Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Table A1. Coordinates and total energy for 1-decene calculated at MP2/def2-TZVP level of theory

1-decene			
atom	x	y	z
C	-0.682288	2.043939	5.355662
C	-1.377988	1.659471	4.286066
H	-1.011243	1.809054	6.359329
H	0.236963	2.608363	5.250630
C	-0.976065	1.920930	2.872618
H	-2.294939	1.093229	4.430791
H	-0.088730	2.560187	2.855381
H	-1.774378	2.466721	2.357942
C	-0.694801	0.629746	2.108324
C	-0.324720	0.874620	0.654545
H	-1.576533	-0.018059	2.155342
H	0.114510	0.089685	2.609310
H	0.554108	1.526904	0.609774
C	-0.037991	-0.407782	-0.109909
H	-1.137851	1.417155	0.160207
H	0.774566	-0.950095	0.385342
H	-0.916851	-1.059984	-0.064759
C	0.333067	-0.165130	-1.564176
C	0.619444	-1.447021	-2.329147
H	1.211949	0.487100	-1.609021
H	-0.479556	0.377697	-2.059005
H	1.431591	-1.990486	-1.834026
C	0.991566	-1.206286	-3.783575
H	-0.259536	-2.099346	-2.284769
C	1.274884	-2.498036	-4.534843
H	0.179820	-0.663206	-4.276505
H	1.869211	-0.554550	-3.826242
H	0.401334	-3.152159	-4.526208
H	1.540203	-2.309785	-5.575697
H	2.100250	-3.042879	-4.073378
E_0	-1030001.218 kJ/mol		

Table A2. Coordinates and total energy for trans-2-decene calculated at MP2/def2-TZVP level of theory

Trans-2-decene			
atom	x	y	z
C	-0.632170	2.626075	5.160870
C	-0.522400	1.443596	4.255048
H	-1.039339	2.341003	6.133394
H	-1.280183	3.389880	4.730919
C	-1.136984	1.331484	3.075995
H	0.104224	0.620644	4.591667
H	-1.763795	2.153595	2.734220
C	-1.007845	0.162528	2.156674
C	-0.351215	0.540405	0.831396
H	-1.998433	-0.257482	1.949349
H	-0.424635	-0.624527	2.643648
H	0.647662	0.940247	1.031969
C	-0.251116	-0.630216	-0.133055
H	-0.921495	1.349945	0.363490
H	0.315701	-1.440168	0.338777
H	-1.253754	-1.026819	-0.326379
C	0.406202	-0.259695	-1.452929
C	0.508109	-1.429364	-2.418462
H	1.408190	0.137797	-1.258755
H	-0.160992	0.550205	-1.924307
H	1.075459	-2.239498	-1.947390
C	1.164695	-1.060264	-3.739285
H	-0.493935	-1.827378	-2.612413
C	1.259427	-2.240525	-4.693948
H	0.597203	-0.251044	-4.208285
H	2.164938	-0.662540	-3.543944
H	0.268281	-2.636161	-4.922303
H	1.731928	-1.960698	-5.636109
H	1.845029	-3.049797	-4.254417
H	0.346907	3.073460	5.345484
E_0	-1030011.8686 kJ/mol		

Table A 3. Coordinates and total energy for trans-3-decene calculated at MP2/def2-TZVP level of theory

