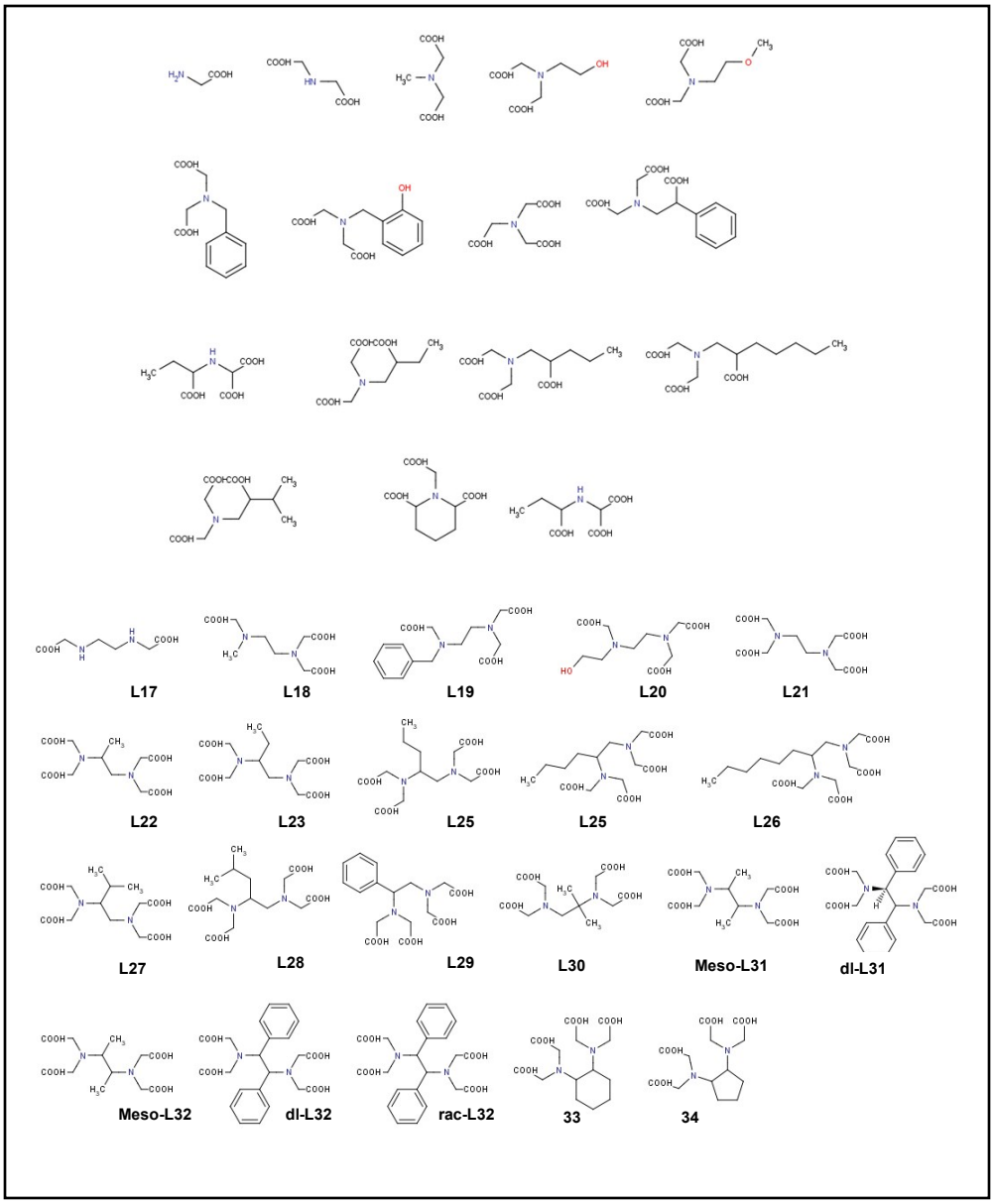
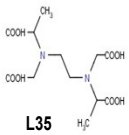
Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Figure S1: Structures of acyclic polyamino-polycarboxylic ligands





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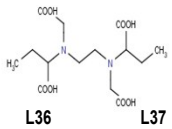

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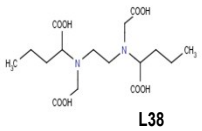

