Supplementary information for

LC-MS Analysis of *p*-Aminosalicylic Acid under Electrospray Ionization Conditions Manifests a Profound Solvent Effect

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Table of Contents

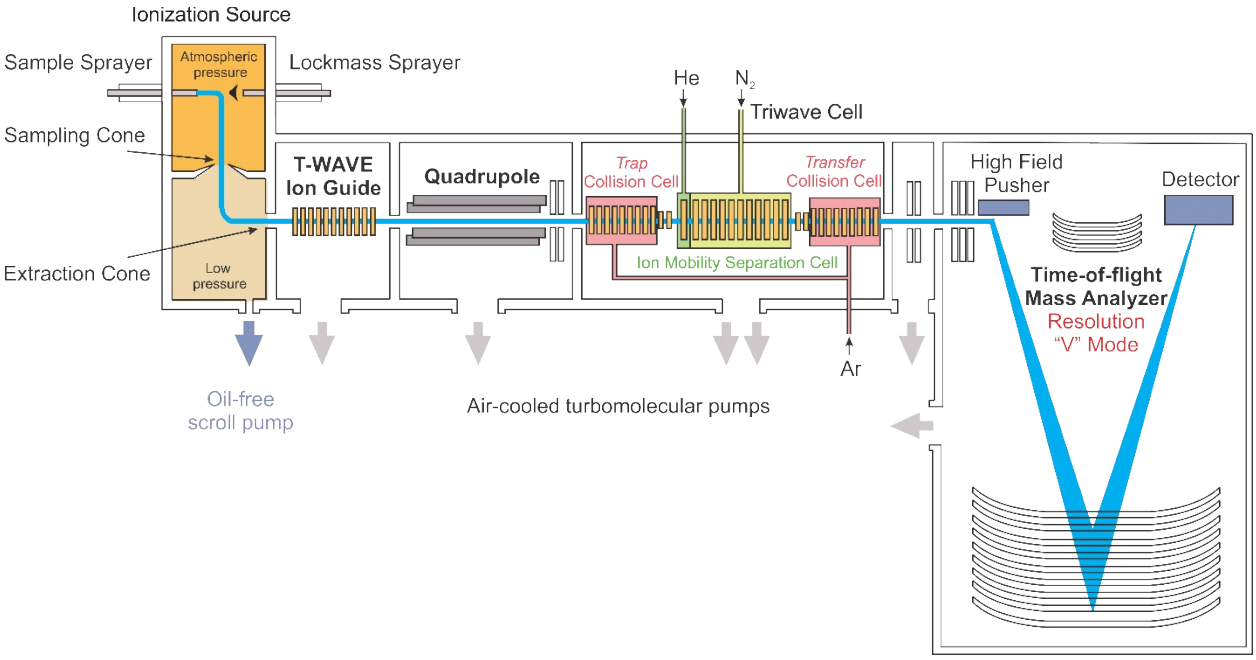


Figure S1. A Schematic diagram of Waters Synapt-G2 HDMS instrument.

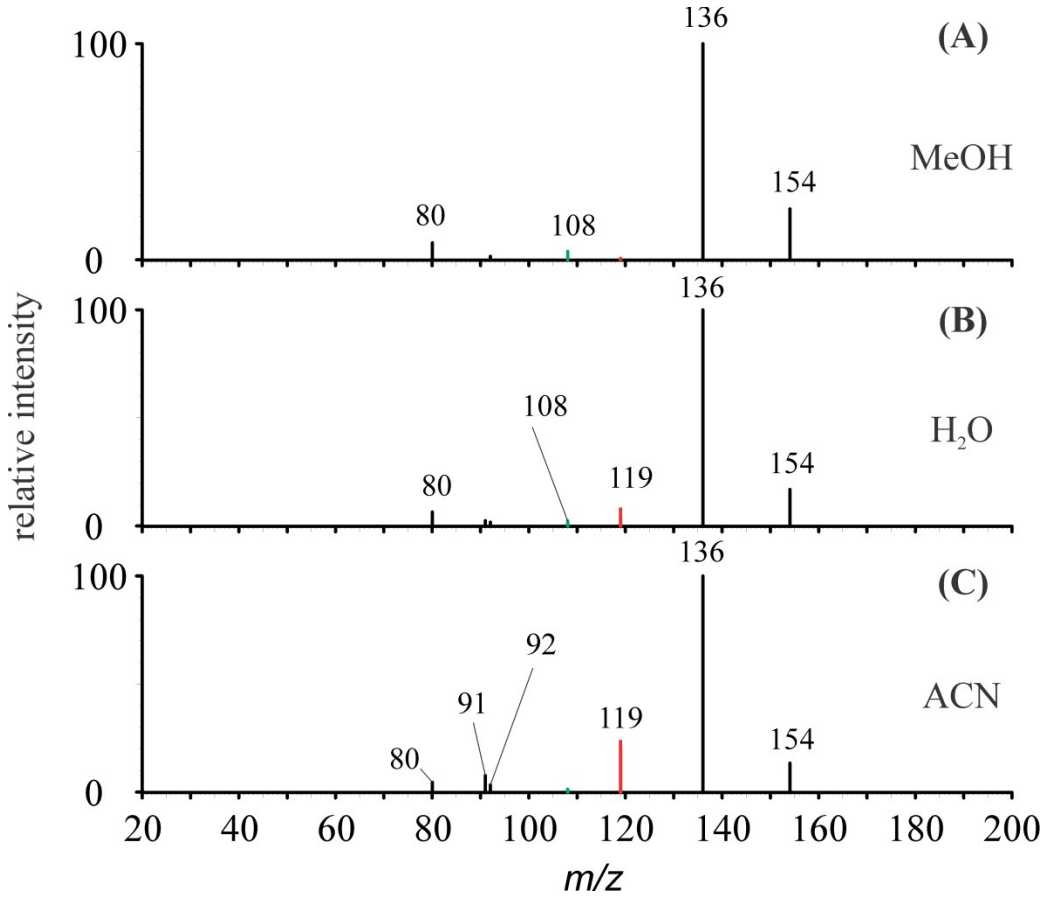


Figure S2. Product-ion mass spectra recorded from mass-selected *m/z* 154 ion of protonated *p*-aminosalicylic acid generated by electrospraying PAS samples dissolved in *neat* methanol (A) or water (B), or acetonitrile containing 1% formic acid (C). Product-ion spectra were recorded from the *m/z* 154 ion on a SYNAPT G2 HDMS instrument, without subjecting them to ion mobility separation, using argon as the collision gas at a *Trap* and *Transfer* collision energy setting of 10 eV and 2 eV, respectively.

