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SUPPLEMENTARY MATERIAL TO

Assessing the pharmacological potential of selected xanthene derivatives

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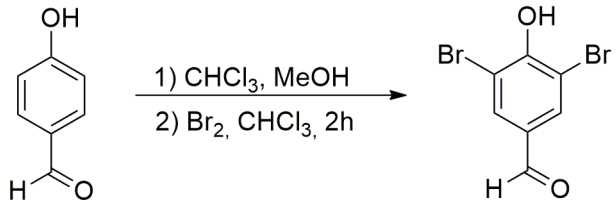
EXPERIMENTAL DETAILS

Synthesis of 3,5-dibromo-4-hydroxybenzaldehyde

The mixture of chloroform (20 mL) and methanol (2 mL) was used for dissolving 4-hydroxybenzaldehyde (2 g, 0.16 mmol) prior to addition of bromine solution (2.84 g, 0.18 mmol in 4 mL of chloroform). Moreover, the reaction mixture was additionally diluted by the dichloromethane and water. After stirring for 2 h, the obtained solution was washed with aqueous sodium thiosulfate and dried over $MgSO_4$. The solvent was removed by evaporation under reduced pressure and a solid 3,5-dibromo-4-hydroxybenzaldehyde was acquired. The crude product was purified by recrystallization from ethanol.[1] The obtained values of melting point and ^{1}H- and ^{13}C-NMR spectra are in accordance with literature data.[2]



Scheme S-1. Synthesis of 3,5-dibromo-4-hydroxybenzaldehyde.

Synthesis of 3-chloro-4-hydroxybenzaldehyde

To a solution of 4-hydroxybenzaldehyde (2 g, 16.36 mmol) in dry chloroform (20 mL) one portion of *N*-chlorosuccinimide (2.2 g, 16.36 mmol) was added. The reaction mixture was stirred under exclusion of light at 50 °C for 23 h. After cooling to a room temperature, the reaction mixture was concentrated and the residue dissolved in CH_2Cl_2 (20 mL). The organic layer was washed with water (30 mL) and dried over Na_2SO_4. The crude product was purified by recrystallization from ethanol.[3] The obtained values of melting point and ^{1}H- and ^{13}C-NMR spectra are in accordance with literature data.[4]

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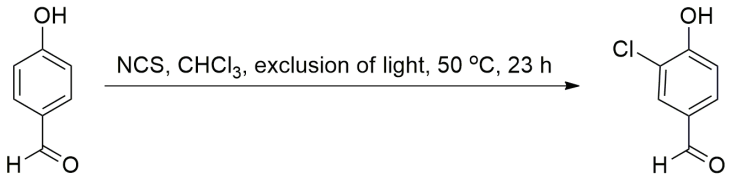
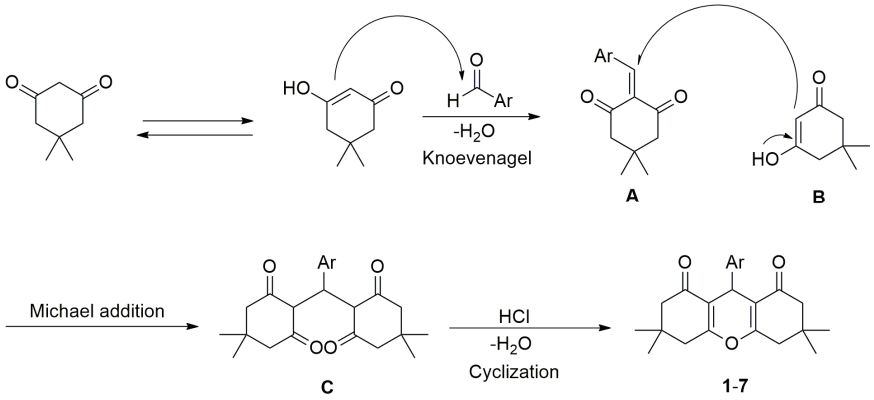
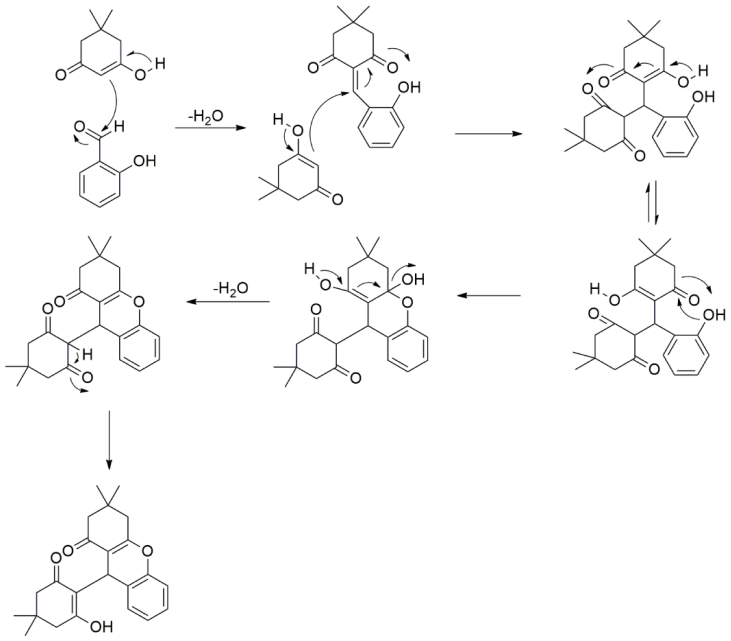


Scheme S-2. Synthesis of 3-chloro-4-hydroxybenzaldehyde.



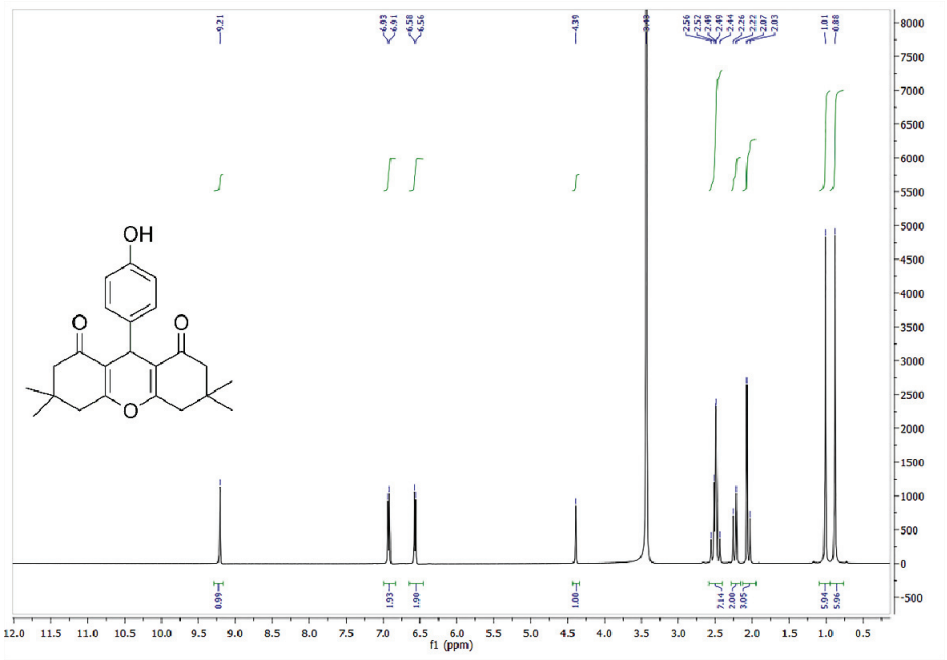
Scheme S3. Proposed mechanism of the synthesized compounds **1**–**7**.



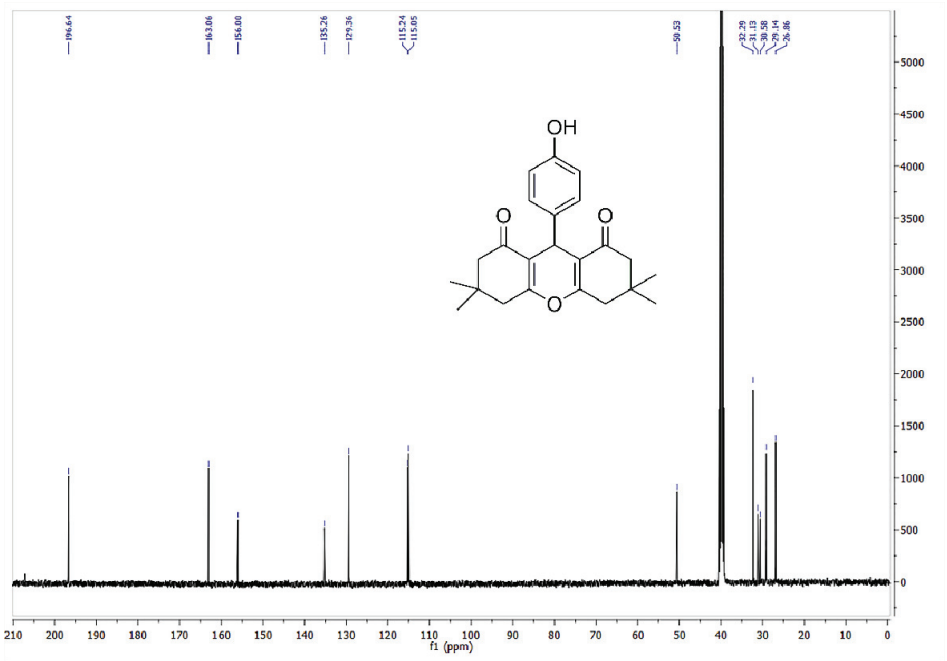
Scheme S-4. Proposed mechanism of the synthesized compound **8**.[5]

