SUPPORTING INFORMATION FOR

Synthesis, Structural Characterization, Solution Behavior and *in vitro* Antiproliferative Properties of a Series of Gold Complexes with 2-(2'-Pyridyl) benzimidazole as Ligand. Comparisons of Gold(III) *vs.* Gold(I) and Mono- *vs.* Binuclear Derivatives.

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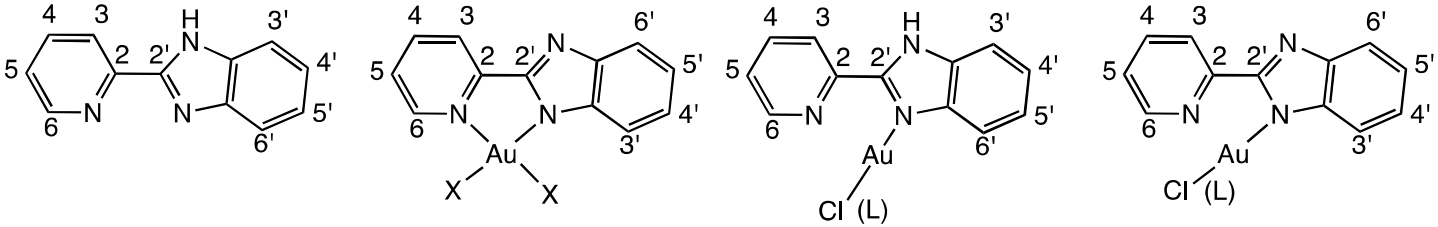
Table S1 ^{1}H and $^{31}P\{^{1}H\}$ NMR chemical shifts for pbiH and its gold complexes in various solvents

