SUPPLEMENTARY INFORMATION

A combined Electrochemical and Theoretical study of pyridine-based Schiff bases as novel corrosion inhibitors for mild steel in hydrochloric acid medium

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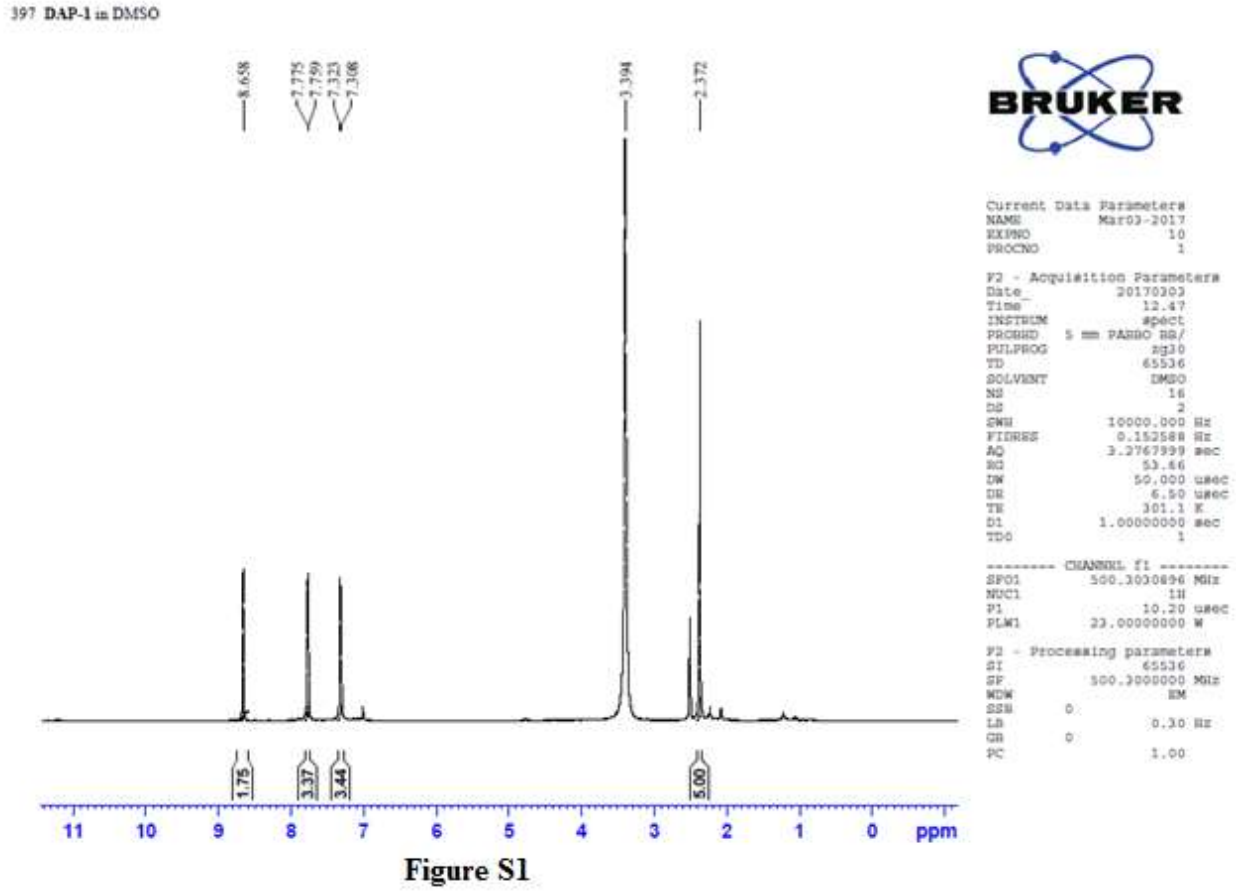