*Characterization of compounds **1**–**8***

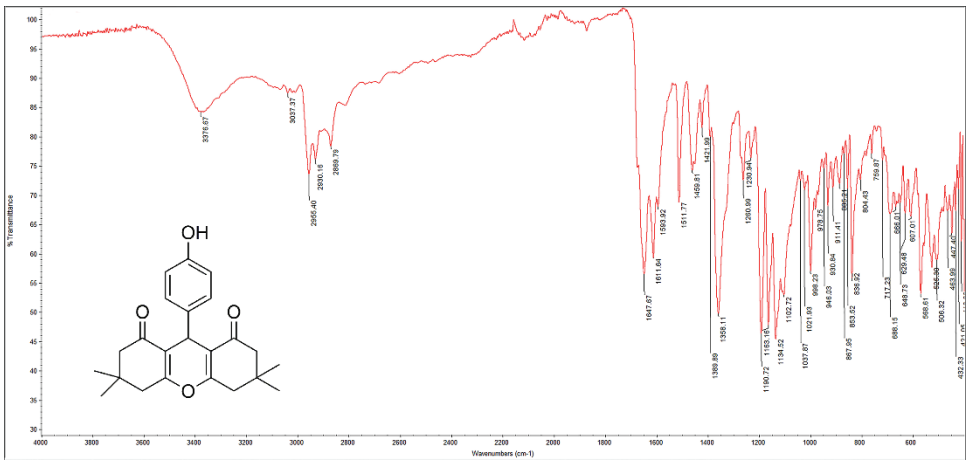
9-(4-Hydroxyphenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**1**). Yield 300 mg (75 %). White solid melts at 240-243 °C. IR (ATR): 3377, 3038, 2955, 2930, 2870, 1648, 1612, 1594, 1512, 1460, 1422, 1390, 1358, 1261, 1231, 1191, 1163, 1134, 1103, 1038, 1022, 979, 946, 931, 911, 868, 853, 834, 804, 760, 717, 688, 666, 649, 630, 607, 569, 525, 506, 464, 447, 432, cm^{-1}. ^1H NMR (400 MHz, DMSO-d_6, δ): 9.21 (*s*, 1H, −OH), 6.92 (*d*, 2H, J = 8.4 Hz, $-C_6H_4$), 6.57 (*d*, 2H, J = 8.4 Hz, $-C_6H_4$), 4.39 (*s*, 1H, −CH), 2.56−2.03 (*m*, 8H, 4x$-CH_2$), 1.01 (*s*, 6H, 2x$-CH_3$), 0.88 (*s*, 6H, 2x$-CH_3$). ^{13}C NMR (100 MHz, DMSO-d_6, δ): 196.6, 163.1, 156.0, 135.3, 129.4, 115.2, 115.0, 50.5, 32.3, 31.1, 30.6, 29.1, 26.9. Elemental analysis for $C_{23}H_{26}O_4$: Calculated C 75.38, H 7.15, Found C 75.43, H 6.97.



(a)



(b)

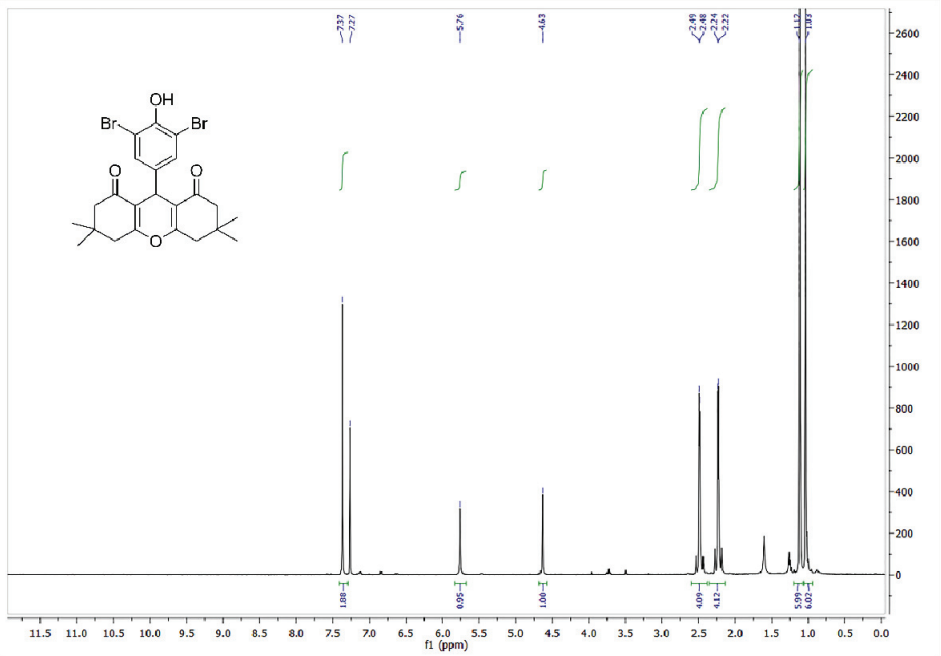


(c)

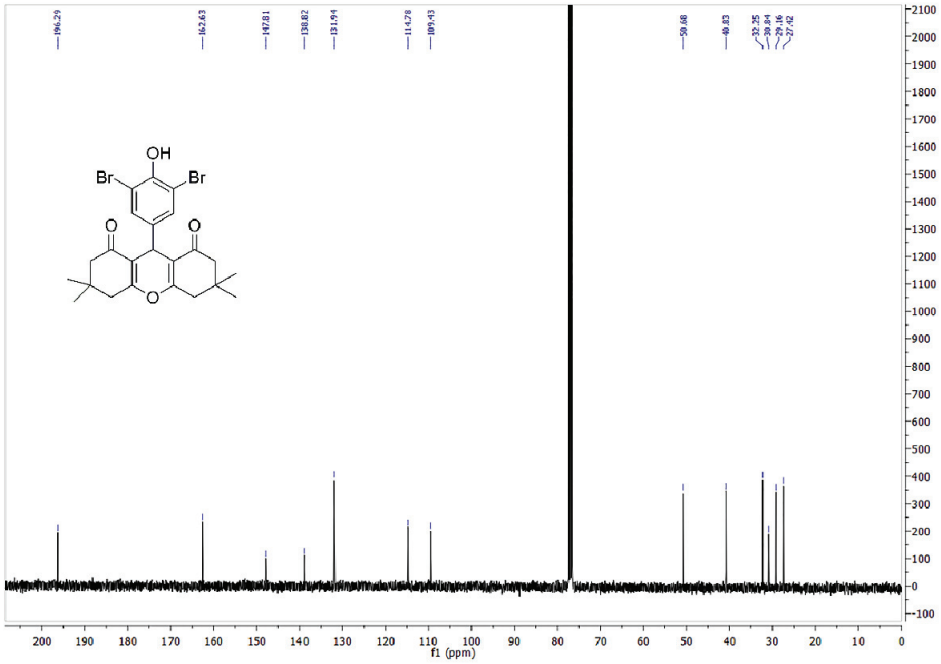
Fig. S-1. Spectra of **1**: a) ^{1}H NMR; b) ^{13}C NMR and c) FTIR.

9-(3,5-Dibromo-4-hydroxyphenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**2**). Yield 580 mg (85 %). White solid melts at 263-266 °C. IR (ATR): 3355, 2956, 2926, 2869, 1673, 1651, 1616, 1562, 1512, 1463, 1424, 1390, 1356, 1307, 1263, 1240, 1219, 1193, 1164, 1134, 1105, 1038, 999, 945, 932, 911, 870, 853, 836,

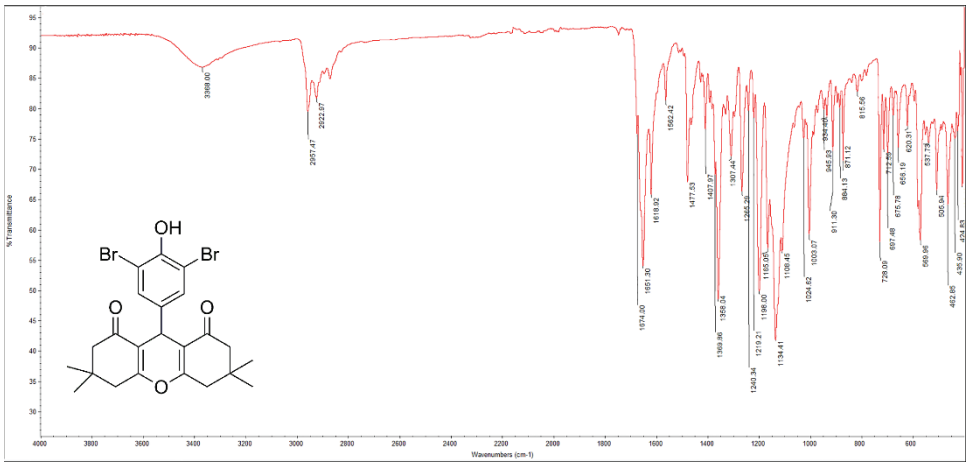
760, 727, 711, 695, 675, 656, 610, 568, 530, 505, 460, 448, 432, cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$, δ): 7.37 (*s*, 2H, −C_6H_2), 5.76 (*s*, 1H, −OH), 4.63 (*s*, 1H, −CH), 2.49 (*d*, 4H, J = 3.6 Hz, 2x −CH_2), 2.23 (*d*, 4H, J = 4.4 Hz, 2x −CH_2), 1.12 (*s*, 6H, 2x−CH_3), 1.03 (*s*, 6H, 2x−CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 196.3, 162.6, 147.8, 138.8, 131.9, 114.8, 109.4, 50.7, 40.8, 32.2, 30.8, 29.2, 27.4. Elemental analysis for $C_{23}H_{24}Br_2O_4$: Calculated C 52.69, H 4.61; Found C 52.59, H 4.71.



