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SUPPLEMENTARY MATERIAL TO

A DFT study of the chemical reactivity of cimetidine A, C and D in the gas phase and in H_2O, MeOH and EtOH solvents

LUIS HUMBERTO MENDOZA HUIZAR[1]*, GUILLERMO SALGADO-MORÁN[2], WILSON CARDONA-VILLADA[2], ALISON GERALDO PACHECO[3] and DANIEL GLOSSMAN-MITNIK[4,5]

[1]Universidad Autónoma del Estado de Hidalgo, Academic Area of Chemistry, Carretera Pachuca-Tulancingo Km. 4.5 Mineral de la Reforma, Hgo, México, [2]Universidad Andrés Bello. Departamento de Ciencias Químicas, Facultad de Ciencias Exactas, Sede Concepción, Autopista Concepción-Talcahuano 7100, Talcahuano, Chile, [3]Instituto Federal de Educação Ciência e Tecnologia do Sul de Minas Gerais, Inconfidentes, Minas Gerais, Brasil, [4]Laboratorio Virtual NANOCOSMOS, Centro de Investigación en Materiales Avanzados, Chihuahua, Miguel de Cervantes 120, Complejo Industrial Chihuahua, Chih 31136, México and [5]Departament de Química, Universitat de les Illes Balears, 07122 Palma de Mallorca, Spain

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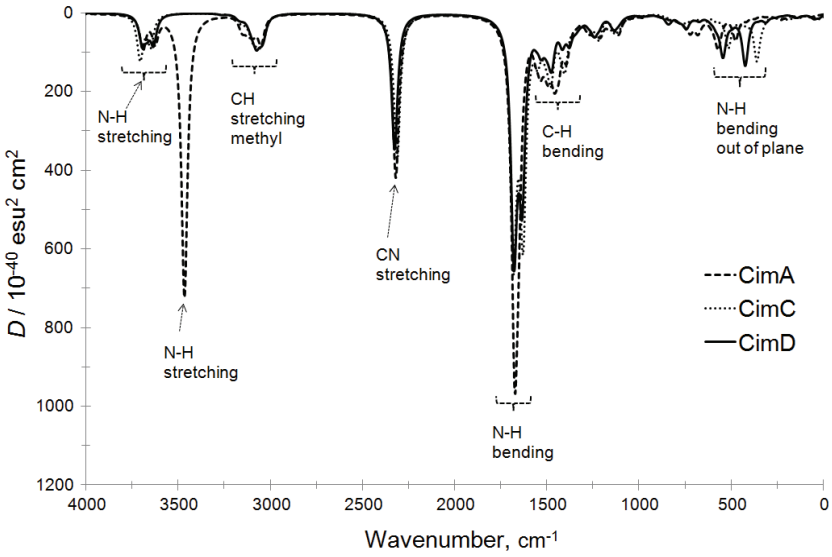

Fig. S-1. Theoretical IR spectra of CimA, CimC and CimD obtained at the wB97XD/def2TZVP level of theory in the gas phase.

