

# Supplementary Materials: An Assessment of New Imidazol Derivatives and an Investigation of Their Corrosion-Reducing Characteristics for Carbon Steel in an HCl Acid Solution

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**Table S1.** Hirshfeld charges, condensed Fukui functions (in e units), local softness in e. eV<sup>-1</sup>, local electrophilicity (in e. eV) and condensed dual Fukui (in e), softness (in e.eV<sup>-1</sup>) and philicity (in e.eV) descriptors for the neutral TIMQ inhibitor obtained at B3LYP/6-31+G(d,p) in aqueous solution using PCM solvation model. Units "e" is the elementary charge.

atom	q(N)	q(N+1)	q(N-1)	f <sub>A</sub> <sup>+</sup>	f <sub>A</sub> <sup>-</sup>	f <sub>A</sub> <sup>2</sup>	s <sub>A</sub> <sup>+</sup>	s <sub>A</sub> <sup>-</sup>	Δs <sub>k</sub>	ω <sub>A</sub> <sup>+</sup>	ω <sub>A</sub> <sup>-</sup>	Δω <sub>k</sub>
O1	-0.1972	-0.2331	-0.1905	0.0359	0.0066	0.0293	0.0198	0.0036	0.0161	0.1460	0.0268	0.1191
N1	-0.2238	-0.2309	-0.1837	0.0071	0.0401	-0.0331	0.0039	0.0221	-0.0182	0.0289	0.1631	-0.1342
N2	-0.0017	0.0003	0.0217	-0.0019	0.0233	-0.0253	-0.0010	0.0128	-0.0139	-0.0077	0.0947	-0.1025
N3	-0.1874	-0.2926	-0.1820	0.1052	0.0054	0.0998	0.0579	0.0030	0.0549	0.4278	0.0220	0.4058
C1	0.0746	0.0726	0.1383	0.0020	0.0637	-0.0617	0.0011	0.0351	-0.0340	0.0081	0.2590	-0.2509