(a)



(b)

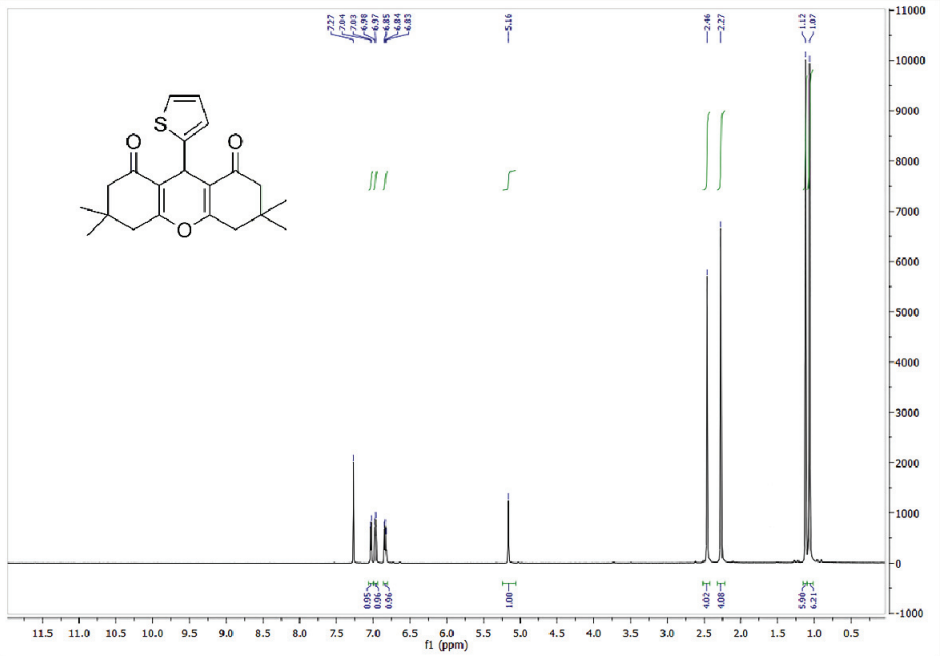


(c)

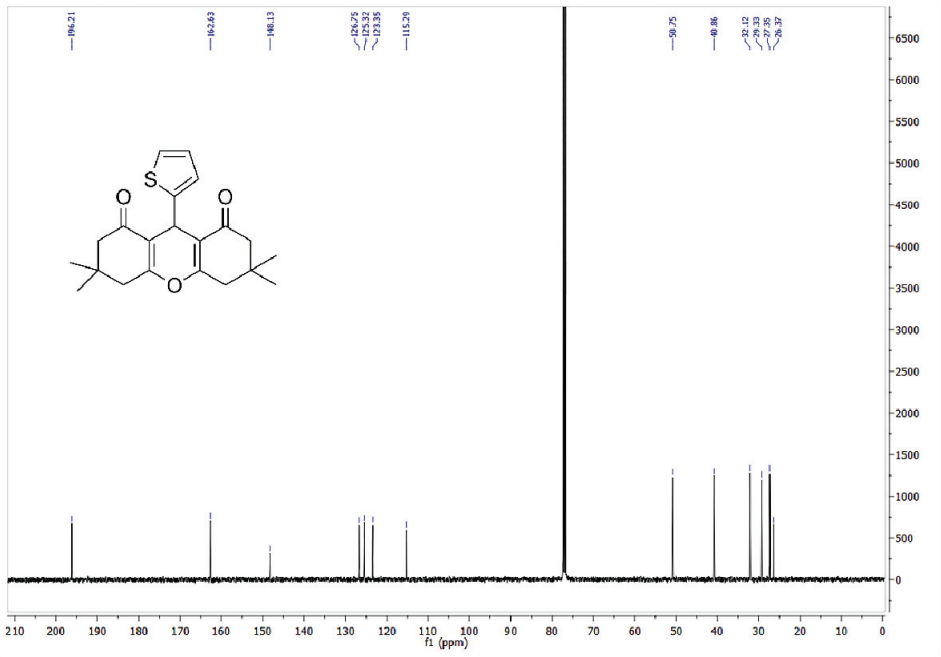
Fig. S-2. Spectra of **2**: a) ^{1}H NMR; b) ^{13}C NMR and c) FTIR.

3,3,6,6-Tetramethyl-9-(thiophen-2-yl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3**). Yield 260 mg (65 %). White solid melts at 155-158 °C. IR (ATR): 3305, 2958, 2931, 2870, 1675, 1660, 1621, 1514, 1464, 1435, 1423, 1389, 1354, 1326, 1282, 1192, 1135, 1104, 1074, 1037, 1022, 1038, 997, 967, 931, 914, 888, 867, 853, 836, 803, 772, 760, 731, 716, 694,

668, 629, 610, 598, 564, 510, 483, 445, 432, cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$, δ): 7.03 (*d*, 1H, *J* = 5.2 Hz, thiophen-2-yl), 6.97 (*d*, 1H, *J* = 2.8 Hz, thiophen-2-yl), 6.84 (*q*, 1H, *J* = 3.2 Hz, thiophen-2-yl), 5.16 (*s*, 1H, −CH), 2.46 (*s*, 4H, 2x $-CH_2$), 2.27 (*s*, 4H, 2x $-CH_2$), 1.12 (s, 6H, 2x $-CH_3$), 1.07 (*s*, 6H, 2x $-CH_3$). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 196.2, 162.6, 148.1, 126.7, 125.3, 123.3, 115.3, 50.7, 40.9, 32.1, 29.3, 27.3, 26.4. Elemental analysis for $C_{21}H_{24}O_3S$: Calculated C 70.75, H 6.79; Found C 70.73, H 6.81.



(a)



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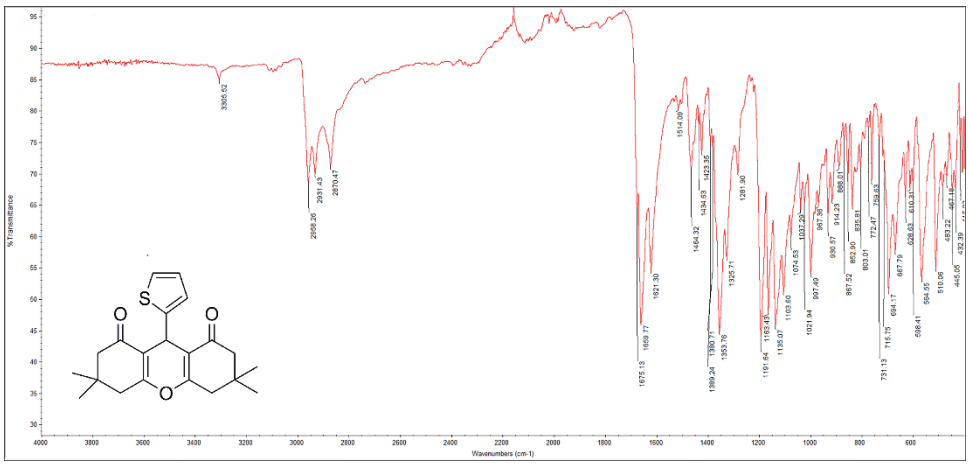
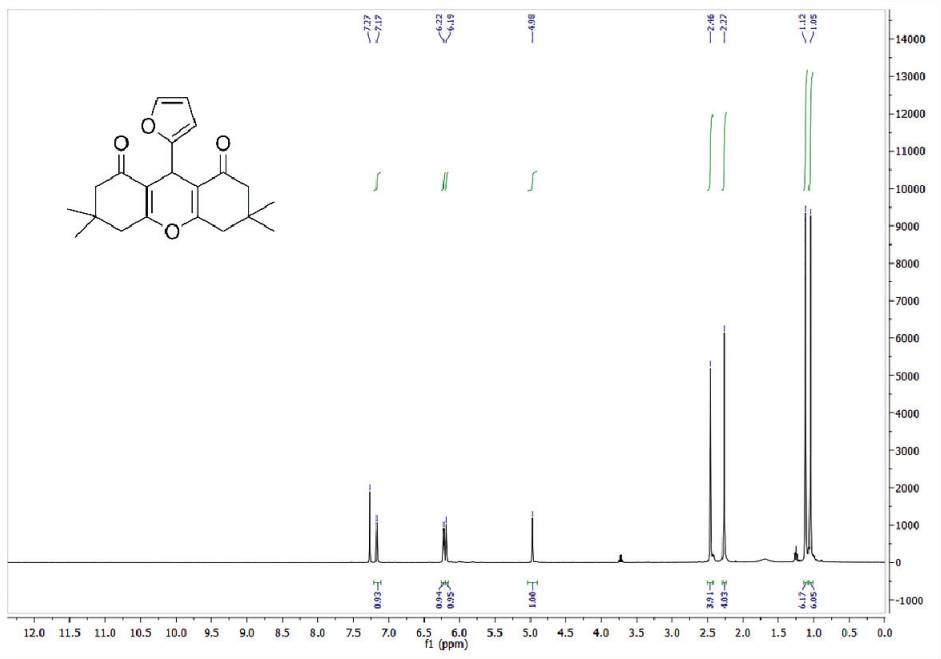


(c)

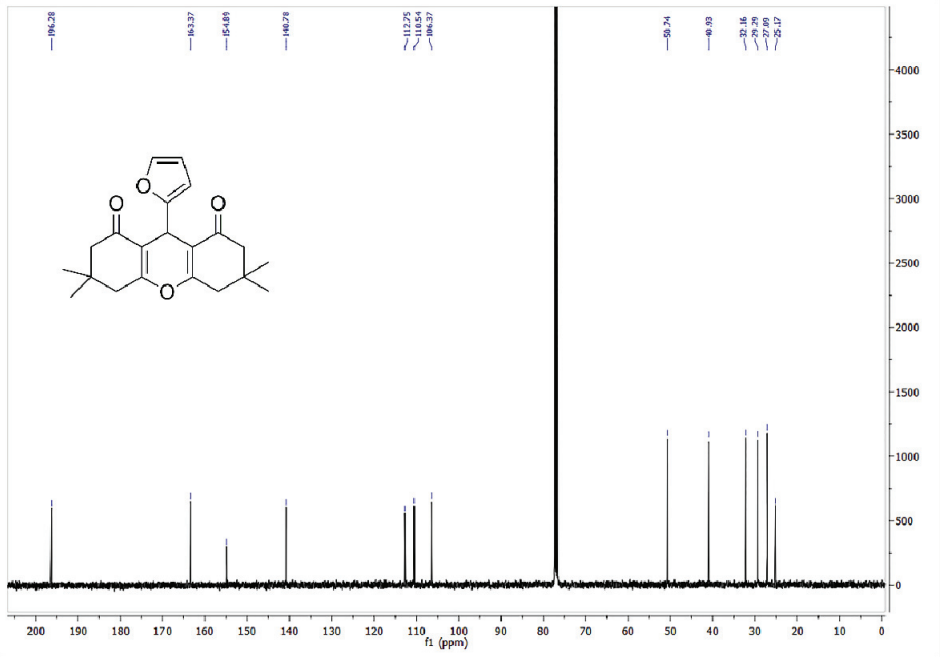
Fig. S-3. Spectra of **3**: a) ^{1}H NMR; b) ^{13}C NMR and c) FTIR.

