Supplementary figures

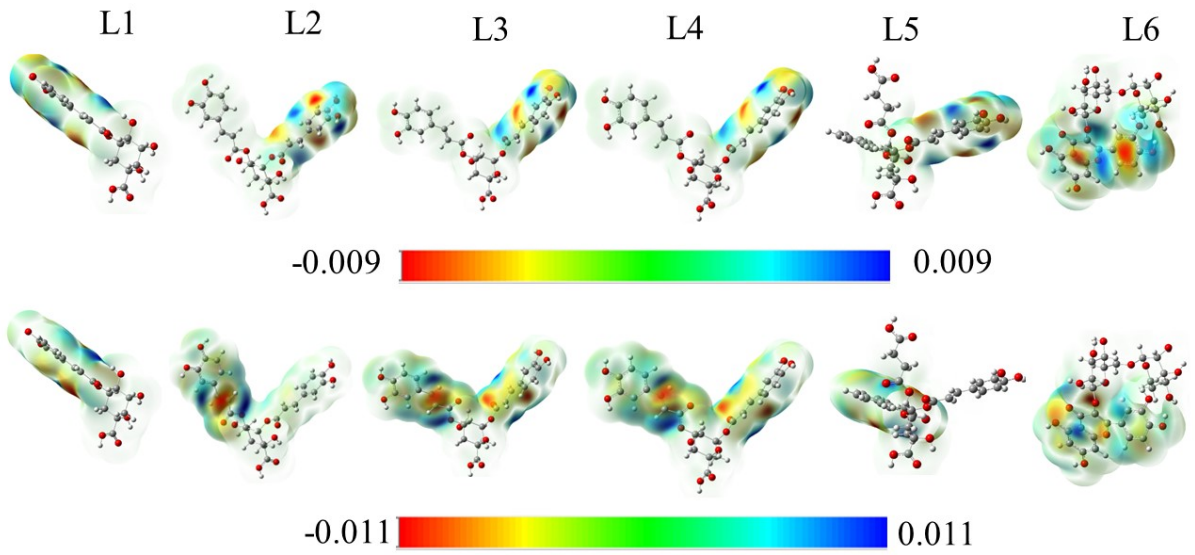

Figure SD1. Total densities at (*upper* raw) HOMOs and (*lower raw*) LUMOs for the components of the *Chrysanthemum Coronarium leaves* extract as obtained using the B3LYP/6-311+G(d,p) level of theory in aqueous solution.