* Corresponding author. E-mail: hhuizar@uaeh.edu.mx

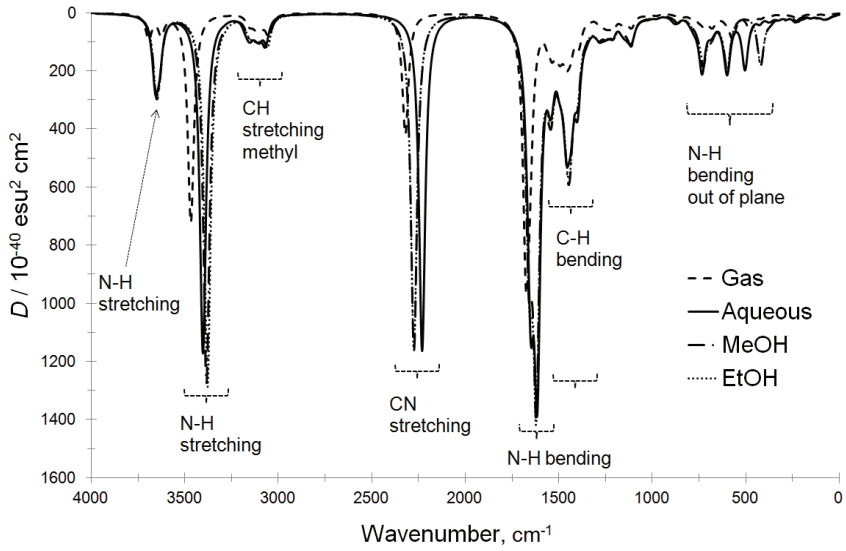

Fig. S-2. Theoretical IR spectra of CimA obtained at the wB97XD/def2TZVP level of theory in different solvents as indicated in the Figure.

TABLE S-I. Electronic energies including the zero-point vibrational energy correction (*ZPE* / / Ha) for CimA, CimC and CimD at the wB97XD/def2TZVP level of theory

Solvent	CimA	CimC	CimD
Gas	–1117.18590	–1117.16810	–1117.17586
H_2O	–1117.21585	–1117.20897	–1117.21457
MeOH	–1117.22783	–1117.21860	–1117.22364
EtOH	–1117.22900	–1117.21939	–1117.22459

TABLE S-II. The *x*, *y* and *z* coordinates for CimA optimized at the wB97XD /def2TZVP level of theory in different solvents

El.	Gas			H_2O			MeOH			EtOH		
	x	*y*	z	*x*	*y*	*z*	*x*	*y*	*z*	*x*	*y*	*z*
S	1.526	2.436	–0.017	1.517	2.447	–0.100	1.494	2.456	–0.146	1.487	2.457	–0.155
N	3.031	–1.928	–0.716	2.943	–1.970	–0.621	3.049	–1.956	–0.584	3.065	–1.952	–0.583
N	1.321	–1.124	0.393	1.342	–1.111	0.607	1.329	–1.075	0.449	1.327	–1.067	0.414
N	–2.292	0.947	0.095	–2.290	0.967	0.273	–2.307	0.958	0.207	–2.311	0.955	0.203
N	–1.654	–1.229	0.579	–1.616	–1.230	0.545	–1.621	–1.235	0.466	–1.622	–1.236	0.463
N	–3.776	–0.849	–0.177	–3.715	–0.820	–0.262	–3.768	–0.834	–0.197	–3.775	–0.839	–0.184
N	–5.517	0.773	–0.865	–5.565	0.698	–0.859	–5.666	0.651	–0.705	–5.676	0.643	–0.690
C	1.769	–2.147	–0.285	1.744	–2.176	–0.046	1.787	–2.145	–0.154	1.793	–2.137	–0.184
C	2.341	–0.199	0.403	2.339	–0.171	0.437	2.354	–0.150	0.404	2.355	–0.147	0.395
C	3.417	–0.681	–0.288	3.346	–0.693	–0.326	3.436	–0.687	–0.239	3.450	–0.686	–0.224
C	4.746	–0.096	–0.603	4.624	–0.121	–0.818	4.775	–0.142	–0.571	4.800	–0.146	–0.521
C	2.176	1.120	1.066	2.235	1.192	1.017	2.204	1.208	0.984	2.198	1.210	0.976
C	–0.030	1.705	–0.568	–0.066	1.697	–0.531	–0.087	1.705	–0.588	–0.094	1.708	–0.596

