Supplementary Information

Single crystal investigation, spectroscopic, DFT studies, and *in-silico* molecular docking of the anticancer activities of acetylacetone coordinated Re(I) tricarbonyl complexes

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1. ^{1}H and ^{13}C NMR spectra (**Figure SI1, SI2 (a, b)**)
2. IR spectra of the complexes (**Figure SI3, SI4**)
3. UV/Vis spectra of complexes (**Figure SI5, SI6**)
4. Crystallographic data (**Tables SI1, SI2)**
5. SCXRD Packing diagrams and Hydrogen bonding diagram (**Figures SI3, SI4**)
6. Geometrical Parameters of (R)-d,d imidazole and 2-M1λ2,3λ2 imidazole (**Table SI3**)
7. Visualized active pocket of the known complexed inhibitors with 2yw6 and 5w9d (**Figure SI 7**)
8. Superimposed lowest binding conformations of the known inhibitors after redocking experiments (**Figure SI 8**)

^{1}H and ^{13}C spectra for Re-1 and Re-2

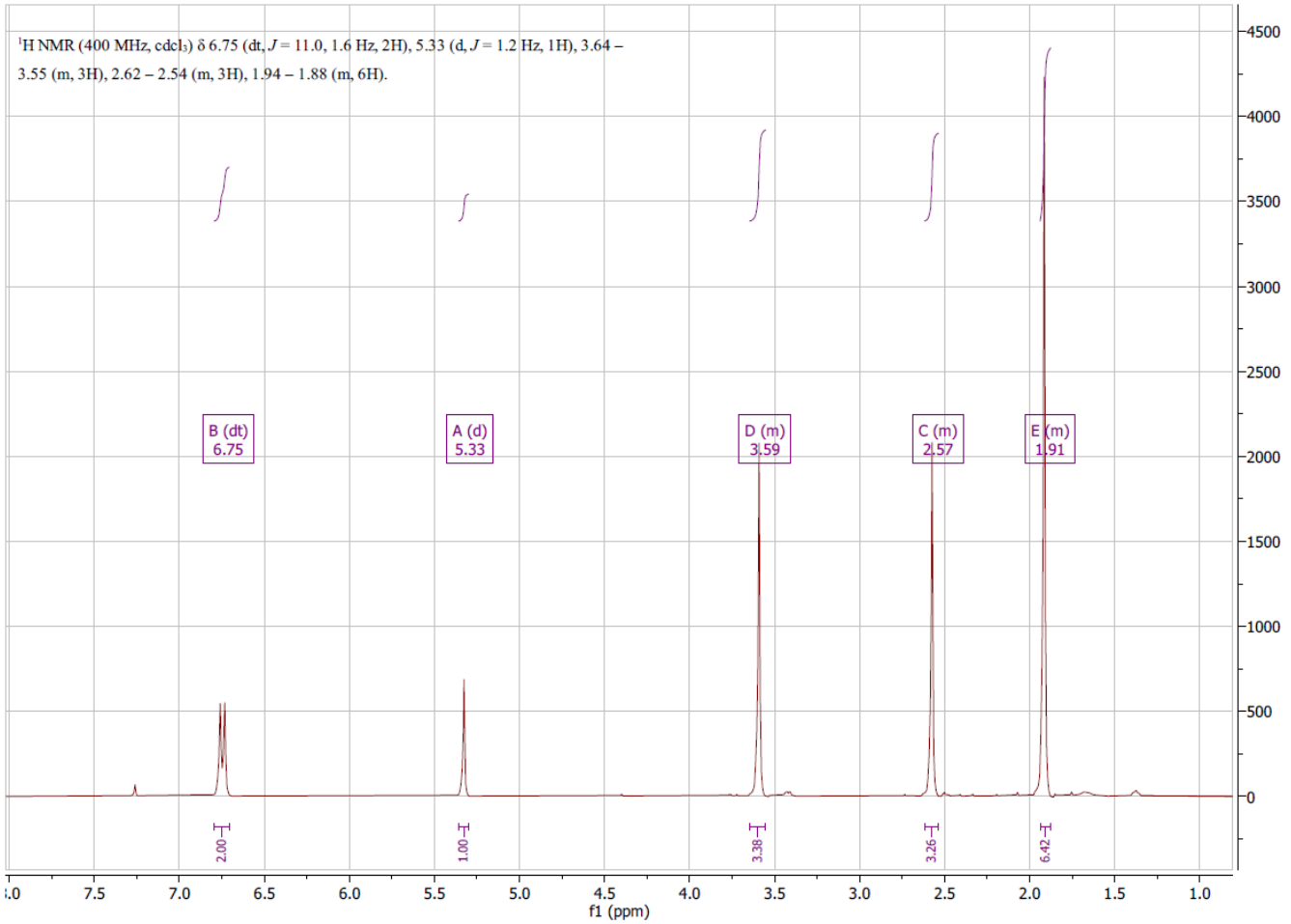


Figure SI 1a: ^{1}H NMR spectrum of **Re-1**

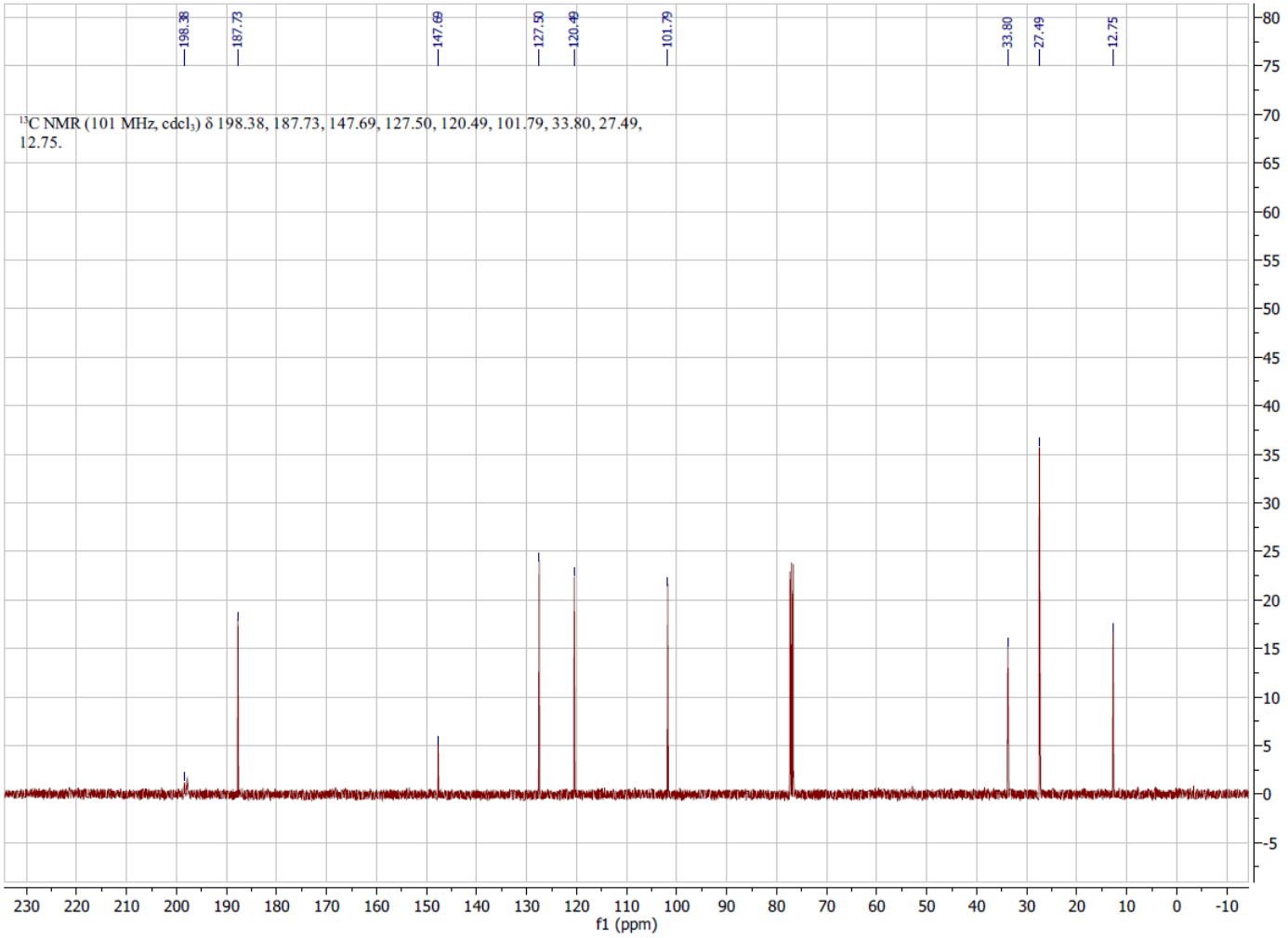


Figure SI 1b: ^{13}C NMR spectrum of **Re-1**

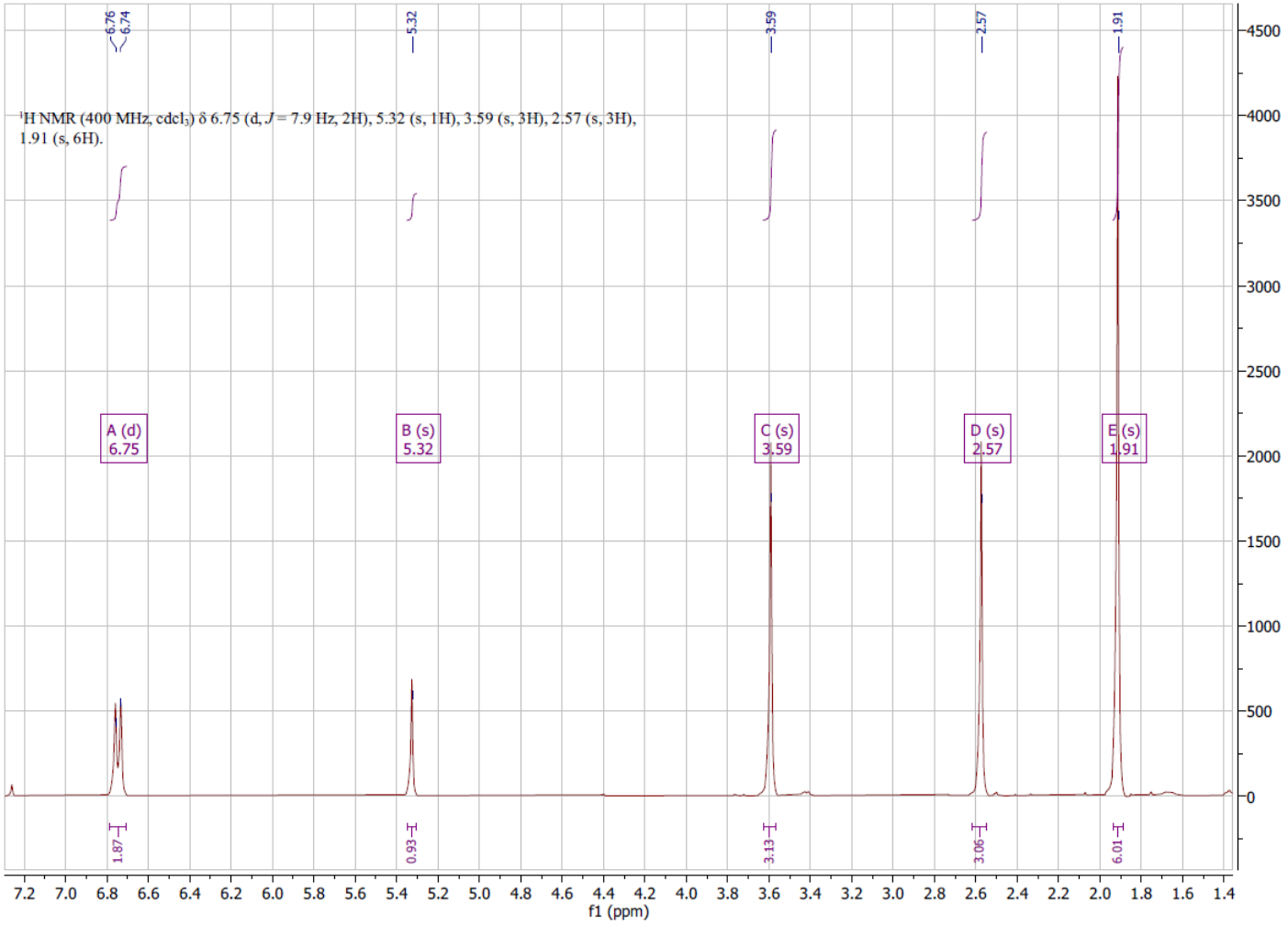


Figure SI 2a: ^{1}H NMR spectrum of **Re-2**

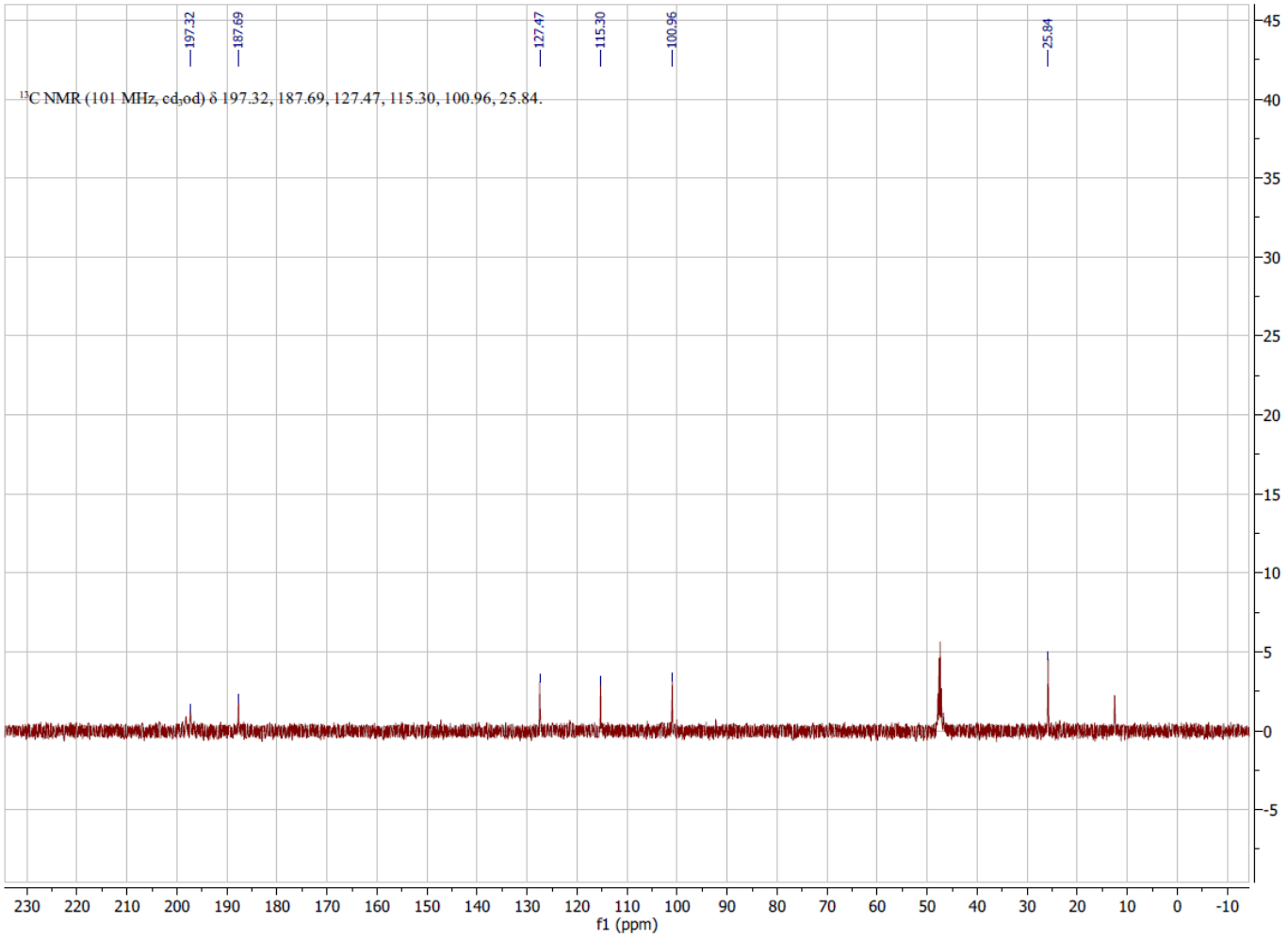


Figure SI 2b: ^{13}C NMR spectrum of **Re-2**

