

Insight into selectivity: Uptake studies of radionuclides  $^{90}\text{Sr}^{2+}$ ,  $^{137}\text{Cs}^+$ , and  $^{233}\text{UO}_2^{2+}$   
with bis-amidoxime polymers

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**Table S1: Counting Methods**

Isotope	Method	Region of Interest (keV)	Time (min.)	Sigma
<sup>90</sup> Sr	Alpha/Beta	0-750	10	0.2
<sup>137</sup> Cs	Gamma	580-754	10	0.3
<sup>233</sup> U	Alpha/Beta	0-750	10	0.2

**Table S2: Cartesian coordinates for optimized Sr, Cs, and U complexes**

Metal	Starting Geometry	Ligand Protonation State		
		bis-AO <sup>-1</sup>	bis-AO	bis-AO <sup>+1</sup>
Sr	(A)	SrA1	SrA2	SrA3
	(B)	SrB1	SrB2	SrB3
	(C)	SrC1	SrC2	SrC3
	(D)	SrD1	SrD2	NA
Cs	(A)	CsA1	CsA2	
	(B)	CsB1	CsB2	
	(C)	CsC1	CsC2	
	(D)	CsD1	CsD2	
U	(B)	UB1	UB2	UB3
	(D)	UD1	UD2	UD3

## SrA1

C	5.012073000000	5.548133000000	-2.398450000000
C	4.464289000000	4.314425000000	-2.741354000000
C	3.296158000000	4.266692000000	-3.502673000000
C	2.668579000000	5.447769000000	-3.922207000000
C	3.230688000000	6.675794000000	-3.560752000000
C	4.399208000000	6.733148000000	-2.804994000000
H	5.920086000000	5.579084000000	-1.805654000000
H	4.939155000000	3.394415000000	-2.422280000000
H	2.746909000000	7.590349000000	-3.886917000000
H	4.827375000000	7.692719000000	-2.537850000000
O	2.674189000000	3.077264000000	-3.827379000000
C	3.441687000000	1.932598000000	-4.055887000000
C	4.426335000000	1.968324000000	-5.042521000000
C	3.162246000000	0.764029000000	-3.326218000000
C	5.181762000000	0.833244000000	-5.314347000000
H	4.597382000000	2.890972000000	-5.586151000000
C	3.935647000000	-0.371933000000	-3.636553000000
C	4.934821000000	-0.342164000000	-4.601081000000
H	5.945940000000	0.864095000000	-6.083478000000
H	3.727943000000	-1.287923000000	-3.097579000000
H	5.508384000000	-1.238958000000	-4.810701000000
C	2.123408000000	0.676034000000	-2.273304000000
N	0.918847000000	1.370224000000	-2.409013000000
H	0.999189000000	2.281969000000	-2.835623000000
H	0.433838000000	1.374599000000	-1.516562000000
N	2.326179000000	-0.133405000000	-1.276321000000
C	1.420739000000	5.403449000000	-4.741320000000
N	0.222399000000	5.402047000000	-4.086730000000
N	1.563101000000	5.433757000000	-6.023170000000
H	0.203977000000	5.163814000000	-3.108347000000
H	-0.605809000000	5.177210000000	-4.617727000000
O	1.302093000000	-0.162437000000	-0.365024000000
O	0.270402000000	5.400913000000	-6.645509000000
H	0.476130000000	5.383463000000	-7.587404000000
Sr	1.320781000000	-2.069404000000	1.260373000000

## SrA2

C	5.292005000000	6.155048000000	-2.776284000000
C	4.893466000000	4.830479000000	-2.624403000000
C	3.658669000000	4.409720000000	-3.111686000000
C	2.777055000000	5.310985000000	-3.731411000000
C	3.200821000000	6.643694000000	-3.868721000000

C	4.443653000000	7.063281000000	-3.407307000000
H	6.257267000000	6.473643000000	-2.398620000000
H	5.532141000000	4.112196000000	-2.122924000000
H	2.548480000000	7.355318000000	-4.360989000000
H	4.744776000000	8.096707000000	-3.537138000000
O	3.255742000000	3.105574000000	-2.871776000000
C	3.791590000000	2.052305000000	-3.577790000000
C	4.813284000000	2.188043000000	-4.516281000000
C	3.252571000000	0.785007000000	-3.291151000000
C	5.321250000000	1.056522000000	-5.153183000000
H	5.217224000000	3.165239000000	-4.746815000000
C	3.784925000000	-0.335188000000	-3.936444000000
C	4.818767000000	-0.209307000000	-4.861012000000
H	6.115907000000	1.174224000000	-5.882210000000
H	3.364525000000	-1.309230000000	-3.715104000000
H	5.215949000000	-1.087950000000	-5.356452000000
C	2.111069000000	0.623927000000	-2.349162000000
N	0.975886000000	1.339102000000	-2.580882000000
H	1.062590000000	2.161781000000	-3.165102000000
H	0.318122000000	1.408866000000	-1.817248000000
N	2.262153000000	-0.266584000000	-1.418937000000
C	1.418431000000	4.939619000000	-4.212170000000
N	0.442256000000	5.897252000000	-4.125636000000
N	1.240432000000	3.779978000000	-4.761555000000
H	0.522049000000	6.588196000000	-3.395695000000
H	-0.499782000000	5.592950000000	-4.321598000000
O	1.020327000000	-0.387411000000	-0.671932000000
H	1.311756000000	-0.702066000000	0.192980000000
O	-0.123470000000	3.651708000000	-5.168819000000
H	-0.149292000000	2.793001000000	-5.607651000000
Sr	-0.884708000000	-2.124389000000	-1.746616000000

### SrA3

C	5.308126000000	6.170840000000	-2.744252000000
C	4.907728000000	4.848379000000	-2.579370000000
C	3.680014000000	4.423416000000	-3.075609000000
C	2.794695000000	5.311774000000	-3.709767000000
C	3.229813000000	6.639094000000	-3.870713000000
C	4.468017000000	7.065321000000	-3.403281000000
H	6.268356000000	6.495576000000	-2.359714000000
H	5.540332000000	4.135322000000	-2.063177000000
H	2.594718000000	7.346157000000	-4.390049000000
H	4.770908000000	8.095590000000	-3.551450000000
O	3.290889000000	3.110881000000	-2.835809000000

C	3.803579000000	2.074750000000	-3.565925000000
C	4.850019000000	2.197879000000	-4.477090000000
C	3.222311000000	0.810514000000	-3.336994000000
C	5.325922000000	1.069317000000	-5.140540000000
H	5.295560000000	3.165329000000	-4.666343000000
C	3.721711000000	-0.313738000000	-4.008861000000
C	4.772571000000	-0.188940000000	-4.908349000000
H	6.139440000000	1.181532000000	-5.848670000000
H	3.255353000000	-1.281120000000	-3.860719000000
H	5.143712000000	-1.060834000000	-5.433071000000
C	2.060167000000	0.672369000000	-2.441713000000
N	1.041123000000	1.494481000000	-2.508058000000
H	1.079573000000	2.287701000000	-3.151073000000
H	0.250163000000	1.395590000000	-1.886498000000
C	1.433885000000	4.942932000000	-4.190346000000
N	0.511802000000	5.945849000000	-4.286480000000
N	1.194793000000	3.723838000000	-4.573507000000
H	0.596512000000	6.740241000000	-3.672418000000
H	-0.434327000000	5.666636000000	-4.497569000000
O	0.917185000000	-0.626872000000	-0.867913000000
H	1.062107000000	-0.353431000000	0.053564000000
O	-0.159069000000	3.625786000000	-5.020326000000
H	-0.204556000000	2.752842000000	-5.429240000000
Sr	-0.748845000000	-3.069391000000	-1.254334000000
N	2.073306000000	-0.329198000000	-1.565356000000
H	2.797475000000	-1.034624000000	-1.535757000000

### SrB1

C	5.218071000000	6.273431000000	-2.730712000000
C	4.862372000000	4.937049000000	-2.572712000000
C	3.673996000000	4.458765000000	-3.120618000000
C	2.804231000000	5.315161000000	-3.814649000000
C	3.177439000000	6.661595000000	-3.952169000000
C	4.373858000000	7.137877000000	-3.426629000000
H	6.146259000000	6.637354000000	-2.303984000000
H	5.496133000000	4.254768000000	-2.017490000000
H	2.519419000000	7.336301000000	-4.487868000000
H	4.641756000000	8.180661000000	-3.555132000000
O	3.292856000000	3.151496000000	-2.853751000000
C	3.824526000000	2.092025000000	-3.580267000000
C	4.890310000000	2.261617000000	-4.461930000000
C	3.250491000000	0.822276000000	-3.355957000000
C	5.435753000000	1.161167000000	-5.120976000000
H	5.303460000000	3.248013000000	-4.630256000000
C	3.826609000000	-0.264415000000	-4.039329000000

C	4.909317000000	-0.110232000000	-4.898706000000
H	6.264562000000	1.306137000000	-5.805863000000
H	3.387183000000	-1.243243000000	-3.890528000000
H	5.321920000000	-0.973518000000	-5.410243000000
C	2.092765000000	0.592184000000	-2.473852000000
N	1.079968000000	1.587134000000	-2.317915000000
H	0.952581000000	2.150893000000	-3.151971000000
H	0.226642000000	1.079453000000	-2.075929000000
N	1.979137000000	-0.534992000000	-1.831194000000
C	1.491195000000	4.874378000000	-4.359669000000
N	0.423175000000	5.713009000000	-4.167895000000
N	1.442984000000	3.780596000000	-5.046362000000
H	0.440842000000	6.321569000000	-3.364082000000
H	-0.485959000000	5.343912000000	-4.404555000000
O	0.853806000000	-0.671505000000	-1.104549000000
O	0.098987000000	3.546406000000	-5.475962000000
H	0.164158000000	2.728601000000	-5.983245000000
Sr	1.557324000000	3.102850000000	-0.070174000000

