ARTICLE

A search of a quantitative quantum-chemical approach for radiation stability prediction

Supporting Information

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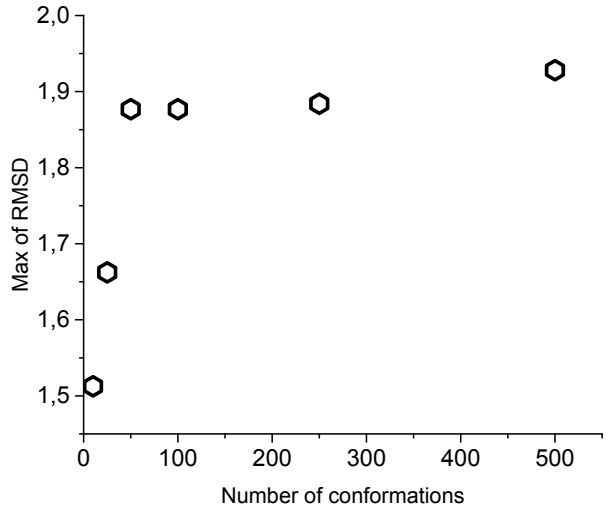

Fig. 1. The dependence of RMSD maximum of CDD on the numbers of conformations for TBP molecule

Table 1. Calculated reactivity descriptors.

TBP			
Atom	CDD_{opt}	CDD_{conf}	conf-CDD×SASA
P1	0.024181	0.053756399	0.000154861
O2	-0.10738	-0.258505331	-0.069822699
O3	-0.1282	-0.031892797	-0.003048318
O4	-0.05259	-0.029671673	-0.001857269
O5	-0.13887	-0.025462418	-0.001788046
C6	0.034027	0.080454707	0.00040286
C7	0.004814	0.039839015	0.000322035
C8	0.091133	0.036882239	0.000354231
C9	0.088953	0.026877797	0.001561276
C10	0.057847	0.077268469	0.000396545
C11	0.089551	0.042150058	0.000353285
C12	0.00562	0.031295654	0.00029042
C13	0.087058	0.029321229	0.001730382
C14	0.034066	0.080093358	0.000462688
C15	0.120459	0.04889372	0.000406795
C16	0.053664	0.037549289	0.000388113
C17	0.195044	0.027479022	0.001624228
PO-1			
Atom	CDD_{opt}	CDD_{conf}	conf-CDD×SASA
C1	0.114684	0.091050758	0.009601581
C2	0.008454	0.007439039	0.000470059
C3	0.018972	0.062595366	0.000494975
N4	0.093825	0.065649413	0.001302405
C5	0.084275	0.058803065	0.000486518
C6	-0.01714	0.010293162	0.000547211

