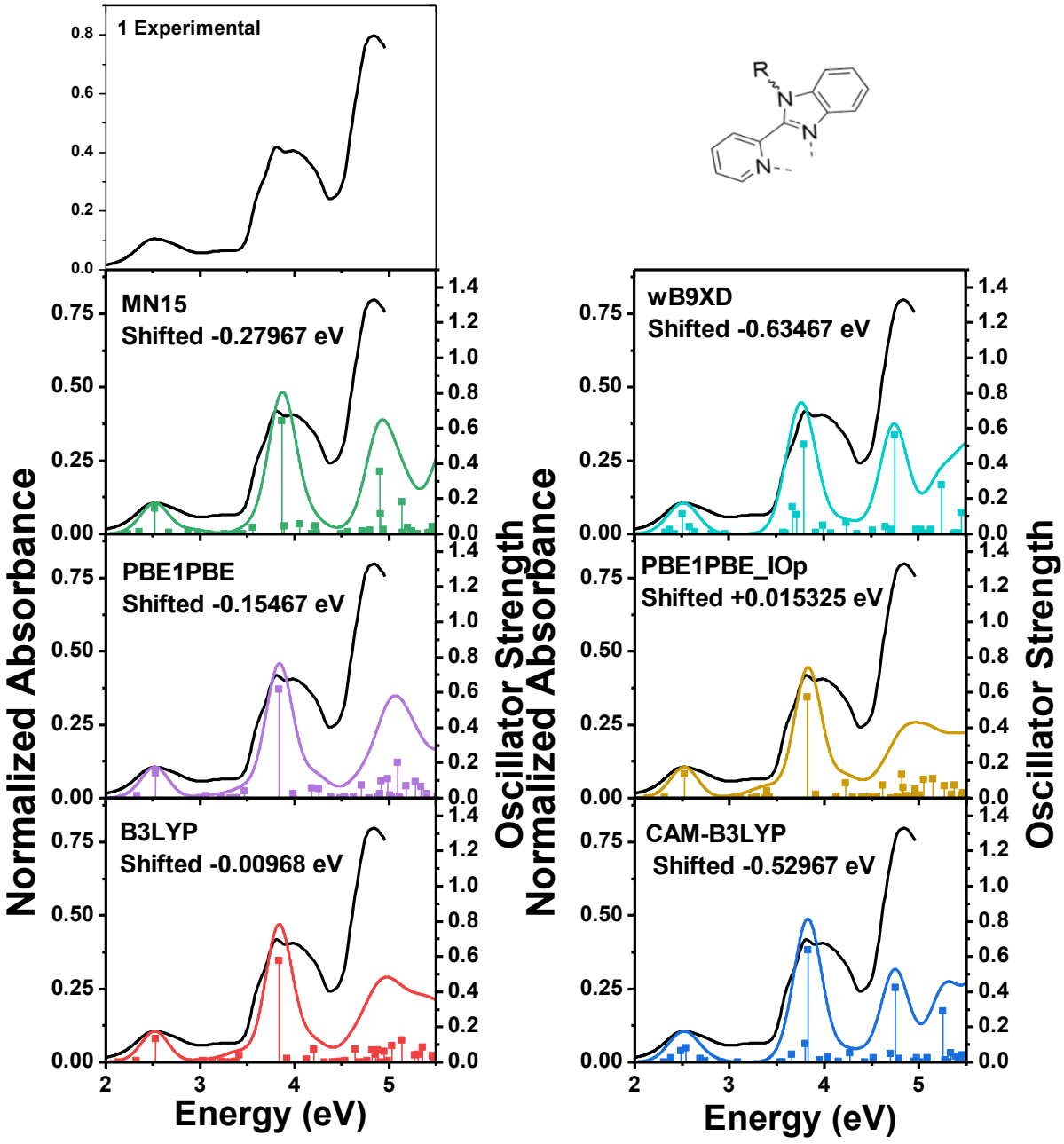


Figure S1: Shows the calculated absorbance spectra using different functionals and the amount of energy needed to shift it to match with the experimental spectra (black line) for L1.

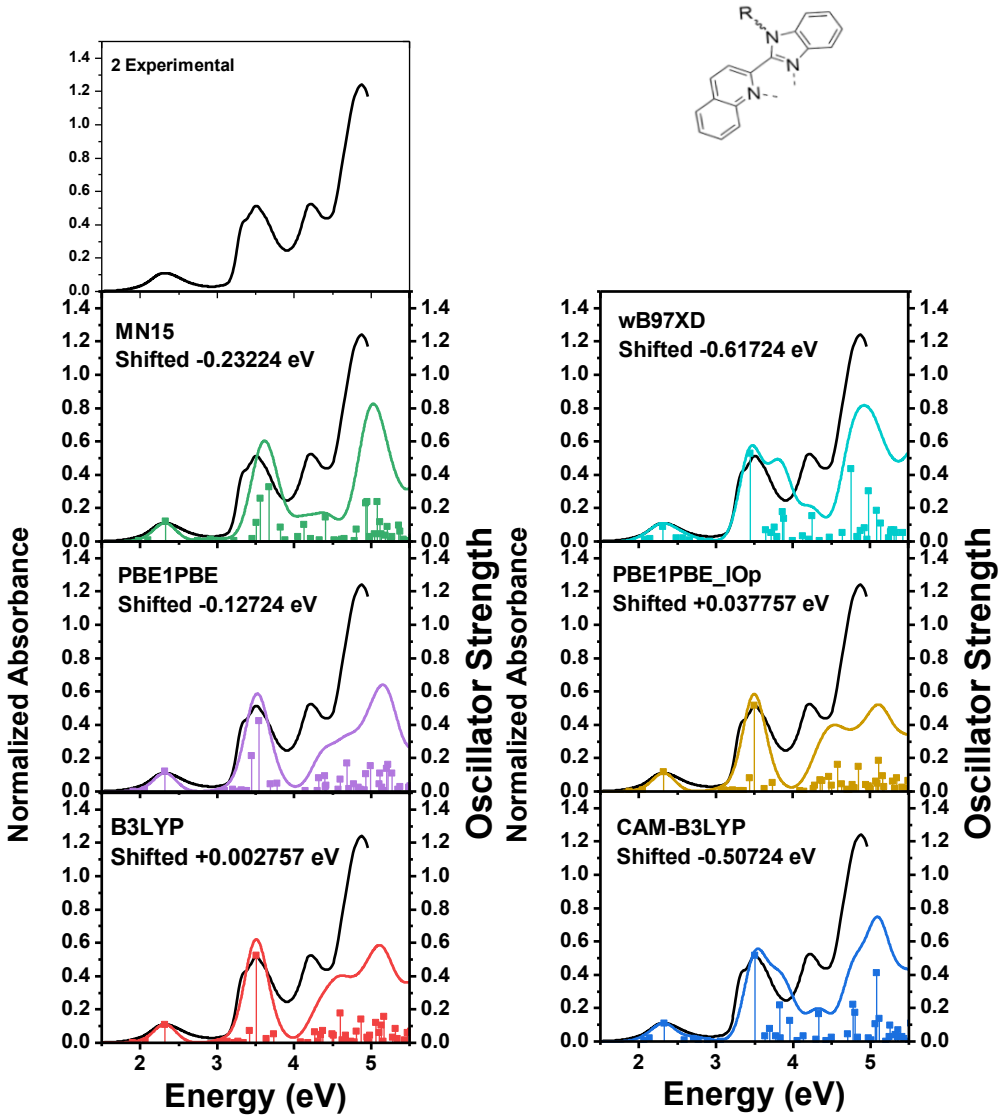


Figure S2: Shows the calculated absorbance spectra using different functionals and the amount of energy needed to shift it to match with the experimental spectra (black line) for L2.

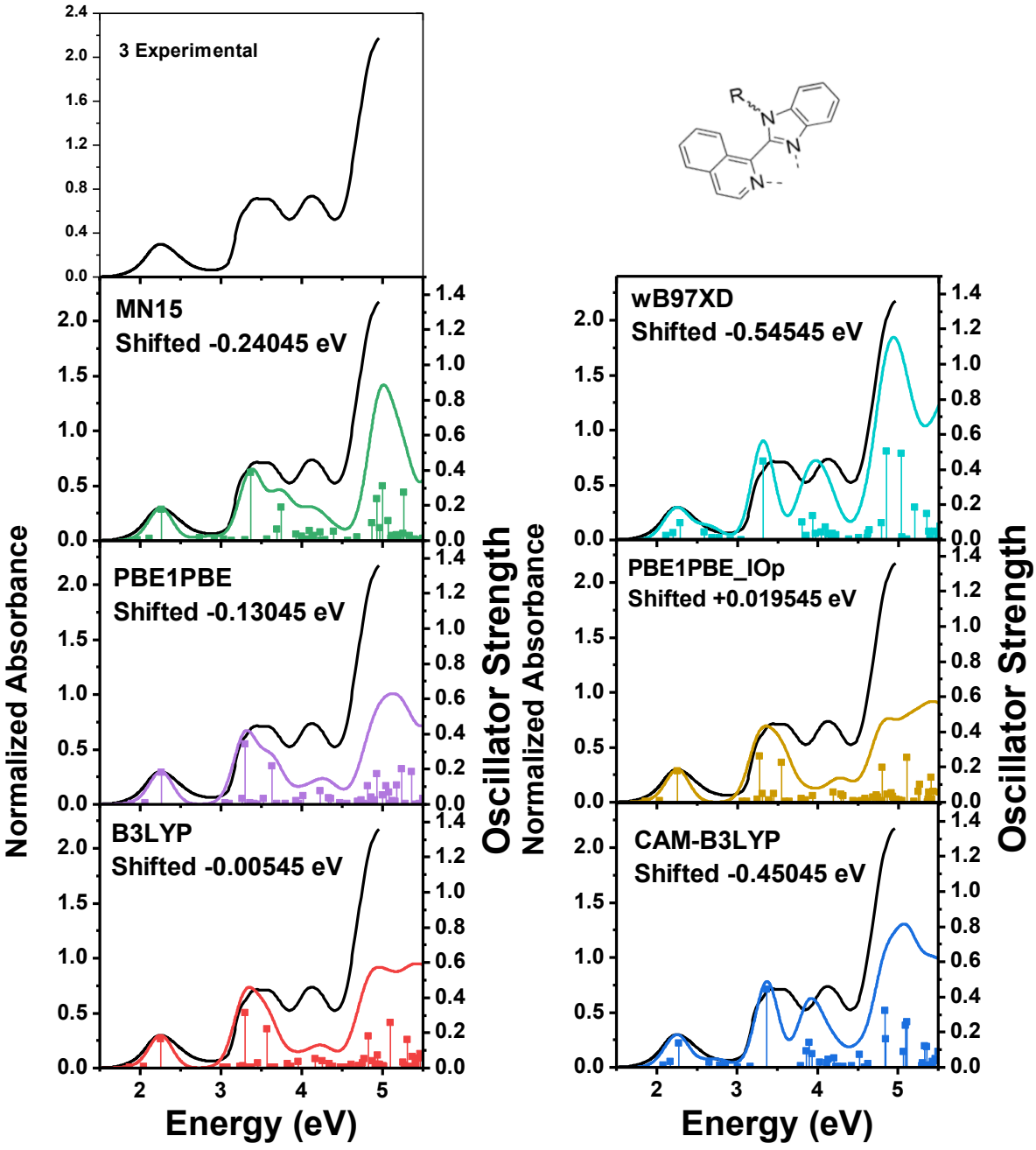


Figure S3: Shows the calculated absorbance spectra using different functionals and the amount of energy needed to shift it to match with the experimental spectra (black line) for L3.

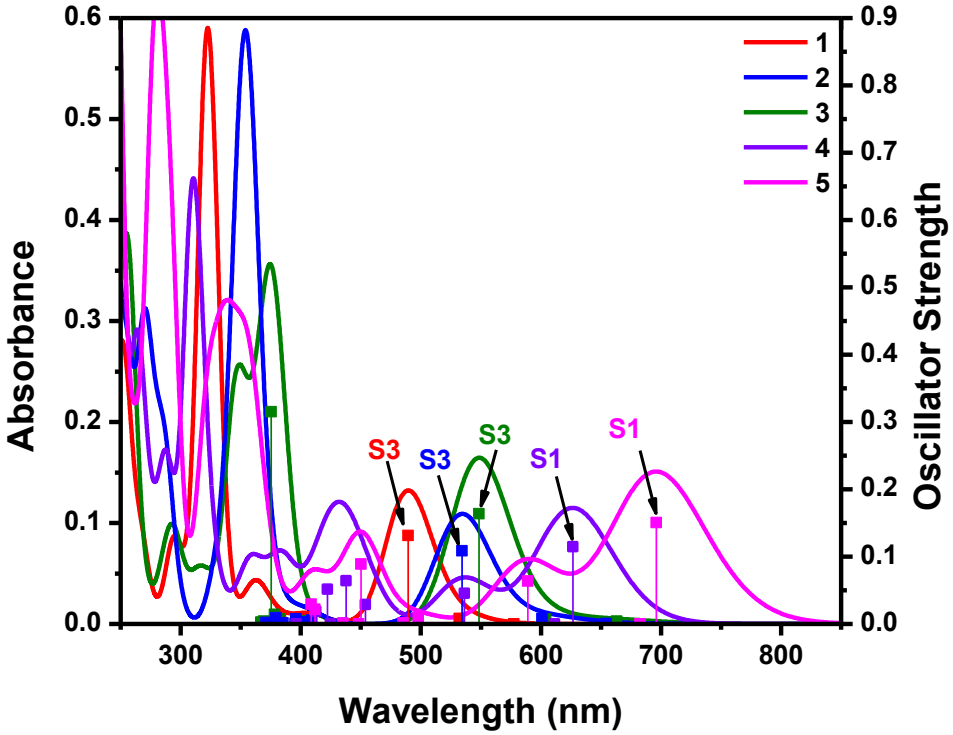


Figure 4-supp: Shows the calculated absorbance spectra for complex 1(red), 2 (blue),3 (green), 4 (purple) and 5 (magenta).

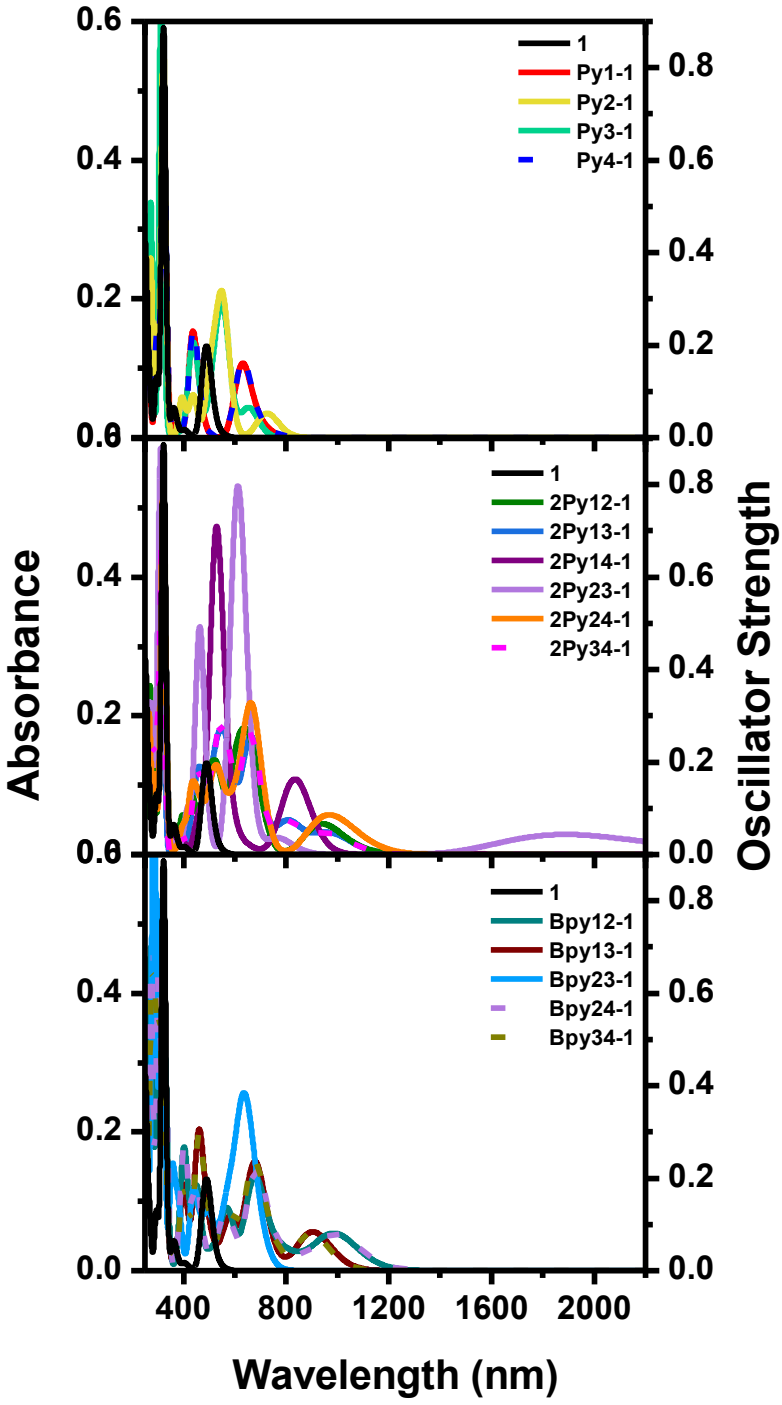


Figure S5: Shows the calculated absorbance spectra of all isomers with L1.

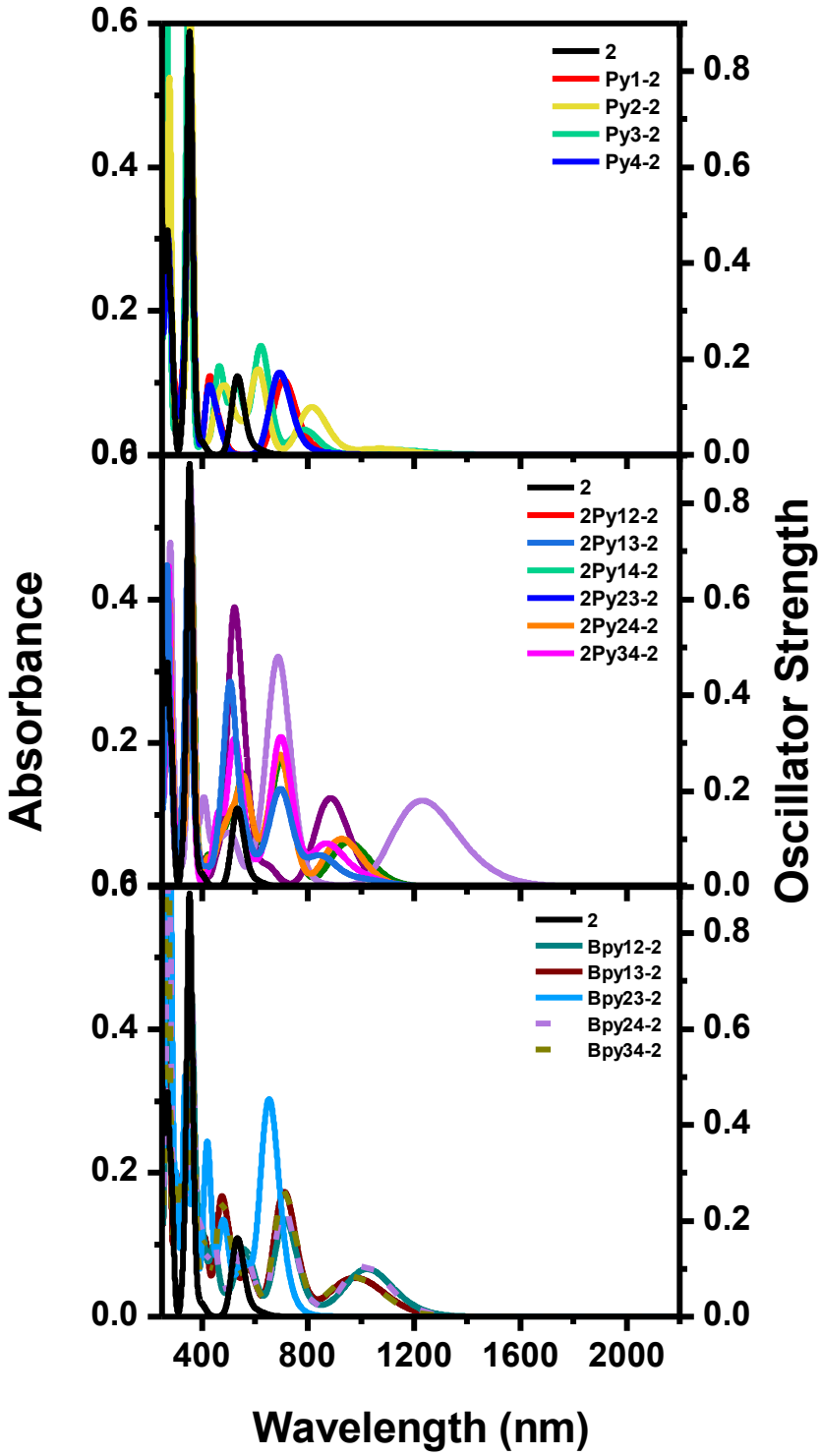


Figure S6: Shows the calculated absorbance spectra of all isomers with L2.