TABLE S-II. Continued

El.	Gas			H_2O			MeOH			EtOH		
	x	*y*	*z*	*x*	*y*	*z*	*x*	*y*	*z*	*x*	*y*	*z*
C	–1.068	1.566	0.544	–1.024	1.569	0.646	–1.047	1.564	0.588	–1.052	1.563	0.581
C	–2.594	–0.373	0.151	–2.541	–0.349	0.170	–2.570	–0.358	0.150	–2.575	–0.360	0.152
C	–1.915	–2.648	0.650	–1.824	–2.660	0.456	–1.841	–2.665	0.436	–1.842	–2.666	0.440
C	–4.696	0.022	–0.537	–4.663	0.019	–0.564	–4.744	–0.014	–0.456	–4.753	–0.022	–0.442
H	3.592	–2.566	–1.251	3.465	–2.642	–1.160	3.618	–2.636	–1.063	3.642	–2.632	–1.052
H	1.229	–3.057	–0.491	1.212	–3.110	–0.130	1.252	–3.069	–0.304	1.257	–3.058	–0.349
H	–3.035	1.540	–0.240	–2.975	1.583	–0.136	–3.029	1.578	–0.120	–3.038	1.575	–0.117
H	–0.675	–0.960	0.602	–0.647	–0.938	0.673	–0.647	–0.942	0.558	–0.647	–0.942	0.542
H	4.869	0.060	–1.677	4.599	0.030	–1.900	4.904	–0.032	–1.651	4.949	–0.016	–1.596
H	5.560	–0.735	–0.255	5.464	–0.781	–0.592	5.570	–0.797	–0.206	5.582	–0.816	–0.155
H	4.850	0.874	–0.120	4.809	0.844	–0.349	4.908	0.840	–0.117	4.933	0.824	–0.045
H	1.539	1.013	1.944	1.664	1.166	1.944	1.608	1.168	1.896	1.600	1.168	1.886
H	0.162	0.738	–1.034	0.107	0.728	–0.999	0.087	0.740	–1.065	0.079	0.743	–1.075
H	–0.401	2.376	–1.344	–0.496	2.356	–1.287	–0.518	2.370	–1.339	–0.527	2.375	–1.344
H	–1.307	2.553	0.943	–1.242	2.555	1.052	–1.270	2.546	1.002	–1.276	2.545	0.997
H	–0.663	0.987	1.375	–0.579	0.990	1.455	–0.600	0.978	1.391	–0.602	0.977	1.383
H	–2.070	–3.088	–0.338	–1.886	–3.002	–0.579	–1.979	–3.036	–0.582	–1.993	–3.041	–0.575
H	–1.057	–3.120	1.128	–0.979	–3.149	0.936	–0.965	–3.144	0.869	–0.959	–3.142	0.863
H	–2.805	–2.845	1.245	–2.733	–2.955	0.978	–2.713	–2.939	1.029	–2.706	–2.939	1.045
H	3.134	1.510	1.410	3.222	1.590	1.253	3.175	1.623	1.253	3.167	1.629	1.249

TABLE S-III. The *x*, *y* and *z* coordinates for CimC optimized at the wB97XD/def2TZVP level of theory in different solvents