IR spectra of Re-1 and Re-2

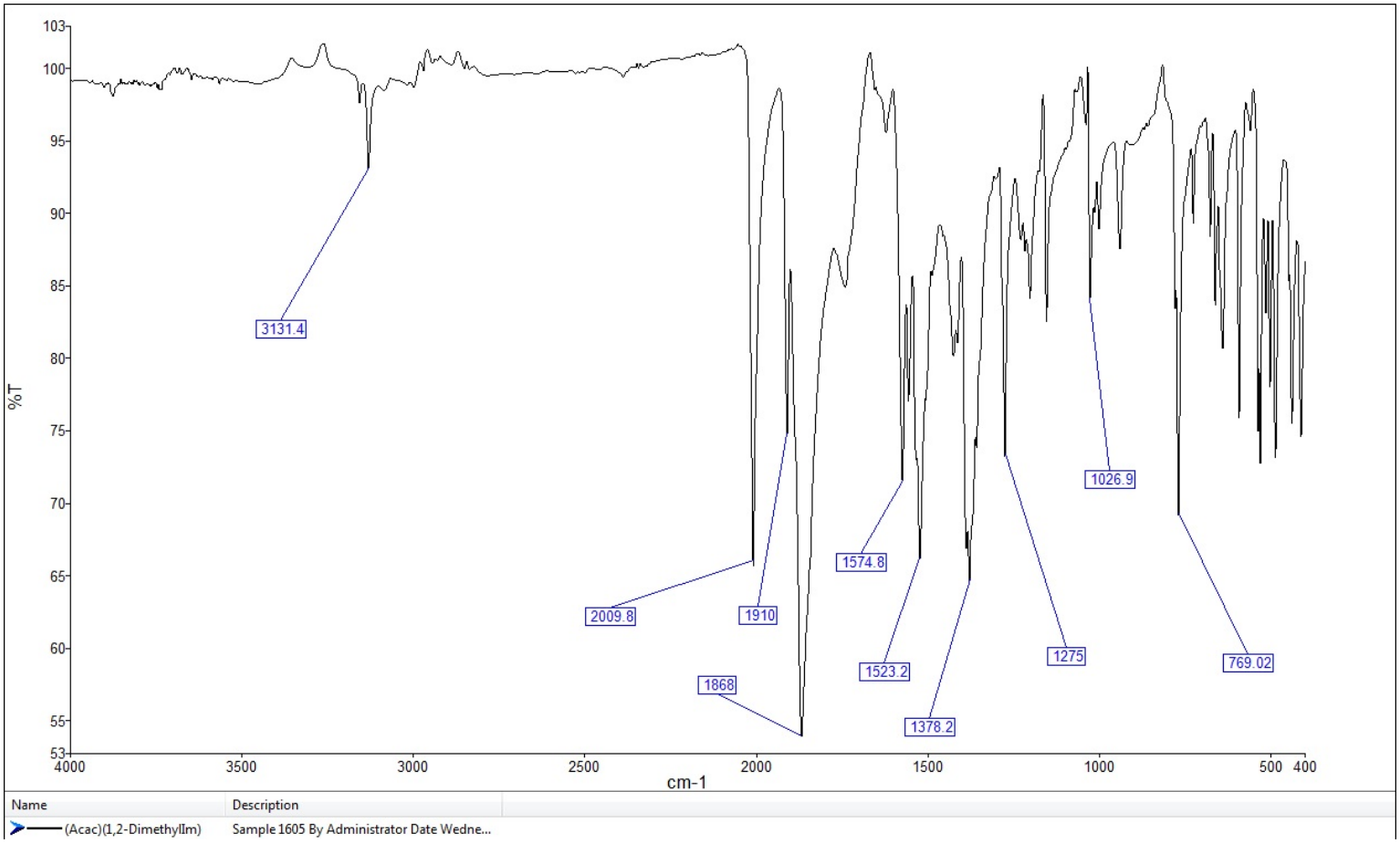


Figure SI 3: IR spectrum of **Re-1**

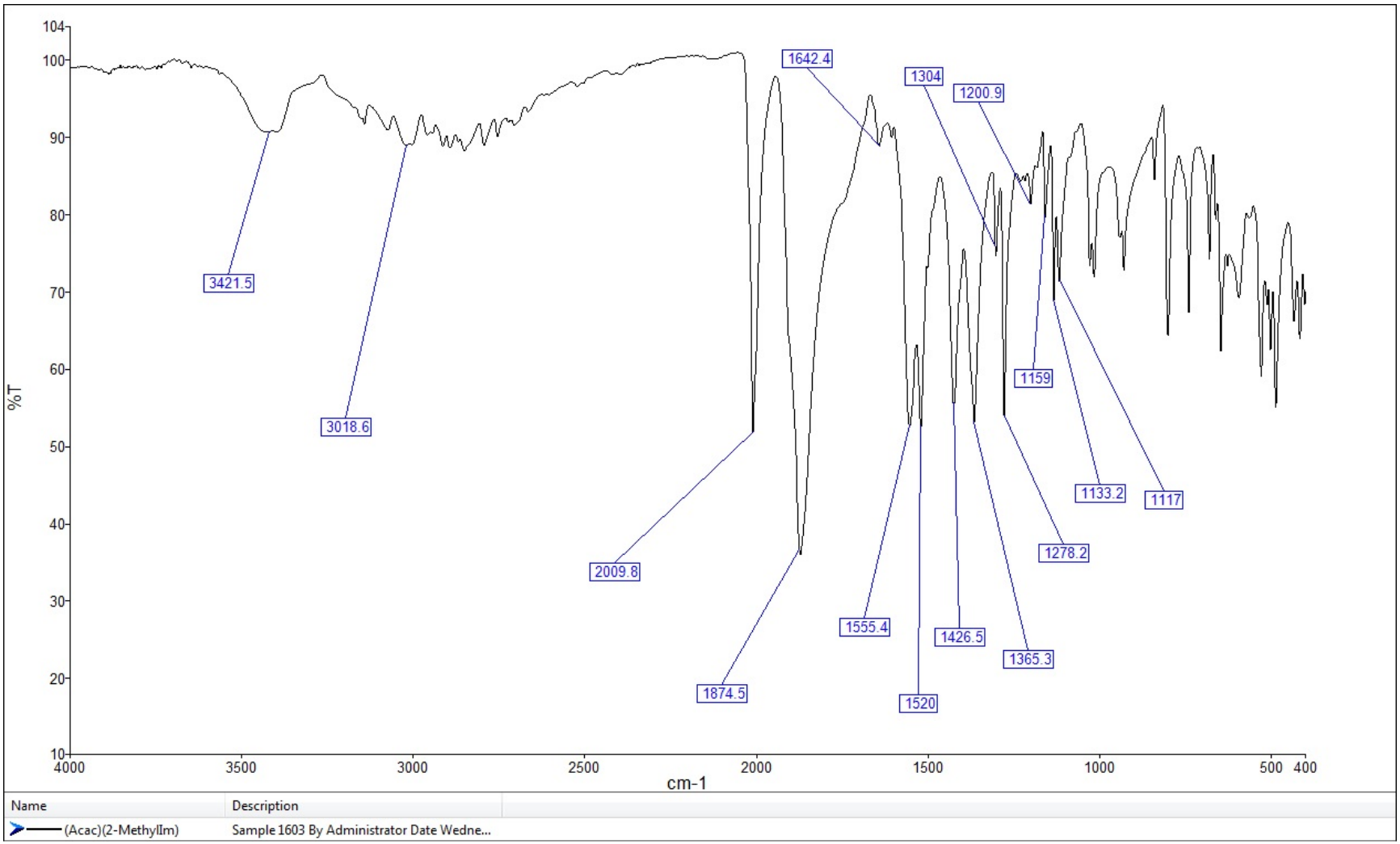


Figure SI 4: IR spectrum of **Re-2**

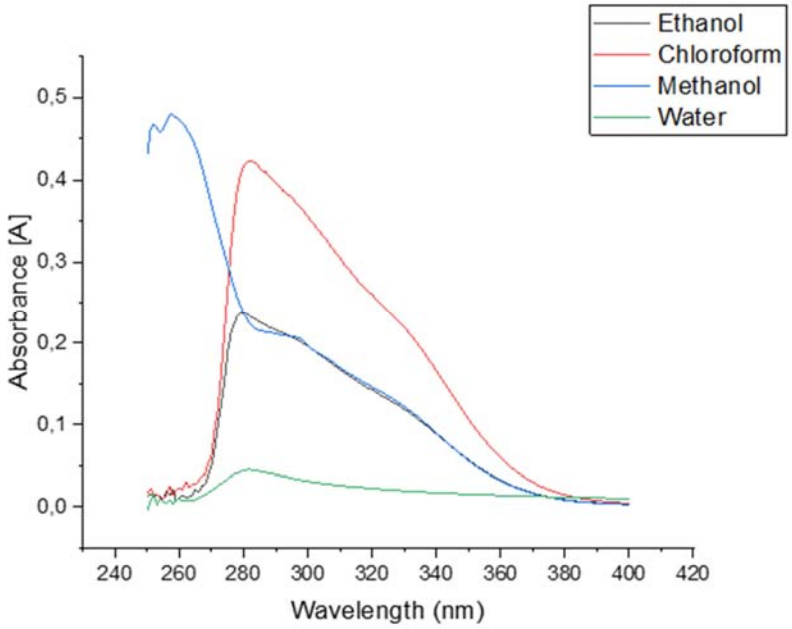


Figure SI 5: UV/Vis spectra of **Re-1** in different solvents.

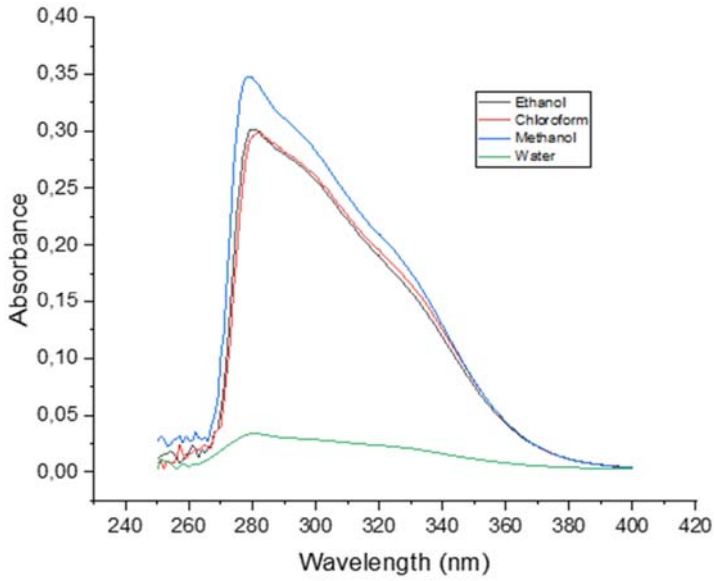


Figure SI 6: UV/Vis spectra of **Re-2** in different solvents.