9-(Furan-2-yl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**4**). Yield 230 mg (63 %). White solid melts at 140-143 °C. IR (ATR): 2962, 2938, 2870, 1677, 1656, 1623, 1514, 1501, 1465, 1423, 1390, 1357, 1289, 1231, 1191, 1163, 1148, 1106, 1073, 1015, 998, 981, 931, 917, 890, 884, 668, 657, 628, 598, 564, 510, 483, 445, 432, cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.17 (*s*, 1H, furan-2-yl), 6.22 (*s*, 1H, furan-2-yl), 6.19 (*s*, 1H, furan-2-yl), 4.98 (*s*, 1H, −CH), 2.46 (*s*, 4H, 2x $-CH_2$), 2.27 (*s*, 4H, 2x $-CH_2$), 1.12 (*s*, 6H, 2x $-CH_3$), 1.05 (*s*, 6H, 2x $-CH_3$). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 196.3, 163.4, 154.9, 140.8, 112.7, 110.5, 106.4, 50.8, 40.9, 32.2, 29.3, 27.1, 25.2. Elemental analysis for $C_{21}H_{24}O_4$: Calculated C 74.09, H 7.11; Found C 74.07, H 7.13.



(a)



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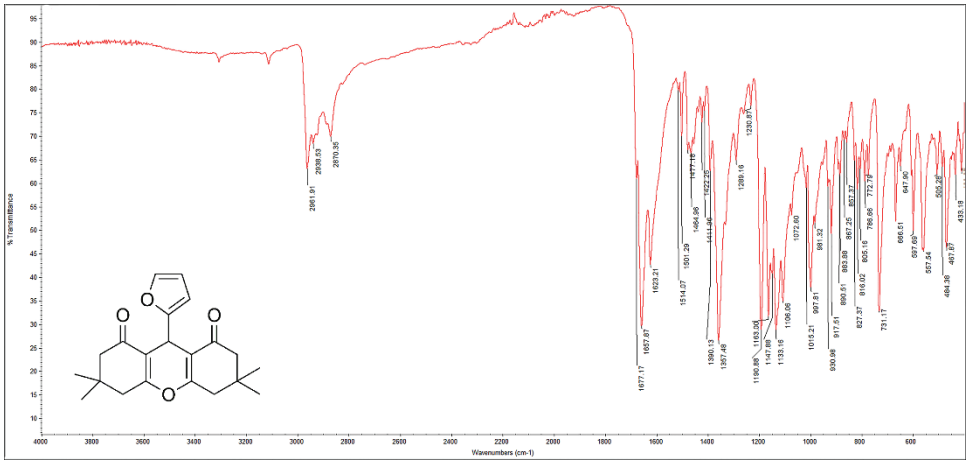
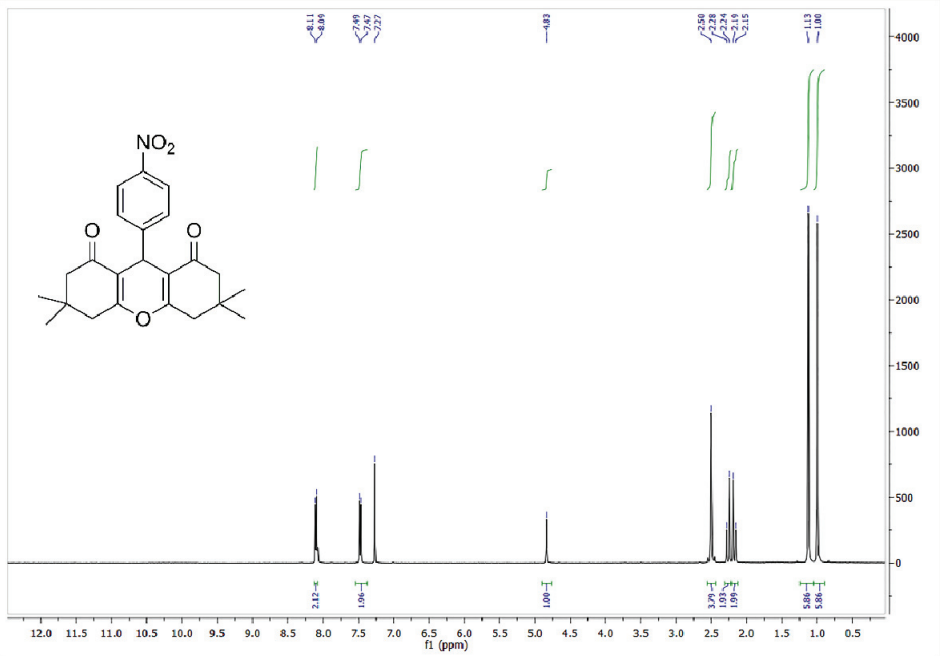


(c)

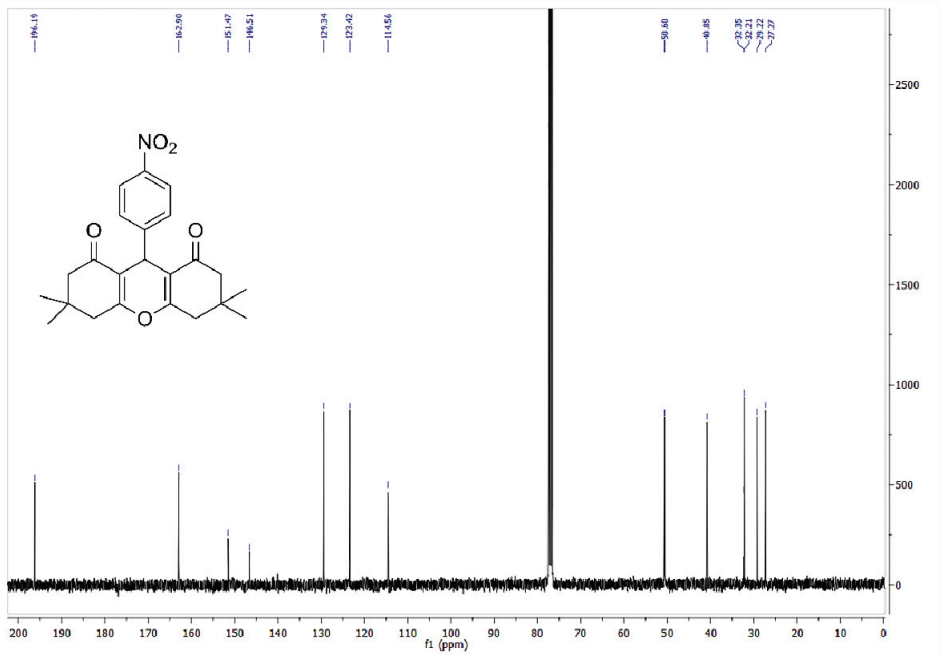
Fig. S-4. Spectra of **4**: a) ^{1}H NMR; b) ^{13}C NMR and c) FTIR.

3,3,6,6-Tetramethyl-9-(4-nitrophenyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**5**). Yield 340 mg (80 %). Yellow solid melts at 190-193 °C. IR (ATR): 2958, 2867, 1660, 1651, 1614, 1601, 1587, 1512, 1470, 1423, 1412, 1390, 1359, 1341, 1314, 1193, 1165, 1137, 1107, 1013, 1000, 982, 934, 913, 891, 831, 815, 740, 706, 695, 667, 633, 610, 596, 563,

520, 501, 490, 437, cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$, δ): 8.10 (*d*, 2H, J = 8.4 Hz, $-C_6H_4$), 7.48 (*d*, 2H, J = 8.8 Hz, $-C_6H_4$), 4.83 (*s*, 1H, −CH), 2.50 (*s*, 4H, 2x $-CH_2$), 2.22 (*q*, 4H, J = 16.4 Hz, 2x $-CH_2$), 1.13 (*s*, 6H, 2x $-CH_3$), 1.00 (*s*, 6H, 2x $-CH_3$). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 196.2, 162.8, 151.5, 146.5, 129.3, 123.4, 114.6, 50.6, 40.8, 32.3, 32.2, 29.2, 27.3. Elemental analysis for $C_{23}H_{25}NO_5$: Calculated C 69.86, H 6.37, N 3.54; Found C 69.84, H 6.39, N 3.48.



(a)



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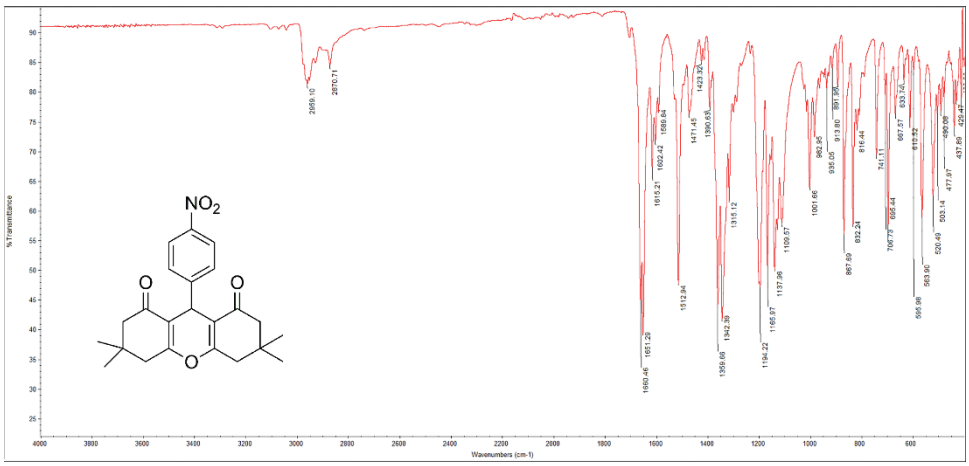
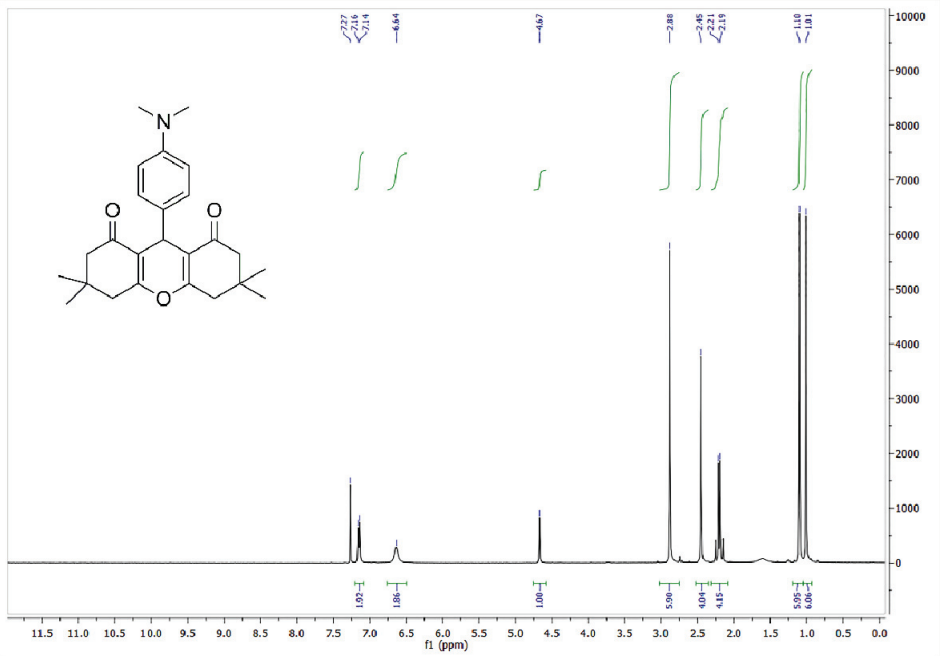


(c)

Fig. S-5. Spectra of **5**: a) ^{1}H NMR; b) ^{13}C NMR and c) FTIR.