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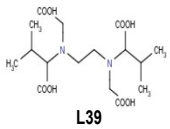

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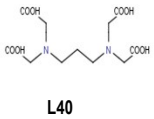

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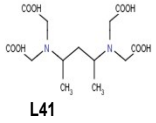

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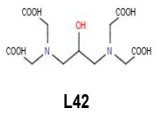

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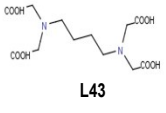

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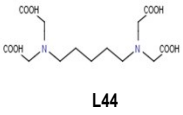

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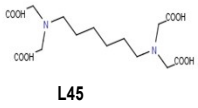

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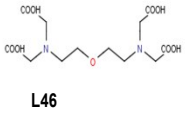

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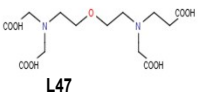

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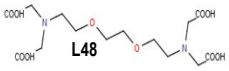

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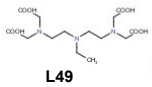

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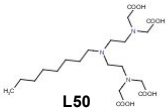

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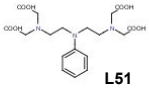

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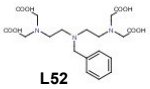

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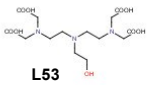

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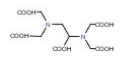

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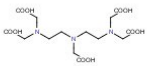

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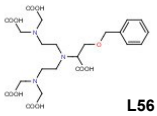

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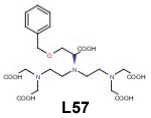

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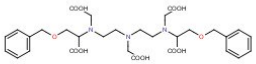

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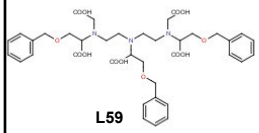

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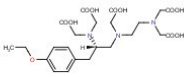

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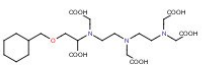

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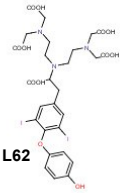

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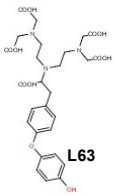

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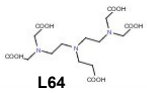

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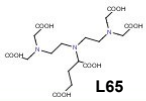

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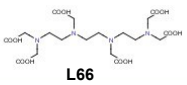

L66

Table S1: Glide XP docking, Binding affinity and Log K_{HSA} values of acyclic polyamino-polycarboxylic ligands with 1H9Z.

Molecules	XP G Score (kcal/mol)	Binding Affinity(kcal/mol in relative terms)	QPlog K_{HSA}
L1	-2.44	-11.83	-1.106
L2	-4.08	-13.51	-1.245
L3	-2.80	-18.51	-1.25
L4	-4.32	-22.93	-1.336
L5	-2.95	-27.88	-1.347
L6	-5.35	-33.15	-0.952
L7	-4.95	-28.87	-1.034
L8	-4.89	-27.11	-1.47
L9	-5.50	-32.23	-1.206
L10	-4.02	-17.21	-1.392
L11	-4.03	-22.25	-1.355
L12	-4.21	-26.51	-1.335
L13	-4.89	-37.71	-1.233
L14	-4.54	-23.33	-1.287
L15	-4.61	-23.43	-1.23
L16	-4.36	-24.36	-1.233
L17	-4.15	-24.34	-1.3
L18	-4.04	-25.97	-1.581
L19	-7.51	-40.95	-1.321
L20	-7.18	-24.95	-1.722
L21	-3.99	-19.30	-1.841
L22	-5.81	-27.22	-1.697
L23	-5.57	-31.93	-1.774
L24	-5.93	-28.523	-1.676
L25	-7.06	-47.71	-1.618
L26	-5.52	-27.56	-1.744
L27	-5.94	-36.92	-1.7
L28	-6.79	-38.85	-1.631
L29	-6.99	-40.22	-1.609
L30	-4.99	-29.80	-1.617
Meso-L31	-5.58	-34.21	-1.612
dl-L31	-5.01	-34.22	-1.668
Meso-L32	-7.48	-38.99	-1.612
Rac-L32	-8.12	-39.11	-1.612
dl-L32.mol	-6.63	-40.89	-1.612
L33	-5.45	-20.90	-1.664
L34	-5.15	-25.62	-1.565
L35	-5.91	-25.55	-1.492
L36	-5.59	-31.20	-1.821
L37	-6.08	-35.31	-1.658
L3	-7.11	-45.62	-1.919
L39	-4.70	-23.68	-1.783