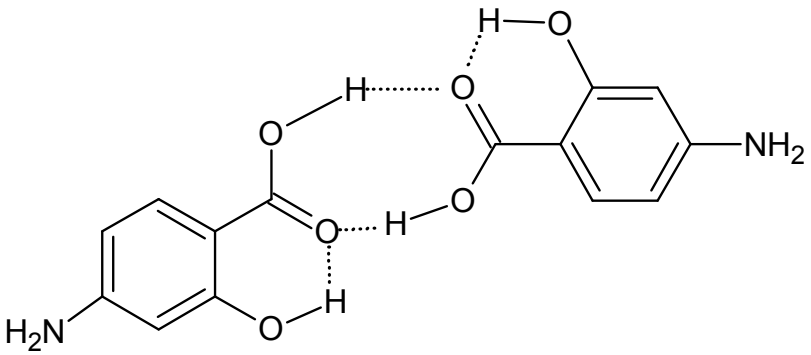


Figure S3. Proposed structure of the hydrogen bonded dimer of PAS that may exist in non-polar solvents.

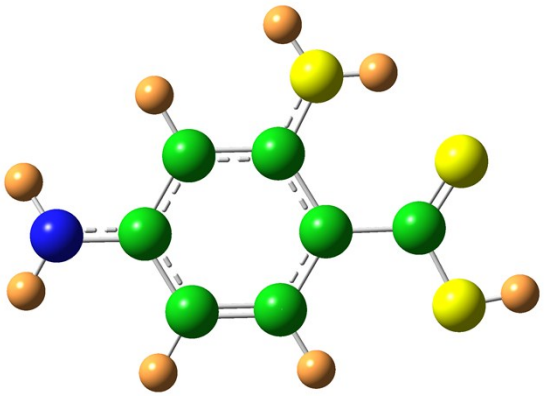
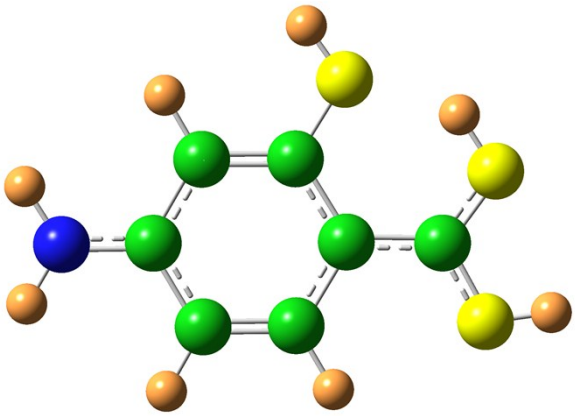
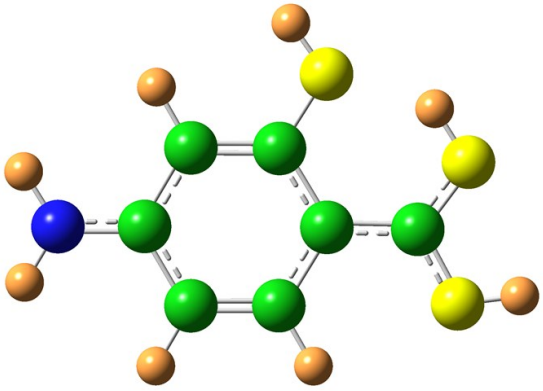
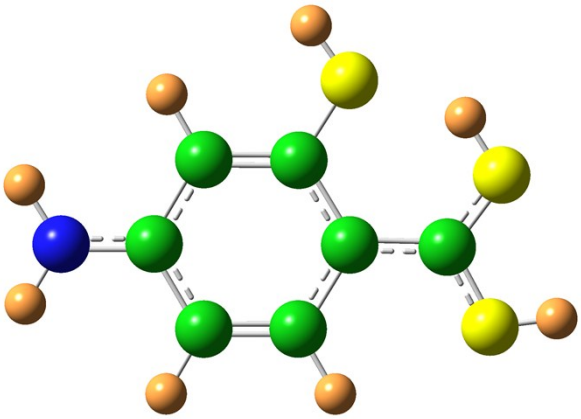
Table S1. Accurate masses and elemental compositions of protonated *p*-aminosalicylic acid and its major fragment ions.

Accurate mass (u)	Elemental Composition	Exact mass (u)	Error in ppm
154.0507	$C_7H_8NO_3$	154.0499	-5.4
136.0400	$C_7H_6NO_2$	136.0393	-5.1
119.0129	$C_7H_3O_2$	119.0128	-1.2
108.0446	C_6H_6NO	108.0444	-1.9
91.0180	C_6H_3O	91.01784	-1.7
80.0496	C_5H_6N	80.04948	-1.6
63.0237	C_5H_3	63.0230	11.1

Table S2. Relative permittivity or dielectric constant of solvents

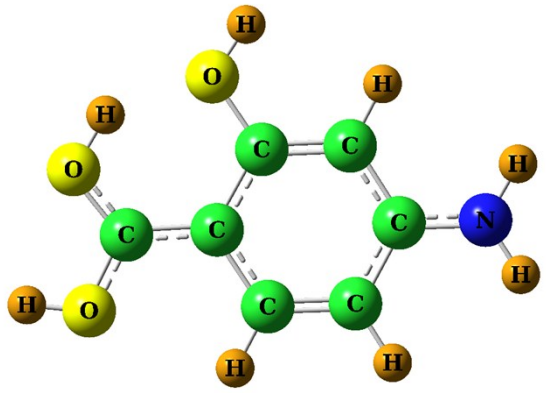
Solvent	Relative permittivity or dielectric constant
Acetonitrile (25 ^oC)	37.5
Methanol (20 ^oC)	33.6
Water (100 ^oC)	55.3
Water (20 ^oC)	80

Table S3. Input and output data for protonation on phenol OH group and carboxy carbonyl group.*

Input Data	Output Data
Protonated on phenol OH group 	Absolute electronic and Gibbs free energy -551.842468 CCS 123.67 A^2 
Protonated on carboxy carbonyl group 	Absolute electronic and Gibbs free energy -551.842467 CCS 123.91 A^2 

*Protonation on the carboxyl OH leads to dissociation.

