

C	0.065195	-0.001050	1.110130
C	-0.646846	-1.277167	0.590028
H	-1.859700	-1.095204	-1.223206
H	-0.462586	-2.135775	-1.410326
H	-1.619857	-1.382345	1.073319
H	-0.056352	-2.154206	0.874182
C	-0.620776	1.302034	-0.959246
H	-0.010077	2.157874	-1.264899
H	-1.616934	1.469372	-1.382012
C	-0.713506	1.236364	0.592156
H	-0.301266	2.146254	1.039459
H	-1.752983	1.170867	0.920477
C	1.495680	0.037389	0.539733
H	1.972531	0.977071	0.831456
H	2.094621	-0.756197	0.991440
C	1.453115	-0.107123	-1.007497
H	2.080203	0.661596	-1.470787
H	1.877644	-1.070305	-1.309605
C	0.102952	0.000046	2.627093
O	-1.142342	0.000805	3.173881
O	1.093555	0.002327	3.316727
Si	-0.050545	0.002352	-3.425572
H	0.669110	1.190105	-3.960644
H	0.596165	-1.224709	-3.964795
H	-1.456905	0.045781	-3.911254
H	-1.033770	0.002883	4.137768

4-silylbicyclo[2.2.2]octylcarboxylate,

B3LYP/6-311G* = -792.14490, Zpe = 138.63

-1 1

C	-0.881639	-1.148248	-0.934736
C	-0.000649	0.000034	-1.493034
C	0.035053	-0.008670	1.162239
C	-0.745531	-1.222156	0.615121
H	-1.926419	-0.974452	-1.222711
H	-0.593441	-2.103201	-1.393148
H	-1.723239	-1.249598	1.099919
H	-0.223490	-2.141207	0.907126
C	-0.548702	1.337743	-0.931264
H	0.110555	2.157835	-1.242893
H	-1.532915	1.554364	-1.366987
C	-0.643460	1.269293	0.622574
H	-0.167749	2.148438	1.070848
H	-1.682857	1.274569	0.958538
C	1.465493	-0.063178	0.599137
H	2.004334	0.836948	0.907375
H	2.002157	-0.897186	1.056933
C	1.442146	-0.194039	-0.954129
H	2.117074	0.540718	-1.412528
H	1.811931	-1.179992	-1.264128
C	-0.009672	-0.000911	2.742404
O	-1.165772	0.005687	3.231244
O	1.095293	0.006765	3.333256
Si	-0.017520	0.006388	-3.382809
H	0.777632	1.140150	-3.943882
H	0.558625	-1.250267	-3.949409
H	-1.401319	0.134618	-3.931595

Table S11. Calculated structures for Bicyclo[1.1.1]carboxylic acids

Bicyclo[1.1.1]pentanecarboxylic acid, B3LYP/6-311+G* = -383.92990

0 1

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.878344
C	1.246745	0.000000	0.933391
C	-0.607113	1.088938	0.933391
H	1.856260	-0.906791	0.945980
H	-1.695936	1.179734	0.945980
H	1.861355	0.902160	0.942710
H	-0.118434	2.065068	0.942710
C	-0.627544	-1.068359	0.946001
H	-1.717094	-1.141142	0.957667
H	-0.160548	-2.055442	0.957667
C	-0.005850	-0.009959	3.371529
H	-0.002933	-0.004993	-1.090384
O	-0.504574	-0.859010	4.068972
O	0.630845	1.073979	3.883844
H	0.591825	1.007550	4.851229

Bicyclo[1.1.1]pentanecarboxylate, B3LYP/6-311+G* = -393.37910

-1 1

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.897613
C	1.239348	0.000000	0.935851
C	-0.606937	1.080560	0.935851
H	1.853002	-0.908144	0.944782
H	-1.699248	1.170853	0.944782

H	1.858252	0.901558	0.953459
H	-0.123979	2.061683	0.953459
C	-0.624914	-1.067751	0.941609
H	-1.716666	-1.145786	0.954183
H	-0.158296	-2.057841	0.954183
C	0.022284	0.038076	3.437523
H	-0.000616	-0.001053	-1.098060
O	-0.539659	-0.922081	4.017753
O	0.606472	1.036240	3.926166