El.	Gas			H_2O			MeOH			EtOH		
	x	*y*	z	*x*	*y*	*z*	*x*	*y*	*z*	*x*	*y*	*z*
S	–1.130	–0.831	–0.683	1.096	–0.717	0.701	1.108	–0.824	0.675	1.112	–0.874	0.662
N	–5.419	0.609	–0.110	5.455	0.606	0.093	5.465	0.497	0.099	5.447	0.518	0.107
C	–4.084	0.911	0.006	4.162	0.927	–0.231	4.161	0.900	–0.024	4.136	0.901	0.003
N	–4.466	–1.202	0.702	4.429	–1.312	–0.231	4.375	–1.253	–0.657	4.383	–1.224	–0.703
C	–2.081	–0.460	0.835	2.119	–0.510	–0.794	2.050	–0.331	–0.807	2.042	–0.338	–0.812
C	–3.514	–0.225	0.513	3.540	–0.275	–0.432	3.498	–0.200	–0.498	3.489	–0.193	–0.505
C	–5.593	–0.668	0.321	5.565	–0.738	0.079	5.545	–0.792	–0.290	5.547	–0.756	–0.327
N	3.074	1.117	–0.293	–3.200	1.095	0.456	–3.126	1.125	0.277	–3.099	1.127	0.263
N	2.925	–1.157	–0.537	–2.923	–1.180	0.394	–2.940	–1.145	0.490	–2.943	–1.143	0.499
C	0.533	–0.889	0.046	–0.523	–0.872	–0.092	–0.546	–0.886	–0.058	–0.548	–0.912	–0.060
C	3.796	2.156	0.086	–3.914	2.154	0.206	–3.799	2.184	–0.067	–3.757	2.193	–0.090
C	1.571	–1.067	–1.056	–1.592	–1.112	0.964	–1.597	–1.062	1.030	–1.596	–1.073	1.033
C	3.610	–0.069	–0.118	–3.667	–0.105	0.111	–3.657	–0.084	0.105	–3.648	–0.076	0.107
C	–3.508	2.226	–0.385	3.673	2.327	–0.290	3.705	2.267	0.332	3.657	2.248	0.408
N	4.416	3.076	0.422	–4.486	3.153	0.018	–4.331	3.179	–0.350	–4.276	3.192	–0.383
N	4.819	–0.269	0.450	–4.850	–0.292	–0.482	–4.867	–0.291	–0.424	–4.864	–0.271	–0.412
C	5.475	–1.548	0.579	–5.383	–1.583	–0.864	–5.489	–1.588	–0.587	–5.502	–1.562	–0.564
H	–6.557	–1.148	0.336	6.494	–1.241	0.295	6.474	–1.339	–0.291	6.486	–1.287	–0.351
H	–6.135	1.224	–0.450	6.194	1.261	0.292	6.232	1.068	0.417	6.206	1.091	0.441

TABLE S-III. Continued

El.	Gas			H_2O			MeOH			EtOH		
	x	*y*	*z*	*x*	*y*	*z*	*x*	*y*	*z*	*x*	*y*	*z*
H	–3.658	2.427	–1.447	3.648	2.780	0.704	3.852	2.468	1.396	3.802	2.414	1.478
H	–3.950	3.047	0.183	4.315	2.945	–0.921	4.251	3.028	–0.229	4.191	3.038	–0.127
H	–2.435	2.227	–0.204	2.663	2.357	–0.697	2.643	2.380	0.114	2.594	2.351	0.193
H	–2.002	–1.301	1.520	2.026	–1.408	–1.404	1.902	–1.086	–1.580	1.903	–1.078	–1.601
H	–1.633	0.418	1.300	1.720	0.334	–1.357	1.641	0.614	–1.167	1.618	0.609	–1.149
H	0.728	0.045	0.572	–0.740	0.045	–0.641	–0.721	0.047	–0.595	–0.712	0.026	–0.592
H	0.588	–1.717	0.755	–0.500	–1.704	–0.799	–0.601	–1.713	–0.769	–0.621	–1.735	–0.773
H	1.378	–1.980	–1.619	–1.413	–2.058	1.473	–1.422	–1.986	1.581	–1.430	–1.998	1.586
H	1.527	–0.229	–1.748	–1.574	–0.323	1.714	–1.550	–0.237	1.741	–1.536	–0.246	1.741
H	3.252	–2.058	–0.246	–3.230	–2.074	0.049	–3.310	–2.064	0.313	–3.326	–2.057	0.332
H	5.314	0.565	0.719	–5.399	0.526	–0.689	–5.399	0.522	–0.686	–5.383	0.546	–0.688
H	4.922	–2.222	1.238	–4.746	–2.077	–1.601	–4.903	–2.233	–1.246	–4.928	–2.216	–1.225
H	6.454	–1.390	1.021	–6.360	–1.425	–1.311	–6.465	–1.438	–1.040	–6.480	–1.403	–1.010
H	5.616	–2.030	–0.391	–5.502	–2.236	0.003	–5.628	–2.088	0.375	–5.639	–2.056	0.401