Trans-3-decene			
atom	x	y	z
C	-1.866927	1.371366	4.607362
C	-0.382681	1.648520	4.381790
H	-2.155847	0.430591	4.137765
H	-2.479657	2.162717	4.172698
C	-0.057800	1.773665	2.929483
H	0.218539	0.848483	4.820294
H	-0.543917	2.585137	2.389633
C	0.754832	0.956098	2.256282
C	1.036519	1.048356	0.793387
H	1.237281	0.142142	2.795396
H	2.115366	1.146398	0.628648
C	0.535591	-0.176740	0.032612
H	0.569155	1.949628	0.385989
H	0.982616	-1.078278	0.464957
H	-0.545531	-0.266045	0.178055
C	0.850455	-0.118910	-1.453367
C	0.348344	-1.334217	-2.215916
H	1.933327	-0.026744	-1.590608
H	0.406651	0.786218	-1.881969
H	0.792124	-2.239454	-1.787327
C	0.660668	-1.279016	-3.703013
H	-0.734355	-1.426679	-2.077575
C	0.152167	-2.501454	-4.451629
H	0.217267	-0.374363	-4.129426
H	1.742170	-1.186293	-3.839404
H	-0.930111	-2.597406	-4.349228
H	0.382941	-2.447747	-5.516087
H	0.603516	-3.413777	-4.057953
H	-2.103062	1.310648	5.670506
H	-0.109064	2.572887	4.899890
E_0	-1030011.9642 kJ/mol		

Table A 4. Coordinates and total energy for trans-4-decene calculated at MP2/def2-TZVP level of theory

Trans-4-decene			
atom	x	y	z
C	-1.241639	1.743319	3.988559
C	-0.650830	2.111484	2.629731
H	0.229164	2.744389	2.791131
H	-1.373216	2.709461	2.066243
C	-0.268588	0.907930	1.834050
C	-0.827467	0.550798	0.675339
C	-0.444413	-0.652036	-0.121183
H	0.277406	-1.250347	0.442459
H	-1.324343	-1.284406	-0.284198
C	0.147533	-0.279952	-1.478331
C	0.504843	-1.494135	-2.319686
H	1.038899	0.334830	-1.319162
H	-0.566941	0.344787	-2.024870
H	1.215407	-2.120127	-1.768884
C	1.100195	-1.129879	-3.670530
H	-0.391067	-2.105837	-2.472536
C	1.453044	-2.353987	-4.501515
H	0.389768	-0.504094	-4.218691
H	1.994128	-0.518717	-3.515623
H	0.568113	-2.964363	-4.689578
H	1.878590	-2.077348	-5.466697
H	2.181588	-2.979161	-3.982475
H	-2.131379	1.128414	3.830223
H	-0.526550	1.120264	4.533411
C	-1.593044	2.969990	4.815700
H	-2.017054	2.695072	5.781955
H	-0.708047	3.581265	5.000638
H	-2.322971	3.593055	4.296062
H	-1.603829	1.187790	0.254016
H	0.508042	0.270944	2.254890
E_0	-1030012.4605 kJ/mol		

Table A5. Coordinates and total energy for trans-5-decene calculated at MP2/def2-TZVP level of theory

Trans-5-decene			
atom	x	y	z
C	-1.242869	1.754251	4.000300
C	-0.648350	2.123512	2.643857
H	0.233661	2.752891	2.807357
H	-1.367423	2.724045	2.079053
C	-0.268579	0.919144	1.847968
C	-0.827219	0.563967	0.688539
C	-0.447526	-0.640421	-0.107357
H	0.271365	-1.241107	0.457513
H	-1.329622	-1.269642	-0.271010
C	0.147213	-0.271186	-1.463711
C	0.500407	-1.486557	-2.305875
H	1.041413	0.339661	-1.304566
H	-0.563636	0.356641	-2.011651
H	1.205875	-2.113706	-1.752808
C	1.097466	-1.107168	-3.652308
H	-0.398117	-2.092055	-2.457378
H	1.346687	-1.987763	-4.245341
H	0.397575	-0.502116	-4.231129
H	2.010066	-0.523196	-3.522028
H	-2.136865	1.143070	3.841288
H	-0.531770	1.126749	4.548287
C	-1.596445	2.969621	4.842304
H	-0.698111	3.575421	4.993728
H	-2.302110	3.596474	4.289155
H	-1.601041	1.203558	0.266469
H	0.505213	0.279540	2.270073
C	-2.193386	2.590222	6.188787
H	-2.443091	3.470821	6.781610
H	-3.105681	2.005756	6.058582
H	-1.493221	1.985656	6.767782
E_0	-1030012.4967 kJ/mol		

