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Supporting Information

Predicted structure and selectivity of glutamic n, n-*bis*(carboxymethyl acid complexes

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Table S1. *Selected geometrical parameters of GLDA complexes (B structure)*

Metal ions			Bond length (Å)						dihedral angle	E(kcal)
		Spin	M-N	$M-O_{17}$	$M-O_{12}$	$M-O_{14}$	$M-O_{16}$	$M-O_{29}$		
Mn^{2+}	Solvent	HS	2.27	2.21	2.14	2.21	2.08	2.30	22.5	- 4839.84
		LS	2.29	2.21	2.15	2.21	2.09	2.29	12.1	-4303.88
Fe^{2+}	solvent	HS	2.21	2.11	2.13	2.09	2.12	2.24	22.9	-4818.83
Co^{2+}	solvent	HS	2.11	2.12	2.08	2.13	2.02	2.22	20.1	- 4783.13
Ni^{2+}	solvent		2.03	2.08	2.04	2.09	2.06	2.17	15.7	- 4727.28
Zn^{2+}	solvent		2.14	2.15	2.10	2.17	2.05	2.19	20.3	- 4654.01

Table S2: *Selected geometrical parameters of GLDA complexes (A structure)*

Metal ions		Bond length (Å)						dihedral angle	E(kcal/mol)
		Spin	M-N	$M-O_{17}$	$M-O_{12}$	$M-O_{14}$	$M-O_{16}$		
Mn^{2+}	gas	H-S	2.23	2.28	2.06	2.18	2.01	37.0	-4331.34
		L-S	2.00	2.03	2.02	1.99	1.92	25.1	-4297.43
	solvent	H-S	2.22	2.22	2.07	2.20	2.03	26.6	-4503.29
Fe^{2+}	gas	H-S	2.19	2.18	2.08	2.08	1.98	33.4	-4301.01
		L-S	1.90	1.99	1.95	1.98	1.93	14.7	-4284.17
	solvent	H-S	2.17	2.12	2.08	2.08	1.98	28.4	-4473.42
		L-S	1.90	1.97	1.94	1.97	1.92	13.4	-4460.66
Co^{2+}	gas	H-S	2.10	2.17	2.01	2.09	1.97	35.0	-4274.47
		L-S	2.07	1.96	1.93	1.96	1.92	14.0	-4272.86
	solvent	H-S	2.07	2.13	2.01	2.09	1.95	23.4	-4446.16
		L-S	2.06	1.93	1.93	1.94	1.91	13.7	-4447.09
Ni^{2+}	gas		2.03	2.15	2.01	2.08	1.95	28.4	-4214.55
	solvent		2.00	2.08	2.00	2.08	1.96	20.0	-4388.50
Cu^{2+}	gas		2.23	2.07	2.01	2.03	1.95	30.2	-4162.18
	solvent		2.17	2.02	1.99	2.03	1.95	22.2	-4333.75
Zn^{2+}	gas		2.11	2.34	2.00	2.15	1.93	41.6	-4145.21
	solvent		2.09	2.21	2.00	2.17	1.95	31.6	-4316.91

Table S3: *Topological data for the BCPs of coordination bonds in the GLDA-M complexes (B structure) when (M= Mn, Fe, Co, Ni, Cu and Zn)*

