Supporting Information

Chiral Recognition of Amino Acids Through Homochiral Metallacycle $[ZnCl_2L]_2$

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Table S1: The E_{int} of the possible orientations of amino acids inside the metallacycle.

Complexes	E_{int} (kcal/mol)
R-ala@metallacycle	-17.05
	-28.38
	-28.38
S-ala@metallacycle	-30.4
	-30.59
	-31.49
R-pro@metallacycle	-26.09
	-30.23
	-26.19
S-pro@metallacycle	-32.17
	-28.33
	-25.65
R-ser@metallacycle	-30.75
	-26.70
	-22.46
S-ser@metallacycle	-33.03
	-32.45
	-33.02
R-val@metallacycle	-30.27
	-21.48
	-20.33
S-val@metallacycle	-27.68
	-15.91
	-27.78

Table S2: Interaction energies of complexes when amino acids are in zwitterionic form in gas phase and solvents (H_2O and DCM).

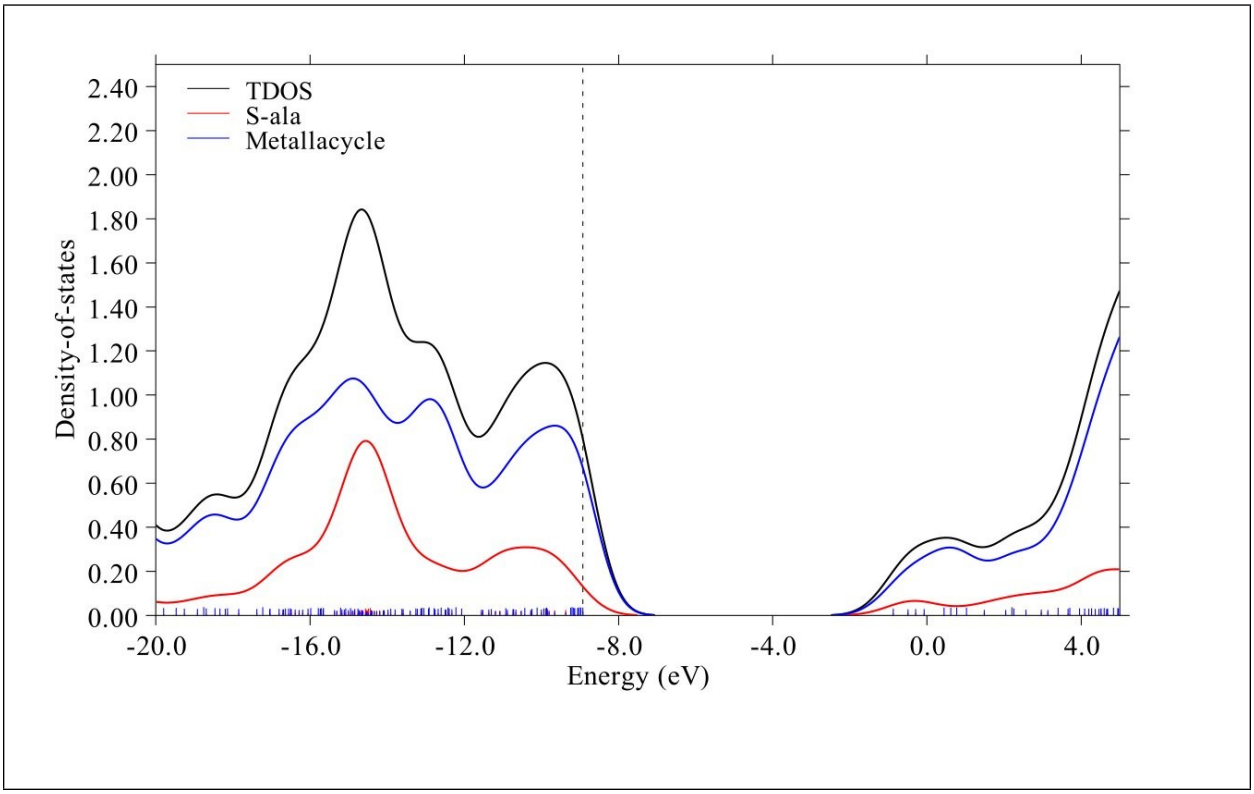
Complexes	E_{int} of zwitterion in gas phase (kcal/mol)	E_{int} of zwitterion in H_2O (kcal/mol)	E_{int} of zwitterion in DCM (kcal/mol)
R-ala@metallacycle	-17.77	-25.01	-23.60
S-ala@metallacycle	-18.09	-24.23	-23.37
R-pro@metallacycle	-18.79	-26.11	-25.41
S-pro@metallacycle	-27.10	-24.41	-23.63
R-ser@metallacycle	-24.46	-16.67	-28.10
S-ser@metallacycle	-18.48	-25.56	-32.59
R-val@metallacycle	-18.24	-22.27	-20.25
R-val@metallacycle	-20.20	-13.86	-13.26

Table S3: QTAIM parameters for R and S enantiomeric complexes of ala@metallacycle, pro@metallacycle, ser@metallacycle and val@metallacycle.

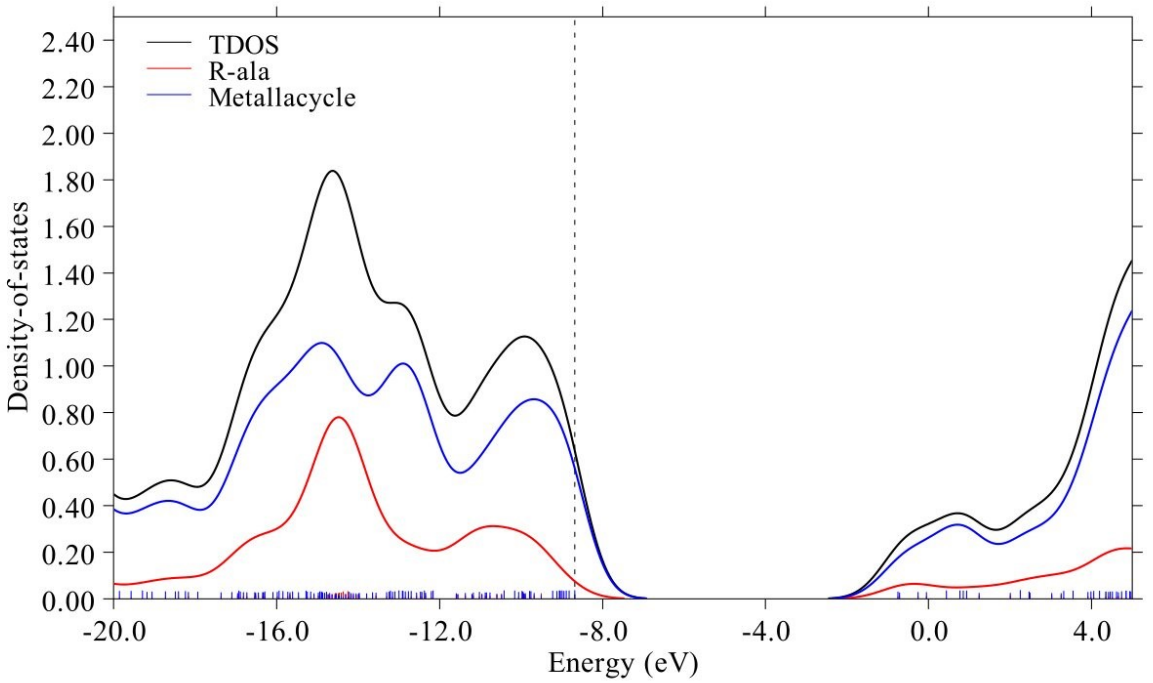
Complexes	Analyte-metallacycle	CPs	ρ (a.u)	$\nabla^2\rho$ (a.u)	G (r) (a.u)	V (r) (a.u)	H (r) (a.u)	-V/G	E_{int} (kcal mol^{-1})
S-ala@metallacycle	N93-C81	232	0.0058	0.016	0.0034	-0.0028	0.0006	0.82	0.88
	098-C47	215	0.0081	0.030	0.0064	-0.0010	0.0010	0.16	0.31
	O98-C39	212	0.0073	0.025	0.0054	-0.0045	0.0009	0.83	1.41
	H92-C31	186	0.0054	0.018	0.0036	-0.0029	0.0007	0.80	0.91
	O97-C69	229	0.0087	0.026	0.0055	-0.0043	0.0011	0.78	1.35
	H90-O9	170	0.0096	0.035	0.0079	-0.0071	0.0008	0.90	2.23
	H90-C67	150	0.0032	0.010	0.0019	-0.0013	0.0006	0.68	0.41
	O97-N5	132	0.0085	0.031	0.0069	-0.0061	0.0007	0.88	1.91
	H88-C76	143	0.0086	0.027	0.0056	-0.0044	0.0012	0.79	1.38
	O97-C16	144	0.0052	0.019	0.0036	-0.0024	0.0011	0.67	0.75
	H94-O12	193	0.0207	0.055	0.0148	-0.0159	-0.0011	1.07	4.99
R-ala@metallacycle	O98-C67	225	0.0085	0.030	0.0066	-0.0057	0.0009	0.86	1.79
	O97-C51	209	0.0039	0.015	0.0029	-0.0021	0.0008	0.72	0.66
	O97-C16	212	0.0092	0.033	0.0073	-0.0062	0.0011	0.85	1.94
	H91-C76	226	0.0061	0.020	0.0039	-0.0028	0.0011	0.72	0.88
	H94-O12	173	0.0186	0.051	0.0135	-0.0143	-0.0008	1.06	4.49
	N93-C81	131	0.0089	0.026	0.0057	-0.0049	0.0008	0.86	1.54
	H88-C31	143	0.0112	0.034	0.0073	-0.0061	0.0012	0.84	1.91
	O98-C69	166	0.0056	0.019	0.0040	-0.0033	0.0008	0.82	1.04
	H99-O9	192	0.0338	0.101	0.0253	-0.0253	-0.0001	1	7.94
	H8-O29	218	0.0116	0.036	0.0086	-0.0082	0.0004	0.95	2.57
	H9-C64	251	0.0063	0.020	0.0039	-0.0028	0.0011	0.72	0.88
	H10-C64	239	0.0058	0.019	0.0039	-0.0029	0.0009	0.74	0.91
	H10-N20	268	0.0060	0.019	0.0038	-0.0027	0.0010	0.71	0.85
	H8-C56	242	0.0072	0.023	0.0048	-0.0039	0.0009	0.81	1.22
	H5-C85	241	0.0085	0.027	0.0055	-0.0043	0.0012	0.78	1.35

