

Highly efficient functionalized MOF-LIC-1 for Extraction of U(VI) and Th(IV) from Aqueous Solution: Experimental and Theoretical Studies

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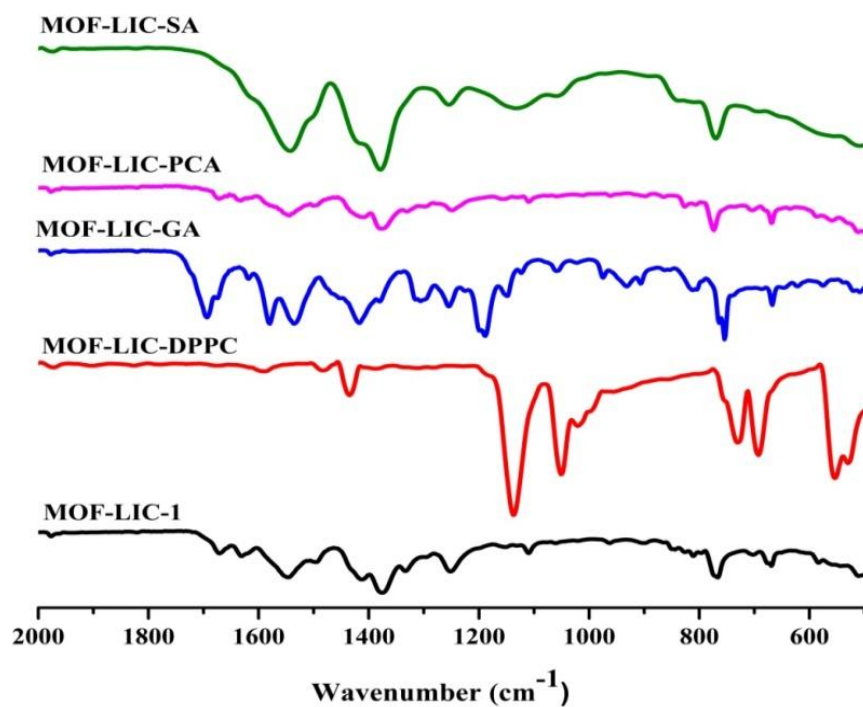


Figure S1. FTIR spectra of MOF-LIC-1 and its PSM MOFs.

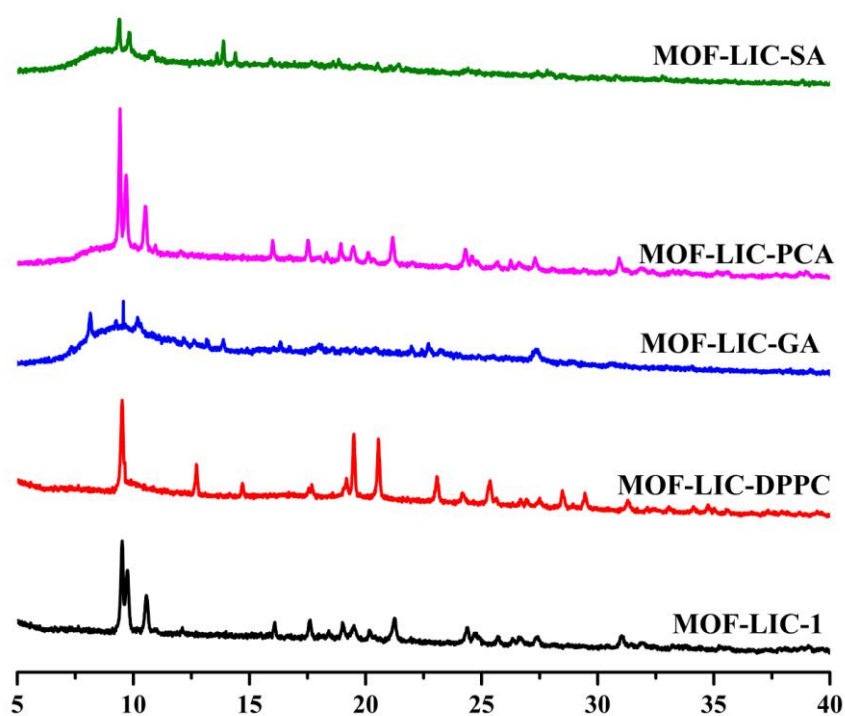


Figure S2. Powder XRD patterns of MOF-LIC-1 and its PSM MOFs.

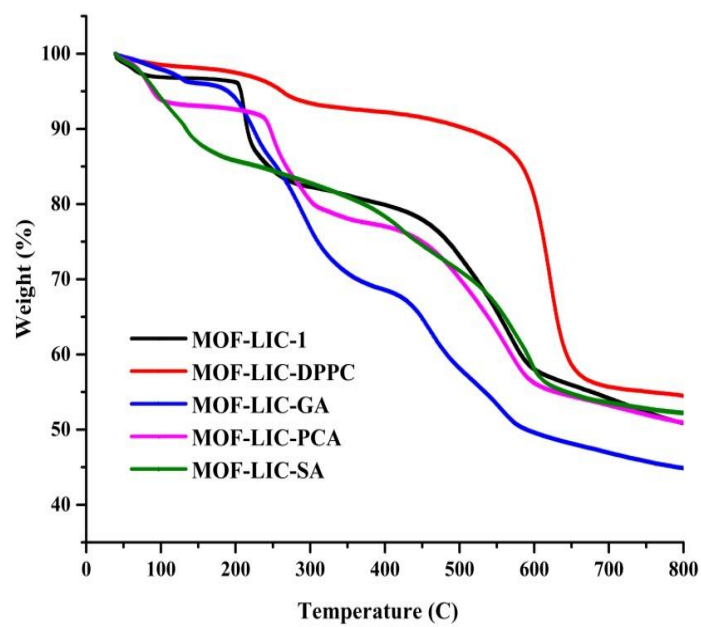
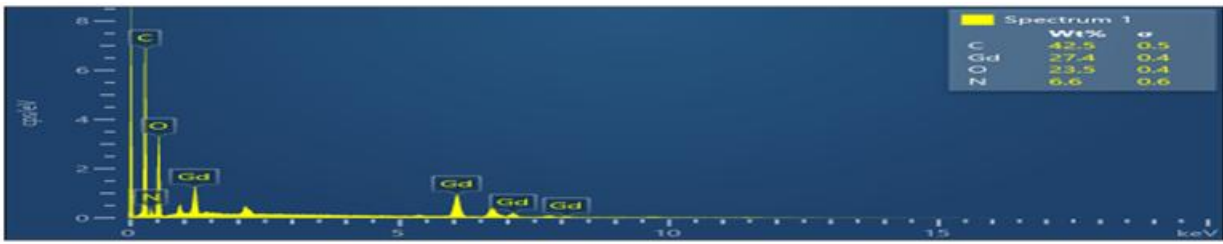
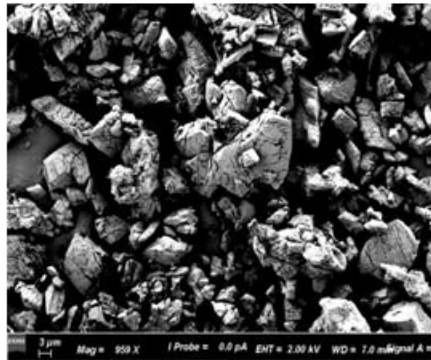


Figure S3. TGA plot of MOF-LIC-1 and its PSM MOFs.

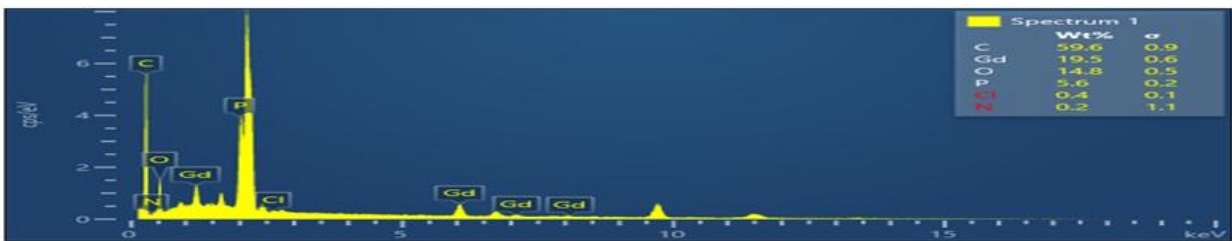


1(a)

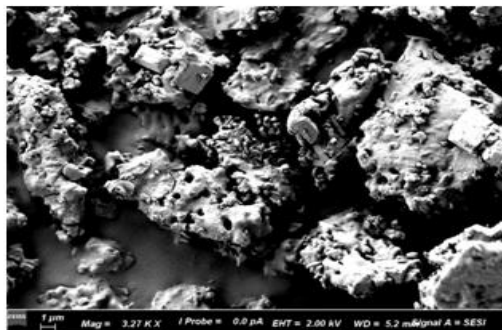


1(b)

Figure S4(a, b). EDX spectra & SEM image of MOF-LIC-1.