## SrB2

C	5.202436000000	6.256394000000	-2.682993000000
C	4.837591000000	4.924837000000	-2.506900000000
C	3.658844000000	4.441270000000	-3.066520000000
C	2.791582000000	5.284050000000	-3.782679000000
C	3.184105000000	6.623493000000	-3.947208000000
C	4.374745000000	7.105599000000	-3.414579000000
H	6.125336000000	6.624704000000	-2.249154000000
H	5.460836000000	4.247545000000	-1.934053000000
H	2.548809000000	7.291922000000	-4.516039000000
H	4.650204000000	8.142987000000	-3.567464000000
O	3.299299000000	3.123283000000	-2.800027000000
C	3.830515000000	2.092372000000	-3.555366000000
C	4.889676000000	2.284125000000	-4.441829000000
C	3.271053000000	0.812951000000	-3.375979000000
C	5.417217000000	1.202876000000	-5.142731000000
H	5.307015000000	3.272232000000	-4.583695000000
C	3.825434000000	-0.257618000000	-4.092998000000
C	4.892299000000	-0.075409000000	-4.964920000000
H	6.239636000000	1.368514000000	-5.830305000000
H	3.388037000000	-1.240163000000	-3.966369000000
H	5.297037000000	-0.919380000000	-5.511873000000
C	2.106023000000	0.555382000000	-2.493626000000
N	1.117843000000	1.530995000000	-2.343898000000
H	1.088204000000	2.199945000000	-3.108662000000
H	0.208052000000	1.124639000000	-2.151024000000

N	2.064010000000	-0.579377000000	-1.883798000000
C	1.477281000000	4.854127000000	-4.333334000000
N	0.483762000000	5.796112000000	-4.387675000000
N	1.353266000000	3.653950000000	-4.805642000000
H	0.495864000000	6.537805000000	-3.704783000000
H	-0.435768000000	5.458800000000	-4.630997000000
O	0.859794000000	-0.690096000000	-1.141490000000
H	0.895397000000	-1.583598000000	-0.779166000000
O	0.024581000000	3.470494000000	-5.295878000000
H	0.042331000000	2.583487000000	-5.675055000000
Sr	1.561176000000	3.155927000000	0.032418000000

### SrB3

C	5.131446000000	6.175956000000	-2.625626000000
C	4.777430000000	4.834224000000	-2.521140000000
C	3.591618000000	4.377716000000	-3.087218000000
C	2.699604000000	5.252253000000	-3.731907000000
C	3.088337000000	6.600017000000	-3.830740000000
C	4.286397000000	7.058415000000	-3.294367000000
H	6.060358000000	6.524435000000	-2.188532000000
H	5.415989000000	4.129247000000	-2.001177000000
H	2.450160000000	7.299060000000	-4.357075000000
H	4.554338000000	8.103737000000	-3.397463000000
O	3.247203000000	3.043089000000	-2.910856000000
C	3.850971000000	2.052874000000	-3.637130000000
C	4.942673000000	2.256271000000	-4.478590000000
C	3.321731000000	0.754293000000	-3.480926000000
C	5.518229000000	1.174914000000	-5.141382000000
H	5.346861000000	3.250380000000	-4.614574000000
C	3.922896000000	-0.321195000000	-4.151563000000
C	5.020493000000	-0.116779000000	-4.976832000000
H	6.365292000000	1.351090000000	-5.795138000000
H	3.498831000000	-1.313796000000	-4.054547000000
H	5.469517000000	-0.952506000000	-5.499663000000
C	2.112994000000	0.516595000000	-2.674792000000
N	1.079465000000	1.320800000000	-2.722233000000
H	1.110979000000	2.150232000000	-3.317618000000
H	0.275620000000	1.153492000000	-2.132094000000
C	1.377344000000	4.847184000000	-4.285141000000
N	0.426715000000	5.820226000000	-4.412691000000
N	1.197831000000	3.627385000000	-4.696701000000
H	0.452811000000	6.606357000000	-3.783068000000
H	-0.498013000000	5.510848000000	-4.671488000000
O	0.970616000000	-0.780374000000	-1.114014000000
H	0.502652000000	-1.562692000000	-1.449067000000



O	-0.127083000000	3.492175000000	-5.211603000000
H	-0.129996000000	2.615751000000	-5.615565000000
Sr	2.408897000000	4.296259000000	0.907184000000
N	2.066980000000	-0.598845000000	-1.940304000000
H	2.914836000000	-1.045818000000	-1.614728000000

### SrC1

C	5.087781000000	5.905398000000	-2.665286000000
C	4.606131000000	4.600621000000	-2.700355000000
C	3.375046000000	4.332525000000	-3.298333000000
C	2.613459000000	5.364898000000	-3.860011000000
C	3.105147000000	6.675489000000	-3.798388000000
C	4.337493000000	6.947282000000	-3.213028000000
H	6.045163000000	6.109002000000	-2.198024000000
H	5.172168000000	3.788459000000	-2.258765000000
H	2.518036000000	7.480541000000	-4.226780000000
H	4.709714000000	7.965062000000	-3.182492000000
O	2.827740000000	3.064776000000	-3.244075000000
C	3.494833000000	1.969958000000	-3.778698000000
C	4.439338000000	2.123068000000	-4.793375000000
C	3.149769000000	0.698227000000	-3.278148000000
C	5.085739000000	1.007642000000	-5.318985000000
H	4.672246000000	3.113034000000	-5.166339000000
C	3.813250000000	-0.405879000000	-3.842015000000
C	4.774768000000	-0.263398000000	-4.836543000000
H	5.818816000000	1.136177000000	-6.108226000000
H	3.550011000000	-1.391474000000	-3.478458000000
H	5.264600000000	-1.140834000000	-5.245340000000
C	2.143380000000	0.476957000000	-2.211323000000
N	0.985150000000	1.258533000000	-2.156265000000
H	1.120746000000	2.234602000000	-2.377702000000
H	0.525927000000	1.102548000000	-1.263369000000
N	2.316099000000	-0.527112000000	-1.403673000000
C	1.288978000000	5.096429000000	-4.491351000000
N	0.196876000000	5.692705000000	-3.937949000000
N	1.290769000000	4.367775000000	-5.559161000000
H	0.261544000000	6.018382000000	-2.986248000000
H	-0.714187000000	5.374952000000	-4.235075000000
O	1.317421000000	-0.676326000000	-0.475740000000
O	-0.071310000000	4.223946000000	-6.042455000000
H	-0.059792000000	3.366737000000	-6.486939000000
Sr	0.853423000000	-2.928499000000	0.515430000000
Sr	-1.108613000000	6.145192000000	-7.766506000000

## SrC2

C	5.157400000000	6.038178000000	-2.750497000000
C	4.727321000000	4.716726000000	-2.682140000000
C	3.480653000000	4.363608000000	-3.194008000000
C	2.636613000000	5.326388000000	-3.764379000000
C	3.082952000000	6.655859000000	-3.809893000000
C	4.333912000000	7.011092000000	-3.316960000000
H	6.129334000000	6.306890000000	-2.351659000000
H	5.347290000000	3.954111000000	-2.224650000000
H	2.443355000000	7.411847000000	-4.251232000000
H	4.662427000000	8.042775000000	-3.371478000000
O	3.017578000000	3.068159000000	-3.027311000000
C	3.614679000000	2.011172000000	-3.677683000000
C	4.536381000000	2.169588000000	-4.711125000000
C	3.231652000000	0.726283000000	-3.253375000000
C	5.094658000000	1.045742000000	-5.317385000000
H	4.820612000000	3.161350000000	-5.039060000000
C	3.807560000000	-0.385804000000	-3.876624000000
C	4.737459000000	-0.235205000000	-4.901790000000
H	5.809689000000	1.180117000000	-6.121953000000
H	3.508708000000	-1.375041000000	-3.550608000000
H	5.170563000000	-1.108753000000	-5.375583000000
C	2.234165000000	0.527757000000	-2.166200000000
N	1.008093000000	1.113953000000	-2.277643000000
H	0.941689000000	1.922707000000	-2.877559000000
H	0.453567000000	1.159423000000	-1.433958000000
N	2.591461000000	-0.277263000000	-1.215316000000
C	1.281718000000	4.995198000000	-4.287421000000
N	0.255505000000	5.820213000000	-3.929823000000
N	1.184216000000	3.997721000000	-5.106285000000
H	0.356340000000	6.361120000000	-3.084807000000
H	-0.681160000000	5.500538000000	-4.129494000000
O	1.477198000000	-0.454470000000	-0.298838000000
H	1.909860000000	-0.628286000000	0.546923000000
O	-0.194907000000	3.864722000000	-5.532732000000
H	-0.273011000000	2.925510000000	-5.744163000000
Sr	-0.202539000000	-2.578967000000	-0.931678000000
Sr	-0.975472000000	5.344153000000	-7.784681000000

## SrC3

C	5.234780000000	6.174890000000	-2.922144000000
C	4.877167000000	4.841168000000	-2.749990000000
C	3.614894000000	4.403112000000	-3.136417000000
C	2.659508000000	5.289428000000	-3.658982000000