S-pro@metallacycle	H5-C39	209	0.0070	0.021	0.0042	-0.0032	0.0010	0.76	1.00
	H17-C52	214	0.0085	0.029	0.0064	-0.0055	0.0009	0.86	1.72
	H14-O26	194	0.0333	0.115	0.0268	-0.0249	0.0020	0.93	7.81
	C11-H69	135	0.0077	0.025	0.0053	-0.0043	0.0010	0.81	1.35
	O12-H41	131	0.0096	0.039	0.0081	-0.0065	0.0016	0.80	2.04
	H6-C40	138	0.0066	0.022	0.0044	-0.0034	0.0010	0.77	1.07
	H4-C94	174	0.0068	0.024	0.0047	-0.0034	0.0013	0.72	1.07
	H7-C35	164	0.0069	0.020	0.0041	-0.0032	0.0009	0.78	1.00
	C58-O26	167	0.0029	0.012	0.0024	-0.0016	0.0007	0.67	0.50
	O13-O26	162	0.0042	0.013	0.0026	-0.0020	0.0007	0.77	0.63
R-pro@metallacycle	H11-C75	253	0.0053	0.017	0.0034	-0.0024	0.0009	0.70	0.75
	H12-N25	265	0.0065	0.022	0.0044	-0.0033	0.0011	0.75	1.03
	H12-C46	270	0.0055	0.018	0.0036	-0.0026	0.0009	0.72	0.82
	H10-C56	235	0.0080	0.026	0.0052	-0.0040	0.0012	0.77	1.26
	H8-C40	232	0.0095	0.030	0.0062	-0.0049	0.0013	0.79	1.53
	H7-O26	215	0.0094	0.031	0.0070	-0.0063	0.0007	0.90	1.98
	H17-O26	198	0.0362	0.124	0.0290	-0.0272	0.0018	0.94	8.53
	O15-H41	129	0.0100	0.040	0.0084	-0.0067	0.0017	0.80	2.10
	H8-N23	138	0.0082	0.027	0.0058	-0.0048	0.0010	0.83	1.51
	H6-C93	171	0.0051	0.016	0.0032	-0.0023	0.0009	0.72	0.72
	H9-C73	163	0.0068	0.020	0.0040	-0.0030	0.0010	0.75	0.94
	H11-C29	219	0.0101	0.031	0.0074	-0.0070	0.0004	0.95	2.20
	O15-C91	126	0.0078	0.028	0.0058	-0.0047	0.0012	0.81	1.48
	O16-C84	149	0.0065	0.024	0.0049	-0.0038	0.0011	0.78	1.19
	N13-N22	140	0.0069	0.023	0.0050	-0.0043	0.0007	0.86	1.35
	H10-C64	227	0.0044	0.015	0.0029	-0.0021	0.0008	0.72	0.66
S-ser@metallacycle	O6-C30	214	0.0054	0.019	0.0038	-0.0029	0.0009	0.76	0.91
	O6-C65	218	0.0082	0.029	0.0062	-0.0052	0.0010	0.84	1.63
	O6-C53	158	0.0025	0.017	0.0034	-0.0024	0.0009	0.71	0.75
	H3-O23	202	0.0167	0.048	0.0124	-0.0130	-0.0004	1.05	4.08
	H4-C55	238	0.0076	0.028	0.0056	-0.0041	0.0015	0.73	1.29
	H14-C53	149	0.0092	0.029	0.0059	-0.0048	0.0012	0.81	1.51
	O7-C61	138	0.0084	0.030	0.0066	-0.0057	0.0009	0.86	1.79
	O7-C70	195	0.0086	0.027	0.0061	-0.0053	0.0008	0.87	1.66
	O12-C47	146	0.0060	0.020	0.0041	-0.0033	0.0008	0.80	1.04
	H12-O26	191	0.0360	0.107	0.0267	-0.0266	0.0002	0.99	8.35
	H11-C90	241	0.0104	0.031	0.0066	-0.0055	0.0011	0.83	1.73
R-ser@metallacycle	N88-C76	227	0.0080	0.025	0.0053	-0.0045	0.0009	0.85	1.41
	O92-C56	193	0.0086	0.029	0.0062	-0.0053	0.0009	0.86	1.66
	H89-O12	190	0.0126	0.038	0.0095	-0.0095	0.0001	1	3.00
	O92-C81	141	0.0074	0.028	0.0060	-0.0051	0.0009	0.85	1.60
	H100-C31	154	0.0077	0.022	0.0045	-0.0034	0.0010	0.76	1.07
	O93-C39	152	0.0062	0.021	0.0045	-0.0037	0.0008	0.82	1.16
	H99-O9	198	0.0370	0.114	0.0280	-0.0280	0.0002	1	8.78
	O9-C74	238	0.0095	0.032	0.0068	-0.0060	0.0011	0.88	1.88
	O93-C51	202	0.0055	0.019	0.0041	-0.0033	0.0008	0.80	1.04
	H96-C23	250	0.0071	0.024	0.0050	-0.0034	0.0013	0.68	1.07
	O3-C88	219	0.0100	0.038	0.0081	-0.0067	0.0014	0.83	2.10
	O2-C86	167	0.0059	0.019	0.0041	-0.0033	0.0007	0.80	1.04

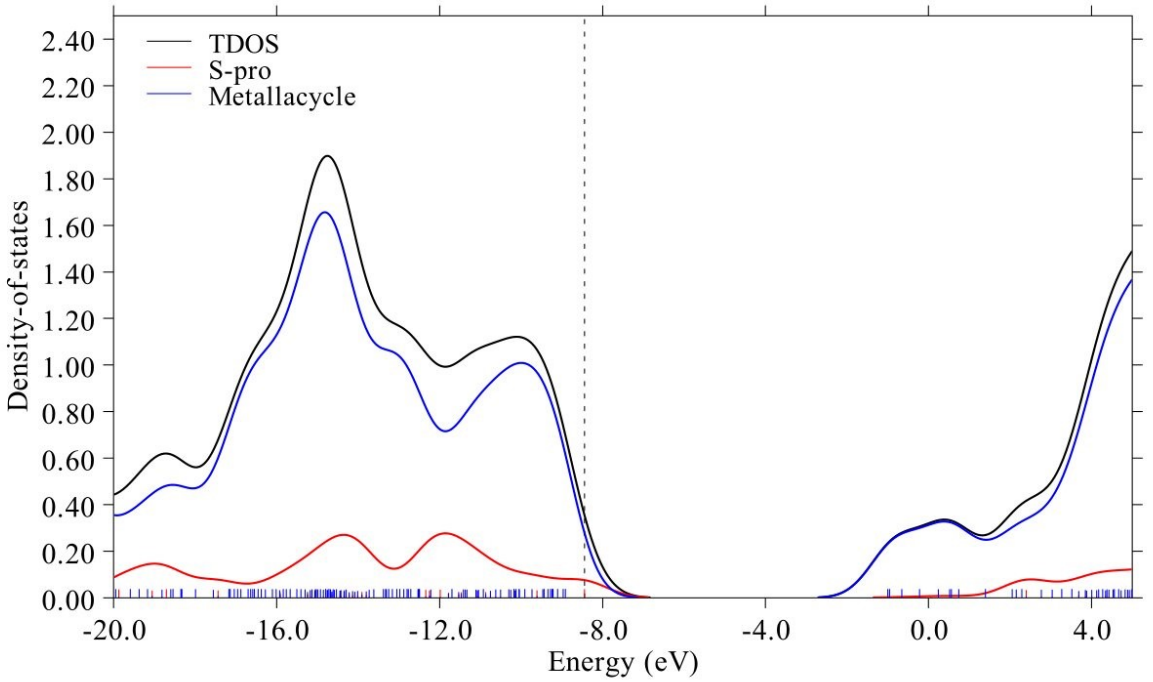
S-val@metallacycle	H4-O28	208	0.0411	0.123	0.0308	-0.0310	0.0007	1.01	9.73
	O3-C60	170	0.0097	0.032	0.0072	-0.0062	0.0009	0.86	1.94
	H7-C58	225	0.0036	0.011	0.0023	-0.0017	0.0006	0.74	0.53
	H8-N22	238	0.0056	0.019	0.0040	-0.0031	0.0008	0.78	0.97
	H9-N27	242	0.0098	0.032	0.0070	-0.0061	0.0010	0.87	1.91
	H10-C48	240	0.0053	0.018	0.0037	-0.0027	0.0009	0.73	0.85
	H15-C75	156	0.0061	0.019	0.0038	-0.0028	0.0010	0.74	0.88
	H15-O32	180	0.0040	0.015	0.0031	-0.0023	0.0008	0.74	0.72
	N16-C70	134	0.0100	0.029	0.0066	-0.0058	0.0008	0.88	1.82
	H19-N25	146	0.0084	0.030	0.0064	-0.0052	0.0011	0.81	1.63
	C81-H14	212	0.0073	0.024	0.0047	-0.0035	0.0012	0.74	1.10
	H4-O30	204	0.0072	0.028	0.0064	-0.0060	0.0005	0.94	1.88
R-val@metallacycle	H13-C100	227	0.0056	0.018	0.0035	-0.0025	0.0010	0.71	0.78
	H9-Cl103	274	0.0025	0.007	0.0014	-0.0010	0.0004	0.71	0.31
	H18-Cl105	125	0.0084	0.026	0.0054	-0.0043	0.0011	0.80	1.35
	O3-C93	154	0.0065	0.024	0.0050	-0.0039	0.0010	0.78	1.22
	O2-C93	160	0.0058	0.021	0.0043	-0.0033	0.0010	0.77	1.04
	O3-C54	210	0.0099	0.034	0.0073	-0.0062	0.0012	0.85	1.94
	H10-C48	259	0.0050	0.018	0.0033	-0.0023	0.0011	0.70	0.72
	H7-C48	251	0.0039	0.013	0.0025	-0.0018	0.0007	0.72	0.56
	N16-C42	144	0.0072	0.025	0.0051	-0.0040	0.0012	0.78	1.26
	H19-N25	151	0.0088	0.028	0.0059	-0.0051	0.0009	0.86	1.60
	H13-O31	200	0.0057	0.021	0.0044	-0.0035	0.0009	0.80	1.10
	H13-C37	184	0.0065	0.021	0.0041	-0.0030	0.0011	0.73	0.94
	H4-O28	196	0.0370	0.110	0.0273	-0.0270	0.0002	0.99	8.47
	C11-C41	218	0.0088	0.032	0.0070	-0.0058	0.0011	0.83	1.82



