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C1' North Hydrogen Abstraction Radical
Charge = 0 Multiplicity = 2

8	-1.04552	-0.09885	-0.21534
6	-1.14069	0.30392	1.13045
6	0.23158	0.34325	1.74818
6	1.16756	-0.03817	0.58773
6	0.28706	0.21126	-0.65626
6	0.57385	-0.65602	-1.86967
1	0.54339	-1.71572	-1.56456
1	1.58194	-0.44504	-2.24608
8	-0.32197	-0.3937	-2.93351
1	-1.21045	-0.45387	-2.55441
1	0.35163	1.27462	-0.92764
1	1.41366	-1.1105	0.6441
8	2.34581	0.75033	0.6248
1	2.97526	0.38872	-0.01218
1	0.3303	-0.33712	2.60638
1	0.49614	1.34611	2.10544
7	-2.25263	-0.12145	1.84609
1	-2.15735	-1.03992	2.28864
1	-3.09882	-0.10474	1.28767

C1' South Hydrogen Abstraction Radical
Charge = 0 Multiplicity = 2

8	-0.98017	-0.10811	-0.32437
6	-0.98194	-0.31271	1.06331
6	0.4257	-0.23702	1.56399
6	1.08705	0.7258	0.56064
6	0.26934	0.5013	-0.7252
6	0.92896	-0.44635	-1.72425
1	1.27137	-1.35255	-1.194
1	1.81115	0.03357	-2.16216
8	0.05463	-0.76721	-2.78751
1	-0.78262	-1.01641	-2.36831
1	0.04823	1.46176	-1.20066
1	2.14909	0.48476	0.40043
8	0.93347	2.09289	0.92013
1	1.37708	2.23077	1.76738
1	0.92536	-1.22454	1.53129
1	0.49122	0.1204	2.59638
7	-1.90105	-1.21991	1.58106
1	-2.81274	-1.12466	1.14618
1	-1.60885	-2.20042	1.51907

C2' North Hydrogen Abstraction Radical
Charge = 0 Multiplicity = 2

8	-1.03511	-0.01544	-0.18973
6	-1.10906	0.45254	1.19007
6	0.29572	0.29876	1.68047
6	1.21694	-0.02773	0.55914
6	0.29597	0.19962	-0.66792
6	0.50788	-0.73797	-1.8454
1	0.44199	-1.77838	-1.48355
1	1.50979	-0.59044	-2.26533
8	-0.41707	-0.49015	-2.88739
1	-1.28836	-0.47516	-2.46551
1	0.42542	1.24378	-0.99375
1	1.52358	-1.09098	0.6046
8	2.37496	0.8042	0.56975
1	3.0467	0.38512	0.0162
1	0.60441	0.46985	2.70343
1	-1.41713	1.5133	1.1752
7	-2.08193	-0.25855	1.96441
1	-3.01348	-0.11138	1.58522
1	-1.88631	-1.25608	1.93343

C2' South Hydrogen Abstraction Radical
Charge = 0 Multiplicity = 2

8	-1.01886	0.19521	-0.32706
6	-1.08789	-0.17421	1.07926
6	0.31022	0.00316	1.5733
6	1.13281	0.7294	0.56636
6	0.33611	0.49265	-0.72388
6	0.8619	-0.68069	-1.55462
1	1.06089	-1.53784	-0.88488
1	1.81065	-0.41188	-2.03303
8	-0.05188	-1.02244	-2.57601
1	-0.92379	-0.9812	-2.1525
1	0.30922	1.40261	-1.33148
1	2.15973	0.34121	0.48649
8	1.16403	2.14999	0.80794
1	1.56022	2.28977	1.67906
1	0.61422	-0.2411	2.58429
1	-1.78448	0.53924	1.54722
7	-1.61021	-1.49088	1.33801
1	-2.55823	-1.57129	0.98037
1	-1.04216	-2.19734	0.87693