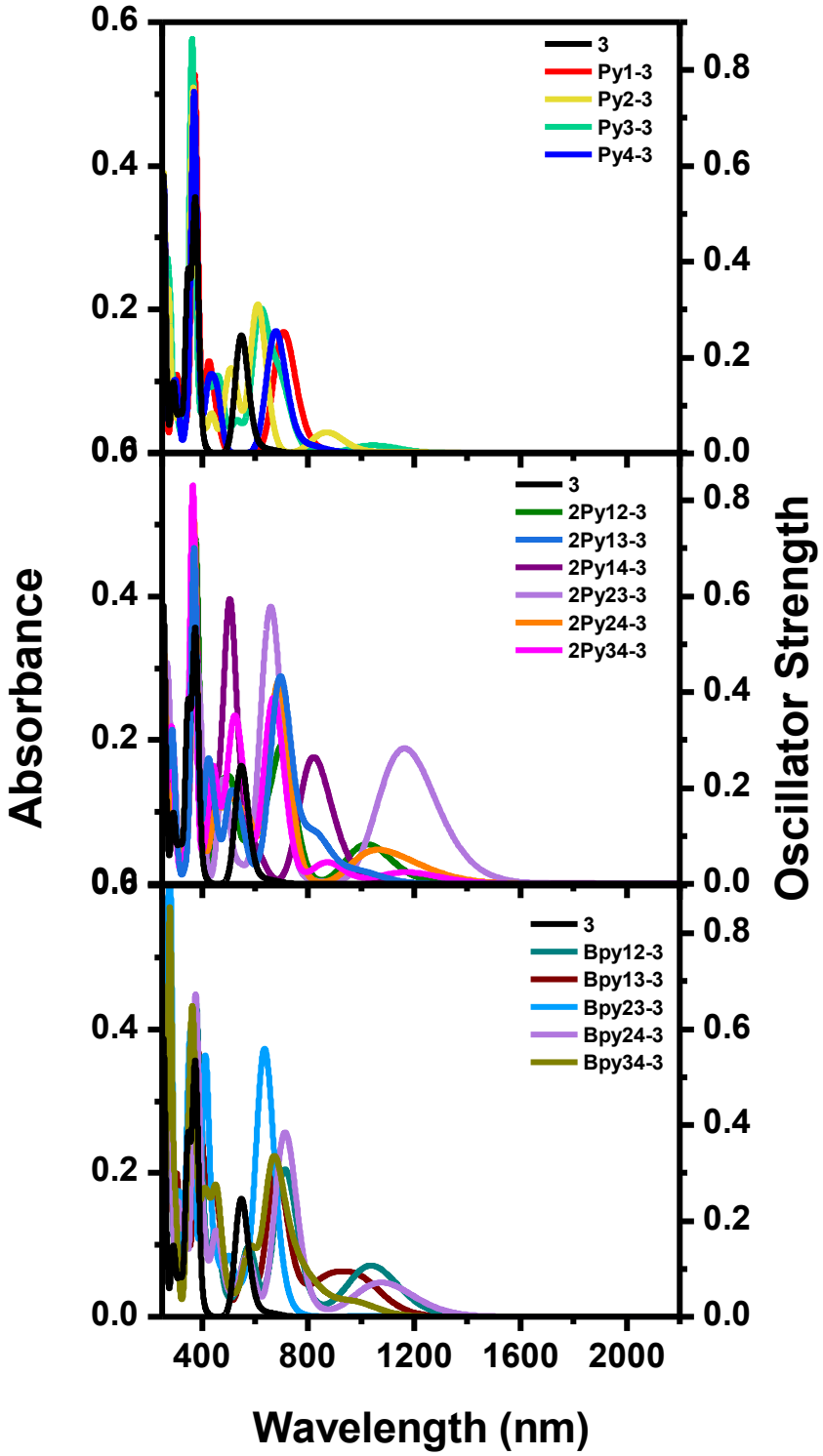


Figure S7: Shows the calculated absorbance spectra of all isomers with L3.

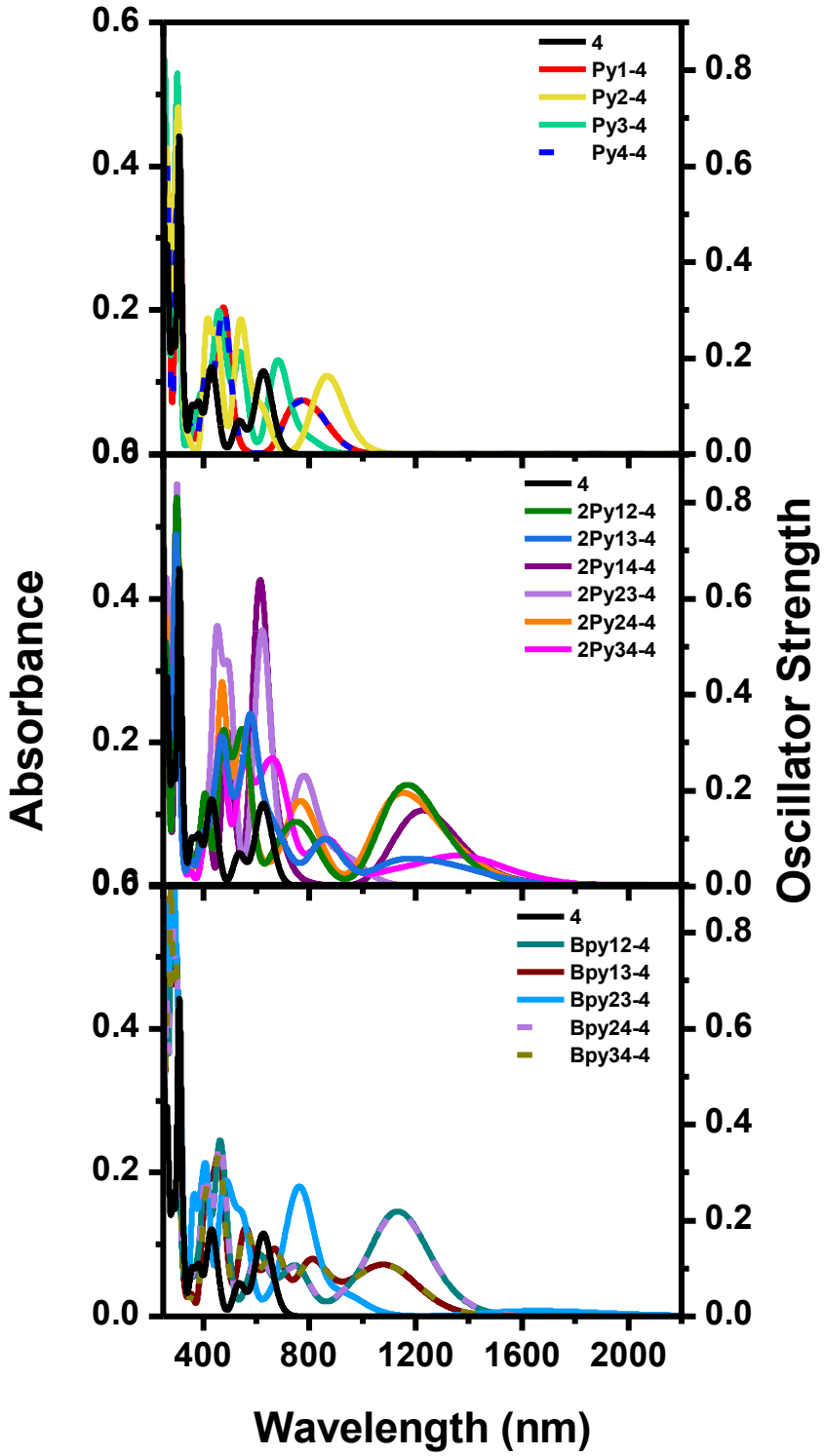


Figure S8: Shows the calculated absorbance spectra of all isomers with L4.

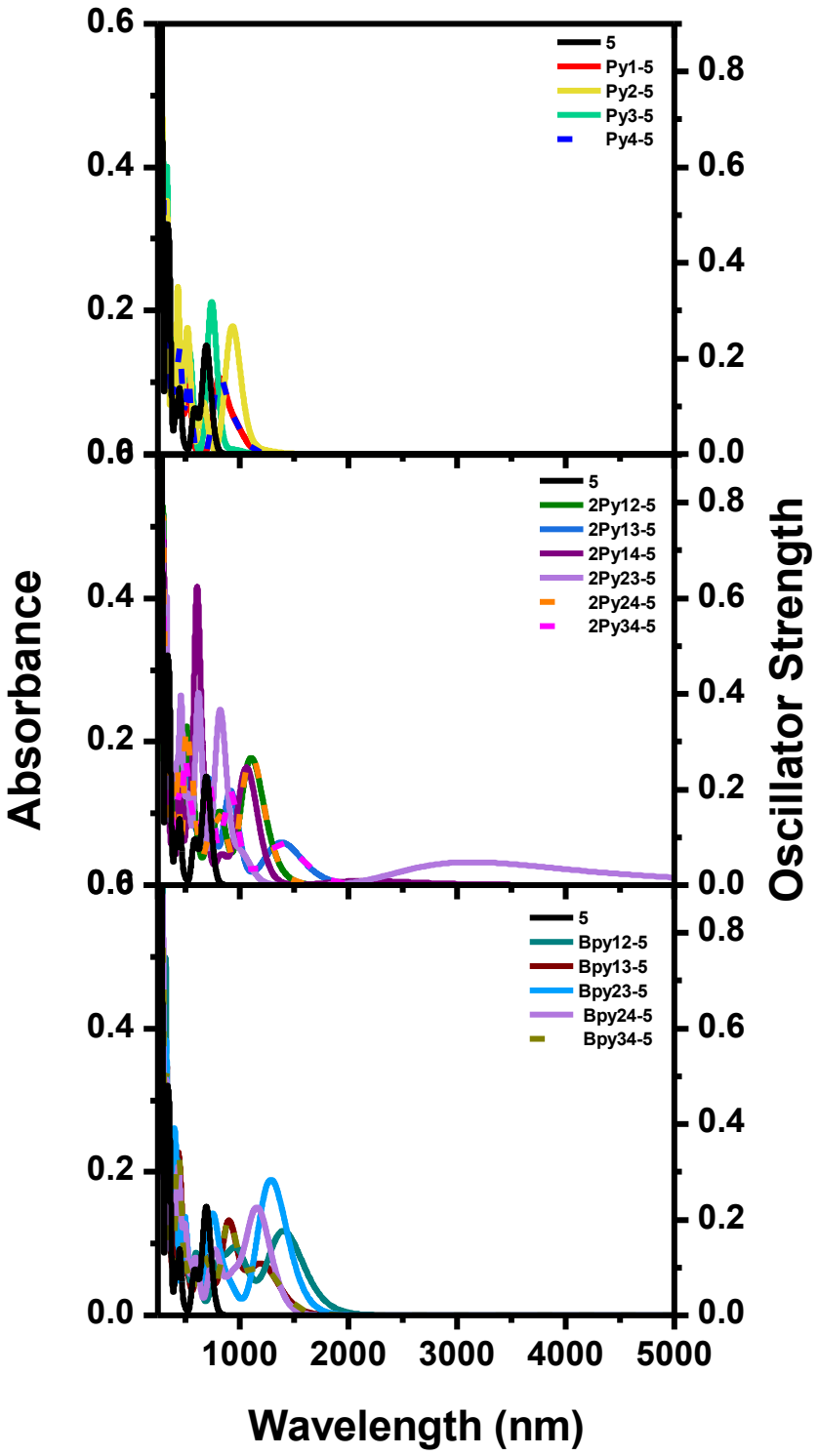


Figure S9: Shows the calculated absorbance spectra of all isomers with L5.

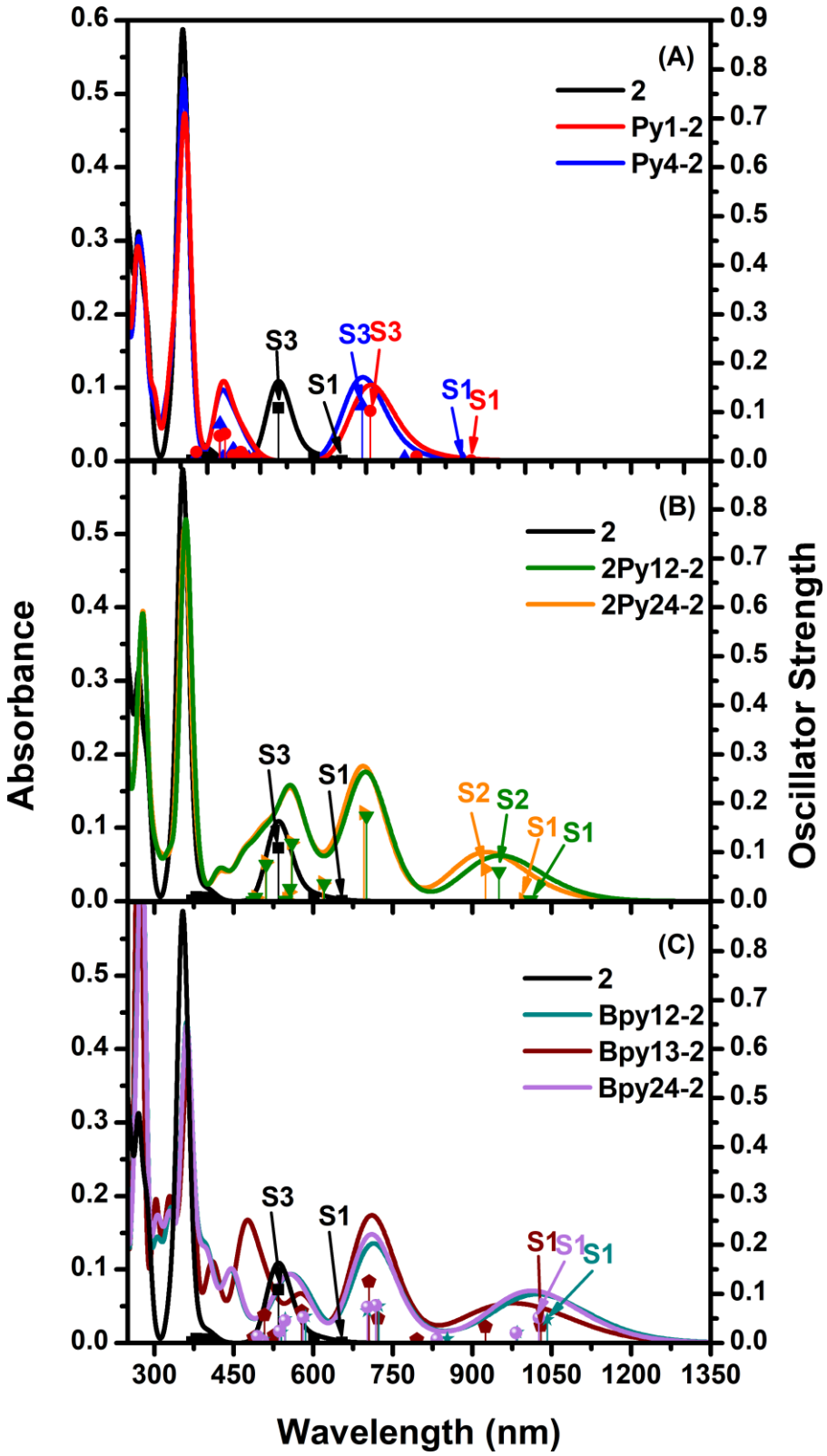
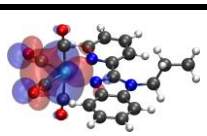
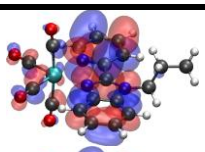
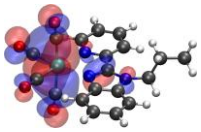
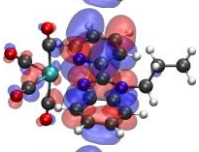
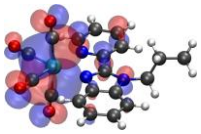
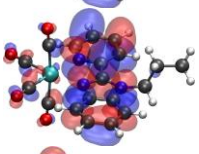
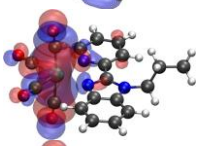
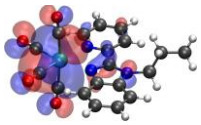
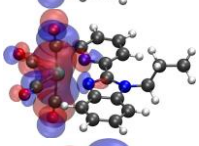
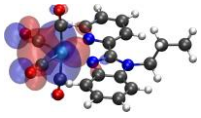
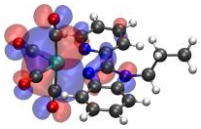
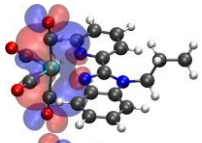
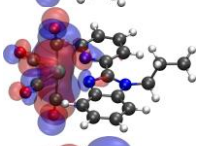
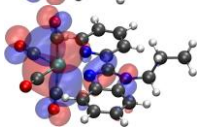
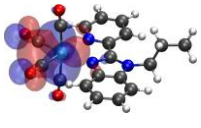
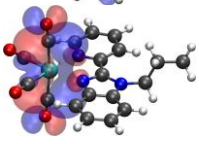
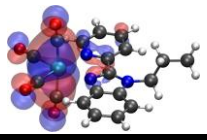
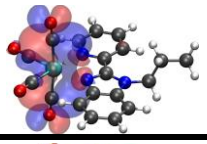
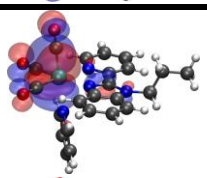
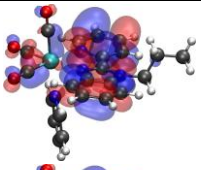
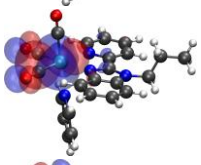
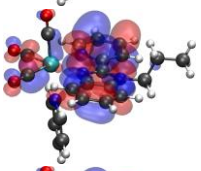
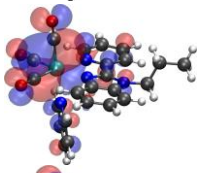
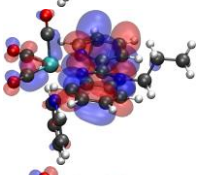
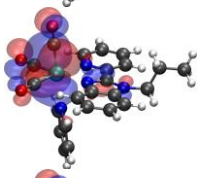
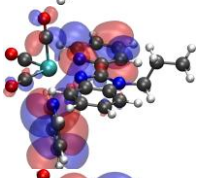
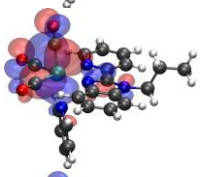
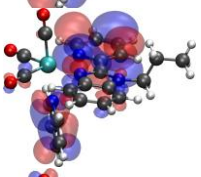
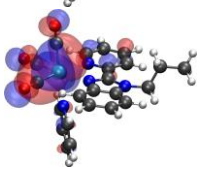
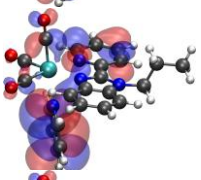
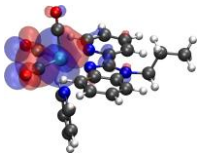
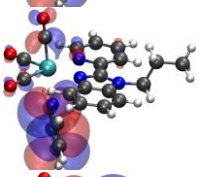
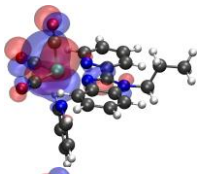
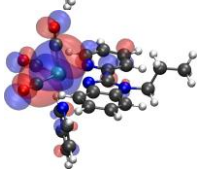
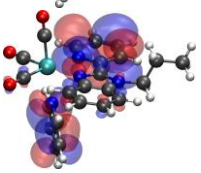
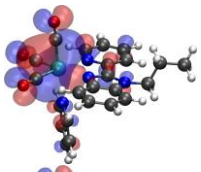
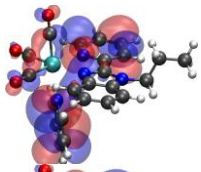
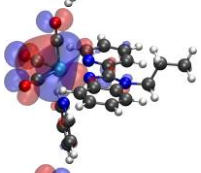
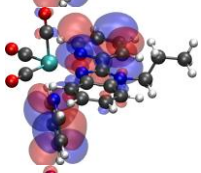
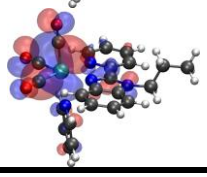
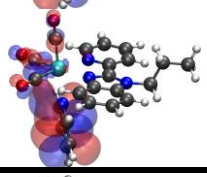
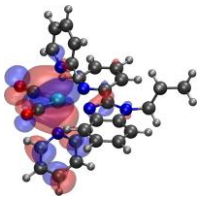
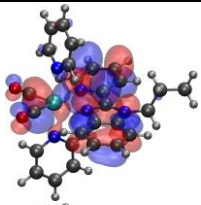
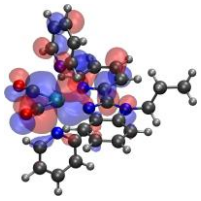
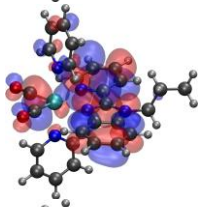
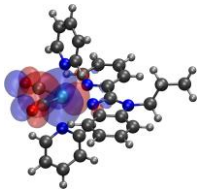
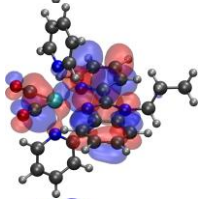
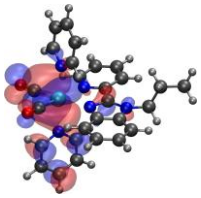
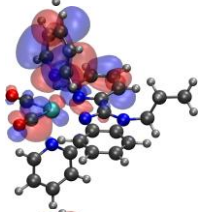
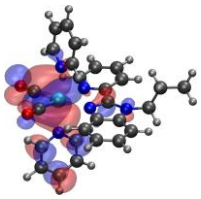
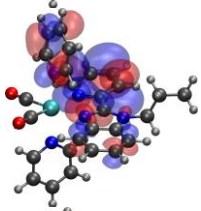
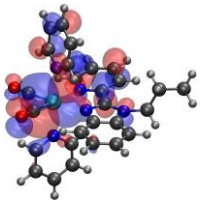
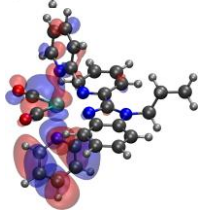


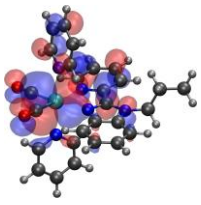
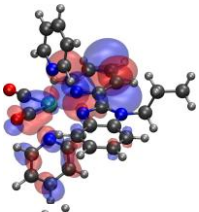
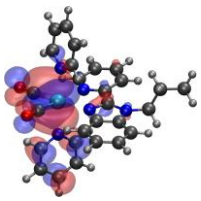
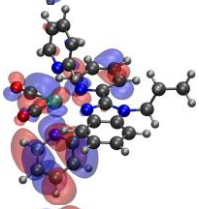
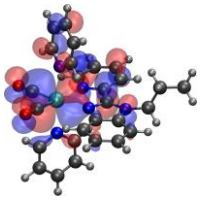
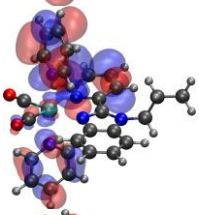
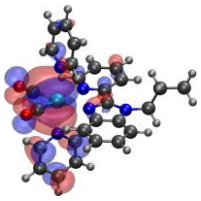
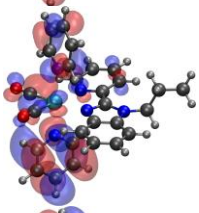
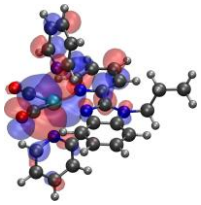
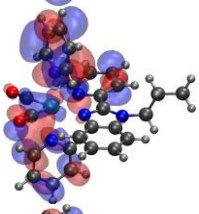
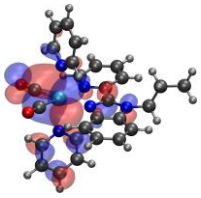
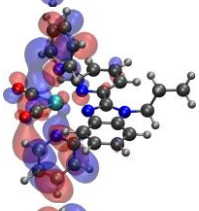
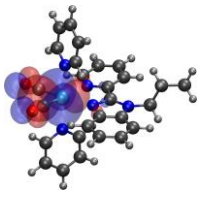
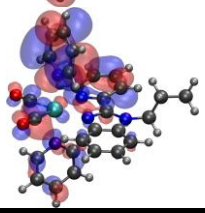
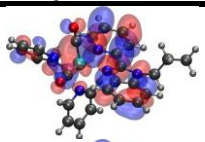
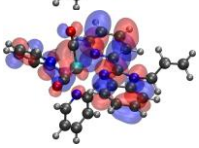
Figure S10: Shows the calculated absorbance spectra of the most energetically favorable isomers of all complexes with L2 for Py (a), 2Py (b), and Bpy (c).

