

Supplementary Material to Article

On the efficiency of the DFT-based computational protocol for ^1H and ^{13}C NMR chemical shifts of natural products: studying the accuracy of the pecS- n ($n = 1, 2$) basis sets

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The pecS-1 basis set for carbon atom with newly optimized contraction coefficients of the *p*-shell (Dalton format)

\$ C

a 6

\$ s functions

7 4 0

1.158704E+03	6.1043E-03	1.0143E-03	0.00000000	0.00000000
1.744210E+02	4.4530E-02	8.1051E-03	0.00000000	0.00000000
4.064338E+01	1.8738E-01	3.1628E-02	0.00000000	0.00000000
1.141525E+01	4.7151E-01	1.1437E-01	0.00000000	0.00000000
3.439092E+00	4.3067E-01	1.1469E-01	0.00000000	0.00000000
3.002996E-01	0.00000000	0.00000000	1.00000000	0.00000000
5.973462E-02	0.00000000	0.00000000	0.00000000	1.00000000

\$ p functions

5 4 0

3.880432E+01	3.8015E-03	0.00000000	0.00000000	0.00000000
6.201621E+00	4.3304E-02	0.00000000	0.00000000	0.00000000
1.332637E+00	0.00000000	1.00000000	0.00000000	0.00000000
3.106991E-01	0.00000000	0.00000000	1.00000000	0.00000000
8.352061E-02	0.00000000	0.00000000	0.00000000	1.00000000

\$ d functions

1 1 0

4.584126E-01	1.00000000
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The pecS-1 basis set for carbon atom with newly optimized contraction coefficients of the p -shell (Gaussian format)

```

C 0
S 5 1.00
1.158704E+03      6.1043E-03
1.744210E+02      4.4530E-02
4.064338E+01      1.8738E-01
1.141525E+01      4.7151E-01
3.439092E+00      4.3067E-01
S 5 1.00
1.158704E+03      1.0143E-03
1.744210E+02      8.1051E-03
4.064338E+01      3.1628E-02
1.141525E+01      1.1437E-01
3.439092E+00      1.1469E-01
S 1 1.00
3.002996E-01      0.1000E+01
S 1 1.00
5.973462E-02      0.1000E+01
P 2 1.00
3.880432E+01      3.8015E-03
6.201621E+00      4.3304E-02
P 1 1.00
1.332637E+00      0.1000E+01
P 1 1.00
3.106991E-01      0.1000E+01
P 1 1.00
8.352061E-02      0.1000E+01
D 1 1.00
4.584126E-01      0.1000E+01
****

```

The pecS-2 basis set for carbon atom with newly optimized contraction coefficients of the *p*-shell (Dalton format)

\$ C

a 6

\$ s functions

10 5 0

7.811885E+03	5.7075E-04	1.0361E-04	0.00000000	0.00000000	0.00000000
1.168486E+03	4.3473E-03	7.7592E-04	0.00000000	0.00000000	0.00000000
2.735860E+02	2.1213E-02	3.9293E-03	0.00000000	0.00000000	0.00000000
7.954210E+01	7.9825E-02	1.4569E-02	0.00000000	0.00000000	0.00000000
2.613539E+01	2.2806E-01	4.6979E-02	0.00000000	0.00000000	0.00000000
9.217097E+00	4.3136E-01	9.9114E-02	0.00000000	0.00000000	0.00000000
3.390089E+00	3.5137E-01	1.5321E-01	0.00000000	0.00000000	0.00000000
1.045814E+00	0.00000000	0.00000000	1.00000000	0.00000000	0.00000000
3.150044E-01	0.00000000	0.00000000	0.00000000	1.00000000	0.00000000
1.155406E-01	0.00000000	0.00000000	0.00000000	0.00000000	1.00000000

\$ p functions

7 5 0

1.844063E+02	2.5812E-04	0.00000000	0.00000000	0.00000000	0.00000000
3.098346E+01	3.5919E-03	0.00000000	0.00000000	0.00000000	0.00000000
7.830746E+00	2.4201E-02	0.00000000	0.00000000	0.00000000	0.00000000
2.308071E+00	0.00000000	1.00000000	0.00000000	0.00000000	0.00000000
7.525987E-01	0.00000000	0.00000000	1.00000000	0.00000000	0.00000000
2.530275E-01	0.00000000	0.00000000	0.00000000	1.00000000	0.00000000
8.574535E-02	0.00000000	0.00000000	0.00000000	0.00000000	1.00000000

\$ d functions

2 2 0

1.566238E+00	1.00000000	0.00000000
3.508371E-01	0.00000000	1.00000000

\$ f functions

1 1 0

1.148503E+00	1.00000000
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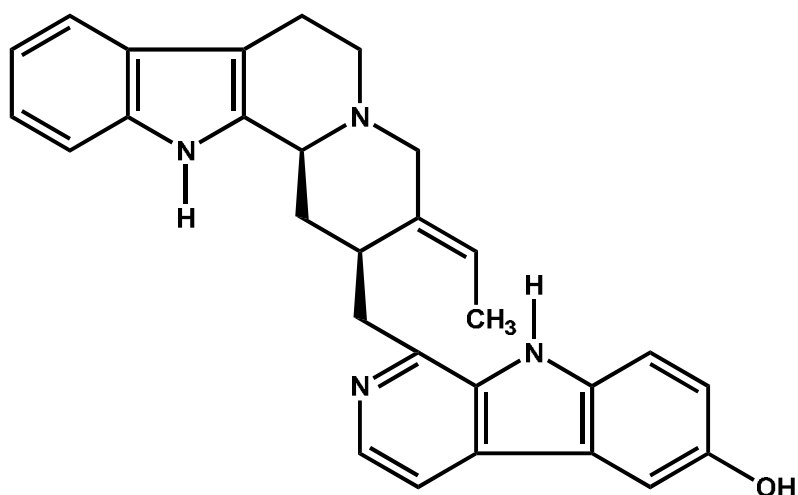
The pecS-2 basis set for carbon atom with newly optimized contraction coefficients of the p -shell (Gaussian format)

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C 0
S 7 1.00
7.811885E+03      5.7075E-04
1.168486E+03      4.3473E-03
2.735860E+02      2.1213E-02
7.954210E+01      7.9825E-02
2.613539E+01      2.2806E-01
9.217097E+00      4.3136E-01
3.390089E+00      3.5137E-01
S 7 1.00
7.811885E+03      1.0361E-04
1.168486E+03      7.7592E-04
2.735860E+02      3.9293E-03
7.954210E+01      1.4569E-02
2.613539E+01      4.6979E-02
9.217097E+00      9.9114E-02
3.390089E+00      1.5321E-01
S 1 1.00
1.045814E+00      0.1000E+01
S 1 1.00
3.150044E-01      0.1000E+01
S 1 1.00
1.155406E-01      0.1000E+01
P 3 1.00
1.844063E+02      2.5812E-04
3.098346E+01      3.5919E-03
7.830746E+00      2.4201E-02
P 1 1.00
2.308071E+00      0.1000E+01
P 1 1.00
7.525987E-01      0.1000E+01
P 1 1.00
2.530275E-01      0.1000E+01
P 1 1.00
8.574535E-02      0.1000E+01
D 1 1.00
1.566238E+00      0.1000E+01
D 1 1.00
3.508371E-01      0.1000E+01
F 1 1.00
1.148503E+00      0.1000E+01
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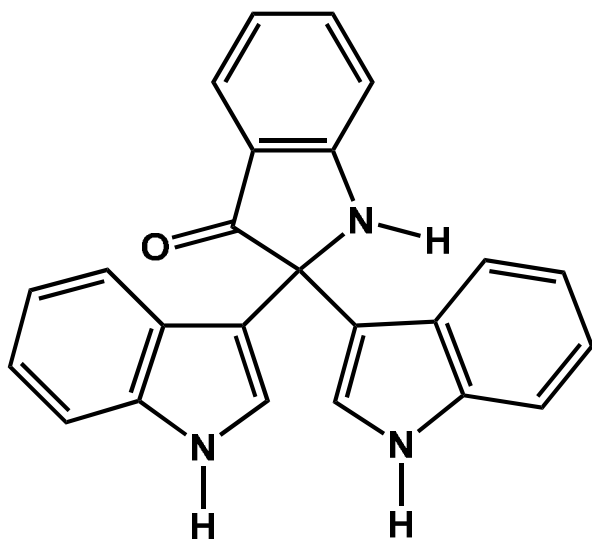
Equilibrium geometry of 10'-hydroxyusambarensine (1)



O	-6.394331	3.027550	0.537892
N	3.301681	-1.346042	0.086243
N	1.494289	1.775900	-0.740848
N	-2.058264	-2.998707	-1.752602
N	-2.427560	-0.724545	1.109050
C	2.227833	-0.657599	-0.630014
C	0.871484	-1.119192	-0.110473
C	0.708798	-2.636136	-0.266311
C	2.443630	0.813684	-0.486650
C	3.206613	-2.788501	-0.131247
C	4.617293	-0.834178	-0.291364
C	1.892856	-3.321182	0.379537
C	3.610171	1.397999	-0.100066
C	4.822825	0.588499	0.223173
C	-0.659313	-3.113844	0.225724
C	3.385501	2.814317	-0.102680
C	2.046188	3.013085	-0.513413
C	1.783415	-4.268274	1.308078
C	-1.786383	-2.498329	-0.554958
C	4.177324	3.929157	0.194415
C	-2.526690	-1.413465	-0.076400
C	1.488309	4.283766	-0.629902
C	2.878703	-5.003666	2.017410
C	-3.557534	-0.848762	-0.850733
C	3.627028	5.190819	0.079053
C	2.294451	5.365318	-0.329122
C	-4.106760	0.237831	-0.077812
C	-3.377722	0.276895	1.123561
C	-3.819119	-1.397720	-2.103348
C	-3.040339	-2.465816	-2.499184
C	-5.135337	1.155202	-0.308814
C	-3.658578	1.223335	2.107007
C	-5.409392	2.089335	0.668121
C	-4.675609	2.121401	1.865367
H	2.278733	-0.915783	-1.705107

H	0.079218	-0.608053	-0.659976
H	0.784221	-0.842591	0.943658
H	0.757882	-2.852632	-1.340524
H	3.294726	-3.018964	-1.207776
H	4.048147	-3.258338	0.367420
H	4.736178	-0.851792	-1.386466
H	5.370766	-1.497791	0.128891
H	5.001382	0.568023	1.300490
H	5.714138	1.016168	-0.238005
H	-0.764930	-2.894498	1.290278
H	-0.727170	-4.194633	0.109504
H	0.551093	1.608350	-1.044305
H	0.787190	-4.571906	1.607418
H	5.204377	3.802867	0.509866
H	0.462819	4.417758	-0.944170
H	3.874897	-4.674550	1.740167
H	2.772524	-4.885610	3.096135
H	2.808968	-6.072813	1.813542
H	4.227366	6.060546	0.305176
H	1.891666	6.364872	-0.409689
H	-1.775853	-0.912896	1.849813
H	-4.596315	-1.012706	-2.746903
H	-3.203940	-2.929417	-3.462797
H	-5.704604	1.135177	-1.229115
H	-3.100089	1.255387	3.030893
H	-4.928830	2.872321	2.599773
H	-6.838818	2.922974	-0.307951

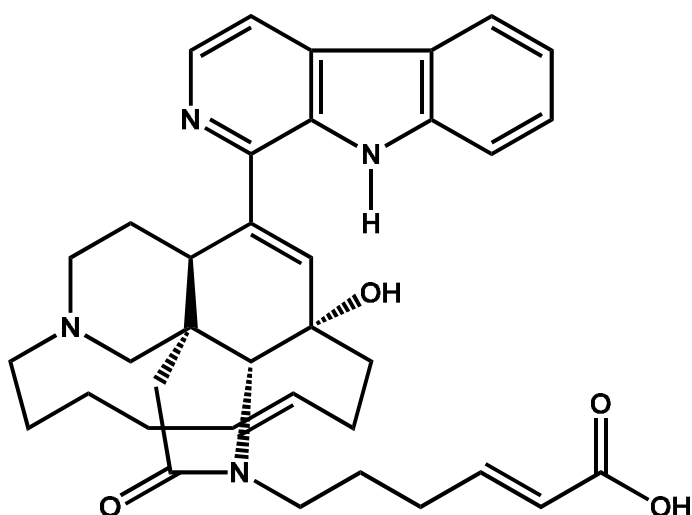
Equilibrium geometry of 2-2-di(3-indolyl)-3-indolone (2)



C	-1.193205	-3.837036	-1.284155
C	-0.576609	-2.537599	-1.244483
C	-1.589002	-1.628975	-1.130284
C	-2.585644	-3.631839	-1.191500
N	-2.795024	-2.278982	-1.097471

C	-3.494560	-4.688643	-1.197118
C	-2.983784	-5.966307	-1.302311
C	-1.600130	-6.194393	-1.392531
C	-0.702827	-5.146363	-1.380177
C	0.900259	-2.271252	-1.361728
C	1.684685	-2.823542	-0.210940
C	3.116328	-2.815573	-0.079180
C	3.413137	-3.376708	1.180834
N	2.219403	-3.701344	1.776990
C	1.188488	-3.362721	0.939141
C	4.168585	-2.379541	-0.894066
C	5.464006	-2.517508	-0.439155
C	5.736906	-3.086601	0.816259
C	4.720324	-3.522367	1.641584
C	1.118815	-0.736906	-1.489947
C	1.520299	-0.483834	-2.868911
C	1.615440	-1.716317	-3.520016
N	1.413305	-2.768697	-2.657161
C	1.769820	0.714126	-3.531990
C	2.096505	0.668631	-4.872113
C	2.165452	-0.568677	-5.530044
C	1.930949	-1.765628	-4.879910
O	0.949821	0.049619	-0.588446
H	-1.540031	-0.555648	-1.056759
H	-3.690505	-1.830233	-1.015051
H	-4.558754	-4.511315	-1.120227
H	-3.660900	-6.809533	-1.309241
H	-1.235717	-7.209955	-1.464692
H	0.363218	-5.333736	-1.424606
H	2.112934	-4.121115	2.683600
H	0.164125	-3.533164	1.225583
H	3.970218	-1.941493	-1.864142
H	6.286811	-2.183872	-1.056611
H	6.763669	-3.182243	1.142323
H	4.928023	-3.956672	2.610372
H	1.002891	-3.615748	-3.021297
H	1.697137	1.651779	-2.996644
H	2.294644	1.578287	-5.420194
H	2.413828	-0.588523	-6.583270
H	1.997671	-2.709842	-5.402319

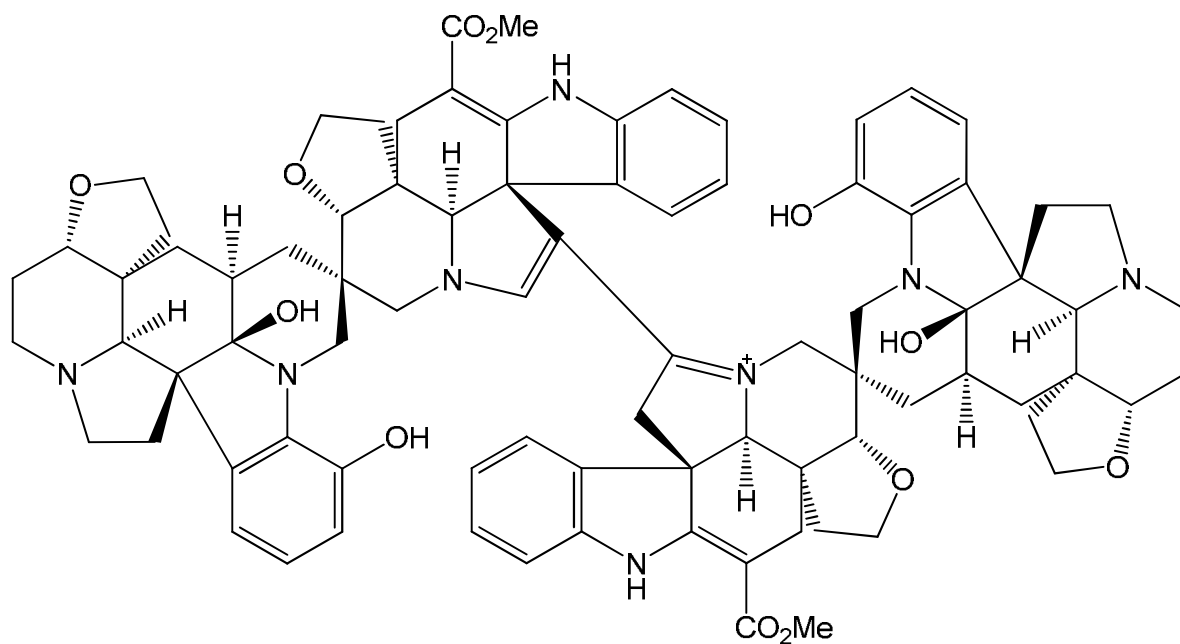
Equilibrium geometry of acantholactam (3)



O	0.011522	-1.314907	-2.910697
O	1.917915	-4.289869	-2.082897
O	6.613205	4.071861	-0.234977
O	7.366689	2.255039	0.820447
N	1.823244	-2.126410	-1.332294
N	1.238886	-1.432266	2.332325
N	-4.084552	-2.274963	0.444987
N	-3.913678	1.292539	-0.448048
C	0.165299	-2.282027	0.285820
C	0.854346	-1.272549	-0.657724
C	-1.192472	-1.829581	0.826271
C	-0.078433	-0.567875	-1.692056
C	1.101968	-2.582006	1.467418
C	0.116903	-3.524169	-0.609334
C	-1.089556	-0.837020	2.005735
C	-2.048429	-1.171843	-0.220926
C	1.381359	-3.399615	-1.441476
C	-1.528683	-0.564533	-1.284024
C	-0.017941	-1.195801	3.018841
C	0.418672	0.861327	-1.963788
C	2.960710	-1.617194	-2.067401
C	2.383963	-1.478129	3.227208
C	-3.509412	-1.148260	0.038687
C	0.368781	1.800748	-0.739554
C	3.853550	-0.759829	-1.183548
C	2.868837	-0.087975	3.634750
C	-4.278843	0.011435	-0.104986
C	3.215984	0.794756	2.430699
C	1.692242	2.447382	-0.447344
C	5.021474	-0.146294	-1.959275
C	-5.662216	-0.014645	0.155716
C	2.050506	1.665897	1.948735
C	2.389796	2.396873	0.684725
C	-5.403324	-2.308482	0.680157
C	-6.145449	1.330166	-0.046182
C	-6.240088	-1.216509	0.548987
C	-5.025111	2.104230	-0.408647
C	5.855169	0.681473	-1.042117

C	-7.400730	1.930114	0.055235
C	-5.133630	3.468767	-0.669944
C	5.913917	2.008376	-1.065447
C	-7.513256	3.281566	-0.203635
C	-6.386935	4.038577	-0.561500
C	6.706840	2.744382	-0.063366
H	1.364452	-0.514012	-0.064163
H	-1.714000	-2.720573	1.184132
H	0.698975	-3.453449	2.011919
H	2.085052	-2.860116	1.089072
H	-0.739362	-3.502754	-1.286100
H	0.102669	-4.463678	-0.060533
H	-2.062803	-0.769564	2.493039
H	-0.868286	0.155716	1.612852
H	-2.186591	-0.073443	-1.997256
H	0.100614	-0.373307	3.723445
H	-0.312971	-2.086100	3.598646
H	-0.177174	1.269456	-2.781879
H	1.442193	0.784432	-2.334998
H	2.617144	-1.046645	-2.934022
H	3.506524	-2.481466	-2.440879
H	3.197438	-1.974102	2.695470
H	2.170064	-2.083183	4.121199
H	-0.615606	-0.942491	-3.538154
H	0.014869	1.257571	0.134028
H	-0.369002	2.584030	-0.921593
H	3.275252	0.057273	-0.749536
H	4.226796	-1.364371	-0.353743
H	3.746272	-0.224526	4.267395
H	2.123188	0.412623	4.256600
H	3.547923	0.156478	1.607165
H	4.057189	1.447218	2.672333
H	2.114719	3.011100	-1.274067
H	5.629870	-0.941826	-2.394025
H	4.638338	0.467093	-2.775588
H	1.816668	2.390244	2.734881
H	1.168942	1.042605	1.820122
H	-2.972774	1.597685	-0.627575
H	3.338284	2.927638	0.705753
H	-5.802192	-3.263121	0.995865
H	-7.295588	-1.302123	0.760769
H	6.409443	0.158090	-0.269239
H	-8.267458	1.346163	0.331884
H	-4.270306	4.056051	-0.946623
H	5.378571	2.594991	-1.799223
H	-8.475745	3.765975	-0.131074
H	-6.503052	5.094898	-0.757898
H	7.144651	4.503842	0.447538

Equilibrium geometry of alasmontamine A (4)



N	-6.469236	-0.974674	2.483841
C	-5.993793	-0.541149	1.279537
C	-1.767896	1.264250	-0.604795
N	-2.648759	0.327001	0.094932
C	-2.574431	-0.993994	-0.000847
C	-3.817697	-1.614627	0.569250
C	-4.478135	-0.462855	1.374619
C	-4.239007	-0.636317	2.856495
C	-3.077322	-0.572441	3.610159
C	-3.155101	-0.844527	4.982488
C	-4.377154	-1.183550	5.566640
C	-5.552922	-1.260039	4.811748
C	-5.456906	-0.979425	3.454591
C	-2.510989	2.534253	-1.072824
C	-3.950993	2.125250	-1.450755
C	-6.620978	-0.183074	0.126588
C	-5.755026	0.440004	-0.938723
C	-5.810148	3.512329	-1.038860
C	-5.577631	2.682279	0.217835
C	-4.787689	1.479767	-0.323530
C	-3.884009	0.816329	0.735610
C	-8.065118	-0.238254	-0.070252
C	-10.148213	-0.858520	0.838669
N	-0.585709	3.708290	-2.251081
C	-0.606098	4.825985	-1.298859
C	0.902731	8.581462	0.343870
N	0.586288	7.472008	-0.546542
C	1.159255	7.633013	-1.885924
C	1.214904	6.205985	-2.456628
C	0.871916	5.277372	-1.255018
C	1.562594	3.941604	-1.427529

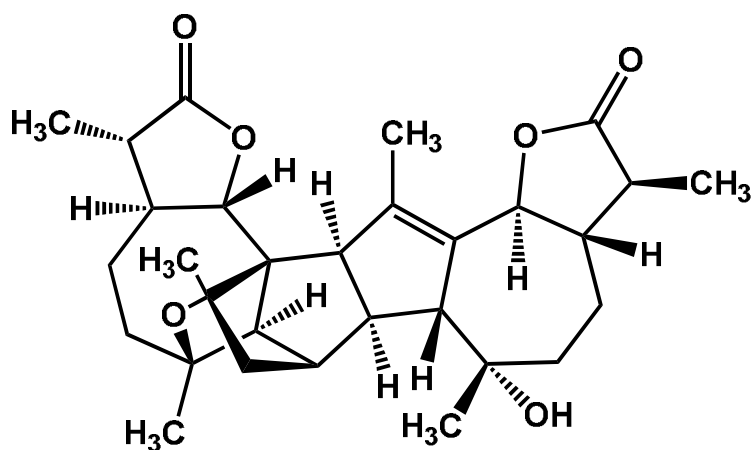
C	2.885049	3.584149	-1.212455
C	3.317246	2.322201	-1.632380
C	2.432165	1.459776	-2.275748
C	1.100062	1.822550	-2.507449
C	0.654388	3.073788	-2.067658
C	0.270747	8.350272	1.708270
C	0.640490	6.992195	2.279427
C	-1.062003	4.288936	0.072670
C	-0.949626	5.374390	1.133153
C	2.500999	5.636432	2.640024
C	1.395179	4.780600	2.001959
C	0.505205	5.816204	1.297996
C	1.137148	6.201877	-0.051819
C	-2.456684	3.672337	-0.033681
C	-1.869186	3.037665	-2.390562
N	-3.678023	-4.307303	-1.052576
C	-2.422541	-4.175071	-0.526811
C	2.004207	-2.242752	-1.384805
N	0.557777	-2.255524	-1.256573
C	-0.199619	-1.330688	-0.699243
C	-1.526445	-1.727650	-0.572032
C	-1.693215	-3.074686	-1.305375
C	-2.637998	-2.852000	-2.473532
C	-2.541846	-2.003135	-3.566257
C	-3.635661	-1.901079	-4.434624
C	-4.805243	-2.623975	-4.184275
C	-4.920002	-3.465618	-3.073152
C	-3.816263	-3.566494	-2.232893
C	2.643174	-3.420529	-0.624732
C	1.856796	-4.704485	-0.929868
C	-1.787453	-4.884753	0.442804
C	-0.297271	-4.668833	0.556771
C	1.150958	-6.090808	-2.634559
C	-0.017648	-5.952633	-1.643056
C	0.313270	-4.669664	-0.856135
C	-0.207108	-3.450743	-1.638565
C	-2.413096	-5.944022	1.228849
C	-4.400829	-7.097082	1.746049
N	3.630242	-2.254913	1.409745
C	5.002806	-2.488867	0.944275
C	9.349836	-2.103978	1.194086
N	7.930568	-2.178373	1.516332
C	7.658204	-1.982483	2.943208
C	6.191685	-1.524367	2.998491
C	5.786112	-1.283099	1.514196
C	4.717452	-0.214260	1.462546
C	4.818781	1.162265	1.589997
C	3.651571	1.918855	1.743186
C	2.415380	1.280122	1.817493
C	2.310300	-0.109133	1.717481
C	3.466650	-0.866509	1.493606

C	9.559219	-2.322937	-0.297551
C	8.690857	-1.400372	-1.134597
C	4.999326	-2.479116	-0.596298
C	6.418564	-2.537106	-1.140570
C	8.098885	0.837564	-1.351248
C	6.812065	-0.004620	-1.390097
C	7.219826	-1.313921	-0.693991
C	7.158048	-1.130119	0.832069
C	4.095722	-3.597958	-1.102694
C	2.627814	-3.186887	0.906116
H	-7.459165	-1.053624	2.675490
H	-0.914149	1.520225	0.042139
H	-1.380028	0.726734	-1.483079
H	-3.588129	-2.481442	1.200993
H	-4.464119	-1.957383	-0.252140
H	-2.121504	-0.312537	3.148143
H	-2.256319	-0.793909	5.596605
H	-4.421034	-1.393494	6.635907
H	-6.505914	-1.523123	5.270771
H	-3.871031	1.415720	-2.294781
H	-6.396218	0.933730	-1.680972
H	-5.170155	-0.311089	-1.499228
H	-5.849540	4.591027	-0.837044
H	-6.737220	3.216656	-1.555100
H	-4.981559	3.243443	0.949694
H	-6.517675	2.384220	0.700389
H	-3.616912	1.535608	1.520064
H	-10.512564	-1.314759	1.763735
H	-10.412108	-1.479456	-0.025848
H	-10.573067	0.144502	0.711691
H	2.003616	8.683597	0.443820
H	0.519688	9.511658	-0.099943
H	2.179820	8.055563	-1.813601
H	0.545875	8.322685	-2.482638
H	2.223428	5.973238	-2.818939
H	0.507950	6.047062	-3.279198
H	3.576905	4.277712	-0.730092
H	4.347000	2.008072	-1.464048
H	2.780381	0.490292	-2.640181
H	0.580536	9.136425	2.411404
H	-0.824712	8.401968	1.618128
H	0.012643	6.778631	3.165221
H	-0.345616	3.495977	0.348729
H	-1.325969	5.000534	2.098286
H	-1.581349	6.233653	0.854080
H	3.430658	5.624345	2.050237
H	2.733953	5.307921	3.663524
H	1.800605	4.033259	1.306897
H	0.812089	4.257269	2.774785
H	2.237138	6.304283	0.083170
H	-2.750022	3.315951	0.965077

H	-3.172376	4.454712	-0.329749
H	-2.558137	3.778031	-2.817285
H	-1.771022	2.212137	-3.104195
H	-4.326221	-5.013225	-0.729122
H	2.256601	-2.317803	-2.454753
H	2.365094	-1.277489	-1.003449
H	0.258305	-0.408786	-0.343300
H	-1.633108	-1.423106	-3.743969
H	-3.577671	-1.249591	-5.306251
H	-5.651429	-2.529337	-4.865692
H	-5.836199	-4.021253	-2.873879
H	2.214984	-5.498538	-0.245498
H	0.141308	-5.473514	1.161396
H	-0.086128	-3.718387	1.070294
H	0.856627	-5.905686	-3.675986
H	1.614914	-7.086126	-2.569828
H	-0.988239	-5.895018	-2.153420
H	-0.055603	-6.804926	-0.950045
H	-0.086529	-3.607751	-2.720380
H	-4.334117	-6.874228	2.817968
H	-3.947672	-8.075671	1.547137
H	-5.443221	-7.081077	1.415160
H	9.754119	-1.115575	1.497730
H	9.883907	-2.874050	1.769300
H	8.319525	-1.194737	3.352541
H	7.851644	-2.911353	3.498375
H	6.103402	-0.582328	3.552789
H	5.527660	-2.261485	3.464781
H	5.797273	1.647622	1.579782
H	3.711060	3.004254	1.825416
H	1.494595	1.842595	1.982050
H	10.614762	-2.165574	-0.561354
H	9.307763	-3.363077	-0.554429
H	8.717529	-1.725559	-2.192151
H	4.573136	-1.507086	-0.902319
H	6.397886	-2.576973	-2.240871
H	6.909982	-3.462157	-0.796129
H	8.292818	1.327579	-2.316676
H	8.070062	1.609447	-0.567807
H	6.514744	-0.216994	-2.427706
H	5.976824	0.502186	-0.889076
H	7.575586	-0.131692	1.091317
H	4.117069	-3.633565	-2.200747
H	4.477252	-4.564587	-0.737872
H	1.648108	-2.829358	1.229826
H	2.811839	-4.153788	1.397870
H	-1.215286	6.645663	-1.339545
H	0.720655	0.274047	-3.580442
H	6.418206	-3.706002	1.394286
H	1.023901	-1.209556	2.655127
O	-3.737376	-6.077741	0.987656

O	5.445555	-3.733053	1.439041
O	9.172803	-0.060152	-1.039655
O	1.054558	-0.690449	1.839878
O	-8.650081	0.156418	-1.064625
O	-4.692911	3.254161	-1.898791
O	-1.491034	5.816241	-1.769934
O	2.016509	6.986108	2.663244
O	-8.724308	-0.781886	0.978978
O	0.224959	0.995703	-3.173329
O	2.109813	-5.088918	-2.276277
O	-1.830740	-6.649323	2.034400

Equilibrium geometry of anabsinthin (5)

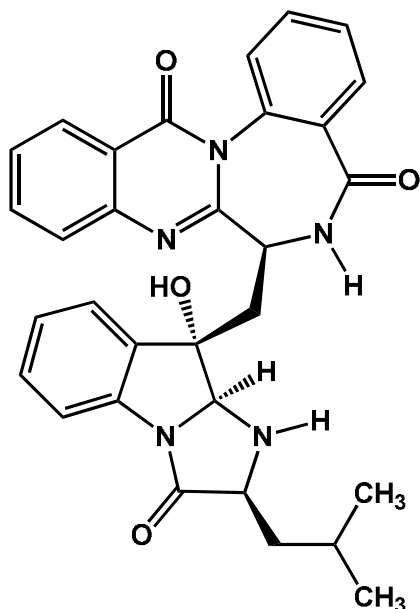


O	-2.352482	1.078412	-2.272179
O	-2.552358	-1.936139	0.706542
O	2.213547	0.406871	3.076285
O	3.089752	-1.673862	-1.182207
O	-3.734299	-3.335790	1.966951
O	4.598536	-2.247297	-2.714927
C	-1.648074	0.145249	-0.264228
C	-1.979303	1.652662	-0.054392
C	-0.505952	2.110477	-0.165333
C	-1.182604	0.431992	-1.726658
C	-0.515706	-0.100270	0.765705
C	0.147845	1.285635	0.949266
C	-2.822210	2.028670	-1.285452
C	-0.108125	1.514567	-1.533576
C	-2.811690	-0.846564	-0.217402
C	1.677773	1.090254	0.847225
C	0.624029	-1.010605	0.404030
C	-4.174455	-0.318123	0.219375
C	-4.335191	1.866783	-1.082082
C	1.791746	-0.364376	0.420992
C	-0.778154	-0.685694	-2.651669
C	-4.875177	0.456707	-0.879750

C	2.466439	1.452444	2.135438
C	-2.594620	3.460431	-1.767657
C	-4.866435	-1.608095	0.653437
C	3.101059	-1.020747	0.122730
C	0.410926	-2.469978	0.167909
C	3.980913	1.599605	1.896545
C	-3.706331	-2.409053	1.201824
C	4.315528	-0.111264	0.049653
C	4.764631	0.386110	1.410305
C	1.987264	2.793265	2.699573
C	-6.017774	-1.469936	1.630079
C	5.287001	-1.000410	-0.722384
C	4.342456	-1.715692	-1.668055
C	6.432402	-0.308584	-1.434437
H	-2.439307	1.913726	0.897284
H	-0.336514	3.181123	-0.069967
H	-0.979876	-0.453956	1.688392
H	-0.139643	1.704111	1.908691
H	0.892665	1.089163	-1.537009
H	-0.166793	2.224289	-2.355837
H	-2.933946	-1.308618	-1.199995
H	2.078642	1.757070	0.075167
H	-4.046914	0.310573	1.107710
H	-4.836896	2.303808	-1.947947
H	-4.607822	2.485109	-0.222645
H	0.143076	-1.148641	-2.300930
H	-1.549496	-1.449293	-2.745722
H	-0.593151	-0.271278	-3.643652
H	-5.939230	0.532040	-0.647304
H	-4.795365	-0.111359	-1.809917
H	-3.123368	3.613231	-2.708404
H	-2.996074	4.162303	-1.034956
H	-1.546213	3.694837	-1.924022
H	-5.197636	-2.145539	-0.244232
H	3.295494	-1.811151	0.856833
H	-0.311880	-2.639861	-0.632188
H	1.333590	-2.986746	-0.083482
H	-0.020208	-2.919397	1.064659
H	4.417919	1.927101	2.843326
H	4.126669	2.423434	1.191964
H	4.070164	0.743222	-0.592091
H	4.693524	-0.427740	2.136798
H	5.817817	0.669477	1.359789
H	0.996401	2.711707	3.137900
H	1.961862	3.552985	1.916713
H	2.669510	3.135428	3.478949
H	-5.695519	-0.943348	2.528787
H	-6.394708	-2.448363	1.922334
H	-6.834205	-0.909343	1.176777
H	2.598598	0.659290	3.922050
H	5.674336	-1.769725	-0.042673

H	6.053601	0.440444	-2.130228
H	7.026837	-1.027368	-1.995404
H	7.083210	0.186916	-0.715295

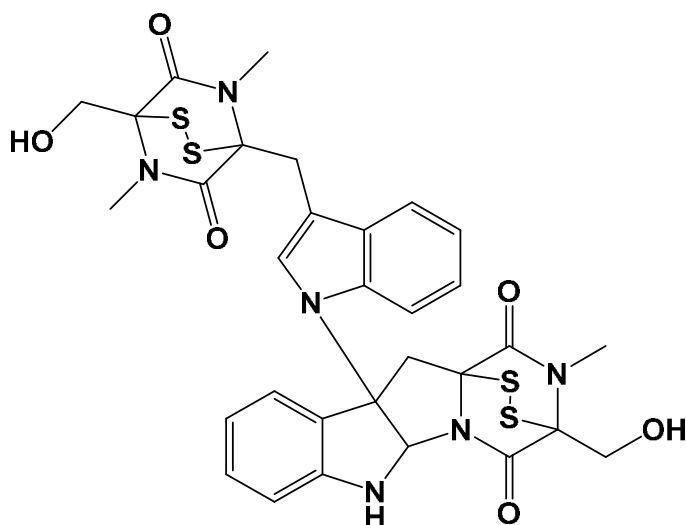
Equilibrium geometry of asperlicin (6)



C	6.394614	0.062583	-1.378436
C	6.598687	-0.596205	-0.159305
C	5.523966	-1.107573	0.533308
C	4.235090	-0.955293	0.015636
C	4.029038	-0.311228	-1.203357
C	5.128361	0.200240	-1.903172
C	3.079455	-1.431078	0.768222
N	1.821263	-1.029988	0.236496
C	1.745759	-0.580628	-1.070988
N	2.768719	-0.233234	-1.762529
C	0.722837	-1.006347	1.166489
C	-0.525470	-1.548277	0.890987
C	-0.896834	-2.188862	-0.396305
N	-0.573234	-1.554431	-1.555653
C	0.455555	-0.575103	-1.892902
C	0.971341	-0.473042	2.426775
C	-0.009792	-0.477592	3.398095
C	-1.259612	-1.016716	3.128777
C	-1.507108	-1.554635	1.882375
O	-1.561352	-3.210482	-0.416592
O	3.148547	-2.073908	1.790402
C	-0.002458	0.822222	-2.357610
C	-0.515169	1.966764	-1.466429
C	0.071664	2.115553	-0.071733
C	-0.938178	2.151125	0.892219
N	-2.168014	1.913104	0.275541
C	-2.038523	1.986183	-1.186114

C	1.381961	2.364330	0.291904
C	1.662641	2.679155	1.619608
C	0.640963	2.735403	2.560449
C	-0.678388	2.465352	2.213993
N	-2.929464	0.966974	-1.697110
C	-4.040416	1.035443	-0.721950
C	-3.331560	1.303863	0.627415
O	-3.724939	1.041871	1.743504
C	-4.987319	-0.147512	-0.687063
C	-4.285230	-1.509770	-0.678291
C	-5.032641	-2.517681	0.186252
C	-4.104768	-2.058144	-2.092684
O	-0.303328	3.170156	-2.211288
H	7.243365	0.459785	-1.918573
H	7.599165	-0.702300	0.235398
H	5.649098	-1.617036	1.478512
H	4.958607	0.686308	-2.853841
H	-0.886500	-2.090232	-2.354760
H	0.852753	-0.967941	-2.827571
H	1.943238	-0.059651	2.646501
H	0.201850	-0.045410	4.366572
H	-2.034322	-1.016818	3.881937
H	-2.463772	-2.004161	1.656194
H	0.881380	1.217673	-2.860054
H	-0.746366	0.670642	-3.142602
H	-2.405759	2.958055	-1.522739
H	2.178738	2.342858	-0.443676
H	2.680027	2.892899	1.916804
H	0.875006	2.989387	3.585713
H	-1.477581	2.505329	2.939817
H	-2.474841	0.060786	-1.594473
H	-4.606609	1.946652	-0.945491
H	-5.584477	-0.027375	0.219113
H	-5.673604	-0.089416	-1.534085
H	-3.297694	-1.373770	-0.230189
H	-4.513751	-3.477077	0.192020
H	-5.118999	-2.163193	1.214564
H	-6.041509	-2.676942	-0.201968
H	-3.508239	-2.969756	-2.075809
H	-5.082230	-2.293270	-2.520977
H	-3.627189	-1.337682	-2.758756
H	0.643109	3.328399	-2.289995

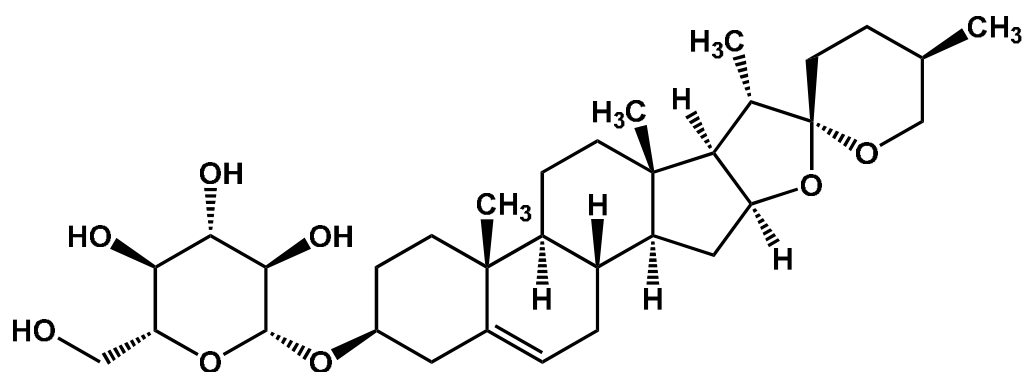
Equilibrium geometry of chetomin (7)



S	5.174918	0.690405	-0.420283
S	6.000094	-1.038296	0.412444
S	-2.867353	-1.100449	0.232448
S	-4.285768	-2.621712	0.069442
O	3.026147	-2.813002	1.244671
O	3.729484	-0.555354	-3.267270
O	5.839832	-3.675966	1.262674
O	-4.399662	1.487021	-1.535818
O	-6.915653	-1.314590	1.854258
O	-7.082400	-3.503944	0.205577
N	2.945435	-0.860616	0.098320
N	0.287532	1.513081	-0.161448
N	1.902710	-0.065754	2.147177
N	4.570871	-2.055087	-1.755640
N	-5.085481	0.002519	1.506467
N	-5.518517	-0.468029	-1.199920
C	1.672586	1.123773	0.082144
C	1.753873	-0.296626	0.730669
C	3.530358	-0.058705	-0.926578
C	2.499756	1.020994	-1.211925
C	2.317521	1.968256	1.164242
C	4.798247	-2.285489	-0.349190
C	3.497472	-2.049311	0.429321
C	3.928837	-0.904857	-2.123644
C	2.454323	1.209151	2.322631
C	-0.182674	2.496582	-1.015852
C	-0.752783	1.131153	0.657022
C	2.726074	3.285855	1.122116
C	5.371531	-3.667546	-0.064694
C	-1.909107	1.758929	0.302623
C	-1.565094	2.655770	-0.764482
C	3.032396	1.749265	3.460801
C	5.278728	-2.816355	-2.780554
C	-3.226783	1.559702	0.989183