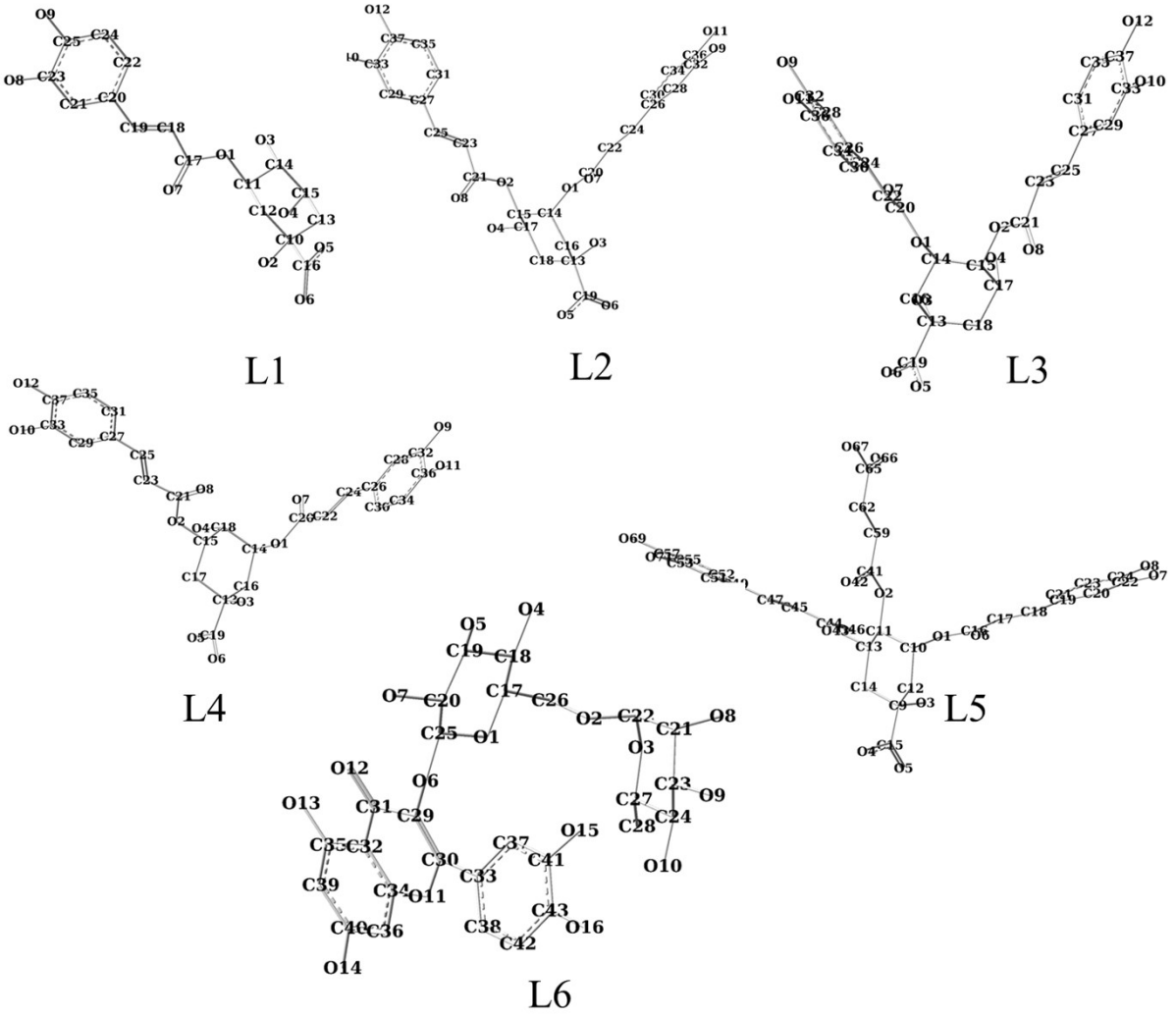

Figure SD2. Optimized structures of the investigated structures with atom numbering.

Supplementary Tables

Table 1. Hirshfeld charges for N, N+1, and N-1 electron systems and the condensed Fukui indices for electrophilic, f^-_k, nucleophilic, f^+_k, and dual attacks, f^2_k, indices for **L1** inhibitor molecule. None-hydrogen atoms are only listed. Units in elementary charges (e).

Atom	q^N_k	q^{N+1}_k	q^{N-1}_k	f^-_k	f^+_k	f^2_k
O1	-0.1186	-0.1540	-0.1048	0.0138	0.0354	0.0216
O2	-0.1972	-0.1984	-0.1967	0.0005	0.0012	0.0006
O3	-0.2503	-0.2547	-0.2483	0.0020	0.0044	0.0024
O4	-0.2705	-0.2728	-0.2694	0.0011	0.0024	0.0013
O5	-0.1376	-0.1388	-0.1371	0.0005	0.0012	0.0007
O6	-0.2804	-0.2836	-0.2790	0.0014	0.0032	0.0018
O7	-0.3130	-0.4037	-0.2723	0.0407	0.0907	0.0501
O8	-0.1832	-0.1989	-0.1199	0.0633	0.0157	-0.0477
O9	-0.1952	-0.2298	-0.1004	0.0948	0.0346	-0.0602
C10	0.0877	0.0863	0.0884	0.0007	0.0015	0.0008
C11	0.0487	0.0414	0.0522	0.0035	0.0073	0.0038
C12	-0.0588	-0.0622	-0.0572	0.0016	0.0034	0.0019
C13	-0.0548	-0.0556	-0.0544	0.0004	0.0008	0.0004
C14	0.0403	0.0380	0.0414	0.0011	0.0023	0.0013
C15	0.0538	0.0520	0.0546	0.0008	0.0018	0.0010
C16	0.2268	0.2252	0.2273	0.0005	0.0015	0.0010
C17	0.1981	0.1120	0.2209	0.0227	0.0862	0.0634
C18	-0.0696	-0.1735	0.0210	0.0905	0.1039	0.0134
C19	-0.0025	-0.1290	0.0306	0.0330	0.1265	0.0935
C20	-0.0148	-0.0480	0.0680	0.0827	0.0332	-0.0495
C21	-0.0493	-0.0979	-0.0119	0.0374	0.0485	0.0111
C22	-0.0390	-0.0932	0.0376	0.0765	0.0542	-0.0223
C23	0.0569	0.0321	0.1290	0.0721	0.0248	-0.0473
C24	-0.0536	-0.0835	-0.0021	0.0514	0.0299	-0.0215
C25	0.0678	0.0139	0.1582	0.0905	0.0538	-0.0367