9-(4-(Dimethylamino)phenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**6**). Yield 320 mg (75 %). Yellow solid melts at 205-208 °C. IR (ATR): 2953, 2937, 2870, 2840, 2784, 1674, 1657, 1620, 1605, 1567, 1514, 1464, 1441, 1357, 1338, 1296, 1283, 1232, 1189, 1159, 1135, 1106, 1058, 1021, 998, 971, 946, 932, 914, 892, 846, 831, 816,

807, 784, 738, 722, 674, 640, 631, 603, 583, 557, 537, 497, 476, 432, cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$, δ): 7.15 (*d*, 2H, J = 8.4 Hz, $-C_6H_4$), 6.64 (*s*, 2H, $-C_6H_4$), 4.67 (*s*, 1H, −CH), 2.88 (*s*, 6H, $-N(CH_3)_2$), 2.45 (*s*, 4H, 2x $-CH_2$), 2.20 (*d*, 4H, J = 8.8 Hz, 2x $-CH_2$), 1.10 (*s*, 6H, 2x $-CH_3$), 1.01 (*s*, 6H, 2x $-CH_3$). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 196.5, 161.8, 150.2, 136.6, 129.0, 116.0, 114.6, 50.8, 40.9, 32.2, 30.7, 29.2, 27.5. Elemental analysis for $C_{25}H_{31}NO_3$: Calculated C 76.30, H 7.94, N 3.56; Found C 76.28, H 7.96, N 3.56.



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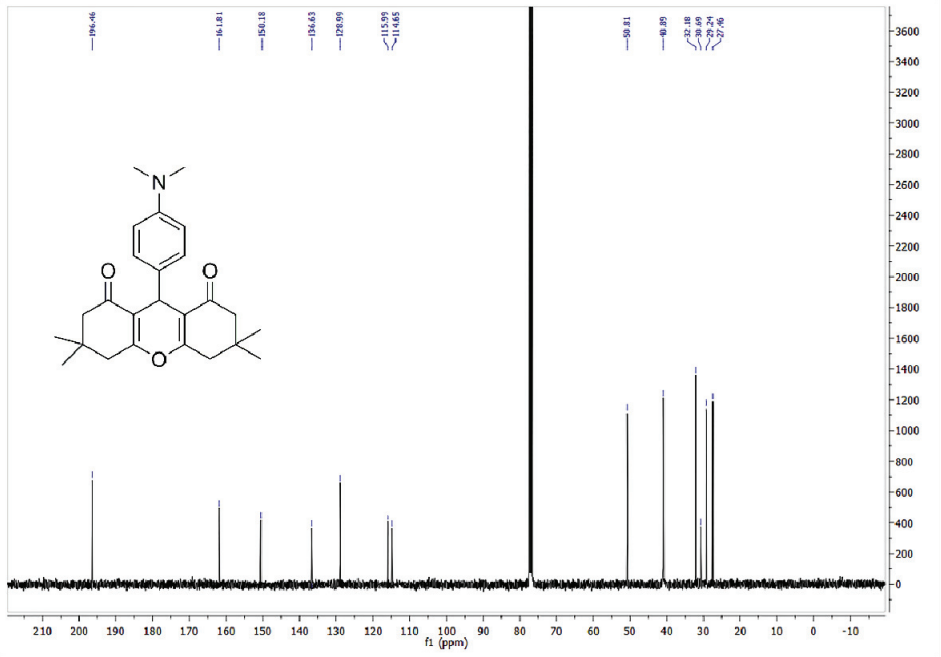
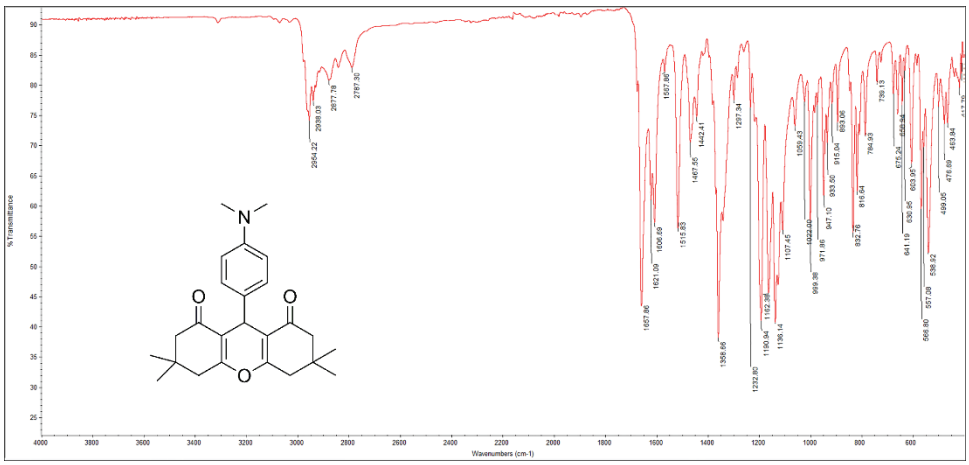


(b)

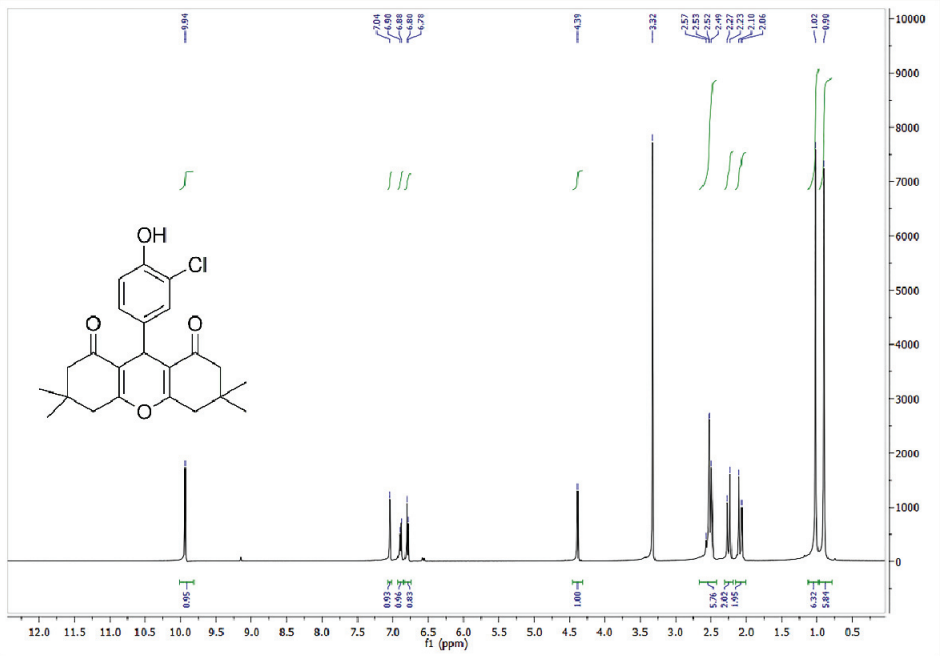


(c)

Fig. S-6. Spectra of **6**: a) ^{1}H NMR; b) ^{13}C NMR and c) FTIR.

9-(3-Chloro-4-hydroxyphenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**7**). Yield 370 mg (85 %). White solid melts at 264-266 °C. IR (ATR): 3614, 2984, 2974, 2848, 2789, 1678, 1652, 1624, 1615, 1569, 1511, 1462, 1440, 1356, 1334, 1292, 1281, 1235, 1187, 1154, 1134, 1102, 1053, 1020, 997, 975, 949, 934, 913, 898, 844, 830, 819,

806, 783, 734, 725, 679, 642, 630, 608, 585, 559, 538, 494, 473, 431, cm^{-1}. ^1H NMR (400 MHz, DMSO-d_6, δ): 9.94 (s, 1H,−OH), 7.04 (*s*, 1H,−C_6H_3), 6.89 (*d*, 1H, J = 8.4 Hz, −C_6H_3), 6.79 (*d*, 1H, J = 8.4 Hz, −C_6H_3), 4.39 (*s*, 1H, −CH), 2.57-2.49 (m, 4H, 2x −CH_2) 2.25 (*d*, 2H, J = 16.4 Hz, −CH_2), 2.08 (*d*, 2H, J = 16.4 Hz, −CH_2), 1.02 (*s*, 6H, 2x −CH_3), 0.90 (*s*, 6H, 2x −CH_3). ^{13}C NMR (100 MHz, DMSO-d_6, δ): 196.6, 163.3, 151.8, 136.6, 129.7, 127.8, 119.3, 116.6, 114.6, 50.5, 32.3, 30.7, 29.1, 26.9. Elemental analysis for $C_{23}H_{25}ClO_4$: Calculated C 68.91, H 6.29; Found C 68.88, H 6.32.