Figure S1

Figure S1. NMR spectrum of DAP-1

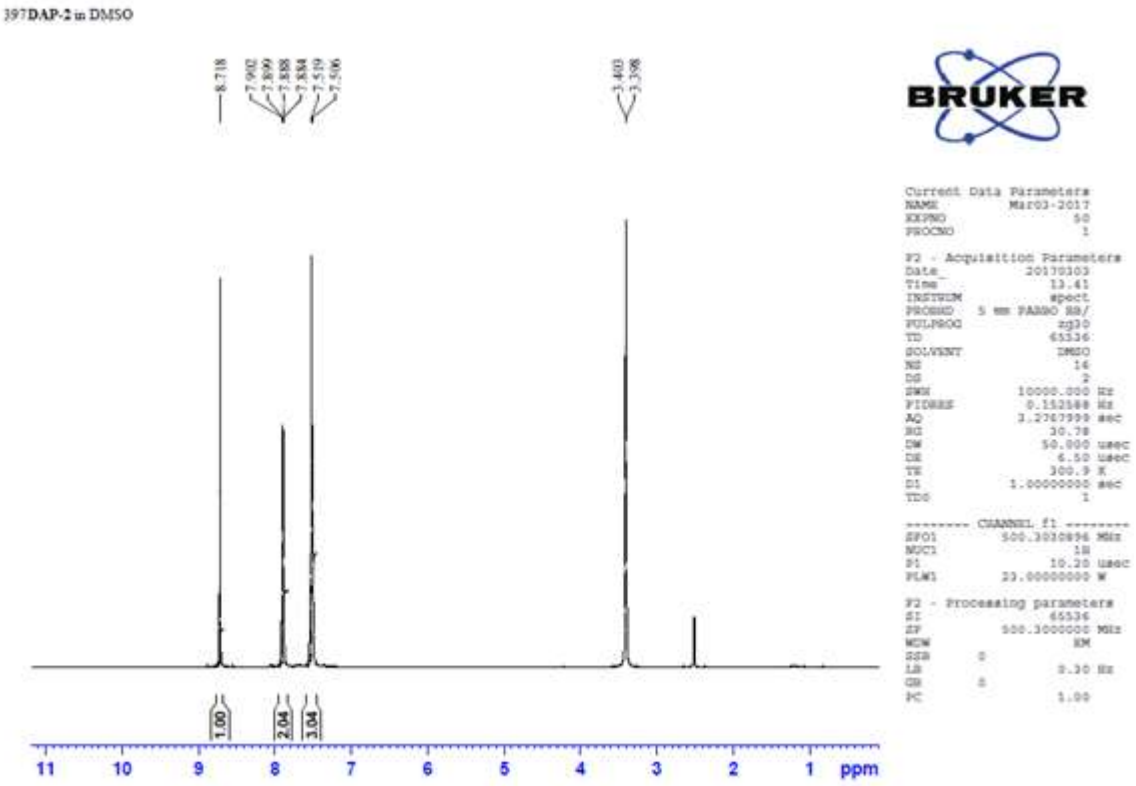

Figure S2

Figure S2. NMR spectrum of DAP-2

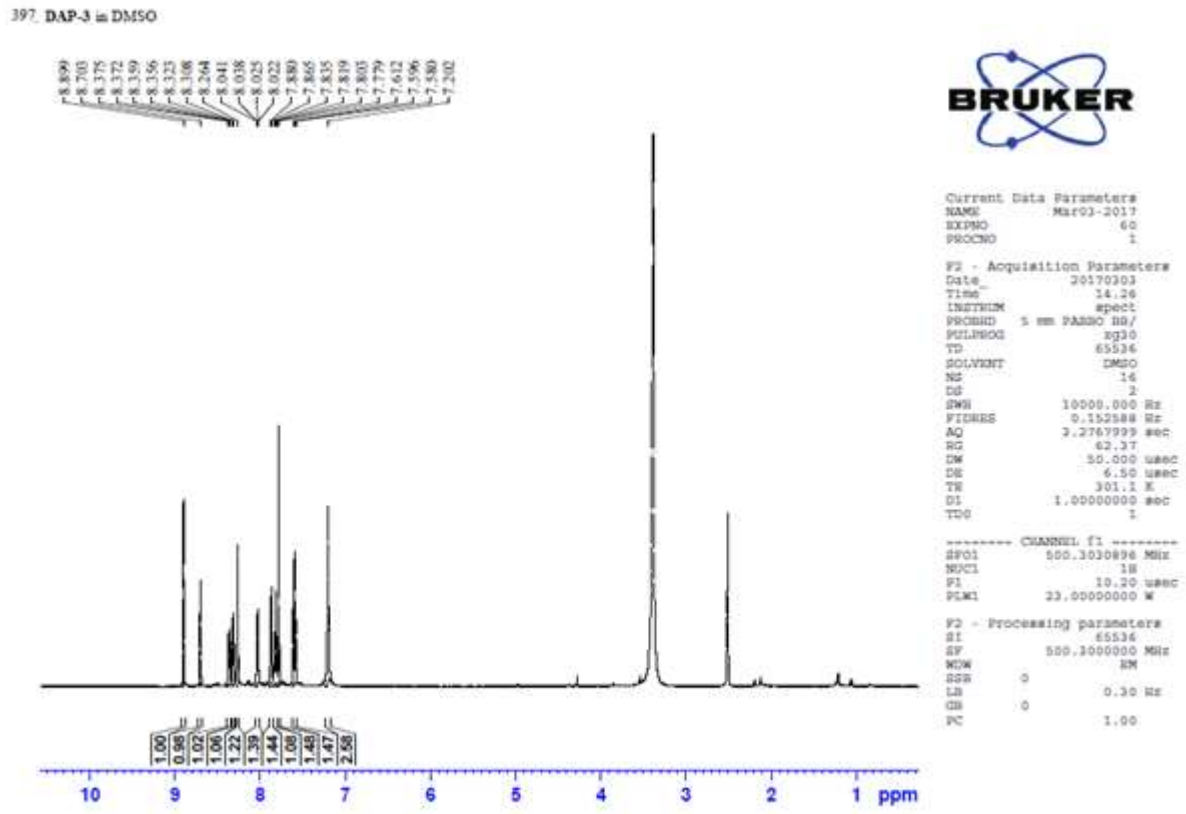

Figure S3

Figure S3. NMR spectrum of DAP-3

Table S1. *fchk* file of DAP-1 NEUTRAL molecule

Summary of Natural Population Analysis: ne

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.46256	1.99904	4.44946	0.01406	6.46256
C	2	0.46813	1.99925	3.50528	0.02734	5.53187
N	3	-0.56684	1.99938	5.55117	0.01629	7.56684
C	4	0.49292	1.99918	3.48061	0.02729	5.50708
C	5	-0.47213	1.99900	4.46053	0.01260	6.47213
C	6	-0.26664	1.99925	4.25176	0.01564	6.26664
N	7	-0.58693	1.99926	5.56059	0.02708	7.58693
N	8	-0.56686	1.99924	5.53956	0.02806	7.56686
C	9	0.10945	1.99915	3.86738	0.02402	5.89055
C	10	0.15856	1.99915	3.81951	0.02279	5.84144
C	11	-0.21792	1.99867	4.19975	0.01951	6.21792
C	12	-0.22236	1.99920	4.20980	0.01336	6.22236
C	13	-0.37233	1.99907	4.36040	0.01286	6.37233
C	14	0.06805	1.99914	3.91767	0.01514	5.93195
C	15	-0.36356	1.99906	4.35133	0.01317	6.36356
C	16	-0.23140	1.99919	4.21731	0.01489	6.23140
C	17	-0.21797	1.99868	4.20007	0.01922	6.21797

C	18	-0.22812	1.99920	4.21540	0.01352	6.22812
C	19	-0.37153	1.99907	4.35960	0.01287	6.37153
C	20	0.06272	1.99914	3.92299	0.01514	5.93728
C	21	-0.36307	1.99906	4.35081	0.01319	6.36307
C	22	-0.23704	1.99919	4.22303	0.01482	6.23704
C	23	-1.05965	1.99941	5.05276	0.00749	7.05965
C	24	-1.05936	1.99941	5.05250	0.00746	7.05936
H	25	0.34804	0.00000	0.65035	0.00161	0.65196
H	26	0.31878	0.00000	0.67876	0.00246	0.68122
H	27	0.34076	0.00000	0.65794	0.00130	0.65924
H	28	0.29527	0.00000	0.70191	0.00283	0.70473
