

Supplementary Information

The Bimetallic and the Anchoring Group Effects on both the Optical and Charge Transport Properties of the Hexaphyrin Amethyrin

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Figure S1a. Optimized molecular structures calculated at the BP86-D3/def2-TZVP level of theory

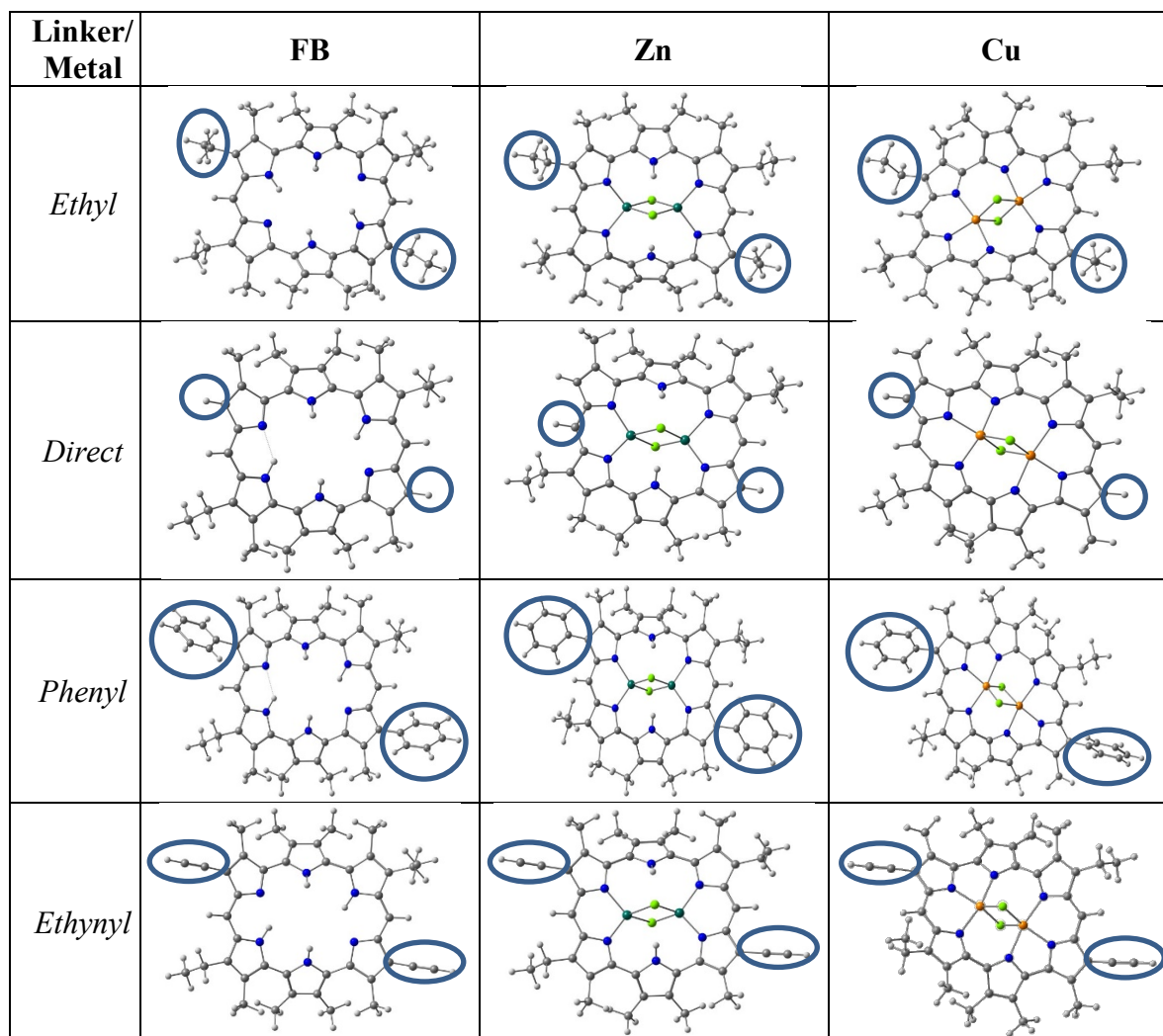


Figure S1b. Comparison of the optimized molecular structures and the RMSD (Å) for the macrocycle between them obtained at the BP86-D3/def2-TZVP level of theory. For simplicity, the metal atoms and substituents of macrocycles have not been included.

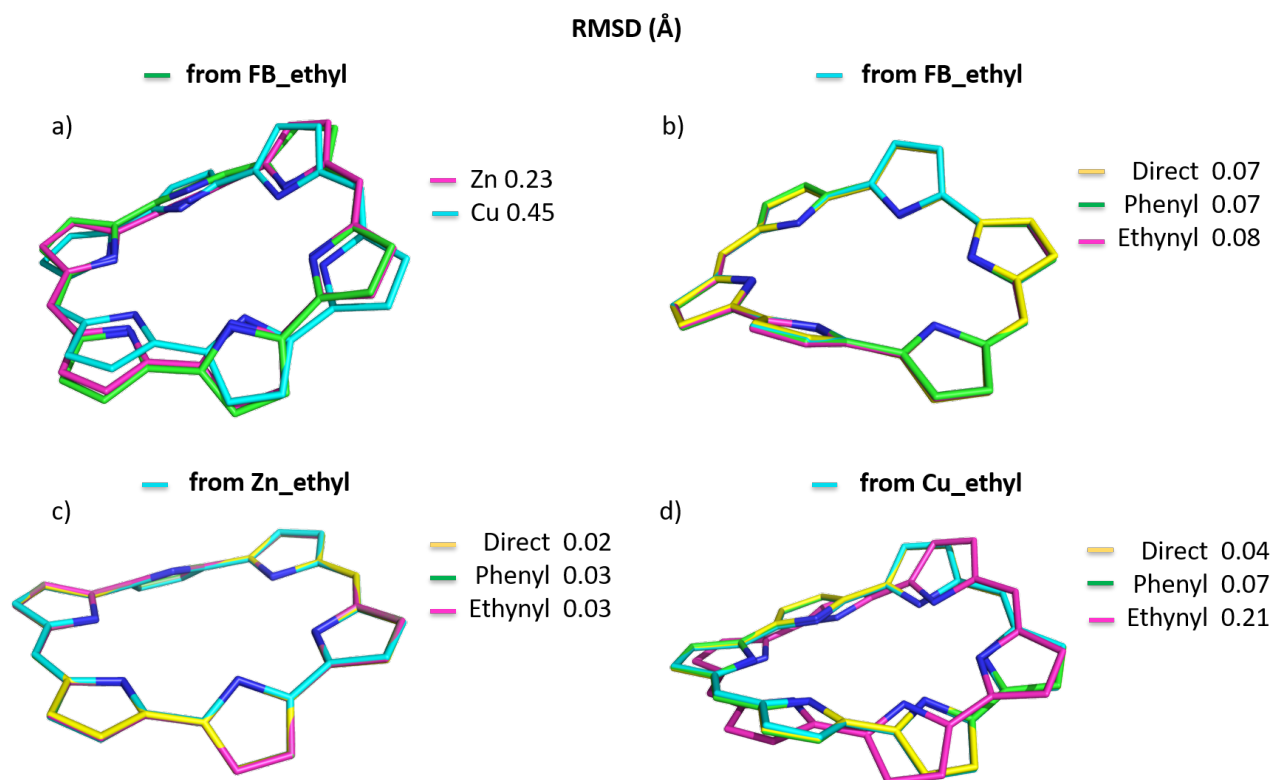


Figure S2. Surface of the frontier molecular orbitals

Figure S2.1. Surface of the frontier molecular orbitals for the singlet state of FB-amethyrin computed with the PWBP95-D3/def2-TZVP level of theory (energy in eV)

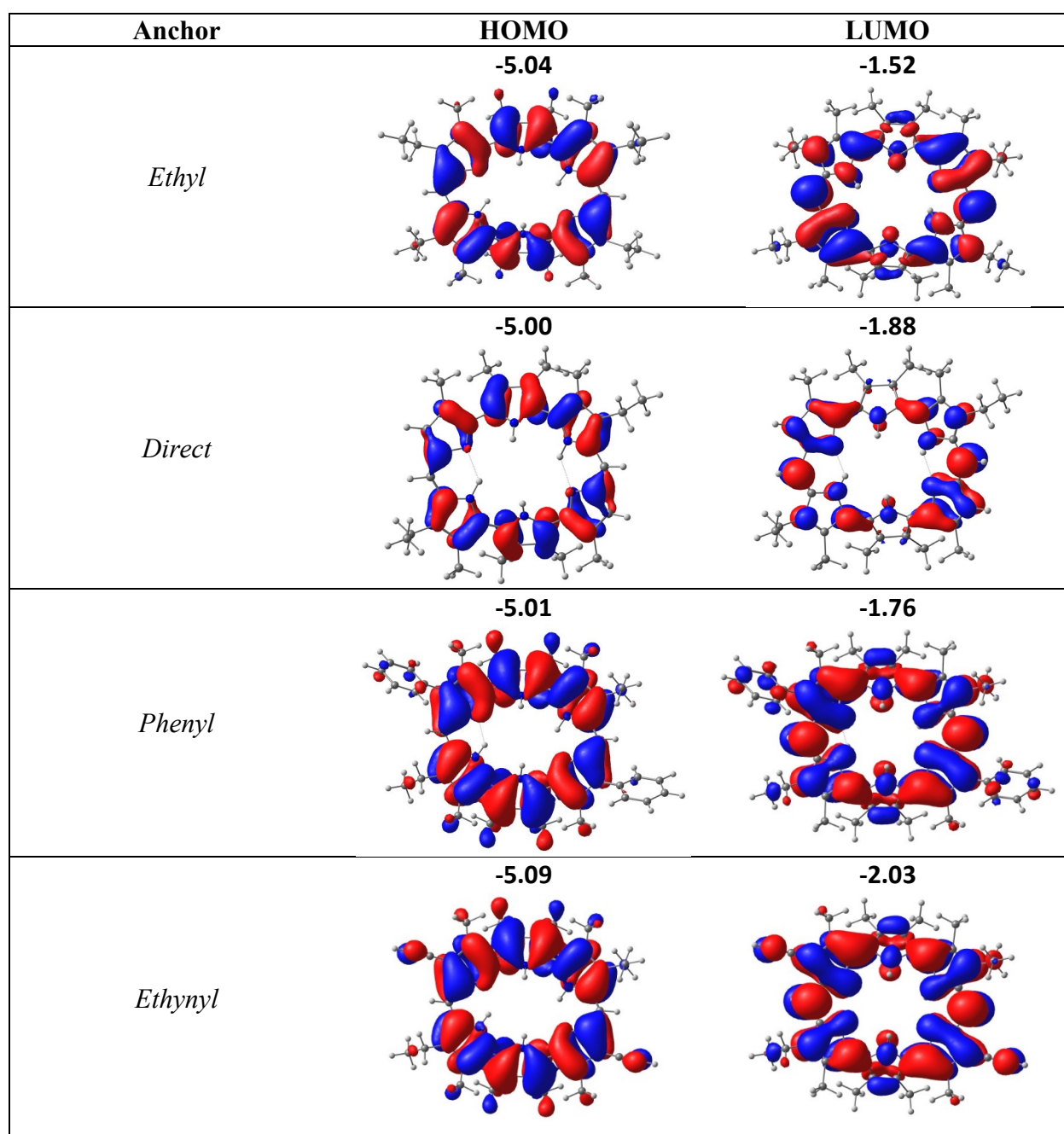


Figure S2.2. Surface of the frontier molecular orbitals for the singlet state of Zn(II)-amethyryn computed with the PWBP95-D3/def2-TZVP level of theory (energy in eV)

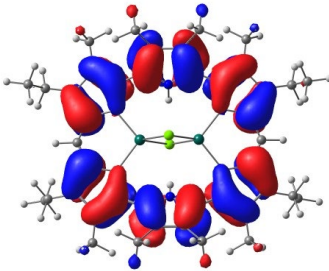
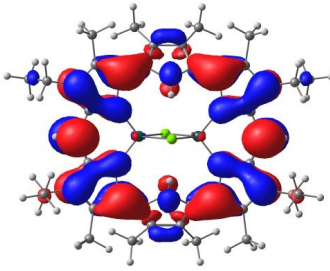
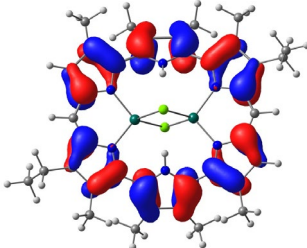
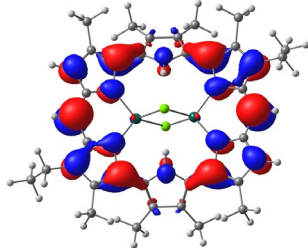
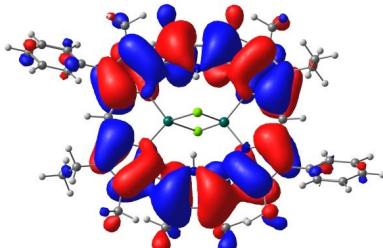
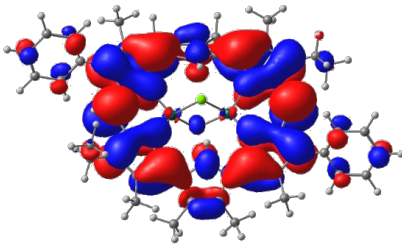
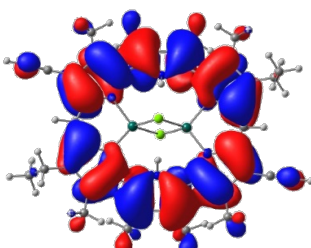
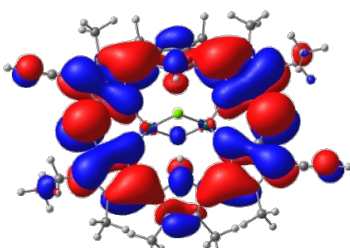
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<i>Direct</i>	-5.18 	-2.00 
<i>Phenyl</i>	-5.14 	-1.93 
<i>Ethynyl</i>	-5.28 	-2.14 

Figure S2.3. Surface of the frontier molecular orbitals for the singlet state of Cu(II)-amethyryn computed with the PWBP95-D3/def2-TZVP level of theory (energy in eV)

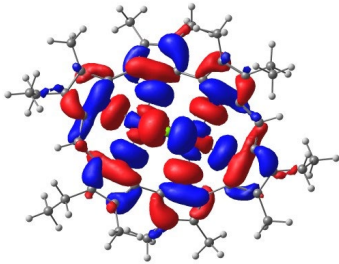
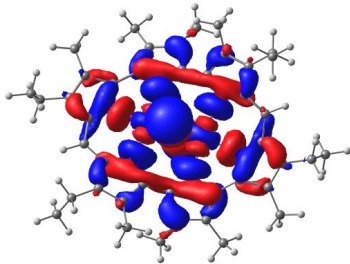
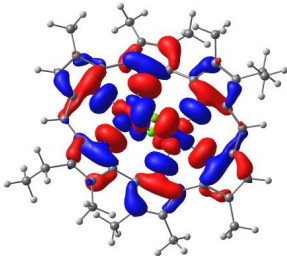
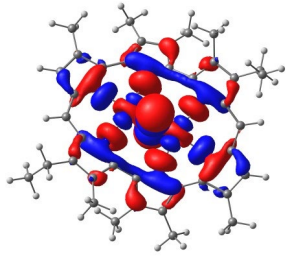
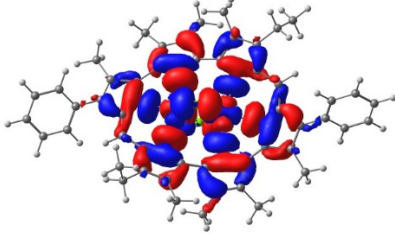
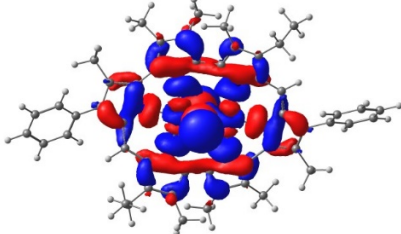
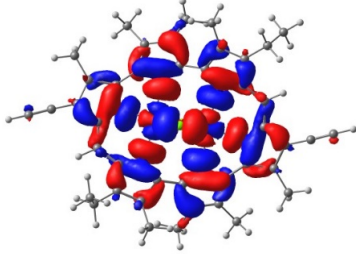
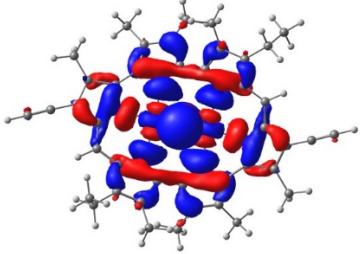
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<i>Direct</i>	-5.47 	-3.19 
<i>Phenyl</i>	-5.37 	-3.09 
<i>Ethynyl</i>	-5.52 	-3.28 

Figure S2.4. Surface of the frontier molecular orbitals for the triplet state of Cu(II)-amethyryn computed with the PWBP95-D3/def2-TZVP level of theory (energy in eV)