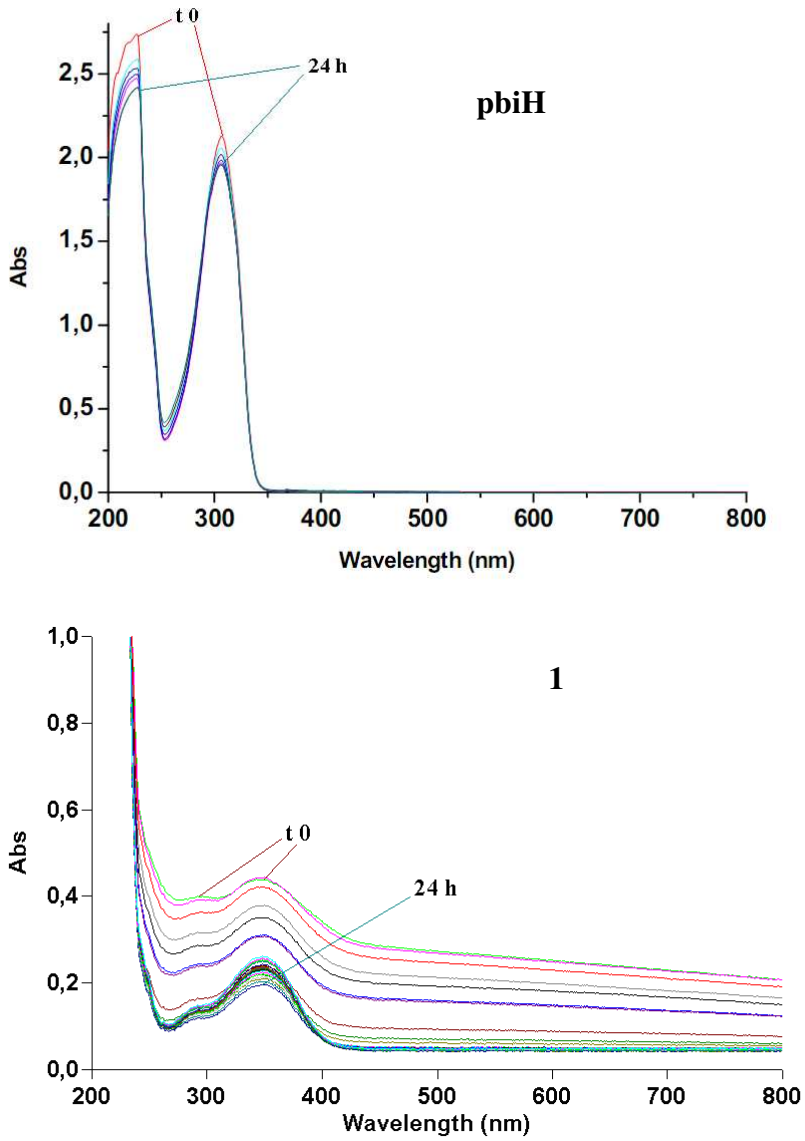


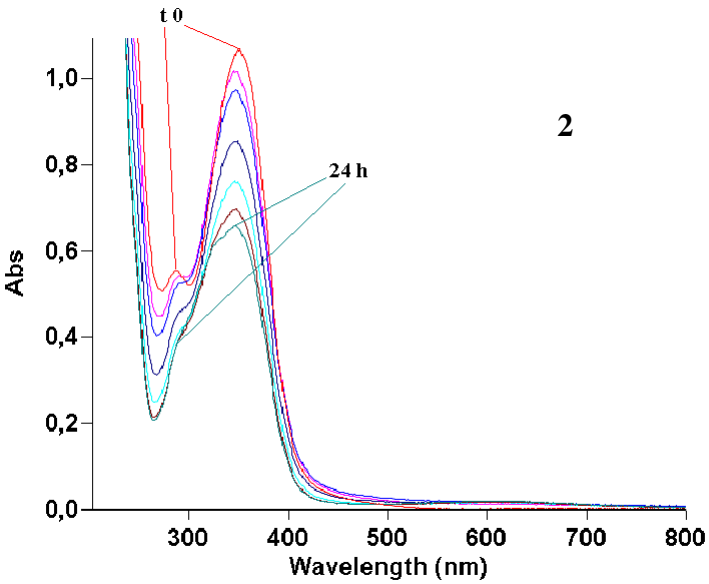
Compound	Solvent	$H^{4'}$,$H^{5'}$	H^{5}	$H^{3'}$	$H^{6'}$	H^{4}	H^{3}	H^{6}	NH	other	δP
pbiH	$CDCl_3$	7.30(m)	7.38(ddd)	7.49(m)	7.86(m)	7.88(td)	8.44(dt)	8.64(dd)	10.77(s,b)		
	CD_3COCD_3	7.26(m,b)	7.47(ddd)	7.63(m,b)	7.72(m,b)	7.98(td)	8,40(d)	8.67(d)	11.9(s,b)		
	DMSO-d_6	7.21(m)	7.51(m)	7.52(m)	7.69(m)	7.99(td)	8.31(d)	8.72(d)	13.10(s,b)		
1	DMSO-d_6	7.27(m)	7.86(td)	8.38(m)	7.75(m)	8.46(t)	8.35(d)	9.24(d)			
2	$CDCl_3$	7.30(m)	7.57(m)	7.76(m)	7.57(m)	8.24(td)	8.36(d)	8.41(d)		2.29(s), 2.36(s) Me	
	CD_3COCD_3	7.28(m)	7.86(td)	7.70(dd)	7.56(dd)	8.54(td)	8.39(dd)	8.67(d)		2.14(s), 2.23(s) Me	
	CD_2Cl_2	7.33(m)	7.62(td)	7.77(m)	7.57(m)	8.28(td)	8.38(d)	8.45(d)		2.28(s), 2.33(s) Me	
3	$CDCl_3$	7.48(m)	7.56(dd)	7.61(m)	8.08(m)	8.00(td)	9.72(d)	8.73(d)	11.12(s,b)		
4-PF_6	$CDCl_3$	7.44(m,b)	7.50(m,b)	7.94(m,b)	7.86(m,b)	7.98(t,b)	8.53(d,b)	8.27(d,b)	13.11(s,b)	7.58-7.70(m) PPh_3	31.4; -143.9
5	$CDCl_3$	7.19(m)	7.21(t)	7.84(m)	7.84(m)	7.77(td)	8.57(d)	8.20(dd)		7.49-7.59(m), 7.67-7.74(m) PPh_3	33.8
6	CD_3COCD_3	7.03((m)	7.40(ddd)	7.59(m)	7.59(m)	7.88(td)	8.43(dt)	8.61(ddd)		4.58(s) N-CH_2-N, 4.67(q,AB) N-CH_2-P	-65.1
	CD_3CN	7.12(m)	7.43(ddd)	7.66(m	7,66(m)	7.88(td)	8.39(d)	8.65(d)		4.44(s) N-CH_2-N, 4.57(q,AB) N-CH_2-P	
7	DMSO-d_6	7.53(m)	7.74(ddd)	7.81(m)	7.81(m)	8.20(td)	8.40(d)	8.90(d,b)			
8-PF_6	DMSO-d_6	7.29(m)	7.88(t)	8.41(m)	7.78(m)	8.47(t)	8.41(m)	9.25(d)		7.54(t,b) H^{p}; 7.59-7.64(m) H^{o}+H^{m} PPh_3	32.8; -143.5
	$CDCl_3$	7.32(m)	7.64(t)	8.53(m)	7.80(m)	8.25(t)	8.42(d)	9.40(d)		7.47-7.56(m) PPh_3	
	CD_3CN	7.31(m)	7.81(t)	8.62(m,br)	7.86(m)	8.32(t)	8.46(d)	9.29(d)		7.54-7.76(m) PPh_3	
9-PF_6	$CDCl_3$	7.39(m)	7.85(t)	7.81(m)	7.81(m)	8.47(t)	8.73(d)	8.49(d)		2.29(s), 2.34(s) Me , 7.59-7.66(m) PPh_3	
	CD_2Cl_2	7.48(m)	7.86(t)	7.91(m)	7.91(m)	8.33(t)	8.77(d)	8.59(d)		2.29(s), 2.34(s) Me, 7.59-7.66(m) PPh_3	30.8
10-PF_6	CD_2Cl_2	7.43(m)	7.51(ddd)	8.01(m)	8.01(m)	7.78(td)	8.93(d)	8.41(d,b)		7.57-7.70(m) PPh_3	32.6; -143.4
	$CDCl_3$	7.34(m)	obscured by PPh_3	7.90(m)	7.90(m)	7.83(t)	8.78(d)	8.29(d)		7.58(b) PPh_3	