Table S4. Atom coordinates and absolute energies of energy-optimized protonated *p*-animosalicylic acid protonated on phenol OH group



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.097971	0.984367	-0.000062
2	6	0	1.467523	1.039766	0.000068
3	6	0	2.226281	-0.151989	0.000039
4	6	0	1.549783	-1.404303	-0.000115
5	6	0	0.190350	-1.448627	-0.000191
6	6	0	-0.594818	-0.261403	-0.000126
7	1	0	1.969773	1.998305	0.000173
8	1	0	2.125606	-2.318499	-0.000178
9	1	0	-0.314936	-2.402293	-0.000268
10	7	0	3.567208	-0.109634	-0.000018
11	1	0	4.069534	0.760896	0.000687
12	1	0	4.112150	-0.954390	0.000567
13	6	0	-1.999918	-0.340102	0.000026
14	8	0	-2.820042	0.673286	0.000035
15	8	0	-2.577744	-1.513176	0.000226
16	1	0	-3.543857	-1.423783	0.000133
17	8	0	-0.670008	2.110283	-0.000136
18	1	0	-2.324913	1.519041	-0.000251
19	1	0	-0.144486	2.918762	0.000417

```
Zero-point correction=                           0.149376
(Hartree/Particle)
 Thermal correction to Energy=                    0.159130
 Thermal correction to Enthalpy=                  0.160074
 Thermal correction to Gibbs Free Energy=         0.114846
 Sum of electronic and zero-point Energies=           -551.807939
 Sum of electronic and thermal Energies=              -551.798184
 Sum of electronic and thermal Enthalpies=            -551.797240
 Sum of electronic and thermal Free Energies=         -551.842468
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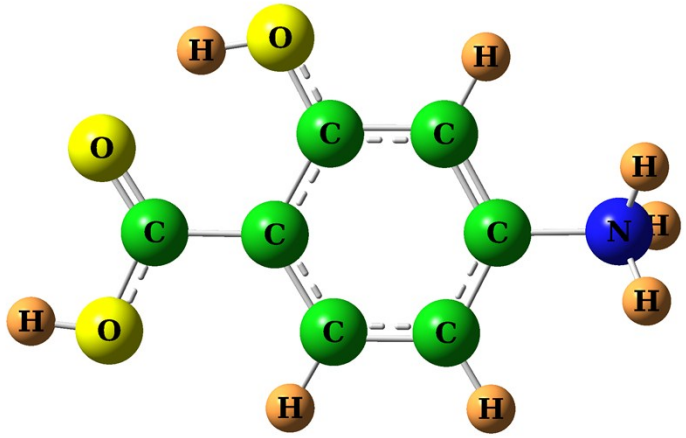
HF=-551.9573141

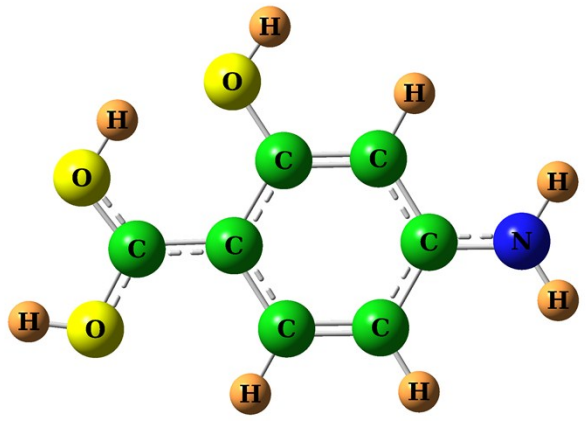
Table S5. Atom coordinates and absolute energies of energy-optimized protonated *p*-animosalicylic acid protonated on amino group



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.407230	1.042311	-0.005905
2	6	0	-2.087605	-0.152716	-0.009080
3	6	0	-1.479242	-1.398841	-0.007819
4	6	0	-0.091813	-1.423584	-0.003581
5	6	0	0.654887	-0.245583	0.000250
6	6	0	-0.002858	1.009463	-0.001573
7	1	0	-1.901292	2.004332	-0.007247
8	1	0	0.425608	-2.370660	-0.005589
9	7	0	-3.582073	-0.098331	0.012032
10	1	0	-3.926276	0.737522	-0.465888
11	1	0	-3.983813	-0.911580	-0.459688
12	6	0	2.135628	-0.258519	0.002366
13	8	0	2.805925	0.758931	0.003113
14	8	0	2.671452	-1.479938	0.003925
15	1	0	3.637202	-1.391006	0.005686
16	8	0	0.632918	2.170224	-0.001703
17	1	0	1.604046	1.990450	-0.000430
18	1	0	-2.048748	-2.317526	-0.011046
19	1	0	-3.945169	-0.082138	0.969358

Zero-point correction= 0.150947 (Hartree/Particle)
Thermal correction to Energy= 0.160706
Thermal correction to Enthalpy= 0.161651
Thermal correction to Gibbs Free Energy= 0.114239
Sum of electronic and zero-point Energies= -551.792811
Sum of electronic and thermal Energies= -551.783051
Sum of electronic and thermal Enthalpies= -551.782107
Sum of electronic and thermal Free Energies= -551.829518
HF=-551.9437571

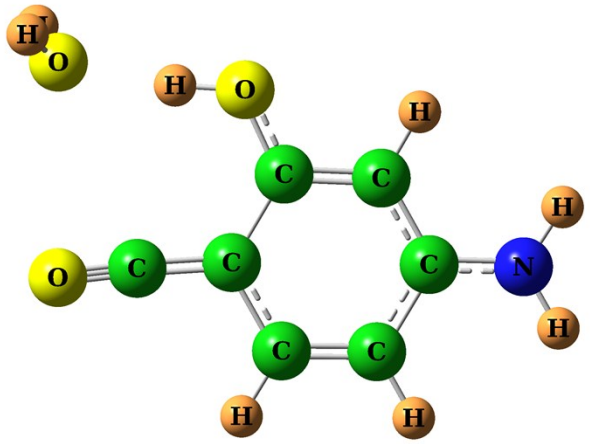
Table S6. Atom coordinates and absolute energies of energy-optimized protonated *p*-aminosalicylic acid protonated on carbonyl oxygen in carboxyl group



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.098000	0.984275	-0.000017
2	6	0	-1.467530	1.039700	0.000037
3	6	0	-2.226259	-0.152094	0.000045
4	6	0	-1.549727	-1.404362	-0.000019
5	6	0	-0.190280	-1.448653	-0.000097
6	6	0	0.594904	-0.261489	-0.000150
7	1	0	-1.969867	1.998187	0.000052
8	1	0	-2.125490	-2.318592	-0.000022
9	1	0	0.314692	-2.402506	-0.000165
10	7	0	-3.567185	-0.109759	0.000113
11	1	0	-4.069506	0.760777	0.000139
12	1	0	-4.112134	-0.954513	0.000108
13	6	0	2.000017	-0.340073	-0.000277
14	8	0	2.578122	-1.513080	0.000076
15	8	0	2.819821	0.673446	0.000238
16	1	0	2.324230	1.518918	0.000536
17	8	0	0.669779	2.110502	-0.000154
18	1	0	0.143632	2.918596	-0.000164
19	1	0	3.544210	-1.423322	0.000316