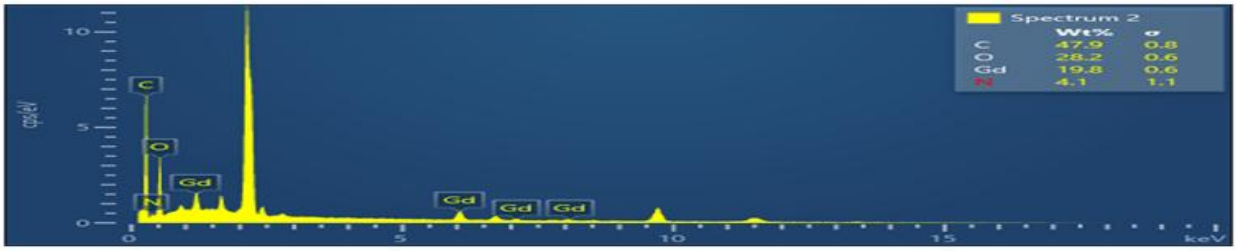


2(a)

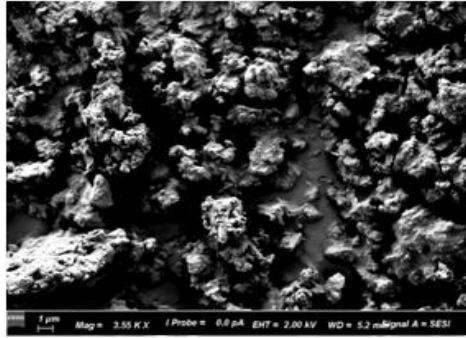


2(b)

Figure S5(a, b). EDX spectra & SEM image of MOF-LIC-DPPC.

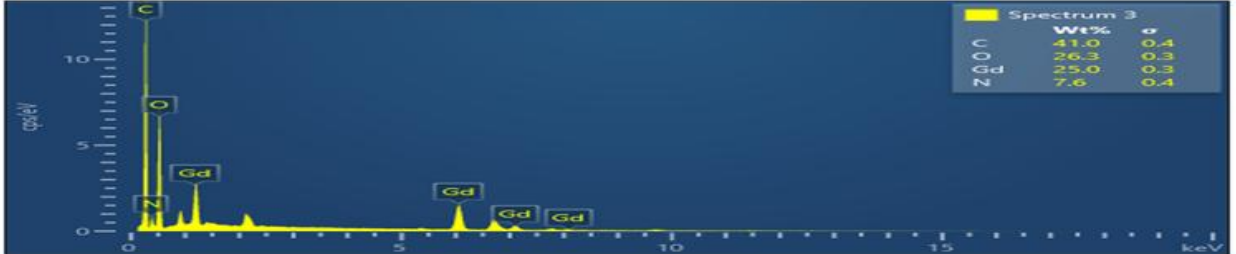


3(a)

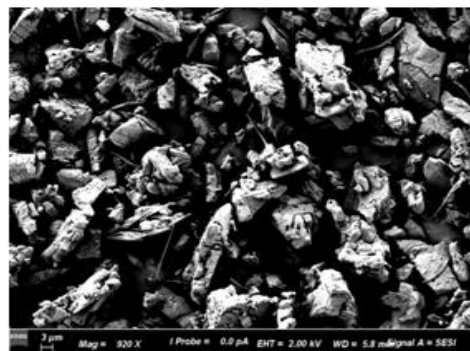


3(b)

Figure S6(a, b). EDX spectra & SEM image of MOF-LIC-GA.

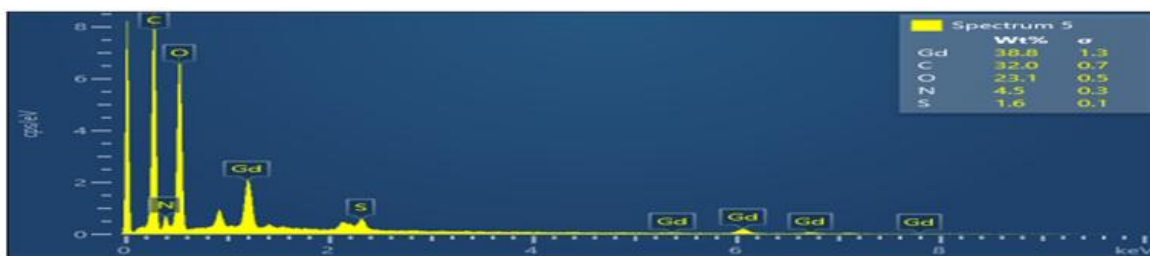


4(a)

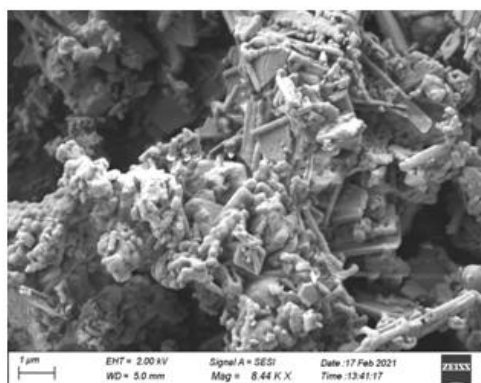


4(b)

Figure S7(a, b). EDX spectra & SEM image of MOF-LIC-PCA.



5(a)



5(b)

Figure S8(a, b). EDX spectra & SEM image of MOF-LIC-SA.

Chemical stability studies:

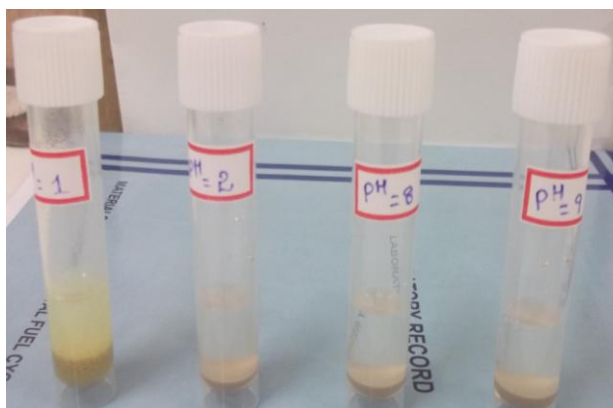


Figure S9. The image of MOF-LIC-1 with different pH solutions.

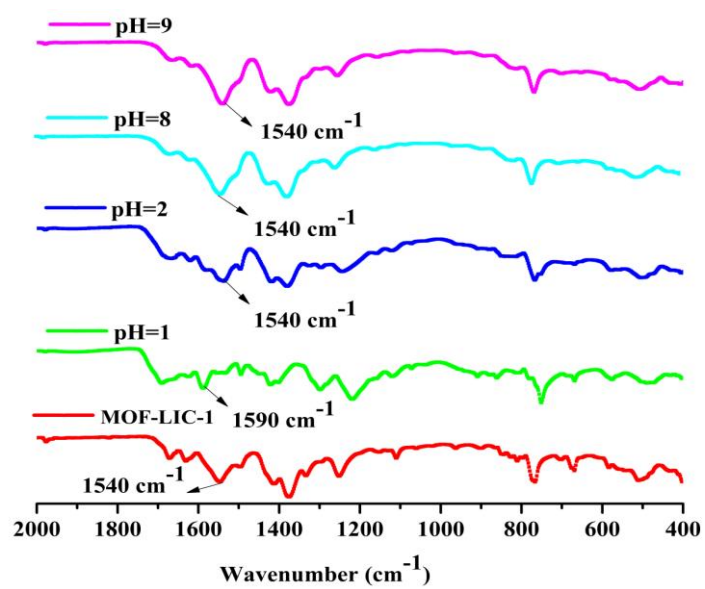


Figure S10. FTIR spectra of MOF-LIC-1 with different pH solutions.

Kinetic Model

The kinetic study of sorption of U(VI) & Th(IV) on MOF-LIC-1 MOFs was appropriate for the linear form of pseudo-second-order kinetic model and is represented as:

$$\frac{t}{q_t} = \frac{1}{K_2 q_e^2} + \frac{t}{q_e}$$

Here, q_e (mg g^{-1}) and q_t (mg g^{-1}) are the amounts of U(VI) & Th(IV) sorption at equilibrium and time t , respectively, K_2 ($\text{g mg}^{-1} \text{min}^{-1}$) is the pseudo-second-order sorption rate constant. The model parameters and the correlation coefficient obtained are shown in Table S1.

