Support information

BTLYP

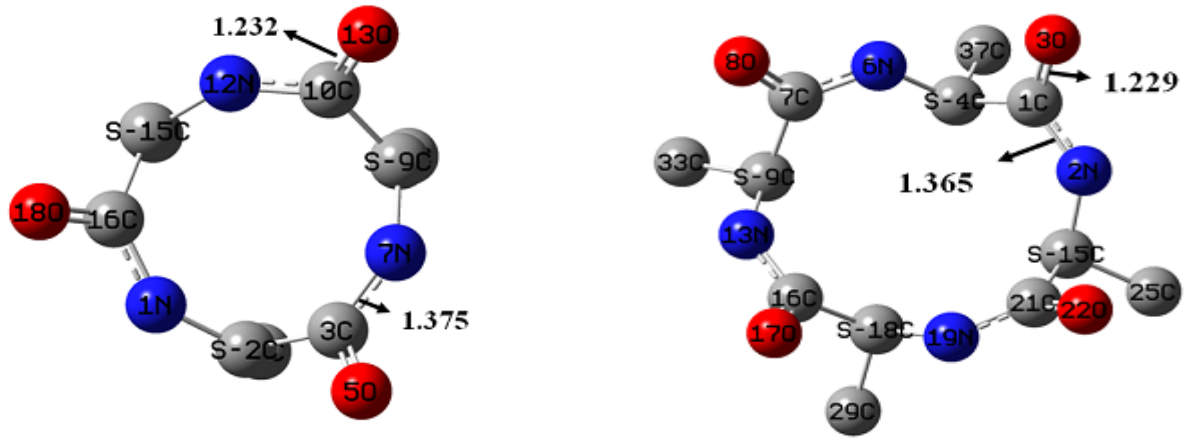

Figure.S1. The optimized structures of **CyAla3** and **CyAla4** obtained at the B3LYP/6–31+G(d) levels of theory (H atoms are omitted for clarity).

