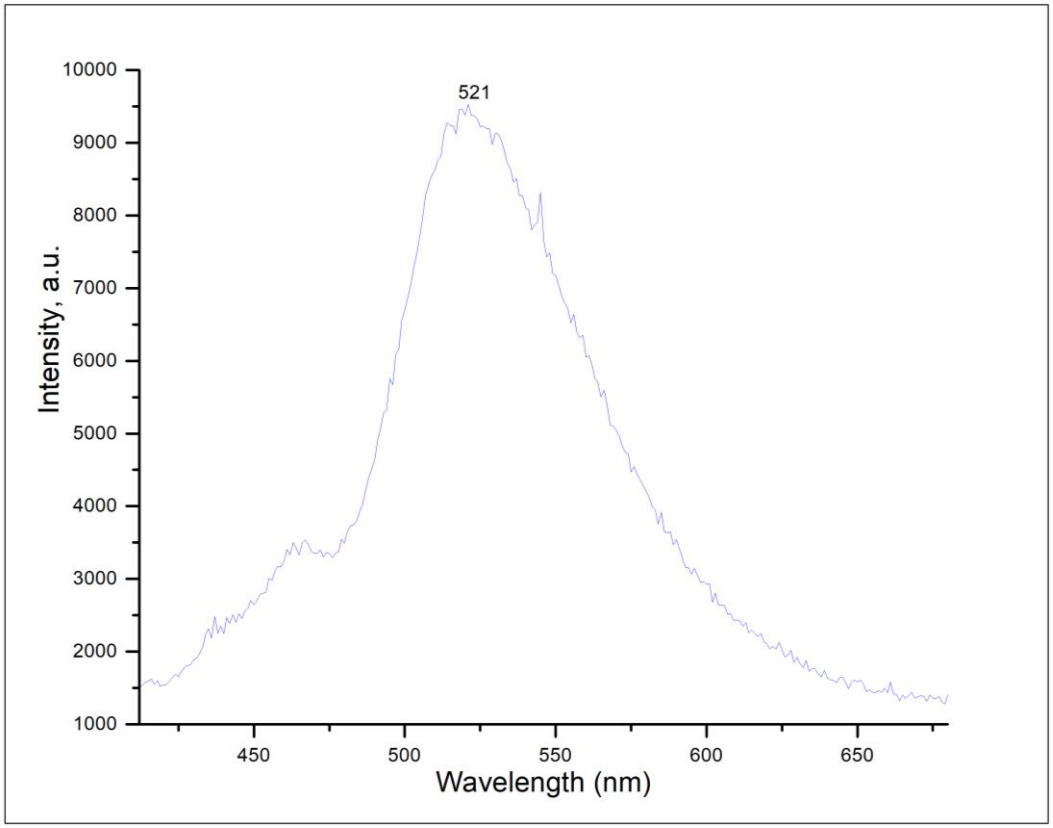


Figure S28. Fluorescence emission spectrum of **8** in solid state at room temperature.

Table S1.

Optical properties of compounds **5a-f**, **7**, **8** in solid state (powder).

Compound	Emission, λ_{max} (nm)	Φ_F[a], %
5a	493	3.0
5b	506	< 1
5c	476	4.2
5d	501	2.3
5e	508	1.6
5f	512	< 1
7	568	< 1
8	521	3.8

[a]Quantum yield in solid state was measured by the integrated sphere method.

4. Aggregation-induced emission of compounds 5a-f, 7, 8

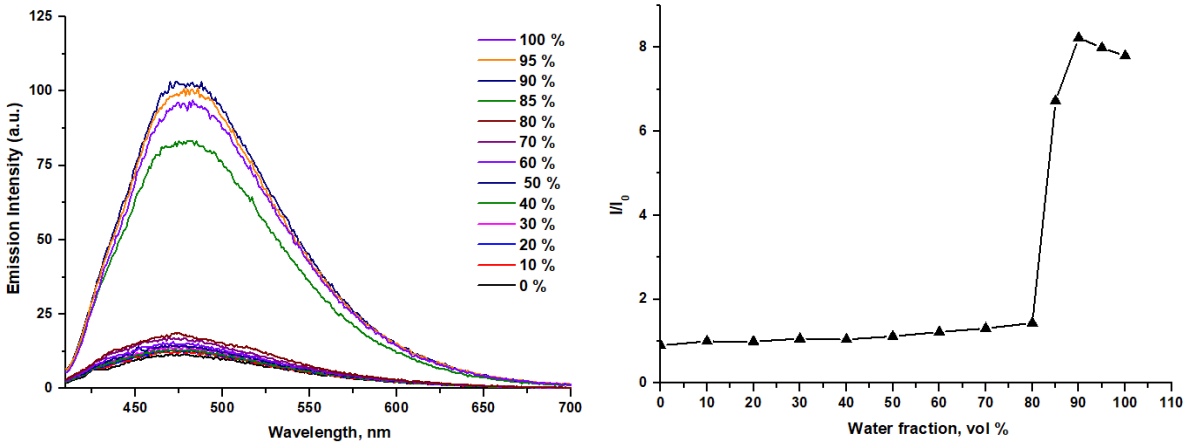


Figure S29. (a) Fluorescence spectra of 10 μM **5a** in the MeCN/H_2O mixtures with different water fractions (f_w). (b) Plot of the I/I_0 at 480 nm versus the composition of the MeCN/H_2O mixture for **5a** (E_{ex} = 378 nm).