Zero-point correction= 0.149377 (Hartree/Particle)
Thermal correction to Energy= 0.159130
Thermal correction to Enthalpy= 0.160075
Thermal correction to Gibbs Free Energy= 0.114847
Sum of electronic and zero-point Energies= -551.807937
Sum of electronic and thermal Energies= -551.798184
Sum of electronic and thermal Enthalpies= -551.797239
Sum of electronic and thermal Free Energies= -551.842467
HF=-551.957314

Table S7. Atom coordinates and absolute energies of energy-optimized protonated *p*-aminosalicylic acid protonated on hydroxyl oxygen in carboxyl group



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.818887	1.626944	0.089805
2	6	0	2.088626	1.168026	0.104624
3	6	0	2.346712	-0.240000	0.018945
4	6	0	1.274745	-1.144054	-0.068608
5	6	0	-0.035245	-0.717312	-0.078807
6	6	0	-0.288583	0.707346	-0.009766
7	1	0	0.616535	2.686274	0.148570
8	1	0	2.915056	1.860001	0.178890
9	1	0	1.454987	-2.208023	-0.122929
10	7	0	3.611706	-0.676547	0.029072
11	1	0	3.828458	-1.656927	-0.031535
12	1	0	4.384681	-0.036992	0.095853
13	6	0	-1.523506	1.251483	-0.082413
14	8	0	-2.536456	1.764828	-0.151017
15	8	0	-3.553994	-1.088902	0.220783
16	1	0	-4.171305	-1.287610	-0.492151
17	8	0	-0.978401	-1.638841	-0.169264
18	1	0	-1.916552	-1.353681	-0.043569
19	1	0	-3.932816	-1.478482	1.016677

Zero-point correction= 0.144884 (Hartree/Particle)
Thermal correction to Energy= 0.156798
Thermal correction to Enthalpy= 0.157742
Thermal correction to Gibbs Free Energy= 0.105863
Sum of electronic and zero-point Energies= -551.788703
Sum of electronic and thermal Energies= -551.776789
Sum of electronic and thermal Enthalpies= -551.775845
Sum of electronic and thermal Free Energies= -551.827724
HF=-551.9335871

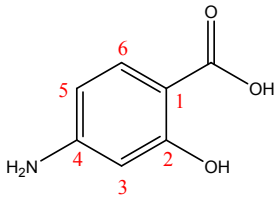
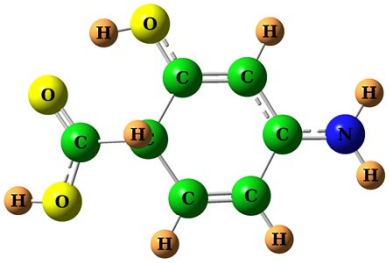


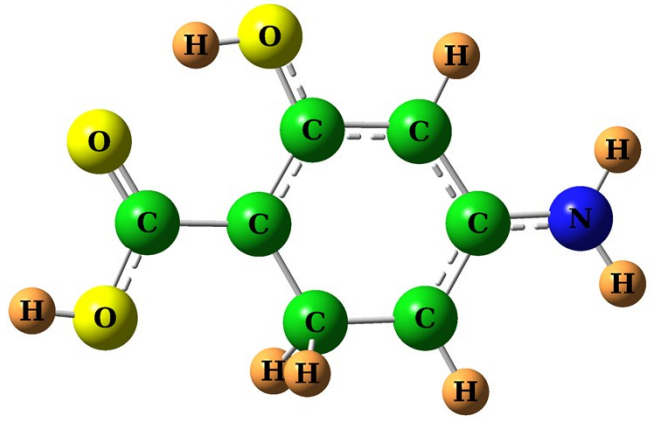
Table S8. Atom coordinates and absolute energies of energy-optimized protonated *p*-aminosalicylic acid protonated on C1 position



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.157018	-1.417339	-0.016032
2	6	0	1.529532	-1.387295	-0.013364
3	6	0	2.205862	-0.145483	-0.009397
4	6	0	1.465033	1.038194	-0.008291
5	6	0	0.076179	1.005517	-0.011018
6	6	0	-0.608991	-0.237712	-0.014955
7	1	0	-0.357172	-2.366676	-0.019020
8	1	0	2.097515	-2.307531	-0.014291
9	1	0	1.955833	2.001509	-0.005340
10	7	0	3.573376	-0.111468	-0.007026
11	1	0	4.069321	0.758937	-0.001740
12	1	0	4.108932	-0.957797	-0.005232
13	6	0	-2.057415	-0.249522	-0.017653
14	8	0	-2.767885	0.754437	-0.015793
15	8	0	-2.623677	-1.479131	-0.021919
16	1	0	-3.580074	-1.336205	-0.023080
17	8	0	-0.577647	2.177526	-0.009839
18	1	0	-1.540030	1.974498	-0.012415
19	1	0	-0.617596	-0.247278	1.054968

Zero-point correction= 0.149404 (Hartree/Particle)
Thermal correction to Energy= 0.158811
Thermal correction to Enthalpy= 0.159755
Thermal correction to Gibbs Free Energy= 0.114443
Sum of electronic and zero-point Energies= -551.792394
Sum of electronic and thermal Energies= -551.782987
Sum of electronic and thermal Enthalpies= -551.782043
Sum of electronic and thermal Free Energies= -551.827355
HF=-551.9417982

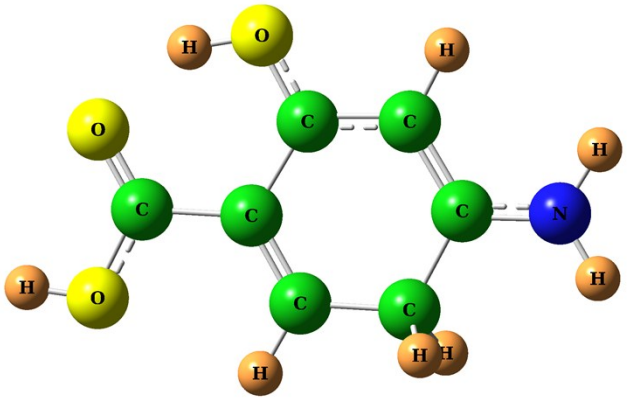
Table S9. Atom coordinates and absolute energies of energy-optimized protonated *p*-aminosalicylic acid protonated on C2 position



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.134170	-1.448797	-0.000157
2	6	0	-1.582683	-1.363070	-0.000252
3	6	0	-2.247608	-0.135023	-0.000004
4	6	0	-1.438859	1.019754	-0.000072
5	6	0	-0.025760	1.006924	-0.000059
6	6	0	0.647518	-0.211691	-0.000087
7	1	0	0.179026	-2.092415	0.843248
8	1	0	-2.142162	-2.289424	-0.000494
9	1	0	-1.903847	1.998581	-0.000099
10	7	0	-3.598067	-0.043685	0.000553
11	1	0	-4.177115	-0.864117	-0.000712