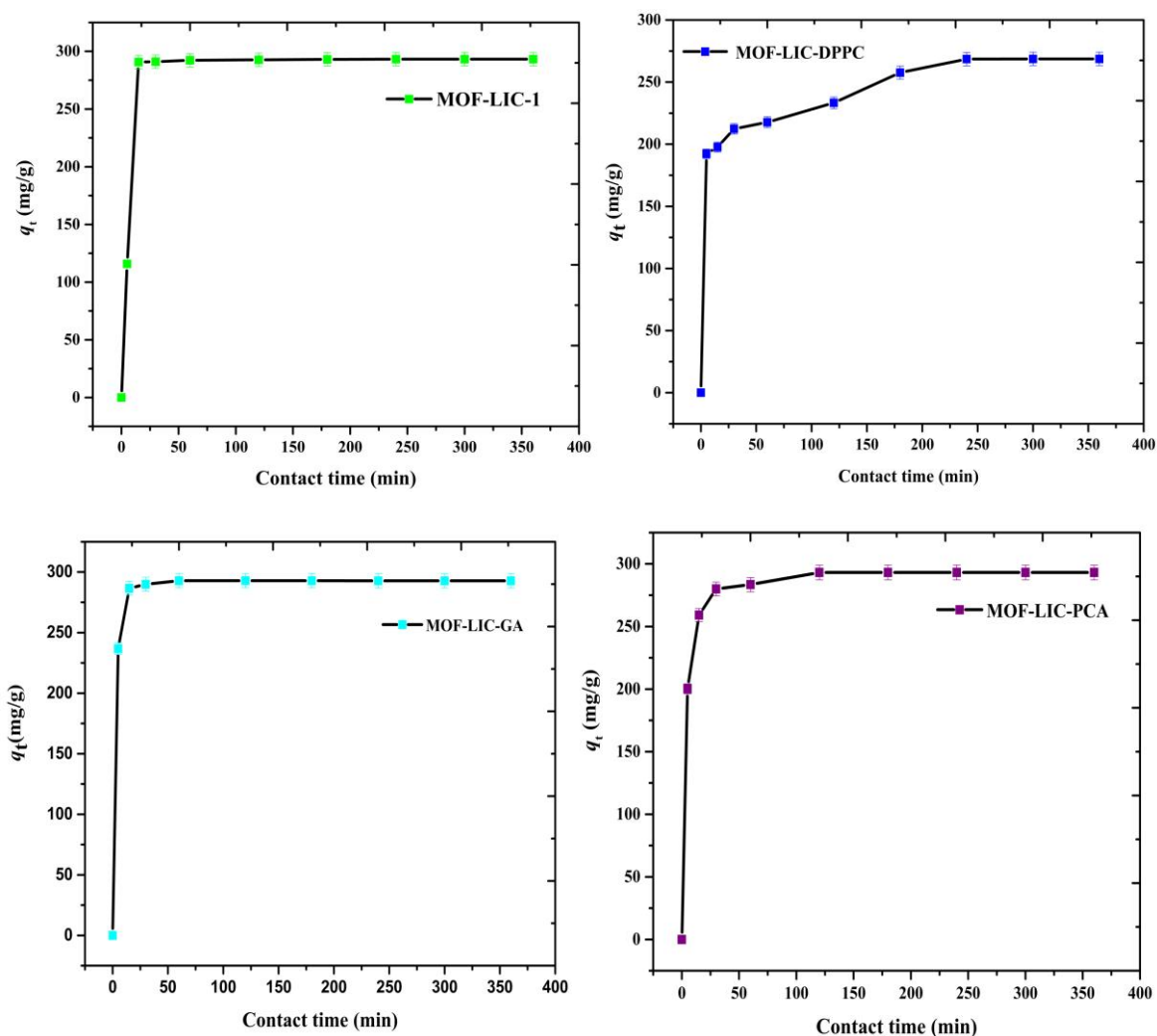


Figure S11. Effect of contact time on U(VI) sorption onto MOF-LIC-1 MOFs; at pH = 6; where $t = 0$ to 300 min, $m_{\text{sorbent}} = 10.0$ mg, $V_{\text{solution}} = 3$ mL, $C_0 = 1000$ mg L^{-1} , $T = 25 \pm 1^\circ\text{C}$.

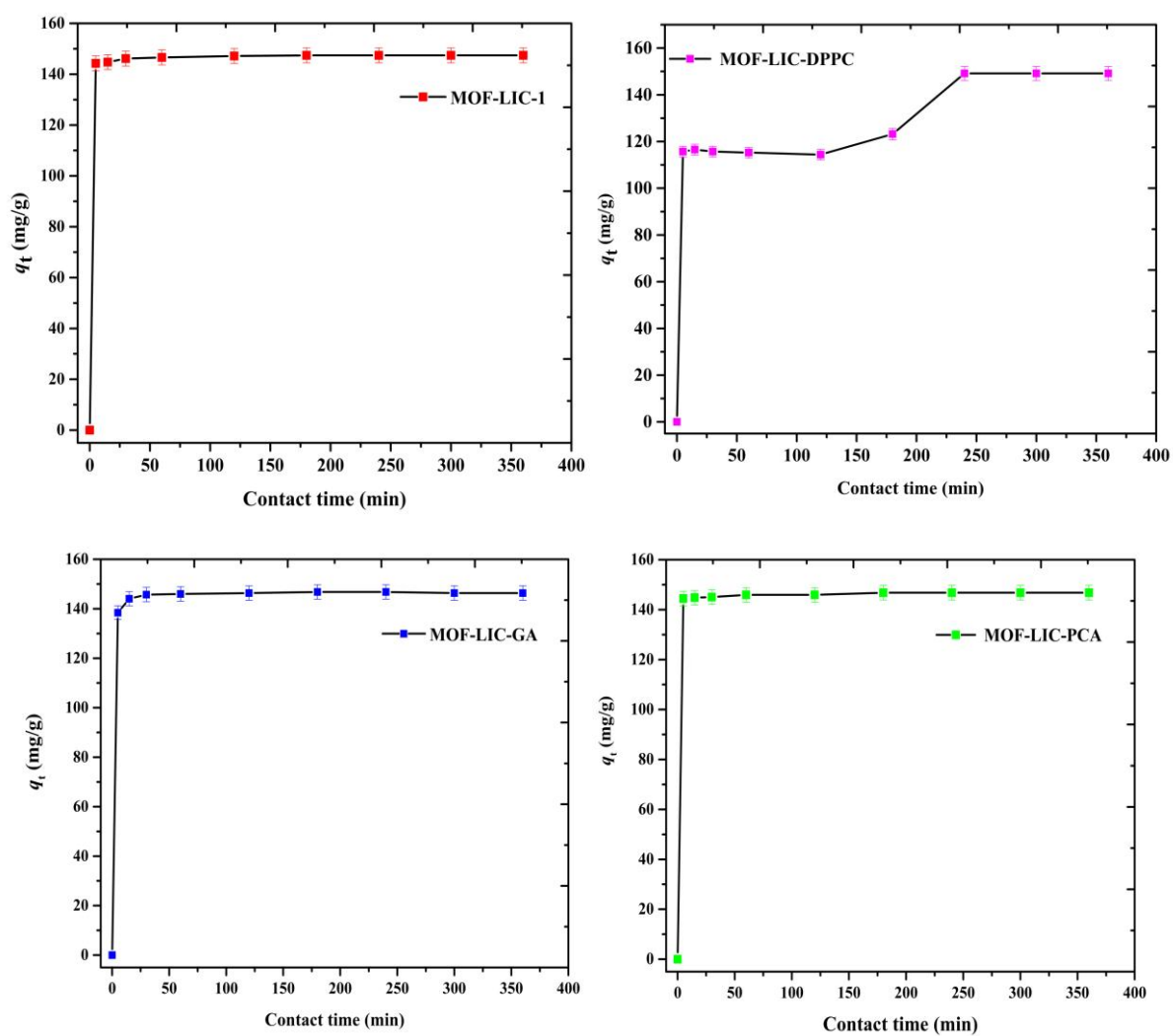


Figure S12. Effect of contact time on Th(IV) sorption onto MOF-LIC-1 MOFs; at pH = 6; where $t = 0$ to 300 min, $m_{\text{sorbent}} = 10.0$ mg, $V_{\text{solution}} = 3$ mL, $C_0 = 500$ mg L⁻¹, $T = 25 \pm 1^\circ\text{C}$.