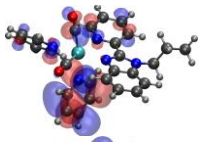
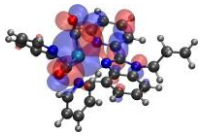
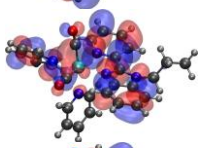
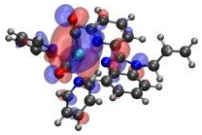
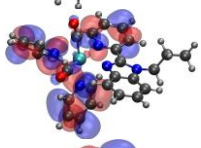
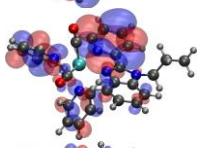
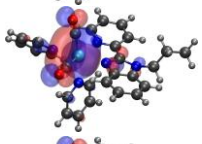
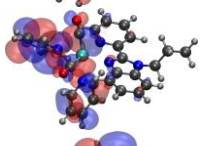
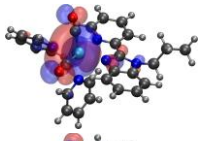
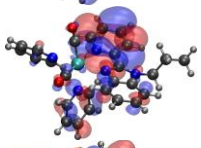
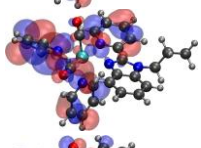
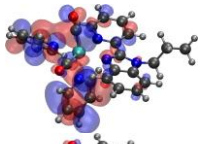
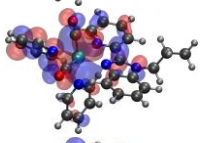
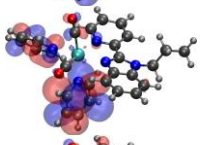
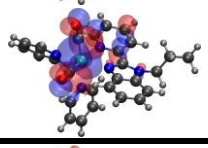
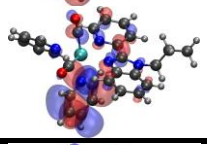
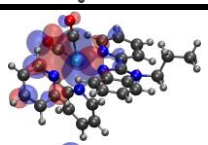
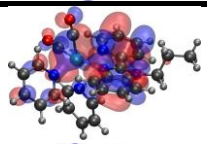
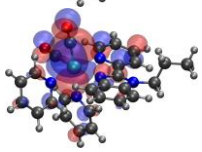
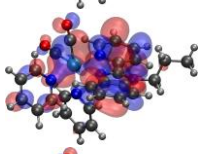
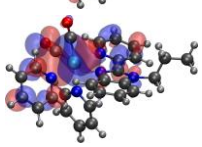
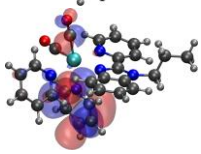
Table S1: Hole and electron NTOs for the first 10 states of all energetically favorable complexes for all complexes with L1. All NTOs are Calculated using TDDFT on the ground state geometry with B3LYP functional and LANL2dz/6-31G* basis set with dichloromethane solvent using the CPCM method.

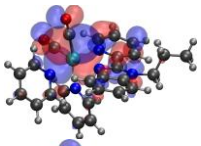
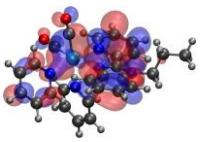
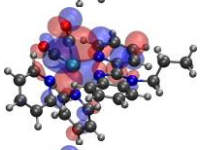
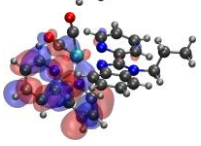
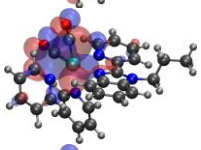
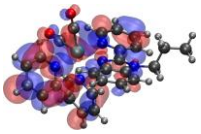
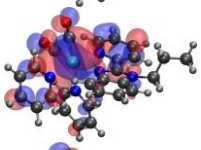
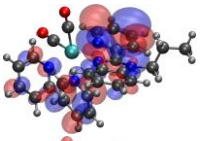
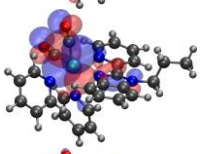
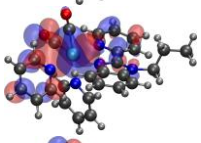
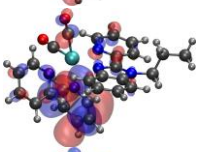
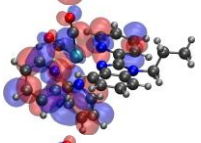
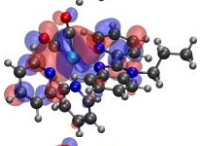
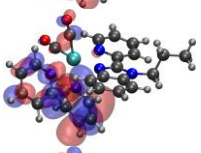
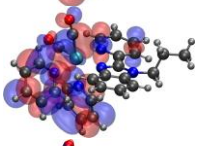
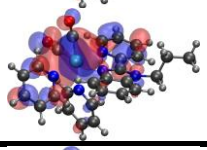
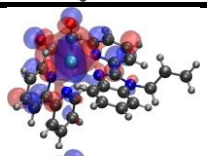
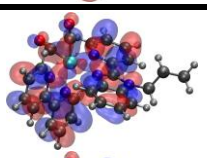
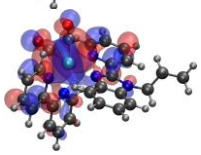
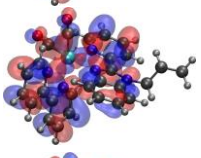
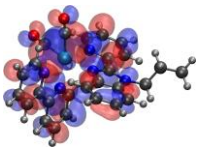
Complex	State/Wavelength/ Oscillator Strength	Hole		Electron
1	**S_1** 578 nm *0.0001*			
	S_2 532 nm *0.0080*			
	S_3 489 nm *0.1312*			
	S_4 408 nm *0.0064*			
	S_5 407 nm *0.0034*			
	S_6 395 nm *0.0006*			
	S_7 383 nm *0.0043*	 	**62%** **37%**	 
	S_8 379 nm *0.0008*			
	S_9 372 nm *0.0005*			

1	**S_{10}** 367 nm *0.0021*			
1-Py4	**S_1** 751 nm *0.0020*			
	S_2 690 nm *0.0149*			
	S_3 631 nm *0.1071*			
	S_4 486 nm *0.0025*			
	S_5 465 nm *0.0092*			**58%**
				**42%**
	S_6 459 nm *0.0261*			**66%**
				**34%**
	S_7 445 nm *0.0424*			

1-Py4	S_8 435 nm *0.0890*		
	S_9 424 nm *0.0243*		
	S_{10} 380 nm *0.0115*		
1-2Py14	**S_1** 1358 nm *0.0013*		
	S_2 836 nm *0.1057*		
	S_3 773 nm *0.0064*		
	S_4 659 nm *0.0076*		
	S_5 615 nm *0.0117*		
	S_6 577 nm *0.0380*		

1-2Py14	**S_7** 547 nm *0.1462*		**69%**	
			**30%**	
	S_8 525 nm *0.3485*		**70%**	
			**30%**	
	S_9 499 nm *0.0474*		**66%**	
			**33%**	
	S_{10} 478 nm *0.0040*			
1-2Py24	**S_1** 1035 nm *0.0269*			
	S_2 938 nm *0.0416*			

1-2Py24	**S_3** 680 nm *0.0341*			
	S_4 664 nm *0.1733*			
	S_5 611 nm *0.0473*			
	S_6 592 nm *0.0164*			
	S_7 567 nm *0.0347*			
	S_8 533 nm *0.0238*			
	S_9 529 nm *0.0759*		**56%**	
			**42%**	
	S_{10} 505 nm *0.0127*		**65%**	
			**34%**	
1-2Py34	**S_1** 971 nm *0.0290*			
	S_2 809 nm *0.0467*			
	S_3 678 nm *0.0219*			

1-2Py34	**S_4** 659 nm *0.1532*			
	S_5 582 nm *0.0797*			
	S_6 556 nm *0.0366*			
	S_7 547 nm *0.0832*			
	S_8 519 nm *0.0357*	 	**50%** **44%**	 
	S_9 518 nm *0.0470*	 	**57%** **39%**	 
	S_{10} 491 nm *0.0160*			
1-Bpy34	**S_1** 899 nm *0.0528*			
	S_2 870 nm *0.0006*	 	**69%** **31%**	 

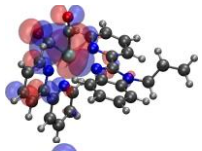
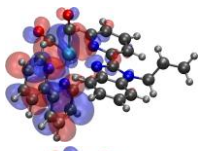
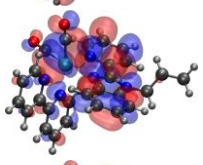
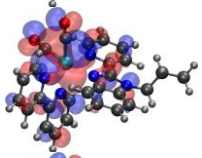
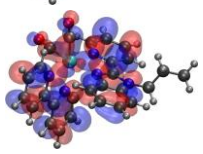
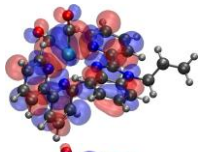
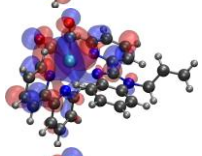
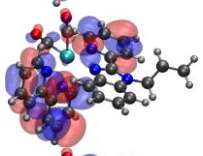
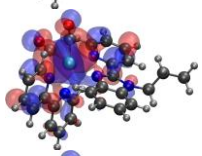
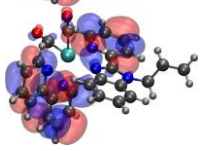
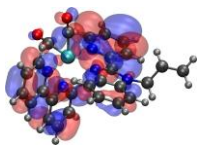
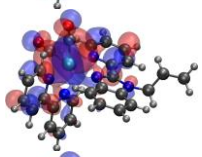
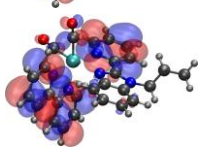
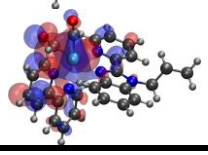
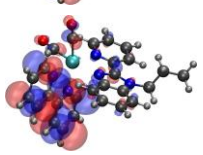
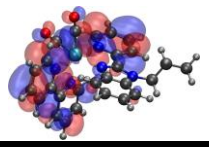
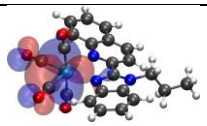
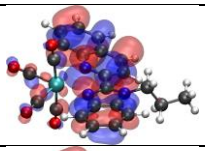
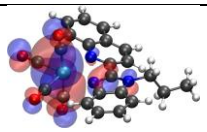
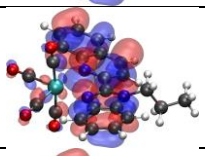
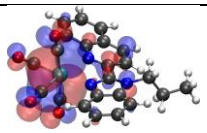
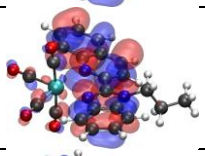
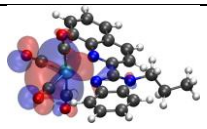
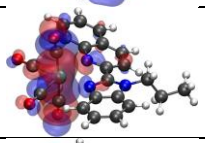
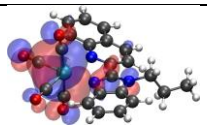
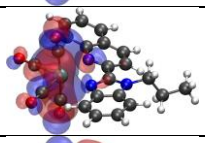
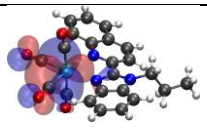
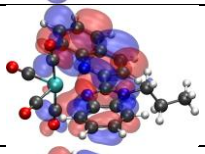
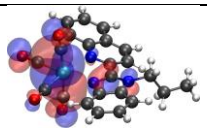
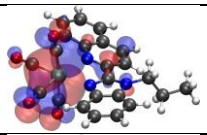
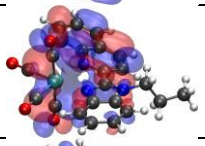
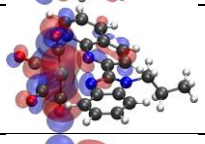
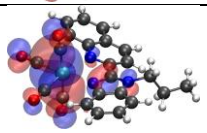
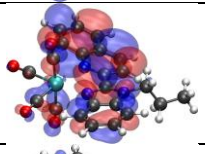
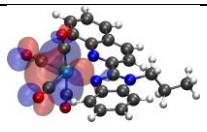
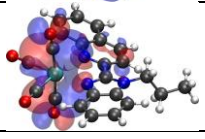
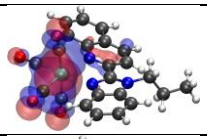
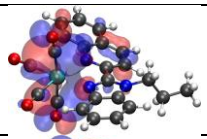
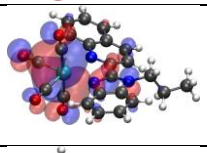
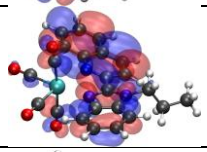
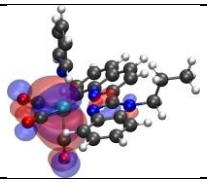
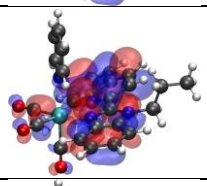
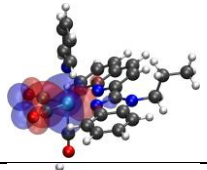
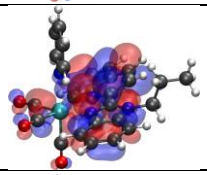
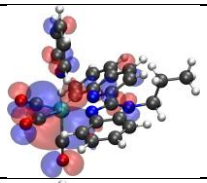
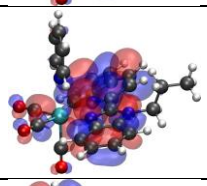
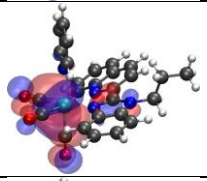
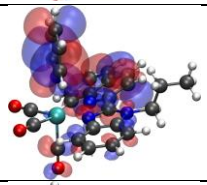
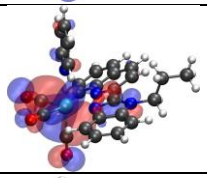
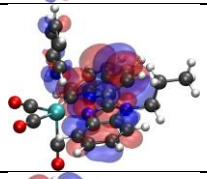
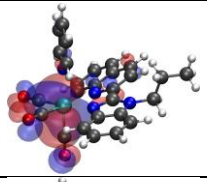
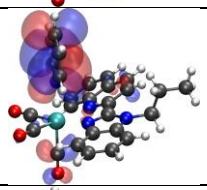
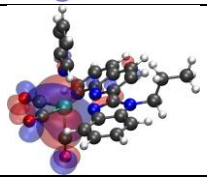
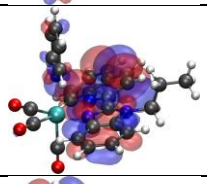
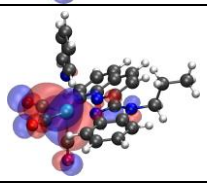
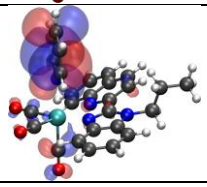
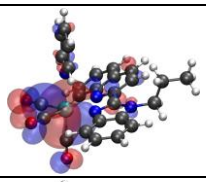
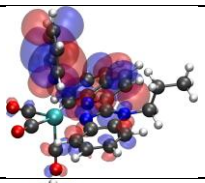
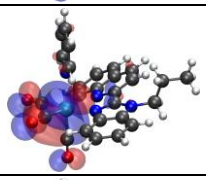
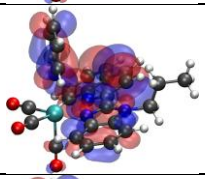
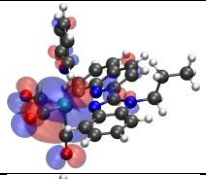
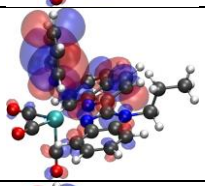
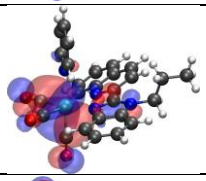
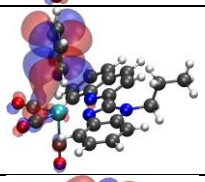
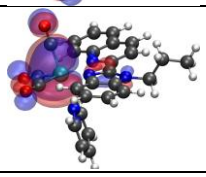
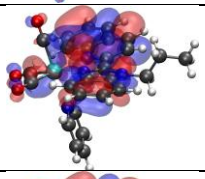
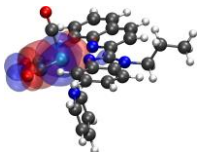
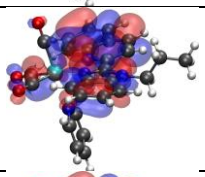
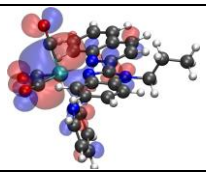
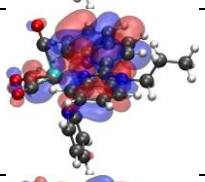
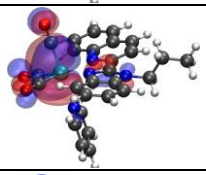
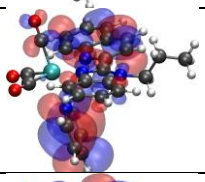
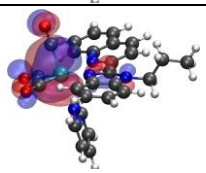
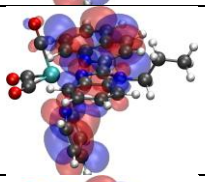
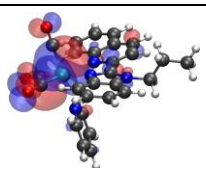
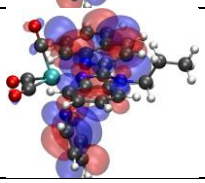
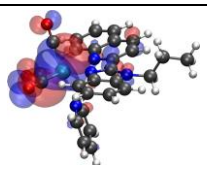
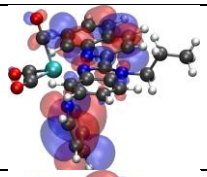
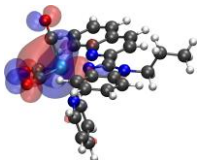
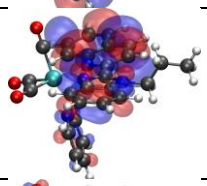
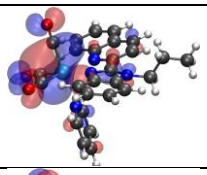
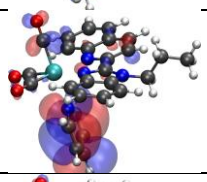
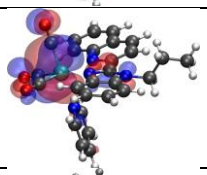
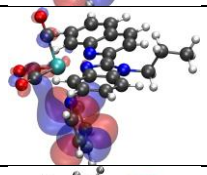
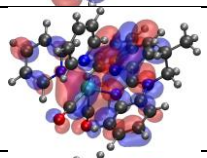
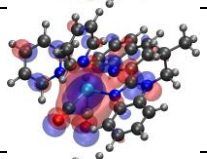
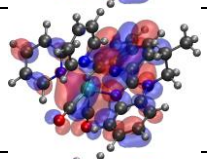
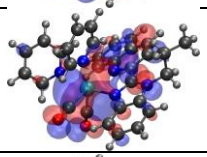
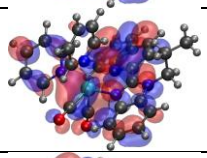
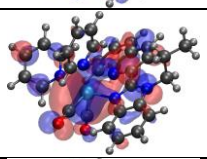
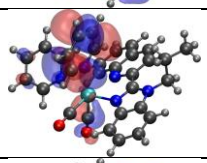
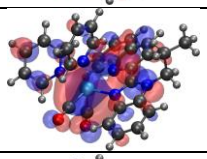
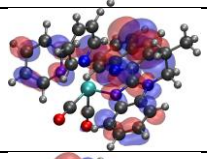
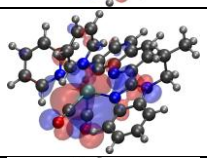
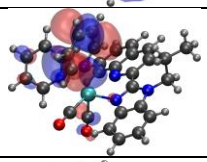
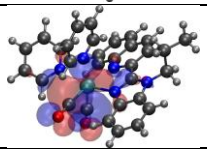
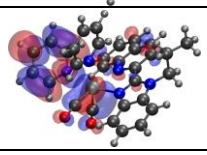
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	S_4 715 nm *0.0254*			
	S_5 672 nm *0.1357*			
	S_6 582 nm *0.0750*			
	S_7 538 nm *0.0196*			
	S_8 503 nm *0.0013*	 	**67%** **33%**	 
	S_9 495 nm *0.0519*			
	S_{10} 483 nm *0.0066*	 	**65%** **33%**	 