H	29	0.25563	0.00000	0.74146	0.00290	0.74437
H	30	0.34286	0.00000	0.65585	0.00129	0.65714
H	31	0.34708	0.00000	0.65157	0.00135	0.65292
H	32	0.34733	0.00000	0.65132	0.00134	0.65267
H	33	0.34341	0.00000	0.65447	0.00211	0.65659
H	34	0.34294	0.00000	0.65574	0.00132	0.65706
H	35	0.34702	0.00000	0.65163	0.00135	0.65298
H	36	0.34721	0.00000	0.65144	0.00135	0.65279
H	37	0.34346	0.00000	0.65450	0.00204	0.65654
H	38	0.35757	0.00000	0.64132	0.00111	0.64243
H	39	0.36800	0.00000	0.63091	0.00110	0.63200
H	40	0.36800	0.00000	0.63091	0.00110	0.63200
H	41	0.35756	0.00000	0.64133	0.00111	0.64244
H	42	0.36776	0.00000	0.63114	0.00110	0.63224

H 43 0.36777 0.00000 0.63113 0.00110 0.63223

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* Total * 0.00000 47.97936 117.58296 0.43768 166.00000

Summary of Natural Population Analysis:

Table S2. ***fchk* file of** DAP-1 CATION molecule

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.19111	1.99903	4.17837	0.01371	6.19111
C	2	0.51611	1.99924	3.45543	0.02922	5.48389
N	3	-0.57593	1.99938	5.56083	0.01572	7.57593
C	4	0.52805	1.99916	3.44577	0.02702	5.47195
C	5	-0.19504	1.99899	4.18275	0.01330	6.19504
C	6	-0.30875	1.99923	4.29410	0.01542	6.30875
N	7	-0.53694	1.99915	5.51211	0.02568	7.53694
N	8	-0.50595	1.99923	5.47886	0.02785	7.50595
C	9	0.16372	1.99914	3.81291	0.02422	5.83628
C	10	0.19336	1.99914	3.78445	0.02305	5.80664
C	11	-0.20134	1.99865	4.18345	0.01924	6.20134
C	12	-0.20019	1.99920	4.18772	0.01327	6.20019
C	13	-0.36991	1.99906	4.35805	0.01280	6.36991
C	14	0.10924	1.99914	3.87654	0.01508	5.89076
C	15	-0.36601	1.99906	4.35382	0.01313	6.36601