Table S2. Absorption characteristics in various solvents of pbiH and of the gold complexes **1**–**10**-PF_6.

Compound	λ_{max}, nm (ε, $L \cdot mol^{-1} \cdot cm^{-1}$)				
	CH_2Cl_2	CH_3COCH_3	CH_3CN	DMSO	BP 10 mM pH 7.4
pbiH	310	326	308 (74405)	313	227, 307
1	–	361	292 (7087), 358 (7087)	313, 325, 354 (s)	290, 343
2	–	–	290 (12411), 350 (17603)	–	287, 352
3	–	–	307 (24604), 240 (sh 295, 319)	–	307
4-PF_6	268, 276, 312	–	268 (9566), 275 (10340), 308 (19147)	268, 276, 313, 324	312
5	268, 275, 325	–	236 (26941), 268 (17682), 275 (18372), 296 (19640), 306 (19993)	268, 275, 325	340, 353
6	–	328	308 (14878), 321 (16800)	313, 325	306
7	–	329	307 (22050), 321 (17145), (sh 350)	313, 325	365
8- PF_6	–	351	267 (5205), 275 (5589), 291 (6118), 353 (10926)	269, 276, 313, 325	349
9-PF_6	268, 275, 355	–	267 (13788), 275 (13932), 345 (14833)	268, 275, 346	347
10-PF_6	268, 275, 311	–	237 (–), 267 (13788), 275 (13932), 308 (18982)	268, 275, 325	247, 326

Figure S1. Hydrolysis profiles of complexes **1** – **10-PF$_6$** dissolved in phosphate buffer 10 mM pH 7.4 (1% DMSO). Spectra were recorded at different times over 24 h at room temperature. Concentration of the complexes is 10^{-4} M for **1**, **2**, **6**, **7**, **8**-PF$_6$, and **9**-PF$_6$ and 10^{-5} M for **3**, **4**-PF$_6$, **5**, and **10**-PF$_6$

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2
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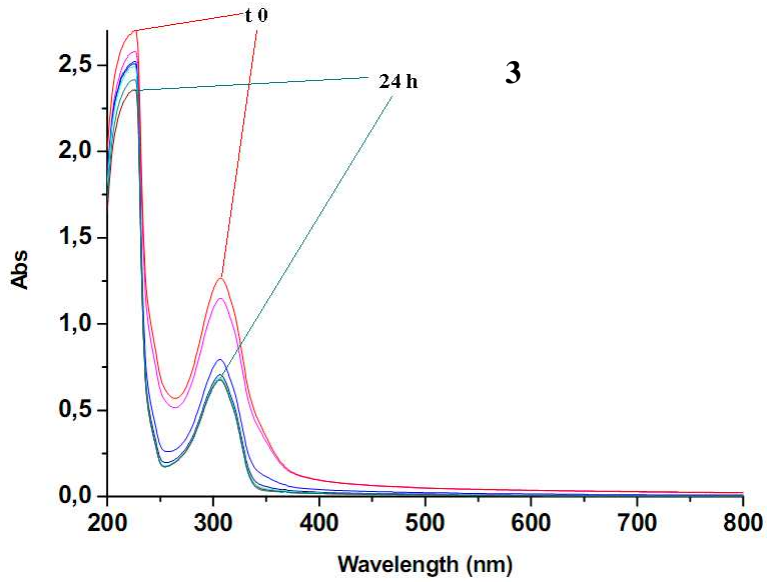
0,6
0,4
0,2
0,0
300
400
500
600
700
800
Wavelength (nm)