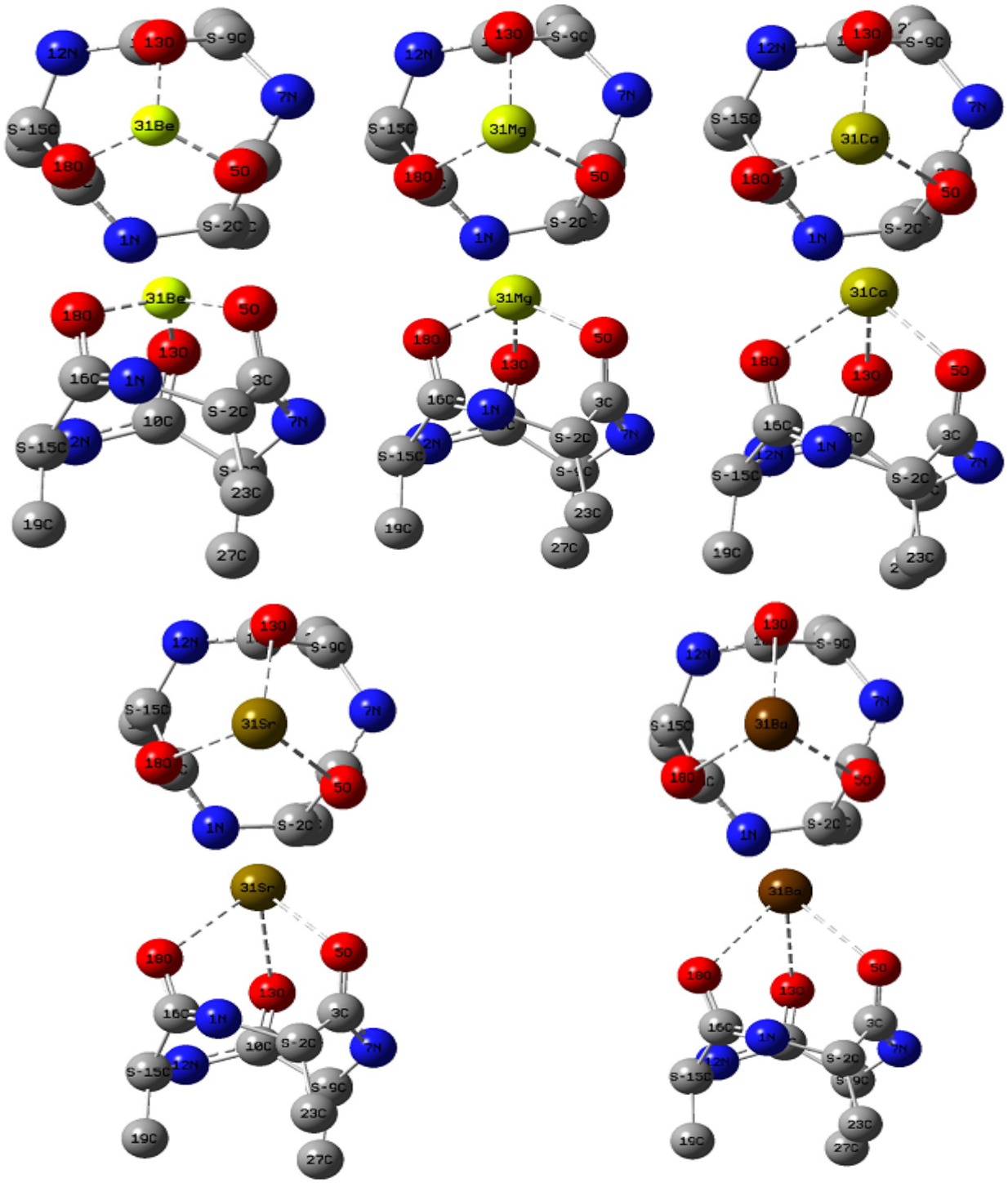

Figure S.2. Optimized structures and important geometrical parameters of M/**CyAla3** complexes calculated at the B3LYP level of theory, M= Be^{2+}, Mg^{2+}, Ca^{2+},Sr^{2+} and Ba^{2+} .