3-cf3bicyclo[1.1.1]acid, B3LYP/6-311+G* = 721.08671

O 1			
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.865713
C	1.250799	0.000000	0.941469
H	1.859717	-0.904288	0.940995
H	1.854961	0.908408	0.938575
C	-0.629432	1.072746	0.928224
C	-0.610039	-1.091922	0.941408
H	-1.697747	-1.176273	0.938521
H	-0.117628	-2.064584	0.940965
H	-1.717789	1.140595	0.925873
H	-0.157742	2.055904	0.925896
C	-0.008211	0.014324	-1.493503
C	-0.005425	0.008965	3.363931
O	0.625279	-1.068001	-2.005744
H	0.588409	-1.004562	-2.973591
O	-0.508451	0.869350	-2.180226
F	0.629144	-1.072151	3.874883

F	0.613671	1.105516	3.859597
F	-1.264742	0.002865	3.859354

cf3bicyco[1.1.1]pentanecarboxylate, B3LYP/6-311+G* = -720.54976

-1 1

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.883617
C	1.242806	0.000000	0.951488
H	1.854956	-0.903707	0.946248
H	1.853858	0.905908	0.949172
C	-0.633385	1.070204	0.954574
C	-0.622605	-1.078107	0.957960
H	-1.712080	-1.152549	0.953077
H	-0.141058	-2.059407	0.958102
H	-1.722575	1.135796	0.947163
H	-0.162112	2.056910	0.955193
C	-0.033455	-0.020737	-1.540159
C	0.002993	0.004553	3.377040
O	1.052913	-0.300526	-2.097549
O	-1.156374	0.231162	-2.037209
F	0.635115	-1.080193	3.906525
F	0.629481	1.097214	3.897094
F	-1.252582	0.002947	3.906794

3-chobicyclo[1.1.1]acid, B3LYP/6-311+G* = -497.28274

0 1

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.876590

C	1.244229	0.000000	0.946902
H	1.856898	-0.901791	0.948182
H	1.851844	0.906227	0.944925
C	-0.643050	1.068409	0.919961
C	-0.622234	-1.087546	0.935214
H	-1.711114	-1.167702	0.920344
H	-0.136134	-2.064306	0.939544
H	-1.732470	1.130278	0.907731
H	-0.178578	2.055783	0.922406
C	-0.018043	0.005524	-1.494008
C	-0.036315	0.016011	3.365695
O	0.741422	-0.991803	-2.008049
H	0.680337	-0.943065	-2.975512
O	-0.630981	0.783703	-2.181901
H	-1.054257	-0.000971	3.814104
O	0.942061	0.048458	4.072723

3-Formylbicyclo[1.1.1]pentanecarboxylate, B3LYP/6-311+G*=-496.74343

-1 1

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.896155
C	1.246830	0.000000	0.944016
H	1.856337	-0.906018	0.945670
H	1.862170	0.904839	0.932789
C	-0.610779	1.086983	0.944037
C	-0.625195	-1.068324	0.966571
H	-1.715646	-1.140001	0.966021
H	-0.153703	-2.054194	0.966052
H	-1.699218	1.174569	0.945677

H	-0.123359	2.066674	0.932798
C	-0.017706	-0.030091	-1.537602
C	0.045372	0.077540	3.371940
O	0.953311	-0.620421	-2.067003
O	-1.009875	0.524254	-2.066698
O	-0.422132	-0.721452	4.158493
H	0.574025	0.981045	3.762379

3-chlorobicyclo[1.1.1]acid B3LYP/6-311+G* = -843.56166

O 1			
C	-0.118003	-1.183896	0.000000
C	0.000000	0.655667	0.000000
C	0.573366	-0.321735	1.082212
C	0.573366	-0.321735	-1.082212
H	0.094193	-0.289473	2.061624
H	0.094193	-0.289473	-2.061624
H	1.659088	-0.392477	1.147489
H	1.659088	-0.392477	-1.147489
C	-1.303677	-0.186977	0.000000
H	-1.909366	-0.146956	-0.905682
H	-1.909366	-0.146956	0.905682
C	0.087537	2.145370	0.000000
Cl	-0.242814	-2.962241	0.000000
O	-0.850626	2.902133	0.000000
O	1.375105	2.567568	0.000000
H	1.368631	3.538127	0.000000

