

# Supplementary Material

## Predicting octanol-water partition coefficients of fluorinated drug-like molecules: A combined experimental and theoretical study

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**Table S1.** SMD-M06-2X/6-31G(d) optimised geometries in water and 1-octanol. All minimum energy structures have zero imaginary frequencies.

**M1 (water)**

H	-4.2489458912	3.0433466252	1.0439537274
C	-5.0792124828	2.8896413983	0.3609484391
C	-6.3090316626	2.4585744406	0.8564071095
H	-6.4351652382	2.2888020473	1.9220419371
C	-7.3873893121	2.2663132232	-0.0096935008
C	-8.7221623512	1.754271167	0.4911312389
C	-7.2175602197	2.5119785367	-1.3740954134
H	-8.0576910754	2.3732295918	-2.0507586926
C	-5.9859085702	2.9316032262	-1.8708954458
H	-5.8672200123	3.117009454	-2.934221217
C	-4.9119377347	3.1231023761	-1.0026293869
H	-3.952860986	3.4574142134	-1.3861154042
O	-8.9406888778	1.9722660041	1.8720828473
C	-9.1742213815	3.3334775897	2.1992436203
C	-9.3280990904	3.4199456746	3.7051524415
C	-8.1058093574	2.8797576727	4.4324218855
C	-7.9157841031	1.3905444457	4.2699319362
O	-6.8511084931	0.8873804821	3.9833068345
F	-6.9618775158	3.5193369027	3.9850597158
H	-8.7756927051	0.669400504	0.3521472967
H	-9.536795843	2.204343328	-0.0939828225
H	-10.0841388494	3.688079139	1.6972275644
H	-8.3347785944	3.9566240555	1.8662065529
H	-10.2027123784	2.8465770568	4.0309314486
H	-9.4837032214	4.4621940715	3.9959617606
H	-8.2039055724	3.066159352	5.5107701935
H	-8.8079714804	0.779419422	4.4918613332

**M1 (1-octanol)**

H	-4.232204119	2.9475784722	1.0909641243
C	-5.0697370872	2.8695667138	0.4035139713
C	-6.2983582672	2.4015580057	0.8651490398
H	-6.418663587	2.1256854114	1.909529397
C	-7.3854111104	2.3049424866	-0.006594132
C	-8.716871744	1.7565965596	0.463113489
C	-7.2255589578	2.6836072942	-1.3407771836
H	-8.0724594638	2.6203592534	-2.0208742907
C	-5.9941191044	3.1403071943	-1.8050350901
H	-5.8825036867	3.4298779162	-2.8460295361
C	-4.9121245353	3.2359185496	-0.9319174097
H	-3.952980631	3.5991338687	-1.2892265838
O	-8.9502169161	1.9271433977	1.8469622798
C	-9.1714857315	3.2740773201	2.2273142046
C	-9.337102679	3.2936315335	3.7349050817
C	-8.1297695499	2.6952203749	4.4421543236
C	-7.9639604278	1.210588847	4.2063648915
O	-6.9068425167	0.702861658	3.912616362
F	-6.9736862302	3.3363848409	4.035160026
H	-8.7529415731	0.675033132	0.2928003155
H	-9.5341169272	2.2114855144	-0.116089728
H	-10.0738770639	3.6624613405	1.7346223794
H	-8.322597248	3.9031381045	1.9302477695
H	-10.2264648691	2.7229271365	4.0252639332
H	-9.4760389933	4.3240300795	4.0744139301
H	-8.2324278166	2.8301303992	5.5285150649
H	-8.8721491636	0.6061395954	4.3853693706

**M2 (water)**

H	-5.736697	0.560952	1.946137
C	-6.0698	1.261122	1.185787
C	-7.42768	1.547858	1.058793

H -8.147333 1.07707 1.722915  
 C -7.868222 2.45337 0.090965  
 C -9.34191 2.747274 -0.095012  
 C -6.932732 3.066942 -0.744569  
 H -7.270641 3.780854 -1.492081  
 C -5.576349 2.771874 -0.625839  
 H -4.85902 3.254487 -1.282794  
 C -5.140981 1.868266 0.342178  
 H -4.083749 1.642669 0.442105  
 O -10.117808 2.53868 1.071521  
 C -9.877664 3.501407 2.086921  
 C -10.735076 3.113633 3.274656  
 C -10.442065 1.704767 3.729611  
 C -10.848625 0.596827 2.753332  
 O -10.098622 -0.301972 2.461019  
 F -9.124837 1.555746 4.027129  
 H -9.762425 2.075298 -0.850136  
 H -9.475238 3.777781 -0.453087  
 H -10.146728 4.503228 1.729352  
 H -8.816987 3.508213 2.366817  
 H -11.797505 3.171945 3.018703  
 H -10.54299 3.781649 4.11928  
 F -11.144099 1.445332 4.877518  
 H -11.890086 0.649261 2.396838

## M2 (1-octanol)

H -5.7408922171 0.521885987 1.9153430028  
 C -6.0748667992 1.2391361271 1.171042785  
 C -7.43463032 1.5091950414 1.0352320237  
 H -8.1560789172 1.0083406468 1.6756435464  
 C -7.8763312968 2.4355843974 0.0873900927  
 C -9.3534631753 2.7094987628 -0.1009743512  
 C -6.9403479805 3.0867013226 -0.7177734114  
 H -7.2783770844 3.817321804 -1.4494391621  
 C -5.5811094819 2.8080579218 -0.5902503874  
 H -4.862642069 3.3201272031 -1.2238855548  
 C -5.1449129358 1.883930093 0.3568779217  
 H -4.0853609462 1.6709489379 0.4639238335  
 O -10.1203402653 2.5310762419 1.0753598751  
 C -9.866296047 3.5046239766 2.0741772299  
 C -10.7143475821 3.1292584364 3.2732277208  
 C -10.4301736695 1.7167650849 3.7259773783  
 C -10.8548744944 0.6110850079 2.7535772647  
 O -10.1215600429 -0.2982963324 2.461171747  
 F -9.1131722506 1.5579770692 4.0137275399  
 H -9.7737654501 2.0081442584 -0.8296523733  
 H -9.4999720506 3.726538487 -0.4929227863  
 H -10.1361411391 4.5046819138 1.7094300055  
 H -8.8029806684 3.5123816042 2.3450596886  
 H -11.7791194525 3.1999701962 3.0286378321  
 H -10.5072596684 3.7966312094 4.1153498267  
 F -11.1279888634 1.4660131714 4.8791209621  
 H -11.8988641321 0.6769534302 2.4026867498