Molecules	XP G Score (kcal/mol)	Binding Affinity(kcal/mol in relative terms)	QPlog K_{HSA}
L40	-5.47	-22.98	-1.736
L41	-6.05	-19.60	-1.998
L42	-4.70	-22.98	-1.979
L43	-3.54	-12.32	-1.975
L44	-2.03	-18.04	-1.959
L45	-4.91	-18.77	-1.531
L46	-6.80	-37.40	-1.709
L47	-3.65	-21.07	-2.066
L48	-4.89	-27.55	-2.05
L49	-6.34	-39.40	-2.322
L50	-4.65	-42.36	-2.187
L51	-6.84	-31.76	-2.191
L52	-5.45	-19.64	-2.028
L53	-4.77	-15.20	-1.978
L54	-5.69	-24.28	-2.071
L55	-5.30	-57.34	-1.677
L56	-8.46	-57.36	-2.299
L57	-10.42	-68.10	-2.566
L58	-10.67	-68.11	-2.716
L59	-7.80	-51.55	-1.512
L60	-7.86	-72.76	-2.13
L61	-8.13	-44.89	-1.711
L62	-9.07	-66.59	-1.718
L63	-6.54	-34.92	-2.57
L64	-6.38	-30.83	-2.72
L65	-6.87	-36.82	-2.72
L66	-6.17	-35.71	-2.78

Table S2: Glide XP docking, binding affinity and Khsa values of acyclic polyamino-polycarboxylic ligands with 1E7A

Molecules	XP G Score (kcal/mol)	Binding Affinity(kcal/mol in relative terms)	QPlog Khsa
L1	-1.53	-7.84	-1.11
L2	-3.29	-18.35	-1.25
L3	0.37	-18.4	-1.25
L4	-3.47	-26.06	-1.34
L5	-3.71	-26.81	-1.35
L6	-6.32	-24.44	-0.95
L7	-6.36	-32.01	-1.03
L8	0.24	-1.16	-1.47
L9	-3.58	-29.01	-1.21

Molecules	XP G Score (kcal/mol)	Binding Affinity(kcal/mol in relative terms)	QPlog Khsa
L10	-3.17	-27.55	-1.39
L11	-4.51	-31.29	-1.36
L12	-4.32	-25.58	-1.34
L13	-2.45	-44.15	-1.23
L14	-4.63	-35.61	-1.29
L15	-3.76	-13.46	-1.23
L16	-5.12	-12.81	-1.23
L17	-4.01	-33.45	-1.3
L18	-4.16	-30.8	-1.58
L19	-5.29	-40.7	-1.32
L20	-1.6	-37.7	-1.72
L21	-4.24	-18.27	-1.84
L22	-6.36	-31.41	-1.7
L23	-3.32	-22.45	-1.77
L24	-3.69	-22.2	-1.68
L25	-4.89	-42.06	-1.62
L26	-3.32	-18.08	-1.74
L27	-3.3	-10.35	-1.7
L28	-4.39	-13.55	-1.63
L29	-5.26	1.19	-1.61
L30	-2.3	-31.35	-1.62
Meso-L31	-5.93	-24.99	-1.71
dl-L31	-4.66	-16.64	-1.72
Meso-L32	-8.23	-48.11	-1.612
Rac-L32	-8.74	-47.10	-1.612
dl-L32.mol	-8.62	-43.21	-1.612
L33	-3.4	1.35	-1.61
L34	-2.16	-23.04	-1.67
L35	-4.34	-26.91	-1.492
L36	-3.98	-24.86	-1.66
L37	-3.68	-29.49	-1.57
L38	-4.1	-45.03	-1.49
L39	-2.84	-25.39	-1.82
L40	-2.95	-27.13	-1.66
L41	-4.91	-21.98	-1.92
L42	-1.32	-31.83	-1.82
L43	-1.21	-30.12	-1.78
L44	-1.53	-30.26	-1.74
L45	-4.54	-34.71	-2
L46	-2.43	-54.13	-1.98

