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Supplementary material for manuscript JP037499E

"Radiation induced damage in serine phosphate – insights into a mechanism for direct DNA strand breakage" by J. Lipfert, J. Llano and L.A. Eriksson

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Optimized coordinates (B3LYP/LanL2DZ or B3LYP/6-31G(d,p))

FIGURE 1, Radical I

C	1.848205	1.159451	-0.061061
C	0.419320	1.558982	0.048057
O	-0.424428	0.742862	-0.808711
P	-1.785085	-0.112187	0.026170
O	-1.697316	0.472557	1.538342
C	2.313829	-0.198907	0.017094
O	3.711953	-0.295177	-0.174715
O	1.664938	-1.254545	0.250691
O	-1.104016	-1.696471	-0.039811
O	-3.094257	-0.050350	-0.873288
H	2.617441	1.917743	-0.192536
H	0.269308	2.507723	-0.487689
H	0.105841	1.720412	1.108213
H	3.967878	-1.242405	-0.106911
H	-0.127304	-1.688834	0.121761

FIGURE 1, Radical II

C	1.783614	-0.527752	-0.759207
C	0.341032	-0.247484	-1.030003
N	1.861551	-1.777784	0.143964
O	-0.403881	-0.342585	0.143972
P	-2.089907	0.073654	0.280499
O	-2.568929	0.071301	1.771382
O	-2.630679	-1.055963	-0.838134
O	-2.169073	1.494418	-0.631338
C	2.535641	0.629337	-0.042722
O	2.372287	1.816403	-0.285981
O	3.443969	0.107332	0.866308
H	2.740360	-1.746242	0.689049
H	1.049909	-1.727196	0.787125
H	2.317770	-0.733591	-1.693724
H	-0.027103	0.311961	-1.881949
H	3.995922	0.784258	1.322517
H	-2.284446	2.357875	-0.180496
H	-3.581228	-1.116226	-1.068852
H	1.795285	-2.643016	-0.406991

FIGURE 1, Radical III

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.495453
N	1.455762	0.000000	2.082851
C	-0.752706	-1.196666	2.110973
O	-0.219762	-1.480166	3.360630
O	-1.693050	-1.777953	1.588591
H	2.039221	-0.680551	1.574627
H	-0.694955	-2.189020	3.853074
H	-0.457005	0.915720	1.902640
H	1.394439	-0.289065	3.076235
H	1.886022	0.930431	1.997478
H	-0.585322	-0.741945	-0.533868
H	0.292615	0.891565	-0.548968

FIGURE 2a, SerPH+ before electron attachement

C	0.31788	-0.23272	-1.09253
O	-0.38383	-0.25282	0.154
P	-1.98854	0.07709	0.27206
O	-2.5077	-0.96065	-0.83669
C	1.76292	-0.57449	-0.72307
C	2.47024	0.60678	-0.03689
O	3.25425	0.17982	0.97397
N	1.73471	-1.77329	0.21086
O	2.34542	1.73778	-0.41227
O	-2.1619	1.49404	-0.46486
O	-2.44493	-0.02246	1.66286
H	2.58826	-1.81086	0.78344
H	0.91775	-1.64251	0.83504
H	2.34308	-0.85012	-1.60912
H	-0.10588	-0.96949	-1.78302
H	0.29577	0.76009	-1.5494
H	3.71581	0.94694	1.36957
H	-2.33463	2.21475	0.16703
H	-3.47017	-0.93407	-0.98048
H	1.61853	-2.66105	-0.29109

FIGURE 2b, SerPH+ after electron uptake and deamination

C	0.28888	-0.42717	1.67877
C	1.60172	0.00722	1.10287
N	1.11367	2.28917	-0.20573
O	-0.86724	0.30421	1.19297
P	-1.58888	-0.00967	-0.21928
O	-1.4055	1.06293	-1.23401
O	-3.12298	-0.20285	0.233
O	-1.15807	-1.49048	-0.61912
C	2.11317	-0.56113	-0.11848
O	1.51118	-1.34052	-0.87018
O	3.37848	-0.18405	-0.4064
H	1.79908	2.67365	-0.85226
H	0.26248	2.04599	-0.72009
H	2.25127	0.66975	1.65736
H	0.28397	-0.24993	2.75556
H	0.12703	-1.49508	1.50006
H	3.60558	-0.62536	-1.24585
H	-0.18354	-1.53786	-0.82787
H	-3.69238	0.31952	-0.35498
H	0.87433	3.0128	0.46829

FIGURE 3a, SerP + H2O, prior to electron emission

C	0.61521	-0.23596	-1.44368
O	-0.32409	-1.00851	-0.65068
P	-1.6483	-0.33879	-0.01231
O	-2.7916	-1.43937	-0.19766
C	1.96337	-0.05173	-0.71037
C	1.74739	0.07238	0.81447
O	2.21371	-0.714	1.60119
N	2.87724	-1.13156	-1.05889
O	0.94977	1.08138	1.2547
O	-2.00057	0.97417	-0.61753
O	-1.41929	-0.38189	1.57344
H	3.77918	-0.95512	-0.61788
H	2.54128	-1.98697	-0.61449
H	2.39466	0.89044	-1.07519

H	0.80342	-0.8109	-2.35197
H	0.16299	0.71871	-1.70985
H	0.69811	1.75967	0.5532
H	-0.61444	0.12976	1.82113
H	-2.70166	-2.1782	0.42709
O	-0.03788	2.82748	-0.4812
H	-0.26186	3.66861	-0.05435
H	-0.89404	2.34457	-0.60148

