

		Atstumo pokytis					
		0%	10%	15%	-10%	-15%	Tinka
Molekulės būsenos energija (Ha)	beh2	-15.5571	-15.5570	-15.5476	-15.5151	-15.4672	+
	bf3	-318.5031	-318.3820	-318.3186	-318.5989	-318.6242	-
	bh3	-25.8708	-25.7784	-25.7311	-25.9523	-25.9847	-
	brf3	-2838.3956	-2838.3974	-2838.4054	-2838.2932	-2838.1460	-
	c2h2	-75.8505	-75.8231	-75.7359	-75.8012	-75.6825	+
	c2h3n	-130.2673	-130.2574	-130.2231	-130.2596	-130.2101	+
	c2h4	-77.1151	-77.0809	-77.0494	-77.0933	-77.0507	+
	c2h6	-78.3045	-78.2647	-78.2303	-78.2892	-78.2514	+
	caffeine	-667.6840	-667.6391	-667.5458	-667.4700	-667.2339	+
	ccln	-545.6557	-545.5814	-545.5675	-545.4721	-545.1529	+
	cf2cc12	-1180.0029	-1179.9566	-1179.9164	-1179.9036	-1179.7744	+
	cf4	-429.5829	-429.5582	-429.5254	-429.5154	-429.4200	+
	ch2cl2	-947.7127	-947.6869	-947.6608	-947.6854	-947.6424	+
	ch5n	-94.0309	-94.0118	-93.9860	-93.9877	-93.9316	+
	cl2o	-982.8846	-982.8758	-982.8574	-982.8279	-982.7582	+
	clf3	-748.2083	-748.2424	-748.2661	-748.0596	-747.8792	-
	co2	-185.0878	-185.0478	-185.0054	-184.9202	-184.6733	+
	cos	-504.4016	-504.3860	-504.3630	-504.3011	-504.2018	+
	cs2	-823.7079	-823.7304	-823.7081	-823.6067	-823.4863	-
	ethanol	-152.1252	-152.0929	-152.0556	-152.0822	-152.0252	+
	etoh	-152.1242	-152.0966	-152.0622	-152.0789	-152.0228	+
	form	-112.3547	-112.3281	-112.3025	-112.3307	-112.2905	+
	geh4	-2054.0825	-2054.0477	-2054.0216	-2054.0919	-2054.0794	-
	h2	-1.1373	-1.1328	-1.1284	-1.1326	-1.1255	+
	h2s	-394.3114	-394.2923	-394.2753	-394.2985	-394.2744	+
	h2se	-2374.6923	-2374.6753	-2374.6593	-2374.6794	-2374.6565	+
	h3po4	-633.8805	-633.8875	-633.8688	-633.7992	-633.7229	-
	hbr	-2545.2273	-2545.2097	-2545.1960	-2545.2216	-2545.2043	+
	hcl	-455.1364	-455.1262	-455.1155	-455.1192	-455.0947	+
	hcn	-91.6769	-91.6420	-91.6115	-91.6413	-91.6055	+
	hn3	-161.6471	-161.6567	-161.6463	-161.5778	-161.5107	-
	hno2	-201.8532	-201.9051	-201.8925	-201.6292	-201.4018	-
	hno3	-275.7012	-275.7258	-275.7190	-275.6111	-275.5353	-
	i2	-13701.4062	-13701.3938	-13701.3777	-13701.3603	-13701.2942	+
	icl	-7305.2693	-7305.2616	-7305.2472	-7305.2171	-7305.1494	+
	n2	-107.5009	-107.4791	-107.4570	-107.4214	-107.3214	+
	nocl	-582.0630	-582.0910	-582.0820	-582.0240	-581.9647	-
	p4s3	-2527.3133	-2527.2612	-2527.2055	-2527.2415	-2527.1344	+
	pcl5	-2609.7935	-2609.7853	-2609.7595	-2609.6396	-2609.4225	+
	propanol	-190.7029	-190.6635	-190.6181	-190.6515	-190.5841	+
	sbh3	-6253.0811	-6253.0526	-6253.0305	-6253.0784	-6253.0609	+
	seocl2	-3356.4236	-3356.4198	-3356.4027	-3356.3336	-3356.2261	+
	snh4	-5965.6168	-5965.5871	-5965.5619	-5965.6171	-5965.5971	-
	ticl4	-2658.5552	-2658.5040	-2658.4593	-2658.5065	-2658.4145	+