C2	-0.0020	-0.0074	0.0772	0.0054	0.0791	-0.0737	0.0030	0.0435	-0.0406	0.0220	0.3216	-0.2997
C3	0.0155	0.0155	0.0990	0.0000	0.0835	-0.0836	0.0000	0.0460	-0.0460	0.0000	0.3395	-0.3395
C4	-0.0028	-0.0010	0.0049	-0.0018	0.0077	-0.0095	-0.0010	0.0042	-0.0052	-0.0073	0.0313	-0.0386
C5	-0.0346	-0.0360	-0.0146	0.0014	0.0200	-0.0186	0.0008	0.0110	-0.0102	0.0057	0.0813	-0.0756
C6	-0.0349	-0.0365	-0.0130	0.0016	0.0219	-0.0203	0.0009	0.0121	-0.0112	0.0065	0.0891	-0.0825
C7	-0.0377	-0.0406	-0.0192	0.0029	0.0185	-0.0155	0.0016	0.0102	-0.0086	0.0118	0.0752	-0.0634
C8	-0.0375	-0.0405	-0.0183	0.0030	0.0192	-0.0162	0.0017	0.0106	-0.0089	0.0122	0.0781	-0.0659
C9	-0.0373	-0.0409	-0.0045	0.0036	0.0328	-0.0293	0.0020	0.0181	-0.0161	0.0146	0.1334	-0.1187
C10	-0.0103	-0.0107	0.0157	0.0004	0.0260	-0.0256	0.0002	0.0143	-0.0141	0.0016	0.1057	-0.1041
C11	-0.0481	-0.0496	-0.0135	0.0015	0.0346	-0.0331	0.0008	0.0190	-0.0182	0.0061	0.1407	-0.1346
C12	-0.0510	-0.0527	-0.0142	0.0017	0.0368	-0.0351	0.0009	0.0203	-0.0193	0.0069	0.1496	-0.1427
C13	-0.0464	-0.0479	-0.0213	0.0015	0.0251	-0.0236	0.0008	0.0138	-0.0130	0.0061	0.1021	-0.0960
C14	-0.0467	-0.0480	-0.0194	0.0013	0.0272	-0.0259	0.0007	0.0150	-0.0143	0.0053	0.1106	-0.1053
C15	-0.0491	-0.0514	0.0032	0.0023	0.0523	-0.0500	0.0013	0.0288	-0.0275	0.0094	0.2127	-0.2033
C16	-0.0126	-0.0113	-0.0045	-0.0013	0.0081	-0.0094	-0.0007	0.0045	-0.0052	-0.0053	0.0329	-0.0382
C17	-0.0412	-0.0448	-0.0213	0.0035	0.0199	-0.0164	0.0019	0.0110	-0.0090	0.0142	0.0809	-0.0667
C18	-0.0379	-0.0383	-0.0214	0.0003	0.0166	-0.0163	0.0002	0.0091	-0.0090	0.0012	0.0675	-0.0663
C19	-0.0400	-0.0437	-0.0255	0.0037	0.0145	-0.0109	0.0020	0.0080	-0.0059	0.0150	0.0590	-0.0439
C20	-0.0381	-0.0422	-0.0239	0.0041	0.0142	-0.0102	0.0023	0.0078	-0.0056	0.0167	0.0577	-0.0411
C21	-0.0390	-0.0444	-0.0129	0.0054	0.0261	-0.0207	0.0030	0.0144	-0.0114	0.0220	0.1061	-0.0842
C22	0.0132	0.0043	0.0197	0.0089	0.0065	0.0024	0.0049	0.0036	0.0013	0.0362	0.0264	0.0098
C23	-0.0168	-0.0629	-0.0182	0.0460	-0.0014	0.0474	0.0253	-0.0008	0.0261	0.1871	-0.0057	0.1927
C24	-0.0070	-0.0321	-0.0056	0.0251	0.0014	0.0238	0.0138	0.0008	0.0130	0.1021	0.0057	0.0964
C25	0.0272	-0.0072	0.0306	0.0344	0.0035	0.0310	0.0189	0.0019	0.0170	0.1399	0.0142	0.1257
C26	0.0715	0.0104	0.0794	0.0611	0.0079	0.0532	0.0336	0.0043	0.0293	0.2485	0.0321	0.2163
C27	-0.0626	-0.1187	-0.0561	0.0561	0.0065	0.0496	0.0309	0.0036	0.0273	0.2281	0.0264	0.2017
C28	-0.0335	-0.0863	-0.0271	0.0528	0.0064	0.0463	0.0291	0.0035	0.0255	0.2147	0.0260	0.1887
C29	-0.0204	-0.1267	-0.0198	0.1063	0.0006	0.1057	0.0585	0.0003	0.0582	0.4323	0.0024	0.4298
C30	-0.0381	-0.1180	-0.0321	0.0799	0.0060	0.0740	0.0440	0.0033	0.0407	0.3249	0.0244	0.3005
C31	0.0224	-0.0684	0.0270	0.0908	0.0046	0.0862	0.0500	0.0025	0.0475	0.3692	0.0187	0.3505

Table S2. As Table S1 but for the protonated form of TIMQ inhibitor.

atom	q(N)	q(N+1)	q(N-1)	$f_A^+$	$f_A^-$	$f_A^2$	$s_A^+$	$s_A^-$	$\Delta s_k$	$\omega_A^+$	$\omega_A^-$	$\Delta\omega_i$
O1	-0.1545	-0.1803	-0.1500	0.0258	0.0045	0.0213	0.0164	0.0029	0.0135	0.2073	0.0362	0.1711
N1	0.0046	0.0007	0.0235	0.0039	0.0189	-0.0150	0.0025	0.0120	-0.0095	0.0313	0.1518	-0.1205
N2	0.0272	0.0294	0.0425	-0.0022	0.0153	-0.0175	-0.0014	0.0097	-0.0111	-0.0177	0.1229	-0.1406
N3	0.0427	-0.0418	0.0453	0.0846	0.0026	0.0820	0.0537	0.0017	0.0520	0.6797	0.0209	0.6588
C1	0.1435	0.1417	0.1880	0.0018	0.0444	-0.0426	0.0011	0.0282	-0.0270	0.0145	0.3567	-0.3423
C2	0.0530	0.0484	0.1105	0.0045	0.0575	-0.0530	0.0029	0.0365	-0.0336	0.0362	0.4620	-0.4258