C	3.048325000000	6.629457000000	-3.826764000000
C	4.319078000000	7.068727000000	-3.472736000000
H	6.221830000000	6.510041000000	-2.624318000000
H	5.569789000000	4.132362000000	-2.311127000000
H	2.350181000000	7.334945000000	-4.260848000000
H	4.588358000000	8.107912000000	-3.622687000000
O	3.257281000000	3.084204000000	-2.890722000000
C	3.783796000000	2.048395000000	-3.612221000000
C	4.774040000000	2.187285000000	-4.581665000000
C	3.269317000000	0.768542000000	-3.315944000000
C	5.263039000000	1.059572000000	-5.236955000000
H	5.165845000000	3.165958000000	-4.824006000000
C	3.780705000000	-0.353594000000	-3.983160000000
C	4.777175000000	-0.212763000000	-4.939900000000
H	6.032230000000	1.183906000000	-5.991021000000
H	3.364466000000	-1.334824000000	-3.785455000000
H	5.157481000000	-1.084128000000	-5.458813000000
C	2.164336000000	0.608349000000	-2.355497000000
N	1.122324000000	1.406152000000	-2.364410000000
H	1.105370000000	2.200491000000	-3.001878000000
H	0.371425000000	1.291686000000	-1.697479000000
C	1.265255000000	4.902247000000	-4.017328000000
N	0.308230000000	5.865903000000	-3.910754000000
N	1.037015000000	3.711774000000	-4.490908000000
H	0.467378000000	6.630339000000	-3.273511000000
H	-0.652091000000	5.564376000000	-3.985973000000
O	1.135274000000	-0.708827000000	-0.720923000000
H	1.325571000000	-0.438837000000	0.193218000000
O	-0.350798000000	3.618433000000	-4.874268000000
H	-0.497572000000	2.669719000000	-4.981028000000
Sr	-0.530309000000	-3.154891000000	-1.097389000000
Sr	-1.032506000000	4.758134000000	-7.508691000000
N	2.246611000000	-0.388522000000	-1.478125000000
H	2.987818000000	-1.076773000000	-1.482543000000

### SrD1

C	5.023446000000	6.348345000000	-2.152401000000
C	4.601607000000	5.022228000000	-2.156496000000
C	3.523020000000	4.631062000000	-2.946174000000
C	2.819632000000	5.564309000000	-3.725708000000
C	3.261208000000	6.897927000000	-3.701381000000
C	4.353418000000	7.288241000000	-2.934057000000
H	5.867111000000	6.643622000000	-1.538410000000
H	5.100621000000	4.277775000000	-1.546295000000
H	2.744437000000	7.633529000000	-4.306707000000

H	4.675713000000	8.323433000000	-2.943769000000
O	3.078239000000	3.320356000000	-2.856440000000
C	3.727519000000	2.303543000000	-3.537232000000
C	4.908057000000	2.522609000000	-4.247073000000
C	3.147775000000	1.019394000000	-3.468292000000
C	5.551127000000	1.463522000000	-4.882485000000
H	5.330423000000	3.517738000000	-4.300031000000
C	3.821255000000	-0.024874000000	-4.126551000000
C	5.010283000000	0.180527000000	-4.815765000000
H	6.468223000000	1.649185000000	-5.431346000000
H	3.377225000000	-1.012188000000	-4.096658000000
H	5.498588000000	-0.650286000000	-5.313489000000
C	1.879921000000	0.724540000000	-2.768367000000
N	0.887917000000	1.717935000000	-2.588551000000
H	0.884545000000	2.417375000000	-3.323390000000
H	-0.008415000000	1.237011000000	-2.510260000000
N	1.664793000000	-0.470813000000	-2.318441000000
C	1.616000000000	5.221260000000	-4.530096000000
N	0.624219000000	6.167651000000	-4.606040000000
N	1.596273000000	4.101669000000	-5.177220000000
H	0.518635000000	6.798986000000	-3.826692000000
H	-0.243363000000	5.866564000000	-5.024991000000
O	0.436446000000	-0.687316000000	-1.755434000000
O	0.363411000000	3.982741000000	-5.887937000000
H	0.441371000000	3.130889000000	-6.333554000000
Sr	1.456259000000	-3.056994000000	-1.631134000000
Sr	1.093740000000	3.014595000000	-0.097755000000

## SrD2

C	5.357169000000	6.210281000000	-2.836253000000
C	4.957816000000	4.889882000000	-2.651754000000
C	3.723659000000	4.460153000000	-3.131312000000
C	2.845808000000	5.344451000000	-3.778104000000
C	3.268669000000	6.673383000000	-3.946466000000
C	4.510506000000	7.103205000000	-3.491119000000
H	6.321505000000	6.537983000000	-2.464177000000
H	5.593854000000	4.183805000000	-2.129969000000
H	2.615618000000	7.372786000000	-4.455272000000
H	4.812313000000	8.133282000000	-3.643739000000
O	3.315072000000	3.163285000000	-2.850343000000
C	3.797026000000	2.094869000000	-3.569202000000
C	4.811876000000	2.203302000000	-4.518496000000
C	3.220675000000	0.844293000000	-3.281869000000
C	5.274695000000	1.062696000000	-5.171266000000
H	5.244352000000	3.169077000000	-4.745102000000

C	3.710398000000	-0.287937000000	-3.945112000000
C	4.733594000000	-0.188131000000	-4.882626000000
H	6.063023000000	1.160757000000	-5.909858000000
H	3.260400000000	-1.249152000000	-3.728749000000
H	5.092688000000	-1.075269000000	-5.391549000000
C	2.088561000000	0.688313000000	-2.330935000000
N	1.027082000000	1.578641000000	-2.377991000000
H	0.981508000000	2.141175000000	-3.221361000000
H	0.136934000000	1.169724000000	-2.120852000000
N	2.171843000000	-0.301601000000	-1.506321000000
C	1.488172000000	4.958126000000	-4.250623000000
N	0.495932000000	5.891833000000	-4.121802000000
N	1.329419000000	3.809481000000	-4.827681000000
H	0.578856000000	6.580311000000	-3.390291000000
H	-0.444122000000	5.586144000000	-4.323319000000
O	0.935665000000	-0.420594000000	-0.759695000000
H	1.231027000000	-0.648807000000	0.132259000000
O	-0.042015000000	3.655518000000	-5.207141000000
H	-0.044510000000	2.841090000000	-5.724309000000
Sr	-0.555392000000	-2.678486000000	-1.588569000000
Sr	0.967309000000	3.585683000000	-0.154499000000

### CsA1

C	4.969773000000	5.454945000000	-2.353278000000
C	4.428106000000	4.239510000000	-2.765967000000
C	3.273135000000	4.229108000000	-3.548965000000
C	2.653363000000	5.432233000000	-3.919102000000
C	3.211059000000	6.639876000000	-3.490628000000
C	4.366358000000	6.659457000000	-2.712341000000
H	5.867422000000	5.454927000000	-1.743988000000
H	4.899473000000	3.305714000000	-2.484928000000
H	2.733002000000	7.569613000000	-3.780373000000
H	4.790507000000	7.604280000000	-2.391597000000
O	2.658819000000	3.063968000000	-3.958016000000
C	3.416680000000	1.894730000000	-4.096890000000
C	4.418505000000	1.868027000000	-5.065483000000
C	3.117107000000	0.776754000000	-3.297513000000
C	5.180696000000	0.719597000000	-5.249205000000
H	4.598698000000	2.755920000000	-5.662024000000
C	3.901615000000	-0.375049000000	-3.518333000000
C	4.920291000000	-0.405339000000	-4.461737000000
H	5.959401000000	0.700305000000	-6.003990000000
H	3.683844000000	-1.255394000000	-2.926157000000
H	5.498728000000	-1.313114000000	-4.599555000000
C	2.055198000000	0.757034000000	-2.271236000000

N	0.849885000000	1.445559000000	-2.480027000000
H	0.951705000000	2.334547000000	-2.949052000000
H	0.359634000000	1.512784000000	-1.591615000000
N	2.223117000000	0.011374000000	-1.214520000000
C	1.417435000000	5.430011000000	-4.756785000000
N	0.211762000000	5.345230000000	-4.122559000000
N	1.574105000000	5.570731000000	-6.029858000000
H	0.185176000000	5.047229000000	-3.161133000000
H	-0.605995000000	5.146370000000	-4.679205000000
O	1.199954000000	0.029564000000	-0.325472000000
O	0.289153000000	5.565723000000	-6.669722000000
H	0.506310000000	5.623310000000	-7.607429000000
Cs	3.006239000000	-2.093058000000	1.122967000000

## CsA2

C	5.135494000000	5.706771000000	-2.393471000000
C	4.533547000000	4.457631000000	-2.519663000000
C	3.366498000000	4.330957000000	-3.270024000000
C	2.780369000000	5.441966000000	-3.887522000000
C	3.399021000000	6.689203000000	-3.746139000000
C	4.571910000000	6.825086000000	-3.008381000000
H	6.043573000000	5.804221000000	-1.808459000000
H	4.965902000000	3.584385000000	-2.044977000000
H	2.950054000000	7.553344000000	-4.222928000000
H	5.040043000000	7.798010000000	-2.909578000000
O	2.710275000000	3.112919000000	-3.375255000000
C	3.398707000000	1.976374000000	-3.762526000000
C	4.461203000000	2.030456000000	-4.663125000000
C	2.947631000000	0.747543000000	-3.252490000000
C	5.096389000000	0.855023000000	-5.054877000000
H	4.789615000000	2.986555000000	-5.052406000000
C	3.597993000000	-0.421339000000	-3.669660000000
C	4.668341000000	-0.375157000000	-4.557691000000
H	5.920651000000	0.905376000000	-5.758075000000
H	3.245698000000	-1.372778000000	-3.289006000000
H	5.155971000000	-1.292625000000	-4.867302000000
C	1.812062000000	0.653386000000	-2.294807000000
N	0.626412000000	1.263607000000	-2.601088000000
H	0.664068000000	2.046436000000	-3.235360000000
H	-0.032408000000	1.363717000000	-1.841934000000
N	1.998658000000	-0.092670000000	-1.253305000000
C	1.521999000000	5.309754000000	-4.677295000000
N	0.351407000000	5.118719000000	-4.002015000000
N	1.621798000000	5.452874000000	-5.956441000000
H	0.385393000000	4.838151000000	-3.035714000000