C	16	-0.20807	1.99919	4.19401	0.01488	6.20807
C	17	-0.19643	1.99867	4.17899	0.01877	6.19643
C	18	-0.19763	1.99919	4.18504	0.01340	6.19763
C	19	-0.36972	1.99906	4.35783	0.01283	6.36972
C	20	0.11796	1.99914	3.86777	0.01514	5.88204
C	21	-0.36551	1.99906	4.35330	0.01315	6.36551
C	22	-0.20650	1.99919	4.19243	0.01489	6.20650
C	23	-1.06139	1.99940	5.05455	0.00744	7.06139
C	24	-1.06172	1.99940	5.05489	0.00743	7.06172
H	25	0.33850	0.00000	0.66006	0.00144	0.66150
H	26	0.30818	0.00000	0.68934	0.00247	0.69182
H	27	0.34097	0.00000	0.65763	0.00140	0.65903
H	28	0.29406	0.00000	0.70321	0.00272	0.70594
H	29	0.25452	0.00000	0.74246	0.00302	0.74548
H	30	0.34206	0.00000	0.65666	0.00128	0.65794
H	31	0.34690	0.00000	0.65174	0.00136	0.65310
H	32	0.34733	0.00000	0.65131	0.00136	0.65267
H	33	0.34280	0.00000	0.65521	0.00199	0.65720
H	34	0.34186	0.00000	0.65684	0.00130	0.65814
H	35	0.34684	0.00000	0.65179	0.00137	0.65316
H	36	0.34718	0.00000	0.65146	0.00136	0.65282
H	37	0.34260	0.00000	0.65547	0.00193	0.65740
H	38	0.35759	0.00000	0.64129	0.00112	0.64241
H	39	0.37001	0.00000	0.62890	0.00108	0.62999
H	40	0.37001	0.00000	0.62890	0.00108	0.62999

H	41	0.35760	0.00000	0.64128	0.00112	0.64240
H	42	0.37047	0.00000	0.62845	0.00108	0.62953
H	43	0.37047	0.00000	0.62844	0.00108	0.62953

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* Total * 1.00026 47.97908 116.58443 0.43622 164.99974

ummary of Natural Population Analysis:

Table S3- *fchk* file of DAP-1 ANION molecule

Natural Population

Natural ----------

Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.56050	1.99905	4.54666	0.01479	6.56050
C	2	0.43863	1.99927	3.53450	0.02760	5.56137
N	3	-0.56516	1.99939	5.54900	0.01677	7.56516
C	4	0.48504	1.99920	3.48804	0.02772	5.51496
C	5	-0.60339	1.99900	4.59001	0.01438	6.60339
C	6	-0.26257	1.99926	4.24725	0.01605	6.26257
N	7	-0.61890	1.99927	5.59232	0.02732	7.61890
N	8	-0.62885	1.99925	5.60068	0.02893	7.62885
C	9	-0.02850	1.99916	4.00452	0.02481	6.02850
C	10	0.02089	1.99916	3.95560	0.02434	5.97911
C	11	-0.21975	1.99869	4.20108	0.01997	6.21975
C	12	-0.27340	1.99920	4.26067	0.01353	6.27340
C	13	-0.36893	1.99909	4.35665	0.01320	6.36893

C	14	-0.00648	1.99914	3.99197	0.01537	6.00648
C	15	-0.35611	1.99908	4.34362	0.01341	6.35611
C	16	-0.29394	1.99919	4.27897	0.01578	6.29394
C	17	-0.21952	1.99871	4.20222	0.01859	6.21952
C	18	-0.28772	1.99920	4.27434	0.01418	6.28772
C	19	-0.36670	1.99909	4.35432	0.01329	6.36670
C	20	-0.02020	1.99914	4.00565	0.01541	6.02020
C	21	-0.35542	1.99909	4.34282	0.01352	6.35542
C	22	-0.30275	1.99919	4.28808	0.01548	6.30275
C	23	-1.05606	1.99942	5.04908	0.00756	7.05606
C	24	-1.05544	1.99942	5.04855	0.00747	7.05544
H	25	0.34955	0.00000	0.64876	0.00169	0.65045
H	26	0.32157	0.00000	0.67592	0.00251	0.67843
H	27	0.34059	0.00000	0.65812	0.00129	0.65941
H	28	0.29762	0.00000	0.69953	0.00286	0.70238
H	29	0.25912	0.00000	0.73793	0.00295	0.74088
H	30	0.34368	0.00000	0.65501	0.00132	0.65632
H	31	0.34694	0.00000	0.65173	0.00133	0.65306
H	32	0.34713	0.00000	0.65154	0.00132	0.65287
H	33	0.34443	0.00000	0.65335	0.00222	0.65557
H	34	0.34395	0.00000	0.65470	0.00135	0.65605
H	35	0.34686	0.00000	0.65182	0.00133	0.65314
H	36	0.34703	0.00000	0.65165	0.00132	0.65297
H	37	0.34452	0.00000	0.65333	0.00215	0.65548
H	38	0.35750	0.00000	0.64140	0.00110	0.64250