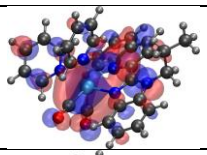
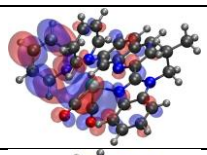
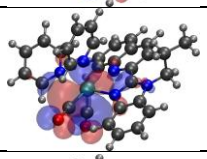
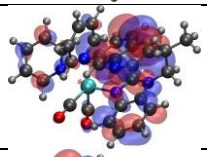
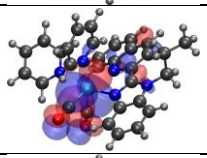
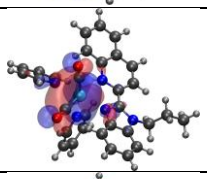
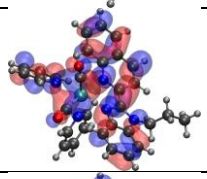
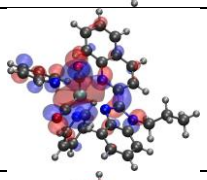
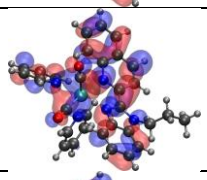
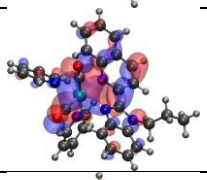
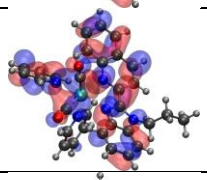
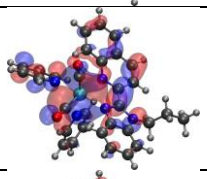
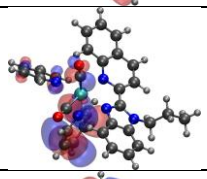
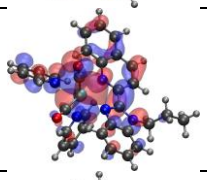
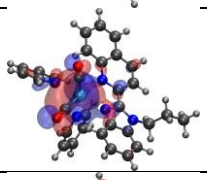
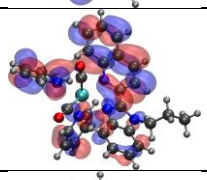
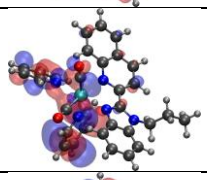
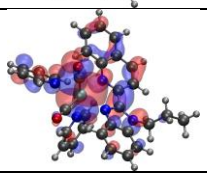
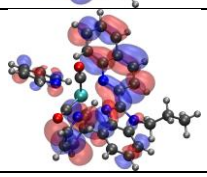
Table S2: Hole and electron NTOs for the first 10 states of all energetically favorable complexes for all complexes with L2. All NTOs are Calculated using TDDFT on the ground state geometry with B3LYP functional and LANL2dz/6-31G* basis set with dichloromethane solvent using the CPCM method.

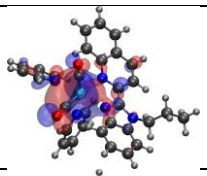
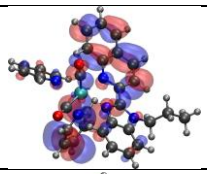
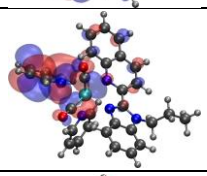
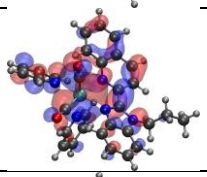
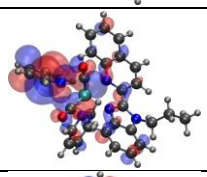
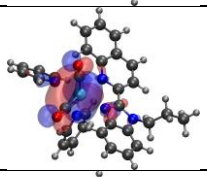
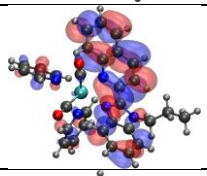
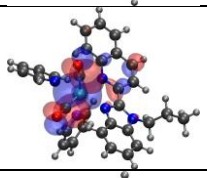
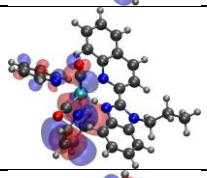
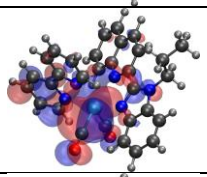
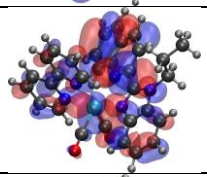
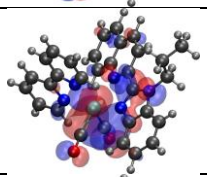
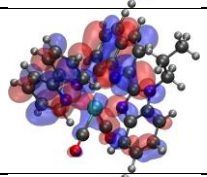
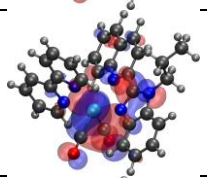
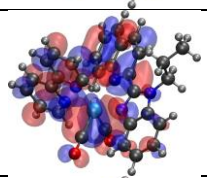
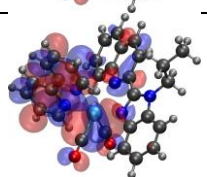
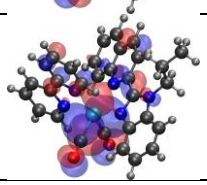
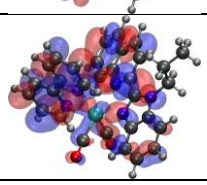
Complex	State/Wavelength/ Oscillator Strength	Hole	Electron
2	**S_1** 654 nm *0.0006*		
	S_2 601 nm *0.0081*		
	S_3 534 nm *0.1087*		
	S_4 409 nm *0.0058*		
	S_5 403 nm *0.0028*		
	S_6 396 nm *0.0076*		
	S_7 385 nm *0.0017*	 **65%**  **33%**	 
	S_8 379 nm *0.0090*		
	S_9 376 nm *0.0016*		

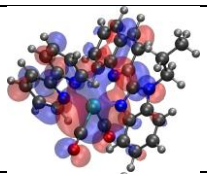
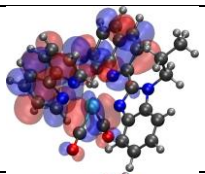
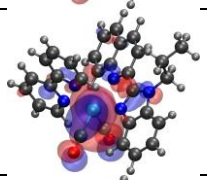
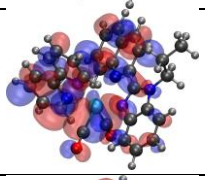
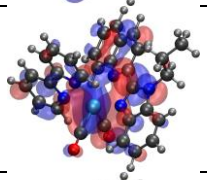
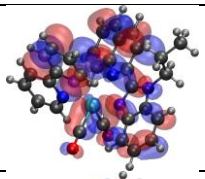
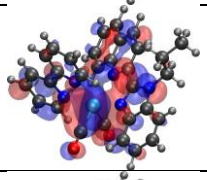
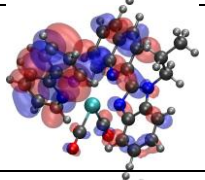
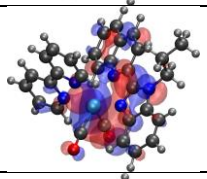
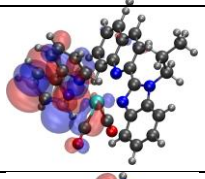
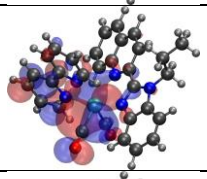
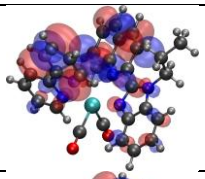
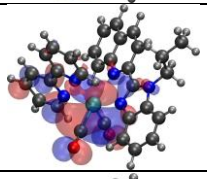
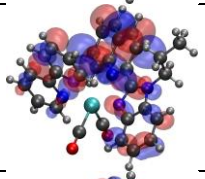
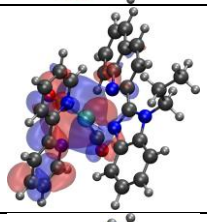
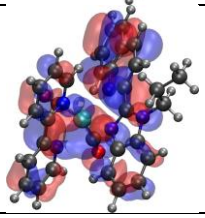
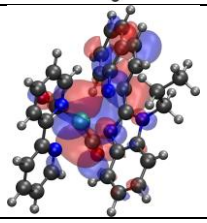
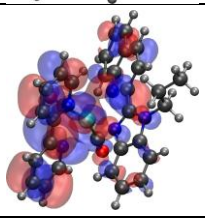
2	**S_{10}** 371 nm *0.0019*		**67%**  **29%**  
2-Py1	**S_1** 898 nm *0.0015*		
	S_2 794 nm *0.0092*		
	S_3 707 nm *0.1024*		
	S_4 490 nm *0.0060*		
2-Py1	**S_5** 469 nm *0.0114*		**61%**  **39%**  
	S_6 463 nm *0.0193*		**64%**  **36%**  

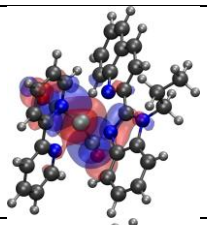
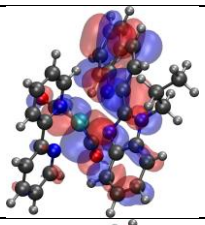
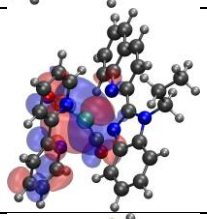
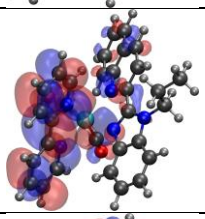
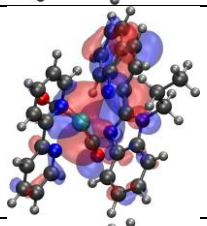
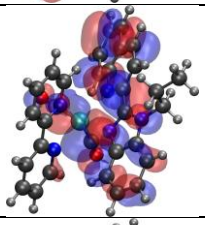
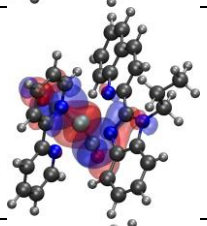
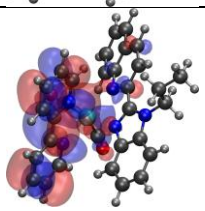
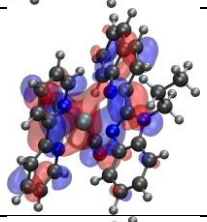
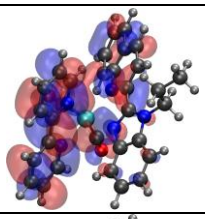
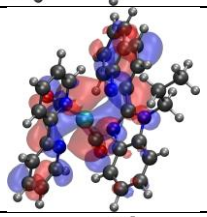
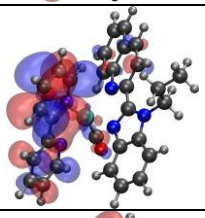
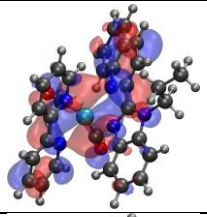
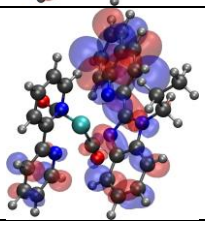
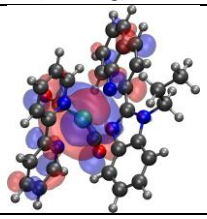
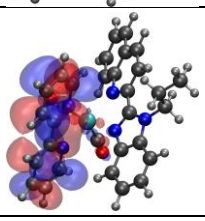
	S_7 449 nm *0.0120*		
	S_8 433 nm *0.0558*		
	S_9 423 nm *0.0515*		
	S_{10} 379 nm *0.0193*		
2-Py4	**S_1** 883 nm *0.0018*		
	S_2 772 nm *0.0072*		
	S_3 693 nm *0.1130*		
	S_4 478 nm *0.0063*		
	S_5 471 nm *0.0108*		
	S_6 451 nm *0.0207*		

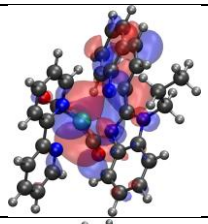
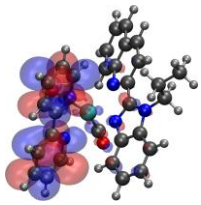
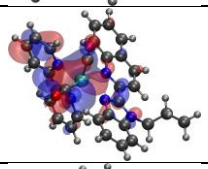
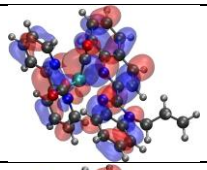
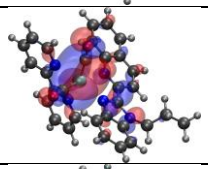
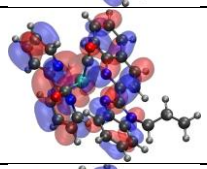
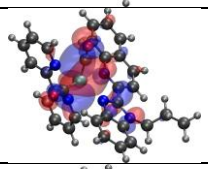
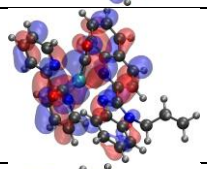
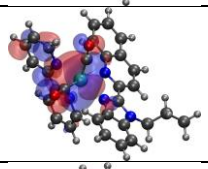
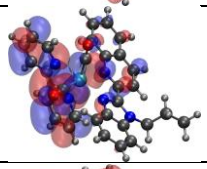
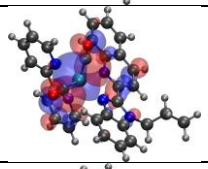
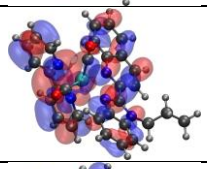
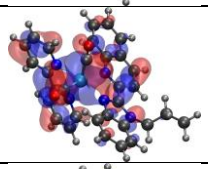
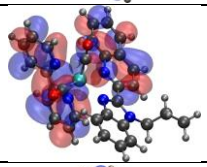
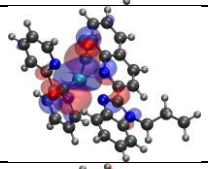
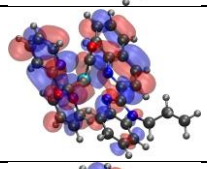
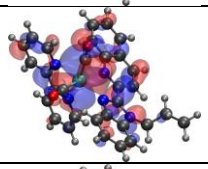
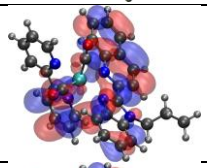
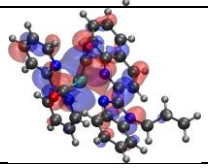
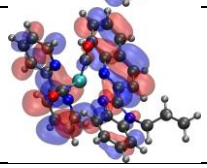
	S_7 449 nm *0.0237*		
	S_8 430 nm *0.0068*		
	S_9 424 nm *0.0762*		
	S_{10} 378 nm *0.0089*		
2-2Py12	**S_1** 1010 nm *0.0028*		
	S_2 950 nm *0.0601*		
	S_3 700 nm *0.1733*		
	S_4 620 nm *0.0354*		
	S_5 560 nm *0.1185*		
	S_6 556 nm *0.0256*		
	S_7 548 nm *0.0020*		

	S_8 511 nm *0.0753*		
	S_9 491 nm *0.0079*		
	S_{10} 487 nm *0.0010*		
2-2Py24	**S_1** 997 nm *0.0024*		
	S_2 925 nm *0.0655*		
	S_3 695 nm *0.1807*		
	S_4 619 nm *0.0369*		
	S_5 559 nm *0.1203*	 **65%**  **35%**	 
	S_6 554 nm *0.0189*	 **69%**	

		 **31%**	
	S_7 551 nm *0.0031*		
	S_8 510 nm *0.0792*		
	S_9 492 nm *0.0082*		
	S_{10} 487 nm *0.0016*		
2-Bpy12	**S_1** 1041 nm *0.0477*		
	S_2 985 nm *0.0215*		
	S_3 853 nm *0.0086*		
	S_4 724 nm *0.0749*		
	S_5 702 nm *0.0650*		

	S_6 585 nm *0.0543*		**66%** 
			**32%** 
	S_7 547 nm *0.0493*		
	S_8 540 nm *0.0216*		
	S_9 506 nm *0.0069*		**69%** 
			**31%** 
	S_{10} 494 nm *0.0129*		
2-Bpy13	**S_1** 1029 nm *0.0351*		
	S_2 925 nm *0.0328*		

	S_3 795 nm *0.0072*		
	S_4 722 nm *0.0501*		
	S_5 705 nm *0.1253*	 **53%**	
		 **48%**	
	S_6 578 nm *0.0647*		
	S_7 526 nm *0.0156*		
	S_8 508 nm *0.0568*		
	S_9 498 nm *0.0055*		

	S_{10} 488 nm *0.0115*		
2-Bpy24	**S_1** 1025 nm *0.0520*		
	S_2 982 nm *0.0208*		
	S_3 833 nm *0.0079*		
	S_4 718 nm *0.0767*		
	S_5 702 nm *0.0737*		
	S_6 581 nm *0.0530*	 **67%**	
		 **31%**	
	S_7 546 nm *0.0458*		
	S_8 536 nm *0.0246*		