12	1	0	-4.064008	0.846050	-0.000498
13	6	0	2.119640	-0.224515	0.000036
14	8	0	2.783473	0.795860	-0.000020
15	8	0	2.642721	-1.452996	0.000209
16	1	0	3.610806	-1.384314	0.000247
17	8	0	0.565628	2.190517	-0.000038
18	1	0	1.541374	2.055631	-0.000059
19	1	0	0.179361	-2.092748	-0.843134

Zero-point correction= 0.145634 (Hartree/Particle)
Thermal correction to Energy= 0.155978
Thermal correction to Enthalpy= 0.156922
Thermal correction to Gibbs Free Energy= 0.110046
Sum of electronic and zero-point Energies= -551.757274
Sum of electronic and thermal Energies= -551.746930
Sum of electronic and thermal Enthalpies= -551.745986
Sum of electronic and thermal Free Energies= -551.792862
HF=-551.902908

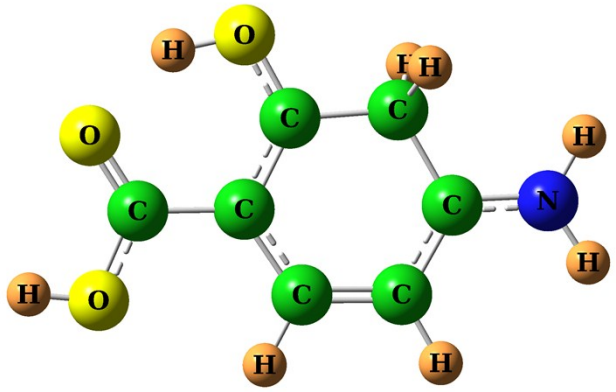
Table S10. Atom coordinates and absolute energies of energy-optimized protonated *p*-aminosalicylic acid protonated on C3 position



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.457350	1.081192	-0.000394
2	6	0	-2.215044	-0.079339	-0.000040
3	6	0	-1.548454	-1.422894	0.000189
4	6	0	-0.063913	-1.400332	-0.000034
5	6	0	0.644552	-0.260280	-0.000014
6	6	0	-0.069726	1.023699	-0.000124
7	1	0	-1.923797	2.055982	-0.000635
8	1	0	-1.888596	-2.001391	0.867705
9	1	0	0.444568	-2.354291	-0.000359
10	7	0	-3.544406	-0.053783	0.000107
11	1	0	-4.050207	0.817771	0.000162
12	1	0	-4.092304	-0.898259	-0.000068
13	6	0	2.132278	-0.240763	-0.000057
14	8	0	2.770540	0.796566	0.000155
15	8	0	2.690145	-1.444634	-0.000124
16	1	0	3.655863	-1.346280	0.000026
17	8	0	0.595245	2.142439	0.000200
18	1	0	1.572654	1.942382	0.000160
19	1	0	-1.888836	-2.002107	-0.866741

Zero-point correction= 0.149034 (Hartree/Particle)
Thermal correction to Energy= 0.158579
Thermal correction to Enthalpy= 0.159524
Thermal correction to Gibbs Free Energy= 0.114202
Sum of electronic and zero-point Energies= -551.802836
Sum of electronic and thermal Energies= -551.793291
Sum of electronic and thermal Enthalpies= -551.792346
Sum of electronic and thermal Free Energies= -551.837668
HF=-551.95187

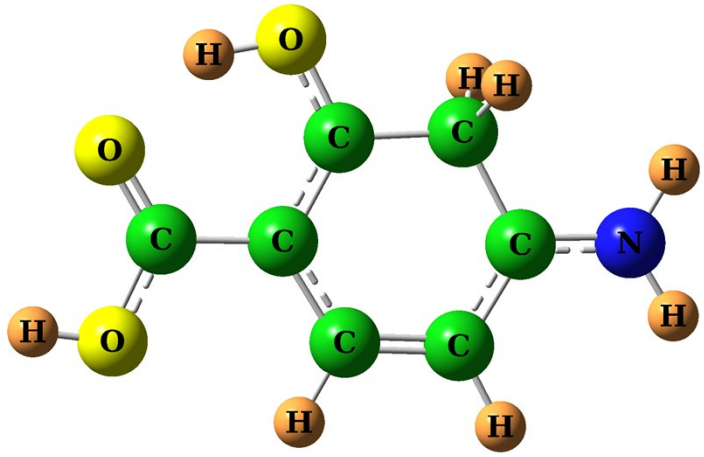
Table S11. Atom coordinates and absolute energies of energy-optimized protonated *p*-aminosalicylic acid protonated on C4 position (the proton relocates to C5 position)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.131274	-1.419894	-0.015703
2	6	0	-1.525939	-1.383693	-0.024107
3	6	0	-2.191897	-0.158250	-0.027295
4	6	0	-1.463146	1.031749	-0.020879
5	6	0	-0.068821	0.995479	-0.011997
6	6	0	0.597194	-0.230421	-0.009805
7	1	0	0.393586	-2.386155	-0.013641
8	1	0	-2.099955	-2.321626	-0.029533
9	1	0	-1.988450	1.997847	-0.023334
10	7	0	-3.661368	-0.120000	-0.036998
11	1	0	-4.138659	0.758742	-0.039282
12	1	0	-4.183716	-0.972721	-0.041315
13	6	0	2.136653	-0.270124	-0.000276
14	8	0	2.797966	0.800487	0.005068
15	8	0	2.816994	-1.527911	0.002511
16	1	0	3.765403	-1.379235	0.006315
17	8	0	0.678355	2.214734	-0.005409
18	1	0	1.617356	2.015117	0.000114
19	1	0	-2.199118	-0.159534	1.042680

Zero-point correction= 0.148871 (Hartree/Particle)
Thermal correction to Energy= 0.158389
Thermal correction to Enthalpy= 0.159333
Thermal correction to Gibbs Free Energy= 0.114002
Sum of electronic and zero-point Energies= -551.803303
Sum of electronic and thermal Energies= -551.793784
Sum of electronic and thermal Enthalpies= -551.792840
Sum of electronic and thermal Free Energies= -551.838171
HF=-551.9521732

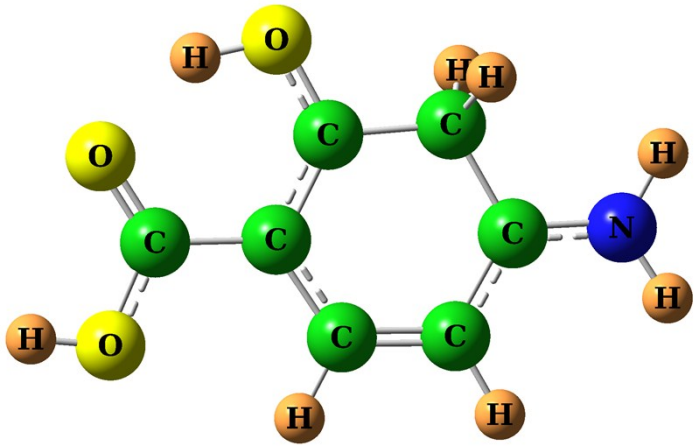
Table S12. Atom coordinates and absolute energies of energy-optimized protonated *p*-aminosalicylic acid protonated on C5 position



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.152924	-1.419097	0.000013
2	6	0	-1.531747	-1.416960	-0.000020
3	6	0	-2.227243	-0.204971	-0.000010
4	6	0	-1.474886	1.093347	0.000082