TABLE S-IV. The *x*, *y* and *z* coordinates for CimD optimized at the wB97XD/def2TZVP level of theory in different solvents

El.	Gas			H_2O			MeOH			EtOH		
	x	*y*	z	*x*	*y*	*z*	*x*	*y*	*z*	*x*	*y*	*z*
S	0.225	–1.868	0.955	0.111	–1.299	1.108	0.409	–1.687	1.043	0.419	–1.705	1.032
N	3.856	0.871	–0.570	4.233	0.313	–0.539	4.155	0.693	–0.682	4.150	0.709	–0.678
N	3.352	–0.802	0.764	3.410	–0.355	1.387	3.625	–0.547	1.050	3.627	–0.550	1.042
N	–1.837	–0.808	–1.217	–2.052	–0.849	–1.220	–1.991	–0.860	–0.996	–1.989	–0.860	–0.988
N	–3.564	–0.035	0.105	–3.703	–0.123	0.209	–3.865	–0.114	0.100	–3.866	–0.112	0.101
N	–1.714	1.323	–0.365	–1.977	1.318	–0.458	–1.967	1.254	–0.102	–1.967	1.255	–0.098
N	–2.712	3.115	1.022	–2.724	3.130	1.037	–2.988	3.130	1.122	–2.990	3.134	1.119
C	4.287	–0.263	0.037	4.489	–0.272	0.649	4.593	–0.176	0.252	4.593	–0.168	0.247
C	2.257	0.020	0.628	2.404	0.211	0.629	2.501	0.118	0.605	2.500	0.115	0.605
C	2.546	1.069	–0.204	2.901	0.636	–0.573	2.815	0.899	–0.475	2.810	0.908	–0.468
C	1.760	2.247	–0.663	2.274	1.302	–1.744	2.012	1.811	–1.332	2.003	1.825	–1.315
C	0.974	–0.249	1.331	1.002	0.293	1.109	1.178	–0.047	1.259	1.178	–0.062	1.259
C	0.350	–1.917	–0.842	0.181	–1.753	–0.638	0.293	–1.809	–0.754	0.295	–1.812	–0.765
C	–0.440	–0.849	–1.596	–0.648	–0.888	–1.580	–0.616	–0.800	–1.442	–0.617	–0.798	–1.442
C	–2.363	0.184	–0.468	–2.573	0.126	–0.458	–2.614	0.109	–0.318	–2.614	0.110	–0.314
C	–4.210	–1.322	0.200	–4.331	–1.423	0.322	–4.608	–1.337	–0.118	–4.608	–1.335	–0.115
C	–2.260	2.267	0.374	–2.407	2.245	0.346	–2.546	2.218	0.549	–2.546	2.221	0.550
H	5.288	–0.645	–0.092	5.474	–0.612	0.924	5.623	–0.494	0.308	5.623	–0.483	0.299
H	4.393	1.466	–1.174	4.903	0.500	–1.267	4.715	1.125	–1.400	4.708	1.149	–1.393
H	1.843	2.381	–1.744	2.072	0.592	–2.549	1.835	1.379	–2.320	1.824	1.400	–2.307
H	0.704	2.121	–0.429	1.331	1.766	–1.457	1.047	2.015	–0.871	1.038	2.023	–0.851
H	0.252	0.538	1.119	0.426	1.009	0.523	0.476	0.712	0.914	0.472	0.696	0.920
H	1.129	–0.284	2.410	0.966	0.616	2.150	1.267	0.060	2.342	1.268	0.037	2.342
H	1.400	–1.852	–1.131	1.220	–1.750	–0.973	1.291	–1.726	–1.190	1.291	–1.726	–1.205
H	0.001	–2.916	–1.115	–0.172	–2.786	–0.675	–0.058	–2.825	–0.944	–0.056	–2.828	–0.961