t 0
24 h
3
Abs
2,5
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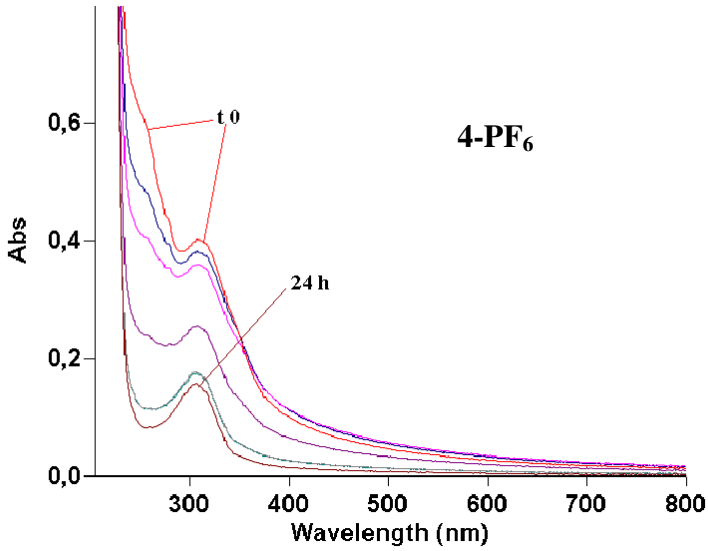
1,5
1,0
0,5
0,0
200
300
400
500
600
700
800
Wavelength (nm)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24 h
4-PF6
Abs
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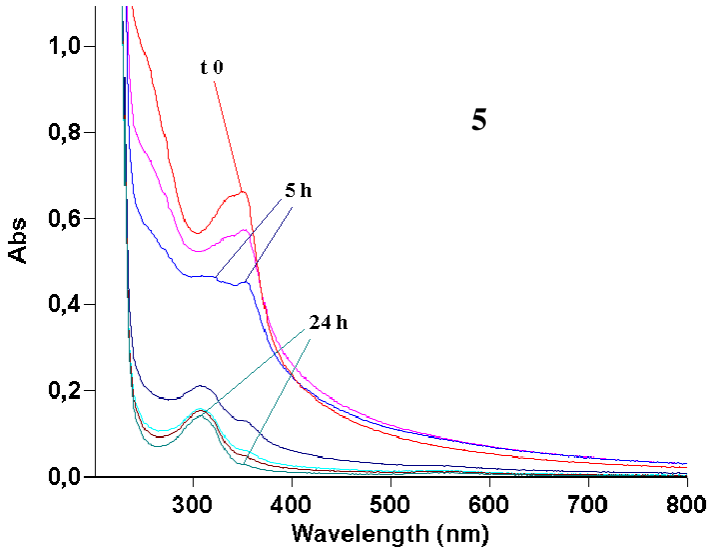
0,4
0,2
0,0
300
400
500
600
700
800
Wavelength (nm)


5
t 0
5 h
24 h
Abs
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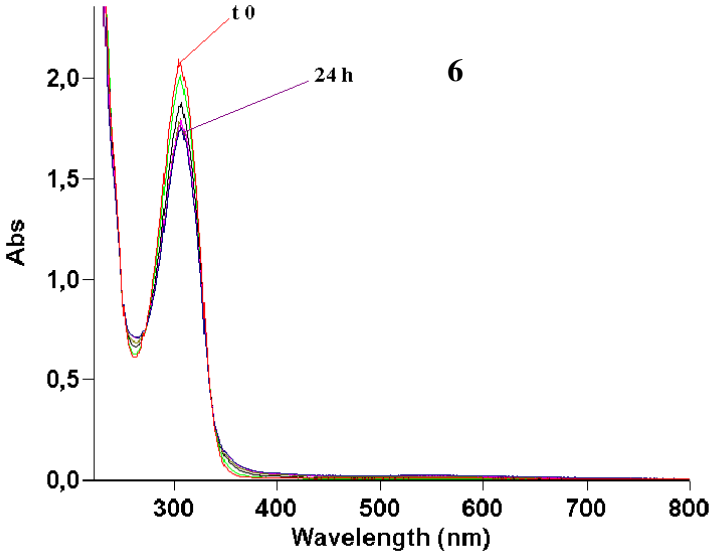
0,6
0,4
0,2
0,0
300
400
500
600
700
800
Wavelength (nm)