Complexes	PC	ρ(r)	∇^2 ρ(r)	|V|/G	H(r)
GLDA-Mn	Mn-O_{16}	0.065	0.3137	1.0983	-0.0085
	Mn-O_{14}	0.051	0.2210	1.0849	-0.0051
	Mn-O_{12}	0.060	0.2705	1.0977	-0.0073
	Mn-O_{17}	0.051	0.2214	1.0852	-0.0052
	Mn-N	0.054	0.1911	1.1628	-0.0093
	Mn-O_{29}	0.041	0.1781	1.0502	-0.0024
	H_{27}-H_{20}	0.016	0.0560	0.8737	0.0016
GLDA-Fe	Fe-O_{16}	0.059	0.4255	1.0486	-0.0054
	Fe-O_{14}	0.065	0.4161	1.0799	-0.0090
	Fe-O_{12}	0.059	0.5226	1.0483	-0.0066
	Fe-O_{17}	0.063	0.418	1.0827	-0.0094
	Fe-O_{29}	0.043	0.3444	1.0171	-0.0015
	Fe-N	0.059	0.531	1.1299	-0.0198
	H_{20}-H_{27}	0.017	0.0385	0.7863	0.0017
GLDA-Co	Co-O_{16}	0.070	0.3100	1.0746	-0.0062
	Co-O_{14}	0.059	0.2911	1.1073	-0.0087
	Co-O_{12}	0.064	0.3521	1.1062	-0.0105
	Co-O_{17}	0.060	0.2940	1.1048	-0.0086
	Co-O_{29}	0.044	0.2147	1.0518	-0.0029
	Co-N	0.071	0.3114	1.1667	-0.0156
	C-H_{27}	0.006	0.1051	0.9064	0.0022
	H_{27}-H_{20}	0.015	0.0576	0.8945	0.0014
GLDA-Ni	Ni-O_{16}	0.061	0.3287	1.0765	-0.0068
	Ni-O_{14}	0.062	0.3037	1.0989	-0.0083
	Ni-O_{12}	0.068	0.3532	1.1021	-0.0100
	Ni-O_{17}	0.062	0.3079	1.0998	-0.0085
	Ni-N	0.084	0.3494	1.1889	-0.0203
	H_{27}-H_{20}	0.017	0.0559	0.8772	0.0015
	Ni-O_{29}	0.048	0.2455	1.0606	-0.0040
	HO_{19}-O_{16}	0.023	0.0977	0.8874	0.0025
GLDA-Zn	Zn-O_{16}	0.064	0.3132	1.1081	-0.0095
	Zn-O_{14}	0.052	0.2568	1.1011	-0.0072
	Zn-O_{12}	0.061	0.2515	1.1010	-0.0071
	Zn-O_{17}	0.064	0.2073	1.0928	-0.0053
	Zn-N	0.065	0.2308	1.1775	-0.0125
	Zn-O_{29}	0.047	0.1759	1.0605	-0.0028
	H_{20}-H_{27}	0.016	0.0385	0.7863	0.0017

Table S4: *Topological data for the BCPs of coordination bonds in the GLDA-M complexes (A structure) when (M= Mn, Fe, Co, Ni, Cu and Zn)*