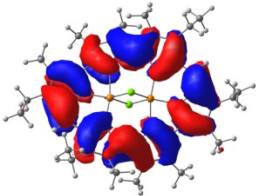
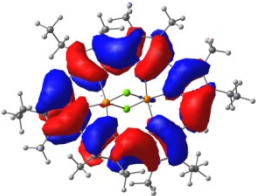
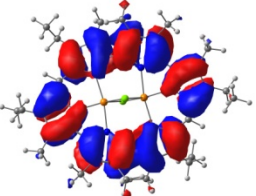
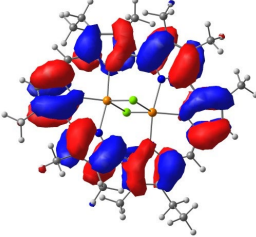
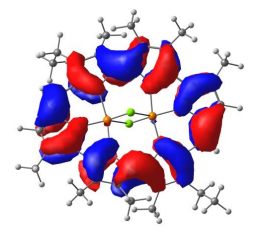
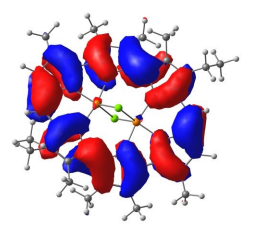
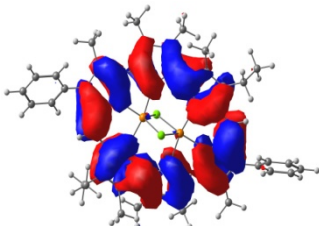
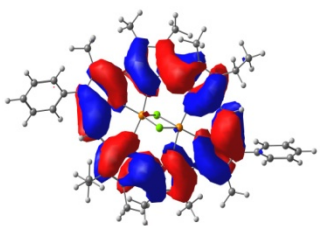
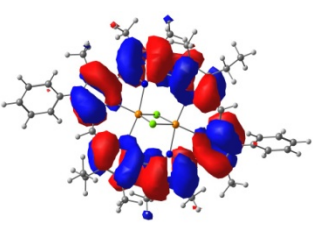
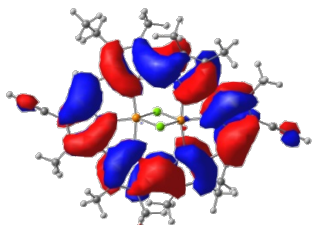
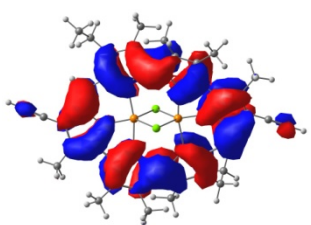
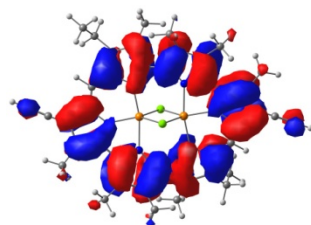
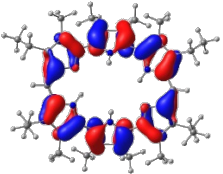
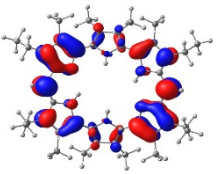
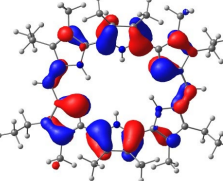
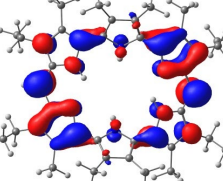
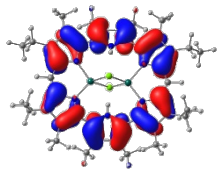
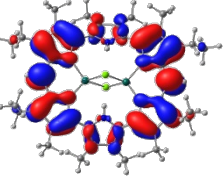
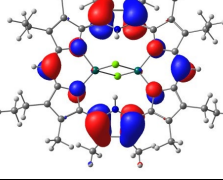
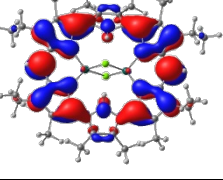
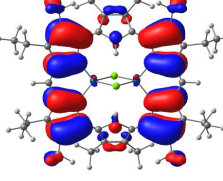
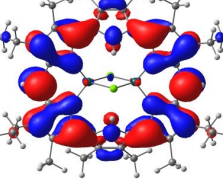
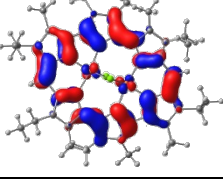
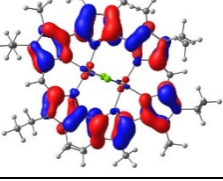
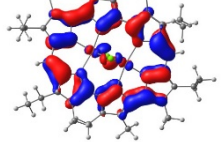
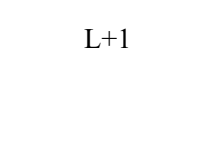
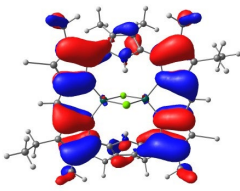
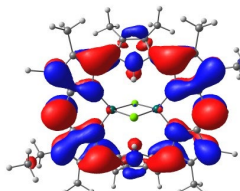
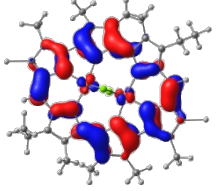
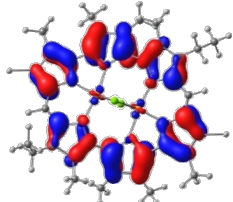
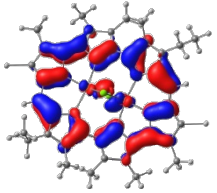
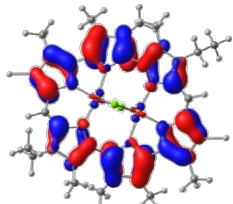
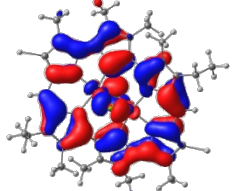
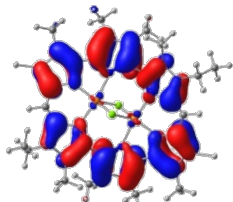
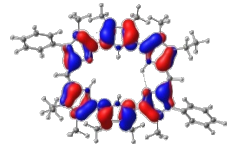
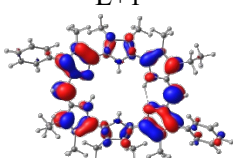
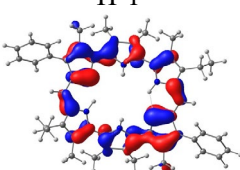
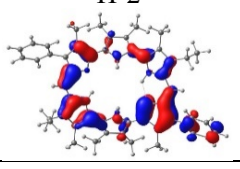
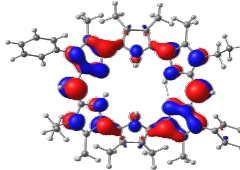
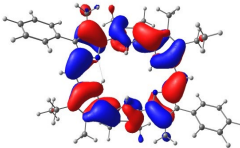
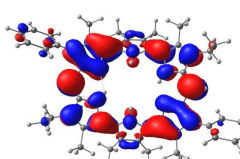
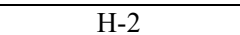
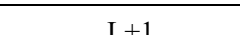
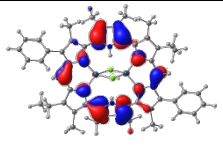
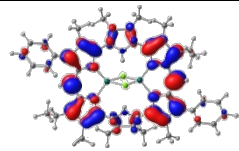
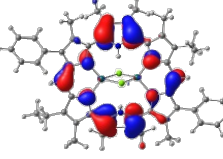
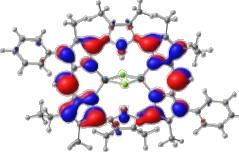
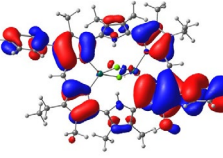
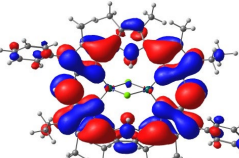
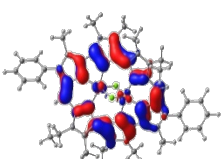
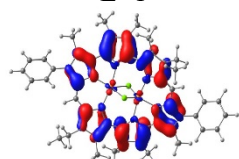
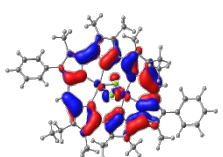
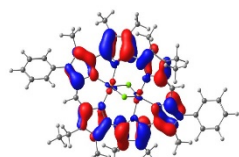
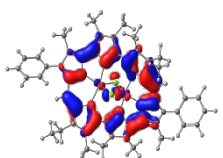
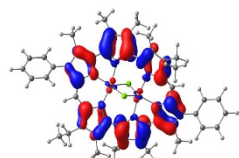
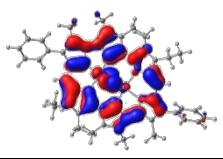
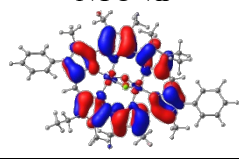
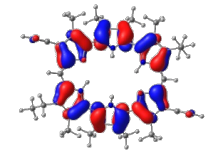
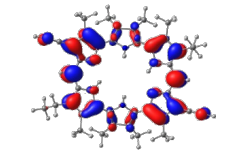
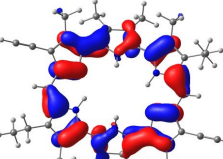
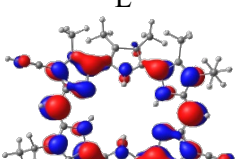
Anchor	SOMO		LUMO
<i>Ethyl</i>	-5.53 	-5.52 	-2.75 
<i>Direct</i>	-5.70 	-5.69 	-2.94 
<i>Phenyl</i>	-5.62 	-5.62 	-2.82 
<i>Ethynyl</i>	-5.73 	-5.72 	-2.99 

Figure S2.5. Surface of the molecular orbitals involved in the absorption bands computed for BF-, Zn(II)- and Cu(II)-amethyrin with the TPSSh/def2-TZVP level of theory in the solution phase (chloroform) (energy in eV).

System/ Anchor	λ/nm (E/eV) <i>f</i>	Assignment	Transition		
Ethyl					
FB	601 (2.06) 0.208	Q	H 	→	L+1 
	493 (2.52) 1.225	Soret	NTO occ 	→	NTO virt 
Zn	642 (1.93) 0.169	Q	H 	→	L+1 
	499 (2.48) 0.306	Q	H-2 	→	L 
	475 (2.61) 0.968	Soret	NTO occ 	→	NTO vir 
Cu	885 (1.40) 0.080	Q	H-1 	→	L+1 
	766 (1.62) 0.091	Q	H-2 	→	L+1 

	491 (2.53) 0.530	Soret	NTO occ 	→	NTO vir
Direct					
FB	640 (1.94) 0.190	Q	H 	→	L+1
	509 (2.44) 0.420	Q	H-1 H-2 	→	L
	458 (2.71) 1.258	Soret	NTO occ 	→	NTO vir
Zn	647 (1.91) 0.175	Q	H 	→	L+1
	508 (2.44) 0.307	Q	H-2 	→	L
	479 (2.59) 1.022	Soret	NTO occ 	→	NTO vir

					
Cu	874 (1.48) 0.152	Q	H-1 	→	L+1 
	776 (1.60) 0.090	Q	H-2 	→	L+1 
	493 (2.51) 0.493	Soret	NTO occ 	→	NTO vir 
Phenyl					
FB	652 (1.90) 0.219	Q	H 	→	L+1 
	518 (2.39) 0.232	Q	H-1  H-2 	→	L 
	462 (2.68) 0.993	Soret	NTO occ 	→	NTO vir 
Zn	657 (1.89) 0.199	Q	H-2 	→	L+1 

					
	510 (2.43) 0.268	Q	H-2 	→	L 
	484 (2.56) 0.782	Soret	NTO occ 	→	NTO vir 
Cu	898 (1.38) 0.126	Q	H-1 	→	L+1 
	779 (1.59) 0.060	Q	H-2 	→	L+1 
	764 (1.62) 0.041	Q	H-2 	→	L+1 
	495 (2.50) 0.373	Soret	NTO occ 	→	NTO vir 
Ethynyl					
FB	698 (1.78) 0.231	Q	H 	→	L+1 
	538 (2.30) 0.103	Q	H-1  H-2	→	L 

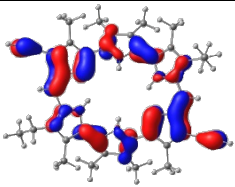
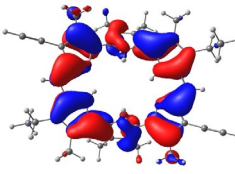
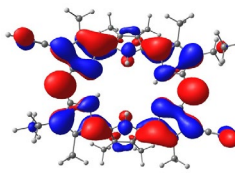
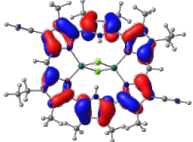
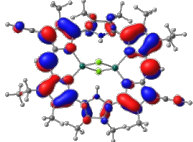
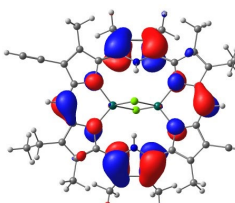
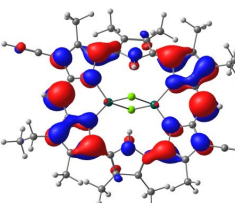
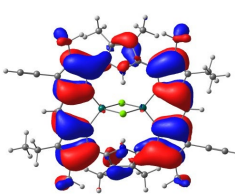
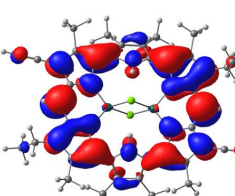
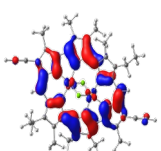
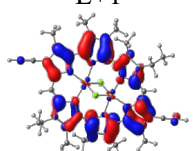
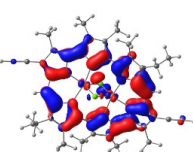
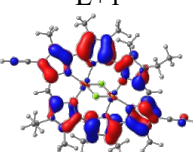
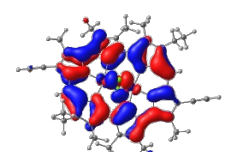
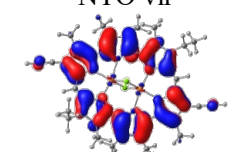
					
	478 (2.59) 1.025	Soret	NTO occ 	→	NTO vir 
Zn	672 (1.85) 0.218	Q	H 	→	L+1 
	520 (2.38) 0.221	Q	H-2 	→	L 
	481 (2.58) 1.157	Soret	NTO occ 	→	NTO vir 
Cu	909 (1.36) 0.121	Q	H-1 	→	L+1 
	780 (1.59) 0.088	Q	H-2 	→	L+1 
	505 (2.46) 0.589	Soret	NTO occ 	→	NTO vir 

Figure S3. UV-Vis absorption spectra of a) FB-, Zn- and Cu- amethyrin with ethyl as an anchoring group (Q bands were plotted as bars) and b) Cu-amethyrin with different anchoring groups calculated at the TPSSh/de2-TZVP level of theory in chloroform.

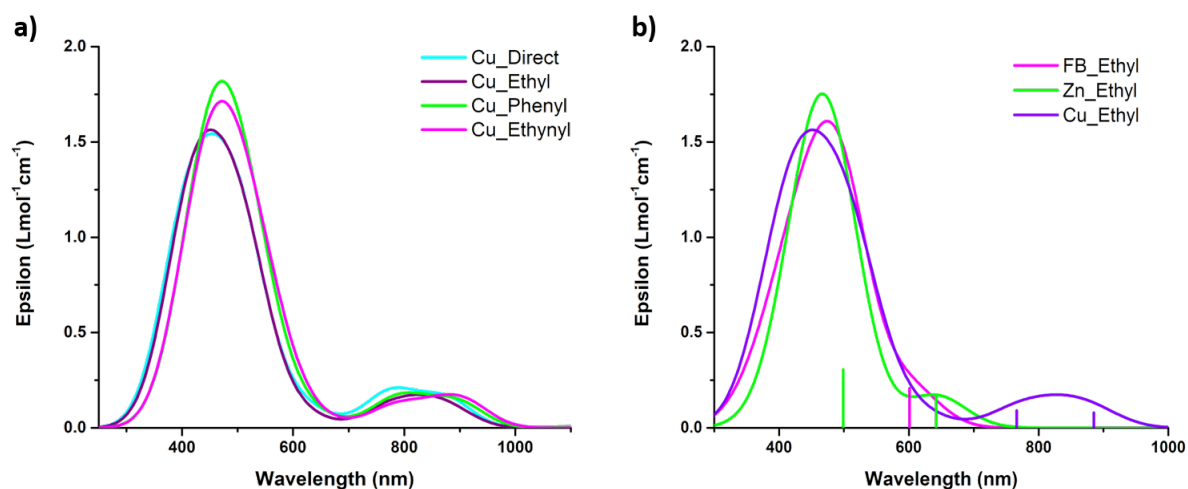


Figure S4. Molecular orbitals-based analysis for free-base-Amethyrin with Spin Degenerate Channels (all energy values are relative to the system's Fermi level)

Ethyl anchor	
Spin Up/Down Transmission function -0.27 eV	Spin Up/Down HOMO -0.28 eV
Phenyl anchor	
Spin Up/Down Transmission function -0.22 eV	Spin Up/Down HOMO -0.44 eV
Ethynyl anchor	
Spin Up/Down Transmission function -0.22 eV	Spin Up/Down HOMO -0.44 eV