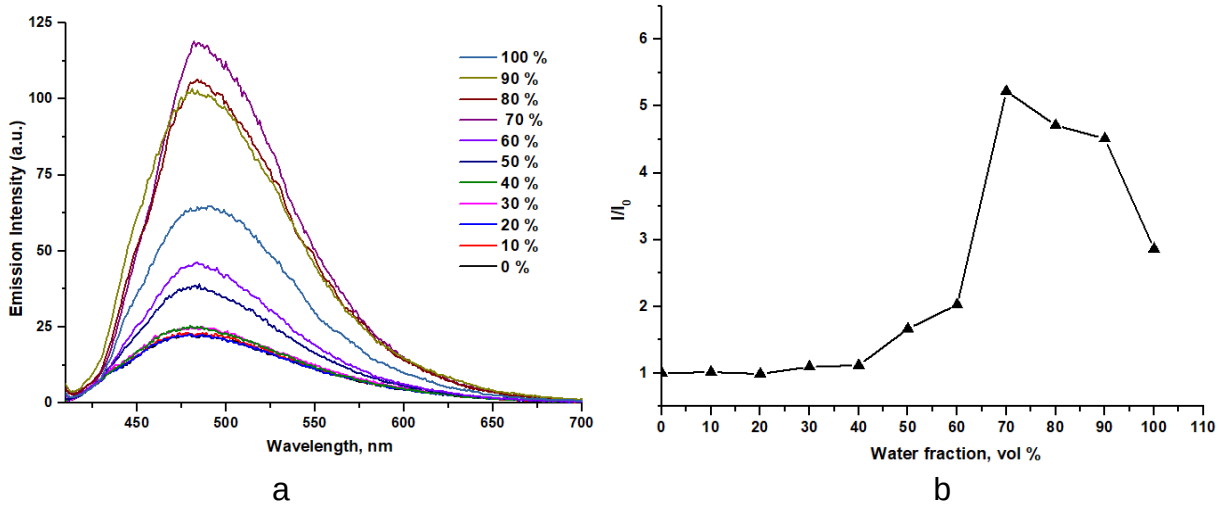


Figure S30. (a) Fluorescence spectra of 10 μM **5b** in the MeCN/H_2O mixtures with different water fractions (f_w). (b) Plot of the I/I_0 at 485 nm versus the composition of the MeCN/H_2O mixture for **5b** (E_{ex} = 385 nm).

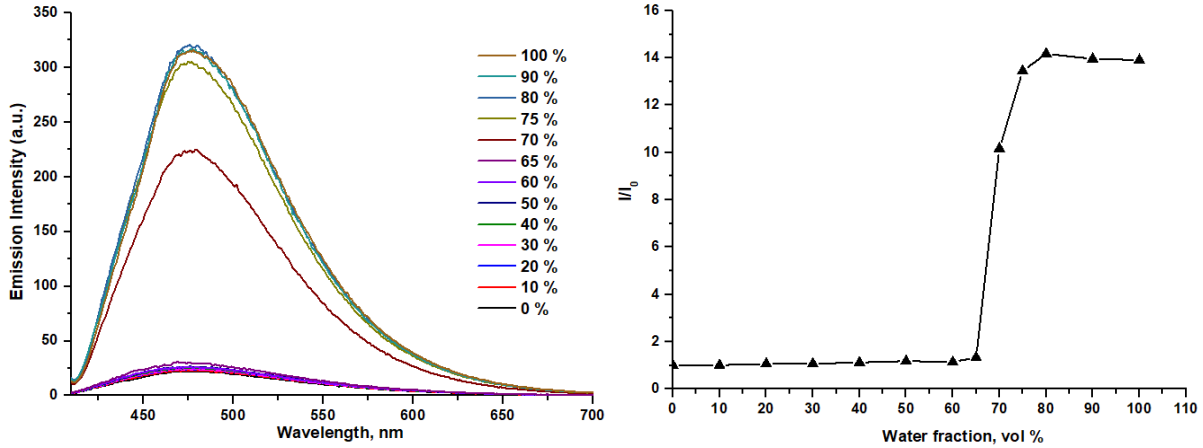


Figure S31. (a) Fluorescence spectra of 10 μM **5c** in the MeCN/H_2O mixtures with different water fractions (f_w). (b) Plot of the I/I_0 at 475 nm versus the composition of the MeCN/H_2O mixture for **5c** (E_{ex} = 385 nm).

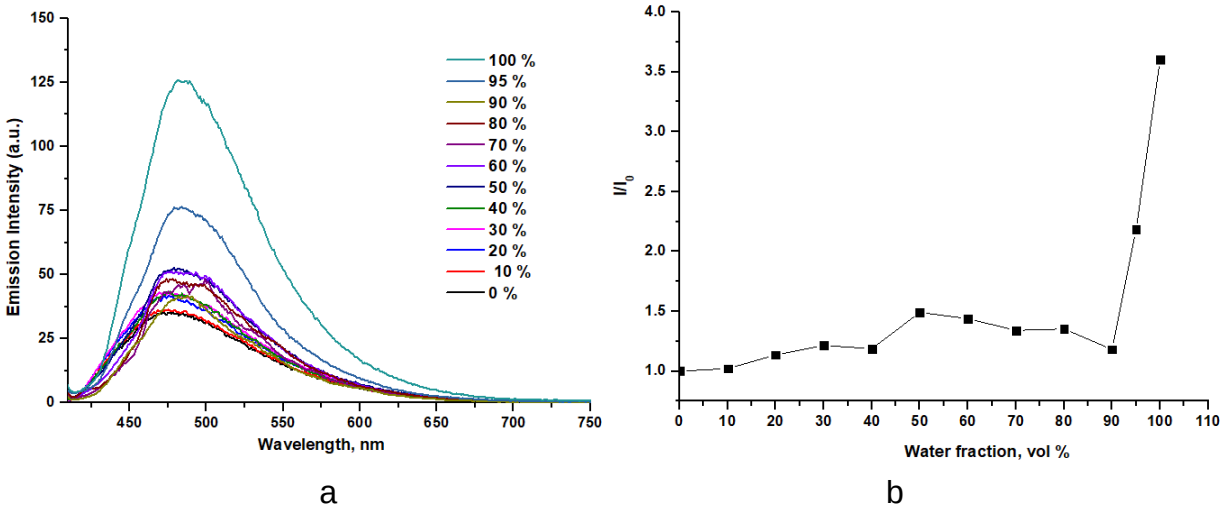


Figure S32. (a) Fluorescence spectra of 10 μM **5d** in the MeCN/H_2O mixtures with different water fractions (f_w). (b) Plot of the I/I_0 at 485 nm versus the composition of the MeCN/H_2O mixture for **5d** (E_{ex} = 390 nm).