5	6	0	0.016575	0.984102	0.000008
6	6	0	0.646312	-0.253081	0.000017
7	1	0	0.359570	-2.371672	0.000032
8	1	0	-2.074200	-2.351161	-0.000055
9	1	0	-1.765738	1.691665	-0.869801
10	7	0	-3.550693	-0.147932	-0.000049
11	1	0	-4.107052	-0.989033	-0.000032
12	1	0	-4.049492	0.727636	-0.000002
13	6	0	2.116284	-0.273552	0.000000
14	8	0	2.780711	0.754524	-0.000006
15	8	0	2.655233	-1.488719	-0.000004
16	1	0	3.622003	-1.405123	0.000044
17	8	0	0.645187	2.118069	-0.000068
18	1	0	1.632073	1.912171	-0.000017
19	1	0	-1.765588	1.691322	0.870264

Zero-point correction= 0.148875 (Hartree/Particle)
Thermal correction to Energy= 0.158393
Thermal correction to Enthalpy= 0.159337
Thermal correction to Gibbs Free Energy= 0.114011
Sum of electronic and zero-point Energies= -551.803298
Sum of electronic and thermal Energies= -551.793780
Sum of electronic and thermal Enthalpies= -551.792836
Sum of electronic and thermal Free Energies= -551.838162
HF=-551.9521733

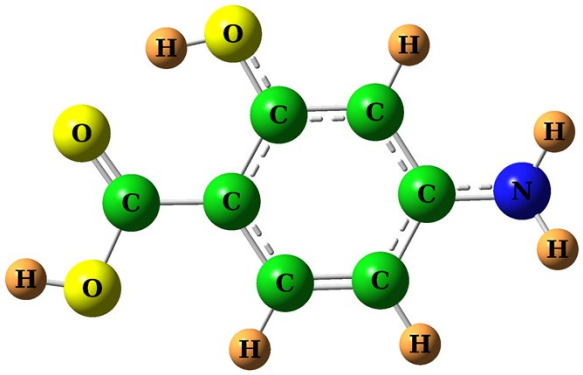
Table S13. Atom coordinates and absolute energies of energy-optimized protonated *p*-aminosalicylic acid protonated C6 position (the proton relocates to C5 position)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.016576	0.984040	0.000093
2	6	0	1.474958	1.093382	0.000401
3	6	0	2.227256	-0.204942	0.000048
4	6	0	1.531733	-1.416947	0.000206
5	6	0	0.152931	-1.419119	0.000164
6	6	0	-0.646342	-0.253081	0.000047
7	1	0	1.765477	1.691157	0.870769
8	1	0	2.074219	-2.351127	0.000242
9	1	0	-0.359568	-2.371690	0.000249
10	7	0	3.550704	-0.147976	-0.000455
11	1	0	4.049611	0.727544	-0.000590
12	1	0	4.107087	-0.989068	-0.000697
13	6	0	-2.116311	-0.273546	-0.000098
14	8	0	-2.780743	0.754538	-0.000227
15	8	0	-2.655261	-1.488693	-0.000042
16	1	0	-3.622039	-1.405105	-0.000141
17	8	0	-0.645152	2.118056	-0.000006
18	1	0	-1.632058	1.912113	-0.000145
19	1	0	1.765697	1.692075	-0.869464

Zero-point correction= 0.148876 (Hartree/Particle)
Thermal correction to Energy= 0.158391
Thermal correction to Enthalpy= 0.159336
Thermal correction to Gibbs Free Energy= 0.114019
Sum of electronic and zero-point Energies= -551.803298
Sum of electronic and thermal Energies= -551.793782
Sum of electronic and thermal Enthalpies= -551.792838
Sum of electronic and thermal Free Energies= -551.838154
HF=-551.9521733

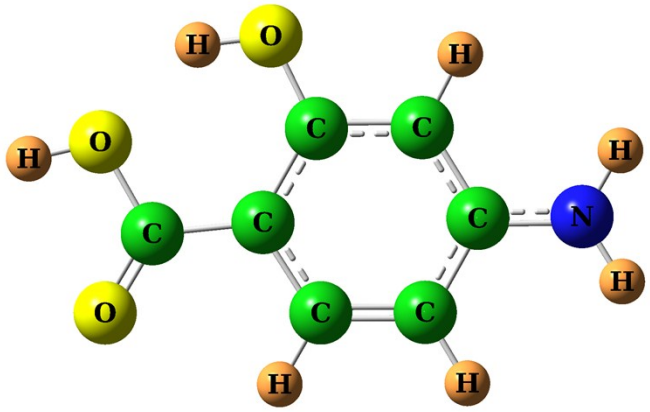
Table S14. Atom coordinates and absolute energies of energy-optimized neutral *p*-aminosalicylic acid hypothetical structure 1.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.066809	1.001914	-0.002416
2	6	0	1.456081	1.034350	-0.003329
3	6	0	2.196037	-0.146887	-0.004255
4	6	0	1.522481	-1.387649	-0.003963
5	6	0	0.150376	-1.419852	-0.001807
6	6	0	-0.615637	-0.241521	-0.001010
7	1	0	1.946825	1.998180	-0.007015
8	1	0	2.092222	-2.307134	-0.009927
9	1	0	-0.363330	-2.369828	-0.000128
10	7	0	3.571066	-0.111553	-0.049977
11	1	0	4.031889	0.749213	0.188377
12	1	0	4.073243	-0.943551	0.205646
13	6	0	-2.064580	-0.253967	0.002148
14	8	0	-2.773156	0.749494	0.004119
15	8	0	-2.628556	-1.481875	0.002738
16	1	0	-3.586021	-1.345082	0.004279
17	8	0	-0.587214	2.171186	0.000003
18	1	0	-1.550284	1.970312	0.001526

Zero-point correction= 0.137002 (Hartree/Particle)
Thermal correction to Energy= 0.146299
Thermal correction to Enthalpy= 0.147243
Thermal correction to Gibbs Free Energy= 0.102796
Sum of electronic and zero-point Energies= -551.487094
Sum of electronic and thermal Energies= -551.477797
Sum of electronic and thermal Enthalpies= -551.476853
Sum of electronic and thermal Free Energies= -551.521300
HF=-551.6240963

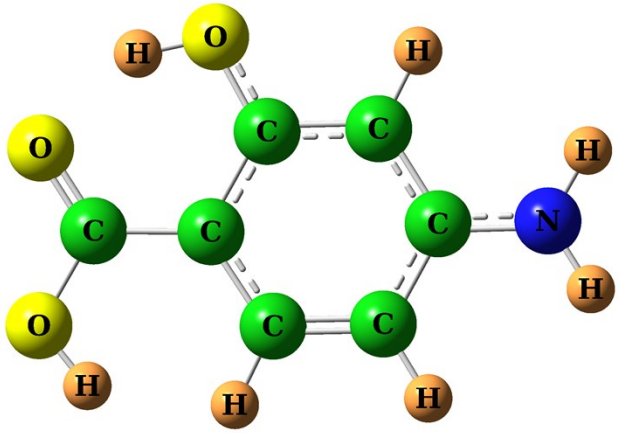