FIGURE 3b, SerP + H2O after electron emission and Decarboxylation (HF/6-31G(d))

C	1.75151	-1.79128	0.9958
O	2.02942	-0.84615	-0.12117
P	1.31451	0.47151	-0.40711
O	1.09521	1.17649	0.93918
C	0.38673	-2.3621	0.88735
C	-3.77299	-0.06606	-0.14484
O	-4.90379	-0.00828	-0.1957
N	0.17119	-3.33186	-0.07057
O	-2.6236	-0.12657	-0.08637
O	-0.00345	0.34865	-1.1946
O	2.20704	1.27826	-1.37932
O	-0.04763	3.57317	0.9792
H	-0.74543	-3.71972	-0.11846
H	0.57498	-3.19147	-0.97219
H	-0.18685	-2.45533	1.79009
H	2.53607	-2.51996	0.86902
H	1.89459	-1.23879	1.90881
H	-0.54605	3.87628	1.72954
H	-0.81501	0.11784	-0.73876
H	3.14679	1.11554	-1.35739
H	0.3127	4.34635	0.55994
H	0.695	2.07176	0.97033

FIGURE 4a, SerP + H3O+, prior to electron uptake

C	0.49515	-0.43167	-1.21191
O	-0.35286	-0.83315	-0.06549
P	-1.80727	-0.29449	0.19924
O	-1.84043	1.19892	0.56943
C	1.9535	-0.62456	-0.80011
C	2.31167	0.19544	0.4544
O	2.74605	-0.26667	1.47428
N	2.25674	-2.03284	-0.67293
O	-2.40269	-1.17146	1.35831
O	-2.74823	-0.52217	-1.04244
O	2.1166	1.55237	0.30367
O	-0.26799	2.7312	-0.65265
H	3.26252	-2.18446	-0.68968
H	1.93219	-2.385	0.2258
H	2.54068	-0.21002	-1.63096
H	0.26327	-1.11151	-2.03179
H	0.26896	0.59956	-1.48704
H	0.65454	2.60584	-0.34541
H	-1.98329	-1.10743	2.23576
H	-3.00638	-1.44125	-1.2424
H	-0.44293	3.68325	-0.73521
H	-1.21731	1.8903	0.08903
H	2.47429	1.96031	1.11873

FIGURE 4b, Phosphoranyl anion intermediate

C	0.78519	-0.44743	-1.47431

C	2.09175	-0.06656	-0.76167
N	2.96647	-1.23004	-0.69164
O	-0.07674	-1.2535	-0.65633
P	-1.43044	-0.43756	0.11141
O	-2.33412	-1.79455	0.08728
O	-2.79304	0.57652	-0.11777
O	-1.06986	-0.35882	1.70165
C	1.86531	0.57605	0.62599
O	0.94244	1.5663	0.75016
O	2.48111	0.22503	1.60404
O	-0.87201	2.59425	-1.04113
H	3.74862	-1.00859	-0.07631
H	2.45799	-1.96865	-0.20342
H	2.58077	0.6968	-1.38773
H	1.05162	-1.04835	-2.34842
H	0.25578	0.44563	-1.82346
H	0.45442	1.82487	-0.07475
H	-0.41385	0.35261	1.84723
H	-1.76121	-2.56328	-0.0699
H	-1.03139	3.46528	-0.64438
H	-1.69595	2.08967	-0.88141
H	-3.63119	0.07339	-0.13035

FIGURE 4c, TS for cleavage of phosphate ester bond

C	0.9799	0.13631	-1.68753
O	-0.62982	-0.79979	-1.27963
P	-1.39556	-0.32822	-0.02409
O	-1.27829	-1.19078	1.34669
C	1.94577	-0.30868	-0.64687
C	1.47669	-0.09239	0.83776
O	1.39424	-1.05281	1.60716
N	2.369	-1.67034	-0.92917
O	-2.96738	-0.71913	-0.30042
O	-1.72687	1.31699	0.011
O	1.47916	1.15298	1.34054
O	0.45054	3.0601	-0.26703
H	2.93212	-2.01368	-0.15357
H	1.53958	-2.26263	-0.9454
H	2.82377	0.35528	-0.73165
H	1.14477	-0.27125	-2.67904
H	0.60767	1.1532	-1.65068
H	1.31618	1.85182	0.65508
H	-0.33989	-1.20207	1.67932
H	-3.17146	-1.57165	0.11606
H	0.42112	3.91608	0.18728
H	-0.43067	2.64989	-0.12762
H	-2.6798	1.45873	-0.17087

FIGURE 4d, Dephosphorylated product complex

C	2.99856	1.06453	-0.91963
O	-1.79822	1.14017	-0.77309
P	-2.14018	-0.18584	-0.16456
O	-1.41962	-1.46545	-0.78066
C	3.02918	-0.0074	0.12754
C	1.59684	-0.50104	0.42874
O	1.21406	-1.62242	0.1427
N	3.93586	-1.07685	-0.26535
O	-3.68711	-0.56086	-0.34361
O	-1.92969	-0.25932	1.42617
O	0.77435	0.33602	1.08962
O	0.25782	2.63837	0.10067

H	3.95499	-1.79268	0.4594
H	3.55817	-1.53797	-1.09257
H	3.40138	0.41319	1.0806
H	3.82314	1.10197	-1.62178
H	2.26361	1.86098	-0.90526
H	0.81131	1.31777	0.81816
H	-0.51913	-1.63719	-0.40659
H	-4.16401	0.20111	-0.70994
H	-0.10557	3.31619	0.69088
H	-0.53387	2.20448	-0.32627
H	-0.97858	-0.11091	1.62498