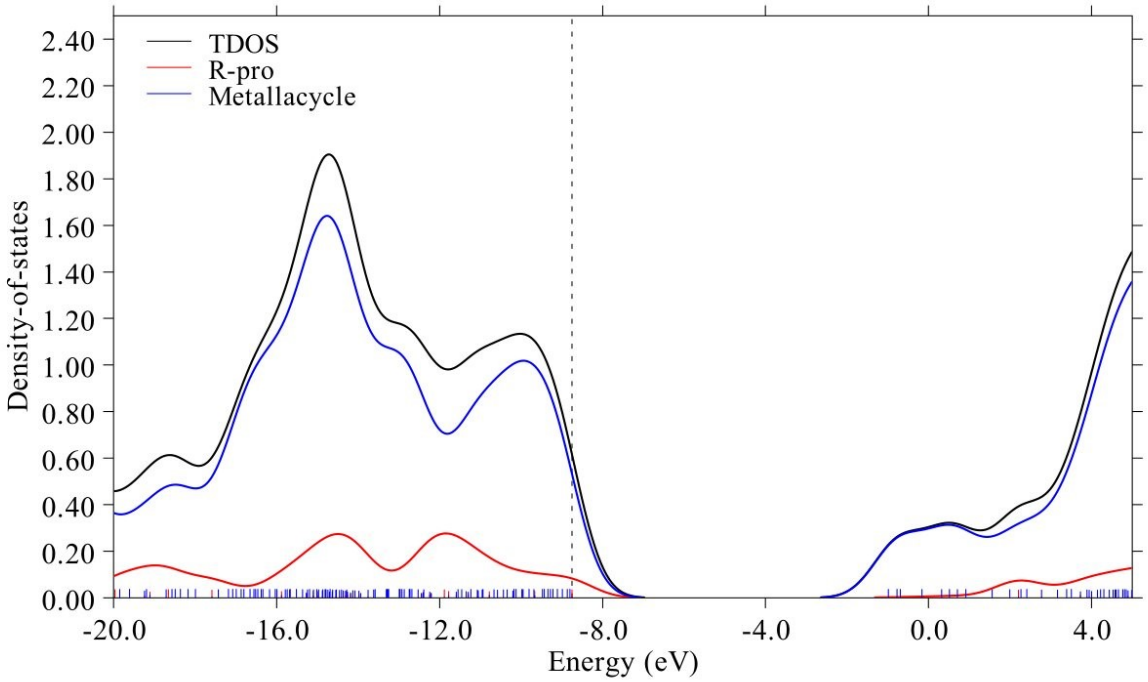
S-ala@metallacycle



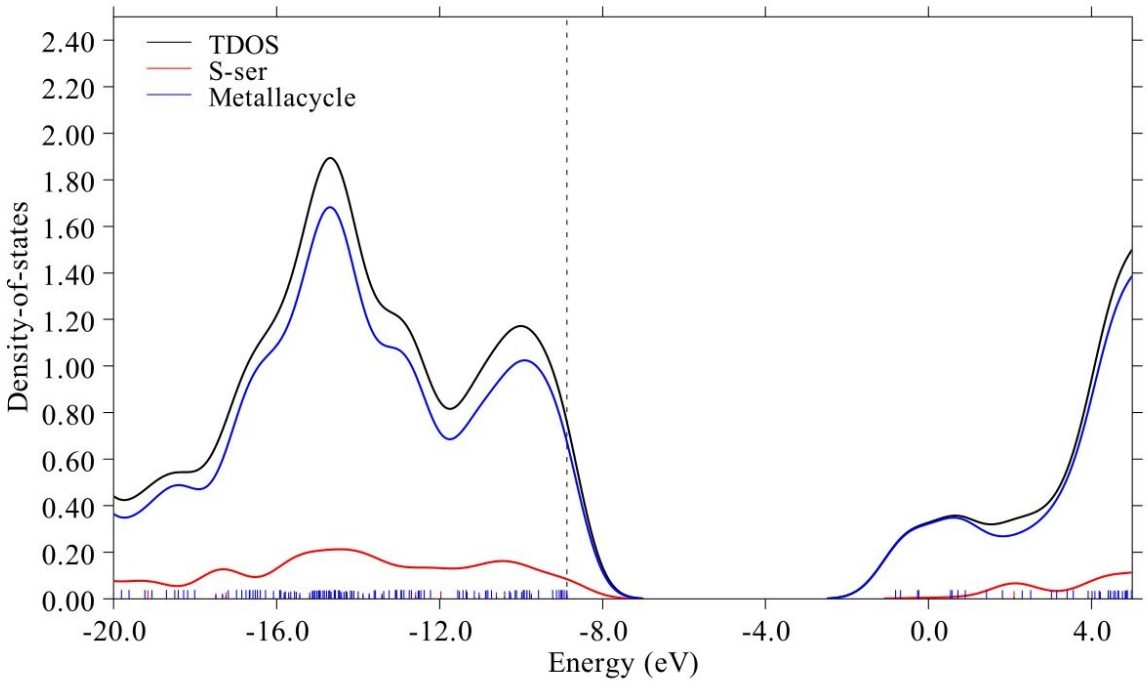
R-ala@metallacycle



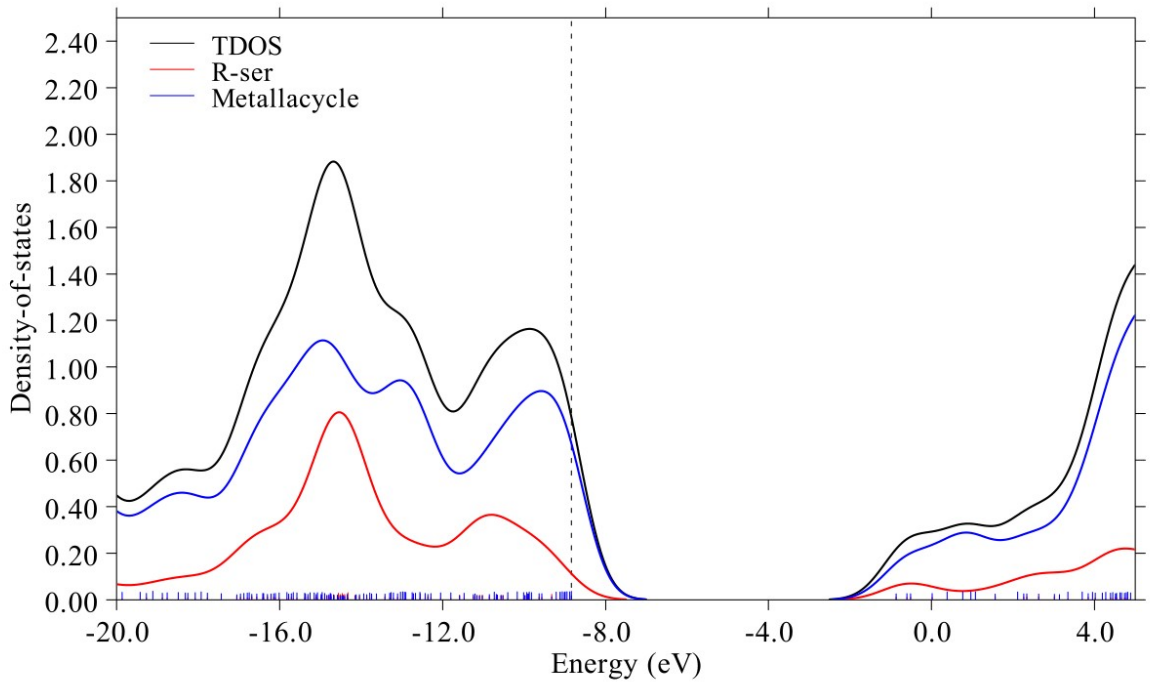
S-pro@metallacycle



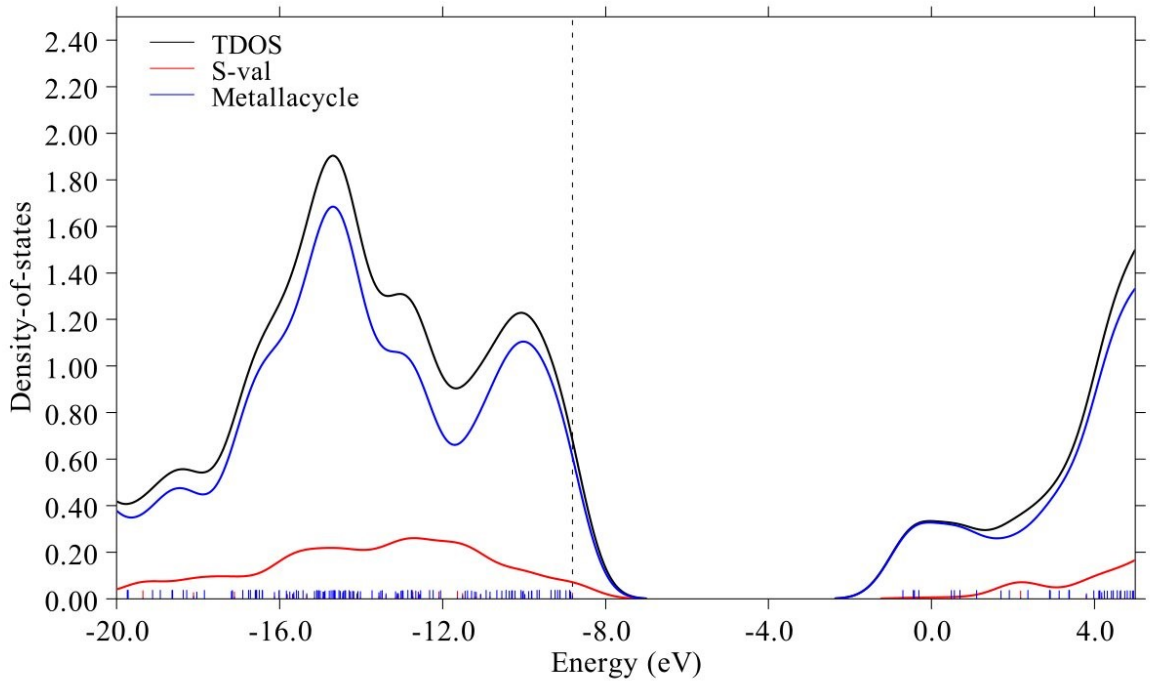
R-pro@metallacycle



S-ser@metallacycle



R-ser@metallacycle



S-val@metallacycle

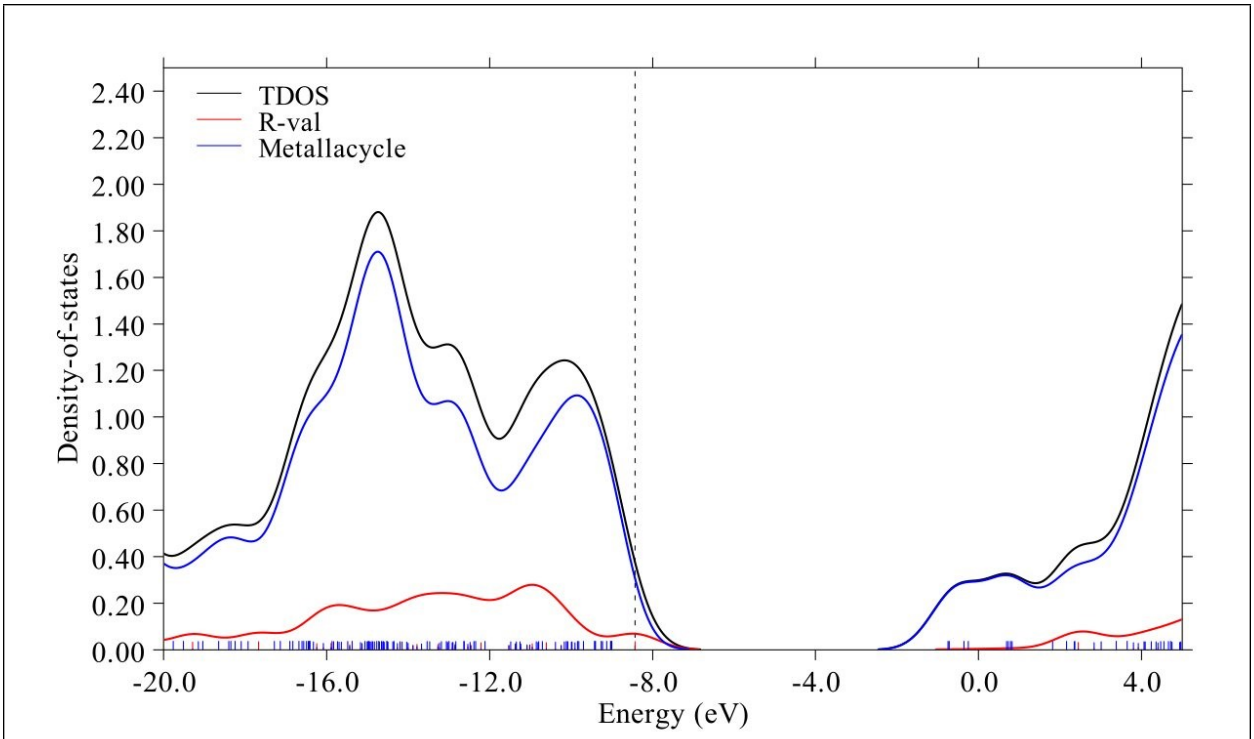


Figure S1: DOS spectra for the complexes of S-amino acids@metallacycle.

1. FMO Analysis

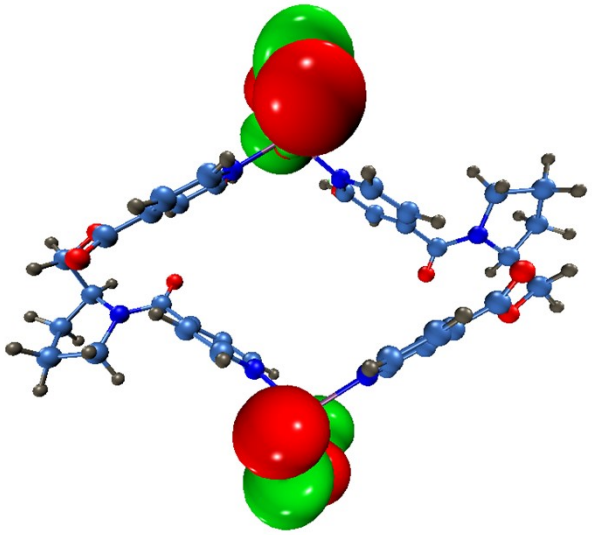
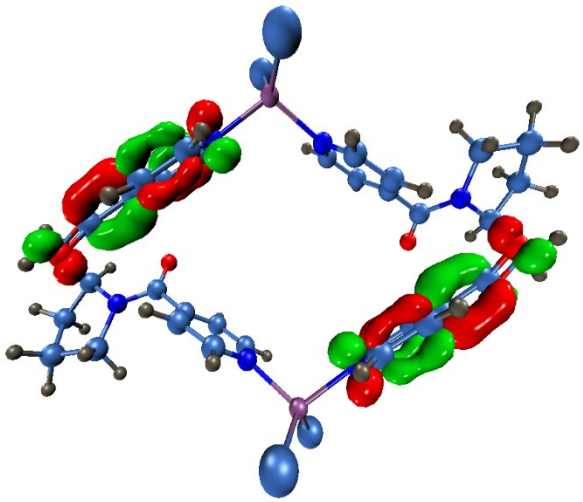
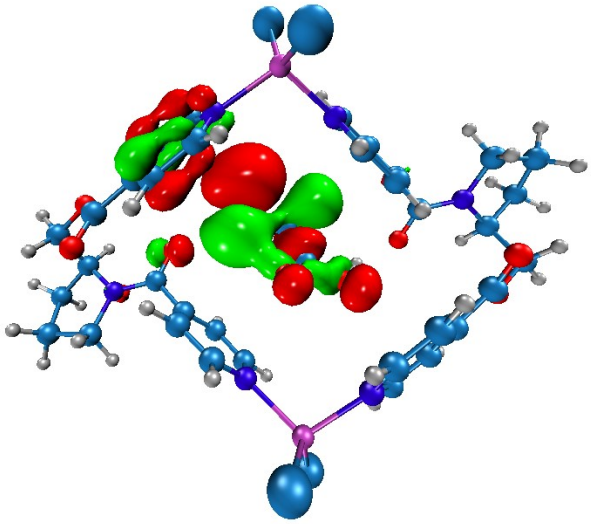
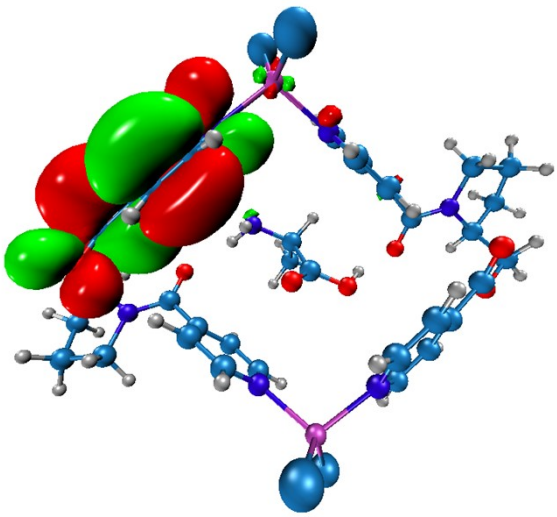
Frontier molecular orbital (FMO) analysis is very important to predict the reactivity of molecules. The HOMO determines the nucleophilic ability, while the LUMO determines the electrophilic ability of molecules. Consequently, the chemical reactivity and stability of the molecule can be determined through FMO analysis. FMO analysis also serves to provide information about the electronic behavior of the molecule *i.e.,* the change in the electronic properties of the guest molecule, after it has been encapsulated inside the cavity of the host. The values of the energies of HOMO, LUMO and HOMO-LUMO energy gaps of the metallacycle, amino acids and the amino-acid@metallacycle complexes are given in Table 2, while the HOMO, LUMO iso-densities are shown in Figure 3. The E_{HOMO}, E_{LUMO}, and E_{gap} of the bare metallacycle are -6.85, -2.66 and 4.19 eV, respectively. The E_{HOMO} of the amino acid enantiomers is smaller than bare metallacycle *i.e.,* ranging between -8.64 and -9.39 eV, while E_{LUMO} is significantly larger than that of the metallacycle *i.e.,* 2.23 to 2.56 eV. Due to this huge difference between the energies of HOMO and LUMO of the amino acids, the energy gaps of amino acids are considerably greater *i.e.,* 10.98 to 11.76 eV. Upon complex formation between amino acids and the metallacycle, the values of energy gap are reduced compared to bare amino acids, *i.e.,* ranging from 7.44-8.10 eV. This