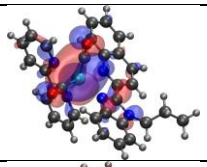
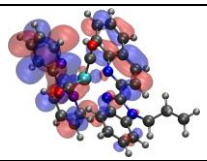
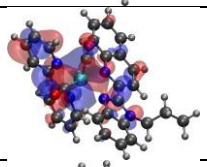
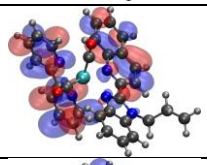
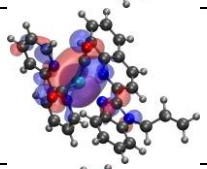
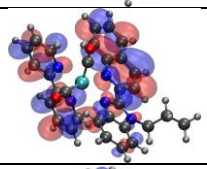
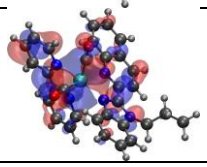
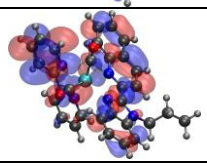
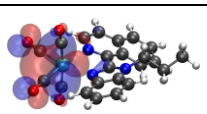
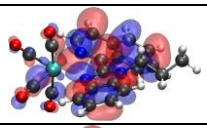
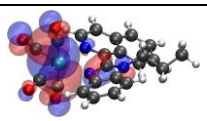
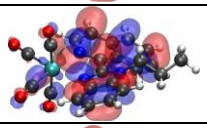
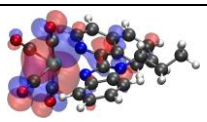
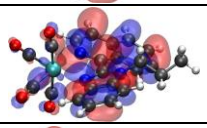
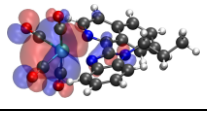
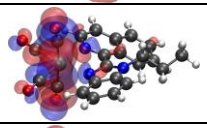
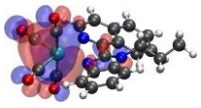
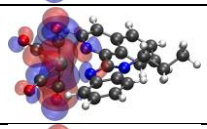
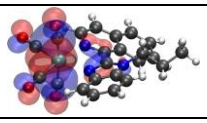
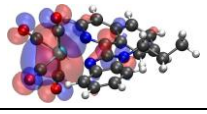
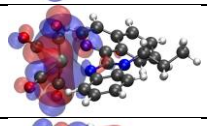
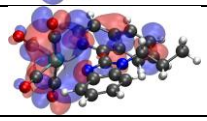
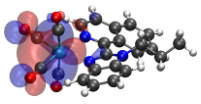
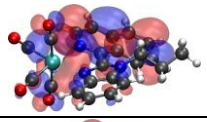
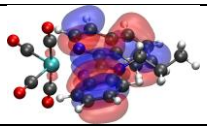
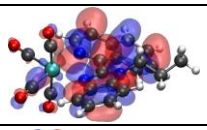
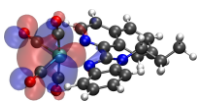
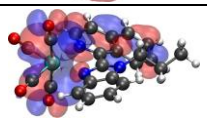
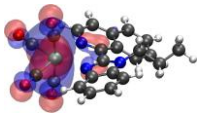
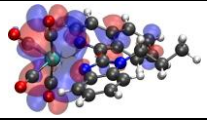
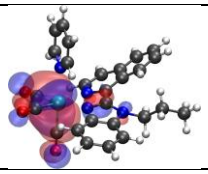
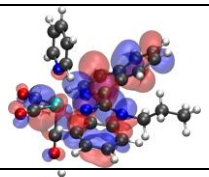
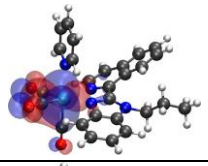
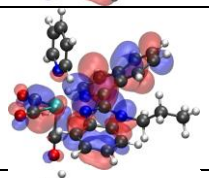
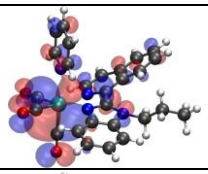
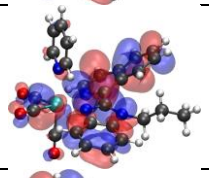
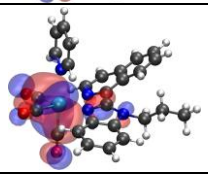
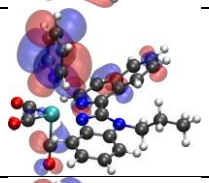
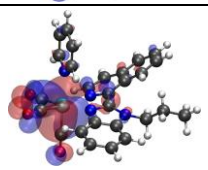
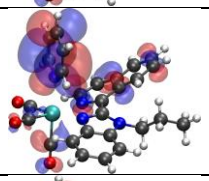
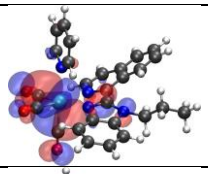
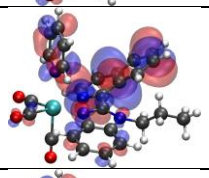
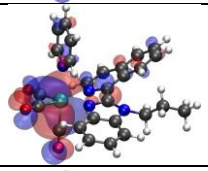
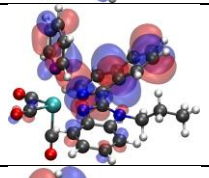
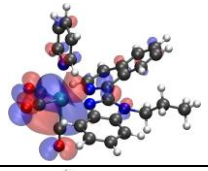
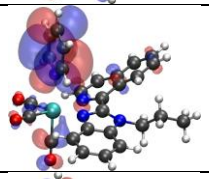
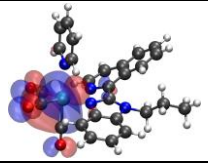
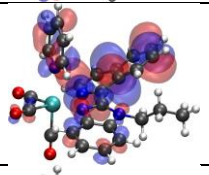
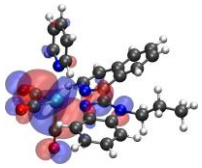
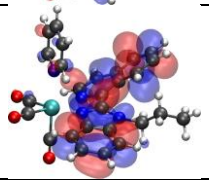
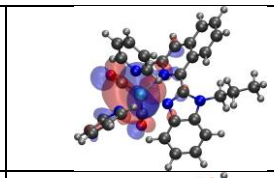
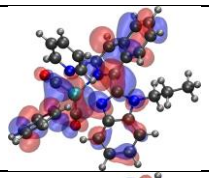
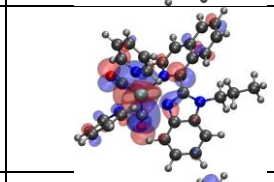
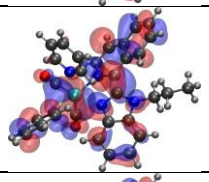
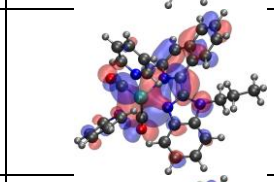
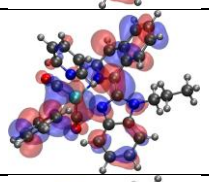
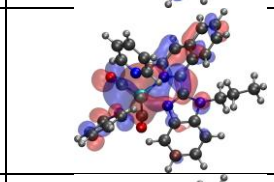
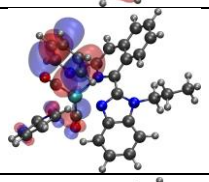
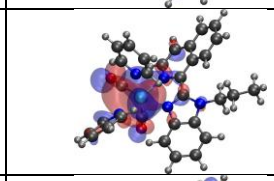
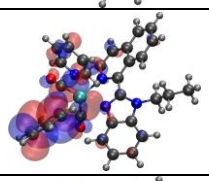
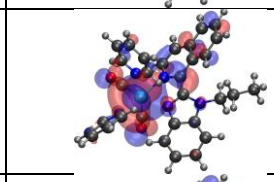
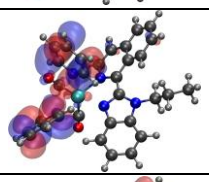
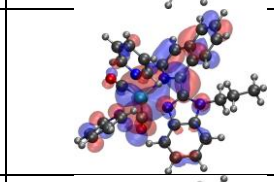
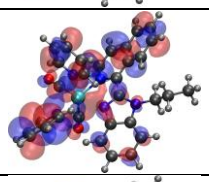
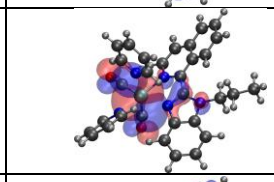
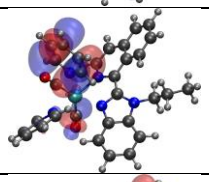
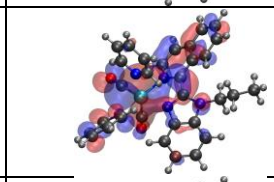
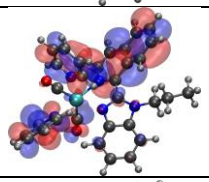
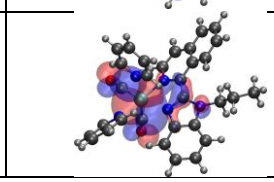
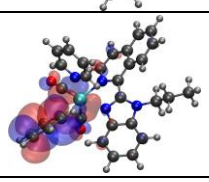
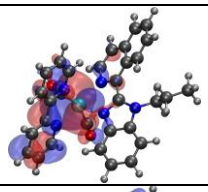
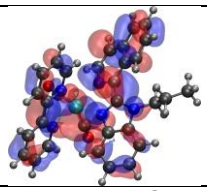
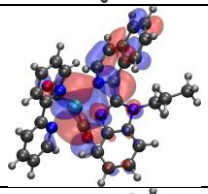
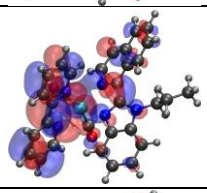
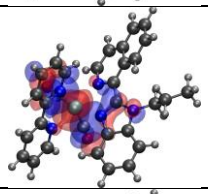
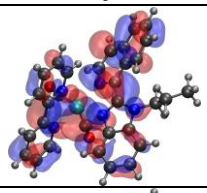
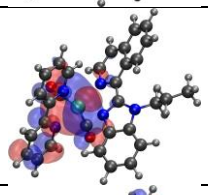
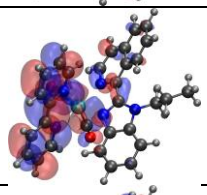
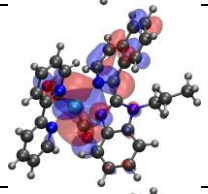
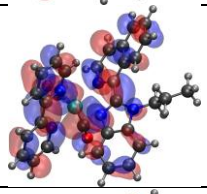
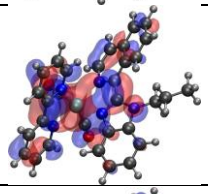
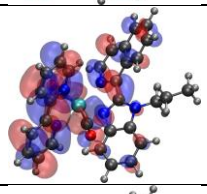
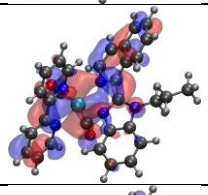
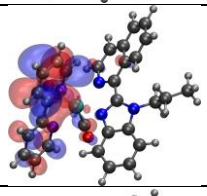
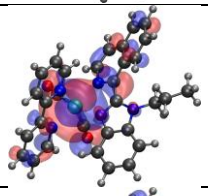
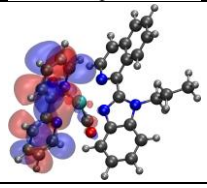
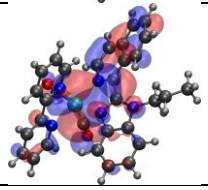
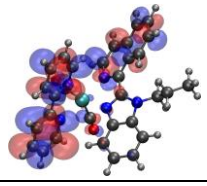
	S_9 505 nm *0.0040*		**61%** 
			**38%** 
	S_{10} 494 nm *0.0138*		**68%** 
			**29%** 

Table S3: Hole and electron NTOs for the first 10 states of all energetically favorable complexes for all complexes with L3. All NTOs are Calculated using TDDFT on the ground state geometry with B3LYP functional and LANL2dz/6-31G* basis set with dichloromethane solvent using the CPCM method.

Complex	State/Wavelength/ Oscillator Strength	Hole	Electron
3	**S_1** 663 nm *0.0039*		
	S_2 604 nm *0.0069*		
	S_3 548 nm *0.1638*		
	S_4 408 nm *0.0051*		
	S_5 403 nm *0.0047*		
	S_6 382 nm *0.0077*	 **50%**  **43%**	 
	S_7 378 nm *0.0139*		
	S_8 375 nm *0.3152*		
	S_9 369 nm *0.0040*		
	S_{10} 367 nm *0.0027*		

3-Py1	**S_1** 886 nm *0.0014*		
	S_2 781 nm *0.0094*		
3-Py1	**S_3** 707 nm *0.1663*		
	S_4 475 nm *0.0017*		
	S_5 454 nm *0.0400*		
	S_6 436 nm *0.0006*		
	S_7 427 nm *0.0300*		
	S_8 425 nm *0.0871*		
	S_9 401 nm *0.0155*		
	S_{10} 386 nm *0.0203*		

3-2Py13	**S_1** 991 nm *0.0165*		
	S_2 826 nm *0.0671*		
3-2Py13	**S_3** 696 nm *0.2866*		
	S_4 616 nm *0.0167*		
	S_5 546 nm *0.0243*		
	S_6 542 nm *0.0540*		
	S_7 506 nm *0.1038*		
	S_8 489 nm *0.0003*		
	S_9 481 nm *0.0041*		
	S_{10} 471 nm *0.0021*		

3-Bpy13	**S_1** 1000 nm *0.0470*		
	S_2 876 nm *0.0456*		
3-Bpy13	**S_3** 770 nm *0.0243*		
	S_4 697 nm *0.0433*		
	S_5 676 nm *0.1629*		
	S_6 569 nm *0.0837*		
	S_7 514 nm *0.0112*		
	S_8 485 nm *0.0029*		
	S_9 475 nm *0.0280*		

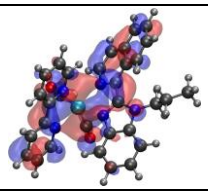
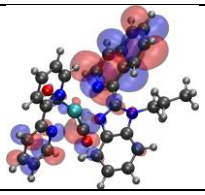
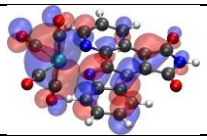
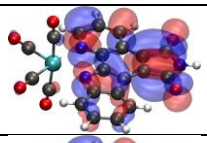
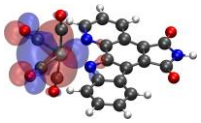
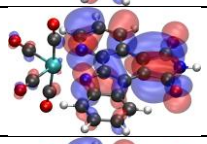
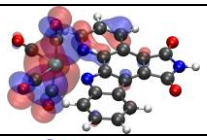
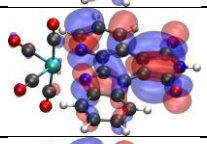
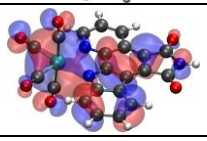
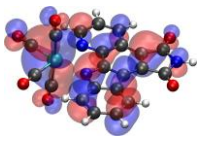
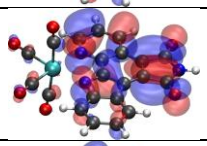
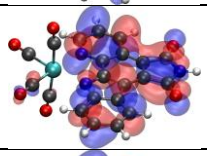
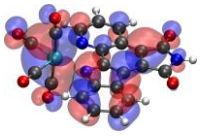
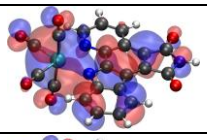
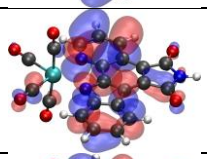
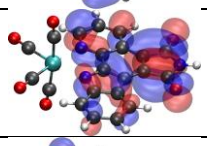
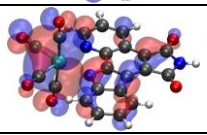
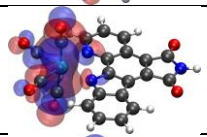
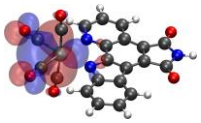
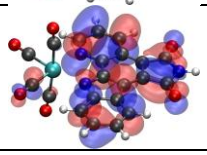
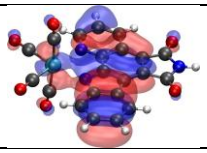
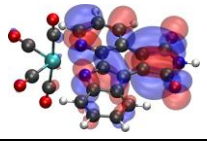
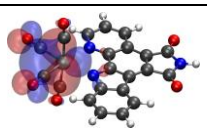
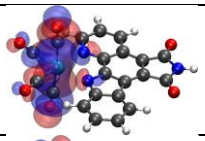
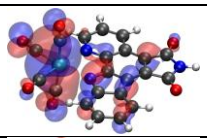
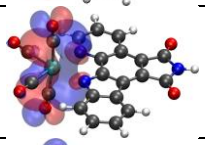
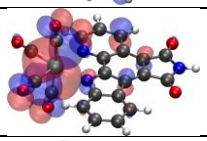
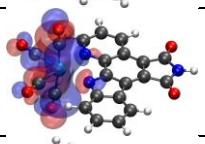
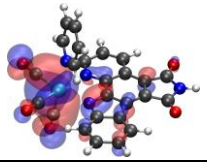
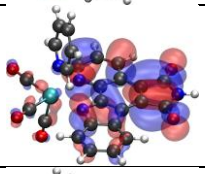
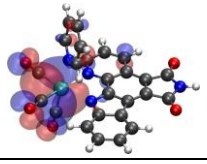
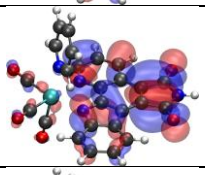
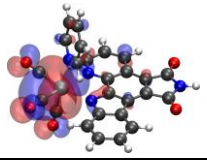
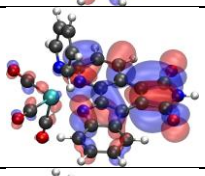
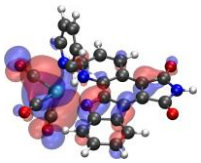
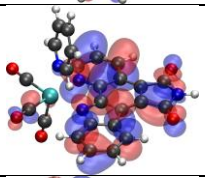
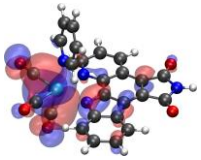
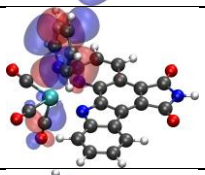
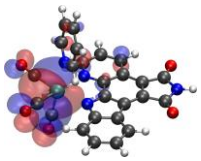
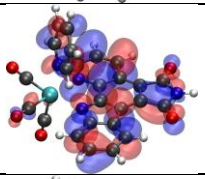
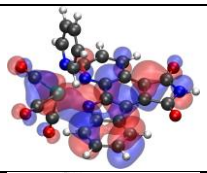
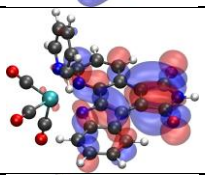
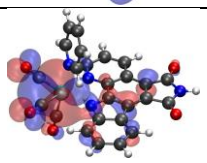
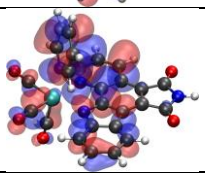
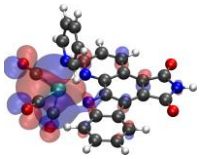
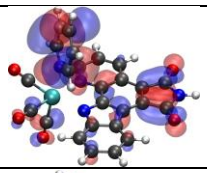
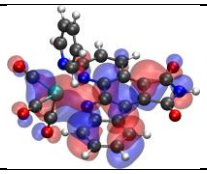
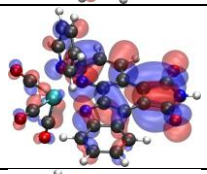
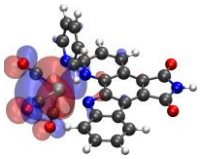
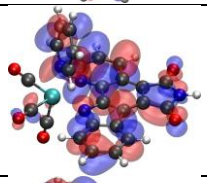
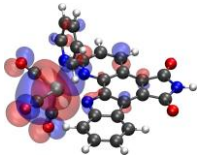
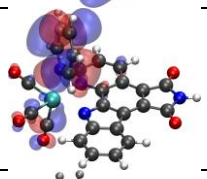
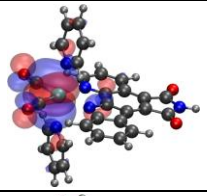
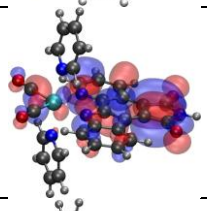
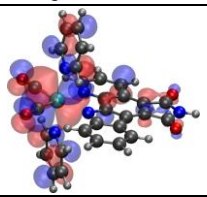
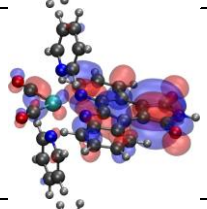
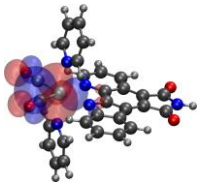
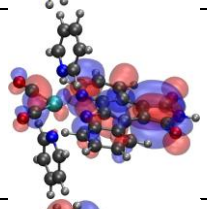
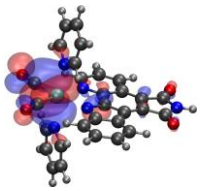
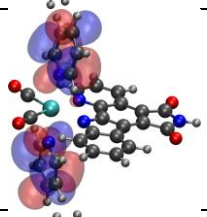
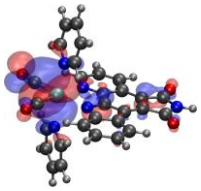
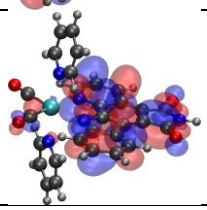
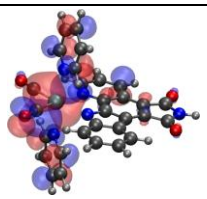
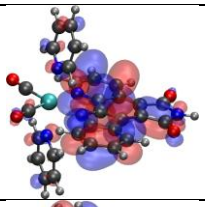
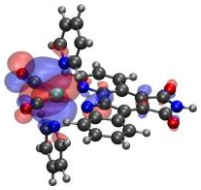
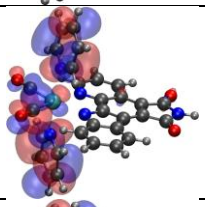
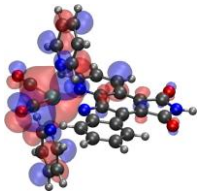
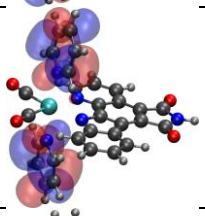
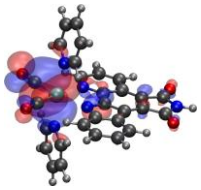
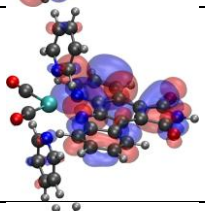
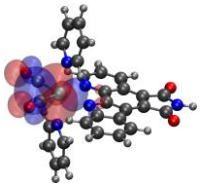
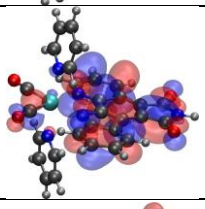
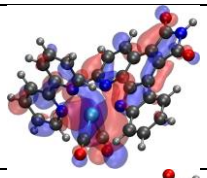
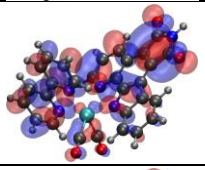
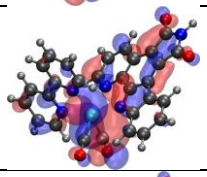
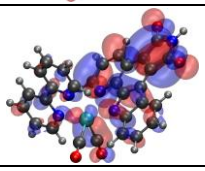
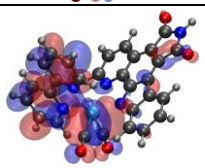
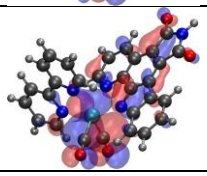
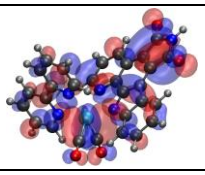
	S_{10} 468 nm *0.0319*		

Table S4: Hole and electron NTOs for the first 10 states of all energetically favorable complexes for all complexes with L4. All NTOs are Calculated using TDDFT on the ground state geometry with B3LYP functional and LANL2dz/6-31G* basis set with dichloromethane solvent using the CPCM method.

