

8	-2.737271874	-1.566446784	-0.712349219
8	-4.001585488	-8.468718201	-3.850424416
8	-5.082096793	-6.278025003	-8.151455884
8	-5.202914534	2.686920125	-8.208107979
8	3.843651638	-1.357382619	9.257128891
6	-1.080413039	-3.628982545	-0.063088502
6	-2.582554338	-6.088065967	-0.236684401
6	0.171817666	-3.063068193	2.449602666
6	-3.536652423	-1.664754110	-3.170151406
6	-3.903486032	-4.028969507	-4.370038592
6	-3.521430680	-6.384116109	-2.926960679
6	-4.028393141	0.624442945	-4.407502409
6	-0.870194251	-3.776619278	4.777361470
6	-4.685770230	-4.088792563	-6.914845653
6	0.337816866	-3.224961019	7.079062842
6	2.452439145	-1.712053951	2.450024075
6	-3.860022334	3.139539735	-3.032626597
6	-4.782694276	0.481462498	-6.958549346
6	-5.094616228	-1.833308219	-8.214850522
6	2.657468745	-1.932813631	7.014175320
6	3.682242583	-1.138164955	4.707554992
6	-0.821460108	-4.063611964	9.565749490
6	-1.217369041	3.956029863	-2.322070728
6	0.229014003	-6.552074955	10.491660423
6	-0.322852126	4.496485827	-0.002859155
6	1.525553114	-7.013532813	12.631756208
6	2.340357607	5.459826562	0.356413660
6	-1.811918411	4.245086130	2.414463211

6	6.258413426	-2.523685594	9.557162576
6	2.419860269	-9.653035934	13.255507513
6	2.213050546	-5.046813719	14.575800480
1	0.440258912	-3.703207203	-1.491039158
1	-1.406840527	-7.727826560	0.260322983
1	-4.256496295	-6.048833365	1.002121692
1	-2.674926034	-4.778196729	4.832337378
1	3.270286097	-1.061067915	0.668326162
1	-4.832031243	-7.642514881	-6.908932701
1	-5.128147525	3.072915555	-1.383761304
1	-4.649393005	4.630140477	-4.252337009
1	-5.644450901	2.313145552	-9.939627998
1	-5.685257644	-1.914900918	-10.190500461
1	6.174392429	-4.560761077	9.133873403
1	7.701000010	-1.607191166	8.363751481
1	6.822477737	-2.289382248	11.544009142
1	-2.878585583	-4.285977911	9.295410960
1	-0.614552120	-2.554571276	10.977633696
1	5.430513132	-0.043845422	4.668350736
1	0.046628989	4.217184326	-3.943725857
1	-0.161577241	-8.149870404	9.230247538
1	3.431099888	4.172609469	1.584826259
1	2.318863863	7.335033786	1.271418983
1	3.360713265	5.645325844	-1.446997205
1	-2.304494387	6.129401833	3.164168534
1	-0.676665523	3.266691838	3.861698521
1	-3.565587908	3.159410204	2.190368165
1	4.504596531	-9.730913432	13.274302728

1	1.747556233	-10.230625013	15.143196377
1	1.740953531	-11.059241513	11.882366470
1	4.237839031	-5.182855093	15.053037550
1	1.132973878	-5.357401524	16.333224862
1	1.863067624	-3.103062354	13.940319645

(A) Bond length (Angstroms and Bohr) of optimized compound CID 14492795.

8	-6.327310000	-2.727140000	2.215810000
6	0.645370000	-0.866990000	0.495850000
6	-0.036600000	-1.313460000	-0.818910000
6	-1.575960000	-1.379690000	-0.800440000
6	-2.190750000	-0.456310000	0.291020000
6	2.141230000	-0.901540000	0.025920000
6	0.103850000	0.536290000	0.867030000
6	-3.731960000	-0.253540000	0.063170000
6	0.771380000	-2.520320000	-1.275810000
6	-1.339920000	0.821370000	0.396170000
6	2.206860000	-2.201030000	-0.829160000
6	-2.196530000	-2.774460000	-0.732390000
6	3.268240000	-0.827890000	1.097660000
6	0.444150000	-1.856950000	1.670330000
6	-4.383520000	-1.618410000	-0.227960000
6	-4.394980000	0.355070000	1.346090000
6	-3.687560000	-2.721150000	-0.567830000
6	-4.001420000	0.710570000	-1.113350000
6	-5.866010000	-1.703310000	0.063730000
6	-5.004410000	-0.706570000	2.264240000
6	3.261820000	0.473540000	1.933100000