Molecules	XP G Score (kcal/mol)	Binding Affinity(kcal/mol in relative terms)	QPlog Khsa
L47	-1.99	-38.36	-1.98
L48	-4.9	-24.36	-1.96
L49	-6.97	-37.11	-2.322
L50	-6.42	-36.89	-2.187
L51	-1.47	-34.87	-1.71
L52	-2.89	-22.57	-2.07
L53	-5.02	-24.78	-2.05
L54	-5.03	-30.78	-2.32
L55	-5.74	-52.63	-2.19
L56	-6.2	-48.83	-2.19
L57	-4.41	-45.18	-2.03
L58	-8.97	-48.99	-2.716
L59	-5.9	-16.74	-1.98
L60	-6.23	-50.56	-2.07
L61	-8.47	-48.26	-1.68
L62	-4.05	-45.65	-2.3
L63	-5.74	-17.25	-2.57
L64	-4.28	-35.33	-2.72
L65	-4.23	-32.12	-2.72
L66	-4.78	-32.98	-2.78

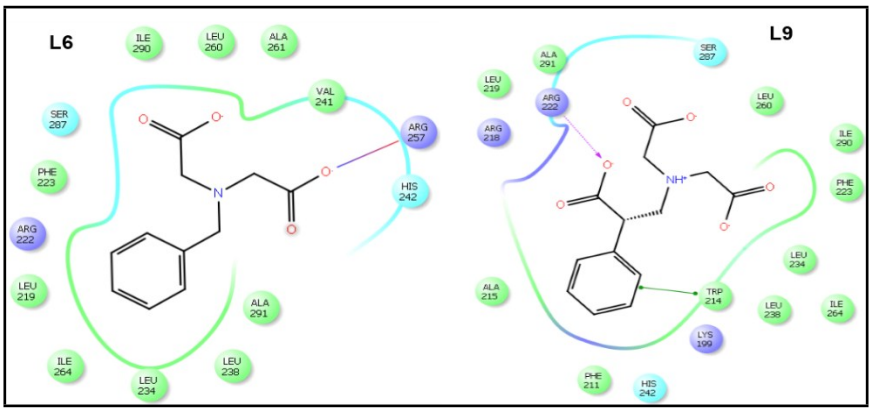

Figure S2: 2D ligand interaction diagram of L6-1H9Z and L9-1H9Z.

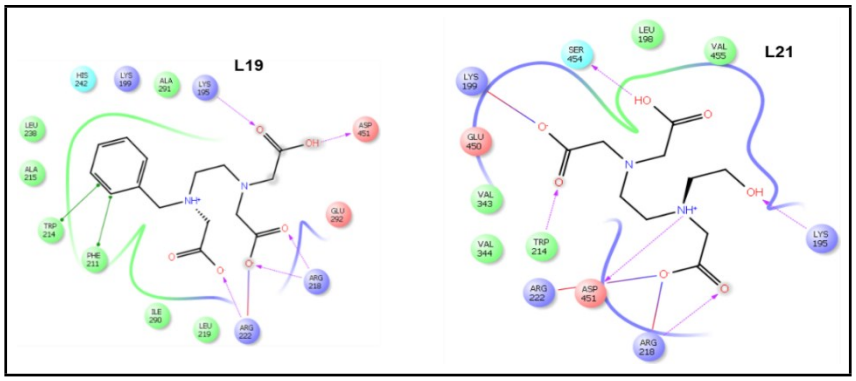

Figure S3: 2D ligand interaction diagram of L19-1H9Z and L21-1H9Z.