Table 2. Hirshfeld charges for N, N+1, and N-1 electron systems and the condensed Fukui indices for electrophilic, f^-_k, nucleophilic, f^+_k, and dual attacks, f^2_k, indices for **L2** inhibitor molecule. None-hydrogen atoms are only listed. Units in elementary charges (e).

Atom	q^N_k	q^{N+1}_k	q^{N-1}_k	f^-_k	f^+_k	f^2_k
O1	-0.1197	-0.1323	-0.1125	0.0072	0.0126	0.0054
O2	-0.1240	-0.1478	-0.1179	0.0061	0.0238	0.0178
O3	-0.2396	-0.2406	-0.2393	0.0003	0.0011	0.0007
O4	-0.2409	-0.2434	-0.2398	0.0010	0.0025	0.0015
O5	-0.1382	-0.1391	-0.1377	0.0004	0.0009	0.0005
O6	-0.2826	-0.2849	-0.2815	0.0011	0.0024	0.0013
O7	-0.3173	-0.3511	-0.2958	0.0215	0.0338	0.0123
O8	-0.3166	-0.3770	-0.2983	0.0184	0.0604	0.0420
O9	-0.2025	-0.2088	-0.1627	0.0398	0.0064	-0.0334
O10	-0.2023	-0.2137	-0.1694	0.0329	0.0115	-0.0214
O11	-0.1938	-0.2062	-0.1435	0.0504	0.0124	-0.0380
O12	-0.1935	-0.2156	-0.1519	0.0416	0.0221	-0.0195
C13	0.0849	0.0846	0.0849	0.0001	0.0003	0.0002
C14	0.0626	0.0582	0.0651	0.0025	0.0044	0.0019
C15	0.0502	0.0444	0.0524	0.0022	0.0058	0.0036
C16	-0.0543	-0.0571	-0.0529	0.0014	0.0028	0.0015
C17	0.0504	0.0485	0.0511	0.0007	0.0020	0.0013
C18	-0.0609	-0.0624	-0.0604	0.0005	0.0015	0.0010
C19	0.2259	0.2249	0.2263	0.0004	0.0010	0.0006
C20	0.1958	0.1645	0.2080	0.0122	0.0313	0.0192
C21	0.1947	0.1381	0.2052	0.0105	0.0565	0.0460
C22	-0.0694	-0.1050	-0.0220	0.0474	0.0356	-0.0118
C23	-0.0695	-0.1365	-0.0305	0.0390	0.0670	0.0280
C24	-0.0041	-0.0504	0.0136	0.0177	0.0463	0.0286
C25	-0.0030	-0.0864	0.0115	0.0145	0.0834	0.0689
C26	-0.0150	-0.0263	0.0290	0.0440	0.0114	-0.0326
C27	-0.0149	-0.0361	0.0214	0.0363	0.0212	-0.0150
C28	-0.0518	-0.0691	-0.0316	0.0202	0.0173	-0.0029
C29	-0.0514	-0.0827	-0.0347	0.0167	0.0313	0.0146
C30	-0.0403	-0.0598	0.0040	0.0443	0.0195	-0.0248
C31	-0.0399	-0.0752	-0.0035	0.0363	0.0354	-0.0009
C32	0.0574	0.0483	0.0984	0.0410	0.0090	-0.0320
C33	0.0575	0.0412	0.0915	0.0339	0.0164	-0.0175
C34	-0.0550	-0.0655	-0.0280	0.0269	0.0105	-0.0164
C35	-0.0548	-0.0738	-0.0327	0.0221	0.0190	-0.0032
C36	0.0673	0.0479	0.1171	0.0498	0.0194	-0.0304

