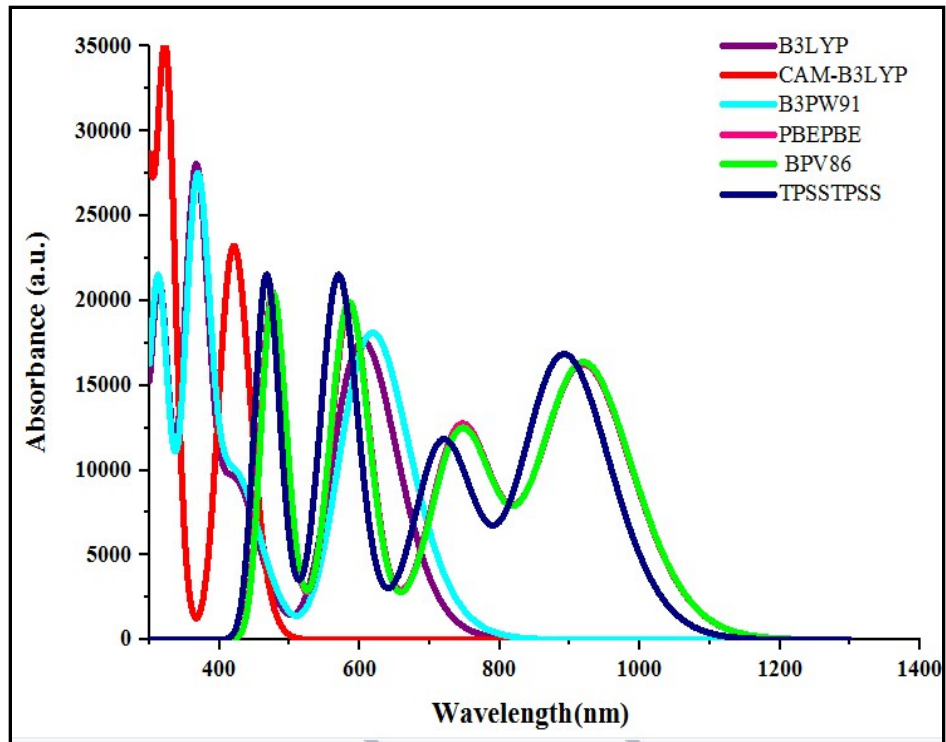


## *Supporting Information*

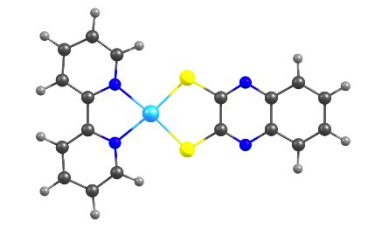
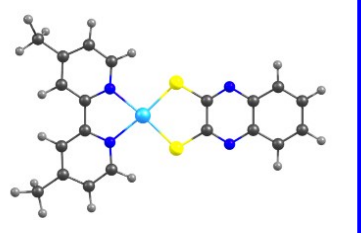
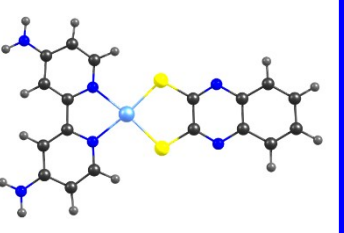
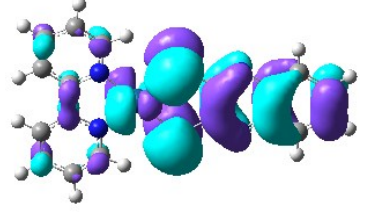
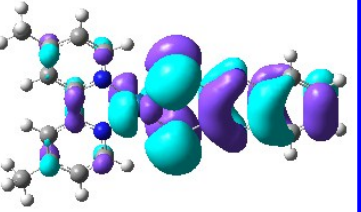
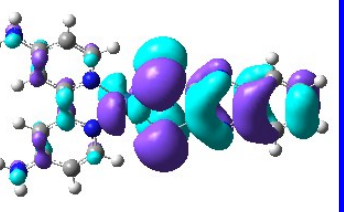
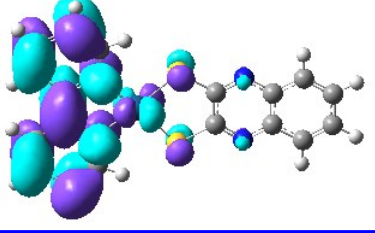
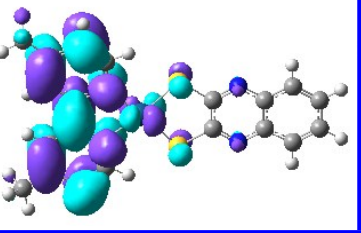
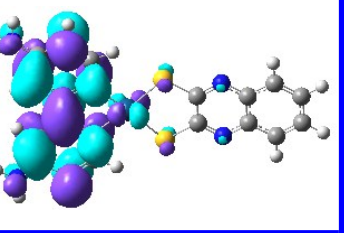
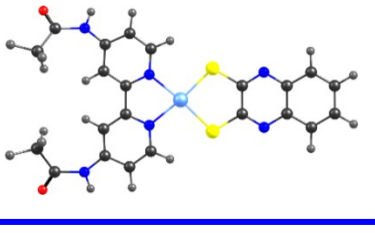
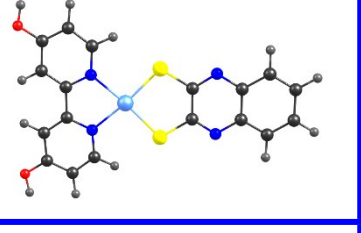
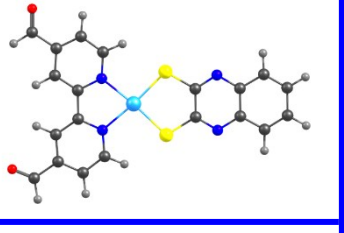
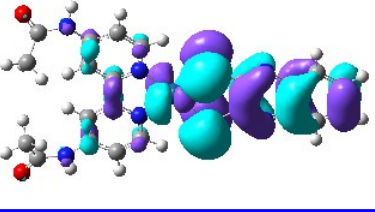
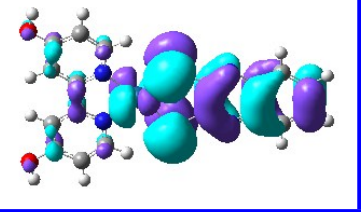
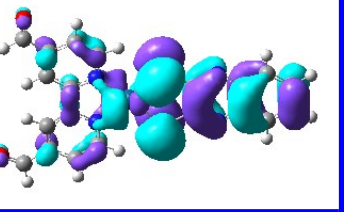
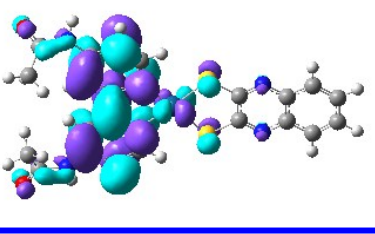
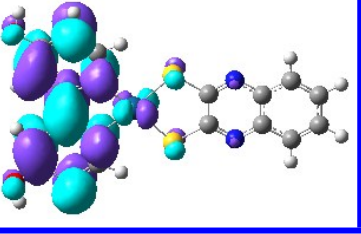
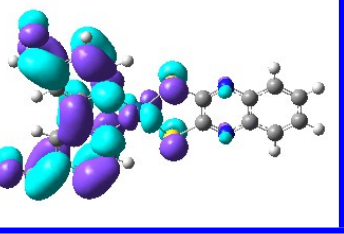
# **A comparative theoretical study on the optoelectronic and nonlinear optical properties of Pt(bpy)(qdt) derivatives with electron-donating and -withdrawing anchors**

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**Figure S1.** Absorption spectra of **2b** complex in acetonitrile solution under different exchange-correlation functional with 6-31G (d)/LanL2DZ basis set.

	R=H	1a	2a
Optimized Structure			
HOMO			
LUMO			
	3a	4a	1b
Optimized Structure			
HOMO			
LUMO			

**Figure S2.** The optimized geometries and calculated isodensity of frontier occupied molecular orbitals for all complexes.