C	3.301342	3.842519	2.260572
C	0.473839	3.280177	-1.969578
C	-4.057031	0.342819	0.551155
C	3.455410	3.073053	3.408877
C	-2.293384	3.606953	-1.487543
C	-5.775030	-1.504390	-0.248998
C	-0.270457	4.212090	-2.663526
C	-4.677011	0.541585	-0.831617
C	-1.643112	4.377317	-2.426463
C	-6.007679	-0.921784	1.138621
C	-4.987329	0.371509	2.916107
C	-6.940564	-2.408942	-0.657226
C	-5.865124	-0.632364	-2.607549
H	0.899393	-0.935056	0.513369
H	1.876367	0.701563	-2.046939
H	2.980233	1.957937	-1.478002
H	2.278513	-0.838448	2.678979
H	-0.584291	0.430292	1.459328
H	2.609503	3.873313	0.218982
H	6.187414	-3.868007	-0.758361
H	4.573531	-4.399251	-0.219819
H	3.152169	1.159909	4.359532
H	6.355863	-2.671782	-2.689200
H	4.948239	-2.440206	-3.742132
H	5.038618	-3.874297	-2.709472
H	-3.859859	2.438905	0.855902
H	-3.029147	1.453833	2.052184
H	3.635509	4.870093	2.250513
H	1.528383	3.186976	-2.171375
H	3.913645	3.512058	4.284934
H	-3.352557	3.722988	-1.310198
H	6.162312	-4.555955	1.473752
H	0.220720	4.829118	-3.403496
H	-2.193216	5.119015	-2.989116
H	-4.060002	-0.013769	3.340632
H	-5.829270	-0.082396	3.425736
H	-5.030758	1.450239	3.039187
H	-6.758015	-2.809079	-1.651344
H	-7.842977	-1.789753	-0.684654
H	-5.383988	-1.524846	-3.009631
H	-5.499357	0.241703	-3.134299
H	-6.942406	-0.704240	-2.737800
H	-7.279464	-3.142613	1.080596

Equilibrium geometry of diosgenin-3-O- β -D-glucopyranoside (8)

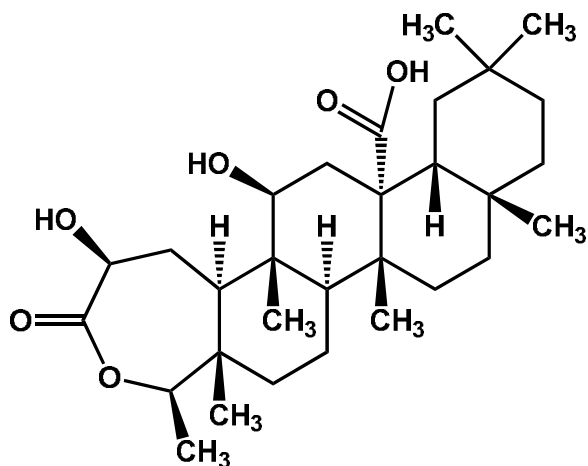


O	5.946016	0.808737	-0.381183
O	7.256757	0.555770	1.515506
O	-5.295839	-0.659263	-1.530560
O	-6.236308	1.100233	-0.445365
O	-6.732577	-2.460162	0.224094
O	-7.843321	-1.211757	2.529288
O	-8.805617	1.386401	2.146078
O	-7.156870	3.746367	-0.943125
C	3.247813	-1.014505	0.118926
C	2.463994	0.297676	-0.062407
C	4.462695	-0.494106	0.921765
C	1.165204	0.162128	-0.842041
C	4.723215	0.924008	0.346538
C	0.275671	-0.905893	-0.178579
C	3.527266	1.289491	-0.539288
C	2.348248	-1.993123	0.867537
C	5.819276	-1.206547	0.799226
C	1.036112	-2.210962	0.108188
C	-1.042782	-1.140530	-0.963708
C	6.768540	-0.081140	0.348043
C	3.680431	-1.608008	-1.228768
C	0.424849	1.494986	-0.889858
C	-1.654182	0.188445	-1.390078
C	-2.052287	-1.850008	-0.031844
C	6.259522	-1.947343	2.051765
C	7.913249	-0.527269	-0.544763
C	-0.999402	1.344750	-1.324031
C	-0.804145	-2.009484	-2.212020
C	-3.077436	0.146533	-1.890883
C	-3.463184	-1.953829	-0.602306
C	-4.002245	-0.571407	-0.918963
C	8.865979	0.623522	-0.846948
C	9.324959	1.290032	0.446241
C	8.097722	1.674039	1.257166
C	10.195622	2.509791	0.184396
C	-6.379163	-0.269340	-0.767152
C	-6.572470	-1.089661	0.515231
C	-7.749492	-0.531589	1.297482

C	-7.378516	1.663443	0.175761
C	-7.606387	0.966050	1.516224
C	-7.134003	3.143094	0.337591
H	2.175613	0.610191	0.952223
H	4.172629	-0.420216	1.972264
H	1.384149	-0.137099	-1.871966
H	4.859028	1.654775	1.146428
H	-0.015763	-0.482100	0.792975
H	3.774040	1.122240	-1.589341
H	3.226575	2.329511	-0.425076
H	2.132828	-1.585033	1.860365
H	2.854332	-2.950994	1.016098
H	5.791414	-1.914987	-0.028203
H	1.255825	-2.721284	-0.830131
H	0.400592	-2.885894	0.682697
H	2.850859	-1.664740	-1.930889
H	4.470790	-1.019374	-1.695446
H	4.058320	-2.622710	-1.093266
H	0.940020	2.185493	-1.562383
H	0.459236	1.966158	0.100826
H	-2.096679	-1.295553	0.911261
H	-1.686231	-2.849282	0.204932
H	5.572487	-2.768453	2.259593
H	7.259871	-2.366829	1.934528
H	6.269155	-1.281243	2.912638
H	7.494318	-0.948141	-1.459265
H	8.445380	-1.326275	-0.022028
H	-1.521252	2.251704	-1.614645
H	-1.671884	-2.013410	-2.869129
H	0.042073	-1.637714	-2.791441
H	-0.601193	-3.044141	-1.934053
H	-3.444047	1.158091	-2.065801
H	-3.134284	-0.388244	-2.844276
H	-3.471766	-2.546811	-1.520573
H	-4.120704	-2.459800	0.105252
H	-4.071808	0.020398	-0.001600
H	9.726245	0.266157	-1.415546
H	8.355243	1.367524	-1.465381
H	9.892739	0.558540	1.030655
H	8.379681	2.067641	2.233548
H	7.532414	2.447168	0.723882
H	10.534662	2.965242	1.115782
H	11.075137	2.239396	-0.400462
H	9.638447	3.262941	-0.377144
H	-7.258530	-0.403366	-1.411617
H	-5.676324	-1.012031	1.134779
H	-8.666954	-0.690346	0.709679
H	-8.262917	1.514390	-0.459003
H	-6.743037	1.146432	2.166036
H	-7.556367	-2.589648	-0.258041
H	-6.163900	3.284953	0.823788

H	-7.914578	3.564456	0.976596
H	-8.542469	-0.784040	3.036776
H	-8.632618	2.139426	2.716489
H	-6.936762	4.676866	-0.851899

Equilibrium geometry of itoaic acid (9)

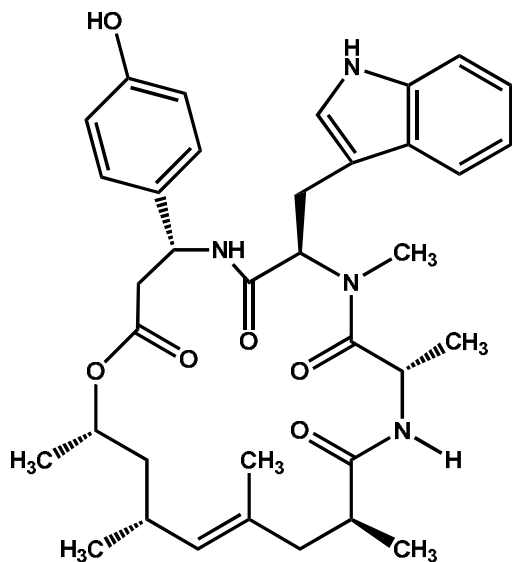


C	-3.407752	-1.105963	-0.224295
C	-2.544170	0.167520	0.056563
C	-1.247516	-0.085103	0.920009
C	-0.415959	-1.139573	0.107067
C	-1.215906	-2.431605	-0.035039
C	-2.496011	-2.189054	-0.820115
C	-0.412654	1.219180	0.992315
C	1.070128	1.018467	1.320820
C	1.790694	0.039619	0.381811
C	1.068151	-1.346848	0.526498
C	3.308724	-0.090404	0.776018
C	4.079641	-1.253570	0.100199
C	3.253460	-2.552442	0.008172
C	1.775316	-2.403157	-0.349397
C	4.141068	1.221370	0.745008
C	5.043947	1.527703	-0.490426
C	4.710036	0.606339	-1.666235
C	4.586138	-0.884832	-1.322712
C	-3.355835	1.372962	0.546364
C	-4.424609	1.915123	-0.411072
C	-5.691312	1.088779	-0.336505
O	-5.654647	-0.170741	-0.737374
C	-4.468828	-0.775162	-1.311549
O	-4.738790	3.243107	-0.071383
O	-6.713564	1.548853	0.112807
C	-5.027426	-1.962191	-2.078442
C	-4.138870	-1.665394	1.002964
C	-1.598193	-0.504716	2.363444
O	-0.953806	2.080853	1.993650
C	1.144997	-1.888592	1.968674

C	5.270194	-1.590115	1.014943
C	6.540230	1.398939	-0.163919
C	4.809209	2.980089	-0.917325
C	1.684920	0.694441	-1.000523
O	1.604066	-0.116492	-2.066306
O	1.698316	1.891270	-1.156459
H	-2.156206	0.458722	-0.929439
H	-0.363960	-0.733074	-0.908088
H	-1.440404	-2.872288	0.937271
H	-0.637734	-3.174967	-0.579709
H	-3.052516	-3.123265	-0.905301
H	-2.214356	-1.892963	-1.836697
H	-0.489835	1.713159	0.017064
H	1.165794	0.678110	2.350465
H	1.533266	2.002142	1.269542
H	3.238834	-0.349722	1.834415
H	3.329935	-3.084212	0.956763
H	3.736070	-3.204046	-0.725326
H	1.311308	-3.374290	-0.177271
H	1.649343	-2.178684	-1.404743
H	4.778075	1.215047	1.630737
H	3.465238	2.063074	0.884403
H	5.479096	0.732946	-2.432963
H	3.789477	0.960975	-2.123991
H	5.554404	-1.373485	-1.455440
H	3.921380	-1.338230	-2.059528
H	-2.683929	2.211417	0.690391
H	-3.820199	1.194846	1.518816
H	-4.043736	1.901003	-1.436526
H	-4.038077	-0.077442	-2.032945
H	-5.656829	3.244668	0.233913
H	-4.271383	-2.412970	-2.714939
H	-5.421165	-2.721526	-1.404028
H	-5.842314	-1.613677	-2.709830
H	-4.628190	-0.888257	1.588297
H	-4.912550	-2.364729	0.685129
H	-3.463439	-2.205921	1.659546
H	-1.618708	-1.582171	2.497834
H	-0.885497	-0.095153	3.074380
H	-2.570270	-0.114967	2.655916
H	-0.462042	2.907075	1.975306
H	0.726523	-1.228307	2.715621
H	0.588453	-2.826256	2.013667
H	2.163479	-2.112009	2.271408
H	4.909357	-1.917323	1.992235
H	5.853958	-2.405490	0.583177
H	5.934760	-0.747384	1.177320
H	6.872282	0.365275	-0.091004
H	7.124870	1.865949	-0.958980
H	6.784684	1.905415	0.771787
H	5.099643	3.664549	-0.116639

H	5.406266	3.222574	-1.799275
H	3.758771	3.149750	-1.150500
H	1.574625	0.450444	-2.851617

Equilibrium geometry of jaspamide Q (10)

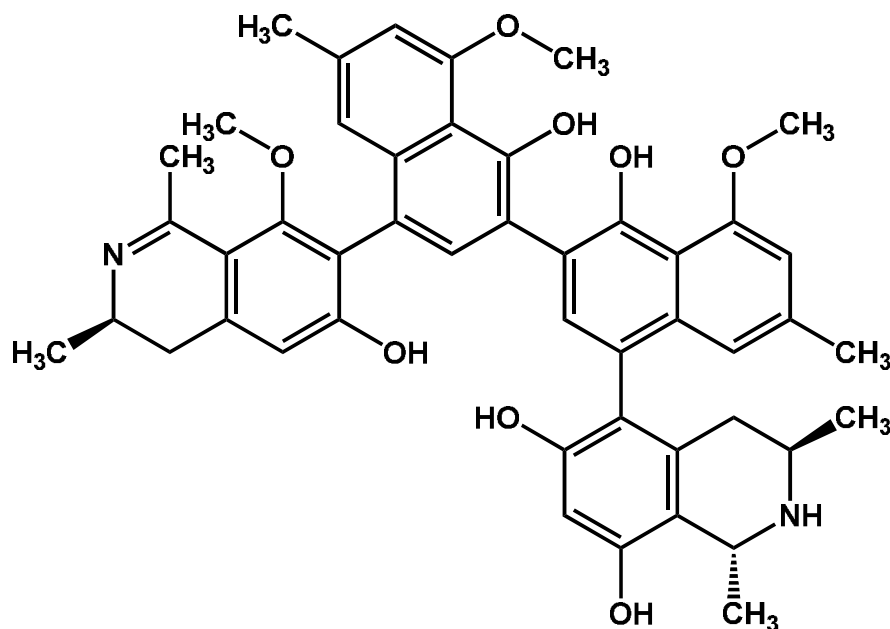


H	-4.571376	-0.713897	-3.879176
O	4.185064	0.291683	-0.973848
O	-0.794533	2.543485	-2.418770
O	-1.441747	0.026352	1.386564
O	0.313452	-4.377678	1.196744
O	2.610094	0.921698	-2.439061
O	0.521335	7.050226	2.860218
N	-1.747424	-0.403372	-0.809692
N	0.176665	1.704484	-0.545181
N	-0.601063	-2.436721	1.893837
N	-5.772499	-1.471786	-2.290232
C	-2.075158	0.998500	-1.069889
C	-3.208307	1.172693	-2.084825
C	4.759529	-2.729754	-0.711548
C	5.626454	-1.598678	-1.283090
C	1.327802	2.598285	-0.552786
C	-4.314520	0.186316	-1.880361
C	-0.833398	1.826508	-1.434684
C	4.868866	-0.486036	-1.983095
C	1.543619	-3.066011	2.810062
C	2.329087	-1.859045	2.224934
C	-1.513732	-2.273825	0.782353
C	-1.551091	-0.782849	0.463916
C	2.828340	-2.052178	0.812643
C	4.099719	-2.379987	0.595013
C	2.600890	1.833468	-0.207389
C	-4.986777	-0.152274	-0.653538
C	0.363690	-3.384582	1.907286

C	5.619115	-3.979279	-0.501239
C	-1.591652	-1.321600	-1.935101
C	1.111662	3.776110	0.375300
C	-4.826398	-0.641991	-2.835326
C	-5.886644	-1.201180	-0.952553
C	5.781762	0.437976	-2.766224
C	2.430685	-4.280783	3.017093
C	3.100938	0.970766	-1.339789
C	-2.937403	-2.737495	1.094708
C	1.831778	-1.843130	-0.299336
C	-4.912191	0.311815	0.667639
C	-6.688627	-1.797997	0.019262
C	1.110144	5.074919	-0.119273
C	0.907384	3.587053	1.739297
C	-5.703898	-0.276633	1.632129
C	-6.581557	-1.326028	1.311470
C	0.913721	6.162412	0.717949
C	0.707518	4.662573	2.588580
C	0.711715	5.955707	2.075550
H	-2.402645	1.393593	-0.110690
H	-2.825352	1.093351	-3.100785
H	-3.563387	2.198571	-1.978776
H	3.995928	-2.971707	-1.452358
H	6.254633	-1.169057	-0.498095
H	6.301712	-2.027146	-2.026333
H	1.414257	2.967734	-1.571116
H	4.112332	-0.909431	-2.643833
H	1.143401	-2.739625	3.772145
H	3.175574	-1.681508	2.887855
H	1.694090	-0.970368	2.269985
H	-1.119746	-2.853972	-0.047294
H	4.755508	-2.456082	1.460402
H	-0.048056	1.228985	0.321412
H	2.474190	1.208205	0.679325
H	3.400058	2.535617	0.031401
H	5.027777	-4.794081	-0.085812
H	6.055742	-4.313720	-1.441132
H	6.432848	-3.766364	0.193815
H	-0.483946	-1.614463	2.467586
H	-1.683035	-0.756359	-2.855995
H	-2.361047	-2.091362	-1.933470
H	-0.605725	-1.781623	-1.921499
H	6.271320	-0.113520	-3.566191
H	5.214882	1.254523	-3.207830
H	6.546993	0.852001	-2.110628
H	1.865641	-5.108749	3.439897
H	2.859579	-4.609944	2.073139
H	3.244882	-4.034193	3.696730
H	-6.290943	-2.170350	-2.792276
H	-2.926294	-3.798583	1.332098
H	-3.331660	-2.183501	1.944864

H	-3.597843	-2.567223	0.243446
H	1.147527	-2.687277	-0.392485
H	2.312939	-1.705018	-1.263812
H	1.226710	-0.951968	-0.103700
H	-4.248545	1.121067	0.937885
H	-7.365772	-2.601802	-0.232714
H	1.263093	5.242119	-1.177296
H	0.900131	2.587468	2.157312
H	-5.649650	0.072378	2.653444
H	-7.186321	-1.768142	2.090263
H	0.911538	7.171256	0.331364
H	0.549130	4.502916	3.646984
H	0.391465	6.784271	3.775197

Equilibrium geometry of korundamine A (11)

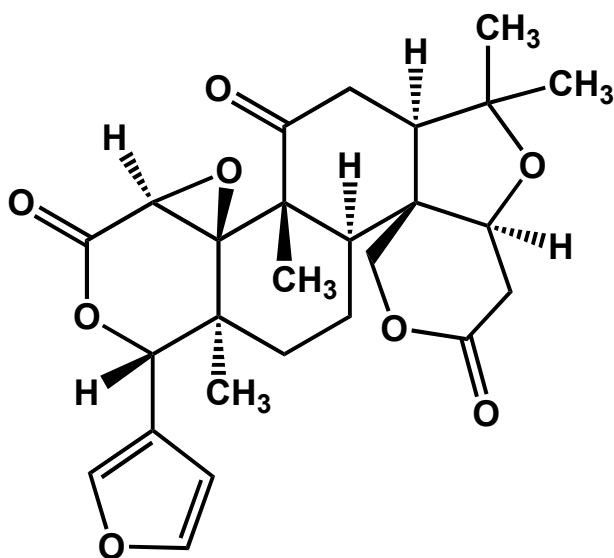


C	6.711090	-4.269977	0.873019
N	6.633041	-3.452999	2.088490
C	5.760378	-2.523900	2.143585
C	4.792621	-2.271343	1.040323
C	4.539675	-3.326252	0.154453
C	5.316183	-4.594082	0.351886
C	4.108574	-1.064660	0.849438
C	3.165399	-0.904542	-0.171863
C	2.909083	-1.997378	-1.002254
C	3.599510	-3.194553	-0.847899
C	2.475162	0.390649	-0.405946
C	1.129265	0.485923	-0.188584
C	0.405822	1.687910	-0.341801
C	1.100600	2.812302	-0.738171
C	2.501148	2.769030	-0.999640
C	3.194552	1.539323	-0.840774

C	4.582982	1.478198	-1.122961
C	5.277162	2.575556	-1.541992
C	4.597096	3.807744	-1.694996
C	3.259824	3.903603	-1.435986
C	-1.062880	1.651659	-0.117753
C	-1.778632	0.593888	-0.719178
C	-3.111991	0.390380	-0.513255
C	-3.821618	1.273923	0.349017
C	-3.135622	2.351208	0.978657
C	-1.742435	2.531836	0.709537
C	-3.905060	3.196033	1.855709
C	-5.245933	2.970382	2.042589
C	-5.916861	1.909173	1.395561
C	-5.209717	1.083893	0.572093
C	-3.801675	-0.748174	-1.182154
C	-4.213340	-0.622164	-2.507143
C	-4.876970	-1.655160	-3.150708
C	-5.129047	-2.830302	-2.464179
C	-4.725315	-3.003177	-1.137478
C	-4.064641	-1.946532	-0.506167
C	-3.661408	-2.070782	0.944175
C	-3.682007	-3.504677	1.461525
N	-4.888758	-4.216925	1.037663
C	-5.012322	-4.312360	-0.416343
C	7.589629	-3.578588	-0.166740
C	5.692459	-1.715780	3.412337
O	1.993833	-1.833058	-1.990862
O	4.447955	-0.004663	1.634894
C	3.426986	0.619655	2.412605
C	6.745343	2.516623	-1.849156
O	2.567078	5.072040	-1.575165
C	3.260038	6.232535	-2.014932
O	0.383201	3.962364	-0.881537
O	-1.086960	3.553393	1.313093
O	-3.255813	4.201537	2.483664
C	-3.996177	5.035259	3.354421
C	-7.386491	1.721723	1.639675
O	-3.957720	0.556248	-3.142922
O	-5.801364	-3.793780	-3.159834
C	-4.126811	-5.448305	-0.939428
C	-3.573738	-3.543262	2.975415
H	-5.695197	-3.720694	1.405815
H	7.197548	-5.202599	1.158268
H	5.370612	-5.160184	-0.578019
H	4.800806	-5.220364	1.086730
H	3.406733	-4.018315	-1.524887
H	0.590134	-0.392882	0.143237
H	5.095308	0.533309	-1.005766
H	5.156518	4.670960	-2.023633
H	-1.240170	-0.079880	-1.375338
H	-5.706873	0.263726	0.071176

H	-5.818139	3.609256	2.697994
H	-5.210240	-1.554846	-4.175681
H	-4.348122	-1.465716	1.548982
H	-2.671016	-1.635434	1.088414
H	-2.829462	-4.039065	1.036985
H	-6.056329	-4.586655	-0.600398
H	7.722500	-4.221179	-1.037129
H	7.140734	-2.639565	-0.492963
H	8.569491	-3.360644	0.255936
H	6.111886	-0.722277	3.264899
H	4.659908	-1.584068	3.736105
H	6.255489	-2.234445	4.183652
H	1.927787	-2.640160	-2.512352
H	2.577828	-0.050828	2.545168
H	3.866006	0.845831	3.382788
H	3.090594	1.540638	1.937779
H	7.142124	1.517647	-1.682421
H	6.932780	2.795497	-2.886992
H	7.297752	3.218090	-1.222547
H	4.048100	6.495152	-1.309714
H	3.684776	6.069386	-3.005083
H	2.520480	7.024756	-2.055261
H	0.980800	4.676697	-1.168726
H	-0.411419	3.884032	0.698817
H	-3.289009	5.759563	3.746207
H	-4.793255	5.555317	2.820078
H	-4.426357	4.462328	4.177933
H	-7.942908	2.611997	1.343003
H	-7.773085	0.871269	1.082149
H	-7.583260	1.558840	2.700328
H	-4.300541	0.522119	-4.041800
H	-5.987980	-4.554245	-2.602069
H	-4.417383	-6.389172	-0.474745
H	-4.202055	-5.553764	-2.021951
H	-3.079855	-5.253348	-0.711099
H	-4.450104	-3.071609	3.425863
H	-3.514935	-4.570326	3.332224
H	-2.689998	-3.002076	3.313097

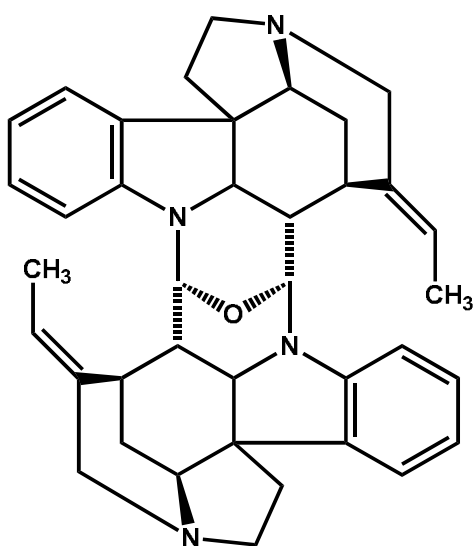
Equilibrium geometry of limonin (12)



O	-1.973063	-1.231342	-2.049429
O	3.984992	0.948083	1.322761
O	-4.222653	-1.048697	-0.223655
O	4.263902	0.724640	-1.564344
O	-0.183371	-2.898039	0.951474
O	-4.177136	-3.249158	-0.210668
O	5.451520	2.567432	-1.443803
O	-5.469064	3.156413	0.535721
C	-1.402377	-0.998736	-0.762088
C	0.132844	-1.141237	-0.676736
C	0.716731	0.255105	-0.261419
C	2.248909	0.244229	-0.098157
C	-2.070106	0.167015	-0.040273
C	-2.234736	-2.178448	-1.028657
C	2.504290	-0.797926	1.008195
C	0.009782	1.333037	-1.075309
C	-1.410783	1.498350	-0.504793
C	2.842733	1.458464	0.628551
C	0.586405	-2.180329	0.364317
C	2.087891	-2.215236	0.645541
C	3.895914	-0.479673	1.552966
C	-3.552696	0.204521	-0.487327
C	0.621612	-1.669696	-2.040234
C	2.990278	0.075447	-1.441527
C	-2.006504	-0.061760	1.477181
C	-3.622156	-2.216719	-0.470294
C	3.342874	2.550916	-0.296204
C	5.036511	-1.191513	0.841726
C	3.984806	-0.723662	3.051243
C	-4.368789	1.254770	0.189295
C	4.443053	1.987321	-1.149839
C	-4.927226	1.234153	1.513010
C	-4.742048	2.439083	-0.348457

C	-5.577718	2.407187	1.660751
H	0.380851	0.431749	0.759863
H	-1.790160	-3.156098	-1.157602
H	1.830807	-0.493153	1.818247
H	-0.030035	1.072647	-2.134503
H	0.523837	2.290134	-1.004394
H	-1.377269	2.177145	0.348387
H	-2.040177	1.976967	-1.255302
H	2.115496	1.862212	1.340876
H	2.252035	-2.908223	1.469025
H	2.634902	-2.587681	-0.222327
H	-3.576879	0.374885	-1.561396
H	0.494964	-0.925963	-2.823125
H	1.656816	-1.982603	-2.015928
H	0.035032	-2.540906	-2.324613
H	3.226707	-0.961184	-1.655662
H	2.357877	0.448539	-2.248889
H	-2.302221	0.841766	2.007590
H	-2.680026	-0.867961	1.770767
H	-1.016595	-0.346491	1.822861
H	3.745287	3.394169	0.258371
H	2.541118	2.916699	-0.939910
H	5.001204	-1.068709	-0.237491
H	5.985617	-0.788758	1.194632
H	5.010155	-2.256567	1.076808
H	3.228012	-0.141715	3.576746
H	3.832980	-1.780521	3.275328
H	4.967569	-0.432553	3.420599
H	-4.861660	0.439831	2.235800
H	-4.578785	2.889180	-1.312359
H	-6.145423	2.840523	2.464357

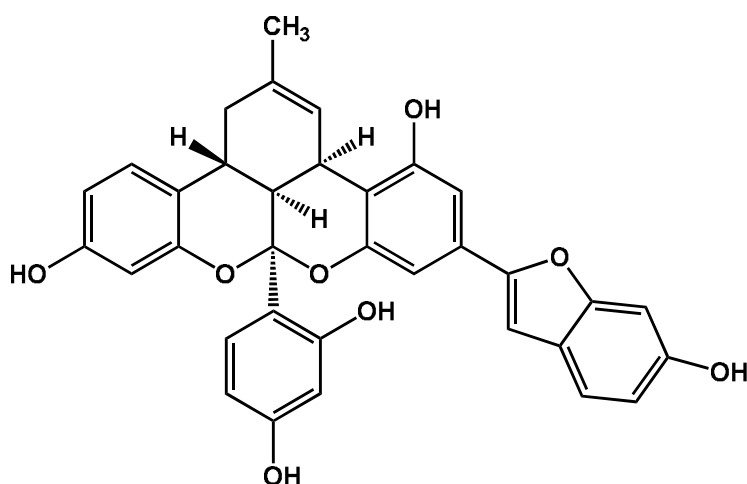
Equilibrium geometry of matopensine (13)



O	0.000000	0.000000	2.415838
N	0.546855	1.412037	0.641547
N	4.247457	0.364652	-1.715275
C	1.879052	0.852221	0.956094
C	2.799674	1.501048	-0.087960
C	1.859927	-0.673920	1.053734
C	-0.476838	1.081532	1.627294
C	2.841561	0.732739	-1.468123
C	2.303187	-1.370187	-0.253873
C	1.950367	-0.499241	-1.463950
C	4.269070	1.553663	0.354113
C	2.119369	2.845074	-0.208717
C	0.805144	2.738349	0.268427
C	5.040300	1.317412	-0.944930
C	3.804224	-1.652086	-0.268249
C	4.542106	-1.045264	-1.439338
C	2.605494	4.050023	-0.663790
C	0.000000	3.864512	0.354665
C	4.440341	-2.415482	0.615797
C	1.785799	5.180175	-0.620776
C	0.505448	5.081727	-0.103897
C	3.837563	-3.175576	1.757148
H	2.181287	1.251929	1.932946
H	2.575675	-0.931796	1.831854
H	-0.596729	1.915794	2.327130
H	2.524848	1.428037	-2.246944
H	1.778277	-2.316938	-0.350937
H	2.084497	-1.054191	-2.391835
H	0.909952	-0.202015	-1.408751
H	4.472234	0.742463	1.055450
H	4.516037	2.494141	0.843009
H	5.110431	2.249952	-1.510523
H	6.051591	0.946670	-0.793746
H	4.282730	-1.619586	-2.332876

H	5.616942	-1.153340	-1.307126
H	3.621135	4.128114	-1.030121
H	-0.993146	3.826173	0.774801
H	5.514014	-2.528033	0.500626
H	2.157480	6.132431	-0.969505
H	-0.117881	5.962617	-0.043121
H	2.751226	-3.136534	1.760808
H	4.133354	-4.223873	1.712614
H	4.186895	-2.790351	2.716985
N	-0.546855	-1.412037	0.641547
N	-4.247457	-0.364652	-1.715275
C	-1.879052	-0.852221	0.956094
C	-2.799674	-1.501048	-0.087960
C	-1.859927	0.673920	1.053734
C	0.476838	-1.081532	1.627294
C	-2.841561	-0.732739	-1.468123
C	-2.303187	1.370187	-0.253873
C	-1.950367	0.499241	-1.463950
C	-4.269070	-1.553663	0.354113
C	-2.119369	-2.845074	-0.208717
C	-0.805144	-2.738349	0.268427
C	-5.040300	-1.317412	-0.944930
C	-3.804224	1.652086	-0.268249
C	-4.542106	1.045264	-1.439338
C	-2.605494	-4.050023	-0.663790
C	-0.000000	-3.864512	0.354665
C	-4.440341	2.415482	0.615797
C	-1.785799	-5.180175	-0.620776
C	-0.505448	-5.081727	-0.103897
C	-3.837563	3.175576	1.757148
H	-2.181287	-1.251929	1.932946
H	-2.575675	0.931796	1.831854
H	0.596729	-1.915794	2.327130
H	-2.524848	-1.428037	-2.246944
H	-1.778277	2.316938	-0.350937
H	-2.084497	1.054191	-2.391835
H	-0.909952	0.202015	-1.408751
H	-4.472234	-0.742463	1.055450
H	-4.516037	-2.494141	0.843009
H	-5.110431	-2.249952	-1.510523
H	-6.051591	-0.946670	-0.793746
H	-4.282730	1.619586	-2.332876
H	-5.616942	1.153340	-1.307126
H	-3.621135	-4.128114	-1.030121
H	0.993146	-3.826173	0.774801
H	-5.514014	2.528033	0.500626
H	-2.157480	-6.132431	-0.969505
H	0.117881	-5.962617	-0.043121
H	-2.751226	3.136534	1.760808
H	-4.133354	4.223873	1.712614
H	-4.186895	2.790351	2.716985

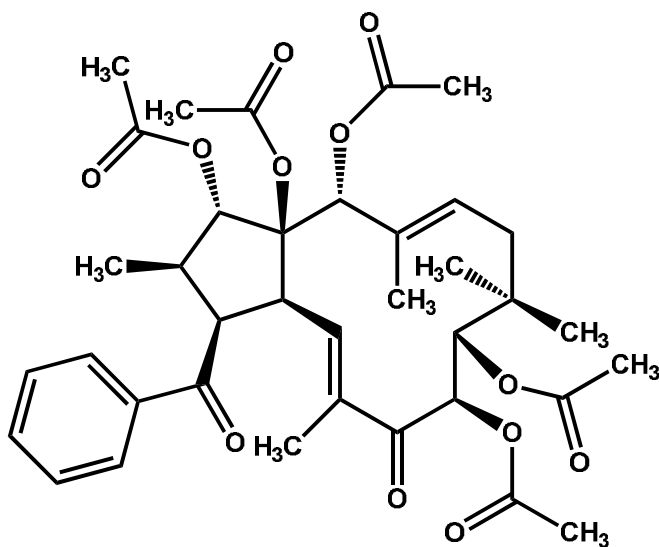
Equilibrium geometry of mulberrofuran G (14)



O	-3.167348	0.347493	-1.355271
O	-1.054098	-0.147690	-0.756672
O	0.923959	0.691685	3.547273
O	-0.594341	1.964002	-2.281951
O	-5.922384	-2.490449	-3.848427
O	4.774994	-0.265103	0.642972
O	-1.468443	6.208455	-0.275245
O	9.504759	-0.809774	-0.154773
C	-2.644899	-0.023646	0.993124
C	-2.845861	-1.532871	0.822177
C	-1.582552	0.259587	2.065746
C	-2.215317	0.573471	-0.346602
C	-3.428336	-2.106211	2.106569
C	-3.676832	-1.822157	-0.401980
C	-0.185117	0.159255	1.469000
C	-1.796354	-0.643441	3.264892
C	-2.645041	-1.666229	3.310813
C	-1.969520	2.074439	-0.336852
C	-3.777459	-0.878210	-1.420655
C	0.001246	-0.091682	0.105326
C	0.972294	0.322635	2.234918
C	-4.357778	-3.022584	-0.585057
C	-2.873886	-2.458366	4.562758
C	1.254385	-0.300558	-0.445877
C	-4.529572	-1.105149	-2.564147
C	-1.176557	2.703538	-1.305803
C	-2.606208	2.893575	0.593020
C	2.237269	0.114675	1.708088
C	2.381454	-0.225417	0.366533
C	-5.110571	-3.280697	-1.718018
C	-5.196751	-2.309483	-2.709765
C	-0.993954	4.083168	-1.286378
C	-2.447434	4.266013	0.618179
C	-1.621426	4.860889	-0.326817
C	3.703304	-0.469864	-0.196001

C	4.114963	-0.885380	-1.416676
C	5.550090	-0.954011	-1.362703
C	5.891041	-0.559735	-0.068398
C	6.576851	-1.301947	-2.244083
C	7.189551	-0.487021	0.405879
C	7.882700	-1.240832	-1.802750
C	8.184528	-0.837041	-0.493029
H	-3.598689	0.412467	1.296316
H	-1.858712	-1.986352	0.686704
H	-1.717949	1.288762	2.416273
H	-3.424005	-3.197423	2.074354
H	-4.477293	-1.808209	2.215547
H	-1.250600	-0.407082	4.170524
H	-4.299578	-3.784831	0.180226
H	-3.933814	-2.448826	4.827406
H	-2.302969	-2.064426	5.401412
H	-2.596962	-3.503481	4.409102
H	1.326440	-0.496352	-1.505955
H	-4.589738	-0.346447	-3.331649
H	-3.264111	2.451681	1.327571
H	3.096223	0.231806	2.351871
H	-5.627593	-4.224451	-1.833245
H	-0.365438	4.547096	-2.037828
H	-2.950454	4.877212	1.352916
H	0.064585	1.063562	3.765670
H	-0.102523	2.541083	-2.875459
H	-6.336596	-3.359271	-3.838817
H	3.482061	-1.125806	-2.253454
H	-0.881823	6.508525	-0.977380
H	6.357782	-1.614038	-3.255933
H	7.412617	-0.177742	1.417948
H	8.703427	-1.502551	-2.455820
H	9.609413	-0.516138	0.755875

Equilibrium geometry of 1 α ,8 β ,9 β ,14 α ,15 β -pentaacetoxy-3 β -benzoyloxy-7-oxojatropha-5,12-
diene (15)

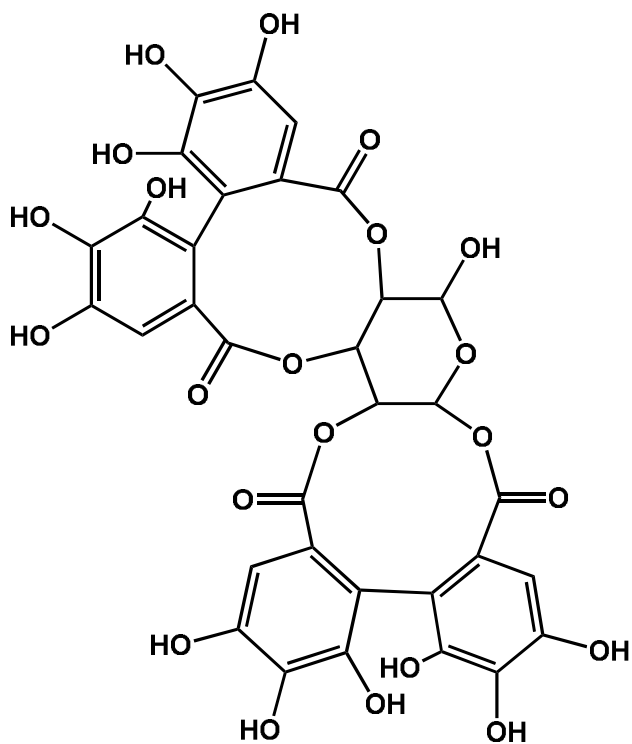


C	2.975370	0.820288	-0.836379
C	3.275052	-0.352941	0.102683
C	1.901057	-0.812702	0.709248
C	0.891778	0.253588	0.211829
C	1.757576	1.456967	-0.172784
C	4.148682	1.766222	-1.028125
O	2.149733	2.132976	1.031543
C	2.437976	3.449153	1.064568
O	3.270409	3.841679	1.834816
C	1.659956	4.377146	0.192231
C	2.327701	5.457142	-0.374509
C	1.627396	6.379596	-1.135199
C	0.256276	6.240108	-1.304103
C	-0.414311	5.173556	-0.719985
C	0.286528	4.233619	0.018975
O	4.096083	-1.422722	-0.341328
C	4.204528	-2.024529	-1.544010
O	4.553853	-3.174927	-1.540750
C	3.977093	-1.275413	-2.826441
O	1.932449	-0.692973	2.137064
C	2.832435	-1.359577	2.885592
O	3.615701	-2.149056	2.437821
C	2.712372	-0.963548	4.325346
C	1.492602	-2.247263	0.309544
C	0.185144	-2.722896	0.916646
C	0.313953	-3.282311	2.310673
C	-0.996496	-2.745460	0.299815
O	1.467740	-2.230509	-1.120077
C	1.531788	-3.376366	-1.841642
O	1.421819	-3.279192	-3.032424
C	1.749434	-4.669110	-1.114733
C	-1.376214	-2.287195	-1.085998