C37	0.0676	0.0327	0.1085	0.0410	0.0348	-0.0061

Table 3. Hirshfeld charges for N, N+1, and N-1 electron systems and the condensed Fukui indices for electrophilic, f_k^-, nucleophilic, f_k^+, and dual attacks, f_k^2, indices for **L3** inhibitor molecule. None-hydrogen atoms are only listed. Units in elementary charges (e).

Atom	q_k^N	q_k^{N+1}	q_k^{N-1}	f_k^-	f_k^+	f_k^2
O1	-0.1219	-0.1402	-0.1153	0.0066	0.0183	0.0117
O2	-0.1231	-0.1417	-0.116	0.0071	0.0186	0.0116
O3	-0.2285	-0.2296	-0.228	0.0005	0.0011	0.0007
O4	-0.2494	-0.2518	-0.2483	0.0011	0.0024	0.0013
O5	-0.1365	-0.1375	-0.1361	0.0004	0.0011	0.0007
O6	-0.2781	-0.2808	-0.2769	0.0011	0.0028	0.0017
O7	-0.3163	-0.363	-0.2971	0.0192	0.0467	0.0275
O8	-0.3165	-0.364	-0.2959	0.0206	0.0475	0.0269
O9	-0.2026	-0.2115	-0.1677	0.0349	0.0089	-0.0261
O10	-0.2022	-0.2112	-0.1644	0.0378	0.0089	-0.0288
O11	-0.1935	-0.2107	-0.1493	0.0442	0.0172	-0.027
O12	-0.1935	-0.2108	-0.1459	0.0476	0.0174	-0.0303
C13	0.0864	0.0855	0.0867	0.0003	0.0009	0.0005
C14	0.0517	0.0466	0.0541	0.0024	0.0051	0.0027
C15	0.0477	0.0426	0.0502	0.0025	0.0051	0.0026
C16	-0.0564	-0.0595	-0.0552	0.0013	0.003	0.0018
C17	0.0576	0.0547	0.0588	0.0013	0.0029	0.0016
C18	-0.0514	-0.0528	-0.0508	0.0006	0.0014	0.0008
C19	0.2274	0.226	0.2278	0.0004	0.0014	0.0009
C20	0.1961	0.1519	0.2072	0.0111	0.0442	0.0331
C21	0.196	0.151	0.2079	0.0119	0.0449	0.033
C22	-0.0693	-0.1203	-0.0276	0.0417	0.051	0.0093
C23	-0.0693	-0.1208	-0.0246	0.0447	0.0515	0.0068
C24	-0.0031	-0.0677	0.0122	0.0153	0.0645	0.0492
C25	-0.0029	-0.0686	0.0135	0.0164	0.0657	0.0492
C26	-0.0149	-0.0307	0.0235	0.0385	0.0158	-0.0227
C27	-0.015	-0.031	0.0265	0.0415	0.016	-0.0255
C28	-0.0515	-0.0755	-0.0338	0.0177	0.024	0.0064
C29	-0.0515	-0.0759	-0.0324	0.0191	0.0243	0.0052
C30	-0.0398	-0.0669	-0.0011	0.0386	0.0272	-0.0115
C31	-0.0398	-0.0672	0.0019	0.0418	0.0274	-0.0143
C32	0.0576	0.0451	0.0936	0.036	0.0126	-0.0234
C33	0.0574	0.0448	0.0963	0.0388	0.0127	-0.0262
C34	-0.0547	-0.0693	-0.0311	0.0236	0.0146	-0.009
C35	-0.0547	-0.0695	-0.0292	0.0255	0.0148	-0.0107
C36	0.0679	0.041	0.1116	0.0436	0.027	-0.0167
C37	0.0676	0.0404	0.1146	0.047	0.0272	-0.0198

Table 4. Hirshfeld charges for N, N+1, and N-1 electron systems and the condensed Fukui indices for electrophilic, f_k^-, nucleophilic, f_k^+, and dual attacks, f_k^2, indices for **L5** inhibitor molecule. None-hydrogen atoms are only listed. Units in elementary charges (e).