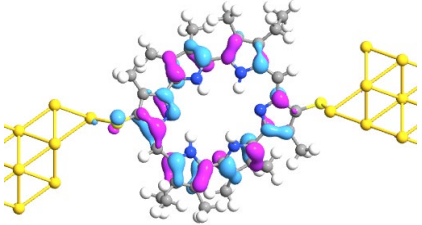
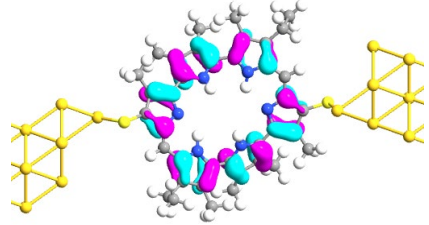
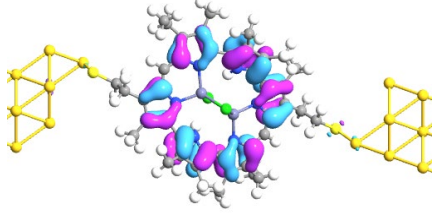
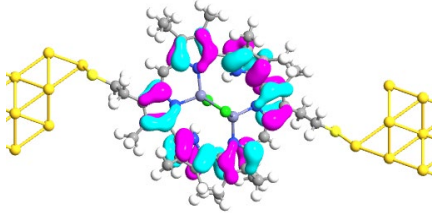
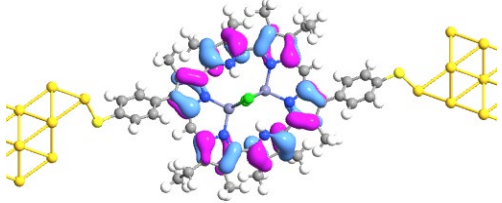
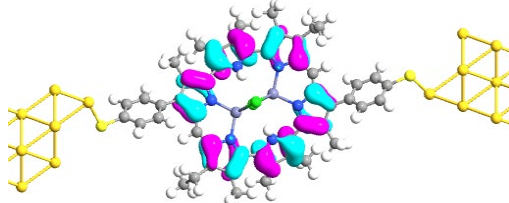
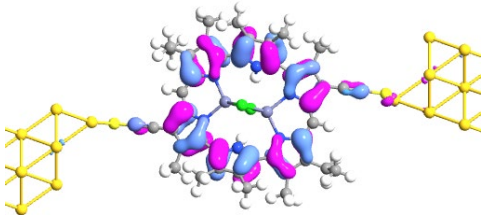
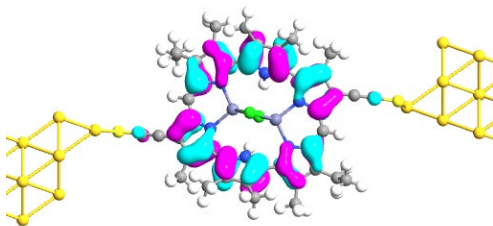
Direct anchor	
	
Spin Up/Down Transmission function -0.23 eV	Spin Up/Down HOMO -0.28 eV

Figure S5. Molecular orbitals-based analysis for Zn(II)-Amethyrin with Spin Degenerate Channels (all energy values are relative to the system's Fermi level)

Ethyl anchor	
	
Spin Up/Down Transmission function -0.28 eV	Spin Up/Down HOMO -0.28 eV
Phenyl anchor	
	
Spin Up/Down Transmission function -0.26 eV	Spin Up/Down HOMO -0.27 eV
Ethynyl anchor	
	
Spin Up/Down Transmission function -0.25 eV	Spin Up/Down HOMO -0.30 eV
Direct anchor	

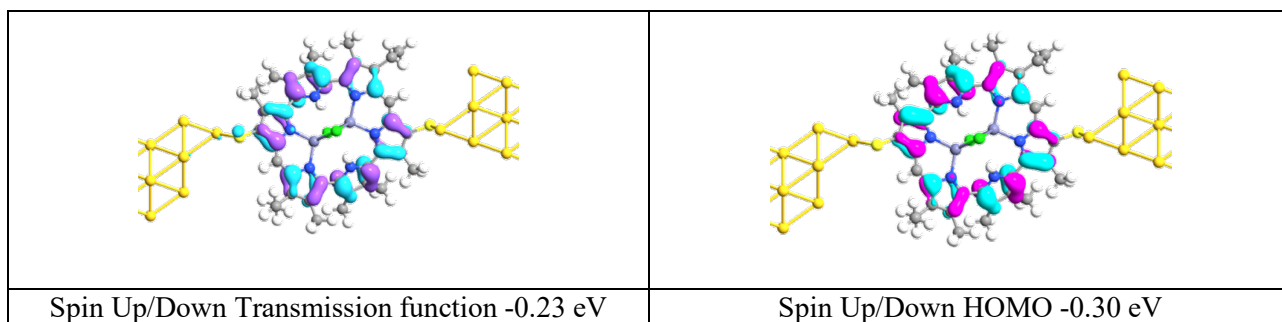
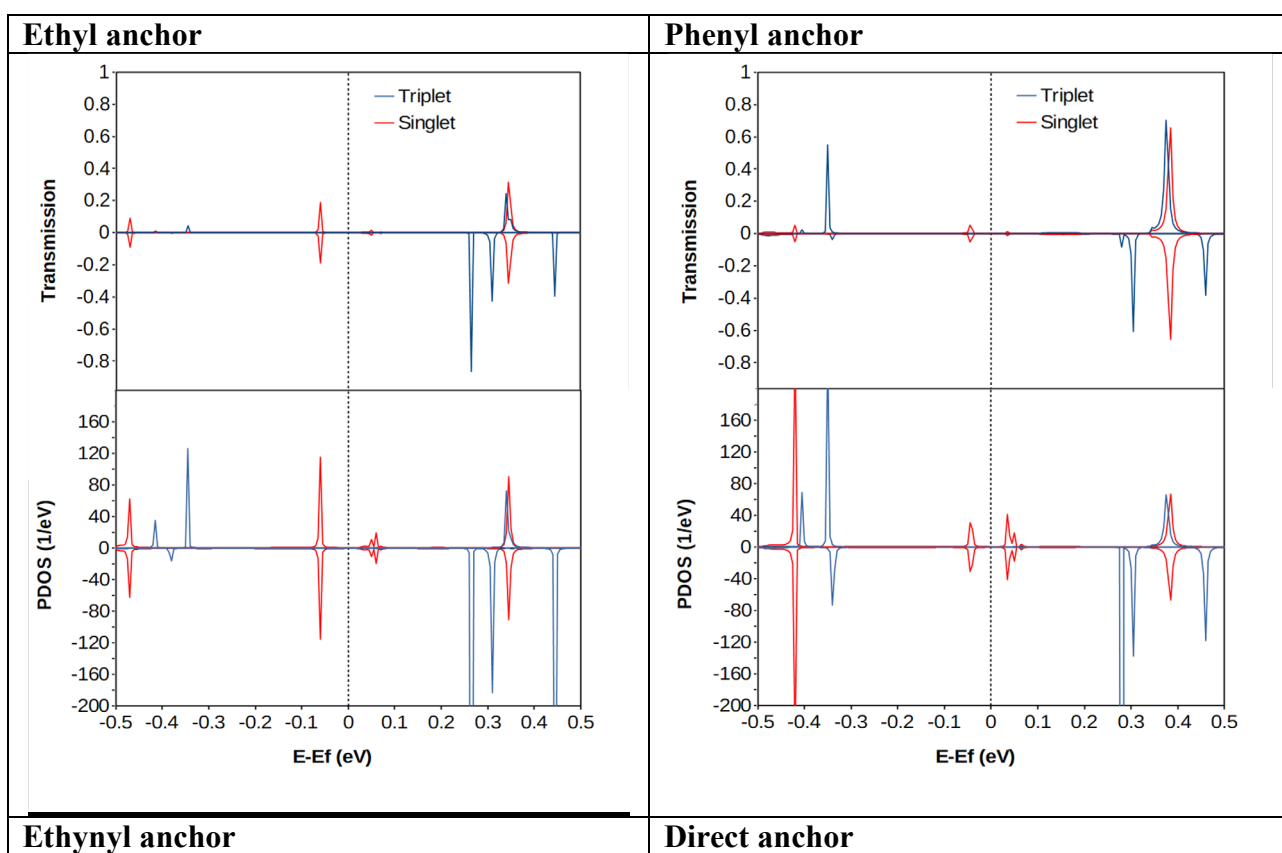


Figure S6. Transmission Spectra and Projected Density of States for Cu(II)-Amethyrin



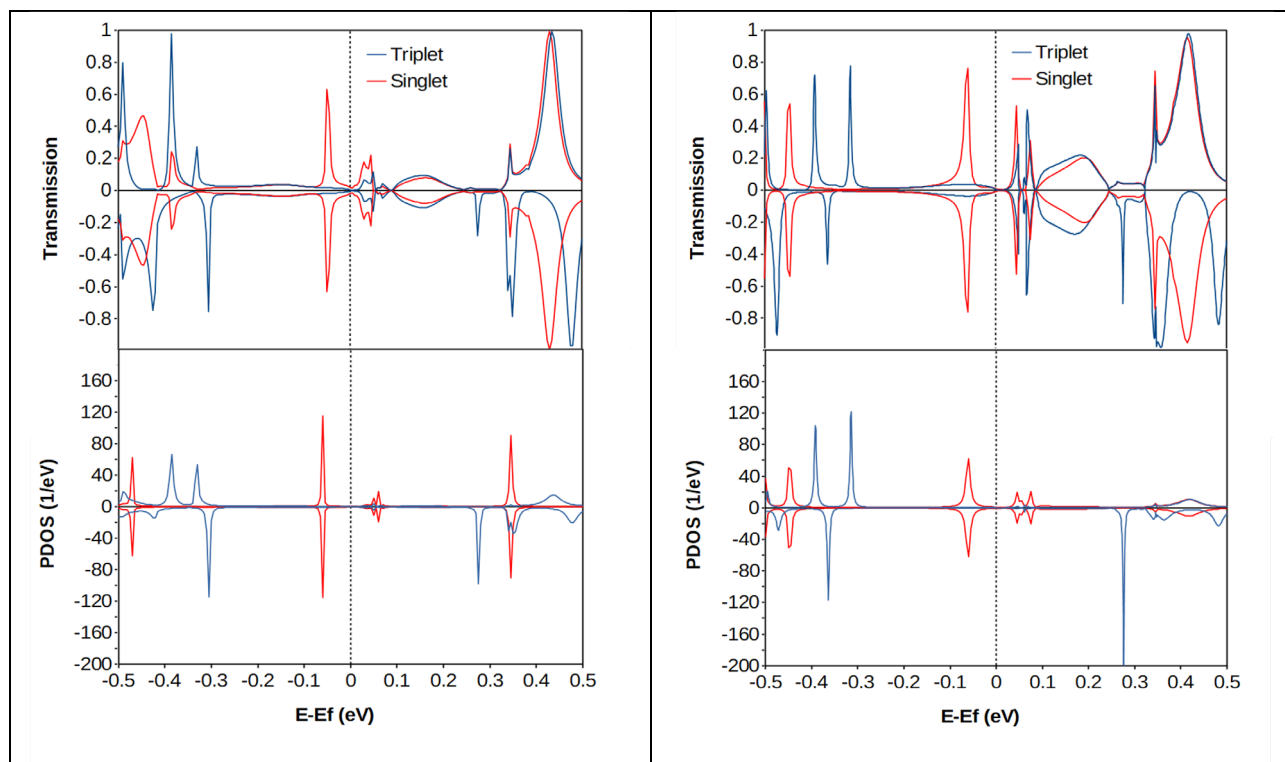
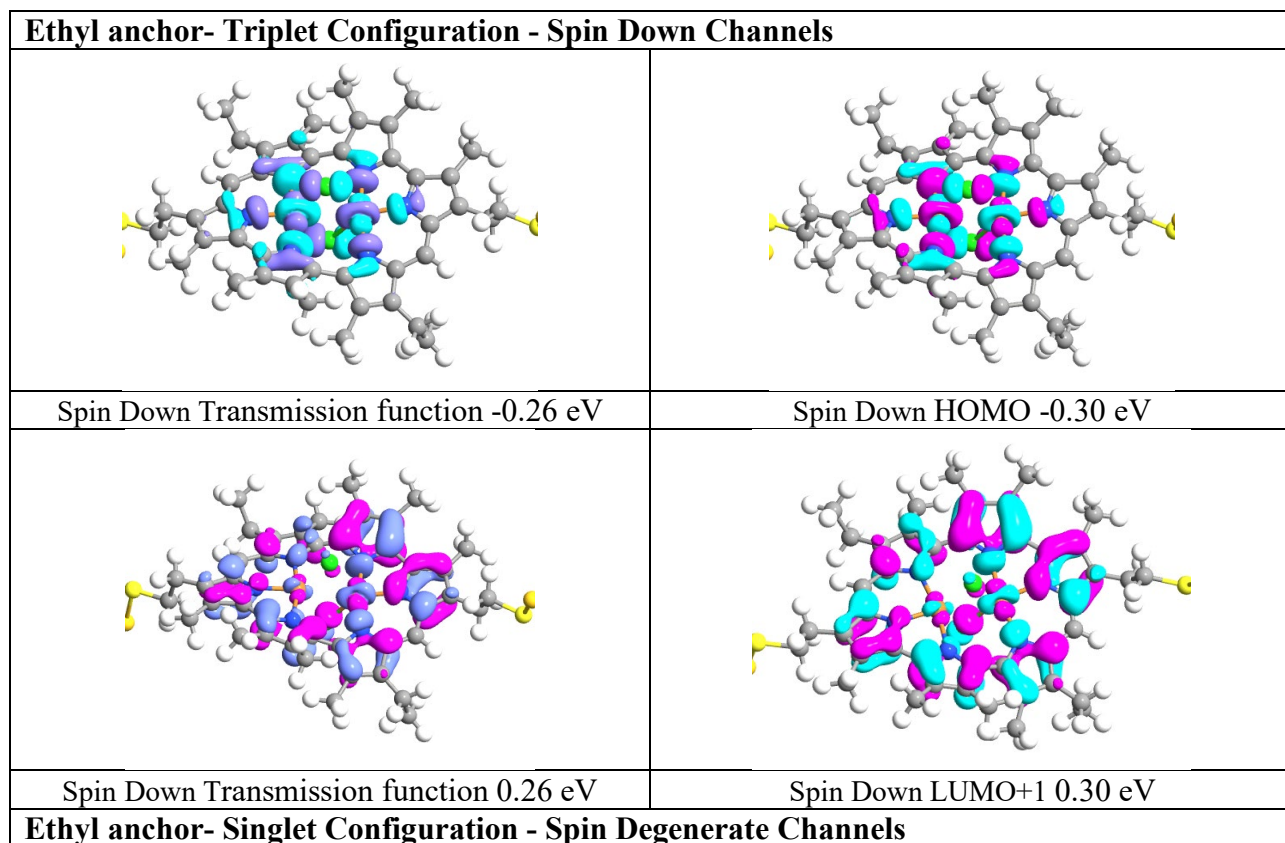
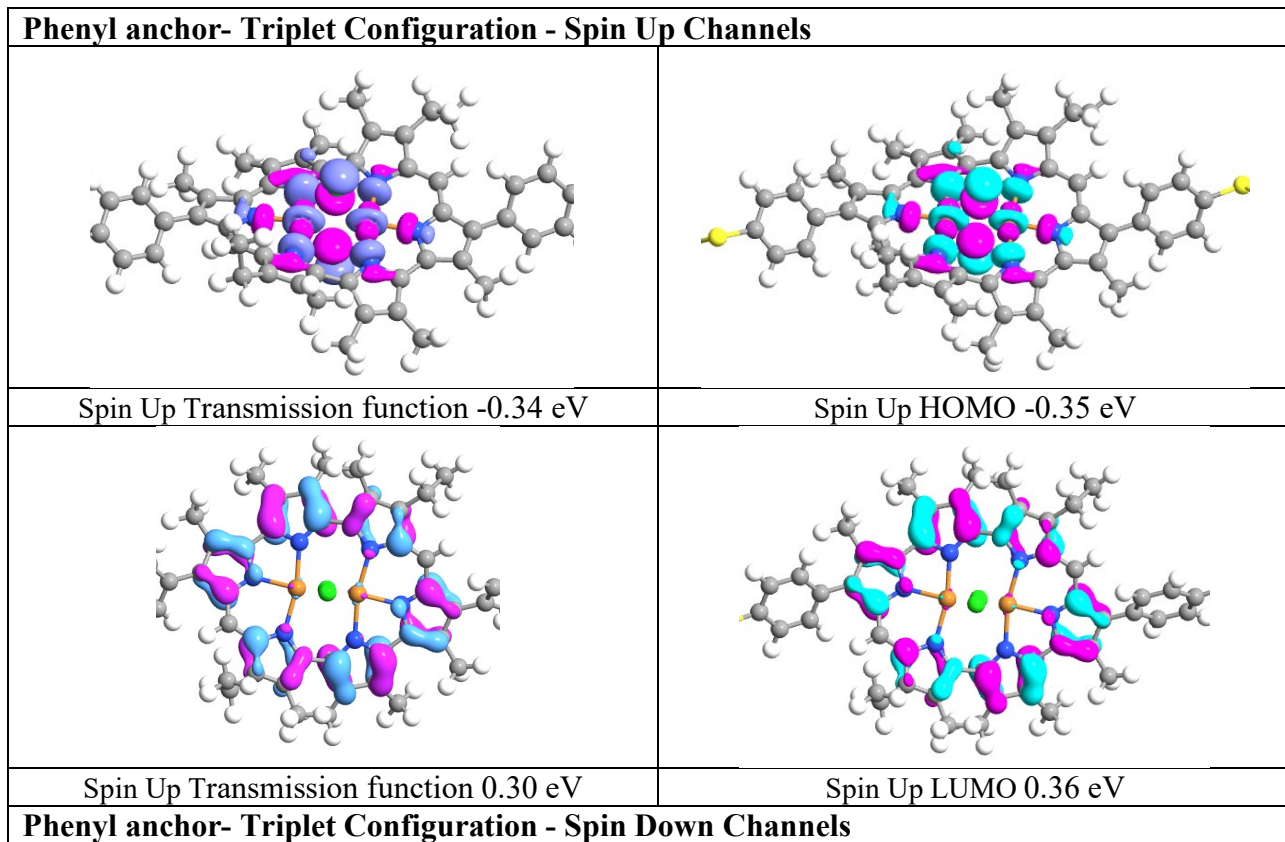
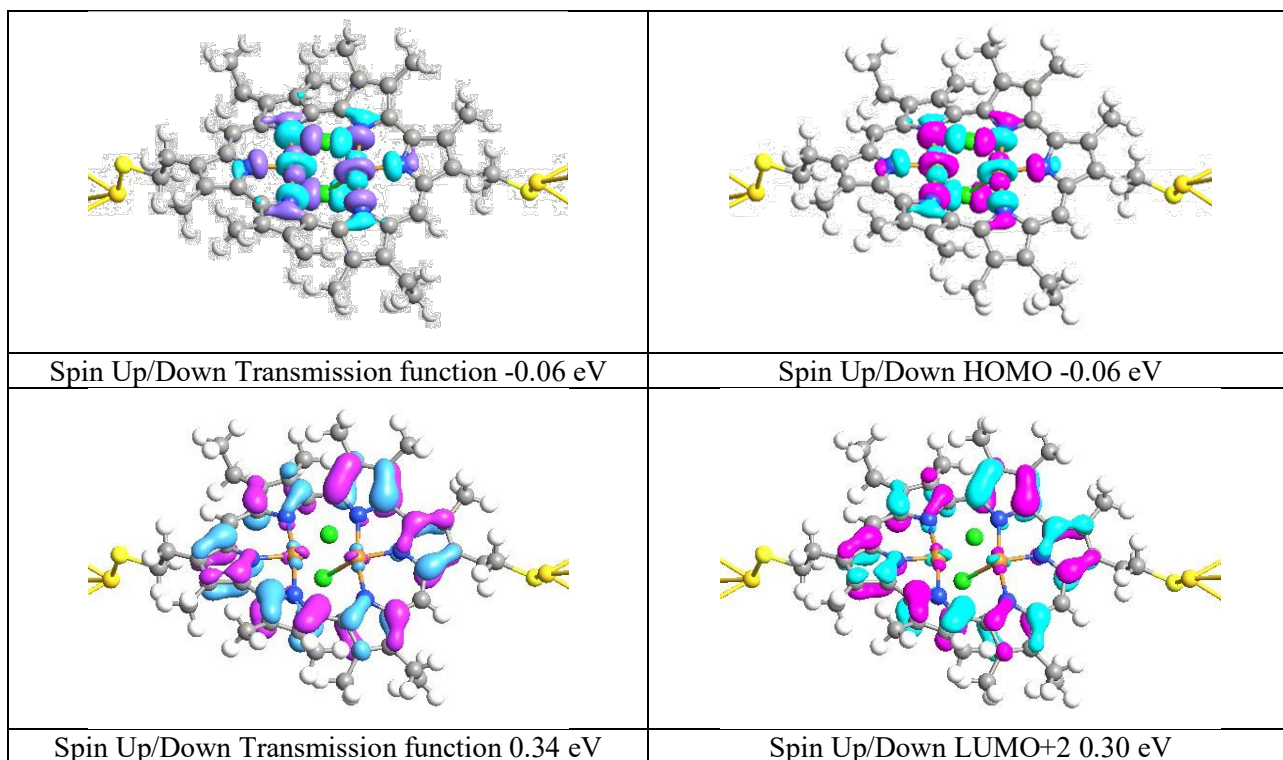
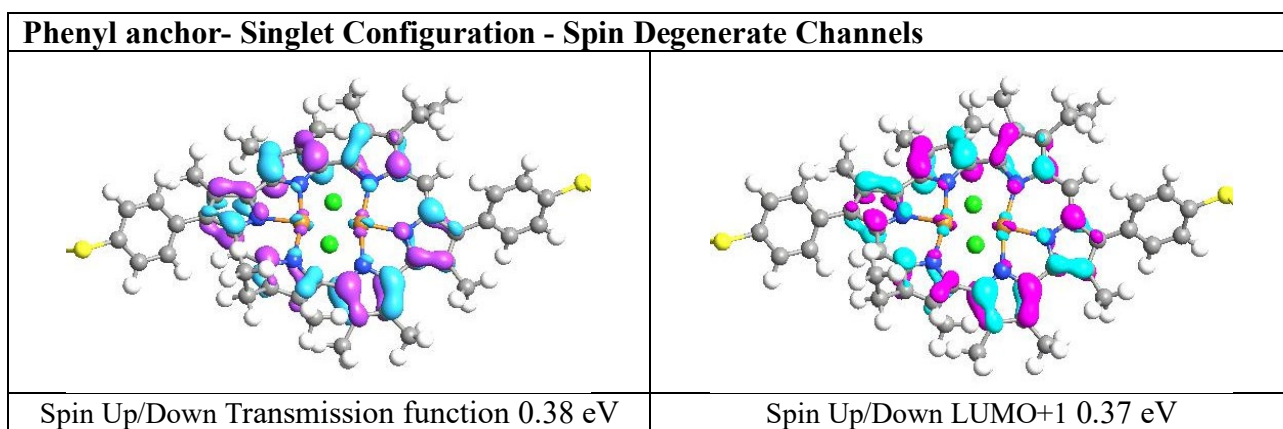
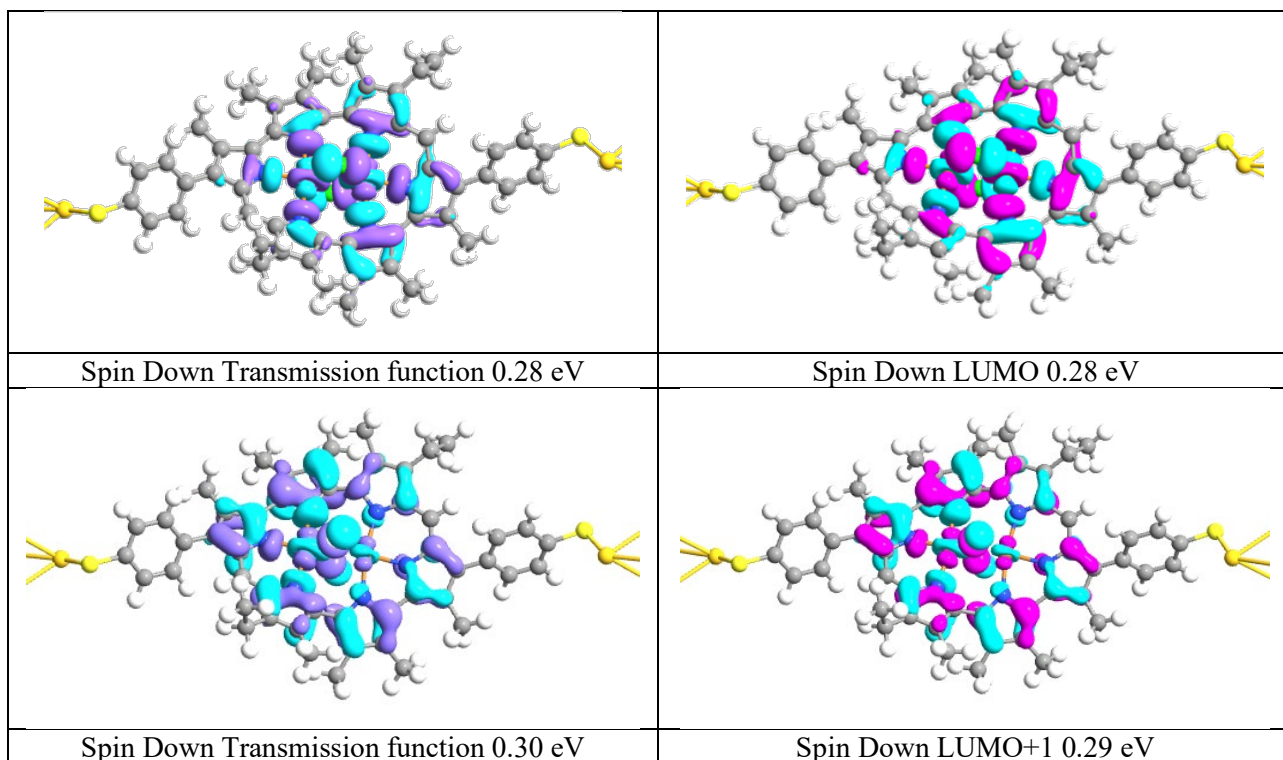