C	-2.882851	-2.179805	-1.401700
C	-3.655992	-1.129150	-0.582371
C	-3.569685	-3.528448	-1.158462
C	-3.013941	-1.831037	-2.888504
O	-3.457446	-1.360890	0.805922
C	-4.448156	-1.605190	1.688963
O	-4.135759	-1.762669	2.836197
C	-5.866047	-1.670942	1.196755
C	-3.375768	0.353104	-0.859705
C	-1.956906	0.848839	-0.524028
C	-1.476884	0.928930	0.884209
O	-1.253256	1.164284	-1.460146
O	-4.363983	1.047723	-0.102977
C	-4.766123	2.304678	-0.412968
O	-5.548267	2.831466	0.323395
C	-4.227192	2.935524	-1.664477
C	-0.205106	0.618281	1.159810
C	-2.406512	1.378228	1.980763
H	2.609415	0.459611	-1.794160
H	3.838973	0.054863	0.940655
H	0.495307	-0.106304	-0.732267
H	1.229919	2.130617	-0.839949
H	5.003114	1.257986	-1.470355
H	3.876627	2.597190	-1.678467
H	4.475440	2.168201	-0.069756
H	3.390891	5.564151	-0.212961
H	2.147810	7.211068	-1.587346
H	-0.291575	6.966071	-1.887431
H	-1.483443	5.076262	-0.839691
H	-0.230460	3.398120	0.473375
H	2.295799	-2.904483	0.641395
H	0.424285	-2.489296	3.049907
H	-0.571198	-3.853733	2.576725
H	1.186878	-3.931794	2.395602
H	-1.799646	-3.187260	0.874649
H	-0.997294	-3.012320	-1.812408
H	-0.884241	-1.355601	-1.350630
H	-4.709039	-1.250452	-0.836817
H	-3.623386	-3.783646	-0.101196
H	-4.585218	-3.516536	-1.555949
H	-3.020942	-4.321099	-1.665650
H	-2.667360	-2.669002	-3.491136
H	-4.051875	-1.631960	-3.159107
H	-2.411489	-0.962440	-3.153228
H	-3.514153	0.532047	-1.923276
H	0.091754	0.671985	2.198816
H	-3.227212	0.686050	2.138702
H	-1.847913	1.468206	2.908613
H	-2.842018	2.351856	1.752760
H	4.426261	-1.859337	-3.621805
H	2.908794	-1.202358	-3.019455

H	4.410962	-0.282114	-2.803762
H	3.361337	-1.586311	4.929094
H	2.997838	0.082049	4.427611
H	1.679800	-1.056872	4.654112
H	2.716495	-4.646348	-0.615253
H	0.974102	-4.828005	-0.368104
H	1.738099	-5.471052	-1.842670
H	-6.501862	-1.883461	2.047237
H	-6.156006	-0.723144	0.748019
H	-5.982739	-2.455775	0.451220
H	-4.580659	3.958332	-1.705717
H	-3.140186	2.913630	-1.694630
H	-4.591653	2.394357	-2.536919

Equilibrium geometry of pedunculagin (16)

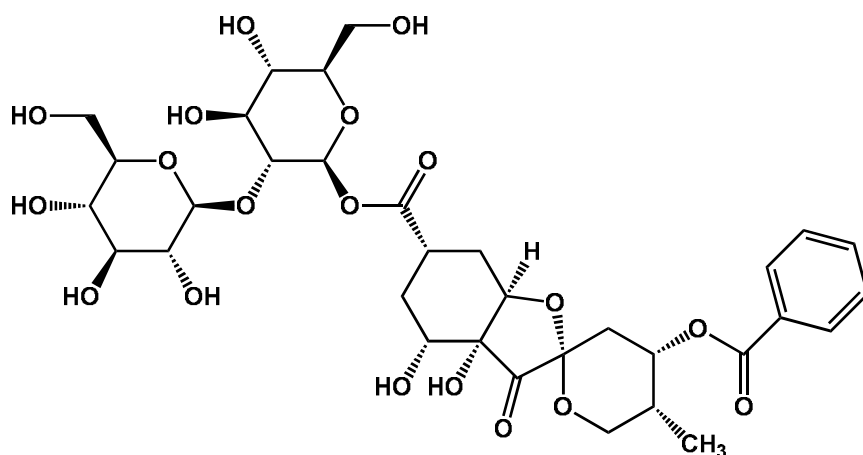


O	-3.109212	-2.666988	-0.936707
C	-4.103065	-2.063602	-0.257714
C	-4.650483	-0.894947	-1.006124
O	-4.494237	-2.421603	0.821285
C	-2.374676	-3.689140	-0.250169
C	-0.640452	-1.812589	-0.179639
C	-0.901401	-3.318478	-0.119155
O	-0.171945	-3.935345	-1.179194
C	1.216644	-3.818180	-1.067534
C	1.604392	-2.341258	-1.040349
C	0.837089	-1.591533	0.048396
H	1.631347	-4.296636	-1.955915
O	1.631323	-4.478527	0.099721

O	2.994479	-2.235349	-0.742386
C	3.676528	-1.185299	-1.274375
O	3.314139	-0.594384	-2.252274
C	4.873889	-0.861211	-0.451788
C	5.718370	-1.904255	-0.096870
C	6.849105	-1.651533	0.656868
C	7.113098	-0.351256	1.064496
C	6.250188	0.685944	0.730530
C	5.098435	0.457677	-0.026725
O	1.159808	-0.208431	-0.083712
C	2.205162	0.260220	0.637092
O	2.630031	-0.274554	1.623400
C	2.766514	1.487856	0.004417
C	4.138176	1.569214	-0.277082
C	4.581685	2.749016	-0.872431
C	3.715968	3.791427	-1.170774
C	2.361752	3.671471	-0.898002
C	1.883603	2.508659	-0.321494
O	5.904167	2.893964	-1.175596
O	4.250095	4.899294	-1.743440
O	1.602866	4.745085	-1.236824
O	6.595365	1.900617	1.250547
O	8.230314	-0.134644	1.800691
O	7.691762	-2.660344	0.984529
O	-1.427352	-1.182547	0.826379
C	-2.102348	-0.068015	0.461598
C	-3.130680	0.302777	1.471999
O	-1.905855	0.515693	-0.569156
C	-2.750761	0.386472	2.803627
C	-3.670863	0.789276	3.755180
C	-4.966422	1.097655	3.361274
C	-5.347889	0.985174	2.029350
C	-4.443603	0.565141	1.054719
C	-4.887407	0.317501	-0.342338
C	-5.492019	1.332251	-1.078013
C	-5.829947	1.163448	-2.413534
C	-5.551073	-0.034314	-3.054611
C	-4.952954	-1.064721	-2.350457
O	-3.305009	0.898652	5.055401
O	-5.838153	1.500361	4.318752
O	-6.662704	1.257399	1.783783
O	-5.757031	2.528044	-0.477552
O	-6.417251	2.209773	-3.045881
O	-5.913910	-0.090802	-4.362497
H	-2.458503	-4.607659	-0.826742
H	-2.812739	-3.834020	0.731424
H	-0.931708	-1.428886	-1.156237
H	-0.540768	-3.712046	0.833318
H	1.395723	-1.896494	-2.012393
H	1.128245	-1.943099	1.037815
H	2.559087	-4.272941	0.265018

H	5.512928	-2.915959	-0.416713
H	0.826506	2.400720	-0.115840
H	6.037525	3.742829	-1.619659
H	3.549665	5.537331	-1.930695
H	0.675356	4.592633	-1.027450
H	6.528679	2.572308	0.553083
H	8.288207	0.810793	1.996084
H	8.422107	-2.304691	1.506462
H	-1.738162	0.160848	3.107088
H	-4.746226	-2.006286	-2.841280
H	-4.065501	1.191928	5.573233
H	-6.685642	1.699119	3.897984
H	-6.729264	1.800826	0.983221
H	-6.145029	3.131936	-1.125595
H	-6.583880	1.977768	-3.968542
H	-5.698815	-0.948312	-4.744010

Equilibrium geometry of phyllaemblicin B (17)

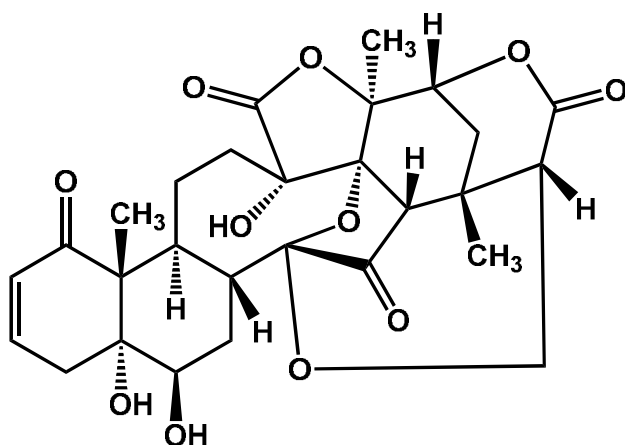


C	5.952244	-2.751371	-0.697872
C	4.773768	-3.099797	-1.597719
O	3.563632	-2.830077	-0.898154
C	3.418332	-1.475716	-0.577265
C	4.507550	-1.051135	0.403427
C	5.867931	-1.298572	-0.250431
O	4.298900	0.277948	0.859859
C	4.679863	1.312113	0.019796
O	6.044114	1.583679	0.247160
C	6.561631	2.593951	-0.605742
C	5.830694	3.902892	-0.327926
C	4.331446	3.700781	-0.483956
C	3.855383	2.538725	0.367438
O	2.171766	-1.329791	0.060043
C	1.079243	-1.299727	-0.739613
C	-0.192042	-1.228895	0.061521
O	1.145617	-1.335864	-1.937619
C	-0.391865	-2.522047	0.860732

C	-1.750839	-2.508800	1.542279
C	-1.911768	-1.286637	2.469655
C	-1.462192	0.034016	1.834740
C	-0.193870	-0.031895	1.013869
O	-2.569037	0.391167	0.999115
C	-3.766332	0.146783	1.701007
C	-3.403045	-1.018246	2.634439
O	-4.129301	-1.568583	3.409721
C	-4.919043	-0.118254	0.732066
C	-5.911285	1.037127	0.787863
C	-5.203022	2.384526	0.733795
C	-4.258924	2.461971	1.952773
O	-4.061449	1.194992	2.589374
C	-4.465186	2.618940	-0.582339
O	-6.811538	0.979527	-0.329347
C	-7.819343	0.105174	-0.270888
O	-7.991108	-0.651545	0.654395
C	-8.703990	0.176746	-1.465885
C	-9.765147	-0.719517	-1.552504
C	-10.617741	-0.678638	-2.643655
C	-10.412440	0.259065	-3.648772
C	-9.353488	1.153949	-3.563685
C	-8.496606	1.114007	-2.474485
C	8.041058	2.674847	-0.322400
O	8.578882	1.383745	-0.563820
C	4.762594	-4.547798	-2.025668
O	4.833967	-5.372676	-0.875594
O	2.489134	2.322366	0.089665
O	3.710239	4.916829	-0.119443
O	6.304901	4.876871	-1.231913
O	6.948620	-1.066903	0.623331
O	7.142540	-2.972208	-1.421984
H	-0.331171	-3.395814	0.209416
O	-1.251518	-1.492866	3.687238
H	5.915553	-3.391109	0.189976
H	4.821206	-2.481585	-2.503437
H	3.430273	-0.869633	-1.489401
H	4.420473	-1.675098	1.294147
H	5.970420	-0.669908	-1.143991
H	4.526172	1.056398	-1.038550
H	6.406725	2.306788	-1.654388
H	6.032629	4.204831	0.707389
H	4.120089	3.470630	-1.536052
H	4.012578	2.767295	1.427160
H	-0.997950	-1.126224	-0.663206
H	0.388048	-2.617327	1.618480
O	-2.813285	-2.464194	0.599601
H	-1.855352	-3.390984	2.181067
H	-1.347620	0.773039	2.632611
H	-0.094083	0.906841	0.465510
H	0.646886	-0.116518	1.706077

H	-5.417772	-1.048240	0.998302
H	-4.517300	-0.224755	-0.273677
H	-6.501466	0.969471	1.700992
H	-5.964750	3.156898	0.844088
H	-4.674649	3.094103	2.733063
H	-3.290648	2.867773	1.652918
H	-4.026725	3.616693	-0.583007
H	-3.656526	1.901344	-0.718845
H	-5.144287	2.546960	-1.430515
H	-9.910368	-1.441100	-0.760758
H	-11.441255	-1.375728	-2.711888
H	-11.078753	0.291644	-4.500107
H	-9.195982	1.883690	-4.345653
H	-7.671639	1.807726	-2.401561
H	8.490840	3.426331	-0.972808
H	8.190339	2.968320	0.720911
H	9.525110	1.402576	-0.397570
H	3.843339	-4.734653	-2.585889
H	5.617327	-4.716562	-2.684092
H	4.786936	-6.290806	-1.153828
H	2.183431	1.605935	0.657286
H	2.764188	4.838611	-0.280401
H	5.752061	5.660455	-1.135177
H	7.194864	-0.133340	0.547843
H	7.863354	-2.598530	-0.901606
H	-1.752521	-2.133696	4.207419
H	-2.854052	-3.303475	0.131165

Equilibrium geometry of physalin D (**18**)

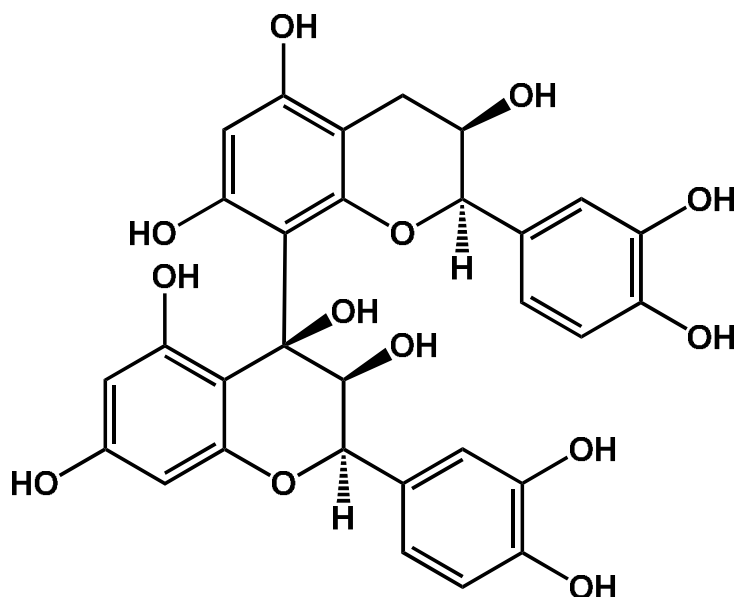


C	-5.942961	0.451842	-0.844269
C	-5.339127	-0.918064	-0.866466
C	-3.816483	-0.873677	-0.762625
C	-3.361891	0.087839	0.379363
C	-3.842978	1.457936	-0.101098
C	-5.265122	1.544774	-0.490017
C	-3.216241	-2.271138	-0.621847

C	-1.699852	-2.199479	-0.548163
C	-1.212279	-1.299199	0.588303
C	-1.824672	0.114374	0.501054
O	-3.108913	2.425727	-0.205480
C	0.307331	-1.182450	0.515089
C	1.010103	-0.636587	1.759106
C	2.111234	0.237686	1.238901
C	1.473145	0.755046	-0.057834
C	0.592769	2.006121	0.206053
C	-0.218495	2.048952	1.491462
C	-1.394387	1.042271	1.670167
O	0.775126	-0.948768	2.892455
O	0.704964	-0.334051	-0.541344
O	0.910469	-2.458193	0.368455
C	3.417448	-0.576228	1.037266
C	3.377784	-1.831015	0.088419
C	2.058099	-2.505648	-0.448132
C	4.391922	0.433374	0.433784
C	3.947984	0.736883	-0.975393
C	2.508288	1.284712	-1.089467
C	1.671218	3.091202	0.135514
O	2.665883	2.668850	-0.665479
O	1.667217	4.177573	0.633586
C	4.122298	-1.648507	-1.219826
O	4.133349	-0.433468	-1.787566
C	2.041556	1.224099	-2.530865
O	4.584877	-2.578460	-1.826564
C	3.913177	-1.028380	2.410796
O	-3.270989	-0.401122	-1.999480
O	-3.774689	-2.886881	0.528807
C	-4.044088	-0.223055	1.728073
O	-0.225352	2.278280	-0.920153
H	-6.973659	0.543801	-1.165427
H	-5.608622	-1.422175	-1.797909
H	-5.762334	-1.523057	-0.062548
H	-5.699553	2.534065	-0.544118
H	-3.507035	-2.825950	-1.519677
H	-1.323072	-1.820918	-1.499921
H	-1.304987	-3.206901	-0.420771
H	-1.449819	-1.759686	1.551760
H	-1.473576	0.511478	-0.443733
H	2.344312	1.026828	1.951589
H	-0.624647	3.061818	1.522635
H	0.450319	1.987466	2.349074
H	-2.242577	1.657419	1.945889
H	-1.195903	0.422713	2.542867
H	3.916452	-2.615315	0.615105
H	2.281338	-3.561973	-0.564387
H	1.815303	-2.107128	-1.431663
H	4.414784	1.346028	1.028946
H	5.406569	0.030938	0.406906

H	4.584476	1.489640	-1.437268
H	2.823989	1.620019	-3.177618
H	1.849995	0.190548	-2.811914
H	1.131541	1.798149	-2.662976
H	3.976079	-0.181612	3.094802
H	3.248504	-1.773846	2.846705
H	4.906120	-1.467743	2.316418
H	-3.860321	0.255550	-2.385161
H	-3.442960	-3.788049	0.581918
H	-3.609107	-1.115058	2.170414
H	-3.919211	0.604119	2.423748
H	-5.111667	-0.389961	1.616300
H	-1.130928	2.460779	-0.621948

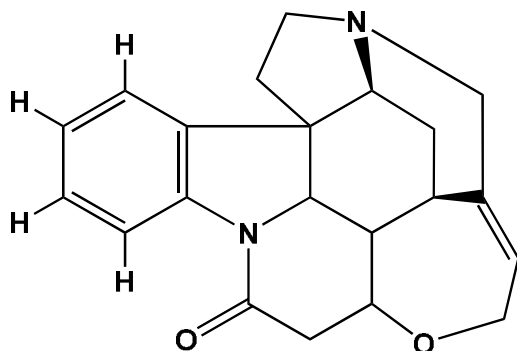
Equilibrium geometry of procyanidin B2 (19)



C	1.259532	3.094442	0.552592
C	0.671982	4.344187	0.683580
C	-0.702691	4.458426	0.569712
C	-1.511641	3.352246	0.304461
C	-0.882536	2.113959	0.197607
C	0.499785	1.941846	0.343059
C	-2.999874	3.495927	0.112038
C	-3.596386	2.240910	-0.514988
C	-3.005355	1.028455	0.190522
O	-1.595967	0.989463	-0.094446
O	-1.225256	5.702966	0.712051
O	2.610516	2.945403	0.631377
C	-3.561560	-0.316830	-0.201850
C	-4.664621	-0.460068	-1.037043
C	-2.950588	-1.451199	0.319261
C	-3.426620	-2.716775	0.010366
C	-4.526032	-2.853517	-0.819066

C	-5.148074	-1.720726	-1.341483
O	-6.227025	-1.847847	-2.161537
O	-5.076169	-4.047936	-1.186807
C	1.182313	0.595443	0.208047
C	1.245163	0.194185	-1.265893
C	0.610074	-0.552279	1.021478
C	0.608657	-1.846424	0.501223
O	1.095986	-2.151337	-0.736666
C	1.891409	-1.188330	-1.418160
C	0.127912	-0.407333	2.330680
C	-0.369265	-1.478254	3.058407
C	-0.373962	-2.742215	2.488779
C	0.119694	-2.938993	1.211024
C	3.342558	-1.230777	-0.992926
C	3.747658	-1.730180	0.238066
C	4.305128	-0.730450	-1.871486
C	5.640506	-0.709609	-1.517409
C	5.092168	-1.715697	0.595322
C	6.036189	-1.202697	-0.272330
O	7.375996	-1.144107	-0.018248
O	6.564528	-0.220947	-2.385548
H	-2.184964	5.683120	0.639349
H	3.026275	3.795059	0.810677
H	1.269191	5.227048	0.868382
H	-3.227713	4.334006	-0.550823
H	-3.495087	3.688469	1.067881
H	-3.117548	1.169487	1.271645
H	-6.422599	-2.786442	-2.272321
H	-4.584097	-4.781535	-0.804946
H	2.217131	0.739453	0.534391
H	0.147370	-3.919550	0.755209
H	1.829022	-1.464442	-2.470584
H	4.023987	-0.362847	-2.850137
H	3.028849	-2.145680	0.929273
H	5.408089	-2.108637	1.553521
H	7.437979	-0.290261	-1.980098
H	7.575448	-1.504009	0.851939
H	-2.944783	-3.598729	0.416090
H	-2.092388	-1.345830	0.968455
H	-5.159031	0.393005	-1.479868
O	-3.349142	2.187549	-1.907932
H	-2.451817	1.864877	-2.051935
H	-4.677686	2.253240	-0.388026
O	1.908005	1.163701	-2.045327
H	2.727891	1.415863	-1.603821
H	-0.744603	-1.321568	4.058981
O	-0.876265	-3.762372	3.236811
H	-0.821051	-4.589314	2.747113
O	0.130621	0.788464	2.978158
H	0.345097	1.504586	2.365299
H	0.231275	0.120580	-1.662277

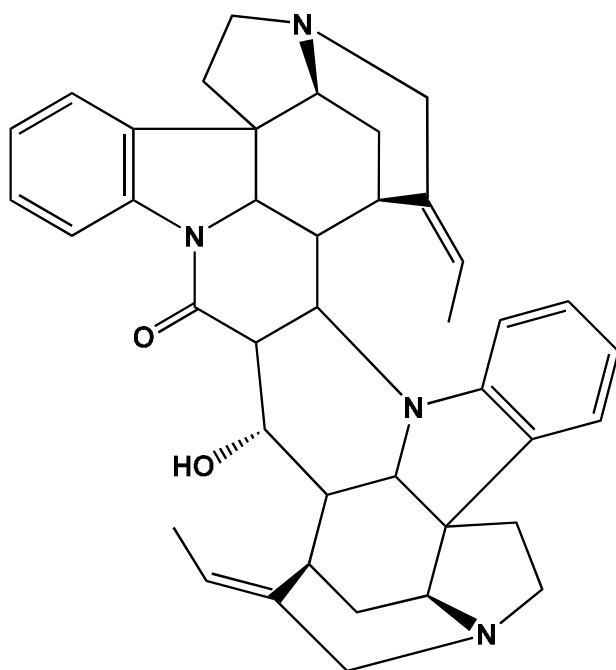
Equilibrium geometry of strychnine (20)



O	-0.433610	6.038797	-0.009786
O	4.162485	6.001808	0.994590
N	2.533037	4.897923	2.166640
N	-1.182535	2.443235	3.222202
C	0.189887	2.081242	2.770606
C	0.232166	1.747976	1.287865
C	-0.223225	2.975923	0.497402
C	0.881655	4.023668	0.660817
C	1.134892	4.409428	2.116061
C	3.338655	3.961534	2.841997
C	4.725223	3.944259	2.986813
C	5.287136	2.877452	3.693057
C	4.492928	1.868911	4.241361
C	3.103674	1.909748	4.098095
C	2.530735	2.960597	3.392051
C	1.083047	3.272531	3.166100
C	0.365431	3.755082	4.436022
C	-1.095176	3.680074	4.019419
C	-2.142351	2.566483	2.116735
C	-1.585913	3.406475	1.002781
C	-2.213573	4.486199	0.515471
C	-1.580067	5.353261	-0.528550
C	0.791555	5.323477	-0.145598
C	1.859095	6.322318	0.343125
C	2.974146	5.733260	1.173485
H	0.528954	1.215432	3.347011
H	-0.402002	0.885077	1.081933
H	1.251190	1.470764	1.009118
H	-0.298540	2.728641	-0.567707
H	1.800771	3.535868	0.308249
H	0.453314	5.217219	2.395731
H	5.334142	4.724921	2.562209
H	6.361323	2.838028	3.814471
H	4.954744	1.055862	4.784347
H	2.485285	1.135557	4.534824
H	0.572158	3.058375	5.250661
H	0.680491	4.753756	4.739421
H	-1.777927	3.637917	4.867963

H	-1.361424	4.558083	3.415356
H	-3.061135	3.003377	2.509436
H	-2.391182	1.566830	1.754289
H	-3.182228	4.770032	0.910912
H	-1.284477	4.765429	-1.405329
H	-2.266070	6.130165	-0.858329
H	0.942686	5.089714	-1.205493
H	2.305773	6.873105	-0.479305
H	1.329257	7.038595	0.976108

Equilibrium geometry of strychnobailonine (21)

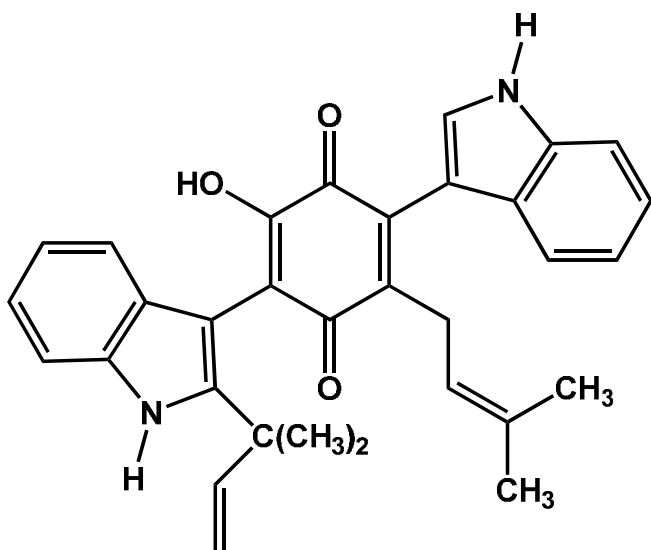


O	1.226924	2.680840	1.849197
O	-1.111705	3.429238	0.772890
N	-2.304949	1.611534	0.132811
N	-4.644151	-2.384122	-0.240140
N	1.116773	-0.748764	0.319312
N	5.200814	-0.129625	-1.459283
C	-5.376803	3.624259	0.823201
C	-6.304697	2.692637	0.378494
C	-5.880006	1.459546	-0.108275
C	-4.526833	1.180701	-0.152370
C	-3.608298	2.128467	0.289286
C	-4.010975	3.360334	0.786520
C	-3.829325	-0.089099	-0.577905
C	-2.363007	0.391194	-0.706021
C	-1.150415	2.281897	0.341456
C	0.093869	1.477757	0.017406
C	-0.117571	0.017778	0.466097
C	-1.227792	-0.615691	-0.401591
C	-4.359219	-0.691615	-1.891234

C	-5.286079	-1.812756	-1.420431
C	-4.082899	-1.233159	0.485834
C	-2.817518	-1.616475	1.238822
C	-1.724052	-1.936551	0.215392
C	-0.054069	-3.224850	-2.034742
C	-1.512349	-3.464317	-1.780683
C	-2.247860	-2.939588	-0.803330
C	-3.652928	-3.424568	-0.537388
C	1.371128	2.164501	0.538485
C	2.539206	1.184338	0.596433
C	2.276272	-0.050177	-0.261501
C	1.621093	-1.604807	1.296787
C	3.421113	-1.088763	-0.171414
C	2.975578	-1.871328	1.042013
C	0.987287	-2.167614	2.396364
C	1.719472	-3.029978	3.212910
C	3.047812	-3.321723	2.948340
C	3.683190	-2.730555	1.853140
C	3.923675	1.807155	0.371221
C	4.947173	0.767331	0.822881
C	4.827853	-0.440883	-0.078108
C	4.829801	-1.357710	-2.169933
C	3.554117	-1.919776	-1.472586
C	4.498725	1.037643	-2.027307
C	4.230866	2.178632	-1.061158
C	4.271078	3.430875	-1.515081
C	3.945191	4.692538	-0.776115
H	-3.290344	4.084825	1.125464
H	-2.511872	-0.789588	1.883580
H	-4.840528	-0.868685	1.181464
H	-6.256180	-1.404449	-1.126631
H	-4.851376	0.055665	-2.512391
H	-3.608945	-4.094528	0.327206
H	-6.604148	0.731046	-0.450069
H	-7.360391	2.923887	0.411036
H	-5.716182	4.578517	1.202646
H	0.168609	1.466858	-1.077589
H	-0.414970	0.021376	1.520569
H	0.438057	-2.730997	-1.197606
H	0.452575	-4.173905	-2.216108
H	-2.242302	0.735720	-1.737498
H	-0.869272	-2.399292	0.708932
H	-4.014998	-4.024112	-1.371704
H	-1.997096	-4.173853	-2.445923
H	-3.530653	-1.120635	-2.458634
H	-5.464276	-2.577616	-2.173676
H	-3.021746	-2.467774	1.888720
H	-0.747099	-0.837510	-1.354152
H	0.102492	-2.611288	-2.926976
H	1.602147	2.981166	-0.156270
H	0.498019	3.315017	1.813535

H	3.612591	4.518639	0.244429
H	4.811888	5.355830	-0.746144
H	3.153132	5.236292	-1.295061
H	4.560735	3.573583	-2.553338
H	5.093683	1.412971	-2.860662
H	3.540603	0.724756	-2.463666
H	4.759548	0.480683	1.859035
H	5.961837	1.161606	0.757668
H	3.996525	2.689303	1.004626
H	2.542296	0.821535	1.630193
H	2.057075	0.213751	-1.294702
H	-0.044561	-1.945668	2.633399
H	1.234965	-3.473439	4.072613
H	3.595366	-3.993753	3.593973
H	4.726534	-2.942102	1.651459
H	3.676385	-2.977873	-1.245198
H	5.645577	-2.074754	-2.074225
H	2.661229	-1.820954	-2.090236
H	4.685803	-1.156359	-3.230042
H	5.517286	-1.221272	0.258906

Equilibrium geometry of terrequinone A (22)

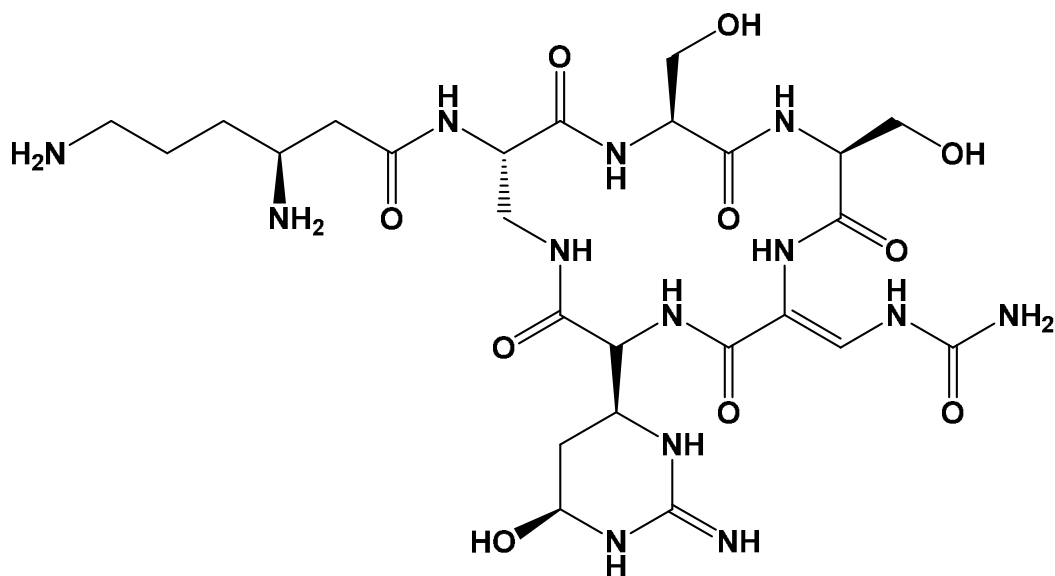


O	-1.109757	0.842247	-1.908403
O	-1.679172	-2.033836	1.747446
O	0.841069	-2.659500	1.499915
N	-4.856105	1.001519	0.279797
N	4.743419	-2.486347	-0.678133
C	-2.847011	2.417670	0.752199
C	-3.486392	1.102770	0.364293
C	-2.938415	-0.118597	0.052502
C	-4.029026	-1.014084	-0.224397
C	-1.523822	-0.500073	-0.029227
C	-5.216920	-0.273438	-0.076796

C	-2.841815	3.360743	-0.455788
C	-3.653816	3.067827	1.894578
C	-1.459960	2.164472	1.297480
C	-0.662144	0.070644	-1.084003
C	0.796418	-0.307860	-1.160900
C	1.321022	-1.203393	-0.309952
C	-0.988850	-1.428294	0.779594
C	-4.102455	-2.362518	-0.588493
C	-6.474594	-0.838712	-0.278740
C	2.752104	-1.549397	-0.275116
C	0.447010	-1.832424	0.700486
C	1.612418	0.412194	-2.197019
C	3.737272	-0.898413	0.541838
C	-5.345836	-2.928677	-0.790175
C	-6.520672	-2.172690	-0.635807
C	4.975089	-1.511486	0.258457
C	3.409773	-2.504631	-0.994639
C	-0.340709	2.748049	0.895844
C	2.099864	1.718402	-1.625158
C	3.687680	0.169651	1.444649
C	6.162970	-1.090339	0.856784
C	3.361174	2.083967	-1.400495
C	4.860786	0.592719	2.033910
C	6.086970	-0.034319	1.742160
C	3.667819	3.411466	-0.766122
C	4.578969	1.271119	-1.729670
H	-5.502521	1.744359	0.484223
H	-2.234051	2.953620	-1.261866
H	-2.449420	4.337128	-0.169520
H	-3.858744	3.500022	-0.822681
H	-4.656289	3.347459	1.569179
H	-3.148299	3.977880	2.215379
H	-3.738540	2.396073	2.748738
H	-1.425967	1.466701	2.130159
H	-3.198500	-2.947208	-0.706038
H	-7.377229	-0.254591	-0.160993
H	2.438943	-0.219238	-2.506045
H	0.978781	0.605730	-3.062028
H	-5.422083	-3.970411	-1.070520
H	-7.479732	-2.644711	-0.799905
H	3.026143	-3.202957	-1.719359
H	0.603323	2.538943	1.382195
H	-0.321982	3.450536	0.072535
H	5.439348	-3.092170	-1.078299
H	1.309176	2.408300	-1.346334
H	-1.068460	-2.641310	2.198707
H	2.746734	0.660703	1.659840
H	7.105875	-1.567600	0.627146
H	4.844604	1.420394	2.729878
H	6.989081	0.321297	2.220972
H	4.199162	3.256367	0.176968

H	2.764145	3.985151	-0.566544
H	4.325745	4.004298	-1.405750
H	4.352483	0.274160	-2.100443
H	5.178792	1.793464	-2.479310
H	5.201761	1.166040	-0.837259

Equilibrium geometry of viomycin (23)



O	6.441226	-3.610173	0.960422
O	2.531476	-3.420217	-0.033416
O	-1.206663	-1.198041	-2.592761
O	2.619322	-0.259604	1.613239
O	-2.095408	-2.561678	2.313012
O	-5.270592	1.983455	-2.829879
O	-2.865375	2.681514	-1.308139
O	-0.212447	0.891800	-0.464688
O	0.861491	4.626766	-2.166782
O	2.547402	3.922850	4.240783
N	5.503255	-0.380676	-0.361011
N	2.797459	0.053045	-0.617970
N	7.401281	-1.769552	-0.194214
N	0.979817	-1.971947	-0.803966
N	-2.516316	-2.851721	0.114892
N	-2.967050	-0.480421	-1.366091
N	7.625750	0.532694	-0.259465
N	-6.486193	-3.835167	1.581042
N	-1.336432	1.772068	-2.723610
N	1.409077	2.460447	-0.393242
N	-7.510256	1.431374	1.152819
N	1.705283	3.800649	2.124305
N	1.390854	5.685505	3.407879
C	4.677119	-1.575126	-0.256333
C	3.301864	-1.279413	-0.880073
C	5.344520	-2.757806	-0.953228

C	6.689321	-3.016010	-0.305545
C	2.239161	-2.329963	-0.505782
C	-1.412233	-2.034028	-0.336379
C	-0.154728	-2.849757	-0.612925
C	6.769822	-0.557851	-0.290779
C	-5.305314	-3.048711	1.223402
C	-4.063969	-3.807308	1.710607
C	-5.391298	-1.661897	1.849197
C	-1.842607	-1.203895	-1.549895
C	2.511322	0.472042	0.636331
C	-2.794579	-3.037104	1.431781
C	-3.394562	0.551992	-2.296504
C	-6.520152	-0.810122	1.281793
C	2.024108	1.872958	0.741548
C	-0.191562	2.516317	-2.246596
C	-2.515454	1.787096	-2.063271
C	-6.446811	0.629953	1.761805
C	-4.859603	0.883772	-2.048886
C	0.313268	1.882659	-0.943075
C	-0.426370	4.022786	-2.124494
C	2.156695	2.529617	1.898437
C	1.921830	4.448160	3.334898
H	4.521047	-1.826399	0.795372
H	3.410180	-1.343200	-1.966258
H	4.734737	-3.653377	-0.882387
H	5.501889	-2.513753	-2.006599
H	7.293659	-3.695313	-0.907966
H	2.901646	0.748643	-1.337630
H	8.404998	-1.787424	-0.125002
H	-1.190745	-1.324182	0.463910
H	0.040356	-3.484745	0.249309
H	-0.309759	-3.490730	-1.484314
H	0.808840	-1.046740	-1.170149
H	-5.222889	-2.917216	0.135492
H	-4.017044	-4.782180	1.219934
H	-4.130324	-3.964533	2.785562
H	-3.078634	-3.330827	-0.571034
H	-5.501600	-1.772874	2.931873
H	-4.443245	-1.139486	1.684686
H	7.283484	-3.798919	1.385639
H	-3.255777	0.181588	-3.311585
H	-7.492116	-1.224646	1.564890
H	-6.475524	-0.819895	0.188297
H	-3.352260	-0.449895	-0.432761
H	7.163439	1.386907	-0.531455
H	8.509706	0.406706	-0.730100
H	0.600309	2.392527	-2.987863
H	-6.438282	-4.749389	1.144687
H	-7.321571	-3.393696	1.214741
H	-6.472775	0.644293	2.857990
H	-5.487360	1.059454	1.463133

H	-5.013953	1.083467	-0.983893
H	-5.471579	0.028495	-2.329912
H	-1.115298	0.888601	-3.165903
H	1.777205	3.297828	-0.830311
H	-0.940924	4.266252	-1.196644
H	-1.040920	4.345867	-2.966389
H	2.661158	2.063230	2.731489
H	-7.450371	2.390614	1.472701
H	-8.413379	1.088285	1.461298
H	-4.857543	2.769880	-2.455071
H	1.167589	4.260711	1.404836
H	0.780464	5.554058	-1.926269
H	0.866760	6.104959	2.660523
H	1.508526	6.199439	4.263021

Table S1. Calculated ^1H NMR shielding constants, together with scaled and experimental chemical shifts – the GIAO-DFT(PBE0) calculations with the first-level basis sets.