C3	0.0438	0.0442	0.1043	-0.0004	0.0605	-0.0609	-0.0003	0.0384	-0.0387	-0.0032	0.4861	-0.4893
C4	-0.0058	-0.0035	0.0151	-0.0023	0.0209	-0.0232	-0.0015	0.0133	-0.0147	-0.0185	0.1679	-0.1864
C5	-0.0275	-0.0280	-0.0029	0.0004	0.0246	-0.0242	0.0003	0.0156	-0.0154	0.0032	0.1976	-0.1944
C6	-0.0266	-0.0279	-0.0022	0.0013	0.0244	-0.0231	0.0008	0.0155	-0.0147	0.0104	0.1960	-0.1856
C7	-0.0283	-0.0310	-0.0057	0.0027	0.0226	-0.0199	0.0017	0.0143	-0.0126	0.0217	0.1816	-0.1599
C8	-0.0280	-0.0309	-0.0026	0.0029	0.0255	-0.0226	0.0018	0.0162	-0.0143	0.0233	0.2049	-0.1816
C9	-0.0245	-0.0277	0.0197	0.0032	0.0442	-0.0410	0.0020	0.0281	-0.0260	0.0257	0.3551	-0.3294
C10	-0.0056	-0.0056	0.0369	0.0000	0.0425	-0.0425	0.0000	0.0270	-0.0270	0.0000	0.3415	-0.3415
C11	-0.0320	-0.0333	0.0084	0.0012	0.0404	-0.0392	0.0008	0.0256	-0.0249	0.0096	0.3246	-0.3149
C12	-0.0348	-0.0359	0.0017	0.0011	0.0364	-0.0353	0.0007	0.0231	-0.0224	0.0088	0.2925	-0.2836
C13	-0.0318	-0.0330	-0.0015	0.0012	0.0303	-0.0291	0.0008	0.0192	-0.0185	0.0096	0.2434	-0.2338
C14	-0.0320	-0.0331	0.0051	0.0011	0.0371	-0.0360	0.0007	0.0235	-0.0229	0.0088	0.2981	-0.2892
C15	-0.0292	-0.0310	0.0364	0.0018	0.0656	-0.0638	0.0011	0.0416	-0.0405	0.0145	0.5271	-0.5126
C16	-0.0103	-0.0081	-0.0005	-0.0022	0.0098	-0.0120	-0.0014	0.0062	-0.0076	-0.0177	0.0787	-0.0964
C17	-0.0234	-0.0256	-0.0074	0.0022	0.0160	-0.0138	0.0014	0.0102	-0.0088	0.0177	0.1286	-0.1109
C18	-0.0226	-0.0226	-0.0080	0.0000	0.0145	-0.0145	0.0000	0.0092	-0.0092	0.0000	0.1165	-0.1165
C19	-0.0241	-0.0271	-0.0104	0.0030	0.0137	-0.0107	0.0019	0.0087	-0.0068	0.0241	0.1101	-0.0860
C20	-0.0220	-0.0250	-0.0089	0.0030	0.0132	-0.0102	0.0019	0.0084	-0.0065	0.0241	0.1061	-0.0820
C21	-0.0169	-0.0208	0.0077	0.0039	0.0246	-0.0207	0.0025	0.0156	-0.0131	0.0313	0.1976	-0.1663
C22	0.0274	0.0199	0.0326	0.0075	0.0052	0.0023	0.0048	0.0033	0.0015	0.0603	0.0418	0.0185
C23	-0.0001	-0.0371	-0.0021	0.0370	-0.0020	0.0390	0.0235	-0.0013	0.0248	0.2973	-0.0161	0.3133
C24	0.0177	-0.0124	0.0189	0.0301	0.0012	0.0289	0.0191	0.0008	0.0183	0.2418	0.0096	0.2322
C25	0.0766	0.0330	0.0793	0.0436	0.0028	0.0408	0.0277	0.0018	0.0259	0.3503	0.0225	0.3278
C26	0.0961	0.0524	0.1017	0.0438	0.0056	0.0382	0.0278	0.0036	0.0242	0.3519	0.0450	0.3069
C27	-0.0222	-0.0794	-0.0180	0.0572	0.0042	0.0530	0.0363	0.0027	0.0336	0.4596	0.0337	0.4258
C28	-0.0054	-0.0516	-0.0010	0.0462	0.0044	0.0418	0.0293	0.0028	0.0265	0.3712	0.0354	0.3358
C29	0.0345	-0.0911	0.0348	0.1255	0.0004	0.1251	0.0797	0.0003	0.0794	1.0083	0.0032	1.0051
C30	0.0016	-0.0674	0.0058	0.0690	0.0042	0.0648	0.0438	0.0027	0.0411	0.5544	0.0337	0.5206
C31	0.1164	-0.0030	0.1199	0.1194	0.0035	0.1159	0.0758	0.0022	0.0736	0.9593	0.0281	0.9312