Complexes	BCP	ρ(r)	∇^2 ρ(r)	|V|/G	H(r)
GLDA-Mn	Mn-O_{16}	0.075	0.3750	1.1202	-0.0128
	Mn-O_{14}	0.052	0.2115	1.0866	-0.0050
	Mn-O_{12}	0.070	0.3446	1.1205	-0.0118
	Mn-O_{17}	0.050	0.1938	1.0905	-0.0048
	Mn-N	0.060	0.2002	1.1642	-0.0098
	H_{27}-H_{20}	0.016	0.0378	0.8043	0.0015
GLDA-Fe	Fe-O_{16}	0.085	0.4831	1.0740	-0.0097
	Fe-O_{14}	0.067	0.4330	1.0778	-0.0091
	Fe-O_{12}	0.066	0.5376	1.0463	-0.0065
	Fe-O_{17}	0.061	0.4358	1.0803	-0.0095
	Fe-N	0.065	0.5518	1.1512	-0.0246
	H_{20}-H_{27}	0.017	0.0573	0.8834	0.0015
GLDA-Co	Co-O_{16}	0.087	0.4977	1.1175	-0.0166
	Co-O_{14}	0.064	0.4523	1.1075	-0.0136
	Co-O_{12}	0.075	0.4702	1.0934	-0.0121
	Co-O_{17}	0.058	0.4439	1.1119	-0.0140
	Co-N	0.077	0.3127	1.1619	-0.0151
	H_{27}-H_{20}	0.016	0.0434	0.8213	0.0016
GLDA-Ni	Ni-O_{16}	0.081	0.5216	1.1293	-0.0194
	Ni-O_{14}	0.064	0.4817	1.1370	-0.0191
	Ni-O_{12}	0.075	0.4918	1.1297	-0.0183
	Ni-O_{17}	0.063	0.4729	1.1441	-0.0199
	Ni-N	0.089	0.1413	1.1394	-0.0057
	H_{27}-H_{20}	0.018	0.5216	1.1293	-0.0194
GLDA-Cu	Cu-O_{16}	0.083	0.4099	1.1444	-0.0173
	Cu-O_{14}	0.071	0.3112	1.1219	-0.0108
	Cu-O_{12}	0.078	0.3637	1.1369	-0.0144
	Cu-O_{17}	0.073	0.0687	1.1259	-0.0108
	Cu-N	0.062	0.2094	1.1456	-0.0089
	H_{27}-H_{20}	0.017	0.0401	0.7969	-0.0017
GLDA-Zn	Zn-O_{16}	0.084	0.4190	1.1417	-0.0173
	Zn-O_{14}	0.052	0.2015	1.0879	-0.0049
	Zn-O_{12}	0.077	0.3718	1.1361	-0.0146
	Zn-O_{17}	0.048	0.1638	1.0832	-0.0037
	Zn-N	0.074	0.2552	1.1798	-0.0140
	H_{27}-H_{20}	0.017	0.0549	0.8682	0.0016

***Table S5**: RCPs electronic densities GLDA-M complexes where (M= Mn, Co, Fe, Ni, Cu and Zn)*

	B				A			
	Ring1	Ring2	Ring3	Ring4	Ring1	Ring2	Ring3	Ring4
Mn^{2+}	0.0062	0.0208	0.0189	0.0218	0.0065	0.0215	0.0201	0.0225
Fe^{2+}	0.0078	0.0225	0.0209	0.0235	0.0097	0.0233	0.0222	0.0243
Co^{2+}	0.0072	0.0239	0.0222	0.0241	0.0081	0.0241	0.0239	0.0248
Ni^{2+}	0.0071	0.0243	0.0238	0.0251	0.0079	0.0247	0.0248	0.0258
Cu^{2+}					0.0072	0.0224	0.0220	0.0234
Zn^{2+}	0.0064	0.0219	0.0207	0.0226	0.0075	0.0223	0.0227	0.0231

Ring1 :7-member cycle (Metal-Oxygen16-four carbon-Nitrogen),
Ring2 : 5-member cycle (Metal-Oxygen14-two carbon-Nitrogen)
Ring3 : 5-member cycle (Metal-Oxygen12-tow carbon-Nitrogen)
Ring4 : 5-member cycle (Metal-Oxygen17-tow carbon-Nitrogen)

***Table S6:** Selected geometrical parameters of hydrated ions in octahedral geometry*

	Ionic radius [48]	M-O equatorial	M-O axial	Exp[a]
Mn	0.830	2.205	2.206	2.175
Fe	0.780	2.144	2.161	2.126
Co	0.745	2.117	2.109	2.092
Ni	0.690	2.086	2.087	2.056
Cu	0.730	2.038	2.350	1.97 and 2.3
Zn	0.740	2.123	2.123	2.092

[a]*RalfAkesson, Lars G. M. Pettersson, Magnus Sandstrom, and Ulf Wahlgred « Ligand Field Effects in the Hydrated Divalent and Trivalent Metal Ions of the First and Second Transition Periods » J. Am. Chem.Soc. 116 (1994) 8691-8704.*

