

### Supplementary Information

A Systematic Study of Spin-Orbit Coupling and Rate of inter system crossing in pristine and donor-acceptor substituted Phospha-Helicenes as a function of position of phosphole ring.

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#### Contents:

1. Optimized cartesian coordinates of  $S_0$ ,  $S_1$  and  $T_n$  geometries (B3LYP/6-311+G(d,p)) of all the systems considered in this work.
2. Energy difference (eV) between singlet and nearest low-lying triplet.
3. Value of spin-orbit coupling matrix element calculated at CAM-B3LYP/cc-PVTZ level of theory.
4. Value of rate of inter system crossing (in  $\text{sec}^{-1}$ ).
5.  $S_0 \rightarrow S_n$  and  $S_0 \rightarrow T_n$  excitation energy (in eV), wavelength (in nm) and oscillator strength (unitless) calculated at CAM-B3LYP/cc-PVTZ level of theory.
6. s and p character (in %) obtained from Natural Transition Orbitals.
7. Root-mean-square deviation values of all systems in vacuum and other solvents.
8. Python code for calculating rate of inter system crossing ( $k_{ISC}$ ) in ( $\text{sec}^{-1}$ ).
9. Structure of experimentally Studied Phosphahelicene (Yavari et al. *Chem. Eur. J.* **2019**, *25*, 5303-5310)
10. Vibronic spectra of each excited state and convoluted for all states.
11. Merged structure and RMSD value between  $S_0$ - $S_1$  and  $S_0$ - $S_2$  geometries of experimentally studied system considered for benchmarked.
12. Optimized Cartesian coordinates of experimentally studied phosphahelicene  $S_0$  geometry (B3LYP/6-311+G(d,p)) in DCM solvent considered for benchmark.
13. Benchmarking the methodology for experimentally available absorption data.
14. Nearest low lying triplet state optimized for all considered systems in vacuum and four solvents.

ST1: Optimized Cartesian coordinates of  $S_0$ ,  $S_1$  and  $T_n$  geometries (B3LYP/6-311+G(d,p)) of all the systems considered in this work.

P1234-vacuum				C1234-vacuum			
C	-2.670114	-3.777477	-1.011761	C	-2.449504	-3.789561	-1.030596
C	-1.900684	-2.878116	-1.771908	C	-1.678897	-2.893765	-1.792814
H	-1.414835	-3.215033	-2.680700	H	-1.181233	-3.238354	-2.692465
C	-3.349945	-3.315252	0.093008	C	-3.147899	-3.318002	0.058914
H	-3.996589	-3.979453	0.657053	H	-3.796850	-3.979999	0.622848
C	-1.767313	-1.562995	-1.376522	C	-1.561407	-1.572241	-1.412288
H	-1.183713	-0.891292	-1.988121	H	-0.978477	-0.901685	-2.025724
C	-3.264190	-1.959922	0.489749	C	-3.079154	-1.957077	0.437937
C	-2.391866	-1.070181	-0.205762	C	-2.203453	-1.069816	-0.256284
C	-4.125555	-1.454478	1.514733	C	-3.963184	-1.444376	1.440494
H	-4.769649	-2.148070	2.044629	H	-4.610857	-2.136023	1.968511
C	-4.202724	-0.119290	1.744268	C	-4.055326	-0.107235	1.649576
H	-4.925491	0.279773	2.448125	H	-4.792802	0.295525	2.335816
C	-3.331559	0.803116	1.078999	C	-3.177303	0.813379	0.989900
C	-2.297092	0.324218	0.223784	C	-2.125424	0.331546	0.155879
C	-3.509303	2.194237	1.269253	C	-3.356245	2.203024	1.174867
H	-4.321512	2.536156	1.901669	H	-4.181376	2.547646	1.788815
C	-2.700328	3.090485	0.624118	C	-2.522920	3.097980	0.557015
H	-2.882782	4.156670	0.705106	H	-2.699982	4.164680	0.642429
C	-1.566964	2.644181	-0.095622	C	-1.374111	2.649075	-0.132924
C	-1.287316	1.259689	-0.197130	C	-1.108328	1.262809	-0.246959
C	-0.699677	3.631055	-0.711007	C	-0.476124	3.648938	-0.697993
H	-1.035040	4.663019	-0.693840	H	-0.816145	4.679241	-0.672363
C	0.469303	3.303587	-1.303129	C	0.720474	3.341138	-1.239299
H	1.086989	4.054789	-1.782608	H	1.361391	4.104836	-1.665570
C	0.950449	1.950658	-1.208727	C	1.173316	1.977143	-1.169635
C	0.084739	0.910607	-0.601973	C	0.266407	0.917582	-0.648687
C	2.213291	1.520706	-1.513215	C	2.401116	1.452936	-1.403541
H	2.986369	2.136340	-1.952319	H	3.276533	1.980768	-1.756145
H	-2.755502	-4.814827	-1.314926	H	-2.522406	-4.831581	-1.320668
C	0.764059	-0.257756	-0.373820	C	0.995006	-0.220896	-0.517438
P	2.344677	-0.240471	-1.216163	C	3.508077	-0.414631	-0.063517
C	3.681164	-0.492190	0.033445	C	3.573324	0.140036	1.220955
C	3.678494	0.169000	1.269710	C	4.480463	-1.342096	-0.443032
C	4.725611	-1.371544	-0.269463	C	4.587275	-0.225251	2.100384
C	4.706190	-0.047968	2.181953	H	2.821792	0.859682	1.527779
H	2.870658	0.849518	1.512818	C	5.499413	-1.710506	0.437672
C	5.757366	-1.585054	0.646225	H	4.442680	-1.782499	-1.434418
H	4.731732	-1.891255	-1.221256	C	5.555671	-1.153188	1.711525
C	5.748054	-0.924675	1.871377	H	4.622997	0.212621	3.091924
H	4.695804	0.466360	3.136641	H	6.245293	-2.433217	0.125551
H	6.562640	-2.268450	0.401003	H	6.344857	-1.438092	2.398159
H	6.547266	-1.091489	2.584912	H	0.665055	-1.172187	-0.130371
H	0.348956	-1.143536	0.080768	C	2.399069	-0.004448	-1.024077
				H	2.517548	-0.606355	-1.940296
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P1234-CCl4				C1234- CCl4			
C	-2.670152	-3.779606	-1.012537	C	-2.449434	-3.792017	-1.028840
C	-1.898857	-2.880001	-1.771241	C	-1.675894	-2.896977	-1.789675

H	-1.411369	-3.217043	-2.679107	H	-1.175238	-3.242662	-2.687212
C	-3.352068	-3.317439	0.091469	C	-3.150908	-3.319245	0.058684
H	-4.000039	-3.981385	0.654188	H	-3.801906	-3.980261	0.621330
C	-1.765820	-1.564726	-1.375153	C	-1.558760	-1.574940	-1.409676
H	-1.180596	-0.893438	-1.985741	H	-0.972934	-0.905952	-2.022094
C	-3.266611	-1.961778	0.488518	C	-3.082408	-1.957632	0.436705
C	-2.392925	-1.071833	-0.205484	C	-2.204288	-1.071072	-0.255920
C	-4.130070	-1.456983	1.512579	C	-3.969501	-1.444398	1.436786
H	-4.774657	-2.151021	2.041168	H	-4.618738	-2.135770	1.963110
C	-4.208041	-0.121505	1.742278	C	-4.061989	-0.106788	1.644924
H	-4.932191	0.277382	2.444754	H	-4.801476	0.296705	2.328515
C	-3.335841	0.801228	1.077982	C	-3.181638	0.813208	0.986673
C	-2.299675	0.322815	0.224211	C	-2.127369	0.330880	0.155498
C	-3.515169	2.192601	1.267877	C	-3.361844	2.203235	1.170288
H	-4.327994	2.533987	1.899622	H	-4.188418	2.547952	1.782064
C	-2.706513	3.089590	0.622679	C	-2.527442	3.098259	0.553331
H	-2.890262	4.155524	0.702954	H	-2.705623	4.164823	0.636985
C	-1.571840	2.643719	-0.096056	C	-1.376484	2.648968	-0.133533
C	-1.290263	1.259295	-0.196047	C	-1.109572	1.262491	-0.245864
C	-0.705365	3.631548	-0.711889	C	-0.477801	3.649577	-0.697132
H	-1.041803	4.663110	-0.695656	H	-0.817789	4.679829	-0.671376
C	0.464567	3.304581	-1.303298	C	0.719893	3.341685	-1.236892
H	1.081808	4.055998	-1.782989	H	1.361550	4.105398	-1.662057
C	0.947173	1.951986	-1.206868	C	1.172738	1.977461	-1.166235
C	0.082900	0.911608	-0.598501	C	0.266282	0.917791	-0.644720
C	2.211092	1.523510	-1.510478	C	2.401025	1.453537	-1.399984
H	2.983938	2.139480	-1.949670	H	3.275703	1.981734	-1.754031
H	-2.755202	-4.816802	-1.316244	H	-2.521930	-4.834187	-1.318411
C	0.763830	-0.255345	-0.366922	C	0.995720	-0.220136	-0.511760
P	2.344691	-0.236452	-1.208260	C	3.510454	-0.413835	-0.061866
C	3.685832	-0.490568	0.034935	C	3.572847	0.131915	1.226875
C	3.685371	0.165024	1.274509	C	4.489248	-1.332032	-0.449000
C	4.732096	-1.365269	-0.276555	C	4.590171	-0.232751	2.103481
C	4.717573	-0.052743	2.182020	H	2.817035	0.844235	1.540452
H	2.876791	0.841922	1.525177	C	5.511571	-1.699754	0.428644
C	5.768298	-1.579338	0.634389	H	4.453909	-1.765260	-1.443529
H	4.737305	-1.880842	-1.230534	C	5.564966	-1.151327	1.707068
C	5.761434	-0.924560	1.863032	H	4.623361	0.198182	3.098141
H	4.709026	0.457067	3.139063	H	6.262207	-2.414978	0.110729
H	6.574863	-2.258763	0.382750	H	6.356548	-1.435826	2.391129
H	6.563973	-1.091965	2.572597	H	0.666027	-1.171843	-0.125434
H	0.350286	-1.141278	0.088883	C	2.399076	-0.003798	-1.019900
	*****			H	2.515749	-0.605945	-1.936077
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P1234-DCM				C1234-DCM			
C	-2.666450	-3.782778	-1.014053	C	-2.441575	-3.796811	-1.026868
C	-1.894624	-2.881987	-1.771629	C	-1.666024	-2.901317	-1.785856
H	-1.405724	-3.218669	-2.678862	H	-1.160726	-3.247358	-2.680573
C	-3.350561	-3.321584	0.089512	C	-3.147755	-3.323996	0.058145
H	-3.998571	-3.986265	0.651164	H	-3.799851	-3.985266	0.619087
C	-1.763073	-1.566471	-1.374649	C	-1.551842	-1.578481	-1.406493
H	-1.176986	-0.894878	-1.984213	H	-0.963332	-0.910515	-2.017474
C	-3.266898	-1.965440	0.486936	C	-3.082086	-1.961498	0.435181
C	-2.392852	-1.074295	-0.205724	C	-2.202585	-1.074102	-0.255473

C	-4.132843	-1.462152	1.510233	C	-3.973536	-1.449208	1.432476
H	-4.777194	-2.157098	2.037744	H	-4.623463	-2.141218	1.956959
C	-4.212918	-0.126415	1.740063	C	-4.068542	-0.111264	1.639786
H	-4.938683	0.271584	2.441249	H	-4.810814	0.291687	2.320550
C	-3.340568	0.797531	1.076742	C	-3.187042	0.809642	0.983433
C	-2.302216	0.320646	0.224343	C	-2.129266	0.328652	0.155331
C	-3.522810	2.189021	1.266484	C	-3.370723	2.199764	1.166239
H	-4.336735	2.528984	1.897380	H	-4.199398	2.543007	1.775804
C	-2.714931	3.087581	0.621785	C	-2.536402	3.096406	0.550813
H	-2.900862	4.153074	0.701465	H	-2.717106	4.162534	0.633394
C	-1.578189	2.643251	-0.095556	C	-1.382504	2.648744	-0.133080
C	-1.293776	1.259072	-0.194962	C	-1.112157	1.262453	-0.244208
C	-0.712694	3.633212	-0.710174	C	-0.484864	3.651844	-0.694947
H	-1.050462	4.664211	-0.693161	H	-0.826936	4.681293	-0.669185
C	0.458670	3.308014	-1.300645	C	0.714655	3.346098	-1.232849
H	1.075451	4.060613	-1.779007	H	1.355588	4.111059	-1.656844
C	0.943316	1.955854	-1.203547	C	1.169962	1.982433	-1.161336
C	0.080819	0.913931	-0.595097	C	0.265477	0.920761	-0.640254
C	2.208676	1.529863	-1.506472	C	2.399562	1.460779	-1.395287
H	2.980734	2.147148	-1.945361	H	3.272174	1.990855	-1.751805
H	-2.750028	-4.819894	-1.318257	H	-2.511555	-4.839295	-1.315774
C	0.764063	-0.251597	-0.361659	C	0.997531	-0.215703	-0.507189
P	2.345318	-0.229167	-1.201766	C	3.513277	-0.408721	-0.061845
C	3.690317	-0.487512	0.035477	C	3.582473	0.138749	1.226252
C	3.693639	0.164373	1.277356	C	4.487242	-1.331747	-0.451209
C	4.735857	-1.361150	-0.282817	C	4.601429	-0.228827	2.100604
C	4.729105	-0.056051	2.181097	H	2.831413	0.855181	1.542248
H	2.886522	0.840819	1.534024	C	5.511113	-1.702500	0.424054
C	5.775213	-1.577807	0.624389	H	4.447101	-1.765949	-1.444985
H	4.739347	-1.873606	-1.238387	C	5.571236	-1.152436	1.702080
C	5.772247	-0.926873	1.855581	H	4.639902	0.203708	3.094367
H	4.723683	0.450883	3.139590	H	6.257769	-2.421098	0.104456
H	6.581192	-2.255904	0.367734	H	6.364011	-1.439186	2.383797
H	6.577221	-1.096235	2.561777	H	0.669351	-1.169226	-0.124037
H	0.352230	-1.138696	0.093530	C	2.399798	0.003143	-1.016812
	*****			H	2.514761	-0.597363	-1.934107
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P1234-DMSO				C1234-DMSO			
C	-2.662709	-3.784705	-1.014614	C	-2.435117	-3.799509	-1.026084
C	-1.891372	-2.882995	-1.771918	C	-1.659506	-2.903222	-1.784350
H	-1.401826	-3.219306	-2.678934	H	-1.152037	-3.248970	-2.677904
C	-3.347950	-3.324283	0.088760	C	-3.143483	-3.327316	0.057991
H	-3.995368	-3.989735	0.650110	H	-3.795392	-3.989298	0.618241
C	-1.761225	-1.567279	-1.374673	C	-1.547542	-1.579986	-1.405235
H	-1.175240	-0.895205	-1.983877	H	-0.958410	-0.912039	-2.015644
C	-3.265955	-1.967838	0.486195	C	-3.079984	-1.964435	0.434729
C	-2.392289	-1.075730	-0.206005	C	-2.200682	-1.075971	-0.255226
C	-4.133279	-1.465524	1.509045	C	-3.973380	-1.453243	1.431100
H	-4.777214	-2.161076	2.036188	H	-4.623007	-2.145955	1.954971
C	-4.214999	-0.129703	1.738731	C	-4.070323	-0.115257	1.638216
H	-4.941700	0.267605	2.439266	H	-4.813864	0.286840	2.318025
C	-3.343000	0.795161	1.075879	C	-3.189158	0.806744	0.982588
C	-2.303397	0.319386	0.224198	C	-2.129776	0.327145	0.155453
C	-3.527112	2.186612	1.265548	C	-3.375118	2.196750	1.165410

H	-4.341831	2.525588	1.895876	H	-4.204744	2.538715	1.774332
C	-2.719689	3.086185	0.621425	C	-2.541520	3.094723	0.550662
H	-2.906961	4.151418	0.700877	H	-2.723855	4.160546	0.633192
C	-1.581667	2.643018	-0.094997	C	-1.386308	2.648630	-0.132422
C	-1.295624	1.259038	-0.194468	C	-1.113654	1.262607	-0.243416
C	-0.716613	3.634320	-0.708359	C	-0.489928	3.653434	-0.693658
H	-1.055101	4.665003	-0.690478	H	-0.833720	4.682247	-0.667938
C	0.455593	3.310416	-1.298215	C	0.710512	3.349512	-1.230899
H	1.072169	4.063893	-1.775419	H	1.350446	4.115488	-1.654542
C	0.941365	1.958520	-1.201377	C	1.167867	1.986423	-1.159201
C	0.079743	0.915470	-0.593541	C	0.264882	0.923152	-0.638658
C	2.207457	1.533970	-1.504055	C	2.398320	1.466560	-1.393468
H	2.979040	2.152161	-1.942558	H	3.269595	1.998044	-1.751236
H	-2.744982	-4.821882	-1.318870	H	-2.503273	-4.842162	-1.314733
C	0.764237	-0.249447	-0.359919	C	0.998714	-0.212360	-0.506315
P	2.345656	-0.224795	-1.199526	C	3.514416	-0.404758	-0.062835
C	3.692066	-0.485524	0.035325	C	3.591879	0.150107	1.221818
C	3.698159	0.166247	1.277396	C	4.479847	-1.338121	-0.449359
C	4.735869	-1.360729	-0.284867	C	4.610344	-0.220384	2.095848
C	4.734634	-0.055936	2.179774	H	2.848069	0.875044	1.535758
H	2.892837	0.844235	1.535713	C	5.503143	-1.711913	0.425569
C	5.776169	-1.579190	0.621012	H	4.433577	-1.777853	-1.440365
H	4.737805	-1.872817	-1.240595	C	5.571451	-1.154543	1.700243
C	5.775972	-0.928473	1.852503	H	4.655408	0.218175	3.086686
H	4.731479	0.450986	3.138242	H	6.243093	-2.438353	0.108170
H	6.580821	-2.258280	0.362995	H	6.363916	-1.443480	2.381378
H	6.581731	-1.099127	2.557424	H	0.671788	-1.167229	-0.125448
H	0.353169	-1.137449	0.094238	C	2.400387	0.008678	-1.016538
*****				H	2.514730	-0.590460	-1.934719
				*****			

P1234-n-hexane				C1234-n-hexane			
C	-2.670264	-3.779193	-1.012317	C	-2.449841	-3.791427	-1.029204
C	-1.899245	-2.879679	-1.771266	C	-1.676829	-2.896297	-1.790337
H	-1.412016	-3.216723	-2.679270	H	-1.176849	-3.241805	-2.688326
C	-3.351825	-3.316963	0.091786	C	-3.150628	-3.318835	0.058741
H	-3.999622	-3.980907	0.654731	H	-3.801275	-3.979980	0.621661
C	-1.766125	-1.564428	-1.375337	C	-1.559493	-1.574374	-1.410226
H	-1.181166	-0.893098	-1.986113	H	-0.974226	-0.905105	-2.022868
C	-3.266273	-1.961365	0.488757	C	-3.081946	-1.957365	0.436958
C	-2.392787	-1.071504	-0.205507	C	-2.204250	-1.070744	-0.256002
C	-4.129361	-1.456407	1.512947	C	-3.968376	-1.444167	1.437543
H	-4.773896	-2.150345	2.041756	H	-4.617348	-2.135552	1.964203
C	-4.207147	-0.120981	1.742597	C	-4.060695	-0.106640	1.645858
H	-4.931056	0.277975	2.445297	H	-4.799754	0.296771	2.329973
C	-3.335090	0.801651	1.078135	C	-3.180743	0.813402	0.987298
C	-2.299233	0.323102	0.224135	C	-2.126995	0.331083	0.155554
C	-3.514081	2.192982	1.268069	C	-3.360608	2.203369	1.171143
H	-4.326792	2.534504	1.899919	H	-4.186870	2.548143	1.783341
C	-2.705333	3.089796	0.622874	C	-2.526363	3.098308	0.553974
H	-2.888813	4.155785	0.703263	H	-2.704277	4.164910	0.637924
C	-1.570916	2.643798	-0.096030	C	-1.375854	2.648995	-0.133474
C	-1.289723	1.259356	-0.196236	C	-1.109269	1.262540	-0.246112
C	-0.704278	3.631391	-0.711854	C	-0.477214	3.649381	-0.697351
H	-1.040517	4.663032	-0.695559	H	-0.817098	4.679683	-0.671603

C	0.465465	3.304273	-1.303383	C	0.720238	3.341399	-1.237416
H	1.082789	4.055601	-1.783115	H	1.361838	4.105049	-1.662778
C	0.947783	1.951619	-1.207245	C	1.172955	1.977177	-1.166955
C	0.083232	0.911365	-0.599093	C	0.266342	0.917619	-0.645514
C	2.211487	1.522821	-1.510992	C	2.401110	1.453109	-1.400717
H	2.984421	2.138669	-1.950171	H	3.276002	1.981163	-1.754416
H	-2.755407	-4.816420	-1.315913	H	-2.522527	-4.833557	-1.318887
C	0.763834	-0.255842	-0.368037	C	0.995528	-0.220461	-0.512796
P	2.344634	-0.237346	-1.209583	C	3.509973	-0.414195	-0.062100
C	3.685001	-0.490923	0.034722	C	3.572388	0.132677	1.226094
C	3.684078	0.165576	1.273753	C	4.488141	-1.333429	-0.448068
C	4.731078	-1.366257	-0.275340	C	4.589150	-0.231943	2.103219
C	4.715559	-0.051933	2.182037	H	2.816924	0.845805	1.538621
H	2.875502	0.842943	1.523154	C	5.509905	-1.701102	0.430125
C	5.766575	-1.580100	0.636376	H	4.452721	-1.767585	-1.442213
H	4.736466	-1.882524	-1.228957	C	5.563327	-1.151547	1.707953
C	5.759213	-0.924405	1.864436	H	4.622397	0.199856	3.097502
H	4.706629	0.458602	3.138707	H	6.260100	-2.417187	0.113100
H	6.573011	-2.260092	0.385800	H	6.354510	-1.435997	2.392495
H	6.561222	-1.091620	2.574665	H	0.665735	-1.172024	-0.126213
H	0.349995	-1.141696	0.087637	C	2.399038	-0.004225	-1.020644
*****				H	2.516049	-0.606420	-1.936772
				*****			

1P234-vacuum				1C234-vacuum			
C	5.573218	1.031547	0.103795	C	5.522619	0.987974	0.021353
C	4.508203	1.715755	-0.507429	C	4.451143	1.711479	-0.528949
H	4.670141	2.699053	-0.934562	H	4.617614	2.704875	-0.930396
C	5.375328	-0.252036	0.565148	C	5.315962	-0.307426	0.445915
H	6.201224	-0.816654	0.985344	H	6.145254	-0.900771	0.817029
C	3.256815	1.136859	-0.582926	C	3.186681	1.157173	-0.579393
H	2.463479	1.671269	-1.085504	H	2.389304	1.716495	-1.046179
C	4.113153	-0.879695	0.459702	C	4.039156	-0.907533	0.366407
C	2.999933	-0.149364	-0.053679	C	2.923565	-0.139545	-0.082487
C	3.967609	-2.270853	0.766577	C	3.875774	-2.305249	0.634963
H	4.820362	-2.807524	1.168592	H	4.733039	-2.871903	0.982621
C	2.815141	-2.922053	0.469545	C	2.696483	-2.922011	0.373675
H	2.735423	-3.994561	0.612187	H	2.598049	-3.995778	0.493764
C	1.666375	-2.221579	-0.027686	C	1.540380	-2.182559	-0.046572
C	1.695712	-0.798056	-0.138978	C	1.603452	-0.756856	-0.134386
C	0.514767	-2.948966	-0.406600	C	0.345433	-2.871995	-0.350497
H	0.534776	-4.031162	-0.334199	H	0.342840	-3.955329	-0.294439
C	-0.595589	-2.301440	-0.898535	C	-0.793924	-2.189934	-0.721930
H	-1.448158	-2.865025	-1.260849	H	-1.700758	-2.722528	-0.985231
C	-0.640679	-0.901393	-0.847247	C	-0.781776	-0.794356	-0.670736
C	0.445813	-0.139328	-0.380596	C	0.362885	-0.070206	-0.307904
C	-1.255555	1.567564	-0.581665	C	-1.415537	1.460449	-0.454907
H	6.549967	1.496152	0.176916	H	6.510267	1.431703	0.075499
C	-3.433507	-0.297974	-0.280472	C	-3.278980	-0.291174	-0.306048
C	-4.378398	-0.741780	1.906677	C	-4.602381	-0.832871	1.653920
C	-4.688299	-0.533821	-0.852353	C	-4.402860	-0.527869	-1.101030
C	-5.627784	-0.974439	1.326938	C	-5.719837	-1.066625	0.849887
C	-5.782049	-0.870068	-0.052226	C	-5.617115	-0.913096	-0.529392
H	-4.810149	-0.454514	-1.927489	H	-4.329969	-0.410521	-2.177803
H	-6.749312	-1.049914	-0.508210	H	-6.478376	-1.092076	-1.163576

P	-2.034351	0.138676	-1.418985	C	-0.061238	1.336430	-0.081479
C	0.041431	1.264172	-0.106977	C	0.568233	2.427103	0.531743
C	0.699953	2.227333	0.673467	C	-0.129488	3.623268	0.694065
C	0.108761	3.464478	0.910010	C	-1.449553	3.750942	0.259102
C	-1.143453	3.774799	0.374306	C	-2.103554	2.656519	-0.308103
C	-1.828798	2.820062	-0.371898	H	1.580863	2.352937	0.901730
H	1.663408	2.012718	1.113806	H	0.362180	4.462653	1.173303
H	0.628792	4.192490	1.522697	H	-1.974937	4.690479	0.387975
H	-1.589459	4.745869	0.557245	H	-3.145838	2.729268	-0.599615
H	-2.816926	3.040671	-0.761534	C	-3.394441	-0.448772	1.081090
C	-3.288910	-0.405505	1.109819	H	-6.660798	-1.365778	1.297734
H	-6.475113	-1.236095	1.950956	H	-4.674326	-0.950230	2.729611
H	-4.255478	-0.822652	2.981187	H	-2.531577	-0.268507	1.713285
H	-2.322852	-0.225564	1.567910	C	-1.959925	0.128374	-0.933927
	*****			H	-2.109783	0.175214	-2.021583
	*****				*****		

1P234-CCI4				1C234-CCI4			
C	5.575285	1.033735	0.102923	C	5.523193	0.990155	0.026457
C	4.509616	1.718214	-0.507713	C	4.451856	1.714409	-0.524059
H	4.671116	2.701943	-0.933927	H	4.618378	2.708645	-0.923287
C	5.378025	-0.250519	0.563861	C	5.316534	-0.306324	0.449074
H	6.204179	-0.815186	0.983323	H	6.145574	-0.899922	0.820187
C	3.258099	1.138881	-0.582985	C	3.187359	1.159649	-0.576637
H	2.464779	1.673890	-1.084966	H	2.390658	1.720125	-1.043157
C	4.115527	-0.878384	0.458375	C	4.039546	-0.906658	0.367082
C	3.001763	-0.147924	-0.054324	C	2.923975	-0.138142	-0.082026
C	3.971095	-2.270196	0.764723	C	3.876815	-2.305234	0.633639
H	4.824300	-2.806581	1.165972	H	4.733843	-2.871920	0.981641
C	2.818585	-2.921945	0.467668	C	2.697842	-2.922249	0.369729
H	2.739253	-3.994566	0.609073	H	2.599518	-3.996198	0.487699
C	1.669086	-2.221139	-0.028505	C	1.541796	-2.182139	-0.050737
C	1.697527	-0.797274	-0.139251	C	1.603823	-0.755999	-0.136043
C	0.517715	-2.949700	-0.406929	C	0.347716	-2.872476	-0.357643
H	0.538590	-4.031802	-0.334668	H	0.346235	-3.955878	-0.304103
C	-0.593650	-2.302538	-0.898011	C	-0.791948	-2.190318	-0.728881
H	-1.445693	-2.866959	-1.260151	H	-1.697255	-2.723799	-0.995542
C	-0.639389	-0.902275	-0.845917	C	-0.781526	-0.794546	-0.674106
C	0.446859	-0.139197	-0.379802	C	0.362539	-0.069917	-0.309471
C	-1.256026	1.567009	-0.579228	C	-1.417282	1.459296	-0.456096
H	6.551857	1.498662	0.175914	H	6.510584	1.434179	0.082396
C	-3.435903	-0.300264	-0.280988	C	-3.278760	-0.293452	-0.304814
C	-4.382121	-0.755886	1.903642	C	-4.597450	-0.843156	1.656944
C	-4.693010	-0.521757	-0.854231	C	-4.406406	-0.520508	-1.097746
C	-5.634058	-0.973767	1.322839	C	-5.718957	-1.067103	0.855109
C	-5.788766	-0.856317	-0.055649	C	-5.620344	-0.904776	-0.523968
H	-4.816193	-0.432953	-1.928402	H	-4.336941	-0.396542	-2.173879
H	-6.757673	-1.024857	-0.512315	H	-6.484489	-1.076232	-1.156300
P	-2.034399	0.137061	-1.415308	C	-0.062865	1.336322	-0.081977
C	0.041587	1.264074	-0.105465	C	0.565727	2.427561	0.531667
C	0.699949	2.227423	0.675052	C	-0.132717	3.623679	0.693873
C	0.108213	3.464482	0.912576	C	-1.452864	3.750614	0.257618
C	-1.144678	3.774451	0.377365	C	-2.105939	2.655474	-0.310174
C	-1.830151	2.819357	-0.369035	H	1.578389	2.354995	0.901828
H	1.663772	2.013770	1.115035	H	0.358360	4.463340	1.173191

H	0.628212	4.192482	1.525236	H	-1.978835	4.689936	0.385658
H	-1.591097	4.745211	0.560756	H	-3.147613	2.728692	-0.603718
H	-2.818490	3.040147	-0.758000	C	-3.389758	-0.459892	1.081905
C	-3.290577	-0.420998	1.108374	H	-6.659513	-1.365534	1.304305
H	-6.482794	-1.234277	1.945323	H	-4.665833	-0.967466	2.732080
H	-4.258701	-0.847134	2.977198	H	-2.524405	-0.287829	1.713100
H	-2.323060	-0.252981	1.568010	C	-1.960854	0.126949	-0.935334
*****				H	-2.112960	0.174081	-2.022417
*****				*****			

1P234-DCM				1C234-DCM			
C	5.577660	1.035931	0.101421	C	5.522675	0.992932	0.038399
C	4.510995	1.721183	-0.507467	C	4.452233	1.718637	-0.512901
H	4.671819	2.705756	-0.931848	H	4.619184	2.714433	-0.907834
C	5.381191	-0.249217	0.561433	C	5.315588	-0.305312	0.456786
H	6.207782	-0.814057	0.979539	H	6.143912	-0.899554	0.828210
C	3.259211	1.141588	-0.582008	C	3.187812	1.163374	-0.570314
H	2.465586	1.677954	-1.082065	H	2.392510	1.725831	-1.036769
C	4.118226	-0.877148	0.456380	C	4.038590	-0.905940	0.369448
C	3.003631	-0.146220	-0.054746	C	2.923537	-0.136308	-0.080402
C	3.974943	-2.269690	0.761931	C	3.876426	-2.305893	0.631390
H	4.828592	-2.805903	1.162250	H	4.732772	-2.873072	0.980043
C	2.822276	-2.921980	0.465123	C	2.698307	-2.923009	0.361990
H	2.743583	-3.994704	0.605431	H	2.600424	-3.997374	0.475697
C	1.671965	-2.220670	-0.029758	C	1.542716	-2.181698	-0.059085
C	1.699362	-0.796309	-0.139248	C	1.603453	-0.754863	-0.139470
C	0.520945	-2.950270	-0.408575	C	0.350129	-2.872763	-0.372139
H	0.542605	-4.032311	-0.337427	H	0.350050	-3.956323	-0.323740
C	-0.591344	-2.303220	-0.898697	C	-0.789485	-2.190048	-0.743381
H	-1.442480	-2.868449	-1.261602	H	-1.692458	-2.724080	-1.016663
C	-0.638106	-0.902739	-0.844644	C	-0.781397	-0.794184	-0.682145
C	0.447775	-0.138815	-0.378389	C	0.361468	-0.069257	-0.313502
C	-1.256748	1.566667	-0.575664	C	-1.419994	1.458302	-0.460908
H	6.554074	1.501094	0.174161	H	6.509595	1.437324	0.098473
C	-3.438452	-0.302678	-0.281678	C	-3.277408	-0.296314	-0.302725
C	-4.385277	-0.776293	1.899476	C	-4.584642	-0.855618	1.665113
C	-4.698606	-0.505066	-0.855857	C	-4.411480	-0.513197	-1.089735
C	-5.640534	-0.974682	1.317948	C	-5.712875	-1.069300	0.869224
C	-5.796398	-0.838565	-0.059123	C	-5.623018	-0.897049	-0.509781
H	-4.823761	-0.402566	-1.928479	H	-4.349168	-0.381736	-2.165219
H	-6.767500	-0.992094	-0.516191	H	-6.492109	-1.060629	-1.137348
P	-2.034498	0.136020	-1.411284	C	-0.065872	1.336457	-0.084405
C	0.041492	1.264142	-0.102732	C	0.560982	2.428573	0.530124
C	0.699721	2.227738	0.677853	C	-0.138439	3.624684	0.691119
C	0.107464	3.464742	0.916336	C	-1.458062	3.750815	0.251651
C	-1.146079	3.774389	0.381579	C	-2.109335	2.654807	-0.317479
C	-1.831688	2.818969	-0.365094	H	1.573505	2.358364	0.901009
H	1.664050	2.015325	1.117275	H	0.351622	4.464867	1.170450
H	0.627484	4.192870	1.528699	H	-1.984490	4.690193	0.377188
H	-1.592737	4.744937	0.565142	H	-3.149580	2.728774	-0.615866
H	-2.819988	3.040222	-0.753869	C	-3.379262	-0.472658	1.083797
C	-3.291639	-0.442041	1.106083	H	-6.651402	-1.367543	1.322726
H	-6.490665	-1.234766	1.938551	H	-4.645799	-0.987840	2.739732
H	-4.260891	-0.882315	2.971486	H	-2.509217	-0.309280	1.711040
H	-2.322007	-0.289769	1.566920	C	-1.962557	0.125640	-0.939874

*****	H	-2.119893	0.172793	-2.025887	*****		
1P234-DMSO	1C234-DMSO						
C	C	5.578717	1.035943	0.100403	5.522162	0.993971	0.045354
C	C	4.511704	1.721670	-0.507665	4.452359	1.720576	-0.506347
H	H	4.672368	2.706550	-0.931325	4.619649	2.717226	-0.898868
C	C	5.382354	-0.249439	0.560264	5.314692	-0.305189	0.461223
H	H	6.209047	-0.814412	0.977860	6.142557	-0.899894	0.832804
C	C	3.259679	1.142236	-0.581626	3.187988	1.165190	-0.566581
H	H	2.465937	1.679364	-1.080686	2.393524	1.728757	-1.033061
C	C	4.119061	-0.877156	0.455689	4.037722	-0.905856	0.370855
C	C	3.004217	-0.145894	-0.054798	2.923070	-0.135503	-0.079372
C	C	3.975943	-2.269882	0.761249	3.875659	-2.306489	0.630072
H	H	4.829629	-2.806095	1.161403	4.731581	-2.874099	0.978974
C	C	2.823091	-2.922253	0.464723	2.698009	-2.923480	0.357634
H	H	2.744521	-3.994951	0.605014	2.600335	-3.998077	0.468956
C	C	1.672597	-2.220647	-0.029877	1.542758	-2.181458	-0.063727
C	C	1.699820	-0.796082	-0.138999	1.603001	-0.754278	-0.141381
C	C	0.521621	-2.950444	-0.409028	0.350960	-2.872680	-0.380231
H	H	0.543314	-4.032467	-0.338390	0.351514	-3.956329	-0.334782
C	C	-0.590857	-2.303265	-0.898967	-0.788508	-2.189579	-0.751506
H	H	-1.441608	-2.868747	-1.262364	-1.690294	-2.723649	-1.028544
C	C	-0.637861	-0.902675	-0.844101	-0.781477	-0.793735	-0.686778
C	C	0.447988	-0.138607	-0.377690	0.360757	-0.068753	-0.315854
C	C	-1.256867	1.566865	-0.574310	-1.421378	1.458127	-0.463871
H	H	6.555156	1.501018	0.172901	6.508858	1.438456	0.107810
C	C	-3.439434	-0.303048	-0.281944	-3.276463	-0.297608	-0.301650
C	C	-4.386787	-0.781675	1.898161	-4.576863	-0.861371	1.669965
C	C	-4.700155	-0.500808	-0.856662	-4.413913	-0.510423	-1.085017
C	C	-5.642688	-0.975467	1.316121	-5.708599	-1.070921	0.877682
C	C	-5.798538	-0.834473	-0.060623	-5.623760	-0.894384	-0.501300
H	H	-4.825718	-0.394738	-1.928840	-4.355659	-0.375699	-2.160221
H	H	-6.770000	-0.984418	-0.518004	-6.495470	-1.054818	-1.126002
P	C	-2.034582	0.136144	-1.409798	-0.067483	1.336725	-0.085972
C	C	0.041563	1.264331	-0.101611	0.558414	2.429312	0.529038
C	C	0.699928	2.228056	0.678828	-0.141474	3.625426	0.689169
C	C	0.107699	3.465200	0.917431	-1.460655	3.751267	0.247787
C	C	-1.146020	3.774869	0.382771	-2.110983	2.654858	-0.322020
C	H	-1.831864	2.819324	-0.363848	1.570829	2.360298	0.900384
H	H	1.664464	2.016113	1.117996	0.348101	4.465905	1.168414
H	H	0.627904	4.193438	1.529440	-1.987145	4.690817	0.371654
H	H	-1.592519	4.745501	0.566092	-3.150366	2.729219	-0.623289
H	C	-2.820018	3.040936	-0.752787	-3.373135	-0.478265	1.084841
C	H	-3.292512	-0.447183	1.105446	-6.645753	-1.369351	1.333859
H	H	-6.493219	-1.235821	1.935989	-4.633953	-0.997068	2.744371
H	H	-4.262408	-0.891588	2.969750	-2.500511	-0.318445	1.709534
H	C	-2.322518	-0.298813	1.566896	-1.963520	0.125259	-0.942662
*****	H	-2.123845	0.172299	-2.028092	*****		

1P234-n-hexane	1C234-n-hexane						
C	C	5.574892	1.033237	0.103100	5.523117	0.989785	0.025166
C	C	4.509384	1.717632	-0.507749	4.451706	1.713844	-0.525287
H	H	4.671002	2.701237	-0.934228	4.618183	2.707884	-0.925045
C	C	5.377474	-0.250856	0.564194	5.316503	-0.306462	0.448258

H	6.203553	-0.815509	0.983860	H	6.145623	-0.899978	0.819361
C	3.257889	1.138393	-0.583082	C	3.187222	1.159145	-0.577337
H	2.464601	1.673238	-1.085285	H	2.390347	1.719342	-1.043907
C	4.115034	-0.878670	0.458703	C	4.039555	-0.906775	0.366866
C	3.001410	-0.148253	-0.054214	C	2.923945	-0.138406	-0.082174
C	3.970363	-2.270342	0.765215	C	3.876730	-2.305170	0.633915
H	4.823471	-2.806771	1.166647	H	4.733833	-2.871814	0.981837
C	2.817859	-2.921976	0.468158	C	2.697681	-2.922161	0.370630
H	2.738412	-3.994569	0.609828	H	2.599336	-3.996068	0.489087
C	1.668516	-2.221239	-0.028261	C	1.541596	-2.182218	-0.049771
C	1.697165	-0.797452	-0.139201	C	1.603807	-0.756176	-0.135655
C	0.517080	-2.949578	-0.406696	C	0.347330	-2.872411	-0.355959
H	0.537771	-4.031694	-0.334313	H	0.345650	-3.955796	-0.301820
C	-0.594091	-2.302354	-0.897965	C	-0.792309	-2.190312	-0.727208
H	-1.446272	-2.866614	-1.260053	H	-1.697943	-2.723651	-0.993053
C	-0.639650	-0.902131	-0.846144	C	-0.781550	-0.794569	-0.673240
C	0.446670	-0.139238	-0.379999	C	0.362646	-0.070011	-0.309054
C	-1.255898	1.567120	-0.579807	C	-1.416916	1.459468	-0.455678
H	6.551505	1.498093	0.176112	H	6.510558	1.433769	0.080657
C	-3.435440	-0.299770	-0.280871	C	-3.278854	-0.293037	-0.305085
C	-4.381549	-0.752297	1.904350	C	-4.598756	-0.841253	1.656098
C	-4.691960	-0.524752	-0.853927	C	-4.405702	-0.521743	-1.098589
C	-5.632845	-0.973760	1.323684	C	-5.719413	-1.066876	0.853670
C	-5.787324	-0.859615	-0.055029	C	-5.619823	-0.906118	-0.525422
H	-4.814774	-0.438362	-1.928352	H	-4.335427	-0.398957	-2.174832
H	-6.755802	-1.030899	-0.511615	H	-6.483357	-1.078860	-1.158244
P	-2.034390	0.137344	-1.416035	C	-0.062500	1.336306	-0.081773
C	0.041599	1.264094	-0.105876	C	0.566293	2.427421	0.531777
C	0.700001	2.227409	0.674611	C	-0.132010	3.623541	0.694061
C	0.108382	3.464496	0.911929	C	-1.452174	3.750607	0.258147
C	-1.144378	3.774538	0.376622	C	-2.105462	2.655605	-0.309494
C	-1.829843	2.819502	-0.369716	H	1.578957	2.354520	0.901878
H	1.663743	2.013552	1.114679	H	0.359193	4.463139	1.173372
H	0.628400	4.192492	1.524595	H	-1.978054	4.689946	0.386440
H	-1.590715	4.745362	0.559920	H	-3.147300	2.728705	-0.602487
H	-2.818155	3.040248	-0.758782	C	-3.390895	-0.457905	1.081688
C	-3.290402	-0.417187	1.108755	H	-6.660141	-1.365379	1.302458
H	-6.481310	-1.234447	1.946485	H	-4.667969	-0.964321	2.731325
H	-4.258325	-0.840934	2.978160	H	-2.526088	-0.284431	1.713215
H	-2.323287	-0.246299	1.568158	C	-1.960637	0.127165	-0.934903
	*****			H	-2.112169	0.174261	-2.022118
					*****		

12P34-vacuum				12C34-vacuum			
C	2.775817	2.978695	1.398924	C	3.081528	2.963083	1.144164
C	2.374669	4.240189	0.909278	C	2.655546	4.227221	0.682034
H	2.870399	5.139854	1.255864	H	3.219868	5.116790	0.937976
C	2.173476	1.827056	0.946626	C	2.388679	1.823262	0.805660
H	2.481385	0.878326	1.360621	H	2.711917	0.874728	1.208043
C	1.326263	4.320721	0.025810	C	1.501112	4.325255	-0.055178
H	0.972455	5.286654	-0.319411	H	1.134137	5.295880	-0.372606
C	4.488732	-1.376276	-0.122797	C	4.252331	-1.905865	-0.118063
C	3.296456	-0.719787	-0.324979	C	3.171400	-1.067619	-0.268022
C	4.504430	-2.722330	0.302447	C	4.065961	-3.272443	0.183918
H	5.448925	-3.224202	0.479525	H	4.924782	-3.919949	0.319796

C	3.319427	-3.401791	0.446040	C	2.793063	-3.781904	0.260406
H	3.318658	-4.452012	0.718823	H	2.636153	-4.840549	0.439857
C	2.073777	-2.767965	0.197138	C	1.655151	-2.954378	0.067171
C	2.047905	-1.367589	-0.121793	C	1.838892	-1.541151	-0.128728
C	0.871632	-3.523720	0.174891	C	0.355895	-3.522302	-0.004467
H	0.911543	-4.578011	0.427281	H	0.244793	-4.589692	0.153945
C	-0.300567	-2.951183	-0.250163	C	-0.731240	-2.748625	-0.334116
H	-1.193049	-3.555081	-0.373284	H	-1.712397	-3.193826	-0.457704
C	-0.346559	-1.567716	-0.516582	C	-0.561764	-1.364094	-0.493630
C	0.769157	-0.740830	-0.332599	C	0.664103	-0.732396	-0.285913
C	-0.797279	0.876992	-1.132946	C	-0.846673	0.936352	-0.876642
H	3.558315	2.915286	2.146874	H	3.954402	2.889934	1.783369
C	-3.076491	-0.556629	-0.147438	C	-2.923444	-0.380751	-0.198713
C	-3.946627	-0.131005	2.073544	C	-4.155360	-0.165725	1.879675
C	-4.377448	-0.818710	-0.589993	C	-4.129947	-0.612754	-0.863217
C	-5.242701	-0.391147	1.622463	C	-5.356098	-0.398145	1.205971
C	-5.457356	-0.734356	0.290908	C	-5.340441	-0.621720	-0.167460
H	-4.546259	-1.091023	-1.626485	H	-4.125262	-0.789168	-1.934353
H	-6.461060	-0.939175	-0.064727	H	-6.266873	-0.804134	-0.700792
P	-1.697590	-0.697664	-1.383145	C	0.444391	0.733474	-0.391385
C	0.438009	0.696728	-0.505205	C	1.227884	1.874573	-0.012209
C	1.128930	1.862556	-0.016969	C	0.738151	3.174166	-0.386323
C	0.651959	3.155350	-0.424024	C	-0.529473	3.306979	-1.012432
C	-0.528879	3.264764	-1.205158	C	-1.335515	2.210997	-1.205156
C	-1.268240	2.150557	-1.510107	H	-0.874662	4.299154	-1.282954
H	-0.866554	4.250623	-1.506721	H	-2.337811	2.323070	-1.604085
H	-2.209854	2.244652	-2.040055	C	-2.951094	-0.157011	1.183645
C	-2.870675	-0.211988	1.195459	H	-6.293957	-0.404719	1.749850
H	-6.079289	-0.326577	2.309305	H	-4.159146	0.009088	2.949918
H	-3.776523	0.135813	3.110865	H	-2.022680	0.024288	1.714611
H	-1.867679	-0.007472	1.552882	H	5.255637	-1.515353	-0.247334
H	5.423658	-0.857519	-0.303051	H	3.341453	-0.036821	-0.541379
H	3.311875	0.301313	-0.677791	C	-1.606500	-0.371909	-0.961496
	*****			H	-1.829590	-0.598137	-2.013110
					*****		

12P34-CCI4				12C34-CCI4			
C	2.775550	2.981670	1.399691	C	3.075477	2.970028	1.145570
C	2.373325	4.243038	0.909357	C	2.647258	4.233444	0.682355
H	2.868612	5.143074	1.255513	H	3.209697	5.124168	0.938333
C	2.173792	1.829224	0.947870	C	2.385072	1.828408	0.806820
H	2.482836	0.881117	1.362488	H	2.710869	0.881044	1.209842
C	1.324392	4.322609	0.025861	C	1.492913	4.328852	-0.056104
H	0.969645	5.288001	-0.319736	H	1.124232	5.298486	-0.374484
C	4.491790	-1.373176	-0.125544	C	4.255950	-1.900728	-0.114375
C	3.298538	-0.717220	-0.325500	C	3.173668	-1.063712	-0.264451
C	4.508959	-2.720115	0.298249	C	4.071106	-3.268535	0.184728
H	5.454103	-3.221305	0.473588	H	4.930739	-3.914916	0.320669
C	3.324395	-3.400888	0.442647	C	2.798487	-3.780188	0.258545
H	3.324509	-4.451367	0.714171	H	2.642855	-4.839342	0.435864
C	2.077772	-2.767206	0.195894	C	1.659489	-2.953487	0.065117
C	2.050467	-1.366320	-0.121855	C	1.841308	-1.539319	-0.128309
C	0.876191	-3.524484	0.174867	C	0.361048	-3.523838	-0.009382
H	0.917383	-4.578855	0.426435	H	0.251365	-4.591705	0.146435
C	-0.297403	-2.952302	-0.247985	C	-0.726944	-2.750872	-0.339002

H	-1.189420	-3.556969	-0.370249	H	-1.706694	-3.198145	-0.466016
C	-0.344467	-1.568408	-0.513466	C	-0.559665	-1.365461	-0.495721
C	0.770798	-0.740374	-0.330675	C	0.665181	-0.731958	-0.285932
C	-0.797345	0.876622	-1.130640	C	-0.848100	0.934360	-0.877614
H	3.558402	2.919294	2.147312	H	3.948220	2.898878	1.785130
C	-3.078666	-0.559605	-0.147323	C	-2.922219	-0.385110	-0.197633
C	-3.952717	-0.144463	2.074563	C	-4.152188	-0.176378	1.883347
C	-4.379973	-0.811075	-0.595950	C	-4.129715	-0.612308	-0.862584
C	-5.249232	-0.393787	1.617667	C	-5.354149	-0.403692	1.209319
C	-5.462079	-0.726281	0.282637	C	-5.339832	-0.621733	-0.165544
H	-4.548410	-1.075330	-1.634515	H	-4.126165	-0.784469	-1.934272
H	-6.465817	-0.922562	-0.077496	H	-6.266990	-0.800214	-0.698924
P	-1.696662	-0.699016	-1.378668	C	0.443144	0.733826	-0.391248
C	0.438421	0.697059	-0.503321	C	1.224439	1.876769	-0.011869
C	1.128700	1.863573	-0.015483	C	0.732462	3.175552	-0.387032
C	0.650795	3.156045	-0.423191	C	-0.534943	3.306085	-1.014869
C	-0.530687	3.264901	-1.204013	C	-1.338732	2.208176	-1.208004
C	-1.269830	2.149875	-1.508039	H	-0.881568	4.297361	-1.286653
H	-0.869025	4.250416	-1.505737	H	-2.340014	2.318441	-1.609882
H	-2.211771	2.243683	-2.037389	C	-2.948179	-0.167029	1.185908
C	-2.874434	-0.225553	1.198715	H	-6.291643	-0.410737	1.753829
H	-6.087406	-0.329243	2.302487	H	-4.154647	-0.006102	2.954316
H	-3.783935	0.113780	3.114204	H	-2.019468	0.010322	1.717827
H	-1.871634	-0.029477	1.561501	H	5.258859	-1.508345	-0.240746
H	5.426173	-0.853528	-0.305841	H	3.343488	-0.032119	-0.534791
H	3.313366	0.304358	-0.676932	C	-1.606075	-0.374812	-0.962515
*****				H	-1.830688	-0.600643	-2.013615
*****				*****			

12P34-DCM				12C34-DCM			
C	2.766973	2.990570	1.401171	C	3.062885	2.980849	1.149161
C	2.359876	4.251025	0.911328	C	2.631689	4.242871	0.683726
H	2.852106	5.152546	1.257787	H	3.190823	5.135444	0.940281
C	2.169196	1.835855	0.948989	C	2.376642	1.836484	0.809729
H	2.482384	0.889076	1.363495	H	2.705718	0.890944	1.214255
C	1.310134	4.327352	0.027913	C	1.478495	4.334089	-0.057855
H	0.951569	5.291428	-0.317169	H	1.107393	5.302106	-0.378133
C	4.497865	-1.360604	-0.127410	C	4.260496	-1.891789	-0.103727
C	3.302303	-0.707803	-0.325978	C	3.176397	-1.056903	-0.255810
C	4.519262	-2.708480	0.294534	C	4.077887	-3.261566	0.189422
H	5.466026	-3.206747	0.469088	H	4.938642	-3.906019	0.326966
C	3.336602	-3.393394	0.438529	C	2.805912	-3.776965	0.255767
H	3.339883	-4.444126	0.708732	H	2.652130	-4.837063	0.428585
C	2.087771	-2.762625	0.192946	C	1.665479	-2.951917	0.060424
C	2.055986	-1.361082	-0.123114	C	1.844236	-1.536198	-0.127688
C	0.888559	-3.524310	0.171785	C	0.368802	-3.526280	-0.021415
H	0.933331	-4.578754	0.421987	H	0.261755	-4.595151	0.128778
C	-0.287437	-2.955088	-0.249539	C	-0.720250	-2.754742	-0.351988
H	-1.177290	-3.562837	-0.371919	H	-1.697471	-3.205191	-0.486763
C	-0.338814	-1.570626	-0.513182	C	-0.556571	-1.367884	-0.502562
C	0.773969	-0.738858	-0.330545	C	0.666131	-0.731354	-0.287550
C	-0.799710	0.873938	-1.129432	C	-0.850445	0.931142	-0.882462
H	3.550551	2.930940	2.148164	H	3.934792	2.912947	1.790103
C	-3.078470	-0.569513	-0.146875	C	-2.918970	-0.391723	-0.196306
C	-3.952143	-0.179534	2.080333	C	-4.140656	-0.190432	1.891388

C	-4.381925	-0.796942	-0.602806	C	-4.129474	-0.614158	-0.857970
C	-5.250994	-0.404269	1.616271	C	-5.345843	-0.412964	1.220707
C	-5.465007	-0.711948	0.275026	C	-5.336965	-0.624853	-0.155715
H	-4.552485	-1.042328	-1.645540	H	-4.130500	-0.781300	-1.930244
H	-6.470236	-0.889187	-0.090502	H	-6.266382	-0.799582	-0.686325
P	-1.694674	-0.704614	-1.375729	C	0.440277	0.734319	-0.392455
C	0.436862	0.697901	-0.502309	C	1.217503	1.880150	-0.011820
C	1.123354	1.866706	-0.013983	C	0.722616	3.177506	-0.389666
C	0.640716	3.157914	-0.421266	C	-0.543218	3.304206	-1.022390
C	-0.541503	3.263581	-1.202061	C	-1.343280	2.203465	-1.216927
C	-1.277054	2.145835	-1.506577	H	-0.890991	4.294014	-1.297766
H	-0.882985	4.248017	-1.503430	H	-2.342209	2.310435	-1.625411
H	-2.219240	2.237004	-2.035894	C	-2.939096	-0.179839	1.188643
C	-2.872722	-0.260228	1.205155	H	-6.281231	-0.421213	1.768780
H	-6.089840	-0.340301	2.300188	H	-4.138562	-0.025254	2.963151
H	-3.782426	0.058871	3.124478	H	-2.008463	-0.006600	1.718812
H	-1.868564	-0.083525	1.574277	H	5.262907	-1.496080	-0.222907
H	5.430674	-0.837759	-0.306248	H	3.345979	-0.023842	-0.520350
H	3.314762	0.314637	-0.674963	C	-1.605647	-0.379452	-0.967136
	*****			H	-1.834532	-0.604967	-2.016986
					*****		

12P34-DMSO				12C34-DMSO			
C	2.760279	2.996121	1.402324	C	3.054904	2.987048	1.151366
C	2.349947	4.255930	0.913088	C	2.621959	4.248180	0.684711
H	2.839991	5.158428	1.259998	H	3.179100	5.141853	0.941649
C	2.165340	1.840023	0.949601	C	2.371200	1.841124	0.811477
H	2.481189	0.893994	1.363769	H	2.702098	0.896580	1.216787
C	1.299907	4.330180	0.029626	C	1.469581	4.336929	-0.058734
H	0.938869	5.293469	-0.314944	H	1.097056	5.303988	-0.380128
C	4.501320	-1.351822	-0.127708	C	4.263047	-1.885942	-0.097481
C	3.304323	-0.701322	-0.326024	C	3.177869	-1.052476	-0.250906
C	4.525488	-2.700132	0.293166	C	4.081950	-3.256757	0.192354
H	5.473276	-3.196369	0.467758	H	4.943426	-3.899968	0.330946
C	3.344184	-3.387823	0.436404	C	2.810520	-3.774464	0.254297
H	3.349637	-4.438680	0.705947	H	2.657944	-4.835113	0.424567
C	2.093992	-2.759319	0.190959	C	1.669185	-2.950661	0.057710
C	2.059222	-1.357449	-0.124087	C	1.845974	-1.534110	-0.127420
C	0.896443	-3.523856	0.169097	C	0.373688	-3.527451	-0.028403
H	0.943529	-4.578359	0.418408	H	0.268409	-4.596905	0.118636
C	-0.280916	-2.956789	-0.251758	C	-0.716079	-2.757043	-0.359664
H	-1.169239	-3.566644	-0.374650	H	-1.691815	-3.209333	-0.498854
C	-0.335289	-1.572037	-0.514178	C	-0.554646	-1.369411	-0.506797
C	0.775736	-0.737829	-0.331136	C	0.666660	-0.730962	-0.288728
C	-0.801525	0.872048	-1.129409	C	-0.851930	0.929160	-0.885641
H	3.544210	2.938152	2.149027	H	3.926267	2.921043	1.793185
C	-3.077414	-0.576027	-0.146510	C	-2.916863	-0.395806	-0.195759
C	-3.949408	-0.202419	2.084439	C	-4.133075	-0.198841	1.896062
C	-4.382366	-0.788172	-0.605788	C	-4.129294	-0.615534	-0.854999
C	-5.249825	-0.411487	1.617065	C	-5.340262	-0.418745	1.227801
C	-5.465359	-0.703239	0.272324	C	-5.334983	-0.627077	-0.149392
H	-4.554617	-1.021394	-1.650978	H	-4.133339	-0.779755	-1.927612
H	-6.471692	-0.868404	-0.095680	H	-6.265854	-0.799747	-0.678078
P	-1.693517	-0.708383	-1.375259	C	0.438410	0.734581	-0.393398
C	0.435443	0.698426	-0.502201	C	1.213090	1.882083	-0.011862

C	1.119219	1.868698	-0.013267	C	0.716468	3.178538	-0.391240
C	0.633443	3.159057	-0.420092	C	-0.548377	3.302904	-1.026790
C	-0.548977	3.262499	-1.201149	C	-1.346193	2.200552	-1.222245
C	-1.281927	2.143021	-1.506353	H	-0.896781	4.291889	-1.304207
H	-0.892494	4.246233	-1.502360	H	-2.343840	2.305453	-1.634354
H	-2.224117	2.232230	-2.035980	C	-2.933224	-0.187484	1.189943
C	-2.869973	-0.282716	1.208944	H	-6.274231	-0.427792	1.778253
H	-6.088596	-0.348006	2.301052	H	-4.128054	-0.036602	2.968266
H	-3.778477	0.023242	3.131189	H	-2.001217	-0.016653	1.718623
H	-1.864733	-0.118409	1.580948	H	5.265092	-1.488200	-0.212573
H	5.433080	-0.826758	-0.305317	H	3.347029	-0.018590	-0.512320
H	3.315092	0.321627	-0.673562	C	-1.605348	-0.382373	-0.970179
	*****			H	-1.836687	-0.607913	-2.019287
	*****				*****		

12P34-n-hexane				12C34-n-hexane			
C	2.776691	2.980319	1.399492	C	3.076845	2.968636	1.145189
C	2.375181	4.241824	0.909145	C	2.649022	4.232204	0.682247
H	2.870886	5.141631	1.255323	H	3.211853	5.122701	0.938186
C	2.174386	1.828224	0.947665	C	2.385946	1.827372	0.806505
H	2.482827	0.879910	1.362263	H	2.711275	0.879766	1.209348
C	1.326416	4.321895	0.025608	C	1.494596	4.328136	-0.055870
H	0.972235	5.287491	-0.320035	H	1.126226	5.297972	-0.374020
C	4.490776	-1.375139	-0.124947	C	4.255315	-1.901720	-0.115520
C	3.297923	-0.718683	-0.325266	C	3.173270	-1.064473	-0.265441
C	4.507229	-2.721934	0.299083	C	4.070216	-3.269262	0.184302
H	5.452093	-3.223574	0.474691	H	4.929713	-3.915860	0.320121
C	3.322360	-3.402057	0.443347	C	2.797551	-3.780476	0.258924
H	3.321945	-4.452496	0.715078	H	2.641701	-4.839516	0.436781
C	2.076120	-2.767917	0.196258	C	1.658734	-2.953627	0.065654
C	2.049551	-1.367125	-0.121697	C	1.840907	-1.539664	-0.128401
C	0.874186	-3.524509	0.175061	C	0.360113	-3.523494	-0.008031
H	0.914801	-4.578882	0.426770	H	0.250149	-4.591244	0.148457
C	-0.298993	-2.951850	-0.248100	C	-0.727750	-2.750407	-0.337587
H	-1.191317	-3.556053	-0.370491	H	-1.707808	-3.197272	-0.463693
C	-0.345374	-1.568033	-0.513753	C	-0.560045	-1.365187	-0.495030
C	0.770264	-0.740593	-0.330826	C	0.665027	-0.732032	-0.285822
C	-0.796990	0.877056	-1.130999	C	-0.847824	0.934745	-0.877189
H	3.559423	2.917514	2.147212	H	3.949658	2.897082	1.784623
C	-3.078550	-0.558035	-0.147383	C	-2.922547	-0.384294	-0.197848
C	-3.952342	-0.139051	2.073786	C	-4.153259	-0.174513	1.882417
C	-4.379540	-0.813331	-0.594595	C	-4.129746	-0.612227	-0.862977
C	-5.248510	-0.392313	1.618278	C	-5.354881	-0.402595	1.208192
C	-5.461338	-0.728678	0.284302	C	-5.340073	-0.621530	-0.166424
H	-4.547777	-1.080484	-1.632465	H	-4.125781	-0.785093	-1.934581
H	-6.464867	-0.928001	-0.074784	H	-6.267012	-0.800610	-0.699993
P	-1.697018	-0.698099	-1.379362	C	0.443441	0.733754	-0.391188
C	0.438621	0.696951	-0.503593	C	1.225199	1.876330	-0.011906
C	1.129443	1.863112	-0.015771	C	0.733611	3.175276	-0.386769
C	0.652249	3.155777	-0.423516	C	-0.533927	3.306265	-1.014082
C	-0.529058	3.265120	-1.204421	C	-1.338171	2.208730	-1.207083
C	-1.268703	2.150509	-1.508468	H	-0.880353	4.297729	-1.285476
H	-0.866882	4.250803	-1.506224	H	-2.339734	2.319371	-1.608174
H	-2.210558	2.244689	-2.037915	C	-2.949065	-0.165305	1.185487
C	-2.874390	-0.220113	1.197643	H	-6.292552	-0.409521	1.752400

H	-6.086465	-0.327771	2.303384	H	-4.156157	-0.003498	2.953268
H	-3.783574	0.122282	3.112669	H	-2.020500	0.012657	1.717423
H	-1.871776	-0.020949	1.559232	H	5.258281	-1.509726	-0.242712
H	5.425431	-0.855976	-0.305277	H	3.343075	-0.033060	-0.536510
H	3.313188	0.302787	-0.677000	C	-1.606132	-0.374260	-0.962100
	*****			H	-1.830275	-0.600177	-2.013340
					*****		

1-A-13-D-P1234-vacuum				1-A-13-D-P1234-CCl4			
C	2.588991	-3.620543	0.317555	C	2.605104	-3.622563	0.314820
C	2.063116	-2.756316	1.288890	C	2.064841	-2.762899	1.282881
C	3.123791	-3.104668	-0.839316	H	1.762547	-3.180102	2.233797
H	3.622268	-3.746251	-1.557128	C	3.147983	-3.101650	-0.836719
C	1.972223	-1.384151	1.074956	H	3.658991	-3.738562	-1.549904
C	3.049393	-1.719033	-1.096987	C	1.970405	-1.389662	1.072225
C	2.339560	-0.856191	-0.209565	C	3.066540	-1.715349	-1.093013
C	3.753119	-1.164550	-2.214961	C	2.344721	-0.857129	-0.209638
H	4.294651	-1.840603	-2.867583	C	3.775591	-1.156554	-2.205945
C	3.822578	0.178791	-2.396022	H	4.325438	-1.829145	-2.855144
H	4.446365	0.605298	-3.174230	C	3.838885	0.187602	-2.385428
C	3.028372	1.063065	-1.599038	H	4.465785	0.618351	-3.158715
C	2.130574	0.525299	-0.630707	C	3.035993	1.067110	-1.591555
C	3.114171	2.464386	-1.779132	C	2.134321	0.525157	-0.629296
H	3.831421	2.854673	-2.493275	C	3.120725	2.469438	-1.768404
C	2.341426	3.314507	-1.029566	H	3.840024	2.861996	-2.479092
H	2.472647	4.388919	-1.098271	C	2.345679	3.317117	-1.018433
C	1.305273	2.798976	-0.217163	H	2.477181	4.391602	-1.083356
C	1.103370	1.398941	-0.139795	C	1.307921	2.798408	-0.209352
C	0.475652	3.706194	0.551140	C	1.105501	1.397830	-0.138255
H	0.752990	4.755339	0.550255	C	0.478515	3.703670	0.561887
C	-0.575702	3.277089	1.284084	H	0.755633	4.752702	0.564497
H	-1.154436	3.959731	1.895841	C	-0.572373	3.271357	1.294012
C	-1.011714	1.910134	1.150608	H	-1.150762	3.950833	1.909421
C	-0.203812	0.969456	0.348890	C	-1.008322	1.905050	1.153686
C	-2.216157	1.409208	1.561294	C	-0.202404	0.968389	0.346304
H	2.630193	-4.685556	0.516242	C	-2.213197	1.402718	1.562418
C	-0.909322	-0.181709	0.040355	H	-2.939144	1.947982	2.150911
P	-2.395404	-0.305035	1.080902	H	2.652132	-4.687436	0.513285
C	-3.864054	-0.375559	-0.033597	C	-0.911707	-0.179557	0.030306
C	-4.020399	0.492182	-1.122935	P	-2.396598	-0.307608	1.072526
C	-4.846458	-1.335850	0.227396	C	-3.869270	-0.375980	-0.035941
C	-5.146253	0.397772	-1.933992	C	-4.033989	0.498778	-1.118865
H	-3.258708	1.233024	-1.336835	C	-4.846733	-1.342084	0.224253
C	-5.976962	-1.424910	-0.585771	C	-5.163520	0.404796	-1.925496
H	-4.726117	-2.016954	1.062503	H	-3.277439	1.245127	-1.331957
C	-6.126848	-0.559472	-1.665357	C	-5.980775	-1.430389	-0.584519
H	-5.258832	1.068589	-2.778379	H	-4.721019	-2.027734	1.054755
H	-6.732795	-2.173640	-0.377431	C	-6.139065	-0.558495	-1.658235
H	-7.002156	-0.631075	-2.301173	H	-5.283056	1.080939	-2.764576
H	1.766731	-3.169560	2.243466	H	-6.732750	-2.183136	-0.377072
N	1.570598	-0.511037	2.117119	H	-7.017084	-0.629512	-2.290262
C	0.838060	-1.091097	3.232737	N	1.559292	-0.522405	2.113726
H	0.411719	-0.279606	3.827577	C	2.579140	0.420550	2.584772
H	0.018571	-1.710524	2.867130	H	2.098592	1.219711	3.154755
H	1.469785	-1.698743	3.903299	H	3.316426	-0.075884	3.236431

C	2.600141	0.422315	2.583476	H	3.109765	0.870207	1.748713
H	2.129092	1.226721	3.154442	C	0.830396	-1.110784	3.228556
H	3.336873	-0.079335	3.232358	H	0.398150	-0.303511	3.824503
H	3.130460	0.866708	1.744271	H	0.016217	-1.736381	2.861796
H	-2.943634	1.957946	2.144585	H	1.467118	-1.714259	3.897329
C	-0.599056	-1.190034	-0.891160	C	-0.610618	-1.174539	-0.916006
N	-0.459808	-2.016816	-1.692703	N	-0.484362	-1.989262	-1.732887
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1-A-13-D-P1234-DCM				1-A-13-D-P1234-DMSO			
C	2.609259	-3.624965	0.310503	C	2.616775	-3.623499	0.309699
C	2.060265	-2.768387	1.276974	C	2.063576	-2.768431	1.275387
H	1.753630	-3.188851	2.224958	H	1.757484	-3.189987	2.223018
C	3.159510	-3.100800	-0.836947	C	3.167408	-3.097973	-0.837363
H	3.680588	-3.734600	-1.545712	H	3.693368	-3.730083	-1.544094
C	1.967513	-1.393400	1.070565	C	1.968922	-1.393021	1.069805
C	3.075828	-1.713391	-1.091144	C	3.079816	-1.710484	-1.091821
C	2.346965	-0.857748	-0.209959	C	2.348045	-0.856419	-0.211070
C	3.789355	-1.151987	-2.200500	C	3.792665	-1.147640	-2.201165
H	4.346136	-1.822168	-2.846268	H	4.352706	-1.816335	-2.845669
C	3.848431	0.192927	-2.379200	C	3.847821	0.197588	-2.380502
H	4.478464	0.626483	-3.148242	H	4.477706	0.632654	-3.148751
C	3.039159	1.069319	-1.587938	C	3.036002	1.072041	-1.589545
C	2.135381	0.524895	-0.629204	C	2.133581	0.525821	-0.630664
C	3.122856	2.472505	-1.763659	C	3.117198	2.475703	-1.765228
H	3.843303	2.866336	-2.472301	H	3.836568	2.870873	-2.474147
C	2.346531	3.318786	-1.013459	C	2.340690	3.320595	-1.013667
H	2.478183	4.393212	-1.076188	H	2.471122	4.395126	-1.075883
C	1.308224	2.798262	-0.205359	C	1.304138	2.798308	-0.204029
C	1.105800	1.397240	-0.137260	C	1.103435	1.396902	-0.136939
C	0.479279	3.703266	0.566967	C	0.475614	3.702017	0.570351
H	0.756205	4.752126	0.570290	H	0.751445	4.751062	0.574188
C	-0.570923	3.269262	1.299369	C	-0.572768	3.265855	1.304228
H	-1.149025	3.946737	1.916951	H	-1.150516	3.941578	1.923908
C	-1.006011	1.902982	1.156067	C	-1.006313	1.899200	1.159723
C	-0.201627	0.968185	0.346163	C	-0.202501	0.966406	0.347620
C	-2.210644	1.399702	1.565265	C	-2.209905	1.394063	1.570047
H	-2.934782	1.942841	2.157934	H	-2.933298	1.935301	2.165326
H	2.659673	-4.689754	0.508980	H	2.671369	-4.687902	0.509323
C	-0.913404	-0.179266	0.028556	C	-0.914191	-0.181611	0.029548
P	-2.397676	-0.308767	1.072675	P	-2.397717	-0.313460	1.075364
C	-3.870294	-0.376267	-0.035929	C	-3.869673	-0.378967	-0.034476
C	-4.040339	0.507865	-1.110942	C	-4.045018	0.516264	-1.099657
C	-4.842137	-1.350641	0.216396	C	-4.835243	-1.362612	0.206501
C	-5.169556	0.414175	-1.918764	C	-5.173090	0.424033	-1.909521
H	-3.290314	1.262940	-1.316388	H	-3.301086	1.279978	-1.295173
C	-5.975650	-1.438668	-0.593855	C	-5.967435	-1.449404	-0.606064
H	-4.714523	-2.041331	1.042322	H	-4.704894	-2.060432	1.025939
C	-6.139157	-0.558100	-1.660266	C	-6.136161	-0.558023	-1.662865
H	-5.294360	1.098681	-2.750170	H	-5.302707	1.118051	-2.732225
H	-6.723841	-2.196596	-0.392100	H	-6.711190	-2.213808	-0.412712
H	-7.017285	-0.627964	-2.292121	H	-7.013789	-0.626097	-2.295540
N	1.552344	-0.531250	2.111828	N	1.551913	-0.533037	2.110721
C	0.830384	-1.125555	3.229352	C	2.556911	0.429155	2.578962
H	0.396582	-0.321077	3.827457	H	2.062724	1.223993	3.142527

H	0.018653	-1.755782	2.865189	H	3.296540	-0.053828	3.236997
H	1.473513	-1.725705	3.893932	H	3.085497	0.880895	1.742998
C	2.562874	0.423509	2.582155	C	0.834319	-1.129671	3.230317
H	2.073667	1.219186	3.149120	H	0.399284	-0.326377	3.828884
H	3.301624	-0.065197	3.237271	H	0.024111	-1.763120	2.868320
H	3.092191	0.875537	1.746716	H	1.481169	-1.727066	3.893311
C	-0.618896	-1.165426	-0.925850	C	-0.621772	-1.163468	-0.928444
N	-0.500486	-1.973498	-1.751877	N	-0.505476	-1.968242	-1.758723
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1-A-13-D-P1234-N-HEXANE				3-A-12-D-P1234-VAC			
C	2.602565	-3.622239	0.315611	C	3.474459	-2.808431	-0.493798
C	2.064698	-2.761736	1.284139	C	2.548379	-2.409168	0.511863
H	1.763402	-3.178176	2.235725	C	3.977589	-1.888103	-1.379411
C	3.143952	-3.102241	-0.836907	H	4.725723	-2.198861	-2.101578
H	3.652723	-3.739990	-1.550933	C	2.131764	-1.073561	0.518820
C	1.970701	-1.388741	1.072763	H	1.452619	-0.740381	1.284748
C	3.063597	-1.716110	-1.093574	C	3.588787	-0.530405	-1.351894
C	2.343840	-0.857050	-0.209543	C	2.580506	-0.129994	-0.427324
C	3.771731	-1.158136	-2.207406	C	4.274940	0.443704	-2.136915
H	4.320031	-1.831390	-2.857231	H	5.033431	0.109108	-2.837019
C	3.836196	0.185863	-2.387188	C	4.049369	1.768964	-1.937992
H	4.462539	0.615818	-3.161383	H	4.636612	2.517744	-2.458064
C	3.034887	1.066256	-1.592770	C	3.021661	2.213649	-1.045977
C	2.133812	0.525106	-0.629478	C	2.157434	1.272002	-0.412465
C	3.119937	2.468395	-1.770152	C	2.872692	3.598395	-0.787403
H	3.838945	2.860499	-2.481413	H	3.564070	4.292204	-1.253311
C	2.345346	3.316567	-1.020265	C	1.908484	4.047456	0.073422
H	2.476892	4.391031	-1.085858	H	1.843864	5.098560	0.332887
C	1.307765	2.798491	-0.210689	C	0.930410	3.156275	0.575160
C	1.105304	1.398020	-0.138570	C	0.979531	1.782265	0.236977
C	0.478355	3.704114	0.560041	C	-0.119975	3.677081	1.423569
H	0.755594	4.753150	0.562157	H	-0.034320	4.712573	1.736965
C	-0.572725	3.272408	1.292197	C	-1.170897	2.930758	1.837017
H	-1.151160	3.952459	1.906965	H	-1.933990	3.337056	2.490058
C	-1.008806	1.906041	1.152936	C	-1.325564	1.610163	1.304204
C	-0.202570	0.968661	0.346539	C	-0.264856	1.029246	0.460149
C	-2.213702	1.404041	1.561873	C	-2.456690	0.819589	1.406921
H	-2.939950	1.949968	2.149369	H	3.820089	-3.830973	-0.548122
H	2.648607	-4.687126	0.514157	C	-0.664163	-0.135785	-0.144281
C	-0.911269	-0.179768	0.031686	P	-2.179965	-0.760342	0.566861
P	-2.396391	-0.306892	1.073469	C	-3.438087	-0.900154	-0.772615
C	-3.868584	-0.375814	-0.035666	C	-3.596285	0.087572	-1.754455
C	-4.031903	0.497220	-1.120103	C	-4.255936	-2.034199	-0.797792
C	-4.847075	-1.340537	0.225405	C	-4.561654	-0.062627	-2.744344
C	-5.161035	0.403048	-1.927146	H	-2.966634	0.969574	-1.740176
H	-3.274268	1.242234	-1.333984	C	-5.224736	-2.179849	-1.791282
C	-5.980748	-1.429064	-0.583755	H	-4.138260	-2.801308	-0.040653
H	-4.722167	-2.025104	1.056938	C	-5.377115	-1.195985	-2.763838
C	-6.137643	-0.558777	-1.658876	H	-4.680447	0.705265	-3.500522
H	-5.279356	1.077800	-2.767532	H	-5.857280	-3.060147	-1.801645
H	-6.733496	-2.180867	-0.375615	H	-6.129700	-1.308153	-3.536165
H	-7.015351	-0.630031	-2.291329	H	-0.065712	-0.710738	-0.833964
N	1.561182	-0.520346	2.114352	N	2.076873	-3.324506	1.443834
C	2.582973	0.420543	2.584823	C	1.299345	-2.845074	2.577640