Atom	q_k^N	q_k^{N+1}	q_k^{N-1}	f_k^-	f_k^+	f_k^2
O1	-0.1181	-0.1350	-0.1067	0.0114	0.0168	0.0054
O2	-0.1228	-0.1430	-0.1196	0.0032	0.0202	0.0170
O3	-0.2395	-0.2406	-0.2392	0.0003	0.0011	0.0008
O4	-0.2263	-0.2307	-0.2235	0.0028	0.0043	0.0015
O5	-0.1382	-0.1393	-0.1377	0.0005	0.0011	0.0006
O6	-0.2836	-0.2863	-0.2825	0.0011	0.0027	0.0015
O7	-0.3148	-0.3587	-0.2831	0.0317	0.0438	0.0121
O8	-0.3171	-0.3651	-0.3103	0.0067	0.0481	0.0413
O9	-0.2023	-0.2107	-0.1417	0.0606	0.0084	-0.0522
O10	-0.2009	-0.2103	-0.1898	0.0111	0.0093	-0.0017
O11	-0.1935	-0.2097	-0.1173	0.0762	0.0162	-0.0599
O12	-0.1922	-0.2110	-0.1765	0.0156	0.0189	0.0032
C13	0.0861	0.0854	0.0862	0.0001	0.0007	0.0006
C14	0.0593	0.0550	0.0625	0.0032	0.0043	0.0011
C15	0.0520	0.0478	0.0529	0.0009	0.0042	0.0033
C16	-0.0567	-0.0586	-0.0554	0.0013	0.0019	0.0006
C17	-0.0618	-0.0637	-0.0613	0.0005	0.0019	0.0014
C18	0.0469	0.0442	0.0483	0.0015	0.0026	0.0011
C19	0.2258	0.2247	0.2263	0.0004	0.0012	0.0007
C20	0.1970	0.1557	0.2150	0.0179	0.0414	0.0234
C21	0.1961	0.1500	0.2002	0.0041	0.0461	0.0419
C22	-0.0690	-0.1166	0.0027	0.0717	0.0476	-0.0240
C23	-0.0708	-0.1244	-0.0550	0.0158	0.0535	0.0377
C24	-0.0031	-0.0642	0.0231	0.0262	0.0611	0.0348
C25	-0.0044	-0.0719	0.0015	0.0059	0.0674	0.0615
C26	-0.0149	-0.0301	0.0517	0.0666	0.0152	-0.0514
C27	-0.0154	-0.0328	-0.0016	0.0138	0.0174	0.0036
C28	-0.0516	-0.0744	-0.0212	0.0304	0.0228	-0.0076
C29	-0.0537	-0.0821	-0.0476	0.0061	0.0285	0.0224
C30	-0.0399	-0.0657	0.0272	0.0672	0.0258	-0.0414
C31	-0.0388	-0.0655	-0.0253	0.0135	0.0266	0.0131
C32	0.0575	0.0456	0.1197	0.0622	0.0119	-0.0503
C33	0.0607	0.0471	0.0722	0.0114	0.0137	0.0022
C34	-0.0548	-0.0687	-0.0141	0.0407	0.0139	-0.0268
C35	-0.0579	-0.0747	-0.0489	0.0090	0.0168	0.0078
C36	0.0676	0.0421	0.1428	0.0752	0.0256	-0.0496
C37	0.0695	0.0392	0.0848	0.0153	0.0303	0.0150

Table 5. Hirshfeld charges for N, N+1, and N-1 electron systems and the condensed Fukui indices for electrophilic, f_k^-, nucleophilic, f_k^+, and dual attacks, f_k^2, indices for **L5** inhibitor molecule. None-hydrogen atoms are only listed. Units in elementary charges (e).