3-chlorobicyclo[1.1.1]ate, B3LYP/6-311+G* = 843.02518

-1 1

C	-0.048330	-1.112488	0.000000
C	0.000000	0.718123	0.000000
C	0.607474	-0.246699	1.080742
C	0.607474	-0.246699	-1.080742
H	0.126790	-0.236091	2.061474
H	0.126790	-0.236091	-2.061474
H	1.695911	-0.267326	1.144879
H	1.695911	-0.267326	-1.144879
C	-1.273724	-0.189488	0.000000
H	-1.880652	-0.170059	-0.906594
H	-1.880652	-0.170059	0.906594
C	0.089596	2.274913	0.000000
Cl	-0.105563	-2.972463	0.000000
O	-1.007654	2.871636	0.000000
O	1.259595	2.714972	0.000000

fluorobicyclo[1.1.1]acid, B3LYP/6-311+G* = -483.20690

0 1

C	-0.349668	-1.547006	0.000000
C	0.000000	0.252658	0.000000
C	0.445028	-0.790653	1.084128
C	0.445028	-0.790653	-1.084128
H	-0.024369	-0.689953	2.063998
H	-0.024369	-0.689953	-2.063998
H	1.514392	-0.992912	1.149258
H	1.514392	-0.992912	-1.149258
C	-1.402545	-0.418160	0.000000
H	-1.996960	-0.293776	-0.905890

H	-1.996960	-0.293776	0.905890
C	0.274360	1.716013	0.000000
F	-0.616289	-2.888042	0.000000
O	-0.559575	2.586468	0.000000
O	1.605459	1.973010	0.000000
H	1.720189	2.936641	0.000000

fluorobc[1.1.1]ate, B3LYP/6-311+G* = - 482.66668

-1 1

C	-0.127345	-1.526373	0.000000
C	0.000000	0.306874	0.000000
C	0.564060	-0.687899	1.079917
C	0.564060	-0.687899	-1.079917
H	0.086084	-0.648380	2.062446
H	0.086084	-0.648380	-2.062446
H	1.651819	-0.749057	1.145864
H	1.651819	-0.749057	-1.145864
C	-1.310683	-0.551826	0.000000
H	-1.917639	-0.497375	-0.906372
H	-1.917639	-0.497375	0.906372
C	0.151780	1.848846	0.000000
F	-0.228336	-2.929145	0.000000
O	-0.918662	2.496079	0.000000
O	1.339070	2.246620	0.000000

3-Aminobicyclo[1.1.1]pentanecarboxylic acid, B3LYP/6-311+G*
= -439.30081

0 1

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.877012
C	1.246010	0.000000	0.929215
C	-0.606680	1.085289	0.932680
H	1.855503	-0.907546	0.944430
H	-1.696530	1.174021	0.946912
H	1.856638	0.904534	0.927341
H	-0.117484	2.060661	0.929879
C	-0.627136	-1.079326	0.966059
H	-1.717311	-1.154512	0.984230
H	-0.154166	-2.063911	0.983273
C	0.024702	-0.007791	3.366821
N	0.044129	0.079435	-1.425916
O	-0.305367	-0.928592	4.073718
O	0.486125	1.166102	3.868823
H	-0.886165	0.139801	-1.827520
H	0.509033	-0.725915	-1.832985
H	0.492016	1.088475	4.836105

3-Aminobicyclo[1.1.1]pentanecarboxylate B3LYP/6-311++G**
= -438.75056

-1 1

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.888428
C	1.239539	0.000000	0.926346
C	-0.604781	1.081334	0.927397
H	1.852483	-0.909063	0.936248
H	-1.697437	1.173508	0.937197
H	1.853675	0.903993	0.931468

H	-0.115934	2.058500	0.933543
C	-0.627474	-1.072424	0.948566
H	-1.720040	-1.147419	0.965078
H	-0.159650	-2.062433	0.965936
C	0.030200	0.035569	3.430354
N	0.036798	0.064372	-1.450077
O	-0.479593	-0.953106	4.009377
O	0.570217	1.057964	3.917352
H	-0.911116	0.066357	-1.819693
H	0.493790	-0.765420	-1.821315

3-hydroxybicyclo[1.1.1]pentanecarboxylic acid, B3LYP/6-311+G*
 = -459.17424

O 1

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.858838
C	1.256986	0.000000	0.926072
C	-0.607950	1.086717	0.911068
H	1.864406	-0.908499	0.947572
H	-1.696578	1.170720	0.913449
H	1.865562	0.905459	0.932572
H	-0.117339	2.060887	0.911444
C	-0.626919	-1.078451	0.939648
H	-1.716124	-1.149883	0.948629
H	-0.152809	-2.062510	0.959439
C	0.012099	-0.012253	3.347397
O	-0.048631	0.072050	-1.383386
O	-0.351016	-0.925451	4.047315
O	0.501795	1.146962	3.854632