H	2.104260	1.220806	3.154904	H	0.969025	-3.699632	3.166894
H	3.319906	-0.077073	3.236113	H	1.874035	-2.173635	3.232853
H	3.113872	0.869119	1.748324	H	0.405454	-2.315272	2.240831
C	0.831277	-1.107147	3.229124	C	2.760228	-4.600590	1.603550
H	0.400066	-0.299067	3.824811	H	3.807546	-4.486947	1.919787
H	0.016121	-1.731493	2.862344	H	2.237637	-5.187045	2.358108
H	1.466836	-1.711512	3.898379	H	2.742708	-5.177772	0.675755
C	-0.608505	-1.177125	-0.912100	C	-3.614235	1.148289	2.135992
N	-0.480096	-1.993855	-1.726443	N	-4.579631	1.410936	2.723084
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3-A-12-D-P1234-CCI4				3-A-12-D-P1234-DCM			
C	3.471525	-2.808084	-0.490339	C	-3.468784	2.809617	-0.488609
C	2.548901	-2.406145	0.518687	C	-2.547831	2.406144	0.522543
C	3.970942	-1.890540	-1.381114	C	-3.966923	1.893486	-1.381794
H	4.716513	-2.203396	-2.104997	H	-4.711023	2.207827	-2.106483
C	2.131872	-1.069548	0.522773	C	-2.131629	1.068140	0.525763
H	1.455455	-0.734638	1.290533	H	-1.455981	0.732704	1.294141
C	3.581832	-0.532279	-1.356196	C	-3.578455	0.534381	-1.357753
C	2.577011	-0.129278	-0.428345	C	-2.575559	0.129644	-0.427815
C	4.265595	0.439430	-2.146483	C	-4.261976	-0.435741	-2.150539
H	5.021788	0.102507	-2.847939	H	-5.016900	-0.097094	-2.852491
C	4.040977	1.766033	-1.951199	C	-4.038653	-1.763491	-1.957142
H	4.626975	2.513105	-2.475024	H	-4.624695	-2.509339	-2.482532
C	3.015738	2.213263	-1.057295	C	-3.014473	-2.212491	-1.062445
C	2.153921	1.273055	-0.417564	C	-2.153161	-1.273336	-0.419532
C	2.867454	3.599457	-0.803219	C	-2.867415	-3.599883	-0.810957
H	3.556988	4.291644	-1.274072	H	-3.556441	-4.290788	-1.284249
C	1.906035	4.051601	0.059451	C	-1.907424	-4.054381	0.052429
H	1.842050	5.103339	0.315928	H	-1.844450	-5.106399	0.307429
C	0.929660	3.161103	0.566816	C	-0.931087	-3.164544	0.562287
C	0.977733	1.785809	0.233042	C	-0.977890	-1.788298	0.231277
C	-0.117917	3.683593	1.416854	C	0.115071	-3.688811	1.412367
H	-0.031864	4.719758	1.727599	H	0.028958	-4.725501	1.720828
C	-1.168517	2.938079	1.835136	C	1.166089	-2.944005	1.833149
H	-1.928129	3.348666	2.489462	H	1.923498	-3.358273	2.487647
C	-1.325661	1.617586	1.304315	C	1.324833	-1.623749	1.303925
C	-0.265930	1.033960	0.462039	C	0.265728	-1.037869	0.463534
C	-2.457664	0.825637	1.408269	C	2.457647	-0.830556	1.408275
H	3.817619	-3.830549	-0.542235	H	-3.814695	3.832132	-0.539675
C	-0.666395	-0.132870	-0.138524	C	0.667116	0.130105	-0.134648
P	-2.181801	-0.756828	0.572362	P	2.182063	0.754089	0.575593
C	-3.438427	-0.905235	-0.767180	C	3.438966	0.907049	-0.763103
C	-3.632655	0.101426	-1.723382	C	3.651913	-0.107876	-1.707031
C	-4.215728	-2.066892	-0.819673	C	4.195795	2.081936	-0.827989
C	-4.594271	-0.057557	-2.715938	C	4.612355	0.056196	-2.700471
H	-3.034950	1.004835	-1.688423	H	3.069989	-1.021191	-1.663530
C	-5.179639	-2.221838	-1.817001	C	5.157958	2.242047	-1.826728
H	-4.070815	-2.848367	-0.082301	H	4.036056	2.870253	-0.101144
C	-5.368596	-1.219055	-2.763995	C	5.366073	1.231086	-2.761582
H	-4.741415	0.724596	-3.452142	H	4.773589	-0.731516	-3.427640
H	-5.779979	-3.123797	-1.849807	H	5.741307	3.154540	-1.870321
H	-6.117715	-1.338282	-3.538552	H	6.113335	1.354682	-3.537140
H	-0.071072	-0.708634	-0.830269	H	0.074013	0.706773	-0.827548
N	2.082435	-3.317996	1.454019	N	-2.083144	3.315949	1.458372

C	1.315259	-2.835371	2.594657	C	-1.325876	2.831151	2.605807
H	0.987096	-3.688686	3.186360	H	-1.000192	3.683806	3.199309
H	1.898526	-2.166363	3.244193	H	-1.917524	2.165153	3.250323
H	0.421025	-2.301642	2.265281	H	-0.431540	2.293027	2.284073
C	2.764497	-4.596893	1.611773	C	-2.760482	4.599624	1.611958
H	3.812589	-4.483262	1.923704	H	-3.808095	4.489863	1.925360
H	2.243972	-5.180735	2.369330	H	-2.236744	5.183170	2.367131
H	2.742072	-5.174211	0.684559	H	-2.736933	5.172734	0.682590
C	-3.613275	1.154958	2.136992	C	3.613435	-1.160558	2.132829
N	-4.580345	1.416011	2.723586	N	4.584764	-1.419949	2.714770
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3-A-12-D-P1234-DMSO				3-A-12-D-P1234-n-hexane			
C	-3.467523	2.810665	-0.489227	C	3.472162	-2.807879	-0.491139
C	-2.547357	2.406964	0.523004	C	2.549152	-2.406460	0.517525
C	-3.965376	1.894642	-1.382782	C	3.971932	-1.889825	-1.381138
H	-4.708777	2.209352	-2.107993	H	4.717803	-2.202215	-2.104919
C	-2.131787	1.068329	0.526722	C	2.132007	-1.070124	0.522142
H	-1.456288	0.733057	1.295357	H	1.455295	-0.735537	1.289749
C	-3.577518	0.535113	-1.358230	C	3.582751	-0.531699	-1.355684
C	-2.575399	0.130046	-0.427298	C	2.577474	-0.129242	-0.428225
C	-4.261213	-0.434760	-2.151337	C	4.266682	0.440493	-2.145177
H	-5.015532	-0.095746	-2.853742	H	5.023175	0.104058	-2.846550
C	-4.038731	-1.762867	-1.957703	C	4.041837	1.766837	-1.949191
H	-4.624953	-2.508431	-2.483243	H	4.627899	2.514257	-2.472469
C	-3.014997	-2.212221	-1.062453	C	3.016308	2.213520	-1.055423
C	-2.153462	-1.273254	-0.419163	C	2.154259	1.272971	-0.416660
C	-2.868777	-3.599920	-0.810870	C	2.867838	3.599429	-0.800467
H	-3.557998	-4.290553	-1.284214	H	3.557574	4.291972	-1.270533
C	-1.909093	-4.054909	0.052746	C	1.906029	4.050921	0.062041
H	-1.846789	-5.106862	0.307984	H	1.841888	5.102535	0.319096
C	-0.932211	-3.165284	0.562435	C	0.929486	3.160218	0.568504
C	-0.978407	-1.788832	0.231753	C	0.977807	1.785175	0.233906
C	0.113899	-3.690180	1.412024	C	-0.118557	3.682309	1.418359
H	0.027895	-4.727005	1.719811	H	-0.032590	4.718340	1.729645
C	1.165391	-2.945641	1.832835	C	-1.169179	2.936614	1.835781
H	1.922415	-3.361104	2.487005	H	-1.929405	3.346393	2.489917
C	1.324455	-1.625532	1.303992	C	-1.325877	1.616121	1.304519
C	0.265383	-1.038940	0.464443	C	-0.265917	1.033021	0.461931
C	2.457578	-0.831965	1.408012	C	-2.457718	0.824417	1.408155
H	-3.813050	3.833262	-0.540719	H	3.818190	-3.830350	-0.543511
C	0.666964	0.129308	-0.133256	C	-0.666118	-0.133523	-0.139276
P	2.181817	0.753461	0.576385	P	-2.181657	-0.757591	0.571517
C	3.439063	0.906807	-0.762038	C	-3.438258	-0.904536	-0.768272
C	3.650655	-0.106821	-1.707916	C	-3.624894	0.098303	-1.729905
C	4.197180	2.081143	-0.824821	C	-4.223686	-2.060878	-0.815261
C	4.611303	0.057984	-2.701299	C	-4.586945	-0.059152	-2.722198
H	3.067426	-1.019423	-1.666705	H	-3.020800	0.997602	-1.699104
C	5.159637	2.241844	-1.823403	C	-5.188276	-2.214187	-1.812091
H	4.037936	2.868899	-0.097301	H	-4.084533	-2.839434	-0.073684
C	5.366531	1.232225	-2.760247	C	-5.369529	-1.215231	-2.764514
H	4.771053	-0.728262	-3.430346	H	-4.728153	0.720131	-3.462616
H	5.743550	3.153994	-1.865717	H	-5.795123	-3.111949	-1.840369
H	6.113496	1.356600	-3.535918	H	-6.119115	-1.333211	-3.538827
H	0.074378	0.706370	-0.826258	H	-0.070237	-0.709105	-0.830689

N	-2.083085	3.316357	1.458562	N	2.082269	-3.318953	1.452488
C	-1.330116	2.831034	2.608990	C	1.313147	-2.837128	2.591919
H	-1.005409	3.683604	3.202953	H	0.984357	-3.690773	3.182913
H	-1.925388	2.166685	3.251714	H	1.894837	-2.167914	3.242774
H	-0.435875	2.290703	2.290773	H	0.419072	-2.303928	2.261240
C	-2.757530	4.602490	1.609352	C	2.764757	-4.597245	1.610368
H	-3.804886	4.495504	1.924076	H	3.812981	-4.483449	1.922110
H	-2.231617	5.186492	2.362534	H	2.244609	-5.181361	2.368057
H	-2.733760	5.172796	0.678432	H	2.742425	-5.174869	0.683250
C	3.614362	-1.162316	2.129401	C	-3.613622	1.153595	2.137103
N	4.588441	-1.421040	2.707688	N	-4.580213	1.414902	2.724080
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1-A-11-D-P1234-vac				1-A-11-D-P1234-CCI4			
C	-3.630620	-1.863981	-0.333280	C	-3.632287	-1.870863	-0.333418
C	-2.574306	-1.494427	-1.213515	C	-2.570658	-1.501495	-1.209369
H	-2.329717	-2.116306	-2.063128	H	-2.323665	-2.123676	-2.058062
C	-3.968364	-0.946874	0.665030	C	-3.973575	-0.951585	0.663685
H	-4.817624	-1.122628	1.311100	H	-4.826489	-1.125985	1.305269
C	-1.848244	-0.344298	-1.016145	C	-1.845187	-0.351173	-1.009870
H	-1.067304	-0.110560	-1.726209	C	-3.257836	0.245966	0.849083
C	-3.252644	0.250750	0.848643	C	-2.112518	0.541769	0.053230
C	-2.110911	0.546293	0.049090	C	-3.729394	1.223425	1.786840
C	-3.720827	1.227835	1.787585	H	-4.586227	0.980263	2.406194
H	-4.575776	0.984806	2.409639	C	-3.171067	2.459812	1.835270
C	-3.162145	2.463696	1.834732	H	-3.587253	3.228876	2.477481
H	-3.576317	3.232685	2.478417	C	-2.024109	2.790432	1.042271
C	-2.016759	2.793644	1.039908	C	-1.384790	1.778707	0.266121
C	-1.380414	1.781566	0.261979	C	-1.555333	4.122517	0.992717
C	-1.544699	4.124175	0.991542	H	-2.072256	4.879539	1.572921
H	-2.059501	4.881877	1.572867	C	-0.514432	4.468631	0.166654
C	-0.502710	4.468044	0.166412	H	-0.222295	5.506226	0.049307
H	-0.207254	5.505014	0.050420	C	0.228868	3.467725	-0.497212
C	0.237978	3.465919	-0.497840	C	-0.109665	2.099729	-0.320034
C	-0.104827	2.099195	-0.323239	C	1.317524	3.855321	-1.371509
C	1.328439	3.850320	-1.370990	H	1.449122	4.915525	-1.560874
H	1.462833	4.910373	-1.559901	C	2.116227	2.947791	-1.975293
C	2.125385	2.941740	-1.974894	H	2.890526	3.248176	-2.671713
H	2.901107	3.241590	-2.670110	C	2.013182	1.563498	-1.592694
C	2.018882	1.557077	-1.594809	C	0.937748	1.143122	-0.670219
C	0.939542	1.138460	-0.675132	C	2.926927	0.585509	-1.877101
C	2.930841	0.577458	-1.877508	H	3.782361	0.715627	-2.526598
H	3.789134	0.706550	-2.523376	C	1.174656	-0.125150	-0.156708
C	1.170393	-0.130188	-0.162416	P	2.465199	-0.966695	-1.121444
P	2.460861	-0.974451	-1.123988	C	3.835231	-1.423416	0.025347
C	3.827648	-1.427096	0.029484	C	4.377856	-0.513709	0.943597
C	4.344866	-0.524551	0.968640	C	4.337015	-2.727782	-0.031264
C	4.353711	-2.720626	-0.043772	C	5.409734	-0.908430	1.788988
C	5.375366	-0.914965	1.817124	H	3.989289	0.496589	0.999199
H	3.935806	0.476780	1.037563	C	5.374473	-3.119067	0.816395
C	5.390377	-3.107694	0.806346	H	3.915969	-3.438602	-0.733422
H	3.950611	-3.426591	-0.761339	C	5.910317	-2.210897	1.725358
C	5.900703	-2.206268	1.735865	H	5.822694	-0.201695	2.499953
H	5.767882	-0.213603	2.544915	H	5.756447	-4.132397	0.767667
H	5.791172	-4.113080	0.744151	H	6.713340	-2.514991	2.387239

H	6.702725	-2.507318	2.400465	H	-1.061871	-0.118637	-1.717797
N	-4.296455	-3.069046	-0.482945	N	-4.298064	-3.072503	-0.486509
C	-4.100519	-3.864758	-1.684777	C	-5.492643	-3.331586	0.301790
H	-3.045966	-4.116964	-1.821125	H	-6.319427	-2.649611	0.054566
H	-4.648302	-4.800735	-1.580814	H	-5.824324	-4.352743	0.119300
H	-4.455331	-3.358756	-2.594750	H	-5.279687	-3.238087	1.369798
C	-5.483531	-3.329744	0.313181	C	-4.092929	-3.873255	-1.685499
H	-6.315115	-2.650095	0.073296	H	-3.037777	-4.126579	-1.812932
H	-5.814684	-4.352215	0.134704	H	-4.642891	-4.807595	-1.582420
H	-5.262112	-3.235400	1.379602	H	-4.440811	-3.368574	-2.598207
C	0.524279	-0.783021	0.903193	C	0.538901	-0.775512	0.914655
N	0.090666	-1.354488	1.814488	N	0.117178	-1.346271	1.832784
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1-A-11-D-P1234-DCM				1-A-11-D-P1234-DMSO			
C	-3.633308	-1.876021	-0.332451	C	-3.633169	-1.878723	-0.331824
C	-2.567839	-1.506239	-1.205779	C	-2.565575	-1.509097	-1.203594
H	-2.320544	-2.127101	-2.055336	H	-2.317856	-2.129322	-2.053473
C	-3.975616	-0.955768	0.665416	C	-3.976387	-0.957932	0.665992
H	-4.831950	-1.128123	1.302974	H	-4.834786	-1.129004	1.301120
C	-1.842043	-0.356172	-1.004213	C	-1.839885	-0.358967	-1.001164
H	-1.057714	-0.124424	-1.711338	H	-1.055050	-0.127562	-1.707822
C	-3.259310	0.241944	0.852198	C	-3.260122	0.240197	0.853261
C	-2.111732	0.538213	0.058212	C	-2.111121	0.536289	0.060644
C	-3.733094	1.219533	1.789695	C	-3.735430	1.218155	1.790009
H	-4.591893	0.976921	2.406474	H	-4.595785	0.976291	2.404884
C	-3.174420	2.456347	1.838937	C	-3.176387	2.455098	1.839632
H	-3.592304	3.225743	2.479529	H	-3.595600	3.224942	2.478762
C	-2.026511	2.787421	1.046733	C	-2.027611	2.786046	1.048356
C	-1.385591	1.776364	0.271045	C	-1.385733	1.775092	0.273400
C	-1.560290	4.121115	0.996373	C	-1.562346	4.120455	0.997467
H	-2.078064	4.877241	1.576771	H	-2.080513	4.876306	1.577758
C	-0.521562	4.469335	0.168206	C	-0.524663	4.469393	0.168278
H	-0.232265	5.507459	0.049946	H	-0.236680	5.507746	0.049324
C	0.223240	3.469622	-0.496975	C	0.220736	3.470055	-0.497419
C	-0.111463	2.100374	-0.317750	C	-0.112109	2.100346	-0.316649
C	1.310033	3.860509	-1.372316	C	1.306297	3.861899	-1.373864
H	1.439254	4.920818	-1.561534	H	1.434318	4.922132	-1.563685
C	2.110533	2.953948	-1.975797	C	2.107242	2.955463	-1.977229
H	2.883789	3.254844	-2.672910	H	2.879482	3.256263	-2.675379
C	2.010365	1.570041	-1.591179	C	2.008639	1.571947	-1.590980
C	0.938086	1.147677	-0.667432	C	0.938316	1.149371	-0.665934
C	2.926044	0.593616	-1.876929	C	2.924885	0.595884	-1.877113
H	3.779208	0.724872	-2.529155	H	3.776856	0.726999	-2.530890
C	1.179363	-0.121495	-0.154696	C	1.181624	-0.119818	-0.152485
P	2.470534	-0.959692	-1.122542	P	2.472110	-0.957438	-1.122259
C	3.840235	-1.422772	0.021218	C	3.842300	-1.422553	0.019793
C	4.405973	-0.508236	0.921241	C	4.418877	-0.505545	0.910678
C	4.317747	-2.737260	-0.019051	C	4.309426	-2.741160	-0.012910
C	5.436463	-0.908969	1.766193	C	5.449408	-0.908295	1.754914
H	4.039208	0.510876	0.962352	H	4.061979	0.517337	0.944456
C	5.353248	-3.134477	0.828798	C	5.344718	-3.140369	0.834488
H	3.881862	-3.450714	-0.709241	H	3.866967	-3.455892	-0.697528
C	5.911987	-2.221973	1.720162	C	5.913997	-2.225654	1.717157
H	5.868911	-0.198357	2.461420	H	5.891212	-0.195594	2.442031

H	5.717169	-4.154838	0.792310	H	5.701164	-4.163502	0.803372
H	6.714566	-2.530189	2.380528	H	6.717161	-2.535139	2.376153
N	-4.299531	-3.074867	-0.488251	N	-4.299366	-3.076853	-0.488337
C	-4.095742	-3.873707	-1.691094	C	-5.509757	-3.326111	0.283679
H	-3.040719	-4.123878	-1.822496	H	-6.325014	-2.637236	0.021404
H	-4.643679	-4.808804	-1.587715	H	-5.846250	-4.344102	0.095648
H	-4.448101	-3.366669	-2.600102	H	-5.313557	-3.232505	1.354575
C	-5.504389	-3.328069	0.289641	C	-4.096872	-3.874405	-1.693271
H	-6.323874	-2.641916	0.032428	H	-3.041753	-4.121508	-1.828150
H	-5.838713	-4.347302	0.103616	H	-4.642265	-4.810747	-1.588905
H	-5.302306	-3.234340	1.359489	H	-4.453385	-3.366889	-2.600108
C	0.551281	-0.768777	0.920262	C	0.556494	-0.763859	0.924763
N	0.135247	-1.337058	1.843696	N	0.141219	-1.328384	1.851465
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1-A-11-D-P1234-n-hexane				3-A-10-D-P1234-vac			
C	-3.632118	-1.869749	-0.333502	C	-3.390802	-2.076838	-1.511746
C	-2.571162	-1.500515	-1.209926	C	-2.252610	-1.492027	-2.090553
H	-2.324281	-2.122837	-2.058548	C	-3.985887	-1.501548	-0.402637
C	-3.972997	-0.950735	0.663616	C	-1.673210	-0.374192	-1.534212
H	-4.825316	-1.125383	1.305926	H	-0.825288	0.077868	-2.025366
C	-1.845629	-0.350210	-1.010771	C	-3.390579	-0.343883	0.192484
H	-1.062522	-0.117601	-1.718886	C	-2.183259	0.197269	-0.344468
C	-3.257282	0.246797	0.848759	C	-4.030403	0.318962	1.287387
C	-2.112399	0.542466	0.052497	H	-4.889895	-0.151949	1.744664
C	-3.728370	1.224232	1.786599	C	-3.601096	1.540821	1.695717
H	-4.584945	0.981103	2.406332	H	-4.140887	2.086505	2.462606
C	-3.169975	2.460506	1.834882	C	-2.415152	2.133017	1.158116
H	-3.585856	3.229556	2.477326	C	-1.590326	1.383271	0.272304
C	-2.023185	2.790974	1.041724	C	-2.061366	3.456566	1.516463
C	-1.384266	1.779143	0.265403	H	-2.724860	4.016853	2.166225
C	-1.553859	4.122777	0.992373	C	-0.928755	4.032278	1.008636
H	-2.070511	4.879930	1.572676	H	-0.695252	5.071269	1.213894
C	-0.512687	4.468498	0.166576	C	-0.000692	3.253232	0.276584
H	-0.219986	5.505988	0.049429	C	-0.267286	1.888354	0.011598
C	0.230220	3.467367	-0.497239	C	1.226239	3.872596	-0.177785
C	-0.109018	2.099605	-0.320442	H	1.317075	4.945848	-0.045595
C	1.319135	3.854367	-1.371422	C	2.230899	3.175005	-0.757209
H	1.451157	4.914544	-1.560803	H	3.131109	3.663843	-1.110172
C	2.117487	2.946656	-1.975289	C	2.139284	1.745993	-0.800249
H	2.891924	3.246953	-2.671628	C	0.896450	1.076699	-0.375792
C	2.013936	1.562314	-1.593046	C	3.169352	0.874076	-1.106032
C	0.937937	1.142296	-0.670857	H	-3.831248	-2.951692	-1.973704
C	2.927338	0.584024	-1.877182	C	1.052315	-0.281964	-0.262640
H	3.783255	0.713928	-2.526080	P	2.573564	-0.833085	-1.019520
C	1.173940	-0.125901	-0.157278	C	3.579311	-1.705155	0.254863
P	2.464357	-0.967997	-1.121527	C	3.708272	-1.222419	1.564444
C	3.834195	-1.423854	0.026003	C	4.231744	-2.886513	-0.111760
C	4.373271	-0.514986	0.947059	C	4.480921	-1.916294	2.489596
C	4.339583	-2.726651	-0.032932	H	3.206812	-0.306513	1.854625
C	5.405157	-0.908863	1.792716	C	5.007632	-3.578327	0.818921
H	3.981540	0.493977	1.004606	H	4.136229	-3.264092	-1.123607
C	5.377137	-3.117117	0.814893	C	5.131713	-3.094543	2.118006
H	3.920922	-3.436949	-0.737068	H	4.578357	-1.537476	3.500821
C	5.909419	-2.209708	1.726584	H	5.513212	-4.491346	0.525849

H	5.815183	-0.202756	2.506023	H	5.734782	-3.631185	2.841724
H	5.761844	-4.129341	0.764336	H	0.288185	-0.967003	0.071079
H	6.712424	-2.513217	2.388780	C	4.460412	1.254233	-1.516347
N	-4.297964	-3.071940	-0.486035	N	5.532471	1.553683	-1.842623
C	-4.093685	-3.872414	-1.684949	H	-1.843080	-1.911715	-3.002657
H	-3.038606	-4.125977	-1.812951	N	-5.197640	-2.011511	0.159117
H	-4.643682	-4.806808	-1.581792	C	-5.380125	-3.455683	0.076735
H	-4.441846	-3.367806	-2.597713	H	-6.201467	-3.742828	0.738695
C	-5.491156	-3.331400	0.303688	H	-5.630263	-3.814922	-0.936051
H	-6.318741	-2.649697	0.057969	H	-4.475576	-3.964519	0.412966
H	-5.822854	-4.352717	0.121695	C	-6.401445	-1.292060	-0.268944
H	-5.276599	-3.238050	1.371431	H	-6.666486	-1.515164	-1.316016
C	0.536571	-0.776665	0.913305	H	-7.242641	-1.580454	0.367560
N	0.113235	-1.347546	1.830436	H	-6.255412	-0.215802	-0.179085
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3-A-10-D-P1234-CCI4				3-A-10-D-P1234-DCM			
C	-3.384157	-2.078590	-1.511504	C	-3.382051	-2.079493	-1.510594
C	-2.247542	-1.490866	-2.090940	C	-2.246425	-1.490373	-2.091080
C	-3.981838	-1.504163	-0.402684	C	-3.980884	-1.505372	-0.401578
C	-1.670035	-0.371471	-1.535194	C	-1.669173	-0.370187	-1.536114
H	-0.823120	0.081890	-2.027039	H	-0.822321	0.082866	-2.028497
C	-3.388457	-0.344023	0.191589	C	-3.388089	-0.343144	0.191534
C	-2.181689	0.198978	-0.345453	C	-2.181451	0.200255	-0.346344
C	-4.028413	0.318744	1.286768	C	-4.026925	0.320733	1.287137
H	-4.888735	-0.150445	1.743994	H	-4.888663	-0.144799	1.745274
C	-3.600726	1.541208	1.696080	C	-3.599211	1.543531	1.696649
H	-4.141797	2.086121	2.462443	H	-4.140776	2.088755	2.462244
C	-2.415303	2.134689	1.158387	C	-2.413954	2.136821	1.158031
C	-1.590273	1.385575	0.271962	C	-1.589903	1.387120	0.270863
C	-2.063314	3.459109	1.517114	C	-2.062253	3.461898	1.516570
H	-2.727403	4.018384	2.166984	H	-2.725746	4.020939	2.167054
C	-0.931574	4.036708	1.008895	C	-0.931115	4.039963	1.006941
H	-0.699711	5.076095	1.213381	H	-0.699470	5.079479	1.210256
C	-0.002875	3.257727	0.276847	C	-0.002962	3.259915	0.274555
C	-0.267727	1.892393	0.011839	C	-0.267524	1.894284	0.010024
C	1.222864	3.877775	-0.178595	C	1.222054	3.879576	-0.182340
H	1.313391	4.950984	-0.046881	H	1.313358	4.952558	-0.050625
C	2.228506	3.180826	-0.758756	C	2.227644	3.182134	-0.763617
H	3.126600	3.673267	-1.111889	H	3.124293	3.676865	-1.117097
C	2.139230	1.752137	-0.799144	C	2.139027	1.753959	-0.801740
C	0.896887	1.082563	-0.375575	C	0.897007	1.085071	-0.377927
C	3.169811	0.878173	-1.103980	C	3.169212	0.877230	-1.106194
H	-3.821423	-2.954931	-1.973245	H	-3.817060	-2.956994	-1.971825
C	1.053866	-0.276073	-0.261608	C	1.054096	-0.273549	-0.262376
P	2.574440	-0.829581	-1.016241	P	2.573395	-0.830988	-1.015355
C	3.577886	-1.706311	0.255962	C	3.576941	-1.706353	0.257498
C	3.719839	-1.218488	1.562634	C	3.727247	-1.211440	1.560945
C	4.213329	-2.897619	-0.109501	C	4.202641	-2.904346	-0.104165
C	4.489223	-1.917895	2.486820	C	4.495977	-1.910855	2.486257
H	3.231545	-0.295434	1.852635	H	3.245845	-0.284133	1.848933
C	4.985472	-3.594963	0.820608	C	4.973841	-3.601638	0.827324
H	4.107612	-3.279405	-1.118669	H	4.089506	-3.292557	-1.109987
C	5.122971	-3.106392	2.116965	C	5.120158	-3.106187	2.120573
H	4.596594	-1.535914	3.495758	H	4.609007	-1.524370	3.492779

H	5.477307	-4.515897	0.529168	H	5.457015	-4.528251	0.539687
H	5.722926	-3.647335	2.839960	H	5.718514	-3.647483	2.844525
H	0.292078	-0.961775	0.076247	H	0.294098	-0.959132	0.079809
C	4.458960	1.256867	-1.516039	C	4.457647	1.252311	-1.517431
N	5.532262	1.552059	-1.844886	N	5.533892	1.540978	-1.845524
H	-1.837597	-1.910339	-3.002962	H	-1.836797	-1.910600	-3.002878
N	-5.189901	-2.019226	0.160274	N	-5.184989	-2.025074	0.164002
C	-6.397216	-1.294210	-0.252962	C	-6.396046	-1.293254	-0.231490
H	-6.666848	-1.507434	-1.300521	H	-6.671464	-1.494964	-1.279372
H	-7.234211	-1.590402	0.384950	H	-7.228198	-1.598119	0.408092
H	-6.251950	-0.218944	-0.152849	H	-6.251044	-0.219405	-0.118917
C	-5.376049	-3.462956	0.056960	C	-5.376832	-3.467771	0.037797
H	-6.196235	-3.756829	0.716996	H	-6.195150	-3.768364	0.696703
H	-5.630191	-3.805129	-0.960124	H	-5.637202	-3.790507	-0.983334
H	-4.471895	-3.979347	0.382584	H	-4.473157	-3.993302	0.349897
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3-A-10-D-P1234-DMSO				3-A-10-D-P1234-n-hexane			
C	-3.383655	-2.079550	-1.509783	C	-3.384955	-2.078430	-1.511584
C	-2.247989	-1.490778	-2.090691	C	-2.248143	-1.491052	-2.090906
C	-3.982265	-1.505278	-0.400425	C	-3.982266	-1.503944	-0.402734
C	-1.669979	-0.370693	-1.536090	C	-1.670447	-0.371875	-1.535034
H	-0.822813	0.081534	-2.028738	H	-0.823433	0.081409	-2.026751
C	-3.388658	-0.342810	0.192371	C	-3.388705	-0.344167	0.191690
C	-2.181933	0.200117	-0.346238	C	-2.181906	0.198672	-0.345293
C	-4.026104	0.321660	1.288640	C	-4.028789	0.318534	1.286764
H	-4.888288	-0.141984	1.747831	H	-4.888888	-0.151152	1.743945
C	-3.597665	1.544434	1.697961	C	-3.601011	1.540961	1.695894
H	-4.138690	2.089948	2.463648	H	-4.141966	2.085943	2.462327
C	-2.412693	2.137335	1.158137	C	-2.415538	2.134352	1.158295
C	-1.589625	1.386982	0.270480	C	-1.590399	1.385223	0.272042
C	-2.060690	3.462729	1.515963	C	-2.063405	3.458665	1.516950
H	-2.723498	4.022034	2.166841	H	-2.727527	4.018064	2.166710
C	-0.929935	4.040540	1.004952	C	-0.931534	4.036046	1.008898
H	-0.697997	5.080114	1.207337	H	-0.699512	5.075393	1.213532
C	-0.002477	3.259660	0.272283	C	-0.002791	3.257147	0.276945
C	-0.267326	1.893881	0.008534	C	-0.267788	1.891866	0.011941
C	1.222223	3.878820	-0.185852	C	1.223128	3.877180	-0.178229
H	1.314055	4.951721	-0.054401	H	1.313583	4.950419	-0.046495
C	2.227356	3.180775	-0.767759	C	2.228720	3.180213	-0.758159
H	3.123489	3.675945	-1.121911	H	3.127147	3.672107	-1.111240
C	2.138620	1.752796	-0.804629	C	2.139194	1.751449	-0.798953
C	0.896850	1.084490	-0.379757	C	0.896780	1.081827	-0.375340
C	3.168301	0.874761	-1.109007	C	3.169796	0.877942	-1.103894
H	-3.818512	-2.957073	-1.970922	H	-3.822665	-2.954559	-1.973382
C	1.053900	-0.274033	-0.262751	C	1.053658	-0.276817	-0.261536
P	2.572351	-0.833585	-1.015607	P	2.574429	-0.829671	-1.016486
C	3.577500	-1.705733	0.258333	C	3.578220	-1.706157	0.255681
C	3.733124	-1.204850	1.559035	C	3.718674	-1.219312	1.562818
C	4.198794	-2.907251	-0.099688	C	4.215788	-2.896114	-0.110258
C	4.503057	-1.901901	2.485375	C	4.488547	-1.918237	2.486864
H	3.254705	-0.275253	1.844634	H	3.228788	-0.297171	1.853034
C	4.971069	-3.602193	0.832917	C	4.988484	-3.592988	0.819652
H	4.080996	-3.300575	-1.102953	H	4.111324	-3.277031	-1.119899
C	5.122929	-3.100804	2.123423	C	5.124406	-3.105341	2.116441

H	4.619738	-1.511193	3.489820	H	4.594839	-1.536850	3.496156
H	5.450213	-4.531843	0.548465	H	5.482108	-4.512818	0.527703
H	5.721680	-3.640478	2.848219	H	5.724892	-3.645882	2.839316
H	0.294587	-0.959307	0.081578	H	0.291479	-0.962469	0.075511
C	4.456840	1.247700	-1.519444	C	4.459241	1.257102	-1.515745
N	5.534701	1.532869	-1.846395	N	5.532204	1.553290	-1.844256
H	-1.838808	-1.911682	-3.002368	H	-1.838219	-1.910482	-3.002952
N	-5.184930	-2.026164	0.166390	N	-5.191046	-2.018103	0.159986
C	-6.397019	-1.290033	-0.219931	C	-6.397721	-1.294171	-0.256218
H	-6.676257	-1.486099	-1.267709	H	-6.666391	-1.509424	-1.303676
H	-7.226853	-1.597881	0.421011	H	-7.235544	-1.588778	0.381433
H	-6.250774	-0.217052	-0.101684	H	-6.252307	-0.218695	-0.158258
C	-5.380844	-3.467950	0.029569	C	-5.376455	-3.461970	0.060709
H	-6.198117	-3.771065	0.688445	H	-6.197010	-3.754519	0.720939
H	-5.645104	-3.781403	-0.993157	H	-5.629630	-3.807444	-0.955609
H	-4.477666	-3.998508	0.334588	H	-4.472312	-3.976924	0.388621
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1-D-13-A-1P234-vac				1-D-13-A-1P234-CCl4			
C	-5.318457	-0.236886	-0.270490	C	-5.314603	-0.253459	-0.256397
C	-4.327582	-0.898346	-1.002093	C	-4.324648	-0.913594	-0.990553
H	-4.576011	-1.767712	-1.598224	H	-4.573524	-1.786514	-1.581152
C	-5.007648	0.948885	0.361219	C	-5.006046	0.937300	0.367569
H	-5.782432	1.524040	0.857174	H	-5.781277	1.511025	0.864250
C	-3.015432	-0.428244	-1.013599	C	-3.014811	-0.436450	-1.009761
C	-3.696419	1.470895	0.333500	C	-3.696987	1.464993	0.332127
C	-2.635179	0.724257	-0.261397	C	-2.635051	0.720107	-0.263283
C	-3.448581	2.800862	0.808051	C	-3.452970	2.798222	0.800220
H	-4.266458	3.350332	1.261097	H	-4.271545	3.346269	1.253374
C	-2.248886	3.391972	0.586570	C	-2.255732	3.392879	0.573169
H	-2.091724	4.435864	0.836071	H	-2.101479	4.438382	0.817244
C	-1.143383	2.652756	0.050217	C	-1.148704	2.654121	0.038538
C	-1.279058	1.246844	-0.185385	C	-1.280771	1.247064	-0.192099
C	0.075480	3.310115	-0.217538	C	0.068785	3.313579	-0.231969
H	0.141643	4.379906	-0.051949	H	0.132263	4.384101	-0.070785
C	1.145179	2.607251	-0.730067	C	1.140815	2.611021	-0.740926
H	2.048157	3.122340	-1.038626	H	2.042294	3.127720	-1.051008
C	1.082426	1.210412	-0.768434	C	1.081244	1.213478	-0.773573
C	-0.067287	0.499774	-0.362109	C	-0.067476	0.501990	-0.366110
C	1.465112	-1.317122	-0.720282	C	1.465085	-1.315556	-0.721684
H	-6.330645	-0.623231	-0.256238	H	-6.324580	-0.644753	-0.234822
C	3.815306	0.299115	-0.306844	C	3.816283	0.301699	-0.305083
C	4.845207	0.397293	1.885329	C	4.837663	0.428564	1.890045
C	5.065963	0.539451	-0.886149	C	5.073563	0.507790	-0.883794
C	6.089316	0.638293	1.297740	C	6.088886	0.634160	1.303219
C	6.198885	0.708824	-0.087817	C	6.205982	0.673238	-0.083387
H	5.153859	0.592996	-1.966169	H	5.168135	0.538553	-1.964064
H	7.162121	0.893872	-0.550209	H	7.174302	0.831578	-0.544935
P	2.363630	0.100525	-1.448247	P	2.365533	0.103367	-1.446658
C	0.230140	-0.940370	-0.142932	C	0.230551	-0.937631	-0.143623
C	-0.470418	-1.912439	0.625767	C	-0.470011	-1.908371	0.628326
C	-0.003835	-3.235511	0.602592	C	-0.007508	-3.233763	0.598838
C	1.150574	-3.600743	-0.085061	C	1.145658	-3.600040	-0.090853
C	1.913484	-2.633037	-0.727019	C	1.911809	-2.632370	-0.730668
H	-0.536330	-3.993993	1.160528	H	-0.540601	-3.992505	1.155706

H	1.473518	-4.635887	-0.076351	H	1.466122	-4.636008	-0.084315
H	2.844934	-2.896734	-1.214882	H	2.843485	-2.897175	-1.217547
C	3.716650	0.228526	1.089700	C	3.709588	0.263080	1.092388
H	6.967433	0.768527	1.920473	H	6.966348	0.762054	1.927260
H	4.757404	0.340061	2.964864	H	4.743790	0.396579	2.970041
H	2.755515	0.037109	1.553302	H	2.743209	0.100574	1.556252
N	-1.592814	-1.557208	1.408307	N	-1.584882	-1.551552	1.417470
C	-2.510380	-2.616699	1.797223	C	-1.320384	-0.616304	2.512912
H	-3.431108	-2.159674	2.167894	H	-2.258585	-0.161304	2.839966
H	-2.762177	-3.234438	0.934287	H	-0.862621	-1.127372	3.375446
H	-2.116077	-3.269037	2.594665	H	-0.651441	0.179111	2.193076
C	-1.333491	-0.632015	2.512249	C	-2.496581	-2.611262	1.822934
H	-2.273351	-0.179743	2.839099	H	-3.411616	-2.153166	2.205428
H	-0.878125	-1.148751	3.373210	H	-2.760572	-3.232486	0.966229
H	-0.664591	0.166904	2.200686	H	-2.089713	-3.259430	2.616682
C	-2.141891	-1.072231	-1.947725	C	-2.146536	-1.074634	-1.952288
N	-1.539297	-1.603067	-2.779491	N	-1.551967	-1.599138	-2.794306

1-D-13-A-1P234-DCM				1-D-13-A-1P234-DMSO			
C	-5.308799	-0.283257	-0.242866	C	-5.306505	-0.299203	-0.235329
C	-4.317939	-0.940339	-0.978611	C	-4.315001	-0.955275	-0.971052
H	-4.564451	-1.818864	-1.561711	H	-4.559839	-1.837128	-1.549760
C	-5.006375	0.914382	0.371514	C	-5.007276	0.902119	0.373641
H	-5.783584	1.484415	0.868950	H	-5.785427	1.470567	0.871179
C	-3.011908	-0.452305	-1.006121	C	-3.010891	-0.461897	-1.002855
C	-3.701219	1.451864	0.327341	C	-3.704180	1.444522	0.324891
C	-2.636504	0.710922	-0.267251	C	-2.637928	0.705435	-0.268928
C	-3.464731	2.789658	0.787054	C	-3.471759	2.784705	0.779930
H	-4.285288	3.334352	1.240252	H	-4.293367	3.327601	1.233224
C	-2.271713	3.391070	0.553581	C	-2.281074	3.389622	0.542922
H	-2.123521	4.438742	0.791395	H	-2.136088	4.438377	0.777590
C	-1.160985	2.655149	0.021741	C	-1.168446	2.655389	0.012341
C	-1.285743	1.246271	-0.201649	C	-1.289025	1.245441	-0.206938
C	0.053562	3.319221	-0.252946	C	0.044129	3.322324	-0.265046
H	0.112068	4.390820	-0.098001	H	0.099706	4.394486	-0.113365
C	1.129737	2.618718	-0.757039	C	1.122551	2.623389	-0.766835
H	2.028453	3.138811	-1.069322	H	2.019708	3.145424	-1.080308
C	1.077008	1.220200	-0.781191	C	1.073939	1.224447	-0.786492
C	-0.069009	0.505992	-0.371151	C	-0.070151	0.508173	-0.374649
C	1.466219	-1.309998	-0.722882	C	1.467790	-1.305734	-0.725081
H	-6.315048	-0.682888	-0.212549	H	-6.310848	-0.702972	-0.200508
C	3.815814	0.310227	-0.303744	C	3.814599	0.316579	-0.303075
C	4.823922	0.490038	1.894144	C	4.814621	0.522927	1.896232
C	5.083497	0.451541	-0.879710	C	5.087383	0.423629	-0.875379
C	6.086173	0.628654	1.310417	C	6.082204	0.626126	1.316441
C	6.215070	0.608920	-0.076014	C	6.217668	0.576046	-0.068786
H	5.188075	0.439086	-1.959333	H	5.197460	0.388641	-1.953926
H	7.191495	0.716680	-0.534836	H	7.198117	0.657024	-0.524420
P	2.366680	0.111592	-1.445505	P	2.367334	0.117776	-1.446258
C	0.232516	-0.932046	-0.142881	C	0.234553	-0.928812	-0.143390
C	-0.465711	-1.901433	0.634876	C	-0.460900	-1.898141	0.637877
C	-0.006388	-3.229140	0.598283	C	-0.001644	-3.226498	0.598126
C	1.144939	-3.595547	-0.094894	C	1.148183	-3.592058	-0.098100
C	1.912873	-2.627349	-0.733993	C	1.915518	-2.622975	-0.737583
H	-0.538095	-3.988391	1.155545	H	-0.531310	-3.986277	1.156500

H	1.464332	-4.631887	-0.089584	H	1.468123	-4.628245	-0.093351
H	2.845090	-2.892570	-1.219781	H	2.847927	-2.887536	-1.223469
C	3.696534	0.331286	1.093390	C	3.688351	0.368364	1.092769
H	6.962708	0.751664	1.936576	H	6.957688	0.746004	1.944595
H	4.720662	0.505415	2.973543	H	4.706167	0.562760	2.974444
H	2.721747	0.222759	1.555670	H	2.709491	0.288081	1.552305
N	-1.571224	-1.543774	1.431913	N	-1.561979	-1.541185	1.438768
C	-2.474394	-2.603925	1.858819	C	-2.459708	-2.602027	1.876751
H	-3.383071	-2.144833	2.254157	H	-3.366100	-2.143098	2.277152
H	-2.752011	-3.230950	1.010742	H	-2.742638	-3.233200	1.033534
H	-2.052014	-3.245165	2.649160	H	-2.029430	-3.238397	2.666377
C	-1.303999	-0.592250	2.514135	C	-1.295726	-0.579803	2.513196
H	-2.241138	-0.132412	2.836543	H	-2.232908	-0.116573	2.830228
H	-0.846497	-1.093458	3.381847	H	-0.840667	-1.074831	3.385370
H	-0.633406	0.197102	2.183620	H	-0.623106	0.205536	2.177666
C	-2.145483	-1.082820	-1.954425	C	-2.144881	-1.089993	-1.952442
N	-1.551417	-1.598303	-2.803038	N	-1.549596	-1.602216	-2.802500
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1-D-13-A-1P234-N-HEXANE				3-D-13-A-1P234-vac			
C	-5.315481	-0.249708	-0.258919	C	5.447360	1.375586	0.505139
C	-4.325429	-0.910241	-0.992563	C	4.439511	1.779488	-0.375347
H	-4.574350	-1.782438	-1.584235	H	4.525016	2.715289	-0.913683
C	-5.006302	0.940070	0.366493	C	5.393658	0.109845	1.052379
H	-5.781372	1.514238	0.862966	H	6.215524	-0.259393	1.656704
C	-3.015078	-0.434618	-1.010315	C	3.333862	0.963803	-0.615872
C	-3.696741	1.466476	0.332529	C	4.303489	-0.750029	0.803001
C	-2.635029	0.721112	-0.262783	C	3.175035	-0.283684	0.062645
C	-3.451849	2.799056	0.801856	C	4.368831	-2.128317	1.193455
H	-4.270257	3.347483	1.254925	H	5.235287	-2.467898	1.750184
C	-2.254059	3.392879	0.575890	C	3.419502	-3.003601	0.778497
H	-2.099103	4.438065	0.820971	H	3.523727	-4.065074	0.976451
C	-1.147424	2.653893	0.040928	C	2.227833	-2.553805	0.118804
C	-1.280330	1.247068	-0.190709	C	2.014275	-1.152204	-0.069139
C	0.070384	3.312858	-0.228998	C	1.251446	-3.485531	-0.292948
H	0.134445	4.383229	-0.066904	H	1.452627	-4.544122	-0.170119
C	1.141907	2.610182	-0.738672	C	0.066205	-3.055215	-0.854489
H	2.043724	3.126504	-1.048427	H	-0.655067	-3.772370	-1.230806
C	1.081578	1.212785	-0.772526	C	-0.236748	-1.689974	-0.838476
C	-0.067392	0.501512	-0.365340	C	0.678839	-0.731817	-0.360696
C	1.465085	-1.315959	-0.721492	C	-1.298097	0.629994	-0.581391
H	-6.325954	-0.639891	-0.238793	H	6.291789	2.026419	0.697535
C	3.816158	0.301028	-0.305410	C	-3.088898	-1.616344	-0.291760
C	4.839349	0.421381	1.889164	C	-3.970074	-2.173690	1.896684
C	5.072021	0.514863	-0.884290	C	-4.241388	-2.155369	-0.873715
C	6.089054	0.634984	1.302132	C	-5.116576	-2.710648	1.306259
C	6.204544	0.681183	-0.084308	C	-5.251566	-2.700967	-0.078859
H	5.165196	0.550813	-1.964536	H	-4.349063	-2.147582	-1.953310
H	7.171772	0.845558	-0.546067	H	-6.139419	-3.115552	-0.543452
P	2.365217	0.102689	-1.446982	P	-1.793425	-0.919880	-1.425916
C	0.230444	-0.938252	-0.143601	C	0.029541	0.567961	-0.108190
C	-0.470164	-1.909282	0.627622	C	0.491786	1.659634	0.638613
C	-0.006903	-3.234218	0.599337	C	-0.305459	2.772702	0.852595
C	1.146508	-3.600292	-0.089962	C	-1.617583	2.859891	0.327930
C	1.912077	-2.632608	-0.730097	C	-2.095539	1.751223	-0.402321

H	-0.539951	-3.992927	1.156322	H	0.101343	3.586562	1.436077
H	1.467399	-4.636118	-0.083115	H	-3.098190	1.753553	-0.807591
H	2.843677	-2.897206	-1.217217	C	-2.963706	-1.630420	1.104620
C	3.711182	0.255165	1.091918	H	-5.899283	-3.133326	1.926479
H	6.966648	0.763393	1.925905	H	-3.862449	-2.179478	2.975952
H	4.746763	0.383660	2.969101	H	-2.078022	-1.213378	1.570587
H	2.745941	0.086115	1.555781	H	1.482209	1.651276	1.074322
N	-1.586564	-1.552772	1.415469	N	-2.410028	3.976477	0.548898
C	-2.499358	-2.612499	1.817686	C	-3.654398	4.122493	-0.190965
H	-3.415523	-2.154679	2.197956	H	-4.149720	5.039517	0.125596
H	-2.761001	-3.233023	0.959743	H	-3.496960	4.171248	-1.278120
H	-2.094866	-3.261503	2.612123	H	-4.335394	3.293056	0.018786
C	-1.322894	-0.619734	2.512765	C	-1.811173	5.180311	1.104435
H	-2.261368	-0.165333	2.840028	H	-1.022273	5.597192	0.461587
H	-0.865476	-1.132111	3.374816	H	-2.585946	5.935733	1.229423
H	-0.654024	1.076461	2.194635	H	-1.381398	4.986714	2.091077
C	-2.146036	-1.074118	-1.951355	C	2.477609	1.373412	-1.688375
N	-1.550510	-1.600146	-2.791633	N	1.884538	1.736586	-2.611755
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3-D-13-A-1P234-CCl4				3-D-13-A-1P234-DCM			
C	5.444564	1.382982	0.512972	C	-5.442924	1.390973	-0.517322
C	4.439885	1.784923	-0.372124	C	-4.440720	1.790870	0.371493
H	4.527245	2.720910	-0.909737	H	-4.529253	2.727143	0.908290
C	5.391025	0.116626	1.059584	C	-5.390000	0.124386	-1.064112
H	6.211283	-0.250872	1.666879	H	-6.209049	-0.240767	-1.674126
C	3.336649	0.966228	-0.615271	C	-3.339552	0.969228	0.615926
C	4.303166	-0.745649	0.806423	C	-4.304099	-0.740366	-0.808604
C	3.176322	-0.281518	0.062672	C	-3.178503	-0.278772	-0.061996
C	4.369946	-2.123870	1.197784	C	-4.372447	-2.118210	-1.201971
H	5.235429	-2.461636	1.756881	H	-5.237067	-2.453643	-1.763467
C	3.422677	-3.000895	0.780821	C	-3.427088	-2.997440	-0.784363
H	3.527924	-4.062083	0.979094	H	-3.533474	-4.058150	-0.983842
C	2.231425	-2.552204	0.118773	C	-2.235949	-2.550251	-0.120249
C	2.016692	-1.150776	-0.071017	C	-2.019985	-1.149131	0.072447
C	1.256326	-3.485474	-0.293636	C	-1.262047	-3.485521	0.292056
H	1.458411	-4.543746	-0.170305	H	-1.465270	-4.543298	0.167422
C	0.070565	-3.056387	-0.855969	C	-0.075599	-3.058442	0.855236
H	-0.649388	-3.774967	-1.232014	H	0.642907	-3.778936	1.230321
C	-0.233807	-1.691101	-0.840665	C	0.230487	-1.692992	0.841340
C	0.680893	-0.731150	-0.364014	C	-0.683374	-0.730962	0.366545
C	-1.298125	0.629230	-0.584486	C	1.297776	0.628129	0.588040
H	6.286723	2.035456	0.708718	H	-6.282851	2.045150	-0.715808
C	-3.089168	-1.619790	-0.292381	C	3.090132	-1.623457	0.293461
C	-3.961980	-2.193003	1.895832	C	3.954728	-2.213898	-1.893906
C	-4.252744	-2.136360	-0.873171	C	4.265163	-2.115329	0.873074
C	-5.120201	-2.706779	1.306791	C	5.125065	-2.702274	-1.306340
C	-5.264856	-2.677939	-0.077495	C	5.279454	-2.652519	0.076711
H	-4.368571	-2.115012	-1.951660	H	4.389435	-2.078951	1.950108
H	-6.161378	-3.074705	-0.540826	H	6.184939	-3.029845	0.538582
P	-1.792924	-0.923668	-1.424622	P	1.792071	-0.928710	1.422384
C	0.030993	0.568810	-0.113223	C	-0.032521	0.569336	0.118088
C	0.492557	1.663021	0.631391	C	-0.493589	1.666249	-0.624245
C	-0.305894	2.775411	0.845835	C	0.305658	2.778430	-0.838041
C	-1.620737	2.860339	0.324322	C	1.622953	2.861528	-0.318483

C	-2.097754	1.748881	-0.405124	C	2.099281	1.747158	0.410081
H	0.100581	3.590374	1.427981	H	-0.100055	3.594040	-1.419791
H	-3.101531	1.749488	-0.807563	H	3.104335	1.745709	0.809488
C	-2.953912	-1.653161	1.102982	C	2.944491	-1.678056	-1.100464
H	-5.904178	-3.126533	1.927279	H	5.910541	-3.118837	-1.926899
H	-3.846618	-2.213890	2.974041	H	3.831645	-2.251483	-2.970706
H	-2.059537	-1.254686	1.568671	H	2.040787	-1.300430	-1.565703
H	1.483377	1.657374	1.066341	H	-1.484454	1.663022	-1.059084
N	-2.413707	3.972449	0.547023	N	2.415394	3.969928	-0.541449
C	-3.666468	4.113843	-0.182106	C	3.679321	4.104824	0.171531
H	-4.161113	5.029323	0.138580	H	4.171297	5.020435	-0.151350
H	-3.517051	4.163229	-1.269850	H	3.542650	4.150717	1.260647
H	-4.342620	3.282008	0.033208	H	4.350358	3.271708	-0.054542
C	-1.821097	5.176311	1.112833	C	1.831353	5.170911	-1.125458
H	-1.033285	5.599323	0.473568	H	1.039325	5.600439	-0.496820
H	-2.599521	5.927120	1.239375	H	2.612844	5.918248	-1.249774
H	-1.392671	4.978397	2.099037	H	1.411202	4.965250	-2.113539
C	2.487428	1.370195	-1.694763	C	-2.495118	1.366946	1.700280
N	1.901440	1.726934	-2.625564	N	-1.910526	1.715080	2.635777
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3-D-13-A-1P234-DMSO				3-D-13-A-1P234-N-HEXANE			
C	5.442552	1.395380	0.516090	C	5.444914	1.381926	0.511799
C	4.441103	1.793365	-0.374415	C	4.439704	1.784139	-0.372560
H	4.529803	2.729148	-0.911986	H	4.526735	2.720069	-0.910346
C	5.390244	0.129367	1.064525	C	5.391364	0.115677	1.058517
H	6.209051	-0.233844	1.675897	H	6.211896	-0.252112	1.665321
C	3.340840	0.970116	-0.618089	C	3.336097	0.965928	-0.615324
C	4.305155	-0.736839	0.809475	C	4.303156	-0.746218	0.805956
C	3.179916	-0.277177	0.061486	C	3.176037	-0.281750	0.062732
C	4.374152	-2.114099	1.205190	C	4.369715	-2.124448	1.197148
H	5.238349	-2.447961	1.768112	H	5.235353	-2.462509	1.755878
C	3.429605	-2.994775	0.788360	C	3.422146	-3.001195	0.780465
H	3.536543	-4.055051	0.989541	H	3.527243	-4.062430	0.978693
C	2.238416	-2.548983	0.123077	C	2.230852	-2.552381	0.118737
C	2.021907	-1.148194	-0.072035	C	2.016261	-1.150932	-0.070710
C	1.264945	-3.485402	-0.288384	C	1.255602	-3.485411	-0.293618
H	1.468588	-4.542864	-0.162269	H	1.457561	-4.543737	-0.170376
C	0.078203	-3.059659	-0.852264	C	0.069950	-3.056142	-0.855879
H	-0.639720	-3.781264	-1.226300	H	-0.650190	-3.774487	-1.232031
C	-0.228677	-1.694108	-0.839933	C	-0.234236	-1.690893	-0.840454
C	0.684875	-0.730935	-0.366511	C	0.680540	-0.731221	-0.363527
C	-1.297128	0.627505	-0.589036	C	-1.298148	0.629301	-0.584127
H	6.281501	2.050588	0.714837	H	6.287449	2.034144	0.706975
C	-3.090869	-1.624892	-0.294521	C	-3.088901	-1.619268	-0.292297
C	-3.952816	-2.224881	1.891410	C	-3.962917	-2.189690	1.896070
C	-4.271481	-2.103230	-0.874257	C	-4.250605	-2.139838	-0.873166
C	-5.129014	-2.699404	1.303892	C	-5.119168	-2.707560	1.306907
C	-5.287481	-2.638128	-0.078388	C	-5.262300	-2.682109	-0.077526
H	-4.399213	-2.058427	-1.950519	H	-4.365102	-2.120903	-1.951859
H	-6.197331	-3.004897	-0.540060	H	-6.157368	-3.082029	-0.540996
P	-1.790948	-0.931223	-1.420767	P	-1.792937	-0.923054	-1.425103
C	0.033592	0.569565	-0.119520	C	0.030664	0.568647	-0.112409
C	0.494604	1.667882	0.621452	C	0.492194	1.662340	0.632774
C	-0.304913	2.780063	0.834513	C	-0.306142	2.774770	0.847146

C	-1.623293	2.862261	0.315695	C	-1.620419	2.860081	0.324884
C	-2.099333	1.746570	-0.412389	C	-2.097477	1.749144	-0.404782
H	0.100512	3.596060	1.415912	H	0.100242	3.589514	1.429661
H	-3.105101	1.743857	-0.810110	H	-3.100987	1.750043	-0.807881
C	-2.940838	-1.691119	1.098541	C	-2.955247	-1.649233	1.103250
H	-5.915733	-3.114370	1.923859	H	-5.902850	-3.127841	1.927437
H	-3.826515	-2.271710	2.967427	H	-3.848768	-2.207897	2.974472
H	-2.032504	-1.324858	1.563958	H	-2.062347	-1.247438	1.568895
H	1.485484	1.665784	1.056207	H	1.482896	1.656186	1.067968
N	-2.415370	3.969184	0.538014	N	-2.413342	3.972996	0.547191
C	-3.684499	4.100408	-0.167022	C	-3.664809	4.115057	-0.183559
H	-4.173293	5.018505	0.152915	H	-4.159739	5.030656	0.136586
H	-3.554320	4.139603	-1.256996	H	-3.514174	4.164500	-1.271212
H	-4.354710	3.268945	0.067867	H	-4.341603	3.283471	0.030800
C	-1.837246	5.167137	1.135078	C	-1.819804	5.176783	1.111505
H	-1.042601	5.602442	0.514152	H	-1.031394	5.598580	0.472031
H	-2.620897	5.911868	1.259807	H	-2.597535	5.928530	1.237320
H	-1.422180	4.954838	2.123869	H	-1.391721	4.979629	2.098051
C	2.497725	1.363077	-1.704614	C	2.485757	1.370871	-1.693759
N	1.912089	1.704634	-2.642167	N	1.899027	1.728953	-2.623478
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2-D-10-A-12P34-vacuum				2-D-10-A-12P34-CCl4			
C	-2.834334	-2.529415	0.403321	C	-2.828256	-2.538643	0.404635
C	-2.560473	-3.813090	-0.160820	C	-2.549014	-3.821674	-0.160771
H	-3.243924	-4.635791	-0.005969	H	-3.229142	-4.647032	-0.005772
C	-1.924590	-1.500945	0.154938	C	-1.920851	-1.506210	0.157051
H	-2.086230	-0.535834	0.604110	H	-2.087266	-0.542365	0.607292
C	-1.410200	-4.031979	-0.869973	C	-1.397916	-4.035939	-0.870032
H	-1.199236	-5.027031	-1.248204	H	-1.183017	-5.029999	-1.248598
C	-3.389713	2.127255	-1.014964	C	-3.396581	2.117530	-1.013065
C	-2.307016	1.278052	-1.065999	C	-2.310006	1.272960	-1.063666
C	-3.261645	3.411160	-0.458611	C	-3.272964	3.402284	-0.458446
H	-4.117885	4.071162	-0.393905	H	-4.132447	4.057899	-0.393587
C	-2.022601	3.852663	-0.028368	C	-2.034202	3.847909	-0.029850
C	-0.863267	3.015378	-0.123115	C	-0.870769	3.015696	-0.123370
C	-1.031697	1.662404	-0.574693	C	-1.035613	1.661644	-0.573420
C	0.435345	3.521567	0.135266	C	0.426361	3.525815	0.134125
H	0.548266	4.540293	0.486058	H	0.539046	4.545018	0.483471
C	1.539026	2.756048	-0.152817	C	1.532508	2.762823	-0.152868
H	2.532068	3.183536	-0.066544	H	2.524087	3.193569	-0.066752
C	1.386268	1.414114	-0.549258	C	1.383062	1.420110	-0.548000
C	0.125798	0.808883	-0.630213	C	0.124211	0.810970	-0.628514
C	1.483462	-1.025485	-1.327989	C	1.486685	-1.019884	-1.326176
C	3.783089	-0.126527	0.142639	C	3.786098	-0.114547	0.143936
C	4.168816	-0.897400	2.406804	C	4.174801	-0.862386	2.415796
C	5.166309	-0.035835	-0.046107	C	5.169442	-0.048861	-0.055746
C	5.548461	-0.805252	2.209546	C	5.554681	-0.796129	2.207613
C	6.046362	-0.375163	0.983171	C	6.051067	-0.390192	0.971938
H	5.556211	0.302117	-1.000358	H	5.559167	0.270881	-1.016259
H	7.116420	-0.300887	0.824474	H	7.120993	-0.335843	0.804839
P	2.685557	0.354871	-1.274352	P	2.685296	0.363571	-1.270984
C	0.209584	-0.648783	-0.889187	C	0.211607	-0.646710	-0.886844
C	-0.760511	-1.685173	-0.629907	C	-0.755974	-1.686098	-0.627231
C	-0.457014	-3.007542	-1.096209	C	-0.447969	-3.007420	-1.095316

C	0.799167	-3.296914	-1.682900	C	0.809044	-3.293143	-1.682004
C	1.777442	-2.335328	-1.753549	C	1.785212	-2.328551	-1.752466
H	0.994966	-4.307957	-2.024995	H	1.007536	-4.303544	-2.024346
H	2.763743	-2.577197	-2.133124	H	2.772152	-2.567715	-2.132081
C	3.291339	-0.561492	1.380972	C	3.295625	-0.525191	1.391316
H	6.229677	-1.068022	3.011183	H	6.237115	-1.059888	3.007822
H	3.778483	-1.231874	3.361728	H	3.785556	-1.177720	3.377590
H	2.221726	-0.638307	1.540870	H	2.226190	-0.582171	1.560636
H	-2.422584	0.303210	-1.517198	H	-2.423126	0.297313	-1.513548
N	-3.978383	-2.326867	1.165975	N	-3.971100	-2.341144	1.165886
C	-4.710681	-3.475983	1.682326	C	-4.709969	-3.492788	1.671356
H	-4.107411	-4.097209	2.360325	H	-4.111132	-4.117540	2.349178
H	-5.581356	-3.118967	2.231058	H	-5.582409	-3.136297	2.216967
H	-5.077668	-4.108840	0.871120	H	-5.072903	-4.120031	0.854311
C	-4.125463	-1.076609	1.896410	C	-4.124102	-1.091927	1.898747
H	-5.104049	-1.058525	2.374927	H	-5.100412	-1.081688	2.381226
H	-3.357139	-0.944565	2.673098	H	-3.353471	-0.957404	2.672097
H	-4.074237	-0.221873	1.218320	H	-4.081021	-0.235778	1.221740
C	-1.900536	5.183779	0.480628	C	-1.918871	5.179961	0.476396
N	-1.809036	6.258967	0.896243	N	-1.835643	6.257166	0.889592
H	-4.345618	1.810477	-1.415259	H	-4.351819	1.796158	-1.410570
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2-D-10-A-12P34-DCM				2-D-10-A-12P34-DMSO			
C	-2.815093	-2.554351	0.406124	C	-2.806685	-2.563286	0.407058
C	-2.526515	-3.836491	-0.159325	C	-2.512991	-3.844955	-0.157810
H	-3.201276	-4.666185	-0.004242	H	-3.184741	-4.677017	-0.002381
C	-1.912709	-1.515553	0.159133	C	-1.907427	-1.521000	0.160005
H	-2.086945	-0.552905	0.609054	H	-2.085998	-0.558875	0.609369
C	-1.373797	-4.043520	-0.868068	C	-1.359423	-4.048100	-0.866281
H	-1.152419	-5.036199	-1.246399	H	-1.134445	-5.040094	-1.244215
C	-3.408983	2.099822	-1.009517	C	-3.415966	2.089406	-1.007386
C	-2.316644	1.262553	-1.060537	C	-2.320586	1.256133	-1.059168
C	-3.292689	3.385839	-0.456855	C	-3.303602	3.376095	-0.455667
H	-4.157045	4.034698	-0.391060	H	-4.170496	4.021353	-0.388901
C	-2.055196	3.838999	-0.031104	C	-2.066912	3.833645	-0.031855
C	-0.885865	3.014485	-0.124213	C	-0.894543	3.013291	-0.125449
C	-1.043722	1.658974	-0.572449	C	-1.048383	1.657002	-0.572710
C	0.408562	3.532209	0.131513	C	0.398358	3.535489	0.128864
H	0.517861	4.552403	0.479013	H	0.505208	4.556273	0.475390
C	1.519170	2.774732	-0.154399	C	1.511417	2.781346	-0.156829
H	2.508114	3.211491	-0.069021	H	2.498869	3.221539	-0.072170
C	1.376476	1.430550	-0.547383	C	1.372697	1.436304	-0.548467
C	0.120776	0.814309	-0.627354	C	0.118863	0.815953	-0.627795
C	1.493073	-1.009745	-1.324474	C	1.496971	-1.004257	-1.324146
C	3.788512	-0.093487	0.145997	C	3.788742	-0.081328	0.147311
C	4.180279	-0.807709	2.428784	C	4.180890	-0.772705	2.437362
C	5.171289	-0.064877	-0.067610	C	5.170794	-0.076424	-0.073345
C	5.559643	-0.779881	2.206485	C	5.559482	-0.769352	2.207866
C	6.054070	-0.409329	0.958449	C	6.053279	-0.422134	0.952687
H	5.560587	0.227850	-1.036774	H	5.560104	0.198538	-1.047648
H	7.123268	-0.384472	0.780558	H	7.121782	-0.416045	0.769295
P	2.684650	0.380084	-1.267509	P	2.684454	0.389359	-1.266705
C	0.215776	-0.643366	-0.884671	C	0.218441	-0.641752	-0.884209
C	-0.746289	-1.688471	-0.624040	C	-0.740265	-1.690141	-0.622663

C	-0.429876	-3.008349	-1.092912	C	-0.419058	-3.009341	-1.091344
C	0.828732	-3.287293	-1.679400	C	0.840446	-3.284434	-1.677695
C	1.799901	-2.316695	-1.750660	C	1.808518	-2.310370	-1.749779
H	1.032851	-4.296670	-2.021373	H	1.047903	-4.293293	-2.019172
H	2.788024	-2.550610	-2.130532	H	2.797330	-2.541271	-2.129737
C	3.299723	-0.468194	1.405624	C	3.300465	-0.432389	1.414078
H	6.243009	-1.045422	3.005206	H	6.242688	-1.035399	3.006506
H	3.792611	-1.094770	3.399958	H	3.793780	-1.041104	3.414054
H	2.231004	-0.494856	1.586985	H	2.232446	-0.439463	1.601530
H	-2.425496	0.285682	-1.508576	H	-2.427124	0.278559	-1.506124
N	-3.958034	-2.364806	1.164260	N	-3.949705	-2.377965	1.163948
C	-4.699378	-3.520657	1.660587	C	-4.691161	-3.536023	1.656330
H	-4.102816	-4.145264	2.339646	H	-4.094867	-4.160681	2.335250
H	-5.575089	-3.167033	2.202043	H	-5.568090	-3.184384	2.196804
H	-5.055174	-4.145653	0.838990	H	-5.044129	-4.160014	0.832808
C	-4.125598	-1.114167	1.893373	C	-4.125950	-1.125940	1.889324
H	-5.101204	-1.114394	2.376539	H	-5.101725	-1.131127	2.371801
H	-3.356024	-0.970160	2.665443	H	-3.357865	-0.975567	2.661435
H	-4.092439	-0.259645	1.213735	H	-4.097473	-0.273239	1.207230
C	-1.948275	5.172148	0.471938	C	-1.964128	5.167346	0.469745
N	-1.871973	6.251180	0.882605	N	-1.890856	6.247320	0.878837
H	-4.363214	1.771318	-1.402845	H	-4.369741	1.756981	-1.398231
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2-D-10-A-12P34-N-HEXANE				2-D-12-A-12P34-VACUUM			
C	-2.829176	-2.537084	0.404413	C	-2.636687	-2.324314	0.537681
C	-2.550838	-3.820213	-0.160762	C	-2.441864	-3.543066	-0.183168
H	-3.231456	-4.645162	-0.005654	H	-3.143247	-4.358374	-0.077737
C	-1.921439	-1.505321	0.156617	C	-1.733987	-1.282214	0.311245
H	-2.086938	-0.541252	0.606701	H	-1.860209	-0.355600	0.844968
C	-1.399920	-4.035251	-0.870069	C	-1.344975	-3.710373	-0.983711
H	-1.185685	-5.029496	-1.248545	H	-1.189393	-4.661729	-1.482109
C	-3.395416	2.119079	-1.013612	C	-3.180061	2.490594	-0.398537
C	-2.309487	1.273731	-1.064184	C	-2.128291	1.614692	-0.608511
C	-3.271103	3.403691	-0.458672	C	-2.962943	3.739000	0.244449
H	-4.130031	4.060076	-0.393943	H	-3.799518	4.403755	0.419554
C	-2.032348	3.848612	-0.029656	C	-1.688527	4.097599	0.593965
C	-0.869592	3.015579	-0.123310	H	-1.502181	5.069551	1.037687
C	-1.034985	1.661714	-0.573671	C	-0.581247	3.241999	0.348013
C	0.427766	3.525034	0.134447	C	-0.812021	1.930618	-0.193572
H	0.540450	4.544127	0.484127	C	0.744204	3.701892	0.549906
C	1.533511	2.761642	-0.152723	H	0.900648	4.689482	0.969591
H	2.525335	3.191829	-0.066481	C	1.807514	2.942807	0.125548
C	1.383564	1.419090	-0.548186	H	2.815470	3.340850	0.172486
C	0.124460	0.810584	-0.628831	C	1.593472	1.639806	-0.364075
C	1.486160	-1.020799	-1.326520	C	0.317247	1.061872	-0.404143
C	3.785556	-0.116473	0.143721	C	1.583857	-0.726102	-1.347220
C	4.173723	-0.868180	2.414296	C	3.993595	0.007908	0.037171
C	5.168910	-0.046429	-0.054087	C	4.507132	-0.975942	2.190833
C	5.553591	-0.797413	2.207985	C	5.363879	0.115134	-0.223562
C	6.050268	-0.387349	0.973882	C	5.873381	-0.865520	1.922347
H	5.558673	0.276480	-1.013538	C	6.300915	-0.320592	0.715215
H	7.120248	-0.329523	0.808225	H	5.699021	0.540518	-1.163565
P	2.685323	0.362159	-1.271577	H	7.360236	-0.232854	0.500944
C	0.211267	-0.647061	-0.887324	P	2.817426	0.623269	-1.260402

C	-0.756730	-1.685946	-0.627825	C	0.350654	-0.369707	-0.789049
C	-0.449468	-3.007422	-1.095595	C	-0.622928	-1.410848	-0.556092
C	0.807405	-3.293720	-1.682302	C	-0.379315	-2.688380	-1.163833
C	1.783917	-2.329641	-1.752738	C	0.827796	-2.942856	-1.857958
H	1.005445	-4.304212	-2.024652	C	1.821494	-1.995639	-1.907050
H	2.770761	-2.569225	-2.132333	H	0.976405	-3.920655	-2.304520
C	3.294840	-0.531296	1.389568	H	2.774917	-2.217237	-2.373038
H	6.235823	-1.060932	3.008459	C	3.572917	-0.543361	1.255250
H	3.784259	-1.186789	3.374932	H	6.598925	-1.204614	2.653344
H	2.225346	-0.591765	1.557251	H	4.171471	-1.401254	3.130289
H	-2.422942	0.298207	-1.514286	H	2.514096	-0.636409	1.469160
N	-3.972229	-2.338806	1.165940	H	-2.318342	0.684238	-1.122200
C	-4.709597	-3.490154	1.673537	N	-3.677798	-2.208010	1.443581
H	-4.109714	-4.114121	2.351310	C	-3.952230	-0.917844	2.058252
H	-5.581716	-3.133769	2.219849	H	-4.280895	-0.162985	1.331129
H	-5.073279	-4.118508	0.857625	H	-4.738371	-1.040187	2.802175
C	-4.124164	-1.089473	1.898492	H	-3.066838	-0.537827	2.575030
H	-5.100765	-1.078020	2.380496	C	-4.750044	-3.194178	1.449119
H	-3.353800	-0.955341	2.672278	H	-5.452285	-2.944103	2.242983
H	-4.079893	-0.233481	1.221376	H	-5.304026	-3.223777	0.500554
C	-1.915999	5.180518	0.477152	H	-4.366432	-4.196538	1.657139
N	-1.831673	6.257338	0.890910	C	-4.497181	2.138484	-0.831379
H	-4.350708	1.798494	-1.411751	N	-5.568684	1.857709	-1.163673
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2-D-12-A-12P34-CCI4				2-D-12-A-12P34-DCM			
C	-2.656032	-2.326043	0.455082	C	-2.643645	-2.337740	0.452322
C	-2.438128	-3.542923	-0.263876	C	-2.422361	-3.549764	-0.275415
H	-3.126599	-4.369301	-0.159228	H	-3.105261	-4.380844	-0.171917
C	-1.742933	-1.284461	0.266052	C	-1.736089	-1.290257	0.264519
H	-1.863938	-0.373993	0.828400	H	-1.859007	-0.383315	0.832221
C	-1.336025	-3.694029	-1.060944	C	-1.322536	-3.691490	-1.077829
H	-1.165536	-4.642659	-1.559607	H	-1.149237	-4.636933	-1.581441
C	-3.201199	2.496604	-0.396927	C	-3.213901	2.487736	-0.400516
C	-2.146694	1.624446	-0.611480	C	-2.155610	1.619128	-0.612376
C	-2.995169	3.732113	0.275014	C	-3.017822	3.722122	0.276906
H	-3.834274	4.392294	0.454588	H	-3.860003	4.378310	0.455883
C	-1.725390	4.085367	0.646083	C	-1.751161	4.079252	0.655314
H	-1.546103	5.047877	1.112286	H	-1.578428	5.040272	1.126558
C	-0.613586	3.237629	0.391441	C	-0.634590	3.237061	0.401267
C	-0.835378	1.936230	-0.177745	C	-0.847933	1.936231	-0.172726
C	0.708592	3.698993	0.612012	C	0.684818	3.704551	0.627221
H	0.858044	4.678423	1.052465	H	0.828265	4.682931	1.071574
C	1.778099	2.953252	0.178502	C	1.759456	2.965737	0.193412
H	2.783560	3.355474	0.239613	H	2.762214	3.373790	0.258496
C	1.572601	1.659220	-0.338612	C	1.561835	1.672123	-0.329109
C	0.299208	1.076596	-0.397952	C	0.291583	1.083390	-0.393540
C	1.578500	-0.688149	-1.368305	C	1.579370	-0.670652	-1.372461
C	3.980730	0.028486	0.040940	C	3.977979	0.045425	0.043146
C	4.490257	-0.979163	2.185071	C	4.489895	-0.933426	2.200642
C	5.351425	0.124289	-0.223317	C	5.346800	0.094059	-0.243968
C	5.857079	-0.880912	1.912962	C	5.854877	-0.884111	1.905178
C	6.286733	-0.329873	0.708877	C	6.282254	-0.371177	0.683050
H	5.689227	0.555020	-1.159844	H	5.684062	0.496595	-1.193044
H	7.346186	-0.251127	0.492085	H	7.339982	-0.329490	0.448655