Table SI1: Crystal data and structure refinement for **Re-1** and **Re-2**.

Complex	Re-1	Re-2
Emp. formula	$C_{13}H_{15}N_2O_5Re$	$C_{24}H_{22}N_4O_{10}Re_2$
CCDC Identifier	2194486	2194485
Form. weight (g.mol^{-1})	465.47	896.89
Crystal system	monoclinic	triclinic
Space group	$P2_1/c$	P-1
Crystal descr.	yellow block	yellow block
a (Å)	8.0388(2)	8.06516(15)
b (Å)	12.4323(3)	13.9029(3)
c (Å)	15.6301(5)	13.9924(3)
α (°)	90	113.5529(18)
β (°)	104.513(3)	100.4679(16)
γ (°)	90	90.3151(15)
Volume (Å^3)	1512.24(7)	1408.99(5)
Z	4	2
Abs. coeff. (m.mm^{-1})	8.057	8.640
F(000)	888	850
Independent refl.	3091	5749
Completeness (%)	99.9	99.9
Data/Restr/Para	3091/0/195	5749/0/367
Goodness of fit on F^2	1.168	1.095
Final R_1 indexes	0.0261	0.0406
wR_2 indices (all data)	0.0684	0.1116
Largest diffr. peak and hole (e.Å^{-3})	2.29/-1.89	3.17/-2.23

Table SI2: Selected bond lengths (Å) and angles (°) for **Re-1** and **Re-2**.

Description	Re-1	Re-2[c]
Re1-C_{eq}[a]	1.909(5)	1.896(7)
Re1-C8	1.908(4)	1.925(8)
Re1-O_{ave}	2.128(3)	2.137(4)
Re1-N1	2.197(3)	2.211(5)
C6-O3	1.158(5)	1.164(8)
C7-O4	1.148(6)	1.164(8)
C8-O5	1.167(5)	1.143(9)
O1-C1	1.276(5)	1.277(8)
O2-C3	1.282(5)	1.274(8)
C1-C2	1.389(5)	1.390(9)
N1-C9	1.340(5)	1.321(8)
N2-C9	1.343(5)	1.332(8)
C6-Re1-C7	89.14(16)	86.1(3)
C8-Re1-C6	88.67(17)	87.3(3)
C8-Re1-O1	93.03(14)	95.4(2)
C6-Re1-N1	96.26(14)	95.3(2)
C8-Re1-N1	175.05(14)	175.0(2)
N1-C9-N2	109.6(3)	109.6(5)
O1-C1-C2	126.3(3)	126.2(6)
O1-Re1-O2	85.67(10)	85.34(16)
C12-C9-N1-Re1	6.49(8)	4.38(7)
O1-C1-C2-C3	4.38(7)	1.03(9)
Re1-O1-C1-C2	-0.50(9)	12.18(5)
N1-C9-N2-C10	0.78(8)	0.27(9)

[a] C_{eq} = average of C6+C7 (equatorial CO ligands), [b] Re1-O_{ave} = average of Re1-O1 and Re1-O2. [c] Values indicated of only one of the two independent molecules in the asymmetric unit.

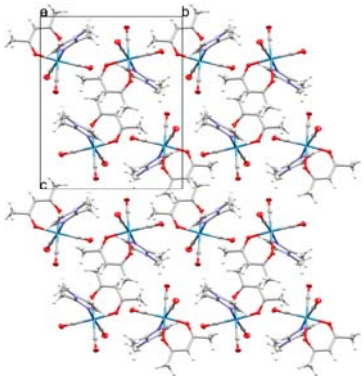
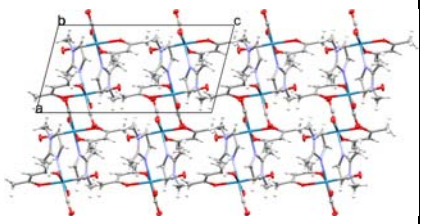
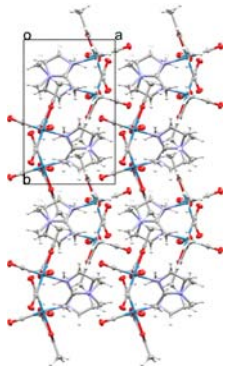
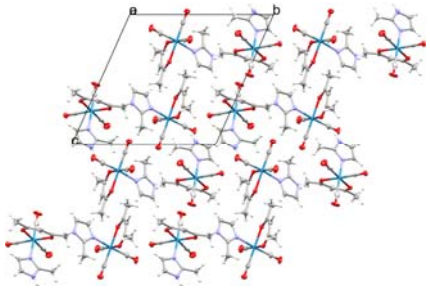
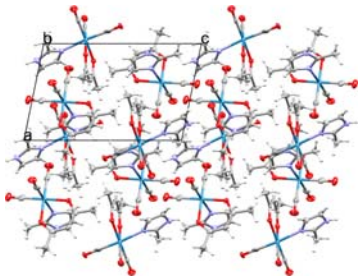
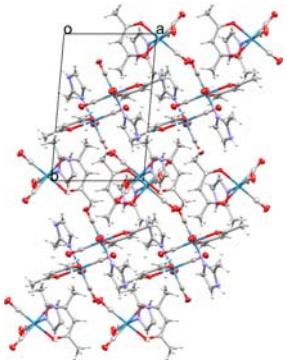
		
Packing of **Re-1** as viewed down *a*	Packing of **Re-1** as viewed down *b*	Packing of **Re-1** as viewed down *c*
		
Packing of **Re-2** as viewed down *a*	Packing of **Re-2** as viewed down *b*	Packing of **Re-2** as viewed down *c*

Figure SI 5: SCXRD Packing diagrams of **Re-1** and **Re-2**.

