Supplementary material:

Table S1. Energies and geometries of optimized structures

Orotic acid

B3LYP/6-31G(d)

E = -603.385856 Hartree

Zero-point correction=	0.102063 (Hartree/Particle)
Thermal correction to Energy=	0.111024
Thermal correction to Enthalpy=	0.111969
Thermal correction to Gibbs Free Energy=	0.067305
Sum of electronic and zero-point Energies=	-603.283793
Sum of electronic and thermal Energies=	-603.274832
Sum of electronic and thermal Enthalpies=	-603.273887
Sum of electronic and thermal Free Energies=	-603.318551

HF/6-311++G(2d,2p)

E = -603.0817693 Hartree

Optimized geometry (B3LYP/6-31G(d))

Center Number	Atomic Number	Coordinates (Å) X	Y	Z
1	7	2.011486	0.023676	-0.000004
2	6	1.360960	1.252834	-0.000004
3	7	-0.024187	1.126697	-0.000001
4	6	-0.683443	-0.080434	0.000001
5	6	-0.019319	-1.259621	0.000001
6	6	1.444833	-1.265297	-0.000002
7	1	3.024599	0.067696	-0.000006
8	8	1.932825	2.324684	-0.000005
9	1	-0.573503	1.978754	0.000000
10	6	-2.170430	0.063829	0.000004
11	8	-2.815132	-1.114355	0.000006
12	8	-2.721981	1.144983	0.000005
13	1	-0.537486	-2.207665	0.000002
14	8	2.147982	-2.261136	-0.000003
15	1	-3.769855	-0.912675	0.000008

Tables S1, continued

Hydroorotate anion

B3LYP/6-31G(d)

E = -602.8581565 Hartree

Zero-point correction=	0.088913 (Hartree/Particle)
Thermal correction to Energy=	0.09755
Thermal correction to Enthalpy=	0.098494
Thermal correction to Gibbs Free Energy=	0.054454
Sum of electronic and zero-point Energies=	-602.769243
Sum of electronic and thermal Energies=	-602.760606
Sum of electronic and thermal Enthalpies=	-602.759662
Sum of electronic and thermal Free Energies=	-602.803703

HF/6-311++G(2d,2p)

E = -603.0817693 Hartree

Optimized geometry (B3LYP/6-31G(d))

Center Number	Atomic Number	Coordinates (Å) X	Y	Z
1	7	-1.949920	0.117421	0.000022
2	6	-1.213048	1.296879	-0.000006
3	7	0.141234	1.061528	0.000007
4	6	0.726633	-0.179630	0.000011
5	6	-0.029932	-1.309436	0.000014
6	6	-1.472788	-1.218251	0.000009
7	1	-2.955755	0.228482	-0.000012
8	8	-1.732152	2.408714	-0.000034
9	1	0.833016	1.815407	0.000009
10	6	2.285403	-0.109083	0.000001
11	8	2.872315	-1.205710	-0.000047
12	8	2.715854	1.075662	0.000036
13	1	0.452462	-2.277196	0.000011
14	8	-2.286832	-2.141442	-0.000003