P	2.805874	0.664600	-1.246976	P	2.801200	0.687075	-1.239411
C	0.341025	-0.346651	-0.810379	C	0.340376	-0.337454	-0.812825
C	-0.631194	-1.394084	-0.602678	C	-0.626812	-1.390383	-0.608712
C	-0.379591	-2.660671	-1.230354	C	-0.370645	-2.652520	-1.244110
C	0.832820	-2.898841	-1.921696	C	0.842382	-2.882052	-1.938015
C	1.823513	-1.946647	-1.950056	C	1.829692	-1.925224	-1.961297
H	0.988112	-3.868661	-2.383095	H	1.001558	-3.848699	-2.404628
H	2.779853	-2.156968	-2.415286	H	2.786707	-2.129646	-2.427854
C	3.557659	-0.528761	1.255749	C	3.556859	-0.473146	1.275948
H	6.581255	-1.233687	2.638744	H	6.579214	-1.244166	2.627094
H	4.152975	-1.408645	3.121985	H	4.154459	-1.331840	3.151760
H	2.498747	-0.612376	1.473257	H	2.499708	-0.517835	1.513017
H	-2.329494	0.703897	-1.145435	H	-2.332287	0.699024	-1.149033
N	-3.740954	-2.200254	1.302958	N	-3.725675	-2.222138	1.305245
C	-4.523454	-3.374512	1.668417	C	-4.483598	-3.409844	1.686696
H	-3.929989	-4.128021	2.204600	H	-3.872957	-4.143428	2.230584
H	-5.342215	-3.062757	2.314618	H	-5.307251	-3.106673	2.330516
H	-4.966114	-3.846590	0.787732	H	-4.916888	-3.900947	0.812649
C	-3.851351	-1.024324	2.153241	C	-3.820360	-1.062877	2.182463
H	-4.791678	-1.068079	2.700007	H	-4.757780	-1.111064	2.733502
H	-3.029757	-0.952273	2.880618	H	-2.993983	-1.014910	2.906051
H	-3.860610	-0.109612	1.555473	H	-3.823886	-0.135479	1.605189
C	-4.509899	2.160547	-0.865129	C	-4.516124	2.148399	-0.882081
N	-5.575200	1.900310	-1.232859	N	-5.575346	1.884940	-1.265717
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2-D-12-A-12P34-DMSO				2-D-12-A-12P34-N-HEXANE			
C	-2.638240	-2.342602	0.451051	C	-2.657560	-2.324217	0.455365
C	-2.414673	-3.553107	-0.278968	C	-2.440035	-3.541882	-0.262123
H	-3.095305	-4.386099	-0.176196	H	-3.129325	-4.367570	-0.157369
C	-1.732959	-1.292646	0.263921	C	-1.743600	-1.283602	0.266328
H	-1.857038	-0.386924	0.833300	H	-1.864273	-0.372588	0.827848
C	-1.315009	-3.691439	-1.082452	C	-1.337462	-3.694454	-1.058154
H	-1.139959	-4.636002	-1.587058	H	-1.167278	-4.643599	-1.555952
C	-3.219978	2.482320	-0.402724	C	-3.199610	2.497235	-0.396506
C	-2.159568	1.615979	-0.613587	C	-2.145420	1.624876	-0.611478
C	-3.028327	3.717069	0.275282	C	-2.992158	3.733227	0.273992
H	-3.872126	4.371114	0.454095	H	-3.830960	4.393810	0.453636
C	-1.762902	4.077104	0.655339	C	-1.721910	4.086411	0.643457
H	-1.593184	5.038104	1.127525	H	-1.541769	5.049381	1.108464
C	-0.644015	3.237594	0.402039	C	-0.610669	3.238013	0.388927
C	-0.853335	1.936367	-0.172593	C	-0.833530	1.936309	-0.179060
C	0.674074	3.708381	0.629631	C	0.711857	3.698745	0.608479
H	0.814665	4.686769	1.074704	H	0.862054	4.678504	1.048017
C	1.751099	2.972358	0.196705	C	1.780706	2.951969	0.175370
H	2.752607	3.383113	0.263237	H	2.786526	3.353435	0.235803
C	1.557240	1.678270	-0.326653	C	1.574236	1.657651	-0.340460
C	0.288514	1.086553	-0.392829	C	0.300457	1.075778	-0.398909
C	1.580799	-0.663778	-1.372793	C	1.578783	-0.690653	-1.367472
C	3.976953	0.054360	0.045129	C	3.981047	0.026446	0.041047
C	4.490884	-0.898141	2.214163	C	4.489833	-0.982499	2.184639
C	5.343452	0.069169	-0.256902	C	5.351877	0.125916	-0.220914
C	5.853422	-0.883650	1.903524	C	5.856764	-0.880419	1.914850
C	6.278555	-0.400877	0.668172	C	6.286875	-0.326878	0.712169
H	5.679562	0.449082	-1.215621	H	5.689839	0.558477	-1.156557

H	7.334345	-0.385644	0.422267	H	7.346477	-0.245239	0.497119
P	2.799741	0.696856	-1.236264	P	2.806826	0.661564	-1.248100
C	0.340845	-0.333822	-0.813413	C	0.341462	-0.347952	-0.809924
C	-0.624089	-1.389239	-0.610328	C	-0.631372	-1.394647	-0.601618
C	-0.365222	-2.650082	-1.247584	C	-0.380344	-2.661934	-1.227984
C	0.848600	-2.876350	-1.941549	C	0.832049	-2.901395	-1.918771
C	1.834112	-1.917297	-1.963146	C	1.823153	-1.949807	-1.947906
H	1.009933	-3.842113	-2.409220	H	0.986911	-3.871723	-2.379260
H	2.791698	-2.119420	-2.429556	H	2.779438	-2.161023	-2.412837
C	3.557930	-0.433700	1.291148	C	3.557569	-0.533351	1.254484
H	6.577603	-1.246592	2.624092	H	6.580706	-1.232276	2.641328
H	4.157271	-1.272106	3.175763	H	4.152188	-1.414048	3.120485
H	2.502822	-0.450445	1.540828	H	2.498501	-0.619980	1.470001
H	-2.333492	0.695425	-1.150268	H	-2.329047	0.704016	-1.144619
N	-3.720609	-2.230679	1.304349	N	-3.743187	-2.196804	1.302272
C	-4.465406	-3.424897	1.695126	C	-4.529393	-3.368870	1.665258
H	-3.845345	-4.147714	2.242407	H	-3.938993	-4.124995	2.201297
H	-5.290819	-3.126017	2.338600	H	-5.348098	-3.055631	2.310872
H	-4.894688	-3.926232	0.825194	H	-4.972555	-3.838712	0.783494
C	-3.811372	-1.076698	2.190145	C	-3.856180	-1.018283	2.148194
H	-4.749076	-1.126112	2.740545	H	-4.797336	-1.061037	2.693695
H	-2.985027	-1.037035	2.914059	H	-3.035830	-0.942739	2.876698
H	-3.811495	-0.145437	1.619467	H	-3.865607	-0.105585	1.547291
C	-4.519773	2.138868	-0.887155	C	-4.509405	2.160705	-0.861675
N	-5.576356	1.870826	-1.275263	N	-5.575685	1.899811	-1.225927
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Singlet optimization coordinates:

C1234-S1-VACUUM				C1234-S1-CCl4			
C	-2.43464500	-3.77479000	-1.01077300	C	-2.45364000	-3.77442600	-1.00784500
C	-1.66769400	-2.87580000	-1.78222500	C	-1.68143700	-2.87924900	-1.77923700
H	-1.17670100	-3.22351500	-2.68445000	H	-1.19048100	-3.22991700	-2.68030000
C	-3.13722100	-3.30604500	0.07572300	C	-3.15366500	-3.30176900	0.07871100
H	-3.78025200	-3.97224700	0.64176700	H	-3.80040100	-3.96396700	0.64519200
C	-1.55722900	-1.55442800	-1.41171600	C	-1.56370700	-1.55818400	-1.40847900
H	-0.99633400	-0.87643700	-2.03926400	H	-0.99495300	-0.88520200	-2.03431100
C	-3.08037900	-1.94249400	0.45324900	C	-3.08965700	-1.93745600	0.45525200
C	-2.20480700	-1.04854400	-0.25076200	C	-2.20941700	-1.04809900	-0.24888000
C	-3.93769800	-1.42854600	1.46323100	C	-3.94662900	-1.41951700	1.46355900
H	-4.58543900	-2.11193600	2.00172400	H	-4.59767500	-2.09974700	2.00196900
C	-3.99878800	-0.08138600	1.69267200	C	-4.00368100	-0.07090100	1.69032800
H	-4.71491800	0.32113800	2.40155500	H	-4.72001800	0.33521000	2.39692700
C	-3.12570200	0.82660000	1.03073400	C	-3.12682500	0.83265100	1.02817000
C	-2.11106100	0.33442600	0.16530700	C	-2.11115400	0.33689700	0.16524400
C	-3.28569300	2.23572700	1.21317200	C	-3.28434600	2.24364300	1.21029400
H	-4.10152500	2.58423900	1.83719500	H	-4.10031300	2.59393300	1.83304100
C	-2.48033300	3.13180600	0.56095600	C	-2.47620300	3.13638600	0.55896300
H	-2.66735500	4.19752100	0.64192500	H	-2.66024000	4.20271700	0.63832300
C	-1.36071400	2.69420000	-0.18134700	C	-1.35530200	2.69467100	-0.18209400
C	-1.08749800	1.25983500	-0.26943600	C	-1.08425200	1.25830200	-0.26811600
C	-0.47715900	3.63260600	-0.76174100	C	-0.47208600	3.63100800	-0.76336300
H	-0.75385900	4.68107500	-0.72315800	H	-0.74657400	4.68002500	-0.72521900
C	0.73979300	3.26381000	-1.31950400	C	0.74526800	3.25926500	-1.32232900
H	1.40869300	4.00750600	-1.73616500	H	1.41474000	4.00182500	-1.74015000

C	1.14893200	1.91524300	-1.20923100	C	1.15267300	1.91111400	-1.21066900
C	0.24784500	0.90814000	-0.63842600	C	0.25116200	0.90414600	-0.63867000
C	2.35836800	1.31220400	-1.50294900	C	2.36278300	1.30818600	-1.50435800
H	3.21810300	1.80930100	-1.93493500	H	3.22163000	1.80500100	-1.93833800
H	-2.50211200	-4.81773900	-1.29887900	H	-2.52612200	-4.81709800	-1.29572600
C	0.98126600	-0.26737300	-0.50751900	C	0.98370400	-0.27110600	-0.50797200
C	3.47828900	-0.45850300	-0.07796600	C	3.48321700	-0.46119400	-0.07579900
C	3.54122500	0.21836800	1.14791200	C	3.54322800	0.20894600	1.15390600
C	4.44448600	-1.42795300	-0.36261100	C	4.45446100	-1.42406800	-0.36680200
C	4.54784500	-0.07012900	2.06578400	C	4.55188600	-0.07979200	2.07012000
H	2.79561100	0.97135500	1.37824500	H	2.79451300	0.95707300	1.39016500
C	5.45304900	-1.71755600	0.55426300	C	5.46534800	-1.71377700	0.54821600
H	4.40408900	-1.95971600	-1.30828000	H	4.41676200	-1.95067000	-1.31537100
C	5.50727000	-1.03871100	1.77170500	C	5.51662100	-1.04179900	1.76989900
H	4.58350600	0.46017000	3.01096800	H	4.58503900	0.44521600	3.01834200
H	6.19523300	-2.47287100	0.32024200	H	6.21128700	-2.46377100	0.30918300
H	6.29125200	-1.26392500	2.48590900	H	6.30204800	-1.26702300	2.48249100
H	0.64362600	-1.17276300	-0.02503500	H	0.64497900	-1.17826800	-0.02951800
C	2.36855100	-0.13239500	-1.07983400	C	2.37246300	-0.13565100	-1.07786200
H	2.51660000	-0.81102500	-1.94137300	H	2.52091000	-0.81468300	-1.93783900
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C1234-S1-DCM				C1234-S1-DMSO			
C	-2.46611100	-3.77630100	-1.00455900	C	-2.46476200	-3.77874800	-1.00342300
C	-1.68873200	-2.88427200	-1.77509900	C	-1.68615700	-2.88692100	-1.77319900
H	-1.19538100	-3.23765600	-2.67369900	H	-1.19057700	-3.24075100	-2.67034200
C	-3.16592700	-3.30029300	0.08086200	C	-3.16602700	-3.30236900	0.08100000
H	-3.81598800	-3.95929300	0.64715700	H	-3.81669800	-3.96110800	0.64683400
C	-1.56627900	-1.56311800	-1.40451600	C	-1.56418100	-1.56547400	-1.40282200
H	-0.98897000	-0.89520700	-2.02790100	H	-0.98401200	-0.89888700	-2.02495500
C	-3.09711900	-1.93499500	0.45609500	C	-3.09764200	-1.93657000	0.45567600
C	-2.21245700	-1.04921600	-0.24739000	C	-2.21207200	-1.05092900	-0.24708700
C	-3.95548100	-1.41396200	1.46176200	C	-3.95779000	-1.41549500	1.45988000
H	-4.60955200	-2.09160700	1.99963700	H	-4.61240700	-2.09298000	1.99724400
C	-4.01019200	-0.06388900	1.68585900	C	-4.01347700	-0.06495700	1.68303500
H	-4.72778500	0.34495900	2.38950600	H	-4.73240300	0.34392600	2.38524000
C	-3.12998400	0.83623800	1.02440400	C	-3.13279800	0.83508500	1.02241000
C	-2.11177800	0.33814800	0.16468100	C	-2.11253800	0.33746400	0.16432700
C	-3.28683800	2.24896900	1.20678500	C	-3.29123000	2.24826500	1.20510500
H	-4.10379300	2.59971700	1.82783900	H	-4.10932500	2.59804400	1.82515500
C	-2.47620900	3.13947000	0.55769500	C	-2.48027000	3.13903500	0.55764200
H	-2.65812000	4.20620700	0.63592000	H	-2.66257300	4.20570100	0.63564100
C	-1.35280000	2.69500500	-0.18152000	C	-1.35494700	2.69501400	-0.18037100
C	-1.08228800	1.25683600	-0.26628800	C	-1.08293100	1.25648700	-0.26501700
C	-0.47086400	3.63059600	-0.76242600	C	-0.47423200	3.63148000	-0.76028400
H	-0.74427900	4.67980200	-0.72376700	H	-0.74838600	4.68043700	-0.72105600
C	0.74766700	3.25785200	-1.32252700	C	0.74538600	3.25998000	-1.32048500
H	1.41666600	4.00042700	-1.74107900	H	1.41338500	4.00358400	-1.73880900
C	1.15496300	1.91061700	-1.20999800	C	1.15410500	1.91346500	-1.20808200
C	0.25394400	0.90207600	-0.63810700	C	0.25414600	0.90315300	-0.63689100
C	2.36676900	1.30958800	-1.50388300	C	2.36721600	1.31447000	-1.50216200
H	3.22372000	1.80726800	-1.94051200	H	3.22286000	1.81332100	-1.93997500
H	-2.54144300	-4.81894200	-1.29169000	H	-2.53936800	-4.82153700	-1.29011800
C	0.98694700	-0.27225700	-0.50896500	C	0.98850100	-0.27021800	-0.50880900
C	3.48862300	-0.46079000	-0.07452900	C	3.49096600	-0.45790500	-0.07464900

C	3.54977800	0.20542400	1.15733900	C	3.55678500	0.20985200	1.15620400
C	4.46029900	-1.42228500	-0.37000900	C	4.45842600	-1.42374700	-0.37029800
C	4.55980100	-0.08568600	2.07201600	C	4.56720000	-0.08381000	2.06991900
H	2.80178900	0.95300800	1.39791100	H	2.81257300	0.96112400	1.39718800
C	5.47264400	-1.71452500	0.54341900	C	5.47104300	-1.71880500	0.54225100
H	4.42251500	-1.94552300	-1.32027300	H	4.41745000	-1.94793800	-1.31982600
C	5.52502900	-1.04657100	1.76761000	C	5.52812500	-1.04926500	1.76550000
H	4.59386500	0.43664400	3.02168400	H	4.60506700	0.44011800	3.01856600
H	6.21876000	-2.46312000	0.30074700	H	6.21380300	-2.47063500	0.29936300
H	6.31142300	-1.27353400	2.47854700	H	6.31478000	-1.27823700	2.47548600
H	0.64748000	-1.18322500	-0.03830200	H	0.64948700	-1.18348900	-0.04229000
C	2.37711000	-0.13405900	-1.07630800	C	2.37891900	-0.12946200	-1.07554700
H	2.52599800	-0.81152200	-1.93614500	H	2.52774900	-0.80514700	-1.93629800
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C1234-S1-n-hexane				1C234-S1-VACUUM			
C	-2.45018100	-3.77444200	-1.00841900	C	5.54555500	0.97299300	-0.30018800
C	-1.67900800	-2.87853600	-1.77985800	C	4.42256400	1.68257100	-0.78125200
H	-1.18815100	-3.22863200	-2.68120800	H	4.56256500	2.66587400	-1.21816000
C	-3.15060600	-3.30253300	0.07817900	C	5.37713400	-0.31595300	0.18259000
H	-3.79663300	-3.96548200	0.64460200	H	6.23536400	-0.89621000	0.50588900
C	-1.56259700	-1.55742500	-1.40912700	C	3.15564700	1.14556300	-0.72498500
H	-0.99540400	-0.88345500	-2.03532000	H	2.32454600	1.69453200	-1.14461700
C	-3.08791300	-1.93836900	0.45491800	C	4.10509300	-0.91365200	0.23239800
C	-2.20858100	-1.04814900	-0.24921900	C	2.92941100	-0.15831700	-0.16980000
C	-3.94491000	-1.42118100	1.46357300	C	3.93784500	-2.26574400	0.63573100
H	-4.59532000	-2.10201400	2.00201000	H	4.81060600	-2.82311600	0.96052100
C	-4.00272200	-0.07284200	1.69083600	C	2.71443100	-2.88103200	0.57875500
H	-4.71900500	0.33259500	2.39788500	H	2.61873200	-3.92771800	0.84889600
C	-3.12659200	0.83154300	1.02868700	C	1.54143800	-2.17154000	0.17061200
C	-2.11115000	0.33645200	0.16528100	C	1.64823900	-0.75637500	-0.06737200
C	-3.28456400	2.24218300	1.21082400	C	0.32744500	-2.84829800	-0.03171500
H	-4.10049600	2.59217200	1.83380800	H	0.30917500	-3.92410800	0.10917800
C	-2.47695400	3.13553600	0.55927400	C	-0.84674800	-2.18507000	-0.46393700
H	-2.66156800	4.20175400	0.63890000	H	-1.75511700	-2.74104500	-0.65986100
C	-1.35631300	2.69458400	-0.18201100	C	-0.80871300	-0.81473800	-0.56718000
C	-1.08486600	1.25859700	-0.26836300	C	0.38062300	-0.06951300	-0.22636900
C	-0.47299800	3.63127600	-0.76315100	C	-1.39738000	1.44256800	-0.29359200
H	-0.74788400	4.68019900	-0.72499200	H	6.53150200	1.41969600	-0.34483600
C	0.74427000	3.26003300	-1.32185300	C	-3.31967500	-0.26022400	-0.38707000
H	1.41367000	4.00278700	-1.73944100	C	-4.81468200	-0.86523400	1.42636600
C	1.15196600	1.91178800	-1.21044400	C	-4.38367300	-0.40611500	-1.28160600
C	0.25051400	0.90486000	-0.63860100	C	-5.87004600	-1.00733300	0.52399600
C	2.36190800	1.30877200	-1.50411600	C	-5.65126500	-0.77710300	-0.83201200
H	3.22097200	1.80559500	-1.93767600	H	-4.21925400	-0.22932600	-2.33994000
H	-2.52176900	-4.81715900	-1.29637200	H	-6.46424400	-0.88617200	-1.54123200
C	0.98318800	-0.27044900	-0.50776100	C	-0.02292600	1.26840200	0.07399100
C	3.48228200	-0.46076100	-0.07614800	C	0.65390400	2.33420300	0.72726500
C	3.54272100	0.21051200	1.15291200	C	-0.01224700	3.53662000	0.91280800
C	4.45276800	-1.42464000	-0.36610300	C	-1.34033300	3.70790700	0.49347100
C	4.55107800	-0.07809300	2.06937400	C	-2.04492800	2.64248400	-0.09522000
H	2.79442600	0.95935700	1.38818300	H	1.66147400	2.20142400	1.09642300
C	5.46330800	-1.71422600	0.54919100	H	0.49704400	4.35634300	1.40769100
H	4.41463000	-1.95213500	-1.31418100	H	-1.83425300	4.66052900	0.64708700
C	5.51501800	-1.04108900	1.77015500	H	-3.08636400	2.76239000	-0.37330600

H	4.58459500	0.44778300	3.01710200	C	-3.55160700	-0.49544500	0.97490000
H	6.20868800	-2.46504800	0.31099100	H	-6.85389400	-1.29536000	0.87684400
H	6.30023300	-1.26623900	2.48300800	H	-4.97744200	-1.04268700	2.48368500
H	0.64469100	-1.17714700	-0.02827600	H	-2.73743500	-0.38640200	1.68296900
C	2.37165500	-0.13518300	-1.07814100	C	-1.94577800	0.14696000	-0.88111100
H	2.51999900	-0.81423000	-1.93835600	H	-1.99897100	0.25984600	-1.97408900
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IC234-S1-CCl4				IC234-S1-DCM			
C	5.54344800	0.97320300	-0.33234900	C	5.54573200	0.97061200	-0.34755400
C	4.41442900	1.68406700	-0.80259600	C	4.41377600	1.68462000	-0.80880500
H	4.54980500	2.66642800	-1.24280700	H	4.54720900	2.66742900	-1.24834400
C	5.38156000	-0.31325700	0.15644700	C	5.38557700	-0.31495400	0.14262200
H	6.24427200	-0.89047300	0.47336700	H	6.24962300	-0.89281100	0.45460200
C	3.15057700	1.14633100	-0.72930000	C	3.15051300	1.14785300	-0.72568900
H	2.31323800	1.69474400	-1.13716200	H	2.31051300	1.69944600	-1.12359100
C	4.11099000	-0.91344000	0.22213700	C	4.11421000	-0.91437200	0.21735300
C	2.93136700	-0.15861300	-0.17034400	C	2.93311500	-0.15772400	-0.16742400
C	3.94958600	-2.26452700	0.63531400	C	3.95547600	-2.26544200	0.63402300
H	4.82584600	-2.81908100	0.95515900	H	4.83334000	-2.81986900	0.94932300
C	2.72723700	-2.87796100	0.59382800	C	2.73285000	-2.87712000	0.59993000
H	2.63151000	-3.92302300	0.86959000	H	2.63697900	-3.92210000	0.87549000
C	1.54857400	-2.16755300	0.19193000	C	1.55200800	-2.16482100	0.20262700
C	1.65252100	-0.75514900	-0.05491900	C	1.65445300	-0.75267600	-0.04571300
C	0.33525800	-2.84371700	-0.00484200	C	0.33957200	-2.84151900	0.00598100
H	0.31525000	-3.91874200	0.14112700	H	0.31834400	-3.91620100	0.15345200
C	-0.84144100	-2.18098500	-0.44456900	C	-0.83746200	-2.17752400	-0.43934500
H	-1.74790900	-2.74193200	-0.63586900	H	-1.74185600	-2.74135900	-0.63241000
C	-0.80794700	-0.81495500	-0.55966500	C	-0.80707500	-0.81373800	-0.55690900
C	0.38137500	-0.06569800	-0.21727400	C	0.38099500	-0.06074800	-0.20906300
C	-1.39982900	1.44030600	-0.28189500	C	-1.40282000	1.44035400	-0.27880500
H	6.52903500	1.41976500	-0.38925700	H	6.53158700	1.41582400	-0.41116900
C	-3.32276400	-0.26198600	-0.39196100	C	-3.32375100	-0.26426400	-0.39363100
C	-4.83369500	-0.86822200	1.40844800	C	-4.84115200	-0.86864800	1.40286800
C	-4.37884000	-0.40760400	-1.29619900	C	-4.37550400	-0.41542300	-1.30227300
C	-5.88136200	-1.01031300	0.49650700	C	-5.88478600	-1.01642800	0.48654700
C	-5.65054700	-0.77936400	-0.85771000	C	-5.64844100	-0.78919800	-0.86773400
H	-4.20551300	-0.22988800	-2.35284500	H	-4.19836300	-0.24027300	-2.35855900
H	-6.45712800	-0.88825900	-1.57421600	H	-6.45154600	-0.90225400	-1.58744900
C	-0.02192000	1.26513900	0.08712500	C	-0.02322300	1.26545300	0.09473500
C	0.65450000	2.33342500	0.74396400	C	0.65044600	2.33809300	0.75287700
C	-0.01211100	3.53437000	0.92923100	C	-0.01766600	3.53782000	0.93443500
C	-1.34116900	3.70578400	0.50788500	C	-1.34657700	3.70825400	0.50758300
C	-2.04602800	2.63946300	-0.08289600	C	-2.04904000	2.63940400	-0.08455800
H	1.66103100	2.20095200	1.11611500	H	1.65627000	2.20890200	1.12807000
H	0.49539100	4.35405500	1.42600900	H	0.48709900	4.35894200	1.43161800
H	-1.83526300	4.65826300	0.66163900	H	-1.84146900	4.66088800	0.65747700
H	-3.08663600	2.76163400	-0.36293600	H	-3.08784100	2.76247600	-0.37070200
C	-3.56654400	-0.49764300	0.96794600	C	-3.57276700	-0.49613000	0.96616000
H	-6.86816100	-1.29877300	0.84067400	H	-6.87231100	-1.30631600	0.82738000
H	-5.00553400	-1.04616000	2.46424500	H	-5.01698800	-1.04365100	2.45848800
H	-2.75939700	-0.38922300	1.68419000	H	-2.76966000	-0.38380100	1.68647600
C	-1.94516300	0.14647100	-0.87571500	C	-1.94517000	0.14647300	-0.87422400
H	-1.99220800	0.26427900	-1.96819200	H	-1.99065900	0.26549100	-1.96621800
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1C234-S1-DMSO				1C234-S1-n-hexane			
C	5.54690200	0.97070400	-0.34943200	C	5.52311700	0.98978500	0.02516600
C	4.41408600	1.68610900	-0.80743500	C	4.45170600	1.71384400	-0.52528700
H	4.54697400	2.66960100	-1.24549700	H	4.61818300	2.70788400	-0.92504500
C	5.38715200	-0.31507500	0.13958400	C	5.31650300	-0.30646200	0.44825800
H	6.25134800	-0.89360800	0.44979400	H	6.14562300	-0.89997800	0.81936100
C	3.15093800	1.14943200	-0.72238200	C	3.18722200	1.15914500	-0.57733700
H	2.31033700	1.70264500	-1.11671600	H	2.39034700	1.71934200	-1.04390700
C	4.11532600	-0.91435900	0.21591600	C	4.03955500	-0.90677500	0.36686600
C	2.93386100	-0.15680100	-0.16591000	C	2.92394500	-0.13840600	-0.08217400
C	3.95762400	-2.26591300	0.63184300	C	3.87673000	-2.30517000	0.63391500
H	4.83604600	-2.82057500	0.94501800	H	4.73383300	-2.87181400	0.98183700
C	2.73488200	-2.87730300	0.59892400	C	2.69768100	-2.92216100	0.37063000
H	2.63923100	-3.92270500	0.87278100	H	2.59933600	-3.99606800	0.48908700
C	1.55344600	-2.16411600	0.20381200	C	1.54159600	-2.18221800	-0.04977100
C	1.65508500	-0.75165700	-0.04331200	C	1.60380700	-0.75617600	-0.13565500
C	0.34139500	-2.84136100	0.00635400	C	0.34733000	-2.87241100	-0.35595900
H	0.32005200	-3.91606300	0.15335500	H	0.34565000	-3.95579600	-0.30182000
C	-0.83572300	-2.17676100	-0.44031100	C	-0.79230900	-2.19031200	-0.72720800
H	-1.73909300	-2.74163300	-0.63527600	H	-1.69794300	-2.72365100	-0.99305300
C	-0.80668200	-0.81354000	-0.55704700	C	-0.78155000	-0.79456900	-0.67324000
C	0.38077400	-0.05904800	-0.20635300	C	0.36264600	-0.07001100	-0.30905400
C	-1.40424000	1.44005600	-0.27870100	C	-1.41691600	1.45946800	-0.45567800
H	6.53277500	1.41572400	-0.41416000	H	6.51055800	1.43376900	0.08065700
C	-3.32386300	-0.26577300	-0.39365600	C	-3.27885400	-0.29303700	-0.30508500
C	-4.84118400	-0.87302900	1.40239100	C	-4.59875600	-0.84125300	1.65609800
C	-4.37594500	-0.41462800	-1.30241600	C	-4.40570200	-0.52174300	-1.09858900
C	-5.88523200	-1.01853700	0.48592900	C	-5.71941300	-1.06687600	0.85367000
C	-5.64902600	-0.78873500	-0.86809800	C	-5.61982300	-0.90611800	-0.52542200
H	-4.19909600	-0.23740300	-2.35833200	H	-4.33542700	-0.39895700	-2.17483200
H	-6.45233300	-0.89996000	-1.58784400	H	-6.48335700	-1.07886000	-1.15824400
C	-0.02422600	1.26546000	0.09716600	C	-0.06250000	1.33630600	-0.08177300
C	0.64781500	2.33999200	0.75586400	C	0.56629300	2.42742100	0.53177700
C	-0.02114200	3.53919500	0.93557800	C	-0.13201000	3.62354100	0.69406100
C	-1.34972300	3.70911700	0.50575300	C	-1.45217400	3.75060700	0.25814700
C	-2.05070400	2.63914500	-0.08711000	C	-2.10546200	2.65560500	-0.30949400
H	1.65340700	2.21256900	1.13229200	H	1.57895700	2.35452000	0.90187800
H	0.48232600	4.36104400	1.43285800	H	0.35919300	4.46313900	1.17337200
H	-1.84495700	4.66190700	0.65335400	H	-1.97805400	4.68994600	0.38644000
H	-3.08849300	2.76243600	-0.37676500	H	-3.14730000	2.72870500	-0.60248700
C	-3.57261800	-0.50024000	0.96584900	C	-3.39089500	-0.45790500	1.08168800
H	-6.87278500	-1.30867500	0.82643200	H	-6.66014100	-1.36537900	1.30245800
H	-5.01677600	-1.05012200	2.45770000	H	-4.66796900	-0.96432100	2.73132500
H	-2.76947400	-0.39010300	1.68654700	H	-2.52608800	-0.28443100	1.71321500
C	-1.94535500	0.14594400	-0.87436700	C	-1.96063700	0.12716500	-0.93490300
H	-1.99123400	0.26527000	-1.96613200	H	-2.11216900	0.17426100	-2.02211800
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12C34-vacuum				12C34-CCl4			
C	3.15637200	2.88230800	1.19835300	C	3.15583300	2.87523600	1.21173100
C	2.78191100	4.14186200	0.72574200	C	2.79443500	4.13424600	0.72589300

H	3.37296300	5.01639500	0.97311200	H	3.38938700	5.00639400	0.97250800
C	2.41013700	1.75225600	0.85159200	C	2.40458200	1.74783200	0.86443600
H	2.70791100	0.79139000	1.24698500	H	2.69382400	0.78756700	1.26761700
C	1.63254800	4.27365600	-0.04097300	C	1.65392900	4.26900400	-0.05273500
H	1.31367200	5.25405100	-0.37896600	H	1.34575100	5.24924600	-0.40086400
C	4.23406300	-1.98274500	-0.16506000	C	4.22477000	-1.99653800	-0.14892700
C	3.14858900	-1.11792300	-0.33693000	C	3.14201700	-1.12763900	-0.32165000
C	4.01720400	-3.32005700	0.17228600	C	4.00154800	-3.33578600	0.17918500
H	4.85722300	-3.98716100	0.32943900	H	4.83869300	-4.00633000	0.33730700
C	2.71886700	-3.80059100	0.27822100	C	2.70184700	-3.81305700	0.27504800
H	2.54329600	-4.84759700	0.50194100	H	2.52196200	-4.86090900	0.49120200
C	1.60008600	-2.95739200	0.06552400	C	1.58592000	-2.96480900	0.05989200
C	1.82362600	-1.55411400	-0.17751200	C	1.81599500	-1.56028200	-0.17415600
C	0.28760800	-3.48865400	0.01854100	C	0.27370400	-3.49295500	-0.00071200
H	0.14990600	-4.54985200	0.19628500	H	0.13127600	-4.55472700	0.16951000
C	-0.80569800	-2.69378500	-0.34029700	C	-0.81651600	-2.69101300	-0.36393700
H	-1.78930500	-3.13743900	-0.44921900	H	-1.79980600	-3.13260200	-0.48309500
C	-0.62268800	-1.34165000	-0.55183700	C	-0.62926300	-1.33972300	-0.56463600
C	0.65541300	-0.70855600	-0.33421400	C	0.64911400	-0.70823300	-0.33578200
C	-0.86792500	0.96294100	-0.86852500	C	-0.86633000	0.96905100	-0.87382700
H	4.02820500	2.77353800	1.83316800	H	4.02087500	2.76468600	1.85533300
C	-2.96290900	-0.33581000	-0.21262100	C	-2.96204800	-0.32430900	-0.20929600
C	-4.15268500	-0.20756000	1.89807800	C	-4.14117000	-0.18612500	1.90739400
C	-4.18958400	-0.45772900	-0.87076800	C	-4.19176100	-0.45515700	-0.86041800
C	-5.37263700	-0.32878500	1.23063900	C	-5.36454800	-0.31636700	1.24708900
C	-5.38804100	-0.45488500	-0.15642600	C	-5.38670400	-0.45185300	-0.13930400
H	-4.20723600	-0.55810200	-1.95172900	H	-4.21526400	-0.56226500	-1.94043600
H	-6.33061500	-0.55286500	-0.68381200	H	-6.33158600	-0.55643300	-0.66118900
C	0.46240100	0.70706300	-0.37451400	C	0.46112100	0.70476700	-0.37238700
C	1.27691800	1.83902600	0.02665200	C	1.28074200	1.83666900	0.02952400
C	0.83286500	3.15132600	-0.37113200	C	0.84779900	3.14943400	-0.38140500
C	-0.41838900	3.31606700	-1.01522600	C	-0.39715300	3.31873000	-1.03462500
C	-1.28541600	2.23596200	-1.20271500	C	-1.27212800	2.24073100	-1.21970500
H	-0.72698800	4.31512400	-1.30382400	H	-0.69806300	4.31762300	-1.33176900
H	-2.27769900	2.39872400	-1.60974700	H	-2.25991700	2.40818600	-1.63550700
C	-2.95917100	-0.21122700	1.18291400	C	-2.95121700	-0.19052500	1.18552400
H	-6.30215300	-0.32567500	1.78873900	H	-6.29108100	-0.31290100	1.81010200
H	-4.13274000	-0.10993500	2.97795500	H	-4.11564400	-0.08110900	2.98643800
H	-2.01528400	-0.11689700	1.70882600	H	-2.00557500	-0.08922500	1.70707100
H	5.24278600	-1.60797600	-0.29483000	H	5.23522800	-1.62355600	-0.26939400
H	3.33983400	-0.09265600	-0.62119200	H	3.33934600	-0.10084500	-0.59574200
C	-1.65699200	-0.32717300	-0.99794900	C	-1.66085900	-0.31805900	-1.00258500
H	-1.91260200	-0.50605000	-2.05419300	H	-1.92134700	-0.49241200	-2.05687500
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12C34-DCM				12C34-DMSO			
C	3.12999900	2.88548500	1.23230300	C	3.11310400	2.89516600	1.24118000
C	2.77593300	4.14143500	0.73186300	C	2.75963100	4.14911800	0.73490100
H	3.36787500	5.01502200	0.98055200	H	3.34852300	5.02447500	0.98451500
C	2.38257500	1.75587700	0.88184400	C	2.36967600	1.76312600	0.88939400
H	2.66747000	0.79840700	1.29474600	H	2.65466500	0.80744200	1.30638500
C	1.64688700	4.27156600	-0.06390000	C	1.63515200	4.27502000	-0.06804300
H	1.34410600	5.24958600	-0.42276900	H	1.33250500	5.25142900	-0.43135900
C	4.22532000	-1.98733100	-0.12267100	C	4.22888200	-1.97620900	-0.11028100
C	3.14106300	-1.12053800	-0.29870400	C	3.14258800	-1.11223400	-0.28786900

C	4.00290200	-3.33090200	0.19055400	C	4.00931100	-3.32218900	0.19538000
H	4.84055100	-4.00006800	0.35163600	H	4.84832600	-3.98928000	0.35777100
C	2.70421600	-3.81329000	0.26818500	C	2.71191600	-3.80923000	0.26396400
H	2.52553000	-4.86373600	0.47227800	H	2.53563200	-4.86122000	0.46198700
C	1.58725600	-2.96613000	0.04851400	C	1.59317200	-2.96449300	0.04247900
C	1.81561500	-1.55828100	-0.17090500	C	1.81805300	-1.55473900	-0.16962800
C	0.27849900	-3.49923000	-0.03173500	C	0.28687300	-3.50217300	-0.04688400
H	0.13766600	-4.56294100	0.12707600	H	0.14887500	-4.56707500	0.10621400
C	-0.81214800	-2.69595600	-0.39982900	C	-0.80523900	-2.70031100	-0.41667400
H	-1.79175800	-3.14124100	-0.53443700	H	-1.78233000	-3.14884200	-0.55868600
C	-0.62890600	-1.34347500	-0.58435100	C	-0.62630700	-1.34676700	-0.59335400
C	0.64587100	-0.70659600	-0.33986100	C	0.64576800	-0.70545000	-0.34174600
C	-0.86975900	0.96716000	-0.88710400	C	-0.87293800	0.96396500	-0.89329600
H	3.98618700	2.77889400	1.88811700	H	3.96581000	2.79190500	1.90195800
C	-2.95660900	-0.32773600	-0.20473800	C	-2.95328100	-0.33433200	-0.20274700
C	-4.11409400	-0.19382800	1.92509300	C	-4.10010100	-0.20900700	1.93383300
C	-4.19309900	-0.45551500	-0.84400000	C	-4.19328700	-0.45470000	-0.83683700
C	-5.34462300	-0.32107800	1.27670200	C	-5.33425900	-0.32884400	1.29061300
C	-5.38081800	-0.45279900	-0.11015800	C	-5.37746200	-0.45253400	-0.09696400
H	-4.22818700	-0.55928200	-1.92380300	H	-4.23408600	-0.55214300	-1.91693000
H	-6.33095200	-0.55486500	-0.62282300	H	-6.33031800	-0.54889400	-0.60561900
C	0.45489500	0.70257000	-0.37316900	C	0.45094400	0.70187200	-0.37370200
C	1.27116800	1.83928200	0.03173400	C	1.26334700	1.84201200	0.03276800
C	0.84394100	3.14948700	-0.39540800	C	0.83609500	3.15029700	-0.40100200
C	-0.39222200	3.31523900	-1.06537400	C	-0.39658100	3.31223600	-1.07830200
C	-1.26839600	2.23454300	-1.25001900	C	-1.27092300	2.22886200	-1.26334600
H	-0.68846100	4.31159100	-1.37545600	H	-0.69243400	4.30703700	-1.39366900
H	-2.24995000	2.40010000	-1.68098600	H	-2.24990400	2.39156400	-1.70118000
C	-2.93130000	-0.19771500	1.19054100	C	-2.92078400	-0.21228900	1.19324500
H	-6.26532700	-0.31838100	1.84915500	H	-6.25214000	-0.32684300	1.86755700
H	-4.07729500	-0.09197200	3.00410600	H	-4.05772100	-0.11364800	3.01323600
H	-1.98085000	-0.09915400	1.70405700	H	-1.96773500	-0.11976400	1.70321600
H	5.23561300	-1.60939600	-0.22717500	H	5.23836300	-1.59417700	-0.20696200
H	3.33958900	-0.09021500	-0.55788500	H	3.33981100	-0.07994600	-0.53991600
C	-1.66376400	-0.32054100	-1.01258200	C	-1.66440400	-0.32535000	-1.01741200
H	-1.93422900	-0.49256200	-2.06334700	H	-1.93951100	-0.49695500	-2.06653000
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12C34-n-hexane				P1234-VACUUM			
C	3.15814200	2.87515400	1.20847500	C	-2.64108900	-3.75984500	-0.98573700
C	2.79465500	4.13449500	0.72535700	C	-1.87811000	-2.86000000	-1.75769300
H	3.38943800	5.00678100	0.97188200	H	-1.40081000	-3.20203600	-2.66904400
C	2.40713400	1.74763700	0.86150900	C	-3.31799500	-3.29935900	0.12084400
H	2.69773500	0.78706300	1.26295100	H	-3.95643300	-3.96618900	0.69101300
C	1.65220100	4.26933400	-0.05047300	C	-1.74576700	-1.54406100	-1.37455700
H	1.34238500	5.24978000	-0.39657700	H	-1.18378600	-0.86756300	-2.00145300
C	4.22573800	-1.99586900	-0.15303900	C	-3.23777400	-1.94219400	0.51385300
C	3.14282400	-1.12722600	-0.32539100	C	-2.37024600	-1.04661500	-0.19639800
C	4.00313100	-3.33451200	0.17744700	C	-4.06678500	-1.43529400	1.55262900
H	4.84055200	-4.00478500	0.33525000	H	-4.70624100	-2.12240600	2.09630600
C	2.70350800	-3.81169100	0.27603500	C	-4.11476700	-0.09327300	1.80249900
H	2.52400000	-4.85921200	0.49410400	H	-4.81173200	0.30417500	2.53282900
C	1.58735700	-2.96390300	0.06146300	C	-3.25396600	0.81768700	1.12665600
C	1.81688900	-1.55979900	-0.17485300	C	-2.26307200	0.33041700	0.23522500
C	0.27482800	-3.49194500	0.00409600	C	-3.41858100	2.22487400	1.31490800

H	0.13275300	-4.55347500	0.17615100	H	-4.21421400	2.56770200	1.96741500
C	-0.81571000	-2.69086000	-0.35820500	C	-2.64979300	3.12317700	0.62692300
H	-1.79934000	-3.13236700	-0.47490500	H	-2.84320700	4.18767900	0.70550900
C	-0.62855900	-1.33961300	-0.56153800	C	-1.54949100	2.68965500	-0.15089200
C	0.65010600	-0.70839000	-0.33528500	C	-1.24937400	1.26291100	-0.22222100
C	-0.86621900	0.96858400	-0.87199100	C	-0.69994900	3.62602300	-0.77606000
H	4.02470800	2.76448200	1.85002900	H	-0.97925400	4.67374100	-0.74847400
C	-2.96260800	-0.32527700	-0.21003500	C	0.49775600	3.24400700	-1.36229000
C	-4.14486300	-0.18796200	1.90482000	H	1.14504400	3.98306300	-1.82099800
C	-4.19137900	-0.45528800	-0.86302800	C	0.93472300	1.90644300	-1.24902700
C	-5.36721900	-0.31739300	1.24263500	C	0.07711800	0.91012700	-0.61351300
C	-5.38736100	-0.45202000	-0.14381000	C	2.16465500	1.38487300	-1.65032500
H	-4.21319700	-0.56182700	-1.94317300	H	2.92142600	1.97425500	-2.15393000
H	-6.33151300	-0.55600700	-0.66714900	H	-2.72444900	-4.79804500	-1.28632000
C	0.46181200	0.70519800	-0.37250000	C	0.76158900	-0.30416600	-0.43842200
C	1.28117800	1.83672600	0.02905600	P	2.33070800	-0.37977300	-1.31587700
C	0.84650800	3.14965800	-0.37904400	C	3.63510000	-0.52618200	0.03256500
C	-0.39988900	3.31877700	-1.02978400	C	3.58896000	0.24954900	1.19765100
C	-1.27391700	2.24076600	-1.21511500	C	4.68175300	-1.43567200	-0.14488400
H	-0.70204600	4.31790800	-1.32485300	C	4.57697800	0.11526700	2.16972700
H	-2.26272700	2.40788200	-1.62864200	H	2.77799300	0.95594600	1.34028200
C	-2.95386600	-0.19229300	1.18483200	C	5.67191900	-1.56990500	0.82826400
H	-6.29460600	-0.31394000	1.80424600	H	4.71891900	-2.03942500	-1.04637300
H	-4.12096700	-0.08359600	2.98396700	C	5.61983800	-0.79433800	1.98558800
H	-2.00886200	-0.09158300	1.70762100	H	4.53540600	0.71816300	3.07063200
H	5.23601900	-1.62316300	-0.27594800	H	6.48062100	-2.27827700	0.68443900
H	3.33938500	-0.10090900	-0.60187700	H	6.38895000	-0.89793500	2.74305900
C	-1.66017200	-0.31882200	-1.00115200	H	0.36936100	-1.14088300	0.12140000
H	-1.91920000	-0.49383400	-2.05596100				
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P1234-CCI4				P1234-DCM			
C	-2.68544300	-3.75111800	-0.97907400	C	-2.71839400	-3.74546800	-0.97536200
C	-1.91602700	-2.85959200	-1.75520600	C	-1.94634600	-2.85912200	-1.75573000
H	-1.44659000	-3.20747500	-2.66844100	H	-1.48473100	-3.21060800	-2.67159400
C	-3.35165000	-3.28263200	0.13071700	C	-3.37469100	-3.27208600	0.13839000
H	-3.99488000	-3.94158300	0.70455000	H	-4.01969100	-3.92588500	0.71596200
C	-1.76702200	-1.54484800	-1.37294500	C	-1.78464300	-1.54547900	-1.37334800
H	-1.19790100	-0.87604200	-2.00177700	H	-1.21084400	-0.88202900	-2.00378100
C	-3.25452000	-1.92528800	0.52194700	C	-3.26518900	-1.91454200	0.52853800
C	-2.38093200	-1.03959600	-0.19314200	C	-2.38867600	-1.03546000	-0.19108200
C	-4.07492200	-1.40919600	1.56311800	C	-4.07851800	-1.39247300	1.57243200
H	-4.71853100	-2.08927300	2.11058000	H	-4.72401100	-2.06761800	2.12357100
C	-4.11027200	-0.06550700	1.81009500	C	-4.10567500	-0.04733000	1.81692300
H	-4.80144700	0.33964300	2.54160400	H	-4.79231200	0.36291100	2.54969500
C	-3.24418800	0.83593700	1.12882300	C	-3.23724000	0.84771200	1.13086300
C	-2.25979200	0.33861200	0.23519300	C	-2.25746600	0.34399400	0.23494000
C	-3.39741200	2.24591000	1.31597800	C	-3.38354100	2.25989800	1.31803400
H	-4.18778200	2.59558200	1.97105000	H	-4.17023100	2.61333600	1.97529200
C	-2.62467600	3.13624200	0.62342200	C	-2.60856400	3.14496700	0.62287100
H	-2.80912300	4.20242200	0.69976400	H	-2.78689500	4.21218400	0.69780100
C	-1.52963000	2.69129700	-0.15767800	C	-1.51640700	2.69237000	-0.16065800
C	-1.24012800	1.26135500	-0.22665800	C	-1.23408700	1.26000900	-0.22971300
C	-0.67761200	3.61989400	-0.78902900	C	-0.66335700	3.61644900	-0.79469600
H	-0.94967600	4.66950700	-0.76371600	H	-0.93006800	4.66732200	-0.76884800

C	0.51621800	3.22815700	-1.37972400	C	0.52820000	3.21913000	-1.38961100
H	1.16570600	3.96172100	-1.84395300	H	1.17878600	3.95004400	-1.85626800
C	0.94548000	1.88888700	-1.26228300	C	0.95248900	1.87893600	-1.27111500
C	0.08366300	0.89852400	-0.62142900	C	0.08806300	0.89090000	-0.62842000
C	2.17338700	1.36127600	-1.66346900	C	2.18040500	1.34931900	-1.67217900
H	2.93201700	1.94591300	-2.16976600	H	2.93988100	1.93247800	-2.17891200
H	-2.78144800	-4.78843300	-1.27885500	H	-2.82366000	-4.78193700	-1.27479800
C	0.76132600	-0.31820600	-0.44289100	C	0.76142500	-0.32730200	-0.44973400
P	2.33420700	-0.40178100	-1.31483100	P	2.33907600	-0.41273800	-1.31551100
C	3.63672800	-0.53894200	0.03533900	C	3.63939500	-0.54567600	0.03592800
C	3.57970200	0.23215800	1.20338000	C	3.58178400	0.22845100	1.20236500
C	4.69416800	-1.43627700	-0.14313500	C	4.69672200	-1.44447300	-0.13909100
C	4.56750500	0.10583100	2.17721200	C	4.56856500	0.10376400	2.17797800
H	2.76099100	0.92911100	1.34791600	H	2.76414000	0.92690700	1.34554400
C	5.68475800	-1.56187900	0.83130400	C	5.68636800	-1.56852400	0.83711900
H	4.74068100	-2.03760100	-1.04574200	H	4.74524600	-2.04840800	-1.03976300
C	5.62169200	-0.79091800	1.99157800	C	5.62253700	-0.79461800	1.99579500
H	4.51703400	0.70491600	3.08011500	H	4.51756600	0.70525800	3.07913400
H	6.50183100	-2.26021300	0.68625100	H	6.50298200	-2.26771600	0.69442500
H	6.39063700	-0.88813700	2.74997100	H	6.39043500	-0.89058300	2.75527500
H	0.36297200	-1.15383100	0.11423600	H	0.35830700	-1.16467100	0.10132300
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P1234-DMSO				P1234-n-hexane			
C	-2.72730500	-3.74432400	-0.97467000	C	-2.67784900	-3.75257100	-0.98013400
C	-1.95552700	-2.85896700	-1.75677100	C	-1.90939700	-2.85968100	-1.75547900
H	-1.49694400	-3.21116400	-2.67389800	H	-1.43849100	-3.20660900	-2.66831800
C	-3.38003800	-3.27000800	0.14084700	C	-3.34600900	-3.28538900	0.12901200
H	-4.02473400	-3.92269900	0.71993700	H	-3.98853800	-3.94564300	0.70215400
C	-1.79028200	-1.54564600	-1.37414000	C	-1.76326600	-1.54471300	-1.37311700
H	-1.21561800	-0.88346400	-2.00520900	H	-1.19533400	-0.87460800	-2.00161400
C	-3.26729000	-1.91234000	0.53073300	C	-3.25176000	-1.92807500	0.52053600
C	-2.39074100	-1.03472400	-0.19063900	C	-2.37911400	-1.04073200	-0.19367000
C	-4.07832800	-1.38897400	1.57583800	C	-4.07367400	-1.41350700	1.56124700
H	-4.72373800	-2.06294300	2.12842800	H	-4.71663800	-2.09477900	2.10801100
C	-4.10382400	-0.04333000	1.81944700	C	-4.11112100	-0.07011400	1.80874000
H	-4.78908200	0.36802100	2.55279000	H	-4.80329900	0.33375100	2.54003200
C	-3.23550300	0.85028900	1.13163400	C	-3.24585300	0.83292700	1.12843500
C	-2.25694400	0.34523200	0.23476600	C	-2.26035500	0.33725600	0.23522100
C	-3.38062200	2.26315400	1.31898500	C	-3.40094300	2.24241800	1.31570900
H	-4.16645500	2.61715300	1.97689200	H	-4.19220900	2.59100900	1.97031500
C	-2.60530000	3.14703400	0.62335900	C	-2.62884000	3.13407500	0.62387800
H	-2.78226500	4.21446200	0.69787800	H	-2.81480100	4.19998300	0.70057500
C	-1.51344000	2.69267100	-0.16072300	C	-1.53294900	2.69103400	-0.15665300
C	-1.23281900	1.25963400	-0.23051600	C	-1.24166800	1.26163900	-0.22591000
C	-0.66026800	3.61599800	-0.79459100	C	-0.68129500	3.62087900	-0.78706600
H	-0.92543800	4.66718100	-0.76761500	H	-0.95459700	4.67017900	-0.76151200
C	0.53091800	3.21778200	-1.39096100	C	0.51316600	3.23070200	-1.37693400
H	1.18171000	3.94853600	-1.85749600	H	1.16231300	3.96511500	-1.84032700
C	0.95403600	1.87740700	-1.27310800	C	0.94369900	1.89169800	-1.26007100
C	0.08900200	0.88922300	-0.63080200	C	0.08256700	0.90045300	-0.61998900
C	2.18249500	1.34811500	-1.67415800	C	2.17185300	1.36495700	-1.66128100
H	2.94201100	1.93158800	-2.18048900	H	2.93019800	1.95027100	-2.16722800
H	-2.83503000	-4.78052300	-1.27407700	H	-2.77170300	-4.79005300	-1.28004100
C	0.76144700	-0.32933500	-0.45302800	C	0.76134700	-0.31588400	-0.44187900

P	2.34119400	-0.41377500	-1.31631100	P	2.33345400	-0.39836300	-1.31490900
C	3.64058800	-0.54649600	0.03550100	C	3.63635600	-0.53693000	0.03495300
C	3.58664100	0.23211600	1.19932100	C	3.58079400	0.23465000	1.20267600
C	4.69394300	-1.45080200	-0.13633100	C	4.69240700	-1.43577400	-0.14357200
C	4.57294200	0.10627900	2.17548900	C	4.56870900	0.10723700	2.17616100
H	2.77260200	0.93517000	1.34063500	H	2.76303100	0.93276200	1.34703500
C	5.68294900	-1.57627000	0.84058000	C	5.68302500	-1.56254000	0.83057900
H	4.74038600	-2.05800900	-1.03487400	H	4.73757100	-2.03730800	-1.04612200
C	5.62271400	-0.79793600	1.99662000	C	5.62144600	-0.79109600	1.99053300
H	4.52490900	0.71138400	3.07433900	H	4.51943600	0.70672100	3.07888300
H	6.49623700	-2.27972800	0.70025500	H	6.49904300	-2.26213600	0.68555700
H	6.39009100	-0.89482000	2.75644900	H	6.39049500	-0.88918000	2.74873000
H	0.35679400	-1.16820200	0.09463200	H	0.36405100	-1.15153500	0.11596400
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1P234-vacuum				1P234-CCI4			
C	5.60966300	0.96461200	-0.14584400	C	5.60568800	0.96654400	-0.15434000
C	4.50173900	1.67157000	-0.66939500	C	4.49604100	1.67377800	-0.67479600
H	4.65124000	2.65955600	-1.09138400	H	4.64404100	2.66139200	-1.09799500
C	5.43551000	-0.32385400	0.32344300	C	5.43430300	-0.32223600	0.31778700
H	6.28513500	-0.89527700	0.68302100	H	6.28611700	-0.89090700	0.67649900
C	3.24180700	1.12220600	-0.66736000	C	3.23721800	1.12304800	-0.66731600
H	2.42003100	1.66860200	-1.10833400	H	2.41303800	1.66782700	-1.10567800
C	4.16789900	-0.93828800	0.31329800	C	4.16821600	-0.93844600	0.31274000
C	3.00679300	-0.19007400	-0.13762300	C	3.00540300	-0.19088600	-0.13573900
C	3.99857300	-2.29173500	0.70410200	C	4.00146500	-2.29262400	0.70963200
H	4.86024100	-2.84111500	1.06898300	H	4.86509100	-2.83962500	1.07315200
C	2.78447800	-2.91553000	0.58511500	C	2.78916300	-2.91589300	0.59629000
H	2.68214800	-3.96417300	0.84444000	H	2.68638100	-3.96429100	0.85589200
C	1.62781900	-2.21210100	0.12362500	C	1.62963800	-2.21140800	0.13472100
C	1.72474900	-0.79918100	-0.09693800	C	1.72584900	-0.79899600	-0.08950900
C	0.43401400	-2.89854300	-0.16738400	C	0.44009000	-2.89710400	-0.16397000
H	0.41038100	-3.97498700	-0.03329000	H	0.41393700	-3.97341700	-0.02997800
C	-0.68876400	-2.24305400	-0.71795100	C	-0.68114600	-2.23993700	-0.72680500
H	-1.55052400	-2.81898400	-1.03474800	H	-1.53947200	-2.81930100	-1.04683900
C	-0.68229100	-0.86834700	-0.80037300	C	-0.67764600	-0.86784100	-0.81097200
C	0.45870100	-0.11082500	-0.30738300	C	0.45674600	-0.10821100	-0.30844700
C	-1.22050900	1.59409200	-0.41633400	C	-1.22467200	1.59298100	-0.41782500
H	6.59260800	1.42068600	-0.14538800	H	6.58867000	1.42275500	-0.15757600
C	-3.47801600	-0.26365600	-0.36500200	C	-3.47817100	-0.26124300	-0.36526200
C	-4.53737600	-0.90594100	1.71893900	C	-4.53618000	-0.89114100	1.72340600
C	-4.72145800	-0.34604000	-1.00323300	C	-4.71896700	-0.36300100	-1.00590000
C	-5.77315500	-0.98506800	1.07347900	C	-5.76979800	-0.99018700	1.07553100
C	-5.86400900	-0.70630300	-0.28843000	C	-5.86007200	-0.72708300	-0.28960000
H	-4.79333100	-0.12860800	-2.06390800	H	-4.79164600	-0.15798000	-2.06891200
H	-6.82061900	-0.76974300	-0.79516000	H	-6.81462400	-0.80526600	-0.79800600
P	-2.01577900	0.24159400	-1.38753000	P	-2.01761700	0.24284500	-1.39097900
C	0.08490200	1.21197700	0.05997700	C	0.08261100	1.20904100	0.06114300
C	0.80194800	2.13845200	0.87579000	C	0.79947600	2.13726700	0.88021000
C	0.27153800	3.39228400	1.12190500	C	0.26860000	3.39035500	1.12482000
C	-0.97212200	3.77041600	0.59043200	C	-0.97471200	3.76959200	0.59012700
C	-1.72139400	2.85822700	-0.16960000	C	-1.72356500	2.85743600	-0.17297000
H	1.73650300	1.84240500	1.33316900	H	1.73309300	1.84170100	1.33955500
H	0.81845700	4.08932200	1.74725300	H	0.81356500	4.08747000	1.75177000
H	-1.36144700	4.76453100	0.77815400	H	-1.36485200	4.76308900	0.77912700

H	-2.69356800	3.14873000	-0.55410600	H	-2.69438600	3.14998400	-0.55919500
C	-3.39689700	-0.54964400	1.00593500	C	-3.39756900	-0.53058500	1.00905600
H	-6.65999700	-1.26359100	1.63181100	H	-6.65504000	-1.27185800	1.63472700
H	-4.46439500	-1.12257800	2.77916400	H	-4.46353800	-1.09541800	2.78602600
H	-2.44103400	-0.49259400	1.51413900	H	-2.44417600	-0.45817300	1.52003100
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1P234-DCM				1P234-DMSO			
C	5.60880300	0.96617800	-0.16577200	C	5.61011700	0.96785700	-0.16805600
C	4.49698900	1.67478600	-0.68123600	C	4.49735800	1.67684000	-0.68171200
H	4.64390500	2.66221800	-1.10506100	H	4.64365000	2.66456600	-1.10499000
C	5.43840700	-0.32189900	0.30910200	C	5.44030100	-0.32019400	0.30681100
H	6.29124000	-0.89032000	0.66555600	H	6.29339000	-0.88869600	0.66239000
C	3.23799300	1.12474000	-0.66646700	C	3.23845200	1.12658800	-0.66516800
H	2.41178300	1.67123400	-1.09879100	H	2.41156400	1.67397300	-1.09509800
C	4.17152200	-0.93732900	0.31073500	C	4.17313000	-0.93572800	0.30999200
C	3.00734300	-0.18920900	-0.13366200	C	3.00832600	-0.18754200	-0.13280800
C	4.00672000	-2.29156300	0.71198900	C	4.00946200	-2.29014500	0.71178300
H	4.87183600	-2.83758000	1.07312300	H	4.87516900	-2.83564400	1.07216900
C	2.79463400	-2.91437500	0.60372700	C	2.79760200	-2.91339100	0.60441400
H	2.69217100	-3.96269300	0.86328200	H	2.69577200	-3.96185400	0.86344900
C	1.63330300	-2.20904800	0.14342100	C	1.63558500	-2.20807900	0.14467400
C	1.72844700	-0.79643400	-0.08273000	C	1.72968600	-0.79515800	-0.08111400
C	0.44625400	-2.89580200	-0.15816300	C	0.44954700	-2.89579500	-0.15817100
H	0.41914600	-3.97192100	-0.02389500	H	0.42262900	-3.97193800	-0.02450400
C	-0.67464100	-2.23759300	-0.72798100	C	-0.67157600	-2.23741900	-0.72972100
H	-1.53044000	-2.81960000	-1.05010400	H	-1.52619500	-2.82056400	-1.05294700
C	-0.67324500	-0.86742400	-0.81344100	C	-0.67146800	-0.86784500	-0.81476100
C	0.45681500	-0.10417600	-0.30455800	C	0.45701500	-0.10289600	-0.30325000
C	-1.22889000	1.59212400	-0.41566900	C	-1.23089600	1.59103300	-0.41524500
H	6.59217400	1.42150500	-0.17378800	H	6.59340000	1.42331900	-0.17697900
C	-3.47967300	-0.26282100	-0.36717800	C	-3.48005500	-0.26479100	-0.36790600
C	-4.54091700	-0.89264200	1.72032500	C	-4.54084000	-0.89980600	1.71848600
C	-4.71859900	-0.36852100	-1.01100600	C	-4.71986500	-0.36484100	-1.01102800
C	-5.77309500	-0.99557200	1.06937500	C	-5.77408100	-0.99683000	1.06830500
C	-5.86082500	-0.73434200	-0.29649600	C	-5.86246900	-0.73013100	-0.29656200
H	-4.79060000	-0.16534000	-2.07431100	H	-4.79286700	-0.15766100	-2.07344600
H	-6.81388500	-0.81521600	-0.80708300	H	-6.81621700	-0.80643000	-0.80648800
P	-2.01776800	0.24204800	-1.38997400	P	-2.01795700	0.24058700	-1.38998100
C	0.08080400	1.20889300	0.06487400	C	0.07958800	1.20841700	0.06634800
C	0.79512700	2.14086700	0.88568000	C	0.79209600	2.14185600	0.88835900
C	0.26116400	3.39187800	1.12981100	C	0.25648400	3.39186800	1.13237000
C	-0.98334900	3.76966600	0.59324900	C	-0.98829700	3.76888500	0.59450300
C	-1.72957400	2.85561300	-0.17199500	C	-1.73283500	2.85398000	-0.17201800
H	1.72997900	1.84914800	1.34483400	H	1.72735400	1.85188200	1.34777100
H	0.80347200	4.09034700	1.75753300	H	0.79730100	4.09083100	1.76080700
H	-1.37589200	4.76201400	0.78289100	H	-1.38204000	4.76072300	0.78413600
H	-2.70006200	3.14747200	-0.55951200	H	-2.70308200	3.14535500	-0.56048400
C	-3.40142200	-0.52980500	1.00788200	C	-3.40104600	-0.53716100	1.00614100
H	-6.65882600	-1.27887200	1.62681300	H	-6.65995900	-1.27995600	1.62552500
H	-4.47017600	-1.09564400	2.78323300	H	-4.46953100	-1.10729800	2.78045700
H	-2.44986700	-0.45461100	1.52200600	H	-2.44890800	-0.46684200	1.51995200
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1P234-n-hexane				12P34-vacuum			
C	5.60578800	0.96634900	-0.15273000	C	2.77165800	2.86443100	1.58805500
C	4.49651600	1.67340200	-0.67396100	C	2.52452400	4.12283900	1.03391500
H	4.64474600	2.66106100	-1.09701100	H	3.05968600	4.99413600	1.39347800
C	5.43408900	-0.32245900	0.31891800	C	2.10325500	1.73906100	1.10472000
H	6.28562400	-0.89137700	0.67791600	H	2.30283200	0.77801900	1.55930800
C	3.23760500	1.12273500	-0.66766000	C	1.56637300	4.25375400	0.03840400
H	2.41384200	1.66745400	-1.10689100	H	1.33697500	5.23194300	-0.37107400
C	4.16793500	-0.93858100	0.31281700	C	4.39975200	-1.54446500	0.00703000
C	3.00541000	-0.19102800	-0.13629500	C	3.23453300	-0.82440500	-0.25478000
C	4.00077400	-2.29263900	0.70886400	C	4.32862400	-2.89263700	0.36647900
H	4.86408800	-2.83991900	1.07275500	H	5.23177000	-3.44791700	0.59186900
C	2.78824700	-2.91598800	0.59468200	C	3.09374100	-3.52482100	0.40158000
H	2.68551900	-3.96438800	0.85439700	H	3.03022400	-4.58209600	0.63669500
C	1.62916000	-2.21170300	0.13302500	C	1.90236800	-2.82720800	0.09944800
C	1.72555700	-0.79927900	-0.09086000	C	1.96303600	-1.41627200	-0.16437000
C	0.43889400	-2.89731500	-0.16453000	C	0.66919900	-3.52150100	-0.03509800
H	0.41303000	-3.97365400	-0.03050300	H	0.64454100	-4.58633100	0.17058300
C	-0.68255000	-2.24042600	-0.72552200	C	-0.46068600	-2.87874300	-0.52336800
H	-1.54149200	-2.81923100	-1.04488200	H	-1.35910800	-3.45294900	-0.72452700
C	-0.67854700	-0.86792200	-0.80957100	C	-0.45279600	-1.50545200	-0.74517500
C	0.45696500	-0.10885200	-0.30864700	C	0.71677900	-0.70880100	-0.41826500
C	-1.22383100	1.59316300	-0.41759900	C	-0.78254200	0.95345200	-1.21088200
H	6.58872600	1.42263700	-0.15516500	H	3.48572400	2.75522800	2.39641300
C	-3.47813600	-0.26124200	-0.36512400	C	-3.08100700	-0.47932200	-0.11772700
C	-4.53624500	-0.89259600	1.72298800	C	-3.74564900	-0.35624900	2.21082800
C	-4.71929400	-0.36057900	-1.00540700	C	-4.43030200	-0.44747400	-0.48689000
C	-5.77014000	-0.98918300	1.07545600	C	-5.08897800	-0.32288600	1.83248100
C	-5.86054000	-0.72417900	-0.28927000	C	-5.43065200	-0.37019900	0.48207500
H	-4.79182600	-0.15400200	-2.06814200	H	-4.69696900	-0.48697400	-1.53864300
H	-6.81538300	-0.80055800	-0.79743500	H	-6.47327700	-0.35148700	0.18341200
P	-2.01737800	0.24290200	-1.39056000	P	-1.80588900	-0.53421900	-1.49501900
C	0.08311400	1.20927900	0.06083800	C	0.44774600	0.68783900	-0.48790900
C	0.80035700	2.13698600	0.87936600	C	1.17476300	1.82557800	0.05330100
C	0.26984000	3.39032500	1.12424400	C	0.84637700	3.13533700	-0.44081200
C	-0.97346700	3.76961600	0.59020300	C	-0.23754800	3.29920800	-1.34549900
C	-1.72270500	2.85767600	-0.17235100	C	-1.06838500	2.23242100	-1.67101000
H	1.73400200	1.84099900	1.33841900	H	-0.45491900	4.29253000	-1.72365800
H	0.81531400	4.08731700	1.75089300	H	-1.94766600	2.40175400	-2.28415900
H	-1.36325300	4.76327600	0.77914100	C	-2.74775400	-0.43502400	1.24279100
H	-2.69370900	3.15012500	-0.55821000	H	-5.86454600	-0.26189600	2.58795200
C	-3.39742800	-0.53262200	1.00877500	H	-3.47726600	-0.32082500	3.26134700
H	-6.65557300	-1.27043800	1.63458200	H	-1.70692700	-0.46387400	1.54569600
H	-4.46353200	-1.09835900	2.78533100	H	5.36155200	-1.05064300	-0.07093600
H	-2.44366900	-0.46211300	1.51931400	H	3.31714400	0.21391900	-0.54441000
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12P34-CCl4				12P34-DCM			
C	2.76953700	2.86368200	1.59030400	C	2.75307900	2.87295600	1.59365300
C	2.52482200	4.12248000	1.03517200	C	2.50720900	4.13067500	1.03573800
H	3.06089400	4.99303300	1.39523400	H	3.04034000	5.00275400	1.39636600
C	2.09998900	1.73892400	1.10493900	C	2.08757100	1.74579300	1.10666800
H	2.29957700	0.77754800	1.55870800	H	2.28968100	0.78550800	1.56153000
C	1.56849100	4.25526700	0.03843600	C	1.55402500	4.26076300	0.03576100
H	1.34082900	5.23384600	-0.37089700	H	1.32518600	5.23845200	-0.37484500

C	4.40097800	-1.54472900	0.00665800	C	4.40679200	-1.53009300	0.01194300
C	3.23537400	-0.82453900	-0.25746900	C	3.23854100	-0.81407700	-0.25503800
C	4.32875300	-2.89232200	0.36908700	C	4.33851900	-2.87827100	0.37424300
H	5.23152000	-3.44734900	0.59661000	H	5.24276300	-3.42965100	0.60456200
C	3.09400600	-3.52431000	0.40459100	C	3.10640900	-3.51523400	0.40664000
H	3.02999700	-4.58115700	0.64108000	H	3.04571400	-4.57228900	0.64262800
C	1.90246200	-2.82645400	0.09857200	C	1.91244800	-2.82129700	0.09665100
C	1.96470400	-1.41528000	-0.16744000	C	1.97070700	-1.40924200	-0.16904500
C	0.67098500	-3.52144600	-0.03967500	C	0.68549300	-3.52200700	-0.04702100
H	0.64550000	-4.58627700	0.16547600	H	0.66333000	-4.58708400	0.15678400
C	-0.45920300	-2.87819200	-0.53463600	C	-0.44740300	-2.88177100	-0.54731300
H	-1.35540300	-3.45431300	-0.73981300	H	-1.33936500	-3.46296400	-0.75651900
C	-0.45082300	-1.50695300	-0.75526200	C	-0.44389900	-1.51216200	-0.76555900
C	0.71640500	-0.70661900	-0.42412700	C	0.71823800	-0.70388800	-0.42969800
C	-0.78870600	0.95836300	-1.20566900	C	-0.79703100	0.95706900	-1.20433300
H	3.48267700	2.75321400	2.39916900	H	3.46428900	2.76491800	2.40436000
C	-3.07974400	-0.47727300	-0.11853900	C	-3.07611200	-0.48578800	-0.11780400
C	-3.74052200	-0.37173500	2.21248100	C	-3.73111300	-0.39461800	2.21607100
C	-4.42979500	-0.43945300	-0.48542000	C	-4.42709900	-0.43937600	-0.48146700
C	-5.08477800	-0.33173500	1.83650100	C	-5.07642700	-0.34527100	1.84339400
C	-5.42871500	-0.36682900	0.48613600	C	-5.42365200	-0.36855100	0.49337100
H	-4.69978500	-0.47040000	-1.53648200	H	-4.70128900	-0.46135000	-1.53153200
H	-6.47155500	-0.34242500	0.18898800	H	-6.46684300	-0.33649300	0.19862700
P	-1.80763300	-0.53244600	-1.49544500	P	-1.80814700	-0.53961200	-1.49594400
C	0.44511900	0.68693000	-0.48855400	C	0.44016700	0.68549800	-0.49007500
C	1.17356500	1.82699800	0.05371300	C	1.16484200	1.83080800	0.05342300
C	0.84592600	3.13719600	-0.44086100	C	0.83445700	3.13974600	-0.44395800
C	-0.24004600	3.30415300	-1.34109300	C	-0.25189000	3.30450300	-1.34329200
C	-1.07534500	2.23596700	-1.66295700	C	-1.08722100	2.23172500	-1.66210200
H	-0.45866500	4.29771800	-1.71755500	H	-0.47391700	4.29695100	-1.72043400
H	-1.95694800	2.40802300	-2.27187600	H	-1.97029800	2.40274900	-2.26911200
C	-2.74417400	-0.44488800	1.24195800	C	-2.73710100	-0.46510000	1.24239600
H	-5.85894600	-0.27542300	2.59368800	H	-5.84850400	-0.29133600	2.60276100
H	-3.47016900	-0.34599300	3.26268000	H	-3.45812700	-0.37860100	3.26568100
H	-1.70325600	-0.47895200	1.54383600	H	-1.69599100	-0.50643000	1.54268500
H	5.36286800	-1.05114200	-0.07071300	H	5.36683700	-1.03254500	-0.06149100
H	3.31977300	0.21351800	-0.54753200	H	3.32108800	0.22485900	-0.54235700
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12P34-DMSO				12P34-n-hexane			
C	2.73981800	2.88118700	1.59507000	C	2.77066200	2.86325200	1.58981600
C	2.49148400	4.13786400	1.03563400	C	2.52567300	4.12207000	1.03500500
H	3.02167300	5.01159600	1.39651800	H	3.06178600	4.99263200	1.39498500
C	2.07833900	1.75170900	1.10745300	C	2.10104500	1.73855600	1.10477200
H	2.28300300	0.79239200	1.56317800	H	2.30052300	0.77714500	1.55853600
C	1.53983300	4.26487900	0.03378600	C	1.56891600	4.25478100	0.03862700
H	1.30899000	5.24169300	-0.37770500	H	1.34108300	5.23337000	-0.37062100
C	4.41124900	-1.51702200	0.01658100	C	4.40050500	-1.54542400	0.00643400
C	3.24091100	-0.80474600	-0.25217900	C	3.23509500	-0.82504300	-0.25730500
C	4.34688000	-2.86578600	0.37790600	C	4.32820900	-2.89304000	0.36854900
H	5.25253500	-3.41405300	0.60996100	H	5.23094100	-3.44827800	0.59570300
C	3.11699900	-3.50710600	0.40750000	C	3.09330600	-3.52479300	0.40415100
H	3.05926400	-4.56444500	0.64279000	H	3.02917100	-4.58167200	0.64054300
C	1.92111000	-2.81679500	0.09542800	C	1.90192300	-2.82678100	0.09877200
C	1.97518100	-1.40418300	-0.16935100	C	1.96416900	-1.41569500	-0.16700800