C7	0.01402	-0.000869385	-2.16E-05
C8	0.003452	-0.000183227	3.18E-05
C9	0.005552	-0.006488199	-0.000723896
C10	0.000602	-0.001358646	-9.93234E-05
C11	-0.01191	0.000890916	6.54E-05
C12	0.000997	-0.010565068	-0.000122988
C13	0.009722	0.000560504	5.47E-05
C14	0.005095	-0.000215287	-1.22E-05
C15	-0.00441	-0.003144274	-0.000303447
C16	0.009506	-0.000733053	2.48E-06
C17	-0.01505	0.0018098	0.000142517
C18	-0.04007	-0.007136589	-9.43962E-05
C19	0.010652	0.000636665	0.00010691
C20	-0.04144	0.000821445	4.62E-05
C21	0.004941	-0.005531715	-7.40E-05
C22	-0.03494	0.003748735	0.000209905
C23	0.00515	0.000386098	6.64E-05
C24	-0.02465	-0.001854559	-0.000156607
C25	-0.02184	0.002178575	8.82102E-05
C26	-0.08287	-0.012642173	-0.000145949
C27	0.003456	-0.000451284	-1.27E-05
C28	-0.0154	0.000979465	0.000153461
C29	-0.06744	-0.008036695	-0.000797611
C30	-0.00158	-0.000472119	-1.93E-05
P31	0.013244	0.018307309	0
P32	0.015918	0.019588378	0
O33	0.020291	-0.138327411	-0.035177495
O34	-0.02542	-0.142471841	-0.036052898
HDEHP			
Atom	CDD_{opt}	CDD_{conf}	conf-CDD×SASA
P1	0.040893	0.070759703	0.000263855
O2	-0.10431	-0.154885101	-0.052536333
O3	0.032894	0.208211059	0.047725982
O4	-0.03035	-0.015141796	-0.001032031
O5	0.038889	-0.011977598	-0.000723832
C6	0.022681	0.069920019	0.000175554
C7	0.047784	-0.001615067	0
C8	0.046077	-0.002684001	-5.71E-06
C9	0.054598	-0.001080076	8.39E-07
C10	0.065952	-0.00101626	-1.64E-05
C11	0.06604	-0.000345619	-2.90E-05
C12	0.062805	0.005425499	3.89E-05
C13	0.064521	0.011339094	0.000617225
C14	0.036552	0.068360266	0.000158306
C15	0.055113	0.001219089	0
C16	0.057314	0.000459923	-6.82E-06
C17	0.06439	-0.005242573	-2.69E-05
C18	0.077704	-0.000790881	-8.18E-06
C19	0.072539	0.000986623	4.95E-05

C20	0.075223	0.006323975	3.91E-05
C21	0.045151	0.010209017	0.000496667
EDTA			
Atom	CDD_{opt}	CDD_{conf}	conf-CDD×SASA
C1	0.004392	0.044139	0.001728
C2	0.02506	0.037969	0.00044
N3	-0.2291	-0.18009	-0.00065
C4	0.239555	0.028879	0.000125
C5	0.123787	0.041186	0.00013
N6	-0.12383	-0.21831	-0.00064
C7	0.042044	0.05588	0.000379
C8	0.513702	0.039697	0.001471
C9	0.008458	0.047495	0.000328
C10	0.003593	0.041814	0.001561
C11	0.041445	0.065167	0.000406
C12	0.001925	0.046866	0.00175
O13	-0.00724	-0.00192	-0.00179
O14	-0.02022	0.044971	0.010904
O15	0.038869	-0.01295	-0.0055
O16	-0.00308	0.026575	0.007365
O17	-0.08092	-0.01899	-0.00753
O18	-0.03378	0.035096	0.007561
O19	-0.09826	-0.01303	-0.00457
O20	-0.02943	0.025917	0.006087
DOTA			
Atom	CDD_{opt}	CDD_{conf}	conf-CDD×SASA
N1	-0.08235	-0.11539	-0.00068147
C2	0.009427	0.015461	6.73879E-05
C3	0.011067	0.020181	7.92292E-05
N4	-0.09932	-0.1064	-0.0004392
C5	0.042559	0.014253	7.19109E-05
C6	0.146171	0.019417	6.04924E-05
N7	-0.06382	-0.11477	-0.00060509
C8	0.274754	0.018221	6.29484E-05
C9	0.080255	0.022013	9.76824E-05
N10	-0.11741	-0.1173	-0.00068545
C11	0.024336	0.017995	7.96266E-05
C12	0.003045	0.018083	4.48958E-05
C13	0.007547	0.037014	0.000264825
C14	0.025046	0.039935	0.000255653
C15	0.19803	0.037314	0.000280249
C16	0.023971	0.042102	0.000272482
C17	0.002128	0.040527	0.001492097
C18	0.011013	0.035316	0.001373666
C19	0.044222	0.041917	0.001566155
C20	0.003917	0.037839	0.001443138
O21	-0.05839	0.004093	0.000405034
O22	-0.03021	0.049558	0.010610392
O23	-0.03312	0.005641	0.001210923