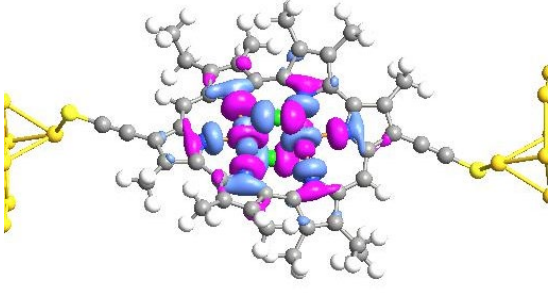
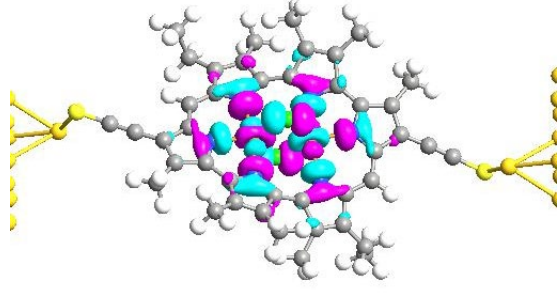
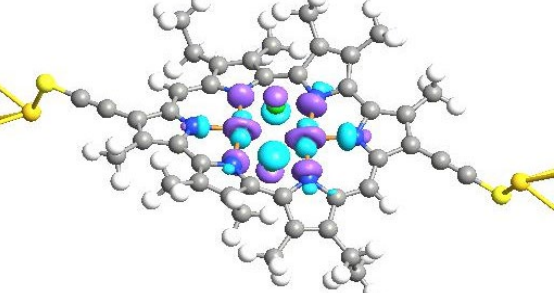
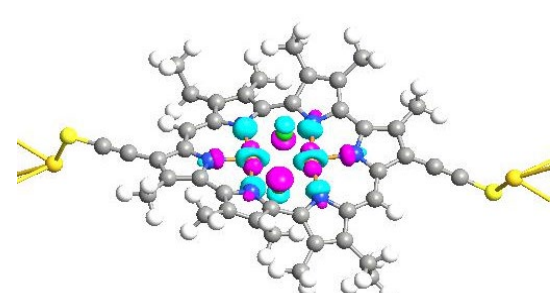
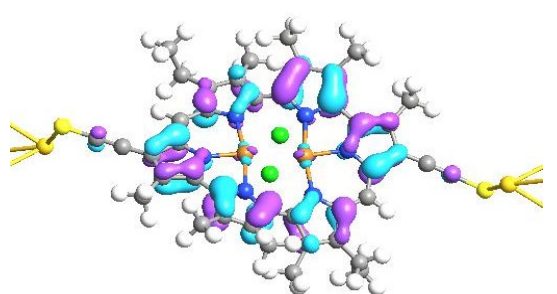
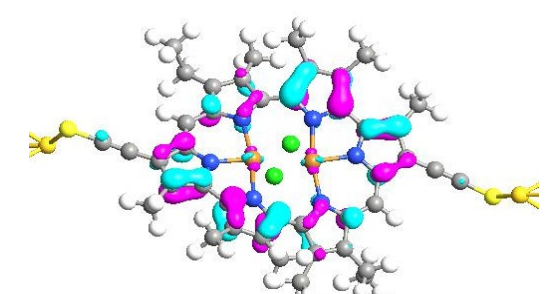
Figure S7. Molecular orbitals-based analysis for Cu(II)-Amethyrin (all energy values are relative to the system's Fermi level)

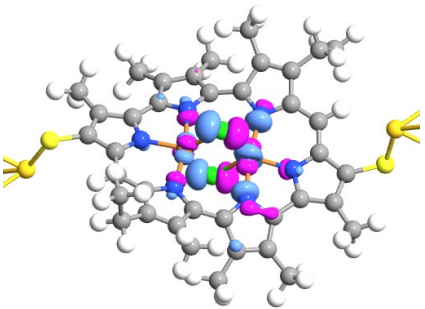
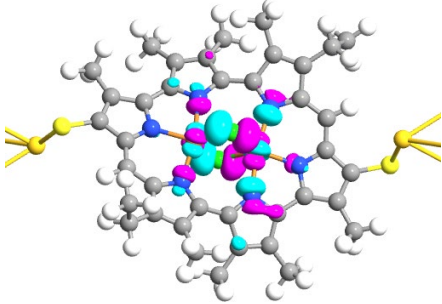
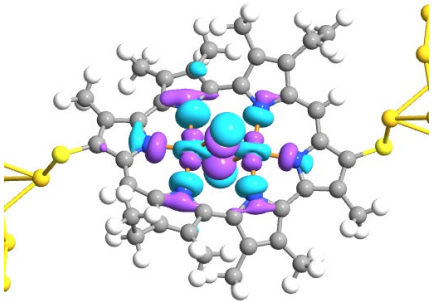
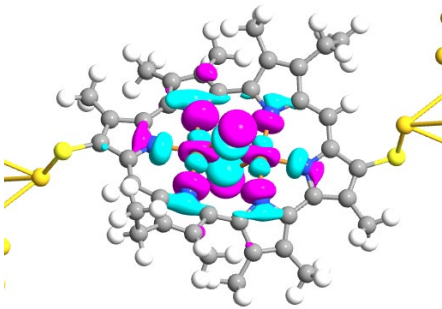
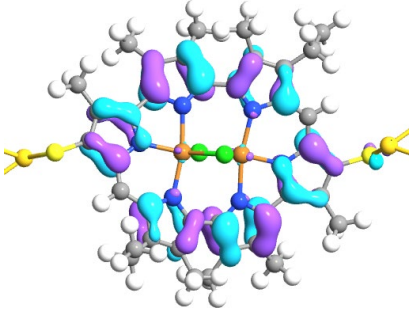
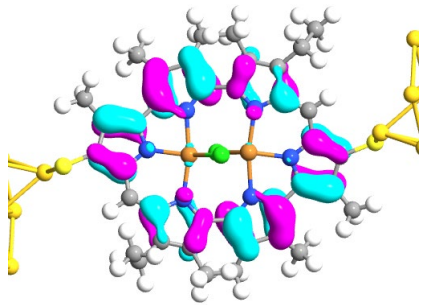


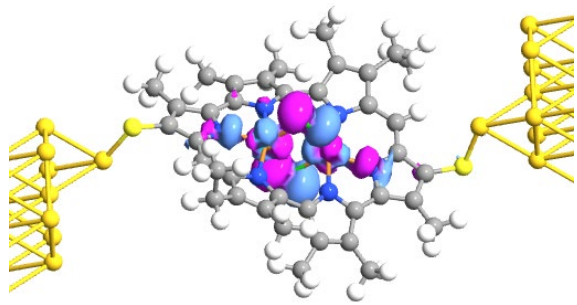
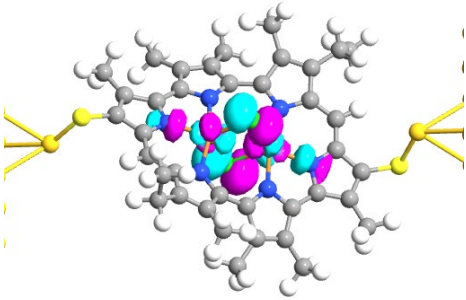
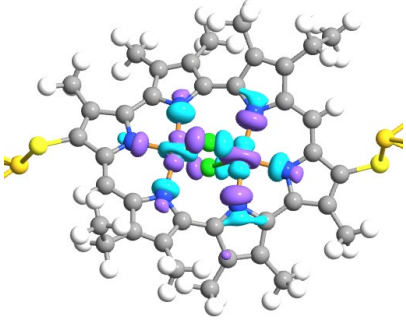
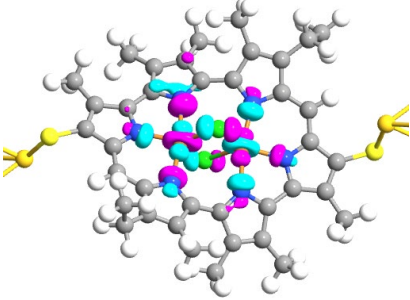




Ethynyl anchor- Triplet Configuration - Spin Up Channels	
Spin Up Transmission function -0.39 eV	Spin Up HOMO-1 -0.40 eV
Spin Up Transmission function 0.43 eV	Spin Up LUMO 0.36 eV
Ethynyl anchor- Triplet Configuration - Spin Down Channels	
Spin Down Transmission function -0.30 eV	Spin Down HOMO -0.32 eV
Spin Down Transmission function 0.35 eV	Spin Down LUMO+1 0.31 eV