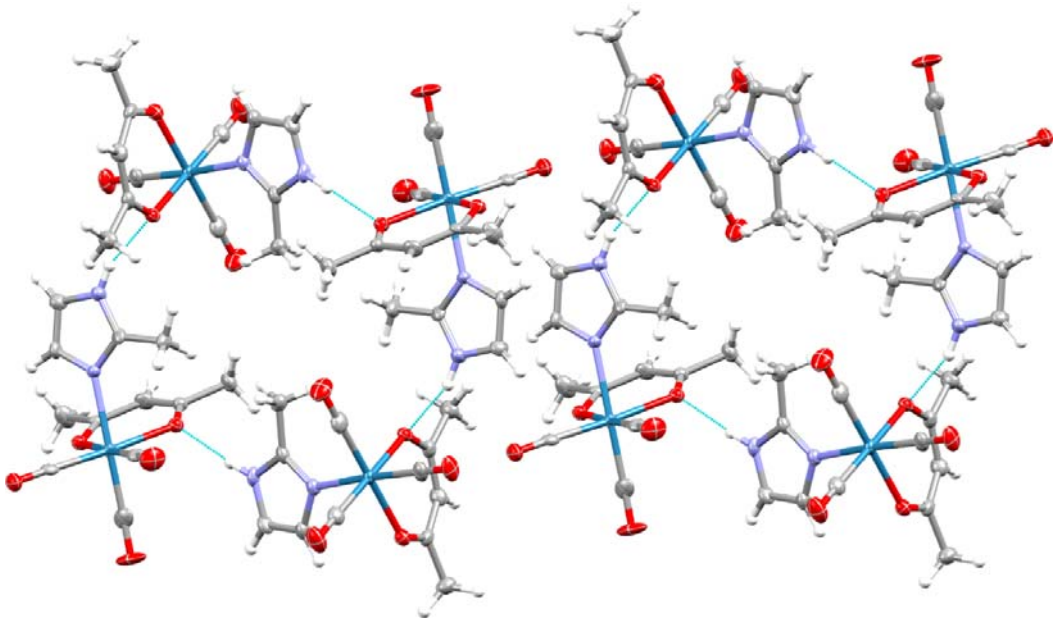


Figure SI 6: Hydrogen bonding interactions in complex **Re-2**.

Table SI3. Geometrical Parameters of (R)-d,d imidazole and 2-M1λ²,3λ² imidazole

Compounds	Atoms	Bond length(XRD)	Bond length(Theoretical) ωB97XD	mO6x-D3	PbeO-D3
A~Re-Im1					
	C(22)-C(26)	1.501	1.2823	1.5099	1.5124
	C(16)-C(18)	1.485	1.5236	1.5219	1.5287
	C(14)-C(31)	1.362	1.4667	1.392	1.3939
	C(12)-C(27)	1.511	1.5064	1.5097	1.5125
	C(10)-C(12)	1.390	1.3999	1.4109	1.4143
	C(10)-C(26)	1.388	1.406	1.402	1.4082
	N(9)-C(14)	1.375	1.2823	1.3261	1.345
	N(9)-C(16)	1.343	1.4684	1.4562	1.4785
	O(8)-C(13)	1.162	1.1461	1.1425	1.1656
	N(6)-C(33)	1.466	1.5236	1.4442	1.4474
	N(6)-C(31)	1.376	1.2774	1.3552	1.3673
	N(6)-C(16)	1.346	1.4433	1.4691	1.4785
	O(5)-C(7)	1.156	1.1509	1.1475	1.1703
	O(4)-C(17)	1.155	1.1461	1.1475	1.1708
	O(3)-C(26)	1.278	1.2676	1.2649	1.2865
	O(2)-C(12)	1.276	-	1.2578	1.2803
	Re(1)-N(9)	2.197	-	2.223	2.1788
	Re(1)-O(2)	2.130	2.1643	2.1897	2.1688
	Re(1)-O(3)	2.120	2.1676	2.1859	2.1647
	Re(1)-C(13)	1.914	1.9224	1.9228	1.9311
	Re(1)-C(17)	1.909	1.9058	1.9002	1.9081
	Re(1)-C(7)	1.904	1.9012	1.9009	1.9109
RMSD					
			0.074682	0.044722	0.045741
		Bond Angles(XRD)			
	O(4)-C(17)-Re(1)	179.015	-	-	-
	O(8)-C(13)-Re(1)	176.615	-	-	-
	O(5)-C(7)-Re(1)	177.626	-	-	-
	C(14)-C(31)-N(6)	105.300	107.2014	107.8437	
	C(22)-C(26)-C(10)	119.421	119.0791	119.0275	
	C(22)-C(26)-O(3)	114.341	114.9081	114.6762	108.2349
	C(10)-C(26)-O(3)	126.194	126.0113	126.29	114.3503
	C(33)-N(6)-C(31)	124.217	123.2179	125.7162	125.5672

	C(33)-N(6)-C(16)	126.634	112.2223	121.6774	121.7728
	C(31)-N(6)-C(16)	109.026	106.4387	108.3932	108.2538
	C(18)-C(16)-N(9)	127.048	-	113.1915	113.5693
	C(18)-C(16)-N(6)	123.510	-	113.1492	113.0583
	N(9)-C(16)-N(6)	109.440	107.2014	103.6615	103.881
	C(31)-C(14)-N(9)	109.966	109.3994	111.7549	111.6948
	C(12)-C(10)-C(26)	125.812	-	125.4048	126.2995
	C(27)-C(12)-C(10)	118.893	-	118.688	119.2762
	C(27)-C(12)-O(2)	114.433	114.6306	115.1484	114.64
	C(10)-C(12)-O(2)	126.670	125.926	126.1588	126.0818
	C(14)-N(9)-C(16)	106.258	106.285	107.8753	107.6059
	C(14)-N(9)-Re(1)	122.293	126.2289	126.3115	126.3793
	C(16)-N(9)-Re(1)	131.109	127.3249	125.6773	125.6515
	C(26)-O(3)-Re(1)	127.910	178.4671	-	17j8.0646
	C(12)-O(2)-Re(1)	127.337	129.4927	129.5623	128.175
	N(9)-Re(1)-O(2)	81.955	81.0885	80.3434	82.0704
	N(9)-Re(1)-O(3)	83.181	83.0363	81.1203	83.5163
	N(9)-Re(1)-C(13)	174.967	93.7676	-	-
	N(9)-Re(1)-C(17)	92.849	95.1155	94.3111	93.4845
	N(9)-Re(1)-C(7)	96.430	94.0595	95.7609	95.6177
	O(2)-Re(1)-O(3)	85.655	83.3674	82.781	85.1247
	O(2)-Re(1)-C(13)	93.078	93.333	94.0647	92.3314
	O(2)-Re(1)-C(17)	93.545	93.9082	93.5548	92.3416
	O(3)-Re(1)-C(13)	97.313	94.0595	94.511	92.6596
	O(3)-Re(1)-C(17)	176.021	-	-	-
RMSD			16.93513	4.08528	53.92996

B~Re-Im2		Bond Length(XRD)	Bond length(Theoretical)		
	C(41)-C(56)	1.504	1.5069	1.2606	1.5109
	C(34)-C(39)	1.518	1.5236	1.5245	1.531
	C(28)-C(30)	1.362	1.4667	1.4751	1.4608
	C(27)-C(46)	1.509	1.5064	1.5085	1.5112
	N(23)-C(39)	1.338	1.4684	1.4467	1.4501
	N(23)-C(30)	1.364	1.2823	1.2757	1.2979
	C(16)-C(41)	1.390	1.406	1.4018	1.4081
	C(16)-C(27)	1.415	1.5069	1.4093	-
	N(15)-C(39)	1.322	1.4433	1.4689	1.4838
	N(15)-C(28)	1.385	1.2774	1.2795	1.3057