O24	-0.01518	0.052108	0.011022578
O25	0.034412	0.003136	0.000351256
O26	0.011784	0.052401	0.010950463
O27	-0.06583	0.003326	0.000134514
O28	-0.02465	0.04431	0.010586875
TOPO			
Atom	CDD_{opt}	CDD_{conf}	conf-CDD×SASA
P1	0.02748	0.083352	0
C2	9.32E-05	0.035267	0.000271
C3	0.00671	0.056571	0.000381
C4	0.04065	0.050682	0.000245
C5	0.01352	0.052524	0.000288
C6	0.03346	0.026026	0.000171
C7	0.01530	0.017748	0.000135
C8	0.03696	0.009711	7.19E-05
C9	0.02166	0.041646	0.000255
C10	0.03211	0.02348	0.000156
C11	0.04513	0.020174	0.000135
C12	0.01012	0.010345	7.24E-05
C13	0.01674	0.05547	0.000346
C14	0.0083	0.027518	0.000204
C15	0.00327	0.018789	0.000114
C16	0.00933	0.010372	9.11E-05
O17	0.0203	-0.42037	-0.09358
C18	0.01323	0.010144	7.99E-05
C19	0.00394	0.008976	0.000109
C20	0.00122	0.008686	0.000614
C21	0.02131	0.01158	9.86E-05
C22	0.00666	0.008095	0.000105
C23	0.00082	0.007778	0.000564
C24	0.00018	0.010918	9.53E-05
C25	0.00018	0.00995	0.000125
C26	7.6E-05	0.01291	0.000927

Table 2. Determination coefficients for different estimation of distribution.

Type of analysis	**Determination coefficient for dependence analysis on:**	
	D (dose constant), kGy^{-1}	**Ln(d)**
Average	<0.1	<0.1
Average values more 0,005	0.29	0.59
Average values more 0,001	0.16	0.62
Quartile 1	0.53	0.42
Quartile 2	0.96	0.72
Quartile 3	0.95	0.77
Excess	0.4	0.58
Quantile 0,8	0.96	0.77
Quantile 0,85	0.97	0.76

Quantile 0,9	0.30	0.51

HPLC-MS data:

There are chromatograms for all investigated substances for non-irradiated and one of the irradiated samples for demonstration the changes of concentration. Products of radiolysis were determined by scanning mass-spectrums of each peak for each irradiation dose.

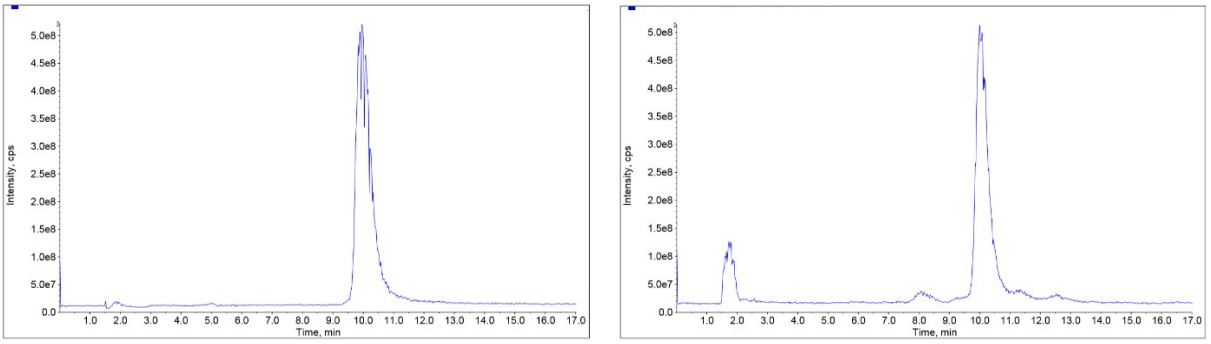

Fig. 2. Chromatograms of non-irradiated and irradiated at 50 kGy HDEHP.