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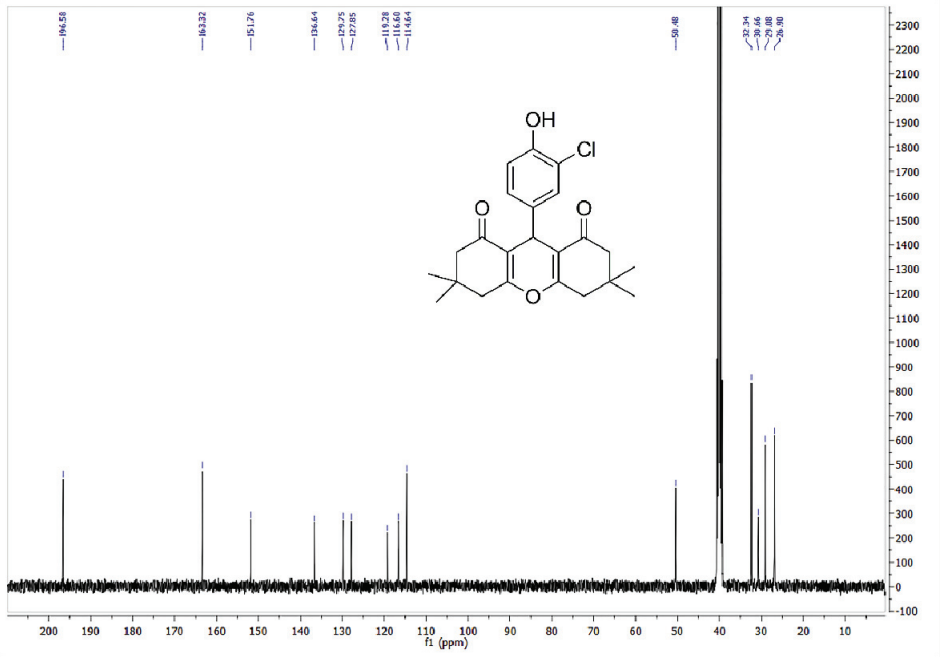

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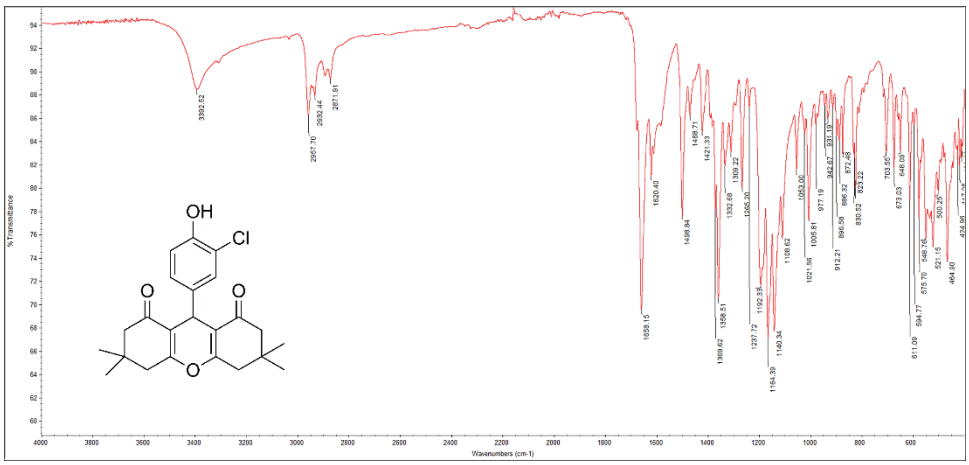
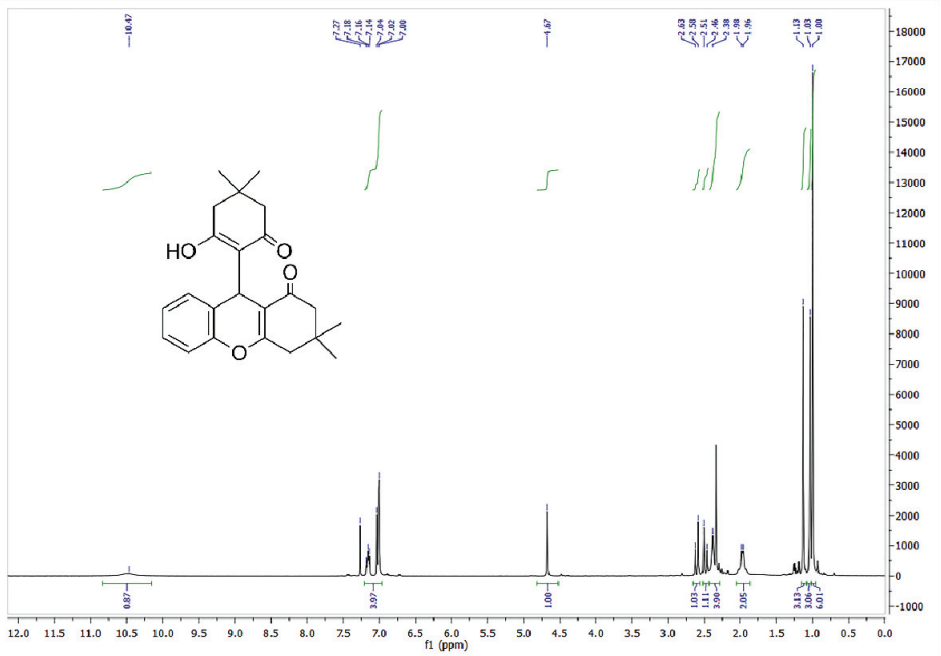


(c)

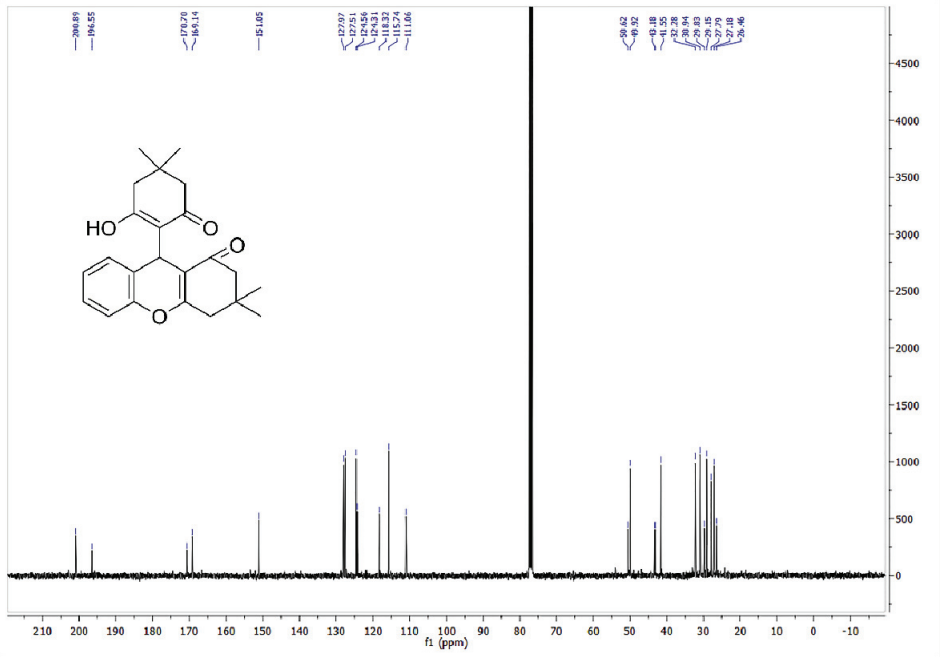
Fig. S-7. Spectra of **7**: a) ^{1}H NMR; b) ^{13}C NMR and c) FTIR.

9-(2-Hydroxy-4,4-dimethyl-6-oxocyclohex-1-enyl)-3,3-dimethyl-2,3,4,9-tetrahydro-1H-xanthen-1-one (**8**). Yield 340 mg (80 %). White solid melts at 190-193 °C. IR (ATR): 3182, 2958, 2928, 2867, 1651, 1587, 1423, 1412, 1376, 1235, 1193, 1165, 1137, 1107, 1013, 1000, 982, 934, 913, 891, 831, 815, 740, 706, 695, 667, 633, 610, 596, 563, 520, 501, 490, 437, cm^{-}

[1]. ^{1}H NMR (400 MHz, $CDCl_3$, δ): 10.47 (*bs*, 1H, −OH), 7.18–7.00 (*m*, 4H), 4.67 (*s*, 1H, −CH), 2.63–2.38 (*m*, 6H, 3x $-CH_2$), 1.97 (*d*, 2H, J = 4.8 Hz,$-CH_2$), 1.13 (*s*, 3H,$-CH_3$), 1.03 (*s*, 3H,$-CH_3$), 1.00 (*s*, 6H, 2x $-CH_3$). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 200.9, 196.5, 170.7, 169.1, 151.0, 128.0, 127.5, 124.6, 124.3, 118.3, 115.7, 111.1, 50.6, 49.9, 43.2, 41.5, 32.3, 30.9, 29.8, 29.1, 27.8, 27.2, 26.5. Elemental analysis for $C_{23}H_{25}NO_5$: Calculated C 69.86, H 6.37; Found C 69.84, H 6.32. Obtained data are in accordance with literature.[5]



(a)



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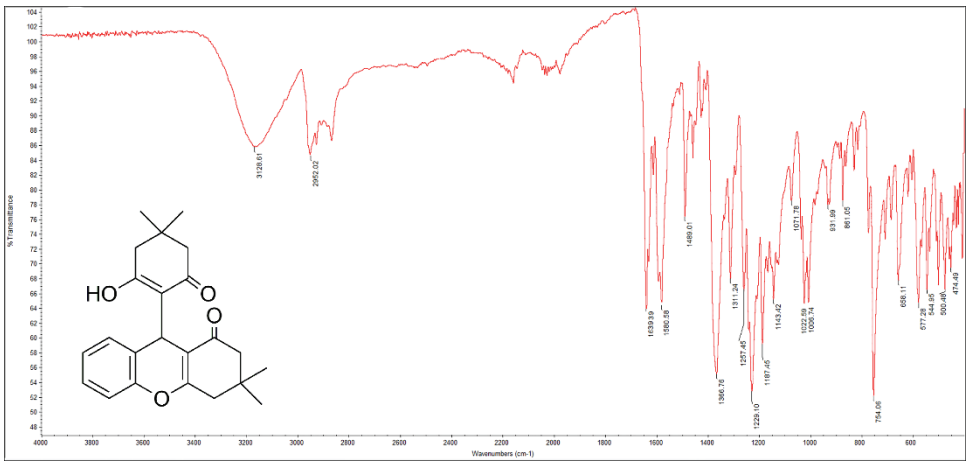

(c)

Fig. S-8. Spectra of **8**: a) ^{1}H NMR; b) ^{13}C NMR and c) FTIR.