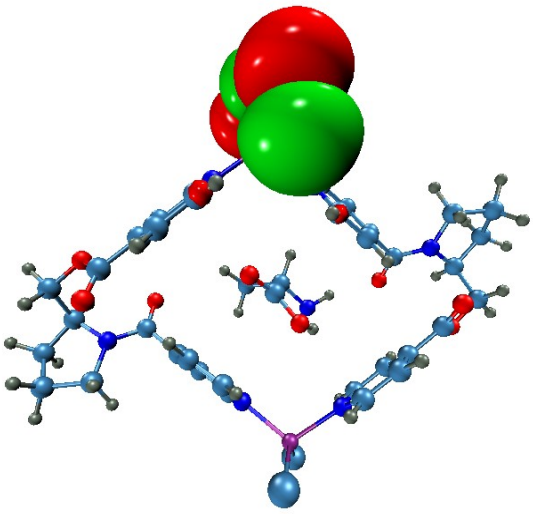
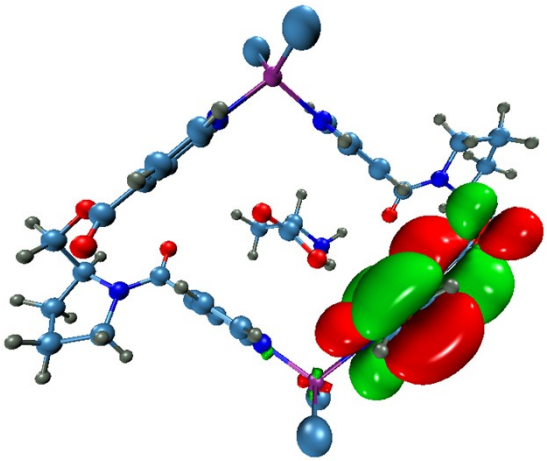
reduction in E_{gap} is due to the substantial decrease in the position and energy of the LUMO after complexation *i.e.,* -0.70 to -1.00 eV. In comparison of the energy gaps of R and S enantiomeric complexes, it is observed that except for S-pro@metallacycle, in all the other cases, R-amino acid@metallacycle has comparatively lower energy gap. The reason behind this is the lower energy gap, and the relative positions of HOMO and LUMO of the amino acid enantiomer forming the complex.

It can be seen in the visual representations of FMO that, the HOMO iso-densities in case of bare metallacycle resides on $ZnCl_2$ group, whereas the LUMO iso-densities are located on the pyridine rings present on the opposite walls of the metallacycle. A significant change in the iso-densities is experienced upon the complexation of amino acid enantiomers with the metallacycle. In the R-ala@metallacycle complex, the HOMO iso-densities are present mainly on the alanine along with one side of the metallacycle, while the LUMO iso-densities exist merely on the metallacycle. This behavior is due to the fact that the HOMO level of the metallacycle and R-alanine are close enough that they can interact, resulting in the presence of iso-densities on both the species in the resulting complex. On the other hand, the LUMO levels of both the species are far away from each other in terms of their energies, so they can not interact, hence the LUMO iso-densities exist only on one specie *i.e.,* metallacycle in the resulting complex. In the S-ala@metallacycle complex, both the HOMO and LUMO iso-densities lie on the metallacycle, due to the significant difference in the positions of HOMO and LUMO of metallacycle and S-alanine from each other. The behavior seen in the R-pro@metallacycle is similar to that observed for the R-ala@metallacycle, whereas for S-pro@metallacycle, the HOMO and LUMO iso-densities are present on amino acid and metallacycle, respectively.

For the R-ser@metallacycle, the HOMO iso-densities are observed on serine (amino acid), along with one pyridine unit and $ZnCl_2$ (in metallacycle). This is again due to the closer HOMO levels of the serine and metallacycle, whereas due to the greater difference in the values and positions of LUMO, the iso-densities appear only on one side of the metallacycle *i.e.,* on pyridine unit present along the side wall. Similarly, the HOMO and LUMO of S-ser@metallacycle show a similar pattern, due to the same reason as mentioned above. In case of R-val@metallacycle, the HOMO iso-densities are present mostly on the amino acid along with two small patches observed on the Cl of $ZnCl_2$ (on metallacycle), because of considerably greater difference in the HOMO positions,

and the greater value of HOMO for the valine, due to which the newly formed HOMO closely resembles that of the valine. The LUMO iso-densities reside on the pyridine unit of metallacycle, alike the aforementioned complexes. For S-val@metallacycle, the HOMO iso-densities are seen on the valine as well as the metallacycle *i.e.,* on $ZnCl_2$ and pyridine unit, due to closer HOMO levels, while the LUMO iso-densities are seen on the pyridine unit of the metallacycle. Overall, a general trend is that the E_{gap} after complexation is reduced, and the HOMO and LUMO iso-densities after complexation are observed on both the species and on the metallacycle, respectively.

HOMO	LUMO
	
Metallacycle	
	

R-ala@metallacycle	
	
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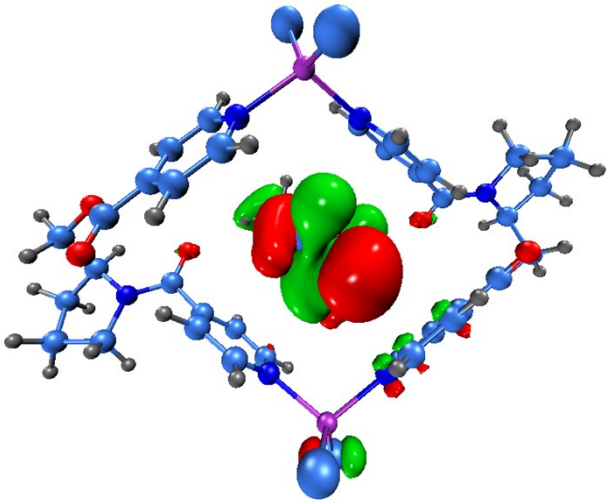	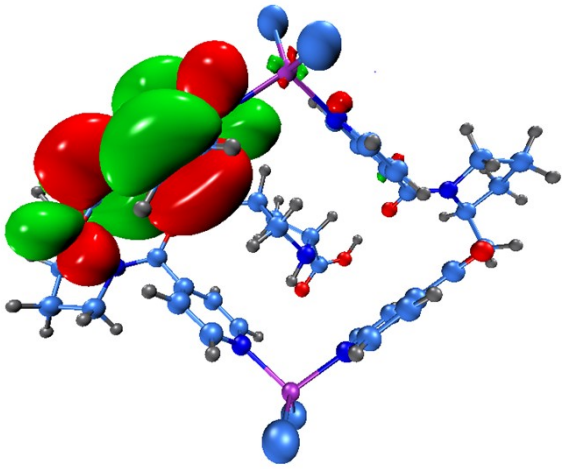
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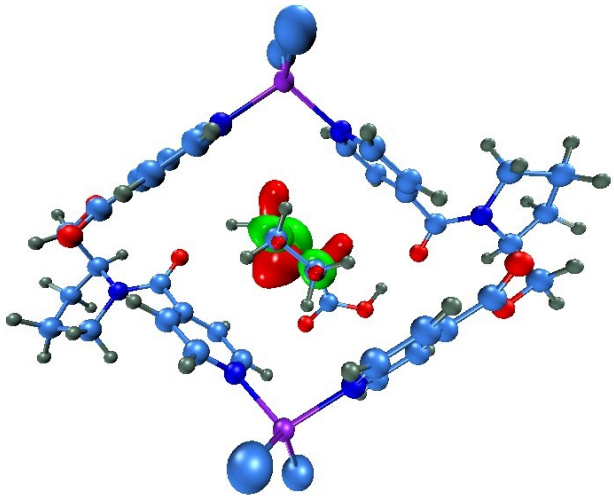	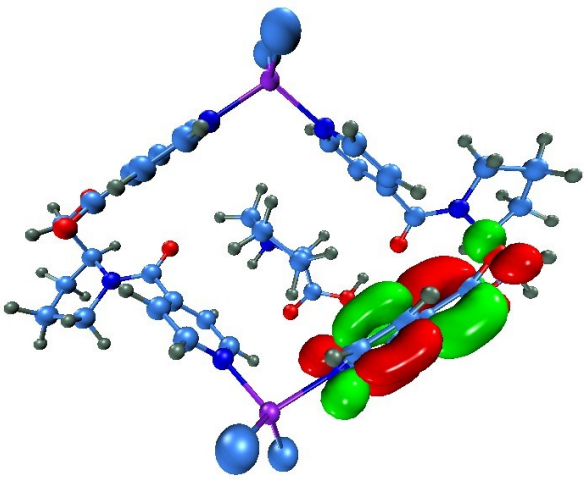

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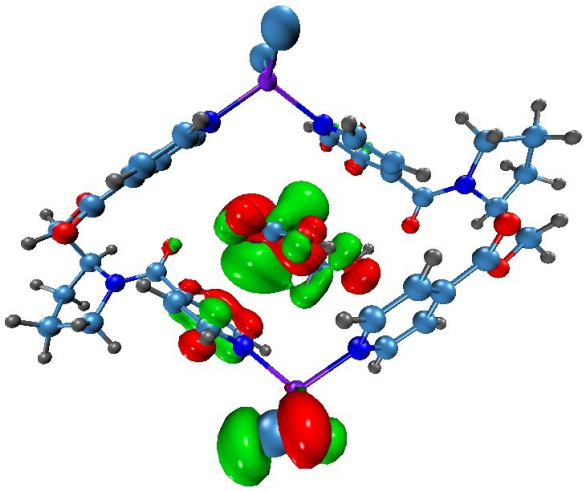	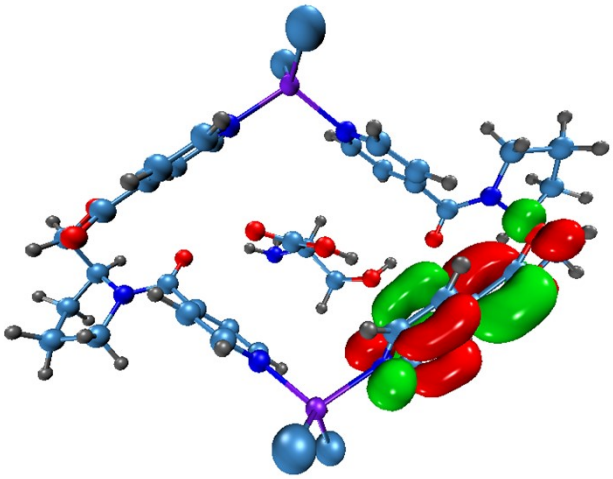
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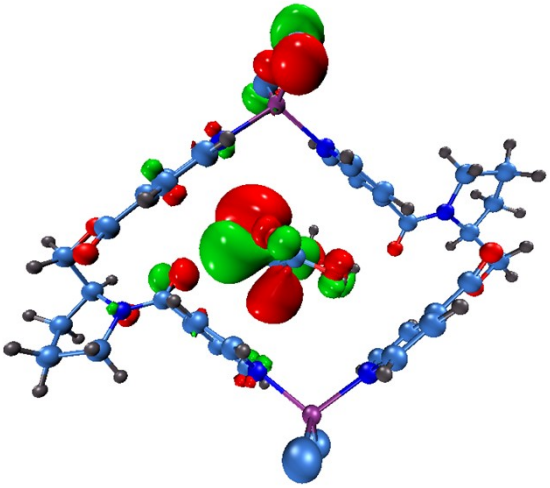	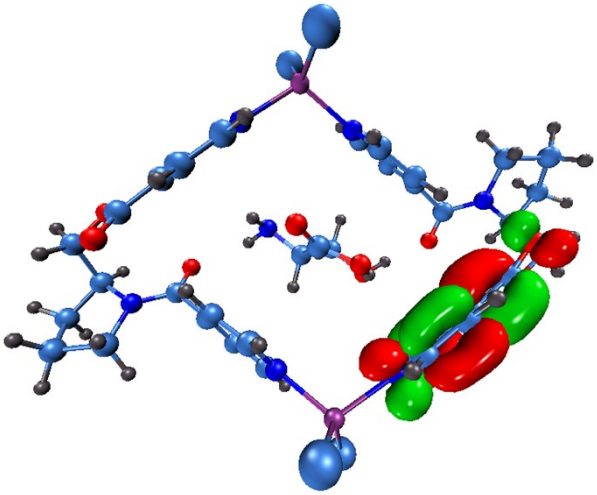
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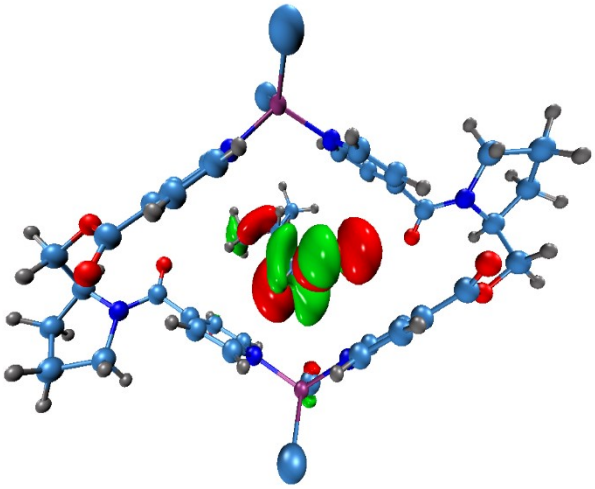
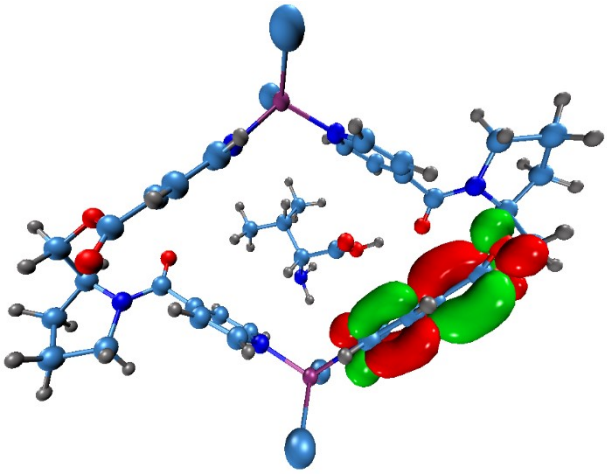
	