Table S15. Atom coordinates and absolute energies of energy-optimized neutral *p*-aminosalicylic acid hypothetical structure 2.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.431336	1.039941	-0.000093
2	6	0	-2.207050	-0.120570	0.000093
3	6	0	-1.561467	-1.376461	-0.000060
4	6	0	-0.190993	-1.434278	0.000056
5	6	0	0.612619	-0.278634	-0.000087
6	6	0	-0.042999	0.977220	-0.000261
7	1	0	-1.895155	2.016603	-0.000109
8	1	0	0.313606	-2.389471	0.000241
9	7	0	-3.573390	-0.047574	0.000286
10	1	0	-4.044990	0.836193	0.000270
11	1	0	-4.132196	-0.878735	0.000305
12	6	0	2.059779	-0.478667	0.000057
13	8	0	2.640960	-1.538719	0.000210
14	8	0	2.786645	0.697592	0.000177
15	1	0	3.719498	0.443354	0.000399
16	8	0	0.599193	2.166686	-0.000513
17	1	0	1.555926	2.013874	-0.000651
18	1	0	-2.148662	-2.284590	0.000315

Zero-point correction= 0.135722 (Hartree/Particle)
Thermal correction to Energy= 0.144947
Thermal correction to Enthalpy= 0.145891
Thermal correction to Gibbs Free Energy= 0.101265
Sum of electronic and zero-point Energies= -551.463702
Sum of electronic and thermal Energies= -551.454476
Sum of electronic and thermal Enthalpies= -551.453532
Sum of electronic and thermal Free Energies= -551.498159
HF=-551.5994234

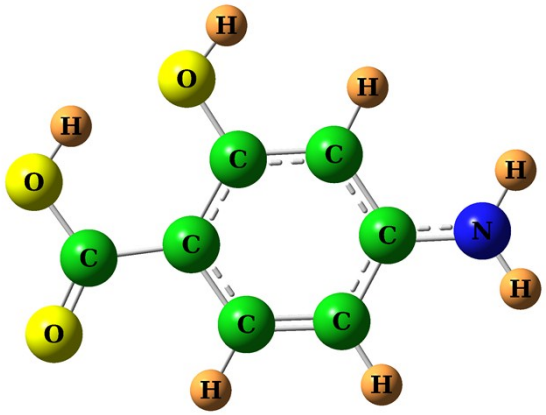
Table S16. Atom coordinates and absolute energies of energy-optimized neutral *p*-aminosalicylic acid hypothetical structure 3



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.443759	1.037442	-0.000035
2	6	0	-2.196900	-0.136314	0.000150
3	6	0	-1.528221	-1.381427	0.000254
4	6	0	-0.154980	-1.415848	0.000186
5	6	0	0.631542	-0.250367	0.000023
6	6	0	-0.053615	0.996600	-0.000115
7	1	0	-1.923881	2.006134	-0.000142
8	1	0	0.310690	-2.394147	0.000302
9	7	0	-3.563915	-0.092359	0.000253
10	1	0	-4.052786	0.782119	-0.000036
11	1	0	-4.106830	-0.933973	0.000166
12	6	0	2.094396	-0.248564	0.000033
13	8	0	2.765106	0.774204	-0.000064
14	8	0	2.760998	-1.426425	-0.000115
15	1	0	2.149592	-2.169403	-0.000162
16	8	0	0.600481	2.164073	-0.000404
17	1	0	1.565346	1.951865	-0.000617
18	1	0	-2.098195	-2.300025	0.000405

Zero-point correction= 0.135257 (Hartree/Particle)
Thermal correction to Energy= 0.144567
Thermal correction to Enthalpy= 0.145511
Thermal correction to Gibbs Free Energy= 0.099903
Sum of electronic and zero-point Energies= -551.461360
Sum of electronic and thermal Energies= -551.452051
Sum of electronic and thermal Enthalpies= -551.451106
Sum of electronic and thermal Free Energies= -551.496715
HF=-551.5966172

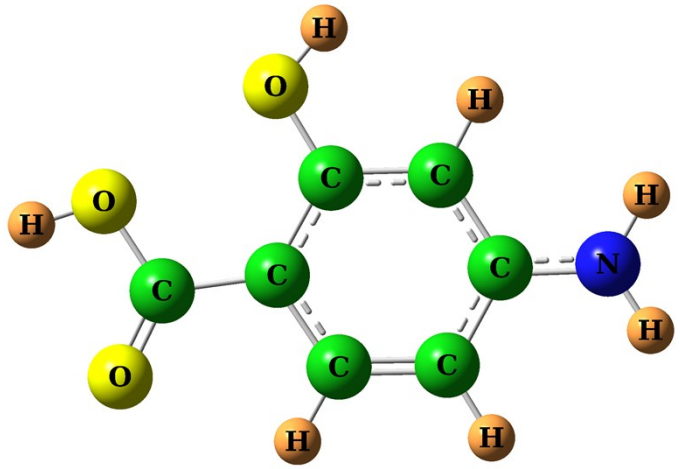
Table S17. Atom coordinates and absolute energies of energy-optimized neutral *p*-aminosalicylic acid hypothetical structure 4



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.424598	1.024643	0.000000
2	6	0	2.197475	-0.142845	-0.000220
3	6	0	1.534839	-1.383489	-0.000337
4	6	0	0.158793	-1.428458	-0.000212
5	6	0	-0.637951	-0.274423	0.000006
6	6	0	0.039402	0.953772	0.000092
7	1	0	1.909784	1.993889	0.000072
8	1	0	-0.356910	-2.377565	-0.000281
9	7	0	3.565774	-0.078886	-0.000522
10	1	0	4.048017	0.798750	0.000874
11	1	0	4.116340	-0.915566	0.000557
12	6	0	-2.118760	-0.471004	0.000132
13	8	0	-2.621125	-1.568104	0.000048
14	8	0	-2.909826	0.625062	0.000311
15	1	0	-2.374642	1.432234	0.000367
16	8	0	-0.703321	2.113743	0.000329
17	1	0	-0.129489	2.884934	0.000332
18	1	0	2.110301	-2.299252	-0.000527

Zero-point correction= 0.134900 (Hartree/Particle)
Thermal correction to Energy= 0.144575
Thermal correction to Enthalpy= 0.145519
Thermal correction to Gibbs Free Energy= 0.099672
Sum of electronic and zero-point Energies= -551.453499
Sum of electronic and thermal Energies= -551.443824
Sum of electronic and thermal Enthalpies= -551.442880
Sum of electronic and thermal Free Energies= -551.488727
HF=-551.5883987

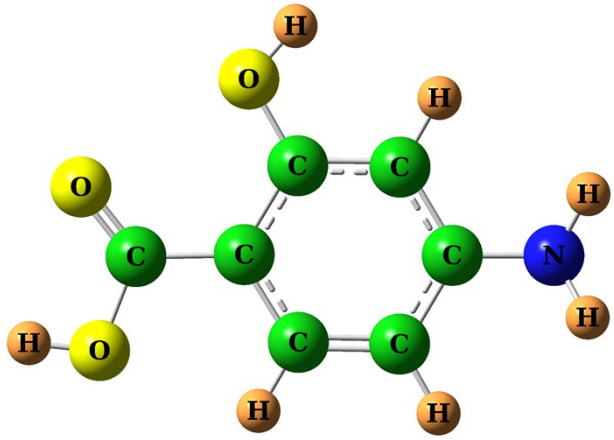