***Table S7:** Energies and free energy of the 4 $HGLDA^{3-}$ isomers (kcal/mol)*

	Free energy		E	
	gas	solvent	gas	solvent
$O16(HGLDA)^{3-}$	-3979.13	-4343.33	-4065.97	-4433.63
$O12(HGLDA)^{-3}$	-3990.43	-4342.85	-4076.64	-4433.05
$O14(HGLDA)^{-3}$	-3997.95	-4343.59	-4084.41	-4433.85
$O17(HGLDA)^{-3}$	-4001.23	-4341.81	-4089.80	-4432.98
$(GLDA)^{-4}$	-3762.62	-4347.38	-3842.51	-4431.28
$N(HGLDA)^{3-}$	-4021.98	-4360.98	-4110.56	-4451.94

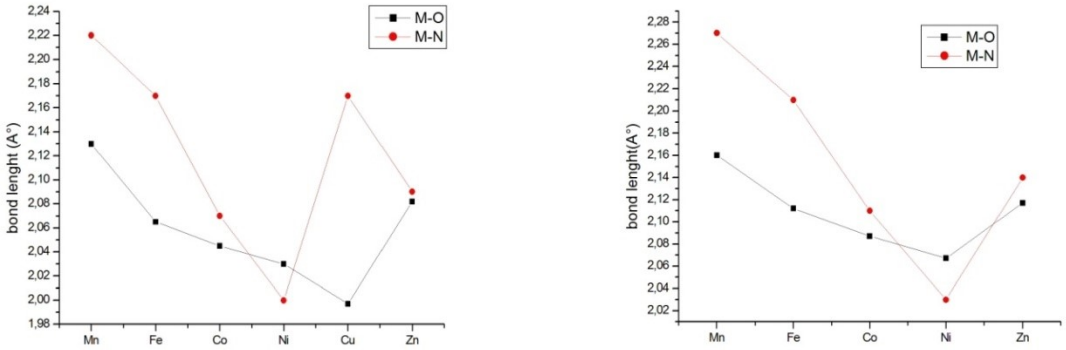
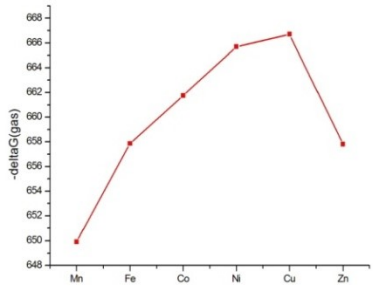


Fig. S1: *Dependence of M-O and M-N bond length with the late first-row transition series divalent metal ions for A and B structures, respectively. Both graphs agree with the Irving-Williams series.*

1



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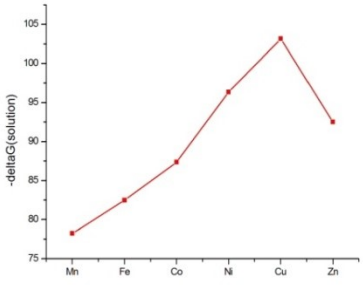

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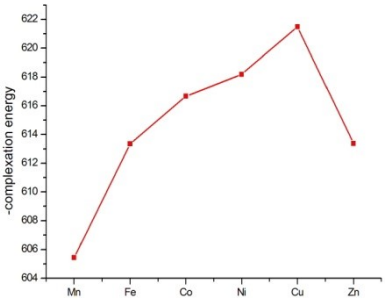

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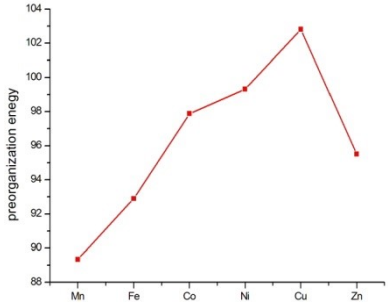

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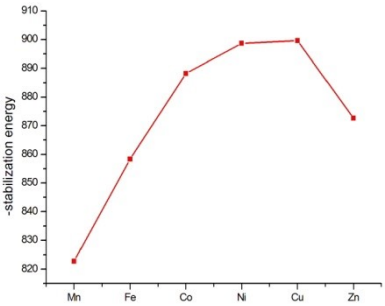