Pseudo-second order fitting of MOF-LIC-1MOFs for U(VI) & Th(IV)

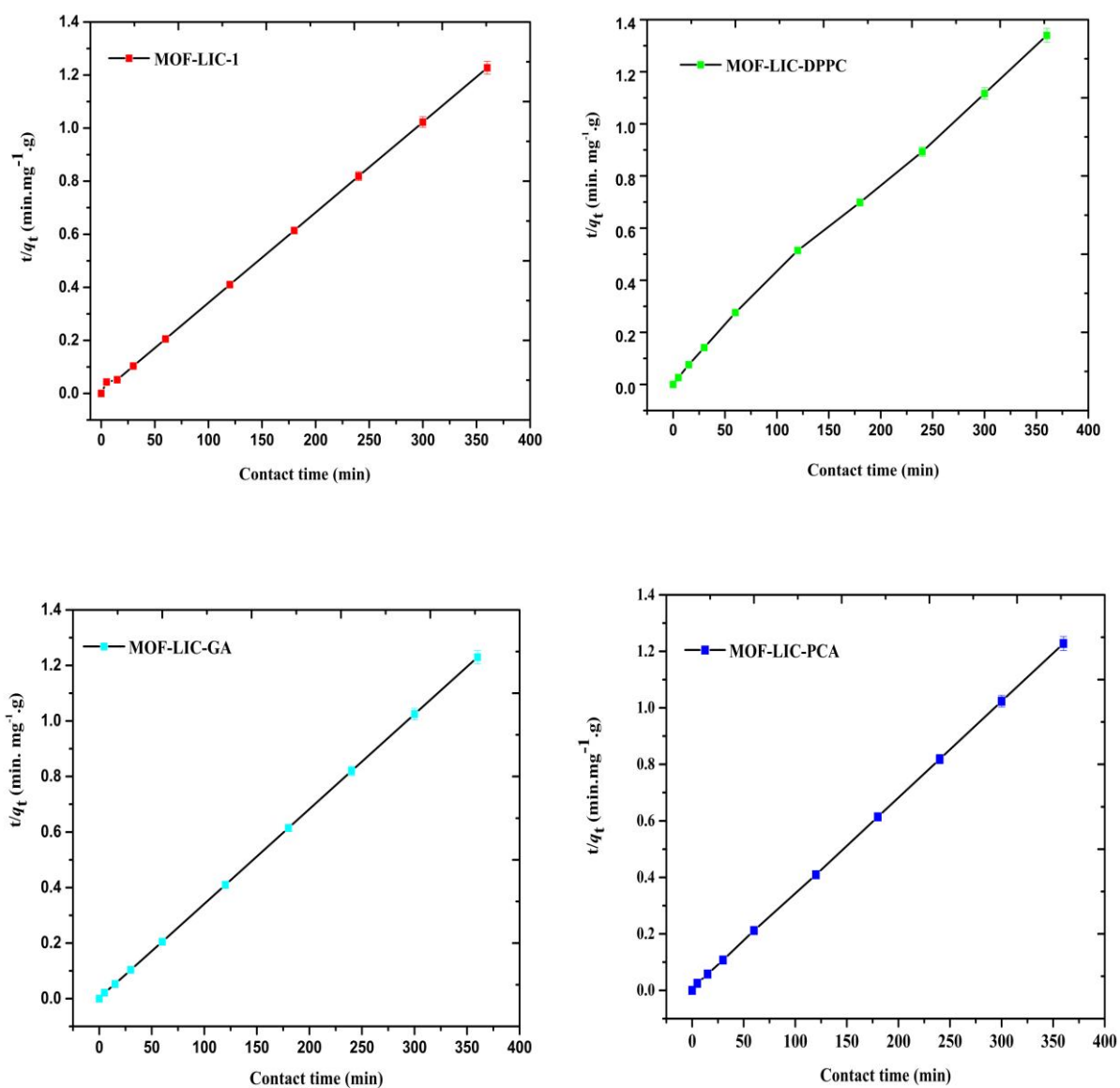


Figure S13. The plot of contact time vs t/q_t for U(VI) sorbed on MOF-LIC-1 and its PSM MOFs (pseudo second order); $m_{\text{sorbent}}=10$ mg, $t = 0$ to 360 min, $V_{\text{solution}}= 3$ mL, $C_o= 1000$ mg L⁻¹, $T = 25$ °C±1.

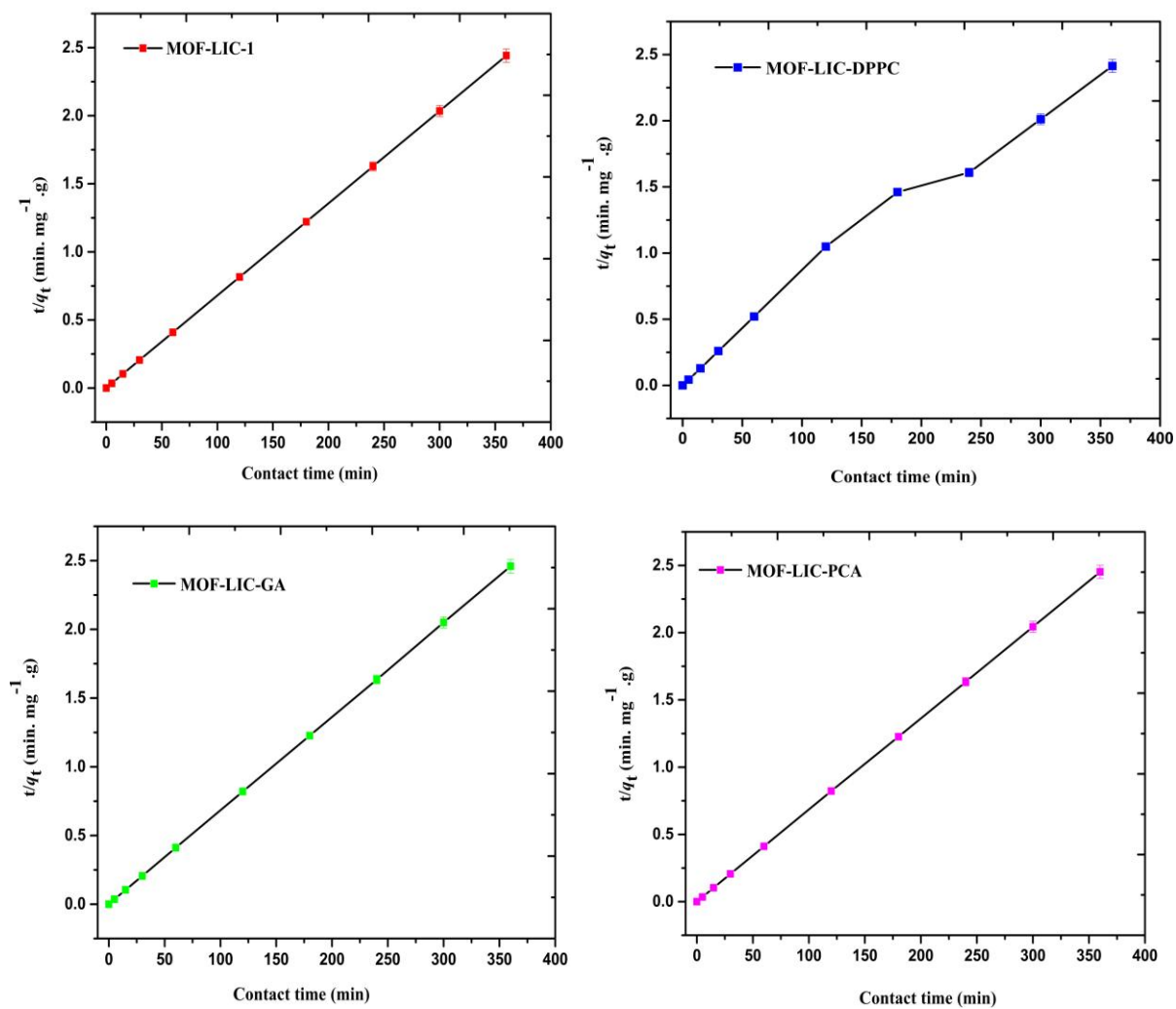


Figure S14. The plot of contact time vs t/q_t for Th(IV) sorbed on MOF-LIC-1 and its PSM MOFs (pseudo second order); $m_{\text{sorbent}}=10$ mg, $t = 0$ to 360 min, $V_{\text{solution}}= 3$ mL, $C_o= 500$ mg L⁻¹, $T = 25$ °C±1.

Table S1: Kinetic parameters for U(VI)/Th(IV) sorption onto MOF-LIC-1 MOFs:

MOFs	Pseudo-second-order kinetic model for U(VI)			Pseudo-second-order kinetic model for Th(VI)		
	q_e (mg g ⁻¹)	K_2 (g mg ⁻¹ min ⁻¹)	R ²	q_e (mg g ⁻¹)	K_2 (g mg ⁻¹ min ⁻¹)	R ²
MOF-LIC-1	238	0.00197	0.9998	128	0.03355	0.9999
MOF-LIC-DPPC	260	0.002326	0.9999	145	0.00057	0.9935
MOF-LIC-GA	263	0.00977	0.9999	136	0.05881	0.9999
MOF-LIC-PCA	254	0.009066	0.9999	146	0.02650	0.9999
MOF-LIC-SA	282	0.000473	0.9988	149	0.02473	0.9999

Table S1. Leaching (%) of U(VI) sorbed onto MOFs:

MOF	Eluents	Leaching (%)
MOF-LIC-1	0.01 M HNO ₃	93
MOF-LIC-DPPC	0.01 M Na ₂ CO ₃	91
MOF-LIC-PCA	0.01 M HNO ₃	95
MOF-LIC-SA	0.01 M HNO ₃	93
MOF-LIC-GA	0.01 M HNO ₃	95

Table S2. Leaching (%) of Th(IV) sorbed onto MOFs:

MOF	Eluents	Leaching (%)
MOF-LIC-1	0.01 M Na ₂ CO ₃	91
MOF-LIC-DPPC	0.01 M Na ₂ CO ₃	94
MOF-LIC-GA	0.01 M HNO ₃	93
MOF-LIC-PCA	0.01 M HNO ₃	98
MOF-LIC-SA	0.01 M HNO ₃	91