H	-0.457698000000	4.824625000000	-4.528315000000
O	0.322574000000	5.335875000000	-6.549039000000
H	0.501394000000	5.390964000000	-7.495047000000
Cs	4.992963000000	-0.823324000000	0.279386000000
O	0.797486000000	-0.135830000000	-0.479356000000
H	1.040234000000	-0.655276000000	0.296061000000

### CsB1

C	4.975307000000	5.529986000000	-2.580119000000
C	4.624121000000	4.325880000000	-3.188519000000
C	3.420749000000	4.227598000000	-3.890798000000
C	2.556902000000	5.333625000000	-3.979619000000
C	2.937028000000	6.532091000000	-3.367438000000
C	4.138341000000	6.640478000000	-2.671210000000
H	5.912993000000	5.594859000000	-2.038257000000
H	5.287814000000	3.473089000000	-3.127965000000
H	2.267660000000	7.382078000000	-3.436212000000
H	4.412083000000	7.577647000000	-2.199377000000
O	3.040541000000	3.090683000000	-4.568377000000
C	3.750373000000	1.904542000000	-4.365566000000
C	4.755396000000	1.591260000000	-5.274329000000
C	3.427496000000	1.059008000000	-3.290924000000
C	5.498104000000	0.423397000000	-5.114248000000
H	4.958443000000	2.277311000000	-6.089711000000
C	4.199545000000	-0.107335000000	-3.148485000000
C	5.226436000000	-0.419505000000	-4.036216000000
H	6.281555000000	0.178783000000	-5.823510000000
H	3.963809000000	-0.780884000000	-2.332817000000
H	5.797792000000	-1.331782000000	-3.899718000000
C	2.320795000000	1.338503000000	-2.353176000000
N	1.058739000000	1.719701000000	-2.862643000000
H	0.780333000000	1.200995000000	-3.688419000000
H	0.387393000000	1.594752000000	-2.104791000000
N	2.517833000000	1.226667000000	-1.072157000000
C	1.254925000000	5.254842000000	-4.699025000000
N	0.341360000000	4.330865000000	-4.290127000000
N	1.054776000000	6.142853000000	-5.621144000000
H	0.665830000000	3.521088000000	-3.758307000000
H	-0.436398000000	4.165620000000	-4.912679000000
O	1.424561000000	1.451023000000	-0.300830000000
O	-0.264105000000	5.973432000000	-6.164186000000
H	-0.291182000000	6.612576000000	-6.885529000000
Cs	2.357062000000	4.138635000000	0.988286000000

## CsB2

C	5.133188000000	5.464023000000	-2.718726000000
C	4.737646000000	4.246157000000	-3.269658000000
C	3.487127000000	4.135629000000	-3.876033000000
C	2.618081000000	5.239428000000	-3.932238000000
C	3.041917000000	6.451445000000	-3.377824000000
C	4.290727000000	6.571961000000	-2.773146000000
H	6.107590000000	5.539613000000	-2.247992000000
H	5.402703000000	3.392526000000	-3.234218000000
H	2.370436000000	7.301175000000	-3.417505000000
H	4.597572000000	7.518844000000	-2.343451000000
O	3.042497000000	2.976053000000	-4.479906000000
C	3.763437000000	1.796587000000	-4.331793000000
C	4.699108000000	1.456558000000	-5.302730000000
C	3.501533000000	0.949240000000	-3.246400000000
C	5.404132000000	0.259531000000	-5.192107000000
H	4.872123000000	2.135237000000	-6.130316000000
C	4.226785000000	-0.244213000000	-3.147327000000
C	5.173208000000	-0.588105000000	-4.109522000000
H	6.132794000000	-0.006126000000	-5.950085000000
H	4.030617000000	-0.907661000000	-2.312893000000
H	5.720387000000	-1.519763000000	-4.018524000000
C	2.470108000000	1.279055000000	-2.223919000000
N	1.167642000000	1.473237000000	-2.643303000000
H	0.897082000000	0.950830000000	-3.465643000000
H	0.479785000000	1.427330000000	-1.901946000000
N	2.869727000000	1.388317000000	-1.004436000000
C	1.269092000000	5.148252000000	-4.558541000000
N	0.394981000000	4.207399000000	-4.109287000000
N	0.997646000000	6.046021000000	-5.454534000000
H	0.749131000000	3.401729000000	-3.605315000000
H	-0.442493000000	4.057795000000	-4.651819000000
O	-0.343288000000	5.842892000000	-5.938470000000
H	-0.530271000000	6.652930000000	-6.428009000000
Cs	1.208975000000	4.142180000000	-8.507266000000
O	1.759462000000	1.654123000000	-0.152388000000
H	2.150057000000	1.684330000000	0.729078000000

## CsC1

C	4.900700000000	5.370258000000	-2.462272000000
C	4.367954000000	4.139163000000	-2.838640000000
C	3.193380000000	4.096112000000	-3.590555000000
C	2.545785000000	5.283029000000	-3.965723000000



C	3.095823000000	6.507137000000	-3.575966000000
C	4.269884000000	6.558594000000	-2.827919000000
H	5.813654000000	5.395248000000	-1.876752000000
H	4.861767000000	3.218075000000	-2.554217000000
H	2.596582000000	7.423784000000	-3.871319000000
H	4.687518000000	7.515489000000	-2.535792000000
O	2.591367000000	2.913973000000	-3.967730000000
C	3.374824000000	1.761416000000	-4.112118000000
C	4.321013000000	1.732119000000	-5.134589000000
C	3.157077000000	0.663840000000	-3.260610000000
C	5.108104000000	0.601101000000	-5.323237000000
H	4.439252000000	2.604196000000	-5.768802000000
C	3.965064000000	-0.470259000000	-3.485589000000
C	4.929395000000	-0.502558000000	-4.484886000000
H	5.843448000000	0.578828000000	-6.120236000000
H	3.809054000000	-1.335935000000	-2.853543000000
H	5.528473000000	-1.396417000000	-4.625346000000
C	2.153737000000	0.649760000000	-2.177096000000
N	0.902892000000	1.260489000000	-2.360274000000
H	0.933432000000	2.127006000000	-2.879028000000
H	0.454376000000	1.351368000000	-1.451817000000
N	2.415930000000	-0.022688000000	-1.091371000000
C	1.291334000000	5.245607000000	-4.773899000000
N	0.104607000000	5.099701000000	-4.117057000000
N	1.416162000000	5.417917000000	-6.047302000000
H	0.115546000000	4.793951000000	-3.157578000000
H	-0.708561000000	4.845980000000	-4.658830000000
O	1.437742000000	-0.007074000000	-0.152884000000
O	0.112352000000	5.399442000000	-6.659360000000
H	0.310592000000	5.317138000000	-7.599928000000
Cs	3.505946000000	-1.728414000000	1.452110000000
Cs	-1.460911000000	8.363958000000	-6.424210000000

### CsC2

C	5.018035000000	5.570387000000	-2.474645000000
C	4.441667000000	4.309475000000	-2.602570000000
C	3.260656000000	4.163243000000	-3.327323000000
C	2.635869000000	5.268842000000	-3.918099000000
C	3.230471000000	6.527990000000	-3.776117000000
C	4.416056000000	6.682662000000	-3.063254000000
H	5.936780000000	5.681252000000	-1.908997000000
H	4.905740000000	3.441237000000	-2.149306000000
H	2.751205000000	7.386458000000	-4.232850000000
H	4.864068000000	7.664866000000	-2.963343000000
O	2.633993000000	2.930919000000	-3.438750000000

C	3.364794000000	1.811106000000	-3.801084000000
C	4.383144000000	1.879222000000	-4.750289000000
C	3.003979000000	0.586475000000	-3.217603000000
C	5.063091000000	0.721469000000	-5.118572000000
H	4.642653000000	2.832940000000	-5.194174000000
C	3.697013000000	-0.565807000000	-3.610989000000
C	4.723377000000	-0.504997000000	-4.548760000000
H	5.852742000000	0.781426000000	-5.859678000000
H	3.414332000000	-1.515505000000	-3.172004000000
H	5.246313000000	-1.409097000000	-4.839485000000
C	1.918409000000	0.482078000000	-2.204304000000
N	0.671264000000	0.948740000000	-2.514902000000
H	0.605710000000	1.648381000000	-3.237342000000
H	0.030033000000	1.068473000000	-1.743746000000
N	2.213104000000	-0.136848000000	-1.106661000000
C	1.367182000000	5.122779000000	-4.686751000000
N	0.223792000000	4.809760000000	-4.007791000000
N	1.426828000000	5.381953000000	-5.950879000000
H	0.310945000000	4.433856000000	-3.077234000000
H	-0.557398000000	4.465576000000	-4.547594000000
O	0.113241000000	5.265170000000	-6.521614000000
H	0.281230000000	5.271175000000	-7.471667000000
Cs	5.311512000000	-0.704707000000	0.281119000000
Cs	-1.751173000000	7.991445000000	-5.926167000000
O	1.050409000000	-0.210898000000	-0.277580000000
H	1.370352000000	-0.622986000000	0.533521000000