Mol.	pcS-1		pecS-1		pecS-1 mod		$\delta_{exp}^{[b]}$
	σ	$\delta_{scaled}^{[a]}$	σ	$\delta_{scaled}^{[a]}$	σ	$\delta_{scaled}^{[a]}$	
1	28.71	2.88	28.3	3.39	28.4	3.36	4.38
	30.19	1.52	30.1	1.74	30.1	1.75	2.51
	30.60	1.15	30.5	1.36	30.6	1.34	2.31
	29.09	2.53	28.9	2.89	28.9	2.88	3.53
	28.92	2.69	28.9	2.85	29.0	2.84	3.21
	27.69	3.82	27.8	3.91	27.8	3.96	4.03
	29.15	2.48	29.0	2.71	29.1	2.72	3.18
	28.63	2.96	28.7	3.02	28.8	3.01	3.34
	28.66	2.93	28.9	2.87	28.9	2.88	3.24
	28.98	2.64	29.1	2.63	29.1	2.66	2.80
	28.67	2.92	28.6	3.11	28.7	3.09	3.00
	28.31	3.25	28.3	3.37	28.4	3.37	3.27
	25.71	5.64	25.9	5.71	25.9	5.69	5.42
	23.79	7.42	24.2	7.31	24.2	7.30	7.45
	24.38	6.87	24.7	6.76	24.8	6.76	7.25
	29.33	2.31	29.6	2.15	29.7	2.17	0.99
	29.71	1.96	30.2	1.67	30.2	1.69	0.99
	29.75	1.93	30.2	1.65	30.2	1.67	0.99
	24.26	6.98	24.5	6.94	24.6	6.93	7.01
	24.29	6.96	24.6	6.92	24.6	6.90	7.05
	23.37	7.80	23.7	7.72	23.7	7.71	7.81
	22.81	8.32	23.1	8.26	23.2	8.22	8.11
	23.60	7.59	24.1	7.34	24.1	7.37	7.47
	23.81	7.39	24.3	7.21	24.3	7.20	7.40
	24.06	7.17	24.5	7.02	24.5	7.02	7.10
2	24.33	6.92	24.53	6.96	24.57	6.94	6.94

	23.84	7.37	24.22	7.25	24.23	7.26	7.62
	24.00	7.23	24.28	7.20	24.31	7.18	7.09
	24.12	7.11	24.40	7.08	24.44	7.06	7.19
	23.68	7.52	23.81	7.64	23.81	7.65	7.36
	24.91	6.38	24.94	6.58	24.95	6.58	6.94
	23.97	7.25	24.15	7.32	24.19	7.29	7.36
	24.31	6.94	24.60	6.90	24.64	6.87	7.19
	24.12	7.11	24.40	7.09	24.43	7.07	7.09
	23.98	7.24	24.36	7.12	24.38	7.12	7.62
	23.40	7.78	23.70	7.75	23.72	7.73	7.73
	24.30	6.95	24.64	6.86	24.66	6.86	6.89
	23.70	7.50	24.00	7.46	24.03	7.44	7.51
	24.34	6.91	24.71	6.79	24.70	6.81	6.91
3	27.33	4.16	26.94	4.69	27.00	4.67	4.18
	28.38	3.19	28.25	3.46	28.32	3.44	2.88
	29.55	2.11	29.52	2.26	29.63	2.21	2.20
	28.77	2.83	28.80	2.94	28.81	2.98	2.60
	28.88	2.72	28.91	2.84	28.97	2.83	2.35
	29.87	1.82	29.90	1.91	29.97	1.89	1.81
	30.17	1.54	30.23	1.59	30.30	1.59	1.51
	30.05	1.65	30.03	1.78	30.09	1.79	2.34
	25.38	5.95	25.43	6.12	25.43	6.14	6.40
	28.82	2.79	28.92	2.83	28.93	2.87	2.80
	29.94	1.76	29.98	1.83	30.06	1.81	1.97
	29.48	2.18	29.73	2.07	29.79	2.06	1.94
	29.84	1.84	29.90	1.91	29.96	1.90	1.57
	28.57	3.02	28.67	3.07	28.72	3.06	3.24
	27.63	3.88	27.65	4.03	27.66	4.06	3.80
	29.40	2.25	29.47	2.31	29.51	2.32	2.44
	29.16	2.47	29.34	2.43	29.40	2.43	2.54
	29.24	2.40	29.20	2.57	29.22	2.60	2.07
	29.24	2.40	29.39	2.39	29.45	2.38	2.31
	29.33	2.31	29.43	2.35	29.45	2.38	1.70
	30.22	1.49	30.27	1.56	30.36	1.53	1.61
	30.24	1.47	30.46	1.38	30.51	1.39	1.47
	30.31	1.41	30.46	1.38	30.51	1.39	1.47
	30.54	1.20	30.46	1.38	30.53	1.37	1.38
	30.13	1.58	30.29	1.54	30.36	1.53	1.38
	25.75	5.61	25.91	5.66	25.97	5.64	5.58
	29.22	2.41	29.46	2.32	29.50	2.33	2.56
	29.33	2.32	29.45	2.33	29.51	2.33	2.58
	29.90	1.79	30.06	1.75	30.14	1.74	1.86
	28.56	3.03	28.55	3.17	28.59	3.18	2.43
	26.02	5.37	26.17	5.42	26.24	5.38	5.47
	22.77	8.36	23.12	8.29	23.16	8.25	8.33
	23.27	7.89	23.58	7.85	23.61	7.84	8.02
	23.98	7.24	24.00	7.46	24.03	7.45	6.24
	22.84	8.29	23.28	8.14	23.30	8.13	8.23
	23.66	7.54	24.02	7.44	24.04	7.44	7.64
	25.40	5.93	25.61	5.95	25.64	5.94	5.75

	23.84	7.37	24.19	7.28	24.21	7.27	7.25
	23.58	7.61	23.89	7.57	23.92	7.55	7.56
4	27.62	3.89	27.55	4.12	27.62	4.09	4.11
	27.16	4.32	26.74	4.88	26.84	4.81	4.26
	28.61	2.97	28.39	3.33	28.48	3.29	2.76
	28.56	3.02	28.23	3.48	28.31	3.45	2.95
	24.02	7.20	24.12	7.34	24.15	7.34	7.56
	24.18	7.05	24.48	7.01	24.50	7.00	6.91
	23.77	7.44	24.06	7.40	24.10	7.38	7.19
	24.12	7.12	24.53	6.96	24.54	6.97	6.96
	28.54	3.04	28.39	3.33	28.48	3.29	2.79
	28.71	2.88	28.59	3.14	28.67	3.11	2.51
	30.68	1.07	30.53	1.32	30.65	1.26	0.72
	27.21	4.26	27.49	4.18	27.53	4.17	3.83
	27.37	4.12	27.58	4.09	27.60	4.11	4.05
	29.97	1.72	29.79	2.01	29.90	1.96	1.56
	29.77	1.91	29.77	2.03	29.82	2.03	1.62
	27.33	4.15	27.10	4.54	27.13	4.55	4.49
	27.35	4.14	27.84	3.85	27.85	3.88	3.78
	27.36	4.12	27.80	3.88	27.81	3.91	3.78
	27.40	4.09	27.81	3.88	27.82	3.90	3.78
	29.16	2.47	29.12	2.64	29.17	2.64	2.37
	28.59	3.00	28.76	2.98	28.78	3.01	2.88
	29.20	2.43	29.26	2.51	29.30	2.52	2.31
	28.35	3.22	28.54	3.19	28.58	3.20	3.09
	30.27	1.45	30.31	1.52	30.38	1.51	1.20
	28.44	3.13	28.57	3.16	28.62	3.16	2.74
	24.41	6.84	24.64	6.86	24.63	6.88	6.65
	25.13	6.18	25.44	6.11	25.44	6.13	5.85
	24.91	6.38	25.27	6.26	25.26	6.29	6.22
	29.45	2.21	29.67	2.12	29.73	2.12	1.95
	29.48	2.18	29.69	2.10	29.72	2.13	1.99
	27.90	3.63	27.97	3.73	28.04	3.70	3.54
	29.42	2.23	29.09	2.67	29.14	2.67	2.28
	30.63	1.12	30.60	1.25	30.69	1.22	1.07
	29.54	2.12	29.49	2.29	29.54	2.30	1.90
	27.01	4.45	27.37	4.29	27.37	4.32	4.01
	27.15	4.32	27.58	4.09	27.59	4.12	4.23
	28.61	2.98	28.74	3.00	28.77	3.02	2.07
	29.56	2.10	29.61	2.18	29.70	2.15	2.59
	28.95	2.66	28.50	3.23	28.59	3.19	2.80
	30.21	1.50	30.16	1.66	30.23	1.65	1.49
	29.20	2.43	29.06	2.70	29.21	2.61	2.15
	27.67	3.85	27.61	4.06	27.68	4.03	3.71
	27.63	3.87	27.58	4.09	27.68	4.04	3.83
	27.57	3.94	27.65	4.02	27.70	4.02	3.82
	27.42	4.07	27.44	4.22	27.50	4.20	3.92
	23.64	7.55	23.69	7.75	23.76	7.70	7.68
	23.74	7.46	23.92	7.53	23.96	7.51	7.26
	23.95	7.27	24.19	7.28	24.23	7.26	7.11

	23.70	7.50	23.95	7.51	23.99	7.48	7.33
	24.17	7.06	24.55	6.94	24.54	6.96	7.02
	28.05	3.50	27.97	3.73	28.06	3.68	3.46
	28.74	2.86	28.66	3.07	28.72	3.06	2.36
	29.05	2.57	29.01	2.75	29.07	2.73	2.66
	27.49	4.01	27.84	3.84	27.86	3.87	3.75
	27.43	4.06	27.72	3.96	27.76	3.96	3.75
	29.99	1.71	29.99	1.83	30.05	1.82	1.43
	29.84	1.84	29.86	1.94	29.93	1.93	1.60
	27.21	4.26	26.88	4.75	26.91	4.75	4.29
	27.64	3.87	28.06	3.64	28.08	3.66	3.69
	27.47	4.03	27.89	3.80	27.90	3.83	3.69
	27.50	4.00	27.98	3.72	27.98	3.75	3.69
	29.12	2.50	29.13	2.63	29.17	2.64	2.37
	28.57	3.02	28.77	2.98	28.77	3.01	2.88
	29.18	2.45	29.27	2.50	29.30	2.52	2.31
	28.34	3.23	28.56	3.17	28.58	3.19	3.09
	30.29	1.43	30.36	1.48	30.41	1.48	1.21
	28.47	3.10	28.64	3.09	28.68	3.10	2.75
	24.10	7.13	24.33	7.14	24.31	7.18	6.83
	24.74	6.54	25.00	6.52	25.00	6.54	6.35
	24.66	6.61	25.00	6.52	25.05	6.49	6.41
	29.42	2.23	29.67	2.12	29.72	2.13	1.95
	29.42	2.23	29.65	2.14	29.67	2.18	1.99
	27.88	3.65	27.94	3.75	28.00	3.73	3.51
	29.57	2.09	29.35	2.43	29.37	2.45	1.99
	30.51	1.22	30.55	1.29	30.62	1.29	0.97
	29.50	2.15	29.56	2.23	29.58	2.26	2.00
	27.21	4.26	27.60	4.08	27.61	4.10	3.94
	27.09	4.38	27.42	4.24	27.42	4.28	4.16
	29.58	2.09	29.69	2.11	29.75	2.10	1.74
	28.69	2.91	28.93	2.82	28.94	2.85	2.56
	28.89	2.72	28.45	3.28	28.52	3.25	2.79
	29.75	1.93	29.86	1.94	29.92	1.95	1.67
	29.18	2.46	29.24	2.52	29.33	2.49	2.20
	26.74	4.70	26.79	4.84	26.80	4.86	4.73
	28.26	3.30	28.25	3.46	28.30	3.46	3.20
5	29.35	2.30	29.27	2.50	29.37	2.46	2.48
	29.52	2.14	29.60	2.19	29.68	2.16	2.23
	28.16	3.39	28.07	3.63	28.16	3.58	3.41
	28.84	2.77	28.87	2.88	28.96	2.84	2.75
	30.09	1.61	30.15	1.67	30.19	1.69	1.67
	29.96	1.74	30.19	1.64	30.28	1.61	1.55
	27.52	3.98	27.46	4.20	27.52	4.19	4.23
	29.20	2.43	29.05	2.71	29.14	2.67	2.57
	30.00	1.69	29.71	2.08	29.79	2.06	1.95
	29.96	1.73	30.11	1.71	30.17	1.71	1.76
	30.20	1.51	30.33	1.51	30.42	1.48	1.56
	30.50	1.24	30.74	1.12	30.81	1.11	1.15
	30.25	1.47	30.59	1.26	30.66	1.25	1.15

	30.30	1.42	30.66	1.19	30.74	1.17	1.15
	29.96	1.73	30.04	1.78	30.11	1.76	1.84
	30.18	1.53	30.29	1.54	30.37	1.52	1.64
	30.43	1.30	30.78	1.08	30.83	1.09	1.25
	30.45	1.28	30.70	1.16	30.75	1.17	1.25
	30.11	1.60	30.49	1.35	30.52	1.38	1.25
	29.57	2.09	29.47	2.32	29.52	2.32	2.29
	26.90	4.55	26.84	4.79	26.93	4.73	4.74
	29.72	1.95	29.90	1.90	29.99	1.87	1.89
	29.18	2.45	29.40	2.38	29.46	2.37	1.89
	29.70	1.97	29.99	1.83	30.06	1.81	1.89
	30.02	1.68	30.18	1.64	30.24	1.65	1.63
	30.02	1.68	30.18	1.64	30.26	1.62	1.78
	29.94	1.75	29.70	2.10	29.79	2.07	1.98
	29.99	1.71	30.07	1.74	30.16	1.71	1.64
	29.92	1.77	30.08	1.74	30.15	1.73	1.84
	30.02	1.68	30.49	1.36	30.52	1.38	1.22
	30.33	1.40	30.61	1.24	30.67	1.25	1.22
	30.51	1.22	30.89	0.97	30.93	0.99	1.22
	30.86	0.91	31.13	0.75	31.20	0.75	1.16
	30.03	1.67	30.34	1.50	30.40	1.49	1.16
	30.31	1.41	30.69	1.17	30.75	1.17	1.16
	29.51	2.14	29.48	2.31	29.54	2.30	2.31
	30.87	0.90	31.18	0.70	31.25	0.70	1.18
	30.01	1.69	30.37	1.47	30.44	1.46	1.18
	30.28	1.44	30.69	1.16	30.75	1.17	1.18
6	23.35	7.82	23.72	7.73	23.73	7.72	7.82
	23.63	7.57	24.00	7.46	24.03	7.44	7.55
	22.92	8.21	23.29	8.13	23.30	8.13	8.27
	23.51	7.67	24.01	7.45	24.01	7.47	7.67
	26.56	4.86	26.52	5.09	26.54	5.10	4.56
	25.05	6.26	25.19	6.34	25.20	6.35	7.58
	24.19	7.04	24.44	7.04	24.46	7.04	7.69
	23.89	7.32	24.16	7.31	24.20	7.29	7.66
	23.80	7.41	23.92	7.53	23.93	7.53	7.96
	28.32	3.25	28.41	3.31	28.43	3.34	2.58
	28.32	3.24	28.44	3.28	28.54	3.23	2.71
	26.74	4.70	26.68	4.94	26.72	4.93	5.49
	24.60	6.67	24.88	6.63	24.86	6.67	7.23
	24.67	6.60	24.98	6.54	24.99	6.54	7.09
	24.20	7.04	24.44	7.05	24.47	7.04	7.27
	24.42	6.84	24.67	6.83	24.69	6.83	7.48
	28.13	3.42	28.10	3.60	28.19	3.56	4.25
	29.62	2.05	29.58	2.20	29.63	2.21	1.73
	30.10	1.60	30.17	1.66	30.26	1.63	1.51
	30.52	1.22	30.22	1.61	30.25	1.63	1.84
	30.27	1.45	30.57	1.28	30.61	1.30	0.95
	30.27	1.45	30.59	1.26	30.65	1.26	0.95
	30.62	1.13	30.88	0.99	30.96	0.97	0.95
	30.01	1.69	30.33	1.50	30.36	1.53	0.90

	30.92	0.85	31.11	0.77	31.21	0.74	0.90
	30.23	1.48	30.52	1.32	30.56	1.34	0.90
7	25.48	5.86	25.42	6.12	25.46	6.11	6.17
	27.47	4.02	27.39	4.27	27.46	4.24	4.49
	27.96	3.58	28.04	3.66	28.10	3.64	3.09
	23.78	7.42	23.86	7.59	23.86	7.60	7.34
	23.74	7.46	24.00	7.46	24.00	7.47	7.22
	27.17	4.30	27.47	4.20	27.51	4.19	4.72
	26.82	4.62	27.06	4.58	27.11	4.57	4.72
	24.44	6.82	24.86	6.65	24.87	6.66	6.75
	28.99	2.63	29.37	2.41	29.42	2.41	2.93
	27.63	3.88	27.96	3.73	27.95	3.79	2.93
	29.42	2.23	29.74	2.06	29.77	2.08	2.93
	27.79	3.73	27.78	3.90	27.82	3.91	2.62
	28.18	3.37	28.11	3.59	28.15	3.60	2.62
	24.47	6.79	24.81	6.70	24.84	6.69	6.90
	23.53	7.66	23.74	7.71	23.73	7.72	7.29
	24.00	7.22	24.31	7.16	24.35	7.14	7.23
	22.93	8.21	23.36	8.06	23.36	8.07	7.64
	23.91	7.30	24.25	7.22	24.29	7.20	7.19
	24.01	7.22	24.38	7.10	24.40	7.10	7.19
	28.90	2.71	29.23	2.54	29.27	2.55	3.14
	27.49	4.01	27.81	3.87	27.78	3.94	3.14
	28.99	2.63	29.33	2.44	29.35	2.47	3.14
	27.53	3.97	27.90	3.79	27.95	3.78	4.72
	27.04	4.42	27.32	4.33	27.37	4.32	4.72
	29.24	2.39	29.67	2.13	29.71	2.14	3.14
	27.85	3.67	28.19	3.52	28.18	3.57	3.14
	29.41	2.24	29.78	2.02	29.82	2.03	3.14
8	30.32	1.40	30.56	1.29	30.57	1.33	0.82
	30.74	1.01	30.85	1.01	30.89	1.04	0.82
	31.18	0.61	31.40	0.50	31.45	0.51	0.82
	30.55	1.19	30.86	1.01	30.95	0.98	1.13
	30.66	1.09	30.99	0.88	31.05	0.89	1.13
	30.52	1.22	30.83	1.04	30.89	1.03	1.13
	25.77	5.59	26.07	5.51	26.10	5.51	5.42
	30.01	1.68	30.22	1.61	30.28	1.61	1.05
	30.71	1.04	30.96	0.91	31.02	0.92	1.05
	30.81	0.95	30.98	0.89	31.05	0.89	1.05
	30.65	1.10	30.98	0.90	31.05	0.88	0.68
	30.61	1.13	30.94	0.93	31.00	0.94	0.68
	31.08	0.70	31.35	0.55	31.41	0.55	0.68
9	30.67	1.08	30.43	1.41	30.60	1.31	1.44
	30.28	1.44	30.04	1.78	30.18	1.70	1.69
	30.04	1.66	30.27	1.56	30.34	1.55	1.69
	29.97	1.72	30.09	1.73	30.16	1.72	1.59
	30.25	1.47	30.25	1.58	30.34	1.55	1.52
	30.75	1.01	30.73	1.12	30.85	1.07	1.52
	28.05	3.50	28.07	3.63	28.16	3.59	3.64
	30.19	1.52	30.37	1.47	30.44	1.46	2.21

	29.24	2.39	29.45	2.33	29.47	2.36	1.52
	29.83	1.85	29.70	2.09	29.77	2.08	1.77
	29.96	1.73	30.07	1.75	30.12	1.75	1.52
	30.23	1.48	30.36	1.47	30.46	1.44	1.52
	30.44	1.29	30.48	1.36	30.58	1.33	1.98
	29.00	2.61	29.12	2.64	29.23	2.59	1.28
	29.93	1.76	30.04	1.78	30.13	1.74	1.31
	29.68	1.99	29.76	2.04	29.77	2.08	1.77
	30.48	1.26	30.57	1.28	30.69	1.23	1.48
	30.44	1.29	30.53	1.31	30.57	1.34	1.49
	30.20	1.51	30.27	1.56	30.37	1.52	1.81
	29.76	1.92	29.88	1.92	30.00	1.87	1.28
	28.52	3.06	28.61	3.12	28.69	3.09	3.10
	29.92	1.77	30.16	1.67	30.25	1.63	1.74
	27.34	4.15	27.52	4.15	27.59	4.12	4.43
	27.73	3.79	27.64	4.04	27.73	3.99	4.26
	30.51	1.23	30.76	1.10	30.82	1.10	1.21
	30.08	1.62	30.56	1.29	30.60	1.31	1.21
	30.49	1.24	30.94	0.93	31.00	0.93	1.21
	30.79	0.97	31.03	0.84	31.10	0.84	0.88
	30.79	0.97	30.97	0.90	31.05	0.89	0.88
	30.69	1.06	30.91	0.96	30.97	0.96	0.88
	30.75	1.01	30.98	0.89	31.05	0.89	0.95
	30.41	1.32	30.58	1.27	30.69	1.23	0.95
	30.69	1.06	30.83	1.04	30.92	1.01	0.95
	30.43	1.30	30.60	1.25	30.66	1.25	1.13
	31.06	0.72	31.17	0.71	31.27	0.68	1.13
	30.22	1.50	30.39	1.45	30.42	1.48	1.13
	30.89	0.88	31.19	0.70	31.26	0.69	1.22
	30.70	1.05	30.94	0.93	31.01	0.92	1.22
	29.47	2.18	29.70	2.10	29.75	2.10	1.22
	29.63	2.03	29.98	1.84	30.03	1.84	0.99
	30.94	0.83	31.18	0.70	31.26	0.69	0.99
	30.77	0.99	31.06	0.82	31.14	0.80	0.99
	30.46	1.27	30.76	1.10	30.82	1.10	0.96
	31.01	0.77	31.27	0.62	31.35	0.61	0.96
	30.29	1.43	30.66	1.19	30.71	1.20	0.96
10	26.09	5.29	25.90	5.67	25.91	5.69	5.63
	28.19	3.36	28.27	3.44	28.29	3.47	3.43
	28.49	3.09	28.66	3.08	28.68	3.10	3.17
	29.33	2.31	29.18	2.59	29.22	2.60	2.23
	30.14	1.57	30.25	1.58	30.35	1.54	1.32
	30.32	1.40	30.29	1.54	30.34	1.55	1.10
	26.48	4.94	26.19	5.40	26.19	5.43	5.25
	26.70	4.73	26.69	4.93	26.72	4.93	4.64
	29.30	2.34	29.25	2.52	29.29	2.53	2.51
	29.48	2.18	29.44	2.34	29.53	2.31	1.90
	29.03	2.59	29.15	2.61	29.20	2.62	2.37
	27.68	3.83	27.47	4.19	27.49	4.21	4.77
	26.32	5.09	26.42	5.19	26.48	5.15	4.79

	28.96	2.65	29.11	2.66	29.17	2.64	2.67
	29.32	2.32	29.45	2.33	29.49	2.34	2.61
	30.64	1.11	31.00	0.87	31.06	0.88	0.83
	30.52	1.22	30.90	0.97	30.95	0.98	0.83
	30.60	1.14	31.00	0.87	31.05	0.89	0.83
	28.95	2.67	29.16	2.60	29.16	2.65	2.97
	29.68	1.99	29.86	1.94	29.90	1.96	2.97
	29.16	2.47	29.40	2.38	29.43	2.40	2.97
	30.63	1.12	30.93	0.94	30.99	0.94	1.06
	30.14	1.56	30.54	1.31	30.60	1.31	1.06
	30.59	1.15	30.97	0.90	31.04	0.89	1.06
	30.72	1.03	31.04	0.83	31.10	0.84	1.15
	30.24	1.47	30.47	1.37	30.53	1.37	1.15
	31.15	0.64	31.40	0.50	31.48	0.48	1.15
	31.11	0.67	31.47	0.43	31.55	0.42	1.04
	31.63	0.19	31.97	-0.04	32.04	-0.04	1.04
	32.88	-0.95	33.05	-1.05	33.10	-1.02	1.04
	29.97	1.73	30.13	1.69	30.19	1.69	1.59
	30.05	1.65	30.09	1.73	30.16	1.71	1.59
	30.89	0.88	30.97	0.90	31.05	0.88	1.59
	23.81	7.40	24.04	7.43	24.07	7.41	7.61
	23.87	7.34	24.28	7.19	24.30	7.19	7.35
	24.01	7.21	24.30	7.18	24.33	7.17	6.90
	24.00	7.22	24.25	7.22	24.24	7.25	6.90
	24.27	6.97	24.54	6.95	24.56	6.94	7.11
	24.12	7.11	24.40	7.08	24.44	7.06	7.18
	24.44	6.82	24.86	6.65	24.89	6.64	6.69
	24.39	6.87	24.81	6.70	24.78	6.74	6.69
11	27.53	3.97	27.63	4.05	27.68	4.03	3.78
	29.14	2.49	29.17	2.59	29.24	2.58	2.97
	28.69	2.91	28.83	2.91	28.88	2.91	2.77
	24.78	6.51	25.32	6.21	25.28	6.27	6.45
	23.84	7.37	23.96	7.49	24.01	7.46	7.35
	24.36	6.89	24.61	6.88	24.62	6.89	6.97
	24.43	6.83	24.72	6.78	24.72	6.80	6.84
	24.02	7.20	24.18	7.29	24.24	7.24	7.30
	24.72	6.55	24.93	6.59	24.94	6.59	6.73
	24.68	6.60	24.88	6.63	24.90	6.63	6.84
	24.95	6.34	25.57	5.99	25.54	6.03	6.44
	30.00	1.70	29.90	1.91	30.00	1.87	2.10
	29.47	2.18	29.34	2.43	29.40	2.43	2.75
	28.77	2.83	28.67	3.06	28.71	3.07	3.65
	27.65	3.86	27.68	4.00	27.67	4.05	4.76
	30.88	0.89	31.11	0.77	31.17	0.78	1.45
	30.54	1.20	30.84	1.03	30.85	1.07	1.45
	30.38	1.35	30.76	1.10	30.82	1.10	1.45
	28.59	3.00	28.96	2.79	29.01	2.79	2.44
	29.54	2.12	29.64	2.15	29.68	2.17	2.44
	29.59	2.08	29.82	1.98	29.88	1.98	2.44
	28.96	2.65	28.96	2.79	28.98	2.82	3.28

	28.06	3.49	28.37	3.34	28.42	3.34	3.28
	29.26	2.38	29.45	2.33	29.46	2.37	3.28
	29.49	2.16	29.69	2.10	29.73	2.12	2.38
	28.86	2.74	29.15	2.61	29.21	2.61	2.38
	28.83	2.78	29.10	2.66	29.15	2.66	2.38
	27.40	4.09	27.79	3.89	27.80	3.92	4.09
	27.47	4.02	27.86	3.83	27.87	3.86	4.09
	26.96	4.50	27.38	4.28	27.40	4.30	4.09
	27.11	4.35	27.54	4.12	27.60	4.11	4.08
	27.65	3.86	27.99	3.71	28.04	3.70	4.08
	27.74	3.78	28.06	3.64	28.11	3.63	4.08
	28.92	2.69	29.19	2.58	29.25	2.56	2.33
	29.61	2.06	29.79	2.02	29.83	2.02	2.33
	28.91	2.70	29.16	2.60	29.23	2.59	2.33
	30.30	1.42	30.50	1.34	30.57	1.34	1.62
	30.36	1.37	30.49	1.35	30.50	1.40	1.62
	30.08	1.63	30.38	1.46	30.40	1.50	1.62
	31.01	0.77	31.42	0.47	31.48	0.48	1.10
	30.41	1.31	30.79	1.07	30.87	1.06	1.10
	30.68	1.07	31.02	0.85	31.08	0.86	1.10
12	29.58	2.09	29.25	2.52	29.25	2.56	2.56
	28.32	3.24	28.42	3.30	28.45	3.31	4.04
	29.64	2.03	29.46	2.32	29.48	2.35	2.23
	29.31	2.33	29.39	2.39	29.45	2.38	2.47
	28.65	2.94	28.85	2.90	28.90	2.90	2.85
	30.34	1.39	30.56	1.29	30.60	1.31	1.07
	30.92	0.85	31.09	0.79	31.14	0.80	1.07
	31.13	0.66	31.24	0.64	31.31	0.65	1.07
	26.80	4.64	27.12	4.52	27.13	4.55	4.76
	27.30	4.18	27.34	4.31	27.38	4.32	4.46
	30.63	1.11	30.93	0.94	30.99	0.95	1.17
	30.24	1.48	30.42	1.42	30.46	1.44	1.17
	30.48	1.26	30.81	1.06	30.86	1.06	1.17
	28.80	2.80	29.01	2.75	29.07	2.73	2.98
	29.06	2.56	29.27	2.50	29.30	2.52	2.68
	29.87	1.82	30.21	1.62	30.23	1.66	1.18
	30.39	1.33	30.73	1.13	30.80	1.12	1.18
	30.87	0.90	31.10	0.78	31.16	0.79	1.18
	30.52	1.22	30.98	0.89	31.03	0.91	1.29
	30.25	1.47	30.58	1.27	30.63	1.28	1.29
	30.07	1.63	30.45	1.39	30.51	1.39	1.29
13	24.77	6.51	25.17	6.36	25.16	6.39	6.34
	24.04	7.18	24.38	7.10	24.41	7.09	7.41
	23.97	7.25	24.44	7.05	24.42	7.08	7.40
	27.86	3.67	27.59	4.08	27.65	4.06	4.11
	28.95	2.66	28.68	3.06	28.74	3.04	1.84
	28.28	3.28	28.26	3.45	28.28	3.47	3.14
	28.51	3.07	28.26	3.45	28.28	3.47	2.98
	29.68	2.00	29.80	2.00	29.87	1.98	2.16
	28.83	2.77	28.94	2.81	28.98	2.82	2.16

	29.55	2.11	29.49	2.30	29.52	2.31	2.48
	29.89	1.80	29.89	1.92	29.95	1.92	2.48
	28.21	3.34	28.39	3.33	28.41	3.35	3.12
	28.69	2.90	28.82	2.92	28.86	2.93	3.12
	27.72	3.80	27.85	3.84	27.85	3.87	3.55
	28.89	2.72	28.94	2.81	28.97	2.83	3.55
	24.11	7.12	24.38	7.10	24.40	7.10	7.14
	24.53	6.73	24.69	6.81	24.70	6.81	6.20
	25.99	5.39	26.13	5.46	26.16	5.45	5.35
	24.46	6.80	24.82	6.69	24.84	6.68	6.66
	24.27	6.97	24.52	6.97	24.56	6.95	7.12
	29.47	2.18	29.59	2.20	29.64	2.20	1.83
	29.79	1.89	30.12	1.70	30.16	1.71	1.83
	29.75	1.93	30.08	1.74	30.12	1.76	1.83
	26.30	5.10	26.28	5.31	26.30	5.32	5.30
	29.55	2.11	29.49	2.30	29.52	2.31	2.48
	29.89	1.80	29.89	1.92	29.95	1.92	2.48
	28.21	3.34	28.39	3.33	28.41	3.35	2.90
	28.69	2.90	28.82	2.92	28.86	2.93	2.90
	27.72	3.80	27.85	3.84	27.85	3.87	3.13
	28.89	2.72	28.94	2.81	28.97	2.83	3.13
14	29.25	2.39	28.81	2.94	28.89	2.90	2.99
	28.72	2.88	28.36	3.36	28.43	3.33	3.36
	27.94	3.59	27.87	3.82	27.89	3.83	3.50
	28.92	2.69	28.95	2.80	29.01	2.79	2.72
	29.60	2.06	29.62	2.17	29.69	2.16	2.04
	25.30	6.03	25.48	6.07	25.46	6.10	6.38
	24.08	7.15	24.38	7.10	24.38	7.12	7.14
	29.49	2.16	29.87	1.94	29.92	1.95	1.78
	29.64	2.03	29.93	1.88	29.97	1.89	1.78
	29.61	2.06	29.97	1.84	30.02	1.85	1.78
	24.34	6.91	24.75	6.76	24.76	6.76	6.94
	24.83	6.46	25.30	6.23	25.32	6.24	6.42
	23.91	7.30	24.13	7.34	24.14	7.34	7.24
	24.26	6.99	24.74	6.76	24.74	6.78	6.98
	24.84	6.45	25.34	6.20	25.31	6.25	6.51
	25.37	5.96	25.87	5.70	25.80	5.79	6.23
	24.90	6.39	25.34	6.20	25.35	6.21	6.46
	24.25	6.99	24.69	6.81	24.70	6.81	7.05
	23.65	7.54	24.14	7.33	24.18	7.30	7.41
	24.40	6.86	24.87	6.64	24.86	6.67	6.97
	24.37	6.89	24.78	6.72	24.81	6.72	6.81
15	29.12	2.51	28.95	2.80	28.96	2.84	2.23
	26.81	4.63	26.82	4.81	26.85	4.81	5.41
	27.97	3.57	27.55	4.12	27.55	4.16	3.58
	26.55	4.87	26.27	5.32	26.28	5.34	5.68
	30.25	1.47	30.64	1.21	30.71	1.20	1.02
	30.68	1.07	30.98	0.90	31.06	0.88	1.02
	30.26	1.46	30.58	1.27	30.63	1.28	1.02
	23.50	7.68	23.82	7.63	23.81	7.65	8.01

	23.68	7.51	24.07	7.40	24.08	7.39	7.42
	23.73	7.47	24.02	7.44	24.04	7.43	7.54
	24.07	7.16	24.42	7.07	24.43	7.07	7.42
	24.05	7.18	24.28	7.19	24.27	7.22	8.01
	25.82	5.54	25.71	5.85	25.73	5.85	6.36
	29.47	2.18	29.81	2.00	29.86	2.00	1.68
	29.81	1.87	30.08	1.74	30.12	1.76	1.68
	29.95	1.74	30.26	1.57	30.29	1.60	1.68
	25.38	5.95	25.50	6.05	25.49	6.08	5.39
	29.88	1.81	29.74	2.06	29.78	2.07	1.99
	29.22	2.41	29.20	2.57	29.24	2.58	2.37
	27.33	4.15	27.11	4.53	27.17	4.51	5.48
	29.85	1.84	30.22	1.60	30.25	1.63	0.97
	30.71	1.04	30.92	0.95	31.02	0.92	0.97
	30.93	0.84	31.14	0.74	31.21	0.73	0.97
	30.58	1.16	30.79	1.07	30.85	1.08	1.02
	30.74	1.02	30.89	0.98	30.97	0.96	1.02
	30.47	1.26	30.62	1.23	30.68	1.23	1.02
	26.88	4.57	26.66	4.96	26.70	4.95	5.39
	24.49	6.77	24.65	6.85	24.67	6.84	6.75
	28.51	3.07	28.85	2.89	28.90	2.89	1.73
	29.60	2.07	29.85	1.96	29.90	1.96	1.73
	29.60	2.07	29.93	1.88	29.99	1.88	1.73
	29.60	2.07	29.83	1.98	29.88	1.98	2.05
	28.79	2.81	29.17	2.60	29.18	2.63	2.05
	29.76	1.92	30.06	1.76	30.08	1.80	2.05
	29.60	2.07	29.90	1.91	29.95	1.92	2.27
	28.94	2.67	29.37	2.40	29.40	2.43	2.27
	29.12	2.50	29.57	2.22	29.59	2.25	2.27
	28.91	2.70	29.31	2.46	29.32	2.51	2.18
	29.60	2.07	29.91	1.90	29.90	1.96	2.18
	29.81	1.87	30.00	1.81	30.09	1.78	2.18
	29.43	2.22	29.68	2.12	29.73	2.12	2.02
	28.88	2.73	29.24	2.53	29.27	2.55	2.02
	29.40	2.25	29.74	2.06	29.78	2.07	2.02
	29.38	2.27	29.65	2.14	29.71	2.13	2.00
	29.31	2.33	29.73	2.07	29.72	2.13	2.00
	29.18	2.45	29.56	2.23	29.61	2.23	2.00
16	27.50	4.00	28.01	3.68	28.04	3.70	3.75
	25.84	5.53	26.13	5.45	26.10	5.51	5.21
	26.37	5.04	26.38	5.22	26.39	5.24	5.04
	26.84	4.60	26.83	4.80	26.90	4.76	4.57
	26.41	5.00	26.46	5.14	26.48	5.16	5.03
	25.87	5.50	25.95	5.62	25.98	5.62	5.44
	24.37	6.88	24.93	6.58	24.93	6.60	6.62
	24.81	6.48	25.42	6.12	25.39	6.17	6.30
	24.42	6.83	25.00	6.52	25.02	6.52	6.58
17	24.47	6.79	25.10	6.43	25.06	6.49	6.49
	29.69	1.99	29.99	1.83	30.06	1.82	1.77
	27.66	3.85	27.73	3.95	27.84	3.89	3.46

	28.33	3.23	28.21	3.50	28.31	3.45	3.39
	26.00	5.38	25.99	5.59	26.05	5.55	5.59
	27.96	3.57	28.14	3.57	28.22	3.53	4.08
	27.94	3.60	27.94	3.76	28.03	3.71	3.62
	27.28	4.20	27.14	4.50	27.23	4.46	4.18
	28.05	3.49	27.96	3.73	28.05	3.69	2.76
	28.17	3.38	28.33	3.38	28.43	3.33	3.25
	27.98	3.56	28.25	3.46	28.37	3.39	3.23
	28.24	3.32	28.50	3.22	28.59	3.19	3.11
	28.45	3.12	28.34	3.37	28.40	3.36	2.94
	29.54	2.12	29.63	2.16	29.69	2.16	2.04
	27.52	3.98	27.89	3.80	27.93	3.80	3.93
	27.32	4.17	27.40	4.26	27.47	4.23	4.29
	29.42	2.23	29.66	2.13	29.69	2.16	2.36
	29.48	2.18	29.54	2.25	29.57	2.27	1.90
	28.71	2.88	28.72	3.02	28.77	3.02	2.28
	29.72	1.95	29.85	1.96	29.94	1.92	2.01
	26.52	4.90	26.48	5.13	26.51	5.13	5.36
	29.27	2.36	29.33	2.45	29.38	2.45	2.18
	27.28	4.20	27.67	4.01	27.68	4.03	4.03
	27.72	3.79	27.93	3.76	27.93	3.80	3.58
	30.58	1.17	30.82	1.04	30.90	1.02	0.89
	29.75	1.93	29.92	1.89	29.98	1.89	0.89
	30.02	1.68	30.34	1.49	30.40	1.49	0.89
	23.12	8.03	23.36	8.06	23.35	8.08	8.16
	23.66	7.54	24.01	7.45	24.02	7.45	7.57
	23.58	7.61	23.83	7.62	23.86	7.60	7.66
	23.69	7.50	24.04	7.42	24.06	7.42	7.57
	23.06	8.09	23.32	8.10	23.30	8.12	8.16
	27.24	4.24	27.69	3.99	27.72	4.00	3.62
	27.72	3.80	28.18	3.53	28.21	3.54	3.56
	27.50	4.00	27.98	3.71	28.03	3.71	3.75
	27.38	4.11	27.68	3.99	27.74	3.98	3.89
18	24.20	7.04	24.57	6.93	24.58	6.93	6.62
	29.27	2.37	29.41	2.37	29.49	2.34	1.98
	27.85	3.67	28.03	3.67	28.08	3.66	3.11
	25.24	6.08	25.50	6.05	25.52	6.05	5.70
	27.71	3.80	27.90	3.79	28.00	3.73	3.49
	29.02	2.60	28.98	2.77	29.07	2.74	2.20
	28.51	3.07	28.22	3.49	28.26	3.49	3.11
	29.60	2.06	29.37	2.41	29.46	2.37	2.77
	29.29	2.35	29.49	2.29	29.55	2.29	2.11
	30.26	1.46	30.40	1.44	30.44	1.45	0.94
	28.76	2.84	28.60	3.13	28.66	3.11	2.87
	27.20	4.27	27.66	4.02	27.70	4.01	3.58
	27.67	3.84	27.89	3.80	27.90	3.83	4.25
	29.78	1.90	29.88	1.93	29.94	1.93	1.93
	29.65	2.02	29.76	2.04	29.84	2.02	2.10
	27.05	4.42	27.23	4.42	27.28	4.41	4.56
	29.96	1.73	30.24	1.58	30.32	1.57	1.81

	29.64	2.03	29.91	1.90	29.97	1.90	1.81
	29.00	2.61	29.32	2.45	29.36	2.47	1.81
	30.48	1.25	30.85	1.02	30.91	1.02	1.17
	29.96	1.73	30.35	1.48	30.39	1.50	1.17
	30.37	1.36	30.80	1.06	30.85	1.07	1.17
	29.71	1.97	29.83	1.97	29.89	1.97	1.11
	30.63	1.12	30.80	1.06	30.87	1.05	1.11
	30.41	1.32	30.52	1.32	30.59	1.32	1.11
19	25.14	6.17	25.82	5.74	25.77	5.82	5.97
	28.93	2.68	29.23	2.53	29.26	2.56	2.91
	28.84	2.77	29.12	2.64	29.14	2.67	2.74
	27.16	4.31	26.88	4.75	26.94	4.73	4.97
	27.93	3.60	27.77	3.91	27.80	3.92	4.74
	25.14	6.17	25.76	5.80	25.72	5.87	6.00
	26.47	4.95	26.53	5.07	26.60	5.04	5.11
	24.48	6.78	24.73	6.77	24.76	6.76	6.99
	24.70	6.58	24.97	6.54	24.96	6.58	6.99
	24.57	6.70	25.09	6.43	25.08	6.46	6.73
	24.62	6.65	25.18	6.35	25.12	6.42	6.71
	26.40	5.01	26.35	5.25	26.38	5.25	6.99
	24.15	7.08	24.47	7.01	24.50	7.01	6.99
	27.07	4.39	27.19	4.45	27.25	4.44	4.31
	25.26	6.06	25.76	5.80	25.78	5.81	6.01
	27.54	3.96	27.42	4.24	27.44	4.25	4.02
20	27.80	3.72	27.69	3.99	27.74	3.98	3.96
	29.36	2.29	29.43	2.35	29.50	2.34	2.35
	30.31	1.41	30.38	1.46	30.41	1.48	1.44
	28.65	2.94	28.43	3.29	28.50	3.27	3.13
	31.02	0.75	30.48	1.37	30.53	1.38	1.26
	28.01	3.53	27.57	4.10	27.60	4.11	3.85
	23.00	8.14	23.37	8.05	23.36	8.07	8.08
	23.97	7.25	24.25	7.22	24.30	7.19	7.24
	24.12	7.11	24.42	7.06	24.45	7.06	7.08
	24.02	7.21	24.31	7.17	24.31	7.18	7.16
	29.73	1.95	29.80	2.00	29.86	2.00	1.89
	29.89	1.80	29.96	1.85	30.01	1.86	1.87
	28.53	3.05	28.76	2.98	28.81	2.98	3.21
	28.75	2.85	28.68	3.05	28.69	3.09	2.87
	28.94	2.67	29.03	2.72	29.08	2.72	2.74
	27.86	3.67	28.06	3.64	28.08	3.66	3.71
	25.24	6.08	25.50	6.05	25.50	6.07	5.92
	27.55	3.95	27.62	4.06	27.63	4.08	4.05
	27.43	4.06	27.78	3.91	27.81	3.91	4.14
	27.45	4.05	27.51	4.16	27.56	4.14	4.27
	28.63	2.96	28.73	3.01	28.77	3.01	3.11
	28.97	2.64	29.22	2.55	29.26	2.56	2.66
21	22.91	8.22	23.33	8.09	23.28	8.14	8.23
	29.74	1.94	29.77	2.03	29.83	2.03	1.72
	28.32	3.25	28.23	3.48	28.24	3.51	3.24
	28.12	3.43	28.27	3.44	28.30	3.45	3.18

	29.69	1.99	29.69	2.11	29.74	2.11	2.46
	27.70	3.81	27.79	3.90	27.80	3.92	3.62
	23.90	7.31	24.20	7.27	24.19	7.29	7.26
	24.10	7.13	24.42	7.06	24.45	7.05	7.18
	24.02	7.20	24.35	7.13	24.38	7.12	7.29
	29.32	2.32	29.05	2.71	29.11	2.70	2.88
	27.96	3.57	27.68	4.00	27.73	3.99	3.86
	28.98	2.64	29.13	2.63	29.12	2.69	1.78
	30.32	1.40	30.60	1.25	30.65	1.26	1.78
	27.37	4.12	27.23	4.42	27.28	4.41	4.45
	28.43	3.14	28.14	3.57	28.18	3.57	2.74
	28.81	2.79	28.88	2.87	28.91	2.89	3.36
	26.00	5.38	26.18	5.41	26.21	5.41	5.43
	29.43	2.22	29.37	2.41	29.40	2.43	2.14
	28.59	2.99	28.73	3.01	28.78	3.01	3.03
	29.43	2.22	29.54	2.25	29.63	2.22	1.73
	28.88	2.73	28.60	3.13	28.69	3.09	2.57
	30.02	1.68	30.29	1.54	30.35	1.54	1.78
	27.39	4.10	27.37	4.29	27.44	4.26	4.62
	29.38	2.27	29.61	2.18	29.63	2.21	1.72
	29.86	1.83	30.24	1.59	30.28	1.61	1.72
	29.95	1.74	30.35	1.49	30.39	1.50	1.72
	25.78	5.58	25.99	5.58	26.02	5.59	5.62
	28.07	3.47	28.16	3.54	28.20	3.55	3.59
	28.66	2.93	28.45	3.27	28.49	3.28	2.91
	29.93	1.76	30.04	1.78	30.06	1.81	1.62
	29.70	1.97	29.79	2.01	29.86	2.00	2.04
	28.74	2.86	28.58	3.15	28.61	3.16	3.03
	30.20	1.51	29.77	2.03	29.83	2.02	1.61
	28.41	3.16	28.17	3.54	28.25	3.51	3.06
	24.78	6.51	24.95	6.57	24.95	6.58	6.52
	24.23	7.01	24.46	7.03	24.49	7.01	7.17
	24.53	6.73	24.84	6.67	24.87	6.66	6.85
	24.22	7.02	24.44	7.04	24.46	7.04	7.09
	28.50	3.08	28.73	3.01	28.76	3.03	3.18
	28.89	2.72	29.12	2.64	29.14	2.67	2.71
	28.37	3.20	28.17	3.53	28.23	3.52	3.51
22	29.49	2.16	29.59	2.20	29.65	2.20	1.52
	30.15	1.55	30.26	1.57	30.33	1.56	1.52
	30.09	1.62	30.28	1.56	30.35	1.54	1.52
	29.69	1.98	29.97	1.85	30.01	1.86	1.52
	30.40	1.33	30.64	1.21	30.71	1.20	1.52
	30.06	1.64	30.29	1.54	30.37	1.53	1.52
	24.90	6.40	25.02	6.50	25.06	6.48	6.16
	23.86	7.35	24.20	7.28	24.23	7.25	7.21
	23.80	7.40	24.17	7.30	24.19	7.30	7.32
	28.60	2.99	28.50	3.22	28.51	3.26	3.27
	28.36	3.21	28.47	3.26	28.50	3.27	3.35
	24.09	7.14	24.39	7.09	24.44	7.06	6.93
	24.01	7.21	24.30	7.17	24.35	7.15	7.03

	24.19	7.05	24.44	7.05	24.48	7.02	7.48
	25.88	5.49	26.24	5.35	26.30	5.32	5.10
	25.91	5.46	26.20	5.39	26.25	5.37	4.99
	23.99	7.23	24.24	7.24	24.26	7.23	7.39
	23.73	7.47	24.15	7.32	24.16	7.32	7.49
	24.11	7.12	24.42	7.07	24.45	7.05	7.10
	23.95	7.27	24.24	7.23	24.28	7.21	7.19
	30.15	1.56	30.47	1.37	30.51	1.39	1.57
	30.02	1.67	30.27	1.56	30.32	1.56	1.57
	30.18	1.54	30.47	1.37	30.50	1.40	1.57
	31.66	0.17	31.61	0.30	31.67	0.31	1.29
	31.18	0.61	31.40	0.50	31.47	0.50	1.29
	33.19	-1.24	33.17	-1.17	33.22	-1.14	1.29
23	27.33	4.16	27.14	4.50	27.19	4.49	4.62
	28.68	2.91	28.59	3.14	28.67	3.11	5.01
	28.88	2.73	28.80	2.94	28.86	2.93	2.05
	31.02	0.76	30.83	1.04	30.92	1.01	1.60
	26.57	4.86	26.70	4.92	26.74	4.91	5.58
	26.83	4.61	26.67	4.94	26.73	4.93	4.68
	28.07	3.47	28.21	3.49	28.26	3.49	3.90
	28.45	3.12	28.62	3.11	28.70	3.08	3.09
	28.59	2.99	28.56	3.17	28.61	3.16	3.70
	29.04	2.58	29.32	2.45	29.37	2.45	2.80
	29.70	1.97	29.82	1.98	29.89	1.97	2.71
	30.53	1.21	30.50	1.35	30.60	1.31	1.81
	30.58	1.16	30.61	1.24	30.66	1.25	1.81
	27.25	4.23	27.15	4.50	27.21	4.47	4.85
	30.11	1.59	30.25	1.58	30.31	1.58	1.81
	30.37	1.35	30.46	1.38	30.56	1.35	1.81
	28.02	3.52	27.93	3.76	27.98	3.75	4.32
	28.63	2.96	28.89	2.85	28.95	2.85	3.06
	29.09	2.54	29.41	2.37	29.45	2.38	3.06
	27.51	3.99	27.89	3.80	27.96	3.78	3.95
	27.63	3.88	28.13	3.58	28.21	3.54	3.92
	26.64	4.79	26.98	4.66	26.98	4.69	4.13
	27.31	4.18	27.68	4.00	27.72	4.00	3.85
	23.83	7.37	23.84	7.61	23.85	7.61	8.03

^[a] Parameters of linear regression models are presented in Table 2 in main text.