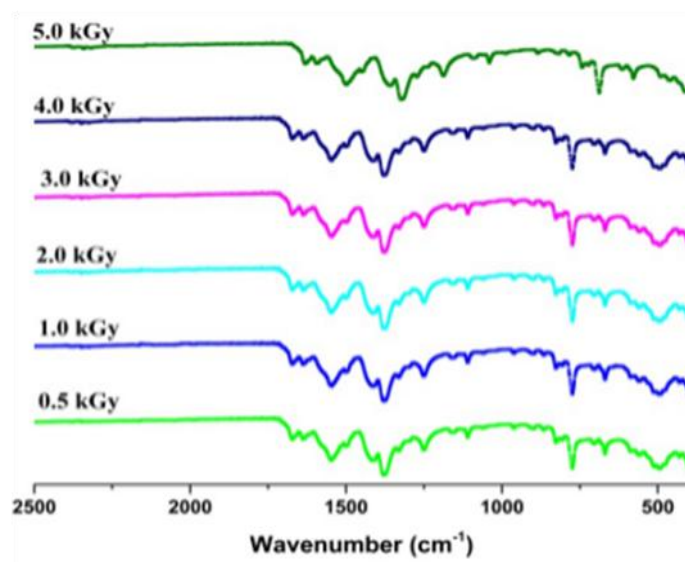


Figure S15. FTIR spectra of MOF-LIC-1 at different gamma dosage.

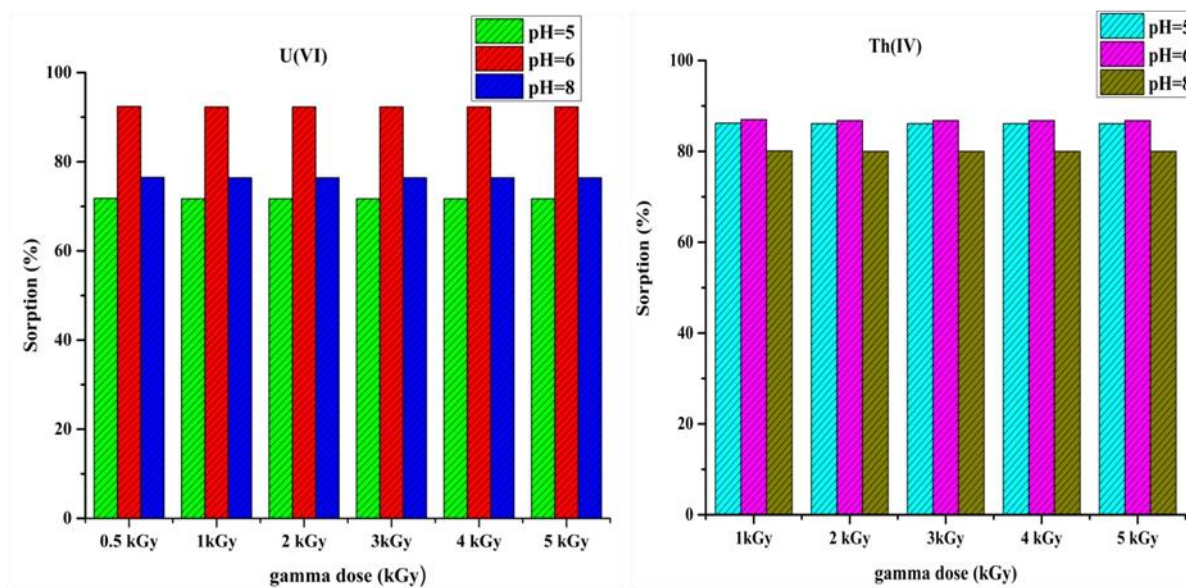


Figure S16. Sorption(%) of U(VI) &Th(IV) on irradiated MOF-LIC-1 at different pH(acidic/basic/neutral)

Coordinates of Optimized Geometries of Ligands:

Ligand-1

C	-0.91520004293151	-0.37225520755908	-0.96754187724197
C	-2.05667066665584	-0.78347009944378	-0.27214872604962
C	0.20730309109141	0.09533684387999	-0.28454780394622
H	-2.93144900654206	-1.15041662516617	-0.80957123378380
H	1.09155703752725	0.41571927128359	-0.84107325406633
C	-2.05637508164746	-0.71786641566004	1.12471878999143
C	0.21236242882729	0.16250434519110	1.12155226943480
H	-2.93708987476703	-1.03521218831707	1.68635863300632
C	-0.93975608174012	-0.25067554808113	1.81736617389624
H	-0.95636322625674	-0.19712117400173	2.90905493163086
H	-0.89397711622568	-0.41787770097069	-2.05836375567270
N	1.31025025766882	0.68776782335136	1.80884907720803
H	1.41169989820928	0.37382290309248	2.76973883284569
H	2.19143129044237	0.65882621440117	1.30398229274727

Ligand-2

C	0.78713450235333	1.53782060846457	-0.91971513843155
C	-0.47061263083047	0.98108196648269	-0.63129023693462
C	1.44254308317631	2.34253277545818	0.02345309274983
H	-0.97963195525451	0.34510491355684	-1.37110958737064
H	2.43446453583545	2.76514824610480	-0.20424083222264
C	-1.07323286456347	1.25464110971532	0.60855069152210
C	0.83275777346437	2.62444415085169	1.26831267948391
H	-2.06485797866488	0.83769205347596	0.84265845610137
C	-0.44111829042733	2.07767884998889	1.55373257074719
H	-0.93276454615016	2.32512714521082	2.50533770756987

H	1.27264206478449	1.33706146707106	-1.88737943922009
N	1.49157263103041	3.46880069012470	2.18864714519146
H	2.40866165224837	3.82222958686371	1.89574447667887
S	1.53042685143584	3.16432532418449	3.88581192866691
O	2.66875758197882	3.96881520172090	4.34550331629029
O	0.16078967430132	3.29821002532814	4.39566206376753
N	1.94065144586289	1.54290003416613	4.13085988596027
H	1.19988970525147	0.90834341459286	3.80444674141026
H	2.85538643416771	1.30960537563818	3.72377646703960

Ligand-3

C	-5.81142482731717	-1.91859138400016	4.57741785529102
C	-6.25534772429940	-1.49826557559547	5.84279671289589
C	-4.60264940453804	-1.44148289233569	4.05002384607458
H	-7.20292903021263	-1.87585771654065	6.25442357074043
H	-4.25996140278183	-1.78492532418163	3.06066283104309
C	-5.47516693151237	-0.58075194442957	6.56793554662647
C	-3.81488834462791	-0.52011405070288	4.78063472245194
H	-5.81277763520606	-0.22895413842582	7.55500689390669
C	-4.27034704982227	-0.08419478367214	6.04877760894120
H	-3.69207112169849	0.67112295254382	6.60060485956945
H	-6.41086146887307	-2.63093797205266	3.98842028795069
N	-2.60390987753479	-0.05678879331228	4.23334077885003
H	-2.41680837529931	-0.31300627551303	3.26156185053465
P	-1.39090362588814	0.87077961711545	5.02592406149898
O	-1.86280885983138	2.13885928393877	5.70444963505304
C	-0.57911283993814	-0.26869894684615	6.20884112088337
C	-0.10246206766891	0.28276920668137	7.41710173899858

C	-0.43037197278913	-1.64958664335217	5.95938396386438
C	0.53409213539295	-0.54065092980203	8.36008186990658
C	0.20833854024275	-2.46872974187260	6.90508103643084
C	0.69318867741960	-1.91380324522532	8.10300220960952
H	-0.25533103221629	1.35668586178035	7.60623826835760
H	-0.83219396409326	-2.08433208664135	5.03080900182539
H	0.90067058537978	-0.11060239559892	9.30509629444060
H	0.32037295626919	-3.54690911927461	6.71026778513006
H	1.18891631923163	-2.55868889211223	8.84554157067671
C	-0.25244894587181	1.15897754297271	3.61503232822378
C	0.95171376734869	0.45059571257067	3.42145205836474
C	-0.60232918042378	2.19878806218235	2.72382784865402
C	1.78837218042115	0.76729561575193	2.33703854992936
C	0.23237470685888	2.50549701399514	1.63798844010589
C	1.42780380748215	1.79012516525184	1.44354337102990
H	1.23952391575577	-0.34775127192133	4.12311286913365
H	-1.52148943709411	2.77869435957694	2.90216238810708
H	2.73008377202301	0.21530463152732	2.19492016114048
H	-0.04339012495154	3.31617631177102	0.94544784347527
H	2.08672492666437	2.03779407074901	0.59661429328373

Ligand-4

C	0.64122850635404	2.50579082193309	-1.85227395886186
C	-0.73612617115841	2.77871069856241	-1.77533717806951
C	1.36495691865017	2.16757385447183	-0.69951390011213
H	-1.29855229139780	3.04614184346052	-2.68292597106160
H	2.43680765338374	1.92672913629427	-0.77101098436355
C	-1.39352490299802	2.68921979063145	-0.53429872121124
C	0.71226279292657	2.08787566623468	0.55747033981266

