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Supplementary Material

The Bioreductive Alkylation of DNA by Kalafungin: A Theoretical Investigation

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Scheme S1 2-electron reduction of kalafungin.

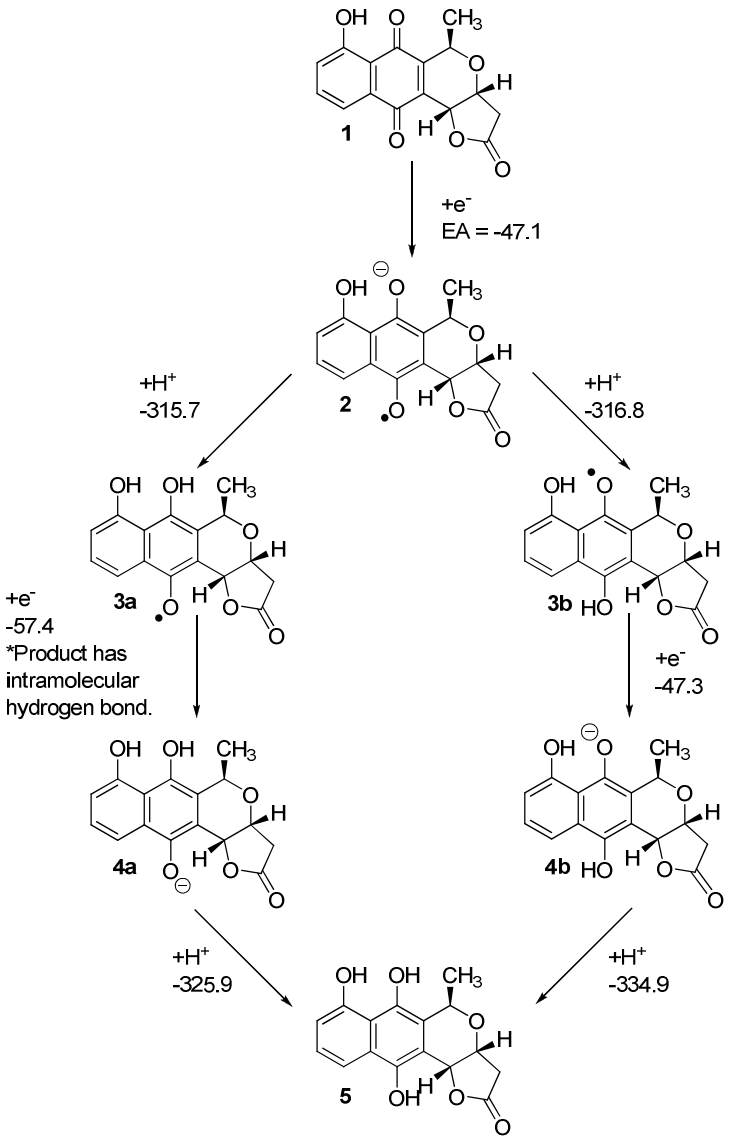

Table S1. The single point and zero point vibrational energies (ZPE) of the structurally optimized molecules in Hartrees (a.u.). The molecular structures are shown in Scheme S1.

System	Energy / a.u.	ZPE / a.u.
1	-1068.5972533	0.25089612
2	-1068.67000164	0.24860983
3a	-1069.18599342	0.26153543
3b	-1069.18702931	0.26085209
4a	-1069.27568785	0.25978541

4b	-1069.26108186	0.25949031
5	-1069.80829624	0.27296395

Scheme S2 Monoalkylation of singly-rearranged kalafungin.