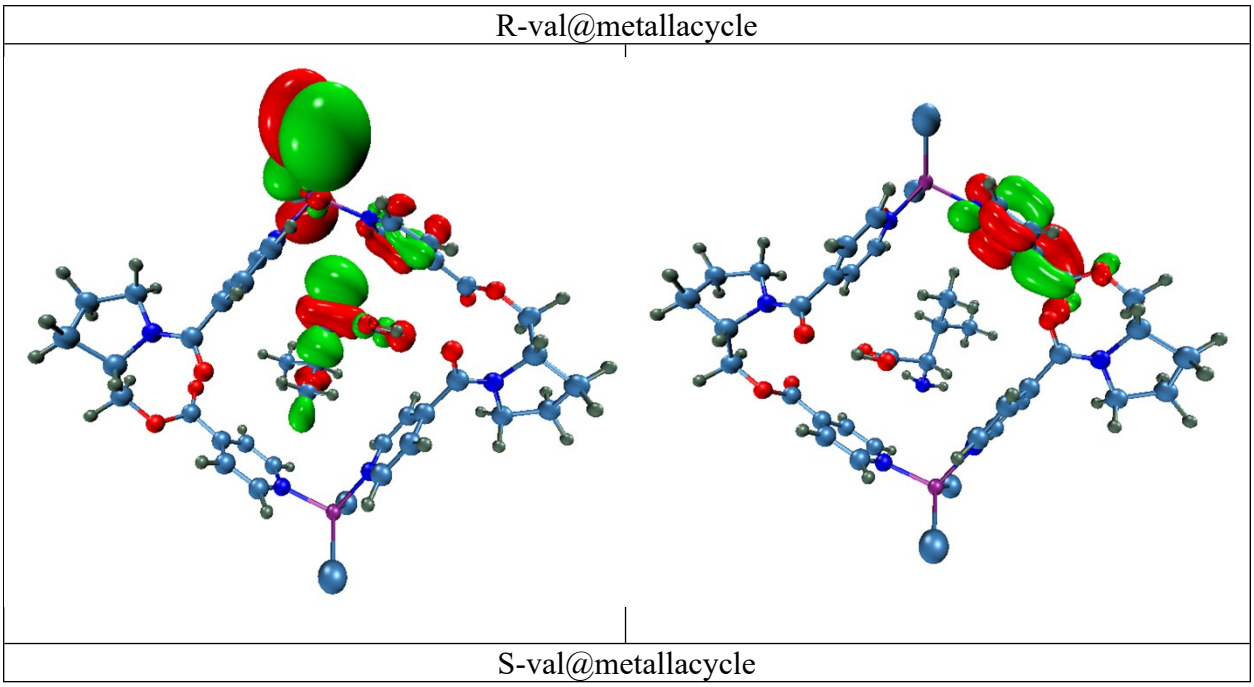
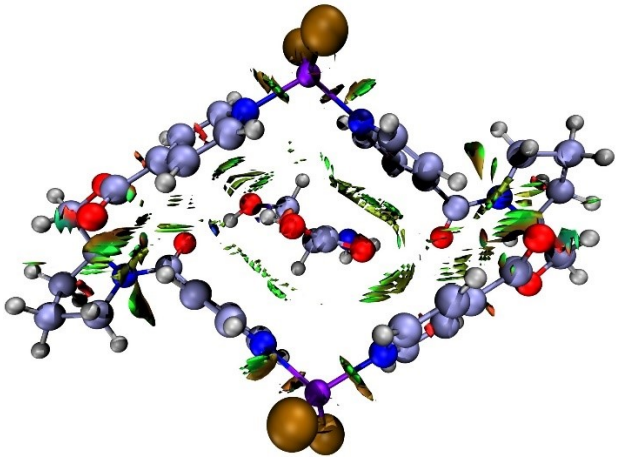
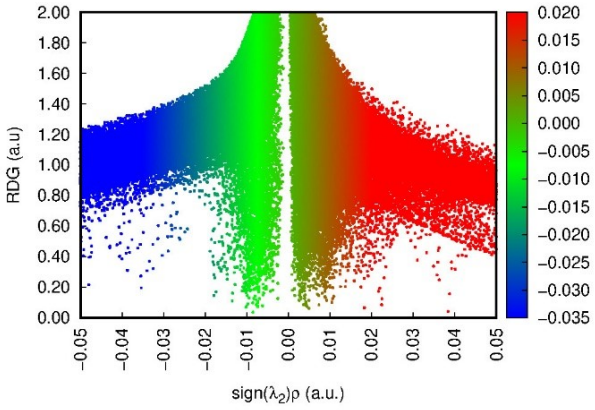


Figure S2: HOMO and LUMO isosurfaces of metallacycle and R and S enantiomers of amino acids@metallacycle complexes.

Table S4: Energy of HOMO (E_{HOMO}), energy of LUMO (E_{LUMO}), energy gap (E_{gap}), and NBO charges (Q) for metallacycle, R and S amino acids and R and S amino acids@metallacycle.

Complexes	E_{HOMO} (eV)	E_{LUMO} (eV)	E_{gap} (eV)	Q |e|	E (2)
Metallacycle	-6.85	-2.66	4.19	-	-
R-alanine	-9.06	2.33	11.39	-	-
R-ala@metallacycle	-8.68	-0.75	7.93	-0.058	LP_O-BD^*_{O-H}=10.64
S-alanine	-8.72	2.56	11.28	-	-
S-ala@metallacycle	-8.92	-0.87	8.04	-0.012	LP_O-BD^*_{N-H}=5.53
R-proline	-9.39	2.37	11.76	-	-
R-pro@metallacycle	-8.75	-0.98	7.76	-0.036	LP_O-LP^*_H=16.99
S-proline	-9.39	2.37	11.76	-	-
S-pro@metallacycle	-8.44	-1.00	7.44	-0.291	LP_O-BD^*_{O-H}=14.99
R-serine	-9.02	2.37	11.40	-	-
R-ser@metallacycle	-8.83	-0.86	7.96	-0.041	LP_O-BD^*_{O-H}=12.71
S-serine	-9.07	2.56	11.63	-	-
S-ser@metallacycle	-8.87	-0.81	8.06	-0.042	LP_O-BD^*_{O-H}=12.41
R-valine	-8.64	2.33	10.98	-	-

R-val@metallacycle	-8.42	-0.75	7.67	-0.052	LP_O-LP^*_H=24.79
S-valine	-8.84	2.23	11.08	-	-
S-val@metallacycle	-8.81	-0.70	8.10	-0.036	LP_O-LP^*_H=19.67

2D	**3D**
	
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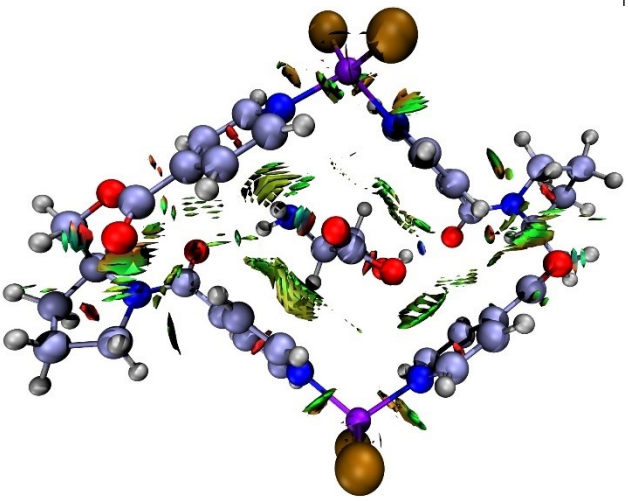	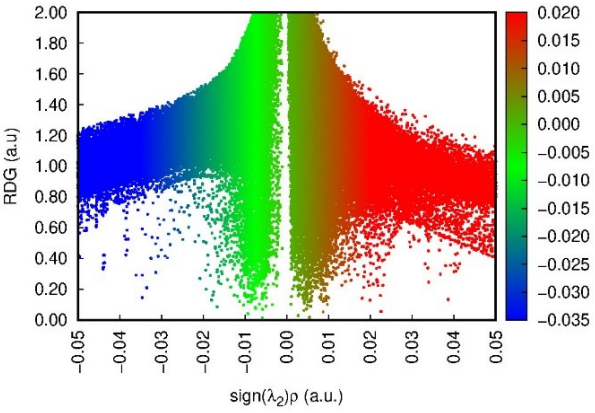
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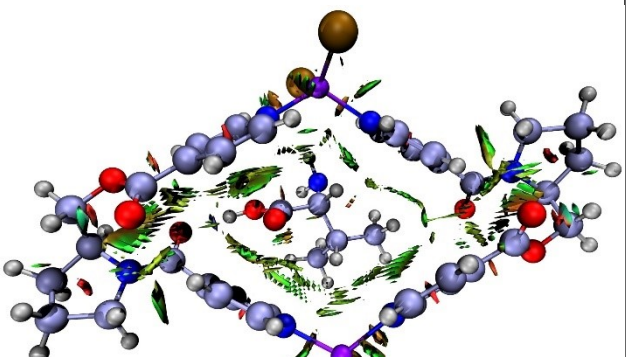	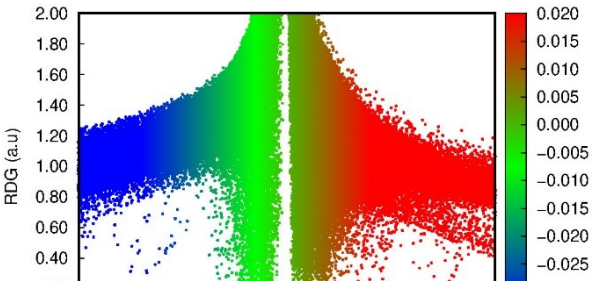

