Artificial bees collect diverse conformers of small organic molecules

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Supplementary Information

Here we would like to provide additional information to the main text of the article to clarify all the discussed issues more thoroughly.

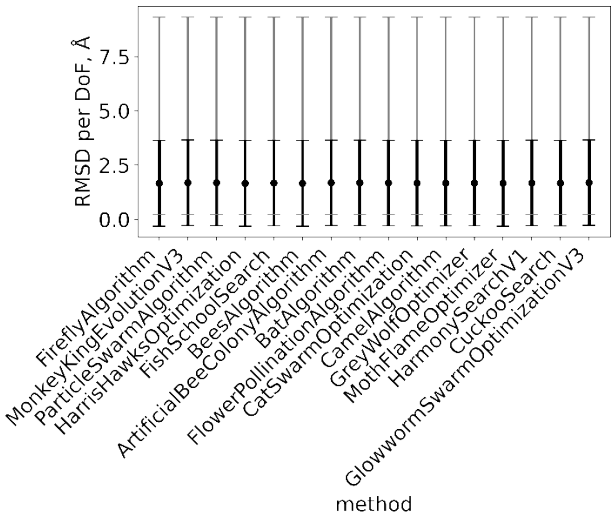

Fig. S1. RMSD of gminorg database geometries and the structures obtained by different approaches optimization.

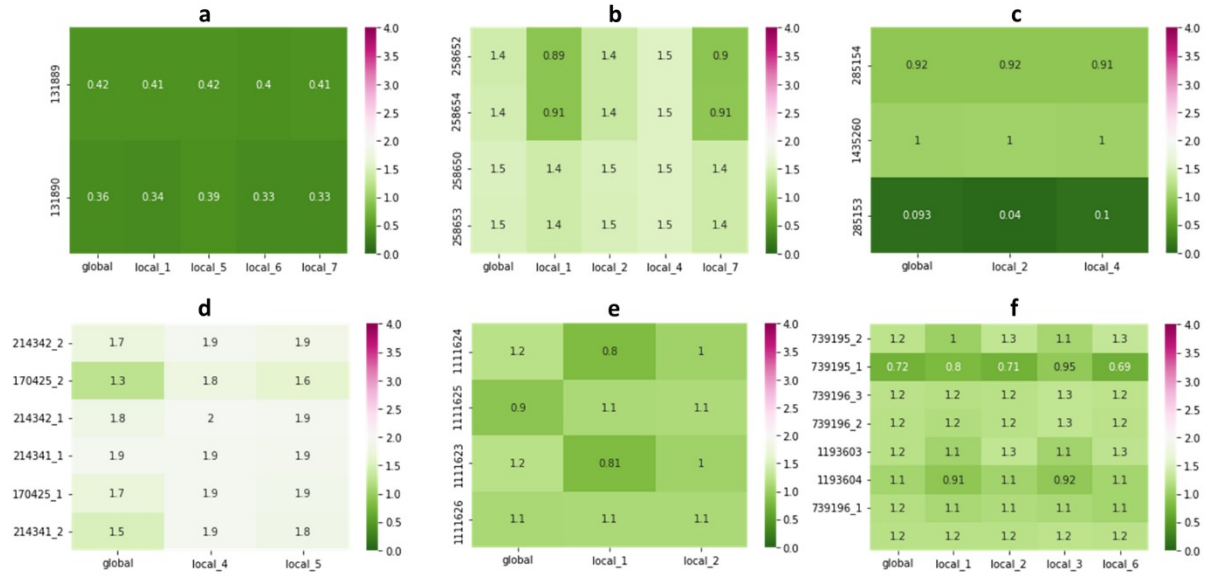

Fig. S2. RMSD per DoF for crystal database geometries (molecules a-f).