H	39	0.36472	0.00000	0.63413	0.00115	0.63528
H	40	0.36473	0.00000	0.63412	0.00115	0.63527
H	41	0.35750	0.00000	0.64141	0.00110	0.64250
H	42	0.36415	0.00000	0.63468	0.00117	0.63585
H	43	0.36416	0.00000	0.63467	0.00117	0.63584

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* Total *	-1.00000	47.97965	118.57041	0.44994	167.00000

Summary of Natural Population Analysis:

Table S4- *fchk* file of DAP-2 NEUTRAL molecule

Summary of Natural Population Analysis:

Natural Population

		Natural	Core	Valence	Rydberg	Total
Atom	No	Charge				
C	1	-0.45290	1.99904	4.44005	0.01381	6.45290
C	2	0.47440	1.99922	3.49888	0.02750	5.52560
N	3	-0.56822	1.99939	5.55482	0.01402	7.56822
C	4	0.49976	1.99915	3.47348	0.02761	5.50024
C	5	-0.46350	1.99900	4.45185	0.01265	6.46350
C	6	-0.26720	1.99922	4.25287	0.01511	6.26720
N	7	-0.58022	1.99928	5.55580	0.02515	7.58022

N	8	-0.55760	1.99925	5.53293	0.02542	7.55760
C	9	0.11903	1.99910	3.85857	0.02331	5.88097
C	10	0.16998	1.99909	3.80843	0.02250	5.83002
C	11	-0.21352	1.99901	4.19750	0.01700	6.21352
C	12	-0.23369	1.99914	4.22165	0.01291	6.23369
C	13	-0.35004	1.99917	4.33726	0.01361	6.35004
C	14	-0.28199	1.99917	4.26942	0.01340	6.28199
C	15	-0.34663	1.99917	4.33383	0.01364	6.34663
C	16	-0.24045	1.99914	4.22738	0.01393	6.24045
C	17	-0.21268	1.99902	4.19696	0.01670	6.21268
C	18	-0.23930	1.99914	4.22720	0.01296	6.23930
C	19	-0.34938	1.99917	4.33661	0.01361	6.34938
C	20	-0.28736	1.99917	4.27478	0.01341	6.28736
C	21	-0.34604	1.99917	4.33322	0.01365	6.34604
C	22	-0.24642	1.99913	4.23334	0.01394	6.24642
H	23	0.34697	0.00000	0.65144	0.00159	0.65303
H	24	0.31601	0.00000	0.68136	0.00263	0.68399
H	25	0.33964	0.00000	0.65895	0.00141	0.66036
H	26	0.29267	0.00000	0.70421	0.00312	0.70733
H	27	0.25093	0.00000	0.74548	0.00359	0.74907
H	28	0.34082	0.00000	0.65766	0.00152	0.65918
H	29	0.34489	0.00000	0.65374	0.00137	0.65511
H	30	0.34164	0.00000	0.65701	0.00134	0.65836
H	31	0.34445	0.00000	0.65416	0.00139	0.65555
H	32	0.34207	0.00000	0.65597	0.00196	0.65793

H	33	0.34099	0.00000	0.65748	0.00152	0.65901
H	34	0.34484	0.00000	0.65379	0.00137	0.65516
H	35	0.34179	0.00000	0.65686	0.00135	0.65821
H	36	0.34430	0.00000	0.65431	0.00139	0.65570
H	37	0.34195	0.00000	0.65605	0.00199	0.65805

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* Total *	0.00000	43.98131	105.61531	0.40337	150.00000

Table S5- *fchk* file of DAP-2 CATION molecule

Natural Population

Natural	----------				
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.18442	1.99903	4.17166	0.01373	6.18442
C	2	0.53721	1.99921	3.43616	0.02742	5.46279
N	3	-0.57820	1.99938	5.56485	0.01397	7.57820
C	4	0.54352	1.99913	3.42987	0.02747	5.45648
C	5	-0.18685	1.99899	4.17507	0.01279	6.18685
C	6	-0.30601	1.99919	4.29169	0.01513	6.30601
N	7	-0.54202	1.99927	5.51778	0.02498	7.54202
N	8	-0.50361	1.99925	5.47905	0.02531	7.50361
C	9	0.18566	1.99909	3.79188	0.02337	5.81434
C	10	0.21214	1.99908	3.76606	0.02272	5.78786
C	11	-0.20212	1.99900	4.18617	0.01694	6.20212