### CsD1

C	4.914701000000	5.271139000000	-2.383539000000
C	4.545373000000	4.126404000000	-3.088323000000
C	3.377093000000	4.129391000000	-3.851423000000
C	2.568037000000	5.277614000000	-3.906093000000
C	2.964012000000	6.416295000000	-3.199188000000
C	4.131309000000	6.422013000000	-2.438679000000
H	5.824945000000	5.257567000000	-1.793256000000
H	5.167527000000	3.241100000000	-3.052815000000
H	2.336674000000	7.299454000000	-3.243922000000
H	4.420248000000	7.312275000000	-1.891398000000
O	2.976653000000	3.061074000000	-4.623219000000
C	3.603761000000	1.825375000000	-4.451271000000
C	4.606972000000	1.483119000000	-5.352332000000
C	3.206531000000	0.962017000000	-3.414360000000
C	5.270780000000	0.264442000000	-5.225815000000
H	4.871357000000	2.185891000000	-6.135111000000
C	3.900881000000	-0.256808000000	-3.307206000000

C	4.922272000000	-0.600607000000	-4.188116000000
H	6.052672000000	-0.001895000000	-5.928785000000
H	3.606555000000	-0.944854000000	-2.523257000000
H	5.430689000000	-1.552775000000	-4.077501000000
C	2.114153000000	1.270798000000	-2.469470000000
N	0.887955000000	1.787415000000	-2.955669000000
H	0.549893000000	1.281718000000	-3.768728000000
H	0.224393000000	1.703711000000	-2.183515000000
N	2.290081000000	1.053312000000	-1.199306000000
C	1.301931000000	5.290539000000	-4.691828000000
N	0.318026000000	4.421480000000	-4.342160000000
N	1.218056000000	6.187148000000	-5.625663000000
H	0.566048000000	3.588156000000	-3.802572000000
H	-0.463419000000	4.331235000000	-4.974872000000
O	1.221384000000	1.302231000000	-0.409573000000
O	-0.063143000000	6.071867000000	-6.275806000000
H	-0.085776000000	6.838153000000	-6.861303000000
Cs	1.807300000000	3.845523000000	-8.255309000000
Cs	3.205608000000	0.374373000000	1.848533000000

### CsD2

C	5.174243000000	5.260874000000	-2.453470000000
C	4.706635000000	4.100519000000	-3.068107000000
C	3.486443000000	4.117501000000	-3.741728000000
C	2.711919000000	5.290477000000	-3.798166000000
C	3.208115000000	6.441643000000	-3.174936000000
C	4.430886000000	6.437239000000	-2.509116000000
H	6.124863000000	5.236760000000	-1.931493000000
H	5.294211000000	3.192295000000	-3.029064000000
H	2.610243000000	7.344427000000	-3.211058000000
H	4.791772000000	7.340409000000	-2.030034000000
O	2.976220000000	3.016204000000	-4.403848000000
C	3.611595000000	1.783612000000	-4.306919000000
C	4.673224000000	1.484977000000	-5.154115000000
C	3.124024000000	0.840087000000	-3.394379000000
C	5.276830000000	0.230871000000	-5.081488000000
H	5.021320000000	2.234244000000	-5.856097000000
C	3.743965000000	-0.412532000000	-3.331898000000
C	4.817491000000	-0.715727000000	-4.166260000000
H	6.104854000000	-0.004012000000	-5.741161000000
H	3.370258000000	-1.151192000000	-2.631714000000
H	5.286112000000	-1.691737000000	-4.108791000000
C	1.943072000000	1.144239000000	-2.536854000000
N	0.733760000000	1.342759000000	-3.160774000000
H	0.617248000000	0.894542000000	-4.058597000000

H	-0.079783000000	1.277122000000	-2.563000000000
N	2.139276000000	1.243550000000	-1.266552000000
C	1.390155000000	5.343698000000	-4.482286000000
N	0.435342000000	4.402302000000	-4.183910000000
N	1.188505000000	6.364278000000	-5.251010000000
H	0.753922000000	3.482066000000	-3.900627000000
H	-0.350780000000	4.380594000000	-4.819649000000
O	-0.144412000000	6.323206000000	-5.765280000000
H	-0.168155000000	7.059393000000	-6.387793000000
Cs	-0.564461000000	4.753993000000	-0.681750000000
Cs	5.066743000000	1.252916000000	0.595634000000
O	0.899605000000	1.528248000000	-0.611139000000
H	1.103062000000	1.418458000000	0.325746000000

### UB1

C	3.909698000000	3.290433000000	1.588155000000
C	3.696969000000	1.917383000000	1.683938000000
C	2.635756000000	1.324482000000	1.007016000000
C	1.758886000000	2.092395000000	0.222316000000
C	2.000532000000	3.471928000000	0.129823000000
C	3.060355000000	4.069396000000	0.804969000000
H	4.736926000000	3.745457000000	2.121591000000
H	4.349291000000	1.289371000000	2.279939000000
H	1.328495000000	4.084401000000	-0.460333000000
H	3.214726000000	5.139535000000	0.724826000000
O	2.444342000000	-0.034519000000	1.197282000000
C	2.753430000000	-0.934937000000	0.199737000000
C	3.549512000000	-0.607901000000	-0.896740000000
C	2.271025000000	-2.243738000000	0.373963000000
C	3.873097000000	-1.590225000000	-1.831902000000
H	3.926411000000	0.400853000000	-1.013728000000
C	2.616398000000	-3.211616000000	-0.574271000000
C	3.412163000000	-2.895175000000	-1.673439000000
H	4.493322000000	-1.327858000000	-2.682397000000
H	2.241733000000	-4.220257000000	-0.443935000000
H	3.663223000000	-3.659446000000	-2.400381000000
C	1.411279000000	-2.608870000000	1.534494000000
N	0.262528000000	-1.905822000000	1.747890000000
H	0.177262000000	-0.981745000000	1.332709000000
H	-0.181745000000	-2.030562000000	2.645743000000
N	1.788666000000	-3.639108000000	2.223112000000
C	0.595861000000	1.522667000000	-0.508481000000
N	0.349407000000	1.999431000000	-1.758241000000
N	-0.179721000000	0.677290000000	0.112130000000
H	1.106585000000	2.401567000000	-2.287570000000

H	-0.373592000000	1.534536000000	-2.287209000000
O	-1.227948000000	0.271677000000	-0.713128000000
O	0.828666000000	-3.894948000000	3.257780000000
H	1.231238000000	-4.610621000000	3.763264000000
U	-3.189232000000	-0.440082000000	-0.260737000000
O	-3.537412000000	-0.500952000000	-2.005285000000
O	-2.804881000000	-0.289265000000	1.465097000000

**UB2**

C	4.054330000000	3.284680000000	1.532233000000
C	3.766390000000	1.926934000000	1.648727000000
C	2.659147000000	1.390606000000	0.999202000000
C	1.810086000000	2.199127000000	0.227194000000
C	2.127327000000	3.560637000000	0.110981000000
C	3.234944000000	4.102481000000	0.756365000000
H	4.916552000000	3.697801000000	2.043918000000
H	4.394372000000	1.269168000000	2.238797000000
H	1.479424000000	4.202541000000	-0.475046000000
H	3.449773000000	5.160808000000	0.659875000000
O	2.390065000000	0.044238000000	1.198537000000
C	2.680228000000	-0.877972000000	0.215207000000
C	3.510729000000	-0.594042000000	-0.867799000000
C	2.136139000000	-2.163620000000	0.386542000000
C	3.809841000000	-1.595515000000	-1.790269000000
H	3.933243000000	0.396491000000	-0.983372000000
C	2.457114000000	-3.151526000000	-0.550650000000
C	3.288375000000	-2.877878000000	-1.634217000000
H	4.457941000000	-1.365947000000	-2.629331000000
H	2.035259000000	-4.141507000000	-0.422874000000
H	3.519816000000	-3.657105000000	-2.351662000000
C	1.241009000000	-2.488635000000	1.530282000000
N	0.157477000000	-1.694168000000	1.774066000000
H	0.156162000000	-0.750658000000	1.396691000000
H	-0.287271000000	-1.809261000000	2.673578000000
N	1.515705000000	-3.573461000000	2.184086000000
C	0.594172000000	1.686980000000	-0.462380000000
N	0.378670000000	2.105131000000	-1.744581000000
N	-0.236614000000	0.964226000000	0.218252000000
H	1.174423000000	2.381305000000	-2.298059000000
H	-0.376603000000	1.668908000000	-2.251404000000
O	0.528934000000	-3.781654000000	3.196686000000
H	0.866830000000	-4.539367000000	3.688484000000
U	-2.633455000000	-3.215390000000	-0.409104000000
O	-2.012018000000	-3.521696000000	-2.013900000000
O	-3.251964000000	-2.906036000000	1.195135000000