## M3 (water)

H -5.4502791175 0.4222821939 0.2472076168  
 C -6.1930108573 1.2133319803 0.2843406308  
 C -7.4745170064 0.9873982994 -0.2196265175  
 H -7.7301124088 0.0213930739 -0.6481285101  
 C -8.4370529063 1.9952554274 -0.1799201015  
 C -9.8259346469 1.7775786322 -0.7309463096  
 C -8.1074271243 3.2341682889 0.3805016135  
 H -8.8624628894 4.0171295229 0.4230136131  
 C -6.8329871214 3.4597402688 0.891407884  
 H -6.5859352659 4.4237372058 1.3257603302  
 C -5.8714657475 2.4485748187 0.840738141  
 H -4.8758643944 2.6251920238 1.2360801291  
 O -10.8392495437 2.0340633379 0.234034495  
 C -10.9804771012 0.9897684987 1.1946118254  
 C -11.9908915004 1.4368056951 2.2396190088  
 C -11.4032636291 2.3045628919 3.3440026203

C -10.5677872377 3.4771234216 2.8682066214  
 F -12.481561266 2.7998578037 4.087746523  
 H -9.9322220504 0.7548699557 -1.1160640943  
 H -10.0224141584 2.4753980907 -1.550125786  
 H -10.0064392011 0.761703387 1.6518824268  
 H -11.3316576926 0.0862378879 0.6808687368  
 H -12.4542619445 0.5598591082 2.7000972929  
 H -12.7845840042 2.0009387688 1.7368482423  
 H -10.7918722876 1.699340706 4.0235979707  
 H -9.5963954165 3.0964455502 2.525312494  
 O -11.1998271511 4.2476674403 1.8604873444  
 H -10.3849200585 4.1380331586 3.720799279  
 H -11.151932271 3.7007865615 1.0518134798

### M3 (1-octanol)

H -6.4555297393 -0.4717007058 0.6787002373  
 C -6.5923840001 0.5836010803 0.4612890268  
 C -7.8719629708 1.0894686002 0.2563409736  
 H -8.7382371783 0.4331567901 0.3232273665  
 C -8.0606671195 2.4475801301 -0.0220814679  
 C -9.4604717648 2.9711463951 -0.2414087509  
 C -6.9513914045 3.289072114 -0.0911302191  
 H -7.0939946688 4.3467918605 -0.3002517326  
 C -5.666207156 2.7830938854 0.1062947209  
 H -4.8087211016 3.4472743747 0.0499165634  
 C -5.4857226747 1.4308940671 0.383242316  
 H -4.4865092475 1.0355725279 0.5405593187  
 O -10.3237077813 2.6940546794 0.8526320121  
 C -10.0975009697 3.5327773789 1.9816611988  
 C -11.018741674 3.0776394809 3.1026962911  
 C -10.4923418154 1.9040049022 3.9147354538  
 C -9.9288439594 0.7500030527 3.0933623642  
 F -9.4292613103 2.3590399053 4.7047973182  
 H -9.9195595996 2.4785819228 -1.1043194095  
 H -9.4422259243 4.0525761027 -0.43430551  
 H -10.3165981136 4.5711008061 1.6987312012  
 H -9.0442163869 3.481856599 2.2938387905  
 H -11.9924964309 2.8169132234 2.6734604819  
 H -11.1852908627 3.9071038036 3.7977723385  
 H -11.2735596389 1.5493015721 4.5955553258  
 H -9.6932422799 -0.0846532032 3.7603366738  
 O -10.844575476 0.2811278147 2.1252906835  
 H -8.9885535509 1.0848147695 2.6337771668  
 H -10.8552312004 0.9622230703 1.4256352665

### M4 (water)

H -4.854112238 1.3238064615 1.4914282981  
 C -5.6030347309 1.8742400214 0.9302915861  
 C -6.8881687628 1.350763443 0.7864108582  
 H -7.1411037843 0.3929184576 1.2348328485  
 C -7.8601832885 2.0502253854 0.069006775  
 C -9.2851406281 1.5641908455 -0.0012619785  
 C -7.5272696161 3.2772050576 -0.5153101634  
 H -8.2830398595 3.8232793793 -1.0754153962  
 C -6.2470130974 3.8029992782 -0.3720258867  
 H -5.9975607873 4.7564075604 -0.8276987292  
 C -5.2833678245 3.1020557182 0.3552140964  
 H -4.2841307803 3.5114300183 0.4680635862  
 O -10.1101032543 2.2844437233 0.9195532097  
 C -10.0497025294 1.7802240613 2.2520154017  
 C -10.6060565854 2.8406688327 3.1880986692  
 C -9.583351314 3.8823399929 3.5914574642  
 C -8.7487328948 4.4985632882 2.4821071427  
 F -10.2350992599 4.8769232544 4.2742723798  
 H -9.3521638621 0.4899314902 0.208950551  
 H -9.7111422529 1.7558118539 -0.9893021305  
 H -9.0144755715 1.5332715945 2.5245158515  
 H -10.6447445965 0.8616147108 2.3124460286  
 H -10.9722220662 2.3802524613 4.1102541232  
 H -11.4482981482 3.344768539 2.7052516861