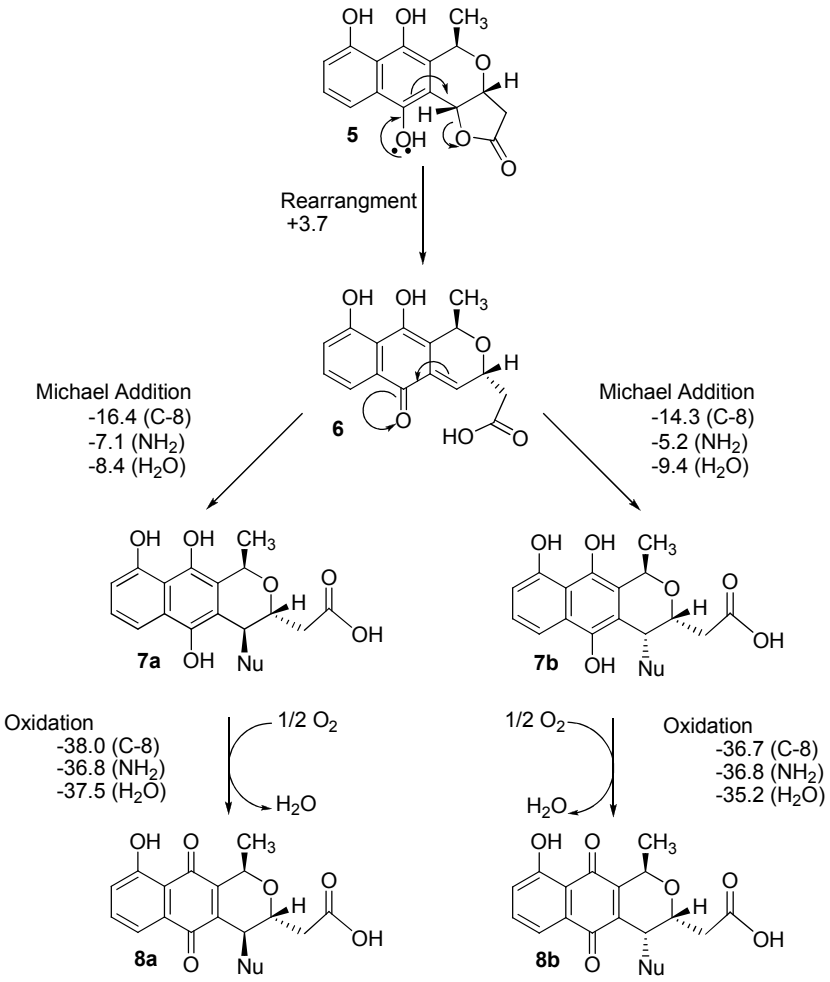

Table S2. The single point and zero point vibrational energies (ZPE) of the structurally optimized molecules in Hartrees (a.u.). The molecular structures are shown in Scheme S2.

System	Energy / a.u.	ZPE / a.u.
H_2O	-76.44970039	0.02094625
9-methyl guanine	-582.05152215	0.141935449
O_2	-150.37272458	0.00370787
5	-1069.80829624	0.27296395
6	-1069.80102435	0.27153354
7a (C-8)	-1651.88299584	0.417710204
7a (NH_2)	-1651.86827323	0.417900402
7a (H_2O)	-1146.27112987	0.29957298
7b (C-8)	-1651.87907093	0.417229808
7b (NH_2)	-1651.86490254	0.417567066
7b (H_2O)	-1146.27204003	0.29877886
8a (C-8)	-1650.67732841	0.395789441
8a (NH_2)	-1650.66034016	0.395593361
8a (H_2O)	-1145.06448081	0.27739928
8b (C-8)	-1650.67100521	0.39495512
8b (NH_2)	-1650.65693774	0.395236495
8b (H_2O)	-1145.06200849	0.27695320