Atom	q_k^N	q_k^{N+1}	q_k^{N-1}	f_k^-	f_k^+	f_k^2
O1	-0.1200	-0.1198	-0.1070	0.0130	-0.0003	-0.0133
O2	-0.1179	-0.1182	-0.1179	0.0000	0.0003	0.0002
O3	-0.2376	-0.2391	-0.2373	0.0003	0.0015	0.0012
O4	-0.1370	-0.1381	-0.1364	0.0006	0.0011	0.0005
O5	-0.2794	-0.2824	-0.2783	0.0012	0.0029	0.0017
O6	-0.3161	-0.3174	-0.2774	0.0388	0.0013	-0.0375
O7	-0.2023	-0.2024	-0.1287	0.0735	0.0002	-0.0734
O8	-0.1935	-0.1937	-0.1014	0.0920	0.0002	-0.0918
C9	0.0862	0.0848	0.0863	0.0001	0.0014	0.0013
C10	0.0623	0.0611	0.0656	0.0034	0.0012	-0.0022
C11	0.0530	0.0511	0.0540	0.0010	0.0019	0.0010
C12	-0.0527	-0.0532	-0.0510	0.0016	0.0006	-0.0011
C13	0.0548	0.0479	0.0549	0.0001	0.0069	0.0068
C14	-0.0576	-0.0605	-0.0574	0.0002	0.0028	0.0026
C15	0.2270	0.2256	0.2274	0.0005	0.0014	0.0009
C16	0.1968	0.1962	0.2184	0.0216	0.0006	-0.0210
C17	-0.0690	-0.0689	0.0173	0.0862	-0.0001	-0.0863
C18	-0.0029	-0.0036	0.0285	0.0315	0.0006	-0.0308
C19	-0.0149	-0.0150	0.0656	0.0805	0.0000	-0.0804
C20	-0.0515	-0.0517	-0.0148	0.0367	0.0002	-0.0365
C21	-0.0398	-0.0399	0.0413	0.0811	0.0001	-0.0810
C22	0.0575	0.0574	0.1328	0.0753	0.0002	-0.0751
C23	-0.0547	-0.0548	-0.0056	0.0491	0.0001	-0.0490
C24	0.0677	0.0674	0.1584	0.0907	0.0003	-0.0904
C41	0.2278	0.2263	0.2284	0.0006	0.0016	0.0010
O42	-0.2897	-0.2924	-0.2882	0.0015	0.0027	0.0012
O43	-0.1127	-0.1394	-0.1123	0.0004	0.0267	0.0262
C44	0.1997	0.1169	0.2000	0.0003	0.0828	0.0826
C45	-0.0603	-0.1642	-0.0603	0.0000	0.1039	0.1039
O46	-0.3175	-0.4150	-0.3172	0.0003	0.0975	0.0972
C47	-0.0032	-0.1237	-0.0029	0.0003	0.1205	0.1202
C49	-0.0044	-0.0432	-0.0044	0.0000	0.0387	0.0387
C51	-0.0305	-0.0799	-0.0304	0.0001	0.0494	0.0493
C52	-0.0309	-0.0874	-0.0309	0.0001	0.0565	0.0564
C53	-0.0377	-0.0758	-0.0376	0.0001	0.0380	0.0379
C55	-0.0359	-0.0694	-0.0358	0.0001	0.0335	0.0334
C57	-0.0296	-0.1008	-0.0294	0.0002	0.0712	0.0710
C61	-0.0433	-0.0440	-0.0431	0.0002	0.0007	0.0004
C64	-0.0421	-0.0423	-0.0419	0.0002	0.0003	0.0001
C67	0.2266	0.2265	0.2267	0.0001	0.0001	0.0000
O68	-0.3166	-0.3168	-0.3167	0.0000	0.0002	0.0002
O69	-0.1701	-0.1704	-0.1700	0.0002	0.0002	0.0001
O71	-0.2023	-0.2024	-0.1287	0.0735	0.0002	-0.0734
O72	-0.1945	-0.1941	-0.1016	0.0929	0.0004	-0.0925

Table 6. Hirshfeld charges for N, N+1, and N-1 electron systems and the condensed Fukui indices for electrophilic, f_k^-, nucleophilic, f_k^+, and dual attacks, f_k^2, indices for **L6** inhibitor molecule. None-hydrogen atoms are only listed. Units in elementary charges (e).