6
t 0
24 h
Abs
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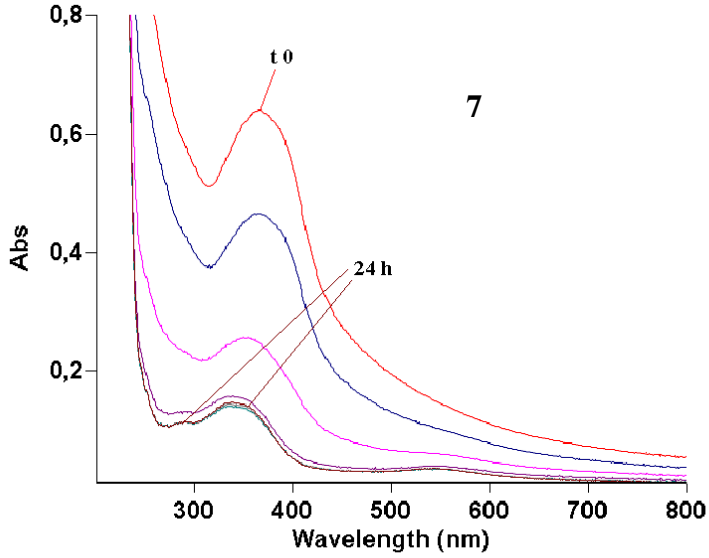
300
400
500
600
700
800
Wavelength (nm)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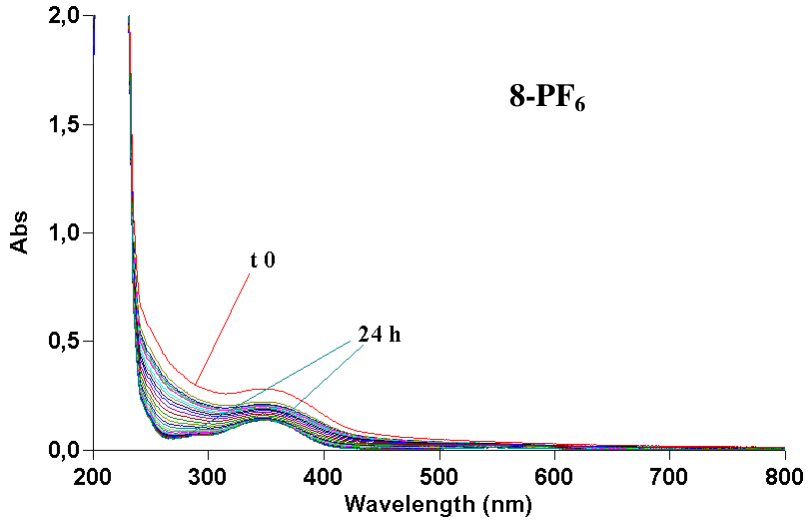
t 0
24 h
Abs
0,8
0,6
0,4
0,2
300
400
500
600
700
800
Wavelength (nm)


8-PF6
Abs
Wavelength (nm)
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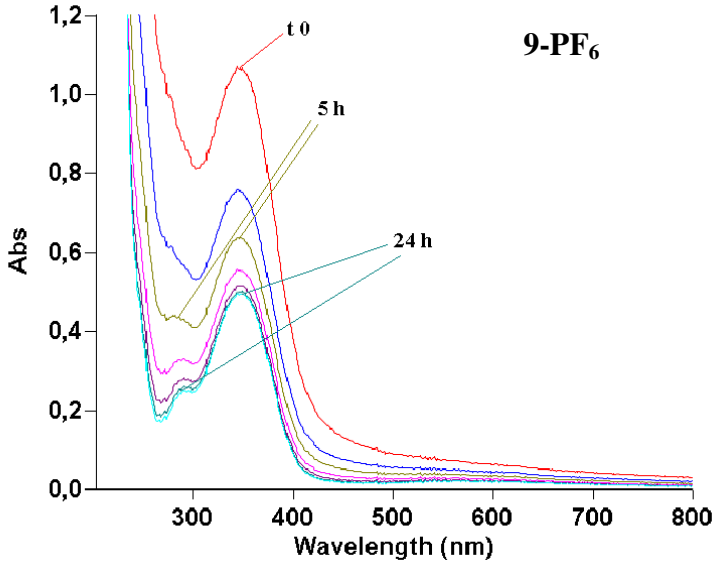
24 h
2,0
1,5
1,0
0,5
0,0
200
300
400
500
600
700
800