Scheme S3 *Bis*-alkylation Scenario 1

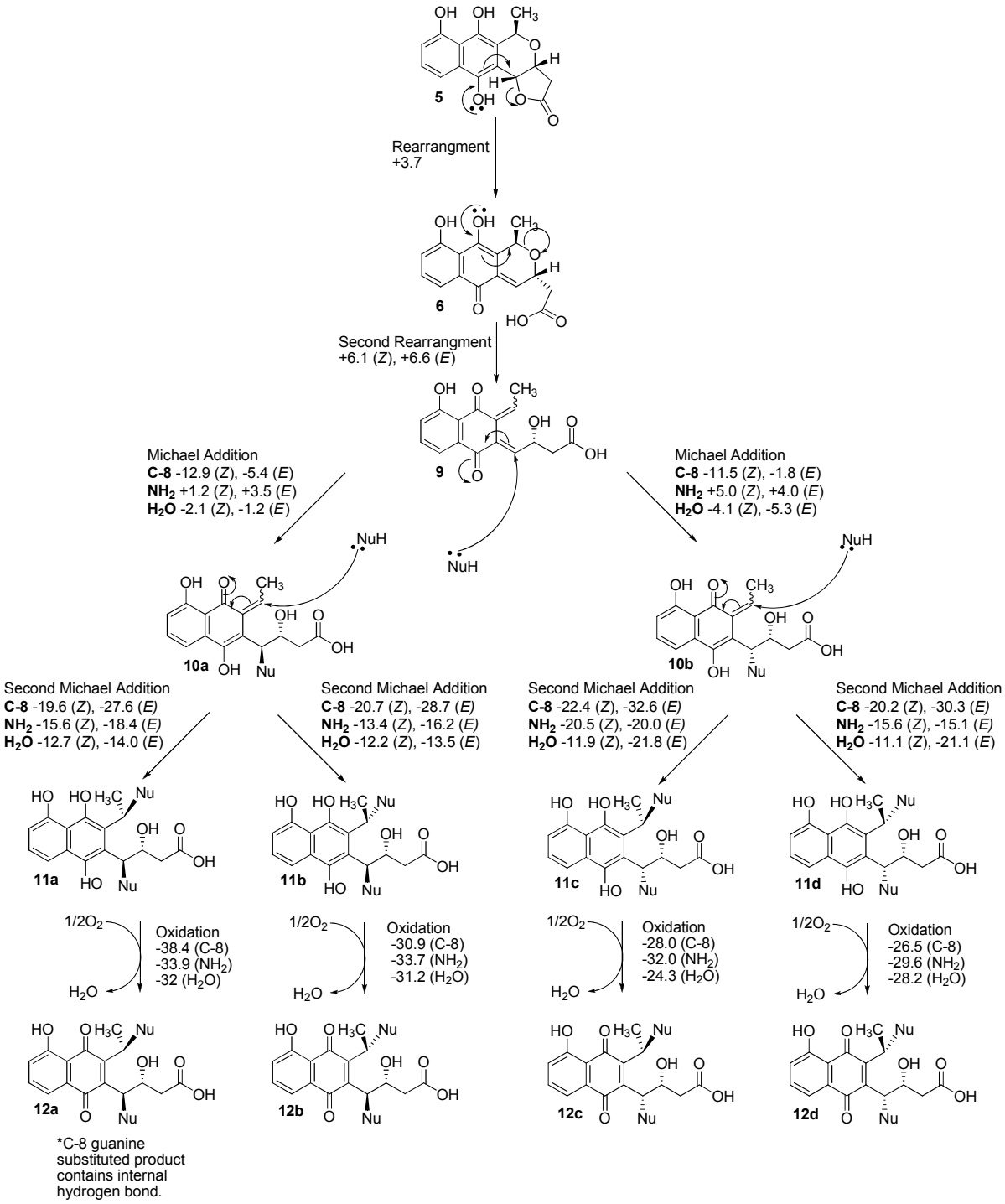

Table S3. The single point and zero point vibrational energies (ZPE) of the structurally optimized molecules in Hartrees (a.u.). The molecular structures are shown in Scheme S3.

System	Energy / a.u.	ZPE / a.u.
H_2O	-76.44970039	0.02094625
9-methyl guanine	-582.05152215	0.141935449
O_2	-150.37272458	0.00370787
5	-1069.80829624	0.27296395
6	-1069.80102435	0.27153354
9*E*	-1069.78855605	0.26955412
9*Z*	-1069.78906471	0.26923255
10a (C-8) *E*	-1651.85231646	0.415067046
10a (NH_2) *E*	-1651.83920157	0.416157251
10a (H_2O) *E*	-1146.24682062	0.29707591
10a (C-8) *Z*	-1651.86525959	0.415255283
10a (NH_2) *Z*	-1651.84323529	0.4157396
10a (H_2O) *Z*	-1146.24823742	0.29637590
10b (C-8) *E*	-1651.84671053	0.41517489
10b (NH_2) *E*	-1651.83857823	0.416339605
10b (H_2O) *E*	-1146.23592254	0.29662100
10b (C-8) *Z*	-1651.86311018	0.415350382
10b (NH_2) *Z*	-1651.83766576	0.416222938