Atom	q_k^N	q_k^{N+1}	q_k^{N-1}	f_k^-	f_k^+	f_k^2
O1	-0.1609	-0.1627	-0.1577	0.0032	0.0018	-0.0014
O2	-0.1538	-0.1539	-0.1537	0.0001	0.0001	0.0000
O3	-0.1752	-0.1755	-0.1747	0.0005	0.0003	-0.0001
O4	-0.2250	-0.2269	-0.2227	0.0024	0.0019	-0.0005
O5	-0.2479	-0.2498	-0.2455	0.0024	0.0020	-0.0004
O6	-0.1373	-0.1510	-0.1036	0.0337	0.0137	-0.0200
O7	-0.2444	-0.2479	-0.2397	0.0046	0.0036	-0.0010
O8	-0.2286	-0.2290	-0.2281	0.0005	0.0004	-0.0001
O9	-0.2584	-0.2587	-0.2580	0.0004	0.0003	-0.0001
O10	-0.2394	-0.2395	-0.2393	0.0001	0.0001	0.0000
O11	-0.0685	-0.1065	-0.0483	0.0202	0.0380	0.0177
O12	-0.3313	-0.4414	-0.2882	0.0431	0.1101	0.0669
O13	-0.1789	-0.2039	-0.1585	0.0204	0.0250	0.0045
O14	-0.1829	-0.2053	-0.1650	0.0179	0.0224	0.0045
O15	-0.1808	-0.1929	-0.1410	0.0398	0.0121	-0.0277
O16	-0.1969	-0.2234	-0.1268	0.0700	0.0266	-0.0434
C17	0.0534	0.0514	0.0561	0.0027	0.0020	-0.0007
C18	0.0401	0.0396	0.0407	0.0006	0.0005	-0.0001
C19	0.0390	0.0380	0.0404	0.0014	0.0010	-0.0003
C20	0.0403	0.0380	0.0426	0.0023	0.0022	0.0000
C21	0.0419	0.0417	0.0421	0.0002	0.0001	0.0000
C22	0.1174	0.1171	0.1178	0.0004	0.0003	-0.0001
C23	0.0353	0.0350	0.0357	0.0004	0.0002	-0.0002
C24	0.0387	0.0386	0.0388	0.0001	0.0001	0.0000
C25	0.1156	0.1109	0.1220	0.0064	0.0046	-0.0018
C26	0.0286	0.0276	0.0299	0.0014	0.0009	-0.0004
C27	0.0473	0.0472	0.0474	0.0001	0.0001	0.0000
C28	-0.0873	-0.0874	-0.0872	0.0001	0.0001	0.0000
C29	0.0260	-0.0170	0.1018	0.0757	0.0431	-0.0327
C30	0.0890	0.0046	0.1250	0.0361	0.0843	0.0483
C31	0.1015	0.0081	0.1215	0.0200	0.0935	0.0734
C32	-0.0540	-0.0727	-0.0382	0.0158	0.0186	0.0029
C33	-0.0241	-0.0472	0.0332	0.0574	0.0230	-0.0343
C34	0.0902	0.0700	0.1003	0.0102	0.0202	0.0100
C35	0.0955	0.0567	0.1154	0.0199	0.0388	0.0189
C36	-0.0871	-0.1165	-0.0552	0.0319	0.0294	-0.0025
C37	-0.0566	-0.0921	-0.0303	0.0263	0.0355	0.0092
C38	-0.0471	-0.0859	0.0106	0.0577	0.0388	-0.0189
C39	-0.0853	-0.1145	-0.0690	0.0162	0.0293	0.0130
C40	0.0916	0.0578	0.1117	0.0200	0.0338	0.0137
C41	0.0566	0.0377	0.1040	0.0473	0.0189	-0.0284
C42	-0.0570	-0.0810	-0.0151	0.0419	0.0240	-0.0180
C43	0.0653	0.0241	0.1334	0.0681	0.0411	-0.0270