9-PF6
Abs
Wavelength (nm)
t 0
5 h
24 h
1,2
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0,6
0,4
0,2
0,0
300
400
500
600
700
800

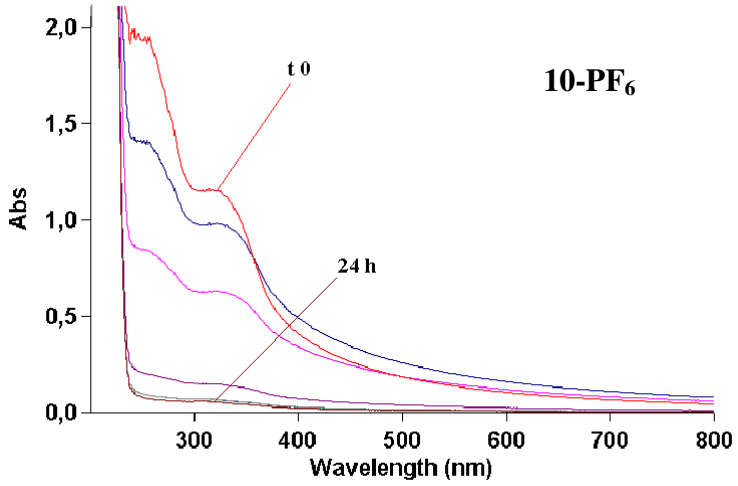
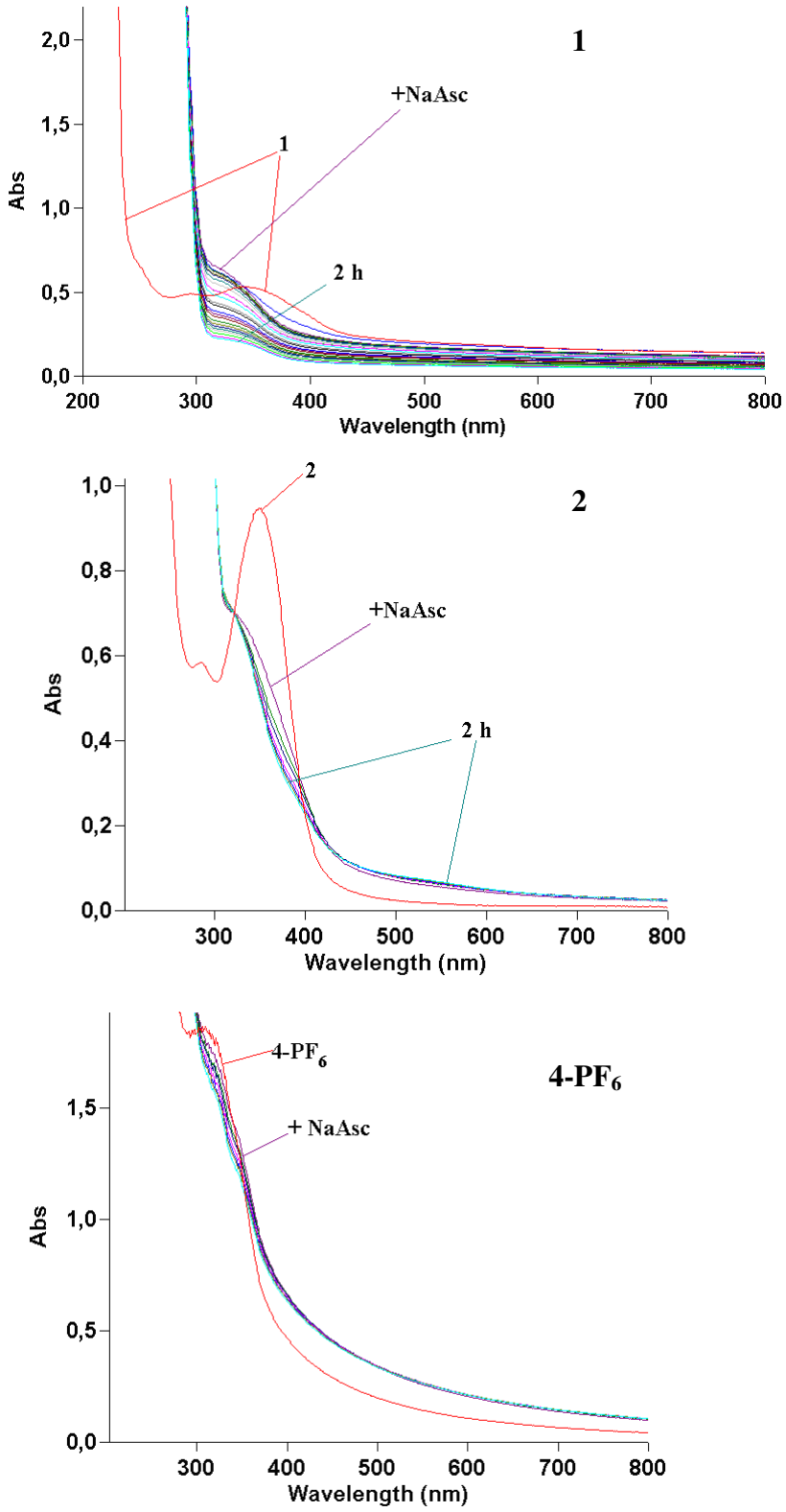
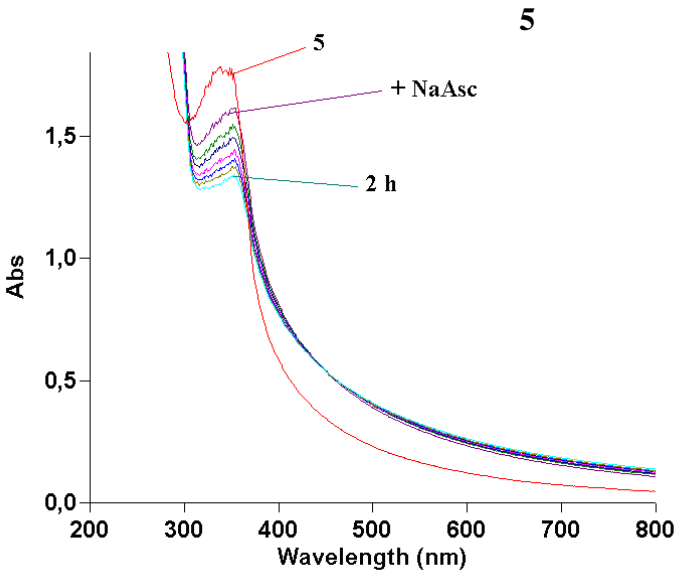