10b (H_2O) *Z*	-1146.25263412	0.29749944
11a (C-8)	-2233.95295169	0.562195674
11a (NH_2)	-2233.92594133	0.563969218
11a (H_2O)	-1222.72609575	0.32530848
11b (C-8)	-2233.95451236	0.561884887
11b (NH_2)	-2233.92169252	0.56331431
11b (H_2O)	-1222.72503054	0.32494868
11c (C-8)	-2233.95501170	0.561963319
11c (NH_2)	-2233.92701492	0.563332938
11c (H_2O)	-1222.72830720	0.32545751
11d (C-8)	-2233.95114589	0.56167214
11d (NH_2)	-2233.91955191	0.563696666
11d (H_2O)	-1222.72737736	0.32573986
12a (C-8)	-2232.74743036	0.539675886
12a (NH_2)	-2232.71173669	0.539970006
12a (H_2O)	-1221.51082542	0.30333674
12b (C-8)	-2232.73789654	0.540330793
12b (NH_2)	-2232.70730983	0.539468041
12b (H_2O)	-1221.50796124	0.30246418
12c (C-8)	-2232.73355338	0.540051379
12c (NH_2)	-2232.70941376	0.539026861
12c (H_2O)	-1221.49916788	0.30187104
12d (C-8)	-2232.72642424	0.538919998
12d (NH_2)	-2232.69860329	0.539817064
12d (H_2O)	-1221.50529102	0.30291517