Ethynyl anchor- Singlet Configuration - Spin Degenerate Channels	
	
Spin Up/Down Transmission function -0.05 eV	Spin Up/Down HOMO -0.05 eV
	
Spin Up/Down Transmission function 0.04 eV	Spin Up/Down LUMO 0.04 eV
	
Spin Up/Down Transmission function 0.43 eV	Spin Up/Down LUMO+1 0.34 eV

Direct anchor- Triplet Configuration - Spin Up Channels	
	
Spin Up Transmission function -0.39 eV	Spin Up HOMO-1 -0.41 eV
	
Spin Up Transmission function -0.31 eV	Spin Up HOMO -0.30 eV
	
Spin Up Transmission function 0.40 eV	Spin Up LUMO 0.30 eV

Direct anchor- Triplet Configuration - Spin Down Channels	
	
Spin Down Transmission function -0.36 eV	Spin Down HOMO -0.39 eV
	
Spin Down Transmission function 0.27 eV	Spin Down LUMO 0.25 eV

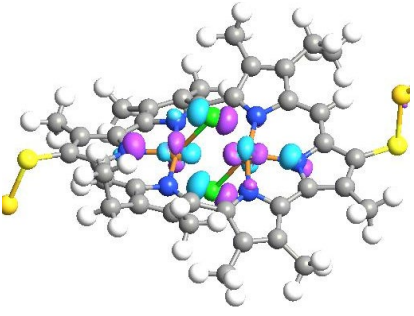
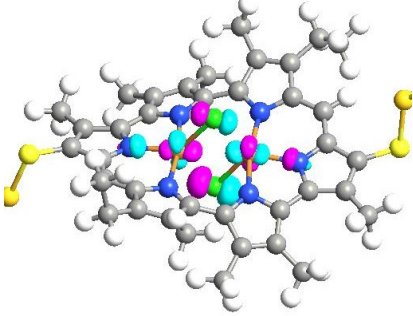
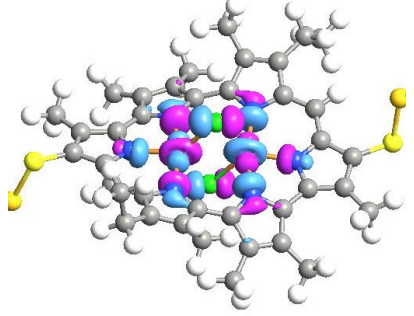
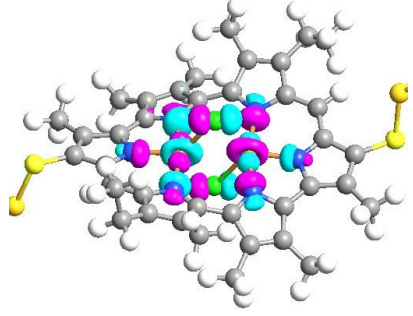
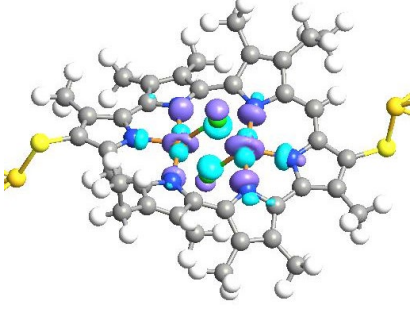
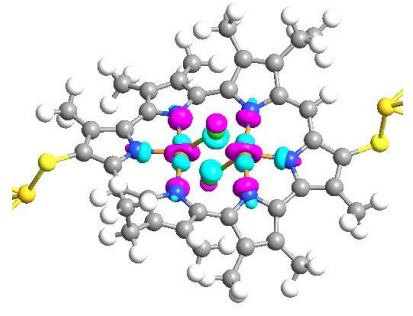
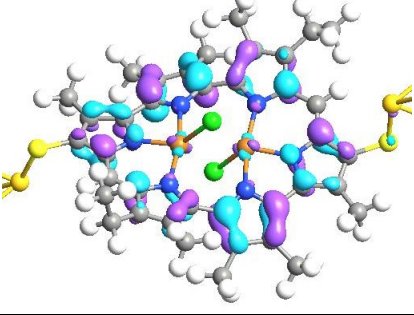
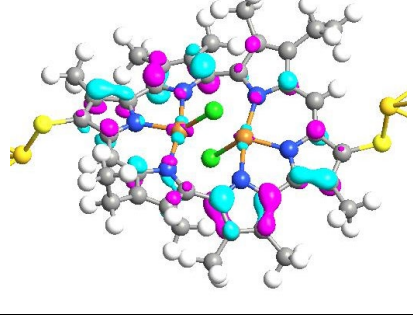
Direct anchor- Singlet Configuration - Spin Degenerate Channels	
	
Spin Up/Down Transmission function -0.44 eV	Spin Up/Down HOMO-1 -0.47 eV
	
Spin Up/Down Transmission function -0.06 eV	Spin Up/Down HOMO -0.06 eV
	
Spin Up/Down Transmission function 0.04 eV	Spin Up/Down LUMO 0.05 eV
	
Spin Up/Down Transmission function 0.41 eV	Spin Up/Down LUMO+1 0.31 eV

Figure S8. Calculated spin resolved current on the Cu(II)-Amethyrin junctions

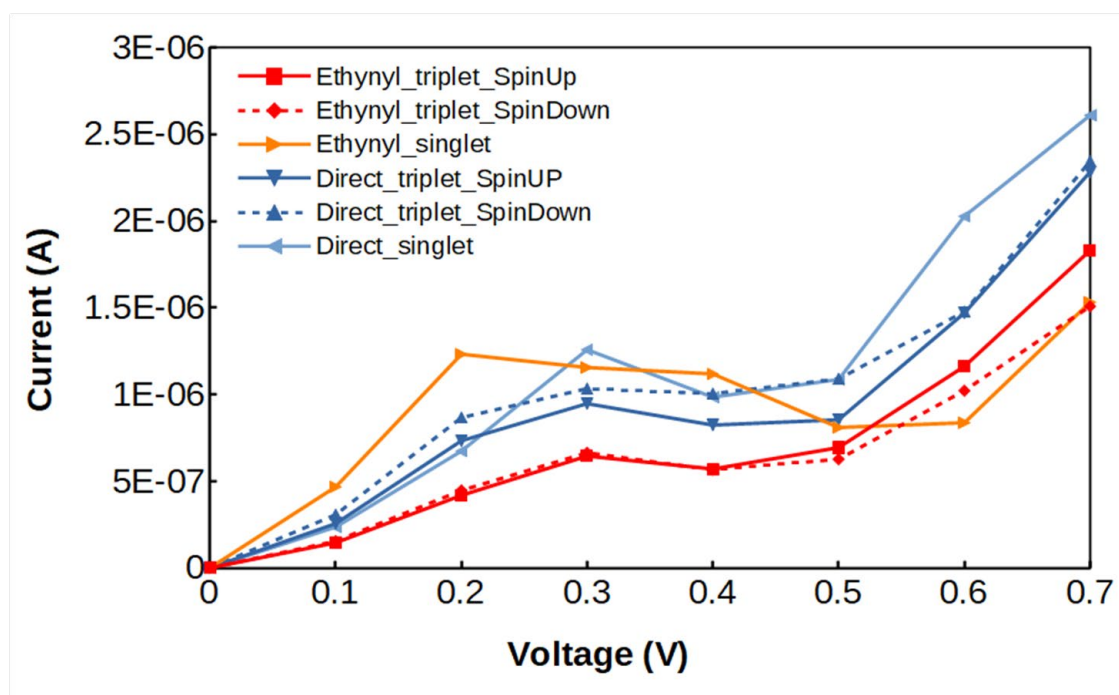


Figure S9. Calculated total current on the Cu(II)-Amethyrin junctions

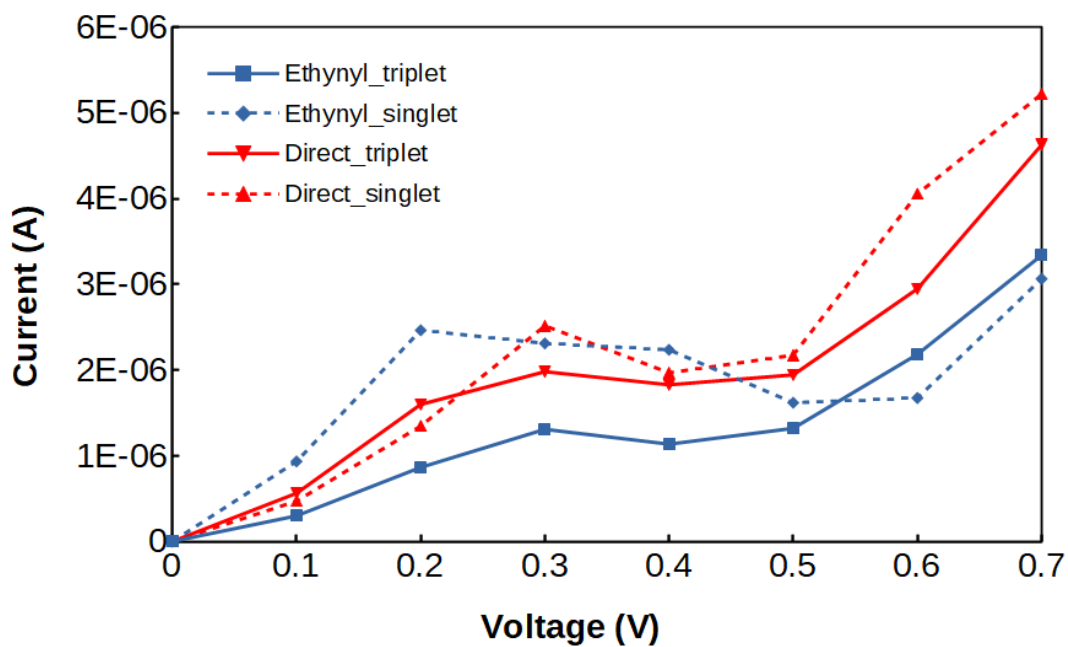


Table S1. Cartesian coordinates of the optimized structures for amethyrins in the ground state.

FB-Amethyrin systems

FB- Ethyl-anchoring

C	14.53994245	18.93001074	25.98566325
C	13.21989636	17.2506467	15.93262499
C	14.02330687	18.67236923	24.65227348
C	13.24134341	18.11212369	17.09517907
C	13.20235314	20.32349909	18.22543442
C	13.17953418	21.72739132	18.3381511
C	12.99320658	20.82345576	20.40175765
C	13.05083068	22.03963079	19.70539461
C	15.23041769	17.79860168	26.33729065
C	13.26159463	16.07298184	17.85274968
C	15.09578851	16.87677742	25.22687772
C	14.64823197	13.98721359	22.05699135
C	15.36269465	14.70071907	24.0648507
C	15.80160547	13.37428355	23.90546287
N	13.11295396	19.81415349	19.50098143
N	13.26964556	17.33725441	18.25206164
N	14.3640602	17.47414597	24.20681722
N	14.67576948	15.04125561	22.91851849
C	13.22719842	19.48682686	17.09299248
C	15.54787892	15.58276359	25.14827428
C	15.36617817	12.93072726	22.64404439
C	13.24542816	15.96300044	16.39836548
C	12.85707507	20.56327405	21.81254114
C	11.99115311	21.10617261	22.7510631
C	12.28414647	20.49791594	24.00196364
C	13.31208349	19.5886094	23.78846984
N	13.61864779	19.61736777	22.45053692
H	14.39887092	19.12318574	22.05357506
C	13.33842488	15.00034951	18.82538228
C	12.78814476	13.72169427	18.88144781
C	13.19565128	13.13320416	20.10842608
C	13.98808609	14.0622822	20.77554855
N	14.0357147	15.19154097	19.99532292
H	14.59267078	16.00901745	20.17452682
C	14.43658821	20.20704533	26.75372666
H	14.40928834	21.0662305	26.08134301
H	13.53406614	20.25561367	27.36877973
H	15.28776756	20.32816157	27.42661873
C	15.98042871	17.57376377	27.61160854
H	16.66363412	16.72811671	27.51497187
H	16.60059367	18.44728548	27.83312246
C	11.50312248	20.68447923	25.2614756
H	11.6473359	19.84406408	25.93980404
H	11.78262921	21.59981708	25.79163737
H	10.4354436	20.75289211	25.04156942
C	10.85245642	22.0275366	22.46318569
H	10.99936001	23.02151664	22.89595196
H	10.71067821	22.14811307	21.39024112
H	9.92254333	21.62649733	22.87623842
C	13.07395163	23.40446355	20.3185023
H	12.10584727	23.90880387	20.25608749
H	13.34205394	23.3476476	21.37385745
H	13.80157365	24.04689584	19.817337
C	13.27486161	22.72185357	17.22604155

H	13.63886273	22.23641764	16.31839842
H	14.02626134	23.47484754	17.48548564
C	13.25042216	17.69933805	14.50577461
H	12.72915985	16.97661273	13.87376978
H	12.72341757	18.64841871	14.38818101
C	13.35238877	14.7208107	15.57072813
H	13.88267831	13.93518293	16.10960355
H	12.37566597	14.31857963	15.29007429
H	13.89368104	14.91681817	14.64413574
C	11.81772546	13.10163147	17.92665162
H	11.33896632	13.85324604	17.30181546
H	12.29428807	12.36928732	17.26962622
H	11.0299013	12.57494191	18.46958746
C	12.73866301	11.81061223	20.6343062
H	13.2991476	10.97432411	20.20718623
H	12.84756803	11.76267202	21.71697722
H	11.68654071	11.64068043	20.39523751
C	15.69282113	11.61626013	22.00638893
H	15.06050078	10.80579632	22.37848173
H	15.55914681	11.66669642	20.92660573
H	16.7276837	11.3314852	22.2040216
C	16.65619698	12.61090076	24.86804639
H	16.42323848	12.90816773	25.893031
H	16.41097954	11.54799058	24.80017301
C	18.15625749	12.80859465	24.61223866
H	18.4269634	13.86132452	24.70772803
H	18.75632978	12.23317108	25.32024553
H	18.42475362	12.49208313	23.60298766
C	14.69711005	17.86059826	14.01090107
H	15.24125956	16.92403277	14.11808196
H	15.20502011	18.6237321	14.59747405
C	11.94466967	23.42803911	16.92775336
H	11.18881534	22.71088143	16.60373619
H	11.5613197	23.93352842	17.81525985
H	12.07307085	24.17577192	16.14203229
C	15.02772756	17.33184708	28.79175772
H	14.43329415	16.43599374	28.62136436
H	14.35737309	18.18070739	28.90458519
H	13.04374651	18.81099768	19.65134308
H	14.19959669	15.9370562	22.85519124
H	16.08835419	15.18443615	25.99761449
H	13.215082	19.98463194	16.13180124
H	15.58168016	17.20190706	29.7462060924
H	14.73591596	18.16347976	12.9425018262

FB-Direct-anchoring

C	16.43527059612278	20.37189409421316	15.16905035656495
C	18.13412510605393	19.24238040926011	25.25576863419417
C	17.03248268534521	20.28687019649881	16.50408476824819
C	17.93798911197223	20.08521049185511	24.09627179631686
C	17.43833784539564	22.23507145870944	22.93044313604253
C	17.10590025002782	23.61402601897440	22.78967940360889
C	17.55354561269530	22.73259314788646	20.72747652161996
C	17.17858839768445	23.92574917811275	21.40947667294479
C	16.08288738012613	19.06973657281497	14.85162093365870
C	18.55885283691058	18.12937393521354	23.33408347517349
C	16.46453561459960	18.24099093980432	15.97488668006012

C	17.77064132946874	15.66295521978708	19.16790227800353
C	16.77529324933717	16.07789224625488	17.18068442942358
C	16.70753879527170	14.67144229080699	17.40383532212530
N	17.68834316610077	21.73811635315207	21.65973344135315
N	18.19798259726944	19.36058024779055	22.93133582937990
N	17.03294889871329	19.02860021194477	16.97769106919823
N	17.41693578308337	16.63945010777027	18.27463449119034
C	17.56941776093480	21.43179819539811	24.08686993226965
C	16.33849429053444	16.85471702656206	16.08324526212936
C	17.32073801458462	14.41285500738381	18.65295205796265
C	18.52783544910884	17.99745424758208	24.79268062322150
C	17.71729808255569	22.49686702478813	19.30943022098092
C	18.30867515972630	23.29140973532142	18.30545227207143
C	18.16028636996173	22.59295841757241	17.06584189826782
C	17.48377014079713	21.38616093018625	17.34056002481412
N	17.26134887096653	21.34084949747175	18.70367858403628
H	16.71433839833667	20.60779939528927	19.15058886440423
C	18.81162997360700	17.08153962734263	22.35972714028173
C	19.69223402159352	15.97971696639830	22.33026550568426
C	19.45052944112244	15.27191257538605	21.11071198049360
C	18.42664676733657	15.95635395310473	20.42327869906229
N	18.08819809719516	17.06058788202809	21.18256086322657
H	17.32132903888740	17.70297075282759	20.99370453232943
C	16.15214632199668	21.61858432624768	14.38311643164105
H	15.98347213633907	22.47969926597857	15.05787477888890
H	16.98809522934796	21.89514062496226	13.70887011506018
H	15.25231216720547	21.48917074348618	13.75324543100052
C	18.76157851088969	23.00984518674492	15.75543745531767
H	18.86722543677945	22.14811832643163	15.07353480454088
H	18.15492244733693	23.78034805898079	15.23733697907099
H	19.76944534894891	23.44427926680252	15.90618973575066
C	19.08554555815835	24.55725244865068	18.51534036600194
H	18.53124349857265	25.45581782622680	18.17537490688962
H	19.33682574697692	24.69750388170584	19.58159338523217
H	20.03561757588786	24.53430902924339	17.94565643181254
C	16.80968521360779	25.23198623687759	20.77120541743931
H	17.64281501723795	25.96378147229200	20.78494090112456
H	16.51730595830374	25.08538850495038	19.71523262339805
H	15.96016846933974	25.70388266274538	21.30165217728061
C	16.77226828790221	24.56863575951325	23.89901530932571
H	16.42392032043269	24.00876296453190	24.78929508224980
H	15.91727131818692	25.20598146650797	23.58870698931601
C	18.74718185494475	16.74950529415742	25.59617090449566
H	18.41969698366592	15.85421457041018	25.03326922545030
H	19.81251807230214	16.59353576920472	25.86013016676335
H	18.17817676034907	16.78994485112342	26.54364235645269
C	20.79309346073403	15.67747398076265	23.30448787367737
H	21.06224132952394	16.57129218567641	23.89434434506961
H	20.51943273949099	14.87109981591899	24.01501584446630
H	21.70463599971497	15.33989982334900	22.77334817497957
C	20.24693333555609	14.11074675855837	20.59323161717004
H	19.98867758691862	13.15968998721938	21.10205078361387
H	20.08566439127175	13.96958535495120	19.50977188856359
H	21.33105826860631	14.27457242775192	20.75389076148796
C	17.37595627802402	13.08963625630896	19.35974782565350
H	18.21225203450200	12.45263290008440	19.00619032773348
H	17.50629276139690	13.23138672755950	20.44803814543375