F	-8.7020623543	3.3285075899	4.4884066376
H	-8.0211564344	3.749168589	2.1445273334
O	-9.5516140134	4.9737278821	1.4231164978
H	-8.2017474592	5.344605428	2.9074209479
H	-9.8561390056	4.1739170819	0.9493093117

### M4 (1-octanol)

H	-4.6147838834	0.6675756092	0.6309932341
C	-5.3835382378	1.4069879293	0.4264467772
C	-6.7252689388	1.0252000235	0.4001990831
H	-7.0004443566	-0.0106623318	0.5848908084
C	-7.7219202701	1.9638297311	0.1373561094
C	-9.1808655553	1.5756854333	0.0986890461
C	-7.3622009214	3.2964105556	-0.0921460369
H	-8.1400124491	4.0331254316	-0.2873405876
C	-6.0259448351	3.6816510967	-0.0584506359
H	-5.7563584662	4.7186840471	-0.2360088755
C	-5.0330010049	2.7347760918	0.1985153316
H	-3.9894024798	3.0344389352	0.2218362238
O	-9.9648703427	2.3252332174	1.0191421821
C	-9.8208959255	1.8937988422	2.3673704802
C	-10.6149086264	2.8397555962	3.2528973119
C	-9.8848792015	4.1258023417	3.5794863079
C	-9.2445747927	4.8685834335	2.4197176041
F	-10.7593915184	4.9586767566	4.2266454649
H	-9.3028915474	0.5023389016	0.2971772697
H	-9.6069380305	1.7917513969	-0.8858154948
H	-8.7601920546	1.8794658081	2.6569083041
H	-10.211085465	0.8721306661	2.4589880363
H	-10.8518399079	2.3566810389	4.2057943253
H	-11.5582068086	3.0891383751	2.7575002754
F	-8.8820546715	3.8601598028	4.4806801985
H	-8.3583917177	4.3033488376	2.1049524849
O	-10.1456418874	5.078496195	1.358375793
H	-8.9164819051	5.8441927839	2.7904626306
H	-10.2459511983	4.2110054539	0.920673348

### M5 (water)

C	-3.6502485596	1.5047871826	-0.2484416678
C	-4.2690074653	0.3187356477	0.1503369198
C	-3.7587473111	-0.4083288112	1.2232378692
C	-2.6415600775	0.0655505207	1.9151857453
C	-2.0330867958	1.2524858056	1.5192864725
C	-2.5251312907	1.9737431694	0.4270834958
C	-1.7582636271	3.1749092418	-0.0568483386
O	-0.5143637162	2.6972056366	-0.5509638413
C	0.3561612985	3.7286874336	-0.9828712948
C	1.7256312998	3.1166730317	-1.2266743555
C	2.4992286361	2.8631183048	0.0570562473
C	1.8324333832	1.9554520142	1.0623177764
O	1.5510050341	0.7051941733	0.4010815205
C	1.0680377715	-0.2663204325	1.1624901579
H	-4.0323656506	2.0593399367	-1.1019436073
H	-5.1398592788	-0.0437630134	-0.3875927986
H	-4.2326750392	-1.3370501494	1.5266416507
H	-2.2458312377	-0.48897577	2.7616771937
H	-1.1617119814	1.6214895431	2.0548361738
H	-1.5738715397	3.8838614535	0.7636494902
H	-2.3063558554	3.7020249472	-0.8497946273
H	0.4128764542	4.5170550872	-0.2161682043
H	-0.0327001459	4.1841633687	-1.9031814958
H	2.3221376541	3.7927965867	-1.8461331674
H	1.6114015206	2.1744260944	-1.7751418858
H	2.7144835018	3.8109044734	0.5630880435
F	3.719585743	2.2806335045	-0.2901729784
H	0.9036233224	2.3952218574	1.4302336011
H	2.5061386069	1.759706108	1.8999697593
O	0.7924917913	-0.1442717633	2.332687054
C	0.9433210167	-1.6140052313	0.4137460889
O	0.9679600521	-2.661771364	1.3459040716

C 2.2392460409 -1.8427922933 -0.3912146576  
C -0.2433017186 -1.6880351228 -0.5463495669  
C -0.7654239046 -0.5580424524 -1.1755427293  
C -0.7641426663 -2.9516176532 -0.8426927254  
C -1.8149460993 -3.0789869019 -1.745229733  
C -2.3436800718 -1.9491655611 -2.3680808745  
C -1.8137338196 -0.6934388803 -2.0848004686  
C -0.1729170963 -2.8213086619 2.1966913061  
F 3.3184222718 -1.6366478498 0.3759499287  
F 2.3261467013 -1.0340411877 -1.4497973783  
F 2.2936929357 -3.0992735993 -0.8402617871  
H -0.3731754389 0.4308341042 -0.9627303153  
H -0.3492200189 -3.8316437575 -0.36108152  
H -2.2187632862 -4.0626650334 -1.9629908008  
H -3.1638339342 -2.0491453507 -3.0722195101  
H -2.2184364335 0.1930742425 -2.5635019089  
H -0.3725456471 -3.8931722489 2.2603816922  
H -1.0533774149 -2.317008349 1.7921153949  
H 0.0480690858 -2.4268200312 3.1897925855