Scheme S4 *Bis*-alkylation Scenario 2

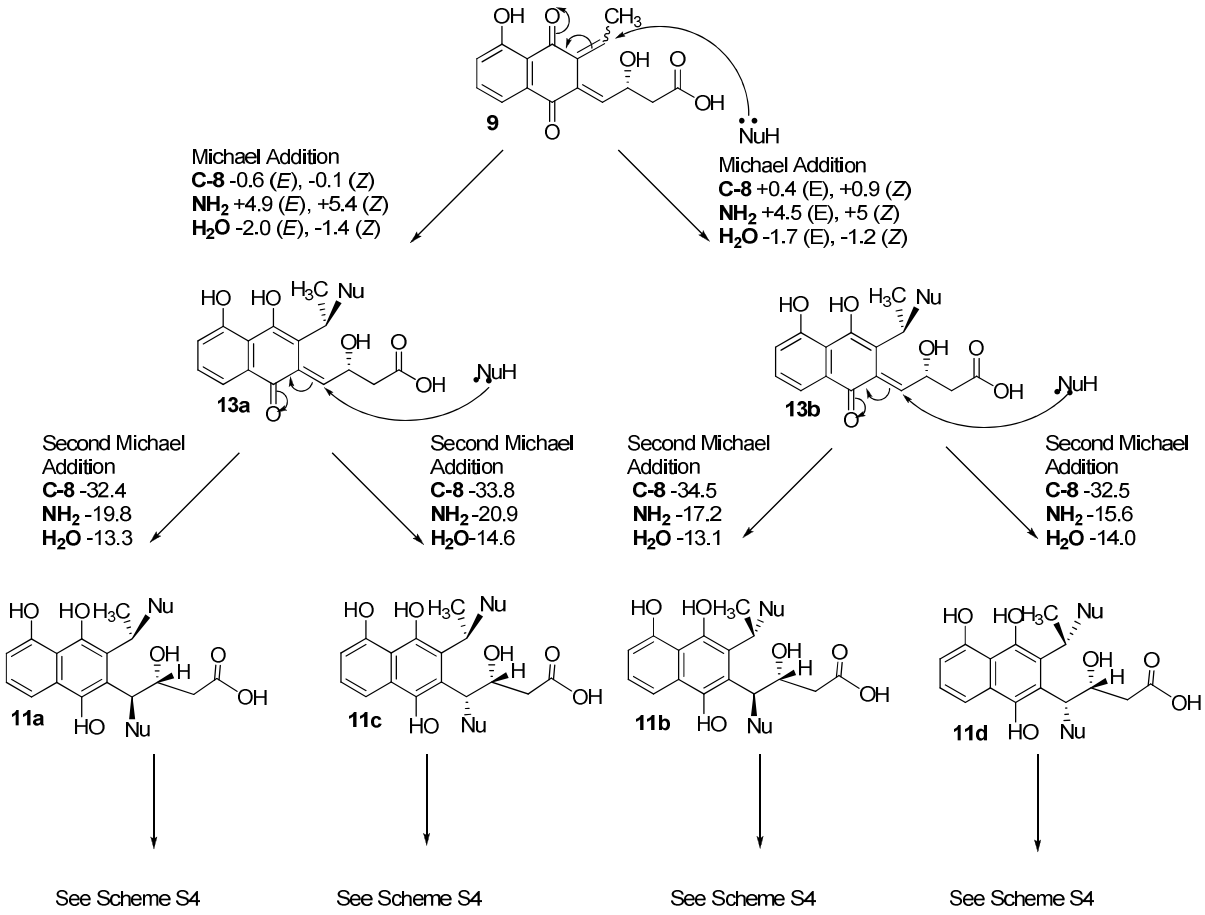

Table S4. The single point and zero point vibrational energies (ZPE) of the structurally optimized molecules in Hartrees (a.u.). The molecular structures are shown in Scheme S4.

System	Energy / a.u.	ZPE / a.u.
H_2O	-76.44970039	0.02094625
9-methyl guanine	-582.05152215	0.141935449
O_2	-150.37272458	0.00370787
9*E*	-1069.78855605	0.26955412
9*Z*	-1069.78906471	0.26923255
13a (C-8)	-1651.845127	0.415526854
13a (NH_2)	-1651.83695148	0.416190584
13a (H_2O)	-1146.24906711	0.29817101
13b (C-8)	-1651.84357743	0.415560187
13b (NH_2)	-1651.8376973	0.416258232
13b (H_2O)	-1146.24846741	0.29795140
11a (C-8)	-2233.95295169	0.562195674
11a (NH_2)	-2233.92594133	0.563969218
11a (H_2O)	-1222.72609575	0.32530848
11b (C-8)	-2233.95451236	0.561884887
11b (NH_2)	-2233.92169252	0.56331431
11b (H_2O)	-1222.72503054	0.32494868
11c (C-8)	-2233.95501170	0.561963319
11c (NH_2)	-2233.92701492	0.563332938
11c (H_2O)	-1222.72830720	0.32545751
11d (C-8)	-2233.95114589	0.56167214
11d (NH_2)	-2233.91955191	0.563696666
11d (H_2O)	-1222.72737736	0.32573986