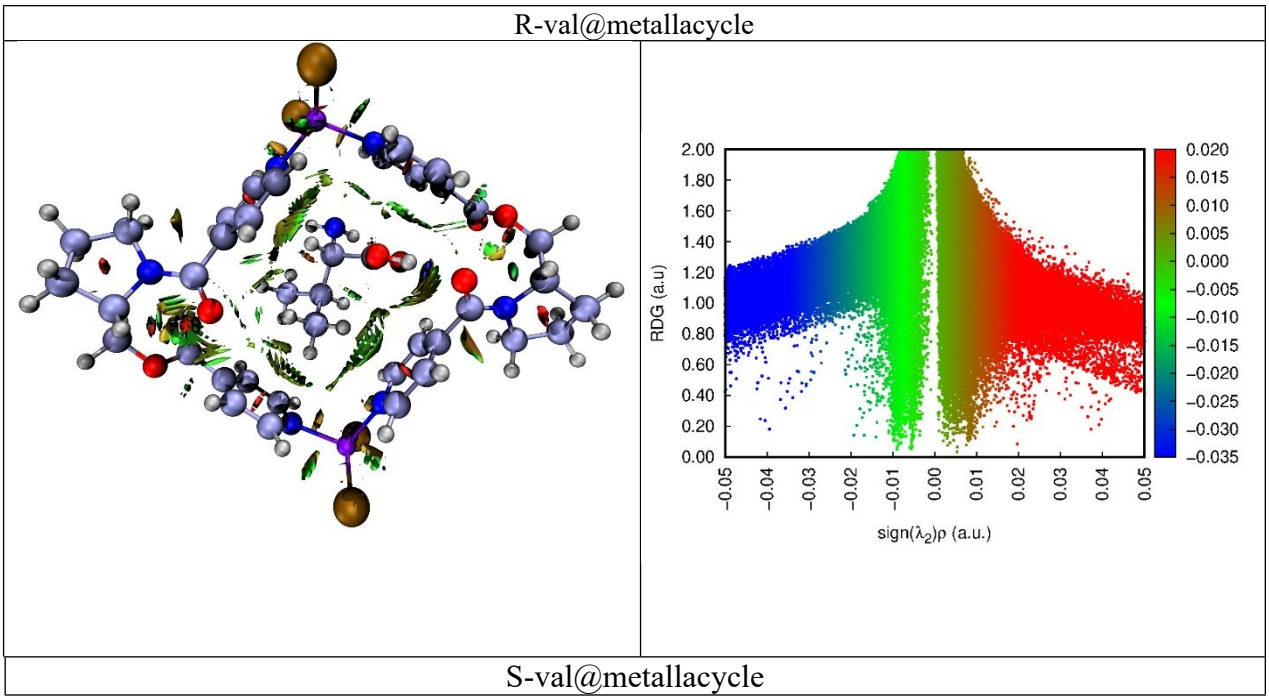

Figure S3: Non-covalent interaction index (NCI) analysis for R and S enantiomeric complexes of serine and valine

1. Cartesian coordinates of optimized structures

R-ala@metallacycle

Zn	-0.44891800	-4.66392000	1.22497500
Zn	0.52553000	4.63383400	1.17867500
N	-1.78714600	-3.35019400	0.35004700
N	-5.65332400	-0.54920500	-1.40103400
N	-1.37442700	3.86435000	1.02568900
N	1.79264700	3.28637800	0.28465500
N	5.64412000	0.50996000	-1.39913000
N	1.41513100	-3.83558800	1.01172700
O	-3.73087000	0.41716000	-2.13861900
O	-5.74976500	2.29254200	-0.61689700
O	-5.46664800	0.99144400	1.20577500
O	3.80631100	-0.44564100	-2.33897900
O	5.78951000	-2.27099700	-0.64335000

O	5.55291900	-1.01964000	1.22268500
C	4.31478500	0.41661500	-1.62499100
C	2.50845100	2.42951000	1.01957200
H	2.38948000	2.51919000	2.09492300
C	3.45112000	1.43792900	-0.93703400
C	-6.38026400	-1.61974400	-0.69997000
H	-6.23410700	-1.52963300	0.37931900
H	-6.00454500	-2.59377200	-1.02221200
C	-4.32102800	-0.47555300	-1.51832300
C	1.87579100	3.23028600	-1.05049900
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C	5.14879200	-1.86754200	0.45678300
C	-7.85083800	-1.40265000	-1.10704400
H	-8.33831400	-2.34202500	-1.37185700
H	-8.41178900	-0.97081500	-0.27457400
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H	-1.84880800	-2.18396400	2.04556200
C	-3.04045300	2.34246800	1.78754200

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C	6.59163200	-0.42131400	-2.00262600
H	6.13538100	-0.85137700	-2.89598500
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C	-3.83134100	2.65252800	0.68607500
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H	2.72193200	2.28709600	-2.78426400
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S-ala@metallacycle

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O	-4.24645500	0.47445700	-2.14053300
O	-5.95964000	2.28469000	-0.22716200
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C	-3.68453600	-1.43102700	-0.84862400
C	6.44021700	1.53680100	-0.01851200
H	6.05441100	1.39293900	0.99348100
H	6.11453400	2.51668800	-0.37902500
C	4.70040900	0.41903200	-1.44653800
C	-2.32542700	-3.36287800	-1.21199900
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H	1.88838300	2.25878100	1.81651700
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H	3.53140900	-2.34357000	2.80122200
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H	-6.69338500	0.79537100	-2.36793300
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Cl	-0.42773700	-6.15649200	-0.99021400
C	-0.34199200	-0.21213800	-1.56851600
H	-0.89211700	-1.15498700	-1.65330900
C	0.89352500	-0.28754800	-2.45952400
H	1.61019100	-1.01212000	-2.07039000
H	0.61551900	-0.57079200	-3.47768500
H	1.40006100	0.68069700	-2.49397600
N	-1.22120300	0.91860800	-1.88007800
H	-2.17873200	0.65434600	-2.10923700
H	-0.85136900	1.48700000	-2.63202200
C	0.06518200	-0.11513300	-0.08645800
O	0.81040200	-0.89750300	0.45723700
O	-0.50219600	0.90687400	0.54299800
H	-1.00702300	1.35479000	-0.19124900

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C	-0.25105800	0.28075100	-2.35143000
C	0.92217700	-0.48263300	-1.70765000
C	-0.31271400	0.38465200	0.08723800
C	-0.79863600	1.11979100	-1.18954000
H	0.05015200	0.88180400	-3.21333300
H	-1.00190800	-0.44148000	-2.68447200
H	1.81182500	0.15271200	-1.68970500

H	-0.08378400	-1.58700300	-0.37334100
H	-1.13979300	0.03378700	0.70988300
H	0.28771100	1.05794100	0.70928500
H	-1.88673800	1.19469400	-1.24709700
H	-0.39231300	2.13517600	-1.22089500
N	0.50733400	-0.76159300	-0.33274600
C	1.22472400	-1.79017700	-2.42744300
O	0.41820800	-2.69487700	-2.45322500
O	2.39771700	-1.90431800	-3.03516800
H	2.98241300	-1.13961500	-2.85429900
Zn	0.47178500	4.62493800	1.08232900
Zn	-0.70329000	-4.45330500	1.34644100
N	1.87088000	3.35032900	0.24461300
N	5.92243000	0.57299700	-1.03533900
N	1.16424100	-3.61702000	1.11338800
N	-2.00734700	-3.14674200	0.41909800
N	-5.89000300	-0.38429300	-1.26644000
N	-1.40329800	3.78536900	0.90233200
O	4.26565600	-0.03811600	-2.45391900
O	5.64261900	-2.20187400	-0.44327100
O	5.43094100	-1.02619300	1.47131100
O	-4.04472300	0.52798400	-2.23984000
O	-5.91644000	2.40682700	-0.54035600
O	-5.65864700	1.17512800	1.33619400
C	-4.56104300	-0.32023800	-1.52037200
C	-2.72593200	-2.27623300	1.14348300
H	-2.58833000	-2.33747200	2.21948700
C	-3.70497100	-1.34922800	-0.83011000

C	6.56775600	1.53013300	-0.12047800
H	6.23564700	1.36393900	0.90570200
H	6.30823700	2.55003800	-0.41524700
C	4.67292000	0.65883300	-1.51953000
C	-2.12878900	-3.14545800	-0.91553600
H	-1.53799900	-3.87802000	-1.45290400
C	-5.25006200	1.98884700	0.53646500
C	8.07374300	1.23995600	-0.27473100
H	8.65562000	2.15974000	-0.35053400
H	8.43762900	0.69702000	0.60107900
C	2.15259200	3.41577900	-1.06415600
H	1.62393300	4.18252000	-1.62268500
C	3.07135300	2.57117500	-1.66368400
H	3.25599500	2.62722400	-2.72984800
C	-3.43368600	3.52236400	-0.32530000
H	-4.02486200	3.75844800	-1.19962600
C	3.74430400	1.64482900	-0.87010100
C	-6.58127100	-1.47494300	-0.56313700
H	-6.20964300	-2.43965800	-0.91931000
H	-6.40799500	-1.41533300	0.51402400
C	2.50866400	2.45245600	1.00594100
H	2.24731400	2.45820500	2.06010200
C	2.89505500	-2.19036200	1.91830200
H	3.28252300	-1.54158800	2.69405300
C	6.87079700	-0.40473100	-1.56294800
H	6.54717000	-0.69495100	-2.56318800
C	-6.82423600	0.57155100	-1.85113400
H	-6.38121400	0.97816700	-2.76216600

C	-1.86113100	2.94108200	1.83677800
H	-1.20184800	2.76745300	2.68177700
C	4.98870500	-1.80759700	0.65520100
C	3.64393100	-2.44690300	0.77371200
C	1.65642800	-2.79379200	2.04777400
H	1.03251000	-2.64810000	2.92432500
C	-7.12318900	1.71965000	-0.88077200
H	-7.76009400	2.46291500	-1.36341400
H	-7.60310100	1.35899300	0.03189000
C	-3.59822600	-1.37246100	0.56079900
H	-4.17422100	-0.68993000	1.17740200
C	-3.90856500	2.64418100	0.64399400
C	-8.06853900	-1.26219000	-0.90569600
H	-8.56789500	-2.20368500	-1.13973200
H	-8.58984500	-0.82305300	-0.05100100
C	-3.10988200	2.34799400	1.74463900
H	-3.46575700	1.67492000	2.51516900
C	6.93957400	-1.64581100	-0.66377800
H	7.51678500	-2.42710500	-1.16104900
H	7.39491000	-1.40950500	0.30045900
C	3.12864100	-3.29331400	-0.20301600
H	3.67196000	-3.50194800	-1.11481100
C	3.45720400	1.58226200	0.49065000
H	3.94417100	0.85958700	1.13657900
C	-8.06759300	-0.28868200	-2.09525400
H	-8.98585200	0.30081700	-2.16003700
H	-7.94880300	-0.82898400	-3.03818800
C	1.88093400	-3.86244200	0.00993800

H	1.43316700	-4.53710700	-0.71207200
C	-2.94750400	-2.24327200	-1.57887300
H	-2.98669800	-2.24263400	-2.66153500
C	8.19057700	0.37088800	-1.53817900
H	9.06461700	-0.28505500	-1.51934100
H	8.25830900	0.99364200	-2.43409600
C	-2.17528700	4.07642100	-0.15302300
H	-1.75610100	4.78265700	-0.86319200
Cl	0.90563200	4.48674600	3.25367000
Cl	0.43632500	6.32084900	-0.35077100
Cl	-1.15622400	-4.19356700	3.51164200
Cl	-0.70229500	-6.24566200	0.05313100

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C	-0.74557000	-0.35585600	2.10976100
C	0.40443600	0.52790300	0.14078800
C	0.89472900	1.15589600	1.47046800
H	1.18068600	-0.45147100	2.70181000
H	-1.59132800	0.29850100	2.34646400
H	-0.29097300	-1.52492500	0.32088300
H	1.23044700	0.05126300	-0.39327000
H	-0.01803500	1.28015600	-0.53037800
H	1.97589700	1.29622100	1.50974600
H	0.42383400	2.13814000	1.61089000
C	-0.95375900	-1.70609100	2.77228500
O	-0.03396200	-2.42727400	3.08631800
O	-2.21815500	-2.09850200	2.91922500
H	-2.84138800	-1.39390300	2.65215000

N	0.48279100	0.27199600	2.55464800
C	-0.64390700	-0.52066900	0.56338000
H	-1.61331500	-0.38765200	0.07570600
Zn	-0.39119100	4.61646400	-1.04789400
Zn	0.56146700	-4.40891300	-1.36074700
N	-1.81105400	3.32542800	-0.26433300
N	-5.88753200	0.60934500	1.04359700
N	-1.30526200	-3.53492100	-1.14774400
N	1.87752100	-3.11103500	-0.45833400
N	5.90075400	-0.50653200	1.17022000
N	1.47260900	3.74368400	-0.90618100
O	-4.14964000	-0.31093700	2.16613300
O	-5.82695600	-2.15178700	0.28030500
O	-5.53232800	-0.88463800	-1.56542400
O	4.10757800	0.44669700	2.19720300
O	5.98297700	2.27701000	0.45771100
O	5.68218800	1.07496500	-1.43198600
C	4.57979500	-0.40633500	1.45306400
C	2.66530000	-2.31350800	-1.19433700
H	2.54685800	-2.40070400	-2.27059900
C	3.67110700	-1.39285800	0.76954600
C	-6.52026000	1.69407900	0.27469100
H	-6.24834200	1.62629400	-0.78055900
H	-6.18638500	2.66070400	0.66089000
C	-4.59310300	0.54511800	1.39600000
C	1.96399100	-3.06249800	0.87750300
H	1.31299200	-3.72773200	1.43417300
C	5.29613200	1.88295700	-0.61532200