Complex	State/Wavelength/ Oscillator Strength	Hole	Electron
4	**S_1** 626 nm *0.1148*		
	S_2 611 nm *0.0000*		
	S_3 536 nm *0.0457*		
	S_4 454 nm *0.0289*	 **54%**  **46%**	 
	S_5 438 nm *0.0643*	 **54%**  **45%**	 
	S_6 435 nm *0.0008*		
	S_7 425 nm *0.0000*		
	S_8 422 nm *0.0516*		

	S_9 413 nm *0.0188*		
	S_{10} 396 nm *0.0000*	 **57%**	
4		 **42%**	
4-Py1	**S_1** 845 nm *0.0336*		
	S_2 777 nm *0.0413*		
	S_3 723 nm *0.0379*		
	S_4 541 nm *0.0041*		
	S_5 514 nm *0.0116*		
	S_6 496 nm *0.0377*		
	S_7 482 nm *0.0614*	 **52%**	
		 **34%**	

	S_8 479 nm *0.0502*		**55%** 
4-Py1			**40%** 
	S_9 474 nm *0.0419*		
	S_{10} 452 nm *0.0821*		
4-2Py14	**S_1** 1768 nm *0.0029*		
	S_2 1226 nm *0.1058*		
	S_3 923 nm *0.0000*		
	S_4 801 nm *0.0001*		
	S_5 783 nm *0.0045*		

	S_6 686 nm *0.0519*		
4-2Py14	**S_7** 651 nm *0.0027*		
	S_8 614 nm *0.4186*		
	S_9 546 nm *0.0086*		
	S_{10} 542 nm *0.0001*		
4-Bpy12	**S_1** 1139 nm *0.1410*		
	S_2 1038 nm *0.0023*	 **68%**  **32%**	 
	S_3 956 nm *0.0300*		

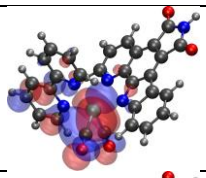
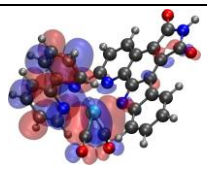
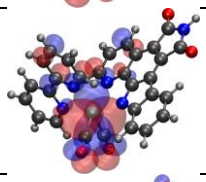
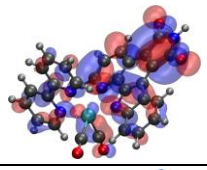
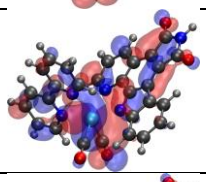
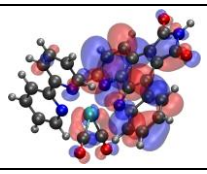
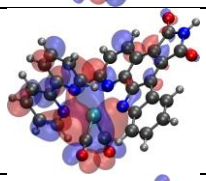
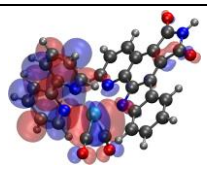
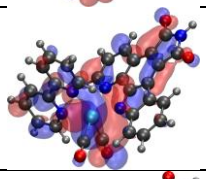
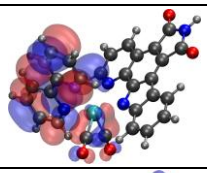
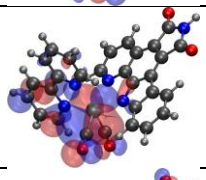
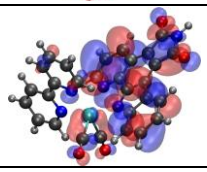
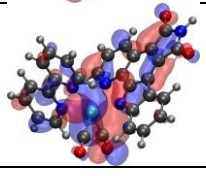
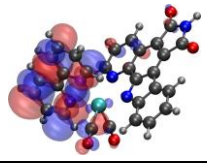
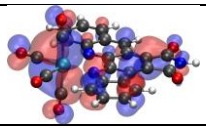
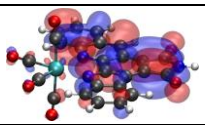
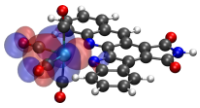
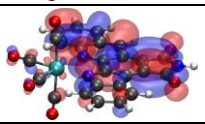
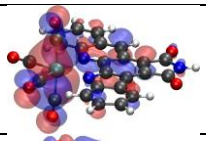
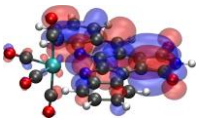
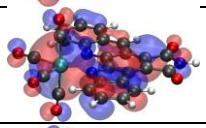
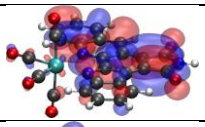
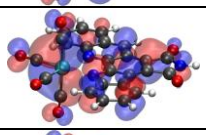
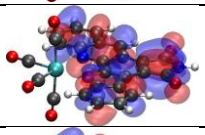
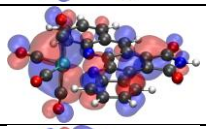
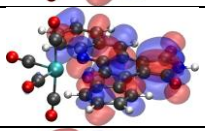
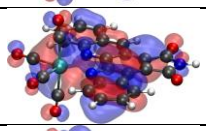
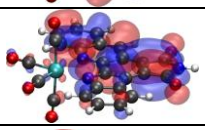
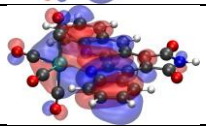
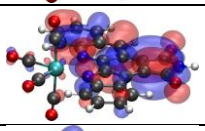
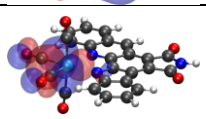
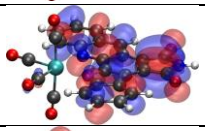
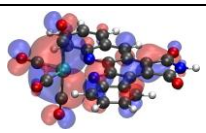
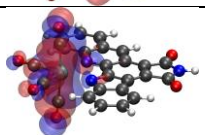
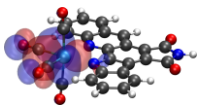
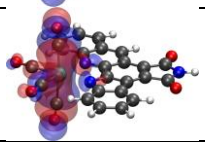
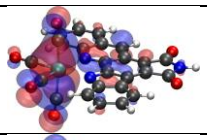
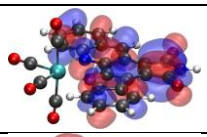
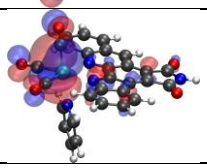
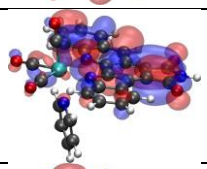
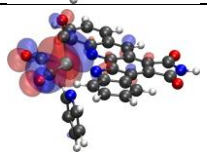
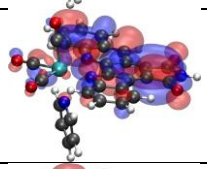
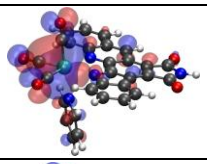
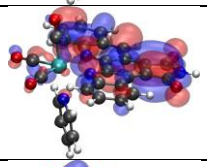
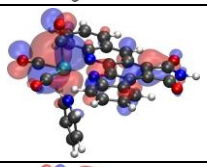
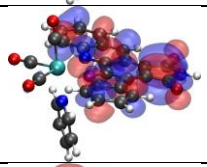
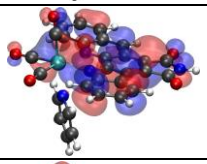
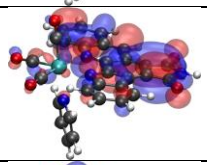
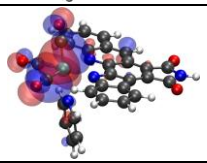
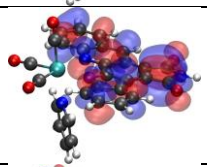
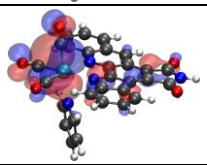
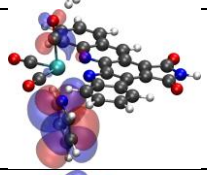
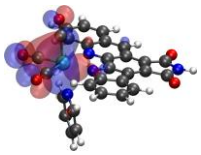
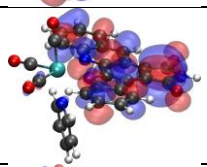
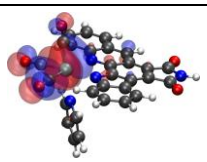
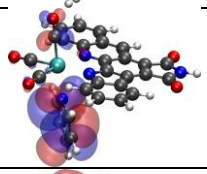
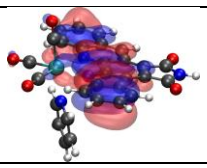
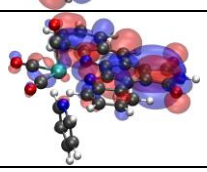
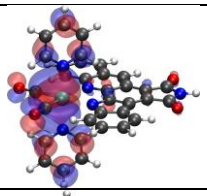
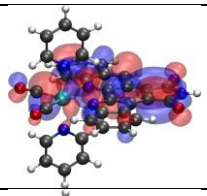
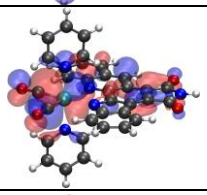
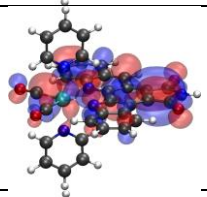
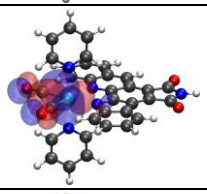
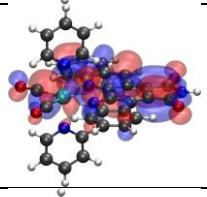
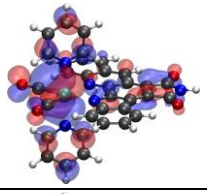
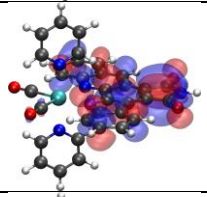
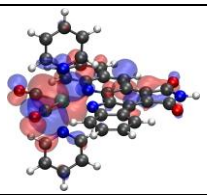
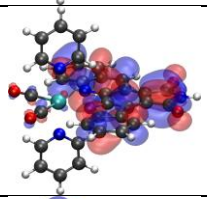
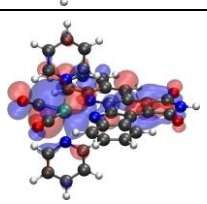
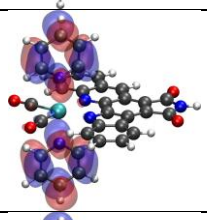
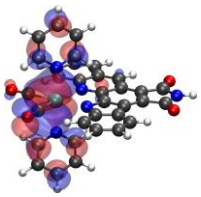
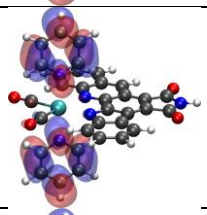
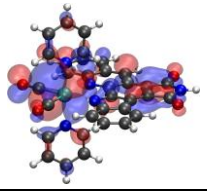
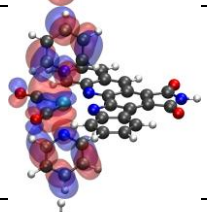
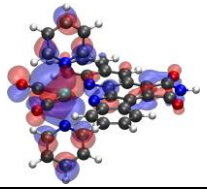
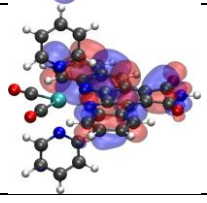
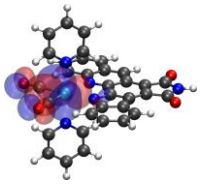
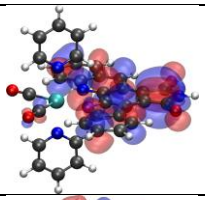
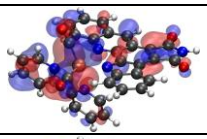
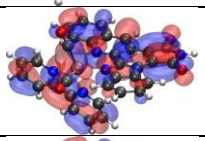
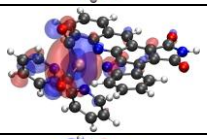
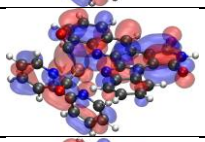
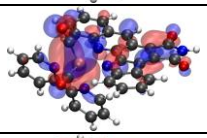
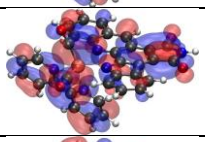
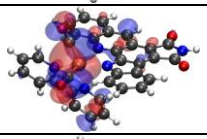
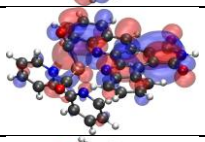
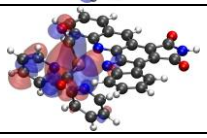
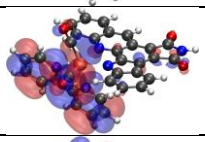
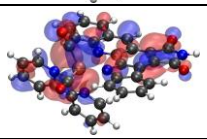
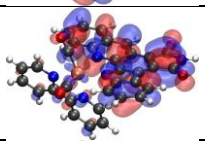
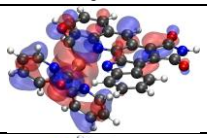
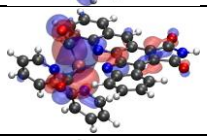
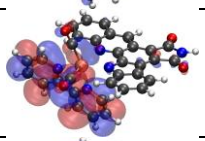
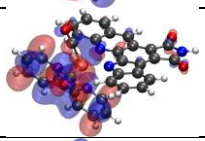
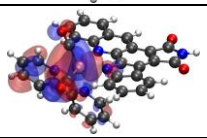
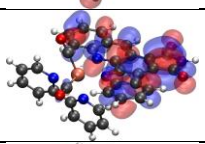
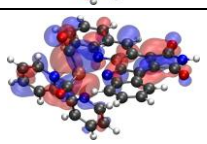
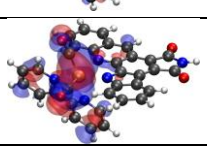
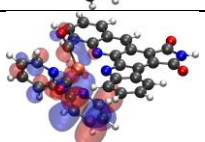
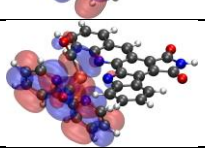
	S_4 767 nm *0.0328*		
4-Bpy12	**S_5** 746 nm *0.0299*		
	S_6 690 nm *0.0282*		
	S_7 620 nm *0.0641*		
	S_8 584 nm *0.0324*		
	S_9 577 nm *0.0014*		
	S_{10} 555 nm *0.0117*		

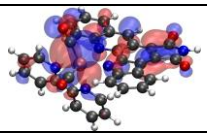
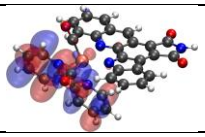
Table S5: Hole and electron NTOs for the first 10 states of all energetically favorable complexes for all complexes with L5. All NTOs are Calculated using TDDFT on the ground state geometry with B3LYP functional and LANL2dz/6-31G* basis set with dichloromethane solvent using the CPCM method.

Complex	State/Wavelength/ Oscillator Strength	Hole	Electron
5	**S_1** 696 nm *0.1506*		
	S_2 683 nm *0.0000*		
	S_3 589 nm *0.0636*		
5	**S_4** 498 nm *0.0090*		
		 **71%**	 **29%**
	S_5 485 nm *0.0014*	 **70%**	
		 **30%**	
	S_6 450 nm *0.0889*		
	S_7 448 nm *0.0000*		
	S_8 435 nm *0.0010*		
	S_9 412 nm *0.0218*		

	S_{10} 409 nm *0.0291*		
5-Py4	**S_1** 976 nm *0.0302*		
	S_2 863 nm *0.0431*		
	S_3 799 nm *0.0788*		
5-Py4	**S_4** 590 nm *0.0041*		
	S_5 532 nm *0.0891*		
	S_6 531 nm *0.0106*		
	S_7 512 nm *0.0097*		
	S_8 504 nm *0.0031*		
	S_9 472 nm *0.0266*		
	S_{10} 458 nm *0.0758*		

5-2Py14	**S_1** 2169 nm *0.0060*		
	S_2 1066 nm *0.1635*		
	S_3 956 nm *0.0000*		
5-2Py14	**S_4** 835 nm *0.0424*		
	S_5 682 nm *0.0243*		
	S_6 678 nm *0.0732*		
	S_7 609 nm *0.4024*		
	S_8 544 nm *0.0117*		
	S_9 538 nm *0.0368*		

	S_{10} 534 nm *0.0001*		
5-Bpy24	**S_1** 1169 nm *0.1408*		
	S_2 1097 nm *0.0094*		
5-Bpy24	**S_3** 944 nm *0.0534*		
	S_4 789 nm *0.0698*		
	S_5 737 nm *0.0182*		
	S_6 725 nm *0.0199*		
	S_7 613 nm *0.0452*	 **67%**  **32%**	 
	S_8 594 nm *0.0022*		
	S_9 585 nm *0.0393*	 **66%**  **28%**	 

	S_{10} 545 nm *0.0223*		

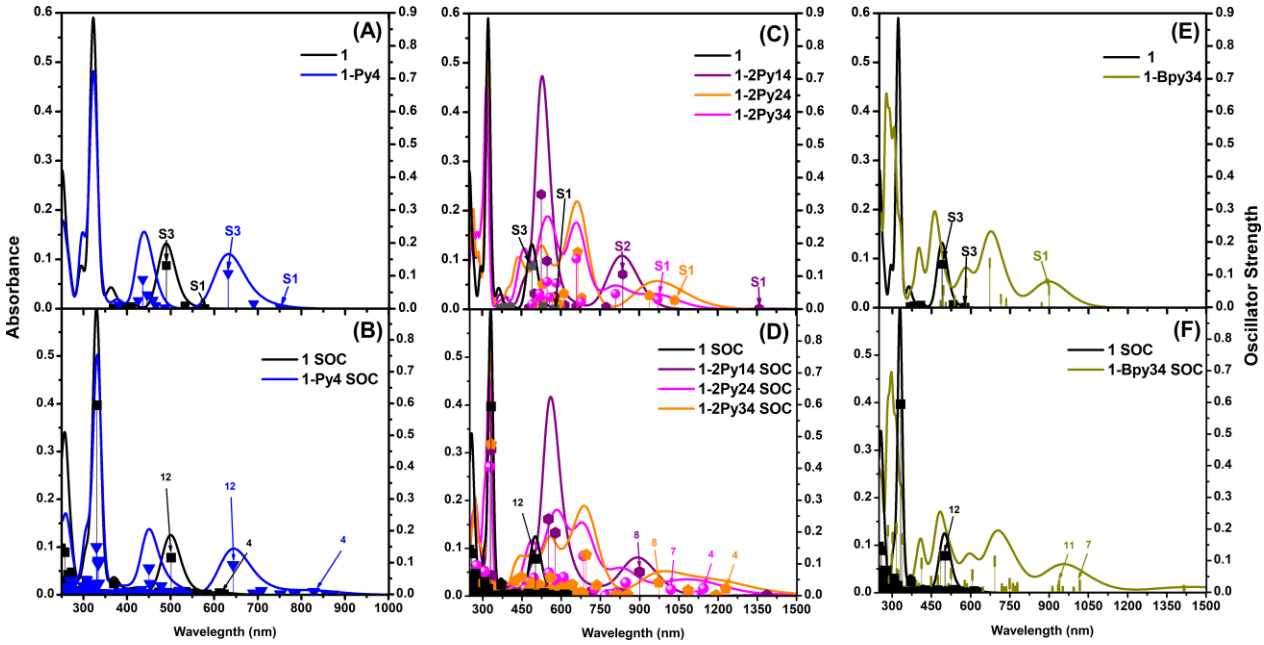


Figure S11: Shows the calculated absorbance spectra of the most energetically favorable isomers of all complexes with L1 for Py (A), 2Py (C), and Bpy (E) and compares them with when spin orbit coupling is considered for Py (B), 2Py (D) and Bpy (F). The first state and most optically active state are shown in the absorbance spectra (A, C, and E) while the corresponding states are labeled in the SOC spectra(B, D, and F)..

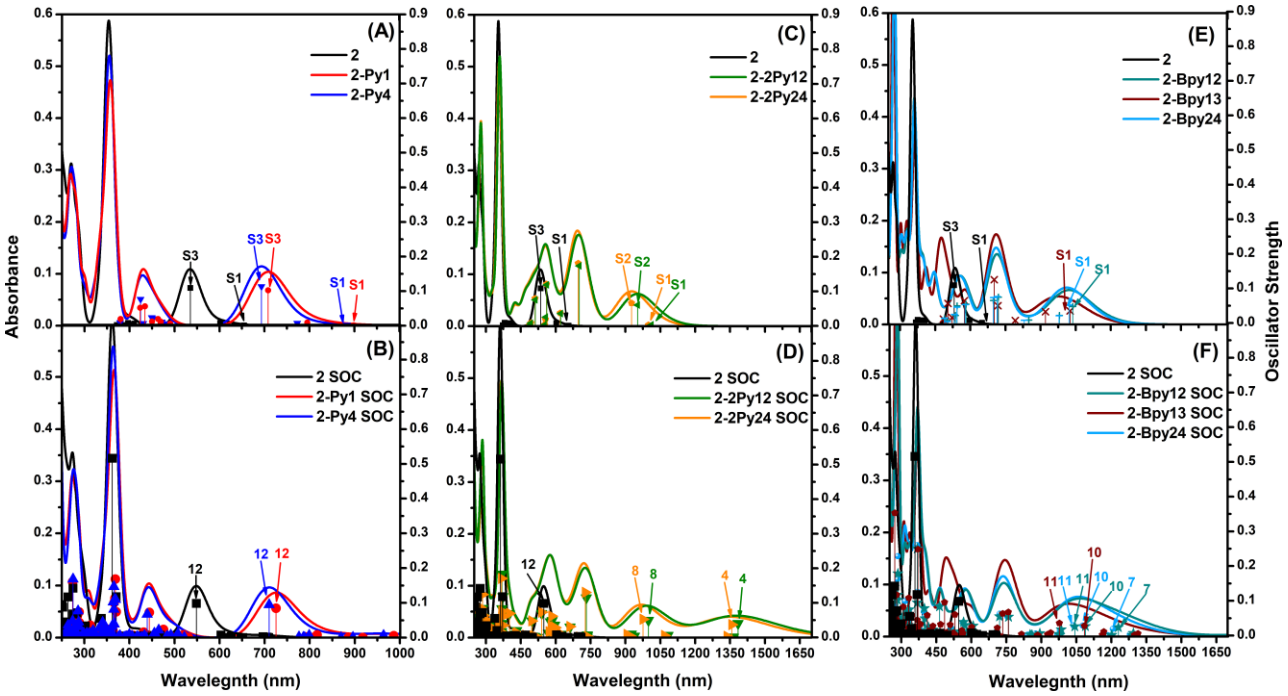


Figure S12: Shows the calculated absorbance spectra of the most energetically favorable isomers of all complexes with L2 for Py (A), 2Py (C), and Bpy (E) and compares them with when spin orbit coupling is considered for Py (B), 2Py (D) and Bpy (F). The first state and most optically active state are shown in the absorbance spectra (A, C, and E) while the corresponding states are labeled in the SOC spectra (B, D, and F).