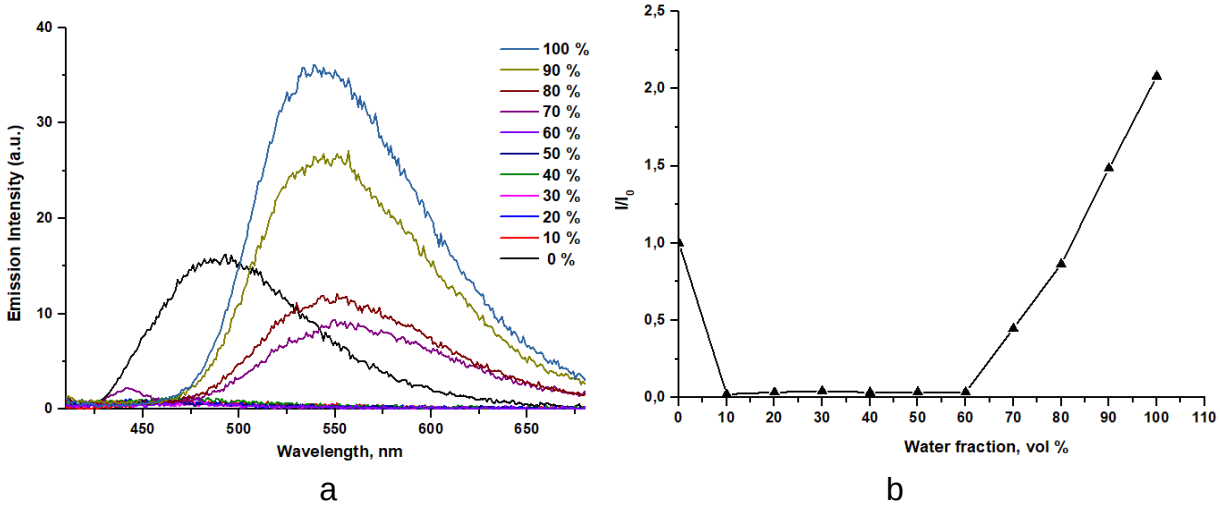


Figure S33. (a) Fluorescence spectra of 10 μM **7** in the MeCN/H_2O mixtures with different water fractions (f_w). (b) Plot of the I/I_0 at 540 nm versus the composition of the MeCN/H_2O mixture for **7** (E_{ex} = 350 nm).

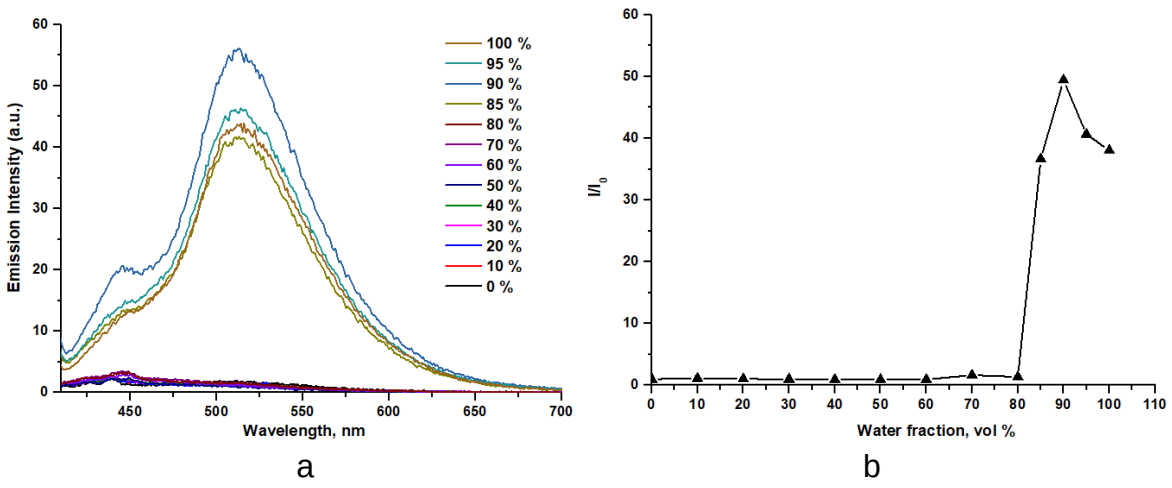


Figure S34. (a) Fluorescence spectra of 10 μM **8** in the MeCN/H_2O mixtures with different water fractions (f_w). (b) Plot of the I/I_0 at 510 nm versus the composition of the MeCN/H_2O mixture for **8** (E_{ex} = 388 nm).