C	12	-0.20991	1.99914	4.19790	0.01288	6.20991
C	13	-0.35035	1.99916	4.33759	0.01359	6.35035
C	14	-0.24244	1.99917	4.22988	0.01339	6.24244
C	15	-0.35038	1.99916	4.33760	0.01362	6.35038
C	16	-0.21340	1.99913	4.20032	0.01394	6.21340
C	17	-0.19895	1.99901	4.18332	0.01662	6.19895
C	18	-0.20728	1.99914	4.19520	0.01295	6.20728
C	19	-0.35061	1.99916	4.33786	0.01359	6.35061
C	20	-0.23504	1.99917	4.22247	0.01340	6.23504
C	21	-0.35055	1.99916	4.33776	0.01363	6.35055
C	22	-0.21118	1.99913	4.19809	0.01396	6.21118
H	23	0.33709	0.00000	0.66138	0.00153	0.66291
H	24	0.30625	0.00000	0.69112	0.00263	0.69375
H	25	0.33996	0.00000	0.65863	0.00141	0.66004
H	26	0.29125	0.00000	0.70564	0.00311	0.70875
H	27	0.25023	0.00000	0.74619	0.00358	0.74977
H	28	0.33994	0.00000	0.65854	0.00151	0.66006
H	29	0.34478	0.00000	0.65385	0.00137	0.65522
H	30	0.34020	0.00000	0.65847	0.00133	0.65980
H	31	0.34447	0.00000	0.65415	0.00139	0.65553
H	32	0.34114	0.00000	0.65691	0.00195	0.65886
H	33	0.33982	0.00000	0.65866	0.00152	0.66018
H	34	0.34472	0.00000	0.65391	0.00137	0.65528
H	35	0.33987	0.00000	0.65879	0.00134	0.66013
H	36	0.34430	0.00000	0.65431	0.00139	0.65570

H	37	0.34073	0.00000	0.65728	0.00198	0.65927

* Total *	1.00000	43.98115	104.61605	0.40280	149.00000

Table S6. *fchk* file of DAP-2 ANION molecule

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.55683	1.99904	4.54345	0.01433	6.55683
C	2	0.45524	1.99924	3.51773	0.02779	5.54476
N	3	-0.56949	1.99939	5.55595	0.01415	7.56949
C	4	0.48593	1.99917	3.48689	0.02800	5.51407
C	5	-0.58826	1.99900	4.57586	0.01340	6.58826
C	6	-0.25902	1.99923	4.24436	0.01542	6.25902
N	7	-0.60280	1.99929	5.57814	0.02538	7.60280
N	8	-0.63472	1.99927	5.60936	0.02609	7.63472
C	9	0.02521	1.99910	3.95218	0.02351	5.97479
C	10	-0.00191	1.99910	3.97941	0.02339	6.00191
C	11	-0.22294	1.99904	4.20638	0.01752	6.22294
C	12	-0.29822	1.99914	4.28595	0.01312	6.29822
C	13	-0.35007	1.99918	4.33693	0.01396	6.35007

C	14	-0.38015	1.99917	4.36712	0.01386	6.38015
C	15	-0.33931	1.99918	4.32621	0.01392	6.33931
C	16	-0.32244	1.99914	4.30885	0.01445	6.32244
C	17	-0.21884	1.99904	4.20275	0.01705	6.21884
C	18	-0.27987	1.99914	4.26759	0.01313	6.27987
C	19	-0.34850	1.99918	4.33551	0.01381	6.34850
C	20	-0.34675	1.99917	4.33390	0.01369	6.34675
C	21	-0.34210	1.99918	4.32910	0.01382	6.34210
C	22	-0.29413	1.99914	4.28079	0.01420	6.29413
H	23	0.34869	0.00000	0.64968	0.00163	0.65131
H	24	0.31856	0.00000	0.67873	0.00270	0.68144
H	25	0.33941	0.00000	0.65917	0.00141	0.66059
H	26	0.29411	0.00000	0.70276	0.00313	0.70589
H	27	0.25472	0.00000	0.74159	0.00368	0.74528
H	28	0.34189	0.00000	0.65657	0.00154	0.65811
H	29	0.34484	0.00000	0.65378	0.00138	0.65516
H	30	0.34345	0.00000	0.65516	0.00139	0.65655
H	31	0.34427	0.00000	0.65434	0.00139	0.65573
H	32	0.34362	0.00000	0.65437	0.00200	0.65638
H	33	0.34168	0.00000	0.65678	0.00154	0.65832
H	34	0.34479	0.00000	0.65383	0.00137	0.65521
H	35	0.34289	0.00000	0.65574	0.00137	0.65711
H	36	0.34420	0.00000	0.65441	0.00139	0.65580
H	37	0.34285	0.00000	0.65514	0.00201	0.65715