TABLE S-IV. Continued

El.	Gas			H_2O			MeOH			EtOH		
	x	*y*	*z*	*x*	*y*	*z*	*x*	*y*	*z*	*x*	*y*	*z*
H	–0.362	–1.043	–2.669	–0.556	–1.296	–2.587	–0.586	–0.997	–2.516	–0.593	–0.989	–2.518
H	–2.302	–1.697	–1.171	–2.498	–1.751	–1.152	–2.474	–1.733	–1.129	–2.474	–1.732	–1.123
H	–0.023	0.137	–1.413	–0.275	0.131	–1.604	–0.258	0.213	–1.286	–0.258	0.213	–1.281
H	–3.917	0.723	0.665	–4.132	0.650	0.690	–4.331	0.638	0.580	–4.330	0.639	0.584
H	–4.497	–1.703	–0.784	–4.729	–1.766	–0.635	–4.742	–1.541	–1.183	–4.740	–1.541	–1.180
H	–5.122	–1.206	0.781	–5.155	–1.336	1.025	–5.590	–1.216	0.331	–5.591	–1.214	0.332
H	2.103	3.168	–0.185	2.927	2.081	–2.141	2.524	2.765	–1.473	2.512	2.782	–1.450
H	–3.575	–2.056	0.705	–3.629	–2.164	0.708	–4.120	–2.192	0.356	–4.121	–2.190	0.360

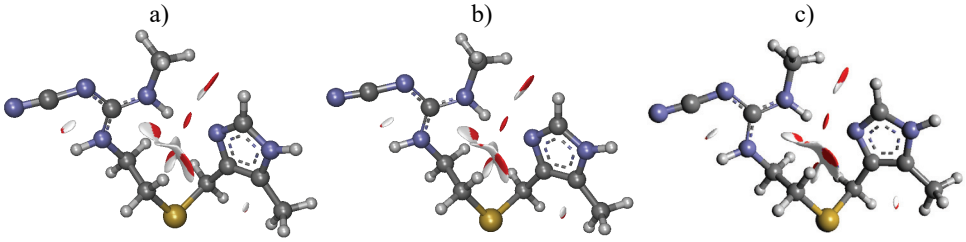

Fig. S-3. NCI Isosurfaces $\rho = 0.3$ for CimA in: a) H_2O, b) MeOH and c) EtOH.

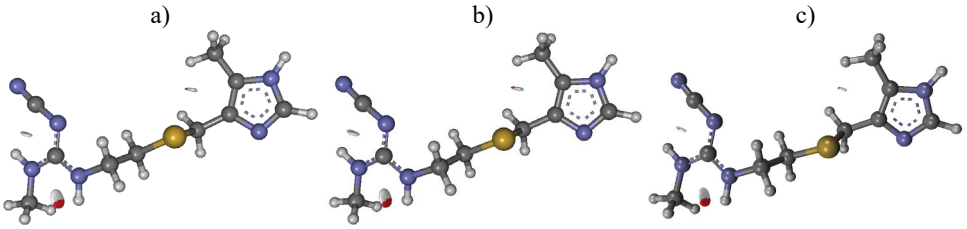

Fig. S-4. NCI Isosurfaces $\rho = 0.3$ for CimC in: a) H_2O, b) MeOH and c) EtOH.