H	-2.47363314725017	2.89323480246935	-0.46659882713128
C	-0.68289031961094	2.32874698766289	0.61810608409615
H	-1.18382274869441	2.23878641280126	1.59380201905568
H	1.15815875886140	2.55122977733524	-2.82401764850515
N	1.36814509603164	1.73645843853152	1.74516213286593
C	2.57350907846079	2.12740696342122	1.98254433491804
H	3.14659249942607	2.81266977403020	1.31359451208374
C	3.30999190742438	1.71525565471501	3.19424236260147
C	2.73143037110553	0.84774285835749	4.15086437262393
C	3.48302608032386	0.49924063142627	5.27810138581068
C	5.26620216261648	1.87774122113602	4.40576189684841
C	4.78103205457194	1.02319198337333	5.41354574613314
H	1.71060845074594	0.47696222870254	3.97905281684315
H	3.06625642957813	-0.17291727415202	6.04485286083425
H	6.28228442670497	2.30538079585387	4.48346272221677
H	5.40968831989737	0.77587550345806	6.28270406939472
N	4.55860506104662	2.22209907428946	3.32017629317752

Ligand-5

C	2.63980429296133	1.83777242984704	0.39496998352410
C	2.90550066194649	2.46435994039612	1.76929541744184
O	2.70229857278458	1.85471991235316	2.81739816881229
N	3.41624137105390	3.75112508224737	1.70655767473074
H	3.50862603642352	4.14372851676134	0.76732827585441
C	3.83909191074403	4.59994942446982	2.75091330585429
C	3.78197711917660	4.23239568037826	4.11601651041259
C	4.34176414054590	5.87520484101385	2.39828033134256
C	4.22601491314163	5.13760939033041	5.09284750877371
C	4.77973499433280	6.76664332365164	3.38658555855986

C	4.72544631751468	6.40369805701863	4.74359305684295
H	3.38854275081157	3.24464001977509	4.38221352212000
H	4.38783267820356	6.16764724600529	1.33570784781408
H	4.17712184865388	4.83993800026261	6.15235119092799
H	5.16651296848691	7.75370977595761	3.08970437181096
H	5.06951536623073	7.10287256679680	5.52056368430043
H	0.48872071479670	0.64044823809896	-3.91853858846795
O	0.69862920905200	0.04432968721869	-3.16580667533267
O	0.82918731822739	2.07516875156714	-2.18284938588440
C	0.91043979395002	0.86168648305396	-2.09983215209410
C	1.24595747294800	0.06825986990115	-0.84911593256133
H	2.16193413758294	-0.52599809715620	-1.06824638651962
H	0.44349034946969	-0.68935722158689	-0.71612603793177
C	1.41352342881250	0.91689294802054	0.41359239246251
H	1.49725057229334	0.25153423980066	1.29653406483568
H	0.50012916199486	1.52976989873818	0.56785957094133
H	3.54764579046465	1.24298585557149	0.13766127538866
H	2.52848036439563	2.61106267150713	-0.39253765795923

Coordinates of Optimized Geometries of Ligands:

Uranyl-Ligand-1(m)

U	-1.07998639474463	-0.20830737342824	-1.22693362402087
H	-2.09757680369819	1.65337671541786	-3.77056038099776
O	-2.48105224746872	-1.29596478384049	-1.12272853835539
H	1.56498358224500	-1.91286000931294	-1.57534412790653
O	0.42325535706173	0.74404514112775	-1.20815680947331
H	-1.98303122594993	-1.83436671392662	-3.77462578185894
H	-2.55269881984119	2.51015607980086	-1.00973268050969
O	-1.44747246622505	1.62839739597428	-3.04359244883959
H	-0.70495646446394	2.20373396893420	-3.30769865114423
O	-1.27260696736372	-1.19777055769077	-3.56976890777259
H	-0.71291673432671	-1.12653060466055	-4.36486889397335
O	0.60730044642095	-2.07600818649359	-1.48752393667142
H	0.45158868848918	-3.00089536272933	-1.75443107276543
O	-2.61535741143848	1.62613903090379	-0.60513159551369
H	-3.04157191555898	1.71977380331603	0.27739252991583
C	-3.35201989773041	0.82749659197142	2.37598694144610
C	-2.72892763332818	2.06078971542756	2.62832180084934
C	-2.60941866027416	-0.24653888465161	1.88668565627917
H	-3.31241843982283	2.88933229657825	3.03125158513283
H	-3.08516065395148	-1.21174693584377	1.70661279755295
C	-1.35399675037983	2.22045640304223	2.39932159307281
C	-1.23014051335229	-0.07563043939376	1.64915636517920
H	-0.86851292047181	3.17009026119621	2.62387210799905
C	-0.59870946575448	1.16036917237252	1.90648616814825
H	0.47429895246936	1.27470716517848	1.74247020991379
H	-4.41417539995612	0.69710689637264	2.58456359360141

N	-0.47928561223167	-1.13755957766962	1.06628701095267
H	0.51639122367214	-1.11554298727659	1.30180447281548
H	-0.85948138102527	-2.06733506369624	1.26329844594399

Uranyl-Ligand-2(m)

C	0.95670762374252	0.47485065108771	0.54023500388367
C	-0.16086043194892	0.71018478481941	-0.26969335239987
C	1.10216057061617	1.15528508221733	1.74648944815119
H	-0.27341452490401	0.17071703103737	-1.20987860634096
H	1.96122609176031	0.96456607779524	2.39174374059292
C	-1.12760722471760	1.64498118589460	0.11861253167306
C	0.12997697495543	2.09416193842102	2.11841681135059
H	-1.98596569125644	1.84230358758785	-0.52319622005025
C	-0.98383750833908	2.35400958549676	1.30994729021942
H	-1.70683326110544	3.12073201409804	1.58749923916670
H	1.71265484451184	-0.24841664882533	0.23531681494610
N	0.31449107013236	2.78699862778994	3.36086162553418
H	1.24834366250334	3.06693572556064	3.65966101570293
S	-0.86824838500896	3.14143445194389	4.40015730333737
O	-0.10191000642057	3.54296556110431	5.61971826216378
O	-1.83760058668536	4.13957147430684	3.96659681313959
N	-1.70348466577583	1.78524080465640	4.63871142338052
H	-2.68515102188805	1.80904802884032	4.36584359127236
H	-1.21609611778683	0.89605643937067	4.53503129150356
U	-0.63325694547655	4.81660068491864	7.62137742204107
H	-1.68354063854827	5.58753789345150	4.89742565182808
O	-2.21938492803735	4.02060645384044	7.68291026185909
H	1.52459081354951	2.64459108411860	8.43038807029082

O	0.95212885207389	5.61430397526916	7.66564018090918
H	0.07442659941851	5.04030597956516	10.73196397666179
H	-1.24212368667209	7.73558433030165	8.79942894987759
O	-1.38738984986171	6.13336783800589	5.67952341420313
H	-0.96135385666833	6.94087830364376	5.33926839934654
O	0.55683649632778	2.75438410604984	8.39370627832914
H	0.15919408594759	1.93580994634028	8.74205713241708
O	-0.66668475523454	4.83756646690871	10.13205265944256
H	-1.45791610477762	4.70847284962348	10.68707730073511
O	-1.68066889148451	6.97526737113553	8.37577949566368
H	-2.59332295294113	7.24798585962396	8.16680253416764

Uranyl-Ligand-2(b)

C	-1.84457118995837	6.78532726993165	0.11127472610180
C	-2.02396353072240	8.14740359082786	0.37881335864697
C	-1.54659929734240	5.90143080547001	1.14855990653460
H	-2.26149663437451	8.83182638078735	-0.43544423279129
H	-1.41030844941775	4.83654914777685	0.95479351218601
C	-1.89187418340330	8.63677424808777	1.68225620778798
C	-1.41144597700151	6.41038453718112	2.44275424643850
H	-2.01959878541660	9.70019543580358	1.88296887289474
C	-1.57397157574281	7.76928601790078	2.72689487472660
H	-1.43598195158461	8.14225404889513	3.74190392001663
H	-1.94257467447040	6.40845783312273	-0.90656068958584
N	-1.08397294425522	5.47886044575380	3.50421926106480
H	-0.18314364693958	4.99543306828002	3.51403372544769
S	-1.95478800360889	5.26253165561187	4.82215733866754
O	-1.40108590635466	4.04077622673657	5.47877002977642

O	-1.94886343099808	6.32011420788451	5.87512162655457
N	-3.44523830188770	5.22415575541687	4.27455129598138
H	-4.20068849424163	5.53987936552402	4.87988737666317
H	-3.66730539852348	4.68521044344622	3.43840134008859
U	-0.96976559585510	4.97107210858362	7.76484272282666
O	-2.59136178655088	4.53029894030667	8.33208562528988
H	0.51277022737946	2.21079425499221	7.52467083831500
O	0.69313550965927	5.40488387241550	7.32657703206103
H	0.70785724361623	4.87980823013734	10.43042749029533
H	-0.68834056721216	8.01150816339369	8.48743557754169
O	-0.34296546337748	2.58880354688062	7.80345011168611
H	-0.96120970181161	1.84201166061655	7.91756865981096
O	-0.19915257945413	4.73635824541498	10.09950669821363
H	-0.74756635294458	4.47844345850266	10.86475338348047
O	-1.30897442401064	7.26614659389510	8.59619592129356
H	-2.14061456019434	7.63475341342189	8.94979783998441