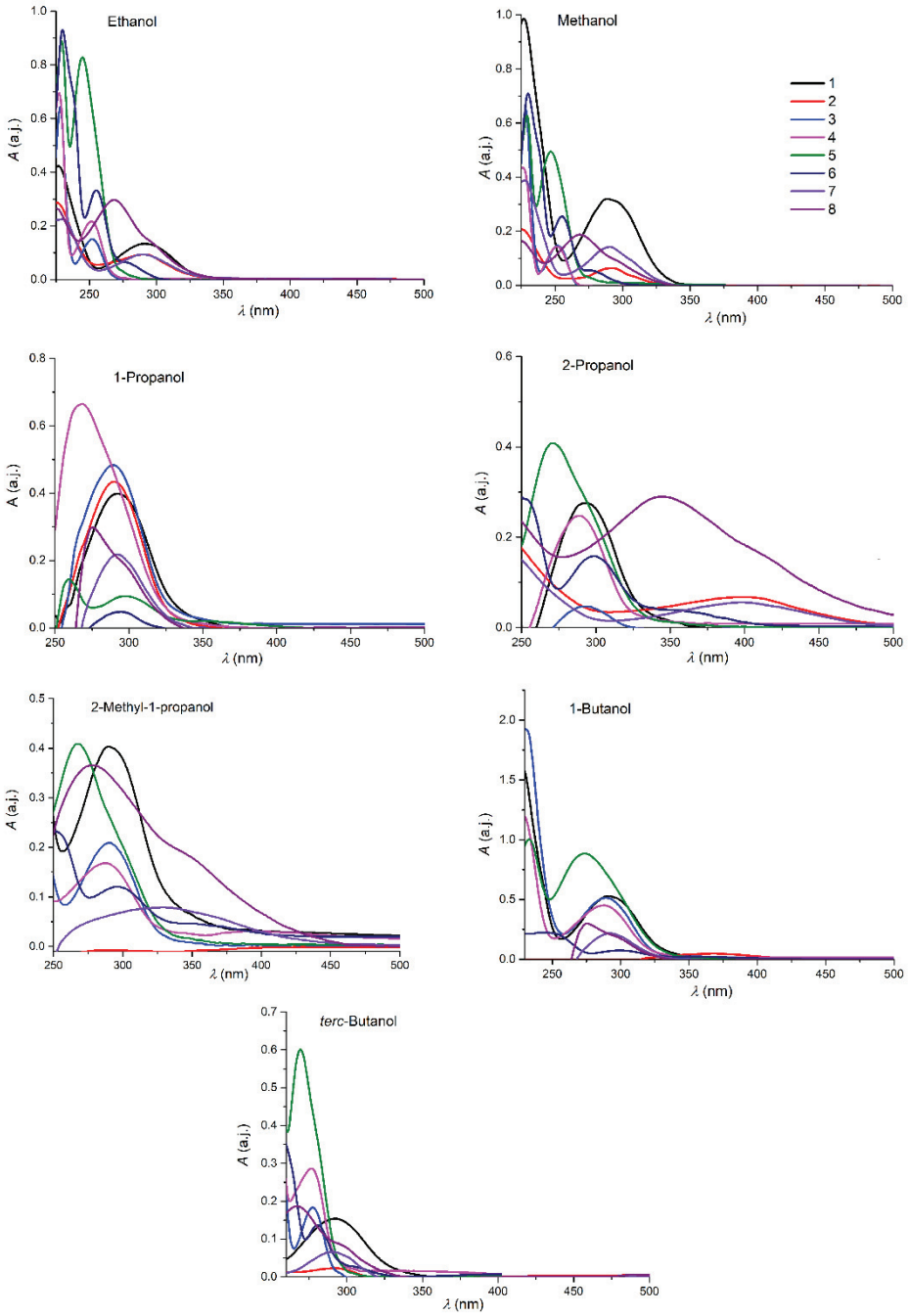

Fig. S-9. The UV-Vis spectra of investigated compounds **1**–**8** in alcohols.

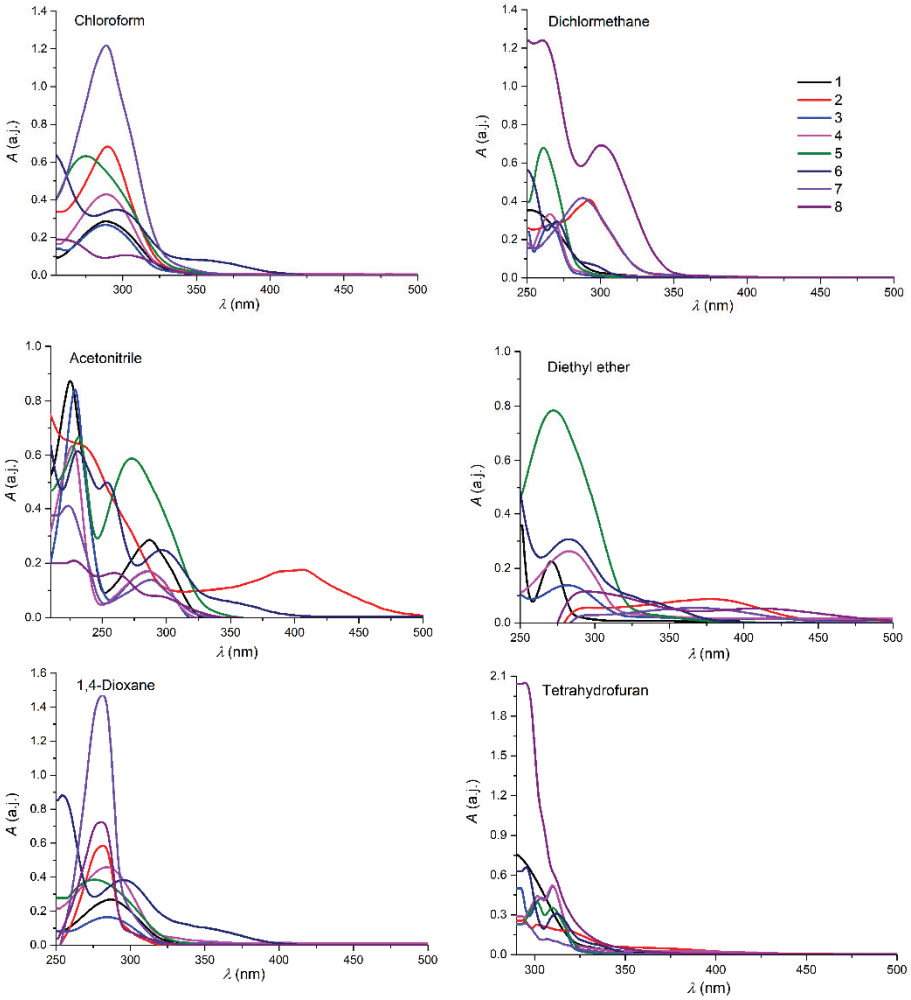

Fig. S-10. The UV-Vis spectra of investigated compounds **1**–**8** in selected solvents.

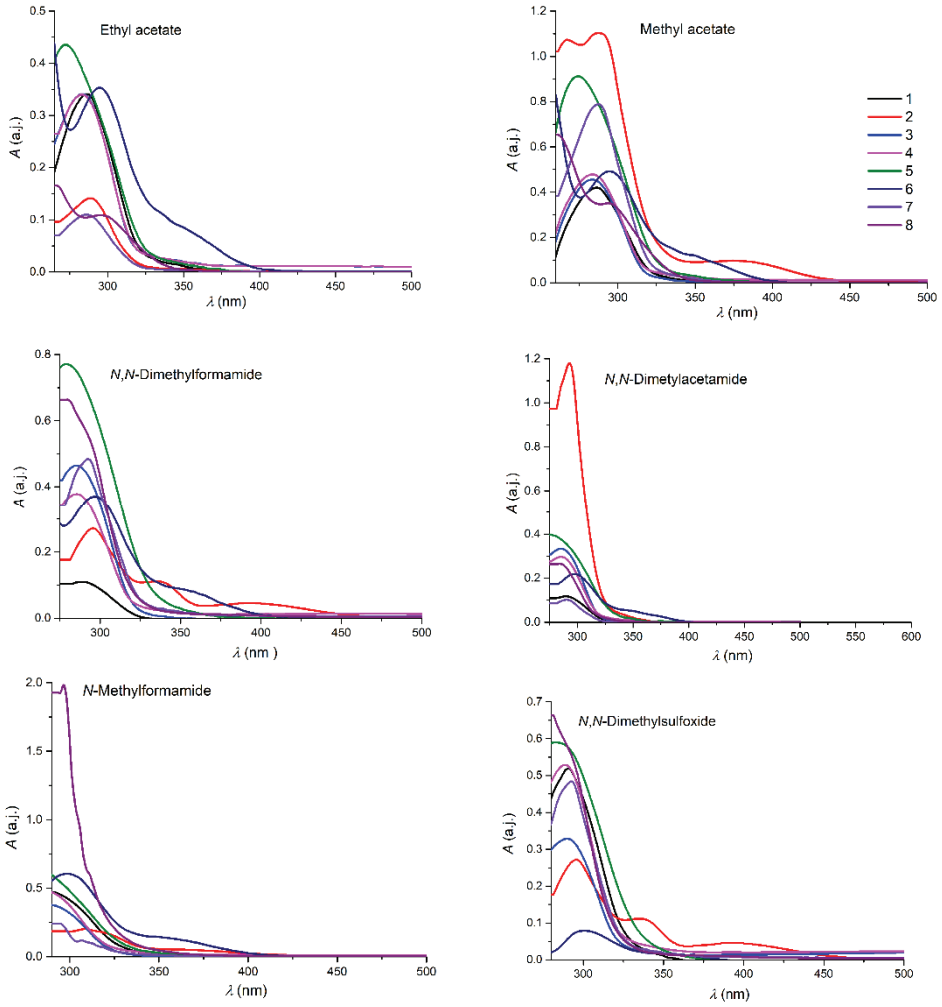

Fig. S-11. The UV-Vis spectra of investigated compounds **1**–**8** in selected solvents.