C	-8.02988100	1.47095100	0.48377800
H	-8.55433500	2.40993100	0.66660900
H	-8.46757100	1.02380800	-0.41227500
C	-2.04798100	3.30243900	1.05340300
H	-1.49038700	4.02021700	1.64761500
C	-2.95770100	2.42750400	1.62563400
H	-3.10098500	2.41459000	2.69973700
C	3.48540100	3.37640500	0.32442100
H	4.06549500	3.54315900	1.22190300
C	-3.66841800	1.56645600	0.79486900
C	6.55153900	-1.61716700	0.45914600
H	6.15888500	-2.57060600	0.82315600
H	6.36573600	-1.55566400	-0.61563500
C	-2.49268800	2.49596600	-1.06557400
H	-2.26683000	2.57571900	-2.12515600
C	-3.04934100	-2.17234700	-2.03388200
H	-3.44231000	-1.56923400	-2.84337600
C	-6.86658500	-0.35133700	1.54996000
H	-6.50478900	-0.74693100	2.50026400
C	6.86976300	0.41948800	1.74713100
H	6.45108800	0.83230700	2.66675400
C	1.93532400	2.96047200	-1.89113000
H	1.28464000	2.85124900	-2.75336300
C	-5.13609100	-1.71586600	-0.77595300
C	-3.79633000	-2.37098500	-0.87519200
C	-1.80727700	-2.77680200	-2.13218800
H	-1.18681200	-2.68405800	-3.01867700
C	7.18085000	1.56456700	0.77707600

H	7.84026900	2.29242900	1.25283800
H	7.63888200	1.19732900	-0.14420400
C	3.58407000	-1.44965500	-0.62183900
H	4.20641300	-0.81875100	-1.24827700
C	3.96335700	2.56027000	-0.69593500
C	8.04904200	-1.44452800	0.77829000
H	8.52699900	-2.39955500	1.00201900
H	8.56754100	-1.01688000	-0.08394800
C	3.17529900	2.34715700	-1.82355200
H	3.53289500	1.72020100	-2.63123500
C	-7.06951800	-1.50620500	0.56251400
H	-7.70600900	-2.26984700	1.01227500
H	-7.51449900	-1.15813500	-0.37229200
C	-3.27173300	-3.15135000	0.15033500
H	-3.81209900	-3.30833500	1.07382400
C	-3.43841100	1.60665000	-0.57924000
H	-3.97042700	0.94630300	-1.25686100
C	8.09295100	-0.47430200	1.96938100
H	9.02751800	0.09035600	2.02056500
H	7.97477200	-1.01335900	2.91307900
C	-2.01765800	-3.71825400	-0.02910500
H	-1.56302800	-4.34590600	0.73148600
C	2.83169200	-2.20010100	1.52987700
H	2.84473300	-2.17098600	2.61286700
C	-8.13001400	0.50440300	1.67504200
H	-9.04568700	-0.09193400	1.65917700
H	-8.10217600	1.05029500	2.62175800
C	2.23348400	3.95320800	0.17592800

H	1.81297600	4.61228500	0.92912900
Cl	-0.83651400	4.57540500	-3.22237100
Cl	-0.33784000	6.24534000	0.45726000
Cl	0.99764100	-4.21784300	-3.53295600
Cl	0.47584600	-6.16010600	-0.01684800

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Zn	-0.27781700	-4.38909400	0.90408000
Zn	0.34561300	4.33511000	0.98665300
N	-1.70318300	-3.08573600	0.14473800
N	-6.00690400	-0.67798600	-1.01739300
N	-1.52900300	3.47298100	0.91108500
N	1.76519100	3.06935700	0.22101800
N	5.99694700	0.59497200	-1.02060400
N	1.57451200	-3.53584900	0.86329300
O	-4.39502000	0.29558600	-2.28633700
O	-6.12234600	2.05412600	-0.21502300
O	-5.70112100	0.79403800	1.61111300
O	4.34113700	-0.40275900	-2.22446500
O	6.15812100	-2.13115400	-0.26203800
O	5.79111900	-0.93755000	1.62253000
C	4.71139300	0.45309300	-1.42649900
C	2.48089800	2.27328500	1.02601500
H	2.24380800	2.33567400	2.08343000
C	3.71825200	1.41003000	-0.82629600
C	-6.53035400	-1.78867100	-0.20377800
H	-6.24741900	-1.66336400	0.84319900
H	-6.12056000	-2.73412500	-0.56737100

C	-4.74158800	-0.54667300	-1.44986800
C	2.00907900	3.05198800	-1.09726700
H	1.42724500	3.74828000	-1.69393500
C	5.42607100	-1.73271800	0.78370900
C	-8.05876300	-1.70196700	-0.38613800
H	-8.49897600	-2.68373100	-0.56658500
H	-8.51923800	-1.30238700	0.52078700
C	-1.97091200	-3.07602900	-1.16783700
H	-1.38353000	-3.76062200	-1.77289300
C	-2.95373600	-2.26823500	-1.71481500
H	-3.13188000	-2.26693500	-2.78395500
C	3.59333200	-3.06627700	-0.31777600
H	4.17261400	-3.13407100	-1.22832700
C	-3.71359000	-1.47113300	-0.86209000
C	6.53278700	1.72227800	-0.24245700
H	6.11435300	2.66118300	-0.61486900
H	6.27386500	1.62317800	0.81417800
C	-2.41562200	-2.30332900	0.96237000
H	-2.15860000	-2.36372600	2.01530100
C	-3.13682200	1.97881900	1.83947200
H	-3.40907800	1.25818600	2.60077500
C	-7.07352600	0.20675700	-1.48100500
H	-6.77599100	0.63663800	-2.43845300
C	7.05570200	-0.27088100	-1.52647800
H	6.72910100	-0.69766100	-2.47640900
C	2.04228600	-2.87137300	1.92782500
H	1.38725200	-2.84014700	2.79256900
C	-5.36936200	1.64283800	0.81125100

C	-4.04344700	2.33051700	0.84076600
C	-1.88792400	2.57463200	1.83946500
H	-1.14751100	2.35616300	2.60156500
C	7.35439300	-1.40490600	-0.53788800
H	8.04702200	-2.12123700	-0.98313000
H	7.76954600	-1.02298200	0.39767800
C	3.47900000	1.44206900	0.54446900
H	4.03793700	0.81057200	1.22665900
C	4.08332000	-2.38724100	0.79264300
C	8.05679500	1.63902100	-0.45552800
H	8.49403000	2.62259100	-0.63489700
H	8.53600700	1.22930700	0.43744400
C	3.29478500	-2.28204200	1.93312100
H	3.65809700	-1.75139100	2.80465100
C	-7.32764100	1.33361800	-0.47068000
H	-8.02699200	2.05767000	-0.89174800
H	-7.72271400	0.94456900	0.47034500
C	-3.67575900	3.27437800	-0.11014300
H	-4.35065900	3.56113300	-0.90503100
C	-3.44284300	-1.49159700	0.50289000
H	-4.01044100	-0.88161700	1.19752000
C	8.24133600	0.68972500	-1.65041100
H	9.20616600	0.17579900	-1.63697900
H	8.16455700	1.23502700	-2.59495200
C	-2.40322800	3.82155100	-0.03811900
H	-2.05371600	4.56309700	-0.74969100
C	2.95742600	2.21913600	-1.66425200
H	3.08346100	2.18492700	-2.73862500

C	-8.27110400	-0.74273600	-1.56949500
H	-9.22899900	-0.21869800	-1.52093500
H	-8.23207700	-1.28224900	-2.51945400
C	2.33125900	-3.62846000	-0.23732400
H	1.90263800	-4.19187200	-1.05993500
Cl	-0.83378900	-4.51548200	3.05096400
Cl	-0.21040500	-5.93998000	-0.69895900
Cl	0.77927800	4.38136200	3.16631900
Cl	0.21363700	5.96128200	-0.53294500
C	0.03516600	-0.08340400	-2.18059100
N	1.23472000	-0.08470000	-2.99164800
H	2.03827900	-0.41193300	-2.45746400
H	1.13376200	-0.68464900	-3.79971000
C	0.38891800	-0.19778500	-0.69075600
O	1.43708200	-0.66320300	-0.30971000
O	-0.55083400	0.18965100	0.16996700
H	-1.29132100	0.60702200	-0.33709200
C	-0.79133200	1.17551000	-2.50302400
H	-0.16885600	2.05533600	-2.32329600
H	-1.05197300	1.16582100	-3.56613100
O	-1.94976000	1.29842000	-1.69259000
H	-2.73911000	0.88405600	-2.09447300
H	-0.61307000	-0.95665800	-2.36508000

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C	-0.44630300	-0.03912400	-1.28379500
N	-1.36593200	1.05833800	-1.47892000
H	-2.15220900	0.79685500	-2.06785300

H	-1.74349400	1.30873100	-0.57081000
C	0.05741000	-0.03406700	0.16158500
O	-0.49218500	0.57733300	1.05120400
O	1.12047300	-0.79449500	0.39862600
H	1.46474300	-1.10954200	-0.47682200
C	0.69410500	0.05329800	-2.30513900
H	0.25954100	0.03434800	-3.31087700
H	1.20198900	1.01316600	-2.17601500
O	1.58853600	-1.04078000	-2.12911400
H	2.50192700	-0.75729600	-2.33660500
H	-0.90546100	-1.03339700	-1.41178800
Zn	-0.46837200	-4.65175700	0.82179000
Zn	0.39130100	4.65904200	0.81812900
N	-1.79672200	-3.25024000	0.07522300
N	-5.92619700	-0.56386700	-1.03229300
N	-1.48624000	3.84153200	0.76914900
N	1.78070200	3.30695400	0.09954700
N	5.90035100	0.58380200	-0.99739700
N	1.43062600	-3.86303200	0.79555900
O	-4.27768300	0.34546800	-2.31297000
O	-6.00799800	2.23424100	-0.40502900
O	-5.58747800	1.07626200	1.48854800
O	4.22892300	-0.31258500	-2.24523800
O	5.93140400	-2.22568400	-0.39304300
O	5.54602800	-1.11716400	1.53841100
C	4.62936200	0.52114000	-1.42417400
C	2.26504600	2.34278800	0.89126700
H	1.87080200	2.31192000	1.90134800

C	3.67788300	1.53512900	-0.85516800
C	-6.45602000	-1.62930400	-0.16739700
H	-6.13343500	-1.48115600	0.86582900
H	-6.09099000	-2.60102700	-0.51095800
C	-4.65683400	-0.47775800	-1.48383000
C	2.23217600	3.41416400	-1.15697300
H	1.81339800	4.23009900	-1.73890600
C	5.20437000	-1.90336700	0.68243500
C	-7.98468100	-1.50211300	-0.30990200
H	-8.46392100	-2.47777200	-0.40446100
H	-8.40315000	-1.01968800	0.57710700
C	-2.20966400	-3.33349900	-1.19787500
H	-1.77699300	-4.14228200	-1.77971500
C	-3.13847500	-2.45474200	-1.73137300
H	-3.43456500	-2.53800300	-2.77051100
C	3.36734300	-3.21950800	-0.44127000
H	3.89377500	-3.17932000	-1.38573800
C	-3.68243700	-1.47155700	-0.90781300
C	6.45451600	1.63458200	-0.12663400
H	6.10786400	2.61395400	-0.46618600
H	6.12628100	1.48632400	0.90444300
C	-2.30577400	-2.29387500	0.86409000
H	-1.94465100	-2.27822300	1.88736000
C	-3.15011700	2.48049400	1.79544000
H	-3.47649600	1.88457800	2.63853000
C	-6.98009100	0.30831800	-1.54054800
H	-6.68392400	0.66789600	-2.52763500
C	6.93680000	-0.30813300	-1.51289800