5. Fe^{3+} cation detection of compounds 5a-d,f and 7

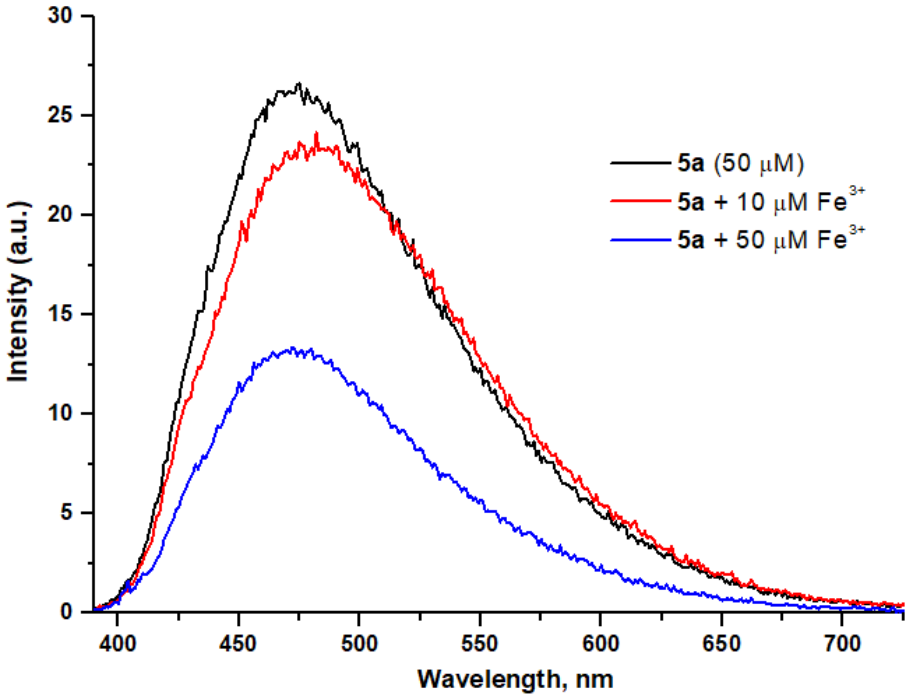


Figure S35. Fluorescence emission spectra (λex = 380 nm) of **5a** acetone solvent with different concentration of Fe^{3+}.

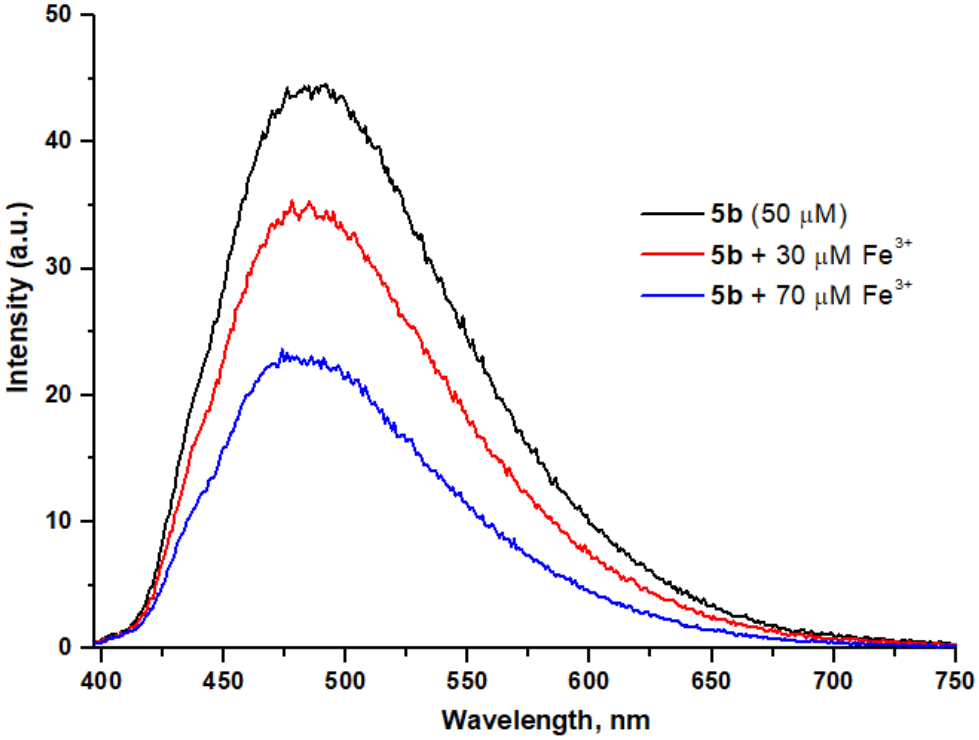


Figure S36. Fluorescence emission spectra (λex = 387 nm) of **5b** acetone solvent with different concentration of Fe^{3+}.

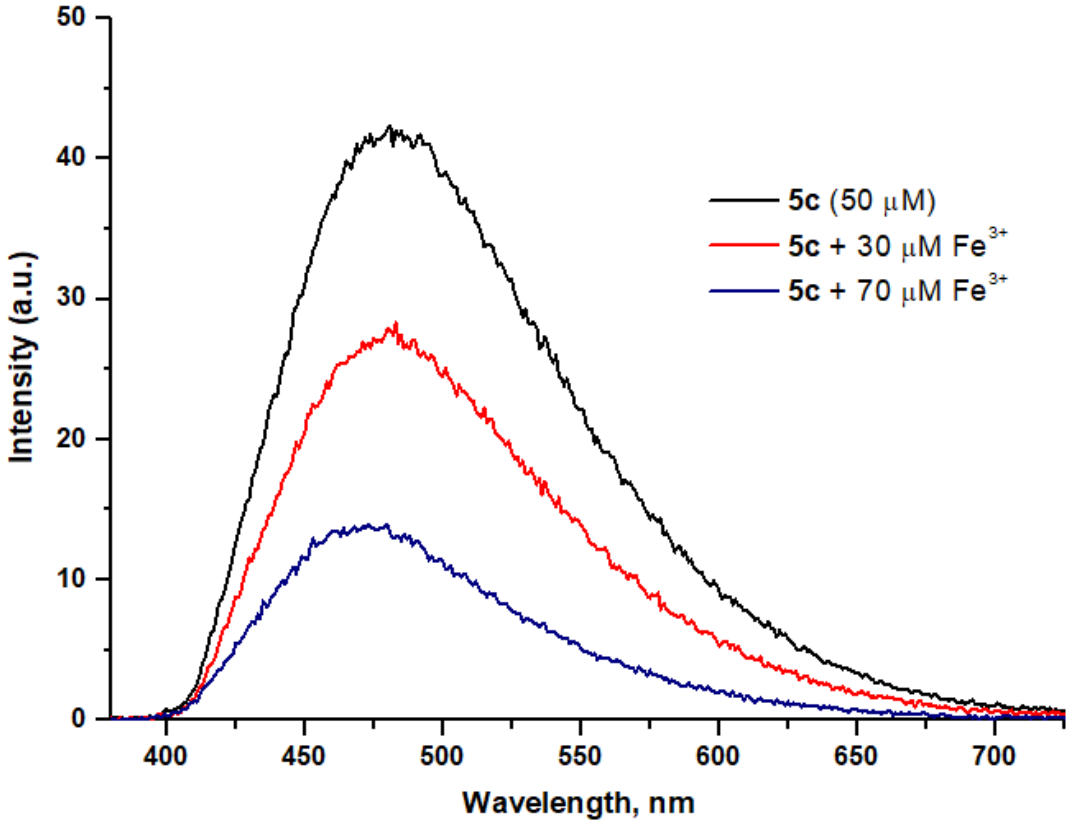


Figure S37. Fluorescence emission spectra (λex = 385 nm) of **5c** acetone solvent with different concentration of Fe^{3+}.