Table S-I. Physicochemical properties of the investigated compounds

No.	Molecular weight, g mol^{-1}	Number of atoms	Number of rotatable bonds	Number of hydrogen bond donors	Number of hydrogen bond acceptors	Molar refractivity	Topological polar surface area, Å^2
1	366.45	27	1	1	4	104.02	63.60
2	524.24	29	1	1	4	119.42	63.60
3	356.48	25	1	0	3	99.87	71.61
4	340.41	25	1	0	4	94.26	56.51
5	395.45	29	2	0	5	110.82	89.19
6	393.52	29	2	0	3	116.20	46.61
7	400.90	28	1	1	4	109.03	63.60
8	366.45	27	1	1	4	104.02	63.60

Table S-II. Partition coefficients of the investigated compounds

No.	$\log P_{o/w}$ (XLOGP3)	$\log P_{o/w}$ (WLOGP)	$\log P_{o/w}$ (MLOGP)
1	3.61	4.79	2.58
2	5.00	6.32	3.74
3	3.69	5.15	2.77
4	3.07	4.68	1.92
5	3.80	5.52	2.07
6	4.09	5.15	3.00
7	4.24	5.45	3.06
8	3.61	4.79	2.58

Table S-III. QSAR pharmacokinetic profiles of the investigated compounds related to absorption properties

	SwissADME	PreADMET	SwissADME	PreADMET	SwissADME	PreADMET
No	Gastrointestinal absorption	Gastrointestinal absorption, %	The compound penetrates the blood-brain barrier	The compound penetrating the blood-brain barrier (c_{brain}/c_{blood})	The compound is a P-gp inhibitor	The compound is a P-gp inhibitor
1	High	95.93	Yes	0.16	Yes	Yes
2	High	97.11	No	1.04	Yes	Yes
3	High	98.60	No	2.25	Yes	Yes
4	High	98.19	Yes	2.02	Yes	Yes
5	High	98.54	No	0.01	No	No
6	High	95.93	Yes	0.77	Yes	Yes
7	High	97.45	Yes	0.05	Yes	No
8	High	96.16	No	0.38	Yes	Yes

Table S-IV. Absorption maxima in nm of the investigated compounds **1**–**8** in selected solvent set

No.	Solvent	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**
1.	Acetonitrile	225, 287	291	229, 287	228, 285	232; 273	231, 254, 297	224, 290	230, 262, 295
2.	1-Butanol	228, 293	289	231, 289	228, 288	234, 274	237, 300	294	275
3.	Chloroform	289	293	287	289	275	297	289	262, 303
4.	Dichlormethane	287	293	286	288	275	256, 299	290	260, 301
5.	Diethyl ether	224, 287	253	227, 283	225, 284	229; 272	228, 252 294	252	251
6.	N,N-Dimethylacetamide	289	293	286	285	277	297	291	294
7.	N,N-Dimethylformamide	289	337	285	286	278	297	292	295
8.	N,N-Dimethylsulfoxide	291	296, 337, 394	289	288	284	301	292	275
9.	1,4-Dioxane	287	281	285	284	276	254, 297	282	279
10.	Ethanol	226, 292	225, 290	230, 290	228, 289	233, 271	234	227, 292	224, 269
11.	Ethyl acetate	285	292	283	283	272	257, 295	288	258, 296
12.	Methanol	227, 288	225, 292	229, 288	229, 288	233, 278	235, 299	227, 290	225, 269
13.	Methyl acetate	287	266, 292	284	285	275	257, 296	287	261, 294
14.	2-Methyl-1-propanol	232, 290	270	234, 290	235, 288	239, 268	247, 298	290	269
15.	N-Methylformamide	289	307	288	287	278	298	303	303
16.	1-Propanol	236, 293	293	239, 290	235, 289	240, 275	261, 298	292	277
17.	2-Propanol	228, 293	225, 292	231, 293	229, 290	233, 272	233, 298	227, 293	224, 270
18.	tert-Butanol	232, 293	292, 353	232, 289	232, 289	234, 268	234, 297	292, 253	268, 358
19.	Tetrahydrofuran	289	296	289	273, 290	269, 291	253, 296	294	292

Table S-V. Solvent parameters

		Kamlet-Taft			Catalán			
No.	Solvent	π*	β	α	SA	SB	SP	SdP
1.	Acetonitrile	0.75	0.31	0.19	0.044	0.286	0.645	0.974
2.	1-Butanol	0.47	0.88	0.79	0.341	0.809	0.674	0.655
3.	Chloroform	0.58	0.00	0.44	0.047	0.071	0.783	0.614
4.	Dichlormethane	0.82	0.00	0.30	0.040	0.178	0.761	0.769
5.	Diethyl ether	0.27	0.47	0.00	0.000	0.562	0.617	0.385
6.	N,N-Dimethylacetamide	0.88	0.76	0.00	0.028	0.650	0.763	0.987
7.	N,N-Dimethylformamide	0.88	0.69	0.00	0.031	0.613	0.759	0.977
8.	N,N-Dimethylsulfoxide	1.00	0.76	0.00	0.072	0.647	0.830	1.000
9.	1,4-Dioxane	0.55	0.37	0.00	0.000	0.444	0.737	0.312
10.	Ethanol	0.54	0,77	0.83	0.400	0.658	0.633	0.783
11.	Ethyl acetate	0.55	0.45	0.00	0.000	0.542	0.656	0.603
12.	Methanol	0.60	0.62	0.93	0.605	0.545	0.608	0.904
13.	Methyl acetate	0.60	0.37	0.00	/	/	/	/
14.	2-Metyl-1-propanol	0.41	0.93	0.41	0.000	0.590	0.710	0.630
15.	N-Methylformamide	0.90	0.80	0.62	/	/	/	/
16.	1-Propanol	0.52	0.90	0.78	0.367	0.782	0.658	0.748
17.	2-Propanol	0.48	0.95	0.76	0.283	0.830	0.633	0.808
18.	tert-Butanol	0.41	1.01	0.68	0.145	0.928	0.632	0.732
19.	Tetrahydrofuran	0.58	0.55	0.00	0.000	0.591	0.714	0.634

Table S-VI. Regression fits to solvatochromic parameters (Eq. (2)) and percentage contribution of solvatochromic parameters

No.	ν_0 / 10^3 cm^{-1}	s / 10^3 cm^{-1}	b / 10^3 cm^{-1}	a / 10^3 cm^{-1}	R^a	s^b	F^c	P_π / %	P_β / %	P_α / %
1	35.14 (±0.06)	–0.12 (±0.04)	–0.59 (±0.05)	–0.52 (±0.04)	0.995	0.004	253	9.76	47.97	42.27
2	45.51 (±0.66)	–13.52 (±0.80)	–5.69 (±0.54)	0.53 (±0.18)	0.985	0.405	99	68.49	28.82	2.68
3	35.49 (±0.10)	–0.41 (±0.14)	–0.14 (±0.04)	–0.82 (±0.07)	0.975	0.081	52	29.93	10.22	59.85
4	35.31 (±0.14)	–0.39 (±0.18)	0.14 (±0.04)	–0.89 (±0.10)	0.951	0.110	25	27.46	9.86	62.68
5	37.77 (±0.30)	–2.59 (±0.39)	0.48 (±0.04)	0.09 (±0.04)	0.944	0.234	22	81.96	15.19	2.85
6	34.16 (±0.06)	–0.62 (±0.08)	0.05 (±0.01)	–0.43 (±0.04)	0.970	0.045	48	55.86	4.50	38.74
7	36.91 (±0.28)	–2.48 (±0.31)	–0.49 (±0.16)	–1.74 (±0.22)	0.963	0.175	34	52.65	10.40	36.94
8.	34.42 (±0.90)	–2.27 (±1.05)	2.12 (±0.57)	2.54 (±0.44)	0.971	0.456	45	32.76	30.59	36.65

[a]Correlation coefficient; [b]Standard error of the estimate; [c]Fisher's test.

Table S-VII. Regression fits to solvatochromic parameters (Eq. (3)) and percentage contribution of solvatochromic parameters

No.	v_0 / 10^3 cm^{-1}	a /10^3 cm^{-1}	b /10^3 cm^{-1}	c /10^3 cm^{-1}	d /10^3 cm^{-1}	R^a	s^b	F^c	P_{SA} / %	P_{SB} / %	P_{SP} / %	P_{SdP} / %
1	35.76 (±0.25)	–0.13 (±0.01)	–0.81 (±0.38)	–1.23 (±0.18)	–0.71 (±0.13)	0.984	0.07	55	4.51	28.12	42.71	24.65
2	57.65 (±2.76)	–0.90 (±0.15)	–2.70 (±1.01)	–22.61 (±3.98)	–8.33 (±1.34)	0.973	0.717	32	2.61	7.82	65.46	24.12
3	36.23 (±0.43)	–0.28 (±0.01)	–1.47 (±0.62)	–2.00 (±0.29)	0.25 (±0.03)	0.949	0.119	15	7.00	36.75	50.0	6.25
4	36.64 (±0.61)	–0.03 (±0.01)	–1.11 (±0.08)	–0.97 (±0.28)	–1.25 (±0.31)	0.936	0.128	12	0.89	33.04	28.87	37.20
5	42.13 (±0.78)	0.27 (±0.03)	–7.53 (±1.13)	0.19 (±0.06)	–1.14 (±0.30)	0.961	0.160	21	2.96	82.47	2.08	12.49
6	36.39 (±0.28)	0.30 (±0.11)	–3.55 (±0.40)	–1.31 (±0.13)	–0.52 (±0.13)	0.978	0.058	38	5.28	62.5	23.06	9.15
7	54.51 (±2.42)	–5.57 (±0.98)	–3.56 (±0.83)	–25.60 (±3.51)	–3.12 (±0.80)	0.983	0.421	50	14.71	9.40	67.64	8.24
8	61.63 (±2.68)	–1.24 (±0.32)	–4.11 (±0.72)	–26.78 (±3.46)	–8.70 (±1.09)	0.972	0.458	30	3.04	10.07	65.59	21.31

[a]Correlation coefficient; [b]Standard error of the estimate; [c]Fisher's test.

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