Uranyl-Ligand-3(m)

C	-10.49458405476441	0.67645698457732	2.79323134142051
C	-11.53749192012534	1.31561280516422	3.46948560464725
C	-9.16593400846829	0.98097500139770	3.08684678104270
H	-12.57414878169241	1.06752510197290	3.24465737077059
H	-8.35970912370028	0.48190053078661	2.54584660333652
C	-11.23624541652266	2.25609449250546	4.45699567170701
C	-8.86132696698690	1.92395264457021	4.07658048121343
H	-12.03784750935298	2.73805002081990	5.01817381543018
C	-9.90416327435906	2.57024416845678	4.76651106101295
H	-9.68728155285508	3.25653397580806	5.58403325903216

H	-10.71418040568902	-0.07096871527559	2.03061245330383
N	-7.49078273335720	2.19678729613995	4.35156947961131
H	-6.85388109226303	1.66902957934550	3.75329109785940
P	-6.88538167901184	3.66719706347431	4.84288877054572
O	-7.26258904877959	4.84168935360703	3.88356822927152
C	-7.49821231511903	4.06224315724908	6.46093966668499
C	-7.86964267972645	5.38382414798403	6.76373067767936
C	-7.53250379384564	3.05869083685200	7.44638950222247
C	-8.28664859656244	5.69370682001657	8.05766995921012
C	-7.95264727121000	3.38361627865738	8.73351304094696
C	-8.32824423683495	4.69738236445173	9.03783090963196
H	-7.83354445794037	6.15355883171043	5.99282382026399
H	-7.24553921890008	2.03465655679615	7.20382995905226
H	-8.57771426972335	6.71496356097666	8.30345151985494
H	-7.98781275521720	2.61216016385234	9.50261151943868
H	-8.65443573864040	4.94550500960481	10.04817860436683
C	-5.10599901245233	3.47574038986137	4.80945901462253
C	-4.46303543847585	2.22975961667578	4.85352697311218
C	-4.34406116988552	4.66450632986295	4.78933507797425
C	-3.06768948362382	2.17237446493521	4.83921454673332
C	-2.95007054540594	4.59306595846334	4.77675060711056
C	-2.31312620454414	3.34722432614845	4.79330787129286
H	-5.03481127849011	1.30363843863828	4.92362505437786
H	-4.84033001615263	5.63715950474303	4.83310349406112
H	-2.56881828129438	1.20380403547070	4.87433010200865
H	-2.36108838185893	5.51066710905886	4.77313411410857
H	-1.22433414185876	3.29374964580599	4.79005907510433
U	-7.82464846168972	5.23526049206064	1.74489452688086

H	-6.69017339521941	5.33183944123507	-1.25711201367253
O	-7.74431394369323	3.50159869074725	1.33106130529910
O	-8.04680564098737	6.98417633234871	1.99086563437875
H	-10.52167758781161	5.54951782197023	3.21722188496935
H	-4.71103900859511	5.33941683905757	1.16403085327886
H	-10.06678016266285	6.20773457170746	-0.30681399354924
O	-6.62439716956472	5.86309155211171	-0.44205143990721
H	-6.55805656999302	6.79443124923071	-0.72499237276777
O	-5.32154449060858	5.32485572876351	1.92165794649857
H	-4.82209541233533	5.03287230190117	2.71821384566266
O	-10.02583634816319	4.83365898345546	2.77950133782616
H	-10.16521187759292	4.01412490930002	3.33255732952207
O	-9.55838117022082	5.40184463429895	-0.10139518531876
H	-10.11971842516935	4.64500434064483	-0.35137397416609

Uranyl-Ligand-3(b)

C	-5.12663661041799	0.33006845898233	3.59146824817191
C	-6.03357424036620	-0.57163347620947	3.02515030816748
C	-5.51630815080731	1.64566214466270	3.85944701204987
H	-5.72802063215230	-1.59770928110165	2.82273571751409
H	-4.81666288347692	2.34154532593462	4.32893028041232
C	-7.33145847303996	-0.15256702142884	2.72199308155257
C	-6.82379348485844	2.05715031551158	3.55596240846693
H	-8.04219585710601	-0.84925542018733	2.27805259476237
C	-7.73252758552073	1.15968821854369	2.97596732833568
H	-8.74566248824028	1.47170124507863	2.72634058978258
H	-4.11473158069788	0.00975064263128	3.83989166490328
N	-7.17574606481920	3.43645619322254	3.76849484142474

H	-6.41251027602300	3.95279381686725	4.21686124142940
P	-8.73096899474412	3.98061172383302	4.35246430918093
O	-9.35170391581464	4.49897877986465	3.02839387069307
C	-9.64004640004028	2.62479365232912	5.02967560567738
C	-10.91383701639801	2.32818621829917	4.51526687591033
C	-9.07614257613483	1.85224361222312	6.06305643398025
C	-11.62632989235079	1.25450228265128	5.04742077320536
C	-9.79842971443641	0.78062233943529	6.57939755544012
C	-11.06978257666778	0.48416739439081	6.07293004570780
H	-11.33518128768976	2.93346274319502	3.71258122881945
H	-8.08457439042960	2.08276546926454	6.45629002491651
H	-12.61856865979103	1.01917589424799	4.66285337781506
H	-9.37221338375238	0.17426383286037	7.37842228068410
H	-11.63132350551357	-0.35533094650373	6.48376982342142
C	-8.38056855206860	5.24567912477620	5.54387769966436
C	-8.98284690815254	5.18214451710102	6.81502003156228
C	-7.52858241288740	6.31981907243332	5.20810052820596
C	-8.71821954733670	6.18325940668963	7.74810871095630
C	-7.27167796349847	7.30745100898910	6.15368721285162
C	-7.86304147572889	7.23863728579477	7.42133894853805
H	-9.65479596709394	4.36260833831964	7.06776835825689
H	-7.08631935845929	6.39784285398007	4.21383958863972
H	-9.18408279828508	6.13948401510653	8.73239344378477
H	-6.61404779856159	8.13948093757270	5.90212388265366
H	-7.65926550314019	8.01831110628095	8.15575958828567
U	-7.83544815413921	4.48556316542664	1.29564335407246
H	-7.07650784102867	4.47911762238334	-1.76943544816421
O	-8.68581568688472	3.13011204012318	0.51970805774869

O	-6.97626168163404	5.94647552006845	1.85475175923109
H	-5.44478870759997	2.47753954558973	1.70146942704715
H	-9.68932777440989	6.92075806237253	0.61766416220894
O	-6.89316930489300	5.00056123377297	-0.96561417771910
H	-6.49880256928580	5.84463548741698	-1.25350312469479
O	-5.64645193109937	3.26264238417101	1.14346092953781
H	-4.80698979461494	3.58742853160860	0.77214611684582
O	-9.56980952013087	5.98545075474711	0.36893195165415
H	-10.41208994377571	5.68026358767686	-0.01665871759313

Uranyl-Ligand-4(m)

C	-2.17192771632913	-4.93606770235657	4.16153850222749
C	-1.21792608208326	-5.66281670040884	3.42540338168326
C	-2.18117589208811	-3.55169910801136	4.11556003986099
H	-1.22120188515290	-6.75231850375355	3.46576236139138
H	-2.93542641586840	-2.98154386422591	4.65967778857021
C	-0.27972161044937	-4.99758352674679	2.62355027446707
C	-1.22505917058147	-2.87222163811776	3.31743893392410
H	0.44683636063624	-5.56860600122307	2.04605283203608
C	-0.29259350735885	-3.61262813255642	2.54883713292540
H	0.41192998275557	-3.06978762272382	1.91911698058602
H	-2.90995740384079	-5.46830944939865	4.76198437885143
N	-1.17933755182566	-1.49883467923716	3.20606728601895
C	-1.54400834388129	-0.67931169801905	4.12754427692328
H	-1.80429448978605	-1.01350225540952	5.14600066057136
C	-1.56890124761344	0.75848869778795	3.87295741196446
C	-0.99629233285147	1.29581158460459	2.70842697248284
C	-0.95814889495475	2.67143615523564	2.53004869283096