	O(14)-C(38)	1.153	1.1526	1.1471	1.17
	O(13)-C(21)	1.156	1.1509	1.1411	1.1637
	O(9)-C(40)	1.119	1.1461	1.1458	1.5109
	Re(2)-C(40)	1.944	1.9224	1.9053	-
	Re(2)-C(38)	1.896	1.9012	1.9013	1.9151
	Re(2)-C(21)	1.912	1.9058	1.9213	1.9319
	Re(2)-N(15)	2.199	2.2204	2.2408	2.1804
RMSD			0.064822	0.086487	0.11965354

		Bond Angles(XRD)			
	C(56)-C(41)-C(16)	118.294	119.4351	114.748	119.6914
	O(9)-C(40)-Re(2)	176.344	-	-	-
	C(34)-C(39)-N(23)	121.898	112.4789	112.0967	112.5234
	C(34)-C(39)-N(15)	126.848	112.2223	111.9393	112.8921
	N(23)-C(39)-N(15)	126.848	107.2014	107.1349	107.7272
	O(14)-C(38)-Re(2)	109.500	-	-	-
	C(28)-C(30)-N(23)	106.045	109.3994	110.5467	111.3289
	C(30)-C(28)-N(15)	109.245	110.675	109.301	109.5348
	C(46)-C(27)-C(16)	118.185		118.8336	119.4235
	C(39)-N(23)-C(30)	107.997	106.285	106.527	105.8091
	O(13)-C(21)-Re(2)	178.013	-	-	-
	C(41)-C(16)-C(27)	125.061	125.5688	125.297	126.2208
	C(39)-N(15)-C(28)	105.455	106.4387	106.4896	105.5991
	C(39)-N(15)-Re(2)	129.989	127.3249	125.9252	126.4375
	C(28)-N(15)-Re(2)	124.515	126.2289	127.5339	127.7369
	C(40)-Re(2)-C(38)	87.088	88.9913	89.3098	89.3657
	C(40)-Re(2)-C(21)	89.161	89.5991	89.5772	89.7504
	C(40)-Re(2)-N(15)	95.484	95.1155	95.0389	94.9928
	C(38)-Re(2)-C(21)	90.000	89.642	89.7044	90.117
	C(38)-Re(2)-N(15)	90.000	93.7676	93.9482	93.2227
RMSD			29.40926	6.817378	
		6.530778			

Table SI4: Docking score, receptor and interacting amino acids during docking.

1g50	Binding Affinity	Interacting amino acids residues	1xyt	Binding Affinity	Interacting amino acid residues	1oqa	Binding Affinity	Interacting amino acid residues	2lwl	Binding Affinity	Interacting amino acid residues	3hb4	Binding Affinity	Interacting amino acid residues
Re-1	-5.9	A:ARG95:HH22 - :UNK0:O B:GLY90:HN - :UNK0:O B:ARG95:HE - :UNK0:O A:GLY89:CA - :UNK0:O	**Re-1**	-5.4	A:GLY45:CA - :UNK0:O :UNK0:C - :UNK0:O : :UNK0:C - :UNK0:O :UNK0:C - :UNK0:O :UNK0:C - :UNK0:O	**Re-1**	-4.9	A:ARG35:HH21 - :UNK0:O A:GLN38:HE22 - :UNK0:O A:SER42:HN - :UNK0:O :UNK0:C - :UNK0:O :UNK0:C - :UNK0:O	**Re-1**	-5.1	A:ARG35:HH21 - :UNK0:O A:ARG35:HH22 - :UNK0:O A:LYS10:CE - :UNK0:O :UNK0:C - :UNK0:O :UNK0:C - :UNK0:O	**Re-1**	-5.5	A:GLY50:HN - :UNK0:N A:GLY45:CA - :UNK0:O :UNK0:C - :UNK0:O :UNK0:C - :UNK0:O :UNK0:C - :UNK0:O
Re-2	-6.1	A:ARG95:HH12 - :UNK0:O A:ARG95:HH22 - :UNK0:O B:GLY90:HN - :UNK0:O :UNK0:C - :UNK0:O :UNK0:C - :UNK0:O	**Re-2**	-3.7	A:LYS169:HZ1 - :UNK0:O A:THR204:HG1 - :UNK0:O :UNK0:C - :UNK0:O :UNK0:C - :UNK0:O :UNK0:C - :UNK0:O	**Re-2**	-5.2	A:SER42:CB - :UNK0:O :UNK0:C - :UNK0:O :UNK0:C - :UNK0:O :UNK0:C - :UNK0:O :UNK0:C - :UNK0:O	**Re-2**	-5.4	A:ARG35:HH21 - :UNK0:O A:GLN38:HE21 - :UNK0:N A:GLY41:CA - :UNK0:N :UNK0:C - :UNK0:O :UNK0:C - :UNK0:O		-5.7	A:GLY48:HN - :UNK0:N :UNK0:C - :UNK0:O :UNK0:C - :UNK0:O :UNK0:C - :UNK0:O :UNK0:C - :UNK0:O