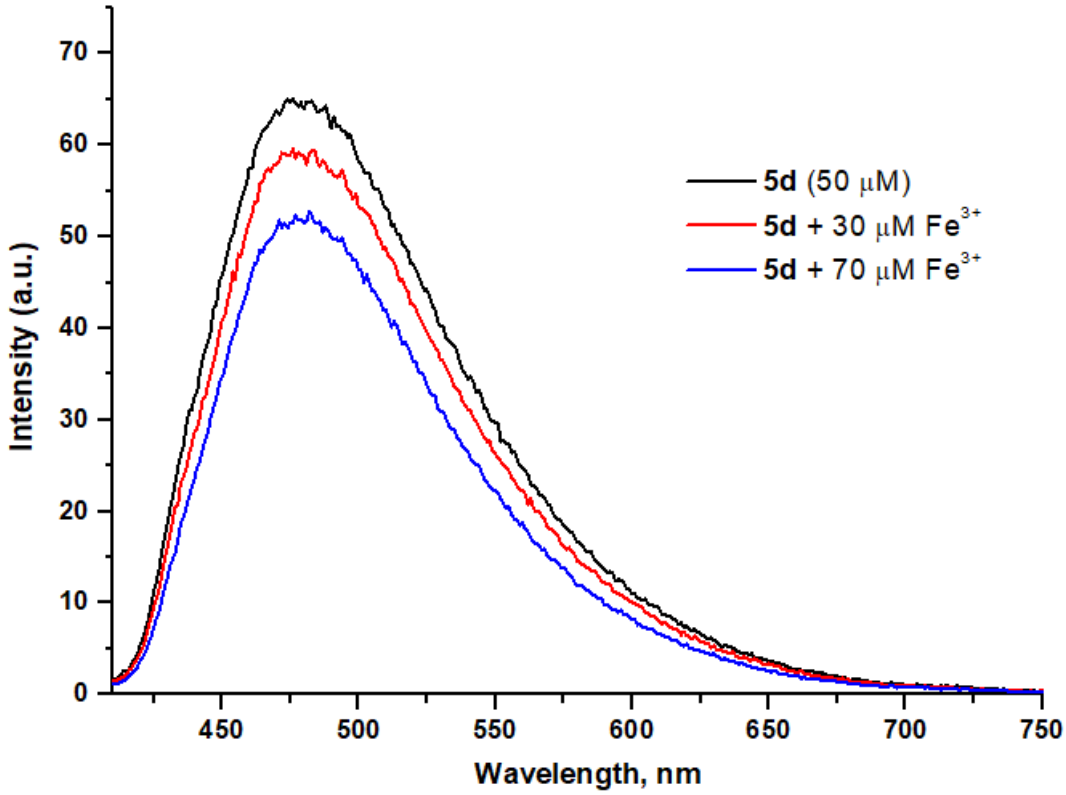


Figure S38. Fluorescence emission spectra (λex = 396 nm) of **5d** acetone solvent with different concentration of Fe^{3+}.

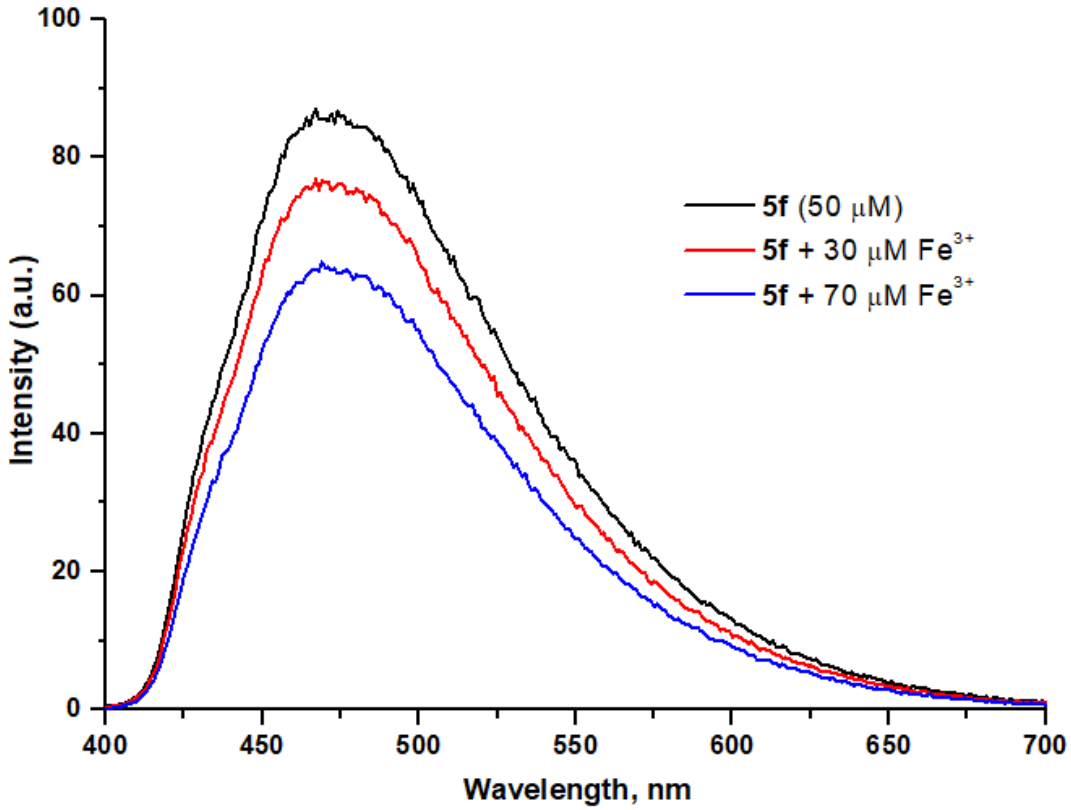


Figure S39. Fluorescence emission spectra (λex = 390 nm) of **5f** acetone solvent with different concentration of Fe^{3+}.