6	-6.134380000	-1.471990000	1.560850000
6	4.655240000	-1.038430000	0.469160000
6	3.625820000	1.745780000	1.150840000
6	3.107080000	3.043200000	1.813260000
6	3.315250000	4.257480000	0.861280000
6	3.717500000	3.248300000	3.203610000
6	2.355430000	5.402450000	1.201320000
6	4.753940000	4.779280000	0.826620000
1	-6.451980000	-2.547500000	3.162920000
1	-7.075700000	-0.918700000	1.660500000
1	0.186810000	-0.524660000	-1.559720000
1	2.292280000	-0.071150000	-0.677750000
1	0.137540000	0.677190000	1.953780000
1	0.743480000	1.318050000	0.441700000
1	-0.600320000	-2.104540000	1.857290000
1	0.955540000	-2.810530000	1.503850000
1	0.842940000	-1.441890000	2.602590000
1	-1.875700000	-0.979720000	-1.780400000
1	0.709800000	-2.666290000	-2.358950000
1	0.439070000	-3.446900000	-0.796410000
1	-2.115550000	-0.960010000	1.261170000
1	-1.780170000	-3.348030000	0.102900000
1	-1.965980000	-3.323110000	-1.653260000
1	-1.786850000	1.553730000	1.075620000
1	-1.291140000	1.309610000	-0.585810000
1	2.859410000	-2.054310000	-1.697170000
1	2.606360000	-3.046500000	-0.257480000
1	3.124110000	-1.654770000	1.804890000

1	-5.193990000	1.055070000	1.066390000
1	-3.675690000	0.944940000	1.922960000
1	-5.075470000	0.833460000	-1.295060000
1	-3.602220000	1.709930000	-0.908440000
1	-3.561540000	0.357500000	-2.050730000
1	-4.208540000	-3.669710000	-0.685230000
1	2.290960000	0.588520000	2.420360000
1	3.982410000	0.358810000	2.754010000
1	4.831290000	-0.345030000	-0.359580000
1	4.765210000	-2.056810000	0.083390000
1	5.446630000	-0.891200000	1.212170000
1	-6.378690000	-0.932380000	-0.523810000
1	-6.284210000	-2.665260000	-0.256310000
1	-5.400800000	-0.236310000	3.172400000
1	-4.226160000	-1.399790000	2.609870000
1	3.208900000	1.691990000	0.140600000
1	4.715210000	1.793270000	1.034780000
1	2.023920000	2.920610000	1.949100000
1	3.060080000	3.936180000	-0.157640000
1	4.811760000	3.232500000	3.169500000
1	3.402310000	4.200020000	3.641560000
1	3.397650000	2.458450000	3.891030000
1	2.459040000	6.218940000	0.478290000
1	2.542830000	5.811370000	2.198440000
1	1.315850000	5.059430000	1.162030000
1	4.864260000	5.540280000	0.046070000
1	5.466270000	3.978610000	0.607540000
1	5.039020000	5.243370000	1.776610000

(B) Bond length (Angstroms and Bohr) of optimized compound CID 10134.