C3' North Hydrogen Abstraction Radical
Charge = 0 Multiplicity = 2

8	-0.95314	0.69441	-0.28088
6	-1.13546	0.47268	1.15307
6	0.27996	0.56409	1.74226
6	1.11321	0.07484	0.60232
6	0.37826	0.34054	-0.68508
6	0.29286	-0.8355	-1.6666
1	-0.07089	-1.72389	-1.1248
1	1.28666	-1.07554	-2.06573
8	-0.53054	-0.51536	-2.76988
1	-1.33764	-0.14161	-2.38456
1	0.80954	1.20382	-1.22507
8	2.47298	0.20359	0.70522
1	2.88317	-0.03628	-0.13673
1	0.37827	-0.02529	2.659
1	0.53184	1.608	1.99034
1	-1.7912	1.28394	1.4791
7	-1.76605	-0.77399	1.49463
1	-2.64411	-0.87673	0.99307
1	-1.1706	-1.55938	1.24133

C3' South Hydrogen Abstraction Radical
Charge = 0 Multiplicity = 2

8	-0.8865	-0.43916	-0.29973
6	-1.19485	-0.23309	1.10364
6	0.16616	0.09407	1.75701
6	0.96339	0.62563	0.5988
6	0.18482	0.43883	-0.67373
6	0.93462	-0.23121	-1.8244
1	1.3758	-1.16961	-1.45292
1	1.74874	0.41884	-2.15967
8	0.08561	-0.45033	-2.93739
1	-0.68702	-0.91815	-2.58952
1	-0.21478	1.40587	-1.03413
8	1.74242	1.75296	0.66915
1	2.1563	1.79607	1.54102
1	0.59433	-0.81891	2.19809
1	0.05475	0.82301	2.56983
1	-1.86712	0.63326	1.18515
7	-1.85297	-1.36154	1.67986
1	-2.75276	-1.51389	1.23211
1	-1.29452	-2.19883	1.52683

C4' North Hydrogen Abstraction Radical
Charge = 0 Multiplicity = 2

8	-1.06704	0.27909	-0.26548
6	-1.18881	0.47412	1.1911
6	0.26047	0.60905	1.67538
6	1.10208	-0.13472	0.6265
6	0.23307	-0.02956	-0.59307
6	0.38461	-0.76666	-1.87991
1	-0.06815	-1.77713	-1.80004
1	1.44874	-0.91369	-2.09857
8	-0.17096	-0.07445	-2.9935
1	-1.04159	0.23622	-2.70914
1	1.26136	-1.19023	0.9261
8	2.37331	0.50749	0.51984
1	2.86244	0.08492	-0.19833
1	0.3825	0.23109	2.69143
1	0.57442	1.65582	1.65072
1	-1.77109	1.39058	1.31119
7	-1.8942	-0.59204	1.83612
1	-2.81927	-0.70796	1.43186
1	-1.40076	-1.47575	1.73523

C4' South Hydrogen Abstraction Radical
Charge = 0 Multiplicity = 2

6	0.09111	-0.7017	0.25069
8	-0.71839	-0.70383	-0.85484
6	-1.50016	0.54612	-0.87591
6	-0.61063	1.53629	-0.11731
7	-2.80791	0.41597	-0.30369
1	-1.61054	0.7783	-1.93738
6	0.16655	0.66062	0.89979
1	-1.19066	2.34008	0.33943
1	0.1216	1.97914	-0.79838
8	1.49243	1.09734	1.16692
1	-0.33653	0.6769	1.87835
1	2.05905	0.68834	0.48917
6	1.21475	-1.66289	0.25835
1	0.91593	-2.59847	-0.23047
1	1.50272	-1.88025	1.29554
8	2.34746	-1.07142	-0.44689
1	3.13399	-1.59668	-0.24028
1	-3.32753	-0.32332	-0.76885
1	-2.75438	0.17684	0.68347

C5' North Hydrogen Abstraction Radical
Charge = 0 Multiplicity = 2

8	-0.75441	0.91061	-0.3342
6	-1.07298	0.45356	1.01497
6	0.30322	0.32715	1.67774
6	1.27584	-0.05122	0.54671
6	0.47445	0.27649	-0.7434
6	0.12969	-0.94023	-1.55515
1	0.90519	-1.58833	-1.95609
8	-0.96414	-0.83674	-2.36236
1	-1.49858	-0.12518	-1.96216
1	1.02185	1.03322	-1.33054
1	1.51809	-1.12352	0.56966
8	2.45859	0.72482	0.7024
1	3.11356	0.40705	0.06724
1	0.29656	-0.38408	2.50523
1	0.62256	1.30176	2.05616
1	-1.67769	1.25681	1.4437
7	-1.83296	-0.7658	1.0933
1	-2.7207	-0.66575	0.60839
1	-1.33183	-1.53533	0.65336