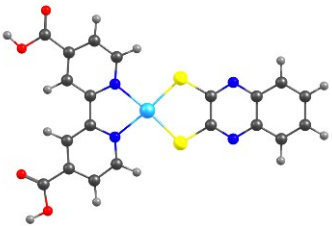
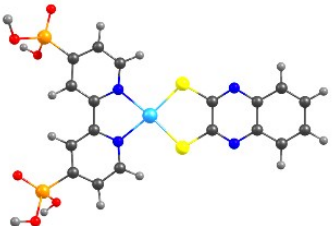
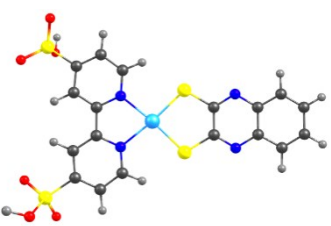
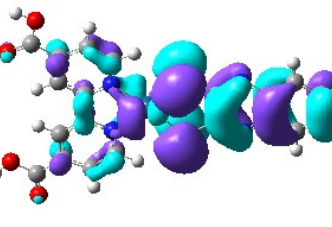
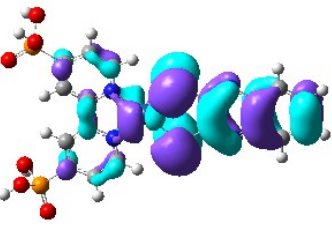
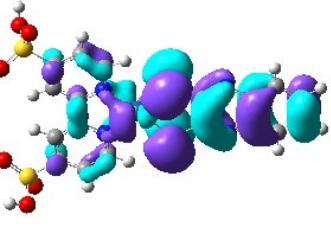
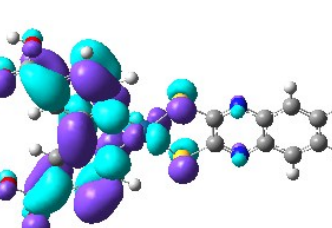
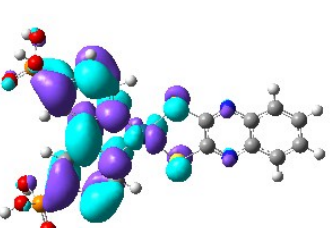
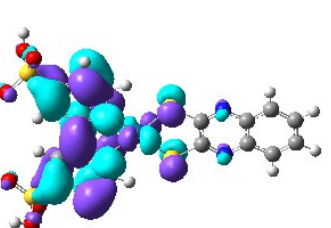
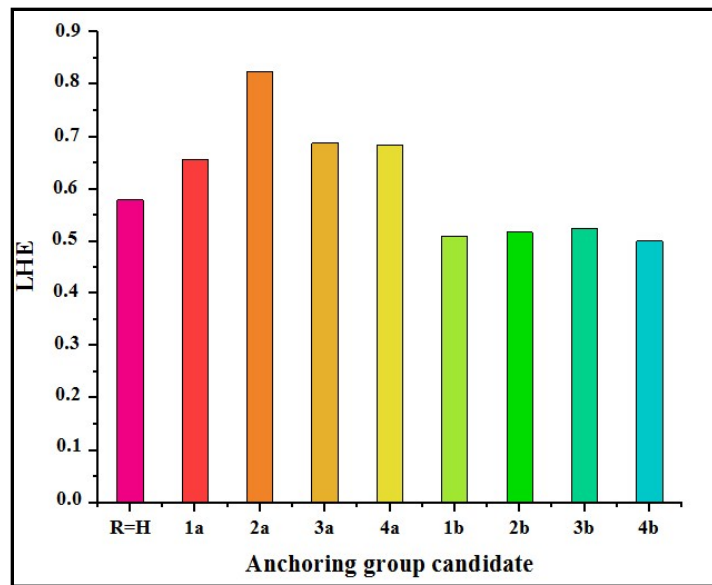
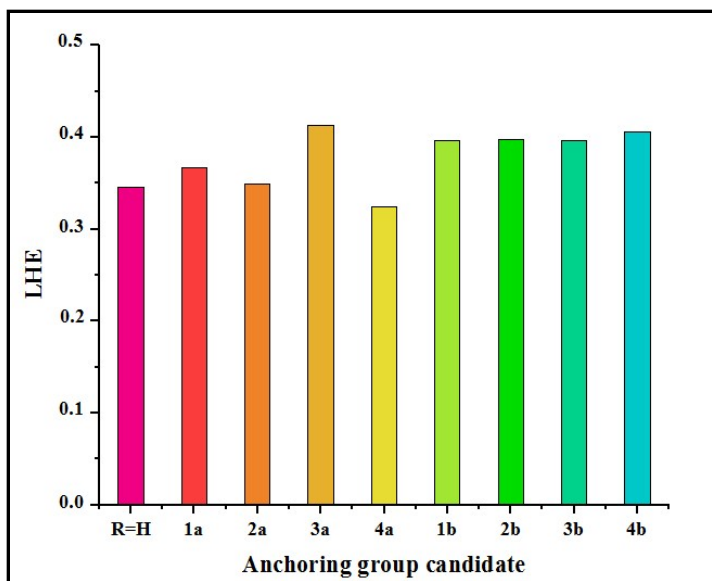
	2b	3b	4b
Optimized Structure			
HOMO			
LUMO			