Table A6. Coordinates and total energy for cis-2-decene calculated at MP2/def2-TZVP level of theory

Cis-2-decene			
atom	x	y	z
C	0.535360	0.536530	4.772196
C	-0.505303	1.449260	4.208267
H	1.489972	1.058747	4.866717
H	0.697241	-0.345524	4.156221
C	-1.222545	1.258661	3.095526
H	-0.685345	2.362211	4.768574
H	-1.928849	2.036413	2.816680
C	-1.126899	0.104147	2.151392
C	-0.378966	0.479273	0.872942
H	-2.135544	-0.227466	1.884509
H	-0.633626	-0.749490	2.619801
H	0.636822	0.790254	1.136885
C	-0.323130	-0.657600	-0.134294
H	-0.859511	1.350517	0.415621
H	0.154353	-1.528199	0.328549
H	-1.342893	-0.964660	-0.390671
C	0.426123	-0.290107	-1.405138
C	0.483943	-1.425664	-2.414057
H	1.445281	0.017690	-1.147656
H	-0.051587	0.580578	-1.867176
H	0.961698	-2.296626	-1.952202
C	1.232650	-1.059330	-3.685731
H	-0.535322	-1.733838	-2.671440
C	1.282186	-2.205276	-4.684577
H	0.754512	-0.189429	-4.145612
H	2.249960	-0.751174	-3.426969
H	0.275740	-2.510694	-4.975827
H	1.821759	-1.927824	-5.590723
H	1.779776	-3.075539	-4.253196
H	0.257549	0.203724	5.774855
E_0	-1030007.0515 kJ/mol		

Table A7. Coordinates and total energy for cis-3-decene calculated at MP2/def2-TZVP level of theory

Cis-3-decene			
atom	x	y	z
C	0.438687	0.506103	4.841911
C	-0.646283	1.378692	4.299203
C	1.790349	1.217668	4.805329
H	0.502498	-0.428546	4.284219
C	-1.354825	1.182917	3.180896
H	-0.847241	2.282084	4.870505
H	-2.082038	1.943603	2.908341
C	-1.216418	0.045875	2.220432
C	-0.423099	0.450236	0.978325
H	-2.211467	-0.288105	1.909700
H	-0.732781	-0.812238	2.690816
H	0.580101	0.761189	1.287190
C	-0.321426	-0.666472	-0.047662
H	-0.890733	1.328048	0.520188
H	0.141786	-1.543699	0.417188
H	-1.328637	-0.972935	-0.350185
C	0.475749	-0.270791	-1.279965
C	0.580700	-1.385506	-2.308771
H	1.482498	0.036602	-0.976665
H	0.012610	0.606657	-1.744306
H	1.043127	-2.260981	-1.843406
C	1.380558	-0.973860	-3.535186
H	-0.425444	-1.691630	-2.610110
H	0.203791	0.240675	5.877150
H	2.068887	1.456693	3.778353
H	1.752251	2.153315	5.365205
H	2.576605	0.598117	5.238752
H	2.397101	-0.689026	-3.258548
H	0.920205	-0.116789	-4.029670
H	1.447428	-1.782725	-4.263517
E_0	-1030007.1366 kJ/mol		

Table A8. Coordinates and total energy for cis-4-decene calculated at MP2/def2-TZVP level of theory