^[b] For the references to the experimental works, please, see the main text.

Table S2. Calculated ¹H NMR shielding constants, together with scaled and experimental chemical shifts – the GIAO-DFT(PBE0) calculations with the second-level basis sets.

Mol.	pcS-2		pecS-2		pecS-2 mod		$\delta_{exp}^{[b]}$
	σ	$\delta_{scaled}^{[a]}$	σ	$\delta_{scaled}^{[a]}$	σ	$\delta_{scaled}^{[a]}$	
1	28.41	3.06	28.34	3.09	28.36	3.11	4.38
	29.89	1.72	29.80	1.76	29.84	1.76	2.51

	30.39	1.26	30.32	1.28	30.36	1.28	2.31
	28.81	2.69	28.77	2.69	28.80	2.70	3.53
	28.79	2.71	28.75	2.71	28.77	2.73	3.21
	27.43	3.95	27.37	3.97	27.42	3.96	4.03
	28.95	2.57	28.91	2.57	28.93	2.58	3.18
	28.40	3.07	28.41	3.02	28.44	3.03	3.34
	28.62	2.87	28.60	2.85	28.64	2.85	3.24
	28.82	2.68	28.81	2.66	28.85	2.66	2.80
	28.40	3.07	28.33	3.10	28.38	3.09	3.00
	28.13	3.32	28.05	3.35	28.10	3.34	3.27
	25.47	5.73	25.43	5.73	25.48	5.73	5.42
	23.67	7.37	23.66	7.35	23.71	7.34	7.45
	24.24	6.85	24.20	6.86	24.23	6.86	7.25
	29.27	2.28	29.21	2.29	29.26	2.28	0.99
	29.79	1.81	29.79	1.77	29.82	1.77	0.99
	29.81	1.79	29.81	1.75	29.84	1.75	0.99
	24.10	6.98	24.11	6.93	24.15	6.94	7.01
	24.13	6.95	24.13	6.92	24.17	6.92	7.05
	23.21	7.78	23.18	7.78	23.23	7.78	7.81
	22.70	8.25	22.66	8.25	22.70	8.26	8.11
	23.55	7.48	23.52	7.47	23.58	7.46	7.47
	23.73	7.32	23.71	7.30	23.75	7.31	7.40
	23.93	7.14	23.92	7.11	23.97	7.10	7.10
2	24.09	6.99	24.09	6.95	24.14	6.95	6.94
	23.70	7.34	23.66	7.34	23.70	7.35	7.62
	23.83	7.22	23.82	7.20	23.86	7.20	7.09
	23.97	7.10	23.96	7.07	24.01	7.07	7.19
	23.46	7.56	23.44	7.54	23.50	7.54	7.36
	24.62	6.51	24.58	6.51	24.65	6.49	6.94
	23.87	7.19	23.85	7.17	23.90	7.17	7.36
	24.18	6.90	24.18	6.87	24.22	6.88	7.19
	23.96	7.10	23.95	7.08	23.99	7.08	7.09
	23.84	7.22	23.80	7.22	23.84	7.23	7.62
	23.27	7.73	23.24	7.72	23.29	7.72	7.73
	24.17	6.91	24.17	6.88	24.21	6.89	6.89
	23.53	7.49	23.52	7.47	23.57	7.47	7.51
	24.25	6.84	24.23	6.82	24.27	6.83	6.91
3	27.04	4.30	26.88	4.41	26.94	4.40	4.18
	28.13	3.32	28.05	3.35	28.10	3.34	2.88
	29.44	2.13	29.39	2.13	29.41	2.15	2.20
	28.66	2.84	28.58	2.87	28.62	2.87	2.60
	28.82	2.69	28.77	2.70	28.80	2.70	2.35
	29.76	1.83	29.69	1.86	29.73	1.86	1.81
	30.04	1.58	30.00	1.58	30.03	1.58	1.51
	29.88	1.72	29.80	1.76	29.85	1.75	2.34
	25.11	6.06	25.03	6.10	25.08	6.09	6.40
	28.63	2.86	28.59	2.86	28.62	2.86	2.80
	29.84	1.76	29.80	1.76	29.82	1.77	1.97
	29.40	2.16	29.40	2.12	29.42	2.14	1.94
	29.77	1.83	29.73	1.82	29.77	1.82	1.57

	28.58	2.91	28.54	2.90	28.58	2.90	3.24
	27.46	3.92	27.42	3.92	27.46	3.92	3.80
	29.26	2.29	29.25	2.26	29.27	2.27	2.44
	29.05	2.48	29.03	2.46	29.06	2.47	2.54
	28.94	2.58	28.83	2.64	28.89	2.62	2.07
	29.10	2.44	29.07	2.42	29.10	2.43	2.31
	29.27	2.28	29.14	2.36	29.19	2.35	1.70
	30.14	1.49	30.08	1.50	30.12	1.50	1.61
	30.15	1.48	30.14	1.45	30.16	1.46	1.47
	30.21	1.43	30.17	1.42	30.20	1.42	1.47
	30.44	1.22	30.37	1.24	30.41	1.24	1.38
	30.01	1.61	29.98	1.59	30.02	1.59	1.38
	25.52	5.68	25.52	5.66	25.55	5.66	5.58
	29.17	2.37	29.16	2.34	29.19	2.35	2.56
	29.19	2.35	29.16	2.34	29.20	2.34	2.58
	29.85	1.76	29.83	1.73	29.85	1.74	1.86
	28.44	3.04	28.31	3.11	28.37	3.09	2.43
	25.84	5.40	25.81	5.39	25.85	5.39	5.47
	22.66	8.29	22.62	8.29	22.66	8.30	8.33
	23.12	7.87	23.10	7.86	23.14	7.86	8.02
	23.67	7.37	23.60	7.40	23.65	7.40	6.24
	22.74	8.21	22.75	8.17	22.80	8.17	8.23
	23.52	7.50	23.50	7.49	23.54	7.50	7.64
	25.09	6.08	25.02	6.11	25.07	6.10	5.75
	23.73	7.32	23.73	7.28	23.77	7.29	7.25
	23.42	7.59	23.42	7.56	23.46	7.56	7.56
4	27.43	3.95	27.35	3.99	27.39	3.99	4.11
	26.94	4.40	26.84	4.45	26.89	4.45	4.26
	28.38	3.09	28.32	3.10	28.37	3.09	2.76
	28.29	3.17	28.17	3.25	28.24	3.21	2.95
	23.80	7.25	23.77	7.25	23.82	7.24	7.56
	24.05	7.02	24.03	7.01	24.06	7.02	6.91
	23.64	7.39	23.64	7.37	23.68	7.37	7.19
	24.05	7.02	24.03	7.01	24.06	7.02	6.96
	28.40	3.07	28.37	3.06	28.41	3.06	2.79
	28.52	2.96	28.45	2.98	28.51	2.97	2.51
	30.54	1.12	30.45	1.16	30.49	1.16	0.72
	27.20	4.16	27.18	4.14	27.21	4.15	3.83
	27.31	4.06	27.32	4.01	27.34	4.03	4.05
	29.77	1.82	29.70	1.85	29.74	1.84	1.56
	29.62	1.96	29.57	1.96	29.63	1.95	1.62
	27.01	4.33	26.93	4.37	26.98	4.37	4.49
	27.41	3.97	27.40	3.94	27.44	3.94	3.78
	27.45	3.94	27.41	3.93	27.45	3.94	3.78
	27.47	3.91	27.43	3.92	27.47	3.92	3.78
	29.04	2.49	29.01	2.48	29.04	2.49	2.37
	28.44	3.04	28.45	2.98	28.48	2.99	2.88
	29.07	2.46	29.05	2.44	29.07	2.45	2.31
	28.25	3.20	28.28	3.14	28.30	3.16	3.09
	30.17	1.46	30.13	1.45	30.17	1.45	1.20

	28.35	3.12	28.30	3.12	28.35	3.11	2.74
	24.19	6.90	24.13	6.92	24.17	6.92	6.65
	24.97	6.18	24.93	6.19	24.98	6.18	5.85
	24.85	6.29	24.78	6.33	24.83	6.32	6.22
	29.39	2.17	29.38	2.14	29.42	2.14	1.95
	29.38	2.18	29.36	2.16	29.38	2.17	1.99
	27.77	3.64	27.74	3.63	27.76	3.65	3.54
	29.05	2.48	28.93	2.55	28.98	2.54	2.28
	30.49	1.17	30.40	1.21	30.43	1.21	1.07
	29.34	2.21	29.30	2.21	29.32	2.23	1.90
	26.92	4.41	26.89	4.41	26.92	4.42	4.01
	27.17	4.19	27.16	4.16	27.19	4.17	4.23
	28.40	3.07	28.30	3.12	28.35	3.11	2.07
	29.43	2.13	29.36	2.16	29.40	2.16	2.59
	28.60	2.88	28.50	2.94	28.54	2.94	2.80
	30.02	1.60	29.95	1.62	29.98	1.63	1.49
	29.14	2.40	29.07	2.42	29.10	2.43	2.15
	27.54	3.85	27.53	3.82	27.56	3.84	3.71
	27.56	3.83	27.53	3.83	27.57	3.83	3.83
	27.55	3.84	27.51	3.84	27.54	3.85	3.82
	27.28	4.09	27.17	4.15	27.23	4.14	3.92
	23.47	7.55	23.36	7.62	23.42	7.60	7.68
	23.60	7.43	23.58	7.42	23.63	7.42	7.26
	23.80	7.25	23.78	7.24	23.82	7.24	7.11
	23.56	7.47	23.55	7.44	23.60	7.45	7.33
	24.09	6.98	24.06	6.98	24.10	6.98	7.02
	27.87	3.55	27.82	3.56	27.84	3.58	3.46
	28.52	2.96	28.42	3.01	28.48	2.99	2.36
	28.86	2.65	28.81	2.66	28.84	2.66	2.66
	27.48	3.90	27.48	3.87	27.50	3.88	3.75
	27.47	3.91	27.46	3.88	27.49	3.90	3.75
	29.79	1.80	29.75	1.81	29.79	1.80	1.43
	29.74	1.85	29.71	1.84	29.73	1.85	1.60
	26.94	4.40	26.85	4.44	26.90	4.43	4.29
	27.73	3.68	27.69	3.68	27.72	3.69	3.69
	27.52	3.87	27.47	3.88	27.51	3.88	3.69
	27.56	3.83	27.55	3.81	27.59	3.81	3.69
	29.01	2.51	28.99	2.50	29.01	2.51	2.37
	28.43	3.04	28.45	2.99	28.47	3.00	2.88
	29.05	2.48	29.03	2.46	29.06	2.47	2.31
	28.25	3.21	28.27	3.15	28.29	3.17	3.09
	30.18	1.45	30.15	1.44	30.19	1.44	1.21
	28.38	3.09	28.33	3.09	28.38	3.08	2.75
	23.86	7.19	23.83	7.19	23.87	7.19	6.83
	24.52	6.59	24.47	6.61	24.51	6.61	6.35
	24.63	6.50	24.54	6.55	24.59	6.54	6.41
	29.36	2.20	29.35	2.16	29.38	2.17	1.95
	29.32	2.24	29.31	2.20	29.34	2.21	1.99
	27.74	3.67	27.71	3.66	27.74	3.67	3.51
	29.23	2.32	29.12	2.38	29.20	2.34	1.99

	30.38	1.27	30.30	1.30	30.34	1.30	0.97
	29.32	2.23	29.28	2.23	29.30	2.25	2.00
	27.22	4.14	27.21	4.11	27.23	4.13	3.94
	26.99	4.35	26.98	4.33	27.01	4.34	4.16
	29.48	2.09	29.42	2.10	29.45	2.11	1.74
	28.51	2.97	28.43	3.00	28.48	2.99	2.56
	28.53	2.95	28.46	2.98	28.48	2.99	2.79
	29.66	1.93	29.61	1.93	29.64	1.93	1.67
	29.14	2.40	29.12	2.37	29.15	2.39	2.20
	26.50	4.80	26.41	4.84	26.46	4.84	4.73
	28.11	3.34	28.08	3.33	28.11	3.33	3.20
5	29.11	2.42	29.04	2.45	29.08	2.45	2.48
	29.36	2.20	29.31	2.20	29.35	2.20	2.23
	28.09	3.35	28.05	3.35	28.08	3.36	3.41
	28.71	2.79	28.65	2.80	28.69	2.80	2.75
	30.00	1.62	29.92	1.65	29.98	1.63	1.67
	29.98	1.63	29.94	1.63	29.97	1.64	1.55
	27.34	4.03	27.26	4.07	27.29	4.08	4.23
	28.92	2.60	28.82	2.65	28.87	2.64	2.57
	29.71	1.88	29.59	1.95	29.64	1.94	1.95
	29.88	1.72	29.85	1.72	29.88	1.72	1.76
	30.10	1.52	30.07	1.51	30.09	1.52	1.56
	30.53	1.13	30.48	1.14	30.53	1.12	1.15
	30.30	1.34	30.27	1.33	30.31	1.33	1.15
	30.43	1.23	30.42	1.19	30.46	1.19	1.15
	29.78	1.81	29.76	1.80	29.79	1.80	1.84
	30.10	1.52	30.07	1.52	30.09	1.52	1.64
	30.50	1.17	30.50	1.12	30.52	1.13	1.25
	30.41	1.24	30.39	1.22	30.43	1.21	1.25
	30.13	1.49	30.10	1.49	30.14	1.48	1.25
	29.32	2.23	29.26	2.25	29.28	2.26	2.29
	26.73	4.59	26.66	4.61	26.69	4.63	4.74
	29.79	1.81	29.74	1.81	29.79	1.80	1.89
	29.19	2.35	29.16	2.34	29.21	2.33	1.89
	29.80	1.79	29.79	1.77	29.82	1.77	1.89
	29.88	1.73	29.85	1.71	29.88	1.72	1.63
	29.83	1.77	29.79	1.77	29.82	1.77	1.78
	29.65	1.94	29.54	2.00	29.58	1.99	1.98
	29.91	1.70	29.89	1.68	29.92	1.69	1.64
	29.77	1.83	29.74	1.82	29.77	1.82	1.84
	30.03	1.59	30.01	1.57	30.05	1.57	1.22
	30.26	1.38	30.24	1.35	30.28	1.35	1.22
	30.53	1.13	30.52	1.10	30.56	1.10	1.22
	30.87	0.82	30.84	0.81	30.88	0.81	1.16
	30.05	1.57	30.03	1.55	30.06	1.55	1.16
	30.31	1.34	30.30	1.30	30.33	1.31	1.16
	29.31	2.24	29.25	2.26	29.27	2.27	2.31
	30.91	0.79	30.87	0.78	30.91	0.78	1.18
	30.05	1.57	30.03	1.55	30.06	1.55	1.18
	30.29	1.35	30.28	1.32	30.31	1.33	1.18

6	23.19	7.80	23.18	7.78	23.22	7.79	7.82
	23.53	7.50	23.53	7.46	23.57	7.47	7.55
	22.78	8.18	22.76	8.17	22.80	8.17	8.27
	23.37	7.64	23.35	7.63	23.40	7.62	7.67
	26.27	5.01	26.23	5.01	26.26	5.02	4.56
	24.86	6.29	24.77	6.34	24.83	6.32	7.58
	24.10	6.98	24.06	6.99	24.10	6.99	7.69
	23.80	7.25	23.79	7.23	23.82	7.24	7.66
	23.62	7.42	23.53	7.46	23.60	7.44	7.96
	28.06	3.38	28.03	3.37	28.06	3.38	2.58
	28.24	3.22	28.19	3.23	28.23	3.22	2.71
	26.56	4.74	26.52	4.74	26.54	4.76	5.49
	24.45	6.66	24.43	6.64	24.47	6.64	7.23
	24.55	6.57	24.54	6.55	24.58	6.55	7.09
	24.06	7.01	24.02	7.02	24.06	7.02	7.27
	24.34	6.76	24.28	6.78	24.32	6.78	7.48
	27.95	3.48	27.90	3.48	27.92	3.51	4.25
	29.48	2.09	29.42	2.10	29.46	2.11	1.73
	30.02	1.60	29.98	1.59	30.01	1.60	1.51
	30.24	1.40	30.09	1.49	30.14	1.48	1.84
	30.26	1.38	30.26	1.34	30.29	1.34	0.95
	30.28	1.36	30.26	1.34	30.29	1.35	0.95
	30.64	1.04	30.64	0.99	30.67	1.00	0.95
	30.03	1.59	30.01	1.56	30.05	1.56	0.90
	30.94	0.76	30.93	0.73	30.96	0.73	0.90
	30.23	1.41	30.18	1.41	30.22	1.41	0.90
7	25.20	5.98	25.14	6.00	25.18	6.00	6.17
	27.21	4.15	27.12	4.20	27.18	4.17	4.49
	27.64	3.76	27.61	3.75	27.65	3.75	3.09
	23.55	7.48	23.49	7.50	23.54	7.50	7.34
	23.61	7.42	23.59	7.41	23.64	7.41	7.22
	27.06	4.29	26.99	4.32	27.03	4.32	4.72
	26.75	4.57	26.69	4.58	26.73	4.59	4.72
	24.39	6.71	24.36	6.71	24.40	6.71	6.75
	29.01	2.52	28.96	2.52	29.00	2.52	2.93
	27.49	3.90	27.43	3.92	27.47	3.91	2.93
	29.35	2.20	29.33	2.19	29.37	2.18	2.93
	27.54	3.86	27.45	3.90	27.50	3.89	2.62
	27.82	3.60	27.73	3.64	27.79	3.62	2.62
	24.39	6.71	24.37	6.70	24.41	6.70	6.90
	23.22	7.78	23.20	7.77	23.24	7.77	7.29
	23.90	7.16	23.88	7.14	23.92	7.15	7.23
	22.83	8.14	22.83	8.10	22.87	8.10	7.64
	23.78	7.27	23.78	7.24	23.82	7.24	7.19
	23.87	7.18	23.89	7.13	23.93	7.14	7.19
	28.86	2.65	28.82	2.65	28.86	2.64	3.14
	27.32	4.05	27.25	4.07	27.31	4.06	3.14
	28.93	2.59	28.91	2.57	28.95	2.57	3.14
	27.45	3.93	27.41	3.93	27.46	3.93	4.72
	26.93	4.41	26.89	4.41	26.91	4.42	4.72

	29.28	2.27	29.24	2.26	29.28	2.26	3.14
	27.73	3.68	27.66	3.71	27.71	3.70	3.14
	29.37	2.19	29.35	2.17	29.38	2.17	3.14
8	30.27	1.37	30.23	1.37	30.29	1.35	0.82
	30.72	0.96	30.67	0.96	30.71	0.96	0.82
	31.17	0.55	31.14	0.54	31.17	0.54	0.82
	30.56	1.11	30.56	1.06	30.59	1.07	1.13
	30.65	1.02	30.64	0.99	30.68	0.99	1.13
	30.56	1.11	30.54	1.08	30.58	1.08	1.13
	25.66	5.56	25.64	5.55	25.68	5.54	5.42
	29.95	1.66	29.93	1.64	29.97	1.63	1.05
	30.69	0.99	30.66	0.98	30.70	0.97	1.05
	30.76	0.93	30.75	0.90	30.78	0.90	1.05
	30.65	1.03	30.66	0.97	30.69	0.98	0.68
	30.60	1.07	30.60	1.03	30.63	1.03	0.68
	31.05	0.66	31.05	0.62	31.07	0.63	0.68
9	30.36	1.29	30.25	1.35	30.28	1.35	1.44
	30.10	1.53	29.98	1.60	30.01	1.60	1.69
	29.99	1.63	29.94	1.63	29.97	1.64	1.69
	29.81	1.79	29.75	1.80	29.79	1.80	1.59
	30.06	1.56	30.01	1.57	30.05	1.56	1.52
	30.56	1.10	30.53	1.09	30.56	1.10	1.52
	27.89	3.54	27.81	3.57	27.84	3.58	3.64
	30.17	1.46	30.13	1.46	30.15	1.47	2.21
	29.19	2.36	29.12	2.38	29.16	2.38	1.52
	29.67	1.92	29.59	1.95	29.62	1.96	1.77
	29.86	1.74	29.83	1.73	29.86	1.74	1.52
	30.18	1.45	30.14	1.44	30.17	1.45	1.52
	30.30	1.34	30.27	1.33	30.30	1.34	1.98
	28.98	2.55	28.93	2.55	28.97	2.55	1.28
	29.90	1.71	29.85	1.71	29.88	1.72	1.31
	29.59	1.99	29.52	2.02	29.56	2.01	1.77
	30.44	1.22	30.41	1.21	30.43	1.21	1.48
	30.35	1.29	30.26	1.34	30.30	1.33	1.49
	30.15	1.48	30.12	1.47	30.15	1.47	1.81
	29.81	1.79	29.77	1.79	29.80	1.79	1.28
	28.51	2.97	28.44	3.00	28.49	2.99	3.10
	29.92	1.69	29.89	1.68	29.91	1.69	1.74
	27.16	4.19	27.09	4.23	27.12	4.23	4.43
	27.38	3.99	27.29	4.04	27.32	4.05	4.26
	30.44	1.22	30.40	1.21	30.44	1.20	1.21
	30.18	1.46	30.16	1.43	30.19	1.43	1.21
	30.60	1.07	30.60	1.03	30.64	1.03	1.21
	30.81	0.88	30.77	0.87	30.81	0.87	0.88
	30.84	0.86	30.79	0.86	30.83	0.86	0.88
	30.67	1.01	30.61	1.02	30.66	1.01	0.88
	30.71	0.97	30.65	0.99	30.70	0.97	0.95
	30.47	1.18	30.43	1.19	30.47	1.18	0.95
	30.69	0.99	30.65	0.98	30.71	0.96	0.95
	30.37	1.28	30.34	1.27	30.37	1.27	1.13

	31.03	0.68	31.01	0.66	31.05	0.66	1.13
	30.18	1.45	30.12	1.47	30.17	1.45	1.13
	30.89	0.80	30.88	0.78	30.91	0.78	1.22
	30.68	1.00	30.68	0.95	30.71	0.97	1.22
	29.39	2.17	29.34	2.18	29.39	2.17	1.22
	29.60	1.98	29.56	1.98	29.61	1.97	0.99
	30.96	0.74	30.95	0.71	30.97	0.72	0.99
	30.76	0.92	30.76	0.89	30.78	0.90	0.99
	30.46	1.20	30.46	1.16	30.48	1.17	0.96
	31.03	0.68	31.02	0.65	31.05	0.65	0.96
	30.35	1.30	30.31	1.29	30.36	1.28	0.96
10	25.73	5.50	25.61	5.57	25.66	5.57	5.63
	28.02	3.42	27.94	3.45	28.00	3.44	3.43
	28.42	3.05	28.38	3.05	28.42	3.05	3.17
	29.13	2.41	29.04	2.45	29.08	2.44	2.23
	30.13	1.50	30.13	1.46	30.15	1.47	1.32
	30.14	1.49	30.10	1.48	30.13	1.49	1.10
	25.99	5.26	25.90	5.31	25.96	5.29	5.25
	26.50	4.80	26.42	4.83	26.47	4.83	4.64
	29.01	2.52	28.94	2.54	28.96	2.55	2.51
	29.26	2.29	29.19	2.31	29.23	2.31	1.90
	28.86	2.65	28.79	2.68	28.83	2.68	2.37
	27.33	4.04	27.21	4.12	27.27	4.10	4.77
	26.22	5.05	26.16	5.07	26.22	5.05	4.79
	28.83	2.68	28.75	2.71	28.79	2.71	2.67
	29.21	2.33	29.14	2.36	29.18	2.36	2.61
	30.69	0.99	30.68	0.95	30.71	0.96	0.83
	30.55	1.11	30.56	1.06	30.59	1.07	0.83
	30.67	1.00	30.68	0.96	30.71	0.96	0.83
	28.87	2.65	28.79	2.68	28.84	2.66	2.97
	29.65	1.93	29.58	1.96	29.63	1.95	2.97
	29.14	2.40	29.07	2.42	29.12	2.41	2.97
	30.63	1.05	30.62	1.01	30.66	1.01	1.06
	30.21	1.42	30.21	1.38	30.25	1.38	1.06
	30.72	0.96	30.71	0.93	30.74	0.93	1.06
	30.75	0.93	30.73	0.91	30.76	0.91	1.15
	30.28	1.36	30.24	1.36	30.28	1.35	1.15
	31.13	0.59	31.12	0.56	31.15	0.56	1.15
	31.20	0.52	31.16	0.52	31.21	0.51	1.04
	31.78	0.00	31.73	0.00	31.77	0.00	1.04
	32.92	-1.04	32.80	-0.98	32.85	-0.98	1.04
	30.05	1.57	29.98	1.59	30.04	1.58	1.59
	29.97	1.64	29.87	1.69	29.94	1.66	1.59
	30.83	0.86	30.74	0.90	30.80	0.88	1.59
	23.68	7.36	23.65	7.35	23.71	7.35	7.61
	23.77	7.28	23.74	7.28	23.77	7.28	7.35
	23.84	7.21	23.82	7.20	23.88	7.19	6.90
	23.77	7.28	23.73	7.28	23.79	7.27	6.90
	24.11	6.97	24.10	6.94	24.14	6.95	7.11
	24.00	7.07	23.96	7.07	24.01	7.07	7.18

	24.32	6.78	24.31	6.75	24.35	6.76	6.69
	24.25	6.84	24.23	6.83	24.28	6.83	6.69
11	27.40	3.98	27.39	3.95	27.42	3.96	3.78
	28.96	2.56	28.91	2.57	28.95	2.56	2.97
	28.57	2.91	28.55	2.90	28.59	2.89	2.77
	24.74	6.40	24.68	6.42	24.72	6.42	6.45
	23.51	7.51	23.48	7.51	23.54	7.50	7.35
	24.15	6.94	24.10	6.94	24.17	6.92	6.97
	24.23	6.86	24.19	6.87	24.24	6.85	6.84
	23.71	7.33	23.70	7.31	23.75	7.30	7.30
	24.48	6.64	24.41	6.66	24.47	6.65	6.73
	24.37	6.73	24.35	6.72	24.40	6.71	6.84
	24.97	6.19	24.92	6.20	24.96	6.20	6.44
	29.76	1.84	29.69	1.85	29.73	1.86	2.10
	29.13	2.40	29.07	2.42	29.11	2.42	2.75
	28.51	2.97	28.47	2.96	28.51	2.96	3.65
	27.36	4.02	27.29	4.04	27.32	4.05	4.76
	30.87	0.82	30.86	0.79	30.89	0.80	1.45
	30.53	1.13	30.49	1.13	30.53	1.13	1.45
	30.44	1.21	30.45	1.16	30.48	1.17	1.45
	28.63	2.86	28.62	2.83	28.65	2.84	2.44
	29.39	2.17	29.32	2.20	29.37	2.19	2.44
	29.57	2.00	29.53	2.00	29.58	1.99	2.44
	28.71	2.78	28.65	2.81	28.69	2.80	3.28
	27.99	3.44	27.96	3.43	28.01	3.42	3.28
	29.14	2.39	29.07	2.43	29.12	2.41	3.28
	29.42	2.14	29.39	2.13	29.43	2.12	2.38
	28.86	2.65	28.86	2.61	28.90	2.61	2.38
	28.82	2.69	28.81	2.66	28.86	2.65	2.38
	27.43	3.95	27.41	3.93	27.46	3.93	4.09
	27.50	3.89	27.48	3.87	27.52	3.87	4.09
	26.99	4.35	27.00	4.31	27.04	4.31	4.09
	27.16	4.20	27.17	4.16	27.21	4.15	4.08
	27.63	3.77	27.61	3.75	27.66	3.75	4.08
	27.71	3.70	27.69	3.67	27.73	3.68	4.08
	28.89	2.62	28.88	2.59	28.93	2.58	2.33
	29.51	2.06	29.48	2.05	29.52	2.04	2.33
	28.88	2.64	28.87	2.60	28.91	2.60	2.33
	30.24	1.40	30.22	1.37	30.26	1.37	1.62
	30.19	1.45	30.13	1.46	30.18	1.45	1.62
	30.04	1.58	30.02	1.56	30.06	1.55	1.62
	31.09	0.63	31.07	0.60	31.11	0.60	1.10
	30.45	1.21	30.45	1.17	30.48	1.17	1.10
	30.69	0.99	30.67	0.97	30.69	0.98	1.10
12	29.11	2.43	28.96	2.52	29.01	2.51	2.56
	28.12	3.32	28.03	3.37	28.07	3.36	4.04
	29.33	2.22	29.21	2.29	29.26	2.29	2.23
	29.18	2.36	29.08	2.41	29.13	2.41	2.47
	28.46	3.01	28.39	3.04	28.42	3.05	2.85
	30.22	1.42	30.16	1.43	30.20	1.43	1.07

	30.71	0.97	30.64	0.99	30.69	0.98	1.07
	31.06	0.65	30.98	0.69	31.02	0.68	1.07
	26.62	4.69	26.55	4.72	26.58	4.72	4.76
	27.10	4.25	27.04	4.27	27.08	4.27	4.46
	30.62	1.06	30.59	1.04	30.62	1.05	1.17
	30.19	1.44	30.15	1.44	30.19	1.44	1.17
	30.43	1.22	30.35	1.26	30.40	1.24	1.17
	28.74	2.76	28.67	2.78	28.71	2.79	2.98
	28.88	2.64	28.82	2.65	28.84	2.66	2.68
	29.95	1.66	29.93	1.64	29.98	1.62	1.18
	30.50	1.16	30.48	1.14	30.52	1.14	1.18
	30.83	0.86	30.80	0.85	30.83	0.85	1.18
	30.69	0.99	30.68	0.95	30.71	0.96	1.29
	30.24	1.40	30.22	1.38	30.25	1.38	1.29
	30.20	1.44	30.18	1.41	30.21	1.42	1.29
	24.64	6.49	24.62	6.47	24.67	6.47	6.34
	23.89	7.17	23.85	7.17	23.89	7.17	7.41
	23.81	7.24	23.81	7.21	23.84	7.22	7.40
13	27.63	3.77	27.60	3.76	27.63	3.77	4.11
	28.55	2.93	28.49	2.95	28.52	2.96	1.84
	28.10	3.34	28.08	3.33	28.11	3.33	3.14
	28.14	3.31	28.05	3.35	28.10	3.34	2.98
	29.58	2.00	29.58	1.96	29.61	1.97	2.16
	28.72	2.78	28.67	2.78	28.72	2.77	2.16
	29.35	2.20	29.30	2.21	29.34	2.21	2.48
	29.71	1.88	29.67	1.88	29.72	1.86	2.48
	28.09	3.35	28.10	3.31	28.12	3.33	3.12
	28.49	2.99	28.47	2.96	28.51	2.96	3.12
	27.62	3.78	27.61	3.75	27.64	3.76	3.55
	28.70	2.80	28.65	2.81	28.68	2.81	3.55
	23.92	7.14	23.91	7.12	23.95	7.12	7.14
	24.23	6.86	24.18	6.87	24.22	6.87	6.20
	25.77	5.46	25.74	5.46	25.78	5.45	5.35
	24.34	6.76	24.34	6.73	24.37	6.74	6.66
	24.09	6.99	24.08	6.96	24.12	6.97	7.12
	29.32	2.24	29.23	2.28	29.29	2.26	1.83
	29.77	1.82	29.77	1.78	29.81	1.78	1.83
	29.70	1.89	29.67	1.87	29.71	1.87	1.83
	26.03	5.22	26.00	5.22	26.03	5.23	5.30
	29.35	2.20	29.30	2.21	29.34	2.21	2.48
	29.71	1.88	29.67	1.88	29.72	1.86	2.48
	28.09	3.35	28.10	3.31	28.12	3.33	2.90
	28.49	2.99	28.47	2.96	28.51	2.96	2.90
	27.62	3.78	27.61	3.75	27.64	3.76	3.13
	28.70	2.80	28.65	2.81	28.68	2.81	3.13
14	28.74	2.76	28.64	2.82	28.68	2.81	2.99
	28.37	3.09	28.29	3.13	28.34	3.12	3.36
	27.55	3.85	27.47	3.88	27.50	3.89	3.50
	28.62	2.87	28.59	2.86	28.63	2.85	2.72
	29.39	2.17	29.37	2.15	29.40	2.15	2.04

	25.02	6.14	24.97	6.16	25.01	6.15	6.38
	23.84	7.21	23.83	7.19	23.88	7.19	7.14
	29.50	2.07	29.50	2.03	29.54	2.03	1.78
	29.57	2.01	29.54	1.99	29.59	1.98	1.78
	29.64	1.94	29.63	1.91	29.67	1.91	1.78
	24.20	6.88	24.15	6.90	24.20	6.90	6.94
	24.76	6.38	24.74	6.36	24.79	6.36	6.42
	23.65	7.39	23.60	7.40	23.65	7.39	7.24
	24.14	6.94	24.08	6.96	24.13	6.96	6.98
	24.76	6.38	24.74	6.37	24.77	6.37	6.51
	25.33	5.86	25.25	5.89	25.30	5.89	6.23
	24.81	6.34	24.77	6.33	24.81	6.34	6.46
	24.13	6.95	24.12	6.93	24.16	6.93	7.05
	23.64	7.39	23.65	7.36	23.69	7.36	7.41
	24.32	6.77	24.29	6.78	24.33	6.78	6.97
15	24.28	6.82	24.28	6.78	24.33	6.78	6.81
	28.72	2.78	28.62	2.83	28.66	2.83	2.23
	26.71	4.61	26.66	4.62	26.68	4.63	5.41
	27.57	3.82	27.46	3.89	27.49	3.89	3.58
	26.06	5.20	25.97	5.25	26.01	5.25	5.68
	30.29	1.35	30.23	1.37	30.27	1.36	1.02
	30.70	0.98	30.67	0.97	30.70	0.97	1.02
	30.30	1.34	30.28	1.32	30.32	1.32	1.02
	23.30	7.70	23.27	7.70	23.32	7.70	8.01
	23.55	7.48	23.53	7.47	23.57	7.47	7.42
	23.57	7.46	23.54	7.45	23.58	7.46	7.54
	23.92	7.14	23.89	7.14	23.93	7.14	7.42
	23.82	7.23	23.75	7.26	23.81	7.25	8.01
	25.56	5.65	25.46	5.71	25.50	5.71	6.36
	29.54	2.04	29.49	2.04	29.54	2.03	1.68
	29.74	1.85	29.70	1.85	29.75	1.84	1.68
	29.88	1.73	29.86	1.71	29.90	1.70	1.68
	25.27	5.91	25.21	5.94	25.27	5.92	5.39
	29.69	1.90	29.60	1.94	29.63	1.94	1.99
	29.08	2.45	28.98	2.50	29.04	2.49	2.37
	26.98	4.36	26.87	4.43	26.90	4.43	5.48
	29.84	1.76	29.80	1.76	29.83	1.76	0.97
	30.71	0.97	30.67	0.97	30.70	0.97	0.97
	30.94	0.76	30.92	0.74	30.95	0.74	0.97
	30.56	1.11	30.54	1.08	30.57	1.09	1.02
	30.65	1.02	30.63	1.00	30.66	1.01	1.02
	30.38	1.27	30.35	1.26	30.38	1.26	1.02
	26.49	4.80	26.37	4.88	26.41	4.88	5.39
	24.35	6.75	24.33	6.74	24.38	6.73	6.75
	28.68	2.81	28.63	2.82	28.68	2.81	1.73
	29.57	2.01	29.52	2.02	29.57	2.00	1.73
	29.63	1.95	29.58	1.95	29.63	1.94	1.73
	29.59	1.99	29.54	2.00	29.59	1.98	2.05
	28.84	2.67	28.74	2.72	28.79	2.71	2.05
	29.68	1.90	29.59	1.95	29.64	1.93	2.05