Table S3. As Table S1 but for the neutral form of CDIQ inhibitor.

atom	q(N)	q(N+1)	q(N-1)	$f_A^+$	$f_A^-$	$f_A^2$	$s_A^+$	$s_A^-$	$\Delta s_k$	$\omega_A^+$	$\omega_A^-$	$\Delta \omega_i$
O1	-0.1966	-0.2323	-0.1901	0.0357	0.0065	0.0291	0.0196	0.0036	0.0160	0.1463	0.0266	0.1197
N1	-0.2223	-0.2297	-0.1826	0.0074	0.0397	-0.0323	0.0041	0.0218	-0.0177	0.0303	0.1627	-0.1324
N2	-0.0009	0.0009	0.0220	-0.0018	0.0229	-0.0247	-0.0010	0.0126	-0.0135	-0.0074	0.0938	-0.1012
N3	-0.1870	-0.2902	-0.1817	0.1033	0.0052	0.0980	0.0566	0.0029	0.0538	0.4233	0.0213	0.4020
C1	0.0745	0.0724	0.1381	0.0021	0.0635	-0.0614	0.0012	0.0348	-0.0337	0.0086	0.2602	-0.2516

C2	-0.0009	-0.0064	0.0773	0.0055	0.0782	-0.0728	0.0030	0.0429	-0.0399	0.0225	0.3205	-0.2979
C3	0.0166	0.0163	0.0990	0.0003	0.0824	-0.0821	0.0002	0.0452	-0.0450	0.0012	0.3377	-0.3364
C4	-0.0029	-0.0012	0.0051	-0.0017	0.0079	-0.0097	-0.0009	0.0043	-0.0053	-0.0070	0.0324	-0.0393
C5	-0.0346	-0.0362	-0.0146	0.0016	0.0201	-0.0185	0.0009	0.0110	-0.0101	0.0066	0.0824	-0.0758
C6	-0.0346	-0.0363	-0.0127	0.0017	0.0219	-0.0202	0.0009	0.0120	-0.0111	0.0070	0.0897	-0.0828
C7	-0.0375	-0.0405	-0.0190	0.0030	0.0185	-0.0155	0.0016	0.0101	-0.0085	0.0123	0.0758	-0.0635
C8	-0.0373	-0.0404	-0.0180	0.0031	0.0193	-0.0162	0.0017	0.0106	-0.0089	0.0127	0.0791	-0.0664
C9	-0.0370	-0.0407	-0.0040	0.0038	0.0329	-0.0291	0.0021	0.0180	-0.0160	0.0156	0.1348	-0.1192
C10	-0.0103	-0.0106	0.0158	0.0004	0.0260	-0.0257	0.0002	0.0143	-0.0140	0.0016	0.1065	-0.1049
C11	-0.0476	-0.0491	-0.0134	0.0015	0.0342	-0.0327	0.0008	0.0187	-0.0179	0.0061	0.1401	-0.1340
C12	-0.0506	-0.0524	-0.0142	0.0017	0.0365	-0.0347	0.0009	0.0200	-0.0191	0.0070	0.1496	-0.1426
C13	-0.0462	-0.0476	-0.0212	0.0015	0.0250	-0.0235	0.0008	0.0137	-0.0129	0.0061	0.1024	-0.0963