Scheme S5 One-electron Reduction and Rearrangement Part1

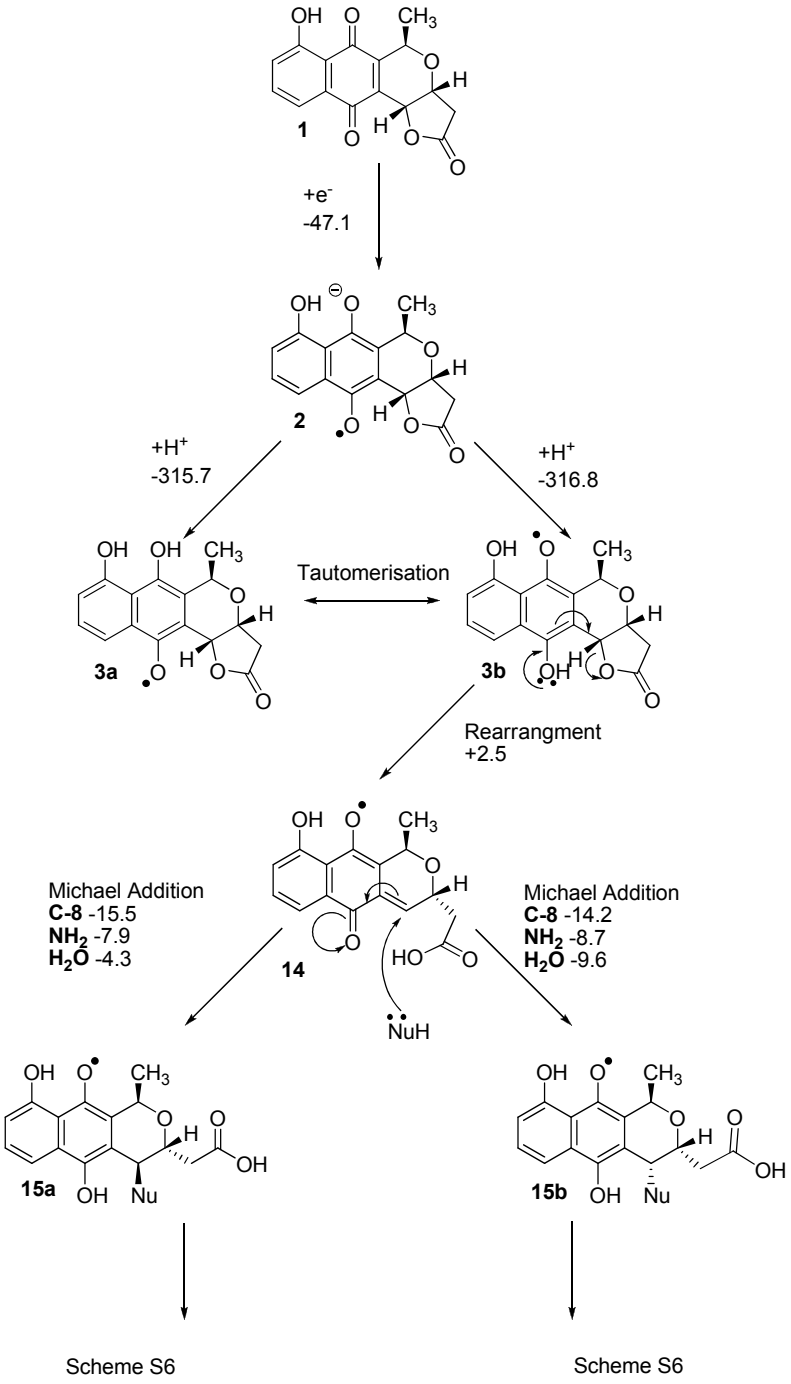

Table S5. The single point and zero point vibrational energies (ZPE) of the structurally optimized molecules in Hartrees (a.u.). The molecular structures are shown in Scheme S5.

System	Energy / a.u.	ZPE / a.u.
H_2O	-76.44970039	0.02094625
9-methyl guanine	-582.05152215	0.141935449
O_2	-150.37272458	0.00370787
1	-1068.5972533	0.25089612
2	-1068.67000164	0.24860983
3a	-1069.18599342	0.26153543
3b	-1069.18702931	0.26085209
14	-1069.1812627	0.25910011
15a (C-8)	-1651.26230988	0.405806188
15a (NH_2)	-1651.25026521	0.405907169
15a (H_2O)	-1145.64475993	0.28706602
15b (C-8)	-1651.25942517	0.405065005
15b (NH_2)	-1651.25201482	0.406370898
15b (H_2O)	-1145.65130896	0.28514444