H	16.44222930726743	12.51806807264320	19.19899213878151
C	15.99563675313041	13.67941723030779	16.52907974447199
H	16.14063107102429	13.94531665657698	15.46213019599241
H	16.45540894194706	12.67943098705798	16.65851558975192
C	14.48660300151825	13.60284820835368	16.83999917859449
H	14.00828502213225	14.58853691607514	16.68168698225917
H	13.97955530757481	12.85881187255152	16.19525137422389
H	14.31784261937381	13.31951691447160	17.89686066413763
C	17.96296917670869	25.46989379244651	24.28285689683259
H	18.81654157974707	24.85890854421939	24.63399734164114
H	18.30815918929753	26.05669883374431	23.41009914744621
H	17.68536716341302	26.17900277689255	25.08674422126681
H	15.58253378789639	18.72390328125829	13.93944842044212
H	17.96782948018052	19.53637664107907	26.29886697905173
H	18.00787691111616	20.75557624707508	21.56523126063465
H	17.60886719085966	17.65880929058454	18.26917071631096
H	15.88161920729774	16.31496547553281	15.24268821861829
H	17.38860337863558	21.91776836172084	25.05501551284758

FB-Phenyl-anchoring

C	20.87268259	15.16533283	27.50292339
C	19.87027978	17.93953438	17.67128531
C	21.10613778	15.50788593	26.10993127
C	20.0286215	16.92570329	18.70542842
C	20.1190127	14.58507385	19.55119468
C	20.01363888	13.16912527	19.49953395
C	20.81678068	13.78082106	21.54144342
C	20.44603749	12.66664084	20.74289597
C	20.51451393	16.35724628	28.12117819
C	20.65740536	18.81612697	19.60372925
C	20.52987412	17.37579313	27.08226048
C	20.71421823	20.54745312	24.17534054
C	20.28784214	19.69894734	26.22295357
C	20.04244715	21.0969995	26.2806229
N	20.58882021	14.91472699	20.8119699
N	20.49698038	17.50765136	19.87609996
N	20.87859687	16.80892027	25.86236738
N	20.67899882	19.40592308	24.92707163
C	19.87065835	15.5510203	18.56068164
C	20.226138	18.72385518	27.23310177
C	20.30082914	21.62560196	25.00130848
C	20.28394109	19.14151872	18.24131759
C	21.29728686	13.82836065	22.89875217
C	22.21430669	13.01582694	23.58355458
C	22.30888357	13.50764222	24.91697826
C	21.44917528	14.61187648	25.02245777
N	20.88567016	14.81009534	23.77904401
H	20.13642033	15.47371637	23.61577767
C	21.05294693	19.73535833	20.65018059
C	21.82301329	20.90961274	20.66235454
C	21.82463216	21.40779005	21.99675833
C	21.05822159	20.52749894	22.7756608
N	20.64143397	19.50512579	21.94658535
H	19.96991171	18.7849963	22.1895195
C	20.97583693	13.80473222	28.11875579
H	20.74630174	13.02390426	27.38013655
H	21.98783566	13.60002583	28.50237154

H	20.28858497	13.69237776	28.96628317
C	23.28139252	13.02165547	25.94605886
H	23.4286632	13.76674186	26.73699881
H	22.95690139	12.08192566	26.42072796
H	24.26324849	12.82509633	25.48883447
C	23.05779015	11.93035258	22.99179159
H	22.71843289	10.92608914	23.2920862
H	23.04745111	11.97394537	21.89520679
H	24.104098	12.02460039	23.32078749
C	20.40690931	11.23737489	21.18614413
H	21.28118486	10.66387307	20.84000833
H	20.3833915	11.16955421	22.28207557
H	19.51323216	10.72990481	20.7934364
C	19.54406612	12.36091557	18.3298316
H	18.90521264	12.97605524	17.67781492
H	18.90681288	11.5359542	18.68968276
C	20.16387379	20.51266376	17.65170106
H	19.96360268	21.2549527	18.437365
H	21.07707309	20.83676598	17.12834796
H	19.34444461	20.54894112	16.91979801
C	22.63532462	21.46629158	19.5346461
H	22.78768735	20.71724013	18.74785741
H	22.16471037	22.34862459	19.0723529
H	23.62759561	21.78277617	19.89095841
C	22.62289038	22.57167531	22.4947383
H	22.17722808	23.53788432	22.20920807
H	22.71145663	22.55211926	23.58829869
H	23.64075858	22.55484366	22.07534358
C	20.07402287	23.04011947	24.56389263
H	20.89216217	23.71008051	24.8726968
H	19.9923001	23.10219962	23.47078127
H	19.146685	23.44155752	24.99787227
C	19.5034445	21.84290264	27.46319533
H	19.92578776	21.42979027	28.39309298
H	19.83672602	22.89121481	27.41456716
C	17.96532249	21.79279728	27.53631727
H	17.61642562	20.75436397	27.62740909
H	17.59016535	22.3606469	28.40001662
H	17.51682074	22.21513205	26.62545849
C	20.71045115	11.77911811	17.50994299
H	21.34362961	12.58516093	17.11293036
H	21.34421238	11.13360479	18.13483121
H	20.34074122	11.18120677	16.6643767
H	19.216722591	17.27144008	33.284373240
H	17.896241862	17.23052757	12.696810775
H	20.8243625	15.8978559	21.01440265
H	20.98177184	18.4481497	24.69805535
H	19.93345768	19.06680532	28.22709926
H	19.56459917	15.17799685	17.582403
C	20.1669	16.58959155	29.5271291
C	20.83996165	17.57496562	30.28076436
C	19.14113103	15.85887319	30.1618403
C	20.50657572	17.81804422	31.60960163
H	21.65120213	18.13538802	29.81314574
C	18.80563202	16.09512211	31.49068327
H	18.58187665	15.11935457	29.5870261
C	19.48220417	17.08182418	32.23269562

H	21.04214194	18.57331653	32.18592643
H	18.00695924	15.52803102	31.97011634
C	19.33755826	17.73680874	16.32701498
C	18.19802037	16.9328322	16.09918534
C	19.93745183	18.3580894	15.20861401
C	17.68625112	16.75484304	14.81834242
H	17.68899899	16.48062936	16.95164482
C	19.43373425	18.17867334	13.92658068
H	20.83009306	18.96661021	15.35755179
C	18.30032779	17.37064152	13.71136025
H	16.79266455	16.15024871	14.6589845
H	19.91169822	18.65666481	13.07077548

FB-Ethynyl anchoring

C	3.98867987	4.89424513	17.56325068
C	1.39233058	3.02834484	27.27777069
C	3.72038303	4.29501569	18.84069788
C	2.38392008	3.22800863	26.22413688
C	4.69170563	3.67662318	25.42046133
C	6.08723925	3.94516985	25.5111667
C	5.53300337	3.60980689	23.32687113
C	6.61200737	3.90434814	24.20751814
C	2.73104736	5.27207596	17.05996996
C	0.5139134	2.69159191	25.22361128
C	1.75699359	4.88022865	18.07485971
C	-1.31948476	3.57537567	20.78103054
C	-0.56521245	4.59050005	18.91053716
C	-1.98771064	4.65722232	18.89096103
N	4.39609075	3.50150558	24.07735201
N	1.80698317	3.03437628	24.99005207
N	2.39780678	4.30563432	19.14828521
N	-0.20384101	3.9433762	20.08225074
C	3.72690293	3.54035708	26.42521606
C	0.37470347	5.02106829	17.96763974
C	-2.45753962	4.03367446	20.05839002
C	0.19519088	2.68665327	26.62433188
C	5.51040024	3.49937785	21.89355633
C	6.41636743	2.91677749	20.99136917
C	5.89329059	3.10324673	19.68113452
C	4.67872862	3.79687826	19.80573989
N	4.4473597	3.98047953	21.15188286
H	3.70270567	4.57199112	21.50461843
C	-0.38692211	2.47542466	24.11029797
C	-1.48116151	1.616708	23.91449858
C	-2.0139623	1.88969095	22.62343262
C	-1.2336365	2.90906599	22.05222359
N	-0.2297674	3.20901214	22.9543327
H	0.4072114	3.9954396	22.88620128
C	5.30789948	5.18778923	16.93071224
H	6.09366735	5.30269014	17.69009386
H	5.62861217	4.38803249	16.24447236
H	5.24521283	6.11078031	16.33713317
C	6.46900569	2.51867679	18.42947476
H	5.72293403	2.48627567	17.62649906
H	7.33764258	3.08781083	18.06245149
H	6.81386325	1.48831194	18.60533893
C	7.62561872	2.10662226	21.33894783

H	8.56312011	2.64616694	21.13033148
H	7.62603343	1.8282289	22.40018371
H	7.65522057	1.17760536	20.74928347
C	8.01432862	4.23685775	23.80369416
H	8.69835227	3.38093334	23.91261879
H	8.05364436	4.5580425	22.75437758
H	8.41603641	5.05074604	24.42485025
C	6.84993889	4.20490068	26.77248925
H	6.17307966	4.59068589	27.54950118
H	7.59262313	4.99945464	26.59168627
C	-1.13272481	2.49520276	27.27710547
H	-1.94867072	2.80198625	26.60802421
H	-1.31428333	1.44527649	27.55612096
H	-1.18641726	3.08601752	28.20246427
C	-1.92223945	0.50456808	24.814209
H	-1.13639321	0.23992973	25.53213774
H	-2.82761635	0.76131029	25.38650675
H	-2.15822114	-0.39745096	24.22927333
C	-3.10113997	1.11341264	21.94891758
H	-4.1014896	1.38322604	22.32282457
H	-3.09164709	1.27487669	20.86387561
H	-2.97561769	0.03459342	22.1278793
C	-3.88239321	3.97396918	20.51645496
H	-4.44851608	3.17042527	20.0196771
H	-3.93879831	3.79768353	21.5983982
H	-4.40222534	4.91795771	20.29851163
C	-2.81211298	5.36766544	17.86176012
H	-2.36036624	5.23913204	16.86561424
H	-3.8086495	4.90268448	17.81049043
C	-2.95652903	6.8714815	18.16585121
H	-1.97154181	7.35874792	18.18029723
H	-3.57727672	7.36968489	17.40758736
H	-3.42139725	7.02938635	19.1497976
C	7.56942417	2.94617778	27.29233396
H	6.84491061	2.148559	27.5087351
H	8.27791413	2.56200866	26.54449202
H	8.12801973	3.16451064	28.21368654
H	3.44935259	3.20529555	23.80246905
H	0.78424885	3.70634088	20.24499158
H	-0.00095117	5.48344877	17.052214
H	4.05232193	3.65849695	27.46076965
C	1.60859899	3.19523666	28.64102893
C	1.85261161	3.34998932	29.8449222
C	2.44622735	5.92316643	15.86477538
C	2.15576312	6.51018483	14.81422919
H	1.91810049	7.01799495	13.8897725879
H	2.04382011	3.48303004	30.9007183252

Cu-Amethyrin systems

Cu-Ethyl anchoring

C	15.75217199	21.10109446	26.68860147
C	13.49935741	17.8785041	16.51784265
C	15.42437572	20.90554959	25.27671166
C	13.8656868	18.83787127	17.55508605
C	14.51415769	21.02516873	18.54605975
C	14.85353862	22.42939239	18.40106813
C	14.74531684	21.82350492	20.59164984

C	15.00675304	22.93217141	19.67229696
C	16.26408419	19.89292575	27.13018247
C	13.73674743	16.8602078	18.53476894
C	16.22081972	18.97210602	25.99906255
C	15.68540393	16.00969616	22.86079529
C	16.45278945	16.82801872	24.76346163
C	16.95173835	15.46645415	24.67224065
N	14.53051305	20.67833188	19.88718852
N	13.97320806	18.18258404	18.72947926
N	15.72112885	19.62590844	24.93169513
N	15.74559177	17.14346061	23.61504259
C	14.15509028	20.20127787	17.47065702
C	16.6204889	17.63774466	25.89401272
C	16.4986512	14.9587042	23.47880078
C	13.42028515	16.63740955	17.12498877
C	14.68030458	21.97977402	22.01632817
C	14.14731419	23.16892066	22.69353233
C	14.35121472	22.98570217	24.04771896
C	14.97312809	21.68938297	24.18714971
N	15.10558231	21.09680541	22.94681779
C	13.98622093	16.06961845	19.68274352
C	13.69236084	14.71108038	20.06887932
C	14.24810331	14.54110374	21.32302795
C	14.90166544	15.80849171	21.67760568
N	14.66057243	16.71392934	20.69983065
C	15.6211836	22.35276175	27.49336125
H	16.08738619	23.20767353	26.98298345
H	14.56832757	22.61756103	27.6718673
H	16.10181527	22.24247878	28.47476931
C	16.72694647	19.52880389	28.50542451
H	17.54699227	18.79584513	28.4497653
H	17.12651747	20.4109698	29.02855421
C	13.88729628	23.89715814	25.13759057
H	13.35359478	23.34643502	25.92473965
H	14.72405575	24.42641378	25.61875242
H	13.20656075	24.66219964	24.74138166
C	13.30777505	24.25394419	22.08612085
H	13.78356982	25.24443138	22.14620999
H	13.0817726	24.04658715	21.03394391
H	12.3450738	24.32463793	22.61604489
C	15.55841997	24.28668026	20.00496886
H	14.86291818	25.10093183	19.75196822
H	15.81301217	24.37233334	21.0674922
H	16.48193545	24.46298972	19.43186673
C	14.9968483	23.17878687	17.1125583
H	15.33991139	22.50555723	16.31175982
H	15.78409399	23.94165336	17.22592804
C	13.35134312	18.21523358	15.066877
H	12.71958045	17.47309981	14.55693315
H	12.84856325	19.18891301	14.95301077
C	13.15267047	15.33217301	16.44782007
H	13.89324785	14.57477142	16.74121411
H	12.16073551	14.92951149	16.70247867
H	13.19713003	15.4369606	15.35581107
C	12.84260677	13.72452237	19.33484327
H	11.9828618	14.21066392	18.85450563
H	13.40642693	13.20125224	18.54637914

H	12.45742196	12.95529902	20.01806936
C	13.9789779	13.37614833	22.22884203
H	14.50764636	12.46243869	21.9180501
H	14.25695378	13.59620104	23.26579346
H	12.90305775	13.1424092	22.2251363
C	16.95900417	13.66859328	22.86540362
H	16.55863095	12.7857273	23.38619952
H	16.67945631	13.5973841	21.80823872
H	18.05610021	13.60479609	22.91993342
C	17.89122809	14.81219224	25.63781223
H	17.5772455	15.02390384	26.67347233
H	17.82880858	13.71937207	25.52140807
C	19.34916716	15.27233836	25.443337
H	19.43752685	16.35825456	25.58835602
H	20.02110988	14.77145422	26.15522602
H	19.6960945	15.04786686	24.42460845
C	14.73784155	18.27025451	14.38817232
H	15.21805868	17.28462889	14.43789538
H	15.37795079	18.9995709	14.90040778
C	13.68519352	23.86554523	16.68598566
H	12.88504974	23.12541448	16.54228648
H	13.34850832	24.5712223	17.45872617
H	13.81489787	24.41924414	15.74480876
C	15.55923824	18.93106118	29.31974122
H	15.16097676	18.04559663	28.80841927
H	14.75671257	19.67271493	29.42016117
Cl	13.10631484	18.83435977	22.34573258
Cl	16.87978371	18.9814406	21.24200413
Cu	15.41943816	19.07371754	23.08483805
Cu	14.62631685	18.74784958	20.48282183
H	17.08949402	17.17448599	26.763188
H	14.1000129	20.67439896	16.48941596
H	15.88367365	18.62850199	30.3387690328
H	14.65890328	18.56496975	13.3197084989

Cu-Direct anchoring

C	15.88651333178213	20.85185129326119	14.99156132470428
C	18.35453792275464	18.44192539767653	25.36691330409496
C	16.23164904256946	20.74880732179451	16.41689803820267
C	17.85066536784308	19.30163995877451	24.30556015556928
C	17.04037450404650	21.37278322526442	23.16839116986125
C	16.60105521680154	22.76242325951572	23.20795152465813
C	16.77407781525508	22.00276825246548	21.06182307872466
C	16.42229303658237	23.15822363709277	21.89458685994831
C	15.45528424258899	19.58642867746346	14.62420148608607
C	18.15055870138093	17.28824105455176	23.41896294906036
C	15.54840608008023	18.72831936210102	15.79718201130831
C	16.27518571753403	16.02617578868039	19.13792729581173
C	15.45121527752872	16.64899416279552	17.17884721258788
C	15.06305730283781	15.25339035558416	17.36311363976279
N	17.06296699189086	20.93278677388486	21.85210063068165
N	17.75516341669923	18.56344873150668	23.17487796385075
N	16.01315229449426	19.47297716757991	16.82726989032397
N	16.12297813765919	17.09509602552376	18.30830071765975
C	17.45484407921387	20.65089689799193	24.30579474857399
C	15.23122009391366	17.37116047572340	15.98854535749101
C	15.55576619336600	14.86611457798119	18.59469962046657