6. Selected bond lengths and angles of compounds 5a,b, and 7

Table S2

Selected bond lengths of compound **5a**.

Bond	Bond length (Å)	Bond	Bond length (Å)
S(1)-C(13)	1.715(4)	C(10)-C(16)	1.487(5)
S(1)-C(14)	1.722(4)	C(11)-C(14)	1.363(5)
N(1)-C(15)	1.303(4)	C(11)-C(12)	1.428(5)
N(1)-C(1)	1.377(5)	C(12)-C(13)	1.346(5)
O(1)-C(7)	1.211(4)	C(14)-C(15)	1.429(5)
C(1)-C(2)	1.398(5)	C(16)-C(21)	1.379(5)
C(1)-C(6)	1.402(5)	C(16)-C(17)	1.390(5)
N(2)-C(15)	1.422(4)	C(17)-C(18)	1.371(6)
N(2)-C(9)	1.434(4)	C(18)-C(19)	1.382(6)
N(2)-C(7)	1.448(5)	C(19)-C(20)	1.359(6)
C(2)-C(3)	1.370(6)	C(20)-C(21)	1.375(5)
C(3)-C(4)	1.396(6)	C(22)-C(23)	1.383(5)
C(4)-C(5)	1.368(5)	C(22)-C(27)	1.386(5)
C(5)-C(6)	1.396(5)	C(23)-C(24)	1.385(5)
C(6)-C(7)	1.459(5)	C(24)-C(25)	1.366(6)
C(9)-C(10)	1.352(5)	C(25)-C(26)	1.380(6)
C(9)-C(22)	1.496(5)	C(26)-C(27)	1.377(5)
C(10)-C(11)	1.446(5)		

Table S3

Selected bond angles of compound **5a**.

Angle	(°)	Angle	(°)
C(13)-S(1)-C(14)	90.48(19)	C(12)-C(11)-C(10)	129.2(3)
C(15)-N(1)-C(1)	118.4(3)	C(13)-C(12)-C(11)	112.4(4)
N(1)-C(1)-C(2)	119.4(3)	C(12)-C(14)-S(1)	113.0(3)
N(1)-C(1)-C(6)	121.7(3)	C(11)-C(14)-C(15)	123.8(3)
C(2)-C(1)-C(6)	118.9(4)	C(11)-C(14)-S(1)	112.6(3)
C(15)-N(2)-C(9)	121.1(3)	C(15)-C(14)-S(1)	123.6(3)
C(15)-N(2)-C(7)	117.6(3)	N(1)-C(15)-N(2)	125.4(3)
C(9)-N(2)-C(7)	121.0(3)	N(1)-C(15)-C(14)	119.3(3)
C(3)-C(2)-C(1)	120.0(4)	N(2)-C(15)-C(14)	115.2(3)
C(2)-C(3)-C(4)	120.8(4)	C(21)-C(16)-C(17)	118.4(4)
C(5)-C(4)-C(3)	120.0(4)	C(21)-C(16)-C(10)	120.0(3)
C(4)-C(5)-C(6)	119.9(4)	C(17)-C(16)-C(10)	121.5(3)
C(5)-C(6)-C(1)	120.3(4)	C(18)-C(17)-C(16)	120.3(4)
C(5)-C(6)-C(7)	119.3(3)	C(17)-C(18)-C(19)	120.1(4)
C(1)-C(6)-C(7)	120.4(3)	C(20)-C(19)-C(18)	120.2(4)
O(1)-C(7)-N(2)	121.0(3)	C(19)-C(20)-C(21)	119.9(4)
O(1)-C(7)-C(6)	124.5(4)	C(20)-C(21)-C(16)	121.1(4)
N(2)-C(7)-C(6)	114.6(3)	C(23)-C(22)-C(27)	118.2(3) .
C(10)-C(9)-N(2)	120.9(3)	C(23)-C(22)-C(9)	121.8(3)
C(10)-C(9)-C(22)	119.7(3)	C(27)-C(22)-C(9)	119.8(3)
N(2)-C(9)-C(22)	119.3(3)	C(22)-C(23)-C(24)	120.8(4)
C(9)-C(10)-C(11)	119.4(3)	C(25)-C(24)-C(23)	119.9(4)
C(9)-C(10)-C(16)	123.8(3)	C(24)-C(25)-C(26)	120.3(4)
C(11)-C(10)-C(16)	116.7(3)	C(27)-C(26)-C(25)	119.5(4)

C(14)-C(11)-C(12)	111.5(3)	C(26)-C(27)-C(22)	121.2(4)
C(14)-C(11)-C(10)	119.3(3)		

Table S4

Selected bond lengths of compound **5b**.