10-PF6
Abs
Wavelength (nm)
t 0
24 h
2,0
1,5
1,0
0,5
0,0
300
400
500
600
700
800

Figure S2. Time dependent spectral profiles of complexes **1 - 10-PF$_6$** dissolved in phosphate buffer 10 mM pH 7.4 (1% DMSO) before (red) and after the addition of NaAsc at the ratio complex:NaAsc of 1:10. Spectra were recorded at different times over 2 h at room temperature. Concentration of the complexes is as in Figure S1.




5
5
+ NaAsc
2 h
Abs
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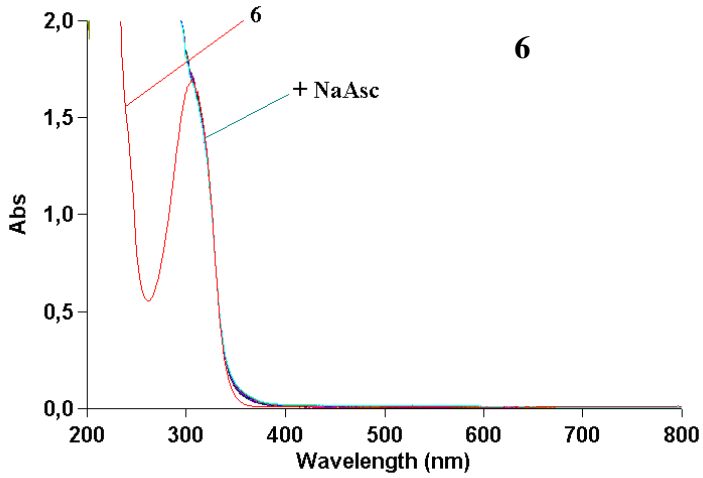
1,0
0,5
0,0
200
300
400
500
600
700
800
Wavelength (nm)


6
6
+ NaAsc
Abs
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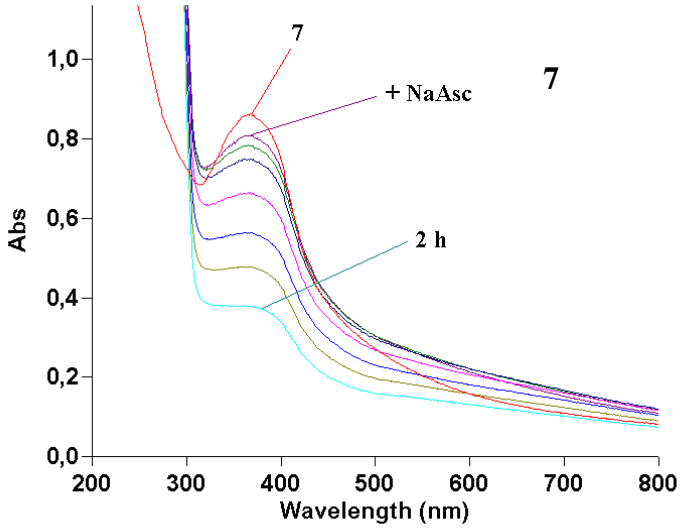
1,0
0,5
0,0
200
300
400
500
600
700
800
Wavelength (nm)