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* Total * -1.00000 43.98155 106.60650 0.41195 151.00000

Summary of Natural Population Analysis:

Table S7. *fchk* file of DAP-3 NEUTRAL molecule

Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.43657	1.99904	4.42373	0.01381	6.43657
C	2	0.47153	1.99922	3.50181	0.02744	5.52847
N	3	-0.55976	1.99939	5.54635	0.01401	7.55976
C	4	0.49721	1.99915	3.47609	0.02755	5.50279
C	5	-0.44785	1.99900	4.43620	0.01265	6.44785
C	6	-0.26939	1.99921	4.25508	0.01510	6.26939
N	7	-0.56625	1.99928	5.54187	0.02510	7.56625
N	8	-0.54319	1.99926	5.51857	0.02537	7.54319
C	9	0.11084	1.99909	3.86677	0.02330	5.88916
C	10	0.16219	1.99909	3.81624	0.02249	5.83781
C	11	-0.18762	1.99902	4.17175	0.01685	6.18762
C	12	-0.24482	1.99914	4.23244	0.01325	6.24482
C	13	-0.29343	1.99912	4.28022	0.01409	6.29343

C	14	0.11468	1.99887	3.86781	0.01864	5.88532
C	15	-0.29415	1.99911	4.28045	0.01459	6.29415
C	16	-0.24999	1.99914	4.23661	0.01425	6.24999
C	17	-0.18642	1.99903	4.17084	0.01655	6.18642
C	18	-0.25057	1.99914	4.23812	0.01331	6.25057
C	19	-0.29285	1.99912	4.27966	0.01408	6.29285
C	20	0.10943	1.99887	3.87306	0.01864	5.89057
C	21	-0.29352	1.99911	4.27980	0.01460	6.29352
C	22	-0.25609	1.99914	4.24270	0.01425	6.25609
N	23	1.01994	1.99921	3.94112	0.03973	5.98006
N	24	1.01991	1.99921	3.94113	0.03975	5.98009
O	25	-0.44924	1.99972	6.43125	0.01827	8.44924
O	26	-0.76429	1.99986	6.75842	0.00600	8.76429
O	27	-0.45056	1.99972	6.43257	0.01827	8.45056
O	28	-0.76532	1.99986	6.75945	0.00600	8.76532
H	29	0.34650	0.00000	0.65192	0.00158	0.65350
H	30	0.31558	0.00000	0.68179	0.00263	0.68442
H	31	0.33967	0.00000	0.65892	0.00141	0.66033
H	32	0.29284	0.00000	0.70406	0.00310	0.70716
H	33	0.25112	0.00000	0.74531	0.00357	0.74888
H	34	0.34159	0.00000	0.65690	0.00151	0.65841
H	35	0.34540	0.00000	0.65264	0.00196	0.65460
H	36	0.34502	0.00000	0.65308	0.00190	0.65498
H	37	0.34324	0.00000	0.65483	0.00194	0.65676
H	38	0.34177	0.00000	0.65671	0.00151	0.65823

H	39	0.34537	0.00000	0.65267	0.00196	0.65463
H	40	0.34487	0.00000	0.65323	0.00190	0.65513
H	41	0.34316	0.00000	0.65487	0.00197	0.65684

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* Total *	0.00000	55.97809	137.47702	0.54489	194.00000

Summary of Natural Population Analysis:

Table S8. *fchk* file of DAP-3 CATION molecule

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.17894	1.99903	4.16618	0.01373	6.17894
C	2	0.53432	1.99921	3.43909	0.02738	5.46568
N	3	-0.56965	1.99938	5.55630	0.01397	7.56965
C	4	0.54104	1.99913	3.43241	0.02742	5.45896
C	5	-0.18185	1.99899	4.17007	0.01279	6.18185
C	6	-0.30684	1.99919	4.29253	0.01512	6.30684
N	7	-0.53149	1.99927	5.50728	0.02495	7.53149
N	8	-0.49315	1.99925	5.46863	0.02527	7.49315
C	9	0.17835	1.99909	3.79920	0.02336	5.82165
C	10	0.20525	1.99908	3.77295	0.02272	5.79475
C	11	-0.17871	1.99901	4.16292	0.01679	6.17871