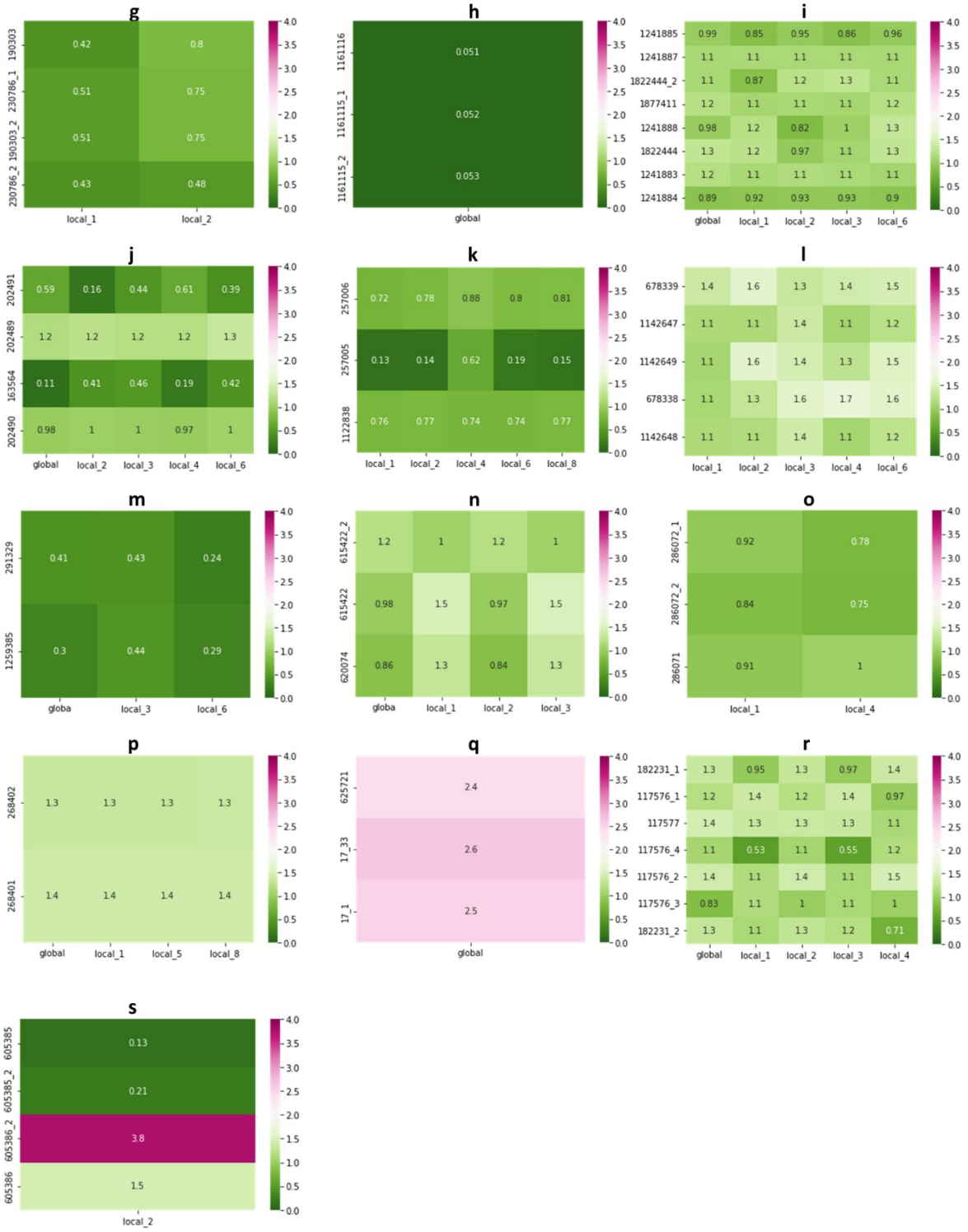

Fig. S3. RMSD per DoF for crystal database geometries (molecules g-s).

Table S1. Operation time for global conformation search for the ABC and CREST approaches.

Molecule	ABC	CREST	DOF	Molecule	ABC	CREST	DOF	Molecule	ABC	CREST	DOF
757	40.949	16	1	1130688	362.401	267	3	CID137997	82.972	63	3
7530	42.360	53	1	1135600	286.237	303	1	CID15277	796.824	319	4
7674	68.707	61	2	1136851	337.471	611	4	CID18724	95.164	134	1
7945	187.180	155	4	1137474	194.954	317	3	CID220186	69.184	54	1
7997	120.778	51	3	1138766	163.906	458	4	CID2272	66.571	142	2
10882	183.714	171	5	1140079	967.155	449	4	CID23514418	89.088	75	2
11583	75.524	77	3	1145908	245.246	569	3	CID2724518	32.350	46	1
12348	257.579	191	5	1157508	663.396	925	4	CID43683	53.299	40	1
69391	40.079	29	2	1160770	4352.572	2226	7	CID6570	32.539	22	1
130547	186.175	298	3	1175256	659.650	975	5	CID68010	72.680	55	2
145751	54.535	29	2	1191799	748.633	1405	4	CID68120	97.590	66	1
185472	229.264	109	3	1201580	270.868	409	1	CID69636	43.292	31	1
195802	107.99	141	2	1286889	245.695	272	4	CID70967	68.875	79	1
262857	133.449	84	2	1306802	868.311	1557	4	CID7166	141.480	93	3
751100	86.311	49	1	CCDC153210	71.820	73	2	CID751	51.592	27	2
757095	1339.090	3295	6	CCDC231363	47.232	28	2	CID97375	110.083	96	2
1110121	1172.495	2589	6	CCDC682820	106.317	58	2	CID9975	32.827	43	1
1124382	393.646	982	3	CID11084236	59.513	64	2				
1128171	2953.685	5759	6	CID11169919	2741.755	2618	4				