O	-1.343534000000	0.600766000000	-0.610489000000
H	-1.969785000000	0.205460000000	0.007672000000

### UB3

C	3.814879000000	2.083005000000	1.846158000000
C	3.410741000000	1.055634000000	0.999066000000
C	2.235752000000	1.183276000000	0.262754000000
C	1.445107000000	2.347838000000	0.386540000000
C	1.883656000000	3.374302000000	1.241529000000
C	3.057757000000	3.247417000000	1.968193000000
H	4.735745000000	1.970951000000	2.407422000000
H	4.010199000000	0.159464000000	0.907447000000
H	1.315369000000	4.294297000000	1.306936000000
H	3.384993000000	4.053716000000	2.613117000000
O	1.780377000000	0.208540000000	-0.589313000000
C	2.539275000000	-0.948490000000	-0.811559000000
C	3.484879000000	-0.926651000000	-1.829019000000
C	2.289557000000	-2.101514000000	-0.056484000000
C	4.218957000000	-2.076979000000	-2.107060000000
H	3.640631000000	-0.011959000000	-2.389584000000
C	3.041552000000	-3.246890000000	-0.354862000000
C	3.998030000000	-3.236902000000	-1.365339000000
H	4.955750000000	-2.064779000000	-2.902328000000
H	2.856730000000	-4.150571000000	0.212911000000
H	4.562387000000	-4.137361000000	-1.580274000000
C	1.277826000000	-2.148172000000	1.034215000000
N	0.009170000000	-1.692287000000	0.799077000000
H	-0.131457000000	-1.061427000000	0.026209000000
H	-0.562849000000	-1.511169000000	1.611411000000
N	1.655507000000	-2.706759000000	2.138738000000
C	0.188426000000	2.526379000000	-0.354641000000
N	-0.026391000000	2.024464000000	-1.549374000000
H	0.675723000000	1.462016000000	-2.004613000000
H	-0.926011000000	2.144374000000	-1.995372000000
O	0.565790000000	-2.729468000000	3.055037000000
H	0.948867000000	-3.102844000000	3.857909000000
U	-1.800773000000	-5.105633000000	1.342911000000
O	-1.788327000000	-5.088359000000	-0.402698000000
O	-1.829322000000	-5.135816000000	3.087002000000
O	-1.980401000000	3.361628000000	-0.443280000000
H	-2.093960000000	4.288464000000	-0.709988000000
N	-0.758651000000	3.291052000000	0.205697000000
H	-0.824086000000	3.378853000000	1.211802000000

### UD1

C	3.867265000000	3.456574000000	1.545524000000
C	3.729686000000	2.079927000000	1.706638000000
C	2.710744000000	1.399394000000	1.049761000000
C	1.800068000000	2.077091000000	0.220990000000
C	1.968146000000	3.461412000000	0.062953000000
C	2.986058000000	4.148152000000	0.717248000000
H	4.661863000000	3.981875000000	2.063489000000
H	4.408214000000	1.518115000000	2.338108000000
H	1.269386000000	4.007449000000	-0.560336000000
H	3.082279000000	5.219939000000	0.586043000000
O	2.593577000000	0.040014000000	1.311712000000
C	2.847444000000	-0.885930000000	0.330808000000
C	3.651140000000	-0.611487000000	-0.773753000000
C	2.306828000000	-2.173541000000	0.512876000000
C	3.907969000000	-1.610551000000	-1.709605000000
H	4.079242000000	0.375730000000	-0.896773000000
C	2.578341000000	-3.161898000000	-0.442897000000
C	3.371917000000	-2.887193000000	-1.550917000000
H	4.533727000000	-1.384053000000	-2.565928000000
H	2.140344000000	-4.144823000000	-0.321525000000
H	3.563616000000	-3.660639000000	-2.285237000000
C	1.425539000000	-2.492065000000	1.662926000000
N	0.459235000000	-1.665720000000	2.016140000000
H	0.305651000000	-0.787698000000	1.507948000000
H	-0.113156000000	-1.888296000000	2.818049000000
N	1.627621000000	-3.656683000000	2.271233000000
C	0.672084000000	1.412155000000	-0.483931000000
N	0.394045000000	1.818546000000	-1.749166000000
N	-0.050295000000	0.546282000000	0.171713000000
H	1.118230000000	2.252461000000	-2.298954000000
H	-0.306322000000	1.295645000000	-2.253920000000
O	-1.070011000000	0.028632000000	-0.626313000000
O	0.736637000000	-3.868201000000	3.365137000000
H	0.110903000000	-4.551871000000	3.074878000000
U	-3.036394000000	-0.620377000000	-0.058925000000
O	-3.313844000000	-1.061267000000	-1.757500000000
O	-2.661937000000	-0.169787000000	1.615178000000
U	3.439732000000	-5.109066000000	2.968030000000
O	3.254238000000	-5.979889000000	1.453050000000
O	3.514821000000	-4.165988000000	4.446203000000

## UD2

C	4.197249000000	3.390869000000	1.330168000000
C	3.961394000000	2.036402000000	1.552552000000

C	2.814937000000	1.437129000000	1.043417000000
C	1.872420000000	2.173788000000	0.307687000000
C	2.138865000000	3.533311000000	0.084827000000
C	3.284884000000	4.139821000000	0.590060000000
H	5.091628000000	3.854013000000	1.731686000000
H	4.659722000000	1.429754000000	2.117455000000
H	1.420987000000	4.125057000000	-0.471368000000
H	3.457796000000	5.195054000000	0.411755000000
O	2.610696000000	0.100250000000	1.361773000000
C	2.654412000000	-0.865519000000	0.389578000000
C	3.325247000000	-0.695180000000	-0.819786000000
C	2.040149000000	-2.095229000000	0.691470000000
C	3.377977000000	-1.743397000000	-1.735573000000
H	3.812683000000	0.246882000000	-1.038680000000
C	2.111487000000	-3.138648000000	-0.242432000000
C	2.771626000000	-2.966761000000	-1.453809000000
H	3.903140000000	-1.599100000000	-2.673398000000
H	1.625466000000	-4.079851000000	-0.017398000000
H	2.810514000000	-3.778822000000	-2.170184000000
C	1.316416000000	-2.310655000000	1.966699000000
N	0.475159000000	-1.408376000000	2.436377000000
H	0.317177000000	-0.534383000000	1.928922000000
H	0.023322000000	-1.559847000000	3.327246000000
N	1.538571000000	-3.477132000000	2.556713000000
C	0.620087000000	1.591580000000	-0.246653000000
N	0.247409000000	1.990798000000	-1.495369000000
N	-0.093545000000	0.811771000000	0.504622000000
H	0.954115000000	2.332205000000	-2.127246000000
H	-0.536252000000	1.520154000000	-1.921353000000
O	0.847995000000	-3.648341000000	3.792850000000
H	0.142591000000	-4.294748000000	3.623364000000
U	-1.877290000000	-3.095120000000	-1.645641000000
O	-2.282628000000	-1.844933000000	-2.797349000000
O	-1.477487000000	-4.349495000000	-0.495453000000
U	3.389965000000	-4.898556000000	3.163180000000
O	2.917264000000	-6.027603000000	1.899973000000
O	3.783764000000	-3.672686000000	4.357734000000
O	-1.247988000000	0.385038000000	-0.218028000000
H	-1.771694000000	-0.095305000000	0.434736000000

### UD3

C	3.554772000000	2.532245000000	1.687431000000
C	3.348817000000	1.241869000000	1.207055000000
C	2.205210000000	0.955818000000	0.470122000000
C	1.247055000000	1.956137000000	0.222636000000



C	1.470814000000	3.248612000000	0.724336000000
C	2.620566000000	3.538582000000	1.446304000000
H	4.450226000000	2.746256000000	2.259707000000
H	4.068330000000	0.459177000000	1.412827000000
H	0.752770000000	4.033101000000	0.516758000000
H	2.787079000000	4.543327000000	1.815054000000
O	1.914389000000	-0.322713000000	0.032719000000
C	2.924992000000	-1.205870000000	-0.322642000000
C	3.882445000000	-0.826875000000	-1.257870000000
C	2.910164000000	-2.507993000000	0.212498000000
C	4.831257000000	-1.746462000000	-1.691075000000
H	3.876873000000	0.182699000000	-1.651088000000
C	3.866874000000	-3.424971000000	-0.262256000000
C	4.817800000000	-3.051709000000	-1.200183000000
H	5.567678000000	-1.444864000000	-2.427095000000
H	3.846828000000	-4.444200000000	0.101067000000
H	5.540123000000	-3.778033000000	-1.552992000000
C	1.977103000000	-2.938752000000	1.276710000000
N	0.806307000000	-2.360443000000	1.478163000000
H	0.514301000000	-1.577724000000	0.914216000000
H	0.228140000000	-2.648312000000	2.254811000000
N	2.386567000000	-3.974781000000	2.008447000000
C	0.012063000000	1.691789000000	-0.539447000000
N	-0.013440000000	1.015385000000	-1.664747000000
H	0.833124000000	0.677890000000	-2.093734000000
H	-0.892227000000	0.835081000000	-2.132148000000
O	1.521883000000	-4.250240000000	3.117387000000
H	1.104623000000	-5.112284000000	2.948131000000
U	-4.630688000000	-0.914542000000	0.489841000000
O	-5.494051000000	-1.509636000000	-0.904743000000
O	-3.765650000000	-0.321173000000	1.884507000000
U	4.098491000000	-4.445248000000	3.643278000000
O	4.033893000000	-6.111491000000	3.080617000000
O	3.957497000000	-2.764035000000	4.138643000000
O	-2.295813000000	1.926865000000	-0.724370000000
H	-2.622870000000	2.761493000000	-1.099517000000
N	-1.115161000000	2.225687000000	-0.070034000000
H	-1.218874000000	2.469175000000	0.907229000000