## M5 (1-octanol)

C -2.2273028244 -0.2886587593 -0.920497054  
C -3.3219427178 -1.1313767834 -0.7278085612  
C -3.5266133424 -1.7339283606 0.5105925076  
C -2.6363294006 -1.4882647668 1.5579534407  
C -1.5548442285 -0.633607194 1.3654785458  
C -1.3411568938 -0.0263279676 0.1237945033  
C -0.1381624727 0.8686888409 -0.0774569194  
O 1.0866973601 0.2182930994 0.2251715437  
C 1.343317173 -0.8760893145 -0.6401902265  
C 2.6988871787 -1.4669066065 -0.2986949696  
C 2.8508517758 -1.8184822382 1.1748040366  
C 1.688301902 -2.5808147022 1.7619261062  
O 1.3284457587 -3.6295711302 0.8455442231  
C 0.1781129138 -4.2453366886 1.0939563776  
H -2.0580508462 0.1695294514 -1.8922669796  
H -4.0071654512 -1.3246554894 -1.5480338798  
H -4.3766181627 -2.3936825847 0.6621667231  
H -2.7896145779 -1.95912802 2.5250057407  
H -0.872430168 -0.4243832513 2.1864808572  
H -0.1837637449 1.7311580683 0.5949646973  
H -0.1186905887 1.2401662548 -1.1125445023  
H 1.3312959643 -0.5391745293 -1.6875860865  
H 0.5563327566 -1.6334186598 -0.5292813332  
H 3.4993015923 -0.773098197 -0.5739632964  
H 2.8314752923 -2.384020529 -0.8813218473  
H 2.9933982001 -0.9200551909 1.7835755751  
F 4.0033963522 -2.5959836577 1.3040497475  
H 0.8309179722 -1.9169541148 1.8951501153  
H 1.9596309062 -3.0202022423 2.7258104482  
O -0.5013255319 -4.0528344083 2.0707460765  
C -0.1355447513 -5.2569933589 -0.0413368735  
O 0.9709958936 -6.0878443316 -0.2655025837  
C -0.2793004625 -4.46035517 -1.3553989118  
C -1.4301657242 -6.0281213911 0.1946139102  
C -2.5985423034 -5.3792259826 0.6035231789  
C -1.4682628001 -7.3911569828 -0.1034428689  
C -2.6529453094 -8.1081310628 0.0435679476  
C -3.8118241828 -7.4644544754 0.4696750081  
C -3.7823576406 -6.0983492353 0.7413818945  
C 1.4963281049 -6.710524224 0.9052331777  
F 0.8743721612 -3.9350933409 -1.7728263134  
F -1.1488188899 -3.4505638017 -1.186669993  
F -0.7351211811 -5.2418714935 -2.3371904091  
H -2.5899389149 -4.3153507348 0.8132220006  
H -0.5709126783 -7.8899088045 -0.455905402  
H -2.6689069185 -9.170011492 -0.182502142  
H -4.7360078258 -8.0231884804 0.583386016  
H -4.6845216079 -5.5860429547 1.0625764974  
H 2.1702919249 -7.4936366859 0.5562939446  
H 0.7032919102 -7.1561428387 1.5150821664  
H 2.0622830492 -5.9886884869 1.5051781455

## M6 (water)

C 2.6080616248 2.8983930799 -0.0698993066  
C 3.748162981 2.2833535579 -0.583779275  
C 3.630406852 1.296984785 -1.562304945  
C 2.3680718328 0.9446981829 -2.0384375528  
C 1.2320614104 1.5798344276 -1.5405084119  
C 1.3412104026 2.55171567 -0.5438303385  
C 0.1139272317 3.2458669092 -0.0098708308  
O -0.9801519924 2.3482682524 -0.0046773675  
C -2.1906773305 2.9885876436 0.3662230293  
C -3.2584886867 1.944525352 0.6404258348  
C -3.7614695055 1.2012814096 -0.5861409316  
C -2.7267440503 0.4281258888 -1.3650309411  
O -2.0001895379 -0.4094672966 -0.4436993989  
C -0.9507697708 -1.0375375411 -0.9495740942  
H 2.7000187077 3.648163379 0.7125670472  
H 4.7276121614 2.5621169361 -0.20661559  
H 4.5174365039 0.8065001321 -1.9515590732  
H 2.2635867001 0.1751967221 -2.7981185745  
H 0.2526926513 1.3156677523 -1.9251659898  
H -0.1303837742 4.1187183441 -0.6357034799  
H 0.3022102224 3.6172054941 1.0087753817  
H -2.5061307663 3.6804952766 -0.4296297756  
H -2.0283665012 3.5797033477 1.2778962053  
H -4.1203645395 2.4448538886 1.092865038  
H -2.8800685027 1.2197107793 1.368154142  
H -4.2460659469 1.8933800845 -1.2838906009  
F -4.7311363153 0.2951901838 -0.1481837493  
H -2.035215459 1.1114060097 -1.8603615709  
H -3.2105516396 -0.2086389434 -2.1100955407  
O -0.6199387398 -0.9876179213 -2.1122543791  
C -0.1892272139 -1.845750472 0.1279225559  
C 0.6101694723 -0.8950952264 1.0174789752  
C 0.6817876285 -2.8730004612 -0.6215027302  
O -1.1844183582 -2.5654429044 0.8210422633  
F 1.5911778211 -2.3118640825 -1.4272013346  
F -0.0866070433 -3.6716524785 -1.3680655889  
F 1.3498655964 -3.6551082108 0.2399799027  
C -0.8606928664 -3.0849252978 2.11620599  
H -1.5871732508 -3.8780906972 2.2963368475  
H 0.1463431552 -3.502278677 2.1535220231  
H -0.9658673919 -2.3149559477 2.8844620628  
C 2.0067664028 -0.8309366716 1.030164085  
C 2.6542183222 0.060879891 1.8829783215  
C 1.9225066403 0.895189715 2.7242765793  
C 0.5307313205 0.8289211583 2.7197398852  
C -0.1191455137 -0.0640109931 1.8744406048  
H 2.6083781582 -1.461127116 0.3865775317  
H 3.7388306862 0.1044511752 1.8799476546  
H 2.4344028162 1.5919031121 3.3809665795  
H -0.0528638319 1.4686262269 3.3747540985  
H -1.2024997735 -0.1275248289 1.8829077327