C5' South Hydrogen Abstraction Radical
Charge = 0 Multiplicity = 2

1	-0.97295	0.12897	-0.41403
6	-0.99899	-0.17888	1.01861
1	0.47783	-0.2596	1.41141
6	1.14287	0.76326	0.48694
6	0.33884	0.58073	-0.80993
6	0.92502	-0.46686	-1.72034
1	1.85966	-0.28807	-2.24497
8	0.03551	-1.22168	-2.4259
1	-0.80036	-1.13697	-1.92796
1	0.22299	1.55979	-1.30305
1	2.21035	0.5578	0.32591
8	0.93806	2.10278	0.93018
1	1.39335	2.20785	1.77589
1	0.86267	-1.26336	1.19622
1	0.63721	-0.05291	2.47334
1	-1.4883	0.66749	1.5133
7	-1.73604	-1.36237	1.32395
1	-2.71071	-1.26465	1.05498
1	-1.35298	-2.1629	0.82648

O3' North Hydrogen Abstraction Radical
Charge = 0 Multiplicity = 2

8	-1.01735	0.15484	-0.25741
6	-1.12349	0.46477	1.15948
6	0.32384	0.57851	1.66342
6	1.13771	-0.15401	0.57409
6	0.35145	0.25627	-0.66989
6	0.50698	-0.63353	-1.88212
1	0.32194	-1.67127	-1.5776
1	1.52307	-0.56391	-2.27089
8	-0.36743	-0.22954	-2.9234
1	-1.24093	-0.17557	-2.51284
1	0.61216	1.29078	-0.92509
1	1.07783	-1.2399	0.73143
8	2.43486	0.30342	0.62087
1	0.44403	0.1511	2.65501
1	0.6492	1.61821	1.68006
1	-1.65559	1.4131	1.25727
7	-1.8659	-0.52907	1.87717
1	-2.80835	-0.58208	1.50637
1	-1.44167	-1.43876	1.72571

O3' South Hydrogen Abstraction Radical
Charge = 0 Multiplicity = 2

8	-0.93746	-0.08761	-0.32773
6	-1.02515	-0.14968	1.13353
6	0.43449	-0.20271	1.57498
6	1.14018	0.74116	0.5863
6	0.2822	0.51816	-0.73373
6	0.98955	-0.42177	-1.7155
1	1.3345	-1.31766	-1.17258
1	1.86553	0.07371	-2.14593
8	0.12622	-0.75429	-2.78105
1	-0.69939	-1.04856	-2.36763
1	0.08247	1.48053	-1.21959
1	2.19481	0.47808	0.39323
8	0.97712	2.057	0.89252
1	0.82218	-1.22337	1.46793
1	0.57108	0.11398	2.61074
1	-1.49194	0.78263	1.473
7	-1.81327	-1.24361	1.58715
1	-2.78067	-1.14509	1.2945
1	-1.46032	-2.12087	1.21296

O5' North Hydrogen Abstraction Radical

Charge = 0 Multiplicity = 2

6	0.70574	-0.03874	-0.28126
8	-0.22855	-1.10557	-0.25468
6	-1.57627	-0.58317	-0.46031
6	-1.46653	0.94299	-0.23232
7	-2.53142	-1.21505	0.40232
1	-1.86534	-0.81364	-1.49286
6	-0.05149	1.14873	0.33327
1	1.00516	0.20875	-1.31668
1	-2.25991	1.3084	0.42238
1	-1.55355	1.47841	-1.18543
8	0.54757	2.4087	0.09704
1	-0.05911	1.0388	1.42436
1	0.53776	2.56779	-0.85752
6	1.96507	-0.43585	0.48787
1	1.70275	-0.7972	1.49979
1	2.55715	0.49373	0.63787
8	2.8058	-1.28665	-0.1706
1	-2.55269	-2.21545	0.22015
1	-2.25002	-1.09985	1.37414