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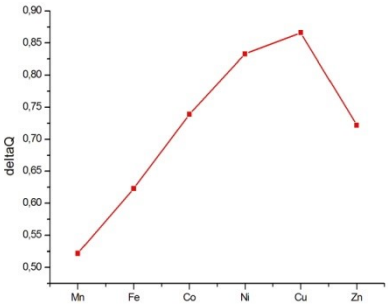

Fig. S2: *Dependence of DFT calculated 1,2 free energy both in gas phase and solution respectively, 3 complexation energy, 4 preorganization energy, 5 stabilization energy and 6 GLDA-metal charge transfer ΔQ on the atomic number of the late first-row transition series divalent metal ions for pentadentate complexes. All the graphs agree with the Irving-Williams series.*

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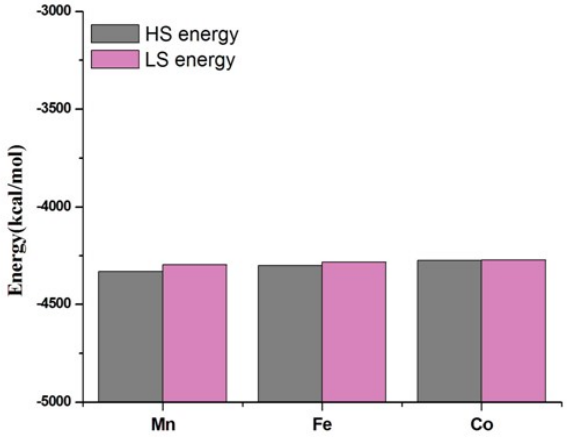