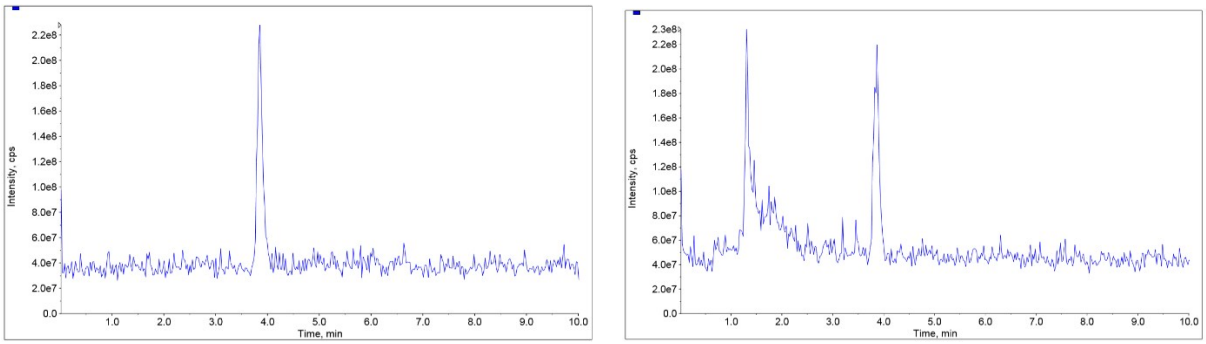

Fig. 3. Chromatograms of non-irradiated and irradiated at 25 kGy PO-1.

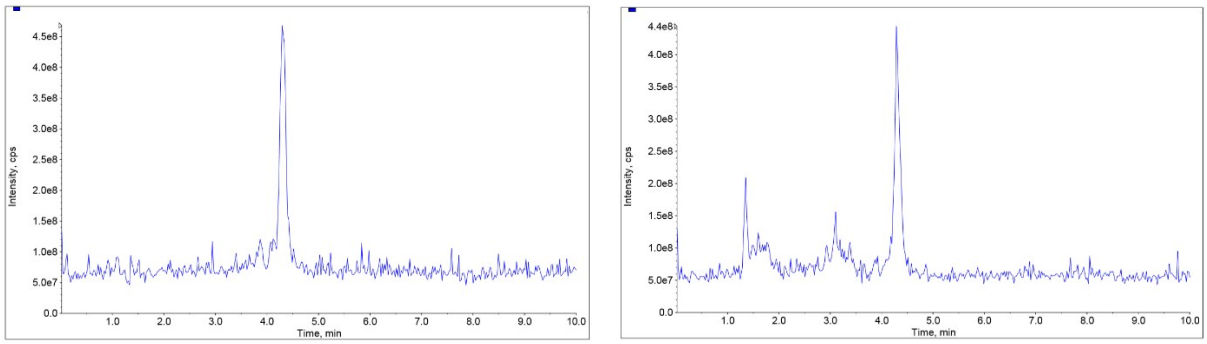

Fig. 4. Chromatograms of non-irradiated and irradiated at 25 kGy TOPO.