O5' South Hydrogen Abstraction Radical

Charge = 0 Multiplicity = 2

8	-0.93572	-0.37282	-0.33865
6	-1.10134	-0.22682	1.0938
6	0.34344	-0.18847	1.59648
6	1.06116	0.63457	0.51989
6	0.20837	0.37202	-0.75145
6	0.93512	-0.43092	-1.83572
1	1.25125	-1.41922	-1.45068
1	1.87229	0.10603	-2.09912
8	0.25894	-0.53096	-3.01953
1	-0.08839	1.3422	-1.17248
1	2.10435	0.31111	0.38332
8	1.00615	2.03788	0.76664
1	1.5307	2.22108	1.55747
1	0.73676	-1.21235	1.62236
1	0.44035	0.24135	2.59712
1	-1.60148	0.7303	1.29798
7	-1.88909	-1.27697	1.65508
1	-2.83694	-1.23906	1.28992
1	-1.50072	-2.17779	1.38287

C5' North Radical Formed Through Breakage
of a Phosphoester Bond

Charge = 0 Multiplicity = 2

8	-1.10462	-0.08295	-0.65639
6	-1.25462	0.40849	0.7045
6	0.18054	0.51281	1.27284
6	1.06835	-0.12767	0.2063
6	0.23847	0.1344	-1.08859
6	0.55601	-0.7392	-2.23939
1	0.11186	-1.72651	-2.30113
1	1.26616	-0.4318	-2.9981
1	0.40744	1.19334	-1.35542
1	1.13372	-1.21591	0.35714
8	2.35306	0.46388	0.20341
1	2.89689	-0.01999	-0.43246
1	0.25711	0.03181	2.25021
1	0.48288	1.55824	1.38773
1	-1.73297	1.395	0.65407
7	-2.11023	-0.44101	1.48439
1	-3.03099	-0.48742	1.05426
1	-1.74045	-1.39008	1.48291

C5' South Radical Formed Through Breakage
of a Phosphoester Bond

Charge = 0 Multiplicity = 2

8	0.17856	1.1216	-0.42531
6	1.25805	0.25807	0.00784
6	0.54772	-0.80362	0.84855
6	-0.74143	-1.03875	0.06186
6	-1.05178	0.38868	-0.49396
6	-2.11517	1.12072	0.24338
1	-1.85335	1.94856	0.89092
1	-3.15805	0.84912	0.11833
1	-1.34525	0.24628	-1.54734
1	-1.564	-1.41556	0.68372
8	-0.53223	-1.88511	-1.06814
1	-0.28906	-2.76101	-0.73982
1	0.31874	-0.39024	1.83881
1	1.14422	-1.71026	0.98472
1	1.71893	-0.20387	-0.87562
7	2.27313	0.97655	0.71635
1	2.71566	1.65281	0.09946
1	1.84531	1.50584	1.47385

C3' North Radical Formed Through Breakage
of a Phosphoester Bond

Charge = 0 Multiplicity = 2

8	-0.53482	0.83201	-0.19279
6	-0.76815	0.54893	1.21344
6	0.64181	0.45544	1.83113
6	1.47703	0.0332	0.67005
6	0.75744	0.33833	-0.59926
6	0.55499	-0.84786	-1.55888
1	0.13788	-1.69987	-0.99657
1	1.51725	-1.16343	-1.97702
8	-0.27657	-0.47775	-2.64029
1	-1.02893	-0.02001	-2.23484
1	1.24006	1.14473	-1.17797
1	2.51703	-0.26489	0.72216
1	0.66359	-0.23554	2.68109
1	0.95303	1.44055	2.21715
1	-1.3436	1.40266	1.58155
7	-1.53068	-0.64423	1.48018
1	-2.4083	-0.62413	0.96748
1	-1.02086	-1.47282	1.18159