	29.62	1.96	29.59	1.94	29.64	1.94	2.27
	29.04	2.48	29.01	2.48	29.05	2.48	2.27
	29.20	2.34	29.14	2.36	29.18	2.36	2.27
	28.97	2.55	28.92	2.56	28.97	2.55	2.18
	29.58	2.00	29.48	2.05	29.54	2.03	2.18
	29.81	1.78	29.77	1.78	29.82	1.77	2.18
	29.41	2.15	29.36	2.16	29.41	2.14	2.02
	28.89	2.63	28.82	2.65	28.87	2.64	2.02
	29.34	2.22	29.27	2.24	29.31	2.24	2.02
	29.37	2.19	29.30	2.21	29.35	2.20	2.00
	29.28	2.27	29.18	2.33	29.23	2.31	2.00
16	29.19	2.35	29.14	2.36	29.18	2.36	2.00
	27.67	3.73	27.66	3.70	27.69	3.72	3.75
	25.76	5.47	25.70	5.49	25.76	5.48	5.21
	26.23	5.04	26.15	5.08	26.20	5.07	5.04
	26.72	4.60	26.68	4.60	26.72	4.60	4.57
	26.21	5.06	26.14	5.09	26.17	5.10	5.03
	25.76	5.47	25.69	5.50	25.74	5.49	5.44
	24.33	6.77	24.27	6.79	24.33	6.78	6.62
	24.80	6.34	24.73	6.38	24.78	6.36	6.30
17	24.43	6.68	24.38	6.69	24.43	6.68	6.58
	24.46	6.65	24.39	6.68	24.45	6.67	6.49
	29.70	1.89	29.64	1.90	29.68	1.90	1.77
	27.65	3.75	27.64	3.73	27.65	3.75	3.46
	28.09	3.35	28.03	3.36	28.06	3.38	3.39
	25.76	5.47	25.72	5.48	25.74	5.49	5.59
	27.92	3.51	27.87	3.51	27.90	3.53	4.08
	27.78	3.63	27.72	3.65	27.76	3.65	3.62
	26.94	4.40	26.87	4.42	26.91	4.43	4.18
	27.86	3.56	27.82	3.56	27.84	3.57	2.76
	28.11	3.33	28.07	3.33	28.10	3.34	3.25
	27.94	3.48	27.92	3.47	27.94	3.48	3.23
	28.23	3.22	28.19	3.22	28.21	3.24	3.11
	28.30	3.16	28.24	3.18	28.27	3.19	2.94
	29.46	2.11	29.43	2.10	29.46	2.10	2.04
	27.52	3.87	27.48	3.87	27.50	3.88	3.93
	27.22	4.14	27.18	4.14	27.21	4.15	4.29
	29.33	2.23	29.28	2.23	29.32	2.23	2.36
	29.35	2.21	29.32	2.20	29.34	2.21	1.90
	28.62	2.87	28.57	2.88	28.61	2.87	2.28
	29.71	1.88	29.68	1.86	29.72	1.86	2.01
	26.34	4.94	26.27	4.97	26.32	4.96	5.36
	29.12	2.41	29.08	2.41	29.11	2.42	2.18
	27.29	4.07	27.29	4.04	27.32	4.05	4.03
	27.66	3.74	27.65	3.72	27.67	3.73	3.58
	30.56	1.11	30.56	1.07	30.58	1.08	0.89
	29.74	1.85	29.71	1.84	29.75	1.84	0.89
	30.01	1.61	30.00	1.57	30.04	1.58	0.89
	22.83	8.13	22.77	8.16	22.82	8.15	8.16
	23.50	7.52	23.49	7.50	23.53	7.50	7.57

	23.38	7.64	23.36	7.62	23.41	7.61	7.66
	23.54	7.49	23.53	7.47	23.57	7.47	7.57
	22.80	8.15	22.78	8.15	22.82	8.15	8.16
	27.27	4.09	27.25	4.08	27.28	4.09	3.62
	27.73	3.68	27.72	3.66	27.74	3.67	3.56
	27.60	3.80	27.59	3.77	27.62	3.78	3.75
	27.36	4.01	27.35	3.99	27.38	4.00	3.89
18	24.08	6.99	24.07	6.97	24.11	6.97	6.62
	29.23	2.31	29.20	2.31	29.23	2.31	1.98
	27.76	3.65	27.74	3.63	27.77	3.64	3.11
	25.14	6.03	25.11	6.02	25.15	6.03	5.70
	27.68	3.72	27.64	3.72	27.66	3.74	3.49
	28.92	2.59	28.86	2.61	28.89	2.62	2.20
	28.36	3.11	28.21	3.21	28.26	3.20	3.11
	29.24	2.31	29.13	2.37	29.17	2.36	2.77
	29.24	2.31	29.17	2.33	29.21	2.33	2.11
	30.01	1.60	29.94	1.63	30.00	1.61	0.94
	28.55	2.93	28.46	2.98	28.49	2.99	2.87
	27.29	4.08	27.26	4.07	27.30	4.07	3.58
	27.67	3.73	27.62	3.74	27.66	3.74	4.25
	29.68	1.90	29.65	1.89	29.69	1.90	1.93
	29.55	2.03	29.48	2.05	29.52	2.05	2.10
	26.95	4.39	26.92	4.38	26.94	4.40	4.56
	30.06	1.56	30.05	1.53	30.07	1.54	1.81
	29.70	1.89	29.65	1.89	29.70	1.88	1.81
	29.05	2.48	29.02	2.47	29.06	2.46	1.81
	30.48	1.18	30.49	1.13	30.52	1.13	1.17
	30.03	1.59	30.01	1.57	30.04	1.57	1.17
	30.47	1.19	30.45	1.17	30.48	1.17	1.17
	29.67	1.91	29.65	1.90	29.68	1.90	1.11
	30.54	1.12	30.49	1.13	30.53	1.12	1.11
	30.31	1.34	30.26	1.34	30.30	1.34	1.11
19	25.20	5.98	25.14	6.00	25.18	6.00	5.97
	28.86	2.65	28.79	2.67	28.83	2.67	2.91
	28.74	2.76	28.69	2.77	28.73	2.77	2.74
	26.73	4.59	26.67	4.61	26.70	4.61	4.97
	27.52	3.87	27.42	3.92	27.48	3.90	4.74
	25.10	6.06	25.06	6.07	25.10	6.08	6.00
	26.24	5.03	26.22	5.01	26.25	5.03	5.11
	24.28	6.82	24.26	6.80	24.32	6.78	6.99
	24.49	6.63	24.44	6.64	24.49	6.63	6.99
	24.48	6.63	24.45	6.63	24.50	6.62	6.73
	24.55	6.57	24.51	6.58	24.55	6.57	6.71
	26.07	5.19	25.92	5.29	25.97	5.28	6.99
	24.03	7.04	24.01	7.03	24.06	7.02	6.99
	26.77	4.56	26.73	4.55	26.77	4.56	4.31
	25.21	5.96	25.17	5.97	25.22	5.97	6.01
	27.24	4.12	27.21	4.12	27.25	4.12	4.02
20	27.55	3.84	27.52	3.84	27.54	3.85	3.96
	29.20	2.35	29.17	2.33	29.21	2.33	2.35

	30.19	1.44	30.19	1.40	30.22	1.41	1.44
	28.30	3.16	28.24	3.18	28.27	3.18	3.13
	30.54	1.13	30.45	1.17	30.49	1.16	1.26
	27.61	3.78	27.53	3.82	27.57	3.82	3.85
	22.85	8.12	22.81	8.12	22.85	8.13	8.08
	23.80	7.25	23.78	7.24	23.82	7.24	7.24
	23.97	7.10	23.96	7.07	23.99	7.08	7.08
	23.83	7.23	23.81	7.21	23.86	7.21	7.16
	29.60	1.98	29.61	1.93	29.64	1.94	1.89
	29.71	1.88	29.69	1.86	29.72	1.86	1.87
	28.48	3.00	28.46	2.98	28.49	2.98	3.21
	28.52	2.96	28.45	2.98	28.49	2.98	2.87
	28.80	2.71	28.78	2.69	28.82	2.69	2.74
	27.77	3.65	27.76	3.61	27.79	3.63	3.71
	25.06	6.11	25.03	6.10	25.08	6.09	5.92
	27.30	4.07	27.29	4.04	27.32	4.05	4.05
	27.36	4.01	27.38	3.96	27.42	3.96	4.14
	27.26	4.10	27.22	4.11	27.25	4.12	4.27
	28.52	2.96	28.46	2.98	28.49	2.98	3.11
	28.89	2.62	28.87	2.61	28.89	2.62	2.66
21	22.79	8.17	22.77	8.16	22.80	8.17	8.23
	29.56	2.01	29.52	2.01	29.56	2.01	1.72
	28.08	3.36	28.04	3.36	28.08	3.36	3.24
	27.97	3.46	27.97	3.42	28.00	3.44	3.18
	29.51	2.06	29.46	2.07	29.51	2.05	2.46
	27.59	3.81	27.59	3.77	27.61	3.79	3.62
	23.72	7.33	23.71	7.30	23.75	7.30	7.26
	23.97	7.09	23.96	7.07	24.00	7.08	7.18
	23.88	7.18	23.86	7.16	23.90	7.17	7.29
	28.95	2.57	28.86	2.61	28.89	2.62	2.88
	27.59	3.81	27.49	3.86	27.54	3.85	3.86
	28.91	2.61	28.84	2.63	28.91	2.61	1.78
	30.28	1.36	30.28	1.32	30.32	1.32	1.78
	27.11	4.24	27.06	4.26	27.09	4.26	4.45
	28.08	3.36	27.99	3.40	28.03	3.40	2.74
	28.62	2.87	28.60	2.85	28.63	2.86	3.36
	25.80	5.43	25.78	5.42	25.82	5.41	5.43
	29.21	2.33	29.15	2.35	29.19	2.35	2.14
	28.39	3.08	28.39	3.04	28.42	3.04	3.03
	29.32	2.24	29.28	2.23	29.32	2.23	1.73
	28.52	2.96	28.43	3.00	28.46	3.01	2.57
	29.95	1.67	29.92	1.64	29.96	1.64	1.78
	27.20	4.16	27.17	4.15	27.19	4.17	4.62
	29.26	2.29	29.21	2.29	29.27	2.28	1.72
	29.91	1.70	29.91	1.66	29.94	1.66	1.72
	29.99	1.62	29.99	1.58	30.03	1.58	1.72
	25.60	5.61	25.57	5.61	25.61	5.61	5.62
	27.89	3.53	27.87	3.52	27.90	3.52	3.59
	28.34	3.12	28.31	3.12	28.34	3.12	2.91
	29.84	1.76	29.81	1.75	29.84	1.75	1.62

	29.61	1.97	29.57	1.97	29.60	1.97	2.04
	28.42	3.05	28.36	3.07	28.40	3.06	3.03
	29.88	1.73	29.82	1.74	29.85	1.74	1.61
	28.00	3.44	27.94	3.45	27.97	3.45	3.06
	24.58	6.54	24.53	6.56	24.58	6.55	6.52
	24.03	7.04	24.02	7.02	24.06	7.02	7.17
	24.37	6.74	24.37	6.70	24.40	6.71	6.85
	24.01	7.06	23.98	7.06	24.02	7.05	7.09
	28.40	3.07	28.42	3.02	28.44	3.03	3.18
	28.73	2.77	28.75	2.71	28.79	2.71	2.71
	28.05	3.39	28.00	3.39	28.03	3.41	3.51
22	29.40	2.16	29.38	2.14	29.43	2.13	1.52
	30.06	1.56	30.01	1.57	30.05	1.56	1.52
	30.00	1.62	29.98	1.59	30.02	1.59	1.52
	29.64	1.95	29.61	1.93	29.65	1.93	1.52
	30.42	1.24	30.40	1.21	30.43	1.22	1.52
	30.01	1.61	30.01	1.57	30.04	1.57	1.52
	24.72	6.41	24.67	6.42	24.73	6.42	6.16
	23.79	7.26	23.80	7.22	23.84	7.22	7.21
	23.68	7.36	23.65	7.36	23.68	7.37	7.32
	28.33	3.13	28.22	3.19	28.29	3.16	3.27
	28.26	3.20	28.21	3.21	28.25	3.20	3.35
	23.97	7.10	23.98	7.06	24.02	7.06	6.93
	23.87	7.18	23.87	7.15	23.92	7.15	7.03
	23.99	7.08	23.94	7.09	23.98	7.10	7.48
	25.85	5.38	25.82	5.38	25.87	5.37	5.10
	25.87	5.37	25.82	5.38	25.87	5.37	4.99
	23.88	7.18	23.84	7.18	23.90	7.17	7.39
	23.63	7.40	23.60	7.40	23.64	7.41	7.49
	23.99	7.08	23.95	7.08	24.00	7.08	7.10
	23.84	7.22	23.80	7.22	23.84	7.22	7.19
	30.18	1.45	30.15	1.44	30.19	1.43	1.57
	29.94	1.67	29.92	1.65	29.96	1.64	1.57
	30.19	1.45	30.18	1.41	30.21	1.42	1.57
	31.48	0.27	31.39	0.31	31.45	0.29	1.29
	31.22	0.51	31.19	0.50	31.23	0.49	1.29
	33.17	-1.27	33.04	-1.19	33.09	-1.21	1.29
23	27.20	4.16	27.19	4.13	27.23	4.13	4.62
	28.48	3.00	28.41	3.02	28.44	3.03	5.01
	28.71	2.79	28.69	2.77	28.73	2.77	2.05
	30.78	0.91	30.77	0.88	30.79	0.89	1.60
	26.37	4.91	26.36	4.88	26.39	4.90	5.58
	26.54	4.76	26.47	4.79	26.51	4.79	4.68
	28.01	3.43	27.97	3.42	28.02	3.41	3.90
	28.49	2.99	28.47	2.97	28.50	2.97	3.09
	28.36	3.11	28.29	3.13	28.32	3.14	3.70
	28.98	2.54	28.94	2.54	28.97	2.55	2.80
	29.69	1.90	29.65	1.90	29.68	1.90	2.71
	30.46	1.20	30.41	1.20	30.45	1.20	1.81
	30.44	1.21	30.37	1.24	30.41	1.23	1.81

	26.91	4.42	26.83	4.46	26.87	4.46	4.85
	30.01	1.60	29.98	1.59	30.01	1.60	1.81
	30.31	1.34	30.25	1.34	30.29	1.34	1.81
	27.70	3.71	27.64	3.73	27.66	3.74	4.32
	28.57	2.92	28.58	2.87	28.59	2.89	3.06
	29.09	2.45	29.08	2.42	29.11	2.42	3.06
	27.65	3.75	27.62	3.75	27.65	3.75	3.95
	27.79	3.63	27.77	3.60	27.81	3.60	3.92
	26.50	4.80	26.45	4.81	26.48	4.82	4.13
	27.31	4.06	27.29	4.04	27.31	4.06	3.85
	23.51	7.52	23.41	7.57	23.47	7.56	8.03

^[a] Parameters of linear regression models are presented in Table 2 in main text.

^[b] For the references to the experimental works, please, see the main text.

Table S3. Calculated ^{13}C NMR shielding constants, together with scaled and experimental chemical shifts – the GIAO-DFT(PBE0) calculations with the first-level basis sets.

Mol.	pcS-1		pecS-1		pecS-1 mod		$\delta_{exp}^{[b]}$
	σ	$\delta_{scaled}^{[a]}$	σ	$\delta_{scaled}^{[a]}$	σ	$\delta_{scaled}^{[a]}$	
1	126.4	58.3	124.3	57.5	124.2	58.4	55.5
	149.4	36.3	147.1	36.3	147.8	36.1	33.3
	141.6	43.8	138.4	44.4	139.3	44.1	35.9
	46.7	134.9	40.4	135.5	42.7	135.4	133.2
	130.2	54.7	128.4	53.6	128.6	54.2	54.6
	132.5	52.5	131.2	51.0	131.5	51.4	52.0
	40.9	140.4	33.5	142.0	36.4	141.3	135.2
	75.9	106.8	70.1	107.9	72.3	107.4	107.3
	164.0	22.3	162.5	21.9	162.8	21.9	19.5
	149.3	36.4	147.1	36.2	147.3	36.5	38.5
	56.7	125.2	49.7	126.9	51.3	127.3	128.1
	48.6	133.1	41.5	134.5	43.8	134.3	138.1
	62.6	119.6	57.5	119.7	60.0	119.1	124.5
	36.9	144.3	31.3	144.1	32.6	144.9	145.0
	64.2	118.0	59.9	117.4	61.4	117.7	118.6
	47.5	134.1	40.8	135.2	43.1	135.0	137.1
	72.2	110.3	67.9	110.0	69.4	110.2	112.2
	172.4	14.2	171.6	13.4	172.1	13.1	13.0
	56.4	125.5	49.8	126.8	51.9	126.7	130.1
	63.5	118.7	58.1	119.1	60.4	118.7	119.8
	61.5	120.7	56.4	120.7	58.6	120.4	122.5
	61.4	120.7	55.1	121.9	56.6	122.2	122.8
	49.4	132.2	42.7	133.4	45.0	133.3	136.9
	69.1	113.4	64.9	112.7	66.4	113.0	114.4
	42.9	138.5	38.5	137.3	40.3	137.6	137.2
	78.6	104.2	75.1	103.3	75.8	104.2	106.7
	69.6	112.9	65.1	112.5	66.6	112.8	113.6

	30.5	150.4	23.2	151.6	26.6	150.6	152.0
	65.2	117.1	60.0	117.3	62.0	117.2	119.3
2	56.6	125.4	49.1	127.5	51.4	127.2	125.7
	68.5	114.0	62.7	114.8	64.6	114.7	115.1
	58.0	124.0	53.8	123.1	55.4	123.4	124.1
	46.6	134.9	39.6	136.3	41.9	136.1	137.0
	71.0	111.6	66.5	111.3	68.0	111.5	111.4
	59.6	122.5	54.2	122.7	56.5	122.4	122.3
	62.5	119.7	57.1	120.0	59.2	119.9	119.9
	61.9	120.3	56.6	120.5	58.3	120.7	120.4
	118.1	66.3	113.3	67.7	113.7	68.3	68.2
	66.5	115.9	61.5	115.9	63.2	116.1	115.1
	57.9	124.1	50.2	126.4	52.3	126.3	125.7
	47.2	134.4	40.1	135.9	42.3	135.8	137.0
	55.1	126.8	50.4	126.3	52.2	126.5	124.1
	61.8	120.3	56.5	120.6	58.3	120.7	120.4
	62.8	119.4	57.3	119.8	59.4	119.6	119.9
	60.2	121.9	54.8	122.2	57.0	121.9	122.3
	72.1	110.5	67.6	110.2	69.2	110.4	111.4
	-22.3	201.1	-26.4	197.7	-24.4	198.9	201.5
	62.9	119.3	55.4	121.6	57.6	121.4	120.8
	20.0	160.5	12.6	161.5	16.2	160.4	160.3
	55.7	126.2	50.2	126.4	52.0	126.6	125.5
	63.5	118.7	58.2	119.0	60.2	118.8	119.4
	43.0	138.4	36.9	138.8	39.4	138.6	137.6
	69.5	113.0	65.1	112.5	66.4	113.0	112.9
3	145.7	39.9	141.5	41.5	142.4	41.1	40.3
	127.7	57.1	124.7	57.1	124.4	58.2	64.8
	147.1	38.5	143.8	39.3	144.6	39.1	39.2
	114.5	69.8	109.8	70.9	111.0	70.8	72.2
	121.4	63.2	119.9	61.6	120.1	62.3	65.5
	143.3	42.1	140.9	42.0	141.1	42.4	41.7
	152.8	33.0	151.4	32.2	151.9	32.1	32.7
	34.3	146.7	29.2	146.0	31.4	146.1	138.6
	6.1	173.9	0.2	173.0	3.0	173.0	172.7
	47.5	134.1	42.8	133.4	44.1	134.1	137.9
	136.5	48.6	135.1	47.4	135.2	48.0	49.5
	143.9	41.6	142.3	40.7	142.8	40.8	41.6
	144.3	41.1	143.1	40.0	143.0	40.5	41.9
	126.0	58.7	125.0	56.8	125.0	57.6	52.9
	39.0	142.2	34.0	141.5	34.8	142.9	143.3
	163.2	23.0	161.1	23.2	162.0	22.6	21.1
	157.7	28.3	156.5	27.5	157.2	27.2	25.9
	161.3	24.8	159.6	24.6	160.7	23.9	24.5
	49.7	132.0	42.4	133.7	45.2	133.1	132.6
	157.0	29.0	155.4	28.5	156.3	28.0	26.5
	49.3	132.3	44.6	131.6	46.8	131.5	128.5
	153.5	32.3	151.7	31.9	152.7	31.4	25.9
	54.4	127.5	47.4	129.1	49.8	128.7	128.5
	154.6	31.3	152.8	30.9	153.7	30.5	25.8

	47.1	134.4	42.3	133.8	44.3	133.9	131.8
	42.7	138.7	38.3	137.5	40.1	137.8	137.8
	61.9	120.2	55.2	121.8	57.0	121.9	121.0
	67.9	114.5	63.6	114.0	65.1	114.2	113.7
	43.3	138.1	36.1	139.6	38.4	139.4	140.6
	21.7	158.9	15.5	158.8	17.6	159.1	148.1
	59.2	122.9	54.6	122.3	56.1	122.8	121.6
	71.0	111.5	66.6	111.1	68.1	111.4	111.9
	61.8	120.3	57.2	119.9	59.5	119.5	121.0
	62.2	120.0	56.6	120.5	58.9	120.1	119.5
	52.3	129.4	46.6	129.8	49.0	129.5	128.2
	14.5	165.8	8.4	165.4	12.1	164.3	167.0
4	18.9	161.6	13.0	161.0	15.0	161.6	161.4
	130.7	54.2	128.5	53.5	128.2	54.6	55.0
	11.5	168.6	6.9	166.7	8.6	167.6	168.2
	135.9	49.3	133.8	48.6	133.8	49.3	48.7
	131.3	53.6	125.8	56.1	127.7	55.1	52.4
	45.7	135.8	38.8	137.1	40.6	137.4	134.9
	57.7	124.3	52.4	124.4	54.2	124.5	122.6
	58.4	123.6	52.9	124.0	54.7	124.1	122.8
	49.5	132.2	43.5	132.7	45.9	132.4	130.0
	70.7	111.8	66.2	111.6	67.5	111.9	111.1
	37.2	144.0	29.8	145.4	32.9	144.7	144.8
	143.9	41.6	139.3	43.5	140.7	42.8	41.8
	97.7	85.9	94.7	85.0	95.1	85.9	87.3
	89.8	93.5	85.5	93.6	86.5	94.0	92.6
	154.8	31.1	152.2	31.5	152.6	31.5	31.1
	114.2	70.1	112.5	68.4	112.6	69.3	69.2
	148.7	37.0	146.5	36.8	146.8	37.0	35.8
	135.6	49.5	130.7	51.5	131.7	51.3	50.8
	107.6	76.4	104.6	75.8	104.6	76.9	76.2
	11.2	168.9	6.3	167.4	9.3	167.0	169.1
	132.2	52.8	131.2	51.1	131.4	51.5	51.7
	89.7	93.6	86.4	92.8	86.1	94.4	93.6
	135.0	50.1	133.4	49.0	133.7	49.4	48.6
	131.1	53.8	129.9	52.3	130.3	52.6	51.6
	152.7	33.1	151.6	32.1	152.2	31.9	30.6
	127.9	56.9	123.0	58.7	124.6	58.0	57.0
	42.4	139.0	36.1	139.6	37.8	140.0	136.6
	63.1	119.1	58.4	118.8	60.1	119.0	116.3
	58.7	123.3	53.5	123.4	55.4	123.4	121.6
	66.5	115.9	61.3	116.1	63.0	116.2	116.5
	40.7	140.6	34.5	141.1	37.4	140.4	142.0
	46.0	135.5	38.6	137.3	41.7	136.3	136.1
	158.3	27.7	156.7	27.3	157.6	26.7	25.5
	102.5	81.3	99.7	80.4	100.2	81.0	80.5
	154.0	31.8	150.5	33.0	151.5	32.5	31.2
	152.0	33.8	149.5	34.0	150.0	34.0	31.6
	117.2	67.2	115.7	65.5	115.9	66.2	65.1
	146.7	38.8	144.5	38.6	145.3	38.4	36.8

	141.3	44.0	136.2	46.4	137.8	45.5	46.3
	121.4	63.1	118.5	62.9	118.2	64.1	64.7
	153.6	32.2	151.2	32.4	151.4	32.6	29.3
	134.4	50.7	132.7	49.7	132.7	50.4	50.7
	21.7	158.8	15.7	158.6	17.6	159.1	158.7
	132.0	53.0	130.5	51.7	130.2	52.7	53.5
	19.1	161.3	14.4	159.8	16.7	160.0	158.7
	78.0	104.8	73.0	105.2	74.6	105.3	104.6
	123.8	60.9	118.1	63.2	119.7	62.6	60.9
	45.5	136.0	39.0	136.8	40.2	137.8	135.4
	54.6	127.2	49.6	127.0	51.2	127.4	124.4
	57.4	124.6	52.0	124.8	53.7	125.0	123.4
	48.8	132.8	43.3	132.9	45.5	132.8	131.2
	70.3	112.2	66.0	111.7	67.1	112.3	111.6
	37.7	143.5	30.8	144.6	33.7	143.9	144.7
	147.0	38.6	142.8	40.2	143.8	39.8	39.8
	98.0	85.6	95.2	84.5	95.6	85.4	87.1
	83.7	99.3	80.1	98.7	80.9	99.3	98.4
	156.8	29.2	154.3	29.5	154.2	30.0	28.2
	119.0	65.5	117.9	63.4	118.1	64.1	64.3
	148.2	37.4	146.3	37.0	146.8	37.0	37.0
	136.8	48.3	131.8	50.5	133.0	50.0	49.1
	112.1	72.1	109.4	71.3	108.8	73.0	72.1
	12.2	168.0	7.0	166.7	10.2	166.1	168.6
	132.1	52.8	131.2	51.0	131.4	51.5	51.9
	89.7	93.6	86.3	92.8	85.9	94.6	93.2
	134.8	50.3	133.4	49.0	133.6	49.5	48.6
	131.3	53.6	130.1	52.1	130.5	52.4	51.6
	151.2	34.5	150.2	33.3	150.8	33.2	31.4
	127.5	57.3	122.8	58.9	124.3	58.3	56.0
	43.3	138.1	37.2	138.6	38.6	139.3	135.9
	60.5	121.6	56.0	121.0	57.6	121.3	115.9
	58.5	123.5	53.2	123.7	55.1	123.7	120.9
	56.6	125.4	51.4	125.4	53.4	125.3	118.9
	42.7	138.7	36.6	139.2	39.1	138.9	142.0
	40.0	141.3	32.9	142.5	36.0	141.7	136.9
	158.3	27.8	156.8	27.2	157.6	26.8	25.5
	102.7	81.1	99.9	80.2	100.5	80.8	80.5
	153.2	32.6	150.1	33.4	150.8	33.2	32.3
	152.3	33.5	150.0	33.6	150.4	33.6	32.1
	117.6	66.8	116.2	65.0	116.4	65.7	64.8
	147.4	38.1	145.5	37.7	146.1	37.6	36.2
	141.3	44.0	136.3	46.3	137.8	45.5	46.1
	121.8	62.8	118.9	62.5	118.5	63.7	64.7
	149.1	36.6	147.2	36.1	147.7	36.2	36.0
	141.2	44.1	139.6	43.2	139.3	44.1	45.2
5	124.1	60.5	119.4	62.0	120.5	61.9	62.3
	122.0	62.6	118.9	62.5	119.0	63.3	63.8
	143.2	42.2	141.3	41.7	141.7	41.8	42.5
	97.1	86.5	93.4	86.2	94.1	86.8	88.0

	131.3	53.7	128.2	53.8	128.8	54.0	53.7
	141.5	43.8	138.4	44.4	139.5	43.9	44.6
	107.8	76.2	103.6	76.7	104.7	76.8	77.7
	150.7	35.0	149.2	34.3	149.5	34.4	35.9
	102.5	81.3	98.9	81.1	99.5	81.7	83.5
	129.2	55.7	125.0	56.8	126.0	56.7	57.5
	31.7	149.2	26.6	148.4	28.4	148.9	145.9
	137.3	47.8	133.7	48.7	134.5	48.7	49.5
	146.4	39.2	144.4	38.7	145.1	38.6	35.9
	45.6	136.0	39.4	136.5	42.4	135.7	133.7
	169.4	17.1	168.3	16.5	168.9	16.1	17.4
	160.3	25.8	158.0	26.1	159.0	25.5	25.0
	111.5	72.6	106.8	73.7	108.3	73.4	73.8
	159.8	26.3	158.5	25.6	159.0	25.5	27.6
	143.0	42.4	139.2	43.6	140.8	42.6	43.2
	103.0	80.8	99.9	80.2	100.3	80.9	82.2
	167.6	18.8	167.0	17.7	167.0	17.9	17.1
	140.6	44.7	138.4	44.3	139.0	44.3	42.1
	0.1	179.6	-6.6	179.4	-3.1	178.7	178.9
	136.9	48.2	133.5	48.9	134.2	48.9	50.1
	162.2	24.0	159.9	24.4	160.8	23.7	24.0
	156.2	29.8	154.8	29.0	155.4	28.9	30.0
	174.5	12.2	173.3	11.9	174.0	11.3	12.7
	143.4	42.1	139.9	42.9	141.3	42.2	43.5
	-0.3	179.9	-6.7	179.5	-3.5	179.1	178.9
	174.7	12.0	173.5	11.6	174.2	11.1	12.9
6	45.4	136.1	39.6	136.3	42.0	136.1	135.3
	54.2	127.6	48.7	127.9	51.0	127.6	128.0
	53.2	128.6	47.5	128.9	49.4	129.1	127.4
	62.7	119.5	54.4	122.5	57.0	121.9	121.3
	37.1	144.1	30.3	145.0	32.6	144.9	146.3
	54.6	127.3	49.6	127.0	51.2	127.4	131.8
	17.9	162.5	13.0	161.1	15.5	161.1	162.2
	23.8	156.8	19.4	155.1	20.7	156.2	155.3
	49.9	131.8	43.3	132.9	45.4	132.9	133.7
	55.2	126.7	48.3	128.2	50.0	128.5	130.4
	14.5	165.8	9.4	164.5	12.3	164.1	168.4
	125.9	58.9	123.0	58.6	123.6	59.0	50.7
	52.4	129.4	46.4	130.0	48.5	129.9	128.6
	47.5	134.0	42.5	133.6	44.3	133.9	127.8
	52.5	129.3	47.4	129.1	49.6	128.9	129.3
	49.6	132.1	44.0	132.3	46.0	132.2	129.9
	140.5	44.8	138.0	44.8	139.1	44.3	42.9
	106.4	77.5	102.2	78.1	103.6	77.8	80.9
	45.0	136.4	38.0	137.8	39.8	138.1	139.6
	44.3	137.2	37.7	138.1	40.2	137.8	136.3
	97.2	86.4	95.1	84.6	94.8	86.2	86.8
	57.1	124.9	52.4	124.4	53.9	124.8	124.0
	57.3	124.7	52.4	124.4	54.2	124.5	126.0
	49.1	132.6	43.7	132.5	45.9	132.4	129.8

	64.4	117.9	59.8	117.5	61.0	118.1	115.9
	117.9	66.5	115.4	65.7	116.0	66.2	62.0
	9.6	170.5	4.7	168.9	7.5	168.7	171.4
	153.4	32.5	151.4	32.2	152.2	31.9	34.5
	161.0	25.1	158.6	25.5	160.0	24.5	25.2
	162.3	23.9	161.4	22.9	161.7	22.9	23.6
	163.0	23.2	161.9	22.5	162.1	22.5	21.4
7	111.7	72.5	108.0	72.7	107.8	73.9	73.8
	100.2	83.5	98.0	82.0	97.3	83.8	80.2
	109.8	74.3	105.7	74.7	105.6	76.0	73.6
	141.2	44.1	138.7	44.0	139.7	43.7	42.7
	52.0	129.8	45.3	131.0	47.3	131.0	126.7
	107.2	76.8	104.0	76.4	103.6	77.9	76.3
	19.7	160.8	15.6	158.6	18.3	158.5	163.1
	16.7	163.7	11.6	162.4	14.7	161.9	165.6
	32.9	148.1	25.7	149.3	28.7	148.7	148.4
	47.4	134.2	40.3	135.7	42.9	135.2	134.1
	53.7	128.2	49.2	127.4	50.8	127.7	127.3
	57.6	124.4	52.2	124.6	54.1	124.6	125.0
	122.1	62.4	120.8	60.7	121.8	60.6	60.4
	73.1	109.5	67.2	110.7	69.4	110.2	107.8
	52.7	129.1	45.4	130.9	47.5	130.8	130.4
	71.1	111.4	66.4	111.4	68.0	111.5	111.1
	160.8	25.3	160.1	24.2	160.4	24.1	27.5
	158.0	28.0	156.0	27.9	156.4	27.9	27.1
	61.9	120.3	56.4	120.7	58.4	120.6	120.3
	72.1	110.5	66.7	111.1	68.5	111.0	111.5
	107.4	76.5	103.5	76.8	103.2	78.2	74.9
	50.0	131.7	44.2	132.0	46.5	131.9	131.4
	57.0	124.9	52.3	124.5	54.2	124.6	119.2
	109.0	75.0	105.1	75.4	104.8	76.7	76.6
	59.6	122.5	54.2	122.7	56.2	122.6	122.8
	17.1	163.3	12.2	161.9	15.0	161.6	165.6
	62.9	119.3	57.5	119.7	59.6	119.5	120.6
	14.2	166.1	9.2	164.7	12.4	164.0	166.8
	160.2	25.9	159.5	24.7	159.9	24.6	28.3
	121.0	63.6	119.2	62.2	120.1	62.3	61.1
	162.0	24.2	161.4	22.9	161.6	23.0	27.5
8	146.4	39.2	141.8	41.1	143.1	40.5	40.5
	129.6	55.3	126.3	55.6	126.6	56.1	56.7
	121.7	62.8	118.7	62.7	119.3	63.0	62.9
	155.0	30.9	151.0	32.6	152.0	32.1	31.7
	103.1	80.8	100.5	79.6	100.8	80.4	81.1
	136.1	49.1	132.4	49.9	133.1	49.9	50.3
	153.2	32.7	151.1	32.5	152.0	32.1	32.2
	145.7	39.8	143.9	39.2	144.3	39.4	39.9
	143.8	41.6	140.7	42.2	142.3	41.3	42.0
	164.7	21.5	162.2	22.1	163.1	21.6	21.1
	149.5	36.2	144.6	38.5	146.3	37.5	37.2
	75.5	107.2	71.3	106.8	72.1	107.6	109.3

	169.9	16.6	168.3	16.5	168.6	16.4	16.3
	152.8	33.1	151.0	32.6	151.5	32.5	32.3
	36.7	144.4	30.0	145.3	32.1	145.4	140.8
	147.8	37.9	145.6	37.6	146.1	37.6	37.5
	172.0	14.6	171.0	14.0	171.5	13.6	15.0
	154.4	31.5	152.4	31.3	153.4	30.7	31.7
	57.1	124.9	53.0	123.8	55.1	123.7	121.8
	166.4	20.0	164.9	19.6	165.2	19.6	19.4
	143.9	41.5	141.6	41.3	142.3	41.2	39.0
	155.3	30.6	153.4	30.3	154.3	29.9	30.4
	112.7	71.5	110.0	70.8	110.5	71.3	78.2
	156.9	29.1	155.4	28.5	155.9	28.4	29.3
	155.7	30.2	152.7	31.1	154.3	29.9	30.6
	118.1	66.3	116.6	64.6	116.9	65.3	66.9
	169.4	17.1	168.3	16.5	168.8	16.2	17.3
	82.4	100.6	80.1	98.6	80.6	99.6	102.5
	114.6	69.7	111.4	69.5	112.7	69.3	71.8
	107.7	76.3	104.9	75.5	106.1	75.4	78.2
	108.5	75.6	105.5	74.9	106.6	75.0	78.2
	112.3	71.9	109.4	71.4	110.4	71.4	75.5
	120.5	64.1	119.1	62.3	120.2	62.1	62.7
9	147.2	38.4	142.8	40.3	143.9	39.8	40.1
	124.9	59.8	121.4	60.1	122.0	60.5	60.9
	143.2	42.2	138.5	44.2	139.7	43.7	44.0
	134.7	50.3	131.4	50.8	131.9	51.1	51.6
	168.5	17.9	165.8	18.8	166.7	18.2	17.3
	148.5	37.1	146.2	37.0	146.7	37.1	37.4
	109.6	74.5	106.9	73.7	107.2	74.4	76.1
	146.2	39.4	143.6	39.5	144.1	39.6	37.9
	132.3	52.7	127.6	54.4	128.4	54.4	53.5
	145.9	39.6	141.9	41.1	142.5	41.1	38.5
	138.2	47.0	134.7	47.7	135.2	48.0	42.6
	157.8	28.2	153.2	30.5	154.5	29.7	30.0
	148.1	37.5	146.0	37.3	146.5	37.3	37.3
	157.9	28.1	155.5	28.4	155.8	28.5	32.1
	154.9	31.0	152.7	31.0	152.9	31.3	35.5
	160.5	25.6	156.2	27.8	157.8	26.6	27.8
	152.9	32.9	150.7	32.9	151.4	32.7	32.2
	155.0	30.9	152.7	31.0	153.4	30.7	35.0
	152.8	33.0	149.9	33.6	151.0	33.0	31.1
	117.4	67.0	113.7	67.3	115.1	66.9	68.7
	1.9	177.8	-3.9	176.9	-0.7	176.4	176.8
	102.4	81.4	99.2	80.9	99.7	81.5	83.8
	170.3	16.2	169.1	15.8	169.8	15.3	15.5
	173.6	13.0	172.0	13.1	172.3	12.9	12.8
	170.9	15.6	169.0	15.8	169.5	15.5	13.1
	168.9	17.5	167.2	17.5	167.6	17.3	21.5
	149.3	36.3	148.1	35.3	148.3	35.6	30.6
	153.3	32.6	152.2	31.5	152.4	31.7	30.0
	150.6	35.1	149.5	34.0	149.7	34.2	34.1

	-0.7	180.4	-5.4	178.2	-3.0	178.6	178.0
10	130.5	54.4	127.5	54.5	128.1	54.7	57.9
	161.7	24.5	159.6	24.6	160.1	24.4	25.2
	151.9	33.9	148.9	34.5	150.5	33.5	30.5
	143.8	41.7	141.8	41.2	142.5	41.0	44.1
	137.8	47.4	134.9	47.6	135.5	47.7	50.5
	72.7	109.9	67.2	110.6	68.9	110.6	110.6
	9.4	170.6	4.7	168.8	7.3	168.9	171.3
	111.8	72.3	109.0	71.7	109.9	71.8	71.7
	146.9	38.7	144.0	39.1	145.1	38.6	40.8
	138.4	46.9	136.1	46.5	136.6	46.6	42.6
	138.1	47.1	135.6	47.0	136.2	47.0	47.1
	2.3	177.5	-2.1	175.2	0.5	175.3	174.9
	49.5	132.2	43.5	132.7	46.1	132.2	134.1
	41.3	140.0	37.0	138.8	38.6	139.3	130.6
	144.2	41.2	142.5	40.5	143.2	40.4	42.1
	56.0	126.0	48.7	127.9	50.6	127.9	128.5
	3.5	176.3	-1.6	174.7	1.3	174.5	177.9
	163.0	23.2	162.4	22.0	162.7	22.0	22.0
	155.6	30.3	154.7	29.2	154.7	29.5	31.1
	46.8	134.8	40.9	135.1	42.7	135.4	132.7
	56.4	125.6	52.5	124.3	54.1	124.6	124.2
	46.7	134.8	40.1	135.9	42.3	135.8	138.1
	166.2	20.1	165.2	19.3	166.1	18.8	19.6
	174.1	12.6	172.9	12.2	173.4	11.9	20.0
	6.9	173.0	2.6	170.8	5.7	170.4	172.1
	169.5	17.0	168.7	16.2	169.3	15.7	18.5
	166.2	20.1	164.2	20.3	164.8	20.0	18.2
	62.0	120.2	57.1	120.0	58.8	120.2	119.3
	70.9	111.7	66.8	111.0	68.2	111.3	112.3
	52.0	129.8	46.2	130.2	48.3	130.1	128.2
	54.0	127.8	48.1	128.4	50.3	128.2	128.2
	62.4	119.8	57.3	119.8	59.3	119.7	119.8
	60.0	122.1	55.1	121.9	57.0	121.9	122.4
	69.0	113.4	63.6	113.9	65.5	113.8	116.2
	67.7	114.7	62.6	114.9	64.2	115.1	116.2
	24.8	155.9	17.2	157.2	20.9	156.0	157.7
11	135.1	50.0	132.4	49.9	133.4	49.7	49.4
	17.5	162.9	12.4	161.6	14.1	162.4	169.4
	68.0	114.4	60.9	116.5	63.2	116.0	106.6
	41.8	139.6	34.5	141.1	37.1	140.7	141.5
	153.0	32.8	151.0	32.6	151.5	32.6	36.9
	21.2	159.4	14.5	159.7	17.9	158.8	165.3
	65.0	117.3	58.8	118.5	60.4	118.7	124.5
	23.6	157.0	17.1	157.3	20.6	156.3	158.1
	73.3	109.3	69.0	108.9	69.8	109.8	117.3
	59.6	122.5	53.3	123.6	55.0	123.8	124.4
	44.0	137.5	39.4	136.5	40.7	137.3	134.8
	62.3	119.9	56.0	121.0	58.0	121.0	120.6
	31.1	149.8	25.9	149.1	27.9	149.4	151.8