H	6.63283600	-0.65587100	-2.50168200
C	1.94975500	-3.31049800	1.89898900
H	1.33947800	-3.38167200	2.79405900
C	-5.26273400	1.88708800	0.64818800
C	-3.95712000	2.61433800	0.67071800
C	-1.91784000	3.11295200	1.80559400
H	-1.24503200	3.04649400	2.65372600
C	7.15178200	-1.51383300	-0.59218900
H	7.83632500	-2.22009500	-1.06516900
H	7.55122400	-1.20721300	0.37699000
C	3.22304000	1.43763500	0.45568000
H	3.58649400	0.66413800	1.12308700
C	3.89944100	-2.63067100	0.70341600
C	7.97924700	1.47506100	-0.27218900
H	8.47854200	2.44095900	-0.36131700
H	8.38896400	0.97801500	0.61069300
C	3.18427000	-2.68151800	1.89485700
H	3.57939300	-2.22367800	2.79323000
C	-7.21785600	1.50622300	-0.61369600
H	-7.90957700	2.20695600	-1.08442000
H	-7.61670800	1.18837500	0.35217900
C	-3.51422300	3.38456600	-0.40245400
H	-4.11179800	3.49067000	-1.29775300
C	-3.25653700	-1.38867500	0.41536400
H	-3.65178000	-0.63384000	1.08680300
C	8.16947000	0.60138800	-1.52311800
H	9.10720000	0.04015500	-1.50827600
H	8.15890200	1.21299800	-2.42927900

C	-2.26682600	3.98141600	-0.31097000
H	-1.86132300	4.59193400	-1.11107400
C	3.17602500	2.54306000	-1.67617000
H	3.50248500	2.64239300	-2.70496300
C	-8.19593400	-0.62349400	-1.55404100
H	-9.14486100	-0.08126800	-1.53236700
H	-8.17592600	-1.22847500	-2.46452900
C	2.12539900	-3.82749500	-0.34911800
H	1.65976800	-4.30883100	-1.20298600
Cl	-0.99920700	-4.76618800	2.97168900
Cl	-0.41369000	-6.19204900	-0.78408600
Cl	0.90151600	4.75890800	2.97908200
Cl	0.35564100	6.23530000	-0.75520400

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C	1.43951800	-0.63765000	-1.41950900
O	2.38178800	-0.95166400	-2.30660700
O	1.67457400	-0.30463500	-0.27352100
H	3.27938400	-0.81905900	-1.91744200
C	0.02577900	-0.70139400	-1.98433100
C	-0.41744300	0.72905000	-2.39227600
H	-0.18084100	1.37646000	-1.53639800
C	0.33723100	1.25633800	-3.61600200
H	0.11524000	2.31799900	-3.76161500
H	1.42058500	1.14280300	-3.51394800
H	0.02772000	0.72452300	-4.52201900
C	-1.92496900	0.76619500	-2.63209800
H	-2.48531200	0.55777000	-1.71734300

H	-2.23761600	1.74805400	-3.00028900
H	-2.20648600	0.01713200	-3.37674000
N	-0.18459400	-1.65903300	-3.05495200
H	0.47204200	-1.48157800	-3.80840900
H	0.00739100	-2.60538100	-2.73265400
H	-0.59831500	-0.99382200	-1.13378800
Zn	0.35636100	4.32836200	0.16603100
Zn	-0.48728000	-4.25221100	0.20764100
N	1.97586200	3.09553500	-0.09662800
N	6.38193500	0.51176500	-0.04730300
N	1.32803500	-3.37715400	0.63448400
N	-2.03113200	-2.94602100	-0.17296700
N	-6.45997800	-0.47507300	-0.05330300
N	-1.41511000	3.33455600	0.54305600
O	4.96355300	-0.53113000	-1.47543300
O	6.10980700	-2.20191100	0.85657300
O	5.26395100	-0.87647400	2.47960400
O	-5.27895400	0.44256300	-1.77076400
O	-6.20956000	2.21198400	0.67520300
O	-5.44155600	1.02831900	2.44390300
C	-5.37814300	-0.37899600	-0.86725800
C	-2.53297300	-2.20916300	0.82820300
H	-2.04812400	-2.31950000	1.79247700
C	-4.23849000	-1.32208200	-0.58915000
C	6.82045400	1.66626800	0.75376100
H	6.30748500	1.68627300	1.71725100
H	6.59167900	2.59216500	0.21997300
C	5.21194000	0.40125500	-0.70010500

C	-2.60879600	-2.88111400	-1.38097800
H	-2.16055800	-3.49234500	-2.15614000
C	-5.26012100	1.77209100	1.50383300
C	8.33518000	1.44892300	0.93377900
H	8.89502100	2.37410300	0.78907900
H	8.54341900	1.09913200	1.94815600
C	2.46182100	2.87219400	-1.32462100
H	1.94559300	3.37704800	-2.13541700
C	3.55269600	2.05018100	-1.54489000
H	3.89996100	1.86136400	-2.55374200
C	-3.63180300	2.76959500	-0.14732800
H	-4.37119800	2.71194300	-0.93602100
C	4.15966500	1.43926600	-0.45216300
C	-6.76582600	-1.59030500	0.85648200
H	-6.56027900	-2.54220200	0.35847600
H	-6.15980800	-1.53624900	1.76326900
C	2.56862000	2.51967200	0.95549700
H	2.14673700	2.75723600	1.92661600
C	2.74473200	-2.20672700	2.15597700
H	2.87380900	-1.68794100	3.09774300
C	7.44417400	-0.48120000	-0.20351700
H	7.32388900	-0.96998200	-1.17171000
C	-7.59192200	0.43015300	-0.21662000
H	-7.57833400	0.81862700	-1.23618500
C	-1.68872000	2.88594700	1.77726500
H	-0.89752200	3.00116400	2.51070200
C	5.12325000	-1.72001100	1.62093600
C	3.80967100	-2.34048200	1.27172300

C	1.52342800	-2.75428000	1.80427500
H	0.67262700	-2.72342100	2.47625800
C	-7.49663600	1.59995500	0.77334300
H	-8.21980300	2.37513900	0.51533200
H	-7.65999800	1.26968500	1.80155500
C	-3.63111600	-1.38343700	0.66517800
H	-3.99732600	-0.79541000	1.50012700
C	-3.91658200	2.31815500	1.13695100
C	-8.26120000	-1.41320700	1.17802100
H	-8.78733900	-2.36904400	1.19491300
H	-8.37592100	-0.96084100	2.16662300
C	-2.92215500	2.35551300	2.11185400
H	-3.12341900	1.99880200	3.11469900
C	7.37090500	-1.53617900	0.90515600
H	8.12484200	-2.30719200	0.73713700
H	7.51070900	-1.09177300	1.89341800
C	3.61519100	-3.00493600	0.06585800
H	4.41923200	-3.10442400	-0.65069300
C	3.66397900	1.68303800	0.82414500
H	4.07639900	1.18403900	1.69406100
C	-8.79245900	-0.46874400	0.08867300
H	-9.67230300	0.09497900	0.41008200
H	-9.06226100	-1.02712600	-0.81181900
C	2.35195700	-3.49697100	-0.21988200
H	2.13327500	-4.00991800	-1.15103800
C	-3.70583200	-2.07315400	-1.63052600
H	-4.12690100	-2.01634500	-2.62656900
C	8.71060500	0.37164900	-0.09582400

H	9.58641500	-0.21027100	0.20192600
H	8.92279400	0.82233500	-1.06895000
C	-2.36062500	3.26520100	-0.40180900
H	-2.07942600	3.64667800	-1.37827400
Cl	0.78967600	5.23392400	2.15612000
Cl	0.03803100	5.21790100	-1.85136700
Cl	-1.07356000	-5.05445800	2.19671400
Cl	-0.13787800	-5.20373500	-1.78342700

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C	1.51806100	-0.66093500	0.23816200
O	1.43939900	-0.74507300	-1.08181900
O	2.51465000	-0.30007100	0.83906000
H	2.27930700	-0.39412600	-1.47269900
C	0.22637000	-0.99211800	0.96236300
C	-0.41987600	0.34791100	1.39764300
H	0.34918900	0.89409200	1.96255800
C	-0.81780800	1.17200600	0.17203000
H	-1.18793000	2.14908700	0.48321900
H	0.02201200	1.33752900	-0.50821500
H	-1.61285700	0.67406200	-0.39484200
C	-1.62641000	0.14140800	2.31075000
H	-1.38867700	-0.47512400	3.18244500
H	-1.97899400	1.10472300	2.68629500
H	-2.46030400	-0.31927600	1.77136000
N	0.56834100	-1.92803300	2.02207300
H	1.25465400	-1.50193800	2.63809600
H	-0.24594500	-2.17054000	2.57326600

H	-0.44624100	-1.48757400	0.25931200
Zn	-0.57286700	5.55403000	0.29908800
Zn	0.45180400	-5.38207700	0.20428900
N	0.89706200	4.15993100	-0.16941500
N	5.24392400	1.68846200	-0.87042800
N	2.21242400	-4.36008000	0.34657600
N	-1.07125200	-4.02586700	-0.17072600
N	-5.44304100	-1.55093900	-0.89801500
N	-2.29872600	4.43842700	0.46790200
O	3.70804000	0.42684100	-1.96226200
O	5.88801800	-1.19417600	-0.48907800
O	5.82175700	-1.19139800	1.76877600
O	-3.80751100	-0.09208000	-1.49879000
O	-6.11757300	1.40281400	-0.27559300
O	-5.23037500	0.55606200	1.62376600
C	-4.14801300	-1.18544900	-1.05632400
C	-1.95320000	-3.69462800	0.77954200
H	-1.81500800	-4.18922200	1.73710400
C	-3.09476200	-2.20356900	-0.70581900
C	5.65809900	2.94959300	-0.22330900
H	5.35464500	2.97339800	0.82468600
H	5.19137400	3.79843300	-0.73261100
C	3.98427600	1.39176200	-1.24118100
C	-1.17122300	-3.45670500	-1.37803500
H	-0.44704800	-3.78260600	-2.11747400
C	-5.24015100	1.37157800	0.73121000
C	7.18391100	2.96607300	-0.37838500
H	7.56304800	3.97957700	-0.51810200

H	7.65964200	2.55700800	0.51735600
C	1.15613300	3.86085600	-1.44813000
H	0.56456700	4.39327700	-2.18699100
C	2.13867400	2.95226400	-1.81193000
H	2.31417500	2.72564100	-2.85685900
C	-3.87404500	3.00511700	-0.61219600
H	-4.29973000	2.61325300	-1.52615800
C	2.90104100	2.34895900	-0.81472000
C	-5.91165900	-2.91130100	-0.57663900
H	-5.44785900	-3.63886300	-1.25166000
H	-5.65963500	-3.19042500	0.44727500
C	1.60437400	3.55293900	0.79361600
H	1.35188100	3.83400100	1.81176800
C	3.80436500	-3.19769400	1.68474200
H	4.19419800	-2.94156100	2.66196600
C	6.38780700	0.95720100	-1.43587500
H	6.08020900	0.52216000	-2.38903700
C	-6.51928000	-0.70008300	-1.42748800
H	-6.13171900	-0.14338900	-2.28479300
C	-2.70352800	3.98170700	1.66117700
H	-2.19989700	4.40894100	2.52350000
C	5.42390000	-1.59573100	0.70346200
C	4.34619400	-2.61980500	0.54330400
C	2.72470100	-4.05341100	1.54472700
H	2.22942800	-4.50490900	2.39763700
C	-7.03286400	0.31252600	-0.40461700
H	-7.96052300	0.76093400	-0.76630100
H	-7.19764500	-0.14824400	0.57222300

C	-2.98280200	-2.79289700	0.55250800
H	-3.67044200	-2.54311300	1.35265300
C	-4.25978900	2.49656700	0.62414700
C	-7.42671900	-2.83547200	-0.78399200
H	-7.83946700	-3.79126100	-1.11065100
H	-7.92170800	-2.56280700	0.15301100
C	-3.68001200	3.00565300	1.78175300
H	-3.97172600	2.62759900	2.75424600
C	6.86768100	-0.16257600	-0.51792800
H	7.78671800	-0.59643500	-0.92335800
H	7.05430100	0.19151400	0.49857600
C	3.83731400	-2.96544500	-0.70557700
H	4.23537800	-2.52481100	-1.60999900
C	2.61466100	2.64533400	0.51626100
H	3.14384500	2.15438000	1.32310000
C	-7.59467200	-1.72151000	-1.82029100
H	-8.59970800	-1.29373200	-1.83163700
H	-7.38206700	-2.10106300	-2.82396500
C	2.77148900	-3.84716000	-0.75708200
H	2.33467600	-4.16473600	-1.69879500
C	-2.15408500	-2.52762200	-1.67987900
H	-2.18915900	-2.06270600	-2.65746700
C	7.44367800	2.05830900	-1.58525400
H	8.46200900	1.66366300	-1.61092800
H	7.27106400	2.60234000	-2.51835300
C	-2.88630600	3.97645200	-0.64427600
H	-2.53392300	4.40686500	-1.57689300
Cl	-0.08235100	6.16316600	2.37281800

Cl	-0.82198800	6.67351600	-1.59880400
Cl	-0.01973600	-6.16276300	2.22934400
Cl	0.59809200	-6.38450100	-1.78478500