## M6 (1-octanol)

C -0.1582764367 -0.794447901 1.5101603353  
C -0.1978742795 -1.9782665517 2.2414775033  
C -1.0811565308 -2.9952656686 1.872721703  
C -1.9298920621 -2.8155280771 0.7832534993  
C -1.8842539913 -1.6287679592 0.0515353909  
C -0.9958812001 -0.6122658368 0.4043461779  
C -0.8396005212 0.6260136617 -0.4475063916  
O 0.4457386193 0.6660567844 -1.0564908796  
C 0.611813987 -0.2934365083 -2.0906897521  
C 2.0745420874 -0.7055660363 -2.1434917726  
C 2.5771813023 -1.2553058469 -0.8200457208  
C 1.9630472829 -2.5763945231 -0.4232200714  
O 2.4919924089 -2.8670887373 0.8814213028  
C 2.207891639 -4.0589599505 1.3784735606  
H 0.5402812877 -0.0068719835 1.7852976912  
H 0.47306728 -2.1183645974 3.08471057  
H -1.1044220394 -3.9260068851 2.4305136169  
H -2.6191524419 -3.6036235816 0.4944855361

H -2.5345077067 -1.4951248227 -0.8103032996  
 H -0.9001993337 1.5313585635 0.1636977909  
 H -1.628428017 0.6726406767 -1.2113654451  
 H 0.304669278 0.1402351865 -3.0520286529  
 H -0.0241512581 -1.1690980049 -1.9080963298  
 H 2.6929116899 0.1630202322 -2.3942051852  
 H 2.2136986465 -1.4539087749 -2.9322797528  
 H 2.4296060805 -0.525520758 -0.0184173072  
 F 3.9551583296 -1.4701142233 -0.9311999597  
 H 2.2624905097 -3.3676531963 -1.1179172523  
 H 0.8714949667 -2.5323630542 -0.3657188115  
 O 1.486191478 -4.874264943 0.8555729339  
 C 2.9804014999 -4.3231978033 2.6884099624  
 C 4.3008187363 -4.9997001316 2.3171575464  
 C 2.0678846303 -5.1854782763 3.5781892824  
 O 3.1323030126 -3.0882867375 3.3453877983  
 F 1.8479591047 -6.408328523 3.0919980512  
 F 0.8780898444 -4.5865927337 3.7323120549  
 F 2.5915492695 -5.3274261915 4.8059801141  
 C 4.245082028 -2.9358723459 4.2268534967  
 H 4.0519325072 -2.0102189444 4.7710452081  
 H 4.3260979249 -3.7620208987 4.9373068217  
 H 5.1806997731 -2.8390708577 3.6684430863  
 C 4.7506906509 -6.1738431174 2.9257574767  
 C 5.988341701 -6.7114816398 2.5773294928  
 C 6.7894070975 -6.0813219622 1.6306678373  
 C 6.3491667519 -4.9038070612 1.0292607581  
 C 5.1133754752 -4.364454776 1.3686247306  
 H 4.1549791825 -6.6845898291 3.6729925122  
 H 6.3239594108 -7.6267053873 3.0551346396  
 H 7.753524711 -6.503230812 1.3637101828  
 H 6.9681969492 -4.4013347845 0.2924311545  
 H 4.7828756841 -3.4433558699 0.8965377651

### LT1 (water)

C 4.7123292594 3.0752357251 0.6395619111  
 C 5.0853035414 4.556795087 0.5940466234  
 C 6.536269741 4.486722467 0.1253929407  
 H 4.4594445713 5.13122107 -0.0885919483  
 H 5.0245751283 4.9854734601 1.5964069545  
 O 7.0514460344 3.2409556723 0.6651593176  
 H 6.6184791746 4.4331444971 -0.9626721613  
 H 7.1675191767 5.2876824733 0.5065920152  
 C 6.0475980927 2.4072824693 0.9661202861  
 O 6.2304595723 1.2983103831 1.4070552796  
 N 3.6819257341 2.6789007971 1.5656005324  
 C 3.9043157961 2.7075564859 2.8878326659  
 C 2.8216384967 2.0966601018 3.7619336177  
 C 3.4059816835 0.9161586501 4.5158096089  
 C 2.3675495562 0.0773112896 5.2284795216  
 C 2.9919394686 -1.1040524771 5.9670995871  
 C 1.9401317315 -1.9525290819 6.6728315654  
 H 2.8404557669 2.2340653277 1.2220148715  
 F 1.7690531636 1.6657594857 2.9662553177  
 H 2.4471574056 2.8491308026 4.4612756896  
 H 4.1651924734 1.2940101274 5.2079381109  
 F 4.0623714502 0.118207472 3.5710080143  
 H 1.6409433352 -0.2789589728 4.4893859216  
 H 1.8293993335 0.7242785671 5.9319408484  
 H 3.7205523309 -0.728542532 6.6960814675  
 H 3.5484100074 -1.7179862972 5.2506291621  
 H 1.3893209931 -1.3585415055 7.4099947008  
 H 2.3962499322 -2.7988337017 7.1947463232  
 H 1.2147512196 -2.3505437015 5.9551779465  
 O 4.9279007414 3.1598722193 3.4021435894  
 H 4.4222490881 2.7240506388 -0.3553232813

### LT1 (1-octanol)

C 4.8061261892 2.6533627894 0.4387612254  
 C 4.8365700222 4.1226901337 0.860812026  
 C 6.330505316 4.4307055313 0.7775859091



H	4.2449936933	4.7669485878	0.2095334704
H	4.4819603018	4.2170092516	1.8892225949
O	6.9986214231	3.1833787216	1.0844038678
H	6.6370683098	4.7334280407	-0.227488674
H	6.6729307787	5.1678156431	1.5031403819
C	6.1737291633	2.144224977	0.9039443329
O	6.5125489922	1.0011491445	1.0701727181
N	3.7356319149	1.8426012875	0.959790967
C	3.6898933456	1.5318325688	2.2664840053
C	2.6363562009	0.512234038	2.6704357751
C	3.3327205223	-0.7605981271	3.1181694835
C	2.3872605858	-1.9187478684	3.3590080776
C	3.1265551865	-3.1880047236	3.7771485786
C	2.1716922493	-4.3533648151	4.0115221858
H	3.1129040353	1.3623287076	0.3234944351
F	1.8154773726	0.2309492432	1.5867038266
H	2.0238512981	0.9216277879	3.478785915
H	3.9271640965	-0.5304928166	4.0088970844
F	4.222427082	-1.1072016196	2.0978389962
H	1.8157357521	-2.0984655159	2.4409708229
H	1.6721788704	-1.6222013986	4.1367310575
H	3.7015198656	-2.9872408019	4.6899926753
H	3.8517898757	-3.4499574251	2.9990385296
H	1.4530052044	-4.1193194894	4.804805316
H	2.7131634664	-5.2578309077	4.3053201649
H	1.6031943599	-4.5826102987	3.1033994746
O	4.4597295138	1.9876272651	3.1069567048
H	4.7923920123	2.566320089	-0.6523729283