C14	-0.0463	-0.0476	-0.0191	0.0013	0.0271	-0.0258	0.0007	0.0149	-0.0141	0.0053	0.1111	-0.1057
C15	-0.0486	-0.0508	0.0034	0.0023	0.0519	-0.0496	0.0013	0.0285	-0.0272	0.0094	0.2127	-0.2033
C16	-0.0091	-0.0089	-0.0012	-0.0002	0.0079	-0.0081	-0.0001	0.0043	-0.0044	-0.0008	0.0324	-0.0332
C17	-0.0300	-0.0346	-0.0107	0.0046	0.0193	-0.0147	0.0025	0.0106	-0.0081	0.0189	0.0791	-0.0602
C18	-0.0275	-0.0284	-0.0113	0.0009	0.0162	-0.0153	0.0005	0.0089	-0.0084	0.0037	0.0664	-0.0627
C19	-0.0417	-0.0459	-0.0283	0.0042	0.0135	-0.0093	0.0023	0.0074	-0.0051	0.0172	0.0553	-0.0381
C20	-0.0402	-0.0449	-0.0269	0.0048	0.0132	-0.0085	0.0026	0.0072	-0.0046	0.0197	0.0541	-0.0344
C21	0.0243	0.0187	0.0445	0.0056	0.0202	-0.0146	0.0031	0.0111	-0.0080	0.0229	0.0828	-0.0598
C22	-0.0173	-0.0629	-0.0187	0.0456	-0.0014	0.0470	0.0250	-0.0008	0.0258	0.1869	-0.0057	0.1926
C23	-0.0068	-0.0314	-0.0054	0.0247	0.0013	0.0233	0.0135	0.0007	0.0128	0.1012	0.0053	0.0959
C24	0.0275	-0.0062	0.0309	0.0337	0.0034	0.0303	0.0185	0.0019	0.0166	0.1381	0.0139	0.1242
C25	0.0722	0.0115	0.0799	0.0607	0.0077	0.0530	0.0333	0.0042	0.0291	0.2487	0.0316	0.2172
C26	-0.0620	-0.1171	-0.0556	0.0551	0.0064	0.0487	0.0302	0.0035	0.0267	0.2258	0.0262	0.1996
C27	-0.0333	-0.0857	-0.0271	0.0525	0.0062	0.0463	0.0288	0.0034	0.0254	0.2151	0.0254	0.1897
C28	-0.0200	-0.1246	-0.0195	0.1046	0.0006	0.1040	0.0573	0.0003	0.0570	0.4286	0.0025	0.4262
C29	-0.0376	-0.1165	-0.0318	0.0789	0.0058	0.0731	0.0433	0.0032	0.0401	0.3233	0.0238	0.2996
C30	0.0227	-0.0666	0.0273	0.0894	0.0045	0.0848	0.0490	0.0025	0.0465	0.3664	0.0184	0.3479
C31	0.0135	0.0046	0.0199	0.0089	0.0064	0.0025	0.0049	0.0035	0.0014	0.0365	0.0262	0.0102
Cl1	-0.0800	-0.0867	-0.0510	0.0068	0.0290	-0.0222	0.0037	0.0159	-0.0122	0.0279	0.1188	-0.0910