Figure S2. Continued



**Figure S3.** Comparison of the calculated LHE values for [Pt(bpy)(qdt)] derivatives vacuum in (left) and in solvent (right).

**Table S1.** The optimized main geometry parameters for all considered structures in ground state

	<b>R=H</b>	<b>1a</b>	<b>2a</b>	<b>3a</b>	<b>4a</b>	<b>1b</b>	<b>2b</b>	<b>3b</b>	<b>4b</b>
<b>Bond length(Å)</b>									
Pt–N	2.097	2.097	2.101	2.096	2.102	2.088	2.089	2.092	2.092
Pt–S	2.319	2.320	2.322	2.318	2.319	2.306	2.306	2.307	2.304
C–C <sup>qdt</sup>	1.446	1.447	1.449	1.446	1.447	1.444	1.444	1.445	1.443
C–C <sup>bpy</sup>	1.471	1.473	1.479	1.476	1.475	1.469	1.469	1.469	1.467
C–N	1.362	1.363	1.361	1.360	1.362	1.366	1.364	1.363	1.364
C–N	1.311	1.311	1.312	1.311	1.311	1.312	1.312	1.311	1.311
C–S	1.764	1.764	1.764	1.765	1.765	1.764	1.764	1.764	1.765
<b>Bond angle(°)</b>									
N–Pt–N	78.17	78.02	80.52	88.70	78.02	78.59	78.50	78.38	78.40
S–Pt–S	88.71	88.73	91.10	90.24	88.73	88.72	88.73	88.73	88.78
S–Pt–N(cis)	96.55	96.61	94.18	94.51	96.63	96.26	96.39	96.44	96.428
S–Pt–N(cis)	96.55	96.63	94.18	94.51	96.61	96.40	96.36	96.42	96.383
N–Pt–S(trans)	174.73	174.65	174.71	175.07	174.63	175.00	174.86	174.81	174.79
N–Pt–S(trans)	174.73	174.63	174.71	175.07	174.65	174.86	174.89	174.82	174.83

**Table S2.** The calculated frontier orbital energies and HOMO–LUMO gap energies (eV) all considered structures.

	R=H	1a	2a	3a	4a	1b	2b	3b	4b
LUMO+5	-0.36	-0.26	0.18	-0.78	-0.22	-1.09	-0.84	-0.67	-1.16
LUMO+4	-0.94	-0.85	-0.59	-1.00	-0.84	-1.28	-1.16	-1.09	-1.37
LUMO+3	-1.05	-0.92	-0.60	-1.11	-0.92	-1.45	-1.30	-1.24	-1.61
LUMO+2	-1.70	-1.52	-0.90	-1.92	-1.36	-2.59	-2.37	-2.20	-2.68
LUMO+1	-1.88	-1.75	-1.20	-2.09	-1.66	-3.15	-2.73	-2.29	-2.77
LUMO	-2.84	-2.68	-2.25	-2.99	-2.65	-3.62	-3.36	-3.18	-3.66
HOMO	-4.94	-4.82	-4.49	-4.97	-4.78	-5.33	-5.19	-5.12	-5.45
HOMO-1	-5.13	-5.02	-4.72	-5.18	-4.99	-5.52	-5.38	-5.31	-5.62
HOMO-2	-5.83	-5.73	-5.46	-5.88	-5.71	-6.19	-6.06	-5.99	-6.29
HOMO-3	-6.17	-6.08	-5.81	-6.21	-6.05	-6.52	-6.39	-6.32	-6.61
HOMO-4	-6.46	-6.32	-5.90	-6.50	-6.25	-6.97	-6.80	-6.71	-7.10
HOMO-5	-6.66	-6.54	-6.16	-6.65	-6.48	-7.04	-6.90	-6.84	-7.15