Fig. S3: *Stability of HS complexes compared to LS ones (A structure)*

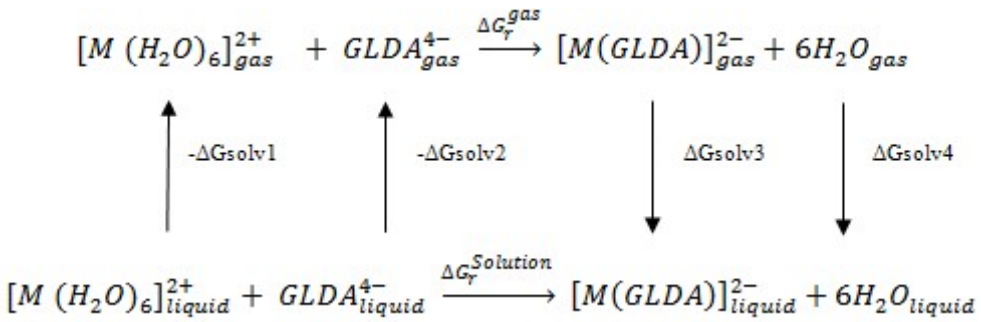


Fig. S4: *The thermodynamic cycle used for the complexation of the metal ion*

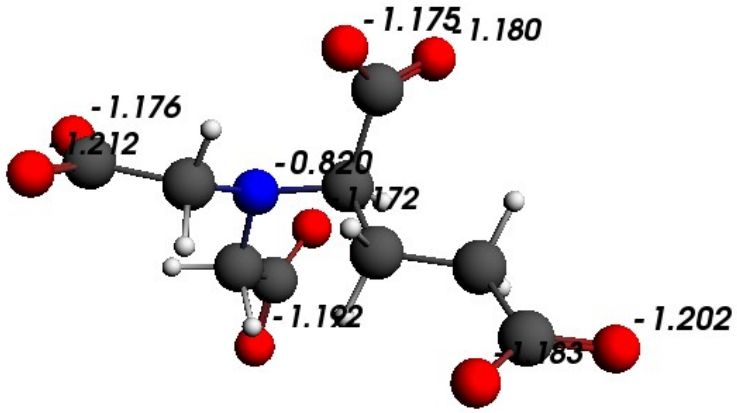


Fig. S5*: GLDA^{4-} Bader charges*

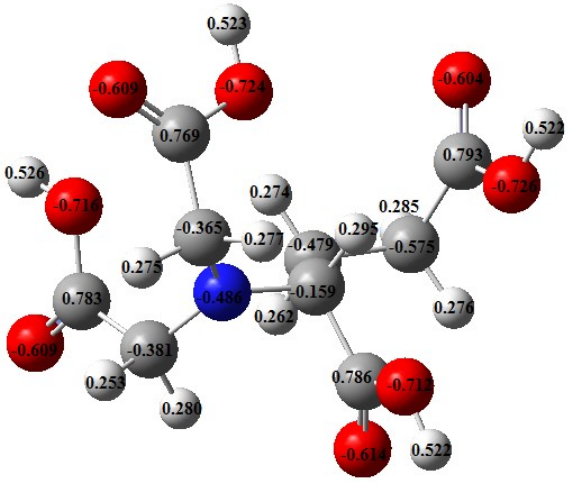


Fig. S6: *GLDA^{4-} NPA numerical charges*

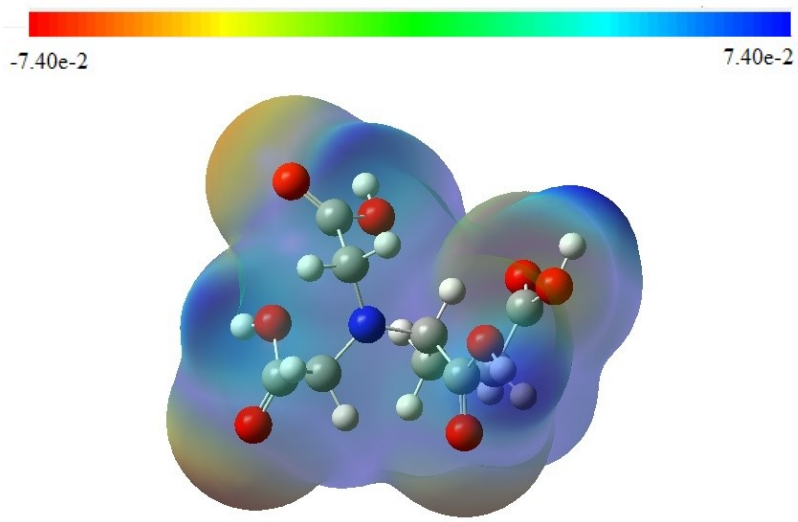


Fig. S7: *GLDA^{4-} MEPS. The largest negative values are depicted in red, the lowest in blue.*

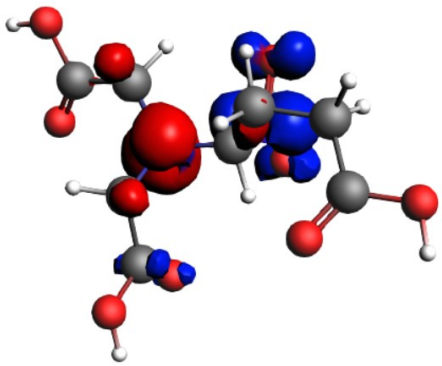


Fig. S8: *GLDA^{4-} Dual descriptors with Negative regions are colored red and positive regions are colored blue.*