C	18.55559091784404	17.18047728977298	24.82765962798900
C	16.86069376688137	22.06952933099334	19.62496667890013
C	17.33460761191004	23.25237154779870	18.88434479451766
C	17.17294739396318	22.96643551429526	17.53312136858391
C	16.62952031109092	21.62466283385629	17.46821058151668
N	16.51074454262852	21.10443084851469	18.74218992135366
C	17.96977210628805	16.41348871920352	22.30883795267755
C	18.39629178632181	15.06720335100188	21.98733209848804
C	17.84808041536099	14.77609254097333	20.74323174476770
C	17.07502850773326	15.96237883365821	20.33389875577278
N	17.22861916818511	16.93330117982287	21.26643732150736
C	15.91758018817955	22.06652455026263	14.11632426567408
H	15.35709711922268	22.90625262648347	14.57229371996078
H	16.95026941906706	22.42513751073560	13.93828663200546
H	15.46350601902949	21.84531994823824	13.13384311942580
C	17.60291958521403	23.82431792159553	16.38377662429249
H	18.19679856574088	23.24668999722293	15.65001966260202
H	16.73855297120081	24.25404795760399	15.83948319202437
H	18.22174887285157	24.67077261873983	16.73133785554815
C	18.09472281209399	24.42481624587446	19.44014017437649
H	17.53769181243115	25.37807026729288	19.35422057851009
H	18.35396186034392	24.27138010125360	20.50140965555426
H	19.04604020399024	24.55337614809994	18.88733886778621
C	15.78335815603992	24.44611945150815	21.45747988780876
H	16.43415757566861	25.32480811874675	21.63268765370057
H	15.51071526114696	24.42631292349520	20.38861498932369
H	14.85219476882214	24.61544931470862	22.03319798724590
C	16.41008069048173	23.60272927661302	24.43691470252533
H	16.11036962777826	22.96921988778607	25.29534984903805
H	15.56661610701894	24.30325224316850	24.26899636698543
C	19.02411619076337	15.96488627184870	25.56573395730792
H	18.31782128645395	15.12053276808176	25.44216162489870
H	20.01053225792977	15.61504964172069	25.20366157533833
H	19.11720686297808	16.18003050909203	26.64516800759832
C	19.33919087620911	14.20479764581423	22.76760329709931
H	20.21970871234541	14.77811172838709	23.11451264605082
H	18.85750449716787	13.76942074307906	23.66564842925129
H	19.70333440725672	13.36106123987792	22.15432657508043
C	18.21227707477949	13.58886230949714	19.89464329393620
H	17.76272229815496	12.64562228707047	20.26162650149042
H	17.90550865624897	13.73041662615114	18.84463951868564
H	19.31090101250529	13.44653107702563	19.89813757578748
C	15.19962830710387	13.59112543338357	19.30813648269242
H	15.66725045384462	12.69952695307281	18.84673165650231
H	15.49219194723709	13.62315075731799	20.37098899469754
H	14.10371444886117	13.43793321129385	19.27150534969416
C	14.16432297284541	14.46555945091405	16.45466639811075
H	14.47676732250303	14.60282438785235	15.39811221698259
H	14.28575276701874	13.38525456616943	16.66618473702782
C	12.68295460358152	14.86797328657069	16.61122774722795
H	12.54315937835885	15.94002924088007	16.37419411629064
H	12.03236394499145	14.27203976451467	15.94223651916788
H	12.34639086122365	14.71436210236934	17.65433921511877
C	17.67655439428177	24.40799596987599	24.79538610852542
H	18.53148898146547	23.73035165823043	24.98345689241722
H	17.96111142850939	25.07681362031195	23.96046941723297
H	17.51543405036628	25.02784041927965	25.69865508288303

H	15.09535465044329	19.28390656250764	13.63430274977192
H	18.52839949432638	18.74050641601752	26.40691541799552
Cl	18.64874436967133	19.03225686159959	19.51592707653884
Cl	14.84369858750596	18.99918212159108	20.55954074339017
Cu	16.34550934753297	19.06236317930377	18.71447803449083
Cu	17.08741216652477	18.97182008727404	21.37670494909631
H	14.79723942559097	16.81878058136045	15.14535018480412
H	17.48125076806719	21.19474120712943	25.25842762592511

Cu-Phenyl anchoring

C	15.97674776	20.9599963	19.40629575
C	15.65893654	18.0680421	29.87882828
C	15.99571971	20.80264747	20.85440641
C	15.46634368	18.97330089	28.74572564
C	14.98152834	21.08265088	27.53805502
C	14.49996455	22.45078897	27.5339743
C	15.29859501	21.85143787	25.49041973
C	14.68356047	22.9329777	26.25932452
C	15.63096784	19.71373424	18.89245047
C	16.12402048	17.03360103	27.91044865
C	15.46776044	18.81606511	20.0345636
C	15.44209083	15.95090536	23.2888698
C	15.02865361	16.70750104	21.25508098
C	14.60331632	15.32010157	21.27199607
N	15.40077438	20.72598034	26.26601455
N	15.76547429	18.30935885	27.61115837
N	15.69987313	19.51261311	21.16456041
N	15.47387577	17.08031896	22.51354079
C	15.06720368	20.30932181	28.70067529
C	15.07144685	17.47942693	20.09024494
C	14.85045725	14.84442057	22.53743044
C	16.08740851	16.85195526	29.35271488
C	15.75360889	21.9966493	24.15024924
C	16.32840862	23.22071565	23.58919763
C	16.53478308	22.99181266	22.24099553
C	16.11101381	21.63594618	21.99542694
N	15.70367691	21.04881437	23.17585812
C	16.28844249	16.21591708	26.76584737
C	16.79811174	14.89136419	26.51817991
C	16.57994489	14.64248399	25.17478212
C	15.92951851	15.83081013	24.61951384
N	15.83725807	16.77775778	25.59111717
C	16.28525613	22.18949841	18.615428
H	15.55653695	22.99194697	18.80778269
H	17.27874955	22.58705979	18.86197938
H	16.27165843	21.9728254	17.5402726
C	17.17135687	23.9435315	21.28094031
H	17.99109129	23.46948133	20.72279989
H	16.45110562	24.32767081	20.54283368
H	17.58414488	24.81115439	21.81187217
C	16.85555628	24.40107511	24.35159444
H	16.29645891	25.32610554	24.14536685
H	16.83218912	24.22246751	25.43244656
H	17.9043693	24.58784184	24.07461151
C	14.13409426	24.23061092	25.74474426
H	14.68421904	25.10496156	26.12316656
H	14.14080963	24.27029436	24.64971864

H	13.08912922	24.34421451	26.07182877
C	13.92983808	23.18673175	28.70657772
H	13.38518411	22.49318284	29.36601048
H	13.18329138	23.9135483	28.34795815
C	16.30117704	15.58080626	30.10946137
H	15.81926395	14.73535886	29.6001835
H	17.36881105	15.33091348	30.21178764
H	15.87978753	15.65626569	31.12038073
C	17.53038923	14.00410479	27.47260678
H	18.14848387	14.58453557	28.16966456
H	16.84515016	13.38676509	28.07519325
H	18.1900911	13.31238969	26.93041599
C	17.14930208	13.48513224	24.41032526
H	16.63361909	12.53739999	24.62683036
H	17.11056925	13.65665921	23.32859075
H	18.20751818	13.34379488	24.67996283
C	14.37885647	13.52010187	23.0637719
H	14.98241571	12.67896329	22.69072188
H	14.39509627	13.48966519	24.15899979
H	13.34213179	13.34041945	22.74311104
C	13.92241085	14.60388234	20.14706594
H	14.43599317	14.81964904	19.19549178
H	14.01323046	13.51759028	20.29827269
C	12.43584872	14.99034386	20.02396123
H	12.32708341	16.06750034	19.83458623
H	11.95207678	14.44306839	19.20217507
H	11.89696483	14.76446863	20.95510907
C	15.01223483	23.92896061	29.51431561
H	15.76398752	23.22549863	29.89976953
H	15.53562042	24.65950852	28.88092123
H	14.57209948	24.46443631	30.36787257
H	14.94250080	18.21344273	13.75444045
H	14.71104671	19.31668722	35.04188937
H	14.78405884	16.99243661	19.15863221
H	14.81488946	20.80047549	29.63973247
C	15.4509226	19.31786249	17.49453332
C	16.05735926	18.14521101	16.99452338
C	14.65226542	20.07873075	16.61525799
C	15.87929381	17.75314208	15.67218474
H	16.69741349	17.55613861	17.65322383
C	14.47454464	19.69233733	15.29101901
H	14.1448978	20.9676395	16.99251027
C	15.08378805	18.5216684	14.80206161
H	16.36388328	16.85347739	15.29153984
H	13.85302409	20.28562605	14.61962666
C	15.40583701	18.40412796	31.27976778
C	14.21950218	19.06971224	31.65939191
C	16.33229159	18.0725828	32.29036886
C	13.972614	19.39419783	32.98833772
H	13.47169278	19.30009313	30.89908473
C	16.08684396	18.39028663	33.6221827
H	17.26669274	17.58204209	32.01445411
C	14.90563512	19.06171816	33.98851888
H	13.0475446	19.89654572	33.27311241
H	16.81102372	18.13213627	34.39551414
Cu	15.57057691	19.03127227	23.06310399
Cu	15.60158267	18.78956263	25.71408518

Cl	13.66596528	18.80988062	24.23677717
Cl	17.75080272	18.92582008	24.21234704

Cu-Ethynyl anchoring

C	0.75129335	6.61618969	27.18535334
C	-0.10692802	4.03400798	16.68288864
C	0.53422294	6.47060677	25.76419318
C	0.07409525	4.93564844	17.82722445
C	0.28938854	7.08953387	19.02867692
C	0.41464976	8.537865	19.02640256
C	0.17051233	7.72562509	21.13729863
C	0.35255269	8.94096426	20.33777667
C	0.10235441	2.86541851	18.62047368
C	1.56779467	4.61254019	26.39184035
C	1.72988949	1.87429621	23.03576007
C	2.22293726	2.64095931	25.04492149
C	2.91118402	1.36682931	24.91221656
N	0.21957498	6.62399531	20.33289497
N	0.18726298	4.19241517	18.93682497
N	1.03160238	5.26622201	25.35186897
N	1.57473999	2.95216273	23.85930042
C	0.17168264	6.32761671	17.86339427
C	2.18076932	3.36812899	26.23698444
C	2.6234295	0.89184411	23.65740782
C	-0.0936246	2.72547285	17.1954492
C	-0.07015993	7.73494095	22.54456917
C	-0.82084589	8.77297656	23.25949007
C	-0.72356953	8.482769	24.60698624
C	0.05512894	7.27149739	24.69765101
N	0.37557846	6.81504744	23.43838751
C	0.34016378	2.011309	19.72608333
C	0.18433422	0.59746088	19.97023751
C	0.64265919	0.38030227	21.25578646
C	1.09308889	1.67703196	21.7730488
N	0.82815556	2.6383502	20.85114532
C	0.43293614	7.76696629	28.07598485
H	0.74109889	8.71967406	27.62376401
H	-0.64611179	7.83815654	28.28134417
H	0.94884387	7.6490635	29.03814584
C	-1.40954013	9.20686952	25.71970492
H	-1.82316626	8.50934845	26.45959651
H	-0.72718849	9.88690865	26.25370338
H	-2.2355091	9.81968756	25.33394432
C	-1.74182293	9.79690189	22.66574423
H	-1.40685745	10.8284769	22.85089602
H	-1.85440922	9.66168959	21.58413151
H	-2.74441585	9.69972713	23.11095325
C	0.64724807	10.32694823	20.82961971
H	-0.15182918	11.04300271	20.58641543
H	0.80825462	10.34794649	21.91340789
H	1.56728626	10.69908347	20.35336096
C	0.57007426	9.40719505	17.81810457
H	1.12146855	8.87280311	17.02942585
H	1.1841905	10.28311295	18.08199509
C	-0.19891168	1.48845568	16.37273522
H	0.58831002	0.76709442	16.63206342
H	-1.16513337	0.98230298	16.51869821

H	-0.11055823	1.73965302	15.30741745
C	-0.46507062	-0.41126914	19.07933019
H	-1.35735308	-0.00041348	18.58803084
H	0.21441823	-0.76142614	18.28680328
H	-0.77321615	-1.29630569	19.6519713
C	0.4548792	-0.88921165	22.03159653
H	1.13820659	-1.68991769	21.71147012
H	0.59297446	-0.73060963	23.10691208
H	-0.57011616	-1.26433846	21.88914211
C	3.2974341	-0.28165851	23.00863364
H	2.94967559	-1.2443188	23.41210785
H	3.14454531	-0.29094377	21.92363927
H	4.38155291	-0.23030483	23.18770168
C	3.85456853	0.77607044	25.91349446
H	3.43544686	0.86912832	26.92864536
H	3.9542992	-0.30361304	25.72486441
C	5.24393598	1.44198223	25.87101426
H	5.16900121	2.51496258	26.09574207
H	5.92408393	0.98168745	26.60178621
H	5.69184302	1.34461364	24.87181112
C	-0.78722339	9.88729902	17.26705392
H	-1.41446747	9.03330698	16.97479316
H	-1.3356674	10.45847568	18.02970318
H	-0.64998669	10.53033841	16.38593498
Cl	-1.20117986	4.34979832	22.44135937
Cl	2.67671619	5.15965748	21.80568861
Cu	0.95467238	4.8466769	23.44216019
Cu	0.56166664	4.67080568	20.79667994
H	2.6479051	2.92840787	27.11886343
H	0.13660875	6.85440915	16.90934088
C	1.4107964	5.4433295	27.59174368
C	1.85621525	5.11161768	28.86716751
C	-0.24027846	4.43185726	15.35659746
C	2.27181646	4.77843494	29.98337807
C	-0.36063482	4.83780206	14.19447969
H	2.62664095	4.49838239	30.965950836
H	-0.46567718	5.17483082	13.172152653

Zn-Amethyrin systems

Zn-Ethyl anchoring

C	16.84317315	17.25356942	25.81516991
C	13.71451224	16.27703999	16.03675578
C	16.12112608	17.2369368	24.57889432
C	13.85875381	16.99581072	17.27166682
C	13.86805668	19.15529233	18.63119944
C	13.71104302	20.57959086	18.75729341
C	14.15543679	19.65962315	20.78501965
C	13.88906845	20.89443963	20.10692089
C	17.42464106	15.98826148	25.95229522
C	14.1481984	14.83064245	17.72745246
C	17.04562463	15.21639406	24.80226074
C	16.09199599	12.40154164	21.52409173
C	17.0253513	13.05268177	23.44438315
C	17.39113375	11.67612589	23.23980703
N	14.14648434	18.63464098	19.89295661
N	14.1236287	16.07403553	18.27989024
N	16.25725607	16.0205246	23.98552017

N	16.23327945	13.45498225	22.37055561
C	13.74134846	18.38381123	17.46629492
C	17.36848887	13.87377499	24.52951071
C	16.81281291	11.27180342	22.03496419
C	13.90552231	14.92134709	16.31937767
C	14.42709039	19.41219742	22.19141678
C	13.80538319	19.87753005	23.36168313
C	14.37444717	19.17049148	24.46230625
C	15.33641141	18.28605562	23.9478495
N	15.33753942	18.44688591	22.57609245
H	16.03260155	18.03529546	21.95137929
C	14.40879088	13.65867202	18.54677225
C	13.79099191	12.39895184	18.60484761
C	14.35642354	11.69195778	19.70757685
C	15.31165417	12.53089546	20.30505463
N	15.31186052	13.71283138	19.58927904
H	16.0131891	14.44704558	19.6994452
C	17.02075737	18.43026397	26.72412729
H	16.78603924	19.36596159	26.19922123
H	16.36969623	18.3795111	27.61138214
H	18.05662467	18.49659656	27.08929968
C	18.25069326	15.50456732	27.10257416
H	19.01147499	14.78356616	26.76532017
H	18.79322279	16.34519971	27.56231592
C	13.9049755	19.24708739	25.88124037
H	14.22243508	18.36431669	26.45058612
H	14.28891115	20.13970726	26.40086979
H	12.80647432	19.2976486	25.92903332
C	12.64582272	20.82033729	23.43936937
H	12.94846707	21.82665294	23.77118065
H	12.15472816	20.92392829	22.46367476
H	11.89307594	20.46033061	24.15701266
C	13.90693478	22.26310136	20.71437033
H	12.89379028	22.65671568	20.89360581
H	14.4340676	22.25812254	21.67758316
H	14.41574721	22.98030127	20.05251966
C	13.38002645	21.53492472	17.65281775
H	13.81996482	21.18831433	16.70450087
H	13.8442872	22.51172715	17.86424299
C	13.51211756	16.89087238	14.68569994
H	13.06723724	16.15758673	13.99666636
H	12.81071406	17.73856865	14.74226972
C	13.95023197	13.79358191	15.3346808
H	14.50501076	12.94023949	15.74749561
H	12.945033	13.43193144	15.06504193
H	14.44536546	14.09975027	14.40144392
C	12.63950558	11.93575576	17.76832983
H	12.12412897	12.78550676	17.30218374
H	12.95647367	11.25430861	16.96241491
H	11.90327444	11.39048425	18.37810902
C	13.88833833	10.3669001	20.22258962
H	14.29502911	9.52500242	19.63957062
H	14.18267824	10.22311823	21.26982201
H	12.7915708	10.29154511	20.16975739
C	16.99479398	9.9505981	21.35171496
H	16.35492782	9.1639849	21.7828669
H	16.74882846	10.02587562	20.28413703