C	0.69738400	-3.52217200	-0.05134300	C	0.67000100	-3.52139000	-0.03875300
H	0.67870300	-4.58746800	0.15147500	H	0.64447000	-4.58621100	0.16652300
C	-0.43761400	-2.88509700	-0.55358400	C	-0.45999000	-2.87807500	-0.53261600
H	-1.32684200	-3.46984000	-0.76458300	H	-1.35668600	-3.45368800	-0.73709800
C	-0.43864000	-1.51593700	-0.77027200	C	-0.45143300	-1.50647500	-0.75349400
C	0.72002300	-0.70246300	-0.43220700	C	0.71635300	-0.70704000	-0.42313500
C	-0.80170700	0.95374000	-1.20570300	C	-0.78750500	0.95781000	-1.20644100
H	3.45007600	2.77562500	2.40685400	H	3.48404100	2.75279300	2.39849900
C	-3.07314200	-0.49418000	-0.11686200	C	-3.08005200	-0.47709300	-0.11847300
C	-3.72433600	-0.40816500	2.21856800	C	-3.74154600	-0.36868600	2.21211300
C	-4.42467700	-0.44302600	-0.47837200	C	-4.42996800	-0.44043900	-0.48576000
C	-5.07021700	-0.35369700	1.84805200	C	-5.08563700	-0.32996800	1.83570800
C	-5.41958000	-0.37194600	0.49839700	C	-5.42915800	-0.36715900	0.48533000
H	-4.70117800	-0.46100800	-1.52785500	H	-4.69933900	-0.47290300	-1.53696000
H	-6.46305700	-0.33587300	0.20531500	H	-6.47196300	-0.34384800	0.18790000
P	-1.80775500	-0.54680100	-1.49663100	P	-1.80738700	-0.53230400	-1.49542600
C	0.43688300	0.68478000	-0.49144900	C	0.44569100	0.68713800	-0.48843900
C	1.15746900	1.83352500	0.05277500	C	1.17413400	1.82661800	0.05365300
C	0.82393500	3.14125800	-0.44625500	C	0.84651000	3.13683800	-0.44065200
C	-0.26223300	3.30281800	-1.34623700	C	-0.23921200	3.30352900	-1.34145800
C	-1.09517600	2.22663000	-1.66440400	C	-1.07390100	2.23576700	-1.66399200
H	-0.48716800	4.29429800	-1.72411600	H	-0.45753500	4.29713400	-1.71804600
H	-1.97868200	2.39548900	-2.27138500	H	-1.95514600	2.40752500	-2.27353100
C	-2.73191800	-0.47858000	1.24302400	C	-2.74491600	-0.44266400	1.24203400
H	-5.84094300	-0.29994700	2.60874900	H	-5.86006700	-0.27296100	2.59259300
H	-3.44968000	-0.39643800	3.26776300	H	-3.47154400	-0.34126400	3.26237800
H	-1.69060000	-0.52392700	1.54207700	H	-1.70400800	-0.47573400	1.54407900
H	5.36963000	-1.01594000	-0.05386900	H	5.36248000	-1.05201500	-0.07122400
H	3.32106300	0.23492500	-0.53744600	H	3.31936200	0.21298600	-0.54751400
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1-A-13-D-P1234				1-A-13-D-P1234-CC14			
C	2.29446000	-3.62906300	0.45043300	C	2.33808200	-3.62492400	0.41105300
C	1.78660500	-2.71032500	1.36026200	C	1.81508200	-2.72290600	1.32889100
C	2.96770800	-3.18079800	-0.67487400	H	1.44408800	-3.08564200	2.27675900
H	3.43433900	-3.89159500	-1.34726900	C	3.00683700	-3.15615800	-0.70967800
C	1.89661100	-1.32371400	1.10981700	H	3.49082400	-3.85283800	-1.38433500
C	3.03315000	-1.80042700	-0.99730300	C	1.91032600	-1.33134000	1.09652300
C	2.33005200	-0.86785300	-0.19506300	C	3.04937400	-1.77332300	-1.01870400
C	3.75833200	-1.33772100	-2.13162300	C	2.33662300	-0.85561200	-0.20431000
H	4.29003700	-2.05410400	-2.74689300	C	3.76799800	-1.29200000	-2.15009300
C	3.82331000	0.00236700	-2.39003800	H	4.30727600	-1.99782900	-2.77083500
H	4.45861900	0.37701400	-3.18563100	C	3.81785200	0.05051900	-2.39869400
C	3.02528900	0.93464400	-1.66876000	H	4.44734200	0.43880000	-3.19219400
C	2.11081200	0.46565600	-0.68870500	C	3.01236900	0.96755500	-1.66570700
C	3.13660700	2.34170500	-1.89748300	C	2.10556200	0.47997300	-0.68439900
H	3.84444600	2.70217300	-2.63502900	C	3.11207300	2.37627200	-1.88101000
C	2.39788800	3.20847900	-1.14452500	H	3.81639000	2.74856200	-2.61598000
H	2.54238500	4.27929800	-1.24897100	C	2.36861400	3.23228500	-1.11769300
C	1.35834100	2.75486900	-0.27762500	H	2.50670300	4.30484500	-1.21149700
C	1.08025700	1.35993700	-0.19190600	C	1.33591400	2.76216700	-0.25383300
C	0.55139200	3.68669800	0.44858800	C	1.07024200	1.36316700	-0.17769100
H	0.81664000	4.73815500	0.41102900	C	0.52342700	3.68201400	0.48192100
C	-0.53412800	3.27022400	1.16565000	H	0.78262900	4.73532800	0.45322700
H	-1.12621300	3.98364500	1.72958200	C	-0.55664300	3.25336400	1.19914800

C	-0.98025800	1.91128000	1.09165600	H	-1.15188500	3.95757500	1.77117100
C	-0.19903200	0.95003700	0.32398400	C	-0.99260500	1.89086500	1.11378300
C	-2.16675000	1.40816700	1.60654900	C	-0.20373000	0.94109800	0.33826400
H	2.22462600	-4.68860600	0.66113800	C	-2.17464000	1.37694700	1.62555000
C	-0.89340800	-0.27758300	0.15490800	H	-2.87360200	1.94368300	2.22588400
P	-2.40731800	-0.31991600	1.18152900	H	2.28744200	-4.68693500	0.61420700
C	-3.83225600	-0.34927300	-0.02828300	C	-0.89307700	-0.28966800	0.15887500
C	-3.88622700	0.49488000	-1.14384200	P	-2.40786600	-0.34975400	1.18597600
C	-4.88157200	-1.24208300	0.20238800	C	-3.83013400	-0.36272900	-0.02873000
C	-4.97324800	0.44431500	-2.01093600	C	-3.86221500	0.46465400	-1.15818900
H	-3.07281700	1.18675500	-1.33189800	C	-4.90242100	-1.22570700	0.21314100
C	-5.97470800	-1.29082900	-0.66504600	C	-4.94902800	0.42776000	-2.02698200
H	-4.84140100	-1.90357500	1.06177300	H	-3.03175200	1.13297500	-1.35701100
C	-6.02095700	-0.44809500	-1.77197000	C	-5.99610300	-1.26018500	-0.65509500
H	-5.00480600	1.09847800	-2.87575400	H	-4.88088200	-1.87583400	1.08191200
H	-6.78337900	-1.98896500	-0.47740400	C	-6.01987100	-0.43394500	-1.77562500
H	-6.86661800	-0.48627900	-2.44994000	H	-4.96260100	1.06867500	-2.90207800
H	1.40979700	-3.05615400	2.31248800	H	-6.82225300	-1.93470500	-0.45765600
N	1.72146300	-0.45163500	2.15295300	H	-6.86523400	-0.46154600	-2.45439900
C	0.85715700	-0.77918000	3.28038800	N	1.73209500	-0.47645300	2.15183100
H	0.42016500	0.15000900	3.64805600	C	2.58756700	0.68937500	2.38458100
H	0.04797300	-1.42936100	2.96049100	H	1.98428200	1.59012500	2.49678300
H	1.42438200	-1.24410600	4.09579800	H	3.14084800	0.51583600	3.31420900
C	2.58842800	0.70611300	2.37624000	H	3.29199200	0.82008000	1.57073000
H	1.99611600	1.61589800	2.47314900	C	0.89919200	-0.84111400	3.29325000
H	3.13772200	0.53759900	3.31034600	H	0.47270500	0.07539900	3.70191600
H	3.29686600	0.81937500	1.56299300	H	0.08525100	-1.48749300	2.97753600
H	-2.86440200	1.98440100	2.19907400	H	1.49065800	-1.32727100	4.07721100
C	-0.61258900	-1.30175900	-0.75163300	C	-0.62629900	-1.29368700	-0.77010300
N	-0.42464900	-2.16769800	-1.50974600	N	-0.46701500	-2.14408700	-1.55409700
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1-A-13-D-P1234-DCM				1-A-13-D-P1234-DMSO			
C	2.35150800	-3.62497900	0.39276800	C	2.35700400	-3.62518400	0.39786200
C	1.82481600	-2.72931200	1.31462500	C	1.83075700	-2.72810000	1.31869100
H	1.46288400	-3.09881700	2.26309000	H	1.47634100	-3.09577000	2.27066500
C	3.01705900	-3.14938100	-0.72832200	C	3.01735200	-3.15154100	-0.72760000
H	3.51201100	-3.84074800	-1.40028300	H	3.51512000	-3.84358300	-1.39673500
C	1.91579600	-1.33576100	1.09024400	C	1.91819900	-1.33499800	1.09068000
C	3.04821300	-1.76708300	-1.03307100	C	3.04344900	-1.77079400	-1.03632500
C	2.33465300	-0.85314000	-0.21123800	C	2.33180400	-0.85479600	-0.21341200
C	3.76172500	-1.27961900	-2.16615100	C	3.75308000	-1.28535800	-2.17329100
H	4.30464800	-1.98232800	-2.78720000	H	4.29638000	-1.98920400	-2.79272600
C	3.80549100	0.06307100	-2.41432100	C	3.79537300	0.05647500	-2.42567200
H	4.43180800	0.45528000	-3.20820600	H	4.42001600	0.44715800	-3.22154700
C	3.00015900	0.97572000	-1.67450900	C	2.99265200	0.97085900	-1.68441800
C	2.09963300	0.48198000	-0.68710700	C	2.09551100	0.47883700	-0.69172200
C	3.09770500	2.38364300	-1.88474700	C	3.09149900	2.37761400	-1.89651300
H	3.80102300	2.75857100	-2.61921600	H	3.79439100	2.75042700	-2.63241800
C	2.35670500	3.23904100	-1.11468000	C	2.35438800	3.23617100	-1.12453100
H	2.49736600	4.31155500	-1.20352400	H	2.49841500	4.30814100	-1.21383500
C	1.32906100	2.76532000	-0.24977000	C	1.32930300	2.76521400	-0.25650500
C	1.06638500	1.36449100	-0.17456500	C	1.06526900	1.36421400	-0.17770300
C	0.51834000	3.68260800	0.49220200	C	0.52219200	3.68487000	0.48709500
H	0.77958400	4.73552700	0.46789000	H	0.78697400	4.73686300	0.46247100

C	-0.55806900	3.25293700	1.21327300	C	-0.55296100	3.25875900	1.21159900
H	-1.14963200	3.95456200	1.79203900	H	-1.14055100	3.96171400	1.79263300
C	-0.99358800	1.88944700	1.12397900	C	-0.99142700	1.89564500	1.12395900
C	-0.20351800	0.94170800	0.34590500	C	-0.20299800	0.94503100	0.34737200
C	-2.17375900	1.37495100	1.63685000	C	-2.17188100	1.38489900	1.63894000
H	-2.86717200	1.93909800	2.24617400	H	-2.86110100	1.95114200	2.25110200
H	2.31364900	-4.68727900	0.59701200	H	2.32629900	-4.68659800	0.60787900
C	-0.89453100	-0.29009300	0.16640600	C	-0.89695800	-0.28675500	0.17252900
P	-2.40733200	-0.35303300	1.19975100	P	-2.40821300	-0.34472200	1.21012100
C	-3.82796600	-0.36316900	-0.01815100	C	-3.82760300	-0.36006300	-0.00948300
C	-3.87521000	0.48982800	-1.12875300	C	-3.89372900	0.51529500	-1.10203700
C	-4.88416100	-1.25283300	0.20010700	C	-4.86273400	-1.27955100	0.18668000
C	-4.95915000	0.45170200	-2.00187200	C	-4.97437500	0.46948200	-1.97915900
H	-3.05944700	1.18141500	-1.30922600	H	-3.09593500	1.23203300	-1.26446800
C	-5.97484600	-1.28990100	-0.67279600	C	-5.94982100	-1.32532900	-0.69073000
H	-4.85433000	-1.92122000	1.05467700	H	-4.82035700	-1.96369400	1.02814700
C	-6.01296500	-0.43811100	-1.77413800	C	-6.00625400	-0.45144800	-1.77399600
H	-4.98482900	1.11406100	-2.86051600	H	-5.01535800	1.15045700	-2.82248600
H	-6.78794500	-1.98467200	-0.49273700	H	-6.74639200	-2.04288800	-0.52730900
H	-6.85632700	-0.46633000	-2.45519800	H	-6.84736300	-0.48530000	-2.45748500
N	1.74363100	-0.48886200	2.15152000	N	1.74871900	-0.48663600	2.15104500
C	0.94413200	-0.87668700	3.31084800	C	2.60257800	0.68339000	2.37743200
H	0.54068500	0.03238200	3.75709400	H	1.99461100	1.57914200	2.50471400
H	0.11773100	-1.51280400	3.00638800	H	3.16555400	0.50685700	3.29903100
H	1.55788200	-1.38557400	4.06122200	H	3.29725700	0.82053600	1.55666100
C	2.59614000	0.68073500	2.38243100	C	0.95990600	-0.87719700	3.31724500
H	1.98824800	1.57702700	2.50603300	H	0.56385600	0.03118300	3.77129900
H	3.15559300	0.50460200	3.30668900	H	0.13003400	-1.51182100	3.01897800
H	3.29432200	0.81837200	1.56460700	H	1.58064500	-1.38976100	4.05874000
C	-0.64933700	-1.27954300	-0.77878800	C	-0.66255300	-1.27386700	-0.77524000
N	-0.52224500	-2.11865400	-1.58338000	N	-0.54840200	-2.11148700	-1.58470500
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1-A-13-D-P1234-n-hexane				3-A-12-D-P1234			
C	2.33280300	-3.62531400	0.41721600	C	3.55270600	2.76954400	0.58410100
C	1.81183700	-2.72084500	1.33383400	C	2.57822800	2.39748300	-0.39723600
H	1.43988600	-3.08108500	2.28234900	C	4.07339700	1.80998600	1.40001800
C	3.00180100	-3.15945800	-0.70435600	H	4.83742600	2.07761000	2.12166600
H	3.48297400	-3.85816700	-1.37896500	C	2.13176700	1.05330600	-0.43778900
C	1.90871100	-1.33001100	1.09854500	H	1.42172000	0.75842900	-1.18933100
C	3.04747300	-1.77687200	-1.01543100	C	3.66708700	0.44175400	1.32650800
C	2.33599900	-0.85714400	-0.20288100	C	2.59434200	0.07939200	0.45087500
C	3.76685100	-1.29818200	-2.14730500	C	4.36597200	-0.56268600	2.02670200
H	4.30494600	-2.00545200	-2.76745700	H	5.16847200	-0.29068600	2.70248300
C	3.81869400	0.04404100	-2.39722000	C	4.08132300	-1.88151400	1.76472000
H	4.44884900	0.43044000	-3.19114200	H	4.67914200	-2.66109400	2.22569400
C	3.01416700	0.96314700	-1.66592500	C	3.01627100	-2.27987000	0.90670900
C	2.10632700	0.47814700	-0.68490800	C	2.13466900	-1.30520600	0.37656400
C	3.11525700	2.37173800	-1.88324800	C	2.84561800	-3.65609200	0.57369600
H	3.81984200	2.74245900	-2.61876900	H	3.53190000	-4.38843500	0.98349800
C	2.37238500	3.22905600	-1.12139700	C	1.86648000	-4.01721100	-0.30399700
H	2.51099100	4.30142500	-1.21685100	H	1.77984900	-5.04716000	-0.63400800
C	1.33877200	2.76110000	-0.25695900	C	0.89305800	-3.08351300	-0.75882500
C	1.07147100	1.36269500	-0.17954300	C	0.92758900	-1.73234000	-0.28959500
C	0.52691600	3.68254800	0.47735400	C	-0.14413100	-3.51346700	-1.64067900

H	0.78672200	4.73566400	0.44727100	H	-0.11298400	-4.52925600	-2.01809200
C	-0.55399400	3.25543700	1.19440900	C	-1.16538600	-2.67066200	-1.99329600
H	-1.14904700	3.96093000	1.76507200	H	-1.94074300	-3.00189400	-2.67590200
C	-0.99121100	1.89342000	1.11072100	C	-1.28329600	-1.38847200	-1.39528400
C	-0.20329400	0.94209100	0.33632600	C	-0.27037900	-0.92599500	-0.46239200
C	-2.17389200	1.38084500	1.62278500	C	-2.37119700	-0.50116200	-1.53176300
H	-2.87302300	1.94887900	2.22165900	H	3.88163000	3.79390900	0.67937800
H	2.27932500	-4.68700400	0.62139700	C	-0.64938200	0.24001400	0.20561700
C	-0.89312500	-0.28823700	0.15829000	P	-2.16106700	0.95149900	-0.45335200
P	-2.40796300	-0.34601200	1.18493900	C	-3.44199700	0.77899000	0.90163200
C	-3.83049100	-0.36123400	-0.02922300	C	-3.40278300	-0.25258800	1.84714000
C	-3.86381700	0.46606800	-1.15857300	C	-4.47971400	1.71356300	0.95656900
C	-4.90132400	-1.22572800	0.21300900	C	-4.38746600	-0.34613900	2.82704600
C	-4.95070700	0.42749500	-2.02705700	H	-2.59907200	-0.97959200	1.80971300
H	-3.03424800	1.13545100	-1.35743300	C	-5.47057100	1.61674800	1.93469000
C	-5.99500800	-1.26186200	-0.65499900	H	-4.51520400	2.51706400	0.22781300
H	-4.87837100	-1.87571900	1.08183200	C	-5.42437300	0.58783800	2.87203100
C	-6.02014500	-0.43574100	-1.77548700	H	-4.35039800	-1.15043200	3.55432300
H	-4.96534400	1.06826200	-2.90225400	H	-6.27523800	2.34358500	1.96296700
H	-6.82011500	-1.93764800	-0.45746400	H	-6.19228400	0.51096500	3.63404000
H	-6.86556800	-0.46465800	-2.45415400	H	-0.08657700	0.71607400	0.99338400
N	1.73044000	-0.47245000	2.15195000	N	2.08603900	3.30928700	-1.28097700
C	2.58747500	0.69216800	2.38354000	C	1.01231000	2.96850700	-2.22348100
H	1.98577800	1.59420300	2.49388900	H	0.59275000	3.88996800	-2.61968400
H	3.14051000	0.51916500	3.31364800	H	1.40115300	2.37386000	-3.05613100
H	3.29227600	0.82073200	1.56962600	H	0.21670200	2.41777200	-1.72450400
C	0.89193400	-0.83142500	3.29073300	C	2.62548500	4.66661200	-1.33259100
H	0.46308500	0.08702300	3.69264500	H	3.71616300	4.64989000	-1.37090600
H	0.07911400	-1.47858700	2.97378000	H	2.25623300	5.15839800	-2.22880100
H	1.47918400	-1.31409700	4.08023100	H	2.30971800	5.24955000	-0.46126700
C	-0.62351300	-1.29546700	-0.76719000	C	-3.45029400	-0.68407800	-2.39988000
N	-0.45878700	-2.14853400	-1.54671600	N	-4.35123100	-0.82607000	-3.12515400
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3-A-12-D-P1234-CCl4				3-A-12-D-P1234-DCM			
C	3.55757600	2.74079800	0.60613800	C	3.56590200	2.71384500	0.62301600
C	2.60972600	2.37637200	-0.40572600	C	2.63975600	2.35618800	-0.41270000
C	4.04886200	1.77870000	1.43533900	C	4.02972700	1.75036200	1.46459200
H	4.79608500	2.04046200	2.17610000	H	4.76243400	2.00662900	2.22124300
C	2.14889900	1.03594100	-0.45469700	C	2.16385700	1.02023500	-0.46759500
H	1.45945700	0.74697700	-1.22775500	H	1.49364900	0.73598500	-1.25943400
C	3.63456500	0.41284100	1.34930400	C	3.60627100	0.38729900	1.36933300
C	2.58004900	0.06049900	0.44793300	C	2.56759700	0.04369600	0.44619400
C	4.31195500	-0.59707100	2.06174800	C	4.26387700	-0.62671800	2.09313800
H	5.10233600	-0.33024100	2.75344600	H	5.04393200	-0.36383900	2.79769300
C	4.02642600	-1.91505100	1.79353100	C	3.97721100	-1.94439300	1.82079600
H	4.61174200	-2.69807800	2.26391500	H	4.55155000	-2.73025500	2.29924800
C	2.97330000	-2.30362900	0.91769400	C	2.93534500	-2.32461700	0.92955700
C	2.11003700	-1.32023000	0.36944500	C	2.08864200	-1.33375300	0.36434900
C	2.79286600	-3.67932400	0.58648300	C	2.74711800	-3.70011400	0.60027600
H	3.46971100	-4.41570100	1.00464000	H	3.41635800	-4.43902700	1.02599200
C	1.81631900	-4.03753900	-0.29557700	C	1.77351200	-4.05671300	-0.28585300
H	1.72208200	-5.06845500	-0.62036500	H	1.67362900	-5.08832900	-0.60649900
C	0.85362000	-3.09593400	-0.75790500	C	0.81993900	-3.10855200	-0.75514700
C	0.90544400	-1.73966500	-0.30403200	C	0.88671600	-1.74733200	-0.31536900

C	-0.18993000	-3.52365100	-1.63179600	C	-0.22842700	-3.53489100	-1.62171600
H	-0.16899500	-4.54335400	-1.99955700	H	-0.21578800	-4.55789200	-1.98085000
C	-1.20860700	-2.67703200	-1.98839000	C	-1.24562000	-2.68516800	-1.98224200
H	-1.98940100	-3.01332300	-2.66235000	H	-2.03065000	-3.02618100	-2.64904700
C	-1.31195000	-1.38912900	-1.40326200	C	-1.33645100	-1.39274100	-1.40917500
C	-0.28484500	-0.92183800	-0.48748700	C	-0.29708900	-0.92015500	-0.50942600
C	-2.39526600	-0.49142400	-1.53960900	C	-2.41720600	-0.48663100	-1.54518500
H	3.89401200	3.76175800	0.70788300	H	3.90945400	3.73170600	0.72952900
C	-0.64645300	0.25771400	0.16458500	C	-0.64352100	0.27188100	0.12691100
P	-2.16100400	0.97525900	-0.48239400	P	-2.16017600	0.99455900	-0.51040100
C	-3.42072200	0.81488200	0.89529100	C	-3.40295800	0.85064400	0.88543700
C	-3.38693600	-0.22605500	1.83155000	C	-3.38134700	-0.19893500	1.81337100
C	-4.43688500	1.77148000	0.97930600	C	-4.39459400	1.83111800	0.99330700
C	-4.35456800	-0.30747100	2.82983700	C	-4.33657100	-0.26646200	2.82506200
H	-2.60038200	-0.97040900	1.77384200	H	-2.61275000	-0.96075400	1.74118000
C	-5.41065000	1.68810100	1.97656400	C	-5.35577900	1.76281300	2.00477700
H	-4.46899500	2.58344100	0.25971200	H	-4.41680600	2.65234700	0.28383700
C	-5.36952200	0.64936900	2.90374600	C	-5.32713500	0.71445700	2.92205300
H	-4.32096800	-1.11882400	3.54930700	H	-4.31097400	-1.08342900	3.53833300
H	-6.19730700	2.43312100	2.02771500	H	-6.12130300	2.52784100	2.07560300
H	-6.12356900	0.58280900	3.68036200	H	-6.07013500	0.66014200	3.71003100
H	-0.06883400	0.74357800	0.93522600	H	-0.05264300	0.76801900	0.88059400
N	2.16055800	3.28876500	-1.30637800	N	2.22963500	3.26896000	-1.32712900
C	1.13650100	2.94707300	-2.30144900	C	1.23244400	2.93793300	-2.35116600
H	0.76555400	3.86520300	-2.74837200	H	0.88512400	3.85969200	-2.80873900
H	1.55950300	2.31823200	-3.09040800	H	1.67312400	2.30451700	-3.12627400
H	0.30057800	2.42853100	-1.83417600	H	0.37885200	2.42739700	-1.90724100
C	2.70009700	4.64960900	-1.32785800	C	2.79019600	4.62333300	-1.34298100
H	3.79089700	4.63281900	-1.33983700	H	3.87941000	4.58872900	-1.31399000
H	2.35174600	5.15172900	-2.22585600	H	2.48256100	5.11859500	-2.25899800
H	2.36063000	5.21703200	-0.45641300	H	2.42504200	5.20253700	-0.49056500
C	-3.48383100	-0.67446700	-2.39007200	C	-3.51845400	-0.67420300	-2.37143000
N	-4.39874100	-0.81439600	-3.10147100	N	-4.45237900	-0.81572700	-3.06126200
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3-A-12-D-P1234-DMSO				3-A-12-D-P1234-N-HEXANE			
C	3.56608500	2.70783600	0.62330000	C	3.55504900	2.74721400	0.60143900
C	2.64819100	2.34952200	-0.41997600	C	2.60293900	2.38064200	-0.40529200
C	4.02112400	1.74619400	1.47108600	C	4.05213200	1.78598700	1.42852400
H	4.74832900	2.00281700	2.23278000	H	4.80219300	2.04937900	2.16590100
C	2.16843000	1.01463100	-0.47463000	C	2.14549700	1.03922400	-0.45251500
H	1.50540300	0.72975000	-1.27240900	H	1.45233300	0.74874700	-1.22160500
C	3.59587000	0.38354500	1.37519600	C	3.64007000	0.41942700	1.34495000
C	2.56340300	0.04000500	0.44483500	C	2.58252000	0.06456200	0.44813200
C	4.24731900	-0.62960500	2.10513700	C	4.32173400	-0.58904000	2.05554000
H	5.02337900	-0.36589300	2.81368500	H	5.11413000	-0.32080000	2.74442500
C	3.96163300	-1.94812200	1.83413500	C	4.03687700	-1.90735800	1.78882400
H	4.53303400	-2.73338800	2.31681200	H	4.62470800	-2.68939700	2.25783800
C	2.92433000	-2.32836900	0.93836600	C	2.98168900	-2.29837800	0.91632100
C	2.08260000	-1.33697000	0.36473200	C	2.11480000	-1.31703400	0.37095600
C	2.73482200	-3.70479700	0.61304000	C	2.80334800	-3.67435700	0.58540400
H	3.40226200	-4.44273300	1.04319200	H	3.48206400	-4.40968900	1.00238100
C	1.76265900	-4.06398600	-0.27362600	C	1.82634000	-4.03373300	-0.29564100
H	1.66194700	-5.09662700	-0.59056100	H	1.73367200	-5.06466900	-0.62083600
C	0.81128400	-3.11559900	-0.74754600	C	0.86145000	-3.09401200	-0.75699200

C	0.88203500	-1.75135300	-0.31607500	C	0.90984600	-1.73843800	-0.30098400
C	-0.23825600	-3.54468900	-1.61023700	C	-0.18095800	-3.52278200	-1.63205700
H	-0.22728700	-4.56960800	-1.96402500	H	-0.15798600	-4.54196600	-2.00108000
C	-1.25619400	-2.69586300	-1.97395300	C	-1.20031100	-2.67727800	-1.98825200
H	-2.04221600	-3.04097300	-2.63757000	H	-1.98009800	-3.01320200	-2.66353500
C	-1.34396200	-1.40076200	-1.40829700	C	-1.30655300	-1.39010100	-1.40138200
C	-0.30041500	-0.92265600	-0.51599000	C	-0.28201900	-0.92302700	-0.48277200
C	-2.42534300	-0.49348200	-1.54562100	C	-2.39081200	-0.49452900	-1.53812500
H	3.91065000	3.72528400	0.72962000	H	3.88964200	3.76897100	0.70174200
C	-0.64256700	0.27520900	0.11129200	C	-0.64698500	0.25427700	0.17173400
P	-2.16018800	0.99704700	-0.52515800	P	-2.16111500	0.97019600	-0.47777100
C	-3.39693600	0.86507900	0.87738300	C	-3.42434800	0.80802800	0.89623400
C	-3.38976400	-0.19209800	1.79731800	C	-3.38982200	-0.23153400	1.83383000
C	-4.36876100	1.86376600	0.99977100	C	-4.44370200	1.76144700	0.97587900
C	-4.33975400	-0.24963900	2.81465600	C	-4.36001000	-0.31459400	2.82939600
H	-2.63548100	-0.96729700	1.71603800	H	-2.60077600	-0.97344000	1.77899800
C	-5.32438700	1.80625800	2.01760200	C	-5.42001900	1.67623700	1.97031800
H	-4.37918800	2.69181500	0.29799100	H	-4.47633500	2.57197800	0.25471700
C	-5.31041800	0.74989800	2.92613300	C	-5.37816700	0.63900700	2.89904500
H	-4.32462700	-1.07184500	3.52211500	H	-4.32602300	-1.12497500	3.54996500
H	-6.07328700	2.58630000	2.10065300	H	-6.20943300	2.41858400	2.01797900
H	-6.04844400	0.70419300	3.71923700	H	-6.13435600	0.57098400	3.67346800
H	-0.04729300	0.77835200	0.85675400	H	-0.07207000	0.73887600	0.94522500
N	2.25081600	3.26039600	-1.34041600	N	2.14566600	3.29241400	-1.30337700
C	1.26192700	2.93124800	-2.37241200	C	1.11533900	2.94844800	-2.29141700
H	0.92103700	3.85368800	-2.83328300	H	0.73919000	3.86587300	-2.73564500
H	1.70830800	2.29656800	-3.14309300	H	1.53398600	2.32063500	-3.08359900
H	0.40378200	2.42268200	-1.93490500	H	0.28358500	2.42823600	-1.81859700
C	2.81711000	4.61296100	-1.35645400	C	2.68151100	4.65423800	-1.32738600
H	3.90511900	4.57392100	-1.30772200	H	3.77240600	4.64058400	-1.34628900
H	2.52760200	5.10176500	-2.28168400	H	2.32620300	5.15629300	-2.22280000
H	2.43834500	5.19896000	-0.51484200	H	2.34650300	5.22081100	-0.45349400
C	-3.53327200	-0.68760500	-2.35866200	C	-3.47744700	-0.67790800	-2.39210500
N	-4.47671700	-0.83422100	-3.03593200	N	-4.38949100	-0.81849200	-3.10636900
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1-A-11-D-P1234				1-A-11-D-P1234-CCI4			
C	-3.27466800	-2.01121000	-0.45772500	C	-3.38332100	-1.94567800	-0.42738700
C	-2.32270800	-1.47801300	-1.37770900	C	-2.38843400	-1.46421600	-1.33323400
H	-2.01208700	-2.04888000	-2.24019700	H	-2.10224400	-2.04978100	-2.19415100
C	-3.75814400	-1.15717000	0.55948200	C	-3.81961000	-1.07073600	0.59567700
H	-4.54336400	-1.49032900	1.22399500	H	-4.63123000	-1.35900600	1.24894100
C	-1.77173600	-0.24941900	-1.16183000	C	-1.77716000	-0.26495300	-1.11399500
H	-1.05303500	0.13463100	-1.86855700	C	-3.24188100	0.18861100	0.78636300
C	-3.24808200	0.13301500	0.74530300	C	-2.10609700	0.57004700	0.00436000
C	-2.12755400	0.55906500	-0.03217200	C	-3.79005000	1.10937400	1.73478400
C	-3.83428500	1.03027800	1.69175500	H	-4.63684700	0.80421900	2.33870200
H	-4.67381100	0.69530200	2.29016500	C	-3.28803200	2.37058600	1.81057600
C	-3.37245700	2.30650500	1.77609000	H	-3.75074100	3.10744400	2.45838400
H	-3.86312900	3.02521700	2.42396000	C	-2.13392000	2.76365100	1.06250600
C	-2.21989100	2.73725400	1.04751400	C	-1.42869100	1.80824400	0.28650800
C	-1.48227800	1.81048600	0.27152600	C	-1.71165000	4.12633800	1.04892600
C	-1.82222400	4.10860800	1.06195500	H	-2.26270500	4.85360600	1.63429000
H	-2.39628900	4.81719000	1.64827200	C	-0.67710500	4.51231700	0.24373400
C	-0.77781100	4.52261800	0.28712100	H	-0.41369300	5.56200400	0.16153100

H	-0.52779200	5.57729500	0.22970700	C	0.12694600	3.56136800	-0.45120500
C	0.05767000	3.59707800	-0.40773600	C	-0.14603600	2.17107800	-0.29003100
C	-0.19770300	2.20102900	-0.27825000	C	1.23045000	3.98677400	-1.25360700
C	1.17191000	4.05370800	-1.17618500	H	1.37673900	5.05106800	-1.40426200
H	1.30780500	5.12244400	-1.30230500	C	2.07767300	3.08115500	-1.82694400
C	2.04301900	3.16957700	-1.74748300	H	2.89174700	3.41339200	-2.46246400
H	2.86677600	3.52512800	-2.35739200	C	1.97020500	1.68965100	-1.51463900
C	1.94724500	1.77128400	-1.46913600	C	0.88891000	1.23957900	-0.65160000
C	0.85567700	1.28744400	-0.63969600	C	2.86449100	0.69102500	-1.88418400
C	2.86234900	0.79198600	-1.84301400	H	3.70518900	0.84421400	-2.54707100
H	3.71310400	0.97130700	-2.48599800	C	1.05934100	-0.11464600	-0.25318200
C	1.03048800	-0.07495900	-0.27455600	P	2.39456800	-0.90574600	-1.22264400
P	2.39513200	-0.82492300	-1.23584900	C	3.69988700	-1.36454000	0.03282800
C	3.67465100	-1.30642700	0.03774700	C	4.22653400	-0.43625300	0.94003600
C	4.18233300	-0.39389000	0.97072000	C	4.17086400	-2.68011500	0.05325500
C	4.14629600	-2.62140000	0.04407800	C	5.20548200	-0.82165900	1.85126800
C	5.14284600	-0.79486600	1.89415700	H	3.86665800	0.58661100	0.92966000
H	3.82210300	0.62879800	0.96932000	C	5.15365500	-3.06748500	0.96687000
C	5.11049100	-3.02420600	0.97000800	H	3.76724400	-3.40434400	-0.64691400
H	3.75721100	-3.33213500	-0.67780800	C	5.67166900	-2.13878800	1.86581600
C	5.60930300	-2.11148300	1.89520900	H	5.60548700	-0.09694900	2.55237800
H	5.52835200	-0.08235400	2.61570100	H	5.51073500	-4.09162500	0.97494200
H	5.46866800	-4.04808500	0.96715600	H	6.43438900	-2.43665700	2.57690600
H	6.35804200	-2.42145200	2.61603700	H	-1.03589100	0.07824700	-1.81839000
N	-3.72636100	-3.29464700	-0.57329900	N	-3.91937000	-3.18938300	-0.56393400
C	-3.16540400	-4.18503400	-1.58682900	C	-4.93136400	-3.67980700	0.37171100
H	-2.08006500	-4.26242600	-1.47746600	H	-5.85053000	-3.09105700	0.30204600
H	-3.59881600	-5.17496300	-1.46943000	H	-5.16574200	-4.71243000	0.12911700
H	-3.39210100	-3.82708200	-2.59532700	H	-4.56105700	-3.64078300	1.39890700
C	-4.67919800	-3.84306100	0.38851000	C	-3.46424300	-4.08080900	-1.63043000
H	-5.61501400	-3.27751500	0.38178400	H	-2.38705800	-4.25097300	-1.55890800
H	-4.90265000	-4.87200500	0.11873300	H	-3.97421000	-5.03531400	-1.53601500
H	-4.26532400	-3.83033100	1.40138600	H	-3.69069500	-3.66230400	-2.61506900
C	0.38614600	-0.81767500	0.71599900	C	0.43801100	-0.81153700	0.78158000
N	-0.10552900	-1.49430000	1.52999900	N	-0.02251700	-1.44702400	1.64664100
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1-A-11-D-P1234-DCM				1-A-11-D-P1234-DMSO			
C	-3.47204400	-1.89630100	-0.40386900	C	-3.49882300	-1.87414200	-0.40071100
C	-2.44299500	-1.45874300	-1.29669800	C	-2.46358700	-1.44654000	-1.29253200
H	-2.18383800	-2.05060400	-2.16189400	H	-2.21608600	-2.03642100	-2.16248700
C	-3.86691600	-1.00969400	0.62802100	C	-3.87811600	-0.98764900	0.63805300
H	-4.69187200	-1.26495600	1.27779100	H	-4.70641100	-1.23397700	1.28690700
C	-1.78498400	-0.28503600	-1.07443300	C	-1.78999800	-0.28240600	-1.06679200
H	-1.02989100	0.02665000	-1.77896800	H	-1.03301100	0.02212800	-1.77258200
C	-3.23555400	0.22115400	0.82428500	C	-3.23014200	0.23318400	0.83791900
C	-2.09046800	0.56948400	0.03592900	C	-2.08409000	0.57347700	0.04565500
C	-3.74845100	1.15567400	1.78084200	C	-3.72911100	1.16919100	1.80124700
H	-4.59828100	0.87204300	2.39071300	H	-4.57915000	0.89122500	2.41329600
C	-3.21594900	2.40430000	1.85145100	C	-3.18583600	2.41298800	1.87354900
H	-3.65430300	3.15277300	2.50261400	H	-3.61492900	3.16327100	2.52869200
C	-2.06662000	2.77170700	1.08172200	C	-2.03919600	2.77407800	1.09599100
C	-1.38912300	1.79619000	0.30030300	C	-1.37332800	1.79398500	0.30801000
C	-1.63109600	4.12766200	1.04409300	C	-1.59802700	4.12701100	1.05422000
H	-2.16407400	4.86749200	1.63019300	H	-2.12357200	4.86976900	1.64319300

C	-0.61045400	4.49590600	0.20907100	C	-0.58239300	4.49116900	0.20920000
H	-0.34307500	5.54251500	0.10515500	H	-0.31331300	5.53685500	0.10114200
C	0.16890700	3.52920100	-0.48810000	C	0.18701900	3.52112100	-0.49229700
C	-0.11113700	2.14179300	-0.30188200	C	-0.09700600	2.13423100	-0.30242500
C	1.25988000	3.93538600	-1.31865300	C	1.27422400	3.92204700	-1.33099800
H	1.40757000	4.99649600	-1.48945600	H	1.42349400	4.98232900	-1.50547500
C	2.09331400	3.01790900	-1.89229000	C	2.10205200	3.00140100	-1.90715600
H	2.89726400	3.33562300	-2.54769100	H	2.90291800	3.31523500	-2.56809200
C	1.98471300	1.63168200	-1.55185400	C	1.99146300	1.61600600	-1.56155200
C	0.91210100	1.20212800	-0.66572300	C	0.92046600	1.19177700	-0.67016500
C	2.86951900	0.62443800	-1.91625500	C	2.87216100	0.60621800	-1.92690500
H	3.70113600	0.76325000	-2.59382200	H	3.70073700	0.74168400	-2.60893700
C	1.08650900	-0.14678500	-0.24551500	C	1.09365300	-0.15771400	-0.24816300
P	2.40557900	-0.96055300	-1.21887900	P	2.40778200	-0.97682400	-1.22497300
C	3.72678700	-1.39950400	0.02720700	C	3.73019300	-1.41549200	0.01990400
C	4.26586000	-0.45807100	0.91428200	C	4.30964200	-0.46279100	0.86912700
C	4.19517200	-2.71628400	0.06388800	C	4.15589200	-2.74527600	0.09708100
C	5.25433500	-0.83107200	1.82111600	C	5.29469700	-0.83745000	1.77936900
H	3.90940300	0.56593500	0.89242600	H	3.98869800	0.57174400	0.81405500
C	5.18727500	-3.09148600	0.97335400	C	5.14352300	-3.12239900	1.01089800
H	3.78382800	-3.45170200	-0.61991800	H	3.71586500	-3.48944800	-0.55884400
C	5.71754800	-2.14953500	1.85177300	C	5.71360700	-2.16923400	1.85179200
H	5.66467600	-0.09599600	2.50512100	H	5.73743600	-0.09336900	2.43269500
H	5.54225800	-4.11604100	0.99346500	H	5.46514700	-4.15675600	1.06239800
H	6.48765900	-2.43772400	2.55867200	H	6.48133600	-2.45870000	2.56065600
N	-4.07657100	-3.10116100	-0.56161600	N	-4.12272500	-3.06649000	-0.56562600
C	-3.65524900	-4.01488400	-1.62477000	C	-5.23111700	-3.46650100	0.30576200
H	-2.57745600	-4.18193300	-1.58246300	H	-6.06269300	-2.76274400	0.22455800
H	-4.15955600	-4.96737600	-1.49143100	H	-5.57845300	-4.44933600	0.00264900
H	-3.91487100	-3.61586800	-2.60979900	H	-4.90544000	-3.51717800	1.34718000
C	-5.17369800	-3.51622700	0.31573700	C	-3.72282500	-3.97865000	-1.63886200
H	-6.01896200	-2.82854700	0.23459100	H	-2.64643000	-4.15580500	-1.61061100
H	-5.50486200	-4.50684200	0.01936500	H	-4.23440400	-4.92679500	-1.50377700
H	-4.84383700	-3.55576300	1.35652600	H	-3.99133300	-3.57135100	-2.61797000
C	0.49088400	-0.81304700	0.81981300	C	0.50508300	-0.81714700	0.82330700
N	0.06214300	-1.42295300	1.72089100	N	0.08449600	-1.42164900	1.73288300
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1-A-11-D-P1234-N-HEXANE				3-A-10-D-P1234			
C	-3.36199300	-1.95852100	-0.43302800	C	-3.22441200	-2.13173000	-1.48676500
C	-2.37491400	-1.46698300	-1.34144000	C	-2.10441900	-1.52728100	-2.02533900
H	-2.08352600	-2.04999300	-2.20236800	C	-3.94625600	-1.49788900	-0.44593400
C	-3.80796700	-1.08702600	0.58841500	C	-1.61184900	-0.34835300	-1.47558100
H	-4.61547600	-1.38375200	1.24308200	H	-0.78709600	0.15100100	-1.95436800
C	-1.77517600	-0.26182600	-1.12278500	C	-3.40598400	-0.30935600	0.18561000
H	-1.03790300	0.08924000	-1.82749400	C	-2.17622500	0.22215900	-0.30139300
C	-3.24321200	0.17859700	0.77810300	C	-4.03056000	0.33618600	1.28632100
C	-2.10989600	0.56843900	-0.00258100	H	-4.87840600	-0.10350400	1.78755000
C	-3.79940300	1.09537400	1.72539300	C	-3.56434100	1.55378100	1.71021200
H	-4.64525500	0.78470400	2.32786400	H	-4.09909000	2.08677900	2.48996900
C	-3.30512000	2.35962100	1.80272300	C	-2.38810500	2.14476400	1.18572900
H	-3.77365700	3.09327100	2.45003500	C	-1.56466900	1.37997600	0.31738700
C	-2.15071000	2.75964000	1.05902900	C	-2.01908900	3.48062500	1.52570100
C	-1.43887600	1.80940600	0.28367000	H	-2.66314700	4.05779500	2.17932100
C	-1.73286200	4.12403100	1.05069100	C	-0.89767500	4.02541600	0.97334500

H	-2.28848400	4.84793800	1.63593800	H	-0.65061800	5.06615800	1.15705300
C	-0.69596600	4.51511500	0.25163900	C	0.02644600	3.24265400	0.22029300
H	-0.43487400	5.56575700	0.17408900	C	-0.22415700	1.85034300	0.02478400
C	0.11426600	3.56868800	-0.44289100	C	1.23300600	3.82957000	-0.26108800
C	-0.15560100	2.17738300	-0.28731700	H	1.37189000	4.89824300	-0.14179000
C	1.22004300	3.99951700	-1.23899400	C	2.21007600	3.06169800	-0.84333200
H	1.36470700	5.06462200	-1.38529000	H	3.11904500	3.51919400	-1.21867800
C	2.07148100	3.09753200	-1.81196400	C	2.09278200	1.64847100	-0.87308300
H	2.88740900	3.43384100	-2.44295800	C	0.88745000	1.00943100	-0.36326000
C	1.96584200	1.70477400	-1.50576100	C	3.08217300	0.73111400	-1.27687600
C	0.88277900	1.24898600	-0.64834400	H	-3.62287000	-3.02258100	-1.95126800
C	2.86338400	0.70915300	-1.87628800	C	1.01535800	-0.37881900	-0.26683200
H	3.70583000	0.86651500	-2.53593200	P	2.51744300	-0.98454100	-1.04274800
C	1.05368700	-0.10654300	-0.25523000	C	3.55134800	-1.67641600	0.35761300
P	2.39338100	-0.89097700	-1.22390800	C	3.58589700	-1.09009200	1.62868100
C	3.69491500	-1.35439200	0.03372300	C	4.32290900	-2.81544200	0.11328700
C	4.22091200	-0.42861800	0.94373500	C	4.37965200	-1.63506300	2.63384400
C	4.16407900	-2.67054500	0.05242200	H	2.99088300	-0.20474200	1.82370700
C	5.19737100	-0.81719500	1.85617100	C	5.12125800	-3.36184100	1.12006900
H	3.86244800	0.59473400	0.93426700	H	4.30284600	-3.27274400	-0.87072600
C	5.14432500	-3.06106700	0.96727400	C	5.14951600	-2.77278500	2.38124900
H	3.76089100	-3.39256600	-0.65027400	H	4.40367400	-1.17103600	3.61432800
C	5.66167100	-2.13491000	1.86911100	H	5.72055800	-4.24283200	0.91667400
H	5.59690800	-0.09442800	2.55957100	H	5.77018400	-3.19367300	3.16483900
H	5.50006500	-4.08570400	0.97404600	H	0.28878600	-1.04276000	0.17527900
H	6.42253600	-2.43523700	2.58118100	C	4.31576000	1.08263000	-1.83278600
N	-3.88201300	-3.21030000	-0.56521700	N	5.34565200	1.36958500	-2.29519600
C	-3.41006400	-4.10129700	-1.62434100	H	-1.62859400	-1.95136000	-2.90017600
H	-2.33100500	-4.25723500	-1.54672700	N	-5.16596000	-2.02937500	-0.09662400
H	-3.90824700	-5.06190500	-1.52761100	C	-5.46051800	-3.44274700	-0.32156500
H	-3.63670600	-3.69140700	-2.61257200	H	-6.18741000	-3.76159700	0.42772400
C	-4.88278600	-3.71225900	0.37578400	H	-5.89668600	-3.61420900	-1.31286300
H	-5.80850600	-3.13299600	0.31301000	H	-4.56211800	-4.04453600	-0.20713400
H	-5.10862900	-4.74684700	0.13301500	C	-6.35528200	-1.22370700	0.18697300
H	-4.50677100	-3.67113700	1.40104000	H	-7.15706400	-1.55949300	-0.47816200
C	0.42761300	-0.81076900	0.77231200	H	-6.69199700	-1.35884200	1.21883800
N	-0.03932900	-1.45235700	1.62912200	H	-6.16280300	-0.17239000	0.00024900
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3-A-10-D-P1234-CCI4				3-A-10-D-P1234-DCM			
C	-3.23939900	-2.11051200	-1.50390300	C	-3.24528700	-2.09824300	-1.51527700
C	-2.12754700	-1.50227700	-2.05147800	C	-2.14341100	-1.48403100	-2.07252000
C	-3.95402400	-1.48284800	-0.45147000	C	-3.95618500	-1.47553600	-0.45471300
C	-1.62476300	-0.32761100	-1.50037300	C	-1.63535900	-0.30991500	-1.52298300
H	-0.80628400	0.17340100	-1.98886100	H	-0.82427600	0.19452800	-2.02101600
C	-3.40129700	-0.29689300	0.18066000	C	-3.39659500	-0.28871500	0.17524600
C	-2.17516600	0.23496800	-0.31812900	C	-2.17511000	0.24613400	-0.33508600
C	-4.01019200	0.34428300	1.29146700	C	-3.99390700	0.34924800	1.29278400
H	-4.85529500	-0.09345100	1.79759500	H	-4.83528600	-0.08832700	1.80395400
C	-3.54078000	1.56031600	1.71791800	C	-3.52515700	1.56622600	1.71971400
H	-4.06983200	2.08997800	2.50337200	H	-4.05179800	2.09341400	2.50796400
C	-2.36843000	2.15066000	1.18499100	C	-2.35711100	2.15738700	1.17966900
C	-1.55645400	1.38880300	0.30270900	C	-1.55298600	1.39847400	0.28641700
C	-1.99298500	3.48380300	1.53063200	C	-1.97838200	3.48908900	1.52930700
H	-2.63404400	4.05866200	2.18922700	H	-2.61909000	4.06175400	2.19008200

C	-0.87137600	4.02945400	0.98004500	C	-0.85590700	4.03636900	0.98237900
H	-0.61980000	5.06813600	1.16875300	H	-0.60216200	5.07371300	1.17491700
C	0.04740700	3.24337300	0.22268600	C	0.06067300	3.24763700	0.22381100
C	-0.21540700	1.85596500	0.01082000	C	-0.21173000	1.86407300	-0.00295400
C	1.25975600	3.82501100	-0.24931000	C	1.27865500	3.82487100	-0.23640600
H	1.40519000	4.89178500	-0.12023100	H	1.42900000	4.88991600	-0.09827700
C	2.23641600	3.05668700	-0.83463800	C	2.25743300	3.05626900	-0.82172900
H	3.14919100	3.51497300	-1.19982100	H	3.17460900	3.51571200	-1.17472100
C	2.10936700	1.64593500	-0.87628900	C	2.12197300	1.64828700	-0.87510400
C	0.89461400	1.01161200	-0.38318700	C	0.89831700	1.01757900	-0.40022200
C	3.09675000	0.72116000	-1.28088800	C	3.10903500	0.71688000	-1.27923900
H	-3.64153500	-2.99813100	-1.97014100	H	-3.64790800	-2.98521300	-1.98096300
C	1.01207300	-0.37713500	-0.29669100	C	1.00681100	-0.37191400	-0.32331700
P	2.51839100	-0.99316000	-1.05740400	P	2.51753000	-0.99672600	-1.06807700
C	3.53099600	-1.68835500	0.35776900	C	3.51193200	-1.69732800	0.35744300
C	3.56599300	-1.09117200	1.62426200	C	3.51906200	-1.11569700	1.63225000
C	4.28539200	-2.84288900	0.13057700	C	4.28193000	-2.84229600	0.13002200
C	4.34287300	-1.63969100	2.64111400	C	4.28465100	-1.66836000	2.65607400
H	2.98394200	-0.19472500	1.80794300	H	2.92205600	-0.22963500	1.81915800
C	5.06645900	-3.39385800	1.14916200	C	5.05210100	-3.39730500	1.15532600
H	4.26554300	-3.31065800	-0.84858300	H	4.28119800	-3.30244500	-0.85301200
C	5.09528800	-2.79321700	2.40523500	C	5.05368300	-2.81121900	2.41908600
H	4.36635600	-1.16735000	3.61756000	H	4.28410100	-1.20963800	3.63914400
H	5.65116200	-4.28744600	0.95892100	H	5.64682800	-4.28415000	0.96523900
H	5.70192800	-3.21754400	3.19781300	H	5.64946500	-3.24001400	3.21728500
H	0.27056600	-1.03984900	0.12160000	H	0.25261600	-1.03349800	0.07340100
C	4.33492300	1.06325100	-1.82274500	C	4.35332600	1.04963500	-1.80136300
N	5.37465000	1.33835600	-2.27577600	N	5.40523900	1.31307300	-2.23927700
H	-1.66607700	-1.92025200	-2.93683800	H	-1.69437100	-1.89738600	-2.96646700
N	-5.16600700	-2.01494500	-0.10124700	N	-5.16079900	-2.00983700	-0.10446900
C	-6.34578500	-1.22212100	0.25546400	C	-6.33300700	-1.23177600	0.30868700
H	-7.17781700	-1.56981000	-0.36229800	H	-7.18344100	-1.58584400	-0.27787400
H	-6.61903200	-1.36539000	1.30430000	H	-6.56027700	-1.38969500	1.36593800
H	-6.17901400	-0.16852100	0.05698100	H	-6.18696600	-0.17500300	0.11088700
C	-5.46874400	-3.42570200	-0.35020200	C	-5.46786700	-3.41852100	-0.37284600
H	-6.18492800	-3.75341300	0.40430100	H	-6.17494500	-3.75425200	0.38564300
H	-5.92077600	-3.57000200	-1.33724400	H	-5.93194200	-3.54147300	-1.35604600
H	-4.57157300	-4.03286200	-0.26136300	H	-4.57094900	-4.02804500	-0.30460800
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3-A-10-D-P1234-DMSO				3-A-10-D-P1234-N-HEXANE			
C	-3.24806600	-2.09637400	-1.51687700	C	-3.23893000	-2.11541200	-1.49923300
C	-2.14966100	-1.48065200	-2.07786200	C	-2.12463100	-1.50923600	-2.04482000
C	-3.95750400	-1.47439700	-0.45403900	C	-3.95450800	-1.48532800	-0.44944500
C	-1.63971400	-0.30621400	-1.52984500	C	-1.62282200	-0.33394400	-1.49440700
H	-0.83125600	0.19902800	-2.03161700	H	-0.80274100	0.16580000	-1.98134300
C	-3.39513700	-0.28729400	0.17469200	C	-3.40232700	-0.29998200	0.18306600
C	-2.17556900	0.24855000	-0.34047200	C	-2.17530300	0.23096900	-0.31380800
C	-3.98798600	0.34970700	1.29456700	C	-4.01304500	0.34167400	1.29281600
H	-4.82736900	-0.08816900	1.80840900	H	-4.85828400	-0.09660600	1.79859400
C	-3.51974800	1.56753000	1.72080500	C	-3.54347600	1.55766200	1.71884200
H	-4.04541300	2.09422500	2.50985200	H	-4.07262300	2.08782300	2.50398100
C	-2.35391000	2.15915500	1.17723700	C	-2.37079800	2.14803700	1.18642900
C	-1.55247500	1.40103100	0.28024000	C	-1.55735300	1.38551600	0.30622200
C	-1.97466600	3.49085900	1.52710600	C	-1.99638800	3.48178300	1.53048800

H	-2.61549500	4.06286400	2.18829100	H	-2.63748300	4.05709900	2.18865100
C	-0.85235400	4.03892700	0.98072900	C	-0.87547200	4.02735800	0.97835200
H	-0.59845000	5.07612600	1.17361200	H	-0.62474100	5.06652500	1.16560600
C	0.06369100	3.24913500	0.22210800	C	0.04374300	3.24182000	0.22119200
C	-0.21148500	1.86649400	-0.00886600	C	-0.21664600	1.85337200	0.01315700
C	1.28311500	3.82497000	-0.23461600	C	1.25444400	3.82456800	-0.25399100
H	1.43462700	4.88959100	-0.09434300	H	1.39847400	4.89181200	-0.12742100
C	2.26314500	3.05617000	-0.81936400	C	2.23086400	3.05633500	-0.83921900
H	3.18147500	3.51634000	-1.16864400	H	3.14240600	3.51460700	-1.20742900
C	2.12541400	1.64919100	-0.87567800	C	2.10609200	1.64501700	-0.87761100
C	0.89893600	1.01955300	-0.40688300	C	0.89362400	1.00975200	-0.38008700
C	3.11294500	0.71536300	-1.27870600	C	3.09386600	0.72167200	-1.28206100
H	-3.65122900	-2.98314900	-1.98192100	H	-3.64127000	-3.00322400	-1.96518200
C	1.00480700	-0.37017800	-0.33251400	C	1.01351300	-0.37876700	-0.29080300
P	2.51701700	-0.99813000	-1.07150500	P	2.51891700	-0.99294000	-1.05469300
C	3.50676600	-1.69940200	0.35679200	C	3.53650400	-1.68540400	0.35814200
C	3.50415000	-1.12348900	1.63449100	C	3.57377600	-1.08706700	1.62392300
C	4.28393200	-2.83971000	0.12861600	C	4.29238400	-2.83860400	0.12973900
C	4.26769300	-1.67637500	2.65997600	C	4.35437000	-1.63335600	2.63902100
H	2.89992900	-0.24267700	1.82336400	H	2.99078400	-0.19136000	1.80809800
C	5.05217200	-3.39488300	1.15552300	C	5.07718700	-3.38723100	1.14657900
H	4.28918700	-3.29764600	-0.85546400	H	4.27086300	-3.30674100	-0.84919900
C	5.04441100	-2.81400800	2.42186300	C	5.10824700	-2.78558500	2.40203600
H	4.25824700	-1.22311700	3.64547300	H	4.37987700	-1.16000800	3.61494600
H	5.65120600	-4.27869400	0.96513900	H	5.66332600	-4.27969300	0.95539000
H	5.63743900	-3.24373400	3.22151400	H	5.71803000	-3.20801600	3.19323800
H	0.24670600	-1.03133700	0.05737800	H	0.27502300	-1.04168800	0.13251200
C	4.36051300	1.04420000	-1.79084000	C	4.33075800	1.06555100	-1.82762900
N	5.41834700	1.30255500	-2.22006400	N	5.36825700	1.34290800	-2.28328800
H	-1.70522700	-1.89320400	-2.97454100	H	-1.66056200	-1.92907800	-2.92793800
N	-5.16045200	-2.00775500	-0.10425000	N	-5.16940000	-2.01446000	-0.10047500
C	-6.32883500	-1.23284000	0.32606900	C	-6.34945200	-1.21587200	0.24151600
H	-7.18514600	-1.58866500	-0.25017100	H	-7.17632800	-1.55910200	-0.38600600
H	-6.54151800	-1.39414400	1.38564400	H	-6.63609400	-1.35672100	1.28716200
H	-6.18795100	-0.17542800	0.12802200	H	-6.17471600	-0.16315600	0.04525900
C	-5.47119800	-3.41511400	-0.37912700	C	-5.47404900	-3.42492300	-0.34570100
H	-6.17511200	-3.75273200	0.38119000	H	-6.19411800	-3.74921000	0.40680000
H	-5.94022500	-3.52995800	-1.36061800	H	-5.92223500	-3.57278900	-1.33422000
H	-4.57522700	-4.02659000	-0.31853200	H	-4.57836900	-4.03354000	-0.25098100
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I-D-13-A-1P234				I-D-13-A-1P234-CCI4			
C	5.21347700	0.57882600	-0.19209200	C	-5.21668700	-0.54708700	-0.17497500
C	4.20425600	1.23380700	-0.86805200	C	-4.21320400	-1.20822400	-0.85424900
H	4.39626700	2.19276300	-1.33635600	H	-4.41128300	-2.16947400	-1.31538100
C	5.00530800	-0.72438400	0.29978100	C	-5.00121100	0.75844000	0.30726000
H	5.82570700	-1.28801300	0.72868500	H	-5.81723000	1.32666200	0.73883700
C	2.91609300	0.64942300	-1.03110800	C	-2.92533800	-0.62663200	-1.02806700
C	3.74268600	-1.33496200	0.18266600	C	-3.73644300	1.36103500	0.18940200
C	2.62887800	-0.61759300	-0.36757100	C	-2.62550300	0.63667500	-0.36068200
C	3.55739200	-2.70965400	0.56132300	C	-3.54272200	2.73401700	0.57165400
H	4.41807400	-3.25014000	0.94231000	H	-4.39904400	3.27955100	0.95523800
C	2.37716300	-3.35882300	0.35711500	C	-2.35646200	3.37216000	0.37319500
H	2.29410600	-4.42547200	0.53904000	H	-2.26249200	4.43657500	0.56264000
C	1.22993200	-2.64691700	-0.10283100	C	-1.21261800	2.65176200	-0.08697500

C	1.33695100	-1.22946300	-0.29824700	C	-1.32952400	1.23548700	-0.28942600
C	0.02273000	-3.31701900	-0.42533400	C	-0.00142300	3.31530800	-0.39850400
H	0.00030700	-4.39859800	-0.33285400	H	0.03052900	4.39546800	-0.29451200
C	-1.08404300	-2.64496700	-0.90817500	C	1.10266400	2.63642100	-0.88605300
H	-1.95851100	-3.18416900	-1.25094800	H	1.98226200	3.17209200	-1.22123600
C	-1.07031900	-1.23672900	-0.86214100	C	1.07732400	1.23107800	-0.85568000
C	0.07384500	-0.54469000	-0.42960100	C	-0.07165600	0.53932900	-0.42465000
C	-1.44573000	1.29203900	-0.64439000	C	1.44066600	-1.30080300	-0.65806500
H	6.18656000	1.04699100	-0.09382200	H	-6.18988600	-1.01277400	-0.06670700
C	-3.80754800	-0.29512100	-0.31438300	C	3.80995500	0.28666500	-0.30991000
C	-4.82628700	-0.85919800	1.81141300	C	4.81757300	0.78507200	1.83761500
C	-5.07903300	-0.01996300	-0.83128500	C	5.08772500	0.08407500	-0.84467800
C	-6.08883600	-0.56766500	1.29211600	C	6.08788700	0.56929300	1.29903700
C	-6.21384500	-0.14777100	-0.02950400	C	6.22168200	0.21845500	-0.04194900
H	-5.18260400	0.28891500	-1.86615300	H	5.19744900	-0.17477500	-1.89238800
H	-7.19251500	0.07082900	-0.44187800	H	7.20551300	0.05713500	-0.46801800
P	-2.35676800	-0.08739900	-1.45356200	P	2.36193000	0.08037400	-1.45101800
C	-0.23850700	0.84006000	-0.08352000	C	0.23231500	-0.84756900	-0.09158400
C	0.49275600	1.74485900	0.76548400	C	-0.50338000	-1.76212200	0.74695800
C	0.19060600	3.13538400	0.67208100	C	-0.20836200	-3.15271900	0.62939100
C	-0.90784200	3.57046900	-0.03496200	C	0.89006700	-3.58259100	-0.08086100
C	-1.76692600	2.64203600	-0.65505600	C	1.75763100	-2.64987600	-0.68496600
H	0.76892800	3.84625000	1.24524400	H	-0.79025900	-3.87074900	1.18922200
H	-1.14253800	4.62743100	-0.06458100	H	1.12017300	-4.64005200	-0.12298900
H	-2.65903100	2.99070800	-1.16239600	H	2.65182000	-2.99611100	-1.19005700
C	-3.69299300	-0.72244700	1.01501700	C	3.68577200	0.64356700	1.03969900
H	-6.97011200	-0.67573900	1.91437200	H	6.96779100	0.68116000	1.92249200
H	-4.72641300	-1.19562900	2.83764100	H	4.71059100	1.06568300	2.87969200
H	-2.71694000	-0.95914100	1.42301100	H	2.70407300	0.81937100	1.46476400
N	1.35658700	1.30864700	1.73470500	N	-1.35960500	-1.33871200	1.72672400
C	2.36922600	2.19337300	2.29674800	C	-1.11576700	-0.13851500	2.52770700
H	3.20530800	1.57774400	2.62985200	H	-2.02727100	0.45522300	2.59871200
H	2.73396500	2.88136500	1.53901700	H	-0.81865100	-0.45350400	3.53601800
H	1.98206700	2.75135500	3.15939100	H	-0.32299800	0.46284300	2.09785800
C	1.11232400	0.10538900	2.52901900	C	-2.33945800	-2.24700800	2.31360100
H	2.02159500	-0.49242000	2.59207500	H	-3.15943700	-1.64711400	2.70810800
H	0.81683400	0.41367500	3.54088400	H	-2.73603000	-2.91909400	1.55730600
H	0.31799200	-0.49181900	2.09576300	H	-1.90500200	-2.82462400	3.13889500
C	2.04975100	1.24061700	-1.97114100	C	-2.08007700	-1.20733400	-1.99086400
N	1.37536900	1.76143700	-2.76828900	N	-1.43298600	-1.71547000	-2.82008000
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1-D-13-A-1P234-DCM				1-D-13-A-1P234-DMSO			
C	-5.22469600	-0.50651500	-0.18106700	C	-5.22853100	-0.49336800	-0.18259800
C	-4.22534100	-1.17302300	-0.86188600	C	-4.23093500	-1.16290800	-0.86334400
H	-4.42937300	-2.13386700	-1.32128600	H	-4.43727100	-2.12428800	-1.32055900
C	-4.99879200	0.79645700	0.30286800	C	-4.99817900	0.80896700	0.30047100
H	-5.81004700	1.36800300	0.73924500	H	-5.80720800	1.38195500	0.73911400
C	-2.93414800	-0.59888800	-1.03291200	C	-2.93844000	-0.59216700	-1.03381000
C	-3.73016000	1.38822300	0.19378500	C	-3.72836100	1.39666500	0.19321900
C	-2.62123500	0.65729300	-0.35629800	C	-2.62029700	0.66260400	-0.35657400
C	-3.52626000	2.75637400	0.59016100	C	-3.52070300	2.76340900	0.59330000
H	-4.37752000	3.30512500	0.98009200	H	-4.36962300	3.31320200	0.98667200
C	-2.33273600	3.38272600	0.40445300	C	-2.32492400	3.38546700	0.41046100
H	-2.22626300	4.44266700	0.61106300	H	-2.21375700	4.44368700	0.62300600

C	-1.19243000	2.65505900	-0.05939300	C	-1.18610900	2.65488300	-0.05522600
C	-1.32078300	1.24107100	-0.27633400	C	-1.31832200	1.24130400	-0.27517800
C	0.02383900	3.31117000	-0.35514400	C	0.03141300	3.30810600	-0.34725300
H	0.06782100	4.38879600	-0.23269300	H	0.07985300	4.38481900	-0.21929600
C	1.12526000	2.62613200	-0.85089900	C	1.13197100	2.62020300	-0.84569100
H	2.01066400	3.15950900	-1.17449500	H	2.01916600	3.15260300	-1.16613500
C	1.08706300	1.22446900	-0.84269500	C	1.08994400	1.22017200	-0.84247000
C	-0.06840600	0.53315900	-0.41558400	C	-0.06757500	0.52921300	-0.41456400
C	1.43403700	-1.31189300	-0.66958200	C	1.43327900	-1.31696600	-0.66917300
H	-6.20004500	-0.96679800	-0.07055100	H	-6.20460900	-0.95138300	-0.07008000
C	3.81641700	0.27012500	-0.30704400	C	3.81962400	0.26625100	-0.30734700
C	4.82083600	0.64143800	1.86750000	C	4.82478400	0.61885100	1.86982700
C	5.09598600	0.20140900	-0.87061300	C	5.09834000	0.22143200	-0.87542100
C	6.09458000	0.56498700	1.29837700	C	6.09792500	0.56750900	1.29618300
C	6.23104700	0.34471300	-0.07007400	C	6.23365800	0.36852800	-0.07576600
H	5.20693700	0.03761900	-1.93701500	H	5.20883900	0.07251500	-1.94400700
H	7.21664500	0.28857400	-0.51811400	H	7.21868700	0.33096200	-0.52691700
P	2.36747300	0.06966400	-1.44553900	P	2.37020900	0.06288700	-1.44336200
C	0.22597500	-0.85491900	-0.09572500	C	0.22447100	-0.85759700	-0.09496000
C	-0.51697100	-1.77615500	0.73139800	C	-0.52126200	-1.77926600	0.72999500
C	-0.23120000	-3.16643700	0.59418200	C	-0.23844200	-3.16951600	0.58979200
C	0.86501400	-3.59474900	-0.12138400	C	0.85773900	-3.59893800	-0.12576800
C	1.74119300	-2.66096500	-0.71384100	C	1.73715700	-2.66606800	-0.71586700
H	-0.81470300	-3.88829700	1.14704600	H	-0.82213800	-3.89119500	1.14263500
H	1.08990400	-4.65292600	-0.17204700	H	1.08161900	-4.65737200	-0.17565800
H	2.63575400	-3.00789700	-1.21770800	H	2.63279000	-3.01430600	-1.21691700
C	3.68863200	0.49445600	1.07101200	C	3.69217700	0.46878000	1.07427500
H	6.97450500	0.68055300	1.92103200	H	6.97796200	0.68506400	1.91826700
H	4.71158700	0.81664500	2.93202100	H	4.71602000	0.77627500	2.93710300
H	2.70502500	0.55838600	1.52241600	H	2.70952100	0.51196900	1.53002000
N	-1.37182100	-1.36018200	1.71477700	N	-1.37697100	-1.36314700	1.71221200
C	-2.34110800	-2.27944700	2.30532800	C	-2.34471100	-2.28403200	2.30372300
H	-3.14978700	-1.68619600	2.73142600	H	-3.15014600	-1.69155300	2.73684600
H	-2.75316800	-2.93904100	1.54610300	H	-2.76026400	-2.94111600	1.54412500
H	-1.88857600	-2.87172500	3.10917200	H	-1.88834000	-2.87930900	3.10274100
C	-1.12170300	-0.16952700	2.52934000	C	-1.12411100	-0.17476300	2.52978800
H	-2.03088100	0.42713500	2.60756600	H	-2.03221400	0.42342200	2.60952600
H	-0.82967800	-0.49866000	3.53371800	H	-0.83413100	-0.50783300	3.53312000
H	-0.32317200	0.43101800	2.10948200	H	-0.32283700	0.42400500	2.11279400
C	-2.10013000	-1.17494600	-2.00568900	C	-2.10754000	-1.16972000	-2.00741900
N	-1.46823600	-1.67329900	-2.85432400	N	-1.48007200	-1.66651800	-2.86101000
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1-D-13-A-1P234-N-HEXANE				3-D-13-A-1P234			
C	5.21549200	0.55461500	-0.17394400	C	-5.35669100	1.36256200	-0.55168100
C	4.21129200	1.21510800	-0.85257900	C	-4.33125000	1.81779300	0.25580300
H	4.40827500	2.17658900	-1.31368300	H	-4.36577600	2.81622400	0.67506000
C	5.00151200	-0.75128600	0.30805400	C	-5.37679800	0.03786500	-1.00354500
H	5.81825200	-1.31898800	0.73888600	H	-6.22239100	-0.34543300	-1.56149200
C	2.92375900	0.63262800	-1.02650800	C	-3.23878200	0.96750000	0.60854700
C	3.73742200	-1.35560000	0.18854100	C	-4.29160200	-0.82916500	-0.71362100
C	2.62614700	-0.63226100	-0.36157600	C	-3.14599100	-0.34746300	-0.00566900
C	3.54545000	-2.72945000	0.56823600	C	-4.34971700	-2.20984700	-1.07525700
H	4.40254900	-3.27427100	0.95112000	H	-5.24200400	-2.56485400	-1.58061800
C	2.36065800	-3.36978900	0.36711000	C	-3.36848700	-3.09321900	-0.71457100

H	2.26897000	-4.43492200	0.55367100	H	-3.48566300	-4.15650200	-0.89462900
C	1.21629500	-2.65080200	-0.09292300	C	-2.17662200	-2.62347600	-0.10776900
C	1.33104100	-1.23402200	-0.29243200	C	-2.00794400	-1.21620000	0.09952100
C	0.00629600	-3.31564800	-0.40809500	C	-1.16941400	-3.53205400	0.33179000
H	-0.02356100	-4.39623000	-0.30759000	H	-1.36950800	-4.59475400	0.23483800
C	-1.09821900	-2.63792900	-0.89461000	C	0.00885500	-3.10605300	0.89756800
H	-1.97646700	-3.17421100	-1.23231700	H	0.73256300	-3.81566600	1.27970100
C	-1.07553300	-1.23200500	-0.85981300	C	0.28990500	-1.72298500	0.87444100
C	0.07206200	-0.54029400	-0.42730400	C	-0.65830600	-0.79891200	0.40360800
C	-1.44192900	1.29907400	-0.65675300	C	1.28906900	0.60483800	0.57576600
H	6.18842100	1.02098600	-0.06608400	H	-6.17694000	2.02902800	-0.79660900
C	-3.80838700	-0.28926700	-0.31102600	C	3.14333700	-1.55880400	0.28123200
C	-4.81574300	-0.80974300	1.83137600	C	3.93708200	-2.32263900	-1.87766900
C	-5.08533300	-0.06402700	-0.83864500	C	4.42657100	-1.75605100	0.80414500
C	-6.08487800	-0.57043100	1.30035900	C	5.21690300	-2.50617800	-1.34984000
C	-6.21835600	-0.19722300	-0.03458200	C	5.46080900	-2.22293300	-0.00875600
H	-5.19509500	0.21118900	-1.88221100	H	4.61559300	-1.55027400	1.85262200
H	-7.20149600	-0.01806100	-0.45511700	H	6.45013700	-2.37264000	0.40914900
P	-2.36106000	-0.08169200	-1.45322800	P	1.83387200	-0.92708100	1.43718100
C	-0.23396500	0.84603600	-0.09110100	C	-0.04479800	0.48157800	0.09065700
C	0.50010800	1.75840600	0.75046900	C	-0.56377900	1.52878000	-0.70905400
C	0.20412200	3.14916900	0.63727300	C	0.15769800	2.68370800	-0.90194400
C	-0.89392300	3.58014900	-0.07281700	C	1.44118300	2.85688100	-0.31230400
C	-1.75982900	2.64832900	-0.68024200	C	2.00470400	1.76408700	0.41372900
H	0.78533000	3.86577000	1.19975000	H	-0.26817400	3.46535600	-1.51401600
H	-1.12467100	4.63756600	-0.11281200	H	2.99289400	1.84811100	0.84434600
H	-2.65349700	2.99512700	-1.18590200	C	2.90689000	-1.85241500	-1.06896400
C	-3.68466800	-0.66887400	1.03232900	H	6.01664000	-2.87571400	-1.98195400
H	-6.96426200	-0.68183800	1.92464400	H	3.74228100	-2.55013200	-2.91999900
H	-4.70907300	-1.10836700	2.86848900	H	1.91444200	-1.72059000	-1.48521600
H	-2.70378400	-0.86352900	1.45099400	H	-1.53240200	1.42226700	-1.17246200
N	1.35610000	1.33224300	1.72946300	N	2.12614800	4.03000500	-0.44770600
C	2.33988300	2.23654300	2.31499100	C	3.47148700	4.18326600	0.10218500
H	3.16194100	1.63404100	2.70132100	H	3.86446500	5.15381900	-0.19013400
H	2.73298700	2.91145100	1.55944200	H	3.46173500	4.12809400	1.19539400
H	1.91102200	2.81078100	3.14577100	H	4.14287200	3.41218900	-0.28339100
C	1.11139900	0.13054600	2.52759300	C	1.50760200	5.18087000	-1.10222400
H	2.02189100	-0.46501200	2.59609100	H	0.54037400	5.41070300	-0.64911400
H	0.81521500	0.44320800	3.53707600	H	2.15630100	6.04573800	-0.98739100
H	0.31751300	-0.46862800	2.09661500	H	1.36038800	4.99803500	-2.17152600
C	2.07577900	1.21587000	-1.98585700	C	-2.40951400	1.38889800	1.66610200
N	1.42500200	1.72715600	-2.80987500	N	-1.76476300	1.79311300	2.55147300
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3-D-13-A-1P234-CCl4				3-D-13-A-1P234-DCM			
C	-5.36794100	1.35508700	-0.54121600	C	-5.38631900	1.34187800	-0.51910300
C	-4.34693500	1.80562400	0.27421900	C	-4.36711400	1.78849200	0.30052900
H	-4.38639500	2.80089200	0.70109900	H	-4.41068000	2.78065100	0.73472700
C	-5.38133500	0.03159300	-1.00268100	C	-5.39234700	0.02023400	-0.99154600
H	-6.22511700	-0.35074600	-1.56439300	H	-6.23544800	-0.36117300	-1.55522400
C	-3.25338900	0.95546300	0.62329700	C	-3.26975400	0.94007000	0.63989600
C	-4.29466700	-0.83185000	-0.72059700	C	-4.30238500	-0.83815600	-0.72296700
C	-3.14844900	-0.35305300	-0.00844000	C	-3.15306000	-0.36127700	-0.00978900
C	-4.34567000	-2.21044800	-1.09871900	C	-4.34540500	-2.21370900	-1.12046800
H	-5.23544500	-2.56539800	-1.60856200	H	-5.23296800	-2.56840800	-1.63420300