Table S18. Atom coordinates and absolute energies of energy-optimized neutral *p*-aminosalicylic acid hypothetical structure 5



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.442152	1.017292	-0.000076
2	6	0	2.201089	-0.156661	-0.000100
3	6	0	1.527302	-1.391957	-0.000117
4	6	0	0.152440	-1.415711	-0.000078
5	6	0	-0.632084	-0.250668	-0.000036
6	6	0	0.050257	0.982793	-0.000059
7	1	0	1.943576	1.978595	-0.000152
8	1	0	-0.373594	-2.359011	-0.000053
9	7	0	3.570286	-0.107858	-0.000775
10	1	0	4.061102	0.765024	0.003569
11	1	0	4.111894	-0.950267	0.003405
12	6	0	-2.094260	-0.448546	0.000046
13	8	0	-2.627860	-1.539554	0.000083
14	8	0	-2.834382	0.686129	0.000116
15	1	0	-3.755115	0.388756	0.000173
16	8	0	-0.652257	2.146177	-0.000033
17	1	0	-0.036549	2.885349	-0.000117
18	1	0	2.091299	-2.314712	-0.000203

Zero-point correction= 0.135075 (Hartree/Particle)
Thermal correction to Energy= 0.144645
Thermal correction to Enthalpy= 0.145590
Thermal correction to Gibbs Free Energy= 0.099905
Sum of electronic and zero-point Energies= -551.452279
Sum of electronic and thermal Energies= -551.442708
Sum of electronic and thermal Enthalpies= -551.441764
Sum of electronic and thermal Free Energies= -551.487449
HF=-551.5873539

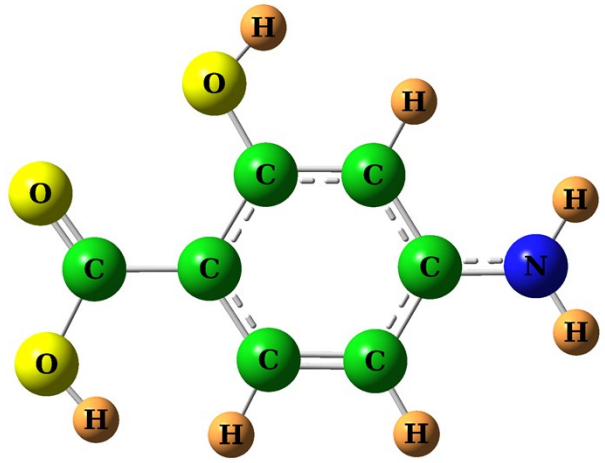
Table S19. Atom coordinates and absolute energies of energy-optimized neutral *p*-aminosalicylic acid hypothetical structure 6



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.477141	0.998471	-0.003925
2	6	0	2.188509	-0.202611	-0.004774
3	6	0	1.471593	-1.410042	-0.005485
4	6	0	0.094133	-1.386690	-0.002917
5	6	0	-0.643610	-0.191820	-0.000991
6	6	0	0.084843	1.016781	-0.002730
7	1	0	2.014778	1.939902	-0.010776
8	1	0	-0.449242	-2.318419	-0.001107
9	7	0	3.571992	-0.203954	-0.059469
10	1	0	4.041376	0.631220	0.247655
11	1	0	4.030702	-1.049131	0.236267
12	6	0	-2.116463	-0.219287	0.003501
13	8	0	-2.864896	0.728816	0.008293
14	8	0	-2.612116	-1.497662	0.001613
15	1	0	-3.573280	-1.397029	0.004309
16	8	0	-0.580750	2.197050	-0.001721
17	1	0	0.055174	2.919317	-0.009767
18	1	0	2.001762	-2.352635	-0.011855

Zero-point correction= 0.136012 (Hartree/Particle)
Thermal correction to Energy= 0.145827
Thermal correction to Enthalpy= 0.146771
Thermal correction to Gibbs Free Energy= 0.100696
Sum of electronic and zero-point Energies= -551.451322
Sum of electronic and thermal Energies= -551.441506
Sum of electronic and thermal Enthalpies= -551.440562
Sum of electronic and thermal Free Energies= -551.486637
HF=-551.5873332

Table S20. Atom coordinates and absolute energies of energy-optimized neutral *p*-aminosalicylic acid hypothetical structure 7.



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.460824	1.000234	-0.000374
2	6	0	2.192052	-0.189797	-0.000341
3	6	0	1.484258	-1.403404	-0.000219
4	6	0	0.106176	-1.386809	-0.000068
5	6	0	-0.659496	-0.209966	-0.000009
6	6	0	0.068466	1.004438	-0.000243
7	1	0	1.984900	1.949206	-0.000771
8	1	0	-0.378711	-2.354396	0.000165
9	7	0	3.561617	-0.176625	-0.002898
10	1	0	4.073659	0.683956	0.012483
11	1	0	4.082850	-1.031649	0.012434
12	6	0	-2.148179	-0.217284	0.000370
13	8	0	-2.844213	0.761273	0.000861
14	8	0	-2.764441	-1.442828	-0.000190
15	1	0	-2.126464	-2.161092	-0.000893
16	8	0	-0.597376	2.182094	-0.000261
17	1	0	0.038033	2.905068	-0.000650
18	1	0	2.018048	-2.343506	-0.000458

Zero-point correction= 0.134174 (Hartree/Particle)
Thermal correction to Energy= 0.143135
Thermal correction to Enthalpy= 0.144079
Thermal correction to Gibbs Free Energy= 0.100365
Sum of electronic and zero-point Energies= -551.440176
Sum of electronic and thermal Energies= -551.431215
Sum of electronic and thermal Enthalpies= -551.430271
Sum of electronic and thermal Free Energies= -551.473984
HF=-551.5743498