Cis-4-decene			
atom	x	y	z
C	-0.618566	0.650647	1.977976
C	-1.232932	0.423052	0.810918
C	-0.942280	-0.706374	-0.127839
H	-0.632727	-1.599285	0.420121
H	-1.854712	-0.974538	-0.668016
C	0.144200	-0.340448	-1.138715
C	0.423350	-1.451850	-2.136528
H	1.061308	-0.093908	-0.593808
H	-0.150224	0.569388	-1.672048
H	0.708879	-2.360925	-1.595532
C	1.515925	-1.097194	-3.132804
H	-0.497347	-1.692459	-2.679277
C	1.786478	-2.217306	-4.125572
H	1.229809	-0.188421	-3.670412
H	2.433740	-0.857157	-2.587952
H	0.888362	-2.454131	-4.698554
H	2.571905	-1.948502	-4.832709
H	2.098876	-3.126869	-3.609686
H	-1.979623	1.141690	0.484512
H	-0.909865	1.533564	2.541820
H	3.840937	0.349702	3.322139
C	0.476191	-0.169442	2.576980
H	1.636722	1.526143	3.215322
H	2.645808	-0.509289	4.293575
H	2.074241	0.911091	1.635006
H	0.196564	-0.471433	3.592531
C	2.907674	-0.212481	3.276480
H	3.093864	-1.122683	2.703619
H	0.632700	-1.087444	2.006385
C	1.791624	0.605342	2.645906
E_0	-1030008.2208 kJ/mol		

Table A9. Coordinates and total energy for cis-5-decene calculated at MP2/def2-TZVP level of theory

Cis-5-decene			
atom	x	y	z
C	-1.231880	-3.962838	3.363300
C	-1.146138	-2.448685	3.247825
C	-0.436139	-2.002755	1.979859
H	-0.955457	-2.406947	1.104887
H	0.574930	-2.423121	1.959671
C	-0.355451	-0.482608	1.846618
C	0.396059	-0.075794	0.620975
H	0.146862	-0.078445	2.731646
H	-1.366182	-0.070250	1.844217
C	-0.122144	0.408710	-0.514147
C	-1.567130	0.650251	-0.807611
C	-2.136742	-0.411730	-1.747210
H	-1.683336	1.632959	-1.276364
H	-2.157921	0.668927	0.110124
H	-1.533139	-0.450069	-2.660210
C	-3.591425	-0.161448	-2.110466
H	-2.039027	-1.393067	-1.271748
C	-4.151094	-1.231122	-3.035622
H	-4.187708	-0.116967	-1.194151
H	-3.679615	0.820698	-2.584299
H	-5.194305	-1.039464	-3.289024
H	-3.583873	-1.274754	-3.966904
H	-4.096378	-2.216030	-2.568813
H	-0.235894	-4.408788	3.371590
H	-1.742269	-4.269286	4.276989
H	-1.776837	-4.386772	2.518167
H	1.471263	-0.233418	0.655333
H	0.564050	0.614874	-1.331905
H	-2.152416	-2.019441	3.265676
H	-0.620804	-2.040476	4.116328
E_0	-1030008.3348 kJ/mol		

Table B1. Relative enthalpies at 378 K with respect to 1-decene. All values are given in kJ/mol.

	MP2	HF	M06-2X	B3LYP-D3	B3LYP	BP86-D3	BP86
1-decene	0	0	0	0	0	0	0
Trans-2-decene	-11.00	-10.02	-11.65	-11.75	-13.68	-13.05	-15.32
Trans-3-decene	-10.71	-9.40	-10.14	-10.66	-12.72	-11.68	-14.11
Trans-4-decene	-11.30	-9.77	-10.71	-10.54	-12.74	-11.51	-14.08
Trans-5-decene	-11.33	-9.76	-10.21	-10.64	-12.84	-11.66	-14.22
Cis-2-decene	-5.67	-2.17	-6.16	-6.39	-7.18	-8.38	-9.43
Cis-3-decene	-5.43	-0.88	-4.33	-5.08	-5.68	-6.86	-7.77
Cis-4-decene	-6.62	-1.27	-4.60	-5.81	-6.07	-7.77	-8.19
Cis-5-decene	-6.67	-1.26	-4.48	-5.67	-5.98	-7.77	-8.09

Table B2. Calculated entropies at 378 K. All values are given in kJ/mol K.