	72.9	109.7	65.8	111.9	67.6	111.9	115.2
	49.2	132.5	42.0	134.1	44.1	134.1	137.2
	63.5	118.7	58.3	118.9	59.4	119.6	120.5
	43.5	137.9	36.5	139.2	39.1	138.8	136.9
	77.6	105.2	71.9	106.2	73.3	106.5	107.9
	24.7	155.9	18.6	155.9	20.6	156.3	157.8
	62.3	119.9	55.6	121.4	57.7	121.2	120.6
	47.8	133.8	43.3	132.9	44.8	133.4	135.0
	55.5	126.4	49.4	127.2	50.7	127.8	124.5
	47.0	134.6	39.8	136.2	41.7	136.4	136.6
	69.1	113.3	61.7	115.8	63.4	115.8	114.9
	28.3	152.5	22.6	152.1	24.9	152.3	152.5
	22.0	158.5	15.7	158.6	17.9	158.8	157.8
	78.5	104.3	72.4	105.7	73.7	106.1	107.7
	43.4	138.0	36.5	139.2	39.1	138.8	136.8
	66.5	115.8	61.2	116.2	62.5	116.7	119.3
	64.2	118.1	58.2	119.0	59.8	119.3	118.9
	26.4	154.3	20.4	154.2	23.9	153.2	155.9
	85.6	97.5	81.7	97.1	82.7	97.6	101.7
	27.6	153.2	20.9	153.7	24.3	152.8	155.5
	67.6	114.8	60.8	116.6	62.4	116.8	116.4
	42.8	138.6	35.7	139.9	38.4	139.5	134.7
	151.6	34.2	149.6	33.9	149.2	34.7	34.7
	144.4	41.1	141.8	41.2	142.7	40.9	44.0
	138.9	46.4	136.8	45.8	136.9	46.4	48.9
	170.9	15.6	170.3	14.7	170.5	14.6	19.2
	124.4	60.3	123.5	58.2	123.6	59.0	61.0
	163.9	22.4	163.0	21.4	163.1	21.6	22.1
	130.4	54.5	129.1	53.0	129.5	53.4	56.9
	131.3	53.6	130.0	52.2	130.3	52.6	56.9
	164.1	22.1	163.3	21.2	163.3	21.4	22.2
	165.8	20.5	164.7	19.8	165.2	19.7	19.7
	164.1	22.2	163.5	21.0	163.8	20.9	20.8
12	123.9	60.7	118.5	62.8	119.5	62.8	65.7
	133.8	51.3	128.3	53.8	129.7	53.1	51.3
	136.9	48.3	133.6	48.8	133.8	49.3	48.1
	141.0	44.3	135.2	47.3	136.7	46.5	45.9
	149.1	36.5	144.1	39.0	145.9	37.9	37.9
	133.4	51.6	130.3	51.9	131.7	51.3	53.9
	124.5	60.1	121.0	60.5	121.9	60.6	60.6
	167.0	19.4	164.4	20.1	165.6	19.2	18.9
	150.9	34.8	149.3	34.2	149.6	34.3	30.8
	105.3	78.6	102.6	77.6	103.4	78.0	79.1
	-32.7	211.0	-37.8	208.4	-36.1	209.9	206.1
	148.5	37.2	145.4	37.8	146.6	37.2	36.4
	105.2	78.7	101.1	79.1	102.6	78.8	80.3
	108.6	75.5	105.4	75.1	105.7	75.9	77.8
	170.0	16.5	167.7	17.0	168.4	16.6	17.6
	119.9	64.6	117.0	64.3	117.3	64.9	65.3
	164.5	21.8	163.0	21.5	163.4	21.3	21.4

	13.2	167.1	7.5	166.2	10.2	166.1	166.6
	150.1	35.6	147.7	35.7	148.6	35.3	35.6
	166.5	19.9	165.2	19.4	165.4	19.4	20.7
	157.3	28.7	156.2	27.7	156.6	27.8	30.2
	60.8	121.3	53.8	123.1	56.1	122.7	120.0
	11.0	169.1	5.1	168.4	8.0	168.2	169.1
	69.8	112.7	64.8	112.9	66.8	112.7	109.7
	40.6	140.7	35.1	140.5	37.6	140.2	141.1
	38.0	143.2	32.2	143.2	34.9	142.8	143.2
13	122.1	62.5	119.6	61.9	119.3	63.0	62.9
	134.9	50.2	129.4	52.7	131.1	51.8	53.5
	142.2	43.2	139.4	43.4	140.8	42.7	41.4
	98.9	84.7	97.0	82.8	97.2	83.9	82.7
	120.9	63.6	118.4	62.9	118.4	63.8	65.4
	158.9	27.2	155.6	28.3	156.5	27.8	29.2
	161.7	24.5	159.4	24.8	160.1	24.4	23.3
	144.8	40.7	142.8	40.2	143.4	40.2	37.3
	38.5	142.8	31.1	144.2	33.4	144.2	133.9
	29.5	151.3	22.4	152.3	25.2	152.0	146.5
	126.9	57.8	125.6	56.3	125.6	57.0	53.8
	31.5	149.5	24.2	150.6	26.8	150.5	141.5
	126.8	58.0	125.0	56.8	124.8	57.8	52.0
	59.7	122.4	54.4	122.5	56.4	122.5	122.7
	74.5	108.2	69.5	108.5	71.3	108.4	103.8
	61.1	121.0	57.3	119.9	59.4	119.6	117.7
	62.4	119.8	57.0	120.1	59.1	119.9	117.2
	55.3	126.6	49.5	127.1	51.7	126.9	128.2
	170.6	16.0	169.7	15.1	170.2	14.9	13.3
14	150.9	34.9	146.8	36.5	147.6	36.2	35.1
	158.1	27.9	154.4	29.5	155.3	28.9	28.5
	151.4	34.3	148.1	35.3	148.7	35.2	37.2
	84.0	99.1	80.4	98.3	80.7	99.5	102.6
	151.2	34.5	148.6	34.8	149.0	34.9	36.2
	66.7	115.7	59.3	118.0	61.6	117.6	116.8
	72.6	110.0	66.2	111.6	67.5	112.0	117.5
	62.6	119.6	57.5	119.7	59.9	119.1	122.9
	40.5	140.8	33.5	142.0	36.6	141.1	133.7
	69.2	113.2	62.3	115.2	64.5	114.8	113.4
	28.3	152.5	21.5	153.2	24.2	152.9	154.5
	27.7	153.1	20.9	153.7	23.8	153.3	155.0
	25.0	155.7	17.8	156.6	21.0	155.9	156.7
	54.0	127.9	47.7	128.7	49.9	128.6	127.9
	161.5	24.7	160.7	23.6	160.9	23.7	23.9
	77.2	105.5	73.0	105.2	73.4	106.4	105.0
	81.5	101.5	77.1	101.5	78.2	101.9	104.6
	23.7	156.9	16.9	157.5	20.3	156.5	159.9
	50.0	131.7	43.9	132.3	46.2	132.1	130.3
	79.4	103.5	75.1	103.2	76.2	103.8	105.4
	53.1	128.7	46.7	129.7	48.5	130.0	131.1
	75.8	107.0	71.2	106.9	72.7	107.0	109.9

	24.3	156.3	17.0	157.3	20.9	156.0	157.9
	82.1	100.9	77.4	101.1	78.4	101.7	103.9
	77.7	105.1	72.9	105.3	74.4	105.5	107.1
	22.2	158.4	14.7	159.5	18.6	158.2	157.7
	27.7	153.1	20.7	153.9	23.2	153.9	156.7
	80.4	102.5	76.1	102.3	77.4	102.6	102.2
	61.3	120.8	53.8	123.1	56.3	122.6	122.5
	27.3	153.5	19.5	155.0	22.3	154.7	153.3
	59.2	122.9	54.8	122.2	56.4	122.5	122.0
	87.4	95.8	83.9	95.1	84.7	95.7	98.4
	71.1	111.5	66.0	111.7	67.9	111.5	113.4
	25.8	154.9	18.3	156.2	22.0	155.0	157.5
15	142.5	42.9	139.1	43.6	140.2	43.3	45.9
	90.6	92.7	87.4	91.8	87.9	92.7	89.4
	96.5	87.0	92.7	86.8	93.2	87.6	84.6
	139.0	46.3	135.6	46.9	136.8	46.5	46.8
	97.8	85.8	94.3	85.4	94.8	86.1	76.5
	173.6	13.1	172.4	12.6	172.9	12.3	12.1
	8.5	171.5	3.6	169.9	6.1	170.0	170.5
	52.6	129.2	45.0	131.3	47.2	131.2	130.0
	49.4	132.3	43.5	132.7	45.5	132.7	130.0
	51.7	130.1	46.1	130.3	48.2	130.2	128.5
	48.6	133.0	43.0	133.1	45.2	133.1	133.1
	8.4	171.6	3.0	170.4	6.1	170.1	169.7
	161.0	25.2	160.0	24.2	160.6	24.0	20.6
	8.7	171.3	3.9	169.6	7.1	169.1	166.2
	163.5	22.7	163.0	21.5	163.4	21.3	22.1
	108.6	75.4	105.0	75.4	105.6	76.0	71.2
	50.2	131.5	44.5	131.8	46.7	131.7	133.9
	160.8	25.3	159.9	24.3	160.1	24.4	20.5
	47.3	134.3	42.9	133.2	44.6	133.6	124.1
	7.2	172.8	2.0	171.4	5.0	171.1	169.0
	166.0	20.3	164.8	19.8	165.4	19.4	13.7
	147.2	38.4	145.3	37.9	145.2	38.5	39.9
	150.1	35.6	146.0	37.2	147.3	36.5	39.2
	97.3	86.3	94.5	85.2	95.1	85.9	74.3
	160.6	25.5	159.3	24.9	159.8	24.7	24.1
	159.3	26.8	158.0	26.0	158.2	26.3	25.5
	9.4	170.7	3.7	169.7	7.1	169.1	170.0
	166.7	19.6	165.6	19.1	166.3	18.6	15.2
	100.7	83.0	97.3	82.6	97.9	83.2	74.1
	-25.2	203.9	-30.1	201.2	-27.2	201.5	197.5
	40.4	140.9	35.1	140.5	37.7	140.2	132.1
	11.3	168.9	5.7	167.9	8.5	167.7	170.2
	165.7	20.6	164.6	19.9	165.3	19.5	20.5
	36.9	144.2	32.1	143.3	34.0	143.6	136.9
	161.5	24.6	160.8	23.4	161.0	23.6	20.5
16	12.4	167.8	7.3	166.4	10.1	166.2	169.3
	56.5	125.5	49.9	126.7	51.9	126.8	125.3
	122.2	62.4	120.9	60.6	121.6	60.9	63.9

	117.0	67.3	114.4	66.7	115.0	67.1	66.8
	116.5	67.8	113.6	67.4	114.4	67.6	69.5
	91.6	91.7	89.2	90.1	90.4	90.3	90.7
	108.5	75.6	105.8	74.7	106.9	74.7	76.9
	110.0	74.1	107.3	73.3	108.0	73.7	75.0
	11.1	169.0	6.2	167.5	8.6	167.6	169.6
	57.9	124.1	51.6	125.1	53.3	125.4	124.8
	74.8	107.9	70.3	107.7	71.4	108.3	107.7
	37.7	143.5	31.1	144.2	34.6	143.1	145.1
	45.0	136.5	38.0	137.8	41.4	136.6	136.3
	40.4	140.9	34.6	141.0	37.2	140.7	144.2
	67.4	115.0	60.2	117.1	62.8	116.4	115.0
	10.3	169.8	5.4	168.2	7.8	168.4	170.5
	56.8	125.1	50.5	126.1	52.1	126.5	125.1
	69.3	113.2	62.8	114.7	65.0	114.4	113.7
	41.1	140.2	35.0	140.6	38.1	139.8	144.1
	49.4	132.3	42.6	133.6	45.9	132.4	135.9
	40.0	141.3	33.4	142.1	36.7	141.0	145.1
	76.7	106.0	72.6	105.6	73.3	106.5	107.2
	10.7	169.4	5.9	167.7	8.7	167.6	170.0
	57.2	124.8	50.8	125.9	52.3	126.3	125.2
	74.7	108.0	70.5	107.6	71.4	108.3	108.3
	37.5	143.7	30.9	144.5	34.4	143.3	145.1
	45.7	135.9	38.7	137.1	42.2	135.9	136.0
	40.4	140.9	34.6	141.0	37.2	140.6	144.2
	66.5	115.8	59.6	117.7	62.2	117.0	115.1
	67.5	114.9	60.9	116.5	63.2	116.0	113.9
	40.8	140.5	34.7	140.9	37.7	140.2	144.1
	49.3	132.4	42.5	133.6	45.7	132.5	136.0
	39.9	141.4	33.3	142.2	36.6	141.1	145.1
	75.9	106.8	71.7	106.4	72.5	107.2	107.2
17	117.8	66.6	114.8	66.3	116.2	65.9	70.8
	109.3	74.7	106.2	74.3	107.2	74.4	78.9
	94.2	89.3	91.4	88.0	92.0	88.8	93.7
	106.6	77.4	103.9	76.4	104.7	76.8	83.1
	112.0	72.2	108.5	72.1	109.4	72.4	77.8
	87.5	95.6	85.1	94.0	85.4	95.0	105.9
	111.1	73.0	107.7	72.9	108.9	72.9	77.6
	113.7	70.5	111.0	69.8	112.3	69.6	70.7
	108.4	75.6	105.6	74.9	106.7	74.9	77.7
	111.2	72.9	109.0	71.7	109.9	71.9	75.9
	3.6	176.2	-1.3	174.4	1.7	174.1	175.8
	152.0	33.7	148.8	34.6	150.3	33.7	32.2
	152.8	33.0	150.7	32.9	151.4	32.6	32.2
	111.0	73.1	108.5	72.1	109.3	72.4	71.5
	112.5	71.7	107.0	73.6	109.1	72.6	75.4
	110.8	73.3	107.3	73.3	108.4	73.3	76.3
	157.9	28.1	155.9	28.1	156.5	27.8	29.3
	85.0	98.0	79.9	98.8	80.9	99.3	100.5
	-39.1	217.2	-45.6	215.6	-43.1	216.6	213.7

	154.7	31.2	152.3	31.4	153.7	30.5	32.7
	115.5	68.8	112.7	68.3	113.2	68.7	70.9
	156.3	29.6	153.6	30.2	155.2	29.1	34.3
	118.8	65.7	117.4	63.9	117.6	64.6	63.4
	172.6	14.0	171.9	13.2	172.2	13.0	13.1
	14.7	165.6	9.9	164.0	12.4	164.0	167.8
	53.6	128.2	45.6	130.7	48.5	129.9	132.1
	51.1	130.6	45.3	131.0	47.1	131.3	130.8
	52.7	129.1	46.9	129.5	49.0	129.4	129.9
	46.8	134.7	41.1	134.9	43.2	134.9	134.4
	52.7	129.1	47.1	129.4	49.2	129.3	129.9
	51.4	130.4	45.8	130.6	47.7	130.7	130.8
	120.7	63.8	119.0	62.4	120.1	62.3	62.0
	123.5	61.1	122.2	59.4	123.3	59.2	62.3
	18	28.1	152.7	23.7	151.1	25.8	151.4
	148.5	37.1	146.0	37.2	146.9	36.9	35.1
	108.5	75.5	104.1	76.3	105.0	76.6	76.3
	130.0	54.9	124.4	57.3	126.0	56.6	53.4
	-32.9	211.3	-38.6	209.1	-36.2	210.0	204.3
	51.7	130.0	46.9	129.5	48.9	129.6	127.1
	109.8	74.3	107.7	72.9	108.5	73.2	72.3
	158.8	27.2	156.6	27.4	157.4	27.0	26.6
	150.7	35.0	147.5	35.8	148.2	35.6	38.2
	155.1	30.8	151.0	32.6	152.1	32.0	29.8
	79.8	103.1	76.3	102.1	76.4	103.5	106.8
	-27.2	205.8	-31.6	202.6	-30.0	204.2	209.8
	127.6	57.2	123.5	58.2	124.0	58.5	53.8
	102.9	80.9	98.2	81.7	98.9	82.2	80.4
	105.3	78.6	100.5	79.6	101.8	79.5	78.5
	161.0	25.2	158.3	25.8	159.5	25.0	25.7
	160.8	25.3	158.5	25.6	159.1	25.4	24.7
	155.3	30.6	150.6	33.0	152.3	31.8	30.4
	133.3	51.7	130.3	51.9	130.4	52.5	49.3
	123.4	61.3	121.4	60.2	122.2	60.3	60.4
	149.6	36.1	147.1	36.2	147.8	36.1	31.2
	106.7	77.3	104.3	76.1	104.6	76.9	76.3
	101.8	82.0	97.7	82.2	98.2	83.0	80.6
	7.3	172.6	1.0	172.3	4.1	171.9	171.8
	8.1	171.9	2.1	171.3	5.1	171.0	167.3
	166.7	19.6	165.8	18.8	166.2	18.7	21.6
	155.6	30.3	154.7	29.1	155.2	29.0	24.4
	170.7	15.8	169.1	15.8	169.5	15.6	13.2
	19	24.5	156.2	18.0	156.5	21.5	155.4
	89.7	93.6	85.5	93.5	86.7	93.8	96.5
	23.7	156.9	17.1	157.3	20.3	156.6	155.5
	85.9	97.2	79.8	98.9	81.2	99.0	100.3
	25.7	155.0	19.2	155.3	22.2	154.8	153.8
	85.2	97.9	79.8	98.9	81.0	99.2	106.7
	157.7	28.3	156.0	27.9	156.4	28.0	28.6
	125.2	59.5	121.7	59.9	123.1	59.4	66.1

	108.9	75.1	105.6	74.9	106.2	75.4	79.0
	53.5	128.4	47.2	129.2	48.8	129.7	130.4
	69.4	113.1	64.2	113.5	65.3	114.0	115.8
	58.9	123.2	53.6	123.3	55.5	123.3	120.3
	69.0	113.5	64.6	113.1	65.8	113.6	115.1
	39.8	141.5	32.8	142.7	36.2	141.6	145.1
	38.4	142.8	31.3	144.0	34.7	142.9	145.1
	154.2	31.7	150.9	32.7	151.4	32.7	36.5
	117.3	67.1	114.2	66.8	115.2	66.9	72.6
	82.5	100.5	76.3	102.2	77.8	102.2	100.3
	23.8	156.8	17.4	157.0	20.5	156.4	155.6
	105.7	78.3	103.2	77.1	103.6	77.9	76.6
	22.7	157.8	16.4	157.9	19.4	157.4	158.0
	89.1	94.2	85.5	93.5	86.5	94.0	96.3
	23.4	157.3	17.3	157.1	20.4	156.5	157.2
	88.9	94.3	85.8	93.3	86.2	94.2	95.9
	52.5	129.3	45.9	130.4	47.2	131.1	132.0
	65.6	116.7	60.2	117.1	62.3	116.9	119.0
	69.7	112.8	64.9	112.8	66.1	113.2	115.1
	37.7	143.5	30.4	144.9	34.1	143.5	145.1
	69.3	113.1	64.5	113.1	66.0	113.4	115.3
	39.4	141.8	32.5	143.0	35.9	141.8	145.1
20	123.5	61.1	121.0	60.5	121.1	61.3	60.1
	159.4	26.7	157.1	26.9	157.7	26.7	26.9
	154.0	31.9	150.3	33.2	151.3	32.7	31.7
	138.5	46.8	134.2	48.2	135.3	47.8	48.2
	123.4	61.2	120.1	61.4	119.8	62.5	60.1
	37.7	143.5	30.3	145.0	33.1	144.4	142.2
	64.6	117.6	59.2	118.0	60.7	118.4	116.3
	52.0	129.8	46.1	130.2	48.3	130.1	128.8
	57.1	124.9	51.3	125.4	53.3	125.4	124.4
	58.2	123.8	52.6	124.3	54.5	124.3	122.8
	46.6	135.0	39.1	136.8	41.2	136.8	132.9
	134.3	50.8	129.3	52.8	130.7	52.2	52.3
	141.7	43.7	140.2	42.6	140.8	42.7	42.7
	134.4	50.6	133.1	49.2	133.4	49.6	50.3
	132.9	52.1	131.1	51.1	131.1	51.8	52.9
	33.0	148.0	25.6	149.4	27.8	149.5	140.0
	49.0	132.7	45.3	131.0	47.0	131.3	127.9
	120.0	64.5	118.5	62.8	118.7	63.6	64.8
	106.3	77.6	103.6	76.7	104.2	77.2	77.6
	141.6	43.7	139.6	43.2	140.5	42.9	42.8
	8.7	171.3	3.1	170.3	5.6	170.5	170.3
21	54.0	127.9	48.1	128.4	50.4	128.2	128.0
	56.6	125.4	50.8	125.9	53.0	125.7	125.3
	59.1	123.0	53.7	123.1	55.7	123.1	122.3
	38.4	142.8	30.9	144.5	33.4	144.2	137.4
	41.4	139.9	34.5	141.1	37.1	140.7	141.4
	65.7	116.6	60.5	116.9	62.0	117.2	117.9
	132.3	52.6	126.6	55.3	128.5	54.3	52.8

	124.2	60.5	120.9	60.6	120.8	61.6	63.7
	8.8	171.3	4.5	169.0	7.0	169.2	167.7
	140.3	45.0	136.1	46.5	137.3	46.0	47.8
	132.0	53.0	129.1	53.0	129.1	53.7	57.5
	139.7	45.6	136.2	46.3	137.8	45.5	39.0
	141.4	43.9	139.4	43.4	140.0	43.4	36.5
	126.2	58.5	124.9	56.9	124.9	57.7	54.1
	117.4	66.9	114.7	66.4	115.0	67.1	66.3
	165.2	21.1	162.7	21.7	163.6	21.2	23.8
	156.7	29.3	153.3	30.4	154.2	30.0	29.3
	171.2	15.4	170.3	14.7	170.6	14.5	13.7
	59.1	123.0	55.4	121.6	57.3	121.6	117.7
	34.5	146.6	27.3	147.8	29.7	147.7	140.5
	126.8	58.0	125.2	56.6	124.9	57.7	52.3
	117.7	66.7	115.4	65.8	116.1	66.0	69.5
	136.3	48.8	132.6	49.7	133.7	49.3	47.9
	116.8	67.5	113.2	67.8	113.3	68.7	69.4
	29.4	151.5	22.6	152.2	25.3	151.9	150.0
	133.4	51.6	128.5	53.5	129.7	53.1	51.8
	46.8	134.8	39.6	136.4	41.5	136.5	134.3
	76.1	106.6	71.3	106.8	72.7	107.1	108.3
	54.2	127.6	48.4	128.2	50.3	128.2	128.2
	63.9	118.4	58.7	118.6	60.5	118.5	119.8
	59.0	123.0	53.5	123.4	55.5	123.3	122.2
	156.2	29.7	152.8	30.9	153.6	30.6	27.7
	156.2	29.7	154.6	29.3	154.8	29.4	28.5
	122.9	61.7	119.9	61.6	119.9	62.4	61.7
	131.0	53.9	129.4	52.7	129.8	53.1	53.7
	143.4	42.0	141.5	41.4	142.2	41.3	41.2
	126.3	58.4	124.8	57.0	124.4	58.2	58.1
	42.8	138.6	35.6	140.0	37.9	139.9	133.8
	57.8	124.2	53.8	123.1	55.9	122.9	122.2
	172.2	14.4	171.4	13.6	171.8	13.4	13.0
22	146.8	38.8	142.7	40.3	143.9	39.7	40.0
	37.1	144.1	31.6	143.8	33.3	144.3	143.4
	81.8	101.1	76.5	101.9	78.4	101.6	102.7
	55.8	126.2	48.6	128.0	50.3	128.2	129.9
	68.6	113.8	62.5	115.0	64.2	115.1	118.0
	48.5	133.1	41.7	134.4	43.8	134.4	136.5
	161.5	24.6	160.3	24.0	160.4	24.1	27.9
	156.7	29.2	155.9	28.0	156.1	28.2	27.3
	31.4	149.5	26.0	149.0	27.9	149.4	146.8
	-7.4	186.8	-13.7	185.9	-11.1	186.3	188.3
	27.3	153.4	21.6	153.1	23.7	153.4	147.1
	46.6	134.9	40.4	135.5	42.4	135.7	135.2
	30.5	150.4	24.4	150.5	27.8	149.5	153.8
	62.7	119.5	57.8	119.3	59.5	119.6	119.7
	71.7	110.8	67.2	110.6	68.8	110.8	111.5
	74.0	108.6	68.9	109.0	70.4	109.2	108.3
	-3.5	183.0	-9.9	182.4	-7.7	183.0	184.4

	157.3	28.7	155.2	28.7	155.8	28.5	28.8
	54.7	127.1	47.3	129.1	49.8	128.7	128.0
	62.7	119.5	57.3	119.8	59.5	119.5	119.6
	60.6	121.5	55.2	121.8	57.5	121.5	121.8
	46.8	134.8	40.0	135.9	42.4	135.7	137.3
	58.2	123.9	54.4	122.5	56.2	122.7	127.6
	65.8	116.5	62.2	115.3	64.3	115.0	111.6
	60.3	121.8	55.3	121.7	57.6	121.3	122.5
	61.1	121.1	55.9	121.1	57.8	121.2	120.8
	70.5	112.0	66.8	111.0	68.0	111.5	112.6
	42.7	138.7	36.1	139.6	38.8	139.0	133.4
	62.0	120.1	57.1	120.0	59.3	119.7	120.5
	59.4	122.7	54.6	122.3	56.7	122.2	122.6
	160.2	25.9	159.5	24.7	159.6	24.9	25.8
	170.1	16.4	168.4	16.4	168.9	16.1	17.8
23	139.9	45.4	137.2	45.4	137.7	45.6	46.9
	124.7	60.0	122.1	59.5	122.7	59.8	55.1
	153.5	32.3	151.2	32.4	152.1	32.0	30.2
	111.6	72.6	109.9	70.8	110.2	71.6	71.1
	10.1	170.0	5.8	167.8	8.7	167.5	171.6
	133.8	51.3	130.9	51.3	131.9	51.1	52.9
	146.3	39.2	144.9	38.3	145.4	38.4	41.4
	33.5	147.5	29.0	146.1	31.7	145.8	154.6
	133.1	51.9	130.4	51.8	131.6	51.4	49.3
	139.2	46.1	138.0	44.7	138.5	44.9	37.3
	152.1	33.7	149.7	33.8	150.4	33.6	23.7
	5.8	174.1	1.2	172.1	3.9	172.1	172.0
	15.2	165.1	10.5	163.4	13.1	163.4	168.1
	9.6	170.5	4.4	169.1	7.5	168.7	172.4
	133.0	52.0	130.3	51.8	130.9	52.1	55.4
	154.8	31.1	152.8	30.9	153.7	30.5	29.8
	74.8	107.8	69.5	108.5	71.9	107.8	105.9
	128.4	56.4	125.7	56.1	126.3	56.3	57.0
	4.0	175.8	-0.2	173.4	2.6	173.3	173.6
	140.3	45.0	139.0	43.7	139.8	43.6	40.0
	123.9	60.7	122.4	59.2	123.4	59.1	63.3
	6.9	173.0	2.7	170.7	5.8	170.3	173.1
	119.2	65.2	117.8	63.5	118.6	63.6	60.0
	52.7	129.1	48.4	128.1	50.6	128.0	135.9
	30.9	150.0	26.3	148.7	29.4	147.9	157.5

^[a] Parameters of linear regression models are presented in Table 2 in main text.

^[b] For the references to the experimental works, please, see the main text.

Table S4. Calculated ^{13}C NMR shielding constants, together with scaled and experimental chemical shifts – the GIAO-DFT(PBE0) calculations with the second-level basis sets.

Mol.	pcS-2		pecS-2		pecS-2 mod		$\delta_{\text{exp}}^{[b]}$
	σ	$\delta_{\text{scaled}}^{[a]}$	σ	$\delta_{\text{scaled}}^{[a]}$	σ	$\delta_{\text{scaled}}^{[a]}$	
1	121.3	59.3	120.9	59.0	121.2	59.0	55.5
	145.5	36.5	145.0	36.5	145.3	36.4	33.3
	136.9	44.6	136.2	44.6	136.5	44.7	35.9
	40.2	135.4	39.4	135.3	40.0	135.4	133.2
	126.3	54.6	125.9	54.3	126.2	54.3	54.6
	128.6	52.3	128.6	51.8	128.6	52.1	52.0
	33.3	141.9	32.4	141.9	33.0	142.0	135.2
	70.0	107.4	68.9	107.7	69.5	107.6	107.3
	160.7	22.2	160.2	22.2	160.6	22.0	19.5
	145.5	36.5	144.9	36.5	145.2	36.5	38.5
	49.4	126.7	48.3	127.0	48.9	126.9	128.1
	41.5	134.2	40.6	134.2	41.1	134.4	138.1
	58.0	118.7	57.2	118.7	57.7	118.7	124.5
	29.6	145.3	28.8	145.3	29.4	145.3	145.0
	59.6	117.1	58.7	117.3	59.3	117.2	118.6
	41.0	134.6	40.1	134.7	40.7	134.7	137.1
	67.5	109.7	66.5	110.0	67.1	109.8	112.2
	171.1	12.6	170.2	12.8	170.6	12.6	13.0
	49.6	126.5	48.4	126.9	49.0	126.9	130.1
	58.9	117.8	57.9	118.0	58.5	118.0	119.8
	56.9	119.7	56.0	119.8	56.5	119.8	122.5
	54.6	121.8	53.5	122.2	54.1	122.1	122.8
	42.5	133.2	41.6	133.2	42.1	133.4	136.9
	64.9	112.1	64.0	112.3	64.6	112.2	114.4
	37.4	137.9	36.8	137.7	37.4	137.8	137.2
	73.8	103.8	72.7	104.1	73.4	104.0	106.7
	64.8	112.2	63.9	112.4	64.5	112.4	113.6
	24.3	150.2	23.6	150.2	24.0	150.4	152.0
	60.4	116.4	59.3	116.7	59.8	116.7	119.3
2	49.6	126.5	48.4	126.9	49.2	126.7	125.7
	62.5	114.4	61.5	114.6	62.1	114.6	115.1
	53.4	122.9	52.8	122.7	53.4	122.8	124.1
	39.7	135.8	38.8	135.9	39.3	136.0	137.0
	66.1	111.1	65.0	111.4	65.7	111.2	111.4
	54.7	121.8	53.8	121.9	54.3	121.9	122.3
	57.7	118.9	56.7	119.1	57.3	119.1	119.9
	56.5	120.1	55.6	120.2	56.2	120.1	120.4
	111.3	68.6	110.5	68.7	111.1	68.5	68.2
	61.0	115.8	60.0	116.0	60.6	116.0	115.1
	50.7	125.5	49.6	125.7	50.3	125.7	125.7
	40.2	135.3	39.3	135.5	39.8	135.5	137.0
	50.1	126.0	49.6	125.8	50.1	125.9	124.1

	56.7	119.9	55.8	120.0	56.5	119.9	120.4
	58.0	118.6	57.0	118.8	57.6	118.8	119.9
	55.3	121.2	54.4	121.3	54.9	121.3	122.3
	67.2	110.0	66.2	110.3	66.8	110.2	111.4
	-28.7	200.0	-29.4	199.7	-28.4	199.7	201.5
	56.2	120.3	55.1	120.7	55.7	120.6	120.8
	13.1	160.8	12.3	160.7	12.9	160.9	160.3
	50.5	125.7	49.5	125.8	50.1	125.9	125.5
	58.8	117.9	57.8	118.1	58.3	118.2	119.4
	37.4	138.0	36.5	138.1	36.9	138.2	137.6
	64.8	112.2	63.8	112.5	64.5	112.4	112.9
3	140.6	41.2	139.8	41.3	140.1	41.3	40.3
	122.6	58.1	122.2	57.8	122.5	57.8	64.8
	142.9	39.0	142.0	39.2	142.4	39.1	39.2
	108.1	71.6	107.4	71.6	107.6	71.8	72.2
	117.3	63.0	117.0	62.7	117.2	62.8	65.5
	139.8	41.9	139.3	41.8	139.5	41.8	41.7
	149.7	32.6	149.2	32.5	149.4	32.5	32.7
	28.1	146.7	27.3	146.6	27.8	146.8	138.6
	-1.4	174.4	-2.0	174.1	-0.9	173.8	172.7
	42.3	133.3	41.7	133.2	42.2	133.3	137.9
	132.4	48.8	132.2	48.4	132.5	48.4	49.5
	140.6	41.2	140.1	41.0	140.3	41.1	41.6
	140.6	41.2	140.3	40.9	140.5	40.9	41.9
	122.0	58.6	121.8	58.1	122.0	58.3	52.9
	32.2	142.9	31.3	142.9	32.0	142.9	143.3
	160.3	22.6	159.6	22.7	159.9	22.6	21.1
	154.8	27.8	154.3	27.7	154.5	27.7	25.9
	158.3	24.5	157.9	24.4	158.1	24.3	24.5
	43.1	132.6	42.3	132.6	42.8	132.7	132.6
	153.9	28.6	153.5	28.4	153.6	28.5	26.5
	44.6	131.3	43.7	131.3	44.4	131.2	128.5
	150.5	31.9	149.8	32.0	150.0	31.9	25.9
	47.6	128.4	46.4	128.8	47.0	128.8	128.5
	151.6	30.8	151.0	30.8	151.3	30.7	25.8
	42.2	133.5	41.4	133.5	42.0	133.5	131.8
	37.2	138.2	36.6	137.9	37.2	138.0	137.8
	55.2	121.3	54.0	121.6	54.7	121.6	121.0
	63.7	113.3	62.7	113.5	63.3	113.4	113.7
	36.1	139.1	35.3	139.2	35.8	139.3	140.6
	15.3	158.7	14.4	158.7	14.9	158.9	148.1
	54.3	122.1	53.4	122.2	54.0	122.2	121.6
	66.3	110.9	65.3	111.1	65.9	111.0	111.9
	57.6	119.0	56.5	119.3	57.1	119.3	121.0
	57.6	119.0	56.6	119.2	57.1	119.2	119.5
	47.3	128.7	46.4	128.8	46.9	128.9	128.2
	8.2	165.4	7.3	165.4	8.2	165.2	167.0
4	11.7	162.1	11.2	161.8	11.8	161.8	161.4
	126.3	54.5	125.9	54.3	126.2	54.3	55.0
	4.6	168.7	4.1	168.4	4.8	168.4	168.2

	132.3	48.9	131.8	48.8	132.1	48.8	48.7
	125.9	54.9	125.3	54.9	125.4	55.1	52.4
	38.9	136.6	37.9	136.7	38.5	136.7	134.9
	52.5	123.8	51.7	123.8	52.3	123.8	122.6
	53.4	122.9	52.4	123.1	53.0	123.1	122.8
	44.3	131.5	43.4	131.6	43.9	131.7	130.0
	66.0	111.1	64.9	111.4	65.6	111.3	111.1
	30.3	144.6	29.7	144.5	30.2	144.6	144.8
	138.7	42.9	138.0	43.0	138.2	43.1	41.8
	92.4	86.3	92.0	86.1	92.4	86.1	87.3
	84.8	93.5	83.6	93.9	84.4	93.7	92.6
	151.4	31.0	150.6	31.1	150.8	31.2	31.1
	110.3	69.6	110.0	69.2	110.4	69.2	69.2
	145.4	36.6	145.0	36.5	145.0	36.6	35.8
	130.2	50.9	129.4	51.0	129.8	50.9	50.8
	102.3	77.1	102.0	76.7	102.3	76.8	76.2
	5.3	168.1	4.7	167.9	5.7	167.6	169.1
	129.6	51.5	129.1	51.3	129.2	51.5	51.7
	83.2	95.0	82.8	94.7	83.3	94.7	93.6
	130.9	50.2	130.8	49.7	130.9	49.9	48.6
	127.5	53.4	127.4	52.9	127.5	53.1	51.6
	150.3	32.0	149.8	32.0	150.1	31.8	30.6
	122.3	58.3	121.5	58.4	122.0	58.3	57.0
	35.7	139.6	34.8	139.7	35.4	139.7	136.6
	58.2	118.4	57.3	118.6	58.0	118.4	116.3
	53.5	122.9	52.7	122.9	53.1	123.0	121.6
	61.4	115.4	60.5	115.6	61.0	115.6	116.5
	34.7	140.5	33.9	140.5	34.5	140.5	142.0
	39.4	136.1	38.7	136.0	39.3	136.0	136.1
	155.3	27.4	154.8	27.3	155.0	27.2	25.5
	97.3	81.8	96.9	81.5	97.2	81.6	80.5
	150.0	32.3	149.2	32.4	149.4	32.5	31.2
	148.2	34.0	147.6	34.0	148.0	33.8	31.6
	113.3	66.8	112.9	66.5	113.2	66.5	65.1
	143.4	38.5	142.9	38.4	143.0	38.5	36.8
	135.9	45.5	135.2	45.6	135.4	45.7	46.3
	116.4	63.9	115.9	63.7	116.3	63.6	64.7
	149.8	32.5	149.2	32.5	149.5	32.4	29.3
	130.5	50.6	130.1	50.4	130.3	50.5	50.7
	14.7	159.3	14.3	158.9	14.9	159.0	158.7
	127.9	53.1	127.5	52.8	127.8	52.8	53.5
	13.5	160.4	13.1	160.0	13.6	160.2	158.7
	72.6	104.9	71.6	105.2	72.3	105.0	104.6
	118.3	62.1	117.6	62.1	117.7	62.3	60.9
	38.8	136.6	38.0	136.6	38.6	136.7	135.4
	49.5	126.6	48.7	126.6	49.3	126.6	124.4
	52.5	123.8	51.5	124.0	52.1	123.9	123.4
	43.9	131.9	43.0	132.0	43.5	132.1	131.2
	65.8	111.3	65.0	111.4	65.5	111.4	111.6
	31.1	143.9	30.5	143.7	31.0	143.8	144.7

	141.5	40.3	140.9	40.3	141.2	40.2	39.8
	92.9	85.9	92.4	85.7	92.8	85.7	87.1
	79.0	98.9	77.9	99.3	78.7	99.0	98.4
	153.3	29.2	152.5	29.4	152.8	29.3	28.2
	115.5	64.7	115.3	64.3	115.4	64.4	64.3
	145.1	36.9	144.6	36.8	144.9	36.7	37.0
	131.4	49.8	130.6	49.9	130.8	50.0	49.1
	107.1	72.6	106.7	72.3	106.9	72.4	72.1
	6.3	167.2	5.5	167.1	6.7	166.7	168.6
	129.6	51.5	129.1	51.3	129.2	51.5	51.9
	83.1	95.1	82.8	94.7	83.2	94.7	93.2
	130.8	50.3	130.6	49.9	130.8	50.0	48.6
	127.7	53.3	127.5	52.8	127.7	52.9	51.6
	148.8	33.4	148.3	33.3	148.7	33.1	31.4
	122.0	58.6	121.2	58.7	121.6	58.6	56.0
	36.5	138.8	35.6	138.9	36.3	138.9	135.9
	55.8	120.7	54.9	120.8	55.6	120.7	115.9
	53.3	123.0	52.5	123.0	53.0	123.1	120.9
	51.8	124.4	51.0	124.5	51.7	124.4	118.9
	36.4	138.9	35.6	138.9	36.3	138.9	142.0
	33.4	141.7	32.7	141.6	33.4	141.6	136.9
	155.2	27.4	154.7	27.3	155.0	27.2	25.5
	97.6	81.5	97.2	81.2	97.4	81.4	80.5
	149.0	33.3	148.2	33.5	148.6	33.3	32.3
	148.5	33.7	147.8	33.8	148.4	33.5	32.1
	113.9	66.2	113.5	65.9	113.8	66.0	64.8
	144.2	37.7	143.7	37.6	143.9	37.7	36.2
	135.9	45.6	135.2	45.6	135.4	45.6	46.1
	116.8	63.5	116.3	63.3	116.7	63.2	64.7
	145.7	36.4	145.0	36.4	145.4	36.2	36.0
	137.2	44.3	136.9	44.0	137.1	44.1	45.2
5	118.6	61.8	118.0	61.7	118.2	61.8	62.3
	117.5	62.8	116.9	62.8	117.1	62.9	63.8
	139.8	41.9	139.3	41.8	139.4	41.9	42.5
	91.4	87.3	91.0	87.0	91.0	87.4	88.0
	127.2	53.7	126.7	53.6	126.9	53.7	53.7
	137.9	43.6	137.5	43.5	137.4	43.8	44.6
	101.9	77.5	101.5	77.2	101.5	77.6	77.7
	148.1	34.1	147.5	34.0	147.8	34.0	35.9
	97.2	81.9	96.6	81.8	96.9	81.9	83.5
	124.3	56.5	123.7	56.4	123.8	56.6	57.5
	25.6	149.1	25.0	148.9	25.6	148.9	145.9
	132.3	48.9	131.7	48.8	132.0	48.9	49.5
	142.9	39.0	142.3	39.0	142.7	38.8	35.9
	39.6	135.9	38.9	135.8	39.4	135.9	133.7
	167.3	16.1	166.7	16.1	167.1	15.9	17.4
	156.9	25.9	156.3	25.9	156.6	25.8	25.0
	105.3	74.2	104.8	74.1	105.0	74.3	73.8
	157.5	25.3	156.9	25.3	157.2	25.2	27.6
	138.5	43.1	137.8	43.2	138.0	43.2	43.2