7
7
+ NaAsc
2 h
Abs
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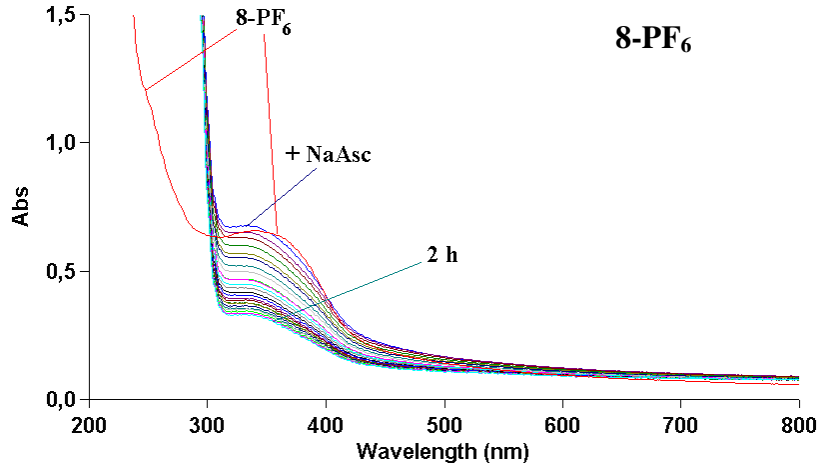
600
700
800
Wavelength (nm)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8-PF6
+ NaAsc
2 h
Abs
Wavelength (nm)
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600
700
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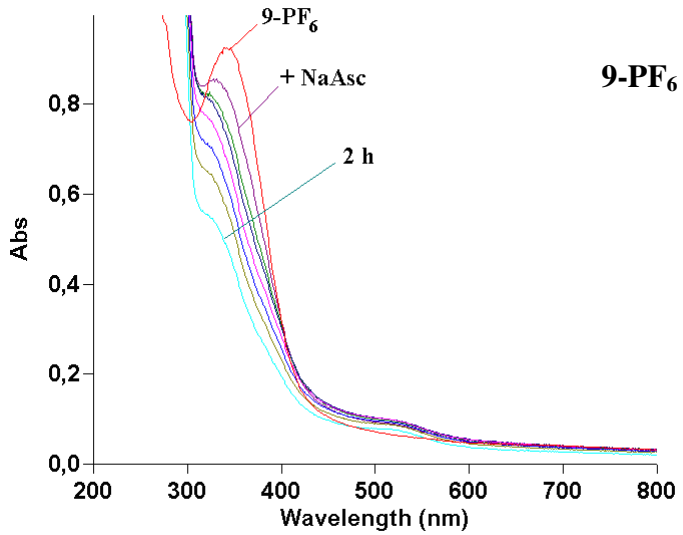
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9-PF6
+ NaAsc
2 h
Abs
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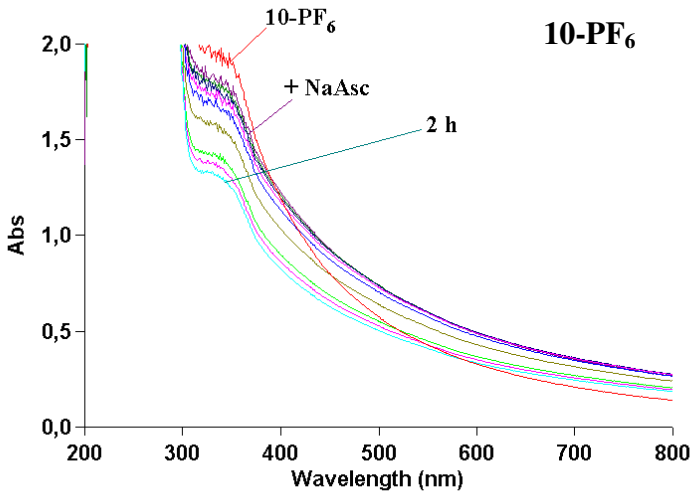
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10-PF6
+ NaAsc
2 h
Abs
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