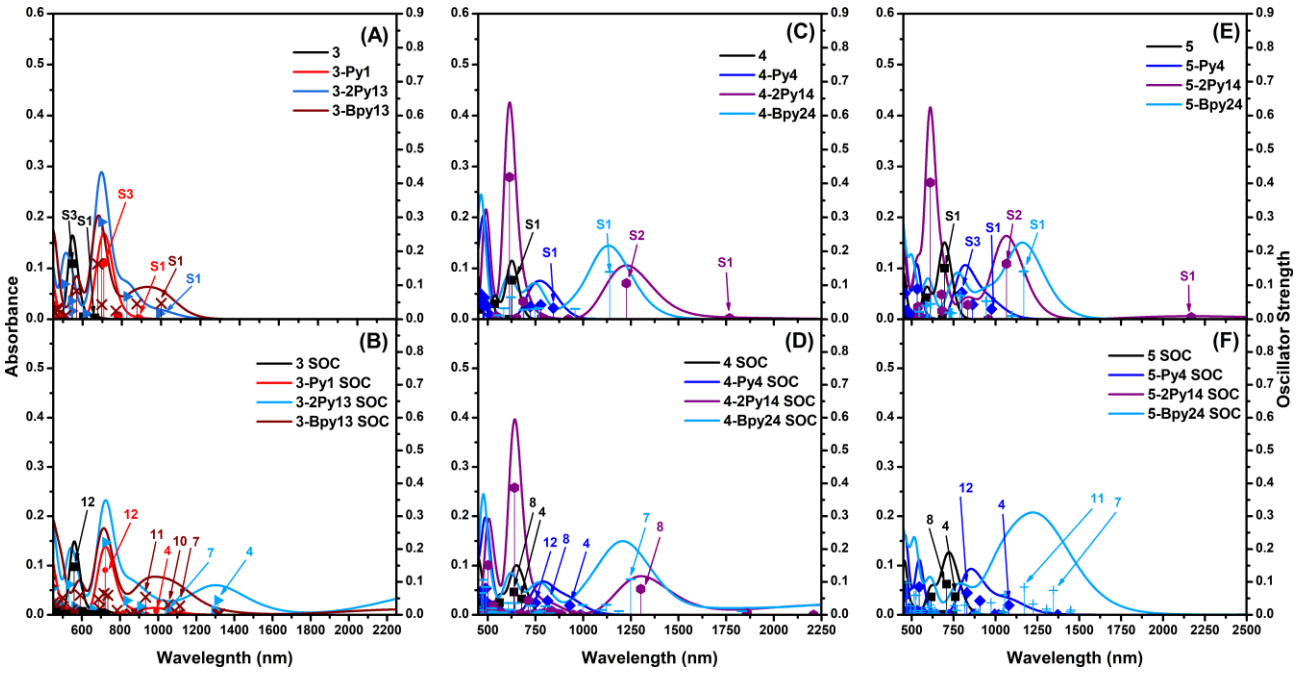
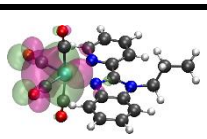
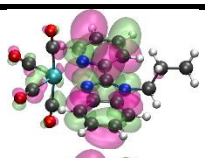
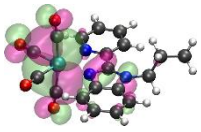
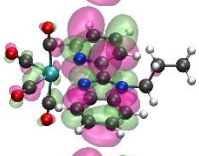
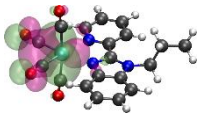
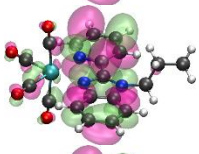
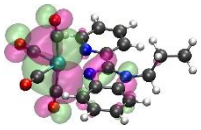
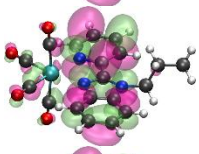
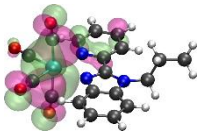
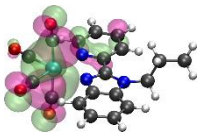
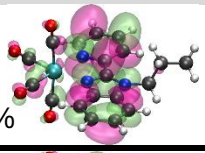
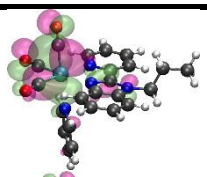
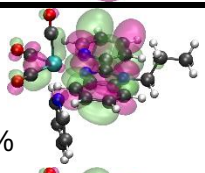
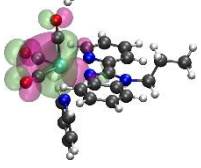
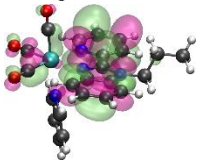
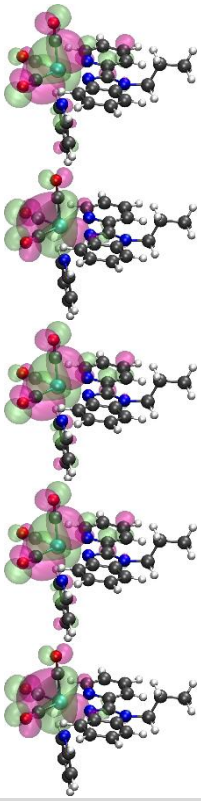
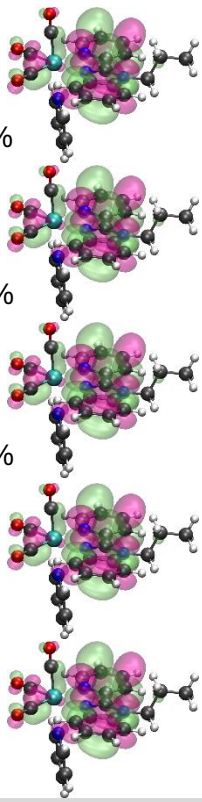
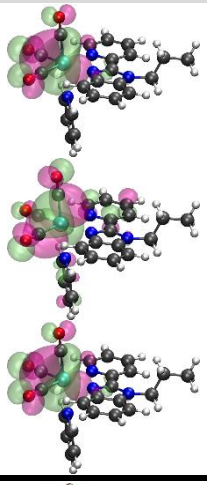
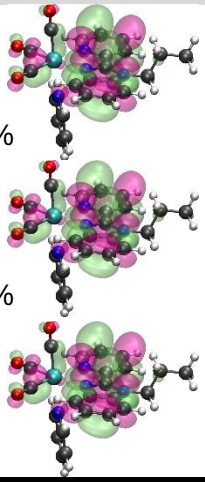
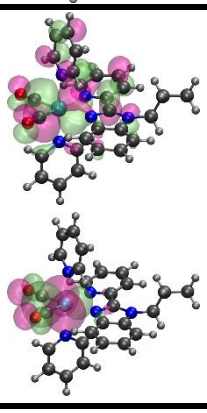
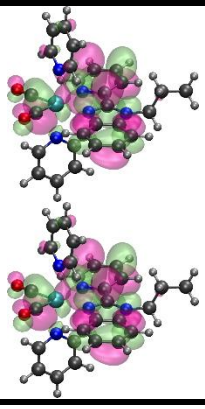


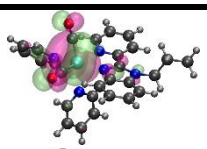
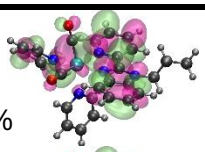
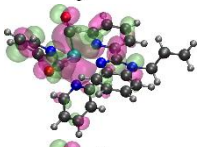
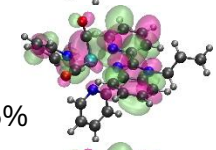
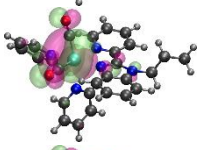
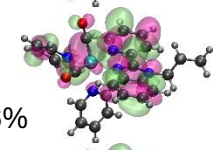
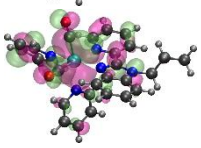
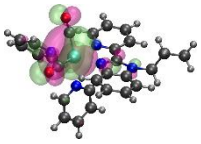
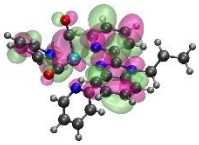
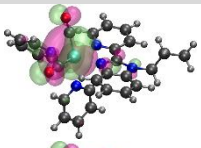
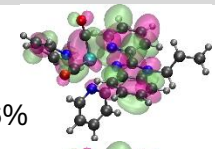
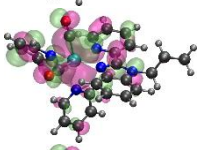
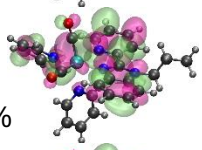
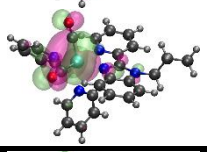
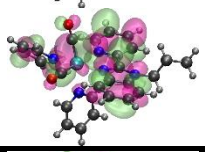
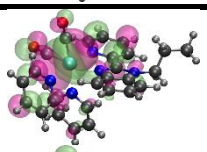
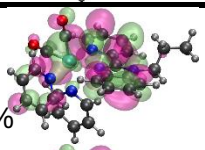
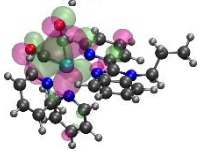
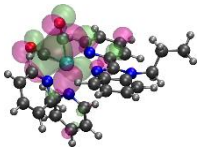
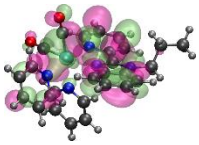
Figure S13: Shows the calculated absorbance spectra of the most energetically favorable isomers

of all complexes for L3 (A), L4 (C), and L5 (E) and compares them with when spin orbit coupling is considered for L3 (B), L4 (D) and L5 (F). The first state and most optically active state are shown in the absorbance spectra (A, C, and E) while the corresponding states are labeled in the SOC spectra (B, D, and F).

Table S6: Hole and electron MOs for the spin orbit coupling excited states that are comparable to the first optically active peak NTO's shown previously; for all energetically favorable complexes for all complexes with L1. All MOs are calculated using SOC-TDDFT on the ground state geometry with B3LYP functional and ZORA-def2-TZVP/SARC-ZORA-TZVP basis set with dichloromethane solvent using the CPCM method.

Complex	SOC State/ Wavelength/ Oscillator Strength	% of Singlet or Triplet		Hole	Electron
1	**4** 612 nm 0.0036	S_1	3		
		S_2	4		
		T_1	68		
		T_2	12		
		T_3	12		
	12 500 nm 0.1150	S_3	94		 71%
1-Py4	**4** 828 nm 0.0077	S_1	4		 74%
	4 828 nm 0.0077	S_2	3		

1-Py4		**S_3**	2		55% 35% 44% 39% 
		T_2 (+1)	39		
		T_2 (-1)	39		
		T_3	8		
	12 642 nm 0.0926	**S_3**	94		44% 39% 
		T_3 (+1)	2		
		T_3 (-1)	2		
1-2Py14	**8** 898 nm 0.0745	**S_2**	82		
		T_3 (+1)	6		
		T_3 (-1)	6		

1-2Py24	**4** 1228 nm 0.0225	**S_1**	8		51% 
					45% 
		S_2	4		46% 
					42% 
		T_2 (0)	75		
		T_2 (+1)	5		
		T_2 (-1)	5		
	8 972 nm 0.0420	**S_2**	88		46% 
					42% 
		T_2 (0)	6		
1-2Py34	**4** 1142 nm 0.0231	**S_1**	7		58% 
					39% 
	4 1142 nm 0.0231	**T_2 (0)**	23		
		T_2 (+1)	33		
		T_2 (-1)	33		

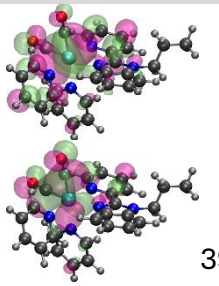
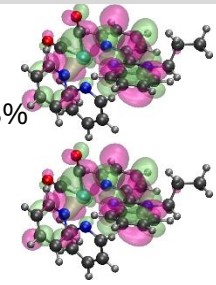
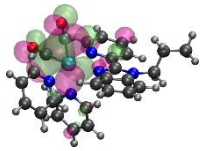
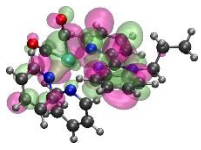
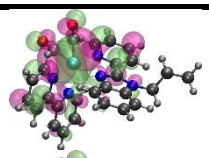
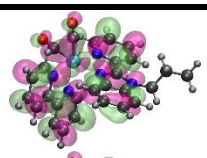
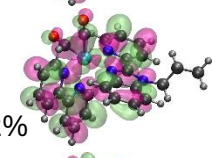
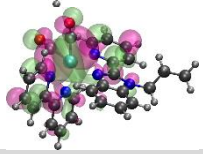
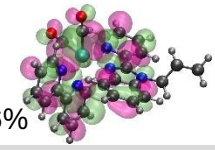
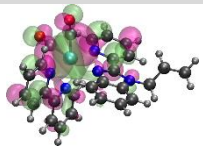
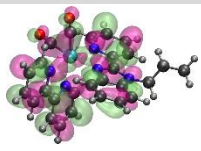
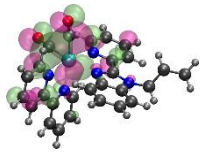
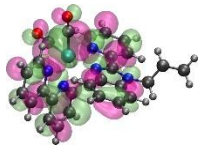
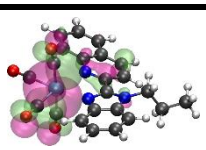
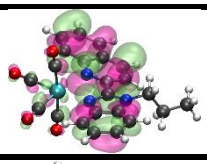
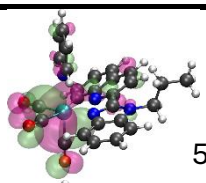
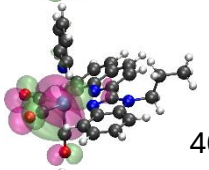
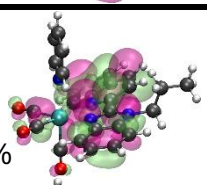
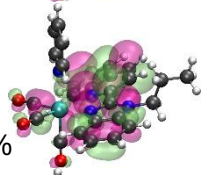
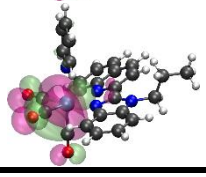
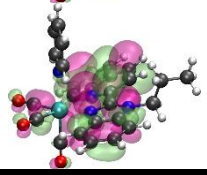
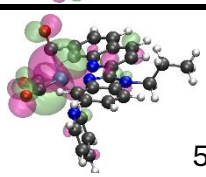
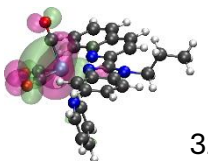
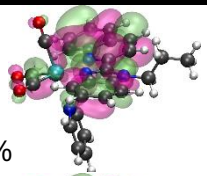
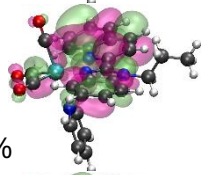
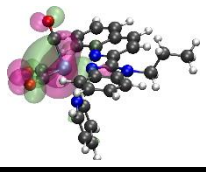
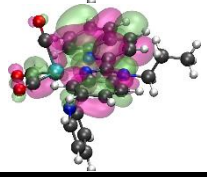
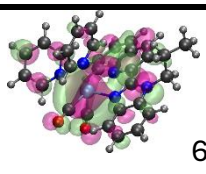
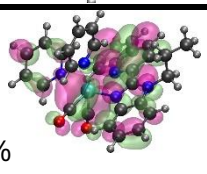
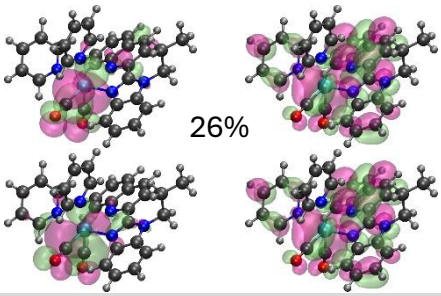
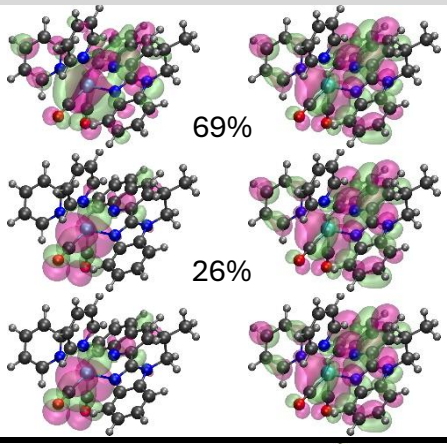
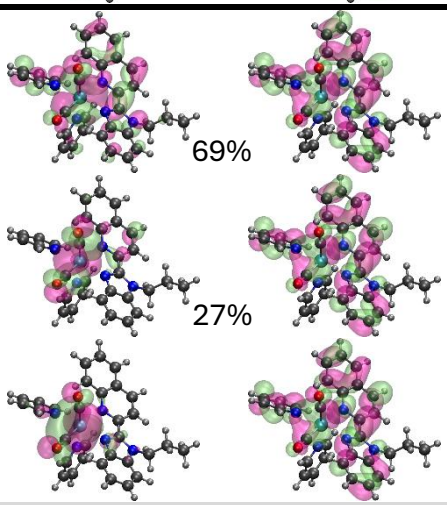
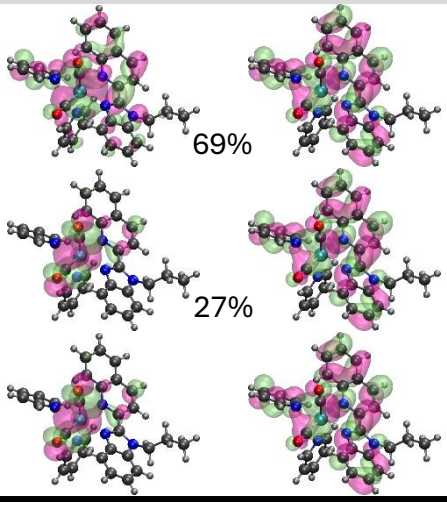
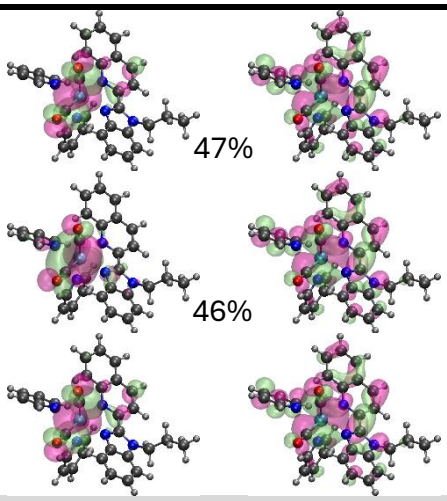
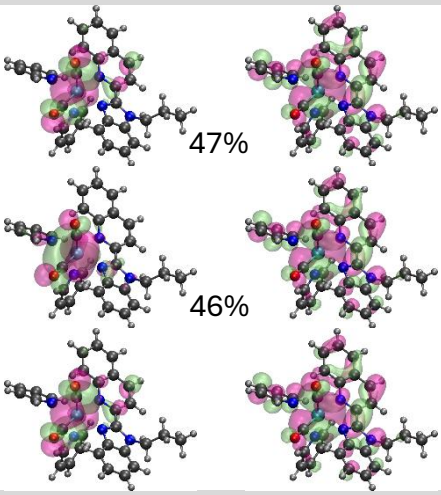
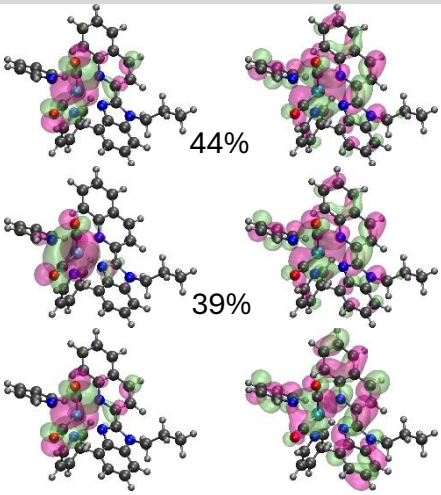
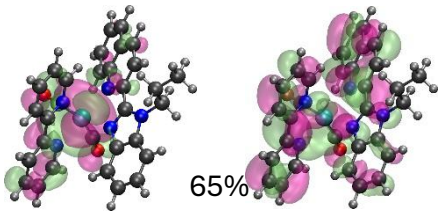
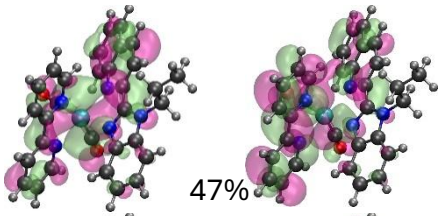
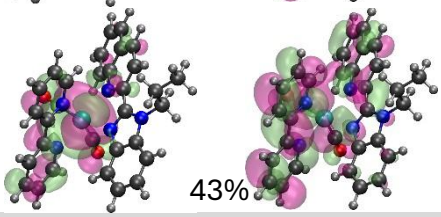
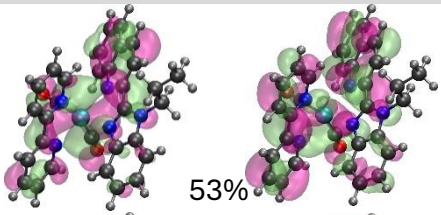
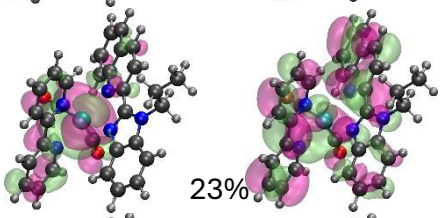
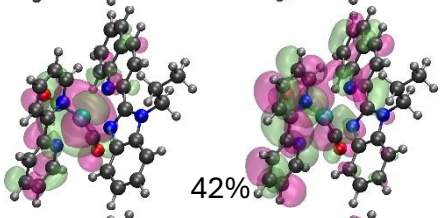
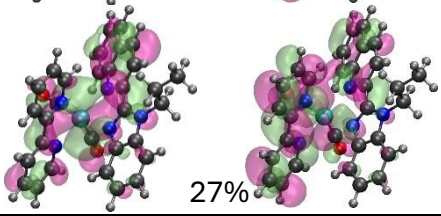
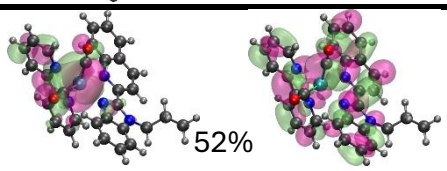
1-2Py34	**7** 1018 nm 0.0198	S_1	88		 58% 39%
		T_2 (0)	3		
		T_2 (+1)	3		
		T_2 (-1)	3		
1-Bpy34	**7** 1015 nm 0.0226	S_1	11		
		T_3 (0)	37		 62%
		T_3 (+1)	23		 36%
		T_3 (-1)	23		
	11 936 nm 0.0211	S_1	41		
		T_4 (0)	22		
		T_4 (+1)	11		
		T_4 (-1)	11		

Table S7: Hole and electron MOs for the spin orbit coupling excited states that are comparable to the first optically active peak NTO's shown previously; for all energetically favorable complexes for all complexes with L2. All MOs are calculated using SOC-TDDFT on the ground state geometry with B3LYP functional and ZORA-def2-TZVP/SARC-ZORA-TZVP basis set with dichloromethane solvent using the CPCM method.