C3' South Radical Formed Through Breakage
of a Phosphoester Bond

Charge = 0 Multiplicity = 2

8	-0.73729	0.03181	-0.18761
6	-0.89769	0.11424	1.25459
6	0.54236	0.12608	1.80278
6	1.31473	0.71149	0.6724
6	0.49187	0.66844	-0.57486
6	1.07345	-0.15664	-1.73084
1	1.34566	-1.15266	-1.34683
1	1.98176	0.32157	-2.1126
8	0.1602	-0.23947	-2.80899
1	-0.675	-0.53671	-2.41925
1	0.27644	1.68129	-0.96481
1	2.32444	1.09902	0.7256
1	0.85613	-0.90674	2.03742
1	0.61815	0.68975	2.7399
1	-1.40025	1.0635	1.48942
7	-1.70071	-0.94827	1.77098
1	-2.64362	-0.89704	1.39526
1	-1.31035	-1.84455	1.48745

C4' Ring-opened Radical
(Figure 4, structure I)

Charge = 0 Multiplicity = 2

8	-2.26941	-1.06171	-0.03035
6	-1.8676	-0.28398	0.82677
6	-0.38961	-0.08093	1.14271
6	0.55745	-0.71775	0.09723
6	0.4344	-0.06806	-1.24994
6	1.61119	0.53487	-1.92521
8	2.21941	1.5088	-1.03444
1	3.09924	1.7122	-1.38166
1	1.31413	1.01642	-2.86578
1	2.35913	-0.24072	-2.16492
1	-0.52719	-0.10957	-1.74818
1	0.26186	-1.77334	0.00951
8	1.89193	-0.7155	0.58773
1	2.24178	0.17357	0.40292
1	-0.17077	-0.54396	2.11354
1	-0.16709	0.98875	1.24068
7	-2.72752	0.46476	1.58076
1	-2.41149	1.05638	2.33174
1	-3.71732	0.30933	1.464

C1' Ring-opened Radical
(Figure 4, structure II)

Charge = 0 Multiplicity = 2

6	-1.9707	-0.06211	0.94535
6	-0.50567	0.06388	1.22263
6	0.37715	-0.8381	0.32933
6	0.29751	-0.4068	-1.1403
6	1.37208	0.54082	-1.68501
8	1.83876	1.42	-0.65965
1	2.57173	1.94031	-1.01193
1	0.93183	1.0891	-2.52589
1	2.18594	-0.09081	-2.07381
1	-0.01384	-1.85948	0.3691
8	1.72035	-0.89573	0.78294
1	2.06956	0.00689	0.70086
1	-0.28571	-0.23459	2.25905
1	-0.14953	1.10605	1.12879
7	-2.85064	0.56729	1.83924
1	-2.61654	0.42511	2.81702
1	-3.82564	0.34048	1.68099
8	-0.56166	-0.82103	-1.89423
1	-2.31512	-0.10608	-0.08338

Ring Breaking Radical
(Figure 4, structure V)

8	- .634324	.002799	-1.711560
6	- .592227	.002839	- .473050
6	.610919	- .003090	.277110
8	.645320	- .002744	1.619236
1	-1.526584	.007657	.138430
1	1.587946	- .008021	- .191550
1	- .261482	.001429	1.967348

Ring Breaking Radical with Phosphorus
(Figure 4, structure III)

8	-1.763780	- .615122	-2.872637
6	-1.802638	- .231733	-1.721261
6	- .470472	- .231590	- .974255
8	- .400684	.137353	.196763
6	-3.024096	.232754	- .983183
1	.420846	- .572228	-1.519035
1	-3.890161	.179006	-1.642355
1	-3.185505	- .386622	- .094049
1	-2.882073	1.258657	- .626146
15	1.412261	.116433	1.148660
8	1.011259	- .805570	2.271286
8	1.447948	1.583734	1.490641
8	2.222284	- .405630	.004432

Dehydroxylated and H2O removal Radical
(Figure 4, structure VIII)

8	- .762804	.042069	- .151143
6	- .825254	.479899	1.274709
6	.613282	.423777	1.702423
6	1.382643	.023321	.624497
6	.546263	- .199024	- .464528
6	.799209	- .639150	-1.863900
1	.283121	-1.597058	-2.048059
1	1.869953	- .805732	-2.008275
8	.398260	.333948	-2.829259
1	- .515478	.567556	-2.614794
1	2.456336	- .112563	.608699
1	.938122	.667142	2.703775
1	-1.236042	1.499391	1.235197
7	-1.704562	- .312916	2.072840
1	-2.654604	- .290648	1.712798
1	-1.389978	-1.278755	2.104788