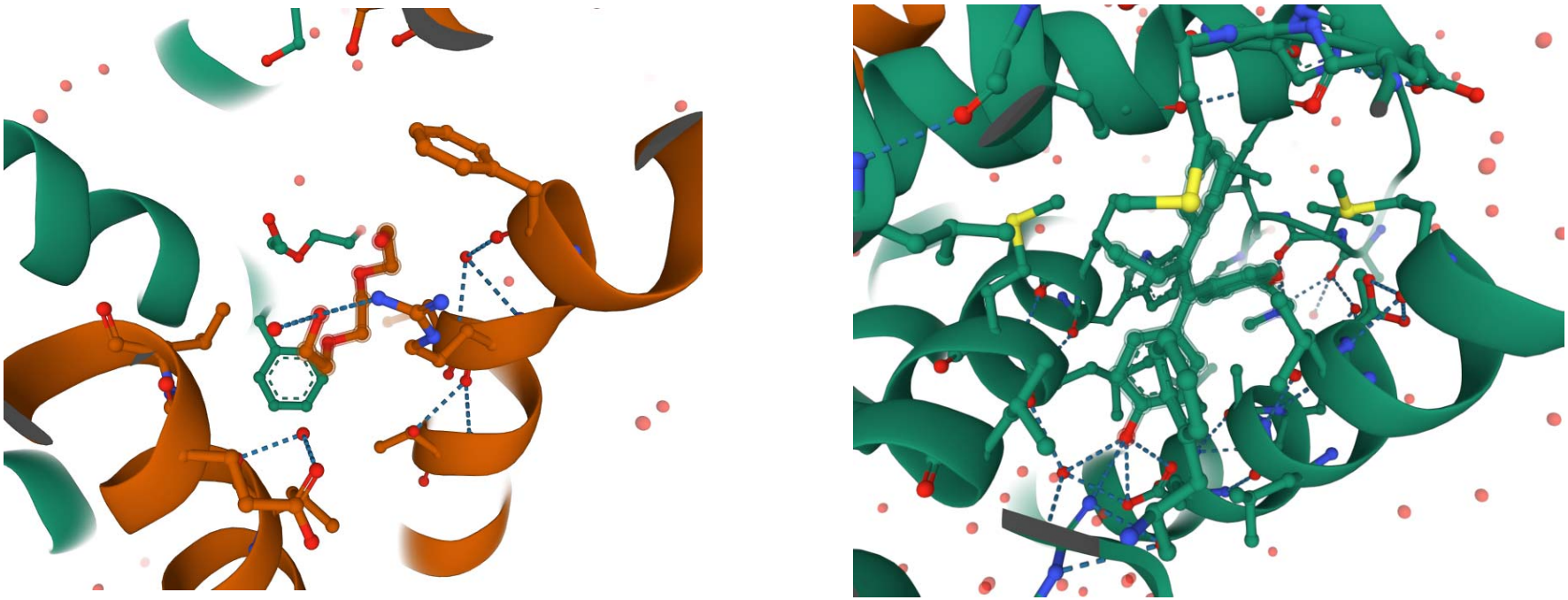
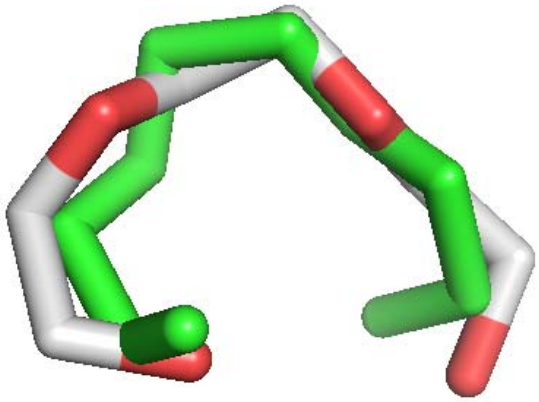
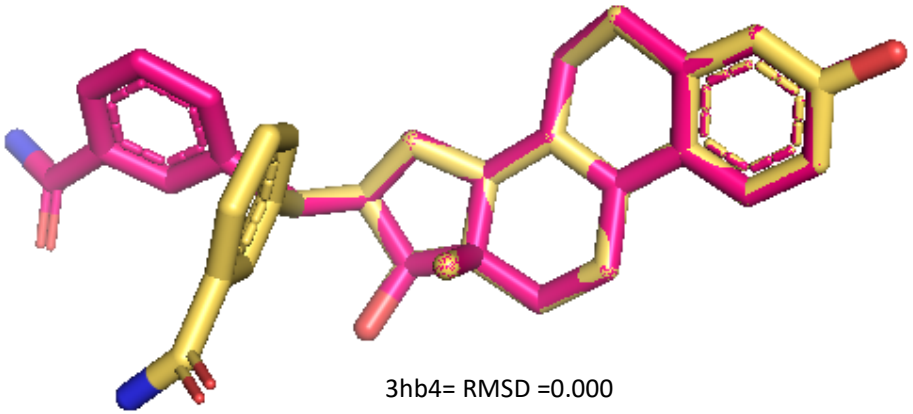


Figure SI 7: Visualized active pocket of the known complexed inhibitors with 2yw6 and 5w9d

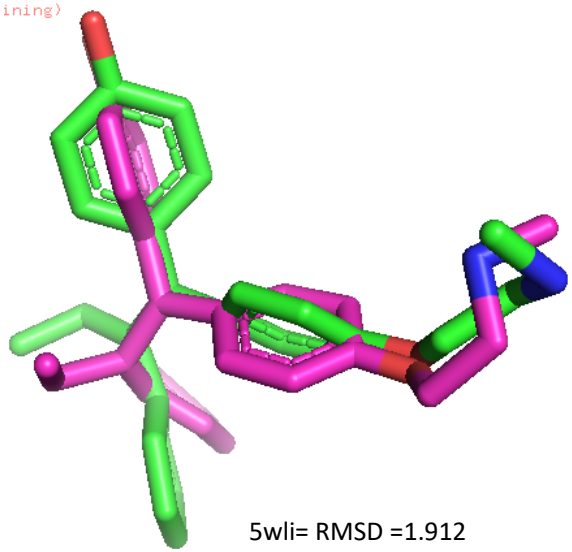
Figure SI 8: Superimposed lowest binding conformations of the known inhibitors after redocking experiments.



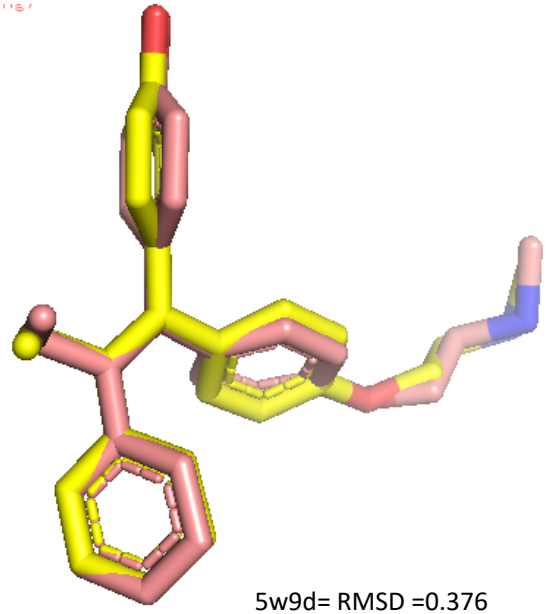
2y6w= RMSD =1.641



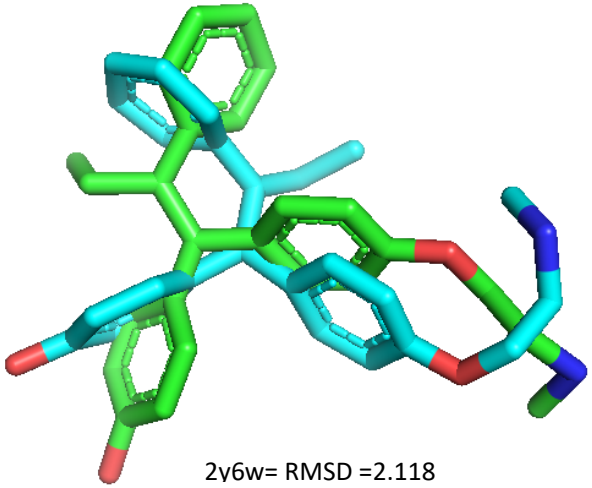
3hb4= RMSD =0.000



5wli= RMSD =1.912



5w9d= RMSD =0.376



2y6w= RMSD =2.118