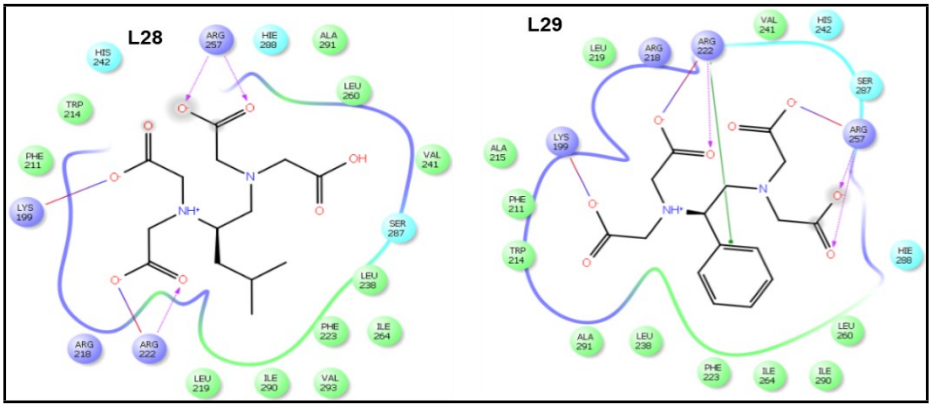

Figure S4: 2D ligand interaction diagram of L28-1H9Z and L29-1H9Z.

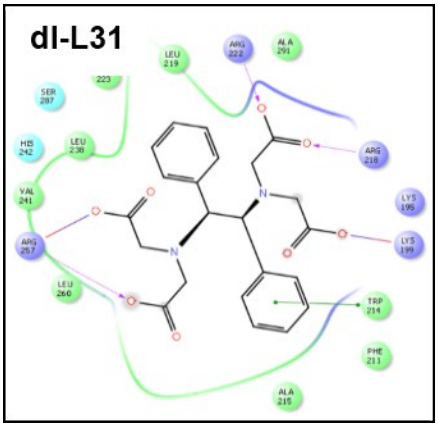

Figure S5: 2D ligand interaction diagram of dl-L31-1H9Z.

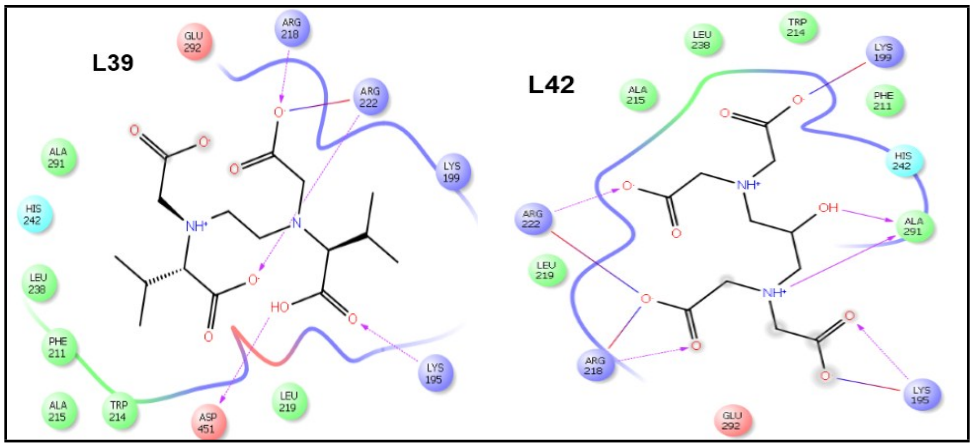

Figure S6: 2D ligand interaction diagram of L39-1H9Z and L42-1E7A.

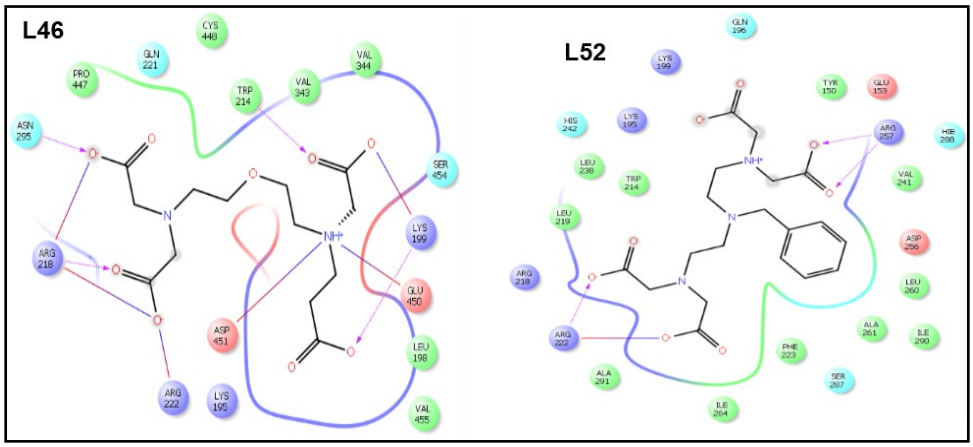

Figure S7: 2D ligand interaction diagram of L46-1H9Z and L52-1H9Z.