Bond	Bond length (Å)	Bond	Bond length (Å)
Br(1)-C(2)	1.878(7)	C(13)-C(12)	1.413(9)
S(1)-C(2)	1.719(7)	C(22)-C(27)	1.386(6)
S(1)-C(15)	1.728(6)	C(22)-C(23)	1.390(8)
O(1)-C(7)	1.208(8)	C(4)-C(3)	1.433(9)
C(1)-C(3)	1.353(9)	C(4)-C(5)	1.454(8)
N(2)-C(14)	1.403(7)	C(27)-C(26)	1.385(8)
N(2)-C(6)	1.444(8)	C(26)-C(25)	1.369(8)
N(2)-C(7)	1.431(8)	C(24)-C(23)	1.38(1)
N(1)-C(14)	1.315(7)	C(24)-C(25)	1.354(7)
N(1)-C(13)	1.375(8)	C(8)-C(7)	1.468(9)
C(15)-C(14)	1.419(8)	C(8)-C(9)	1.39(1)
C(15)-C(4)	1.371(8)	C(17)-C(18)	1.41(1)
C(16)-C(5)	1.466(9)	C(21)-C(20)	1.37(1)
C(16)-C(17)	1.379(8)	C(12)-C(11)	1.37(1)
C(16)-C(21)	1.414(8)	C(9)-C(10)	1.35(1)
C(6)-C(22)	1.492(8)	C(18)-C(19)	1.364(9)
C(6)-C(5)	1.359(8)	C(20)-C(19)	1.37(1)
C(13)-C(8)	1.40(1)	C(10)-C(11)	1.37(1)

Table S5

Selected bond angles of compound **5b**.

Angle	(°)	Angle	(°)
C(2)-S(1)-C(15)	89.5(3)	C(15)-C(4)-C(5)	118.1(5)
Br(1)-C(2)-S(1)	118.9(3)	C(3)-C(4)-C(5)	129.6(5)
Br(1)-C(2)-C(3)	126.3(5)	C(22)-C(27)-C(26)	120.9(5)
S(1)-C(2)-C(3)	114.8(5)	C(27)-C(26)-C(25)	119.1(5)
C(14)-N(2)-C(6)	121.2(4)	C(2)-C(3)-C(4)	110.6(5)
C(14)-N(2)-C(7)	118.5(4	C(23)-C(24)-C(25)	120.5(6)
C(6)-N(2)-C(7)	120.0(4)	C(22)-C(23)-C(24)	120.3(6)
C(14)-N(1)-C(13)	117.6(5)	C(16)-C(5)-C(6)	122.1(5)
S(1)-C(15)-C(14)	122.6(4)	C(16)-C(5)-C(4)	118.5(5)
S(1)-C(15)-C(4)	112.8(4)	C(6)-C(5)-C(4)	119.3(5)
C(14)-C(15)-C(4)	124.6(5)	C(13)-C(8)-C(7)	119.1(6)
C(5)-C(16)-C(17)	121.0(5)	C(13)-C(8)-C(9)	119.5(6)
C(5)-C(16)-C(21)	122.0(5)	C(7)-C(8)-C(9)	121.3(6)
C(17)-C(16)-C(21)	117.0(5)	C(16)-C(17)-C(18)	121.4(6)
N(2)-C(14)-N(1)	125.0(4)	C(16)-C(21)-C(20)	121.2(6)
N(2)-C(14)-C(15)	115.5(4)	C(13)-C(12)-C(11)	120.3(6)
N(1)-C(14)-C(15)	119.5(5)	O(1)-C(7)-N(2)	122.2(5)
N(2)-C(6)-C(22)	119.8(5)	O(1)-C(7)-C(8)	123.0(6)
N(2)-C(6)-C(5)	120.6(5)	N(2)-C(7)-C(8)	114.7(5)
C(22)-C(6)-C(5)	119.5(5)	C(8)-C(9)-C(10)	120.5(6)
N(1)-C(13)-C(8)	122.9(5)	C(17)-C(18)-C(19)	119.5(6)
N(1)-C(13)-C(12)	118.5(5)	C(26)-C(25)-C(24)	120.9(6)
C(8)-C(13)-C(12)	118.6(5)	C(21)-C(20)-C(19)	120.5(6)
C(6)-C(22)-C(27)	118.5(5)	C(9)-C(10)-C(11)	121.2(7)

C(6)-C(22)-C(23)	123.2(5)	C(12)-C(11)-C(10)	119.9(7)
C(27)-C(22)-C(23)	118.2(5)	C(18)-C(19)-C(20)	120.4(7)
C(15)-C(4)-C(3)	112.2(5)		

Table S6

Selected bond lengths of compound **7**.

Bond	Bond length (Å)	Bond	Bond length (Å)
F(1)-C(8)	1.305(7)	C(11)-C(18)	1.394(5)
F(2)-C(8)	1.308(6)	C(12)-C(31)	1.495(6)
F(3)-C(8)	1.313(8)	C(13)-C(23)	1.367(5)
F(4)-C(12)	1.299(7)	C(13)-C(27)	1.389(5)
F(5)-C(12)	1.300(6)	C(14)-C(15)	1.507(5)
F(6)-C(12)	1.335(7)	C(15)-C(25)	1.362(5)
N(1)-C(14)	1.397(4)	C(15)-C(36)	1.367(5)
N(1)-C(3)	1.414(4)	C(16)-C(39)	1.375(5)
N(1)-C(11)	1.433(5)	C(16)-C(28)	1.387(5)
N(2)-C(3)	1.314(4)	C(17)-C(21)	1.398(5)
N(2)-C(6)	1.379(4)	C(18)-C(30)	1.390(6)
O(1)-C(24)	1.180(5)	C(18)-C(24)	1.487(6)
O(2)-C(24)	1.369(4)	C(19)-C(45)	1.365(5)
O(2)-C(31)	1.410(5)	C(20)-C(21)	1.360(6)
C(31)-H(31A)	0.9800	C(22)-C(33)	1.373(7)
C(1)-C(19)	1.348(6)	C(23)-C(32)	1.370(5)
C(1)-C(2)	1.402(7)	C(25)-C(43)	1.375(6)
C(2)-C(40)	1.369(8)	C(27)-C(35)	1.376(6)
C(3)-C(5)	1.409(5)	C(28)-C(34)	1.388(5)
C(4)-C(20)	1.407(6)	C(29)-C(44)	1.330(7)

C(4)-C(7)	1.424(5)	C(29)-C(36)	1.382(6)
C(4)-C(5)	1.425(5)	C(30)-C(37)	1.371(6)
C(5)-C(10)	1.425(5)	C(32)-C(41)	1.350(6)
C(6)-C(7)	1.360(6)	C(33)-C(37)	1.366(6)
C(6)-C(19)	1.491(5)	C(34)-C(42)	1.343(6)
C(7)-C(16)	1.514(5)	C(35)-C(41)	1.375(6)
C(8)-C(31)	1.509(6)	C(38)-C(42)	1.374(6)
C(9)-C(14)	1.334(5)	C(38)-C(39)	1.392(5)
C(9)-C(10)	1.460(5)	C(40)-C(26)	1.326(7)
C(9)-C(13)	1.488(5)	C(43)-C(44)	1.346(7)
C(10)-C(17)	1.386(6)	C(45)-C(26)	1.372(7)
C(11)-C(22)	1.375(6)		

Table S7

Selected bond angles of compound **7**.