C	12	-0.22137	1.99914	4.20901	0.01322	6.22137
C	13	-0.29484	1.99911	4.28166	0.01408	6.29484
C	14	0.15389	1.99887	3.82856	0.01869	5.84611
C	15	-0.29824	1.99910	4.28456	0.01458	6.29824
C	16	-0.22271	1.99914	4.20931	0.01426	6.22271
C	17	-0.17594	1.99901	4.16047	0.01646	6.17594
C	18	-0.21897	1.99914	4.20654	0.01329	6.21897
C	19	-0.29540	1.99911	4.28222	0.01407	6.29540
C	20	0.16121	1.99887	3.82121	0.01870	5.83879
C	21	-0.29861	1.99910	4.28492	0.01458	6.29861
C	22	-0.22067	1.99914	4.20726	0.01427	6.22067
N	23	1.01778	1.99920	3.94340	0.03962	5.98222
N	24	1.01706	1.99920	3.94413	0.03960	5.98294
O	25	-0.44344	1.99972	6.42547	0.01825	8.44344
O	26	-0.75422	1.99986	6.74836	0.00600	8.75422
O	27	-0.44278	1.99972	6.42481	0.01825	8.44278
O	28	-0.75228	1.99986	6.74641	0.00600	8.75228
H	29	0.33694	0.00000	0.66153	0.00153	0.66306
H	30	0.30614	0.00000	0.69123	0.00263	0.69386
H	31	0.33997	0.00000	0.65862	0.00141	0.66003
H	32	0.29137	0.00000	0.70553	0.00309	0.70863
H	33	0.25037	0.00000	0.74606	0.00356	0.74963
H	34	0.34073	0.00000	0.65777	0.00150	0.65927
H	35	0.34539	0.00000	0.65266	0.00196	0.65461
H	36	0.34509	0.00000	0.65301	0.00190	0.65491

H	37	0.34230	0.00000	0.65577	0.00193	0.65770
H	38	0.34062	0.00000	0.65787	0.00151	0.65938
H	39	0.34537	0.00000	0.65267	0.00196	0.65463
H	40	0.34495	0.00000	0.65315	0.00190	0.65505
H	41	0.34194	0.00000	0.65610	0.00196	0.65806

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* Total *	1.00000	55.97791	136.47785	0.54424	193.00000

Summary of Natural Population Analysis:

Table 9- *fchk* file of DAP-3 ANION molecule

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.45288	1.99904	4.43992	0.01393	6.45288
C	2	0.47334	1.99923	3.49969	0.02774	5.52666
N	3	-0.64792	1.99939	5.63432	0.01422	7.64792
C	4	0.47501	1.99916	3.49803	0.02779	5.52499
C	5	-0.45516	1.99900	4.44336	0.01279	6.45516
C	6	-0.27826	1.99921	4.26379	0.01525	6.27826
N	7	-0.58916	1.99928	5.56456	0.02532	7.58916
N	8	-0.62320	1.99927	5.59788	0.02605	7.62320
C	9	0.08034	1.99910	3.89701	0.02356	5.91966
C	10	-0.00191	1.99911	3.97986	0.02294	6.00191
C	11	-0.23259	1.99905	4.21611	0.01744	6.23259

C	12	-0.31782	1.99916	4.30504	0.01362	6.31782
C	13	-0.32106	1.99915	4.30727	0.01464	6.32106
C	14	-0.00276	1.99888	3.98505	0.01883	6.00276
C	15	-0.30827	1.99914	4.29402	0.01511	6.30827
C	16	-0.33073	1.99915	4.31676	0.01482	6.33073
C	17	-0.19355	1.99903	4.17788	0.01664	6.19355
C	18	-0.26193	1.99914	4.24943	0.01336	6.26193
C	19	-0.29781	1.99912	4.28451	0.01418	6.29781
C	20	0.09048	1.99887	3.89198	0.01866	5.90952
C	21	-0.29531	1.99912	4.28151	0.01468	6.29531
C	22	-0.26959	1.99914	4.25609	0.01436	6.26959
N	23	0.98167	1.99924	3.97905	0.04004	6.01833
N	24	1.01377	1.99921	3.94722	0.03980	5.98623
O	25	-0.50706	1.99972	6.48872	0.01862	8.50706
O	26	-0.80195	1.99986	6.79596	0.00612	8.80195
O	27	-0.45991	1.99972	6.44186	0.01833	8.45991
O	28	-0.77133	1.99986	6.76544	0.00602	8.77133
H	29	0.34682	0.00000	0.65159	0.00159	0.65318
H	30	0.31571	0.00000	0.68165	0.00264	0.68429
H	31	0.33988	0.00000	0.65871	0.00141	0.66012
H	32	0.29363	0.00000	0.70324	0.00312	0.70637
H	33	0.25465	0.00000	0.74173	0.00362	0.74535
H	34	0.34297	0.00000	0.65550	0.00153	0.65703
H	35	0.34589	0.00000	0.65212	0.00199	0.65411
H	36	0.34525	0.00000	0.65282	0.00193	0.65475

H	37	0.34493	0.00000	0.65309	0.00198	0.65507
H	38	0.34199	0.00000	0.65650	0.00152	0.65801
H	39	0.34546	0.00000	0.65257	0.00197	0.65454
H	40	0.34490	0.00000	0.65319	0.00191	0.65510
H	41	0.34345	0.00000	0.65457	0.00198	0.65655

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* Total *	-1.00000	55.97835	138.46962	0.55202	195.00000