C	-3.35774300	-3.08892100	-0.74985900	C	-3.34850500	-3.08634000	-0.78858000
H	-3.46602600	-4.15049900	-0.94537100	H	-3.44639400	-4.14533900	-1.00272800
C	-2.16640800	-2.61993800	-0.13628500	C	-2.15655700	-2.61764900	-0.16992200
C	-2.00601000	-1.21302200	0.08785300	C	-2.00538200	-1.21112900	0.07320700
C	-1.15666600	-3.52825200	0.28809400	C	-1.14311600	-3.52466500	0.23626700
H	-1.34695500	-4.59053700	0.17062600	H	-1.32251900	-4.58596100	0.09659400
C	0.01956100	-3.10126000	0.86498200	C	0.03230600	-3.09686200	0.82387400
H	0.74737800	-3.81242700	1.23610200	H	0.76481000	-3.80985100	1.18191600
C	0.29172300	-1.71886500	0.86310900	C	0.29474000	-1.71593500	0.84480600
C	-0.65827600	-0.79006400	0.39863400	C	-0.65873500	-0.78223400	0.38836400
C	1.28576000	0.61570600	0.58388600	C	1.28172300	0.62611000	0.58536000
H	-6.18934900	2.02083300	-0.78397100	H	-6.21037100	2.00594900	-0.75667100
C	3.14768200	-1.55262800	0.28803400	C	3.15700100	-1.54477700	0.29741100
C	3.96309900	-2.26925000	-1.87921300	C	4.00554800	-2.21814400	-1.87098900
C	4.41353600	-1.80362200	0.83015100	C	4.40305700	-1.84186300	0.86181100
C	5.22562600	-2.50916900	-1.33157600	C	5.24819100	-2.50671000	-1.30081400
C	5.44997300	-2.27633500	0.02283800	C	5.44607600	-2.31844900	0.06493000
H	4.58878300	-1.63369800	1.88722900	H	4.55943100	-1.70269800	1.92611100
H	6.42583100	-2.46767900	0.45490600	H	6.40681700	-2.54474500	0.51334700
P	1.83295800	-0.92060100	1.43518700	P	1.83145400	-0.91351600	1.42853100
C	-0.05042200	0.49391500	0.10044100	C	-0.05766800	0.50484600	0.10502900
C	-0.57150400	1.54862200	-0.68946000	C	-0.58382500	1.56823100	-0.67137800
C	0.15336200	2.70037900	-0.88593200	C	0.14176400	2.71910200	-0.86827900
C	1.44431000	2.86807900	-0.30557800	C	1.44113200	2.88103600	-0.30011200
C	2.00483100	1.77199100	0.42167900	C	2.00233900	1.78070400	0.42381800
H	-0.27258400	3.48491100	-1.49383900	H	-0.28448300	3.50582900	-1.47292500
H	2.99752800	1.85079400	0.84214600	H	2.99916000	1.85555700	0.83456100
C	2.93054400	-1.79441000	-1.07595600	C	2.96601800	-1.74042600	-1.07813800
H	6.02725100	-2.88164900	-1.95944300	H	6.05550600	-2.87990000	-1.92077600
H	3.78387100	-2.45576400	-2.93234100	H	3.84780000	-2.36735600	-2.93334700
H	1.95250200	-1.61722800	-1.50917700	H	2.00480900	-1.52288900	-1.53026700
H	-1.54164800	1.44768300	-1.15127600	H	-1.55545100	1.47181800	-1.13154600
N	2.13571900	4.03003300	-0.45283700	N	2.13681700	4.03399600	-0.45749600
C	3.47555400	4.18642400	0.11546100	C	3.48730400	4.18184100	0.09214800
H	3.85270700	5.17335400	-0.13731200	H	3.85856000	5.17288200	-0.15059100
H	3.45211500	4.09296700	1.20459700	H	3.47905800	4.07077900	1.17911800
H	4.16314700	3.44011300	-0.29010800	H	4.16660900	3.44178300	-0.33735800
C	1.54297600	5.16633500	-1.15892700	C	1.55446500	5.16727600	-1.17995300
H	0.59135700	5.45170000	-0.70431200	H	0.60708700	5.46827200	-0.72739900
H	2.22188500	6.01245900	-1.10079800	H	2.24284900	6.00577100	-1.13428400
H	1.37387800	4.92870200	-2.21310500	H	1.38244400	4.91415200	-2.22955900
C	-2.44300000	1.36017100	1.69891300	C	-2.46941800	1.32935300	1.72583500
N	-1.82283700	1.74716900	2.61092100	N	-1.86265600	1.69636300	2.65679300
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3-D-13-A-1P234-DMSO				3-D-13-A-1P234-N-HEXANE			
C	-5.39614200	1.33103500	-0.50353900	C	-5.36523900	1.35659800	-0.54416200
C	-4.37709200	1.77606700	0.31713400	C	-4.34360200	1.80808500	0.26999700
H	-4.42281900	2.76627800	0.75570400	H	-4.38221300	2.80399100	0.69535600
C	-5.39833500	0.01099300	-0.98247700	C	-5.37991400	0.03277000	-1.00354300
H	-6.24127400	-0.36983600	-1.54689500	H	-6.22392400	-0.34983200	-1.56466900
C	-3.27679500	0.92918200	0.64959300	C	-3.25044100	0.95785500	0.62033900
C	-4.30587600	-0.84455500	-0.72211200	C	-4.29364100	-0.83138400	-0.71945400
C	-3.15498000	-0.36805200	-0.00914300	C	-3.14771900	-0.35200400	-0.00792200
C	-4.34441700	-2.21818200	-1.12949100	C	-4.34602200	-2.21048400	-1.09411000

H	-5.23105100	-2.57287600	-1.64473000	H	-5.23626500	-2.56553100	-1.60307200
C	-3.34253200	-3.08777900	-0.80703400	C	-3.35946900	-3.08986800	-0.74264800
H	-3.43517400	-4.14530200	-1.03052900	H	-3.46950800	-4.15184300	-0.93494500
C	-2.15015400	-2.61866500	-0.18687900	C	-2.16809600	-2.62067300	-0.13033000
C	-2.00422900	-1.21255000	0.06568100	C	-2.00613100	-1.21366600	0.09039300
C	-1.13366800	-3.52402300	0.21019900	C	-1.15883300	-3.52903100	0.29707000
H	-1.30723000	-4.58482100	0.06036500	H	-1.35097900	-4.59144700	0.18359400
C	0.04150600	-3.09510100	0.80195600	C	0.01771100	-3.10212400	0.87181900
H	0.77690900	-3.80837600	1.15340600	H	0.74479400	-3.81293300	1.24508800
C	0.29849300	-1.71473900	0.83325800	C	0.29151800	-1.71954200	0.86581500
C	-0.65810900	-0.77996600	0.38130300	C	-0.65810000	-0.79171100	0.40001400
C	1.27921400	0.63179600	0.58189400	C	1.28646500	0.61381900	0.58293000
H	-6.22219500	1.99385000	-0.73718200	H	-6.18633500	2.02249500	-0.78763900
C	3.16459000	-1.53819300	0.30128600	C	3.14660800	-1.55373400	0.28630200
C	4.03364800	-2.19116300	-1.86505600	C	3.95717900	-2.27737900	-1.88039700
C	4.39961600	-1.85687200	0.87807500	C	4.41552600	-1.79686300	0.82478100
C	5.26509500	-2.50262600	-1.28244100	C	5.22276700	-2.50900200	-1.33646200
C	5.44724600	-2.33532800	0.08833200	C	5.45106900	-2.26875800	0.01593800
H	4.54446400	-1.73207700	1.94569500	H	4.59356800	-1.62174900	1.88057900
H	6.39956200	-2.57800900	0.54592900	H	6.42928500	-2.45409600	0.44533700
P	1.83186800	-0.90815100	1.42243400	P	1.83343000	-0.92175000	1.43583000
C	-0.06176800	0.50890300	0.10380900	C	-0.04918200	0.49165100	0.09897700
C	-0.59249100	1.57539100	-0.66587000	C	-0.56965000	1.54471600	-0.69322700
C	0.13120400	2.72744200	-0.86224800	C	0.15467600	2.69696800	-0.88927300
C	1.43395000	2.88884900	-0.29975100	C	1.44398300	2.86600000	-0.30664300
C	1.99821600	1.78717700	0.42114100	C	2.00484900	1.77068500	0.42083200
H	-0.29712200	3.51484500	-1.46449400	H	-0.27140500	3.48098500	-1.49780500
H	2.99711800	1.86151000	0.82660300	H	2.99682500	1.85037500	0.84294200
C	2.98921200	-1.71214800	-1.07933700	C	2.92555900	-1.80320300	-1.07561300
H	6.07636600	-2.87605000	-1.89701500	H	6.02364400	-2.88114500	-1.96550600
H	3.88874400	-2.32262300	-2.93152400	H	3.77477400	-2.47002000	-2.93189300
H	2.03742200	-1.47545500	-1.54165800	H	1.94492700	-1.63283400	-1.50569400
H	-1.56495600	1.47947700	-1.12460200	H	-1.53946500	1.44269500	-1.15541900
N	2.12888600	4.04015100	-0.45989100	N	2.13417300	4.02998000	-0.45160300
C	3.48254800	4.18723300	0.08367300	C	3.47227500	4.18785100	0.11943400
H	3.84955200	5.18092000	-0.15380000	H	3.85013600	5.17431900	-0.13456800
H	3.47975200	4.06796600	1.16958100	H	3.44681500	4.09664000	1.20887000
H	4.16040900	3.45163800	-0.35529700	H	4.16124300	3.44092600	-0.28279400
C	1.54764000	5.17183600	-1.18664100	C	1.53886600	5.16700700	-1.15370400
H	0.60338700	5.47875700	-0.73162500	H	0.58603500	5.44817100	-0.69883800
H	2.23968500	6.00744900	-1.14862100	H	2.21527000	6.01503500	-1.09208700
H	1.37057300	4.91249200	-2.23364600	H	1.37089800	4.93325400	-2.20903000
C	-2.47785500	1.31119700	1.73810700	C	-2.43719100	1.36583000	1.69308900
N	-1.87268100	1.66692900	2.67521800	N	-1.81338600	1.75664000	2.60064600
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2-D-10-A-12P34				2-D-10-A-12P34-CCI4			
C	-2.50033100	-2.72475100	0.49457000	C	-2.53611900	-2.70846900	0.49268200
C	-2.13899700	-4.01499200	-0.00970000	C	-2.19682100	-3.99492700	-0.04013300
H	-2.76159500	-4.87647000	0.18318500	H	-2.83081800	-4.85019600	0.14116100
C	-1.67727800	-1.61918200	0.16667500	C	-1.70110100	-1.60671000	0.17537200
H	-1.90659700	-0.64731800	0.56724600	H	-1.91681400	-0.64054800	0.59731600
C	-0.99018700	-4.16036200	-0.73177500	C	-1.05557400	-4.14398400	-0.77060400
H	-0.70578100	-5.14580900	-1.08484700	H	-0.78728200	-5.12643900	-1.14345000
C	-3.63056100	1.71771800	-1.07819400	C	-3.60639200	1.76889300	-1.05954100

C	-2.43636100	0.98528700	-1.19178900	C	-2.42019900	1.02286400	-1.16996000
C	-3.64938900	2.96429900	-0.48070900	C	-3.60824500	3.02046600	-0.47375400
H	-4.57570400	3.51545300	-0.37560900	H	-4.52841600	3.58195300	-0.36788700
C	-2.44054400	3.55718700	-0.04163000	C	-2.38932300	3.60142600	-0.04243600
C	-1.18652400	2.86311600	-0.21250400	C	-1.14231500	2.89109700	-0.20906600
C	-1.20798000	1.50711500	-0.70357500	C	-1.18499100	1.53012700	-0.68950200
C	0.05226800	3.49888900	0.02237500	C	0.10463200	3.51054600	0.01852000
H	0.04756000	4.52693700	0.36633600	H	0.11986800	4.54106600	0.35483400
C	1.26292400	2.88206500	-0.28097700	C	1.30553100	2.87133400	-0.28501300
H	2.18678200	3.44587100	-0.21774700	H	2.23820900	3.42129700	-0.22763700
C	1.26849900	1.54466400	-0.66060500	C	1.29074800	1.53307000	-0.65740200
C	0.04856600	0.80902100	-0.73360000	C	0.06134800	0.81036500	-0.72040000
C	1.63300800	-0.89762200	-1.32840700	C	1.61663600	-0.91412500	-1.32976300
C	3.77795300	0.25616400	0.15885000	C	3.78102200	0.21043900	0.16318300
C	4.17836700	-0.00587600	2.53465800	C	4.16768400	-0.09310600	2.53698900
C	5.12945200	-0.01786000	-0.08109500	C	5.13722200	-0.04377700	-0.07278700
C	5.52089100	-0.29456400	2.28496400	C	5.51607300	-0.35944300	2.29122500
C	5.99568800	-0.30013000	0.97559900	C	5.99993100	-0.33456300	0.98510200
H	5.50811900	-0.00019900	-1.09811900	H	5.52250500	-0.00676000	-1.08665400
H	7.04070200	-0.51020000	0.77573400	H	7.04847500	-0.52924300	0.78848900
P	2.69254700	0.60811400	-1.31331500	P	2.70005500	0.57296100	-1.30904200
C	0.31253300	-0.61654600	-0.92949300	C	0.30110100	-0.61679200	-0.91977100
C	-0.53685100	-1.74732800	-0.63821200	C	-0.56640200	-1.73764800	-0.63637800
C	-0.12210500	-3.06338100	-1.02568300	C	-0.17227100	-3.05363800	-1.04806100
C	1.14689300	-3.26164500	-1.59393200	C	1.09024900	-3.26350600	-1.62425800
C	2.02694200	-2.19003500	-1.69310500	C	1.98983800	-2.20589800	-1.71306300
H	1.45404000	-4.25732600	-1.89252700	H	1.37886200	-4.25976600	-1.93859300
H	3.03485100	-2.35959000	-2.05713400	H	2.99271400	-2.38770600	-2.08451600
C	3.31141400	0.26640300	1.47951600	C	3.30488900	0.18878000	1.48067700
H	6.19423700	-0.50350900	3.10883600	H	6.18611700	-0.57624500	3.11570400
H	3.80787900	0.01122100	3.55397600	H	3.78950800	-0.10198700	3.55352100
H	2.27252500	0.50218000	1.68071700	H	2.26117700	0.40397100	1.68016000
H	-2.44522300	0.04051600	-1.71639000	H	-2.44524600	0.06765000	-1.67438100
N	-3.60485900	-2.55663300	1.27531200	N	-3.62617400	-2.54231100	1.28719700
C	-4.37159500	-3.71204700	1.73461300	C	-4.41833100	-3.69440500	1.71839000
H	-3.72044300	-4.44894100	2.21118600	H	-3.77811200	-4.46655700	2.14937900
H	-5.10737300	-3.38036400	2.46287100	H	-5.12664300	-3.37049600	2.47603300
H	-4.89856900	-4.19293400	0.90419600	H	-4.97653400	-4.12261500	0.88027900
C	-4.02462600	-1.23339400	1.74839800	C	-4.02031800	-1.22273900	1.79174600
H	-5.07758200	-1.27865400	2.01921000	H	-5.05768200	-1.26934000	2.11404700
H	-3.44937800	-0.93065500	2.63006400	H	-3.40045300	-0.93018700	2.64541500
H	-3.90418600	-0.48252400	0.97000700	H	-3.93597000	-0.46633500	1.01360900
C	-2.46189500	4.85012200	0.52582300	C	-2.39735100	4.89711800	0.51371900
N	-2.47709800	5.91283500	0.99914300	N	-2.40647000	5.96517700	0.97859300
H	-4.54982400	1.30319000	-1.47899000	H	-4.53267800	1.35725300	-1.44601800
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2-D-10-A-12P34-DCM				2-D-10-A-12P34-DMSO			
C	-2.58885800	-2.67710200	0.48800200	C	-2.61570100	-2.65854600	0.48566100
C	-2.27999200	-3.96063100	-0.07293600	C	-2.32150600	-3.94162200	-0.08501800
H	-2.93197700	-4.80461900	0.09562300	H	-2.98290100	-4.77913100	0.07859600
C	-1.73445900	-1.58514200	0.18264500	C	-1.75108900	-1.57285000	0.18472200
H	-1.92874500	-0.62451300	0.62768200	H	-1.93494600	-0.61388700	0.63792900
C	-1.14797600	-4.12007400	-0.81303700	C	-1.19327300	-4.10813000	-0.82849300
H	-0.90280900	-5.10014800	-1.20687000	H	-0.95951700	-5.08777000	-1.23004600

C	-3.57241800	1.84206900	-1.02647600	C	-3.55489400	1.87795200	-1.01204400
C	-2.39925000	1.07555200	-1.14035700	C	-2.38871300	1.10097300	-1.12858000
C	-3.54593000	3.09873400	-0.45368700	C	-3.51391500	3.13608200	-0.44376400
H	-4.45552500	3.67633800	-0.34199800	H	-4.41788600	3.72181700	-0.32855000
C	-2.31124500	3.66001400	-0.03857600	C	-2.27174300	3.68650800	-0.03598800
C	-1.07772400	2.92411900	-0.20256400	C	-1.04556300	2.93803000	-0.19994100
C	-1.15240800	1.55900900	-0.67254500	C	-1.13613700	1.57191000	-0.66639000
C	0.18179900	3.51828700	0.01653500	C	0.22025400	3.51939400	0.01535500
H	0.22430400	4.54984800	0.34755800	H	0.27584300	4.55082100	0.34501400
C	1.36753400	2.84868400	-0.29014500	C	1.39815800	2.83541100	-0.29363900
H	2.31262200	3.37803400	-0.23875000	H	2.34914300	3.35455600	-0.24482100
C	1.32282900	1.51098800	-0.65743700	C	1.33870400	1.49838400	-0.65929300
C	0.07886000	0.80895000	-0.70847800	C	0.08742500	0.80713200	-0.70515800
C	1.59404800	-0.94186100	-1.33398200	C	1.58328400	-0.95723600	-1.33577800
C	3.78313000	0.14120400	0.16786500	C	3.78389700	0.10641200	0.16930400
C	4.14536400	-0.22071600	2.53803100	C	4.13324300	-0.28652200	2.53672400
C	5.14702700	-0.07945500	-0.05760100	C	5.15212200	-0.09315800	-0.04940100
C	5.50307200	-0.44986400	2.30280800	C	5.49603400	-0.49288700	2.30831100
C	6.00282700	-0.37936500	1.00408400	C	6.00436100	-0.39641700	1.01451500
H	5.54376100	-0.01279800	-1.06535700	H	5.55495800	-0.00912500	-1.05336900
H	7.05722900	-0.54837300	0.81575800	H	7.06210300	-0.54934600	0.83150300
P	2.71117600	0.51829300	-1.30683100	P	2.71658000	0.48961700	-1.30701400
C	0.28534300	-0.61971200	-0.91139300	C	0.27783700	-0.62213500	-0.90867200
C	-0.60709500	-1.72534900	-0.63653800	C	-0.62676400	-1.71966200	-0.63678200
C	-0.24279200	-3.04262700	-1.07428800	C	-0.27700600	-3.03827200	-1.08379700
C	1.01091600	-3.27148300	-1.66023200	C	0.97289700	-3.27767000	-1.67282800
C	1.93681100	-2.23403900	-1.73815500	C	1.91129100	-2.25033900	-1.74693600
H	1.27419400	-4.26915700	-1.99148300	H	1.22435200	-4.27653000	-2.00952500
H	2.93284700	-2.43435300	-2.11804400	H	2.90442000	-2.46058900	-2.12903600
C	3.29033100	0.07199800	1.47809800	C	3.28218600	0.01047300	1.47470500
H	6.16684100	-0.67605700	3.12974200	H	6.15656100	-0.72308300	3.13668900
H	3.75400500	-0.26898100	3.54835300	H	3.73487800	-0.35697400	3.54294600
H	2.23892000	0.25398300	1.67054500	H	2.22658200	0.17259100	1.66219900
H	-2.45013700	0.11142200	-1.62519300	H	-2.45250000	0.13396900	-1.60601200
N	-3.66449000	-2.50757000	1.29541700	N	-3.68584100	-2.48484500	1.29742200
C	-4.47551700	-3.65269300	1.71591800	C	-4.50470200	-3.62538300	1.71687600
H	-3.84223900	-4.45550300	2.09541100	H	-3.87523900	-4.43981900	2.07635700
H	-5.14473700	-3.33445300	2.51020000	H	-5.15706800	-3.30799700	2.52531700
H	-5.07510300	-4.03210300	0.88341400	H	-5.12153400	-3.98617700	0.88883500
C	-4.04001800	-1.18996800	1.81763300	C	-4.05359300	-1.16677200	1.82317700
H	-5.07290000	-1.23149700	2.15339000	H	-5.08679800	-1.20352300	2.15828900
H	-3.40568000	-0.91341100	2.66551900	H	-3.41792400	-0.89748500	2.67229900
H	-3.95943500	-0.42821900	1.04430800	H	-3.96835900	-0.40392100	1.05152000
C	-2.29126200	4.96211100	0.49721300	C	-2.23684900	4.99096100	0.49188600
N	-2.27704300	6.03927300	0.94353000	N	-2.20935100	6.07135100	0.93055900
H	-4.51002700	1.43839900	-1.39241000	H	-4.49798500	1.47968600	-1.36919700
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2-D-10-A-12P34-N-HEXANE				2-D-12-A-12P34			
C	-2.52880200	-2.71208500	0.49329300	C	-2.63751600	-2.23916200	0.52669600
C	-2.18523900	-3.99917900	-0.03448700	C	-2.42864300	-3.52743400	-0.06369200
H	-2.81685100	-4.85578500	0.14907100	H	-3.15058100	-4.31907400	0.06876600
C	-1.69632200	-1.60936900	0.17394300	C	-1.67326200	-1.22996500	0.28310600
H	-1.91498600	-0.64211500	0.59173700	H	-1.77727800	-0.26758500	0.75018600
C	-1.04255200	-4.14729900	-0.76339000	C	-1.30368300	-3.76227700	-0.79690700

H	-0.77106600	-5.13028300	-1.13262400	H	-1.13988200	-4.74933900	-1.21580200
C	-3.61120900	1.75858700	-1.06384400	C	-3.24131000	2.39180300	-0.41198900
C	-2.42336600	1.01530900	-1.17440900	C	-2.13654100	1.55862000	-0.74777100
C	-3.61669300	3.00926200	-0.47588700	C	-3.00262700	3.63923000	0.20867700
H	-4.53818100	3.56861700	-0.37048400	H	-3.84298700	4.27032200	0.47454200
C	-2.39989300	3.59270900	-0.04266800	C	-1.71648200	4.05399800	0.45330000
C	-1.15132100	2.88578700	-0.21000600	H	-1.53524200	5.03043800	0.88858100
C	-1.18962700	1.52567200	-0.69230300	C	-0.58674300	3.22786500	0.14096600
C	0.09395200	3.50865200	0.01887600	C	-0.82196500	1.90113600	-0.38456900
H	0.10520300	4.53883500	0.35634200	C	0.72701700	3.70761800	0.27869800
C	1.29685500	2.87387800	-0.28446500	H	0.87303800	4.71569500	0.65330800
H	2.22776800	3.42667100	-0.22610700	C	1.82625400	2.95922300	-0.14508900
C	1.28621700	1.53565400	-0.65793800	H	2.81726500	3.39827000	-0.15025400
C	0.05878600	0.81025800	-0.72281400	C	1.62886200	1.64373400	-0.55236900
C	1.61988000	-0.91065700	-1.32930400	C	0.33540300	1.04905500	-0.54397700
C	3.78046700	0.21986500	0.16235000	C	1.66464500	-0.80343600	-1.29996900
C	4.17015800	-0.07502300	2.53662500	C	4.01128600	0.06702400	0.08736700
C	5.13561000	-0.03883600	-0.07463400	C	4.49267100	-0.34659900	2.42658700
C	5.51726200	-0.34638200	2.28984900	C	5.32662600	-0.29222600	-0.22819200
C	5.99910700	-0.32802600	0.98293700	C	5.79866700	-0.71677300	2.10096600
H	5.51945000	-0.00600100	-1.08922200	C	6.21488400	-0.68887900	0.77231500
H	7.04686000	-0.52616800	0.78549100	H	5.65982400	-0.25333200	-1.26033000
P	2.69848700	0.58021000	-1.30978200	H	7.23146300	-0.96421400	0.51365500
C	0.30334500	-0.61664300	-0.92150600	P	2.89058000	0.56523600	-1.31364300
C	-0.56054600	-1.73953000	-0.63659000	C	0.41101600	-0.39221600	-0.81172700
C	-0.16226500	-3.05548700	-1.04377000	C	-0.55887000	-1.43395900	-0.55167100
C	1.10158100	-3.26295500	-1.61833500	C	-0.31426000	-2.76007000	-1.03417600
C	1.99733200	-2.20254100	-1.70899600	C	0.90576100	-3.07745500	-1.66178800
H	1.39388000	-4.25909900	-1.92969100	C	1.89560300	-2.11290400	-1.74560300
H	3.00125400	-2.38187300	-2.07891100	H	1.07746400	-4.08368200	-2.02585000
C	3.30645600	0.20502700	1.48063000	H	2.86186000	-2.37075500	-2.16659700
H	6.18803000	-0.56164600	3.11415500	C	3.60408400	0.04205300	1.42769500
H	3.79368600	-0.07830200	3.55383800	H	6.48903600	-1.01710300	2.88139700
H	2.26380800	0.42478400	1.68065000	H	4.16786600	-0.35845600	3.46147900
H	-2.44497800	0.06189800	-1.68244200	H	2.59430500	0.33802600	1.68851400
N	-3.62139000	-2.54581300	1.28550500	H	-2.33098100	0.64731000	-1.29229100
C	-4.41000000	-3.69876600	1.71955000	N	-3.74301900	-2.00335100	1.29418900
H	-3.76873300	-4.46483300	2.16028300	C	-4.12387800	-0.68266800	1.79760300
H	-5.12524200	-3.37358500	2.47019300	H	-4.86598800	-0.22346100	1.13457500
H	-4.96049300	-4.13639400	0.88109800	H	-4.55520500	-0.80142700	2.79249300
C	-4.01858900	-1.22571800	1.78635800	H	-3.27039900	-0.01805000	1.87035100
H	-5.05748800	-1.27233900	2.10408300	C	-4.75573600	-3.04335000	1.46473900
H	-3.40290200	-0.93113500	2.64246300	H	-5.52520200	-2.67287700	2.13733800
H	-3.93129100	-0.47018200	1.00772800	H	-5.22583500	-3.29634200	0.50919700
C	-2.41110100	4.88766800	0.51614900	H	-4.31884500	-3.94601800	1.89735900
N	-2.42231500	5.95446600	0.98322300	C	-4.55432300	1.91866500	-0.61856900
H	-4.53600400	1.34622900	-1.45329900	N	-5.61613100	1.45466200	-0.74132100
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2-D-12-A-12P34-CCI4				2-D-12-A-12P34-DCM			
C	-2.55419100	-2.33071100	0.52343100	C	-2.54679900	-2.35045200	0.52732100
C	-2.36743100	-3.57118500	-0.16905900	C	-2.37574400	-3.57397500	-0.19988200
H	-3.07476800	-4.37854700	-0.05099400	H	-3.07635300	-4.38666200	-0.07986600

C	-1.63092200	-1.28090400	0.28378100	C	-1.63323400	-1.29077600	0.28601100
H	-1.72737500	-0.35698100	0.82761000	H	-1.72924600	-0.37501500	0.84423800
C	-1.28164100	-3.73724200	-0.97606600	C	-1.30573800	-3.72266600	-1.03036100
H	-1.12870400	-4.68949700	-1.47218000	H	-1.16055100	-4.66484900	-1.54725200
C	-3.30585800	2.37568100	-0.42828100	C	-3.30186700	2.40162900	-0.42222200
C	-2.19029300	1.53890200	-0.70929700	C	-2.19222400	1.55599400	-0.69508800
C	-3.10019100	3.59951400	0.25161500	C	-3.09362300	3.61620500	0.27816200
H	-3.95214400	4.22696500	0.48761900	H	-3.94207100	4.24812800	0.51479200
C	-1.82950800	4.00098400	0.58271000	C	-1.82390900	4.00138600	0.62725000
H	-1.67277100	4.96018300	1.06369000	H	-1.66446600	4.95164500	1.12494700
C	-0.68259900	3.19834300	0.27336100	C	-0.67979100	3.19698800	0.31056300
C	-0.88902300	1.88830100	-0.30425800	C	-0.89251000	1.89368300	-0.28233700
C	0.62136400	3.69318000	0.45339100	C	0.62529200	3.68542500	0.49589600
H	0.74527700	4.68654700	0.87249100	H	0.75482800	4.67179100	0.92936500
C	1.73874200	2.98488300	0.00321000	C	1.73891400	2.97723700	0.03045100
H	2.72036100	3.44451400	0.02573900	C	2.72233100	3.43318400	0.05777500
C	1.57121100	1.68958200	-0.47200600	C	1.56721200	1.69071500	-0.46321400
C	0.28837400	1.06630500	-0.49135500	C	0.28220800	1.06586200	-0.48322400
C	1.64569400	-0.71106300	-1.36490700	C	1.63191000	-0.69943200	-1.38518100
C	3.98348600	0.12153300	0.07381200	C	3.97555400	0.11505000	0.06854400
C	4.46820100	-0.44255800	2.38141600	C	4.44399600	-0.51905200	2.36195100
C	5.31356700	-0.16282900	-0.25671200	C	5.31886200	-0.11418900	-0.25162800
C	5.79031100	-0.73533400	2.04038400	C	5.78091100	-0.75375900	2.03154200
C	6.21204700	-0.59495200	0.72025000	C	6.21727700	-0.55101300	0.72401700
H	5.65024000	-0.03973300	-1.28098300	H	5.66608500	0.05248700	-1.26602700
H	7.23986400	-0.81124100	0.45040700	H	7.25520400	-0.72458800	0.46251700
P	2.85037300	0.67546700	-1.29585100	P	2.84315000	0.67893200	-1.29683900
C	0.39057800	-0.34834000	-0.83448000	C	0.37745700	-0.33951700	-0.83932400
C	-0.55803100	-1.41676900	-0.61093400	C	-0.57451200	-1.40995200	-0.62446100
C	-0.31265800	-2.70616800	-1.18533000	C	-0.33782200	-2.68809100	-1.23051200
C	0.89257600	-2.96215500	-1.86343600	C	0.85883300	-2.93314600	-1.92455500
C	1.87755300	-1.98285400	-1.90118700	C	1.85247300	-1.95759500	-1.94996100
H	1.06692200	-3.93864200	-2.29977700	H	1.02540600	-3.90121600	-2.38203900
H	2.83630200	-2.20626000	-2.35727900	H	2.80582000	-2.17857300	-2.41816700
C	3.57018300	-0.01759800	1.40557200	C	3.54682700	-0.08798700	1.38765300
H	6.48801900	-1.06408700	2.80254200	H	6.47766500	-1.08786700	2.79212600
H	4.13833200	-0.54346600	3.40977200	H	4.10196100	-0.67118400	3.37987000
H	2.54750100	0.21570600	1.67963600	H	2.51222200	0.09650900	1.65442400
H	-2.35774500	0.63352300	-1.27366500	H	-2.36390900	0.64811200	-1.25464900
N	-3.58683900	-2.16117400	1.39099500	N	-3.55134600	-2.20519700	1.42736400
C	-4.48188800	-3.27280200	1.71135600	C	-4.46238500	-3.31567500	1.71222700
H	-3.91323600	-4.15409300	2.01482100	H	-3.90668700	-4.20006500	2.03159300
H	-5.12859700	-2.97798900	2.53307700	H	-5.13699300	-3.02153900	2.51035000
H	-5.10743800	-3.53108600	0.85149200	H	-5.05508900	-3.56757500	0.82883400
C	-3.83239500	-0.87974800	2.05902000	C	-3.73449100	-0.95618000	2.17270800
H	-4.85237100	-0.87228300	2.43473500	H	-4.67720700	-1.00464500	2.70957200
H	-3.14521600	-0.74154600	2.90027900	H	-2.92543100	-0.81359300	2.89504900
H	-3.72085200	-0.05065200	1.36360100	H	-3.76541500	-0.10176200	1.49696900
C	-4.60760400	1.97372200	-0.79974600	C	-4.59950700	2.03307700	-0.83406700
N	-5.67675000	1.61693900	-1.09419500	N	-5.66962100	1.71870200	-1.17329300
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2-D-12-A-12P34-DMSO				2-D-12-A-12P34-n-hexane			
C	-2.54494200	-2.35611900	0.52641400	C	-2.55811700	-2.32251600	0.51621700
C	-2.37838400	-3.57426600	-0.21126000	C	-2.36129000	-3.57018800	-0.16058000

H	-3.07743300	-4.38834100	-0.09185900	H	-3.07203500	-4.37519600	-0.04602900
C	-1.63439200	-1.29325800	0.28469800	C	-1.63208100	-1.27557700	0.27713000
H	-1.72883700	-0.38112500	0.84930000	H	-1.72584300	-0.35074900	0.81949100
C	-1.31353400	-3.71720600	-1.04918700	C	-1.26945800	-3.74179200	-0.95815200
H	-1.17104600	-4.65599100	-1.57284500	H	-1.11322000	-4.69730700	-1.44699100
C	-3.29988600	2.41025600	-0.41862200	C	-3.30434600	2.36880300	-0.42604400
C	-2.19219200	1.56276500	-0.69135900	C	-2.18657800	1.53679300	-0.71450500
C	-3.09080200	3.62072100	0.29017000	C	-3.09923900	3.59283700	0.25318700
H	-3.93819000	4.25299100	0.52954000	H	-3.95227200	4.21733900	0.49310600
C	-1.82119100	4.00066200	0.64413100	C	-1.82841200	3.99846200	0.57894900
H	-1.66089200	4.94703000	1.14892600	H	-1.67263200	4.95815600	1.05921800
C	-0.67806500	3.19650800	0.32308700	C	-0.68031800	3.19810500	0.26745200
C	-0.89297700	1.89602200	-0.27606900	C	-0.88518700	1.88793500	-0.30998600
C	0.62746800	3.68280700	0.50981800	C	0.62308700	3.69454900	0.44630800
H	0.75917400	4.66622600	0.94916200	H	0.74572700	4.68862800	0.86414400
C	1.73960800	2.97482900	0.03819000	C	1.74140500	2.98693900	-0.00167100
H	2.72367200	3.42946900	0.06744900	H	2.72264900	3.44727600	0.02057600
C	1.56661800	1.69160800	-0.46213900	C	1.57485200	1.69007700	-0.47380000
C	0.28064000	1.06598000	-0.48240400	C	0.29264200	1.06727200	-0.49456400
C	1.62810100	-0.69533200	-1.39278300	C	1.65243800	-0.71350200	-1.35866900
C	3.97281600	0.11288700	0.06792400	C	3.98790200	0.12357200	0.07679900
C	4.43432100	-0.54421200	2.35647700	C	4.47509100	-0.42620500	2.38720200
C	5.32024300	-0.09877600	-0.24731300	C	5.31498300	-0.17285600	-0.25507400
C	5.77584500	-0.76020700	2.03121700	C	5.79389500	-0.73158600	2.04480900
C	6.21771700	-0.53725200	0.72869500	C	6.21292200	-0.60434100	0.72255300
H	5.67146900	0.08164200	-1.25792900	H	5.64981400	-0.05912700	-1.28105600
H	7.25875700	-0.69736500	0.47117000	H	7.23841900	-0.83007200	0.45156200
P	2.84202300	0.67980800	-1.29724800	P	2.85523700	0.67507500	-1.29424400
C	0.37341200	-0.33598300	-0.84200700	C	0.39650200	-0.34996700	-0.83388200
C	-0.58003000	-1.40707800	-0.63018800	C	-0.55175400	-1.41758600	-0.60886100
C	-0.34601600	-2.68150100	-1.24648600	C	-0.30144600	-2.71088500	-1.17116500
C	0.84785400	-2.92296900	-1.94549500	C	0.90745900	-2.97041600	-1.84246600
C	1.84467000	-1.94868800	-1.96687700	C	1.88921600	-1.98954200	-1.88476500
H	1.01211800	-3.88839300	-2.40935400	H	1.08528100	-3.95018800	-2.26999500
H	2.79633600	-2.16932000	-2.43863700	H	2.85024600	-2.21366800	-2.33571900
C	3.53825600	-0.11095500	1.38194200	C	3.57741100	-0.00222000	1.41069300
H	6.47154300	-1.09638200	2.79180200	H	6.49131900	-1.05957700	2.80757200
H	4.08775900	-0.71323200	3.37014400	H	4.14750300	-0.51646600	3.41729100
H	2.49992700	0.05737000	1.64507400	H	2.55738200	0.24141300	1.68560100
H	-2.36558600	0.65452000	-1.25002400	H	-2.35263100	0.63402100	-1.28337300
N	-3.54072900	-2.21942500	1.43606000	N	-3.60294000	-2.14973200	1.36970500
C	-4.44488200	-3.33533500	1.72426700	C	-4.46547500	-3.27107200	1.73878300
H	-3.88218400	-4.21826700	2.03473300	H	-3.87203500	-4.14957300	1.99501300
H	-5.11323300	-3.04743300	2.52972700	H	-5.05478100	-2.98605100	2.60714800
H	-5.04379800	-3.58583300	0.84487400	H	-5.14973500	-3.52541700	0.92278100
C	-3.71670800	-0.97778400	2.19522600	C	-3.92917000	-0.85540400	1.97224400
H	-4.65044700	-1.03469500	2.74655700	H	-5.00656000	-0.80512900	2.12299000
H	-2.89691700	-0.83871800	2.90583000	H	-3.43147900	-0.74358500	2.94154100
H	-3.76121200	-0.11766800	1.52723700	H	-3.64446700	-0.03515900	1.32021700
C	-4.59610700	2.05230500	-0.84256100	C	-4.60680700	1.95968100	-0.78777700
N	-5.66585600	1.75139700	-1.19566100	N	-5.67562400	1.59374500	-1.07164900
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## Triplet Optimized geometry co-ordinates:

C1234-t3				C1234-t3-CCl4			
C	-2.476457	-3.731285	-1.118008	C	-2.477615	-3.732996	-1.117144
C	-1.709803	-2.824454	-1.864137	C	-1.707978	-2.827014	-1.861836
H	-1.223571	-3.151500	-2.776686	H	-1.219033	-3.155017	-2.772572
C	-3.165870	-3.280048	0.007159	C	-3.169289	-3.280681	0.006679
H	-3.802444	-3.961898	0.561624	H	-3.807739	-3.961664	0.559987
C	-1.582975	-1.508610	-1.458867	C	-1.580871	-1.510804	-1.456604
H	-1.025422	-0.817358	-2.073203	H	-1.019760	-0.821285	-2.069699
C	-3.085583	-1.946002	0.425851	C	-3.088428	-1.946153	0.425026
C	-2.219301	-1.027337	-0.270758	C	-2.219898	-1.028259	-0.270277
C	-3.896137	-1.463205	1.511518	C	-3.901144	-1.462764	1.509422
H	-4.522610	-2.171697	2.043003	H	-4.528932	-2.170836	2.039834
C	-3.938692	-0.141882	1.810078	C	-3.943739	-0.140930	1.807416
H	-4.616384	0.232445	2.570380	H	-4.622878	0.234032	2.566098
C	-3.102815	0.804597	1.122937	C	-3.106085	0.805006	1.120997
C	-2.103013	0.318700	0.195915	C	-2.104250	0.318431	0.195965
C	-3.280789	2.173353	1.281940	C	-3.284613	2.174164	1.279134
H	-4.059762	2.533083	1.945374	H	-4.064485	2.534404	1.941150
C	-2.493316	3.100491	0.557610	C	-2.496171	3.100987	0.555040
H	-2.700294	4.161463	0.640814	H	-2.703530	4.161924	0.637280
C	-1.390780	2.675110	-0.181166	C	-1.392097	2.675017	-0.182008
C	-1.089070	1.272143	-0.250621	C	-1.089556	1.271707	-0.249462
C	-0.511504	3.642071	-0.809165	C	-0.512867	3.642090	-0.810326
H	-0.843174	4.673983	-0.840624	H	-0.844591	4.673920	-0.842607
C	0.722442	3.291077	-1.333903	C	0.721862	3.290572	-1.334345
H	1.363100	4.038369	-1.788371	H	1.362623	4.037534	-1.789197
C	1.160387	1.956576	-1.204880	C	1.160008	1.956116	-1.203359
C	0.252952	0.927261	-0.620927	C	0.253071	0.927097	-0.618079
C	2.381565	1.368170	-1.472419	C	2.381562	1.367963	-1.470359
H	3.250527	1.857463	-1.891295	H	3.249430	1.857027	-1.891823
H	-2.561817	-4.764991	-1.431990	H	-2.563216	-4.766735	-1.430951
C	0.971468	-0.237205	-0.482695	C	0.972350	-0.236868	-0.477988
C	3.482398	-0.444946	-0.059106	C	3.484311	-0.444465	-0.057565
C	3.572042	0.187044	1.187474	C	3.571987	0.182130	1.192210
C	4.433044	-1.412899	-0.390547	C	4.439503	-1.406531	-0.394664
C	4.589274	-0.142622	2.077901	C	4.591778	-0.146875	2.080689
H	2.838425	0.938960	1.457873	H	2.835443	0.929410	1.467694
C	5.454479	-1.745237	0.500583	C	5.463553	-1.738122	0.494358
H	4.375053	-1.912741	-1.352389	H	4.383246	-1.902049	-1.358733
C	5.535365	-1.110896	1.737237	C	5.542545	-1.109152	1.734437
H	4.644400	0.354947	3.039909	H	4.645192	0.346440	3.044976
H	6.183660	-2.499812	0.226815	H	6.196122	-2.487822	0.216290
H	6.327145	-1.367814	2.431850	H	6.336131	-1.365527	2.427201
H	0.630148	-1.155950	-0.030976	H	0.631739	-1.155459	-0.025299
C	2.367480	-0.075802	-1.035286	C	2.367624	-0.075716	-1.032118
H	2.482273	-0.731936	-1.914422	H	2.480926	-0.731991	-1.911053
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C1234-t3-DCM				C1234-t3-DMSO			
C	-2.470507	-3.737561	-1.115438	C	-2.463598	-3.740516	-1.114408
C	-1.698286	-2.831493	-1.857944	C	-1.690946	-2.833825	-1.855880

H	-1.204183	-3.160085	-2.765610	H	-1.194011	-3.162283	-2.762000
C	-3.166947	-3.284841	0.005750	C	-3.162790	-3.288137	0.005392
H	-3.806785	-3.965827	0.557348	H	-3.802741	-3.969658	0.556147
C	-1.573885	-1.514411	-1.453276	C	-1.569046	-1.516196	-1.451611
H	-1.008905	-0.826453	-2.064621	H	-1.002854	-0.828531	-2.062185
C	-3.088297	-1.949463	0.423358	C	-3.086365	-1.952314	0.422614
C	-2.218051	-1.031099	-0.269826	C	-2.216003	-1.033055	-0.269539
C	-3.905580	-1.466513	1.505256	C	-3.906301	-1.470168	1.503181
H	-4.534453	-2.174973	2.033765	H	-4.535274	-2.179257	2.030686
C	-3.950702	-0.144143	1.802375	C	-3.953628	-0.147612	1.799884
H	-4.633096	0.230655	2.558166	H	-4.637953	0.226637	2.554170
C	-3.111670	0.802440	1.117801	C	-3.114536	0.799890	1.116407
C	-2.105789	0.316764	0.195920	C	-2.106333	0.315440	0.196043
C	-3.292997	2.171735	1.275275	C	-3.298070	2.169077	1.273819
H	-4.074908	2.530975	1.935318	H	-4.081265	2.527113	1.932949
C	-2.504115	3.099678	0.552813	C	-2.509475	3.098194	0.552527
H	-2.713571	4.160213	0.634193	H	-2.720552	4.158396	0.633725
C	-1.396948	2.674966	-0.181395	C	-1.400532	2.674949	-0.180328
C	-1.091430	1.271604	-0.247232	C	-1.092797	1.271760	-0.245863
C	-0.518713	3.643713	-0.808798	C	-0.523310	3.645142	-0.806914
H	-0.851679	4.675086	-0.840959	H	-0.857424	4.676127	-0.838523
C	0.717562	3.293751	-1.332011	C	0.713832	3.296867	-1.330010
H	1.357426	4.041589	-1.786597	H	1.352737	4.045656	-1.784313
C	1.157708	1.959916	-1.199739	C	1.155705	1.963562	-1.197697
C	0.252526	0.929598	-0.613831	C	0.251941	0.931930	-0.611782
C	2.380180	1.373619	-1.467080	C	2.378812	1.378867	-1.465667
H	3.245565	1.863553	-1.892652	H	3.242639	1.869784	-1.893272
H	-2.553870	-4.771665	-1.428557	H	-2.544947	-4.774898	-1.427083
C	0.974230	-0.233103	-0.473151	C	0.975431	-0.229885	-0.471560
C	3.486763	-0.440109	-0.057438	C	3.487853	-0.436383	-0.058419
C	3.580750	0.189040	1.191012	C	3.590718	0.200461	1.185607
C	4.437281	-1.407032	-0.395534	C	4.429374	-1.413593	-0.392716
C	4.601987	-0.142148	2.077856	C	4.611734	-0.133244	2.072101
H	2.848887	0.940611	1.467680	H	2.866499	0.960544	1.459325
C	5.462665	-1.740886	0.491764	C	5.454387	-1.750111	0.494254
H	4.376687	-1.903964	-1.358451	H	4.362194	-1.916146	-1.352195
C	5.547952	-1.109493	1.730812	C	5.548540	-1.111090	1.728981
H	4.660434	0.353409	3.040692	H	4.677325	0.368606	3.031208
H	6.191488	-2.493934	0.212985	H	6.176197	-2.510936	0.218414
H	6.342615	-1.367529	2.421705	H	6.343096	-1.371034	2.419268
H	0.635370	-1.152834	-0.021392	H	0.637922	-1.150726	-0.021034
C	2.368206	-0.070149	-1.029572	C	2.368620	-0.065098	-1.029307
H	2.479624	-0.725088	-1.909380	H	2.479114	-0.718874	-1.909936
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C1234-t3-n-hexane				1C234-t7			
C	-2.478028	-3.732461	-1.117375	C	5.518034	1.007644	0.096408
C	-1.708913	-2.826396	-1.862384	C	4.464794	1.722538	-0.509380
H	-1.220672	-3.154247	-2.773558	H	4.637544	2.714385	-0.909825
C	-3.169074	-3.280301	0.006820	C	5.303394	-0.278432	0.538126
H	-3.807187	-3.961390	0.560400	H	6.117304	-0.857584	0.961077
C	-1.581618	-1.510287	-1.457102	C	3.184018	1.146322	-0.600180
H	-1.021179	-0.820466	-2.070462	H	2.399090	1.698329	-1.097105
C	-3.088090	-1.945897	0.425264	C	4.022643	-0.897319	0.409430
C	-2.219959	-1.027943	-0.270355	C	2.916022	-0.127363	-0.092822

C	-3.900184	-1.462545	1.510034	C	3.861935	-2.298496	0.665732
H	-4.527702	-2.170653	2.040736	H	4.712098	-2.857544	1.041426
C	-3.942586	-0.140813	1.808167	C	2.696888	-2.934649	0.356738
H	-4.621315	0.234083	2.567253	H	2.608266	-4.009610	0.470325
C	-3.105268	0.805153	1.121505	C	1.543534	-2.202727	-0.103366
C	-2.103973	0.318588	0.195990	C	1.592696	-0.754210	-0.160084
C	-3.283536	2.174253	1.279765	C	0.358111	-2.898049	-0.454577
H	-4.063136	2.534507	1.942115	H	0.368877	-3.982607	-0.438132
C	-2.495269	3.101036	0.555502	C	-0.789867	-2.217298	-0.805780
H	-2.702454	4.162003	0.637890	H	-1.689687	-2.749532	-1.091619
C	-1.391593	2.675049	-0.181958	C	-0.793378	-0.806513	-0.707184
C	-1.089349	1.271783	-0.249738	C	0.360041	-0.079977	-0.322811
C	-0.512293	3.641971	-0.810330	C	-1.412399	1.442334	-0.488676
H	-0.843926	4.673842	-0.842557	H	6.499206	1.460039	0.187093
C	0.722234	3.290405	-1.334500	C	-3.273108	-0.296487	-0.288463
H	1.363033	4.037350	-1.789336	C	-4.543271	-0.810056	1.713268
C	1.160230	1.955903	-1.203832	C	-4.414861	-0.550685	-1.051744
C	0.253107	0.926955	-0.618727	C	-5.679080	-1.062006	0.941363
C	2.381658	1.367569	-1.470896	C	-5.611932	-0.931516	-0.442941
H	3.249834	1.856581	-1.891776	H	-4.368971	-0.450852	-2.131812
H	-2.563782	-4.766165	-1.431261	H	-6.488262	-1.125227	-1.051665
C	0.972130	-0.237168	-0.478892	C	-0.072707	1.326575	-0.102820
C	3.483908	-0.444830	-0.057787	C	0.556913	2.424742	0.516157
C	3.571595	0.182521	1.191538	C	-0.162279	3.652246	0.653958
C	4.438641	-1.407565	-0.393965	C	-1.469584	3.773040	0.206155
C	4.590962	-0.146422	2.080382	C	-2.124031	2.667200	-0.364280
H	2.835269	0.930302	1.466193	H	1.558038	2.349117	0.913699
C	5.462265	-1.739101	0.495450	H	0.329929	4.497354	1.121515
H	4.382309	-1.903726	-1.357722	H	-1.995638	4.714795	0.313424
C	5.541265	-1.109367	1.735031	H	-3.159185	2.732690	-0.677357
H	4.644407	0.347476	3.044370	C	-3.351638	-0.431141	1.103592
H	6.194505	-2.489384	0.218083	H	-6.607166	-1.357639	1.417483
H	6.334548	-1.365697	2.428157	H	-4.587770	-0.909413	2.792220
H	0.631309	-1.155701	-0.026270	H	-2.472558	-0.237620	1.709147
C	2.367566	-0.076128	-1.032716	C	-1.965392	0.115825	-0.954146
H	2.481169	-0.732505	-1.911595	H	-2.154094	0.161658	-2.039936
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1C234-t7-CCI4				1C234-t6-DCM			
C	5.518671	1.007857	0.100351	C	5.495690	1.001302	0.120257
C	4.465622	1.724026	-0.505241	C	4.436336	1.733490	-0.443387
H	4.638515	2.716774	-0.903317	H	4.610214	2.735153	-0.820032
C	5.303686	-0.279149	0.540556	C	5.281526	-0.303029	0.515992
H	6.117275	-0.859005	0.963078	H	6.102400	-0.901412	0.897090
C	3.184584	1.147895	-0.597585	C	3.174019	1.177673	-0.536279
H	2.400125	1.701646	-1.093302	H	2.388255	1.746157	-1.011536
C	4.022462	-0.897632	0.410211	C	4.007455	-0.903560	0.392810
C	2.916000	-0.126713	-0.092053	C	2.901447	-0.129150	-0.070971
C	3.861974	-2.299547	0.665168	C	3.841051	-2.306688	0.633002
H	4.711896	-2.858863	1.040879	H	4.690397	-2.877685	0.992331
C	2.696875	-2.935418	0.354051	C	2.669313	-2.921983	0.331306
H	2.608010	-4.010570	0.465410	H	2.570797	-3.997755	0.429565
C	1.543796	-2.202520	-0.105839	C	1.522440	-2.176865	-0.104825
C	1.592275	-0.753476	-0.160475	C	1.584214	-0.748743	-0.166926
C	0.358933	-2.898357	-0.459191	C	0.337445	-2.866064	-0.451549

H	0.370230	-3.982868	-0.444177	H	0.338136	-3.950049	-0.414961
C	-0.788975	-2.217092	-0.810560	C	-0.794042	-2.180662	-0.840691
H	-1.687598	-2.749772	-1.099349	H	-1.690947	-2.709347	-1.143443
C	-0.793575	-0.806228	-0.709821	C	-0.785910	-0.784676	-0.768175
C	0.359358	-0.079308	-0.323626	C	0.345748	-0.062387	-0.360122
C	-1.413464	1.442162	-0.490755	C	-1.433602	1.463986	-0.535545
H	6.499814	1.460084	0.192176	H	6.480426	1.445927	0.207757
C	-3.272793	-0.297341	-0.287284	C	-3.244626	-0.289738	-0.376438
C	-4.540023	-0.811273	1.716996	C	-4.423362	-0.848110	1.789273
C	-4.415678	-0.551653	-1.049349	C	-4.425189	-0.549692	-1.075234
C	-5.677185	-1.063326	0.946452	C	-5.586717	-1.099861	1.078104
C	-5.611961	-0.932720	-0.438457	C	-5.588948	-0.945419	-0.422021
H	-4.371442	-0.451871	-2.129350	H	-4.431215	-0.440621	-2.156076
H	-6.489141	-1.126432	-1.045927	H	-6.498210	-1.146238	-0.973697
C	-0.073937	1.327025	-0.103657	C	-0.090041	1.337626	-0.122086
C	0.554949	2.425892	0.515723	C	0.517705	2.422299	0.523957
C	-0.164486	3.653562	0.652074	C	-0.189079	3.614462	0.681530
C	-1.471459	3.773979	0.202355	C	-1.497400	3.745033	0.209245
C	-2.125253	2.667277	-0.368255	C	-2.131667	2.655878	-0.390417
H	1.555788	2.351820	0.914224	H	1.519765	2.348993	0.921770
H	0.327279	4.498943	1.119589	H	0.286206	4.449158	1.184729
H	-1.997758	4.715778	0.307954	H	-2.027655	4.682452	0.332889
H	-3.159386	2.733589	-0.684477	H	-3.163673	2.729358	-0.716600
C	-3.349054	-0.432033	1.105162	C	-3.249920	-0.450544	1.138197
H	-6.604558	-1.359072	1.423894	H	-6.496556	-1.405163	1.579065
H	-4.582801	-0.910648	2.796002	H	-4.419664	-0.958794	2.868969
H	-2.469641	-0.238613	1.710369	H	-2.341994	-0.247292	1.690757
C	-1.966294	0.115459	-0.955762	C	-1.970593	0.134270	-1.039800
H	-2.156894	0.160995	-2.040814	H	-2.136446	0.184072	-2.123831
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1C234-t6-DMSO				1C234-t7-n-hexane			
C	5.494878	1.003043	0.125110	C	5.518638	1.007733	0.099163
C	4.435769	1.735618	-0.438792	C	4.465502	1.723621	-0.506423
H	4.609539	2.737971	-0.813535	H	4.638352	2.716149	-0.905087
C	5.280842	-0.302036	0.519074	C	5.303740	-0.279051	0.539797
H	6.101526	-0.900520	0.900302	H	6.117425	-0.858755	0.962364
C	3.173617	1.179385	-0.533702	C	3.184497	1.147489	-0.598288
H	2.388326	1.748583	-1.008839	H	2.399903	1.700860	-1.094222
C	4.006931	-0.902896	0.393718	C	4.022584	-0.897598	0.409958
C	2.900987	-0.128229	-0.070349	C	2.916057	-0.126889	-0.092260
C	3.841051	-2.306557	0.632028	C	3.862050	-2.299344	0.665321
H	4.690267	-2.877637	0.991443	H	4.712051	-2.858589	1.040985
C	2.669763	-2.922113	0.328257	C	2.696915	-2.935270	0.354789
H	2.571780	-3.998052	0.424798	H	2.608069	-4.010375	0.466676
C	1.522925	-2.176748	-0.108007	C	1.543752	-2.202575	-0.105083
C	1.583930	-0.748322	-0.168275	C	1.592395	-0.753646	-0.160266
C	0.338692	-2.866407	-0.457194	C	0.358722	-2.898317	-0.457795
H	0.340202	-3.950430	-0.422870	H	0.369881	-3.982835	-0.442323
C	-0.792878	-2.180982	-0.846407	C	-0.789216	-2.217162	-0.809112
H	-1.688610	-2.709954	-1.152074	H	-1.688136	-2.749771	-1.097102
C	-0.785934	-0.784961	-0.771465	C	-0.793541	-0.806301	-0.708987
C	0.345083	-0.062328	-0.361778	C	0.359531	-0.079455	-0.323285
C	-1.435048	1.463159	-0.538044	C	-1.413183	1.442210	-0.490129
H	6.479268	1.448012	0.214349	H	6.499810	1.459978	0.190612

C	-3.243539	-0.291438	-0.374535	C	-3.272936	-0.297109	-0.287551
C	-4.414831	-0.849643	1.793339	C	-4.541231	-0.810740	1.715965
C	-4.428865	-0.550217	-1.071312	C	-4.415377	-0.551613	-1.050122
C	-5.582826	-1.100029	1.084238	C	-5.677907	-1.062980	0.944895
C	-5.588982	-0.944363	-0.415752	C	-5.611953	-0.932625	-0.439903
H	-4.437278	-0.439903	-2.151934	H	-4.370525	-0.452001	-2.130144
H	-6.500474	-1.143631	-0.964372	H	-6.488793	-1.126497	-1.047820
C	-0.091686	1.337419	-0.123341	C	-0.073610	1.326933	-0.103356
C	0.515187	2.422732	0.522791	C	0.555492	2.425661	0.515899
C	-0.192064	3.614892	0.679280	C	-0.163854	3.653317	0.652546
C	-1.500086	3.744950	0.205433	C	-1.470913	3.773830	0.203286
C	-2.133502	2.655211	-0.394413	C	-2.124910	2.667289	-0.367219
H	1.517197	2.350698	0.920917	H	1.556385	2.351234	0.914212
H	0.282768	4.450076	1.182030	H	0.328039	4.498634	1.120049
H	-2.030365	4.682574	0.327298	H	-1.997155	4.715622	0.309260
H	-3.164718	2.728929	-0.723021	H	-3.159295	2.733440	-0.682660
C	-3.245143	-0.453674	1.139975	C	-3.349991	-0.431575	1.104818
H	-6.491225	-1.404949	1.587923	H	-6.605526	-1.358690	1.421884
H	-4.408690	-0.961669	2.872913	H	-4.584623	-0.909933	2.794966
H	-2.334993	-0.253260	1.690175	H	-2.470827	-0.237973	1.710304
C	-1.971649	0.133019	-1.041614	C	-1.966072	0.115557	-0.955239
H	-2.140245	0.182253	-2.125092	H	-2.156118	0.161165	-2.040471
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12C34-t4				12C34-t4-CCI4			
C	3.173934	2.853179	1.169160	C	3.169328	2.856836	1.171379
C	2.805608	4.110450	0.703906	C	2.801025	4.113656	0.703855
H	3.404712	4.980017	0.948991	H	3.399280	4.983867	0.948715
C	2.403147	1.716329	0.848895	C	2.399379	1.719097	0.851364
H	2.638250	0.767167	1.307237	H	2.635107	0.770699	1.310983
C	1.631796	4.262279	-0.048070	C	1.627743	4.264204	-0.050331
H	1.313017	5.245269	-0.375409	H	1.309038	5.246650	-0.379255
C	4.248322	-1.913518	-0.139575	C	4.249871	-1.910784	-0.133957
C	3.141734	-1.061090	-0.330893	C	3.142777	-1.059035	-0.326782
C	4.061404	-3.253308	0.182515	C	4.063383	-3.251598	0.185603
H	4.916439	-3.902359	0.333401	H	4.918622	-3.900140	0.337458
C	2.764134	-3.778136	0.269658	C	2.765936	-3.778076	0.268899
H	2.610659	-4.831327	0.475185	H	2.612907	-4.831722	0.472222
C	1.612334	-2.939622	0.061451	C	1.613884	-2.939764	0.059483
C	1.798781	-1.547323	-0.154248	C	1.799432	-1.546641	-0.153763
C	0.308577	-3.507931	0.008368	C	0.310683	-3.509754	0.002758
H	0.196599	-4.572955	0.179252	H	0.199453	-4.575216	0.171054
C	-0.788329	-2.734930	-0.328396	C	-0.786512	-2.736753	-0.334756
H	-1.767340	-3.186578	-0.445012	H	-1.764293	-3.189977	-0.455335
C	-0.618883	-1.359859	-0.507595	C	-0.618247	-1.360993	-0.510980
C	0.631792	-0.733375	-0.304383	C	0.631658	-0.733519	-0.305037
C	-0.866772	0.950262	-0.882653	C	-0.867695	0.949086	-0.885288
H	4.046040	2.741298	1.803323	H	4.040613	2.746049	1.806855
C	-2.961500	-0.338529	-0.202956	C	-2.960274	-0.340326	-0.202025
C	-4.174782	-0.127240	1.887288	C	-4.170042	-0.127837	1.890939
C	-4.178214	-0.523787	-0.864205	C	-4.178117	-0.526996	-0.861391
C	-5.385412	-0.312576	1.216731	C	-5.382027	-0.314272	1.222364
C	-5.384029	-0.511200	-0.161122	C	-5.382841	-0.514231	-0.155822
H	-4.184198	-0.680435	-1.938425	H	-4.185945	-0.684684	-1.935292
H	-6.318524	-0.657626	-0.691516	H	-6.318166	-0.661518	-0.684479

C	0.436972	0.712313	-0.392242	C	0.435645	0.712280	-0.392777
C	1.247741	1.825268	-0.002094	C	1.245068	1.826326	-0.002028
C	0.812258	3.124948	-0.377920	C	0.809319	3.125622	-0.379879
C	-0.448510	3.305649	-1.013476	C	-0.450563	3.305288	-1.018263
C	-1.304179	2.236355	-1.208620	C	-1.305244	2.234676	-1.213807
H	-0.755452	4.309451	-1.285873	H	-0.757574	4.308470	-1.292734
H	-2.301391	2.393216	-1.605200	H	-2.301202	2.390612	-1.613859
C	-2.974752	-0.140072	1.184007	C	-2.970981	-0.140798	1.185086
H	-6.320056	-0.302328	1.766047	H	-6.315757	-0.303911	1.773227
H	-4.167555	0.027606	2.960578	H	-4.160851	0.027857	2.964076
H	-2.038589	0.004783	1.712449	H	-2.034420	0.004995	1.712689
H	5.250000	-1.519621	-0.268831	H	5.251464	-1.515621	-0.259906
H	3.299670	-0.053952	-0.687183	H	3.301492	-0.051122	-0.680519
C	-1.649407	-0.347759	-0.974021	C	-1.649673	-0.349328	-0.976247
H	-1.884885	-0.562284	-2.026071	H	-1.887268	-0.563482	-2.027492
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12C34-t4-DCM				12C34-t4-DMSO			
C	3.153884	2.869063	1.177094	C	3.143819	2.877179	1.180410
C	2.782905	4.124345	0.706463	C	2.770618	4.131420	0.708354
H	3.377289	4.996901	0.952270	H	3.362360	5.005556	0.954837
C	2.388849	1.727998	0.855628	C	2.382226	1.733878	0.857903
H	2.627958	0.781047	1.316473	H	2.623838	0.787749	1.319122
C	1.611601	4.270072	-0.052633	C	1.600507	4.273867	-0.053449
H	1.290722	5.250864	-0.384196	H	1.277805	5.253552	-0.386425
C	4.254666	-1.900611	-0.122766	C	4.257883	-1.893490	-0.116702
C	3.145735	-1.051439	-0.318015	C	3.147670	-1.046124	-0.313067
C	4.070699	-3.243512	0.191173	C	4.075854	-3.237595	0.193927
H	4.927113	-3.889980	0.344946	H	4.933167	-3.882606	0.348615
C	2.774138	-3.774381	0.266603	C	2.780114	-3.771289	0.265005
H	2.623243	-4.829136	0.465397	H	2.630783	-4.826731	0.461149
C	1.620549	-2.938167	0.054971	C	1.625369	-2.936715	0.052311
C	1.802689	-1.543315	-0.153025	C	1.805092	-1.540868	-0.152641
C	0.319403	-3.512797	-0.009598	C	0.325649	-3.514347	-0.016671
H	0.211093	-4.579346	0.153192	H	0.219445	-4.581556	0.142951
C	-0.779019	-2.741646	-0.348766	C	-0.773718	-2.744736	-0.356689
H	-1.754047	-3.198497	-0.477450	H	-1.747095	-3.203789	-0.489873
C	-0.614744	-1.364334	-0.518760	C	-0.612162	-1.366525	-0.523162
C	0.632611	-0.733202	-0.307035	C	0.633481	-0.732861	-0.308194
C	-0.870269	0.945022	-0.891954	C	-0.871992	0.942271	-0.895771
H	4.023593	2.761870	1.815278	H	4.012753	2.772351	1.819997
C	-2.956361	-0.347630	-0.200647	C	-2.953849	-0.352835	-0.199987
C	-4.156265	-0.141033	1.899680	C	-4.147800	-0.151920	1.904800
C	-4.177614	-0.530292	-0.855452	C	-4.177224	-0.531150	-0.852274
C	-5.371843	-0.323412	1.235721	C	-5.365546	-0.330024	1.243360
C	-5.379100	-0.518394	-0.143730	C	-5.376744	-0.519965	-0.136994
H	-4.190781	-0.683887	-1.929682	H	-4.193648	-0.680677	-1.926935
H	-6.316997	-0.662536	-0.668597	H	-6.316245	-0.660809	-0.659836
C	0.432323	0.712416	-0.394659	C	0.430234	0.712549	-0.395746
C	1.237024	1.829906	-0.002276	C	1.231775	1.832296	-0.002377
C	0.798459	3.127604	-0.383778	C	0.791001	3.128879	-0.385792
C	-0.459230	3.302874	-1.028590	C	-0.465443	3.301103	-1.034198
C	-1.309979	2.228863	-1.225656	C	-1.313486	2.224944	-1.232251
H	-0.767390	4.304436	-1.307446	H	-0.774551	4.301669	-1.315464
H	-2.303510	2.380963	-1.633101	H	-2.305722	2.374396	-1.643788

C	-2.960238	-0.153164	1.187603	C	-2.953627	-0.163395	1.189141
H	-6.303009	-0.313957	1.790887	H	-6.295177	-0.321308	1.801078
H	-4.141784	0.010419	2.973358	H	-4.130141	-0.004618	2.979008
H	-2.021464	-0.010973	1.712488	H	-2.013345	-0.024926	1.712465
H	5.255591	-1.501694	-0.241660	H	5.258258	-1.492131	-0.231692
H	3.304388	-0.041364	-0.665479	H	3.305798	-0.034729	-0.656853
C	-1.649270	-0.355109	-0.981809	C	-1.648786	-0.359130	-0.985028
H	-1.891632	-0.569485	-2.031392	H	-1.893762	-0.573888	-2.033676
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12C34-t4-n-hexane				P1234-t3			
C	3.170833	2.855640	1.170755	P1234-triplet-opt			
C	2.802689	4.112607	0.703700	C	-2.46798300	-3.82835000	-1.00006800
H	3.401285	4.982596	0.948523	C	-1.85471400	-2.88993100	-1.82559300
C	2.400479	1.718215	0.850807	H	-1.39387500	-3.19462600	-2.75772200
H	2.635925	0.769635	1.310195	C	-3.10222000	-3.40736600	0.16386300
C	1.629222	4.263603	-0.049913	H	-3.62960600	-4.12064300	0.78835100
H	1.310638	5.246214	-0.378487	C	-1.81351400	-1.53289300	-1.44239800
C	4.249386	-1.911723	-0.135342	H	-1.32710100	-0.82332100	-2.09786800
C	3.142465	-1.059736	-0.327822	C	-3.11907000	-2.03532900	0.53633700
C	4.062701	-3.252283	0.184867	C	-2.36089100	-1.09264600	-0.24158300
H	4.917846	-3.901012	0.336472	C	-3.95536700	-1.56651500	1.56927900
C	2.765226	-3.778295	0.269120	H	-4.53962300	-2.27294500	2.14753600
H	2.612016	-4.831819	0.472983	C	-4.16212200	-0.16128500	1.73978600
C	1.613297	-2.939836	0.060000	H	-4.92927200	0.18689100	2.42254900
C	1.799155	-1.546922	-0.153863	C	-3.39344300	0.77054400	1.05178300
C	0.309905	-3.509339	0.004209	C	-2.30140700	0.31965400	0.20043500
H	0.198416	-4.574682	0.173158	C	-3.61691100	2.17737200	1.21102500
C	-0.787184	-2.736232	-0.333102	H	-4.46981200	2.50396100	1.79619300
H	-1.765286	-3.189038	-0.452689	C	-2.78537800	3.07954900	0.62252400
C	-0.618535	-1.360653	-0.510075	H	-2.98248400	4.14354500	0.70027400
C	0.631617	-0.733520	-0.304825	C	-1.60548900	2.65529700	-0.05885400
C	-0.867427	0.949475	-0.884549	C	-1.30858100	1.25184000	-0.16966500
H	4.042316	2.744500	1.805902	C	-0.75147000	3.63663900	-0.65334700
C	-2.960663	-0.339668	-0.202224	H	-1.07910600	4.67079500	-0.61855400
C	-4.171473	-0.126989	1.889949	C	0.42593800	3.31665400	-1.26068300
C	-4.178158	-0.526380	-0.862107	H	1.04244900	4.07732100	-1.72536800
C	-5.383069	-0.313511	1.220841	C	0.90295700	1.96135200	-1.19374700
C	-5.383216	-0.513584	-0.157227	C	0.06065900	0.92302100	-0.60593300
H	-4.185430	-0.684169	-1.936029	C	2.17415300	1.53264500	-1.53206700
H	-6.318279	-0.660936	-0.686336	H	2.93491900	2.16372400	-1.97137600
C	0.436008	0.712274	-0.392588	H	-2.47575600	-4.87732700	-1.27383000
C	1.245883	1.825976	-0.002014	C	0.75220300	-0.26535300	-0.41370600
C	0.810339	3.125413	-0.379396	P	2.33545200	-0.23787600	-1.26807600
C	-0.449785	3.305471	-1.017040	C	3.65055400	-0.45331600	0.02079500
C	-1.304828	2.235230	-1.212438	C	3.62471700	0.24013800	1.23865900
H	-0.756713	4.308829	-1.290990	C	4.70062000	-1.33960700	-0.23850600
H	-2.301089	2.391512	-1.611605	C	4.63431400	0.04763900	2.17655700
C	-2.972105	-0.139987	1.184800	H	2.81299000	0.92738300	1.44841600
H	-6.317071	-0.303108	1.771246	C	5.71394000	-1.52982200	0.70251800
H	-4.162850	0.028841	2.963073	H	4.72514800	-1.88267000	-1.17711500
H	-2.035729	0.005887	1.712679	C	5.68127900	-0.83729100	1.90966900
H	5.251026	-1.516941	-0.262138	H	4.60596500	0.58711300	3.11698400
H	3.301078	-0.052052	-0.682261	H	6.52380300	-2.21921300	0.49116700
C	-1.649662	-0.348791	-0.975626	H	6.46656100	-0.98517800	2.64263600

H	-1.886695	-0.562987	-2.027071	H	0.34638400	-1.15251100	0.04638500
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P1234-CCl4-t3				P1234-DCM-t3			
C	-2.46654800	-3.83062100	-1.00143400	C	-2.46793000	-3.83254800	-1.00196900
C	-1.85331200	-2.89167700	-1.82691600	C	-1.85422100	-2.89362900	-1.82767400
H	-1.39197600	-3.19615500	-2.75887500	H	-1.39318100	-3.19838700	-2.75969400
C	-3.10168400	-3.41006700	0.16270400	C	-3.10314600	-3.41190900	0.16267900
H	-3.62895100	-4.12356600	0.78694500	H	-3.63067200	-4.12521900	0.78678300
C	-1.81287900	-1.53426500	-1.44353000	C	-1.81311200	-1.53583500	-1.44401200
H	-1.32616500	-0.82490900	-2.09910500	H	-1.32523900	-0.82725000	-2.09968200
C	-3.11945900	-2.03762500	0.53490900	C	-3.12053200	-2.03896400	0.53469100
C	-2.36154700	-1.09428600	-0.24296500	C	-2.36232600	-1.09551100	-0.24350500
C	-3.95698800	-1.56968100	1.56772800	C	-3.95834600	-1.57128800	1.56792000
H	-4.54092600	-2.27667500	2.14551600	H	-4.54214700	-2.27828000	2.14570800
C	-4.16614400	-0.16443000	1.73772000	C	-4.16859800	-0.16575200	1.73768300
H	-4.93474300	0.18254400	2.41935800	H	-4.93804000	0.18066300	2.41851000
C	-3.39757600	0.76803000	1.04994500	C	-3.39951600	0.76673100	1.04998700
C	-2.30389300	0.31811500	0.19956700	C	-2.30522100	0.31704800	0.19954200
C	-3.62345500	2.17500900	1.20822400	C	-3.62631300	2.17402500	1.20838300
H	-4.47765600	2.50078000	1.79188900	H	-4.48038800	2.49925300	1.79241600
C	-2.79218300	3.07839200	0.62045200	C	-2.79552500	3.07827400	0.62044000
H	-2.99109800	4.14203600	0.69720000	H	-2.99498100	4.14171300	0.69725100
C	-1.61014800	2.65502100	-0.05874400	C	-1.61278100	2.65499900	-0.05870500
C	-1.31157300	1.25178800	-0.16921400	C	-1.31337300	1.25181900	-0.16915500
C	-0.75594800	3.63808600	-0.65115800	C	-0.75897300	3.63938600	-0.65066400
H	-1.08428000	4.67194700	-0.61571400	H	-1.08784600	4.67293800	-0.61452000
C	0.42299000	3.31948800	-1.25701400	C	0.42064200	3.32166600	-1.25638600
H	1.03974600	4.08102500	-1.71993400	H	1.03724800	4.08371300	-1.71857900
C	0.90069800	1.96414500	-1.19004700	C	0.89886400	1.96624600	-1.18897600
C	0.05888400	0.92468200	-0.60307200	C	0.05782700	0.92601300	-0.60173600
C	2.17294600	1.53718800	-1.52741800	C	2.17197500	1.54077600	-1.52589700
H	2.93400200	2.16922200	-1.96495300	H	2.93272600	2.17355100	-1.96301600
H	-2.47369300	-4.87958800	-1.27521400	H	-2.47551300	-4.88148300	-1.27575200
C	0.75134300	-0.26291600	-0.40924000	C	0.75120800	-0.26074500	-0.40633600
P	2.33534900	-0.23300500	-1.26175800	P	2.33583500	-0.22875700	-1.25773500
C	3.65383400	-0.45203000	0.02214900	C	3.65708300	-0.45081700	0.02194900
C	3.62392000	0.22792400	1.24784800	C	3.63174600	0.23030100	1.24748900
C	4.71131700	-1.32640100	-0.24911700	C	4.71176300	-1.32837000	-0.25168900
C	4.63731400	0.03421600	2.18194800	C	4.64701800	0.03454200	2.17968900
H	2.80695600	0.90571200	1.46788500	H	2.81782100	0.91096500	1.47005400
C	5.72853200	-1.51740000	0.68796200	C	5.73072000	-1.52148900	0.68356900
H	4.73968400	-1.85963700	-1.19318000	H	4.73790900	-1.86231000	-1.19533300
C	5.69201400	-0.83827500	1.90308300	C	5.69883600	-0.84135100	1.89875100
H	4.60581800	0.56298100	3.12825700	H	4.61926400	0.56426200	3.12547600
H	6.54403700	-2.19708100	0.46739900	H	6.54390600	-2.20326700	0.46139400
H	6.48005600	-0.98707500	2.63281300	H	6.48818900	-0.99169200	2.62660900
H	0.34622900	-1.15094400	0.04985600	H	0.34681500	-1.14954700	0.05200000
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P1234-DMSO-t3				P1234-n-hexane-t3			
C	-2.46998000	-3.83311200	-1.00149000	C	-2.46660500	-3.83024200	-1.00120500
C	-1.85562800	-2.89459000	-1.82736100	C	-1.85337700	-2.89136900	-1.82667100
H	-1.39484700	-3.19978500	-2.75936700	H	-1.39204900	-3.19586400	-2.75862800