Complex	SOC State/ Wavelength/ Oscillator Strength	% of Singlet or Triplet		Hole	Electron
2	**12** 548 nm 0.0981	**S_3**	97		
2-Py1	**12** 724 nm 0.0844	**S_3**	94	 50%  40%	 
		T_3 (1)	2		
		T_3 (-1)	2		
2-Py4	**12** 709 nm 0.0945	**S_3**	94	 57%  32%	 
		T_3 (1)	2		
		T_3 (-1)	2		
2-2Py12	**4** 1356 nm 0.0364	**S_2**	3	 69%	

		T_2 (0)	66	
		T_2 (1)	14	
		T_2 (-1)	14	
2-2Py12	**8** 974 nm 0.0522	S_2	75	
		T_3 (0)	6	
		T_3 (1)	7	
		T_3 (-1)	7	
2-2Py24	**4** 1383 nm 0.0405	S_2	3	
		T_2 (0)	86	
		T_2 (1)	4	
		T_2 (-1)	4	
	8 998 nm 0.0494	S_2	73	
		T_3 (1)	11	
		T_3 (-1)	11	

2-Bpy12	**7** 1232 nm 0.0232	**S_1**	7	
		T_3 (0)	53	
		T_3 (1)	16	
		T_3 (-1)	16	
	10 1091 nm 0.0265	**S_1**	88	
		T_3 (0)	3	
		T_3 (1)	1	
		T_3 (-1)	1	
	11 1045 nm 0.0259	**S_2**	72	
		T_4 (0)	15	
		T_4 (1)	2	
		T_4 (-1)	2	

2-Bpy13	**10** 1087 nm 0.0276	**S_1**	89	
		T_3 (1)	2	
		T_3 (-1)	2	
	11 979 nm 0.0355	**S_2**	68	 
		T_4 (0)	7	
		T_4 (1)	7	
		T_4 (-1)	7	
2-Bpy24	**7** 1208 nm 0.0189	**S_1**	5	

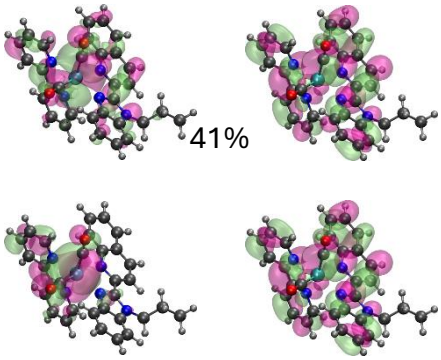
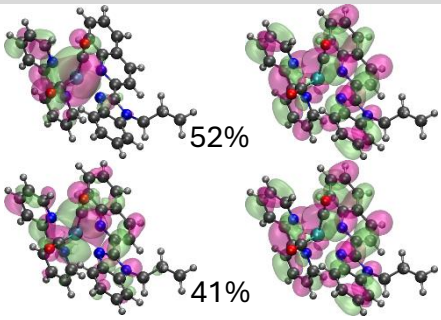
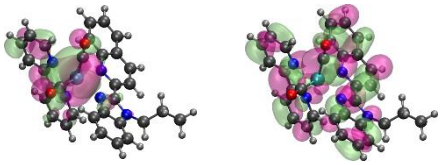
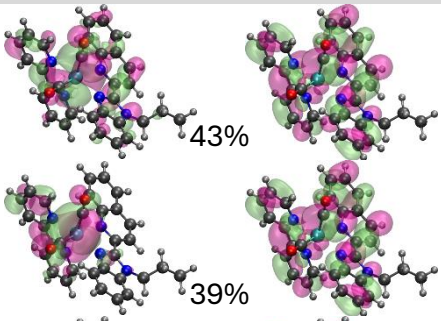
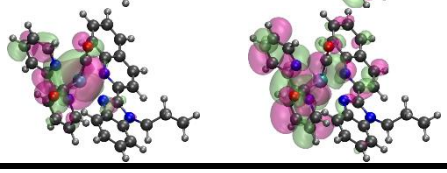
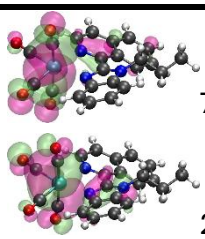
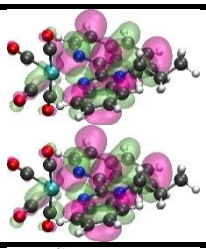
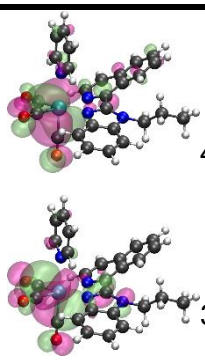
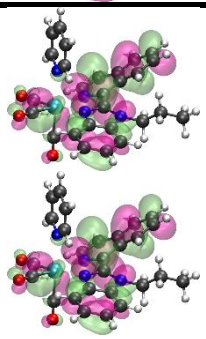
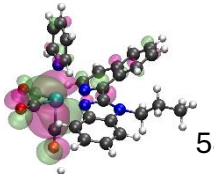
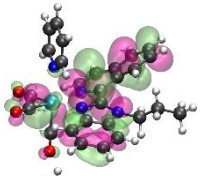
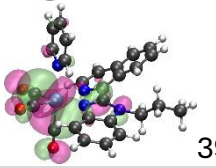
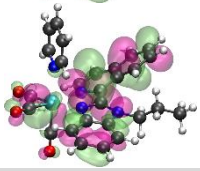
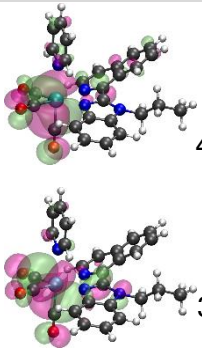
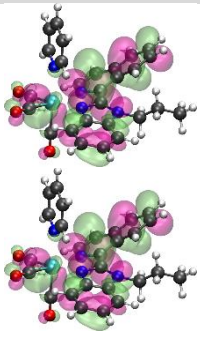
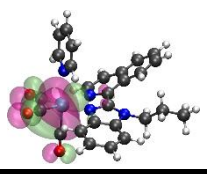
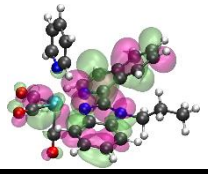
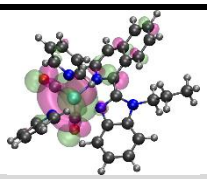
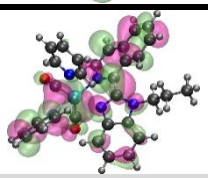
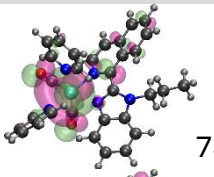
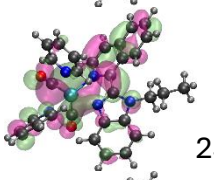
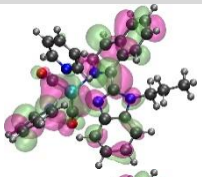
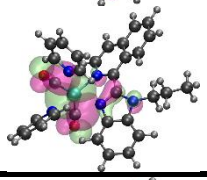
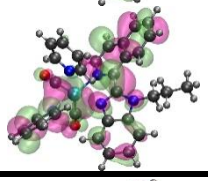
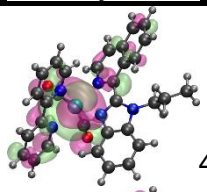
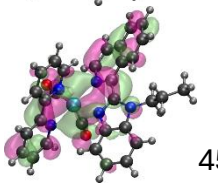
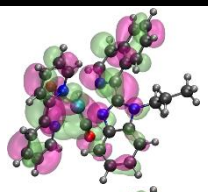
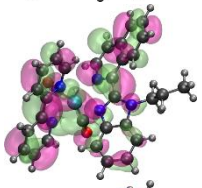
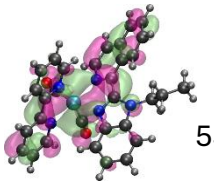
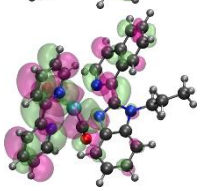
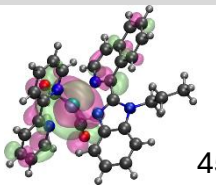
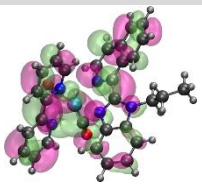
				
		T_3 **(0)**	87	
2-Bpy24	**10** 1078 nm 0.0291	S_1	89	
		T_3 **(0)**	5	
	11 1040 nm 0.0292	S_2	75	
		T_4 **(0)**	14	
		T_4 **(1)**	1	
		T_4 **(-1)**	1	

Table S8: Hole and electron MOs for the spin orbit coupling excited states that are comparable to the first optically active peak NTO's shown previously; for all energetically favorable complexes for all complexes with L3. All MOs are calculated using SOC-TDDFT on the ground state geometry with B3LYP functional and ZORA-def2-TZVP/SARC-ZORA-TZVP basis set with dichloromethane solvent using the CPCM method.

Complex	SOC State/ Wavelength/ Oscillator Strength	% of Singlet or Triplet		Hole	Electron
3	**12** 560 nm 0.1458	**S_3**	96	 71% 26%	
3-Py1	**4** 990 nm 0.0119	**S_3**	2	 47% 31%	
		T_2 (0)	39	 58%	
		T_2 (1)	24	 39%	
		T_2 (-1)	24		
	12 722 nm 0.1363	**S_3**	2	 47% 31%	

3-Py1		**T_3 (1)**	2		
		T_3 (-1)	2		
	4 1313 nm 0.0437	**T_2 (0)**	22		
		T_2 (1)	46		
		T_2 (-1)	46		
3-2Py13	**7** 1054 nm 0.0179	**S_1**	90	 73%  25%	 
		T_3 (0)	4		
		T_3 (1)	1		
		T_3 (-1)	1		
3-Bpy13	**7** 1113 nm 0.0271	**S_1**	9	 45%  45%	 
		T_3 (0)	8	 55%	
		T_3 (1)	39		
		T_3 (-1)	39		
3-Bpy13	**10** 1054 nm 0.0308	**S_1**	84	 45%	

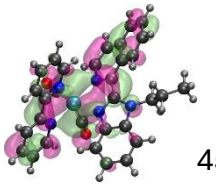
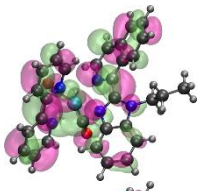
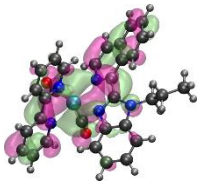
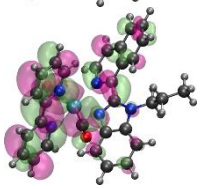
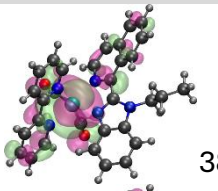
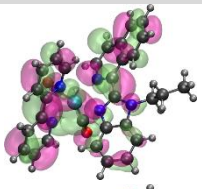
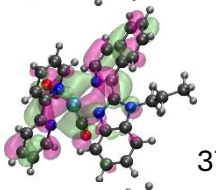
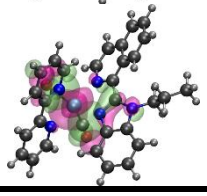
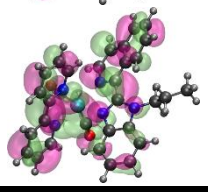
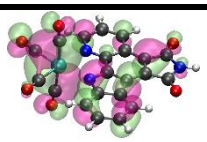
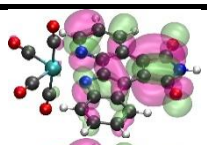
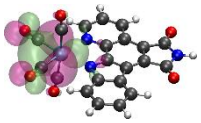
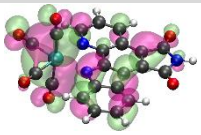
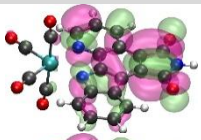
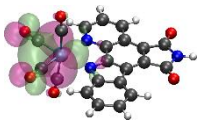
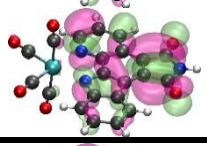
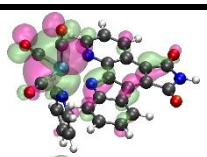
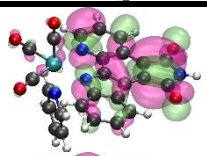
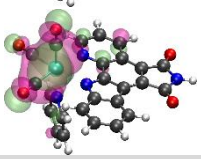
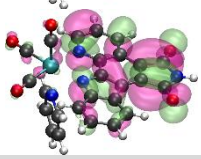
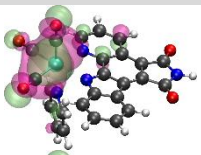
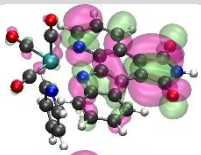
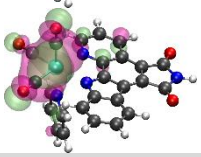
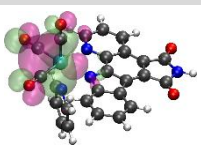
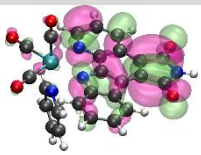
		T_3 **(1)**	5	 45% 	
		T_3 **(-1)**	5	 	
3-Bpy13	**11** 935 nm 0.0537	S_2	71	 38% 	
		T_4 **(0)**	4	 37% 	
		T_4 **(1)**	7	 	
		T_4 **(-1)**	7		

Table S9: Hole and electron MOs for the spin orbit coupling excited states that are comparable to the first optically active peak NTO's shown previously; for all energetically favorable complexes for all complexes with L4. All MOs are calculated using SOC-TDDFT on the ground state geometry with B3LYP functional and ZORA-def2-TZVP/SARC-ZORA-TZVP basis set with dichloromethane solvent using the CPCM method.

Complex	SOC State/ Wavelength/ Oscillator Strength	% of Singlet or Triplet		Hole	Electron
4	**4** 678 nm 0.0481	**S_1**	41		
		T_2 (0) **T_2 (1)** **T_2 (-1)**	7 22 22		
	8 637 nm 0.0695	**S_1**	56		
		T_2 (0) **T_2 (1)** **T_2 (-1)**	4 19 19		
4-Py4	**4** 930 nm 0.0286	**S_1**	38		
		T_2 (0) **T_2 (1)** **T_2 (-1)**	22 13 13		
	8 814 nm 0.0430	**S_2**	51		
		T_2 (0) **T_2 (1)** **T_2 (-1)**	11 5 5		
	12 750 nm 0.0363	**S_3**	84		

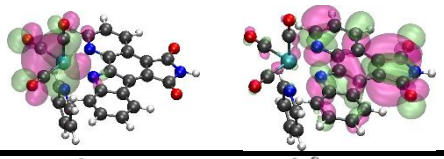
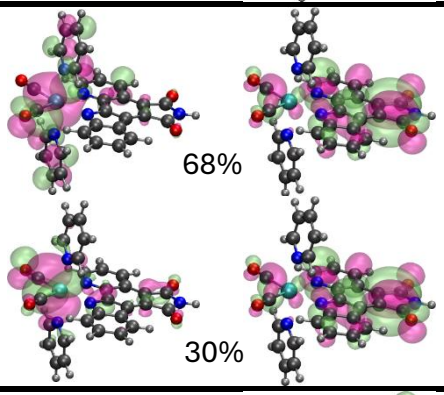
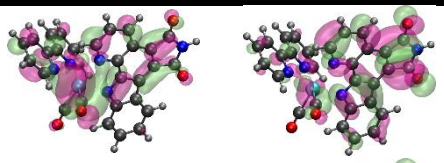
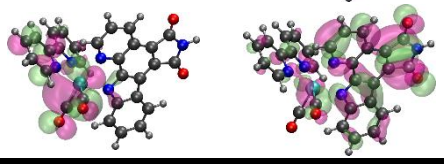
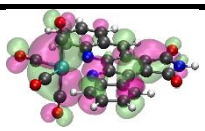
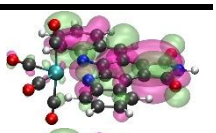
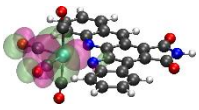
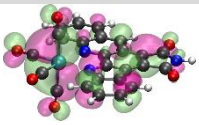
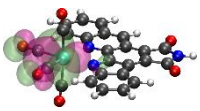
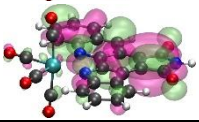
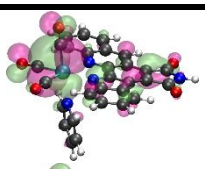
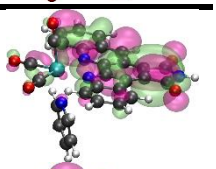
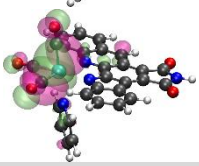
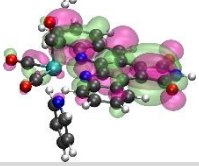
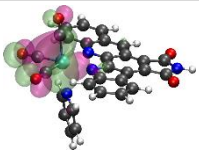
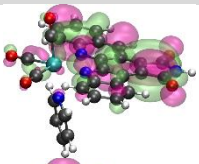
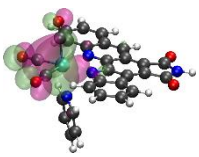
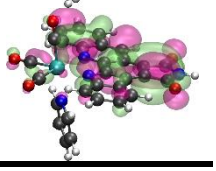
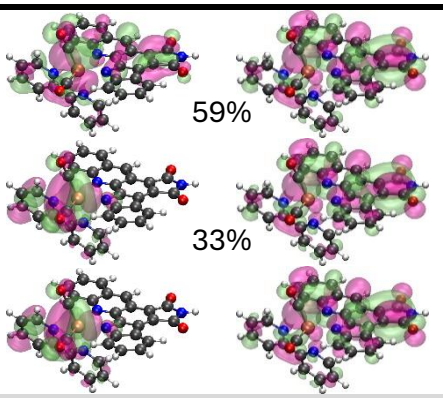
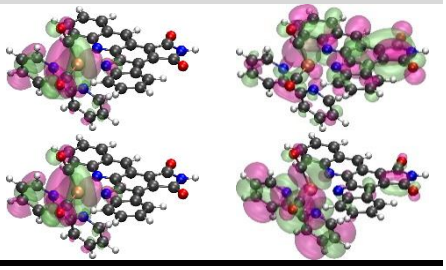
4-Py4		**T_3 (0)**	6	
		T_3 (1)	3	
		T_3 (-1)	3	
4-2Py14	**8** 1304 nm 0.0783	**S_2**	95	
4-Bpy24	**7** 1250 nm 0.1085	**S_1**	63	
		T_4 (0)	4	
		T_4 (1)	13	
		T_4 (-1)	13	

Table S10: Hole and electron MOs for the spin orbit coupling excited states that are comparable to the first optically active peak NTO's shown previously; for all energetically favorable complexes for all complexes with L5. All MOs are calculated using SOC-TDDFT on the ground state geometry with B3LYP functional and ZORA-def2-TZVP/SARC-ZORA-TZVP basis set with dichloromethane solvent using the CPCM method.

Complex	SOC State/ Wavelength/ Oscillator Strength	% of Singlet or Triplet		Hole	Electron
5	4 760 nm 0.0549	S_1	39		
		T_2 (0) T_2 (1) T_2 (-1)	5 24 24		
	8 708 nm 0.0933	S_1	58		
		T_2 (0) T_2 (1) T_2 (-1)	1 20 20		
5-Py4	4 1079 nm 0.0288	S_1	43		
		T_2 (0) T_2 (1) T_2 (-1)	15 15 15		
	12 829 nm 0.0671	S_3	86		
		T_3 (0) T_3 (1) T_3 (-1)	8 1 1		
5-2Py14					

5-Bpy24	7 1347 nm 0.0740	S_1	20		59% 33%
		T_3 (0)	6		
		T_3 (1)	34		
		T_3 (-1)	34		
	11 1172 nm 0.0840	S_2	84		
		T_4 (1)	4		
		T_4 (-1)	4		