Table S4. As Table S1 but for the protonated form of CDIQ inhibitor.

atom	q(N)	q(N+1)	q(N-1)	$f_A^+$	$f_A^-$	$f_A^2$	$s_A^+$	$s_A^-$	$\Delta s_k$	$\omega_A^+$	$\omega_A^-$	$\Delta\omega_A$
o1	-0.1539	-0.1797	-0.1461	0.0258	0.0078	0.0180	0.0153	0.0046	0.0107	0.2034	0.0615	0.1419
N1	0.0053	0.0012	0.0241	0.0040	0.0189	-0.0149	0.0024	0.0112	-0.0089	0.0315	0.1490	-0.1175
N2	0.0285	0.0310	0.0464	-0.0025	0.0179	-0.0204	-0.0015	0.0106	-0.0121	-0.0197	0.1411	-0.1608
N3	0.0431	-0.0413	0.0464	0.0844	0.0033	0.0811	0.0501	0.0020	0.0482	0.6654	0.0260	0.6394

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C1	0.1440	0.1424	0.1903	0.0017	0.0463	-0.0446	0.0010	0.0275	-0.0265	0.0134	0.3650	-0.3516
C2	0.0533	0.0489	0.1094	0.0044	0.0561	-0.0517	0.0026	0.0333	-0.0307	0.0347	0.4423	-0.4076
C3	0.0442	0.0444	0.1111	-0.0002	0.0668	-0.0670	-0.0001	0.0397	-0.0398	-0.0016	0.5267	-0.5282
C4	-0.0074	-0.0056	0.0003	-0.0017	0.0076	-0.0093	-0.0010	0.0045	-0.0055	-0.0134	0.0599	-0.0733
C5	-0.0278	-0.0283	-0.0158	0.0005	0.0120	-0.0115	0.0003	0.0071	-0.0068	0.0039	0.0946	-0.0907
C6	-0.0270	-0.0286	-0.0079	0.0016	0.0191	-0.0175	0.0010	0.0113	-0.0104	0.0126	0.1506	-0.1380
C7	-0.0285	-0.0308	-0.0097	0.0023	0.0189	-0.0166	0.0014	0.0112	-0.0099	0.0181	0.1490	-0.1309
C8	-0.0284	-0.0308	-0.0134	0.0024	0.0150	-0.0126	0.0014	0.0089	-0.0075	0.0189	0.1183	-0.0993
C9	-0.0239	-0.0267	0.0016	0.0027	0.0256	-0.0229	0.0016	0.0152	-0.0136	0.0213	0.2018	-0.1805
C10	-0.0067	-0.0068	0.0457	0.0001	0.0524	-0.0523	0.0001	0.0311	-0.0311	0.0008	0.4131	-0.4123
C11	-0.0331	-0.0341	0.0078	0.0010	0.0409	-0.0399	0.0006	0.0243	-0.0237	0.0079	0.3225	-0.3146
C12	-0.0343	-0.0356	0.0108	0.0012	0.0451	-0.0439	0.0007	0.0268	-0.0261	0.0095	0.3556	-0.3461
C13	-0.0315	-0.0326	0.0089	0.0010	0.0405	-0.0395	0.0006	0.0241	-0.0235	0.0079	0.3193	-0.3114
C14	-0.0314	-0.0326	0.0057	0.0011	0.0372	-0.0361	0.0007	0.0221	-0.0214	0.0087	0.2933	-0.2846
C15	-0.0282	-0.0299	0.0480	0.0017	0.0762	-0.0745	0.0010	0.0453	-0.0443	0.0134	0.6008	-0.5874
C16	-0.0082	-0.0057	0.0000	-0.0025	0.0082	-0.0107	-0.0015	0.0049	-0.0064	-0.0197	0.0646	-0.0844
C17	-0.0131	-0.0155	0.0002	0.0024	0.0134	-0.0110	0.0014	0.0080	-0.0065	0.0189	0.1056	-0.0867
C18	-0.0133	-0.0134	-0.0013	0.0001	0.0120	-0.0119	0.0001	0.0071	-0.0071	0.0008	0.0946	-0.0938
C19	-0.0278	-0.0306	-0.0153	0.0028	0.0125	-0.0097	0.0017	0.0074	-0.0058	0.0221	0.0986	-0.0765
C20	-0.0265	-0.0296	-0.0141	0.0031	0.0124	-0.0093	0.0018	0.0074	-0.0055	0.0244	0.0978	-0.0733
C21	0.0403	0.0371	0.0572	0.0032	0.0169	-0.0137	0.0019	0.0100	-0.0081	0.0252	0.1332	-0.1080
C22	0.0278	0.0203	0.0333	0.0075	0.0055	0.0020	0.0045	0.0033	0.0012	0.0591	0.0434	0.0158
C23	-0.0001	-0.0366	0.0010	0.0365	0.0011	0.0354	0.0217	0.0007	0.0210	0.2878	0.0087	0.2791
C24	0.0175	-0.0121	0.0194	0.0296	0.0019	0.0277	0.0176	0.0011	0.0165	0.2334	0.0150	0.2184
C25	0.0769	0.0336	0.0806	0.0433	0.0036	0.0397	0.0257	0.0021	0.0236	0.3414	0.0284	0.3130
C26	0.0965	0.0528	0.1050	0.0437	0.0085	0.0352	0.0260	0.0050	0.0209	0.3445	0.0670	0.2775
C27	-0.0214	-0.0783	-0.0144	0.0569	0.0070	0.0499	0.0338	0.0042	0.0296	0.4486	0.0552	0.3934
C28	-0.0045	-0.0509	0.0015	0.0464	0.0061	0.0403	0.0276	0.0036	0.0239	0.3658	0.0481	0.3177
C29	0.0353	-0.0898	0.0366	0.1251	0.0013	0.1238	0.0743	0.0008	0.0735	0.9863	0.0102	0.9761
C30	0.0024	-0.0667	0.0078	0.0691	0.0054	0.0637	0.0410	0.0032	0.0378	0.5448	0.0426	0.5022
C31	0.1169	-0.0023	0.1213	0.1192	0.0044	0.1148	0.0708	0.0026	0.0682	0.9398	0.0347	0.9051
C11	-0.0547	-0.0592	-0.0246	0.0045	0.0301	-0.0256	0.0027	0.0179	-0.0152	0.0355	0.2373	-0.2018

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