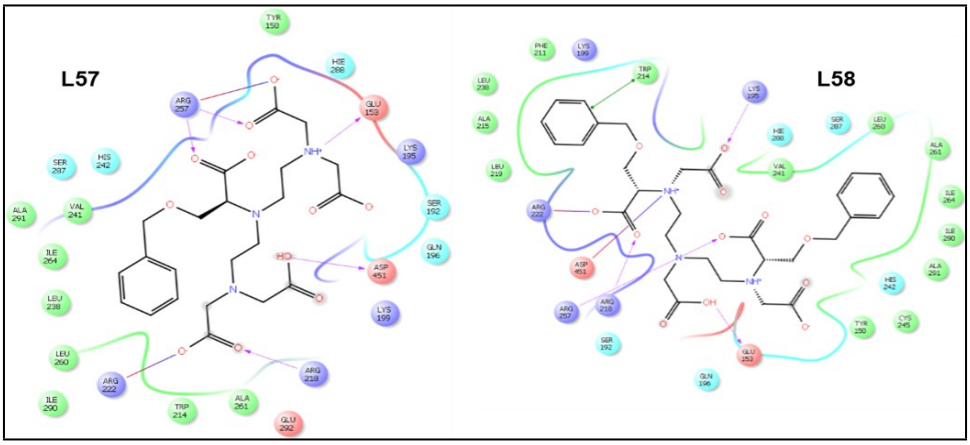

Figure S8: 2D ligand interaction diagram of L57-1H9Z and L58-1H9Z.

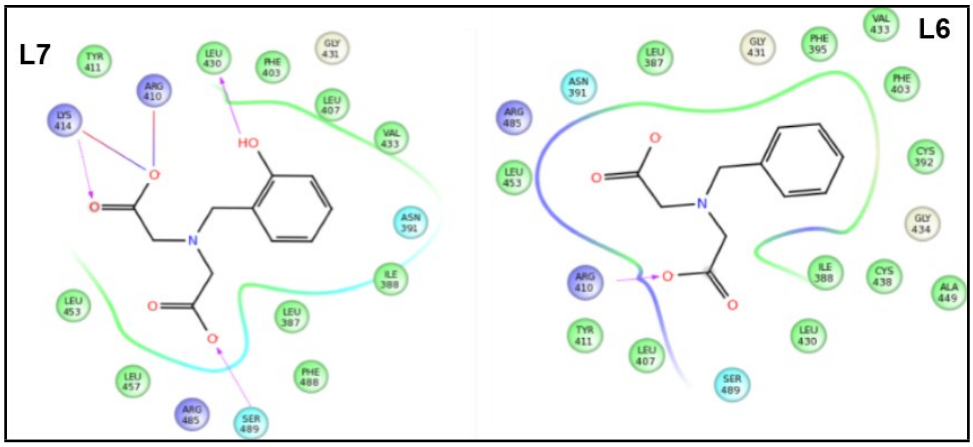

Figure S9: 2D ligand interaction diagram of L6-1E7A and L9-1E7A.

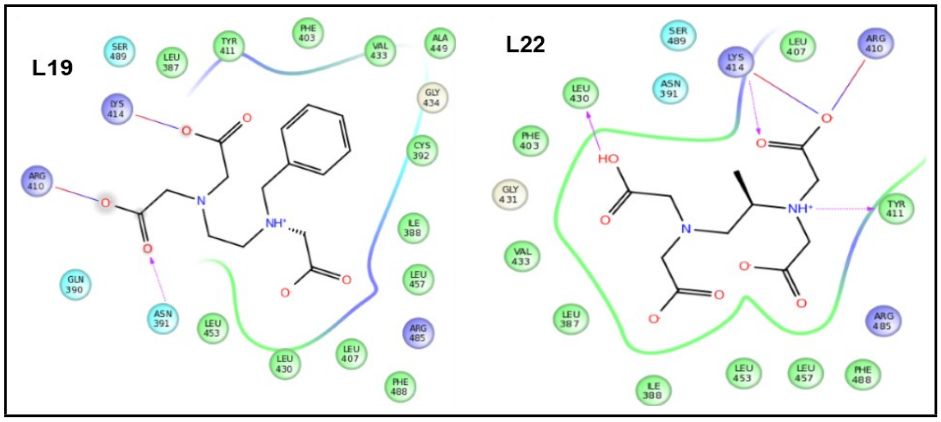

Figure S10: 2D ligand interaction diagram of L19-1E7A and L22-1E7A.