Scheme S6 One-electron Reduction and Rearrangement Part 2

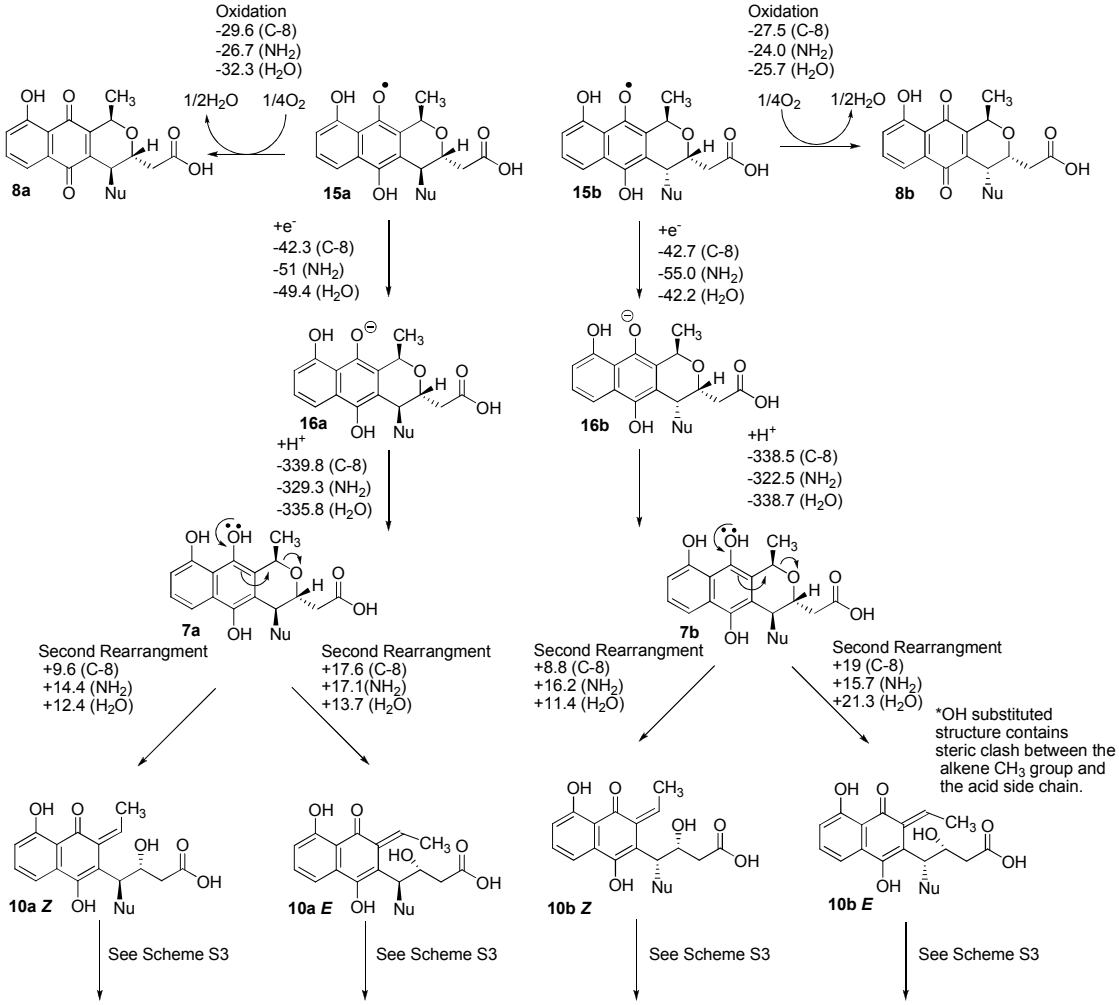

Table S6. The single point and zero point vibrational energies (ZPE) of the structurally optimized molecules in Hartrees (a.u.). The molecular structures are shown in Schemes S6.

System	Energy / a.u.	ZPE / a.u.
H_2O	-76.44970039	0.02094625
9-methyl guanine	-582.05152215	0.141935449
O_2	-150.37272458	0.00370787
15a (C-8)	-1651.26230988	0.405806188
15a (NH_2)	-1651.25026521	0.405907169
15a (H_2O)	-1145.64475993	0.28706602
15b (C-8)	-1651.25942517	0.405065005
15b (NH_2)	-1651.25201482	0.406370898
15b (H_2O)	-1145.65130896	0.28514444
8a (C-8)	-1650.67732841	0.395789441
8a (NH_2)	-1650.66034016	0.395593361
8a (H_2O)	-1145.06448081	0.27739928
8b (C-8)	-1650.67100521	0.39495512
8b (NH_2)	-1650.65693774	0.395236495
8b (H_2O)	-1145.06200849	0.27695320
16a (C-8)	-1651.3283071	0.404471863
16a (NH_2)	-1651.32844354	0.402884596
16a (H_2O)	-1145.72246809	0.28600621
16b (C-8)	-1651.32600299	0.403547346
16b (NH_2)	-1651.3371982	0.403855192
16b (H_2O)	-1145.72051678	0.28704936
7a (C-8)	-1651.88299584	0.417710204
7a (NH_2)	-1651.86827323	0.417900402
7a (H_2O)	-1146.27112987	0.29957298
7b (C-8)	-1651.87907093	0.417229808
7b (NH_2)	-1651.86490254	0.417567066
7b (H_2O)	-1146.27204003	0.29877886
10a (C-8) *E*	-1651.85231646	0.415067046
10a (NH_2) *E*	-1651.83920157	0.416157251
10a (H_2O) *E*	-1146.24682062	0.29707591
10a (C-8) *Z*	-1651.86525959	0.415255283
10a (NH_2) *Z*	-1651.84323529	0.4157396
10a (H_2O) *Z*	-1146.24823742	0.29637590
10b (C-8) *E*	-1651.84671053	0.41517489
10b (NH_2) *E*	-1651.83857823	0.416339605
10b (H_2O) *E*	-1146.23592254	0.29662100
10b (C-8) *Z*	-1651.86311018	0.415350382
10b (NH_2) *Z*	-1651.83766576	0.416222938
10b (H_2O) *Z*	-1146.25263412	0.29749944