Angle	(°)	Angle	(°)
C(14)-N(1)-C(3)	120.5(3)	C(9)-C(14)-N(1)	122.8(3)
C(14)-N(1)-C(11)	121.3(3)	C(9)-C(14)-C(15)	122.3(3)
C(13)-N(1)-C(11)	117.8(3)	N(1)-C(14)-C(15)	114.8(4)
C(3)-N(2)-C(6)	117.0(4)	C(25)-C(15)-C(36)	118.1(4)
C(24)-O(2)-C(31)	116.6(4)	C(25)-C(15)-C(14)	119.7(3)
C(19)-C(1)-C(2)	119.8(5)	C(36)-C(15)-C(14)	122.2(4)
C(40)-C(2)-C(1)	120.2(6)	C(39)-C(16)-C(28)	117.7(3)
N(2)-C(3)-C(5)	124.9(3)	C(39)-C(16)-C(7)	122.7(3)
N(2)-C(3)-N(1)	117.1(4)	C(28)-C(16)-C(7)	119.6(3)
C(5)-C(3)-N(1)	118.0(3)	C(10)-C(17)-C(21)	119.5(4)
C(20)-C(4)-C(7)	125.8(3)	C(30)-C(18)-C(11)	118.4(4)

C(20)-C(4)-C(5)	116.7(4)	C(30)-C(18)-C(24)	121.4(4)
C(7)-C(4)-C(5)	117.5(4)	C(11)-C(18)-C(24)	120.2(4)
C(3)-C(5)-C(4)	117.5(3)	C(1)-C(19)-C(45)	119.0(4)
C(3)-C(5)-C(10)	121.2(3)	C(1)-C(19)-C(6)	120.2(4)
C(4)-C(5)-C(10)	121.2(4)	C(45)-C(19)-C(6)	120.8(4)
C(7)-C(6)-N(2)	123.9(3)	C(21)-C(20)-C(4)	121.9(4)
C(7)-C(6)-C(19)	122.5(3)	C(20)-C(21)-C(17)	121.7(5)
N(2)-C(6)-C(19)	113.6(4)	C(33)-C(22)-C(11)	120.9(5)
C(6)-C(7)-C(4)	119.1(3)	C(13)-C(23)-C(32)	121.9(4)
C(6)-C(7)-C(16)	121.0(3)	O(1)-C(24)-O(2)	122.2(5)
C(4)-C(7)-C(16)	119.6(4)	O(1)-C(24)-C(18)	127.2(4)
F(1)-C(8)-F(2)	108.1(6)	O(2)-C(24)-C(18)	110.6(4)
F(1)-C(8)-F(3)	107.9(5)	C(15)-C(25)-C(43)	120.4(4)
F(2)-C(8)-F(3)	108.1(6)	C(35)-C(27)-C(13)	120.8(4)
F(1)-C(8)-C(31)	111.0(6)	C(16)-C(28)-C(34)	120.2(4)
F(2)-C(8)-C(31)	109.8(5)	C(44)-C(29)-C(36)	121.8(5)
F(3)-C(8)-C(31)	111.9(5)	C(37)-C(30)-C(18)	121.2(5)
C(14)-C(9)-C(10)	119.5(3)	O(2)-C(31)-C(12)	109.1(4)
C(14)-C(9)-C(13)	121.2(3)	O(2)-C(31)-C(8)	107.0(4)
C(10)-C(9)-C(13)	119.3(4)	C(12)-C(31)-C(8)	114.7(5)
C(17)-C(10)-C(5)	119.1(3)	C(41)-C(32)-C(23)	120.6(5)
C(17)-C(10)-C(9)	123.0(4)	C(37)-C(33)-C(22)	120.0(5)
C(5)-C(10)-C(9)	117.9(4)	C(42)-C(34)-C(28)	121.6(4)
C(22)-C(11)-C(18)	119.7(4)	C(41)-C(35)-C(27)	120.2(4)
C(22)-C(11)-N(1)	117.9(4)	C(15)-C(36)-C(29)	119.8(4)
C(18)-C(11)-N(1)	122.3(4)	C(33)-C(37)-C(30)	119.9(5)
F(4)-C(12)-F(5)	107.3(6)	C(42)-C(38)-C(39)	119.9(4)

F(4)-C(12)-F(6)	104.9(5)	C(16)-C(39)-C(38)	121.3(4)
F(5)-C(12)-F(6)	107.2(6)	C(26)-C(40)-C(2)	118.7(6)
F(4)-C(12)-C(31)	113.9(6)	C(32)-C(41)-C(35)	119.3(4)
F(5)-C(12)-C(31)	112.0(5)	C(34)-C(42)-C(38)	119.3(4)
F(6)-C(12)-C(31)	111.0(5)	C(44)-C(43)-C(25)	121.2(5)
C(23)-C(13)-C(27)	117.3(4)	C(29)-C(44)-C(43)	118.6(5)
C(23)-C(13)-C(9)	121.0(3)	C(19)-C(45)-C(26)	120.4(5)
C(27)-C(13)-C(9)	121.7(4)	C(40)-C(26)-C(45)	121.8(6)

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