C	-3.10504800	-3.41203700	0.16331300	C	-3.10166400	-3.40963000	0.16285000
H	-3.63303700	-4.12498600	0.78737800	H	-3.62894300	-4.12310900	0.78712400
C	-1.81361600	-1.53661200	-1.44370600	C	-1.81291500	-1.53402000	-1.44334300
H	-1.32480800	-0.82866800	-2.09942500	H	-1.32629700	-0.82459600	-2.09889600
C	-3.12164300	-2.03883300	0.53516100	C	-3.11937000	-2.03726500	0.53508300
C	-2.36286000	-1.09572600	-0.24327400	C	-2.36142500	-1.09401800	-0.24276500
C	-3.95924200	-1.57082400	1.56861200	C	-3.95675900	-1.56919100	1.56786300
H	-4.54323800	-2.27747000	2.14656000	H	-4.54075900	-2.27611200	2.14569900
C	-4.16917300	-0.16503300	1.73831100	C	-4.16555900	-0.16395800	1.73791800
H	-4.93871100	0.18161800	2.41884600	H	-4.93394600	0.18320500	2.41972100
C	-3.39943600	0.76704400	1.05061600	C	-3.39699000	0.76841700	1.05012700
C	-2.30532400	0.31694700	0.19984900	C	-2.30352700	0.31836500	0.19966200
C	-3.62579200	2.17454800	1.20941900	C	-3.62251900	2.17535700	1.20850900
H	-4.47923200	2.49980000	1.79430200	H	-4.47657900	2.50126100	1.79232200
C	-2.79515500	3.07884800	0.62102900	C	-2.79117500	3.07853600	0.62067300
H	-2.99418700	4.14230300	0.69822800	H	-2.98983600	4.14223700	0.69753500
C	-1.61276000	2.65510900	-0.05889400	C	-1.60943500	2.65505100	-0.05877100
C	-1.31351500	1.25184500	-0.16933500	C	-1.31111100	1.25178800	-0.16927200
C	-0.75921300	3.63968700	-0.65139100	C	-0.75522400	3.63782300	-0.65145400
H	-1.08812400	4.67315200	-0.61507600	H	-1.08344200	4.67173800	-0.61614300
C	0.42028400	3.32193100	-1.25755700	C	0.42349300	3.31900200	-1.25747800
H	1.03676700	4.08391800	-1.71995100	H	1.04023500	4.08040100	-1.72065300
C	0.89848200	1.96643400	-1.18972800	C	0.90108500	1.96367200	-1.19053700
C	0.05776300	0.92619600	-0.60182300	C	0.05916000	0.92439500	-0.60348100
C	2.17178500	1.54127800	-1.52664600	C	2.17315300	1.53641000	-1.52804000
H	2.93230500	2.17413500	-1.96409700	H	2.93419900	2.16828100	-1.96580600
H	-2.47822600	-4.88205500	-1.27516500	H	-2.47378100	-4.87921600	-1.27496800
C	0.75140900	-0.26024800	-0.40569400	C	0.75145200	-0.26334700	-0.40993000
P	2.33620800	-0.22784300	-1.25699500	P	2.33532500	-0.23386300	-1.26274500
C	3.65833200	-0.45059300	0.02135800	C	3.65324100	-0.45225800	0.02201500
C	3.63821100	0.23688300	1.24359700	C	3.62347100	0.22915500	1.24684100
C	4.70799800	-1.33520800	-0.24940500	C	4.71008900	-1.32775900	-0.24774000
C	4.65359000	0.04026200	2.17570700	C	4.63631100	0.03573200	2.18149600
H	2.82867100	0.92347200	1.46403900	H	2.80688500	0.90782500	1.46553800
C	5.72693100	-1.52938000	0.68587300	C	5.72675100	-1.51851400	0.68990300
H	4.73081300	-1.87370000	-1.19050300	H	4.73817000	-1.86206800	-1.19121900
C	5.70021700	-0.84304100	1.89787100	C	5.69034500	-0.83793300	1.90412000
H	4.63003000	0.57506100	3.11870100	H	4.60491200	0.56565300	3.12717800
H	6.53617500	-2.21652300	0.46605800	H	6.54178800	-2.19914800	0.47048500
H	6.48962900	-0.99400700	2.62546800	H	6.47799100	-0.98651500	2.63434100
H	0.34720400	-1.14926800	0.05245200	H	0.34620200	-1.15122500	0.04932200
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1P234-t7				1P234-CC14-t7			
C	5.64026900	0.94035000	-0.26669400	C	5.64156000	0.94050400	-0.26871700
C	4.51786400	1.64774200	-0.76322400	C	4.51858300	1.64811200	-0.76478700
H	4.65609400	2.62686700	-1.20817800	H	4.65677900	2.62715000	-1.20988700
C	5.47763200	-0.32775000	0.23805500	C	5.47926400	-0.32772700	0.23686100
H	6.33520900	-0.89397500	0.58674000	H	6.33707100	-0.89382500	0.58504800
C	3.25927300	1.10255700	-0.69908900	C	3.25969500	1.10307300	-0.69916100
H	2.42090000	1.65067700	-1.10546400	H	2.42131000	1.65176500	-1.10483100
C	4.19967100	-0.93974200	0.28697400	C	4.20077500	-0.93953200	0.28683600
C	3.03849300	-0.19402100	-0.14167200	C	3.03915700	-0.19358800	-0.14123900
C	4.04022400	-2.27837300	0.71230200	C	4.04191000	-2.27854400	0.71251400
H	4.91011700	-2.82866100	1.05495700	H	4.91180300	-2.82891100	1.05480200

C	2.81051900	-2.89197000	0.64737900	C	2.81201100	-2.89248900	0.64782200
H	2.70810400	-3.93704300	0.92014700	H	2.70973900	-3.93759400	0.92020700
C	1.65473600	-2.18328600	0.22677000	C	1.65590500	-2.18350400	0.22738000
C	1.75047000	-0.79659700	-0.05332000	C	1.75105000	-0.79639300	-0.05215300
C	0.41692600	-2.87753100	0.01157700	C	0.41868300	-2.87887800	0.01151200
H	0.38193900	-3.94360300	0.20504700	H	0.38442400	-3.94507500	0.20384200
C	-0.70598900	-2.22979100	-0.58368700	C	-0.70452300	-2.23115800	-0.58400400
H	-1.57601200	-2.81805300	-0.85492600	H	-1.57338700	-2.82054400	-0.85642100
C	-0.68239900	-0.87984600	-0.77158800	C	-0.68159400	-0.88077200	-0.77041000
C	0.47686000	-0.09227500	-0.27841400	C	0.47704600	-0.09239900	-0.27670400
C	-1.22597100	1.58160200	-0.39178600	C	-1.22559500	1.58213200	-0.39124400
H	6.62526900	1.39080100	-0.30985500	H	6.62649100	1.39094500	-0.31294800
C	-3.48774000	-0.25329100	-0.39886700	C	-3.48959800	-0.25357200	-0.39896500
C	-4.62600000	-0.77119300	1.67810100	C	-4.62984300	-0.77176700	1.67737400
C	-4.68402900	-0.47675500	-1.08958000	C	-4.68542800	-0.47619900	-1.09121100
C	-5.81436800	-0.99480100	0.97906500	C	-5.81798000	-0.99461900	0.97695900
C	-5.84249100	-0.84828100	-0.40495100	C	-5.84486200	-0.84751900	-0.40742800
H	-4.70836500	-0.35869800	-2.16798800	H	-4.70999200	-0.35832600	-2.16958600
H	-6.76225300	-1.02029500	-0.95302800	H	-6.76409100	-1.01889700	-0.95646700
P	-2.00044000	0.23782700	-1.39724800	P	-2.00064000	0.23681600	-1.39393900
C	0.08630100	1.21493500	0.08808600	C	0.08630000	1.21501700	0.08947600
C	0.79036900	2.15758300	0.89960000	C	0.79005000	2.15782900	0.90118600
C	0.23640300	3.39658900	1.16021600	C	0.23665000	3.39773700	1.16055900
C	-1.02025100	3.75377600	0.64050600	C	-1.01941800	3.75550800	0.63910200
C	-1.74887000	2.83341200	-0.13247800	C	-1.74825900	2.83468500	-0.13382100
H	1.74343000	1.88709300	1.33409400	H	1.74244400	1.88752800	1.33731400
H	0.77516300	4.10087400	1.78459400	H	0.77519400	4.10210800	1.78494500
H	-1.43203900	4.73546200	0.84367500	H	-1.43074200	4.73760100	0.84097000
H	-2.72587400	3.10947900	-0.51531900	H	-2.72460100	3.11153200	-0.51768700
C	-3.47082400	-0.40468700	0.99469900	C	-3.47367800	-0.40540900	0.99483900
H	-6.71298100	-1.28105400	1.51427800	H	-6.71713400	-1.28072000	1.51123300
H	-4.60196700	-0.88315500	2.75665100	H	-4.60660300	-0.88422300	2.75581800
H	-2.55259000	-0.23425400	1.54541000	H	-2.55626700	-0.23594000	1.54726500
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IP234-DCM-t7				IP234-DMSO-t7			
C	5.62500800	0.98511800	-0.00089700	C	5.62590600	0.98685600	-0.00108700
C	4.57033600	1.67369000	-0.57089600	C	4.57082100	1.67595000	-0.56988600
H	4.72008400	2.66774300	-0.97680100	H	4.72012400	2.67061300	-0.97443800
C	5.41382200	-0.32013600	0.47794400	C	5.41509500	-0.31906900	0.47675700
H	6.23689600	-0.89212300	0.89149300	H	6.23839100	-0.89126400	0.88944000
C	3.27134400	1.09468300	-0.62989500	C	3.27177000	1.09665900	-0.62895900
H	2.47969200	1.65084100	-1.11052300	H	2.47987800	1.65370400	-1.10818500
C	4.12652900	-0.93346700	0.40452700	C	4.12767000	-0.93236200	0.40366600
C	3.00523200	-0.18251400	-0.09476000	C	3.00592200	-0.18123100	-0.09484000
C	3.95694800	-2.28933500	0.74822400	C	3.95856600	-2.28848300	0.74730100
H	4.80714500	-2.85057900	1.11990900	H	4.80875700	-2.84963000	1.11897600
C	2.73878800	-2.94597300	0.50793900	C	2.74063800	-2.94551700	0.50682200
H	2.66280000	-4.01743600	0.65442900	H	2.66535200	-4.01700700	0.65309300
C	1.62299200	-2.23435100	0.04687000	C	1.62461900	-2.23407100	0.04583900
C	1.70009000	-0.80478700	-0.10531200	C	1.70100300	-0.80403900	-0.10547700
C	0.43185700	-2.94351000	-0.32265000	C	0.43413300	-2.94386900	-0.32484200
H	0.42375600	-4.02317800	-0.22347200	H	0.42661200	-4.02358000	-0.22663400
C	-0.65498100	-2.27568100	-0.84343900	C	-0.65308900	-2.27623900	-0.84555000
H	-1.52183600	-2.82344500	-1.19442800	H	-1.51899500	-2.82459600	-1.19788800

C	-0.66062300	-0.86959800	-0.82852200	C	-0.65981800	-0.87000500	-0.82877500
C	0.44040900	-0.11450400	-0.34176700	C	0.44064600	-0.11437300	-0.34149100
C	-1.23899800	1.60378400	-0.50984000	C	-1.23988500	1.60320900	-0.50840300
H	6.60983000	1.43311900	0.06054400	H	6.61067900	1.43489200	0.06054800
C	-3.45762000	-0.26873700	-0.31022600	C	-3.45840500	-0.27036300	-0.31047800
C	-4.45585000	-0.78800100	1.83688300	C	-4.45549700	-0.79975000	1.83496800
C	-4.70097900	-0.46905800	-0.92089600	C	-4.70387700	-0.45964500	-0.92046000
C	-5.69392300	-0.98511300	1.21944600	C	-5.69584600	-0.98546100	1.21830000
C	-5.81565300	-0.82547900	-0.15880600	C	-5.81917800	-0.81522900	-0.15870500
H	-4.79952000	-0.34627400	-1.99413200	H	-4.80399700	-0.32912700	-1.99257500
H	-6.77368100	-0.97739800	-0.64314400	H	-6.77883100	-0.95849700	-0.64234700
P	-2.02747100	0.20312700	-1.39125800	P	-2.02771300	0.20216200	-1.38997800
C	0.06392200	1.25223800	-0.03583300	C	0.06328700	1.25207000	-0.03464300
C	0.76113400	2.20389200	0.75299500	C	0.76010800	2.20393700	0.75434100
C	0.20715000	3.45555700	0.98565000	C	0.20556900	3.45547800	0.98752700
C	-1.04167000	3.80620700	0.45246800	C	-1.04351600	3.80571900	0.45453800
C	-1.76844300	2.86592700	-0.29595100	C	-1.77000200	2.86518000	-0.29419500
H	1.71379600	1.95113500	1.19657700	H	1.71314300	1.95199800	1.19758800
H	0.74737300	4.16988500	1.59718200	H	0.74564000	4.16996200	1.59896200
H	-1.45501300	4.79128700	0.63464400	H	-1.45724100	4.79058400	0.63685000
H	-2.74927000	3.12415800	-0.68091600	H	-2.75080500	3.12337300	-0.67922800
C	-3.34442000	-0.43244700	1.07812000	C	-3.34340500	-0.44481900	1.07655700
H	-6.55778400	-1.26216900	1.81313900	H	-6.56008900	-1.26214900	1.81151800
H	-4.35837700	-0.91198400	2.90973000	H	-4.35678500	-0.93232500	2.90664200
H	-2.38823900	-0.28091000	1.56639100	H	-2.38554700	-0.30257400	1.56440800
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1P234-n-hexane-t7				12P34-t5			
C	5.64129900	0.94036400	-0.26839600	C	3.00506900	2.81549800	1.38286400
C	4.51842900	1.64794400	-0.76455800	C	2.66452500	4.09866800	0.91769100
H	4.65664200	2.62697300	-1.20968300	H	3.22295800	4.96623300	1.24877200
C	5.47892700	-0.32783300	0.23703900	C	2.30906000	1.70138200	0.95191800
H	6.33669100	-0.89397200	0.58530500	H	2.56111400	0.73254700	1.35764100
C	3.25959700	1.10290300	-0.69917800	C	1.57011300	4.25203200	0.06852800
H	2.42121500	1.65146900	-1.10500500	H	1.26136000	5.24185300	-0.25022300
C	4.20053300	-0.93966100	0.28683200	C	4.44626200	-1.52518500	-0.19051700
C	3.03900200	-0.19373900	-0.14132800	C	3.27908600	-0.82737000	-0.41872600
C	4.04153500	-2.27859800	0.71242700	C	4.40738800	-2.85585400	0.29462000
H	4.91141200	-2.82901000	1.05473600	H	5.32564900	-3.39595400	0.48903100
C	2.81165000	-2.89243900	0.64773000	C	3.16867200	-3.49120600	0.44884900
H	2.70933000	-3.93754100	0.92017000	H	3.12842700	-4.53485400	0.74394000
C	1.65560400	-2.18347800	0.22731100	C	1.96116600	-2.81832400	0.18088200
C	1.75090100	-0.79645000	-0.05233700	C	1.99386000	-1.40937500	-0.16241200
C	0.41824300	-2.87857000	0.01163300	C	0.73034200	-3.51389000	0.16656800
H	0.38378200	-3.94473900	0.20419600	H	0.72523500	-4.56619500	0.43249000
C	-0.70488500	-2.23082600	-0.58386900	C	-0.44714800	-2.89777900	-0.25320600
H	-1.57398100	-2.81999200	-0.85603800	H	-1.36238800	-3.46901600	-0.34805400
C	-0.68179300	-0.88052800	-0.77056900	C	-0.43111800	-1.52069100	-0.55223900
C	0.47699100	-0.09236700	-0.27695900	C	0.74534000	-0.73775200	-0.36599900
C	-1.22561400	1.58211700	-0.39129800	C	-0.79510800	0.94613300	-1.06736500
H	6.62625000	1.39079200	-0.31245200	H	3.81195900	2.69694600	2.09712200
C	-3.48925300	-0.25344300	-0.39893900	C	-3.14010200	-0.43688300	-0.16339300
C	-4.62918000	-0.77156800	1.67746500	C	-4.02304600	-0.18939000	2.08088100
C	-4.68512100	-0.47640200	-1.09095500	C	-4.44825200	-0.56612300	-0.64702700
C	-5.81729400	-0.99473500	0.97727100	C	-5.32511300	-0.30553300	1.58836900

C	-5.84435700	-0.84782800	-0.40704900	C	-5.53593500	-0.49306400	0.22294900
H	-4.70957000	-0.35853500	-2.16934300	H	-4.61414400	-0.72462100	-1.70758800
H	-6.76365300	-1.01946200	-0.95592400	H	-6.54433500	-0.58632400	-0.16489900
P	-2.00059400	0.23710800	-1.39453900	P	-1.74447200	-0.58361400	-1.37797300
C	0.08633000	1.21503400	0.08925500	C	0.46396500	0.69466600	-0.46998400
C	0.79019700	2.15776200	0.90093000	C	1.23255200	1.81023900	0.01319300
C	0.23676600	3.39754300	1.16051600	C	0.81347400	3.13498600	-0.36147400
C	-1.01938200	3.75526800	0.63936800	C	-0.38442200	3.31605000	-1.09771000
C	-1.74824600	2.83456200	-0.13355000	C	-1.20584600	2.24250900	-1.40314700
H	1.74268900	1.88735000	1.33676600	H	-0.67677500	4.32322800	-1.37563900
H	0.77539200	4.10186000	1.78491000	H	-2.15694900	2.40386100	-1.89732100
H	-1.43074200	4.73731500	0.84144600	C	-2.93722700	-0.25456700	1.21357900
H	-2.72470500	3.11130700	-0.51721200	H	-6.16897500	-0.25497300	2.26727300
C	-3.47320600	-0.40509600	0.99481200	H	-3.85572300	-0.04672900	3.14297700
H	-6.71634600	-1.28093800	1.51168500	H	-1.92955000	-0.16052000	1.60309300
H	-4.60582900	-0.88384000	2.75594200	H	5.40051200	-1.05619200	-0.40114800
H	-2.55570300	-0.23527700	1.54696200	H	3.33336300	0.16985800	-0.83400900
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12P34-CCL4-t5				12P34-DCM-t5			
C	2.71948000	2.85679100	1.62914300	C	3.09286100	2.77741100	1.49769900
C	2.50278300	4.10803300	1.05405200	C	2.81471600	4.06938100	1.02672300
H	3.03343700	4.97916600	1.42102300	H	3.40334100	4.91314300	1.36866500
C	2.05163800	1.73331500	1.13426800	C	2.35783600	1.68422000	1.03951700
H	2.22876100	0.77241700	1.59877500	H	2.58467400	0.70278000	1.43026100
C	1.57605300	4.23833800	0.02393700	C	1.76196500	4.26398500	0.15024900
H	1.36806700	5.21558900	-0.39892200	H	1.50255800	5.26360700	-0.18168800
C	4.39339400	-1.53195600	0.03974200	C	4.43312700	-1.67820700	-0.20400800
C	3.23038700	-0.81547400	-0.23862400	C	3.27714000	-0.91367800	-0.37477500
C	4.31915900	-2.88113900	0.39248100	C	4.34375100	-3.02901000	0.15902300
H	5.22008800	-3.43609700	0.62804200	H	5.24371000	-3.61369700	0.31260200
C	3.08467700	-3.51654600	0.40662900	C	3.09823100	-3.62139700	0.28494200
H	3.02059700	-4.57576800	0.63252400	H	3.01479800	-4.67783000	0.51675500
C	1.90015700	-2.81910000	0.09259800	C	1.89966200	-2.87921700	0.07368400
C	1.96361400	-1.41364500	-0.17076400	C	1.98914100	-1.46126900	-0.18787800
C	0.66195500	-3.52398500	-0.06103400	C	0.64698300	-3.53912900	0.04268400
H	0.63760600	-4.58772600	0.14687700	H	0.60473300	-4.60507700	0.23376800
C	-0.46620800	-2.88034200	-0.57848000	C	-0.50008100	-2.84602300	-0.34319300
H	-1.35896200	-3.45900500	-0.79173400	H	-1.43220100	-3.37872600	-0.49579500
C	-0.45589200	-1.51661900	-0.80194500	C	-0.43903500	-1.46131000	-0.52874600
C	0.71012400	-0.70076600	-0.45462400	C	0.75948600	-0.70861800	-0.33199800
C	-0.81288200	0.96463400	-1.22354700	C	-0.72065100	1.05587100	-1.00644700
H	3.40737200	2.74801800	2.45976700	H	3.88646200	2.62209900	2.21988600
C	-3.06375100	-0.46341300	-0.11024000	C	-3.22221500	-0.42786800	-0.15238100
C	-3.67830900	-0.34916500	2.23350600	C	-4.31113300	-0.77866400	1.97833800
C	-4.42222100	-0.44855400	-0.44743100	C	-4.44197600	-0.00986100	-0.70220300
C	-5.03069700	-0.32929000	1.88609500	C	-5.52132800	-0.34872600	1.43150500
C	-5.40190000	-0.37923400	0.54439600	C	-5.58554600	0.03568900	0.09164600
H	-4.71520400	-0.49430100	-1.49145800	H	-4.49770400	0.27710400	-1.74654300
H	-6.45059400	-0.36906400	0.26827500	H	-6.52587000	0.36292500	-0.33675000
P	-1.83465200	-0.53384000	-1.51338800	P	-1.72415800	-0.42424800	-1.21933400
C	0.43333600	0.67411200	-0.49679600	C	0.54316000	0.72381400	-0.42966400
C	1.16215900	1.82467900	0.05700700	C	1.32627200	1.82939800	0.08527100

C	0.86602500	3.12444900	-0.46423000	C	0.96351000	3.17364600	-0.30203600
C	-0.20394000	3.29367600	-1.40507500	C	-0.21198800	3.41224100	-1.05469600
C	-1.06659300	2.22702100	-1.71030600	C	-1.07872100	2.36148100	-1.35124900
H	-0.39562900	4.28266400	-1.80550400	H	-0.46190900	4.42655900	-1.34299500
H	-1.93903700	2.40674600	-2.33004300	H	-2.02017500	2.55651700	-1.85271300
C	-2.70175200	-0.41598100	1.24300400	C	-3.16216600	-0.82325900	1.19245100
H	-5.78929700	-0.27788400	2.65919300	H	-6.41273600	-0.31742500	2.04740300
H	-3.38579700	-0.31225000	3.27729400	H	-4.26070700	-1.07942700	3.01866300
H	-1.65523300	-0.43329900	1.52561500	H	-2.22407700	-1.15500700	1.62068500
H	5.35508600	-1.03541700	-0.02046000	H	5.40360200	-1.22008800	-0.35807800
H	3.31372900	0.22477700	-0.52100500	H	3.37586400	0.12086800	-0.67087100
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12P34-DMSO-t4				12P34-n-hexane-t5			
C	3.10241100	2.77357500	1.49905300	C	2.99825200	2.81976100	1.38588900
C	2.82561400	4.06630900	1.02897900	C	2.65663000	4.10256000	0.91932600
H	3.41625700	4.90895400	1.37012700	H	3.21299300	4.97108900	1.25136000
C	2.36454700	1.68175700	1.04159800	C	2.30453800	1.70436200	0.95385600
H	2.59096100	0.69981900	1.43141000	H	2.55731700	0.73622600	1.36083500
C	1.77147400	4.26297300	0.15429500	C	1.56350400	4.25421800	0.06759400
H	1.51319100	5.26315100	-0.17680000	H	1.25405800	5.24344000	-0.25212800
C	4.43282700	-1.68346300	-0.20872200	C	4.44876100	-1.51940400	-0.18891000
C	3.27743100	-0.91695200	-0.37622100	C	3.28039900	-0.82306900	-0.41698700
C	4.34206900	-3.03490700	0.15208000	C	4.41174000	-2.85086100	0.29517700
H	5.24137800	-3.62115900	0.30331300	H	5.33078300	-3.38978700	0.48925600
C	3.09564500	-3.62568900	0.27891900	C	3.17368600	-3.48879200	0.44818300
H	3.01095000	-4.68236600	0.50905300	H	3.13495900	-4.53276900	0.74201100
C	1.89772700	-2.88123200	0.07094900	C	1.96509600	-2.81718300	0.18037500
C	1.98868100	-1.46278200	-0.18816100	C	1.99564900	-1.40757100	-0.16176100
C	0.64399200	-3.53959700	0.04064700	C	0.73558700	-3.51525200	0.16538100
H	0.60046000	-4.60577000	0.23000900	H	0.73210100	-4.56773800	0.43019600
C	-0.50271300	-2.84427600	-0.34253700	C	-0.44304300	-2.90010900	-0.25402100
H	-1.43537700	-3.37583400	-0.49509700	H	-1.35725600	-3.47299500	-0.34899100
C	-0.44057900	-1.45905700	-0.52559900	C	-0.42899300	-1.52255400	-0.55173900
C	0.75959200	-0.70801100	-0.32891200	C	0.74612800	-0.73771800	-0.36568600
C	-0.71965400	1.05923800	-0.99870700	C	-0.79549800	0.94432700	-1.07030400
H	3.89712100	2.61663000	2.21964500	H	3.80400200	2.70268900	2.10166500
C	-3.22629300	-0.42391600	-0.15324700	C	-3.13963600	-0.44162100	-0.16251100
C	-4.33108000	-0.80936500	1.96344200	C	-4.02132700	-0.19119500	2.08204200
C	-4.43740400	0.02362800	-0.69954000	C	-4.44785200	-0.57028500	-0.64597800
C	-5.53228600	-0.34958800	1.42084900	C	-5.32381700	-0.30755700	1.58993900
C	-5.58408300	0.06705100	0.08993900	C	-5.53539700	-0.49622300	0.22477300
H	-4.48402300	0.33585100	-1.73696800	H	-4.61512800	-0.72879600	-1.70626700
H	-6.51739400	0.41757800	-0.33523100	H	-6.54392200	-0.58953900	-0.16262000
P	-1.72449400	-0.41961600	-1.21397000	P	-1.74359500	-0.58671300	-1.37735000
C	0.54532600	0.72458400	-0.42493000	C	0.46292400	0.69451800	-0.47078200
C	1.33145900	1.82885900	0.08909400	C	1.22935600	1.81132400	0.01300700
C	0.97031000	3.17402300	-0.29697400	C	0.80921300	3.13559900	-0.36348800
C	-0.20621600	3.41502100	-1.04778300	C	-0.38724600	3.31509300	-1.10265600
C	-1.07538000	2.36589000	-1.34324000	C	-1.20718700	2.23997400	-1.40869700
H	-0.45488100	4.42978400	-1.33553500	H	-0.68018900	4.32158400	-1.38216300
H	-2.01668000	2.56293300	-1.84398400	H	-2.15706500	2.40022200	-1.90552900
C	-3.17863600	-0.85152600	1.18233600	C	-2.93578600	-0.25765500	1.21398100
H	-6.42640100	-0.32035800	2.03284300	H	-6.16735100	-0.25594000	2.26914300
H	-4.29038100	-1.13546800	2.99650100	H	-3.85344400	-0.04747100	3.14384900

H	-2.24783300	-1.20652000	1.60768900	H	-1.92811000	-0.16349900	1.60356400
H	5.40373300	-1.22639400	-0.36312900	H	5.40241700	-1.04864400	-0.39835000
H	3.37764600	0.11814300	-0.66994700	H	3.33366400	0.17449600	-0.83159300
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1-A-13-D-P1234-t4				1-A-13-D-P1234-t4-CC14			
C	2.255721	-3.653940	0.358814	C	2.310643	-3.716713	0.393018
C	1.732805	-2.767427	1.281912	C	1.764311	-2.844798	1.297844
C	2.969653	-3.170181	-0.734279	H	1.298713	-3.221273	2.197731
H	3.452599	-3.861569	-1.415282	C	2.986766	-3.221881	-0.738762
C	1.872013	-1.366453	1.095279	H	3.455537	-3.907234	-1.435659
C	3.048794	-1.787899	-1.006844	C	1.877192	-1.410154	1.091466
C	2.332767	-0.866468	-0.191018	C	3.021109	-1.825773	-1.027916
C	3.794735	-1.306187	-2.119998	C	2.316306	-0.911596	-0.174174
H	4.334201	-2.014653	-2.737905	C	3.759873	-1.340251	-2.126585
C	3.863366	0.035683	-2.359119	H	4.302462	-2.045701	-2.745299
H	4.507603	0.423230	-3.141049	C	3.905684	0.042533	-2.332986
C	3.058417	0.956268	-1.631449	H	4.619462	0.415011	-3.059856
C	2.124453	0.472720	-0.663627	C	3.147931	0.946242	-1.594709
C	3.185154	2.359099	-1.837143	C	2.160710	0.453116	-0.635939
H	3.911356	2.723215	-2.554565	C	3.322003	2.358246	-1.732353
C	2.437066	3.226002	-1.085387	H	4.099551	2.720393	-2.397246
H	2.596472	4.296318	-1.172492	C	2.546651	3.231672	-1.033093
C	1.383574	2.773863	-0.246725	H	2.717781	4.300520	-1.103245
C	1.090357	1.375016	-0.178362	C	1.423675	2.768155	-0.265508
C	0.574187	3.709622	0.469577	C	1.156515	1.381687	-0.185518
H	0.853238	4.757881	0.442986	C	0.607477	3.726174	0.430503
C	-0.529758	3.303294	1.162562	H	0.925039	4.763714	0.405873
H	-1.125264	4.019017	1.719648	C	-0.494341	3.366850	1.141953
C	-0.986454	1.948551	1.073199	H	-1.065968	4.091379	1.709702
C	-0.197740	0.978506	0.314037	C	-0.964703	2.014553	1.041608
C	-2.178882	1.454184	1.572634	C	-0.172910	1.021810	0.294495
H	2.169389	-4.719827	0.527096	C	-2.191931	1.558661	1.463345
C	-0.897436	-0.244210	0.147597	H	-2.906496	2.150885	2.019468
P	-2.412717	-0.279772	1.169722	H	2.244466	-4.785696	0.559810
C	-3.836420	-0.329791	-0.037344	C	-0.904212	-0.140512	0.047453
C	-3.897682	0.505941	-1.158999	P	-2.402856	-0.171397	1.077104
C	-4.877558	-1.230721	0.199443	C	-3.866937	-0.293219	-0.037502
C	-4.983873	0.439098	-2.025948	C	-4.016745	0.523583	-1.166879
H	-3.090755	1.204098	-1.351620	C	-4.853114	-1.237455	0.266148
C	-5.969775	-1.295634	-0.668006	C	-5.140751	0.394175	-1.976334
H	-4.831946	-1.885626	1.063511	H	-3.253301	1.252441	-1.413219
C	-6.023318	-0.461255	-1.780887	C	-5.981255	-1.361545	-0.546095
H	-5.021189	1.086854	-2.895298	H	-4.738914	-1.877946	1.133566
H	-6.772062	-1.999742	-0.475561	C	-6.125093	-0.546967	-1.665935
H	-6.868345	-0.512050	-2.458791	H	-5.249008	1.025414	-2.851146
H	1.314210	-3.146541	2.202988	H	-6.740266	-2.097005	-0.304935
N	1.699088	-0.546673	2.170964	H	-6.998814	-0.645596	-2.300211
C	0.876038	-0.945363	3.309589	N	1.630880	-0.575728	2.166976

H	0.470131	-0.040303	3.761822	C	2.508034	0.552308	2.478150
H	0.041980	-1.559156	2.980027	H	1.932810	1.472518	2.611267
H	1.466874	-1.477336	4.064795	H	3.044536	0.341027	3.411988
C	2.504317	0.650953	2.413732	H	3.233330	0.702863	1.684529
H	1.870716	1.535482	2.484007	C	0.821629	-1.009808	3.298386
H	3.028556	0.512414	3.366260	H	0.404276	-0.124032	3.782324
H	3.234105	0.791551	1.623728	H	-0.007396	-1.630904	2.965327
H	-2.876899	2.034071	2.161348	H	1.411428	-1.557224	4.046286
C	-0.615611	-1.277330	-0.748854	C	-0.637389	-1.191914	-0.842261
N	-0.431613	-2.151382	-1.497793	N	-0.546470	-2.066512	-1.601910
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1-A-13-D-P1234-t4-DCM				1-A-13-D-P1234-t4-DMSO			
C	2.346870	-3.644512	0.294934	C	2.349565	-3.646487	0.300481
C	1.795015	-2.787416	1.228890	C	1.796505	-2.787955	1.232594
H	1.395054	-3.194921	2.145639	H	1.401378	-3.194271	2.151945
C	3.045644	-3.123878	-0.793315	C	3.046364	-3.127324	-0.790232
H	3.561759	-3.789513	-1.475259	H	3.566526	-3.793467	-1.468557
C	1.898955	-1.379062	1.069280	C	1.898033	-1.379815	1.069956
C	3.076322	-1.739104	-1.046986	C	3.073292	-1.743766	-1.047464
C	2.342108	-0.844316	-0.210587	C	2.339391	-0.846952	-0.211460
C	3.806185	-1.224996	-2.158841	C	3.801858	-1.231632	-2.161824
H	4.362120	-1.914350	-2.783521	H	4.359298	-1.922283	-2.783731
C	3.843166	0.119340	-2.385287	C	3.837888	0.111755	-2.392514
H	4.474550	0.530864	-3.165104	H	4.469091	0.521654	-3.173254
C	3.025987	1.013321	-1.635211	C	3.022090	1.007755	-1.642248
C	2.109381	0.496430	-0.661066	C	2.107020	0.492694	-0.664285
C	3.132536	2.416948	-1.818698	C	3.130686	2.409997	-1.827724
H	3.850342	2.801006	-2.533985	H	3.848786	2.791741	-2.543913
C	2.379797	3.266974	-1.045201	C	2.381097	3.263661	-1.053252
H	2.530311	4.339670	-1.113558	H	2.535290	4.335717	-1.122259
C	1.341347	2.787120	-0.208998	C	1.343893	2.786839	-0.215173
C	1.068580	1.381393	-0.155219	C	1.068930	1.381248	-0.158112
C	0.524691	3.704590	0.525461	C	0.530270	3.707364	0.519850
H	0.796199	4.755137	0.514608	H	0.805724	4.756834	0.508664
C	-0.569563	3.279452	1.219847	C	-0.563638	3.286312	1.216611
H	-1.167945	3.979556	1.793198	H	-1.158450	3.988051	1.791537
C	-1.009741	1.918752	1.112168	C	-1.006898	1.926064	1.110720
C	-0.208953	0.966516	0.340608	C	-0.207844	0.970786	0.340858
C	-2.194306	1.408240	1.609477	C	-2.192119	1.419504	1.609759
H	-2.891743	1.973946	2.212947	H	-2.885706	1.987451	2.215598
H	2.303703	-4.714010	0.456048	H	2.312171	-4.715401	0.466856
C	-0.899517	-0.263934	0.165046	C	-0.901362	-0.259473	0.169737
P	-2.416999	-0.324922	1.188597	P	-2.417557	-0.315315	1.197102
C	-3.833127	-0.352556	-0.031189	C	-3.832642	-0.348752	-0.023945
C	-3.880655	0.490273	-1.149612	C	-3.899578	0.515992	-1.124956
C	-4.885628	-1.245484	0.191963	C	-4.863730	-1.271559	0.178276
C	-4.961708	0.439156	-2.025522	C	-4.977658	0.456747	-2.004311
H	-3.067618	1.183993	-1.333941	H	-3.104740	1.234835	-1.292219
C	-5.973305	-1.295317	-0.683967	C	-5.948075	-1.330560	-0.701624
H	-4.855479	-1.906107	1.052439	H	-4.820525	-1.947635	1.026092
C	-6.011972	-0.453534	-1.792920	C	-6.005680	-0.467054	-1.793087
H	-4.987833	1.093746	-2.890042	H	-5.019558	1.129609	-2.854029
H	-6.783650	-1.992264	-0.500194	H	-6.741620	-2.050350	-0.533631
H	-6.853094	-0.491784	-2.476231	H	-6.844789	-0.511274	-2.478415

N	1.720308	-0.588690	2.164182	N	1.720151	-0.587835	2.163767
C	0.958041	-1.049984	3.324813	C	2.506858	0.621248	2.420450
H	0.554949	-0.171882	3.828894	H	1.854078	1.488491	2.524464
H	0.129390	-1.679571	3.012439	H	3.043299	0.470945	3.361858
H	1.598413	-1.590039	4.029530	H	3.223757	0.792981	1.625370
C	2.504783	0.621073	2.423056	C	0.964314	-1.049661	3.328769
H	1.851493	1.488207	2.524317	H	0.561140	-0.171696	3.833056
H	3.039610	0.471732	3.365883	H	0.137288	-1.683895	3.021709
H	3.223291	0.793675	1.629504	H	1.610408	-1.585298	4.031072
C	-0.645657	-1.265198	-0.765908	C	-0.657959	-1.257299	-0.765103
N	-0.514664	-2.116310	-1.556277	N	-0.539396	-2.105177	-1.562226
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1-A-13-D-P1234-t4-n-hexane				3-A-12-D-P1234-t4			
C	2.309686	-3.715918	0.394933	C	3.298332	2.980126	0.405715
C	1.765181	-2.843269	1.299956	C	2.440361	2.506552	-0.585328
H	1.300499	-3.218877	2.200721	C	3.860983	2.091079	1.329170
C	2.984410	-3.221945	-0.738157	H	4.563706	2.465730	2.064762
H	3.451107	-3.908004	-1.435739	C	2.121945	1.085805	-0.590441
C	1.877920	-1.408953	1.092004	H	1.489605	0.696036	-1.369675
C	3.019383	-1.826132	-1.028172	C	3.571432	0.694876	1.320712
C	2.315899	-0.911371	-0.174386	C	2.593897	0.204841	0.385803
C	3.756942	-1.341390	-2.128005	C	4.267003	-0.217431	2.133001
H	4.298476	-2.047302	-2.747081	H	5.018528	0.152253	2.821386
C	3.902552	0.041015	-2.335398	C	4.118718	-1.608510	1.938200
H	4.615462	0.413018	-3.063370	H	4.785004	-2.296491	2.448172
C	3.145816	0.945409	-1.596858	C	3.155185	-2.118749	1.070633
C	2.159830	0.452893	-0.636577	C	2.222186	-1.203472	0.422246
C	3.319878	2.357087	-1.735328	C	3.078145	-3.511304	0.789390
H	4.096406	2.718942	-2.401573	H	3.808303	-4.173215	1.243229
C	2.545477	3.230875	-1.035367	C	2.123817	-4.000370	-0.053746
H	2.716658	4.299681	-1.106213	H	2.097731	-5.053354	-0.310820
C	1.423116	2.767801	-0.266745	C	1.075628	-3.151022	-0.534849
C	1.155919	1.381618	-0.185653	C	1.055516	-1.779068	-0.204170
C	0.606930	3.726301	0.428843	C	0.032293	-3.733500	-1.342501
H	0.924695	4.763790	0.403476	H	0.154663	-4.769617	-1.641218
C	-0.494890	3.367689	1.140371	C	-1.064303	-3.040173	-1.743488
H	-1.066595	4.092706	1.707444	H	-1.822412	-3.491593	-2.372209
C	-0.965418	2.015293	1.041222	C	-1.257410	-1.714624	-1.240252
C	-0.173370	1.021709	0.295216	C	-0.210571	-1.080161	-0.427232
C	-2.192710	1.560007	1.463131	C	-2.417739	-0.960195	-1.356898
H	-2.907431	2.153024	2.018210	H	3.563551	4.026028	0.463080
H	2.242758	-4.784783	0.562052	C	-0.634051	0.104808	0.138509
C	-0.904209	-0.141036	0.049750	P	-2.174423	0.655049	-0.575820
P	-2.403227	-0.170694	1.078791	C	-3.425795	0.815855	0.768598
C	-3.866297	-0.293094	-0.037185	C	-3.481615	-0.079008	1.845907
C	-4.013823	0.521653	-1.168257	C	-4.344069	1.868268	0.698487
C	-4.853727	-1.235812	0.266729	C	-4.446646	0.081082	2.834894
C	-5.136786	0.391825	-1.978960	H	-2.772078	-0.895919	1.906512
H	-3.249093	1.249050	-1.414902	C	-5.313093	2.022495	1.690255
C	-5.980857	-1.360357	-0.546752	H	-4.304098	2.564927	-0.131429
H	-4.741015	-1.874981	1.135330	C	-5.363866	1.130954	2.758013
C	-6.122407	-0.547755	-1.668213	H	-4.485688	-0.614796	3.665487
H	-5.243139	1.021382	-2.855231	H	-6.024191	2.838246	1.626191
H	-6.740806	-2.094804	-0.305395	H	-6.115592	1.250876	3.530028

H	-6.995293	-0.646837	-2.303592	H	-0.050266	0.714149	0.810407
N	1.632030	-0.572568	2.166594	N	1.836161	3.332719	-1.514543
C	2.512134	0.553020	2.477618	C	1.272679	2.799506	-2.753170
H	1.938854	1.473943	2.614482	H	0.755138	3.603913	-3.273944
H	3.051842	0.339052	3.409208	H	2.046259	2.396579	-3.420107
H	3.234855	0.704324	1.681801	H	0.539235	2.019335	-2.552668
C	0.821829	-1.004649	3.297678	C	2.158500	4.751158	-1.506833
H	0.404802	-0.118085	3.780614	H	3.198005	4.943323	-1.809056
H	-0.007657	-1.625108	2.964485	H	1.495356	5.272537	-2.195619
H	1.410302	-1.552168	4.046802	H	2.008824	5.168935	-0.509118
C	-0.636079	-1.195410	-0.836543	C	-3.568130	-1.343261	-2.067628
N	-0.543636	-2.073168	-1.592132	N	-4.528906	-1.650286	-2.641753
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3-A-12-D-P1234-t3-CCI4				3-A-12-D-P1234-t3-DCM			
C	3.537841	2.771109	0.368750	C	3.490619	2.808875	0.358348
C	2.589177	2.355921	-0.613113	C	2.552074	2.377498	-0.626537
C	4.037902	1.874458	1.282410	C	4.000557	1.922785	1.277947
H	4.797680	2.199615	1.985561	H	4.752118	2.262580	1.982869
C	2.156065	1.027286	-0.576335	C	2.139322	1.040859	-0.587052
H	1.464262	0.677147	-1.322578	H	1.456100	0.677854	-1.335359
C	3.627085	0.524555	1.306054	C	3.610325	0.567052	1.304692
C	2.601634	0.108309	0.397659	C	2.595352	0.132802	0.392790
C	4.291117	-0.429121	2.134906	C	4.285977	-0.373968	2.139505
H	5.058127	-0.083056	2.819449	H	5.045318	-0.013366	2.825021
C	4.027315	-1.754811	1.994309	C	4.043652	-1.704651	2.003395
H	4.594246	-2.498392	2.543351	H	4.620680	-2.437607	2.555906
C	2.988182	-2.207056	1.115390	C	3.014080	-2.175021	1.122923
C	2.145018	-1.271008	0.441525	C	2.158304	-1.252407	0.442616
C	2.824976	-3.589935	0.885115	C	2.871739	-3.560523	0.895828
H	3.498417	-4.286068	1.372800	H	3.554651	-4.245456	1.385833
C	1.862880	-4.049063	0.008113	C	1.916844	-4.036979	0.019564
H	1.796732	-5.106292	-0.224773	H	1.866778	-5.095761	-0.209484
C	0.905143	-3.171881	-0.531788	C	0.945472	-3.175386	-0.522637
C	0.956783	-1.777834	-0.216720	C	0.977375	-1.779056	-0.213484
C	-0.157032	-3.711376	-1.334093	C	-0.110041	-3.733387	-1.318489
H	-0.102354	-4.757140	-1.615011	H	-0.041591	-4.779208	-1.595552
C	-1.218100	-2.938749	-1.738037	C	-1.185621	-2.976539	-1.721716
H	-2.010073	-3.357446	-2.347777	H	-1.972448	-3.412536	-2.326100
C	-1.309230	-1.603314	-1.301305	C	-1.294749	-1.642379	-1.290945
C	-0.251242	-1.019947	-0.451021	C	-0.241181	-1.039141	-0.449022
C	-2.422537	-0.744137	-1.505449	C	-2.421707	-0.796664	-1.491890
H	3.901711	3.788840	0.382426	H	3.839814	3.831662	0.370060
C	-0.631419	0.194223	0.129576	C	-0.637489	0.173040	0.127627
P	-2.213486	0.688353	-0.457330	P	-2.218615	0.655352	-0.464245
C	-3.473270	0.881480	0.860866	C	-3.474419	0.870936	0.855016
C	-3.090723	0.981710	2.206527	C	-3.099695	0.878054	2.206791
C	-4.826731	1.000668	0.507868	C	-4.813566	1.094999	0.498724
C	-4.058441	1.171591	3.188864	C	-4.064349	1.078728	3.190575
H	-2.047060	0.887447	2.482996	H	-2.066383	0.708411	2.485524
C	-5.787848	1.178431	1.497282	C	-5.772697	1.282330	1.488918
H	-5.129446	0.940259	-0.531653	H	-5.107080	1.115875	-0.545005
C	-5.405477	1.268414	2.837127	C	-5.399269	1.277890	2.834522
H	-3.762268	1.236272	4.229749	H	-3.775276	1.073458	4.235329
H	-6.834164	1.249963	1.223742	H	-6.808876	1.438049	1.212035

H	-6.156192	1.414745	3.605283	H	-6.146985	1.432677	3.603797
H	-0.021746	0.798273	0.778219	H	-0.035533	0.786504	0.774840
N	2.116837	3.251017	-1.558450	N	2.071306	3.261714	-1.575081
C	1.264244	2.763957	-2.633247	C	1.238070	2.758282	-2.658523
H	0.926762	3.610038	-3.229779	H	0.892728	3.597793	-3.259303
H	1.781931	2.056149	-3.296533	H	1.776149	2.059732	-3.315079
H	0.378408	2.266685	-2.229200	H	0.356967	2.245808	-2.263528
C	2.806968	4.517619	-1.770444	C	2.739144	4.542851	-1.781641
H	3.844312	4.382508	-2.106975	H	3.781359	4.426289	-2.108451
H	2.273043	5.084486	-2.531316	H	2.201307	5.097867	-2.548063
H	2.815602	5.122857	-0.860612	H	2.728103	5.147887	-0.872011
C	-3.543227	-1.022755	-2.284663	C	-3.537217	-1.096546	-2.265770
N	-4.480830	-1.240253	-2.942146	N	-4.471322	-1.338116	-2.922355
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3-A-12-D-P1234-t3-DMSO				3-A-12-D-P1234-t3-n-hexane			
C	3.479440	2.818861	0.354525	C	3.546584	2.765261	0.367027
C	2.541834	2.383418	-0.629647	C	2.595513	2.351741	-0.613252
C	3.992940	1.935689	1.275125	C	4.045564	1.867750	1.280145
H	4.743263	2.279359	1.979384	H	4.807171	2.191028	1.982191
C	2.134656	1.044680	-0.588897	C	2.158706	1.024684	-0.575127
H	1.452486	0.678426	-1.336632	H	1.464469	0.676235	-1.319831
C	3.607796	0.578419	1.303582	C	3.631146	0.518853	1.304930
C	2.594518	0.139436	0.392035	C	2.603065	0.104773	0.398469
C	4.287135	-0.359061	2.139572	C	4.293425	-0.435983	2.133562
H	5.045059	0.005375	2.824605	H	5.062156	-0.091737	2.817102
C	4.050230	-1.691127	2.005132	C	4.025835	-1.760957	1.993693
H	4.630300	-2.421135	2.558261	H	4.591272	-2.505740	2.542700
C	3.022457	-2.166316	1.125239	C	2.984597	-2.211016	1.116132
C	2.163015	-1.247413	0.443667	C	2.143444	-1.273549	0.442575
C	2.886071	-3.552657	0.898656	C	2.818472	-3.593741	0.886276
H	3.572080	-4.234470	1.388568	H	3.490665	-4.291093	1.374002
C	1.933056	-4.033801	0.022871	C	1.855479	-4.050860	0.009381
H	1.887755	-5.092836	-0.205669	H	1.787068	-5.107953	-0.223601
C	0.957398	-3.176435	-0.519134	C	0.899732	-3.171760	-0.530765
C	0.983866	-1.779535	-0.211339	C	0.953983	-1.777947	-0.215500
C	-0.096806	-3.739520	-1.312422	C	-0.163742	-3.709398	-1.333102
H	-0.024995	-4.785407	-1.588155	H	-0.111009	-4.755361	-1.613746
C	-1.176384	-2.986815	-1.714989	C	-1.223064	-2.935072	-1.736940
H	-1.961972	-3.427583	-2.317605	H	-2.016172	-3.351647	-2.346646
C	-1.290023	-1.652972	-1.285895	C	-1.311540	-1.599115	-1.300116
C	-0.237733	-1.044605	-0.446430	C	-0.252613	-1.017673	-0.449849
C	-2.420702	-0.810540	-1.485802	C	-2.423217	-0.738599	-1.504934
H	3.825198	3.842767	0.365184	H	3.912946	3.782127	0.379700
C	-0.638186	0.166870	0.129935	C	-0.630047	0.197591	0.129827
P	-2.218259	0.647041	-0.464013	P	-2.212590	0.692642	-0.456659
C	-3.475548	0.868987	0.852361	C	-3.473593	0.884013	0.860503
C	-3.105109	0.868276	2.205416	C	-3.090488	1.011615	2.203684
C	-4.811916	1.104584	0.492359	C	-4.829469	0.975979	0.508424
C	-4.071987	1.070914	3.186853	C	-4.059191	1.201626	3.184883
H	-2.073633	0.692656	2.487081	H	-2.045037	0.937837	2.479764
C	-5.773277	1.293964	1.480159	C	-5.791340	1.154332	1.496948
H	-5.101302	1.135225	-0.552303	H	-5.133247	0.892617	-0.529195
C	-5.404415	1.280496	2.827136	C	-5.408168	1.271736	2.834387
H	-3.786295	1.060190	4.232444	H	-3.762256	1.287215	4.224063

H	-6.807170	1.459683	1.200631	H	-6.839192	1.204416	1.224441
H	-6.153590	1.437433	3.594497	H	-6.159782	1.418278	3.601653
H	-0.038180	0.782481	0.776991	H	-0.019257	0.800585	0.778342
N	2.056372	3.265213	-1.577696	N	2.124146	3.247623	-1.558700
C	1.229564	2.756240	-2.663911	C	1.266354	2.762807	-2.630115
H	0.879145	3.593870	-3.264245	H	0.930520	3.609435	-3.226881
H	1.775140	2.063082	-3.320008	H	1.778887	2.051757	-3.293968
H	0.351774	2.236352	-2.271556	H	0.379656	2.269754	-2.222639
C	2.722857	4.546990	-1.789326	C	2.816322	4.512510	-1.772035
H	3.761698	4.430120	-2.126354	H	3.853238	4.375484	-2.109325
H	2.177385	5.102721	-2.549751	H	2.282927	5.080026	-2.532859
H	2.720744	5.150543	-0.879015	H	2.826862	5.118471	-0.862605
C	-3.535617	-1.116274	-2.256329	C	-3.544808	-1.014727	-2.284601
N	-4.470054	-1.365069	-2.910756	N	-4.483385	-1.229140	-2.941276
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1-A-11-D-P1234-t3				1-A-11-D-P1234-t3-CC14			
C	-3.537591	-1.887173	-0.338848	C	-3.547991	-1.885425	-0.337709
C	-2.544487	-1.437298	-1.259086	C	-2.547530	-1.442084	-1.253208
H	-2.298838	-2.032613	-2.127139	H	-2.303951	-2.038082	-2.121296
C	-3.882698	-1.008954	0.686388	C	-3.892532	-1.001309	0.686413
H	-4.695360	-1.236194	1.362347	H	-4.710572	-1.222092	1.357937
C	-1.858558	-0.245962	-1.070005	C	-1.856742	-0.253159	-1.063216
H	-1.120022	0.040189	-1.805767	C	-3.223912	0.238731	0.861281
C	-3.220644	0.235094	0.861034	C	-2.101359	0.584503	0.029506
C	-2.101089	0.585863	0.026743	C	-3.706630	1.196837	1.769818
C	-3.705449	1.191507	1.768293	H	-4.552430	0.959610	2.404646
H	-4.549046	0.951867	2.405294	C	-3.159671	2.489819	1.787524
C	-3.162723	2.486154	1.782907	H	-3.600759	3.243381	2.431445
H	-3.604986	3.238989	2.427256	C	-2.040229	2.844536	1.009668
C	-2.043751	2.845116	1.005250	C	-1.370715	1.829897	0.251235
C	-1.370751	1.832891	0.249789	C	-1.561136	4.189730	0.979874
C	-1.566831	4.190411	0.977235	H	-2.095456	4.949404	1.539017
H	-2.103236	4.949539	1.535285	C	-0.489642	4.520412	0.182960
C	-0.493512	4.521725	0.184104	H	-0.192037	5.557061	0.066430
H	-0.195997	5.558691	0.069067	C	0.259472	3.522544	-0.472094
C	0.258781	3.525382	-0.469471	C	-0.089939	2.125338	-0.291490
C	-0.089767	2.128606	-0.290719	C	1.346541	3.877305	-1.337034
C	1.348100	3.881240	-1.330378	H	1.527107	4.932004	-1.516817
H	1.529252	4.936142	-1.508340	C	2.126401	2.935855	-1.934726
C	2.129531	2.940344	-1.926883	H	2.924200	3.219733	-2.611490
H	2.929385	3.225980	-2.600601	C	1.984439	1.546851	-1.568879
C	1.987181	1.551079	-1.565259	C	0.927718	1.149802	-0.663695
C	0.928883	1.152493	-0.662620	C	2.859719	0.518040	-1.911915
C	2.862984	0.522427	-1.906352	H	3.699919	0.638674	-2.582791
H	3.705525	0.643201	-2.574162	C	1.114182	-0.169711	-0.188377
C	1.112142	-0.166573	-0.188327	P	2.389076	-1.048321	-1.172309
P	2.387471	-1.043957	-1.170298	C	3.755848	-1.450340	0.022339
C	3.752483	-1.449501	0.025740	C	4.300095	-0.498833	0.895360
C	4.282377	-0.505221	0.914585	C	4.252058	-2.757499	0.040034
C	4.262537	-2.750963	0.027041	C	5.323163	-0.853224	1.769566
C	5.304917	-0.861220	1.788127	H	3.918528	0.516038	0.892276
H	3.888830	0.504976	0.923766	C	5.280240	-3.111657	0.915542
C	5.290693	-3.106569	0.901447	H	3.832372	-3.500603	-0.629703
H	3.852425	-3.488173	-0.655083	C	5.815914	-2.160393	1.779965

C	5.811909	-2.162543	1.781806	H	5.736346	-0.112019	2.444881
H	5.706695	-0.125636	2.476454	H	5.656796	-4.128484	0.922864
H	5.678293	-4.119335	0.895929	H	6.612584	-2.433916	2.462805
H	6.608414	-2.437371	2.464427	H	-1.117392	0.028635	-1.799928
N	-4.126033	-3.131131	-0.485645	N	-4.146149	-3.120497	-0.487200
C	-3.964551	-3.881139	-1.723086	C	-5.251352	-3.483208	0.385425
H	-2.909534	-4.070602	-1.935826	H	-6.141838	-2.859453	0.219628
H	-4.451222	-4.849071	-1.612038	H	-5.521779	-4.522274	0.205047
H	-4.409089	-3.372208	-2.590164	H	-4.959210	-3.391799	1.434944
C	-5.215019	-3.505158	0.399694	C	-3.961455	-3.886852	-1.713115
H	-6.117229	-2.894139	0.245354	H	-2.903375	-4.087054	-1.898279
H	-5.474197	-4.548724	0.226166	H	-4.460118	-4.848273	-1.603076
H	-4.909948	-3.407301	1.445058	H	-4.380893	-3.382115	-2.594226
C	0.462871	-0.769864	0.888536	C	0.481086	-0.770342	0.897583
N	-0.031106	-1.286301	1.808653	N	0.008945	-1.289581	1.828418
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1-A-11-D-P1234-t3-DCM				1-A-11-D-P1234-t3-DMSO			
C	-3.566607	-1.876343	-0.334156	C	-3.515410	-1.955243	-0.418745
C	-2.559338	-1.443615	-1.246604	C	-2.493910	-1.543666	-1.282878
H	-2.322139	-2.039851	-2.116213	H	-2.201981	-2.151746	-2.126814
C	-3.904963	-0.985730	0.690960	C	-3.899989	-1.041957	0.633730
H	-4.729064	-1.196651	1.358166	H	-4.719330	-1.291284	1.293353
C	-1.859360	-0.260035	-1.055678	C	-1.830803	-0.326633	-1.071662
H	-1.118195	0.014353	-1.793616	H	-1.067240	-0.042496	-1.782279
C	-3.225920	0.248429	0.865530	C	-3.249646	0.188133	0.829019
C	-2.100858	0.585168	0.033688	C	-2.125089	0.540643	0.008044
C	-3.701791	1.208088	1.778267	C	-3.740059	1.108789	1.802038
H	-4.549792	0.975368	2.411685	H	-4.588436	0.824630	2.414179
C	-3.146566	2.499534	1.798281	C	-3.235115	2.417924	1.853095
H	-3.584411	3.255826	2.440753	H	-3.726699	3.167298	2.463882
C	-2.027603	2.845177	1.018629	C	-2.138293	2.784381	1.075931
C	-1.365236	1.826116	0.253669	C	-1.427455	1.771630	0.279339
C	-1.541887	4.189200	0.986549	C	-1.721131	4.146749	0.981001
H	-2.071740	4.950612	1.547387	H	-2.273922	4.896817	1.536992
C	-0.471774	4.517250	0.185414	C	-0.683777	4.509150	0.174370
H	-0.171546	5.552880	0.067989	H	-0.416382	5.553538	0.056789
C	0.270231	3.516396	-0.473127	C	0.135820	3.516838	-0.474009
C	-0.085249	2.119244	-0.292542	C	-0.156682	2.144158	-0.292390
C	1.354017	3.869646	-1.344004	C	1.227567	3.946027	-1.301271
H	1.534165	4.924171	-1.524838	H	1.334399	5.011310	-1.477150
C	2.130221	2.928067	-1.945566	C	2.081069	3.066102	-1.895333
H	2.924771	3.209381	-2.626838	H	2.862799	3.397422	-2.567979
C	1.987152	1.539748	-1.574732	C	1.997797	1.681806	-1.531606
C	0.930989	1.143365	-0.667317	C	0.917458	1.224937	-0.643091
C	2.864123	0.512147	-1.917262	C	2.938295	0.717520	-1.822468
H	3.702949	0.633647	-2.589725	H	3.799624	0.874728	-2.457876
C	1.121078	-0.174842	-0.191606	C	1.156079	-0.066545	-0.163360
P	2.396877	-1.053630	-1.176998	P	2.475596	-0.856355	-1.130712
C	3.762181	-1.456362	0.017409	C	3.818611	-1.375945	0.019083
C	4.324443	-0.498525	0.872883	C	4.393134	-0.491483	0.943769
C	4.237782	-2.771308	0.055119	C	4.266170	-2.700389	-0.040431
C	5.344519	-0.854744	1.750511	C	5.402218	-0.932281	1.794912
H	3.961467	0.522999	0.853250	H	4.051113	0.535533	0.998109
C	5.262463	-3.127161	0.934625	C	5.279564	-3.137814	0.814488

H	3.806908	-3.519078	-0.602063	H	3.825732	-3.389748	-0.751837
C	5.815870	-2.169904	1.781843	C	5.846969	-2.255416	1.730730
H	5.772879	-0.108666	2.410675	H	5.842639	-0.244667	2.508002
H	5.623438	-4.149263	0.957196	H	5.620948	-4.165237	0.762727
H	6.610572	-2.444522	2.466355	H	6.633417	-2.594592	2.395254
N	-4.179831	-3.101724	-0.483318	N	-4.154117	-3.159033	-0.543245
C	-3.995192	-3.874257	-1.707278	C	-5.314173	-3.501262	0.279640
H	-2.937737	-4.080011	-1.887646	H	-6.161632	-2.836496	0.082584
H	-4.500242	-4.831795	-1.595262	H	-5.617997	-4.518930	0.047181
H	-4.408375	-3.368445	-2.590161	H	-5.072433	-3.457657	1.343717
C	-5.311074	-3.439706	0.368954	C	-3.788325	-4.057418	-1.631804
H	-6.183774	-2.798401	0.181476	H	-2.713666	-4.257248	-1.621188
H	-5.597919	-4.473353	0.184815	H	-4.314434	-5.001001	-1.510226
H	-5.040210	-3.350934	1.424086	H	-4.050591	-3.633727	-2.608661
C	0.499802	-0.779712	0.896892	C	0.530981	-0.749302	0.886660
N	0.047850	-1.310535	1.832090	N	0.123960	-1.356354	1.791973
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1-A-11-D-P1234-t3-n-hexane				3-A-10-D-P1234-t3			
C	-3.546208	-1.886089	-0.337982	C	-3.363670	-2.065592	-1.583226
C	-2.546426	-1.441805	-1.253785	C	-2.211841	-1.463253	-2.104579
H	-2.301922	-2.037955	-2.121522	C	-4.024615	-1.485763	-0.509502
C	-3.891439	-1.002779	0.685866	C	-1.659279	-0.342048	-1.513756
H	-4.708826	-1.224575	1.357863	H	-0.796576	0.118757	-1.967235
C	-1.856569	-0.252400	-1.063870	C	-3.440277	-0.337149	0.153114
H	-1.117022	0.030015	-1.800114	C	-2.200602	0.207835	-0.332679
C	-3.223906	0.237909	0.860882	C	-4.067710	0.266331	1.268834
C	-2.101435	0.584429	0.029227	H	-4.925822	-0.203529	1.727757
C	-3.707344	1.195864	1.768829	C	-3.607965	1.472581	1.739540
H	-4.553006	0.958291	2.403739	H	-4.148111	1.986988	2.527823
C	-3.161079	2.489011	1.786131	C	-2.419846	2.071228	1.239856
H	-3.602512	3.242466	2.430020	C	-1.595647	1.351432	0.334665
C	-2.041452	2.844524	1.008632	C	-2.060187	3.384953	1.651235
C	-1.371040	1.830287	0.251163	H	-2.717247	3.924821	2.323998
C	-1.562907	4.189769	0.979112	C	-0.925356	3.975844	1.147735
H	-2.097712	4.949359	1.537938	H	-0.693196	5.008456	1.385405
C	-0.491122	4.520574	0.182872	C	-0.004241	3.232487	0.382641
H	-0.193669	5.557305	0.066454	C	-0.261527	1.850511	0.087961
C	0.258715	3.522979	-0.471765	C	1.222341	3.857169	-0.036815
C	-0.090190	2.125850	-0.291104	H	1.338304	4.920444	0.141687
C	1.346002	3.877851	-1.336207	C	2.222241	3.141677	-0.630554
H	1.526589	4.932564	-1.515903	H	3.138557	3.622565	-0.952624
C	2.126064	2.936406	-1.933690	C	2.096932	1.733497	-0.760753
H	2.924053	3.220566	-2.610148	C	0.879502	1.050315	-0.311048
C	1.984293	1.547392	-1.568368	C	3.117157	0.858652	-1.205178
C	0.927703	1.150269	-0.663136	H	-3.784850	-2.928247	-2.082206
C	2.859473	0.518502	-1.911261	C	1.031329	-0.329944	-0.243504
H	3.699775	0.638968	-2.582025	P	2.584112	-0.835835	-0.951681
C	1.113889	-0.169046	-0.187592	C	3.647670	-1.682359	0.293877
P	2.388428	-1.047711	-1.171519	C	3.130495	-2.108376	1.524424
C	3.755539	-1.449813	0.022839	C	4.985002	-1.958120	-0.027525
C	4.298384	-0.498959	0.897297	C	3.948153	-2.782706	2.428158
C	4.253511	-2.756233	0.038632	H	2.100353	-1.890326	1.781198
C	5.321808	-0.853265	1.770998	C	5.800011	-2.618828	0.885872
H	3.915166	0.515284	0.895659	H	5.392873	-1.642754	-0.981866

C	5.282106	-3.110305	0.913577	C	5.282552	-3.037179	2.112730
H	3.834594	-3.498778	-0.632221	H	3.545100	-3.101411	3.383263
C	5.816369	-2.159683	1.779445	H	6.838214	-2.810214	0.639202
H	5.733813	-0.112560	2.447603	H	5.917434	-3.559581	2.819494
H	5.660024	-4.126656	0.919450	H	0.270561	-1.031439	0.054351
H	6.613324	-2.433168	2.461993	C	4.367335	1.241431	-1.695267
N	-4.142579	-3.122694	-0.487193	N	5.413601	1.542475	-2.107831
C	-3.960233	-3.887019	-1.714381	H	-1.769087	-1.862179	-3.010101
H	-2.902393	-4.085808	-1.902652	N	-5.247476	-2.001848	-0.044155
H	-4.457239	-4.849376	-1.604304	C	-5.526017	-3.411546	-0.273480
H	-4.382631	-3.381997	-2.594049	H	-6.333805	-3.719223	0.395008
C	-5.244969	-3.487613	0.387526	H	-5.848402	-3.622567	-1.305227
H	-6.137605	-2.866205	0.223620	H	-4.643055	-4.009773	-0.049560
H	-5.513286	-4.527508	0.208316	C	-6.447584	-1.168712	-0.168413
H	-4.950678	-3.395071	1.436376	H	-6.935758	-1.343875	-1.138950
C	0.478770	-0.769501	0.897658	H	-7.159696	-1.416144	0.623587
N	0.003562	-1.287610	1.827394	H	-6.196479	-0.113826	-0.102061
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3-A-10-D-P1234-t3-CCl4				3-A-10-D-P1234-t3-DCM			
C	-3.360780	-2.055813	-1.598942	C	-3.358049	-2.052737	-1.607615
C	-2.211040	-1.449883	-2.122097	C	-2.209015	-1.445007	-2.131767
C	-4.018131	-1.482946	-0.519130	C	-4.013608	-1.484404	-0.524196
C	-1.655124	-0.333204	-1.528145	C	-1.651237	-0.330665	-1.536765
H	-0.794568	0.129875	-1.983616	H	-0.791373	0.132992	-1.993290
C	-3.431046	-0.337284	0.145381	C	-3.424930	-0.339991	0.140769
C	-2.194183	0.210978	-0.341985	C	-2.190232	0.211098	-0.348425
C	-4.056539	0.259822	1.268804	C	-4.049525	0.253149	1.269174
H	-4.914565	-0.213224	1.724329	H	-4.907271	-0.221957	1.722845
C	-3.600150	1.461171	1.745578	C	-3.597368	1.452544	1.749014
H	-4.138606	1.970661	2.537833	H	-4.135682	1.959087	2.542878
C	-2.412229	2.064214	1.243753	C	-2.410683	2.059623	1.244376
C	-1.591241	1.352206	0.330243	C	-1.590564	1.352573	0.325878
C	-2.056010	3.376226	1.659576	C	-2.059365	3.371847	1.660531
H	-2.712728	3.910298	2.337229	H	-2.717116	3.902243	2.339868
C	-0.924656	3.975356	1.156682	C	-0.931103	3.978099	1.157462
H	-0.695910	5.007272	1.399985	H	-0.707187	5.010485	1.402452
C	-0.002578	3.237112	0.387045	C	-0.006695	3.243185	0.386978
C	-0.258344	1.858982	0.082145	C	-0.259470	1.866596	0.076883
C	1.225439	3.865694	-0.022419	C	1.221378	3.875400	-0.015702
H	1.339558	4.927927	0.162767	H	1.332548	4.937332	0.172311
C	2.230668	3.153892	-0.616145	C	2.232221	3.166164	-0.607862
H	3.147547	3.640256	-0.928274	H	3.148614	3.657998	-0.913031
C	2.105112	1.749714	-0.758553	C	2.108620	1.764896	-0.755979
C	0.883929	1.063753	-0.320813	C	0.885547	1.076042	-0.326399
C	3.128428	0.873280	-1.205190	C	3.136206	0.886192	-1.200692
H	-3.782791	-2.916631	-2.100077	H	-3.779849	-2.912838	-2.109840
C	1.035321	-0.318079	-0.260485	C	1.038867	-0.306685	-0.266848
P	2.593222	-0.820757	-0.949644	P	2.598791	-0.807811	-0.943395
C	3.635788	-1.691998	0.295946	C	3.630268	-1.697854	0.296609
C	3.121166	-2.057009	1.547538	C	3.122383	-2.028301	1.561032
C	4.951118	-2.043571	-0.042295	C	4.928714	-2.095791	-0.056402
C	3.923101	-2.743915	2.456099	C	3.917497	-2.724678	2.468712
H	2.106725	-1.784654	1.814495	H	2.118976	-1.726191	1.837176
C	5.751201	-2.717121	0.875403	C	5.722017	-2.779652	0.860103

H	5.352684	-1.782887	-1.015611	H	5.320885	-1.868739	-1.041899
C	5.237681	-3.072340	2.123962	C	5.216818	-3.097947	2.122319
H	3.523585	-3.015612	3.426926	H	3.524182	-2.970657	3.448695
H	6.772839	-2.969421	0.615154	H	6.730047	-3.070861	0.588048
H	5.859834	-3.604821	2.834369	H	5.832678	-3.638853	2.831651
H	0.274785	-1.021876	0.032086	H	0.279745	-1.012164	0.025194
C	4.375095	1.258796	-1.694033	C	4.380896	1.273558	-1.684391
N	5.418980	1.568800	-2.110087	N	5.425724	1.589728	-2.097948
H	-1.773525	-1.843981	-3.032337	H	-1.774630	-1.837633	-3.044236
N	-5.234727	-2.005251	-0.047859	N	-5.225178	-2.011471	-0.047806
C	-6.440243	-1.176001	-0.156753	C	-6.434848	-1.185056	-0.146186
H	-6.935438	-1.350739	-1.123174	H	-6.933609	-1.358525	-1.110511
H	-7.142799	-1.430446	0.640909	H	-7.131092	-1.446259	0.654269
H	-6.194278	-0.119995	-0.089606	H	-6.193386	-0.128235	-0.075962
C	-5.509668	-3.415957	-0.282927	C	-5.498658	-3.422227	-0.290982
H	-6.312753	-3.728637	0.388377	H	-6.300036	-3.738749	0.380082
H	-5.836799	-3.621067	-1.313740	H	-5.827493	-3.620132	-1.322099
H	-4.623399	-4.012235	-0.067197	H	-4.611137	-4.018818	-0.081184
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3-A-10-D-P1234-t3-DMSO				3-A-10-D-P1234-t3-n-hexane			
C	-3.357208	-2.053652	-1.608725	C	-3.360787	-2.058149	-1.595829
C	-2.207994	-1.445934	-2.132996	C	-2.210862	-1.452683	-2.118915
C	-4.012683	-1.486103	-0.524766	C	-4.018854	-1.483912	-0.517248
C	-1.649866	-0.331868	-1.538247	C	-1.655740	-0.334997	-1.525805
H	-0.789771	0.131356	-1.994908	H	-0.794947	0.127783	-1.981082
C	-3.423701	-0.341658	0.139860	C	-3.432543	-0.337364	0.146551
C	-2.189529	0.210127	-0.349977	C	-2.195261	0.210376	-0.340622
C	-4.048282	0.250841	1.269356	C	-4.058571	0.261131	1.268399
H	-4.905955	-0.224635	1.722691	H	-4.916614	-0.211334	1.724543
C	-3.597851	1.450147	1.749484	C	-3.601763	1.463435	1.743820
H	-4.136373	1.956174	2.543405	H	-4.140615	1.973928	2.535229
C	-2.411786	2.058497	1.243560	C	-2.413729	2.065669	1.242370
C	-1.591419	1.352413	0.324243	C	-1.592109	1.352183	0.330526
C	-2.062768	3.371425	1.658467	C	-2.056977	3.378027	1.657212
H	-2.721409	3.901173	2.337334	H	-2.713802	3.913227	2.333893
C	-0.935588	3.979948	1.155041	C	-0.924945	3.975657	1.154225
H	-0.713843	5.012873	1.399387	H	-0.695622	5.007725	1.396471
C	-0.009845	3.245637	0.385441	C	-0.002975	3.236445	0.385574
C	-0.261048	1.869005	0.074940	C	-0.258968	1.857641	0.082622
C	1.217941	3.879129	-0.015456	C	1.224931	3.864289	-0.025490
H	1.327690	4.941177	0.172462	H	1.339365	4.926728	0.158432
C	2.230998	3.170492	-0.606445	C	2.229304	3.151775	-0.618962
H	3.146883	3.664390	-0.909976	H	3.146164	3.637104	-0.932725
C	2.108685	1.769998	-0.754924	C	2.103707	1.746903	-0.759265
C	0.885341	1.080048	-0.327349	C	0.883086	1.061490	-0.319406
C	3.138104	0.890331	-1.198019	C	3.126410	0.870715	-1.205509
H	-3.778698	-2.913832	-2.110945	H	-3.782453	-2.919568	-2.096281
C	1.039911	-0.302896	-0.266498	C	1.034580	-0.320038	-0.257660
P	2.599840	-0.803801	-0.940062	P	2.591590	-0.823358	-0.950083
C	3.630199	-1.698981	0.296438	C	3.637494	-1.690366	0.295955
C	3.125918	-2.022140	1.564394	C	3.124509	-2.058064	1.547310
C	4.923957	-2.107597	-0.062248	C	4.954373	-2.036001	-0.042106
C	3.921138	-2.720659	2.470494	C	3.929120	-2.742211	2.455555
H	2.125136	-1.714796	1.844127	H	2.109123	-1.789404	1.814482