	MP2	HF	M06-2X	B3LYP-D3	B3LYP	BP86-D3	BP86
1-decene	0.53636	0.52798	0.52632	0.54102	0.54108	0.5457	0.54765
Trans-2-decene	0.53914	0.52958	0.53947	0.54734	0.54779	0.55376	0.55669
Trans-3-decene	0.5382	0.52962	0.53811	0.54841	0.54825	0.55478	0.55705
Trans-4-decene	0.53966	0.52951	0.5439	0.54057	0.54084	0.54576	0.54735
Trans-5-decene	0.53405	0.52378	0.52326	0.53702	0.53704	0.54254	0.54427
Cis-2-decene	0.54613	0.53399	0.54598	0.55502	0.55523	0.55966	0.56628
Cis-3-decene	0.54736	0.5341	0.53756	0.55584	0.5473	0.56139	0.55519
Cis-4-decene	0.54424	0.53415	0.53631	0.55303	0.5524	0.55615	0.55935
Cis-5-decene	0.54032	0.52838	0.52141	0.54204	0.5431	0.55626	0.54954

Table C. Relative Gibbs free energies at 298.15 K with respect to 1-decene. Values obtained after scaling of frequencies. λ is the used scaling factor. All values are given in kJ/mol.

	MP2 λ=0.9946	M06-2X λ=0.9871	B3LYP λ=1.0044	BP86 λ=1.0337
1-decene	0	0	0	0
Trans-2-decene	-11.83	-15.58	-15.70	-18.09
Trans-3-decene	-11.26	-13.66	-14.87	-16.96
Trans-4-decene	-12.28	-15.97	-12.68	-14.01
Trans-5-decene	-12.35	-11.02	-13.37	-14.96
Cis-2-decene	-8.60	-12.03	-11.42	-15.05
Cis-3-decene	-8.71	-7.70	-7.54	-10.06
Cis-4-decene	-8.97	-7.58	-9.45	-11.71
Cis-5-decene	-9.57	-4.75	-8.31	-10.40

Table D. Number of QM optimized conformers in an energy window of 5 kJ/mol for each of the nine positional and geometrical decene isomers; calculated entropy without (S (single conformer)) and with correction for mixing (Scorr); calculated Gibbs free energy differences with respect to 1-decene at 298.15 K including the corrected entropy; energy and Gibbs free energy differences after Boltzmann weighting of conformers. MUE = mean unsigned error with respect to experiment. Calculations done on B3LYP-D3 level of theory. S given in J/K mol, ΔG given in kJ/mol.

	n (5 kJ/mol)	S (single conformer) (298.15 K)	S_{corr} (298.15 K)	ΔG with Scorr (298.15 K)	Boltzmann-weighted ΔE (0 K)	Boltzmann-weighted ΔG (378.15 K)
1-decene	51	486.9	519.6	0.0	0.00	0.00
Trans-2-decene	44	492.7	524.1	-13.3	-12.12	-15.75
Trans-3-decene	66	493.8	528.6	-13.5	-11.70	-15.26
Trans-4-decene	52	486.1	519.0	-10.5	-12.68	-12.68
Trans-5-decene	27	488.3	515.7	-9.6	-12.92	-11.71
Cis-2-decene	37	500.5	530.5	-9.8	-7.98	-13.82
Cis-3-decene	13	501.4	522.7	-6.1	-8.41	-14.08
Cis-4-decene	20	498.6	523.5	-7.1	-9.59	-14.22
Cis-5-decene	24	493.4	519.8	-5.8	-9.69	-9.92
MUE					2.60	5.39