## LT2 (water)

C	4.726309	3.476615	0.817387
C	6.209048	3.383921	1.179472
C	6.829971	3.041921	-0.171776
H	6.603115	4.31285	1.59106
H	6.365288	2.57182	1.892867
O	5.817821	2.270972	-0.870827
H	7.038226	3.93168	-0.770453
H	7.721303	2.419838	-0.10852
C	4.606007	2.49445	-0.346048
O	3.603431	1.986903	-0.787551
H	4.49142	4.466152	0.413575
N	3.780507	3.189859	1.865917
C	3.673603	1.955007	2.376079
C	2.669124	1.780331	3.503999
C	3.380258	1.288772	4.749764
C	2.507005	1.291866	5.985768
C	3.25758	0.799523	7.220692
C	2.379021	0.82466	8.466433
H	3.195781	3.928502	2.235361
H	1.905878	1.060872	3.193705
F	2.052003	2.994841	3.770254
F	4.465913	2.146216	4.961416
H	3.78496	0.292764	4.543369
H	1.635693	0.65469	5.791231
H	2.137716	2.31098	6.147947
H	4.14175	1.427839	7.373839
H	3.620354	-0.219631	7.038988
H	2.025961	1.840526	8.67377
H	2.925385	0.471998	9.34608
H	1.499184	0.185349	8.336793
O	4.340337	0.993659	1.990168

## LT2 (1-octanol)

C	4.7305118597	3.4904084223	0.8276810695
C	6.2123735558	3.3662974143	1.1872094972
C	6.8262732165	3.0059018017	-0.1640016461
H	6.6295534713	4.2859825887	1.5984737291
H	6.3492311018	2.5521281835	1.9022663074
O	5.7963809042	2.2749708857	-0.8719491073
H	7.0734989763	3.8898826806	-0.7582140955
H	7.6967052317	2.3540258039	-0.096604484

C	4.589071284	2.5233065873	-0.3504340228
O	3.5743783874	2.0558711951	-0.7994505658
H	4.5073521869	4.4894674044	0.4397842608
N	3.7843786831	3.199437069	1.873966113
C	3.6704795609	1.9561826212	2.3683263015
C	2.6643201011	1.7746827784	3.495074675
C	3.3841576465	1.3095157285	4.7465096541
C	2.5050408549	1.2815187482	5.9789837271
C	3.2676480194	0.8228951885	7.2200562633
C	2.3837190154	0.8148311239	8.4623821501
H	3.1959553808	3.9340836886	2.2443277342
H	1.9159589433	1.0377038496	3.1883948869
F	2.0227272092	2.9790291294	3.7507053968
F	4.4354507496	2.2059117334	4.962724391
H	3.8260017507	0.3285407646	4.5416635185
H	1.6596708137	0.6099615278	5.78299524
H	2.0944928026	2.2858386401	6.1357415108
H	4.1252999539	1.4864943961	7.3761872365
H	3.6729466398	-0.1816302086	7.0441719002
H	1.9884428637	1.8157407673	8.6680883487
H	2.9414158323	0.4865388591	9.3448782516
H	1.5308059617	0.1392905428	8.3332691974
O	4.3357080417	1.0009380846	1.9775525608

### LE1 (water)

C	4.8358294476	3.6071386909	1.054101581
C	6.1097197562	3.9945164501	1.807225356
C	7.0954942429	4.181535873	0.6572065167
H	6.4245428472	3.1703079312	2.4526939523
O	6.6630981931	3.2496531637	-0.3684900929
H	7.0499480936	5.1860915743	0.2302911661
H	8.1250533071	3.9303093642	0.9069946183
C	5.3816732572	2.9041718781	-0.1861925172
O	4.7941373132	2.1667893415	-0.9401754402
N	3.8854396646	2.7882165021	1.7635138826
C	4.2095288071	1.5423969327	2.1453245033
C	3.1692903195	0.8106639841	2.9789202214
C	3.7626535651	0.1635443486	4.2212851721
C	3.9618303265	1.1069966039	5.3951618324
C	5.0000128288	2.2100342799	5.1770491972
C	6.4205586498	1.6880655383	4.9711923249
H	3.0337267848	3.2041115702	2.1189094294
H	2.7326140861	0.0276422992	2.3499493426
F	2.1561781004	1.6876008674	3.3379005874
H	4.6863049318	-0.3461332583	3.9329310539
F	2.852911774	-0.8158545022	4.6264093918
H	4.2608236521	0.4884987695	6.2490404575
H	2.9881508823	1.5455605551	5.6354495468
H	4.9804277435	2.8589524481	6.0589764694
H	4.7041857963	2.8454542518	4.3326643343
H	6.7194680949	1.0458558092	5.8071347573
H	7.1333972593	2.5163993735	4.9127453358
H	6.5123978759	1.1053596135	4.049435752
O	5.2566044015	0.981388357	1.8194509077
H	5.9913468367	4.8999371193	2.4024351172
H	4.312231161	4.5004172704	0.6995102431