**Table S3:** Strontium Complex bond distances, bond indices, natural population analysis, and selected metrics

Species	Moiety	Bond	Distance (Å)	$\rho$	$\nabla^2\rho$	H	WBI	LBO	NPA
Sr (A)	bis-AO <sup>-1</sup>	Sr-O(neg)	2.506	0.0322	0.1713	0.0045	0.32865152	0.05751686	1.99175
		Sr-N	3.346	NA			0.06980665	0.00005902	
	bis-AO	Sr-O	2.793	0.0168	0.0773	0.0026	0.18898451	0.01375858	1.99557
		Sr-N	3.669				0.03146014	0.00000194	
	bis-AO <sup>+1</sup>	Sr-O (pos1)	2.982	0.0100	0.0469	0.0019	0.13909775	0.00649217	1.99788
		Sr-N	3.946				0.01465325	0.00000023	
Sr (B)	bis-AO <sup>-1</sup>	Sr-O	3.976	NA			0.01320934	0.00000491	1.99130
		Sr-N(amine)	2.753	0.0234	0.1009	0.0026	0.25683126	0.02636668	
		Sr-COC	3.281	NA			0.05199987	0.00083532	
	bis-AO	Sr-O	4.082				0.00788816	0.00000113	1.99360
		Sr-N (amine)	2.913	0.0167	0.0684	0.0021	0.18944448	0.01130221	
		Sr-COC	3.323				0.05058409	0.00060454	
	bis-AO <sup>+1</sup>	Sr-O (pos1)	5.650				0.00066480	0.00000000	1.99538
		Sr-N (amine, pos1)	4.878				0.00226256	0.00000001	
Sr-COC		4.105	0.0007	0.0037	0.0002	0.00638374	0.00000377		

**Table S4:** Strontium Complex bond distances, bond indices, natural population analysis, and selected metrics

Species	Moiety	Bond	Distance (Å)	$\rho$	$\nabla^2\rho$	H	WBI	LBO	NPA	
Sr (C)	bis-AO <sup>-1</sup>	Sr1-O (neutral AO)	2.782	0.0171	0.0796	0.0027	0.19601602	0.01411671	1.99620	
		Sr1-N	3.713				0.02904177	0.00000107		
		Sr2-O (neg1)	2.504	0.0319	0.1717	0.0046	0.33013523	0.05701231	1.99239	
		Sr2-N	3.404				0.06051120	0.00002402		
	bis-AO	Sr1-O	2.805	0.0164	0.0751	0.0025	0.18776967	0.01257322	1.99590	
		Sr1-N	3.695				0.03064843	0.00000144		
		Sr2-O	2.781	0.0173	0.0799	0.0027	0.19215682	0.01418740	1.99629	
		Sr2-N	3.631				0.03437380	0.00000327		
	bis-AO <sup>+1</sup>	Sr1-O	2.950	0.0120	0.0524	0.0018	0.14568394	0.00602898	1.99672	
		Sr1-N	3.806				0.02432740	0.00000065		
		Sr2-O (pos1)	2.983	0.0100	0.0467	0.0019	0.13833443	0.00649902	1.99848	
		Sr2-N (pos1)	3.938				0.01494250	0.00000024		
	Sr (D)	bis-AO <sup>-1</sup>	Sr1-N (amine)	2.816				0.10272001	0.00094531	1.99418
			Sr1-COC	3.412				0.02114502	0.00007146	
Sr2-O (neg1)			2.583	0.0106	0.0423	0.0012	0.14216036	0.00830183	1.99310	
Sr2-N			2.684	0.0060	0.0234	0.0009	0.03623261	0.00001239		
bis-AO		Sr1-N (amine)	2.996	0.0139	0.0557	0.0018	0.17225615	0.00607635	1.99397	
		Sr1-COC	3.600	0.3011	-0.7083	-0.2935	0.02478947	0.00008883		
		Sr2-O	2.830	0.0157	0.0706	0.0023	0.17846674	0.00988804	1.99635	
		Sr2-N	3.619				0.03647295	0.00000665		

**Table S5:** Cesium Complex bond distances, bond indices, natural population analysis, and selected metrics

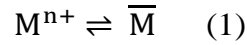
Species	Moiety	Bond	Distance (Å)	$\rho$	$\nabla^2\rho$	H	WBI	LBO	NPA
Cs (A)	bis-AO <sup>-1</sup>	Cs-O(neg1)	3.141	0.0137	0.0477	0.0008	0.16514419	0.00587800	0.99323
		Cs-N	3.241	0.0108	0.0443	0.0015	0.20490154	0.00388807	
	bis-AO	Cs-O	4.319				0.00803927	0.00000022	0.99691
		Cs-N	3.442	0.0082	0.0279	0.0011	0.16318213	0.00442364	
Cs (B)	bis-AO <sup>-1</sup>	Cs-N (neg)	4.101				0.03517797	0.00000050	0.99703
		Cs-O (neg)	3.069	0.0152	0.0554	0.0012	0.23479744	0.01110819	
	bis-AO	Cs-O	3.450	0.0073	0.0258	0.0008	0.08783593	0.00063882	0.99668
		Cs-N	3.604				0.10291157	0.00024087	
		Cs-COC	4.576				0.00553921	0.00000067	
Cs (C)	bis-AO <sup>-1</sup>	Cs1-O (neg1)	3.133	0.0140	0.0485	0.0008	0.16856339	0.00619772	0.99322
		Cs1-N (neg1)	3.251				0.20199844	0.00361153	
		Cs2-O	3.364	0.0088	0.0301	0.0009	0.12721263	0.00175665	0.99776
	bis-AO	Cs2-N	4.135				0.03239509	0.00000120	
		Cs1-O	3.356	0.0089	0.0306	0.0009	0.12734578	0.00182081	0.99774
		Cs1-N	4.112				0.03290230	0.00000131	
		Cs2-O	4.326				0.00795912	0.00000021	0.99680
Cs2-N	3.442	0.0083	0.0280	0.0011	0.16446641	0.00459225			
Cs (D)	bis-AO <sup>-1</sup>	Cs1-O	3.518	0.0063	0.0233	0.0008	0.07141039	0.00034135	0.99567
		Cs1-N	3.570	0.0056	0.0214	0.0009	0.10151949	0.00025808	
		Cs1-COC	3.895	0.0026	0.0106	0.0005	0.02890720	0.00005417	
		Cs2-O (neg1)	3.146	0.0136	0.0475	0.0008	0.16461656	0.00574462	0.99335
	bis-AO	Cs2-N (neg1)	3.254				0.20345897	0.00364111	
		Cs1-COC	4.115				0.01794670	0.00003049	0.99677
		Cs2-N	3.479	0.0076	0.0268	0.0011	0.15765724	0.00390318	0.99714
		Cs2-O	4.328	0.0015	0.0068	0.0004	0.00822881	0.00000021	

**Table S6:** Uranium Complex bond distances, bond indices, natural population analysis, and selected metrics

Species	Moiety	Bond	Distance (Å)	$\rho$	$\nabla^2\rho$	H	WBI	LBO	NPA	
U (B)	bis-AO <sup>-1</sup>	U-O(neg1)	2.135	0.0715	0.6498	0.0008	0.64001891	0.73558179	2.67806	
		U-N	3.232				0.07145278	0.00010100		
	bis-AO	U-O	4.033	0.0007	0.0057	0.0004	0.01065062	0.00000662	3.20123	
		U-N(amine)	3.856				0.02909088	0.00056431		
	bis-AO <sup>+1</sup>	U-O	3.765	0.0027	0.0129	0.0004	0.02101695	0.00088926	3.20880	
		U-N (amine)	3.902	0.0014	0.0093	0.0006	0.02262312	0.00020839		
U (D)	bis-AO <sup>-1</sup>	U1-O	3.001				0.11131410	0.00535803	2.84862	
		U1-N	2.425	0.0414	0.3240	0.0028	0.41045325	0.67007929		
		U2-O (neg)	2.147	0.0700	0.6282	0.0012	0.62423302	0.72479006		2.69393
		U2-N	3.214				0.07233575	0.00014380		
	bis-AO	U1-O	2.902				0.01891316	0.00021571	2.82422	
		U1-N	2.412	0.0422	0.3305	0.0024	0.00173916	0.00000001		
		U1-COC	5.370				0.00122908	0.00000000		
		U2-O	3.814	0.0011	0.0094	0.0006	0.13580676	0.01221387		3.23066
		U2-N	4.803				0.41055592	0.63604155		
		bis-AO <sup>+1</sup>	U1-O	2.637				0.22489598		0.07081355
	U1-N		2.413	0.0406	0.3137	0.0018	0.38561948	0.51704990		
	U2-O(pos)		3.873	0.0009	0.0078	0.0005	0.01567582	0.00114698	3.24122	
	U2-N		4.747				0.00273638	0.00000004		