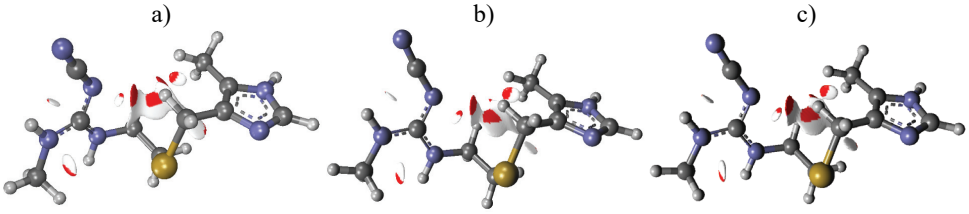

Fig S-5. NCI Isosurfaces $\rho = 0.3$ for CimD in: a) H_2O, b) MeOH and c) EtOH

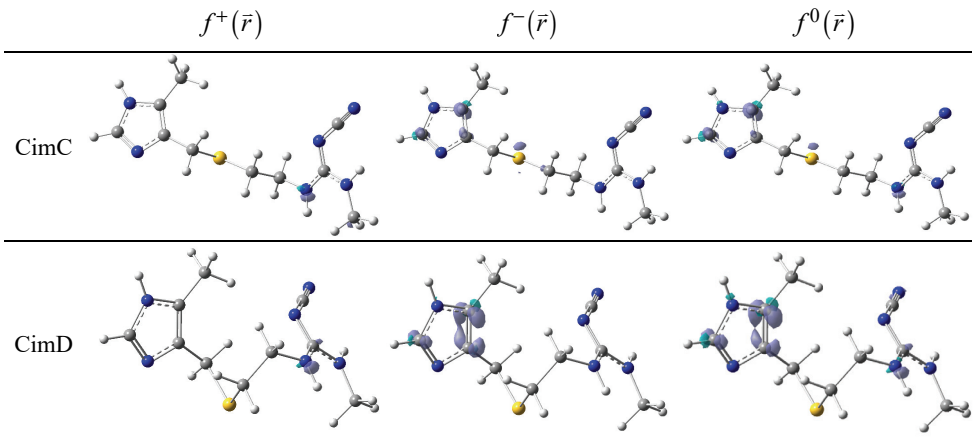

Fig. S-6. Local reactivities for CimC and CimD in the gas phase at the wB97XD/ /def2TZVP level of theory according to Eqs. (6)–(8).

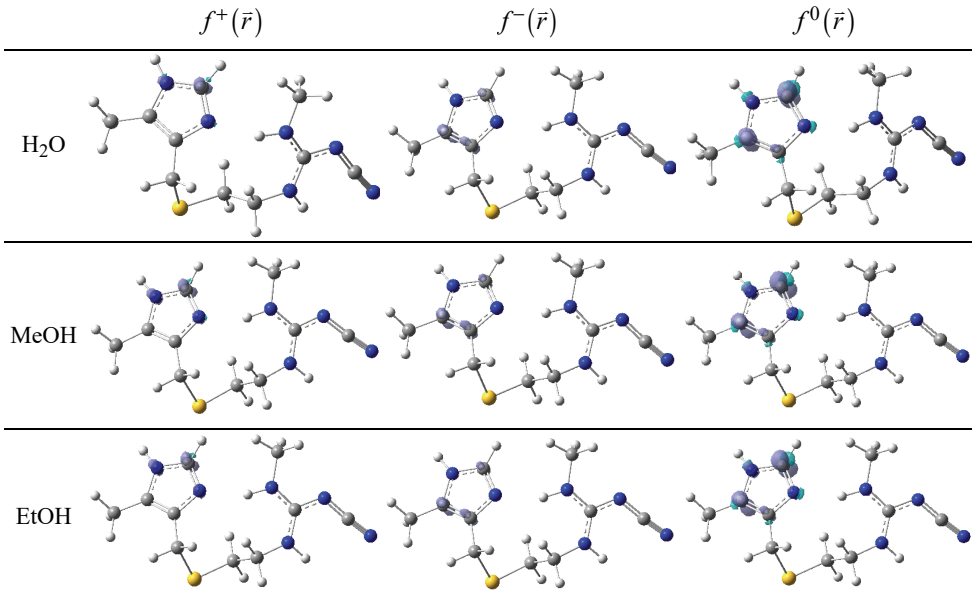

Fig. S-7. Local reactivities for CimA at the wB97XD/def2TZVP level of theory according to Eqs. (6)–(8) in different solvents.