### LE11 (1-octanol)

C	4.8594690227	3.617762596	0.9968560373
C	6.1664248345	4.0048370637	1.6916475542
C	7.1020354727	4.1910678157	0.4985520584
H	6.5076664659	3.1779524793	2.3195382575
O	6.6203850404	3.274711855	-0.5134207167
H	7.0505767181	5.201351342	0.0834232602
H	8.1399482506	3.9304756387	0.7032086867
C	5.349591779	2.9264998948	-0.2776740563
O	4.7234137992	2.2022143136	-1.007401295
N	3.9517176081	2.783970867	1.7417698185
C	4.2881808991	1.5234163906	2.0678042964
C	3.2428888944	0.7404221719	2.8495334301
C	3.8256569865	0.0339319428	4.0643177708

C 3.9588341864 0.90623592 5.3012679732  
 C 4.9413957108 2.0728745829 5.1751564519  
 C 6.3891386253 1.639198924 4.952213613  
 H 3.0593794856 3.1519344861 2.0448727997  
 H 2.8248849764 -0.0137465977 2.1736173625  
 F 2.2134934957 1.5879100342 3.2344929718  
 H 4.775294857 -0.4213242594 3.7678572253  
 F 2.9465422934 -1.0030308136 4.3824535214  
 H 4.2743289859 0.2486458216 6.1196781602  
 H 2.9597896417 1.2780900148 5.5509070741  
 H 4.8797571234 2.6572777916 6.0998364036  
 H 4.6201642573 2.7494199823 4.3726917237  
 H 6.7136059565 0.9554288878 5.745079742  
 H 7.060269239 2.5040806634 4.9637606701  
 H 6.5209644304 1.128609823 3.9931195989  
 O 5.3476480112 0.9965101723 1.7384794271  
 H 6.0784471869 4.909471372 2.2944654978  
 H 4.311226766 4.5098468235 0.6771856817

### IT1 (water)

C 3.070935 0.684325 1.255108  
 C 2.062633 -0.252058 1.572154  
 C 0.915024 -0.355053 0.805718  
 C 0.770317 0.497744 -0.30154  
 C 2.954951 1.529553 0.164407  
 C 1.794527 1.421795 -0.61042  
 C -0.251445 0.684579 -1.287951  
 C 0.160029 1.687211 -2.145089  
 H 3.957161 0.741031 1.879291  
 H 2.194306 -0.900439 2.432579  
 H 0.140888 -1.076966 1.050237  
 H 3.728393 2.248966 -0.085231  
 N -1.442636 -0.069164 -1.338364  
 N 1.409671 2.106056 -1.734951  
 H 1.915981 2.88036 -2.146113  
 C -0.497843 2.297908 -3.306448  
 C -1.89635 2.329181 -3.38906  
 C -2.525864 2.89841 -4.489561  
 C -1.770105 3.460169 -5.518494  
 C -0.379051 3.442598 -5.439442  
 C 0.255411 2.862112 -4.344413  
 C -1.891069 -0.719223 -2.428594  
 C -3.206799 -1.463333 -2.249486  
 C -4.271907 -0.863228 -3.147703  
 C -5.643157 -1.471147 -2.946695  
 C -6.697703 -0.824052 -3.841111  
 C -8.07552 -1.442115 -3.631059  
 O -1.346183 -0.719013 -3.530014  
 H -1.958883 -0.201534 -0.474717  
 H -2.493835 1.910132 -2.587868  
 H -3.610591 2.902762 -4.539075  
 H -2.261833 3.906328 -6.377238  
 H 0.21796 3.873263 -6.237204  
 H 1.340979 2.831993 -4.31088  
 F -3.626016 -1.383227 -0.928713  
 H -3.052066 -2.515645 -2.505058  
 H -3.937551 -0.949457 -4.186441  
 F -4.339953 0.503318 -2.841962  
 H -5.921812 -1.362392 -1.89214  
 H -5.573445 -2.545037 -3.158512  
 H -6.395134 -0.931684 -4.890024  
 H -6.733887 0.250278 -3.630574  
 H -8.061784 -2.513245 -3.859289  
 H -8.825601 -0.970376 -4.272524  
 H -8.400085 -1.32641 -2.591396

### IT1 (1-octanol)

C 3.0615 0.6973 1.261874  
 C 2.059224 -0.245966 1.574647

C 0.91233 -0.35193 0.807666  
 C 0.761452 0.504495 -0.295325  
 C 2.941019 1.545272 0.1738  
 C 1.781998 1.433746 -0.602312  
 C -0.261708 0.688814 -1.281302  
 C 0.147554 1.69046 -2.139511  
 H 3.947895 0.756616 1.886212  
 H 2.195291 -0.898587 2.431638  
 H 0.14447 -1.082467 1.047809  
 H 3.712647 2.268346 -0.072622  
 N -1.4475 -0.070887 -1.342078  
 N 1.394825 2.114919 -1.728076  
 H 1.892465 2.897907 -2.132375  
 C -0.50763 2.288934 -3.308629  
 C -1.90547 2.320505 -3.395506  
 C -2.530644 2.880932 -4.502631  
 C -1.771519 3.431959 -5.534601  
 C -0.381021 3.411344 -5.452831  
 C 0.248942 2.840153 -4.350641  
 C -1.871007 -0.735236 -2.437643  
 C -3.186975 -1.484896 -2.272069  
 C -4.262092 -0.84693 -3.132404  
 C -5.628346 -1.477108 -2.960906  
 C -6.693731 -0.788912 -3.811501  
 C -8.068582 -1.421059 -3.623967  
 O -1.312819 -0.736572 -3.527095  
 H -1.987802 -0.185785 -0.49138  
 H -2.504704 1.908255 -2.591772  
 H -3.615523 2.887232 -4.55527  
 H -2.260592 3.871239 -6.398912  
 H 0.218915 3.831197 -6.254729  
 H 1.334563 2.801444 -4.316389  
 F -3.594111 -1.458784 -0.944877  
 H -3.034366 -2.52619 -2.571472  
 H -3.929617 -0.870707 -4.175695  
 F -4.342381 0.497906 -2.74862  
 H -5.902056 -1.43058 -1.900197  
 H -5.552716 -2.53742 -3.232926  
 H -6.400485 -0.839439 -4.867781  
 H -6.731917 0.273004 -3.544827  
 H -8.056432 -2.479401 -3.907291  
 H -8.824127 -0.918406 -4.23556  
 H -8.388157 -1.359441 -2.577783