H	18.03485381	9.602863	21.43500552
C	18.30629356	10.86766538	24.10843047
H	18.11796705	11.09600764	25.16994419
H	18.07778821	9.79794898	23.98289353
C	19.79286834	11.11893431	23.78959105
H	20.04699503	12.17804024	23.93918689
H	20.44559781	10.51178635	24.43356398
H	20.01417252	10.87075336	22.74157771
C	14.86234151	17.38284862	14.11822077
H	15.52785238	16.55197768	14.01029134
H	15.2911716	18.09864249	14.78802963
C	11.86076622	21.72315268	17.47792248
H	11.37773035	20.76546634	17.23683675
H	11.40700433	22.09979864	18.40580099
H	11.63860952	22.43623469	16.67069074
C	17.34658431	14.83897799	28.16424104
H	16.82990267	14.01154142	27.7245948
H	16.63552645	15.55246687	28.52511545
Zn	15.55747032	15.26941871	22.34318151
Zn	14.38620248	16.72045181	20.0948114
Cl	13.34705661	15.6255264	21.82382247
Cl	16.74638303	16.40270733	20.55412595
H	17.97629517	13.38643942	25.29611153
H	13.49950888	18.95305454	16.56534557
H	17.93714883	14.46569895	29.0281722246
H	14.73801642	17.86216661	13.1235689854

Zn-Direct anchoring

C	16.14041596083101	20.41673894076849	15.14500385914761
C	17.43726785053728	18.80776183462638	25.28421642014553
C	16.60390824767322	20.36159790936232	16.50754857102234
C	17.39513515606289	19.63931149648345	24.11560459706707
C	17.23616427885785	21.92652033551284	22.96148558623267
C	17.13212278641135	23.36865736136595	22.97840698028764
C	17.28869012695362	22.61344005676652	20.83362790411604
C	17.17072256302093	23.79830810113754	21.64157345308794
C	15.83277186464577	19.09718600808478	14.79149346275888
C	17.61736263437167	17.52014772951875	23.42693557565192
C	16.10435039606694	18.26021468228373	15.92475594341585
C	16.87793508074590	15.27389661237940	19.11029850580419
C	16.22867629260210	15.97996794328855	17.09004906157562
C	16.06598173395250	14.54476147858581	17.11068590630379
N	17.32343263928521	21.51342840302675	21.63202735877885
N	17.50708605923113	18.81039897204768	23.00133840317948
N	16.57116064350236	19.07501866038238	16.95301458196487
N	16.72420746446232	16.37885446104469	18.33171163115196
C	17.27423210598752	21.04916991076339	24.06481596361119
C	15.96246343212817	16.85560757497158	16.01816065166446
C	16.46852162632140	14.10295321922363	18.38011982397866
C	17.57424374152825	17.47868635847353	24.86612671257918
C	17.35735570055863	22.48370626533218	19.38407836910079
C	18.10518513703916	23.19007802098876	18.41748067145351
C	17.90913529872419	22.53338882101203	17.15954556158709
C	17.04544359122763	21.43992352397999	17.38341231769369
N	16.73598743201159	21.43486128779074	18.73092348104984
H	16.04113214462509	20.81636235092663	19.16161754282068
C	17.72638083555671	16.42434550037768	22.47087606670146

C	18.54819451590056	15.27502845834353	22.44270818067399
C	18.32886284529272	14.62187595615233	21.18690905095422
C	17.37727980897525	15.38392376904253	20.47407627787716
N	17.03956408019572	16.46151988122810	21.27175461647143
H	16.28000684216732	17.11797787916097	21.06338584753343
C	15.94561187265698	21.65908245120248	14.32437500464675
H	15.80809278438040	22.54132358395521	14.97760825710978
H	16.81445240065835	21.87129732722824	13.66846577852793
H	15.05676013625804	21.56743126915295	13.67236496953216
C	18.61932972446334	22.85268940003156	15.87747683728850
H	18.6669993092662	21.96592169285553	15.22014720174813
H	18.12194988770723	23.66659360110345	15.31103739977948
H	19.65794136717240	23.18395114388785	16.07112836446490
C	19.06010872998922	24.31582562698175	18.68522595004836
H	18.63428770131967	25.30336007203373	18.41309956624697
H	19.34115431103685	24.35189234215836	19.75290646714087
H	19.99041813646499	24.19508512316088	18.09643262715622
C	17.01181846012975	25.20273117806205	21.13763741036642
H	17.96066119596843	25.77561654145573	21.17383846673325
H	16.66466964582918	25.20556746602343	20.08811803300221
H	16.27481941653080	25.76201389827012	21.74587788866452
C	17.05664400523274	24.24398665892549	24.19549904851327
H	16.58215257913828	23.69461378431307	25.03325727113059
H	16.39385472494065	25.10919640981321	23.98635723085371
C	17.57245482786242	16.24408754076632	25.72094767019691
H	17.16462791876175	15.38071106840603	25.16203516296014
H	18.59068650297329	15.96235302824751	26.05776627076901
H	16.95625596169761	16.39414534799174	26.62696647536488
C	19.58445370089672	14.90306507325250	23.46183274510697
H	19.89964059502203	15.78692390425068	24.04533238020061
H	19.21936370393419	14.13901589651601	24.17841772990472
H	20.48598873138259	14.48260430437418	22.97568701451111
C	19.09387283724247	13.44441489106955	20.65829665605643
H	18.67921463278578	12.47820641144788	21.01193586403280
H	19.08262421772763	13.42989911734484	19.55349229109310
H	20.15139835622616	13.47943617396084	20.98462943045273
C	16.37816152947086	12.70500655879321	18.92041172213728
H	17.24969869297238	12.08118657617777	18.63479973223674
H	16.33079145368108	12.71606469780465	20.02484527636730
H	15.47319643918110	12.19134165241540	18.54421371764690
C	15.45681314049816	13.71075856864411	16.02014926432818
H	15.77383066755096	14.09337729910690	15.02831645773684
H	15.84872182325196	12.67625927832894	16.08571459148907
C	13.91573893208911	13.68832616328665	16.09434846152998
H	13.50685676326411	14.71271758607201	16.00038057936247
H	13.48331260191576	13.06256453449878	15.28946143481070
H	13.57761655076655	13.28533995017650	17.06838133472299
C	18.44356573633005	24.75947010467275	24.63171330101690
H	19.11188723301933	23.91349370559314	24.88272622784997
H	18.92210089872842	25.33119375094745	23.81356890667787
H	18.36598448596576	25.41999402129561	25.51715935073745
H	15.42737491258739	18.75405059206525	13.83289212418819
H	17.34599083760029	19.16168962315878	26.31746860170758
Zn	17.06323390223529	18.26112667387720	18.64293771279815
Zn	17.49016186189916	19.62307164304958	21.24127810203067
Cl	19.02829474694680	18.91505302472255	19.66861945843214
Cl	15.36208127716680	18.97495317773365	20.23810581311869

H	15.59689478674965	16.37132200623755	15.10167947766917
H	17.20895168735838	21.53392914166472	25.04875904335831

Zn-Phenyl anchoring

C	19.93695353	17.19851525	28.22079003
C	19.35080095	18.9891186	18.07880975
C	20.15862132	17.26086451	26.8136335
C	19.48132567	18.13577744	19.23468832
C	19.51110741	15.83926616	20.35168473
C	19.39558137	14.40381676	20.31420994
C	19.93733186	15.09134704	22.4101841
C	19.66391434	13.93652163	21.60205017
C	19.85530351	18.53078567	28.66969395
C	19.98188163	20.21528975	19.88143871
C	19.98703716	19.37558397	27.50897527
C	20.27378013	22.38265371	24.27673413
C	19.9910553	21.65953212	26.36788904
C	19.91034312	23.09773365	26.40121403
N	19.83289163	16.21438728	21.65437254
N	19.86031361	18.92588878	20.30886486
N	20.16834779	18.55996615	26.40302565
N	20.21200325	21.26745284	25.0486698
C	19.3653211	16.73067225	19.28071068
C	19.89489356	20.78204938	27.45489968
C	20.08480274	23.54887058	25.09328651
C	19.67802433	20.29541025	18.49009286
C	20.28015768	15.17816446	23.81814562
C	21.19301943	14.45455038	24.60270312
C	21.26343767	15.08909334	25.87814751
C	20.38797061	16.18604186	25.85524976
N	19.82024043	16.22320267	24.59810823
H	19.05621625	16.8455598	24.3314209
C	20.35233105	21.27054738	20.80883744
C	21.2459619	22.34863229	20.6917723
C	21.32502975	22.98376562	21.9660054
C	20.4823962	22.28085941	22.84336929
N	19.91877112	21.24750993	22.11951036
H	19.14570942	20.6722694	22.4578671
C	19.79179561	15.94840465	29.03386995
H	19.97741639	15.05913253	28.42031232
H	20.48775183	15.93391225	29.88645575
H	18.77717381	15.85104389	29.44729373
C	22.22416376	14.73821523	26.97105414
H	22.2925937	15.54436391	27.71289313
H	21.93670987	13.81537971	27.500354
H	23.23410229	14.57084491	26.56574077
C	22.06359241	13.32686207	24.14480086
H	21.70894352	12.35113557	24.51415653
H	22.1011682	13.27657814	23.04938093
H	23.09413165	13.45212952	24.51014986
C	19.57916941	12.52032908	22.08076285
H	20.48539856	11.9408865	21.84355067
H	19.43946465	12.48229641	23.16938039
H	18.73317691	11.99676584	21.61056127
C	19.08022556	13.57410619	19.10862604
H	18.42579059	14.13445779	18.42254696
H	18.5082347	12.68416679	19.41756337

C	19.55965465	21.55516939	17.6890721
H	19.35107453	22.41075802	18.34641491
H	20.47921414	21.79260665	17.13141766
H	18.74810611	21.47323521	16.95200888
C	22.08805794	22.67825862	19.49939047
H	22.18770567	21.8093936	18.83588753
H	21.66691635	23.50551193	18.90569806
H	23.09947366	22.9846653	19.80547666
C	22.26353923	24.09136053	22.32927559
H	21.90174515	25.07293546	21.9834294
H	22.40745715	24.14996821	23.41538461
H	23.25164773	23.93524994	21.87019574
C	19.98703068	24.96421049	24.61143718
H	20.90621129	25.53791551	24.81132135
H	19.80699598	24.99734282	23.52880045
H	19.16089744	25.49404055	25.10765142
C	19.60158324	23.9341068	27.60525183
H	20.11138219	23.52053737	28.49048454
H	20.01149244	24.94580545	27.46209521
C	18.08894153	24.02310239	27.8857864
H	17.6684464	23.02299722	28.06334293
H	17.88575398	24.64524307	28.76938645
H	17.55795798	24.45906299	27.02730315
C	20.34956245	13.12683976	18.35855003
H	20.9208656	13.99922464	18.0107959
H	21.00456179	12.54088997	19.01909284
H	20.09711665	12.50808969	17.48527078
H	19.24737584	20.30997028	33.73337044
H	17.79180999	17.44760669	13.146116301
H	19.7195519	21.26227885	28.41990872
H	19.15279487	16.26221615	18.31778404
C	19.69102307	18.99970194	30.04801171
C	20.53411164	20.00533462	30.57077544
C	18.69596112	18.46817189	30.89480838
C	20.38016672	20.46999727	31.87260062
H	21.33865929	20.39834475	29.94727629
C	18.53710387	18.92973532	32.19674938
H	18.01847235	17.70594257	30.50981927
C	19.37286174	19.9436163	32.70216853
H	21.04499624	21.23837169	32.26865877
H	17.75602551	18.51961608	32.83779435
C	18.91836712	18.57472028	16.74539284
C	17.81939455	17.70671294	16.56456328
C	19.58622568	19.04211635	15.59197242
C	17.41642757	17.31101839	15.29292586
H	17.25407406	17.37593197	17.43713233
C	19.19476311	18.6413016	14.32083664
H	20.44632663	19.70239105	15.70815016
C	18.10669965	17.76286741	14.15290782
H	16.55343016	16.65656867	15.16549209
H	19.73026135	18.99421822	13.43884107
Zn	20.15014186	18.08558075	22.03449874
Zn	20.35386299	19.37500437	24.65243735
Cl	18.46949414	18.85896587	23.59506467
Cl	22.0179299	18.64961329	23.24988113

Zn-Ethynyl anchoring

C	3.88619157	4.92307621	0.08255069
C	-2.68314039	-2.82037107	-1.6400025
C	2.86569936	3.94282567	0.15955882
C	-2.35123073	-1.46489708	-1.26959613
C	-2.98212119	0.96994587	-0.87449687
C	-3.93431549	2.05408261	-0.83789966
C	-1.89195892	2.77842544	-0.15438677
C	-3.25512959	3.18155497	-0.3817232
C	5.07643037	4.22534426	-0.22516725
C	-0.48717193	-2.6942952	-1.10839255
C	4.74493835	2.82260888	-0.31802701
C	4.26967259	-1.54848464	-0.69150481
C	5.38802818	0.38290669	-0.6632792
C	6.35589153	-0.66655041	-0.87574348
N	-1.74659297	1.46297902	-0.45558252
N	-1.01309606	-1.43625616	-0.94267352
N	3.38870594	2.70025368	-0.10496728
N	4.12685516	-0.20425692	-0.56403473
C	-3.22615734	-0.35888538	-1.2297887
C	5.63585046	1.7534177	-0.55029323
C	5.65737004	-1.87039206	-0.90160595
C	-1.49641526	-3.58485652	-1.55350625
C	-0.75971376	3.56531568	0.29213053
C	-0.61792186	4.50684528	1.32713469
C	0.76580454	4.83308277	1.42618381
C	1.44805884	4.09209261	0.44670848
N	0.50711637	3.32539055	-0.20896167
H	0.689479	2.80965155	-1.07145168
C	0.91297322	-2.94949454	-0.80907271
C	1.53506984	-3.98684001	-0.09411383
C	2.91719658	-3.6605483	0.02262139
C	3.11918705	-2.42619585	-0.62147946
N	1.88691981	-2.01765097	-1.10084632
H	1.75623357	-1.23959335	-1.74945043
C	3.75540576	6.40021678	0.22813017
H	2.70680388	6.71599568	0.15680366
H	4.15516607	6.74624872	1.19650799
H	4.34460362	6.91120604	-0.54764942
C	1.38607457	5.68470765	2.4887396
H	2.46773932	5.51261292	2.5519529
H	1.22592092	6.75934544	2.30688827
H	0.95236155	5.45932324	3.47516031
C	-1.68490051	4.96327214	2.2716627
H	-2.0349485	5.98213994	2.04050339
H	-2.55455095	4.29530463	2.24181632
H	-1.31120786	4.98124673	3.30648092
C	-3.8005372	4.57048048	-0.26038776
H	-4.36242507	4.71950525	0.67503026
H	-2.99273795	5.31370436	-0.28272546
H	-4.49154834	4.79347587	-1.08700394
C	-5.38616293	1.96113235	-1.18910742
H	-5.53635793	1.21619187	-1.98555376
H	-5.7235294	2.92531779	-1.60213594
C	-1.33603469	-5.00530268	-1.97809095
H	-0.27609915	-5.27988647	-2.04777826
H	-1.83047018	-5.70010435	-1.28162147

H	-1.80903982	-5.16088778	-2.96121743
C	0.85153923	-5.14557611	0.5612045
H	-0.22803505	-4.96874319	0.64859454
H	0.99091571	-6.08281213	-0.00086987
H	1.24868317	-5.31676259	1.57325202
C	3.91698612	-4.41914928	0.83742806
H	4.32334879	-5.28726542	0.29423904
H	4.75993702	-3.78102708	1.13018418
H	3.45596266	-4.80607783	1.7584876
C	6.21766018	-3.22643832	-1.2054798
H	6.66254072	-3.70511198	-0.31867305
H	5.43316378	-3.89695833	-1.58081248
H	7.0043018	-3.16476557	-1.9709333
C	7.81962276	-0.46914684	-1.12552313
H	8.206679	0.32464462	-0.46705241
H	8.36369408	-1.38608132	-0.85195253
C	8.12020638	-0.10514942	-2.59270839
H	7.60918878	0.82670187	-2.87309585
H	9.19939695	0.03144984	-2.75252407
H	7.76823087	-0.89556362	-3.27122347
C	-6.25730252	1.59691093	0.02892018
H	-5.96203733	0.6201115	0.4373143
H	-6.14037912	2.34320547	0.82771978
H	-7.32076895	1.54910181	-0.24610891
Zn	2.5993197	0.92912792	-0.19621765
Zn	-0.23570899	0.24951564	-0.37363115
Cl	1.1394375	0.28924719	1.4626199
Cl	1.22789861	0.91491938	-2.18986552
H	6.68070915	2.06433601	-0.63349727
H	-4.25103163	-0.6020247	-1.52234598
C	6.47116504	4.84699345	-0.42483573
C	7.55905808	5.33187981	-0.58057714
C	-4.07333403	-3.33830261	-2.05317143
C	-5.15768507	-3.74228921	-2.3754432
H	-6.13255783	-4.11119373	-2.6628348033
H	8.53647825	5.772523671	-0.7203676503