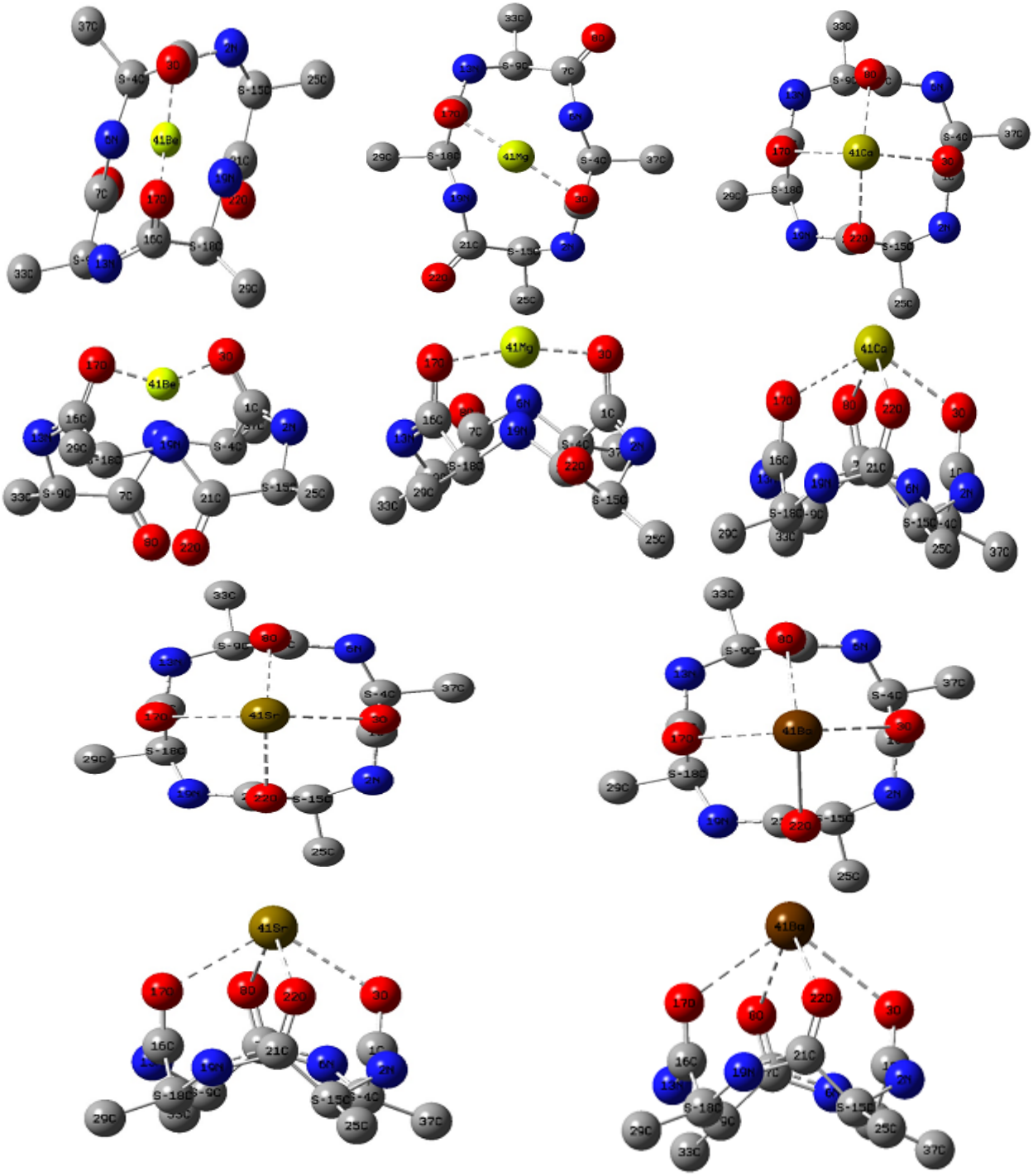

Figure S.3. Optimized structures and important geometrical parameters of M/**CyAla4** complexes calculated at the B3LYP level of theory, M= Be^{2+}, Mg^{2+}, Ca^{2+},Sr^{2+} and Ba^{2+} .

Table S.1

The selected geometrical parameters of M/**CyAla3** complexes calculated at the B3LYP/6-31+G(d) level of theory.

M/CyAla3	C-C(=O)	C-C(H3)	N-H	φ 8-7-3-5	φ 14-12-10-13	φ 6-1-16-18	C=O	C(=O)-N
CyAla3	1.547	1.533	1.015	-4.6	-4.8	-4.8	1.231	1.374
Be^{2+}	1.541	1.520	1.023	23.6	23.5	23.5	1.283	1.357
Mg^{2+}	1.545	1.522	1.021	19.6	19.6	19.6	1.269	1.361
Ca^{2+}	1.546	1.523	1.019	17.1	17.9	17.9	1.259	1.367
Sr^{2+}	1.547	1.524	1.019	16.8	16.8	16.8	1.254	1.369
Ba^{2+}	1.547	1.525	1.019	15.7	15.7	15.6	1.252	1.371

Bond lengths are in Å, diheral angles in degree (H-N-C=O),. All distances are identical in each complexes and in free CyAla3. and are not averaged

Table S.2

The selected geometrical parameters of M/**CyAla4** complexes calculated at the B3LYP level of theory

M/CyAla4	C-C(=O)	C-(CH3)	N-H	φ 12-2-1-3	φ11-6-7-8	φ14-13-16-17	φ20-19-21-22	C=O	C(=O)-N
CyAla4	1.546[a]	1.535	1.018	6.6	4.6	6.5	4.6	1.229	1.365
Be^{2+}	(1.195)[b] 1.286	1.538	1.025	-14.8	119.3	-14.8	119.9	(1.195)[b] 1.286	(1.508)[b] 1.327
Mg^{2+}	(1.558) 1.531	1.533	1.025	-12.0	1.5	-11.1	1.52	(1.191)[b] 1.261	(1.481)[b] 1.337
Ca^{2+}	1.545	1.539	1.022	-13.9	-13.9	-13.9	-13.9	1.250	1.366
Sr^{2+}	1.546	1.539	1.020	-12.2	-12.2	-12.2	-12.2	1.248	1.366
Ba^{2+}	1.546	1.539	1.021	-10.1	-10.1	-10.1	-10.9	1.246	1.366

Bond lengths in Å, diheral angles in degree (H-N-C=O), [a] the average value, [b] the values in parenthesis are the distance between metal ions and faraway atoms.