H	0.494489	1.070160	4.821946
H	0.311416	-0.736871	-1.768378

3-hydroxybicyclo[1.1.1]pentanecarboxylate, B3LYP/6-311+G*
= 458.62791

-1 1

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.867192
C	1.248119	0.000000	0.918459
C	-0.625852	1.068469	0.909451
H	1.860016	-0.906537	0.943701
H	-1.716579	1.139997	0.914471
H	1.857981	0.908730	0.922915
H	-0.154514	2.054703	0.914414
C	-0.610648	-1.088609	0.918502
H	-1.701566	-1.175875	0.923061
H	-0.119326	-2.065785	0.943668
C	0.023560	-0.040458	3.411259
O	-0.035425	0.060495	-1.413787
O	0.611316	-1.038678	3.891893
O	-0.540100	0.916183	3.990256
H	0.421145	-0.719052	-1.754394

3-Mercaptobicyclo[1.1.1]pentanecarboxylic acid, B3LYP/6-311+G*
= -782.14610

0 1

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.867964

C	1.252011	0.000000	0.929784
C	-0.607049	1.090077	0.929445
H	1.857737	-0.908627	0.937576
H	-1.695295	1.176687	0.931681
H	1.862155	0.904076	0.929840
H	-0.115651	2.063764	0.930278
C	-0.629843	-1.072242	0.943858
H	-1.718776	-1.140155	0.945209
H	-0.159616	-2.057154	0.949198
C	0.019661	-0.023337	3.360790
S	-0.068735	0.088366	-1.804472
O	-0.283469	-0.964411	4.051368
O	0.441915	1.158384	3.874673
H	0.447924	1.074577	4.841574
H	0.492123	-1.121614	-2.032750

3-Mercaptobicyclo[1.1.1]pentanecarboxylate, B3LYP/6-311+G*

= -781.60426

-1 1

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.871813
C	1.246419	0.000000	0.919717
C	-0.609894	1.085466	0.921813
H	1.855039	-0.908848	0.924788
H	-1.700053	1.173356	0.924421
H	1.858075	0.905399	0.920907
H	-0.120959	2.061675	0.928609
C	-0.624738	-1.074251	0.926161
H	-1.715427	-1.148561	0.925831

H	-0.150689	-2.058812	0.934487
C	0.048386	0.002350	3.420903
S	-0.066736	0.075610	-1.838608
O	-0.080907	-1.122596	3.956017
O	0.228128	1.128400	3.937677
H	0.534051	-1.116997	-2.064563

3-Methylbicyclo[1.1.1]pentanecarboxylic acid, B3LYP/6-311+G*
= -423.25901

O 1			
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.887066
C	1.244763	0.000000	0.945142
C	-0.607408	1.086504	0.945142
H	1.854890	-0.907196	0.957083
H	-1.696987	1.176374	0.957083
H	1.860350	0.902303	0.954342
H	-0.120213	2.064123	0.954342
C	-0.626245	-1.067565	0.957820
H	-1.716400	-1.141375	0.968806
H	-0.158707	-2.055135	0.968806
C	-0.005148	-0.008777	3.378861
O	-0.502738	-0.857021	4.078527
O	0.631161	1.075944	3.891339
H	0.591504	1.008342	4.858572
C	-0.004554	-0.007763	-1.504722
H	0.497833	-0.898352	-1.895865
H	-1.027064	-0.003831	-1.895865
H	0.510522	0.870292	-1.907361

Mebicyclo[1.1.1]pentanecarboxylate, B3LYP/6-311+G* = -422.70735

-1 1

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.903886
C	1.237753	0.000000	0.944544
C	-0.605528	1.079522	0.944544
H	1.853512	-0.907272	0.951711
H	-1.698056	1.172713	0.951711
H	1.855171	0.903414	0.959492
H	-0.119654	2.059976	0.959492
C	-0.624126	-1.065693	0.949424
H	-1.716494	-1.143691	0.961546
H	-0.157749	-2.056574	0.961546
C	0.020285	0.034637	3.443645
O	-0.542552	-0.926406	4.021155
O	0.604181	1.031638	3.935426
C	-0.001496	-0.002554	-1.511725
H	0.503291	-0.892120	-1.908955
H	-1.024292	0.002512	-1.908955
H	0.514393	0.878324	-1.913706

3-cyanobicyclo[1.1.1]acid, B3LYP/6-311+G* = -476.19822

0 1

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.878357
C	1.248961	0.000000	0.939150
H	1.858959	-0.903440	0.944087

H	1.853912	0.907980	0.941059
C	-0.631298	1.071121	0.927282
C	-0.610909	-1.090835	0.941212
H	-1.698652	-1.174634	0.942817
H	-0.119529	-2.064049	0.945671
H	-1.719579	1.138172	0.930254
H	-0.161031	2.055052	0.929447
C	-0.017519	0.007209	-1.493263
C	-0.002940	0.008388	3.319098
N	-0.004094	0.014117	4.473607
O	0.708444	-1.015501	-2.004405
H	0.654658	-0.966034	-2.972306
O	-0.600973	0.808221	-2.179173