## Calculations for Uptake Studies:

Consider the uptake of a metal ion,  $M^{n+}$  by a solid sorbent. The process can be described by a chemical equilibrium of the type:



where the bar denotes the solid phase species and  $M^{n+}$  is the equilibrium concentration of the metal ion in the aqueous phase. The weight distribution ratio of the metal ion,  $D_w$ , (proportional to the equilibrium constant of reaction 1) can be written as:

$$D_w = \frac{[\bar{M}]}{[M^{n+}]} \quad (2)$$

In the presence of complexing agents in the aqueous phase, we can determine the total concentration of  $M^{n+}$ , given by the sum of all chemical species containing M. The experimentally determined  $D_{w,exp}$  is given by:

$$D_{w,exp} = \frac{[\bar{M}]}{[M^{n+}]_{tot}} \quad (3)$$

In eq. 3, the total equilibrium metal concentration in the aqueous phase can be written as:

$$[M^{n+}]_{tot} = [M^{n+}](1 + \beta_1[L^-]^1 + \dots + \beta_p[L^-]^p) \quad (4)$$

where  $L^-$  represents the aqueous complexing agent (e.g. the anion of a weak acid) and  $\beta_1$  through  $\beta_p$  are the total formation constants for the aqueous phase metal complexes from  $ML$  to  $ML_p$  (charges omitted for simplicity). By substituting equation 4 into equation 3, we obtain:

$$D_w = D_{w,exp}(1 + \beta_1[L^-]^1 + \dots + \beta_p[L^-]^p) \quad (5)$$

From equation 5, the actual value of  $D_w$  for  $M^{n+}$  can be calculated if the  $\beta$  values are known and the concentration of  $L^-$  can be estimated.  $L^-$  in all instances is the anion of the ionic medium used in the experiments (e.g.  $NO_3^-$ ) or another anion introduced in solution for a particular reason (e.g. using a buffer). In the former case, because of the very low complexing power of nitrate ions, the formation of nitrate-complexes can be neglected, unless the  $NO_3^-$  concentration is very high. In the case of a buffer (for example, an acetate/acetic acid buffer), the concentration of the anion,  $[L^-]$ , at each pH value can be calculated knowing the  $pK_a$  of the acid and the buffer concentration.

For an  $HL/L^-$  buffer the following relation holds:

$$K_a = \frac{[H^+][L^-]}{[HL]} \quad (6)$$

where  $K_a$  is the acid dissociation constant,  $[H^+]$  is the concentration of protons in solution,  $[L^-]$  is the concentration of conjugate base, and  $[HL]$  is the initial concentration of acid.

Rearranging gives (7),

$$[H^+] = K_a \frac{[HL]}{[L^-]} \quad (7)$$

The total concentration,  $C$ , of the buffer is known.

Therefore,

$$\frac{[H^+]}{K_a} = \frac{[HL]}{[L^-]} = \frac{C - [L^-]}{[L^-]} \quad (8)$$

Equation (8) can be rearranged as

$$\frac{[H^+]}{K_a} [L^-] + [L^-] = C \quad (9)$$

$$\left(\frac{[\text{H}^+]}{K_a} + 1\right) [\text{L}^-] = C \quad (10)$$

and finally

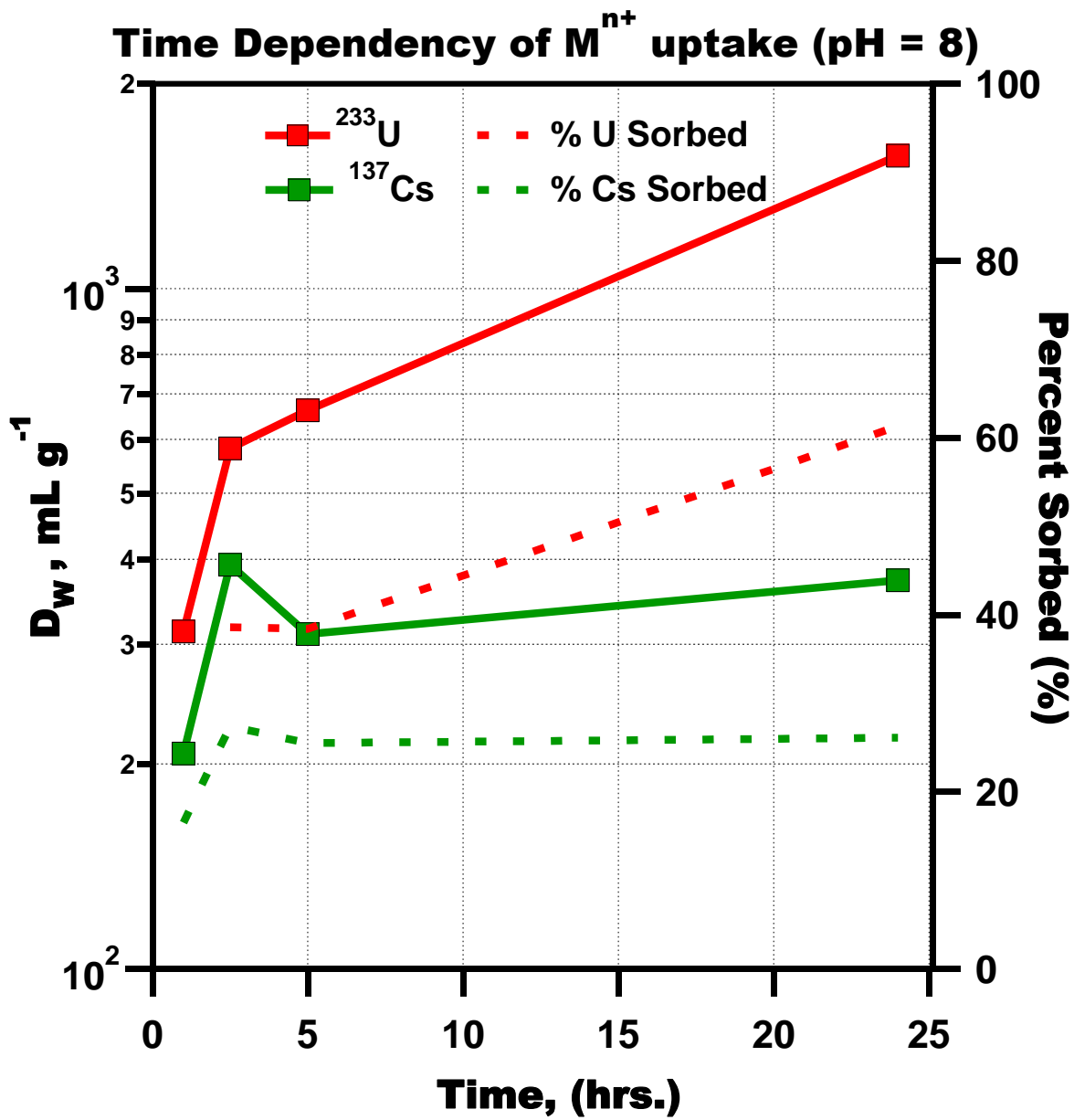
$$[\text{L}^-] = \frac{C}{\frac{[\text{H}^+]}{K_a} + 1} \quad (11)$$



**Table S7:** Percent Sr, Cs, and U sorbed as a function of pH

<b>% Sorbed</b>	<b>Sr<sup>2+</sup></b>	<b>Cs<sup>+</sup></b>	<b>UO<sub>2</sub><sup>2+</sup></b>
pH = 10	0	23	45
pH = 9	0	27	43
pH = 8	0	27	30
pH = 6	0	11	99
pH = 5	1.0	10.	99
pH = 4	0	11	72
pH = 3	1.2	18	38
pH = 2	2.0	10	35

Figure S8: Uptake of  $\text{Cs}^+$  and  $\text{UO}_2^{2+}$  at pH = 8 as a function of time



**Table S9:** Comparison of Advanced Sorbent Materials for U uptake

Adsorbent	Type	U uptake	M <sup>+</sup> Uptake	M <sup>2+</sup> Uptake	Conditions	Uptake Time
Bis-amidoxime functionalized polymer (this work)	Polymer	$D_W^{UO_2^{2+}} = 1.38 \cdot 10^5 mL g^{-1}$	$D_W^{Cs^+} = 1.8 \cdot 10^1 mL g^{-1}$	$D_W^{Sr^{2+}} = 0$	pH = 6, aqueous solution	30 min
Amidoxime Functionalized Porous Aromatic Framework <sup>1</sup>	Polymer	$K_D^{UO_2^{2+}} = 1.05 \cdot 10^6 mL g^{-1}$	U uptake affected by presence of NaCl, and NaHCO <sub>3</sub>		pH = 6, aqueous solution	30 min
Polysulfide/Layered Double Hydroxide <sup>2</sup>	Inorganic	$K_D^{UO_2^{2+}} = 8.4 \cdot 10^5 mL g^{-1} - 3.4 \cdot 10^6 mL g^{-1}$	U uptake not affected by presence of CaCl <sub>2</sub> , NaCl, and NaNO <sub>3</sub>		pH = 6, aqueous solution	24 hrs. – 3 days
Layered metal sulfide <sup>3</sup>	Inorganic	$K_D^{UO_2^{2+}} = 2.7 \cdot 10^4 mL g^{-1}$	$K_D^{Cs^+} = 5.5 \cdot 10^4 mL g^{-1}$	$K_D^{Sr^{2+}} = 2.7 \cdot 10^4 mL g^{-1}$	pH = 7, aqueous solution	15 hrs.
Fe <sub>3</sub> O <sub>4</sub> @MOF composite material <sup>4</sup>	Inorganic	$K_D^{UO_2^{2+}} \sim 2.1 \cdot 10^3 mL g^{-1}$	Not investigated		pH = 5.5, aqueous solution	24 hrs.
Amidoxime functionalized hydrogel particles <sup>5</sup>	Polymer	$K_D^{UO_2^{2+}} \sim 6 \cdot 10^4 mL g^{-1}$	U uptake affected by Na <sup>+</sup> and Mg <sup>+</sup> ,		Artificial groundwater, pH = 5.9	5 min

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