	97.8	81.3	97.3	81.1	97.6	81.2	82.2
	165.9	17.4	165.1	17.6	165.5	17.4	17.1
	136.6	44.9	136.0	44.8	136.4	44.7	42.1
	-7.5	180.1	-8.2	179.9	-7.0	179.5	178.9
	131.9	49.3	131.2	49.3	131.5	49.3	50.1
	158.8	24.1	158.2	24.1	158.5	24.0	24.0
	153.6	28.9	153.0	28.9	153.4	28.7	30.0
	172.8	11.0	172.1	11.0	172.3	11.0	12.7
	138.9	42.7	138.2	42.8	138.5	42.8	43.5
	-7.7	180.3	-8.4	180.1	-7.2	179.8	178.9
	172.9	10.8	172.3	10.8	172.5	10.8	12.9
6	40.0	135.5	39.1	135.6	39.6	135.7	135.3
	49.4	126.7	48.4	126.9	48.9	127.0	128.0
	48.0	128.0	47.1	128.2	47.6	128.2	127.4
	55.4	121.1	54.1	121.6	54.8	121.5	121.3
	29.7	145.2	28.9	145.1	29.4	145.3	146.3
	49.6	126.5	48.7	126.6	49.3	126.6	131.8
	11.5	162.3	10.7	162.2	11.6	162.1	162.2
	16.9	157.2	16.4	156.8	17.2	156.8	155.3
	43.1	132.6	42.4	132.5	42.9	132.6	133.7
	48.6	127.4	47.5	127.8	48.2	127.7	130.4
	7.8	165.7	7.2	165.5	8.2	165.3	168.4
	120.9	59.6	120.3	59.6	120.6	59.6	50.7
	47.0	128.9	46.2	129.0	46.6	129.1	128.6
	42.4	133.2	41.6	133.3	42.1	133.3	127.8
	47.8	128.2	47.0	128.2	47.5	128.3	129.3
	44.5	131.3	43.7	131.3	44.0	131.6	129.9
	137.2	44.3	136.5	44.4	136.8	44.3	42.9
	100.7	78.6	100.0	78.5	100.2	78.8	80.9
	38.0	137.4	37.1	137.5	37.7	137.5	139.6
	37.9	137.5	37.2	137.4	37.7	137.6	136.3
	92.2	86.5	92.1	86.0	92.3	86.2	86.8
	52.2	124.1	51.3	124.2	51.9	124.2	124.0
	52.7	123.6	51.7	123.8	52.3	123.8	126.0
	44.1	131.7	43.2	131.7	43.7	131.9	129.8
	59.6	117.1	58.7	117.3	59.2	117.3	115.9
	113.2	66.8	112.9	66.5	113.1	66.7	62.0
	3.0	170.3	2.4	170.0	3.5	169.7	171.4
	150.3	32.0	149.7	32.0	150.0	31.9	34.5
	157.2	25.5	156.8	25.4	156.8	25.5	25.2
	160.2	22.7	159.6	22.8	159.9	22.6	23.6
	160.8	22.2	160.2	22.2	160.4	22.2	21.4
7	105.3	74.2	105.0	73.9	105.2	74.1	73.8
	94.9	84.1	94.7	83.5	94.9	83.8	80.2
	103.5	76.0	102.8	75.9	103.0	76.2	73.6
	137.6	43.9	137.0	43.9	137.3	43.9	42.7
	45.4	130.4	44.6	130.5	45.0	130.6	126.7
	101.3	78.0	100.6	78.0	100.7	78.3	76.3
	13.4	160.5	12.8	160.3	13.8	160.0	163.1
	9.5	164.1	8.9	163.9	9.9	163.7	165.6

	26.2	148.5	25.6	148.3	26.1	148.4	148.4
	40.6	134.9	39.9	134.9	40.4	134.9	134.1
	48.9	127.2	48.2	127.1	48.8	127.1	127.3
	52.4	123.9	51.6	123.9	52.2	123.9	125.0
	119.0	61.4	118.4	61.4	118.6	61.5	60.4
	67.2	110.0	66.1	110.3	66.8	110.2	107.8
	46.0	129.9	45.0	130.1	45.6	130.1	130.4
	66.4	110.8	65.3	111.1	66.0	110.9	111.1
	158.5	24.3	158.0	24.2	158.1	24.3	27.5
	154.5	28.0	153.7	28.3	154.0	28.1	27.1
	57.1	119.5	56.1	119.7	56.7	119.6	120.3
	66.5	110.6	65.6	110.8	66.2	110.7	111.5
	100.8	78.4	100.1	78.5	100.3	78.7	74.9
	44.9	131.0	44.0	131.0	44.5	131.2	131.4
	52.1	124.1	51.3	124.2	51.9	124.2	119.2
	102.6	76.8	101.9	76.8	102.0	77.1	76.6
	54.7	121.8	53.7	122.0	54.3	121.9	122.8
	10.0	163.7	9.3	163.5	10.3	163.3	165.6
	58.2	118.5	57.2	118.7	57.8	118.7	120.6
	7.4	166.1	6.7	166.0	7.6	165.8	166.8
	157.8	25.0	157.4	24.8	157.5	24.9	28.3
	117.1	63.2	116.5	63.1	116.7	63.2	61.1
	159.8	23.2	159.3	23.0	159.4	23.1	27.5
8	141.1	40.6	140.5	40.7	140.7	40.7	40.5
	124.4	56.3	123.8	56.3	124.1	56.3	56.7
	117.2	63.1	116.8	62.8	117.1	62.8	62.9
	150.4	31.9	149.7	32.0	150.0	31.9	31.7
	98.3	80.9	98.0	80.5	98.1	80.7	81.1
	131.0	50.1	130.4	50.1	130.8	50.0	50.3
	150.3	32.1	149.8	32.0	150.0	31.9	32.2
	142.0	39.9	141.6	39.6	141.9	39.6	39.9
	139.9	41.8	139.3	41.8	139.5	41.8	42.0
	161.8	21.2	161.1	21.3	161.4	21.2	21.1
	144.3	37.7	143.5	37.8	143.8	37.8	37.2
	68.8	108.5	68.6	108.0	68.6	108.5	109.3
	167.7	15.7	167.1	15.7	167.2	15.7	16.3
	149.7	32.6	149.1	32.6	149.4	32.5	32.3
	29.7	145.2	28.8	145.3	29.3	145.4	140.8
	144.3	37.6	143.8	37.6	144.0	37.6	37.5
	170.0	13.5	169.4	13.5	169.7	13.5	15.0
	151.1	31.3	150.5	31.2	151.0	31.0	31.7
	52.6	123.8	51.9	123.6	52.4	123.7	121.8
	164.2	19.0	163.6	19.0	163.8	18.9	19.4
	140.3	41.4	139.6	41.5	140.1	41.3	39.0
	152.2	30.2	151.6	30.2	152.0	30.1	30.4
	107.5	72.2	107.2	71.9	107.4	72.0	78.2
	153.6	29.0	153.1	28.8	153.4	28.7	29.3
	151.4	31.0	151.1	30.7	151.1	30.9	30.6
	114.0	66.1	113.8	65.7	113.9	65.9	66.9
	167.3	16.1	166.8	16.0	167.0	15.9	17.3

	76.8	101.0	76.6	100.5	76.9	100.7	102.5
	109.6	70.2	109.0	70.1	109.2	70.3	71.8
	102.5	76.9	101.9	76.8	102.3	76.8	78.2
	103.2	76.2	103.0	75.8	103.2	75.9	78.2
	107.4	72.2	107.1	71.9	107.3	72.1	75.5
	117.2	63.1	116.8	62.9	116.9	63.1	62.7
9	141.8	40.0	140.9	40.2	141.5	40.0	40.1
	119.6	60.9	118.8	61.0	119.3	60.8	60.9
	138.1	43.4	137.2	43.7	137.6	43.6	44.0
	129.7	51.4	128.9	51.5	129.3	51.4	51.6
	165.4	17.8	164.7	18.0	165.1	17.7	17.3
	144.8	37.2	144.2	37.2	144.4	37.2	37.4
	104.4	75.1	103.7	75.1	104.2	75.0	76.1
	142.7	39.1	141.9	39.3	142.3	39.1	37.9
	126.6	54.3	125.8	54.4	126.3	54.2	53.5
	141.0	40.8	140.0	41.1	140.5	40.9	38.5
	133.8	47.5	133.0	47.6	133.3	47.7	42.6
	153.0	29.5	152.2	29.7	152.5	29.6	30.0
	144.7	37.2	144.2	37.2	144.4	37.2	37.3
	154.4	28.2	153.7	28.3	154.1	28.1	32.1
	151.9	30.5	151.3	30.5	151.5	30.5	35.5
	156.1	26.6	155.3	26.8	155.4	26.9	27.8
	149.5	32.8	149.0	32.7	149.2	32.6	32.2
	151.9	30.6	151.5	30.4	151.5	30.5	35.0
	149.5	32.8	148.7	32.9	149.3	32.6	31.1
	112.3	67.7	111.6	67.7	111.8	67.9	68.7
	-4.9	177.7	-5.6	177.5	-4.3	177.0	176.8
	97.2	81.8	96.8	81.6	96.8	81.9	83.8
	168.5	15.0	167.8	15.0	168.1	14.9	15.5
	171.5	12.2	170.7	12.3	170.9	12.3	12.8
	168.5	14.9	168.0	14.9	168.2	14.8	13.1
	166.8	16.6	166.1	16.7	166.4	16.6	21.5
	146.8	35.3	146.1	35.4	146.4	35.4	30.6
	150.8	31.6	150.2	31.6	150.5	31.4	30.0
	148.2	34.0	147.6	34.0	147.9	33.9	34.1
	-6.5	179.1	-7.2	179.0	-5.9	178.6	178.0
10	125.8	55.0	125.3	54.8	125.5	55.0	57.9
	158.5	24.3	157.7	24.5	158.1	24.3	25.2
	147.9	34.3	147.3	34.3	147.4	34.4	30.5
	140.2	41.5	139.7	41.3	140.0	41.3	44.1
	132.8	48.4	132.5	48.2	132.5	48.3	50.5
	66.5	110.6	65.5	110.9	66.1	110.8	110.6
	2.9	170.4	2.2	170.2	3.2	170.0	171.3
	106.9	72.7	106.6	72.4	106.7	72.7	71.7
	143.1	38.8	142.4	38.9	142.5	39.0	40.8
	134.7	46.7	134.0	46.8	134.3	46.7	42.6
	133.9	47.4	133.4	47.3	133.4	47.5	47.1
	-3.8	176.6	-4.3	176.3	-3.3	176.1	174.9
	43.6	132.1	42.8	132.2	43.4	132.2	134.1
	36.2	139.1	35.6	138.9	36.2	139.0	130.6

	141.3	40.5	140.5	40.6	140.9	40.5	42.1
	49.0	127.1	47.9	127.4	48.6	127.3	128.5
	-3.0	175.9	-3.7	175.7	-2.7	175.5	177.9
	161.1	21.9	160.6	21.8	160.8	21.7	22.0
	152.8	29.7	152.4	29.5	152.5	29.5	31.1
	40.8	134.8	39.6	135.1	40.2	135.2	132.7
	51.8	124.4	51.2	124.2	51.8	124.3	124.2
	40.0	135.5	39.2	135.5	39.7	135.6	138.1
	164.4	18.8	163.8	18.8	164.1	18.7	19.6
	172.4	11.3	171.8	11.4	172.0	11.3	20.0
	1.6	171.6	0.9	171.4	2.0	171.1	172.1
	167.9	15.5	167.2	15.7	167.5	15.5	18.5
	163.7	19.5	163.1	19.5	163.3	19.5	18.2
	57.3	119.3	56.3	119.5	56.9	119.5	119.3
	66.2	110.9	65.2	111.1	65.9	111.0	112.3
	46.6	129.4	45.7	129.4	46.2	129.5	128.2
	48.5	127.6	47.6	127.6	48.1	127.7	128.2
	57.8	118.8	56.9	119.0	57.4	119.0	119.8
	55.4	121.1	54.5	121.2	55.0	121.2	122.4
	64.0	113.0	63.0	113.3	63.5	113.3	116.2
	62.6	114.4	61.5	114.7	62.0	114.6	116.2
	18.4	155.8	17.6	155.7	18.1	155.9	157.7
11	130.6	50.5	130.4	50.1	130.3	50.5	49.4
	10.0	163.7	9.0	163.8	9.8	163.8	169.4
	61.8	115.0	60.6	115.5	61.2	115.4	106.6
	34.6	140.6	33.7	140.6	34.2	140.8	141.5
	149.6	32.7	148.9	32.8	149.1	32.7	36.9
	14.6	159.4	13.9	159.2	14.6	159.3	165.3
	58.6	118.1	57.4	118.4	58.1	118.4	124.5
	17.5	156.6	16.7	156.6	17.3	156.7	158.1
	68.5	108.8	67.4	109.1	68.0	109.0	117.3
	53.0	123.4	51.9	123.6	52.6	123.5	124.4
	38.7	136.8	37.9	136.8	38.5	136.8	134.8
	56.0	120.5	54.9	120.9	55.5	120.8	120.6
	25.2	149.4	24.4	149.4	25.0	149.5	151.8
	66.1	111.1	64.8	111.5	65.5	111.4	115.2
	42.1	133.6	41.0	133.8	41.7	133.8	137.2
	58.4	118.3	57.5	118.4	58.1	118.4	120.5
	36.5	138.8	35.5	139.0	36.0	139.1	136.9
	72.5	105.0	71.5	105.3	72.0	105.2	107.9
	18.1	156.1	17.4	156.0	17.9	156.1	157.8
	55.6	120.9	54.4	121.3	55.0	121.2	120.6
	42.6	133.0	41.8	133.1	42.5	133.0	135.0
	48.9	127.2	47.9	127.4	48.5	127.4	124.5
	39.7	135.8	38.8	135.9	39.4	135.9	136.6
	62.2	114.7	60.9	115.2	61.6	115.0	114.9
	22.4	152.1	21.7	152.0	22.2	152.1	152.5
	15.4	158.6	14.8	158.4	15.3	158.6	157.8
	73.1	104.5	71.9	104.9	72.5	104.8	107.7
	36.5	138.8	35.6	138.9	36.1	139.0	136.8

	61.3	115.6	60.3	115.8	60.9	115.7	119.3
	57.6	119.0	56.5	119.4	57.1	119.3	118.9
	20.9	153.5	20.2	153.3	20.7	153.5	155.9
	81.4	96.7	80.3	97.1	80.8	97.0	101.7
	21.5	152.9	20.7	152.8	21.3	153.0	155.5
	60.6	116.2	59.4	116.6	60.1	116.5	116.4
	36.0	139.3	35.2	139.3	35.6	139.5	134.7
	147.5	34.6	146.8	34.7	147.2	34.5	34.7
	139.8	41.9	139.5	41.5	139.6	41.7	44.0
	134.2	47.2	133.7	47.0	133.7	47.2	48.9
	169.2	14.3	168.6	14.4	168.7	14.4	19.2
	121.1	59.5	120.8	59.1	121.0	59.2	61.0
	161.8	21.3	160.9	21.5	161.3	21.3	22.1
	127.6	53.3	127.2	53.1	127.4	53.2	56.9
	128.3	52.7	128.0	52.4	128.1	52.5	56.9
	161.9	21.1	161.2	21.3	161.6	21.1	22.2
	163.9	19.3	163.2	19.3	163.5	19.3	19.7
	161.9	21.2	161.4	21.1	161.6	21.0	20.8
12	117.2	63.1	116.5	63.1	117.0	63.0	65.7
	127.9	53.0	127.0	53.3	127.3	53.3	51.3
	131.8	49.4	131.0	49.5	131.3	49.5	48.1
	135.1	46.3	134.3	46.4	134.7	46.4	45.9
	144.1	37.8	143.3	38.1	143.5	38.0	37.9
	128.9	52.1	128.3	52.1	128.6	52.1	53.9
	119.4	61.1	118.7	61.1	119.0	61.0	60.6
	163.8	19.4	163.1	19.4	163.4	19.3	18.9
	147.9	34.3	147.4	34.2	147.6	34.2	30.8
	100.4	78.9	100.0	78.5	100.1	78.8	79.1
	-40.1	210.7	-41.1	210.7	-40.1	210.7	206.1
	145.2	36.8	144.3	37.1	144.8	36.9	36.4
	99.4	79.8	98.9	79.6	99.1	79.8	80.3
	103.0	76.4	102.3	76.4	102.7	76.4	77.8
	167.4	15.9	166.6	16.2	166.9	16.1	17.6
	115.5	64.7	114.9	64.6	115.2	64.7	65.3
	162.0	21.0	161.4	21.1	161.6	21.0	21.4
	6.2	167.3	5.5	167.1	6.7	166.7	166.6
	146.7	35.4	146.0	35.5	146.2	35.5	35.6
	164.4	18.8	163.7	18.9	163.9	18.9	20.7
	155.2	27.4	154.5	27.5	154.8	27.4	30.2
	54.5	121.9	53.5	122.2	54.1	122.1	120.0
	3.9	169.4	3.1	169.3	4.2	169.0	169.1
	65.6	111.5	64.6	111.7	65.1	111.7	109.7
	35.5	139.7	34.8	139.6	35.5	139.6	141.1
	32.9	142.2	32.2	142.1	32.8	142.2	143.2
13	117.1	63.2	116.7	62.9	117.0	63.0	62.9
	129.4	51.6	128.9	51.5	128.9	51.7	53.5
	138.2	43.4	137.6	43.3	137.9	43.3	41.4
	93.7	85.2	93.5	84.6	93.7	84.8	82.7
	116.3	63.9	116.1	63.5	116.2	63.7	65.4
	154.8	27.8	154.1	27.9	154.4	27.8	29.2

	158.6	24.2	158.1	24.1	158.2	24.3	23.3
	141.4	40.3	141.2	40.0	141.3	40.1	37.3
	31.4	143.6	30.5	143.7	31.1	143.7	133.9
	22.6	151.8	22.0	151.7	22.6	151.7	146.5
	123.0	57.6	122.8	57.2	122.9	57.4	53.8
	24.1	150.5	23.3	150.4	23.9	150.5	141.5
	122.8	57.8	122.3	57.7	122.6	57.7	52.0
	54.4	122.0	53.6	122.1	54.2	122.0	122.7
	69.3	108.0	68.4	108.2	68.9	108.1	103.8
	56.8	119.8	56.0	119.8	56.7	119.7	117.7
	57.6	119.0	56.7	119.2	57.2	119.2	117.2
	50.3	125.9	49.3	126.0	49.9	126.1	128.2
	168.9	14.6	168.1	14.8	168.4	14.6	13.3
	145.8	36.3	145.0	36.4	145.4	36.2	35.1
14	153.6	29.0	152.8	29.1	153.0	29.1	28.5
	146.6	35.5	145.7	35.7	146.1	35.6	37.2
	77.3	100.6	76.9	100.2	77.2	100.4	102.6
	147.5	34.7	146.9	34.7	147.2	34.6	36.2
	59.9	116.9	58.9	117.1	59.4	117.1	116.8
	66.1	111.0	64.9	111.4	65.7	111.2	117.5
	57.7	118.9	56.9	119.0	57.5	118.9	122.9
	33.6	141.6	32.7	141.6	33.2	141.8	133.7
	62.6	114.4	61.4	114.7	62.2	114.5	113.4
	21.6	152.8	21.0	152.6	21.4	152.8	154.5
	21.0	153.3	20.5	153.0	20.9	153.3	155.0
	18.3	155.9	17.5	155.8	18.1	156.0	156.7
	48.2	127.8	47.3	127.9	47.8	128.0	127.9
	159.4	23.5	158.7	23.6	159.1	23.4	23.9
	72.7	104.8	71.6	105.1	72.4	104.9	105.0
	77.0	100.8	75.8	101.2	76.4	101.1	104.6
	17.4	156.7	16.7	156.6	17.3	156.7	159.9
	44.3	131.4	43.4	131.6	44.0	131.6	130.3
	75.0	102.7	73.9	103.0	74.5	102.9	105.4
	45.8	130.1	44.7	130.4	45.3	130.4	131.1
	71.3	106.2	70.1	106.6	70.8	106.4	109.9
	18.0	156.2	17.3	156.0	17.8	156.3	157.9
	76.9	100.9	75.7	101.4	76.3	101.2	103.9
	73.1	104.5	71.9	104.9	72.6	104.7	107.1
	15.7	158.3	15.0	158.2	15.5	158.4	157.7
	20.6	153.7	19.9	153.6	20.5	153.7	156.7
	76.4	101.4	75.3	101.7	76.0	101.5	102.2
	54.5	121.9	53.3	122.3	53.9	122.3	122.5
	20.0	154.3	19.3	154.2	19.8	154.4	153.3
	54.6	121.9	53.6	122.0	54.2	122.0	122.0
	82.9	95.2	81.7	95.7	82.4	95.5	98.4
	66.7	110.5	65.7	110.7	66.2	110.7	113.4
	19.4	154.8	18.7	154.7	19.2	155.0	157.5
15	138.1	43.5	137.3	43.6	137.6	43.5	45.9
	85.4	92.9	85.0	92.7	85.3	92.8	89.4
	90.9	87.8	90.3	87.7	90.7	87.7	84.6

	134.7	46.7	133.9	46.8	134.3	46.7	46.8
	92.3	86.4	91.8	86.3	92.1	86.4	76.5
	171.6	12.1	170.9	12.2	171.1	12.1	12.1
	2.1	171.1	1.4	170.9	2.6	170.6	170.5
	45.8	130.1	44.6	130.4	45.2	130.5	130.0
	44.0	131.8	43.0	131.9	43.6	132.0	130.0
	46.6	129.3	45.6	129.5	46.2	129.6	128.5
	43.5	132.3	42.5	132.4	43.0	132.5	133.1
	1.9	171.3	1.2	171.1	2.3	170.8	169.7
	159.2	23.7	158.3	24.0	158.6	23.9	20.6
	2.6	170.6	2.1	170.3	3.1	170.0	166.2
	162.1	20.9	161.2	21.2	161.7	21.0	22.1
	103.0	76.4	102.5	76.2	102.9	76.2	71.2
	44.0	131.8	43.1	131.9	43.7	131.9	133.9
	158.8	24.1	158.0	24.3	158.4	24.1	20.5
	42.7	133.0	42.0	132.9	42.6	132.9	124.1
	1.1	172.1	0.5	171.8	1.6	171.5	169.0
	164.3	18.9	163.3	19.3	163.7	19.0	13.7
	143.5	38.4	142.8	38.5	143.1	38.4	39.9
	145.3	36.7	144.5	36.9	144.8	36.8	39.2
	92.2	86.5	91.9	86.2	92.1	86.3	74.3
	158.4	24.4	157.8	24.5	158.1	24.3	24.1
	156.9	25.9	156.2	25.9	156.6	25.8	25.5
	2.9	170.3	2.2	170.1	3.3	169.8	170.0
	165.1	18.1	164.2	18.4	164.5	18.3	15.2
	95.7	83.3	94.9	83.4	95.3	83.3	74.1
	-31.2	202.3	-32.0	202.2	-31.0	202.1	197.5
	35.0	140.2	34.1	140.3	34.8	140.2	132.1
	4.2	169.1	3.6	168.9	4.6	168.6	170.2
	163.9	19.3	163.0	19.6	163.3	19.5	20.5
	31.9	143.2	31.3	142.9	31.8	143.1	136.9
	159.5	23.4	158.7	23.6	159.1	23.3	20.5
16	6.2	167.2	5.6	167.0	6.6	166.8	169.3
	49.4	126.7	48.3	127.0	48.9	127.0	125.3
	119.0	61.4	118.6	61.2	118.8	61.3	63.9
	112.5	67.5	111.9	67.4	112.2	67.5	66.8
	111.6	68.3	111.2	68.1	111.3	68.3	69.5
	86.6	91.8	86.3	91.4	86.5	91.6	90.7
	103.9	75.5	103.4	75.3	103.6	75.5	76.9
	105.2	74.4	104.7	74.2	104.9	74.3	75.0
	4.6	168.7	4.2	168.3	5.1	168.2	169.6
	50.9	125.3	49.8	125.6	50.4	125.6	124.8
	69.8	107.5	68.8	107.8	69.5	107.6	107.7
	31.9	143.1	31.0	143.2	31.6	143.3	145.1
	39.1	136.4	38.1	136.5	38.7	136.6	136.3
	34.3	140.8	33.6	140.8	34.2	140.8	144.2
	60.7	116.1	59.5	116.5	60.1	116.5	115.0
	3.8	169.5	3.4	169.1	4.3	168.9	170.5
	49.7	126.4	48.7	126.7	49.2	126.7	125.1
	62.9	114.0	61.8	114.4	62.4	114.3	113.7

	35.3	139.9	34.4	140.0	35.0	140.1	144.1
	43.6	132.2	42.6	132.3	43.2	132.3	135.9
	34.1	141.1	33.2	141.1	33.8	141.2	145.1
	71.7	105.8	70.6	106.1	71.3	106.0	107.2
	4.9	168.5	4.4	168.2	5.3	168.0	170.0
	50.2	126.0	49.1	126.3	49.6	126.3	125.2
	69.9	107.4	68.9	107.7	69.6	107.6	108.3
	31.6	143.4	30.8	143.4	31.3	143.5	145.1
	39.8	135.7	38.8	135.9	39.4	135.9	136.0
	34.4	140.8	33.6	140.7	34.3	140.7	144.2
	60.0	116.8	58.8	117.1	59.4	117.1	115.1
	61.1	115.8	60.0	116.1	60.6	116.0	113.9
	34.9	140.3	34.0	140.4	34.7	140.4	144.1
	43.4	132.4	42.4	132.5	43.1	132.5	136.0
	33.9	141.3	33.0	141.3	33.6	141.4	145.1
	70.8	106.6	69.8	106.8	70.4	106.8	107.2
17	113.3	66.7	112.6	66.8	112.9	66.9	70.8
	104.0	75.5	103.8	75.0	103.9	75.3	78.9
	88.7	89.8	88.4	89.4	88.7	89.6	93.7
	101.7	77.6	101.3	77.3	101.5	77.5	83.1
	106.4	73.2	106.1	72.9	106.2	73.1	77.8
	81.6	96.5	81.5	95.9	81.7	96.1	105.9
	105.7	73.9	105.4	73.5	105.5	73.8	77.6
	109.0	70.8	108.4	70.7	108.7	70.8	70.7
	103.2	76.2	102.8	75.9	103.1	76.0	77.7
	106.6	73.0	106.2	72.8	106.5	72.8	75.9
	-2.4	175.3	-3.0	175.0	-2.0	174.8	175.8
	148.1	34.1	147.2	34.4	147.5	34.3	32.2
	149.7	32.6	149.0	32.6	149.3	32.6	32.2
	106.3	73.3	105.9	73.1	106.0	73.3	71.5
	106.5	73.2	105.7	73.3	105.9	73.4	75.4
	105.7	73.8	105.3	73.6	105.4	73.8	76.3
	154.8	27.8	154.1	27.9	154.5	27.7	29.3
	78.0	99.9	77.6	99.5	77.8	99.8	100.5
	-48.3	218.4	-49.0	218.1	-47.9	218.0	213.7
	152.2	30.3	151.4	30.4	151.8	30.2	32.7
	111.0	68.9	110.5	68.7	110.6	69.0	70.9
	152.5	29.9	152.1	29.8	152.1	29.9	34.3
	115.2	65.0	114.8	64.7	115.0	64.9	63.4
	170.9	12.7	170.3	12.7	170.5	12.7	13.1
	8.6	165.0	7.9	164.9	8.9	164.6	167.8
	46.7	129.2	45.5	129.6	46.0	129.8	132.1
	45.6	130.3	44.6	130.5	45.2	130.4	130.8
	47.6	128.4	46.5	128.6	47.0	128.7	129.9
	41.6	134.1	40.6	134.2	41.1	134.3	134.4
	47.7	128.3	46.7	128.5	47.2	128.6	129.9
	45.9	130.0	45.0	130.1	45.5	130.2	130.8
	117.0	63.3	116.5	63.1	116.7	63.3	62.0
	120.5	60.0	120.1	59.8	120.2	60.0	62.3
18	23.2	151.3	22.5	151.2	23.0	151.3	142.8

	145.5	36.6	144.7	36.7	145.1	36.5	35.1
	102.1	77.2	101.6	77.1	101.8	77.2	76.3
	124.4	56.3	123.5	56.5	123.9	56.5	53.4
	-40.2	210.8	-41.0	210.6	-40.0	210.6	204.3
	47.5	128.4	46.6	128.6	47.3	128.5	127.1
	105.1	74.5	104.6	74.2	105.0	74.2	72.3
	155.6	27.0	154.9	27.1	155.3	27.0	26.6
	146.9	35.2	146.0	35.5	146.4	35.3	38.2
	150.7	31.7	149.9	31.9	150.1	31.8	29.8
	73.4	104.2	73.1	103.8	73.3	104.1	106.8
	-34.3	205.2	-35.0	205.0	-34.0	204.9	209.8
	122.7	57.9	121.9	58.1	122.1	58.2	53.8
	96.7	82.3	96.2	82.1	96.3	82.4	80.4
	98.7	80.4	98.1	80.3	98.4	80.4	78.5
	157.9	24.9	157.1	25.1	157.3	25.0	25.7
	157.6	25.2	156.9	25.3	157.1	25.2	24.7
	150.5	31.8	149.7	32.0	150.0	32.0	30.4
	128.8	52.2	128.2	52.2	128.3	52.4	49.3
	119.9	60.6	119.5	60.3	119.7	60.5	60.4
	146.0	36.0	145.3	36.2	145.5	36.2	31.2
	101.8	77.5	101.3	77.3	101.5	77.5	76.3
	95.8	83.1	95.3	83.0	95.6	83.1	80.6
	0.0	173.1	-0.7	172.9	0.5	172.5	171.8
	1.3	171.9	0.5	171.8	1.7	171.3	167.3
	164.8	18.4	164.1	18.5	164.5	18.3	21.6
	153.5	29.0	152.8	29.1	153.2	29.0	24.4
	168.8	14.7	168.1	14.8	168.3	14.7	13.2
19	18.4	155.8	17.8	155.6	18.4	155.7	157.4
	85.4	92.9	84.3	93.3	84.8	93.2	96.5
	17.3	156.8	16.6	156.7	17.1	156.9	155.5
	79.8	98.2	78.5	98.7	79.3	98.4	100.3
	19.0	155.2	18.5	154.9	19.1	155.0	153.8
	79.1	98.9	78.0	99.2	78.6	99.1	106.7
	154.6	28.0	153.9	28.1	154.2	28.0	28.6
	119.7	60.7	119.3	60.5	119.5	60.6	66.1
	103.2	76.2	102.7	76.1	103.1	76.1	79.0
	46.6	129.4	45.5	129.6	46.1	129.7	130.4
	64.0	113.0	63.0	113.3	63.6	113.2	115.8
	53.6	122.8	52.5	123.0	53.2	123.0	120.3
	63.9	113.1	62.8	113.4	63.4	113.4	115.1
	33.9	141.3	32.9	141.4	33.5	141.4	145.1
	32.4	142.6	31.5	142.7	32.1	142.8	145.1
	149.5	32.8	148.6	33.1	149.1	32.8	36.5
	111.9	68.0	111.5	67.8	111.7	67.9	72.6
	76.1	101.7	74.9	102.1	75.7	101.8	100.3
	17.6	156.6	17.1	156.2	17.6	156.4	155.6
	100.7	78.6	100.2	78.4	100.5	78.5	76.6
	16.4	157.6	15.8	157.4	16.4	157.6	158.0
	85.4	92.9	84.3	93.3	84.8	93.2	96.3
	17.2	156.9	16.5	156.7	17.0	157.0	157.2

	85.1	93.2	84.0	93.6	84.6	93.4	95.9
	45.6	130.3	44.5	130.6	45.1	130.6	132.0
	60.6	116.2	59.5	116.5	60.0	116.5	119.0
	64.5	112.5	63.5	112.7	64.1	112.7	115.1
	31.6	143.4	30.7	143.5	31.2	143.6	145.1
	64.2	112.8	63.2	113.1	63.7	113.0	115.3
	33.4	141.7	32.5	141.8	33.1	141.9	145.1
20	119.1	61.4	118.7	61.0	118.8	61.2	60.1
	156.1	26.6	155.5	26.6	155.7	26.6	26.9
	149.4	32.8	148.7	32.9	149.1	32.8	31.7
	133.2	48.1	132.4	48.3	132.7	48.2	48.2
	118.4	61.9	117.9	61.8	118.2	61.9	60.1
	30.9	144.0	30.3	143.9	30.8	144.0	142.2
	59.2	117.5	58.2	117.7	58.8	117.7	116.3
	46.8	129.1	45.9	129.3	46.4	129.3	128.8
	52.0	124.3	51.0	124.5	51.6	124.5	124.4
	52.7	123.6	51.8	123.7	52.4	123.7	122.8
	39.6	135.9	38.6	136.1	39.2	136.1	132.9
	128.7	52.3	127.9	52.4	128.1	52.5	52.3
	138.7	42.9	138.3	42.7	138.5	42.8	42.7
	131.0	50.1	130.8	49.7	130.9	49.9	50.3
	129.0	52.0	128.6	51.8	128.8	51.8	52.9
	25.3	149.3	24.4	149.3	25.1	149.4	140.0
	44.5	131.3	43.9	131.1	44.5	131.1	127.9
	116.2	64.0	115.8	63.8	116.0	63.9	64.8
	101.3	78.0	100.9	77.8	101.1	77.9	77.6
	138.6	43.0	138.0	43.0	138.3	42.9	42.8
	1.2	171.9	0.6	171.7	1.6	171.5	170.3
21	48.8	127.2	47.9	127.4	48.4	127.4	128.0
	51.5	124.8	50.5	124.9	51.1	124.9	125.3
	53.8	122.6	52.9	122.7	53.5	122.6	122.3
	31.3	143.7	30.5	143.7	31.0	143.8	137.4
	34.8	140.4	34.2	140.2	34.7	140.3	141.4
	60.4	116.4	59.4	116.6	60.1	116.5	117.9
	126.8	54.1	126.1	54.1	126.2	54.3	52.8
	119.2	61.2	118.6	61.1	118.9	61.2	63.7
	2.3	170.9	1.9	170.5	2.9	170.3	167.7
	135.3	46.1	134.4	46.3	134.8	46.2	47.8
	127.1	53.8	126.6	53.6	126.8	53.7	57.5
	135.3	46.1	134.5	46.2	134.9	46.1	39.0
	137.9	43.6	137.6	43.3	137.8	43.4	36.5
	122.3	58.3	122.1	57.9	122.2	58.1	54.1
	112.7	67.3	112.5	66.9	112.5	67.1	66.3
	162.2	20.9	161.6	20.9	161.6	21.0	23.8
	152.5	30.0	151.8	30.0	152.1	30.0	29.3
	169.3	14.2	168.7	14.3	169.0	14.1	13.7
	54.8	121.7	54.1	121.6	54.7	121.5	117.7
	27.1	147.6	26.3	147.6	26.9	147.7	140.5
	123.0	57.7	122.5	57.5	122.7	57.6	52.3
	113.2	66.8	112.7	66.7	113.0	66.7	69.5

	131.7	49.4	131.1	49.5	131.2	49.6	47.9
	111.3	68.6	110.8	68.5	111.1	68.5	69.4
	22.7	151.7	22.1	151.5	22.7	151.6	150.0
	127.9	53.0	127.1	53.2	127.4	53.2	51.8
	39.8	135.7	38.9	135.8	39.5	135.8	134.3
	71.1	106.4	70.2	106.5	70.8	106.4	108.3
	48.9	127.2	48.0	127.3	48.5	127.3	128.2
	59.1	117.6	58.2	117.7	58.8	117.7	119.8
	53.5	122.9	52.6	122.9	53.3	122.9	122.2
	151.9	30.6	151.1	30.7	151.5	30.5	27.7
	152.9	29.6	152.3	29.6	152.5	29.5	28.5
	117.9	62.5	117.3	62.3	117.7	62.3	61.7
	127.3	53.6	127.2	53.1	127.2	53.4	53.7
	140.3	41.4	139.8	41.3	140.1	41.3	41.2
	122.3	58.3	122.0	58.0	122.1	58.2	58.1
	35.5	139.7	34.6	139.8	35.3	139.7	133.8
	53.4	122.9	52.7	122.9	53.3	122.9	122.2
	170.7	12.9	169.9	13.1	170.2	12.9	13.0
22	141.5	40.3	140.6	40.5	140.9	40.5	40.0
	31.0	144.0	30.4	143.8	30.9	143.9	143.4
	76.4	101.3	75.4	101.7	76.0	101.5	102.7
	48.7	127.4	47.7	127.6	48.3	127.5	129.9
	61.5	115.4	60.3	115.7	61.2	115.4	118.0
	41.5	134.1	40.7	134.2	41.1	134.3	136.5
	159.4	23.5	158.8	23.5	158.9	23.5	27.9
	154.6	28.0	153.9	28.1	154.2	28.0	27.3
	25.8	148.8	25.2	148.7	25.7	148.8	146.8
	-14.8	187.0	-15.7	187.0	-14.8	186.9	188.3
	20.9	153.4	19.9	153.6	20.5	153.7	147.1
	39.5	136.0	38.4	136.3	39.2	136.1	135.2
	24.6	150.0	23.7	150.0	24.4	150.0	153.8
	57.8	118.8	57.0	118.9	57.6	118.8	119.7
	67.0	110.2	66.0	110.5	66.6	110.3	111.5
	68.4	108.9	67.4	109.1	68.0	109.1	108.3
	-11.2	183.5	-12.1	183.6	-11.2	183.5	184.4
	154.6	28.0	153.8	28.2	153.9	28.2	28.8
	48.1	128.0	47.1	128.1	47.7	128.2	128.0
	58.1	118.6	57.1	118.8	57.6	118.8	119.6
	55.9	120.7	54.9	120.8	55.5	120.8	121.8
	40.1	135.4	39.3	135.4	39.9	135.5	137.3
	53.7	122.7	53.1	122.5	53.7	122.5	127.6
	62.6	114.3	61.8	114.4	62.4	114.3	111.6
	55.6	120.9	54.8	120.9	55.3	120.9	122.5
	56.3	120.2	55.5	120.3	56.1	120.2	120.8
	66.1	111.0	65.1	111.3	65.7	111.2	112.6
	36.1	139.2	35.2	139.2	35.7	139.4	133.4
	57.6	119.0	56.7	119.2	57.2	119.2	120.5
	55.0	121.5	54.1	121.6	54.6	121.7	122.6
	158.3	24.5	157.5	24.7	157.8	24.6	25.8
	167.9	15.5	167.2	15.6	167.4	15.5	17.8

23	135.6	45.9	135.1	45.7	135.3	45.7	46.9
	120.1	60.3	119.7	60.1	119.9	60.2	55.1
	150.0	32.3	149.5	32.2	149.7	32.2	30.2
	106.7	72.9	106.5	72.5	106.6	72.8	71.1
	4.2	169.1	3.5	169.0	4.5	168.8	171.6
	129.3	51.7	128.8	51.6	128.9	51.8	52.9
	143.2	38.7	142.6	38.6	142.8	38.7	41.4
	27.1	147.6	26.5	147.4	27.3	147.3	154.6
	128.7	52.3	128.3	52.0	128.4	52.2	49.3
	136.1	45.3	135.6	45.3	135.9	45.2	37.3
	148.4	33.8	147.9	33.7	148.2	33.7	23.7
	-0.5	173.5	-1.0	173.2	-0.1	173.0	172.0
	9.0	164.6	8.4	164.4	9.2	164.3	168.1
	3.0	170.2	2.4	170.0	3.4	169.8	172.4
	128.5	52.5	127.9	52.5	128.1	52.6	55.4
	151.3	31.1	150.9	30.9	151.1	30.9	29.8
	68.8	108.5	67.8	108.7	68.4	108.7	105.9
	123.6	57.1	123.1	56.9	123.3	57.1	57.0
	-1.9	174.8	-2.5	174.6	-1.5	174.4	173.6
	137.3	44.2	137.0	43.9	137.1	44.1	40.0
	120.5	60.0	120.0	59.8	120.1	60.0	63.3
	1.3	171.8	0.7	171.6	1.6	171.4	173.1
	115.7	64.5	115.2	64.3	115.4	64.5	60.0
	48.3	127.7	47.6	127.6	48.1	127.8	135.9
	24.8	149.7	24.1	149.7	24.9	149.5	157.5

^[a] Parameters of linear regression models are presented in Table 2 in main text.

^[b] For the references to the experimental works, please, see the main text.