C	5.717228	-2.793986	0.852604	C	5.757146	-2.706622	0.875308
H	5.311738	-1.889079	-1.051396	H	5.355235	-1.772052	-1.014841
C	5.216293	-3.103868	2.118758	C	5.245025	-3.064947	2.123478
H	3.530813	-2.961558	3.452855	H	3.530665	-3.015975	3.426273
H	6.721139	-3.094826	0.575951	H	6.780055	-2.953917	0.615171
H	5.831728	-3.647087	2.826611	H	5.869378	-3.595155	2.833689
H	0.281520	-1.008933	0.026058	H	0.273960	-1.023453	0.035688
C	4.382457	1.278375	-1.678719	C	4.373710	1.255775	-1.694704
N	5.428265	1.597031	-2.089645	N	5.417835	1.564344	-2.110404
H	-1.774074	-1.839116	-3.045487	H	-1.772406	-1.847703	-3.028287
N	-5.222696	-2.014569	-0.046827	N	-5.236334	-2.005381	-0.046716
C	-6.433690	-1.188963	-0.141925	C	-6.441251	-1.176008	-0.158749
H	-6.933360	-1.361981	-1.105698	H	-6.935047	-1.351420	-1.125871
H	-7.128053	-1.452446	0.659248	H	-7.145464	-1.429183	0.637966
H	-6.193700	-0.131910	-0.070319	H	-6.194822	-0.120065	-0.092215
C	-5.496094	-3.425112	-0.293630	C	-5.511214	-3.416193	-0.279885
H	-6.296965	-3.743102	0.377168	H	-6.314793	-3.728069	0.391293
H	-5.825610	-3.619796	-1.324948	H	-5.837645	-3.623102	-1.310676
H	-4.608327	-4.022243	-0.086317	H	-4.625143	-4.012193	-0.062571
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1-D-13-A-1P234-t5				1-D-13-A-1P234-t4-CCl4			
C	5.173916	0.634314	-0.243561	C	-5.170389	-0.634654	-0.229641
C	4.161189	1.233583	-0.962773	C	-4.157891	-1.235923	-0.947345
H	4.319380	2.166746	-1.487615	H	-4.315039	-2.174351	-1.463033
C	4.988246	-0.633906	0.332550	C	-4.986854	0.638545	0.337518
H	5.807535	-1.126074	0.843960	H	-5.806031	1.131946	0.847719
C	2.882607	0.582848	-1.077750	C	-2.881865	-0.580674	-1.070703
C	3.731514	-1.306854	0.241258	C	-3.729897	1.311143	0.243894
C	2.615530	-0.625261	-0.342823	C	-2.613583	0.629741	-0.337650
C	3.572013	-2.645991	0.665858	C	-3.570766	2.651742	0.666052
H	4.430246	-3.164471	1.079340	H	-4.428971	3.170929	1.078568
C	2.386795	-3.337519	0.433589	C	-2.384952	3.341602	0.435210
H	2.333463	-4.404857	0.618380	H	-2.330559	4.408724	0.621184
C	1.250796	-2.669913	-0.052181	C	-1.248192	2.673027	-0.048810
C	1.321044	-1.237702	-0.241908	C	-1.319620	1.241456	-0.239562
C	0.041190	-3.346945	-0.410830	C	-0.037405	3.351074	-0.402801
H	0.017760	-4.429310	-0.344570	H	-0.012545	4.433039	-0.331216
C	-1.044893	-2.655951	-0.893720	C	1.048163	2.659847	-0.886719
H	-1.917468	-3.194688	-1.247078	H	1.922266	3.198226	-1.236724
C	-1.059366	-1.242856	-0.848344	C	1.059377	1.246092	-0.846756
C	0.067482	-0.539233	-0.375498	C	-0.067419	0.541092	-0.375102
C	-1.425194	1.289926	-0.693494	C	1.420020	-1.289684	-0.706163
H	6.136532	1.126360	-0.157930	H	-6.130823	-1.129470	-0.137320
C	-3.789163	-0.302561	-0.314900	C	3.788453	0.301178	-0.312745
C	-4.791438	-0.824946	1.830070	C	4.784543	0.796129	1.841897
C	-5.065106	-0.041374	-0.827077	C	5.066974	0.060639	-0.829170
C	-6.058862	-0.549036	1.313808	C	6.055172	0.542342	1.320994
C	-6.194338	-0.156701	-0.015347	C	6.195068	0.173973	-0.014949
H	-5.175902	0.248040	-1.867073	H	5.181549	-0.212063	-1.873184
H	-7.176810	0.050807	-0.424861	H	7.179548	-0.017138	-0.427468
P	-2.341761	-0.109501	-1.471325	P	2.342148	0.113338	-1.470546
C	-0.228508	0.851319	-0.071360	C	0.225165	-0.851519	-0.078209
C	0.470281	1.768087	0.789028	C	-0.472564	-1.772128	0.780465
C	0.144711	3.139808	0.680546	C	-0.153260	-3.145305	0.656369

C	-0.932299	3.562318	-0.081112	C	0.920501	-3.565171	-0.111457
C	-1.759072	2.631266	-0.732673	C	1.750785	-2.631608	-0.756298
H	0.689435	3.866712	1.267392	H	-0.698496	-3.875614	1.238193
H	-1.175031	4.617993	-0.118636	H	1.159312	-4.621338	-0.157827
H	-2.641270	2.967923	-1.264998	H	2.632646	-2.967136	-1.289924
C	-3.664648	-0.701128	1.022168	C	3.658937	0.674978	1.031334
H	-6.935379	-0.646293	1.944710	H	6.930475	0.637492	1.953829
H	-4.683073	-1.137370	2.863163	H	4.672634	1.088882	2.880285
H	-2.683787	-0.923005	1.427531	H	2.676052	0.878407	1.441532
N	1.384500	1.333736	1.731274	N	-1.374189	-1.344351	1.734480
C	2.337344	2.269264	2.306230	C	-1.092424	-0.187250	2.585658
H	3.149201	1.699220	2.760189	H	-1.967695	0.462297	2.655771
H	2.760878	2.904558	1.528710	H	-0.832697	-0.535331	3.594062
H	1.886443	2.901569	3.085411	H	-0.259312	0.386895	2.193326
C	1.103794	0.180831	2.586869	C	-2.314392	-2.286330	2.323795
H	1.979795	-0.467664	2.659328	H	-3.118239	-1.720169	2.795791
H	0.840196	0.530373	3.594768	H	-2.749837	-2.921120	1.552653
H	0.273683	-0.397259	2.193754	H	-1.845533	-2.918135	3.091406
C	2.010636	1.084278	-2.073168	C	-2.020081	-1.071540	-2.078902
N	1.388838	1.522464	-2.951948	N	-1.411602	-1.498782	-2.973143
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1-D-13-A-1P234-t4-DCM				1-D-13-A-1P234-t4-DMSO			
C	-5.165307	-0.638641	-0.213919	C	-5.162455	-0.640822	-0.210443
C	-4.152900	-1.242565	-0.929282	C	-4.150183	-1.243967	-0.926709
H	-4.307769	-2.188250	-1.432251	H	-4.303988	-2.191529	-1.426475
C	-4.985202	0.641004	0.341517	C	-4.984151	0.640258	0.342870
H	-5.804229	1.135026	0.850982	H	-5.802979	1.132699	0.853992
C	-2.880353	-0.581717	-1.062946	C	-2.879404	-0.580305	-1.063178
C	-3.728841	1.314082	0.244274	C	-3.728442	1.314355	0.244952
C	-2.611913	0.632972	-0.334019	C	-2.611334	0.634534	-0.333430
C	-3.570542	2.656761	0.663256	C	-3.570404	2.657244	0.664724
H	-4.428441	3.176112	1.075909	H	-4.427907	3.175820	1.079022
C	-2.384847	3.345328	0.433084	C	-2.384904	3.345876	0.435385
H	-2.329651	4.412156	0.620540	H	-2.329443	4.412230	0.625398
C	-1.246945	2.676022	-0.049082	C	-1.246464	2.677096	-0.047105
C	-1.318886	1.244897	-0.239635	C	-1.318646	1.246385	-0.239164
C	-0.035471	3.355277	-0.399281	C	-0.034418	3.356780	-0.394749
H	-0.009367	4.436769	-0.322115	H	-0.007402	4.437958	-0.314036
C	1.050107	2.664011	-0.883549	C	1.051394	2.665664	-0.878944
H	1.925802	3.202296	-1.229622	H	1.928163	3.204176	-1.221930
C	1.058865	1.249434	-0.847423	C	1.059065	1.250671	-0.845194
C	-0.067518	0.543242	-0.375948	C	-0.067771	0.544064	-0.375213
C	1.415602	-1.288888	-0.716638	C	1.413553	-1.288997	-0.718423
H	-6.122554	-1.137404	-0.112153	H	-6.118054	-1.141852	-0.105171
C	3.788835	0.301443	-0.310862	C	3.790449	0.300343	-0.309444
C	4.779094	0.782804	1.849781	C	4.780964	0.772031	1.853174
C	5.068779	0.066538	-0.827000	C	5.070500	0.071270	-0.828256
C	6.051636	0.535872	1.329132	C	6.053819	0.531696	1.329847
C	6.195204	0.177063	-0.009493	C	6.197365	0.180575	-0.011020
H	5.186897	-0.201043	-1.871867	H	5.188724	-0.191389	-1.874329
H	7.180787	-0.009639	-0.421180	H	7.183063	-0.001524	-0.424395
P	2.343395	0.116864	-1.468908	P	2.344064	0.117700	-1.465618
C	0.222075	-0.850795	-0.084058	C	0.219883	-0.850741	-0.085585
C	-0.474997	-1.774475	0.773362	C	-0.478364	-1.775498	0.770307

C	-0.162304	-3.149412	0.634497	C	-0.168929	-3.151228	0.625583
C	0.909369	-3.567078	-0.137539	C	0.903144	-3.568236	-0.146379
C	1.743715	-2.631508	-0.775779	C	1.740419	-2.632088	-0.780531
H	-0.708094	-3.882389	1.212138	H	-0.715898	-3.885045	1.200895
H	1.145225	-4.623585	-0.190104	H	1.137921	-4.624893	-0.200649
H	2.626823	-2.966094	-1.308072	H	2.625097	-2.966444	-1.310426
C	3.654952	0.665077	1.035993	C	3.656245	0.655858	1.039674
H	6.925385	0.628132	1.964412	H	6.927821	0.622635	1.964907
H	4.664227	1.066942	2.890116	H	4.666061	1.049528	2.895229
H	2.671273	0.861880	1.447387	H	2.672595	0.846747	1.453808
N	-1.363613	-1.353736	1.738354	N	-1.362664	-1.357411	1.738522
C	-2.295000	-2.300255	2.338671	C	-2.292349	-2.305272	2.341150
H	-3.092613	-1.736133	2.822823	H	-3.087366	-1.741403	2.829504
H	-2.738342	-2.935826	1.572938	H	-2.738434	-2.939953	1.576361
H	-1.812641	-2.929931	3.098141	H	-1.806163	-2.935227	3.097349
C	-1.086374	-0.188926	2.581956	C	-1.087851	-0.189984	2.580032
H	-1.960355	0.463379	2.639833	H	-1.962215	0.461989	2.634124
H	-0.839879	-0.532162	3.594226	H	-0.845524	-0.532146	3.593235
H	-0.245589	0.377655	2.195231	H	-0.245044	0.374986	2.195492
C	-2.027035	-1.062501	-2.081209	C	-2.028440	-1.053665	-2.086029
N	-1.427903	-1.477872	-2.988476	N	-1.430729	-1.459197	-2.999243
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1-D-13-A-1P234-t4-n-hexane				3-D-13-A-1P234-t3			
C	5.171187	0.633651	-0.232276	C	-5.376922	1.432711	-0.524204
C	4.158720	1.234813	-0.950111	C	-4.362805	1.845885	0.308797
H	4.316235	2.172244	-1.467497	H	-4.380337	2.822981	0.774374
C	4.987042	-0.638682	0.336448	C	-5.384694	0.118861	-1.029338
H	5.806218	-1.132129	0.846655	H	-6.213952	-0.229762	-1.633768
C	2.882081	0.580609	-1.071978	C	-3.274522	0.952608	0.627516
C	3.729948	-1.311029	0.243421	C	-4.305647	-0.782849	-0.760422
C	2.613793	-0.629382	-0.338493	C	-3.155062	-0.324921	-0.047611
C	3.570479	-2.651287	0.666161	C	-4.380741	-2.136318	-1.150445
H	4.428648	-3.170535	1.078709	H	-5.266784	-2.481401	-1.672054
C	2.384590	-3.341126	0.435352	C	-3.391796	-3.035836	-0.785400
H	2.330113	-4.408258	0.621222	H	-3.518271	-4.094623	-0.983550
C	1.248079	-2.672490	-0.048909	C	-2.208238	-2.596799	-0.166990
C	1.319660	-1.240885	-0.239792	C	-2.012933	-1.183541	0.049780
C	0.037304	-3.350133	-0.403501	C	-1.205552	-3.523036	0.269462
H	0.012454	-4.432158	-0.332694	H	-1.402671	-4.583813	0.161632
C	-1.048201	-2.658785	-0.887407	C	-0.038388	-3.081808	0.847337
H	-1.922168	-3.197056	-1.237928	H	0.683393	-3.795083	1.230273
C	-1.059627	-1.245160	-0.846843	C	0.257578	-1.705856	0.852745
C	0.067354	-0.540563	-0.375161	C	-0.666803	-0.754926	0.357779
C	-1.420800	1.290096	-0.703878	C	1.283343	0.623775	0.592810
H	6.132161	1.127725	-0.141297	H	-6.192827	2.106468	-0.759364
C	-3.788601	-0.300910	-0.313015	C	3.110242	-1.596072	0.294901
C	-4.785728	-0.799054	1.840353	C	3.935676	-2.277506	-1.880046
C	-5.066843	-0.059051	-0.829395	C	4.347841	-1.935496	0.851878
C	-6.055994	-0.543742	1.319513	C	5.169522	-2.609360	-1.315637
C	-6.195228	-0.173125	-0.015795	C	5.374763	-2.438224	0.050474
H	-5.180769	0.215040	-1.873130	H	4.507140	-1.808715	1.917743
H	-7.179500	0.019028	-0.428356	H	6.328911	-2.698549	0.495436
P	-2.342115	-0.112156	-1.470588	P	1.801581	-0.925265	1.436082
C	-0.225562	0.851745	-0.077084	C	-0.048292	0.529402	0.093976

C	0.472552	1.771664	0.781743	C	-0.527763	1.613838	-0.672671
C	0.152237	3.144589	0.660380	C	0.235278	2.749421	-0.855238
C	-0.922120	3.565017	-0.106290	C	1.526814	2.879288	-0.275232
C	-1.751946	2.631956	-0.752166	C	2.039347	1.767911	0.441353
H	0.697534	3.874296	1.242963	H	-0.168974	3.548400	-1.460872
H	-1.161447	4.621137	-0.151236	H	3.036844	1.802209	0.858643
H	-2.633811	2.967762	-1.285597	C	2.913177	-1.774787	-1.081368
C	-3.659856	-0.677071	1.030415	H	5.963992	-3.002539	-1.940309
H	-6.931572	-0.639581	1.951879	H	3.771931	-2.412929	-2.943725
H	-4.674356	-1.093737	2.878268	H	1.956971	-1.522563	-1.526005
H	-2.677150	-0.881926	1.440330	H	-1.497805	1.560275	-1.147978
N	1.376519	1.342629	1.733655	N	2.261299	4.035480	-0.420575
C	2.318615	2.283607	2.320704	C	3.608043	4.123369	0.124070
H	3.123852	1.716936	2.789841	H	4.002300	5.121011	-0.059465
H	2.752171	2.918505	1.548546	H	3.611644	3.952822	1.205690
H	1.852587	2.915524	3.090208	H	4.285868	3.396964	-0.340944
C	1.094585	0.186515	2.585816	C	1.740535	5.146618	-1.202273
H	1.970018	-0.462728	2.657081	H	0.774466	5.486392	-0.815194
H	0.833458	0.535047	3.593902	H	2.437063	5.980824	-1.143455
H	0.262378	-0.388650	2.193016	H	1.613732	4.881796	-2.259592
C	2.018790	1.073297	-2.078230	C	-2.486833	1.308305	1.741892
N	1.408569	1.502420	-2.970221	N	-1.925208	1.656073	2.699701
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3-D-13-A-1P234-t3-CCI4				3-D-13-A-1P234-t3-DCM			
C	-5.377443	1.425634	-0.529484	C	-5.372948	1.432802	-0.537865
C	-4.365108	1.840638	0.304352	C	-4.362261	1.847108	0.297981
H	-4.383138	2.819654	0.765826	H	-4.378272	2.828391	0.754601
C	-5.383584	0.110478	-1.033310	C	-5.381531	0.116089	-1.039691
H	-6.211647	-0.239536	-1.638330	H	-6.208738	-0.232313	-1.646490
C	-3.276642	0.946673	0.625533	C	-3.277795	0.949067	0.623479
C	-4.302908	-0.789095	-0.762799	C	-4.302560	-0.784788	-0.766563
C	-3.153474	-0.329841	-0.048969	C	-3.153965	-0.327509	-0.050549
C	-4.376016	-2.143341	-1.151342	C	-4.376765	-2.139656	-1.154879
H	-5.261127	-2.490547	-1.672935	H	-5.261031	-2.486189	-1.678005
C	-3.385842	-3.041836	-0.783647	C	-3.388199	-3.039311	-0.784374
H	-3.511612	-4.100827	-0.980923	H	-3.515284	-4.098033	-0.981895
C	-2.203310	-2.601227	-0.164332	C	-2.206009	-2.600149	-0.162890
C	-2.009617	-1.186629	0.050233	C	-2.010930	-1.185251	0.051568
C	-1.199643	-3.526290	0.272267	C	-1.203920	-3.526945	0.274410
H	-1.394752	-4.587393	0.164347	H	-1.399674	-4.587745	0.165225
C	-0.032805	-3.081905	0.848372	C	-0.036689	-3.083274	0.850371
H	0.690788	-3.793373	1.231244	H	0.686428	-3.795620	1.232566
C	0.260660	-1.704576	0.851458	C	0.258065	-1.705276	0.853346
C	-0.664546	-0.754899	0.356528	C	-0.665860	-0.753976	0.358666
C	1.282860	0.629005	0.592261	C	1.282241	0.629855	0.597938
H	-6.192848	2.098801	-0.767527	H	-6.185102	2.107964	-0.780665
C	3.114801	-1.593052	0.293442	C	3.114888	-1.596248	0.292618
C	3.943790	-2.267516	-1.882792	C	3.940010	-2.272091	-1.885125
C	4.348353	-1.942850	0.853485	C	4.350913	-1.941144	0.850723
C	5.173590	-2.610593	-1.315363	C	5.172474	-2.610561	-1.319851
C	5.375025	-2.448017	0.052764	C	5.377035	-2.444761	0.047854
H	4.506125	-1.822051	1.920182	H	4.512729	-1.817299	1.916362
H	6.326009	-2.716119	0.499690	H	6.330132	-2.708364	0.492668
P	1.804712	-0.921176	1.431086	P	1.805079	-0.924374	1.429007

C	-0.049335	0.532391	0.094608	C	-0.050546	0.534414	0.099965
C	-0.531382	1.617927	-0.669382	C	-0.531302	1.621986	-0.662791
C	0.229452	2.755044	-0.851989	C	0.230159	2.758734	-0.844577
C	1.523623	2.886473	-0.275006	C	1.526047	2.889409	-0.267296
C	2.038065	1.773959	0.441040	C	2.039366	1.774286	0.448108
H	-0.176390	3.553990	-1.456420	H	-0.174057	3.557414	-1.450228
H	3.036010	1.810258	0.856847	H	3.038624	1.808650	0.860771
C	2.921356	-1.762690	-1.084759	C	2.917979	-1.768674	-1.085029
H	5.967938	-3.005083	-1.939251	H	5.966538	-3.003235	-1.945065
H	3.783217	-2.395526	-2.947798	H	3.777305	-2.401823	-2.949494
H	1.969000	-1.501447	-1.532509	H	1.964320	-1.510560	-1.531976
H	-1.501535	1.564486	-1.144573	H	-1.500561	1.570567	-1.140085
N	2.256237	4.039394	-0.423596	N	2.258328	4.038962	-0.415690
C	3.604183	4.131187	0.121901	C	3.612022	4.126621	0.120301
H	4.000361	5.124908	-0.075179	H	4.003254	5.123684	-0.066991
H	3.606773	3.973787	1.205332	H	3.622106	3.955126	1.200941
H	4.278168	3.397280	-0.335200	H	4.282817	3.399880	-0.352044
C	1.725868	5.159130	-1.189789	C	1.736720	5.154671	-1.197115
H	0.765512	5.496005	-0.787103	H	0.771508	5.492255	-0.808482
H	2.424728	5.990872	-1.133019	H	2.434554	5.986358	-1.135731
H	1.586108	4.901320	-2.246486	H	1.611389	4.888449	-2.253066
C	-2.494380	1.300329	1.744111	C	-2.501604	1.295330	1.747846
N	-1.940795	1.645051	2.708044	N	-1.953383	1.630110	2.718906
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3-D-13-A-1P234-t3-DMSO				3-D-13-A-1P234-t3-n-hexane			
C	-5.371922	1.436840	-0.534162	C	-5.377848	1.425607	-0.527915
C	-4.361699	1.848418	0.303565	C	-4.365200	1.840419	0.305703
H	-4.376933	2.829148	0.761350	H	-4.383386	2.818979	0.768151
C	-5.381988	0.120994	-1.039180	C	-5.383909	0.110778	-1.032227
H	-6.209115	-0.224517	-1.647613	H	-6.212152	-0.239151	-1.637101
C	-3.279044	0.947842	0.627501	C	-3.276367	0.946885	0.626095
C	-4.303795	-0.781330	-0.768281	C	-4.303227	-0.788900	-0.762231
C	-3.155371	-0.326743	-0.050702	C	-3.153610	-0.329635	-0.048680
C	-4.378084	-2.135473	-1.160497	C	-4.376388	-2.142992	-1.151057
H	-5.261954	-2.480456	-1.685137	H	-5.261643	-2.490040	-1.672556
C	-3.389880	-3.036261	-0.791805	C	-3.386170	-3.041482	-0.783940
H	-3.517218	-4.094339	-0.992423	H	-3.511876	-4.100466	-0.981352
C	-2.207608	-2.599038	-0.168720	C	-2.203511	-2.600912	-0.164885
C	-2.012518	-1.184676	0.049377	C	-2.009821	-1.186480	0.049982
C	-1.205545	-3.527009	0.266632	C	-1.199767	-3.525917	0.271597
H	-1.400928	-4.587530	0.154376	H	-1.394976	-4.587017	0.163756
C	-0.038336	-3.084512	0.843780	C	-0.032942	-3.081761	0.847900
H	0.684788	-3.797941	1.223970	H	0.690535	-3.793333	1.230795
C	0.256577	-1.706133	0.849868	C	0.260631	-1.704615	0.851257
C	-0.667468	-0.753653	0.357114	C	-0.664653	-0.754973	0.356342
C	1.280615	0.630162	0.598310	C	1.282952	0.628466	0.591574
H	-6.182730	2.113595	-0.776733	H	-6.193617	2.098651	-0.765165
C	3.116732	-1.596454	0.293791	C	3.114488	-1.592984	0.293702
C	3.945537	-2.275881	-1.881528	C	3.943642	-2.268388	-1.882085
C	4.354144	-1.933585	0.853774	C	4.348297	-1.941761	0.853728
C	5.179437	-2.606633	-1.314535	C	5.173680	-2.610329	-1.314657
C	5.382849	-2.435118	0.052805	C	5.375168	-2.446783	0.053271
H	4.515644	-1.805008	1.918858	H	4.505822	-1.820324	1.920406
H	6.337107	-2.692328	0.498733	H	6.326339	-2.714173	0.500266

P	1.803756	-0.925843	1.426160	P	1.804371	-0.921201	1.431604
C	-0.052763	0.535521	0.100871	C	-0.049170	0.531942	0.093919
C	-0.533824	1.624482	-0.660151	C	-0.531161	1.617182	-0.670411
C	0.227908	2.760983	-0.841799	C	0.229820	2.754167	-0.853199
C	1.525168	2.890808	-0.265610	C	1.523665	2.885498	-0.276113
C	2.038377	1.774605	0.449178	C	2.038054	1.773392	0.440116
H	-0.176113	3.559813	-1.447284	H	-0.176049	3.553122	-1.457638
H	3.038629	1.807672	0.859491	H	3.035861	1.809699	0.856294
C	2.920826	-1.774379	-1.083397	C	2.921037	-1.763674	-1.084314
H	5.975598	-2.997470	-1.938144	H	5.968165	-3.004826	-1.938392
H	3.783914	-2.409745	-2.945497	H	3.782983	-2.397290	-2.946986
H	1.966353	-1.522071	-1.531997	H	1.968358	-1.503382	-1.531913
H	-1.503236	1.574248	-1.137264	H	-1.501432	1.563541	-1.145322
N	2.257555	4.038867	-0.414802	N	2.256556	4.038937	-0.424702
C	3.613128	4.125354	0.118151	C	3.603566	4.131075	0.122251
H	4.002009	5.124026	-0.064443	H	4.000381	5.124529	-0.075394
H	3.625684	3.947657	1.197546	H	3.605041	3.974878	1.205957
H	4.283299	3.402108	-0.360163	H	4.278210	3.396582	-0.333094
C	1.740310	5.151671	-1.204603	C	1.725655	5.158717	-1.189828
H	0.774282	5.492426	-0.821347	H	0.765629	5.495758	-0.786233
H	2.439397	5.982200	-1.144945	H	2.424586	5.990550	-1.133627
H	1.618760	4.879142	-2.259162	H	1.584722	4.901528	-2.246616
C	-2.504800	1.285212	1.755557	C	-2.493006	1.301151	1.743796
N	-1.956891	1.608409	2.731033	N	-1.938054	1.646497	2.706636
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2-D-10-A-12P34-t3				2-D-10-A-12P34-t3-CCl4			
C	-2.555194	-2.671906	0.478767	C	-2.599969	-2.645272	0.480567
C	-2.216952	-3.948357	-0.040390	C	-2.284371	-3.920930	-0.055722
H	-2.866382	-4.796926	0.119188	H	-2.943690	-4.761787	0.102140
C	-1.686205	-1.570115	0.209962	C	-1.713495	-1.553957	0.220294
H	-1.849556	-0.626324	0.698506	H	-1.865968	-0.612024	0.716219
C	-1.038053	-4.122759	-0.733915	C	-1.110856	-4.106473	-0.755371
H	-0.769514	-5.111765	-1.087746	H	-0.858024	-5.096075	-1.118736
C	-3.605229	1.615976	-1.031594	C	-3.577059	1.677108	-1.008815
C	-2.395847	0.911870	-1.145326	C	-2.379985	0.954327	-1.123563
C	-3.650953	2.877781	-0.463738	C	-3.599201	2.944744	-0.451758
H	-4.590471	3.407616	-0.367766	H	-4.530368	3.488990	-0.354267
C	-2.452943	3.520713	-0.055701	C	-2.388252	3.569869	-0.053979
C	-1.181311	2.848412	-0.202329	C	-1.127996	2.874088	-0.197279
C	-1.172065	1.489013	-0.657890	C	-1.145367	1.512131	-0.645291
C	0.045643	3.510658	0.037059	C	0.111253	3.515120	0.035968
H	0.022339	4.544149	0.363299	H	0.111456	4.550173	0.358182
C	1.261191	2.900523	-0.229581	C	1.313960	2.879993	-0.231791
H	2.180726	3.470541	-0.159989	H	2.244812	3.431796	-0.165484
C	1.283810	1.547232	-0.583179	C	1.309804	1.525694	-0.583382
C	0.082431	0.815350	-0.674473	C	0.096653	0.813064	-0.666763
C	1.647167	-0.897613	-1.310122	C	1.627542	-0.923232	-1.315296
C	3.820626	0.232664	0.150205	C	3.823772	0.173302	0.150827
C	4.267839	-0.186036	2.494864	C	4.250917	-0.326177	2.483896
C	5.185838	0.083273	-0.119546	C	5.197814	0.090125	-0.102132
C	5.626200	-0.347346	2.214606	C	5.619758	-0.417719	2.220600
C	6.084046	-0.213044	0.906775	C	6.091999	-0.210049	0.927335
H	5.549055	0.207060	-1.134469	H	5.571294	0.265813	-1.105454
H	7.139189	-0.326857	0.684048	H	7.154101	-0.272128	0.717999

P	2.695844	0.614747	-1.277397	P	2.704901	0.566603	-1.277923
C	0.333196	-0.627587	-0.893982	C	0.318702	-0.633649	-0.888124
C	-0.527850	-1.722459	-0.595776	C	-0.560912	-1.715552	-0.591101
C	-0.141195	-3.040823	-0.993556	C	-0.198157	-3.036394	-1.006713
C	1.132369	-3.247677	-1.562254	C	1.068624	-3.259254	-1.586515
C	2.033291	-2.195979	-1.668844	C	1.989381	-2.223501	-1.689082
H	1.424666	-4.248998	-1.858619	H	1.340214	-4.262663	-1.894865
H	3.039752	-2.384831	-2.026572	H	2.989576	-2.427523	-2.055657
C	3.370271	0.100055	1.470494	C	3.358395	-0.034387	1.456624
H	6.323281	-0.568495	3.015156	H	6.312829	-0.643961	3.023145
H	3.909367	-0.280878	3.514083	H	3.880735	-0.480549	3.491515
H	2.318144	0.232094	1.696493	H	2.298042	0.040134	1.670573
H	-2.364988	-0.013561	-1.700740	H	-2.369848	0.017930	-1.660541
N	-3.676562	-2.480067	1.240517	N	-3.715029	-2.443636	1.245210
C	-4.494112	-3.619537	1.640573	C	-4.582150	-3.567635	1.587144
H	-3.884067	-4.384430	2.128963	H	-4.017515	-4.354991	2.094169
H	-5.254339	-3.283770	2.341700	H	-5.368719	-3.221502	2.252007
H	-4.993653	-4.072050	0.777146	H	-5.045398	-3.992221	0.691096
C	-4.068604	-1.155257	1.724166	C	-4.049848	-1.124585	1.785008
H	-5.124180	-1.178149	1.988938	H	-5.071005	-1.147954	2.157400
H	-3.494931	-0.870435	2.613354	H	-3.385367	-0.855526	2.612688
H	-3.925820	-0.397453	0.954139	H	-3.981069	-0.355800	1.014135
C	-2.506482	4.829614	0.467785	C	-2.420682	4.883324	0.456023
N	-2.551308	5.906737	0.906092	N	-2.453930	5.966591	0.883070
H	-4.516713	1.175725	-1.422758	H	-4.498508	1.245418	-1.385042
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2-D-10-A-12P34-t3-DCM				2-D-10-A-12P34-t3-DMSO			
C	-2.640983	-2.619409	0.478624	C	-2.653309	-2.603604	0.484190
C	-2.347963	-3.892935	-0.076519	C	-2.357958	-3.896279	-0.060162
H	-3.019999	-4.724892	0.073871	H	-3.031559	-4.725363	0.099815
C	-1.739609	-1.537680	0.225831	C	-1.764778	-1.544468	0.211135
H	-1.877069	-0.600716	0.735961	H	-1.934113	-0.583257	0.665227
C	-1.181180	-4.087856	-0.784604	C	-1.204767	-4.093079	-0.763168
H	-0.945573	-5.076375	-1.161984	H	-0.971394	-5.084811	-1.134989
C	-3.550153	1.737015	-0.984662	C	-3.544907	1.820585	-0.963280
C	-2.365104	0.996040	-1.101454	C	-2.350816	1.061543	-1.100753
C	-3.548998	3.009150	-0.437066	C	-3.515393	3.080812	-0.421187
H	-4.471885	3.566890	-0.336512	H	-4.422706	3.658073	-0.295195
C	-2.325410	3.616381	-0.049501	C	-2.260254	3.661824	-0.042324
C	-1.076895	2.897766	-0.189873	C	-1.015441	2.934234	-0.213262
C	-1.119978	1.534331	-0.632181	C	-1.093982	1.558843	-0.646010
C	0.173751	3.517957	0.038904	C	0.235107	3.538184	-0.020605
H	0.195862	4.553374	0.359411	H	0.285514	4.578673	0.278183
C	1.363964	2.859635	-0.230577	C	1.420115	2.844556	-0.315997
H	2.305144	3.393954	-0.166053	H	2.367517	3.372036	-0.294673
C	1.334317	1.505454	-0.582386	C	1.365318	1.499683	-0.638707
C	0.109906	0.811436	-0.659476	C	0.116676	0.804325	-0.672087
C	1.608135	-0.945278	-1.323531	C	1.583228	-0.972119	-1.325362
C	3.824594	0.115948	0.152875	C	3.804716	0.078385	0.157427
C	4.233070	-0.454116	2.473634	C	4.155183	-0.443604	2.500109
C	5.204332	0.088464	-0.081085	C	5.187866	0.012776	-0.047283
C	5.608758	-0.486687	2.229805	C	5.534357	-0.512412	2.285159
C	6.093104	-0.216118	0.952403	C	6.049629	-0.284538	1.011055
H	5.586869	0.307972	-1.072151	H	5.594540	0.196207	-1.036267

H	7.159587	-0.235270	0.757981	H	7.119043	-0.332742	0.838706
P	2.713151	0.522030	-1.277612	P	2.727159	0.470804	-1.307276
C	0.304600	-0.637655	-0.885245	C	0.297180	-0.642650	-0.886029
C	-0.592975	-1.707184	-0.591918	C	-0.613935	-1.717832	-0.589682
C	-0.253495	-3.029210	-1.026613	C	-0.273616	-3.039608	-1.015640
C	1.006462	-3.266299	-1.617872	C	0.987757	-3.298420	-1.609132
C	1.945982	-2.246237	-1.714621	C	1.921108	-2.287821	-1.710023
H	1.258196	-4.270668	-1.939381	H	1.226220	-4.306687	-1.927899
H	2.939815	-2.464017	-2.090115	H	2.915017	-2.502459	-2.087723
C	3.346496	-0.156199	1.442630	C	3.296147	-0.151098	1.443860
H	6.296990	-0.718646	3.034787	H	6.201252	-0.740205	3.109100
H	3.853121	-0.660358	3.468164	H	3.751125	-0.618196	3.491257
H	2.280955	-0.131197	1.642302	H	2.227564	-0.098815	1.621118
H	-2.376056	0.050958	-1.622533	H	-2.392682	0.112463	-1.614489
N	-3.745855	-2.413030	1.253103	N	-3.763213	-2.404382	1.256429
C	-4.629415	-3.528781	1.585365	C	-4.671126	-3.509623	1.559398
H	-4.069200	-4.337470	2.061115	H	-4.142736	-4.320631	2.066770
H	-5.394457	-3.183013	2.274422	H	-5.459238	-3.148886	2.213729
H	-5.117728	-3.920780	0.688161	H	-5.129108	-3.903880	0.647715
C	-4.065397	-1.094688	1.802919	C	-4.071915	-1.080239	1.784671
H	-5.077038	-1.117361	2.199033	H	-5.022726	-1.119040	2.308194
H	-3.380536	-0.829964	2.614680	H	-3.300756	-0.746988	2.485953
H	-4.012936	-0.325582	1.030832	H	-4.143986	-0.345263	0.976037
C	-2.334227	4.934038	0.446327	C	-2.247449	4.965423	0.483082
N	-2.349045	6.023769	0.860761	N	-2.243802	6.046813	0.918535
H	-4.481178	1.313833	-1.345654	H	-4.483517	1.398025	-1.302535
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2-D-10-A-12P34-t3-n-hexane				2-D-12-A-12P34-t3			
C	-2.582435	-2.657475	0.475997	C	-2.626294	-2.235249	0.539237
C	-2.259204	-3.931248	-0.060222	C	-2.452604	-3.483940	-0.112562
H	-2.916162	-4.774878	0.093435	H	-3.185091	-4.270009	-0.001806
C	-1.704433	-1.560366	0.213016	C	-1.639017	-1.221583	0.355232
H	-1.858732	-0.620804	0.713024	H	-1.700505	-0.305390	0.913998
C	-1.085454	-4.109655	-0.761188	C	-1.316544	-3.719268	-0.858497
H	-0.828318	-5.097175	-1.127246	H	-1.165549	-4.695251	-1.305704
C	-3.585733	1.659592	-1.018006	C	-3.283581	2.274655	-0.424183
C	-2.384386	0.943137	-1.130500	C	-2.148872	1.460924	-0.709425
C	-3.616725	2.924949	-0.456560	C	-3.095660	3.535359	0.190198
H	-4.550956	3.464182	-0.360792	H	-3.960520	4.150559	0.410282
C	-2.410541	3.555461	-0.052206	C	-1.829851	3.989505	0.476405
C	-1.146063	2.867804	-0.195149	H	-1.692868	4.974851	0.907622
C	-1.154100	1.507129	-0.647269	C	-0.665862	3.194298	0.200882
C	0.088803	3.515642	0.042512	C	-0.847380	1.866411	-0.320710
H	0.081427	4.549760	0.367599	C	0.634096	3.712894	0.369888
C	1.296016	2.888915	-0.224826	H	0.742641	4.724675	0.747190
H	2.223194	3.446490	-0.155461	C	1.758665	2.996751	-0.024653
C	1.301043	1.535634	-0.579904	H	2.738872	3.458561	-0.005971
C	0.092065	0.816281	-0.667768	C	1.599414	1.671136	-0.446180
C	1.633987	-0.909905	-1.317484	C	0.329325	1.061058	-0.474119
C	3.821506	0.193664	0.153077	C	1.664676	-0.749584	-1.318143
C	4.250532	-0.295424	2.487918	C	4.025228	0.084302	0.062418
C	5.194339	0.099061	-0.102395	C	4.542598	-0.554306	2.342387
C	5.617875	-0.399140	2.222005	C	5.367105	-0.116025	-0.280287
C	6.088577	-0.202347	0.926522	C	5.877375	-0.762960	1.988786

H	5.566794	0.267312	-1.107404	C	6.288488	-0.544086	0.676967
H	7.149732	-0.273369	0.715154	H	5.693896	0.069424	-1.298181
P	2.702386	0.586765	-1.275668	H	7.325161	-0.696652	0.397751
C	0.323376	-0.628557	-0.892371	P	2.864781	0.642250	-1.277589
C	-0.550180	-1.715676	-0.597832	C	0.412395	-0.382968	-0.793081
C	-0.178982	-3.034183	-1.012335	C	-0.539773	-1.410074	-0.525902
C	1.089873	-3.249370	-1.590606	C	-0.318779	-2.718755	-1.059614
C	2.004121	-2.208165	-1.691329	C	0.897338	-3.006444	-1.720677
H	1.367985	-4.251080	-1.898744	C	1.894056	-2.047598	-1.800065
H	3.006252	-2.405863	-2.056143	H	1.061252	-4.001924	-2.118104
C	3.357776	-0.002839	1.461099	H	2.852830	-2.301835	-2.239206
H	6.311144	-0.625926	3.024239	C	3.622168	-0.135399	1.386446
H	3.881610	-0.440842	3.497344	H	6.592422	-1.088893	2.735946
H	2.298564	0.081642	1.676879	H	4.220791	-0.717342	3.365251
H	-2.366593	0.009904	-1.672862	H	2.588618	0.030107	1.669412
N	-3.695200	-2.465269	1.247062	H	-2.288378	0.558233	-1.283483
C	-4.527488	-3.600667	1.633356	N	-3.713191	-1.983724	1.332177
H	-3.921648	-4.389247	2.086329	C	-3.857193	-0.715129	2.048056
H	-5.264485	-3.269725	2.360573	H	-3.912134	0.128075	1.355439
H	-5.054013	-4.017187	0.768163	H	-4.775744	-0.743272	2.628139
C	-4.073147	-1.142698	1.747401	H	-3.019868	-0.558315	2.733257
H	-5.122481	-1.164505	2.034116	C	-4.778217	-2.973504	1.448820
H	-3.479332	-0.866632	2.625624	H	-5.585876	-2.559995	2.046583
H	-3.943373	-0.380738	0.979108	H	-5.175828	-3.232662	0.463737
C	-2.451802	4.866630	0.463738	H	-4.416180	-3.887142	1.932298
N	-2.491702	5.947448	0.895801	C	-4.582735	1.819467	-0.750442
H	-4.503382	1.224843	-1.400111	N	-5.642959	1.411024	-1.002710
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2-D-12-A-12P34-t2-CCl4				2-D-12-A-12P34-t2-DCM			
C	-2.660412	-2.306886	0.498555	C	-2.631195	-2.329701	0.498855
C	-2.492119	-3.505808	-0.220181	C	-2.461193	-3.519692	-0.237603
H	-3.202529	-4.313622	-0.120096	H	-3.162534	-4.335347	-0.136768
C	-1.690312	-1.264439	0.317187	C	-1.674181	-1.275684	0.315304
H	-1.766955	-0.366587	0.906712	H	-1.756081	-0.382729	0.911761
C	-1.385772	-3.681943	-1.041978	C	-1.362306	-3.677511	-1.072020
H	-1.248392	-4.628832	-1.552181	H	-1.221878	-4.618312	-1.592755
C	-3.206169	2.478125	-0.397760	C	-3.223946	2.466350	-0.398015
C	-2.125299	1.596276	-0.646446	C	-2.137249	1.589712	-0.642505
C	-2.988393	3.702508	0.257800	C	-3.017685	3.689580	0.264531
H	-3.823776	4.361734	0.458557	H	-3.857039	4.343719	0.464733
C	-1.700400	4.068932	0.610777	C	-1.734131	4.061469	0.625927
H	-1.522279	5.030945	1.077439	H	-1.564528	5.021822	1.098755
C	-0.587187	3.222931	0.340799	C	-0.613947	3.224007	0.354938
C	-0.814147	1.921415	-0.231297	C	-0.830279	1.923067	-0.222884
C	0.731191	3.676357	0.558158	C	0.700314	3.687429	0.575324
H	0.883161	4.659721	0.989434	H	0.844662	4.669749	1.011140
C	1.824429	2.924668	0.122421	C	1.800191	2.946089	0.136415
H	2.823356	3.343332	0.170063	H	2.795202	3.373378	0.187027
C	1.618140	1.645028	-0.385211	C	1.604152	1.666804	-0.377131
C	0.320894	1.065171	-0.431627	C	0.311973	1.076769	-0.427399
C	1.604670	-0.706195	-1.409813	C	1.606261	-0.676713	-1.422687
C	3.991881	0.002718	0.052279	C	3.982173	0.026629	0.058370
C	4.447857	-1.035736	2.194626	C	4.424945	-0.968310	2.224731
C	5.368600	0.146126	-0.153373	C	5.360489	0.094328	-0.175138

C	5.820813	-0.887399	1.981470	C	5.799726	-0.898454	1.982586
C	6.280146	-0.296931	0.807335	C	6.266313	-0.367652	0.782545
H	5.729501	0.604593	-1.068041	H	5.728230	0.509238	-1.107624
H	7.344444	-0.180666	0.635398	H	7.331643	-0.310593	0.588975
P	2.853251	0.626429	-1.278135	P	2.848858	0.661156	-1.271693
C	0.356081	-0.360427	-0.822155	C	0.356930	-0.344838	-0.829254
C	-0.607636	-1.392536	-0.583945	C	-0.598169	-1.386633	-0.594925
C	-0.401434	-2.669570	-1.220840	C	-0.386101	-2.656165	-1.246789
C	0.781933	-2.906930	-1.946141	C	0.795934	-2.877447	-1.980961
C	1.801008	-1.951839	-1.995049	C	1.809024	-1.915433	-2.022098
H	0.925322	-3.875039	-2.413749	H	0.943877	-3.839225	-2.460154
H	2.743341	-2.191076	-2.476043	H	2.751224	-2.144170	-2.508508
C	3.539465	-0.594559	1.237361	C	3.522129	-0.510387	1.269392
H	6.526356	-1.233197	2.728677	H	6.500693	-1.257031	2.727959
H	4.087378	-1.496596	3.107776	H	4.058731	-1.380686	3.158481
H	2.476137	-0.718259	1.409728	H	2.457512	-0.572309	1.466024
H	-2.312006	0.679942	-1.185320	H	-2.316767	0.672226	-1.181801
N	-3.722876	-2.115251	1.351656	N	-3.679390	-2.160557	1.370709
C	-4.671068	-3.197405	1.579255	C	-4.621458	-3.250915	1.593114
H	-4.196723	-4.060846	2.062817	H	-4.138912	-4.114834	2.066598
H	-5.473811	-2.839881	2.220326	H	-5.422052	-2.903437	2.241840
H	-5.114193	-3.531056	0.637012	H	-5.066327	-3.578677	0.650101
C	-3.800641	-0.939533	2.213497	C	-3.749369	-0.999664	2.254973
H	-4.755526	-0.949295	2.734642	H	-4.681013	-1.041032	2.814272
H	-2.999141	-0.925886	2.962108	H	-2.918796	-0.981771	2.969874
H	-3.751130	-0.017592	1.631268	H	-3.742039	-0.067120	1.687199
C	-4.519293	2.122492	-0.814322	C	-4.529614	2.108594	-0.832265
N	-5.590307	1.830119	-1.147767	N	-5.594189	1.815705	-1.186955
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2-D-12-A-12P34-t2-DMSO				2-D-12-A-12P34-t3-n-hexane			
C	-2.625408	-2.335220	0.496119	C	-2.613696	-2.259910	0.532437
C	-2.452730	-3.523657	-0.243306	C	-2.437265	-3.499560	-0.137628
H	-3.151541	-4.341502	-0.142770	H	-3.162262	-4.292552	-0.028314
C	-1.671642	-1.278044	0.312908	C	-1.641341	-1.232869	0.342327
H	-1.753825	-0.387261	0.912517	H	-1.703771	-0.325397	0.915501
C	-1.354980	-3.676879	-1.079661	C	-1.311297	-3.714307	-0.904099
H	-1.212253	-4.616338	-1.602193	H	-1.159497	-4.682016	-1.368577
C	-3.230354	2.461689	-0.399903	C	-3.288646	2.293383	-0.423174
C	-2.141288	1.587190	-0.643263	C	-2.155881	1.473904	-0.698642
C	-3.028113	3.684390	0.265319	C	-3.102099	3.544582	0.215788
H	-3.869087	4.336309	0.465748	H	-3.965828	4.162532	0.432711
C	-1.746223	4.058412	0.629689	C	-1.838905	3.985179	0.527403
H	-1.579709	5.017769	1.105411	H	-1.702245	4.962144	0.977526
C	-0.623485	3.223929	0.358286	C	-0.675105	3.190406	0.247569
C	-0.836114	1.923358	-0.221586	C	-0.857139	1.870931	-0.295770
C	0.689144	3.690891	0.580410	C	0.624554	3.705660	0.429991
H	0.830394	4.672697	1.018131	H	0.732864	4.710483	0.825452
C	1.791399	2.953017	0.140972	C	1.749170	2.995185	0.024519
H	2.785114	3.383092	0.192912	H	2.729946	3.455299	0.053928
C	1.599128	1.673780	-0.374418	C	1.589440	1.677450	-0.422168
C	0.308559	1.080082	-0.426328	C	0.319979	1.066095	-0.460739
C	1.607330	-0.668843	-1.423418	C	1.655572	-0.726802	-1.337851
C	3.980965	0.036413	0.060448	C	4.018845	0.087865	0.059277
C	4.424957	-0.930227	2.239668	C	4.530230	-0.622675	2.319686

C	5.357792	0.067250	-0.189643	C	5.369489	-0.060787	-0.275633
C	5.798168	-0.898607	1.980380	C	5.874762	-0.777735	1.974073
C	6.263332	-0.400495	0.765661	C	6.293220	-0.497134	0.676111
H	5.724939	0.457873	-1.132752	H	5.701585	0.169818	-1.282438
H	7.327362	-0.372445	0.559204	H	7.336684	-0.609158	0.403281
P	2.846933	0.671664	-1.267797	P	2.855706	0.662886	-1.270808
C	0.357022	-0.340316	-0.830474	C	0.402743	-0.370806	-0.802750
C	-0.596150	-1.384934	-0.598303	C	-0.547306	-1.403994	-0.547120
C	-0.381069	-2.652618	-1.252850	C	-0.322983	-2.704146	-1.101705
C	0.802058	-2.870481	-1.986974	C	0.889790	-2.976631	-1.776088
C	1.813244	-1.906304	-2.025217	C	1.885165	-2.014738	-1.844676
H	0.952469	-3.831228	-2.467409	H	1.053976	-3.965107	-2.190264
H	2.756487	-2.132389	-2.510913	H	2.841910	-2.260354	-2.292793
C	3.522245	-0.467215	1.286449	C	3.608040	-0.194601	1.369236
H	6.498991	-1.260674	2.724145	H	6.591137	-1.111036	2.716645
H	4.060000	-1.316059	3.185146	H	4.202271	-0.834853	3.331459
H	2.458918	-0.498347	1.497136	H	2.566906	-0.072708	1.646648
H	-2.318128	0.669584	-1.183217	H	-2.293674	0.573078	-1.276236
N	-3.672830	-2.171949	1.369774	N	-3.684063	-2.034355	1.352230
C	-4.598403	-3.274469	1.606221	C	-4.699493	-3.067650	1.533838
H	-4.099252	-4.128976	2.079141	H	-4.261970	-3.973302	1.964492
H	-5.397250	-2.934262	2.260719	H	-5.467663	-2.698113	2.207124
H	-5.047229	-3.612824	0.669024	H	-5.168138	-3.324078	0.579522
C	-3.741585	-1.017407	2.263560	C	-3.850416	-0.761817	2.055861
H	-4.682424	-1.052015	2.807615	H	-4.789854	-0.783288	2.600933
H	-2.921618	-1.016238	2.990828	H	-3.037587	-0.600451	2.769703
H	-3.714047	-0.081195	1.703416	H	-3.877047	0.075906	1.355449
C	-4.533437	2.103177	-0.839484	C	-4.584012	1.868171	-0.794263
N	-5.595526	1.809417	-1.201554	N	-5.646768	1.497778	-1.094298
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ST2: Energy Difference (eV) between Singlet and nearest low lying triplet:

System	$\Delta E_{st}$	System	$\Delta E_{st}$
C1234	0.195	P1234	0.262
C1234-CCl4	0.164	P1234-CCl4	0.234
C1234-DCM	0.165	P1234-DCM	0.234
C1234-DMSO	0.165	P1234-DMSO	0.234
C1234-n-hexane	0.168	P1234-n-hexane	0.238
1C234	0.031	1P234	0.089
1C234-CCl4	0.004	1P234-CCl4	0.075
1C234-DCM	0.106	1P234-DCM	0.073
1C234-DMSO	0.105	1P234-DMSO	0.072
1C234-n-hexane	0.008	1P234-n-hexane	0.077
12C34	0.105	12P34	0.064
12C34-CCl4	0.037	12P34-CCl4	0.006

12C34-DCM	0.039	12P34-DCM	0.002
12C34-DMSO	0.040	12P34-DMSO	0.023
12C34-n-hexane	0.046	12P34-n-hexane	0.015
1-A-13-D-P1234	0.033	1-D-13-A-1P234	0.009
1-A-13-D-P1234-CCl4	0.012	1-D-13-A-1P234-CCL4	0.087
1-A-13-D-P1234-DCM	0.017	1-D-13-A-1P234-DCM	0.084
1-A-13-D-P1234-DMSO	0.017	1-D-13-A-1P234-DMSO	0.081
1-A-13-D-P1234-n-hexane	0.016	1-D-13-A-1P234-n-hexane	0.090
3-A-12-D-P1234	0.008	3-D-13-A-1P234	0.301
3-A-12-D-P1234-CCl4	0.216	3-D-13-A-1P234-CCl4	0.254
3-A-12-D-P1234-DCM	0.216	3-D-13-A-1P234-DCM	0.246
3-A-12-D-P1234-DMSO	0.214	3-D-13-A-1P234-DMSO	0.245
3-A-12-D-P1234-n-hexane	0.219	3-D-13-A-1P234-n-hexane	0.261
1-A-11-D-P1234	0.238	2-D-10-A-12P34	0.114
1-A-11-D-P1234-CCl4	0.195	2-D-10-A-12P34-CCl4	0.053
1-A-11-D-P1234-DCM	0.182	2-D-10-A-12P34-DCM	0.038
1-A-11-D-P1234-DMSO	0.178	2-D-10-A-12P34-DMSO	0.0307
1-A-11-D-P1234-n-hexane	0.202	2-D-10-A-12P34-n-hexane	0.062
3-A-10-D-P1234	0.261	2-D-12-A-12P34	0.048
3-A-10-D-P1234-CCl4	0.244	2-D-12-A-12P34-CCl4	0.627
3-A-10-D-P1234-DCM	0.257	2-D-12-A-12P34-DCM	0.619
3-A-10-D-P1234-DMSO	0.260	2-D-12-A-12P34-DMSO	0.620
3-A-10-D-P1234-n-hexane	0.246	2-D-12-A-12P34-n-hexane	0.006

ST3: Value of Spin Orbit Coupling Matrix Element calculated at CAM-B3LYP/cc-PVTZ level of theory.

SYSTEM	CCl4	DCM	DMSO	n-hexane	Vacuum
C1234	0.17	0.19	0.20	0.16	0.15
1C234	0.11	0.32	0.33	0.06	0.11
12C34	0.09	0.11	0.11	0.09	0.10
P1234	1.10	1.11	1.11	1.11	1.15
1P234	0.31	0.34	0.36	0.29	0.19

12P34	1.25	1.25	1.08	1.26	1.31
1-A-13-D-P1234	0.46	0.52	0.54	0.44	0.42
3-A-12-D-P1234	1.11	1.18	1.20	1.11	0.44
1-A-11-D-P1234	1.32	1.13	1.06	1.35	1.42
3-A-10-D-P1234	1.00	0.97	0.95	1.01	1.10
1-D-13-A-1P234	1.09	1.14	1.15	1.09	0.69
3-D-13-A-1P234	0.47	0.47	0.48	0.47	0.46
2-D-10-A-12P34	0.74	0.76	0.77	0.74	0.73
2-D-12-A-12P34	0.34	0.35	0.37	0.85	0.81

ST4: Value of Rate of Inter System Crossing (in sec<sup>-1</sup>).

SYSTEM	CCl4	DCM	DMSO	n-hexane	Vacuum
C1234	9.88E+06	9.10E+06	8.99E+06	5.58E+06	6.72E+06
1C234	7.68E+05	7.38E+06	8.51E+06	2.36E+05	1.99E+06
12C34	1.84E+06	4.72E+06	4.53E+06	8.68E+05	1.90E+06
P1234	5.03E+08	5.27E+08	5.32E+08	4.89E+08	5.51E+08
1P234	2.42E+07	6.18E+07	4.06E+07	9.33E+06	1.06E+07
12P34	3.67E+09	7.65E+07	5.17E+07	4.76E+08	6.76E+08
1-A-13-D-P1234	1.77E+07	3.36E+07	2.11E+08	1.83E+07	2.96E+08
3-A-12-D-P1234	5.30E+07	6.02E+07	6.15E+07	6.61E+07	1.27E+07
1-A-11-D-P1234	5.66E+08	4.40E+08	5.55E+08	6.30E+08	5.90E+08
3-A-10-D-P1234	4.32E+07	3.95E+07	3.84E+07	4.39E+07	5.17E+07
1-D-13-A-1P234	1.03E+09	7.44E+08	6.29E+08	7.99E+08	7.75E+07
3-D-13-A-1P234	5.37E+07	4.76E+07	6.28E+07	3.52E+07	3.98E+07

2-D-10-A-12P34	3.08E+08	4.61E+08	6.17E+08	2.12E+08	1.47E+08
2-D-12-A-12P34	1.10E+07	1.69E+08	1.41E+07	2.54E+08	6.75E+07

ST5:  $S_0 \rightarrow S_n$  and  $S_0 \rightarrow T_n$  excitation energy Ex. En. (in eV), wavelength WL (in nm) and Oscillator Strength (unitless) calculated at CAM-B3LYP/cc-PVTZ level of theory.

#### 12C34-OPA-CCl4

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 5:	3.6375	340.85	0.4633	Excited State 1:	2.0239	612.59	0.0000
Excited State 11:	4.2643	290.75	0.0035	Excited State 2:	2.6438	468.96	0.0000
Excited State 12:	4.3394	285.72	0.0008	Excited State 3:	3.5101	353.22	0.0000
Excited State 14:	4.4066	281.36	0.0130	Excited State 4:	3.6007	344.33	0.0000
Excited State 15:	4.8990	253.08	0.0091	Excited State 6:	3.7850	327.57	0.0000
Excited State 16:	5.0329	246.35	0.2860	Excited State 7:	3.8835	319.26	0.0000
Excited State 17:	5.2256	237.27	0.0149	Excited State 8:	4.0673	304.83	0.0000
Excited State 18:	5.3332	232.48	0.4923	Excited State 9:	4.0886	303.25	0.0000
Excited State 19:	5.4046	229.41	0.9805	Excited State 10:	4.2305	293.07	0.0000
Excited State 20:	5.5449	223.60	0.1789	Excited State 13:	4.3570	284.57	0.0000

#### 12C34-OPA-DCM

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 5:	3.6432	340.32	0.4561	Excited State 1:	2.0299	610.78	0.0000
Excited State 11:	4.2683	290.48	0.0032	Excited State 2:	2.6485	468.13	0.0000
Excited State 12:	4.3423	285.53	0.0008	Excited State 3:	3.5153	352.70	0.0000
Excited State 14:	4.4097	281.16	0.0122	Excited State 4:	3.6038	344.03	0.0000
Excited State 15:	4.9025	252.90	0.0089	Excited State 6:	3.7873	327.37	0.0000

Excited State 16:	5.0418	245.91	0.2814	Excited State 7:	3.8850	319.14	0.0000
Excited State 17:	5.2280	237.15	0.0141	Excited State 8:	4.0708	304.57	0.0000
Excited State 18:	5.3405	232.16	0.4039	Excited State 9:	4.0890	303.21	0.0000
Excited State 19:	5.4126	229.06	1.0583	Excited State 10:	4.2344	292.80	0.0000
Excited State 20:	5.5591	223.03	0.0826	Excited State 13:	4.3609	284.31	0.0000

12C34-OPA-DMSO

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 5:	3.6448	340.17	0.4546	Excited State 1:	2.0324	610.03	0.0000
Excited State 11:	4.2698	290.37	0.0030	Excited State 2:	2.6504	467.79	0.0000
Excited State 12:	4.3436	285.44	0.0008	Excited State 3:	3.5175	352.48	0.0000
Excited State 14:	4.4112	281.07	0.0120	Excited State 4:	3.6051	343.92	0.0000
Excited State 15:	4.9035	252.85	0.0091	Excited State 6:	3.7882	327.29	0.0000
Excited State 16:	5.0444	245.78	0.2801	Excited State 7:	3.8857	319.08	0.0000
Excited State 17:	5.2290	237.11	0.0142	Excited State 8:	4.0724	304.45	0.0000
Excited State 18:	5.3427	232.06	0.3801	Excited State 9:	4.0893	303.19	0.0000
Excited State 19:	5.4143	228.99	1.0808	Excited State 10:	4.2361	292.68	0.0000
Excited State 20:	5.5613	222.94	0.0441	Excited State 13:	4.3627	284.19	0.0000

12C34-OPA

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 5:	3.7027	334.85	0.3385	Excited State 1:	2.0187	614.17	0.0000
Excited State 11:	4.2653	290.68	0.0026	Excited State 2:	2.6399	469.66	0.0000
Excited State 12:	4.3466	285.25	0.0001	Excited State 3:	3.5056	353.68	0.0000
Excited State 14:	4.4264	280.10	0.0081	Excited State 4:	3.5980	344.59	0.0000
Excited State 15:	4.9009	252.98	0.0034	Excited State 6:	3.7830	327.74	0.0000
Excited State 16:	5.1103	242.62	0.2291	Excited State 7:	3.8825	319.34	0.0000
Excited State 17:	5.2470	236.30	0.0107	Excited State 8:	4.0646	305.03	0.0000

Excited State 18:	5.3487	231.80	0.0600	Excited State 9:	4.0887	303.24	0.0000
Excited State 19:	5.4659	226.83	0.3610	Excited State 10:	4.2273	293.29	0.0000
Excited State 20:	5.5683	222.66	0.3573	Excited State 13:	4.3538	284.77	0.0000

12C34-OPA-n-hexane

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 5:	3.6465	340.01	0.4449	Excited State 1:	2.0229	612.91	0.0000
Excited State 11:	4.2643	290.75	0.0034	Excited State 2:	2.6430	469.10	0.0000
Excited State 12:	4.3405	285.64	0.0006	Excited State 3:	3.5092	353.31	0.0000
Excited State 14:	4.4093	281.19	0.0123	Excited State 4:	3.6002	344.38	0.0000
Excited State 15:	4.8992	253.07	0.0078	Excited State 6:	3.7846	327.60	0.0000
Excited State 16:	5.0435	245.83	0.2792	Excited State 7:	3.8833	319.28	0.0000
Excited State 17:	5.2286	237.13	0.0138	Excited State 8:	4.0667	304.88	0.0000
Excited State 18:	5.3375	232.29	0.3397	Excited State 9:	4.0885	303.25	0.0000
Excited State 19:	5.4160	228.92	0.9806	Excited State 10:	4.2298	293.12	0.0000
Excited State 20:	5.5452	223.59	0.2174	Excited State 13:	4.3563	284.61	0.0000

12P34-geo-opt-abs

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 6:	3.6210	342.41	0.2286	Excited State 1:	2.0131	615.89	0.0000
Excited State 10:	4.0919	303.00	0.0613	Excited State 2:	2.6097	475.08	0.0000
Excited State 13:	4.2283	293.23	0.0080	Excited State 3:	3.4445	359.95	0.0000
Excited State 14:	4.3941	282.16	0.0294	Excited State 4:	3.5414	350.10	0.0000
Excited State 15:	4.6730	265.32	0.0387	Excited State 5:	3.5573	348.53	0.0000
Excited State 16:	4.8970	253.18	0.2502	Excited State 7:	3.7736	328.56	0.0000
Excited State 17:	4.9460	250.67	0.2851	Excited State 8:	3.9750	311.91	0.0000
Excited State 18:	5.0057	247.69	0.0656	Excited State 9:	4.0121	309.02	0.0000
Excited State 19:	5.0668	244.70	0.0326	Excited State 11:	4.1775	296.79	0.0000

Excited State 20: 5.1656 240.02 0.0714 Excited State 12: 4.1963 295.46 0.0000

12P34-geo-opt-abs-CCl4

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 6:	3.5698	347.32	0.3255	Excited State 1:	2.0153	615.23	0.0000
Excited State 10:	4.0804	303.85	0.1071	Excited State 2:	2.6124	474.60	0.0000
Excited State 13:	4.2245	293.49	0.0123	Excited State 3:	3.4490	359.47	0.0000
Excited State 14:	4.3671	283.91	0.0517	Excited State 4:	3.5447	349.77	0.0000
Excited State 15:	4.6649	265.78	0.0867	Excited State 5:	3.5633	347.95	0.0000
Excited State 16:	4.8513	255.57	0.4272	Excited State 7:	3.7744	328.49	0.0000
Excited State 17:	4.8744	254.36	0.4732	Excited State 8:	3.9752	311.89	0.0000
Excited State 18:	4.9997	247.98	0.0496	Excited State 9:	4.0139	308.88	0.0000
Excited State 19:	5.0709	244.50	0.0177	Excited State 11:	4.1793	296.66	0.0000
Excited State 20:	5.1610	240.23	0.1132	Excited State 12:	4.2009	295.14	0.0000

12P34-geo-opt-abs-DCM

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 6:	3.5717	347.13	0.3184	Excited State 1:	2.0177	614.49	0.0000
Excited State 10:	4.0868	303.38	0.1005	Excited State 2:	2.6155	474.04	0.0000
Excited State 13:	4.2256	293.41	0.0125	Excited State 3:	3.4539	358.97	0.0000
Excited State 14:	4.3717	283.61	0.0495	Excited State 4:	3.5478	349.46	0.0000
Excited State 15:	4.6666	265.69	0.0725	Excited State 5:	3.5697	347.32	0.0000
Excited State 16:	4.8577	255.23	0.4474	Excited State 7:	3.7754	328.40	0.0000
Excited State 17:	4.8816	253.98	0.4560	Excited State 8:	3.9754	311.88	0.0000
Excited State 18:	5.0118	247.39	0.0527	Excited State 9:	4.0162	308.71	0.0000
Excited State 19:	5.0885	243.66	0.0102	Excited State 11:	4.1816	296.50	0.0000
Excited State 20:	5.1820	239.26	0.1096	Excited State 12:	4.2061	294.77	0.0000

12P34-geo-opt-abs-DMSO

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 5:	3.5716	347.13	0.3167	Excited State 1:	2.0186	614.22	0.0000
Excited State 10:	4.0886	303.24	0.0988	Excited State 2:	2.6167	473.82	0.0000
Excited State 13:	4.2261	293.38	0.0127	Excited State 3:	3.4558	358.78	0.0000
Excited State 14:	4.3732	283.51	0.0487	Excited State 4:	3.5490	349.35	0.0000
Excited State 15:	4.6668	265.67	0.0676	Excited State 6:	3.5719	347.11	0.0000
Excited State 16:	4.8593	255.15	0.4591	Excited State 7:	3.7759	328.36	0.0000
Excited State 17:	4.8834	253.89	0.4455	Excited State 8:	3.9755	311.87	0.0000
Excited State 18:	5.0164	247.16	0.0557	Excited State 9:	4.0170	308.65	0.0000
Excited State 19:	5.0965	243.27	0.0083	Excited State 11:	4.1826	296.43	0.0000
Excited State 20:	5.1903	238.88	0.1071	Excited State 12:	4.2083	294.62	0.0000

12P34-geo-opt-abs-n-hexane

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 6:	3.5771	346.60	0.3109	Excited State 1:	2.0149	615.35	0.0000
Excited State 10:	4.0820	303.74	0.0992	Excited State 2:	2.6118	474.70	0.0000
Excited State 13:	4.2250	293.45	0.0115	Excited State 3:	3.4482	359.56	0.0000
Excited State 14:	4.3711	283.65	0.0479	Excited State 4:	3.5442	349.83	0.0000
Excited State 15:	4.6662	265.71	0.0773	Excited State 5:	3.5621	348.07	0.0000
Excited State 16:	4.8587	255.18	0.4053	Excited State 7:	3.7743	328.50	0.0000
Excited State 17:	4.8844	253.84	0.4424	Excited State 8:	3.9752	311.90	0.0000
Excited State 18:	4.9996	247.99	0.0488	Excited State 9:	4.0136	308.91	0.0000
Excited State 19:	5.0693	244.58	0.0201	Excited State 11:	4.1790	296.68	0.0000
Excited State 20:	5.1607	240.24	0.1065	Excited State 12:	4.2000	295.20	0.0000

1C234-OPA-CCl4

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS

Excited State 8:	3.8906	318.68	0.1454	Excited State 1:	2.3127	536.10	0.0000
Excited State 9:	4.0780	304.03	0.1074	Excited State 2:	3.0125	411.57	0.0000
Excited State 12:	4.4575	278.14	0.7888	Excited State 3:	3.4653	357.79	0.0000
Excited State 14:	4.7230	262.51	0.1876	Excited State 4:	3.5130	352.93	0.0000
Excited State 15:	4.9191	252.04	0.1126	Excited State 5:	3.6511	339.58	0.0000
Excited State 16:	5.0543	245.30	0.0908	Excited State 6:	3.7823	327.80	0.0000
Excited State 17:	5.2532	236.02	0.1482	Excited State 7:	3.8868	318.99	0.0000
Excited State 18:	5.3733	230.74	0.0061	Excited State 10:	4.2906	288.97	0.0000
Excited State 19:	5.4678	226.75	0.0041	Excited State 11:	4.3170	287.20	0.0000
Excited State 20:	5.6526	219.34	0.5505	Excited State 13:	4.4581	278.11	0.0000

1C234-OPA-DCM

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 7:	3.8915	318.61	0.1422	Excited State 1:	2.3196	534.51	0.0000
Excited State 9:	4.0856	303.46	0.1042	Excited State 2:	3.0150	411.23	0.0000
Excited State 13:	4.4645	277.71	0.7726	Excited State 3:	3.4682	357.49	0.0000
Excited State 14:	4.7296	262.14	0.1857	Excited State 4:	3.5179	352.43	0.0000
Excited State 15:	4.9231	251.84	0.1096	Excited State 5:	3.6525	339.45	0.0000
Excited State 16:	5.0562	245.21	0.0952	Excited State 6:	3.7851	327.56	0.0000
Excited State 17:	5.2590	235.76	0.1431	Excited State 8:	3.8931	318.47	0.0000
Excited State 18:	5.3762	230.62	0.0055	Excited State 10:	4.2909	288.95	0.0000
Excited State 19:	5.4706	226.64	0.0039	Excited State 11:	4.3209	286.94	0.0000
Excited State 20:	5.6581	219.13	0.5487	Excited State 12:	4.4583	278.09	0.0000

1C234-OPA-DMSO

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 7:	3.8917	318.59	0.1418	Excited State 1:	2.3225	533.84	0.0000
Excited State 9:	4.0887	303.24	0.1032	Excited State 2:	3.0160	411.09	0.0000

Excited State 13:	4.4665	277.59	0.7690	Excited State 3:	3.4694	357.36	0.0000
Excited State 14:	4.7320	262.01	0.1859	Excited State 4:	3.5200	352.23	0.0000
Excited State 15:	4.9244	251.77	0.1088	Excited State 5:	3.6529	339.41	0.0000
Excited State 16:	5.0569	245.18	0.0977	Excited State 6:	3.7863	327.45	0.0000
Excited State 17:	5.2609	235.67	0.1409	Excited State 8:	3.8958	318.25	0.0000
Excited State 18:	5.3772	230.57	0.0052	Excited State 10:	4.2908	288.96	0.0000
Excited State 19:	5.4716	226.60	0.0038	Excited State 11:	4.3224	286.84	0.0000
Excited State 20:	5.6593	219.08	0.5475	Excited State 12:	4.4585	278.08	0.0000

1C234-OPA

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 8:	3.9126	316.88	0.0764	Excited State 1:	2.3072	537.37	0.0000
Excited State 9:	4.0987	302.50	0.0868	Excited State 2:	3.0104	411.85	0.0000
Excited State 13:	4.5418	272.98	0.5635	Excited State 3:	3.4630	358.02	0.0000
Excited State 14:	4.7566	260.66	0.1063	Excited State 4:	3.5086	353.37	0.0000
Excited State 15:	4.9375	251.11	0.0975	Excited State 5:	3.6498	339.70	0.0000
Excited State 16:	5.0647	244.80	0.0647	Excited State 6:	3.7801	327.99	0.0000
Excited State 17:	5.2950	234.15	0.1242	Excited State 7:	3.8817	319.41	0.0000
Excited State 18:	5.3774	230.57	0.0054	Excited State 10:	4.2901	289.00	0.0000
Excited State 19:	5.4686	226.72	0.0043	Excited State 11:	4.3138	287.41	0.0000
Excited State 20:	5.6963	217.66	0.2908	Excited State 12:	4.4581	278.11	0.0000

1C234-OPA-n-hexane

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 8:	3.8941	318.39	0.1335	Excited State 1:	2.3116	536.35	0.0000
Excited State 9:	4.0805	303.85	0.1051	Excited State 2:	3.0121	411.62	0.0000
Excited State 13:	4.4692	277.42	0.7562	Excited State 3:	3.4648	357.84	0.0000
Excited State 14:	4.7281	262.23	0.1739	Excited State 4:	3.5121	353.02	0.0000

Excited State 15:	4.9214	251.93	0.1110	Excited State 5:	3.6509	339.60	0.0000
Excited State 16:	5.0558	245.23	0.0862	Excited State 6:	3.7818	327.84	0.0000
Excited State 17:	5.2592	235.75	0.1458	Excited State 7:	3.8858	319.07	0.0000
Excited State 18:	5.3738	230.72	0.0059	Excited State 10:	4.2905	288.97	0.0000
Excited State 19:	5.4678	226.75	0.0041	Excited State 11:	4.3164	287.24	0.0000
Excited State 20:	5.6595	219.07	0.5058	Excited State 12:	4.4580	278.11	0.0000

1-D-13-A-1P234-OPA-CCl4

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 5:	3.4195	362.58	0.1111	Excited State 1:	2.1368	580.22	0.0000
Excited State 10:	3.7301	332.39	0.0753	Excited State 2:	2.6523	467.46	0.0000
Excited State 12:	3.8909	318.65	0.0016	Excited State 3:	3.2059	386.74	0.0000
Excited State 14:	4.0435	306.62	0.3377	Excited State 4:	3.3328	372.01	0.0000
Excited State 15:	4.2758	289.96	0.4706	Excited State 6:	3.4558	358.77	0.0000
Excited State 16:	4.3674	283.89	0.2159	Excited State 7:	3.4788	356.40	0.0000
Excited State 17:	4.5621	271.77	0.1057	Excited State 8:	3.6070	343.73	0.0000
Excited State 18:	4.7433	261.39	0.0815	Excited State 9:	3.6637	338.42	0.0000
Excited State 19:	4.8689	254.64	0.0237	Excited State 11:	3.7546	330.22	0.0000
Excited State 20:	4.9444	250.76	0.0122	Excited State 13:	4.0295	307.69	0.0000

1-D-13-A-1P234-OPA-DCM

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 5:	3.3963	365.05	0.1075	Excited State 1:	2.1389	579.65	0.0000
Excited State 10:	3.7226	333.06	0.0721	Excited State 2:	2.6408	469.49	0.0000
Excited State 12:	3.8762	319.86	0.0019	Excited State 3:	3.2052	386.82	0.0000
Excited State 14:	4.0368	307.13	0.2564	Excited State 4:	3.3126	374.28	0.0000
Excited State 15:	4.2718	290.24	0.5111	Excited State 6:	3.4602	358.32	0.0000
Excited State 16:	4.3666	283.94	0.2243	Excited State 7:	3.4745	356.84	0.0000

Excited State 17:	4.5564	272.11	0.1188	Excited State 8:	3.5965	344.74	0.0000
Excited State 18:	4.7295	262.15	0.0779	Excited State 9:	3.6540	339.31	0.0000
Excited State 19:	4.8754	254.30	0.0198	Excited State 11:	3.7526	330.40	0.0000
Excited State 20:	4.9593	250.01	0.0179	Excited State 13:	4.0247	308.06	0.0000

1-D-13-A-1P234-OPA-DMSO

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 5:	3.3844	366.34	0.1069	Excited State 1:	2.1400	579.37	0.0000
Excited State 10:	3.7178	333.49	0.0712	Excited State 2:	2.6350	470.53	0.0000
Excited State 12:	3.8707	320.31	0.0024	Excited State 3:	3.2044	386.92	0.0000
Excited State 14:	4.0324	307.47	0.2273	Excited State 4:	3.3036	375.30	0.0000
Excited State 15:	4.2706	290.32	0.5248	Excited State 6:	3.4615	358.18	0.0000
Excited State 16:	4.3666	283.94	0.2291	Excited State 7:	3.4703	357.27	0.0000
Excited State 17:	4.5512	272.42	0.1257	Excited State 8:	3.5887	345.49	0.0000
Excited State 18:	4.7223	262.55	0.0769	Excited State 9:	3.6519	339.51	0.0000
Excited State 19:	4.8778	254.18	0.0188	Excited State 11:	3.7526	330.39	0.0000
Excited State 20:	4.9638	249.77	0.0181	Excited State 13:	4.0212	308.32	0.0000

1-D-13-A-1P234-OPA

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 6:	3.4604	358.29	0.0737	Excited State 1:	2.1347	580.80	0.0000
Excited State 10:	3.7493	330.69	0.0434	Excited State 2:	2.6613	465.89	0.0000
Excited State 12:	3.9123	316.91	0.0013	Excited State 3:	3.2053	386.82	0.0000
Excited State 14:	4.0833	303.64	0.2035	Excited State 4:	3.3490	370.21	0.0000
Excited State 15:	4.3280	286.47	0.3504	Excited State 5:	3.4516	359.21	0.0000
Excited State 16:	4.4116	281.04	0.1322	Excited State 7:	3.4791	356.37	0.0000
Excited State 17:	4.5893	270.16	0.0972	Excited State 8:	3.6105	343.40	0.0000
Excited State 18:	4.7664	260.12	0.0701	Excited State 9:	3.6745	337.42	0.0000

Excited State 19: 4.8744 254.36 0.0170 Excited State 11: 3.7591 329.82 0.0000  
 Excited State 20: 4.9626 249.84 0.0034 Excited State 13: 4.0306 307.61 0.0000