C	-2.07004976723882	2.91226484358687	4.64418940749913
C	-1.49357229682788	3.49783118183431	3.52624135254583
H	-0.57365705992181	0.60527154580047	1.97983671291994
H	-0.50346348492201	3.10130126698055	1.63704693312296
H	-2.50273732406662	3.52580513555323	5.43403311819795
H	-1.46408232107969	4.58352912602546	3.44214871640255
N	-2.13221337590156	1.56577422465000	4.82724516059568
U	-3.76085286031176	0.78949967890459	6.62141210171759
H	-5.49619607611343	0.74993436327332	3.97471964489259
O	-4.00988701520300	-0.91081052664590	6.12733047187784
H	-0.60732146452912	0.90686602199844	7.02177465198725
O	-3.72677020850861	2.47121638480772	7.21256338622074
H	-3.69233851962654	0.56680540586325	9.80601790424906
H	-6.59243219344966	1.51142936890910	7.87677003104259
O	-5.17515155575974	1.38152610719800	4.64393967946665
H	-5.44752524546683	2.27053696246378	4.35179637365380
O	-1.36759112215507	0.40778394346175	7.37045240968044
H	-1.13948944365914	0.12147550706536	8.27384834397315
O	-3.56423504120213	-0.02150903599324	9.03803260241603
H	-3.82986108203956	-0.91421256647708	9.32849023139118
O	-6.11910933564654	0.74552816507621	7.50249734731324
H	-6.77232542009700	0.02907025822418	7.40200129151774

Uranyl-Ligand-4(b)

C	0.26315011320126	0.81702940003642	10.74209586668267
C	-0.35855874689123	-0.28754841232738	11.33362088500721
C	-0.02938706031827	1.16923826722283	9.42441598431415
H	-0.12573596924809	-0.55652428666655	12.36378143548692
H	0.42428689749246	2.05274299169657	8.97281315700818

C	-1.27632785133689	-1.05169095086601	10.60207881028529
C	-0.94699335937910	0.39930137132645	8.69265178132042
H	-1.74091310208031	-1.92885334718485	11.05291467113073
C	-1.58353743936722	-0.71094702501686	9.28309482966326
H	-2.25340868649778	-1.33384222179371	8.68785879932863
H	0.97535912075471	1.41385636620162	11.31221330503781
N	-1.29176265104963	0.75727443214310	7.35944601708109
C	-0.35372617106689	0.97392357551758	6.49151647910186
H	0.70055554198468	0.84156578767088	6.76451313935747
C	-0.67356497285237	1.35438166421379	5.13134691741355
C	0.33780780938488	1.61416271272182	4.20248413409170
C	-0.00939606044977	1.97784089010618	2.90027402334038
C	-2.31892227409478	1.78921040013011	3.55296283779927
C	-1.36016179535025	2.06672140154407	2.57360345744522
H	1.38207394632036	1.53442848381835	4.50521331054828
H	0.76107321854573	2.18740655782182	2.15823801483468
H	-3.38035599367224	1.84425674856711	3.31823049876851
H	-1.68433959856292	2.34370944422788	1.57106665308261
N	-1.99975364662168	1.43363509992824	4.80802052966432
U	-3.71538456048405	1.16069165447476	6.70589635990207
H	-5.46264784478913	0.12076938852767	4.31642681251494
O	-3.83929442204913	-0.61119918846457	6.70929772699218
O	-3.76367322371918	2.93488501255953	6.69632155201613
H	-3.66567122349288	2.28934486598656	9.63813047282006
H	-6.58561201175415	2.02013216625658	7.80452487073844
O	-5.15996133865622	0.98933702955807	4.64426343778235
H	-5.83421475256318	1.64056490512141	4.37232192693367
O	-3.67211414944520	1.43173850471237	9.17360177343319

H	-3.11389491287574	0.80674613929831	9.69514451195307
O	-6.11821270494384	1.23151193705928	7.47136249515614
H	-6.61942264607164	0.45555404587043	7.78536301796260

Uranyl-Ligand-5(m)

C	1.65341120050218	2.81445543740133	-3.71272347497527
C	0.68509129939713	2.11382242477254	-4.63967385654211
O	0.82032193761267	2.14290009449839	-5.90417106983874
N	-0.35944983337138	1.50568788861727	-4.07204228306152
H	-0.35855780769317	1.46261997308657	-3.05239269198742
C	-1.49221825744210	0.93380601507376	-4.73429666631219
C	-2.17528748801243	1.66310122930135	-5.71812620544777
C	-1.92404543603098	-0.33752458703091	-4.34712258258192
C	-3.28767368164442	1.08480278830915	-6.33912552571625
C	-3.04243082297177	-0.89849239945105	-4.96697032909507
C	-3.71873179005497	-0.19587302967294	-5.96738574034521
H	-1.86288136624971	2.67492669224346	-5.97498671509641
H	-1.38702283632764	-0.88854308757006	-3.57376394120496
H	-3.83545198743728	1.65170144451615	-7.09238286900376
H	-3.38510051990606	-1.88774202901873	-4.66427747993427
H	-4.59645769823978	-0.63302892787653	-6.44330300643491
H	7.02702619631661	2.37171208425073	-5.36449121491731
O	6.27362534585329	2.08504136215863	-4.79907889186946
O	5.10824796113298	2.95342516476651	-6.49856781234729
C	5.13212373397391	2.38748948232734	-5.39362020603029
C	3.90801395320322	1.98702795797670	-4.61286047316192
H	4.21880010576787	1.49852914030955	-3.68112955816493
H	3.38299296501717	1.23715120309400	-5.22642949826705

C	2.99696183822062	3.19577298604036	-4.32897124629436
H	2.81574377632167	3.76337184929903	-5.24976967797703
H	3.50603106306025	3.87691259069415	-3.63332763999357
H	1.78641271888806	2.20159360701592	-2.80650774682394
H	1.14070566753334	3.73316154376293	-3.37777095478834
U	1.40815537625315	1.72223004813782	-8.08691661291257
H	2.17961355740098	3.02289694356495	-10.85711302636832
O	0.21869882490740	2.88526689418866	-8.71605904540023
H	-0.72335981010347	-0.47369263484636	-8.37139083881667
O	2.68625616967593	0.59727870038701	-7.55851959696693
H	0.96681416299632	0.02567565030690	-10.79786527040002
H	3.89531383539118	3.25377788970354	-7.17191861412236
O	2.47900338622003	2.23607338338672	-10.36433202551445
H	3.43126717194429	2.14027169821690	-10.55227864610113
O	1.05965652626561	-0.18148570787615	-9.84903181783431
H	1.66215304049081	-0.94761640049157	-9.79837914046677
O	-0.44754082058404	0.12022490924066	-7.64922248278774
H	-1.25899357307497	0.42525939161123	-7.17352377628350
O	2.97965952978087	3.43481482892601	-7.69312784303731
H	2.87934428001621	4.38757572064737	-7.86484372077179

Uranyl-Ligand-5(b)

C	0.16593427134692	3.13244083655227	-4.78418364353161
C	0.04520720388527	1.61337527063369	-4.78717283042064
O	0.29929189958441	0.97342754442660	-5.85600513544715
N	-0.32179990399086	0.95945463285863	-3.68937188598442
H	-0.58438046449493	1.50746222374738	-2.86951604367586
C	-0.42298115497412	-0.47133041983117	-3.60173084231033

C	0.66181060685260	-1.27044355572775	-3.99370055209275
C	-1.59784003181160	-1.03647080715547	-3.10526630594762
C	0.54367474805072	-2.65976539063010	-3.90825985639782
C	-1.69971479737839	-2.42740439155291	-3.02266249500062
C	-0.63815977196486	-3.23831000861383	-3.43115035046302
H	1.60446310164130	-0.80921733919702	-4.29077377447663
H	-2.42989223020087	-0.40193034683088	-2.79694881455348
H	1.39217254512754	-3.29078393005930	-4.17523155757193
H	-2.61461394638373	-2.87613476644408	-2.63633263952269
H	-0.72105053345604	-4.32230684585573	-3.35494379159423
H	1.44654629786515	6.66750122058334	-8.37244779419340
O	1.49011790594085	5.83427604877326	-8.88709721206704
O	1.21049092501990	3.66638344516327	-8.72716217673429
C	1.18062349875670	4.77376218167065	-8.16686075008179
C	0.80345065494121	4.91743416755514	-6.70069026525757
H	-0.07508554325885	5.57691649223316	-6.61446931409500
H	1.63129337954834	5.40508581458304	-6.16092239633622
C	0.53498125067917	3.50209137070425	-6.21443414597651
H	1.46769337728671	2.94884592401291	-6.42817709908048
H	-0.28942555634160	3.12419729801740	-6.84666287859439
H	0.93679938110402	3.43788245301183	-4.05989129873625
H	-0.78509091867128	3.58336267964118	-4.46192427042912
U	0.79498021871485	1.14016895087950	-8.16334469825077
H	0.50462058309946	1.81831525475984	-11.24594767435780
O	-0.93649823315374	1.27397783152766	-8.52575343119959
H	1.08686463342666	-1.95685943311638	-7.58455146785853
O	2.54525742183800	1.06516089039650	-7.89469082978611
H	0.20386677726684	-1.27835074206222	-10.17550913924832

O	1.23965531136834	1.81156787433601	-10.60414613773886
H	1.61194242765797	2.71773397162598	-10.61797063460908
O	0.97024046313067	-0.77782512410656	-9.83879094223547
H	1.62314582885063	-0.72663027014727	-10.56249057419756
O	0.56146076065260	-1.20120386119846	-7.26653704233831
H	0.40303747044401	-1.32078214916450	-6.30216873660582