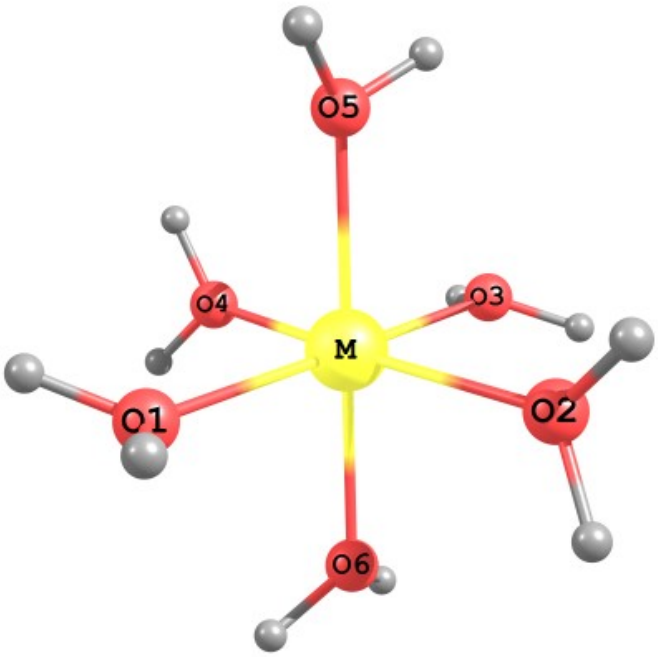


Fig. S9*: Optimized octahedral geometry of hydrated ions with M= Mn, Fe, Co, Ni, Cu and Zn*

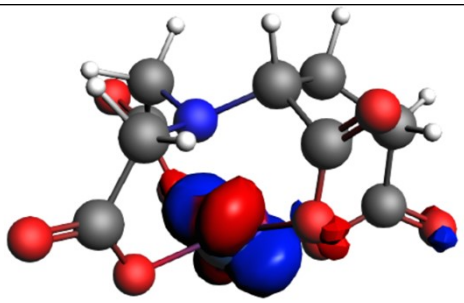
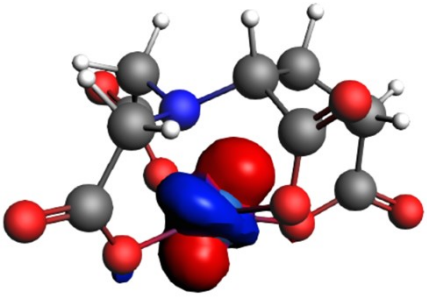
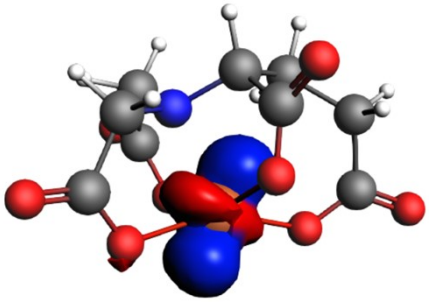
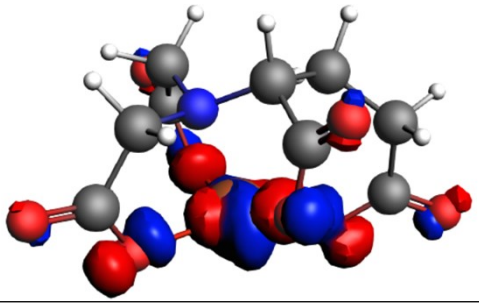
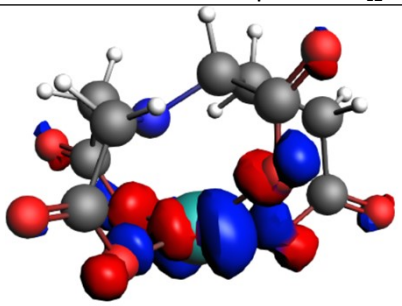
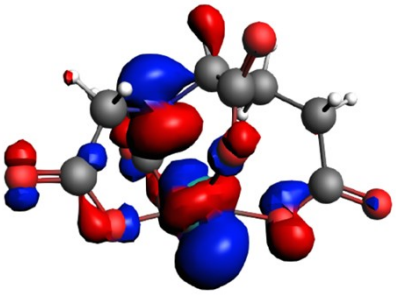
Co		
	HOMO 57β 33.4% d_{yz} 23.9%d_{x2-y2}	HOMO-1 44.3% d_{xy} 35% d_{z2}
Fe		
	HOMO 56β41.5% d_{z2}	HOMO-1 60α 28.6% dxy
Mn		
	HOMO 58α 41.8% d_{x2-y2}	HOMO-1 57α 44.4% d_{z2}

***Fig. S10**: occupancy of HOMO and HOMO-1 of HS complexes*