1-D-13-A-1P234-OPA-n-hexane

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 5:	3.4265	361.84	0.1051	Excited State 1:	2.1364	580.33	0.0000
Excited State 10:	3.7333	332.10	0.0695	Excited State 2:	2.6541	467.14	0.0000
Excited State 12:	3.8946	318.35	0.0015	Excited State 3:	3.2059	386.74	0.0000
Excited State 14:	4.0496	306.16	0.3192	Excited State 4:	3.3361	371.64	0.0000
Excited State 15:	4.2837	289.43	0.4525	Excited State 6:	3.4550	358.86	0.0000
Excited State 16:	4.3741	283.45	0.2010	Excited State 7:	3.4791	356.37	0.0000
Excited State 17:	4.5663	271.52	0.1042	Excited State 8:	3.6080	343.64	0.0000
Excited State 18:	4.7473	261.17	0.0800	Excited State 9:	3.6658	338.22	0.0000
Excited State 19:	4.8696	254.61	0.0228	Excited State 11:	3.7553	330.16	0.0000
Excited State 20:	4.9464	250.66	0.0102	Excited State 13:	4.0300	307.66	0.0000

1-A-13-D-P1234-OPA-CCl4

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 5:	2.7437	451.89	0.0696	Excited State 1:	1.2037	1029.99	0.0000
Excited State 6:	2.8552	434.24	0.0078	Excited State 2:	2.2413	553.17	0.0000
Excited State 11:	3.4968	354.57	0.1956	Excited State 3:	2.5241	491.19	0.0000
Excited State 13:	3.6650	338.29	0.0797	Excited State 4:	2.7314	453.92	0.0000
Excited State 15:	3.7930	326.88	0.4029	Excited State 7:	2.9599	418.88	0.0000
Excited State 16:	3.9170	316.53	0.1084	Excited State 8:	3.1916	388.47	0.0000
Excited State 17:	4.2355	292.73	0.0736	Excited State 9:	3.4526	359.10	0.0000
Excited State 18:	4.3196	287.03	0.0742	Excited State 10:	3.4620	358.13	0.0000
Excited State 19:	4.4762	276.99	0.0704	Excited State 12:	3.5596	348.31	0.0000
Excited State 20:	4.7617	260.38	0.3665	Excited State 14:	3.7497	330.65	0.0000



	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 5:	2.7773	446.43	0.0472	Excited State 1:	1.1905	1041.47	0.0000
Excited State 6:	2.8780	430.80	0.0062	Excited State 2:	2.2477	551.60	0.0000
Excited State 11:	3.5332	350.91	0.0816	Excited State 3:	2.5287	490.30	0.0000
Excited State 13:	3.6858	336.39	0.0511	Excited State 4:	2.7441	451.83	0.0000
Excited State 15:	3.8429	322.63	0.3046	Excited State 7:	2.9637	418.35	0.0000
Excited State 16:	3.9411	314.59	0.1353	Excited State 8:	3.1953	388.02	0.0000
Excited State 17:	4.2596	291.07	0.0587	Excited State 9:	3.4467	359.72	0.0000
Excited State 18:	4.3525	284.86	0.0462	Excited State 10:	3.4541	358.95	0.0000
Excited State 19:	4.4933	275.93	0.0674	Excited State 12:	3.5771	346.60	0.0000
Excited State 20:	4.7861	259.05	0.0150	Excited State 14:	3.7498	330.64	0.0000

1-A-13-D-P1234-OPA-n-hexane

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 5:	2.7492	450.98	0.0661	Excited State 1:	1.2014	1031.98	0.0000
Excited State 6:	2.8595	433.59	0.0076	Excited State 2:	2.2428	552.82	0.0000
Excited State 11:	3.5033	353.90	0.1738	Excited State 3:	2.5248	491.06	0.0000
Excited State 13:	3.6682	338.00	0.0764	Excited State 4:	2.7337	453.54	0.0000
Excited State 15:	3.7997	326.30	0.3939	Excited State 7:	2.9607	418.76	0.0000
Excited State 16:	3.9200	316.28	0.1104	Excited State 8:	3.1922	388.40	0.0000
Excited State 17:	4.2396	292.44	0.0711	Excited State 9:	3.4515	359.22	0.0000
Excited State 18:	4.3246	286.69	0.0690	Excited State 10:	3.4606	358.27	0.0000
Excited State 19:	4.4788	276.82	0.0707	Excited State 12:	3.5630	347.98	0.0000
Excited State 20:	4.7707	259.89	0.3115	Excited State 14:	3.7501	330.62	0.0000

1P234-geo-opt-abs-CCl4

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 8:	3.8370	323.13	0.0694	Excited State 1:	2.2635	547.75	0.0000

Excited State 9:	3.9369	314.93	0.1088	Excited State 2:	2.9789	416.21	0.0000
Excited State 12:	4.3018	288.22	0.9589	Excited State 3:	3.3695	367.96	0.0000
Excited State 14:	4.5017	275.42	0.0966	Excited State 4:	3.4566	358.68	0.0000
Excited State 15:	4.6709	265.44	0.0700	Excited State 5:	3.5615	348.12	0.0000
Excited State 16:	4.9122	252.40	0.1292	Excited State 6:	3.7060	334.55	0.0000
Excited State 17:	5.0541	245.31	0.0435	Excited State 7:	3.7624	329.53	0.0000
Excited State 18:	5.1154	242.37	0.0888	Excited State 10:	4.0314	307.54	0.0000
Excited State 19:	5.1517	240.67	0.0523	Excited State 11:	4.2144	294.19	0.0000
Excited State 20:	5.2612	235.66	0.1396	Excited State 13:	4.3246	286.69	0.0000

1P234-geo-opt-abs-DCM

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 8:	3.8381	323.04	0.0676	Excited State 1:	2.2672	546.86	0.0000
Excited State 9:	3.9394	314.73	0.1058	Excited State 2:	2.9813	415.88	0.0000
Excited State 12:	4.3107	287.62	0.9441	Excited State 3:	3.3709	367.81	0.0000
Excited State 14:	4.5063	275.14	0.0937	Excited State 4:	3.4616	358.17	0.0000
Excited State 15:	4.6751	265.20	0.0673	Excited State 5:	3.5630	347.98	0.0000
Excited State 16:	4.9152	252.25	0.1309	Excited State 6:	3.7110	334.10	0.0000
Excited State 17:	5.0817	243.98	0.0432	Excited State 7:	3.7647	329.33	0.0000
Excited State 18:	5.1201	242.15	0.0906	Excited State 10:	4.0365	307.16	0.0000
Excited State 19:	5.1623	240.17	0.0456	Excited State 11:	4.2176	293.97	0.0000
Excited State 20:	5.2788	234.87	0.1513	Excited State 13:	4.3273	286.51	0.0000

1P234-geo-opt-abs-DMSO

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 8:	3.8381	323.03	0.0675	Excited State 1:	2.2687	546.50	0.0000
Excited State 9:	3.9403	314.66	0.1048	Excited State 2:	2.9822	415.75	0.0000
Excited State 12:	4.3131	287.46	0.9415	Excited State 3:	3.3712	367.77	0.0000

Excited State 14:	4.5077	275.05	0.0927	Excited State 4:	3.4636	357.96	0.0000
Excited State 15:	4.6759	265.16	0.0667	Excited State 5:	3.5635	347.93	0.0000
Excited State 16:	4.9162	252.19	0.1320	Excited State 6:	3.7131	333.91	0.0000
Excited State 17:	5.0924	243.47	0.0434	Excited State 7:	3.7656	329.26	0.0000
Excited State 18:	5.1215	242.09	0.0907	Excited State 10:	4.0380	307.04	0.0000
Excited State 19:	5.1656	240.02	0.0435	Excited State 11:	4.2189	293.88	0.0000
Excited State 20:	5.2856	234.57	0.1577	Excited State 13:	4.3283	286.45	0.0000

1P234-geo-opt-abs

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 8:	3.8494	322.08	0.0296	Excited State 1:	2.2604	548.50	0.0000
Excited State 9:	3.9610	313.01	0.0822	Excited State 2:	2.9765	416.54	0.0000
Excited State 13:	4.3863	282.66	0.6321	Excited State 3:	3.3677	368.16	0.0000
Excited State 14:	4.5228	274.13	0.1265	Excited State 4:	3.4523	359.14	0.0000
Excited State 15:	4.7041	263.57	0.0432	Excited State 5:	3.5597	348.30	0.0000
Excited State 16:	4.9243	251.78	0.0951	Excited State 6:	3.7018	334.93	0.0000
Excited State 17:	5.0396	246.02	0.0242	Excited State 7:	3.7603	329.72	0.0000
Excited State 18:	5.1475	240.86	0.0534	Excited State 10:	4.0256	307.99	0.0000
Excited State 19:	5.1849	239.13	0.0415	Excited State 11:	4.2119	294.36	0.0000
Excited State 20:	5.2607	235.68	0.0880	Excited State 12:	4.3220	286.87	0.0000

1P234-geo-opt-abs-n-hexane

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 8:	3.8391	322.95	0.0616	Excited State 1:	2.2629	547.90	0.0000
Excited State 9:	3.9401	314.67	0.1058	Excited State 2:	2.9784	416.28	0.0000
Excited State 12:	4.3138	287.41	0.9152	Excited State 3:	3.3692	368.00	0.0000
Excited State 14:	4.5042	275.26	0.0974	Excited State 4:	3.4558	358.77	0.0000
Excited State 15:	4.6757	265.17	0.0655	Excited State 5:	3.5612	348.16	0.0000

Excited State 16:	4.9138	252.32	0.1236	Excited State 6:	3.7052	334.63	0.0000
Excited State 17:	5.0510	245.46	0.0393	Excited State 7:	3.7620	329.57	0.0000
Excited State 18:	5.1203	242.14	0.0837	Excited State 10:	4.0304	307.62	0.0000
Excited State 19:	5.1560	240.46	0.0514	Excited State 11:	4.2139	294.23	0.0000
Excited State 20:	5.2604	235.70	0.1303	Excited State 13:	4.3241	286.73	0.0000

2-D-10-A-12P34-OPA-CC14

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	3.2043	386.93	0.2750	Excited State 1:	1.9451	637.41	0.0000
Excited State 9:	3.7054	334.61	0.0842	Excited State 2:	2.4760	500.74	0.0000
Excited State 12:	4.0057	309.52	0.1686	Excited State 3:	3.1513	393.43	0.0000
Excited State 13:	4.0686	304.73	0.0640	Excited State 5:	3.3272	372.64	0.0000
Excited State 15:	4.1917	295.79	0.0236	Excited State 6:	3.4541	358.94	0.0000
Excited State 16:	4.4506	278.58	0.1738	Excited State 7:	3.5415	350.09	0.0000
Excited State 17:	4.6115	268.86	0.2999	Excited State 8:	3.5869	345.66	0.0000
Excited State 18:	4.8086	257.84	0.0636	Excited State 10:	3.8282	323.87	0.0000
Excited State 19:	4.9165	252.18	0.8793	Excited State 11:	3.8579	321.37	0.0000
Excited State 20:	4.9686	249.54	0.0125	Excited State 14:	4.0776	304.06	0.0000

2-D-10-A-12P34-OPA-DCM

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	3.1691	391.23	0.2598	Excited State 1:	1.9442	637.73	0.0000
Excited State 9:	3.6835	336.59	0.0796	Excited State 2:	2.4756	500.83	0.0000
Excited State 12:	3.9734	312.03	0.1897	Excited State 3:	3.1307	396.03	0.0000
Excited State 13:	4.0609	305.31	0.0564	Excited State 5:	3.3113	374.42	0.0000
Excited State 15:	4.1865	296.15	0.0194	Excited State 6:	3.4578	358.56	0.0000
Excited State 16:	4.4416	279.14	0.1591	Excited State 7:	3.5120	353.03	0.0000
Excited State 17:	4.5986	269.61	0.2837	Excited State 8:	3.5765	346.67	0.0000

Excited State 18: 4.8064 257.96 0.0800 Excited State 10: 3.8268 323.99 0.0000  
 Excited State 19: 4.9026 252.90 0.7876 Excited State 11: 3.8372 323.11 0.0000  
 Excited State 20: 4.9577 250.08 0.0023 Excited State 14: 4.0672 304.84 0.0000

2-D-10-A-12P34-OPA-DMSO

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	3.1529	393.23	0.2641	Excited State 1:	1.9439	637.81	0.0000
Excited State 9:	3.6733	337.52	0.0810	Excited State 2:	2.4751	500.93	0.0000
Excited State 12:	3.9602	313.08	0.2022	Excited State 3:	3.1222	397.11	0.0000
Excited State 13:	4.0587	305.48	0.0586	Excited State 5:	3.3056	375.08	0.0000
Excited State 15:	4.1830	296.40	0.0189	Excited State 6:	3.4591	358.43	0.0000
Excited State 16:	4.4354	279.53	0.1603	Excited State 7:	3.5002	354.22	0.0000
Excited State 17:	4.5892	270.17	0.3024	Excited State 8:	3.5739	346.91	0.0000
Excited State 18:	4.8030	258.14	0.1085	Excited State 10:	3.8184	324.70	0.0000
Excited State 19:	4.8917	253.46	0.7580	Excited State 11:	3.8400	322.87	0.0000
Excited State 20:	4.9536	250.29	0.0042	Excited State 14:	4.0655	304.97	0.0000

2-D-10-A-12P34-OPA

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	3.2861	377.30	0.2048	Excited State 1:	1.9476	636.59	0.0000
Excited State 9:	3.7544	330.24	0.0532	Excited State 2:	2.4765	500.63	0.0000
Excited State 12:	4.0521	305.97	0.0603	Excited State 3:	3.1720	390.88	0.0000
Excited State 14:	4.1082	301.80	0.0765	Excited State 5:	3.3431	370.87	0.0000
Excited State 15:	4.2218	293.67	0.0175	Excited State 6:	3.4508	359.29	0.0000
Excited State 16:	4.4989	275.59	0.1227	Excited State 7:	3.5699	347.30	0.0000
Excited State 17:	4.6818	264.82	0.1855	Excited State 8:	3.6027	344.14	0.0000
Excited State 18:	4.8331	256.53	0.0345	Excited State 10:	3.8263	324.03	0.0000
Excited State 19:	4.9792	249.01	0.0645	Excited State 11:	3.8929	318.48	0.0000

Excited State 20: 5.0099 247.48 0.5014 Excited State 13: 4.0975 302.59 0.0000

2-D-10-A-12P34-OPA-n-hexane

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	3.2171	385.39	0.2650	Excited State 1:	1.9455	637.29	0.0000
Excited State 9:	3.7135	333.88	0.0794	Excited State 2:	2.4762	500.70	0.0000
Excited State 12:	4.0150	308.80	0.1506	Excited State 3:	3.1552	392.96	0.0000
Excited State 13:	4.0734	304.37	0.0654	Excited State 5:	3.3302	372.30	0.0000
Excited State 15:	4.1961	295.47	0.0230	Excited State 6:	3.4535	359.01	0.0000
Excited State 16:	4.4580	278.11	0.1673	Excited State 7:	3.5469	349.56	0.0000
Excited State 17:	4.6221	268.24	0.2788	Excited State 8:	3.5895	345.41	0.0000
Excited State 18:	4.8123	257.64	0.0550	Excited State 10:	3.8275	323.93	0.0000
Excited State 19:	4.9299	251.50	0.8332	Excited State 11:	3.8640	320.87	0.0000
Excited State 20:	4.9717	249.38	0.0223	Excited State 14:	4.0805	303.84	0.0000

3-A-12-D-P1234-OPA-CCl4

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	2.6665	464.97	0.0924	Excited State 1:	1.1393	1088.21	0.0000
Excited State 6:	2.9420	421.43	0.0209	Excited State 2:	2.3225	533.84	0.0000
Excited State 9:	3.3883	365.92	0.2391	Excited State 3:	2.4508	505.88	0.0000
Excited State 12:	3.5764	346.67	0.3440	Excited State 5:	2.6899	460.92	0.0000
Excited State 15:	4.0700	304.63	0.1157	Excited State 7:	3.1221	397.11	0.0000
Excited State 16:	4.1930	295.69	0.2571	Excited State 8:	3.2449	382.09	0.0000
Excited State 17:	4.2377	292.57	0.1698	Excited State 10:	3.4531	359.05	0.0000
Excited State 18:	4.4885	276.23	0.0647	Excited State 11:	3.4882	355.44	0.0000
Excited State 19:	4.6665	265.69	0.7803	Excited State 13:	3.5835	345.98	0.0000
Excited State 20:	4.7205	262.65	0.0656	Excited State 14:	3.7021	334.90	0.0000

3-A-12-D-P1234-OPA-DCM

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	2.6415	469.38	0.0843	Excited State 1:	1.1527	1075.56	0.0000
Excited State 6:	2.9138	425.50	0.0286	Excited State 2:	2.3146	535.66	0.0000
Excited State 9:	3.3666	368.28	0.2398	Excited State 3:	2.4258	511.10	0.0000
Excited State 13:	3.5604	348.23	0.3199	Excited State 5:	2.6704	464.28	0.0000
Excited State 15:	4.0636	305.11	0.1036	Excited State 7:	3.1075	398.98	0.0000
Excited State 16:	4.1789	296.69	0.2780	Excited State 8:	3.2351	383.24	0.0000
Excited State 17:	4.2289	293.18	0.1711	Excited State 10:	3.4595	358.39	0.0000
Excited State 18:	4.4702	277.36	0.0599	Excited State 11:	3.4838	355.88	0.0000
Excited State 19:	4.6642	265.82	0.7593	Excited State 12:	3.5581	348.46	0.0000
Excited State 20:	4.7184	262.77	0.0505	Excited State 14:	3.6953	335.52	0.0000

3-A-12-D-P1234-OPA-DMSO

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	2.6323	471.01	0.0819	Excited State 1:	1.1568	1071.77	0.0000
Excited State 6:	2.9062	426.63	0.0315	Excited State 2:	2.3117	536.33	0.0000
Excited State 9:	3.3595	369.06	0.2409	Excited State 3:	2.4180	512.76	0.0000
Excited State 13:	3.5545	348.81	0.3128	Excited State 5:	2.6642	465.37	0.0000
Excited State 15:	4.0609	305.31	0.1000	Excited State 7:	3.1029	399.57	0.0000
Excited State 16:	4.1740	297.04	0.2846	Excited State 8:	3.2319	383.63	0.0000
Excited State 17:	4.2267	293.34	0.1730	Excited State 10:	3.4620	358.13	0.0000
Excited State 18:	4.4635	277.77	0.0575	Excited State 11:	3.4820	356.08	0.0000
Excited State 19:	4.6624	265.92	0.7472	Excited State 12:	3.5503	349.22	0.0000
Excited State 20:	4.7180	262.79	0.0531	Excited State 14:	3.6947	335.57	0.0000

3-A-12-D-P1234-OPA

Singlets			Triplets		
Ex.En	WL	OS	Ex.En	WL	OS

Excited State 5:	2.7210	455.65	0.0671	Excited State 1:	1.1228	1104.21	0.0000
Excited State 6:	2.9950	413.97	0.0118	Excited State 2:	2.3301	532.10	0.0000
Excited State 9:	3.4454	359.85	0.1181	Excited State 3:	2.4813	499.67	0.0000
Excited State 13:	3.6527	339.43	0.3185	Excited State 4:	2.7132	456.97	0.0000
Excited State 15:	4.0992	302.46	0.0933	Excited State 7:	3.1390	394.98	0.0000
Excited State 16:	4.2462	291.99	0.1038	Excited State 8:	3.2564	380.74	0.0000
Excited State 17:	4.2834	289.46	0.1459	Excited State 10:	3.4473	359.66	0.0000
Excited State 18:	4.5272	273.86	0.0373	Excited State 11:	3.4904	355.21	0.0000
Excited State 19:	4.7232	262.50	0.1251	Excited State 12:	3.6123	343.23	0.0000
Excited State 20:	4.7800	259.38	0.4510	Excited State 14:	3.7222	333.09	0.0000

3-A-12-D-P1234-OPA-n-hexane

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	2.6754	463.42	0.0888	Excited State 1:	1.1364	1090.98	0.0000
Excited State 6:	2.9505	420.22	0.0190	Excited State 2:	2.3239	533.51	0.0000
Excited State 9:	3.3981	364.87	0.2183	Excited State 3:	2.4561	504.80	0.0000
Excited State 12:	3.5870	345.64	0.3439	Excited State 5:	2.6939	460.24	0.0000
Excited State 15:	4.0746	304.29	0.1126	Excited State 7:	3.1252	396.73	0.0000
Excited State 16:	4.2028	295.00	0.2253	Excited State 8:	3.2469	381.86	0.0000
Excited State 17:	4.2438	292.15	0.1696	Excited State 10:	3.4520	359.17	0.0000
Excited State 18:	4.4946	275.85	0.0587	Excited State 11:	3.4888	355.38	0.0000
Excited State 19:	4.6802	264.91	0.7298	Excited State 13:	3.5888	345.48	0.0000
Excited State 20:	4.7239	262.46	0.0926	Excited State 14:	3.7046	334.68	0.0000

2-D-12-A-12P34-OPA-CCl4

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 3:	3.1456	394.15	0.2336	Excited State 1:	1.9479	636.50	0.0000
Excited State 10:	3.7018	334.93	0.1099	Excited State 2:	2.5184	492.31	0.0000

Excited State 11:	3.9290	315.56	0.0472	Excited State 4:	3.1469	393.99	0.0000
Excited State 14:	4.0096	309.22	0.1037	Excited State 5:	3.3334	371.95	0.0000
Excited State 16:	4.2663	290.61	0.0679	Excited State 6:	3.4237	362.13	0.0000
Excited State 18:	4.3974	281.95	0.2637	Excited State 7:	3.4560	358.75	0.0000
Excited State 19:	4.6201	268.36	0.0991	Excited State 8:	3.5918	345.19	0.0000
Excited State 20:	4.7297	262.14	0.3469	Excited State 9:	3.6737	337.49	0.0000
Excited State 21:	4.8597	255.13	0.0255	Excited State 12:	3.9855	311.09	0.0000
Excited State 22:	4.9494	250.51	0.2630	Excited State 13:	3.9984	310.09	0.0000
Excited State 23:	5.0404	245.98	0.6446	Excited State 15:	4.1653	297.66	0.0000
Excited State 24:	5.1004	243.09	0.2015	Excited State 17:	4.2733	290.14	0.0000

2-D-12-A-12P34-OPA-DCM

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 3:	3.1365	395.29	0.2253	Excited State 1:	1.9473	636.69	0.0000
Excited State 10:	3.6939	335.64	0.1041	Excited State 2:	2.5175	492.50	0.0000
Excited State 11:	3.9273	315.70	0.0549	Excited State 4:	3.1428	394.50	0.0000
Excited State 14:	3.9959	310.28	0.0951	Excited State 5:	3.3323	372.07	0.0000
Excited State 15:	4.2687	290.45	0.0564	Excited State 6:	3.4109	363.50	0.0000
Excited State 16:	4.3951	282.09	0.2698	Excited State 7:	3.4604	358.29	0.0000
Excited State 17:	4.6209	268.31	0.0889	Excited State 8:	3.5832	346.02	0.0000
Excited State 18:	4.7192	262.72	0.3443	Excited State 9:	3.6633	338.45	0.0000
Excited State 19:	4.8687	254.66	0.0290	Excited State 12:	3.9855	311.09	0.0000
Excited State 20:	4.9521	250.37	0.2775	Excited State 13:	3.9947	310.37	0.0000

2-D-12-A-12P34-OPA-DMSO

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 3:	3.1374	395.18	0.2243	Excited State 1:	1.9476	636.59	0.0000
Excited State 10:	3.6934	335.69	0.1021	Excited State 2:	2.5171	492.56	0.0000

Excited State 11:	3.9296	315.52	0.0563	Excited State 4:	3.1432	394.46	0.0000
Excited State 13:	3.9938	310.44	0.0922	Excited State 5:	3.3335	371.93	0.0000
Excited State 15:	4.2706	290.32	0.0514	Excited State 6:	3.4098	363.61	0.0000
Excited State 16:	4.3956	282.06	0.2768	Excited State 7:	3.4622	358.11	0.0000
Excited State 17:	4.6231	268.18	0.0915	Excited State 8:	3.5809	346.24	0.0000
Excited State 18:	4.7171	262.84	0.3446	Excited State 9:	3.6607	338.69	0.0000
Excited State 19:	4.8750	254.33	0.0345	Excited State 12:	3.9865	311.01	0.0000
Excited State 20:	4.9556	250.19	0.2901	Excited State 14:	3.9957	310.29	0.0000

2-D-12-A-12P34-OPA

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	3.2080	386.48	0.1700	Excited State 1:	1.9490	636.13	0.0000
Excited State 10:	3.7429	331.26	0.0697	Excited State 2:	2.5194	492.11	0.0000
Excited State 11:	3.9489	313.97	0.0185	Excited State 3:	3.1598	392.38	0.0000
Excited State 14:	4.0544	305.80	0.0738	Excited State 5:	3.3406	371.14	0.0000
Excited State 15:	4.2949	288.68	0.0287	Excited State 6:	3.4471	359.67	0.0000
Excited State 16:	4.4318	279.13	0.1720	Excited State 7:	3.4548	358.88	0.0000
Excited State 17:	4.6497	266.65	0.0335	Excited State 8:	3.6007	344.33	0.0000
Excited State 18:	4.7965	258.49	0.1912	Excited State 9:	3.6908	335.93	0.0000
Excited State 19:	4.8708	254.55	0.0350	Excited State 12:	3.9869	310.98	0.0000
Excited State 20:	4.9805	248.94	0.1145	Excited State 13:	4.0123	309.01	0.0000

2-D-12-A-12P34-OPA-n-hexane

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	3.1545	393.04	0.2243	Excited State 1:	1.9482	636.41	0.0000
Excited State 10:	3.7076	334.40	0.1030	Excited State 2:	2.5186	492.28	0.0000
Excited State 11:	3.9322	315.30	0.0413	Excited State 3:	3.1483	393.81	0.0000
Excited State 14:	4.0159	308.74	0.1006	Excited State 5:	3.3341	371.87	0.0000

Excited State 15:	4.2704	290.34	0.0622	Excited State 6:	3.4275	361.73	0.0000
Excited State 16:	4.4037	281.55	0.2471	Excited State 7:	3.4553	358.83	0.0000
Excited State 17:	4.6241	268.13	0.0827	Excited State 8:	3.5937	345.00	0.0000
Excited State 18:	4.7410	261.51	0.3297	Excited State 9:	3.6763	337.25	0.0000
Excited State 19:	4.8602	255.10	0.0261	Excited State 12:	3.9855	311.09	0.0000
Excited State 20:	4.9534	250.30	0.2252	Excited State 13:	4.0005	309.92	0.0000

3-D-13-A-1P234-OPA-CCl4

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	3.2541	381.01	0.2313	Excited State 1:	2.1104	587.49	0.0000
Excited State 7:	3.5193	352.30	0.1587	Excited State 2:	2.6706	464.25	0.0000
Excited State 12:	4.0025	309.77	0.0490	Excited State 3:	3.0004	413.22	0.0000
Excited State 14:	4.1600	298.04	0.4090	Excited State 5:	3.3272	372.64	0.0000
Excited State 15:	4.3396	285.71	0.0887	Excited State 6:	3.4556	358.79	0.0000
Excited State 16:	4.5603	271.88	0.3197	Excited State 8:	3.5199	352.24	0.0000
Excited State 17:	4.6850	264.64	0.1371	Excited State 9:	3.6305	341.51	0.0000
Excited State 18:	4.7417	261.48	0.3970	Excited State 10:	3.6569	339.04	0.0000
Excited State 19:	4.8070	257.92	0.0919	Excited State 11:	3.9039	317.59	0.0000
Excited State 20:	4.8558	255.33	0.1483	Excited State 13:	4.0366	307.15	0.0000

3-D-13-A-1P234-OPA-DCM

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	3.2415	382.49	0.2301	Excited State 1:	2.1117	587.13	0.0000
Excited State 8:	3.5187	352.36	0.1571	Excited State 2:	2.6642	465.37	0.0000
Excited State 12:	3.9875	310.93	0.0361	Excited State 3:	2.9956	413.88	0.0000
Excited State 14:	4.1696	297.35	0.3885	Excited State 5:	3.3083	374.76	0.0000
Excited State 15:	4.3232	286.79	0.1038	Excited State 6:	3.4592	358.42	0.0000
Excited State 16:	4.5542	272.24	0.3251	Excited State 7:	3.4901	355.24	0.0000

Excited State 17:	4.6751	265.20	0.1666	Excited State 9:	3.6367	340.92	0.0000
Excited State 18:	4.7439	261.36	0.3631	Excited State 10:	3.6688	337.95	0.0000
Excited State 19:	4.8051	258.03	0.0812	Excited State 11:	3.9007	317.85	0.0000
Excited State 20:	4.8673	254.73	0.1705	Excited State 13:	4.0356	307.23	0.0000

3-D-13-A-1P234-OPA-DMSO

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	3.2391	382.77	0.2313	Excited State 1:	2.1125	586.90	0.0000
Excited State 8:	3.5193	352.30	0.1565	Excited State 2:	2.6623	465.70	0.0000
Excited State 12:	3.9805	311.48	0.0327	Excited State 3:	2.9943	414.06	0.0000
Excited State 14:	4.1731	297.10	0.3820	Excited State 5:	3.2997	375.74	0.0000
Excited State 15:	4.3170	287.20	0.1130	Excited State 6:	3.4595	358.39	0.0000
Excited State 16:	4.5519	272.38	0.3314	Excited State 7:	3.4787	356.41	0.0000
Excited State 17:	4.6735	265.29	0.1777	Excited State 9:	3.6394	340.68	0.0000
Excited State 18:	4.7444	261.33	0.3340	Excited State 10:	3.6740	337.46	0.0000
Excited State 19:	4.8072	257.91	0.0881	Excited State 11:	3.8994	317.96	0.0000
Excited State 20:	4.8749	254.33	0.1777	Excited State 13:	4.0355	307.23	0.0000

3-D-13-A-1P234-OPA

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	3.3121	374.34	0.1536	Excited State 1:	2.1117	587.14	0.0000
Excited State 8:	3.5548	348.78	0.1171	Excited State 2:	2.6801	462.61	0.0000
Excited State 12:	4.0336	307.38	0.0394	Excited State 3:	3.0113	411.73	0.0000
Excited State 14:	4.1976	295.37	0.2868	Excited State 5:	3.3421	370.98	0.0000
Excited State 15:	4.3839	282.82	0.0377	Excited State 6:	3.4517	359.20	0.0000
Excited State 16:	4.5978	269.66	0.1399	Excited State 7:	3.5471	349.54	0.0000
Excited State 17:	4.7106	263.20	0.0279	Excited State 9:	3.6270	341.84	0.0000
Excited State 18:	4.7925	258.70	0.3070	Excited State 10:	3.6504	339.64	0.0000

Excited State 19: 4.8507 255.60 0.1921 Excited State 11: 3.9072 317.32 0.0000  
 Excited State 20: 4.8863 253.74 0.1324 Excited State 13: 4.0427 306.69 0.0000

3-D-13-A-1P234-OPA-n-hexane

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	3.2624	380.04	0.2195	Excited State 1:	2.1104	587.49	0.0000
Excited State 7:	3.5239	351.83	0.1521	Excited State 2:	2.6721	463.99	0.0000
Excited State 12:	4.0074	309.38	0.0483	Excited State 3:	3.0018	413.04	0.0000
Excited State 14:	4.1647	297.70	0.3901	Excited State 5:	3.3302	372.31	0.0000
Excited State 15:	4.3468	285.23	0.0775	Excited State 6:	3.4548	358.87	0.0000
Excited State 16:	4.5665	271.51	0.2848	Excited State 8:	3.5250	351.73	0.0000
Excited State 17:	4.6893	264.40	0.1110	Excited State 9:	3.6296	341.59	0.0000
Excited State 18:	4.7481	261.12	0.4148	Excited State 10:	3.6552	339.20	0.0000
Excited State 19:	4.8127	257.62	0.1003	Excited State 11:	3.9044	317.55	0.0000
Excited State 20:	4.8590	255.17	0.1427	Excited State 13:	4.0373	307.10	0.0000

1-A-11-D-P1234-OPA-CC14

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	2.6728	463.87	0.0364	Excited State 1:	1.1821	1048.81	0.0000
Excited State 5:	2.8563	434.08	0.2491	Excited State 2:	2.2387	553.82	0.0000
Excited State 11:	3.5629	347.99	0.0732	Excited State 3:	2.4774	500.46	0.0000
Excited State 13:	3.7458	331.00	0.1226	Excited State 6:	2.9059	426.66	0.0000
Excited State 15:	3.9092	317.16	0.1901	Excited State 7:	3.0348	408.54	0.0000
Excited State 16:	4.0061	309.49	0.3966	Excited State 8:	3.2151	385.63	0.0000
Excited State 17:	4.3023	288.18	0.3050	Excited State 9:	3.3346	371.81	0.0000
Excited State 18:	4.5965	269.74	0.0552	Excited State 10:	3.4528	359.09	0.0000
Excited State 19:	4.6715	265.41	0.1112	Excited State 12:	3.6365	340.94	0.0000
Excited State 20:	4.7452	261.28	0.1196	Excited State 14:	3.7477	330.82	0.0000

## 1-A-11-D-P1234-OPA-DCM

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	2.6714	464.12	0.0386	Excited State 1:	1.1972	1035.66	0.0000
Excited State 5:	2.8425	436.19	0.2432	Excited State 2:	2.2193	558.67	0.0000
Excited State 11:	3.5564	348.62	0.0654	Excited State 3:	2.4891	498.10	0.0000
Excited State 14:	3.7500	330.63	0.1370	Excited State 6:	2.8875	429.39	0.0000
Excited State 15:	3.9012	317.81	0.1794	Excited State 7:	3.0307	409.09	0.0000
Excited State 16:	3.9985	310.08	0.3953	Excited State 8:	3.2016	387.25	0.0000
Excited State 17:	4.3020	288.20	0.2979	Excited State 9:	3.3350	371.77	0.0000
Excited State 18:	4.5927	269.96	0.0441	Excited State 10:	3.4598	358.35	0.0000
Excited State 19:	4.6637	265.85	0.0699	Excited State 12:	3.6403	340.59	0.0000
Excited State 20:	4.7386	261.65	0.1581	Excited State 13:	3.7338	332.06	0.0000

## 1-A-11-D-P1234-OPA-DMSO

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	2.6731	463.82	0.0385	Excited State 1:	1.2038	1029.97	0.0000
Excited State 5:	2.8400	436.57	0.2433	Excited State 2:	2.2132	560.20	0.0000
Excited State 11:	3.5557	348.69	0.0622	Excited State 3:	2.4950	496.93	0.0000
Excited State 14:	3.7524	330.42	0.1482	Excited State 6:	2.8813	430.31	0.0000
Excited State 15:	3.9007	317.85	0.1763	Excited State 7:	3.0315	408.99	0.0000
Excited State 16:	3.9946	310.38	0.3910	Excited State 8:	3.1969	387.82	0.0000
Excited State 17:	4.3049	288.01	0.2921	Excited State 9:	3.3349	371.78	0.0000
Excited State 18:	4.5916	270.02	0.0411	Excited State 10:	3.4628	358.05	0.0000
Excited State 19:	4.6593	266.10	0.0608	Excited State 12:	3.6454	340.12	0.0000
Excited State 20:	4.7383	261.67	0.1666	Excited State 13:	3.7289	332.50	0.0000

## 1-A-11-D-P1234-OPA

Singlets				Triplets			
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	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	2.7084	457.77	0.0243	Excited State 1:	1.1682	1061.30	0.0000
Excited State 5:	2.9202	424.57	0.1806	Excited State 2:	2.2635	547.75	0.0000
Excited State 11:	3.5954	344.84	0.0613	Excited State 3:	2.4708	501.79	0.0000
Excited State 14:	3.7711	328.78	0.0712	Excited State 6:	2.9272	423.56	0.0000
Excited State 15:	3.9641	312.77	0.0798	Excited State 7:	3.0477	406.81	0.0000
Excited State 16:	4.0689	304.71	0.3095	Excited State 8:	3.2304	383.81	0.0000
Excited State 17:	4.3464	285.26	0.2757	Excited State 9:	3.3345	371.82	0.0000
Excited State 18:	4.6189	268.43	0.0372	Excited State 10:	3.4467	359.72	0.0000
Excited State 19:	4.6930	264.19	0.0678	Excited State 12:	3.6437	340.27	0.0000
Excited State 20:	4.7550	260.74	0.0151	Excited State 13:	3.7644	329.36	0.0000

1-A-11-D-P1234-OPA-n-hexane

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	2.6780	462.97	0.0344	Excited State 1:	1.1796	1051.07	0.0000
Excited State 5:	2.8658	432.64	0.2391	Excited State 2:	2.2430	552.77	0.0000
Excited State 11:	3.5677	347.52	0.0722	Excited State 3:	2.4758	500.78	0.0000
Excited State 13:	3.7493	330.69	0.1106	Excited State 6:	2.9096	426.12	0.0000
Excited State 15:	3.9179	316.46	0.1706	Excited State 7:	3.0366	408.30	0.0000
Excited State 16:	4.0152	308.79	0.3885	Excited State 8:	3.2178	385.30	0.0000
Excited State 17:	4.3080	287.80	0.3002	Excited State 9:	3.3346	371.82	0.0000
Excited State 18:	4.5999	269.54	0.0527	Excited State 10:	3.4516	359.21	0.0000
Excited State 19:	4.6750	265.21	0.1034	Excited State 12:	3.6372	340.88	0.0000
Excited State 20:	4.7510	260.97	0.1052	Excited State 14:	3.7506	330.57	0.0000

3-A-10-D-P1234-OPA-CC14

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	2.7513	450.63	0.1220	Excited State 1:	1.1385	1088.97	0.0000

Excited State 6:	3.2106	386.18	0.1267	Excited State 2:	2.3580	525.80	0.0000
Excited State 11:	3.6937	335.66	0.2207	Excited State 3:	2.5077	494.42	0.0000
Excited State 13:	3.8343	323.35	0.4819	Excited State 5:	2.9311	422.99	0.0000
Excited State 15:	4.0398	306.91	0.0036	Excited State 7:	3.2231	384.67	0.0000
Excited State 16:	4.2614	290.95	0.2471	Excited State 8:	3.3769	367.15	0.0000
Excited State 17:	4.4029	281.60	0.0487	Excited State 9:	3.4544	358.92	0.0000
Excited State 18:	4.4576	278.14	0.0643	Excited State 10:	3.5407	350.17	0.0000
Excited State 19:	4.5750	271.00	0.2268	Excited State 12:	3.8008	326.20	0.0000
Excited State 20:	4.7467	261.20	0.4397	Excited State 14:	3.8769	319.80	0.0000

### 3-A-10-D-P1234-OPA-DCM

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	2.7461	451.49	0.1239	Excited State 1:	1.1497	1078.37	0.0000
Excited State 6:	3.1774	390.21	0.1181	Excited State 2:	2.3550	526.47	0.0000
Excited State 11:	3.6677	338.05	0.2253	Excited State 3:	2.4892	498.09	0.0000
Excited State 13:	3.8426	322.66	0.4569	Excited State 5:	2.9176	424.96	0.0000
Excited State 15:	4.0311	307.57	0.0043	Excited State 7:	3.2261	384.32	0.0000
Excited State 16:	4.2401	292.41	0.2341	Excited State 8:	3.3775	367.09	0.0000
Excited State 17:	4.3826	282.90	0.0453	Excited State 9:	3.4605	358.28	0.0000
Excited State 18:	4.4492	278.67	0.0896	Excited State 10:	3.5293	351.30	0.0000
Excited State 19:	4.5542	272.24	0.2282	Excited State 12:	3.7969	326.54	0.0000
Excited State 20:	4.7364	261.77	0.2742	Excited State 14:	3.8736	320.07	0.0000

### 3-A-10-D-P1234-OPA-DMSO

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	2.7436	451.90	0.1251	Excited State 1:	1.1533	1075.05	0.0000
Excited State 6:	3.1665	391.54	0.1153	Excited State 2:	2.3538	526.74	0.0000
Excited State 11:	3.6587	338.87	0.2274	Excited State 3:	2.4836	499.21	0.0000

Excited State 13:	3.8445	322.50	0.4499	Excited State 5:	2.9130	425.62	0.0000
Excited State 15:	4.0282	307.79	0.0045	Excited State 7:	3.2269	384.22	0.0000
Excited State 16:	4.2333	292.88	0.2308	Excited State 8:	3.3775	367.09	0.0000
Excited State 17:	4.3753	283.38	0.0433	Excited State 9:	3.4629	358.03	0.0000
Excited State 18:	4.4454	278.90	0.1032	Excited State 10:	3.5255	351.68	0.0000
Excited State 19:	4.5485	272.58	0.2247	Excited State 12:	3.7951	326.69	0.0000
Excited State 20:	4.7324	261.99	0.2218	Excited State 14:	3.8721	320.20	0.0000

### 3-A-10-D-P1234-OPA

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	2.7915	444.14	0.0838	Excited State 1:	1.1238	1103.26	0.0000
Excited State 7:	3.2746	378.63	0.0840	Excited State 2:	2.3603	525.28	0.0000
Excited State 11:	3.7547	330.21	0.0878	Excited State 3:	2.5304	489.99	0.0000
Excited State 14:	3.8846	319.17	0.4497	Excited State 5:	2.9468	420.74	0.0000
Excited State 15:	4.0711	304.55	0.0017	Excited State 6:	3.2183	385.25	0.0000
Excited State 16:	4.3213	286.91	0.1936	Excited State 8:	3.3777	367.06	0.0000
Excited State 17:	4.4355	279.53	0.0323	Excited State 9:	3.4485	359.53	0.0000
Excited State 18:	4.4861	276.37	0.0394	Excited State 10:	3.5538	348.88	0.0000
Excited State 19:	4.6256	268.04	0.1938	Excited State 12:	3.8044	325.90	0.0000
Excited State 20:	4.8106	257.73	0.1359	Excited State 13:	3.8794	319.60	0.0000

### 3-A-10-D-P1234-OPA-n-hexane

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	2.7577	449.59	0.1159	Excited State 1:	1.1362	1091.23	0.0000
Excited State 6:	3.2211	384.92	0.1209	Excited State 2:	2.3585	525.70	0.0000
Excited State 11:	3.7045	334.69	0.1968	Excited State 3:	2.5115	493.67	0.0000
Excited State 13:	3.8400	322.88	0.4827	Excited State 5:	2.9340	422.58	0.0000
Excited State 15:	4.0447	306.54	0.0032	Excited State 7:	3.2223	384.77	0.0000

Excited State 16:	4.2709	290.30	0.2394	Excited State 8:	3.3770	367.14	0.0000
Excited State 17:	4.4091	281.20	0.0473	Excited State 9:	3.4533	359.03	0.0000
Excited State 18:	4.4621	277.86	0.0557	Excited State 10:	3.5429	349.95	0.0000
Excited State 19:	4.5828	270.55	0.2227	Excited State 12:	3.8016	326.14	0.0000
Excited State 20:	4.7573	260.62	0.3980	Excited State 14:	3.8775	319.76	0.0000

C1234-OPA-CCl4

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	3.0131	411.48	0.0717	Excited State 1:	1.2151	1020.36	0.0000
Excited State 9:	3.6145	343.01	0.0056	Excited State 2:	2.5040	495.14	0.0000
Excited State 11:	3.9036	317.62	0.4957	Excited State 3:	2.8496	435.09	0.0000
Excited State 13:	4.2047	294.87	0.1096	Excited State 5:	3.2074	386.55	0.0000
Excited State 15:	4.5246	274.02	0.0303	Excited State 6:	3.4819	356.08	0.0000
Excited State 16:	4.6597	266.08	0.4063	Excited State 7:	3.5039	353.85	0.0000
Excited State 17:	4.6999	263.80	0.0680	Excited State 8:	3.5520	349.05	0.0000
Excited State 18:	5.1117	242.55	0.1926	Excited State 10:	3.8237	324.25	0.0000
Excited State 19:	5.1945	238.68	0.0344	Excited State 12:	4.0898	303.15	0.0000
Excited State 20:	5.2641	235.53	0.0502	Excited State 14:	4.4123	280.99	0.0000

C1234-OPA-DCM

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	3.0172	410.92	0.0703	Excited State 1:	1.2212	1015.26	0.0000
Excited State 9:	3.6161	342.86	0.0067	Excited State 2:	2.5085	494.25	0.0000
Excited State 11:	3.9093	317.15	0.4854	Excited State 3:	2.8523	434.68	0.0000
Excited State 13:	4.2066	294.74	0.1086	Excited State 5:	3.2085	386.42	0.0000
Excited State 15:	4.5274	273.85	0.0318	Excited State 6:	3.4861	355.66	0.0000
Excited State 16:	4.6642	265.82	0.3860	Excited State 7:	3.5094	353.29	0.0000
Excited State 17:	4.7025	263.66	0.0816	Excited State 8:	3.5545	348.81	0.0000

Excited State 18:	5.1197	242.17	0.1932	Excited State 10:	3.8268	323.99	0.0000
Excited State 19:	5.1929	238.76	0.0303	Excited State 12:	4.0890	303.21	0.0000
Excited State 20:	5.2556	235.91	0.0354	Excited State 14:	4.4160	280.76	0.0000

C1234-OPA-DMSO

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	3.0184	410.76	0.0699	Excited State 1:	1.2238	1013.14	0.0000
Excited State 9:	3.6168	342.81	0.0072	Excited State 2:	2.5103	493.90	0.0000
Excited State 11:	3.9108	317.03	0.4822	Excited State 3:	2.8534	434.52	0.0000
Excited State 13:	4.2070	294.71	0.1087	Excited State 5:	3.2087	386.40	0.0000
Excited State 15:	4.5286	273.78	0.0332	Excited State 6:	3.4877	355.49	0.0000
Excited State 16:	4.6656	265.74	0.3772	Excited State 7:	3.5116	353.07	0.0000
Excited State 17:	4.7034	263.60	0.0887	Excited State 8:	3.5557	348.69	0.0000
Excited State 18:	5.1217	242.07	0.1953	Excited State 10:	3.8282	323.87	0.0000
Excited State 19:	5.1925	238.78	0.0275	Excited State 12:	4.0884	303.26	0.0000
Excited State 20:	5.2525	236.05	0.0347	Excited State 14:	4.4178	280.65	0.0000

C1234-OPA

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	3.0424	407.52	0.0484	Excited State 1:	1.2099	1024.77	0.0000
Excited State 9:	3.6157	342.91	0.0025	Excited State 2:	2.5001	495.91	0.0000
Excited State 11:	3.9695	312.34	0.3596	Excited State 3:	2.8472	435.46	0.0000
Excited State 13:	4.2260	293.38	0.0847	Excited State 5:	3.2061	386.72	0.0000
Excited State 15:	4.5320	273.57	0.0144	Excited State 6:	3.4785	356.43	0.0000
Excited State 16:	4.6980	263.91	0.1109	Excited State 7:	3.4991	354.33	0.0000
Excited State 17:	4.7219	262.57	0.2471	Excited State 8:	3.5503	349.22	0.0000
Excited State 18:	5.1309	241.64	0.0633	Excited State 10:	3.8213	324.46	0.0000
Excited State 19:	5.2051	238.20	0.0187	Excited State 12:	4.0899	303.15	0.0000

Excited State 20: 5.2835 234.66 0.0188 Excited State 14: 4.4098 281.15 0.0000

C1234-OPA-n-hexane

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	3.0174	410.90	0.0680	Excited State 1:	1.2141	1021.23	0.0000
Excited State 9:	3.6147	343.00	0.0050	Excited State 2:	2.5032	495.29	0.0000
Excited State 11:	3.9126	316.89	0.4769	Excited State 3:	2.8492	435.16	0.0000
Excited State 13:	4.2077	294.66	0.1050	Excited State 5:	3.2072	386.58	0.0000
Excited State 15:	4.5258	273.95	0.0269	Excited State 6:	3.4812	356.15	0.0000
Excited State 16:	4.6668	265.67	0.3840	Excited State 7:	3.5029	353.94	0.0000
Excited State 17:	4.7014	263.72	0.0718	Excited State 8:	3.5516	349.09	0.0000
Excited State 18:	5.1156	242.37	0.1638	Excited State 10:	3.8232	324.29	0.0000
Excited State 19:	5.1961	238.61	0.0313	Excited State 12:	4.0899	303.15	0.0000
Excited State 20:	5.2673	235.38	0.0385	Excited State 14:	4.4118	281.03	0.0000

P1234-geo-opt-abs

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	2.9545	419.64	0.0326	Excited State 1:	1.3143	943.31	0.0000
Excited State 9:	3.5196	352.26	0.0578	Excited State 2:	2.4670	502.58	0.0000
Excited State 11:	3.8896	318.75	0.4525	Excited State 3:	2.6927	460.45	0.0000
Excited State 14:	4.0586	305.49	0.0985	Excited State 5:	3.1411	394.71	0.0000
Excited State 15:	4.2802	289.67	0.0240	Excited State 6:	3.2556	380.83	0.0000
Excited State 16:	4.5853	270.40	0.0288	Excited State 7:	3.4456	359.83	0.0000
Excited State 17:	4.6556	266.31	0.2724	Excited State 8:	3.4893	355.33	0.0000
Excited State 18:	4.6995	263.82	0.0309	Excited State 10:	3.6084	343.60	0.0000
Excited State 19:	4.7861	259.05	0.0184	Excited State 12:	3.9350	315.08	0.0000
Excited State 20:	5.0377	246.11	0.1672	Excited State 13:	4.0513	306.03	0.0000

P1234-geo-opt-abs-CCl4

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	2.9295	423.23	0.0492	Excited State 1:	1.3188	940.14	0.0000
Excited State 9:	3.5021	354.03	0.1164	Excited State 2:	2.4697	502.02	0.0000
Excited State 11:	3.8153	324.96	0.5614	Excited State 3:	2.6956	459.95	0.0000
Excited State 13:	4.0300	307.65	0.1587	Excited State 5:	3.1435	394.42	0.0000
Excited State 15:	4.2631	290.83	0.0406	Excited State 6:	3.2583	380.52	0.0000
Excited State 16:	4.5676	271.44	0.0955	Excited State 7:	3.4513	359.24	0.0000
Excited State 17:	4.6173	268.52	0.3168	Excited State 8:	3.4915	355.10	0.0000
Excited State 18:	4.6880	264.47	0.0416	Excited State 10:	3.6128	343.18	0.0000
Excited State 19:	4.8030	258.14	0.0264	Excited State 12:	3.9382	314.83	0.0000
Excited State 20:	4.9893	248.50	0.3535	Excited State 14:	4.0518	306.00	0.0000

P1234-geo-opt-abs-DCM

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	2.9326	422.77	0.0481	Excited State 1:	1.3239	936.53	0.0000
Excited State 9:	3.5053	353.70	0.1123	Excited State 2:	2.4722	501.51	0.0000
Excited State 11:	3.8212	324.46	0.5579	Excited State 3:	2.6984	459.48	0.0000
Excited State 13:	4.0313	307.55	0.1503	Excited State 5:	3.1453	394.18	0.0000
Excited State 15:	4.2679	290.50	0.0408	Excited State 6:	3.2613	380.17	0.0000
Excited State 16:	4.5699	271.30	0.0879	Excited State 7:	3.4575	358.59	0.0000
Excited State 17:	4.6237	268.15	0.3148	Excited State 8:	3.4940	354.85	0.0000
Excited State 18:	4.6915	264.27	0.0420	Excited State 10:	3.6183	342.66	0.0000
Excited State 19:	4.8274	256.83	0.0254	Excited State 12:	3.9417	314.54	0.0000
Excited State 20:	4.9885	248.54	0.3223	Excited State 14:	4.0517	306.00	0.0000

P1234-geo-opt-abs-DMSO

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS

Excited State 4: 2.9336 422.64 0.0479 Excited State 1: 1.3262 934.91 0.0000  
 Excited State 9: 3.5063 353.60 0.1117 Excited State 2: 2.4730 501.36 0.0000  
 Excited State 11: 3.8227 324.34 0.5574 Excited State 3: 2.6993 459.33 0.0000  
 Excited State 13: 4.0309 307.58 0.1478 Excited State 5: 3.1458 394.13 0.0000  
 Excited State 15: 4.2697 290.38 0.0411 Excited State 6: 3.2623 380.05 0.0000  
 Excited State 16: 4.5705 271.27 0.0864 Excited State 7: 3.4600 358.34 0.0000  
 Excited State 17: 4.6260 268.01 0.3137 Excited State 8: 3.4950 354.75 0.0000  
 Excited State 18: 4.6928 264.20 0.0424 Excited State 10: 3.6206 342.44 0.0000  
 Excited State 19: 4.8370 256.33 0.0251 Excited State 12: 3.9431 314.44 0.0000  
 Excited State 20: 4.9872 248.61 0.3131 Excited State 14: 4.0515 306.02 0.0000

P1234-geo-opt-abs-n-hexane

Singlets				Triplets			
	Ex.En	WL	OS		Ex.En	WL	OS
Excited State 4:	2.9332	422.69	0.0465	Excited State 1:	1.3179	940.74	0.0000
Excited State 9:	3.5049	353.75	0.1059	Excited State 2:	2.4692	502.12	0.0000
Excited State 11:	3.8250	324.14	0.5487	Excited State 3:	2.6951	460.04	0.0000
Excited State 13:	4.0344	307.32	0.1477	Excited State 5:	3.1431	394.47	0.0000
Excited State 15:	4.2655	290.67	0.0377	Excited State 6:	3.2577	380.58	0.0000
Excited State 16:	4.5709	271.25	0.0801	Excited State 7:	3.4502	359.35	0.0000
Excited State 17:	4.6221	268.24	0.3145	Excited State 8:	3.4911	355.15	0.0000
Excited State 18:	4.6895	264.39	0.0389	Excited State 10:	3.6119	343.26	0.0000
Excited State 19:	4.7995	258.33	0.0252	Excited State 12:	3.9376	314.88	0.0000
Excited State 20:	4.9973	248.10	0.3216	Excited State 14:	4.0517	306.00	0.0000

ST6: s and p character (in %) obtained from Natural Transition Orbitals (NTO).

System / Considered Carbon atom	Percentage of S	Percentage of P
C1234 / C26, C27	29.17, 29.19	70.78, 70.76
1C234 / C21, C31	31.71, 31.56	68.25, 68.40
12C34 / C21, C31	31.71, 31.76	68.25, 68.20
P1234 / C26, C27	30.16, 29.97	69.81, 69.98
1P234 / C21, C32	32.09, 31.71	67.87, 68.26
12P34 / C21, C32	31.95, 31.86	68.01, 68.10

ST7: Root Mean Squared Deviation (RMSD) of all HeIC, HeIP, and DAHeIP systems in vacuum and other solvents.

Systems	RMSD-Values				
	Vacuum	CCl <sub>4</sub>	DCM	DMSO	n-hex
C1234-P1234	0.21	0.21	0.21	0.21	0.21
1C234-1P234	0.28	0.28	0.27	0.27	0.28
12C34-12P34	0.35	0.35	0.34	0.34	0.35
Systems	Vacuum-CCl <sub>4</sub>	Vacuum-DCM	Vacuum-DMSO	Vacuum-n-hex	
C1234	0.009	0.013	0.017	0.008	
1C234	0.007	0.019	0.026	0.006	
12C34	0.005	0.016	0.022	0.004	
P1234	0.008	0.015	0.017	0.006	
1P234	0.008	0.02	0.023	0.006	
12P34	0.008	0.024	0.034	0.005	
1-A-13-D-P1234	0.02	0.03	0.03	0.01	
3-A-12-D-P1234	0.03	0.05	0.05	0.02	
1-A-11-D-P1234	0.02	0.04	0.05	0.02	
3-A-10-D-P1234	0.01	0.03	0.03	0.01	
1-D-13-A-1P234	0.022	0.06	0.08	0.02	
3-D-13-A-1P234	0.02	0.03	0.04	0.01	
2-D-10-A-12P34	0.02	0.04	0.06	0.01	
2-D-12-A-12P34	0.18	0.20	0.21	0.17	

SC1: Python code for calculating rate of inter system crossing ( $k_{ISC}$ ) in ( $\text{sec}^{-1}$ ).

```
# -*- coding: utf-7 -*-
```

```
"""
```

```
Spyder Editor
```

```
This is a temporary script file.
```

```
"""
```

```
import numpy as np
```

```
import pandas as pd
```

```
import scipy.linalg as spl
```

```
from functools import reduce
```

```
def column_to_nxn_matrix(column_matrix, n):
```

```

if len(column_matrix) != n * n:

    print("Error: The column matrix size is incompatible with the desired n x n matrix size.")

    return None

matrix = np.array(column_matrix).reshape((n, n))

return matrix

a = [4]

open("integ-elements.txt","w")

for n in a:

    cm2au = 4.55634E-6

    sec2au = 4.134E+16

    ev2au = 0.0367498

    pi=3.141592654

    nvib = no. of vibrational modes

    deltaeab = energy difference between considered singlet and triplet

    deltaeab = deltaeab * ev2au

    socme = value of calculated socme*cm2au

    socmesq = socme*socme

    eta = 1.0*cm2au

    neg_num = 0.000000000020 # Upper limit of time integration in sec

    m1 = np.add(np.multiply(0.5,nvib),1.0)

    m2 = np.power(2.0,m1)

    kisc1 = np.multiply(m2,socmesq)

    fs = open("/path of the working directory/singlet-ir-text file")

    freqs = np.loadtxt(fs)

    freqs = np.array(freqs)

    freqs = freqs*cm2au

    freqs = np.diag(freqs)

    ft = open("/path of the working directory/triplet-ir-text file ")

```

```

freqt = np.loadtxt(ft)

freqt = np.array(freqt)

freqt = freqt*cm2au

freqt = np.diag(freqt)

j = open("/path of the working directory/duschinsky.dat")

j = np.loadtxt(j)

j = np.array(j)

j = column_to_nxn_matrix(j,nvib)

jdag = np.transpose(j)

d = open("/path of the working directory/displacement.dat")

d = np.loadtxt(d)

ddag = np.asmatrix(d)

d = np.transpose(ddag)

timeau = np.multiply(neg_num,sec2au) # upper limit of time is converted to au

delta = np.divide(timeau,n) # dt = 1E-15 sec = 826800 au

t = np.multiply(delta,-0.9999999) # to start lower limit of time integration in au near zero

integrand = 0.0

for ii in range(n):

    t = np.add(t,delta)

    damping = np.exp(-1.0*eta*eta*t*t)

    freqtt = freqt * t

    st = np.sin(freqtt)

    bt = np.tan(0.5*freqtt)

    sti = np.linalg.inv(st)

    bti = np.linalg.inv(bt)

    p1 = reduce(np.dot,[jdag,freqt,freqt,j])

    p2 = np.dot(freqs,freqs)

    p = np.add(p1,p2)

```

```

q1 = reduce(np.dot,[jdag,freqt,bt,j,freqs])
q2 = reduce(np.dot,[freqs,jdag,freqt,bti,j])
q = np.subtract(q1,q2)
iq = np.dot(1j,q)
piq = np.add(p,iq)
piqi = np.linalg.inv(piq)
c = piqi.real
e = piqi.imag
uprime = reduce(np.dot,[sti,freqs,freqt,e])
vprime = reduce(np.dot,[-1.0,sti,freqs,freqt,c])
iv = np.dot(1j,vprime)
uiv = np.add(uprime,iv)
detuiv = np.linalg.det(uiv)
u = detuiv.real
v = detuiv.imag
asqrtu2v2 = np.power((u*u + v*v),0.25)
ibt = np.dot(1j,bt)
x1 = reduce(np.dot,[jdag,freqt,ibt,j])
x2 = np.add(x1,freqs)
y = np.linalg.inv(x2)
aprime = y.real
bprime = y.imag
f = reduce(np.dot,[ddag,freqt,bt,j,aprime,jdag,freqt,bt,d])
f = np.dot(-1.0,f)
trfs = np.trace(freqs)
k1 = f + trfs*0.5
ek1 = np.exp(k1)
h1 = reduce(np.dot,[ddag,freqt,bt,j,bprime,jdag,freqt,bt,d])

```

```
h1dash = np.multiply(-1.0,h1)
h2 = reduce(np.dot,[ddag,freqt,bt,d])
h = np.subtract(h1dash,h2)
k2 = h + t*deltaeab
z = np.cos(0.5*np.arctan(v/u) + k2)
integrand = integrand + asqrtu2v2*ek1*z*damping
print("rate of intersystem crossing in sec-1")
kisc2 = (kisc1 * integrand * delta* 4.134*1.0E+16)
print(kisc2)
```

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Fig SF1: Experimentally Studied Phosphahelicene (Yavari et al. *Chem. Eur. J.* **2019**, *25*, 5303-5310)

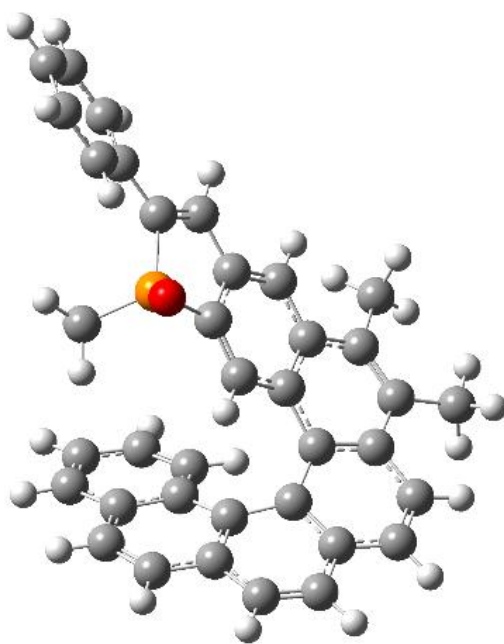


Fig SF2: Vibronic spectra of each excited state and convoluted for all states.

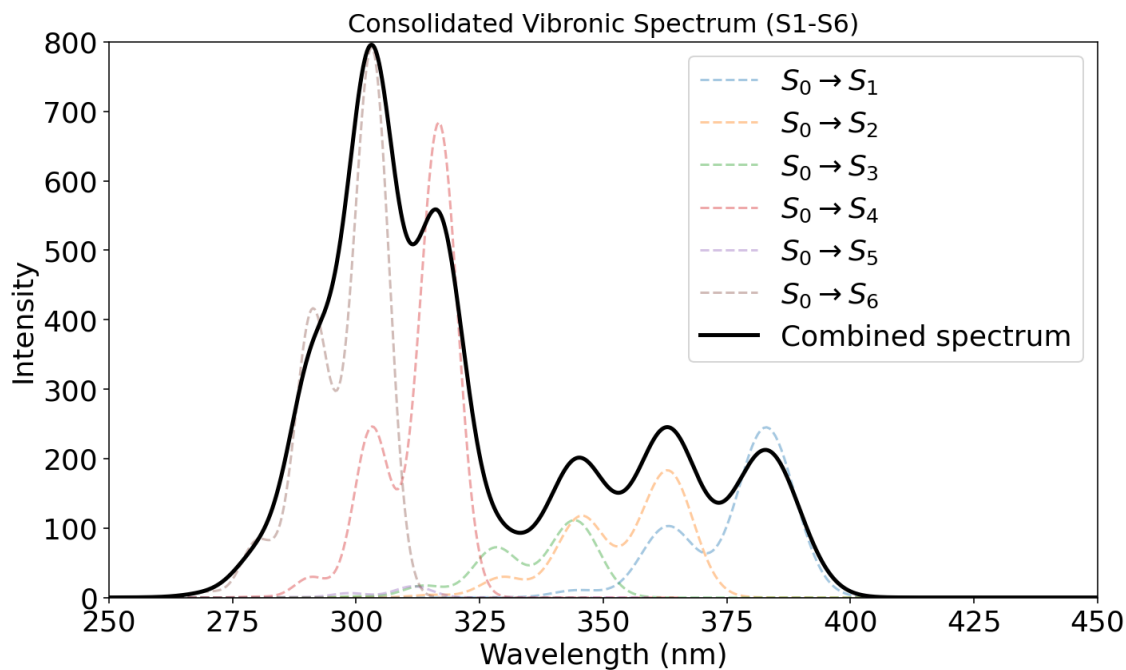
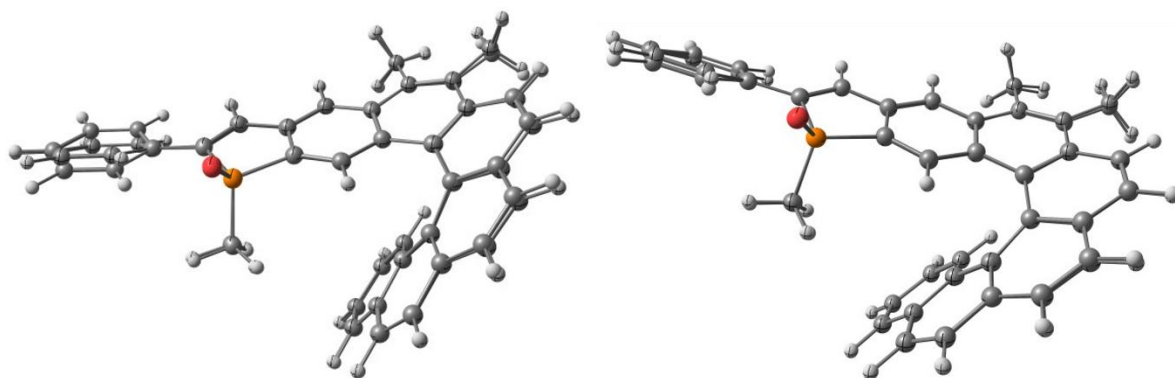


Fig SF3: Merged structure and RMSD value between  $S_0$ - $S_1$  and  $S_0$ - $S_2$  geometries of experimentally studied system considered for benchmarked.



RMSD of  $S_0$ - $S_1$  = 0.22

RMSD of  $S_0$ - $S_2$  = 0.09

ST8: Optimized Cartesian coordinates of experimentally studied P1'  $S_0$  geometry (B3LYP/6-311+G(d,p)) in DCM solvent considered for benchmark

C	-2.61671300	-4.04491900	-0.56140800	H	-4.76760500	4.32873400	0.71696300
C	-3.19439500	-2.76768000	-0.84940200	O	2.58471600	-1.15924500	-2.30582200
C	-2.78133800	-1.61608500	-0.12953600	C	3.72349800	0.55388800	-0.29510000

C	-2.02666800	-1.83340100	1.09903900	C	5.18064400	0.37265300	-0.34696700
C	-1.47900300	-3.12637900	1.36454400	H	3.54125300	-2.61604000	0.17384100
C	-1.74717600	-4.20908000	0.47044000	H	-0.61225100	-0.77868300	-0.97751200
C	-3.24309900	-0.32098000	-0.59706600	H	1.09610700	3.48948700	0.88773700
C	-4.42108800	-0.30089800	-1.39593300	H	-6.04925500	0.90909200	-2.14289000
C	-4.88746400	-1.49559200	-2.01491300	H	-5.28752700	2.96872200	-1.07192100
C	-4.22834000	-2.67331400	-1.82523900	H	-5.75346100	-1.43975600	-2.66537300
C	-5.12712000	0.92032200	-1.57195200	H	-4.53144500	-3.57171200	-2.35147400
C	-4.68550700	2.07472400	-0.99341600	H	-2.36969900	0.10815200	1.99216600
C	-3.39884500	2.13708000	-0.37874700	H	-1.13782300	-0.33709100	4.04248700
C	-2.61280500	0.95804700	-0.32369600	H	-0.03419100	-2.54395100	4.40574600
C	-1.18874600	1.13058300	-0.13114400	H	-0.31641800	-4.33443500	2.71918700
C	-0.69378900	2.37852600	0.35392900	H	-1.30158700	-5.17712500	0.67231200
C	-1.59938800	3.47729700	0.60551200	H	-2.89758700	-4.88600400	-1.18615200
C	-2.89695900	3.38802100	0.15123700	H	-3.40772100	5.44547400	0.63771600
C	0.70773300	2.55129300	0.51437400	H	-4.13404800	4.84961300	-0.84035600
C	1.59241800	1.55959400	0.14813800	H	-1.83971300	5.33021100	1.71205700
C	1.09493300	0.34667800	-0.39336800	C	6.02506700	1.01643200	0.57667400
C	-0.25194900	0.13638200	-0.52863200	C	7.40526100	0.85737500	0.51214400
C	-0.73989700	-3.34962800	2.55152100	C	7.97577600	0.04530000	-0.47024800
C	-0.59068400	-2.35688800	3.49442200	C	7.15114100	-0.60710700	-1.38584300
C	-1.20195300	-1.10663400	3.28143100	C	5.76845700	-0.44845500	-1.32604800
C	-1.89477200	-0.85421300	2.11523000	H	5.59513100	1.62991300	1.35998200
P	2.50316800	-0.70696100	-0.86529300	H	8.03731700	1.35927800	1.23623500
C	2.59303800	-2.09289100	0.31269400	H	9.05139300	-0.08099300	-0.51650800
H	2.51898100	-1.73261400	1.33997200	H	7.58427700	-1.23949800	-2.15267000
C	3.05436200	1.62610500	0.18971800	H	5.13761300	-0.94705000	-2.05280700
H	3.54962000	2.51344200	0.57146600	H	1.77075900	-2.78109600	0.10814100
C	-1.05241700	4.71335400	1.28562100	H	-0.38404600	4.44090400	2.10493400
H	-0.47890100	5.34119900	0.59423700				
C	-3.84628100	4.56552800	0.17672700				

ST9: Benchmarking the methodology for experimentally available absorption data.

i) OPA data of experimentally studied\* HeIP system considered for benchmark.

Wavelength (in nm)	276	292	323	345	375	392
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\* Yavari et al. *Chem. Eur. J.* **2019**, *25*, 5303-5310

ii) OPA data of computationally designed HeIP systems considered for benchmark.

B3LYP/cc-pVDZ			B3LYP/aug-cc-pVDZ			B3LYP/cc-pVTZ		
Ex. State	wavelength	osc.str.	Ex. State	wavelength	osc.str.	Ex. State	wavelength	osc.str.
1	412.97	0.3138	1	420.46	0.339	1	419.61	0.336
2	403.42	0.1269	2	408.74	0.1048	2	408.14	0.1029
3	364.23	0.2198	3	370.01	0.2052	3	369.24	0.2036
4	359.66	0.1384	4	366	0.124	4	365.15	0.1313
5	355.81	0.135	5	360.47	0.155	5	360.04	0.147
6	343.13	0.1185	6	348.33	0.1287	6	347.62	0.1238
7	334.36	0.1641						

8	325.14	0.047	7	338.72	0.15	7	337.83	0.1524
9	322.62	0.0972	8	329.24	0.0388	8	328.6	0.0374
10	311.55	0.0704	9	327.27	0.0916	9	326.25	0.0956
			10	318.12	0.0938	10	316.48	0.0848

Cam-B3LYP/cc-pVDZ			Cam-B3LYP/aug-cc-pVDZ			Cam-B3LYP/cc-pVTZ		
Ex. State	wavelength	osc.str.	Ex. State	wavelength	osc.str.	Ex. State	wavelength	osc.str.
1	360.56	0.2551	1	366.58	0.3119	1	365.98	0.3127
2	351.18	0.3154	2	355.92	0.2664	2	355.58	0.2565
3	323.97	0.2786	3	329.34	0.2511	3	328.74	0.2562
4	308.39	0.2107	4	313.46	0.2485	4	312.45	0.2474
5	304.58	0.1465	5	309.63	0.0791	5	309.03	0.0713
6	291.64	0.5392	6	297.31	0.5356	6	296.33	0.5489
7	278.14	0.3416	7	283.8	0.3565	7	282.48	0.3431
8	271.52	0.0266	8	275.76	0.0452	8	274.7	0.0374
9	265.59	0.2115	9	269.31	0.2699	9	268.41	0.2599
10	259.27	0.1593	10	264.99	0.1615	10	263.54	0.1668

M062X/cc-pVDZ			M062X/aug-cc-pVDZ			M062X/cc-pVTZ		
Ex. State	wavelength	osc.str.	Ex. State	wavelength	osc.str.	Ex. State	wavelength	osc.str.
1	361.17	0.2539	1	367.06	0.3112	1	366.11	0.3323
2	350.66	0.3764	2	355.71	0.3166	2	355.04	0.2855
3	322.87	0.2181	3	328.12	0.1981	3	327.61	0.2138
4	309.24	0.2686	4	314.49	0.2917	4	313.06	0.2964
5	304.6	0.085	5	309.94	0.0347	5	309.02	0.0204
6	293.79	0.5441	6	299.29	0.5421	6	298.03	0.5517
7	277.33	0.2836	7	283.23	0.2512	7	281.69	0.2557
8	275.92	0.0352	8	280.15	0.0965	8	278.55	0.0788
9	267.48	0.2601	9	271.27	0.323	9	269.73	0.3265
10	262.25	0.1142	10	268.15	0.1039	10	266.05	0.1237

WB97XD/cc-pVDZ			WB97XD/aug-cc-pVDZ			WB97XD/cc-pVTZ		
Ex. State	wavelength	osc.str.	Ex. State	wavelength	osc.str.	Ex. State	wavelength	osc.str.

1	356.73	0.1889	1	361.66	0.2385	1	361.16	0.2386
2	346.41	0.3875	2	350.68	0.3475	2	350.31	0.3386
3	321.11	0.2768	3	325.69	0.2487	3	325.21	0.2503
4	305.94	0.2076	4	310.31	0.2385	4	309.45	0.2387
5	301.5	0.1678	5	305.71	0.1127	5	305.23	0.1036
6	287.05	0.5631	6	292.1	0.5458	6	291.12	0.5661
7	276.27	0.3901	7	281.06	0.4244	7	280	0.4086
8	265.48	0.112	8	268.71	0.1275	8	267.79	0.1185
9	259.46	0.2127	9	262.59	0.2774	9	261.79	0.2772
10	255.34	0.1132	10	258.94	0.2236	10	257.75	0.2087

LCWPBE/cc-pVDZ			LCWPBE/aug-cc-pVDZ			LCWPBE/aug-cc-pVTZ		
Ex. State	wavelength	osc.str.	Ex. State	wavelength	osc.str.	Ex. State	wavelength	osc.str.
1	336.65	0.1176	1	341.15	0.1423	1	340.85	0.1542
2	324.77	0.4201	2	328.95	0.4039	2	329.27	0.3791
3	301.66	0.3099	3	306.04	0.2819	3	305.95	0.2916
4	288.61	0.2279	4	292.76	0.2399	4	292.21	0.245
5	282.59	0.2589	5	286.39	0.2261	5	286.36	0.2055
6	263.42	0.4384	6	268.55	0.3774	6	267.88	0.4094
7	260.31	0.8528	7	264.59	0.9102	7	263.92	0.8951
8	248.61	0.0571	8	251.92	0.0587	8	251.24	0.052
9	239.91	0.5516	9	242.88	0.717	9	242.3	0.741
10	236.5	0.0343	10	240.53	0.0718	10	239.2	0.0414

ST10: Nearest low lying triplet state optimized for all considered systems in vacuum and four solvent.

System	CCl <sub>4</sub>	DCM	DMSO	n-hexane	Vacuum
C1234	3	3	3	3	3
1C234	7	6	6	7	7
12C34	4	4	4	4	4
P1234	3	3	3	3	3
1P234	7	7	7	7	7
12P34	5	5	4	5	5
1-A-13-D-P1234	4	4	4	4	4
3-A-12-D-P1234	3	3	3	3	4
1-A-11-D-P1234	3	3	3	3	3
3-A-10-D-P1234	3	3	3	3	3

1-D-13-A-1P234	4	4	4	4	5
3-D-12-A-1P234	3	3	3	3	3
2-D-10-A-12P34	3	3	3	3	3
2-D-12-A-12P34	2	2	2	3	3