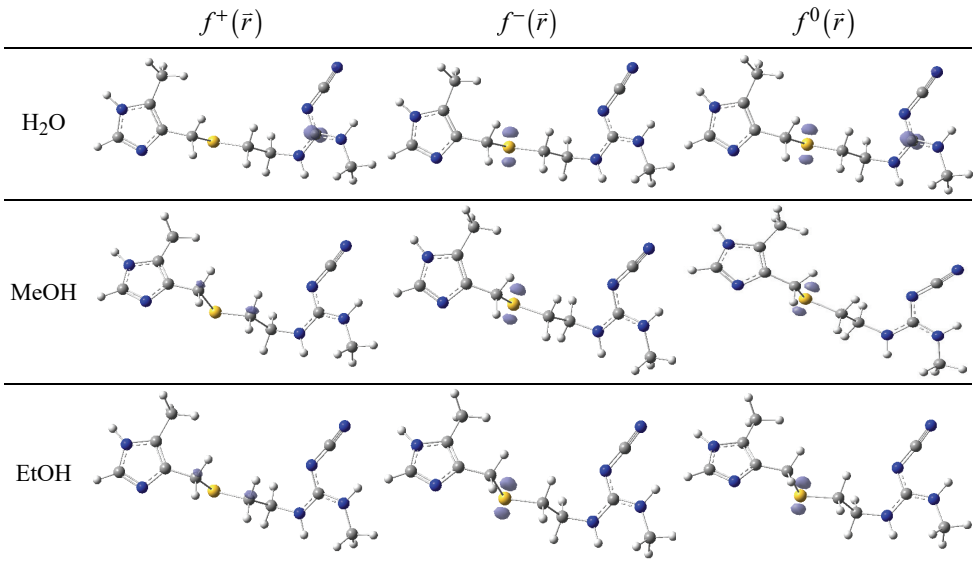

Fig. S-8. Local reactivities for CimC at the wB97XD/def2TZVP level of theory according to Eqs. (6)–(8) in different solvents.

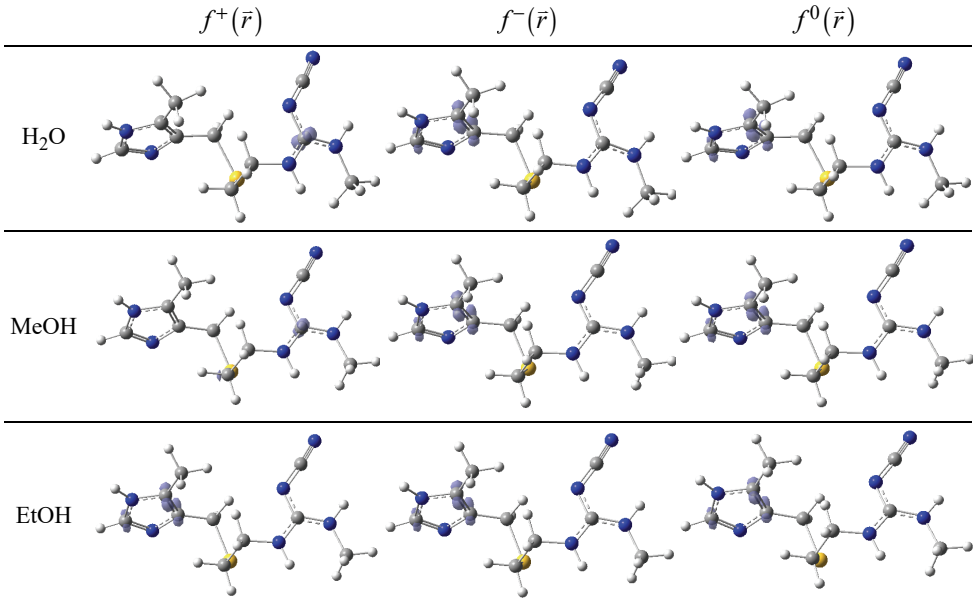

Fig. S-9. Local reactivities for CimD at the wB97XD/def2TZVP level of theory according to Eqs. (6)–(8) in different solvents.