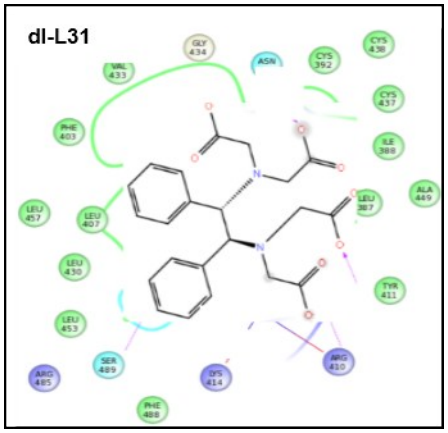

Figure S11: 2D ligand interaction diagram of dl-L31-1E7A.

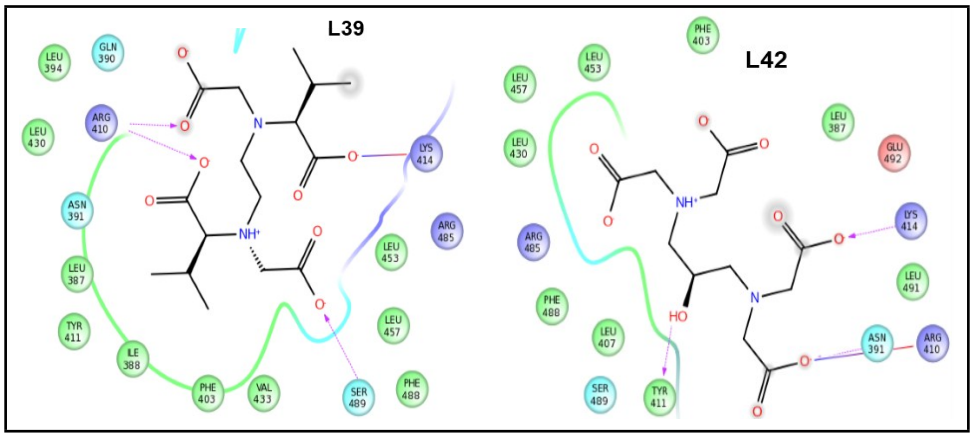

Figure S12: 2D ligand interaction diagram of L39-1E7Aand L42-1E7A.

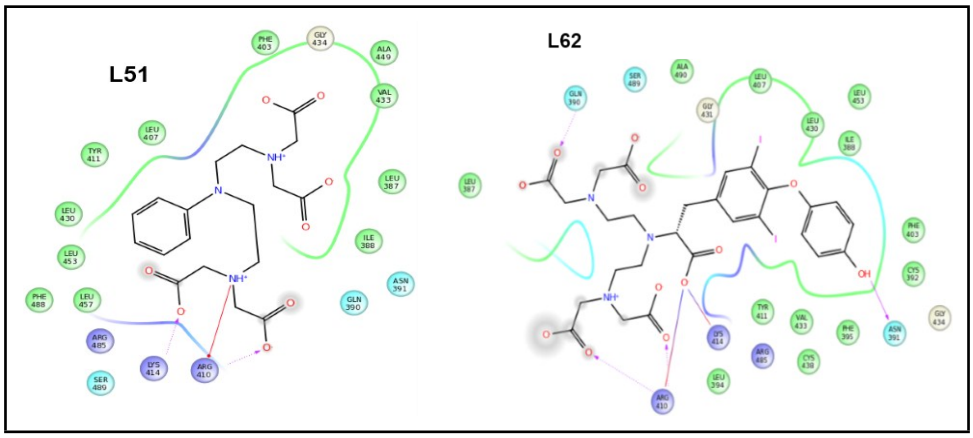

Figure S13: 2D ligand interaction diagram of L51-1E7Aand L62-1E7A.