8	-0.543231971	0.994884041	0.065444990
8	1.526993085	-5.488635435	-0.857701273
8	-7.901053962	-3.960446153	-1.678084237
8	-3.354658582	-5.946122979	-1.505559813
8	-8.518901764	4.911282571	-0.159216973
8	11.249984785	1.787045837	1.572628078
6	-4.165419062	-1.570247023	-0.814940553
6	-3.072558397	0.797770503	-0.263507171
6	1.081471286	-1.015629453	-0.107136125
6	-2.573997659	-3.756994474	-1.022379554
6	0.122255823	-3.371696352	-0.640779627
6	3.723349792	-0.300131951	0.326979288
6	-6.835915578	-1.740127720	-1.155903813
6	-4.528471329	2.981513289	-0.040876663
6	-7.147119433	2.769155331	-0.383466977
6	-8.305283359	0.437019922	-0.936359227
6	4.348130998	2.237641551	0.856146028
6	5.716952128	-2.079482824	0.236918727
6	6.839283070	2.970186271	1.275999679
6	8.205541731	-1.351241009	0.655549725
6	8.794797979	1.181186457	1.179731368
1	-6.523679932	-5.237524866	-1.747267105
1	-3.669800627	4.803076861	0.385475756

1	0.280860525	-6.809637048	-1.238806092
1	2.855525257	3.654299204	0.938800753
1	5.300541558	-4.052122430	-0.166420609
1	-10.348564702	0.293300591	-1.200134740
1	-10.287439625	4.540595811	-0.429619755
1	7.274532318	4.951826642	1.683218622
1	9.737960220	-2.731523327	0.583919661
1	11.396850510	3.576502965	1.910341009

(C) Bond length (Angstroms and Bohr) of optimized compound CID 5280863.

8	0.540879262	6.829471612	1.256843527
8	7.018028472	0.760112043	-6.758206266
8	7.749307076	5.418396209	-5.002894597
6	-1.186403991	0.127027381	1.323751165
6	-0.615394937	-0.552941383	-1.512748331
6	-3.073660107	-1.618820540	2.813168939
6	-0.002628609	-3.409950075	-1.697070314
6	-2.322227576	-4.408199718	2.351355812
6	-1.989713280	-5.097278851	-0.436407651
6	-1.749408165	2.960499536	1.598989756
6	1.668826469	1.056496667	-2.345594037
6	-2.790943871	0.084895940	-3.374708575
6	-2.780047711	-1.098081977	5.670086924
6	-5.882271027	-1.209570142	2.138926044
6	2.012374874	3.533883975	-1.400903008
6	0.299689755	4.661572289	0.519852281
6	3.388830498	0.171307440	-4.159285011
6	4.034032083	5.038789942	-2.261317928

6	5.389967171	1.663724209	-5.017033527
6	5.714992483	4.133265374	-4.045056744
1	0.645675907	-0.192680241	2.280094245
1	-3.535063164	3.476319142	0.648960250
1	-1.982432166	3.525520047	3.584740280
1	0.214240125	-3.961498730	-3.693412753
1	1.843403135	-3.757850519	-0.785602557
1	-4.490451932	-1.062553239	-3.050539310
1	-2.153620554	-0.278496478	-5.323089769
1	-3.346528981	2.086503156	-3.283436700
1	-3.737575649	-5.650292044	3.252044572
1	-0.516515025	-4.776533770	3.338495756
1	-3.874932272	-2.492382283	6.766906564
1	-0.789365002	-1.246376335	6.270078705
1	-3.472617168	0.788282189	6.211143820
1	-6.462209036	0.770979857	2.414776906
1	-6.347606603	-1.732302365	0.184429698
1	-7.077040835	-2.376336100	3.386714004
1	-3.811312757	-4.956590641	-1.443733648
1	-1.404159006	-7.092013134	-0.604459093
1	3.227640650	-1.712499926	-4.974856733
1	4.223274913	6.942382740	-1.474649565
1	8.253741083	2.066729063	-7.115132042
1	7.782511451	7.122898815	-4.349990489

(D) Bond length (Angstroms and Bohr) of optimized compound CID 11119228.

Supplementary Fig. 6. (A) Bond length (Angstroms and Bohr) of optimized compound CID 14492795. (B) Bond length (Angstroms and Bohr) of optimized compound CID 10134. (C)

Bond length (Angstroms and Bohr) of optimized compound CID 5280863. (D) Bond length (Angstroms and Bohr) of optimized compound CID 11119228.