## IE1 (water)

C 5.1623412529 -1.3598799201 0.2842905097  
 C 4.2673977881 -2.3989679677 -0.052574934  
 C 2.9373253171 -2.1365982192 -0.3299694835  
 C 2.4918177375 -0.805432147 -0.2740585565  
 C 4.7447546993 -0.0415487197 0.3555399223  
 C 3.398011249 0.2203524477 0.0798916255  
 C 1.2258821805 -0.168571671 -0.4851380086  
 C 1.3868106326 1.181236536 -0.2507390759  
 H 6.1994147664 -1.6007887651 0.4956609959  
 H 4.6338606933 -3.4199105978 -0.0924563766  
 H 2.2483919672 -2.9362732619 -0.5878373564  
 H 5.4270908424 0.7601020153 0.6196178408  
 N 0.0158116688 -0.8360874412 -0.7846302887  
 N 2.701616543 1.4046674578 0.0883687384  
 H 3.1014225506 2.3216216475 0.2475493703  
 C 0.4020920281 2.2687508703 -0.2603544003  
 C 0.4610158441 3.2745593412 0.7144016772  
 C -0.491994173 4.2874055748 0.7367834691  
 C -1.5172878067 4.306262357 -0.2090200621  
 C -1.5744397814 3.3157903501 -1.1880659038  
 C -0.6164426897 2.3058112831 -1.2200522401  
 C -0.5487596504 -1.6899843305 0.0900068484  
 C -1.8265730877 -2.3765928975 -0.3735420683  
 C -2.977520797 -2.1605868706 0.604235647  
 C -3.8627721871 -0.9693407229 0.2791706818  
 C -3.1381098428 0.3744810756 0.1883971303  
 C -2.4141158849 0.7913916748 1.4674800169  
 O -0.0902239533 -1.9566593932 1.1993198846

H	-0.4510258876	-0.6904741378	-1.6730536885
H	1.2428319851	3.2492783831	1.4683567337
H	-0.4394305097	5.058178737	1.4993545329
H	-2.2639981209	5.0938261924	-0.1867661689
H	-2.361049738	3.3327779677	-1.9362300046
H	-0.6478228036	1.5567100081	-2.0057634281
H	-1.6108379623	-3.4487296448	-0.4280475763
F	-2.1734697103	-1.9431881625	-1.6453673773
H	-2.5613671577	-2.1078587288	1.6144680678
F	-3.785041744	-3.2994917558	0.5535092876
H	-4.6382124501	-0.9268051115	1.052206848
H	-4.3594800175	-1.1863179662	-0.6720718382
H	-3.8831381678	1.1371771942	-0.0645496425
H	-2.4341697965	0.352539059	-0.6504217099
H	-3.0933230579	0.7494669419	2.3267202969
H	-2.0426385393	1.8183510743	1.3824215085
H	-1.5558552288	0.147811244	1.6918185554

### IE1(1-octanol)

C	3.0128757409	0.5594540307	0.9912620912
C	2.0102449536	-0.3622078881	1.361914535
C	0.8006396865	-0.4122707775	0.6920239618
C	0.5861718513	0.4791880139	-0.3716659607
C	2.8282355875	1.4444884916	-0.0575530833
C	1.6062166078	1.3878375412	-0.7366213075
C	-0.5063244797	0.7192008399	-1.2680415615
C	-0.1342614825	1.7316159222	-2.1274623475
H	3.9495406646	0.5738032161	1.5402991032
H	2.1950984357	-1.0402335249	2.1896393915
H	0.0273921552	-1.1189414349	0.9808852191
H	3.5977100071	2.1537836662	-0.3468698812
N	-1.7037656627	-0.0327460193	-1.3179086564
N	1.145695684	2.1187702667	-1.8054669919
H	1.6252803036	2.9042402589	-2.2282253639
C	-0.8537614365	2.3373301771	-3.2556515403
C	-2.2177743589	2.6358763474	-3.1518218485
C	-2.8973186697	3.1883256711	-4.2345913825
C	-2.2227297879	3.4582160148	-5.4243170336
C	-0.860373289	3.179441178	-5.5264546605
C	-0.1781747141	2.621745012	-4.449964727
C	-2.8387297653	0.3367407205	-0.6912657766
C	-3.9971726256	-0.6455347802	-0.8063322381
C	-5.1187795046	-0.0298096035	-1.6268070778
C	-4.8262689788	-0.0021807351	-3.1143982956
C	-5.8955505494	0.7481552375	-3.903603664
C	-5.6127955973	0.7325893211	-5.4018722841
O	-3.0033955331	1.3950279363	-0.0947652212
H	-1.683326934	-0.9587794939	-1.732580248
H	-2.7336623933	2.465060281	-2.2110412991
H	-3.9544265739	3.4226830921	-4.1425872656
H	-2.7550685671	3.8904517835	-6.266391033
H	-0.3285902752	3.3896840656	-6.4495184866
H	0.8787895571	2.3847575611	-4.5405962612
H	-4.3543120789	-0.8807756333	0.2009266199
F	-3.5774404834	-1.8252385252	-1.4052657214
H	-5.3129974841	0.9742685887	-1.2334865134
F	-6.2647579849	-0.7941314154	-1.413135578
H	-4.7484432268	-1.0379373529	-3.4651464215
H	-3.8467213264	0.4667635786	-3.2760926876
H	-5.9472294079	1.7840070182	-3.5432580096
H	-6.8738227249	0.2965262343	-3.7020449379
H	-4.6381039724	1.1837873135	-5.6216686602
H	-6.3747052886	1.2882072236	-5.9574021973
H	-5.598115078	-0.2934374189	-5.7858496974