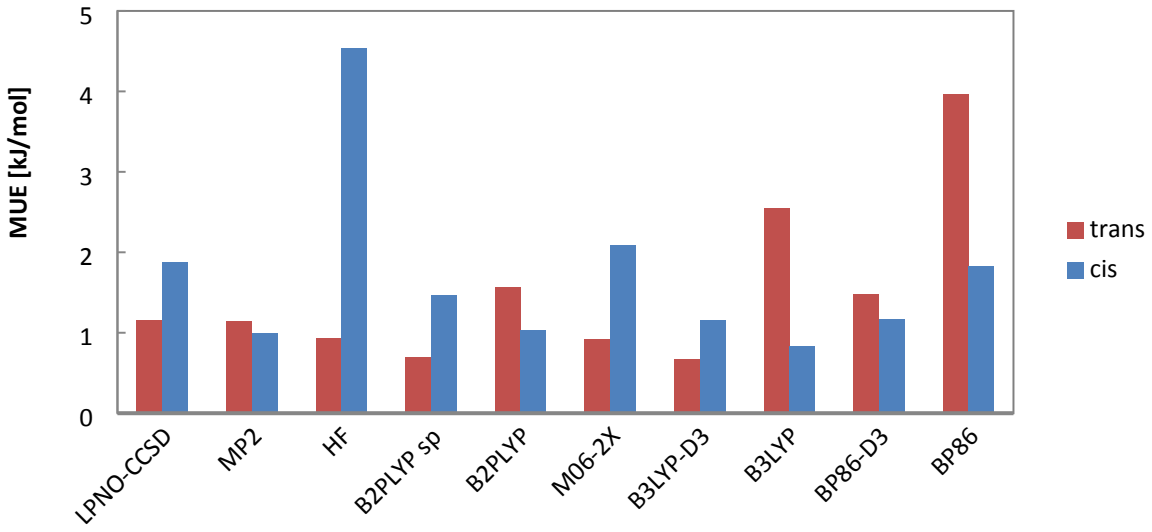

Figure A. Mean unsigned errors for relative energies over all *cis* and *trans* linear decene isomers using def2-TZVP basis set.

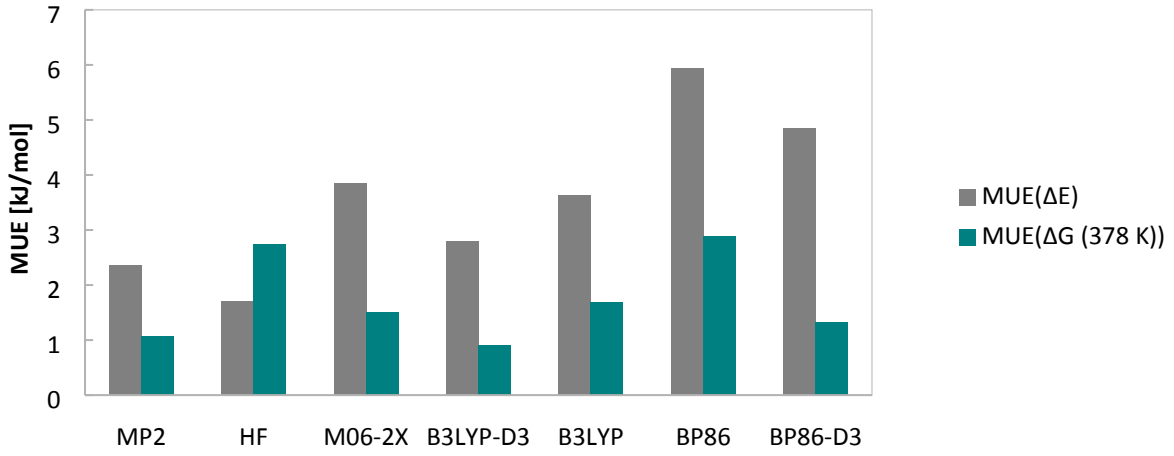

Figure B. Mean unsigned errors for relative electronic energies (grey) and relative Gibbs free energies at 378 K (green) over linear decene isomers using def2-TZVP basis set.