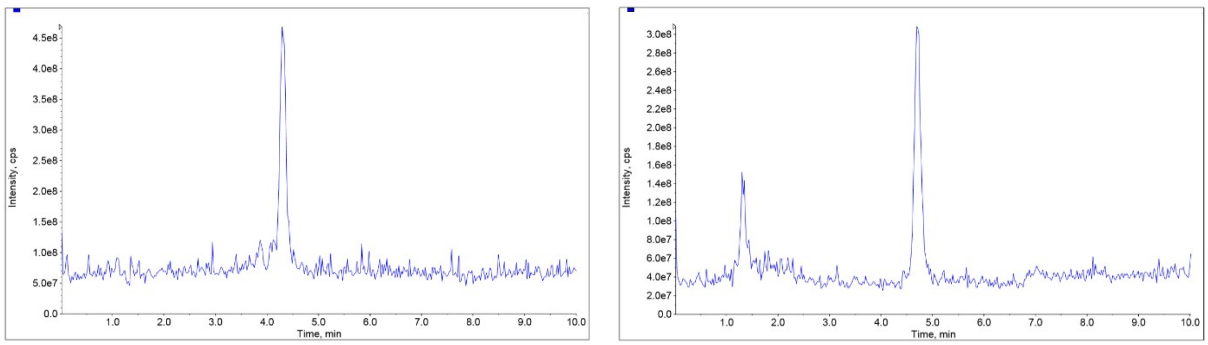

Fig. 5. Chromatograms of non-irradiated and irradiated at 50 kGy TBP.

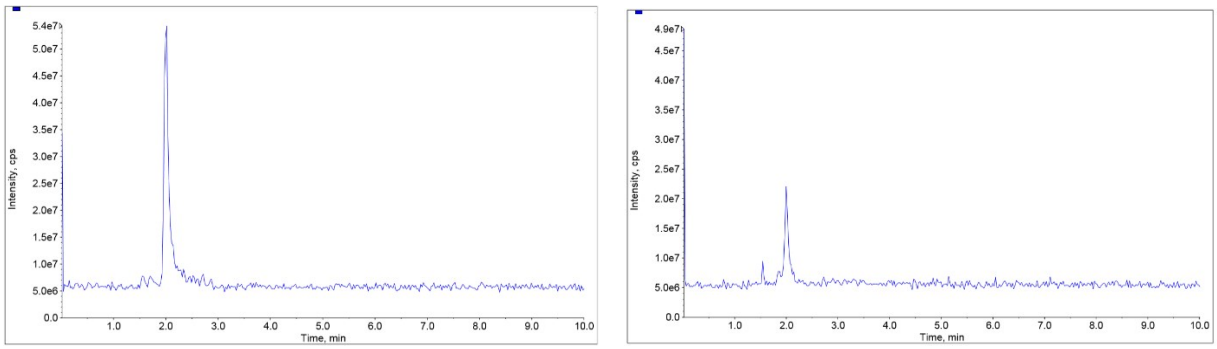

Fig. 6. Chromatograms of non-irradiated and irradiated at 53 kGy DOTA.

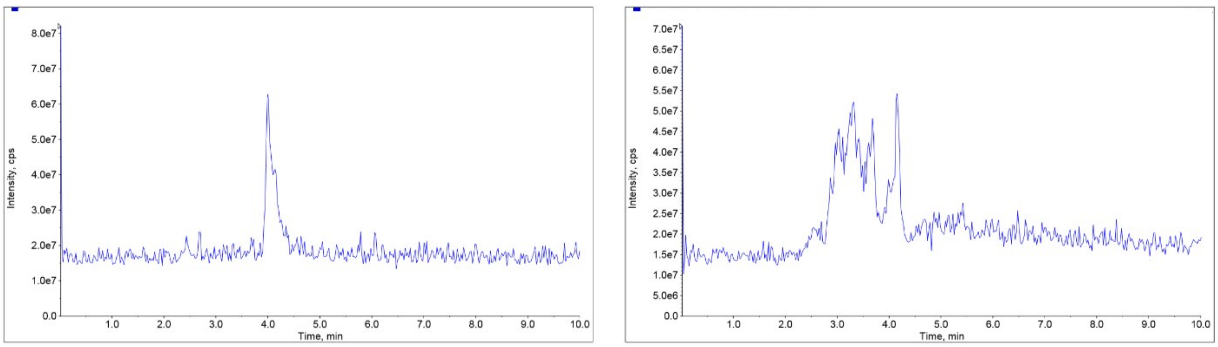

Fig. 7. Chromatograms of non-irradiated and irradiated at 12 kGy EDTA.