3-Cyanobicyclo[1.1.1]pentanecarboxylate, B3LYP/6-311+G*
= -475.66503

-1 1

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.896353
C	1.243269	0.000000	0.954509
H	1.853822	-0.904804	0.953556
H	1.853056	0.907688	0.961454
C	-0.628384	1.070873	0.949275
C	-0.607798	-1.084846	0.954900
H	-1.697726	-1.172656	0.961799
H	-0.116748	-2.059852	0.954418
H	-1.718246	1.142155	0.951937
H	-0.158025	2.056670	0.952131
C	0.015800	-0.031115	-1.538491

C	-0.002035	0.004039	3.340421
N	-0.003770	0.007437	4.498069
O	0.623179	-1.012983	-2.026927
O	-0.575561	0.917634	-2.103113

3-Nitrobicyclo[1.1.1]pentanecarboxylic acid, B3LYP/6-311+G* =
-588.49626

O 1

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.838085
C	1.254212	0.000000	0.890181
H	1.856776	-0.907714	0.890392
H	1.859656	0.905790	0.886533
C	-0.625705	1.088783	0.898442
H	-1.712833	1.159072	0.896592
H	-0.138932	2.063878	0.893082
C	-0.631740	-1.081353	0.915935
H	-1.719229	-1.145842	0.912929
H	-0.152828	-2.060457	0.913335
C	0.009688	-0.015059	3.330346
N	-0.027964	-0.019503	-1.490212
O	-0.409063	-0.910263	4.019108
O	0.560210	1.114510	3.832923
H	0.547562	1.048939	4.801285
O	1.019083	-0.266888	-2.069526
O	-1.106487	0.200621	-2.021654

3-nitrobicyclo[1.1.1]ate, B3LYP/6-311+G* = -587.96653

-1 1

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.848673
C	1.251702	0.000000	0.946444
H	1.855068	-0.908733	0.945054
H	1.858635	0.906722	0.951140
C	-0.624171	1.085431	0.945072
C	-0.623633	-1.080876	0.961975
H	-1.712371	-1.153187	0.962798
H	-0.139336	-2.058662	0.961520
H	-1.712536	1.156908	0.943564
H	-0.139723	2.062989	0.949917
C	-0.024541	-0.043000	-1.544295
N	0.016286	0.026943	3.349222
O	0.883225	-0.732605	-2.059658
O	-0.959659	0.598426	-2.072458
O	0.640002	0.934073	3.892618
O	-0.594872	-0.849684	3.952468

3-Silylbicyclo[1.1.1]pentanecarboxylic acid, B3LYP/6-311+G*
= -674.64699

0 1

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.897748
C	1.244584	0.000000	0.934106
H	1.860437	-0.901186	0.928270
H	1.853849	0.907043	0.924934
C	-0.630797	1.067458	0.924899
C	-0.609121	-1.086626	0.939570

H	-1.697997	-1.175204	0.929609
H	-0.122529	-2.063982	0.931868
H	-1.720061	1.138701	0.917039
H	-0.165050	2.055404	0.915301
C	-0.038139	-0.009164	-1.496541
Si	0.003112	0.011434	3.777982
O	0.761474	-0.974959	-2.014932
O	-0.699573	0.727428	-2.185659
H	0.674043	-1.210211	4.297256
H	0.731092	1.206766	4.280976
H	-1.391005	0.046730	4.294426
H	0.677442	-0.940557	-2.981260

3-Silylbicyco[1.1.1]pentanecarboxylate, B3LYP/6-311+G*
= -694.10141

-1 1

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.914676
C	1.238029	0.000000	0.948884
H	1.856441	-0.901434	0.938654
H	1.854708	0.904358	0.941604
C	-0.631595	1.065724	0.951423
C	-0.619661	-1.074394	0.954575
H	-1.710445	-1.155705	0.945044
H	-0.142063	-2.059676	0.949536
H	-1.722024	1.137241	0.938860
H	-0.165412	2.056964	0.946596
C	-0.030669	-0.020475	-1.541284
Si	0.005761	0.005217	3.784664

O	1.047569	-0.334706	-2.098968
O	-1.143477	0.264920	-2.045821
H	0.705182	-1.187811	4.351807
H	0.694437	1.209231	4.341609
H	-1.375233	0.000928	4.356722