

DFT prediction of radiation stability of conformationally flexible ligands

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Table S1. Summary of radiolysis products of water soluble DGAs.

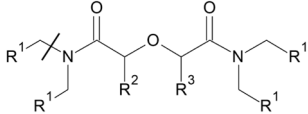
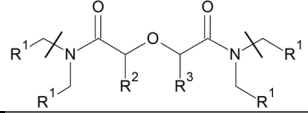
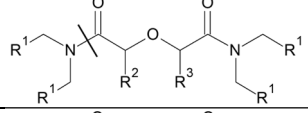
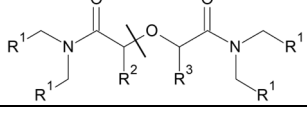
Molecule	Breaking position	TMDGA	TEDGA	MeTEDGA	Me2TEDGA
Single de-alkylation		+	+	+	+
Double de-alkylation		+	+	+	+
De-amination		+	+	+	+
Breaking ether bond		-	+	+	+

Table S2. Calculated Mayer and natural bond orders for TMDGA, TEDGA, MeTEDGA and Me2TEDGA molecules by opt- and conf- approaches. The bold values are the minimum ones for each case. The color row red-orange-yellow-green means the increasing of molecule radiolytic stability.

Molecule	N1-C2	N1-C10	N1-C11	C2-C3	C2-O8	C3-O4	O4-C5	C5-C6	C6-N7
TMDGA_opt_MBO	1.12	0.86	0.86	1.05	1.35	0.56	0.84	0.85	1.21
TMDGA_conf_MBO	1.20	0.93	0.93	0.92	1.96	0.95	0.95	0.93	1.20
TMDGA_opt_NBO	1.21	0.98	0.98	0.95	1.65	0.92	0.97	0.94	1.20
TMDGA_conf_NBO	1.16	0.98	0.98	0.98	1.67	0.95	0.95	0.98	1.15
TEDGA_opt_MBO	1.01	1.00	0.95	0.89	1.35	0.49	0.75	0.79	1.11
TEDGA_conf_MBO	1.19	0.93	0.90	0.94	1.96	1.03	1.03	0.94	1.19
TEDGA_opt_NBO	1.22	0.96	0.97	0.95	1.64	0.92	0.97	0.94	1.21
TEDGA_conf_NBO	1.13	0.97	0.96	0.97	1.67	0.96	0.96	0.97	1.13
MeTEDGA_opt_MBO	0.97	1.01	0.96	0.90	1.37	0.45	0.62	0.84	1.10
MeTEDGA_conf_MBO	1.18	0.91	0.92	0.92	1.96	0.95	1.01	0.93	1.20
MeTEDGA_opt_NBO	1.22	0.96	0.96	0.95	1.64	0.93	0.95	0.97	1.28
MeTEDGA_conf_NBO	1.14	0.97	0.97	0.96	1.68	0.94	0.96	0.98	1.15
Me2TEDGA_opt_MBO	0.94	0.91	1.04	0.27	1.53	0.23	0.58	0.65	1.13
Me2TEDGA_conf_MBO	1.19	0.91	0.91	0.93	1.92	1.00	0.91	0.94	1.17
Me2TEDGA_opt_NBO	1.23	0.96	0.96	0.93	1.64	0.93	0.94	0.93	1.21
Me2TEDGA_conf_NBO	1.14	0.97	0.97	0.95	1.68	0.94	0.93	0.96	1.12
Molecule	C6-O9	N7-C12	N7-C13	C3-C18	C5-C19	C10-C14	C11-C15	C12-C16	C13-C17
TMDGA_opt_MBO	1.43	0.88	0.89	-	-	-	-	-	-
TMDGA_conf_MBO	1.95	0.93	0.93	-	-	-	-	-	-
TMDGA_opt_NBO	1.65	0.97	0.99	-	-	-	-	-	-
TMDGA_conf_NBO	1.68	0.98	0.99	-	-	-	-	-	-
TEDGA_opt_MBO	1.43	0.99	0.93	-	-	0.65	0.62	0.62	0.62
TEDGA_conf_MBO	1.95	0.90	0.93	-	-	0.93	0.93	0.93	0.93

TEDGA_opt_NBO	1.64	0.95	0.97	-	-	1.02	1.02	1.02	1.02
TEDGA_conf_NBO	1.67	0.96	0.97	-	-	1.01	1.02	1.02	1.01
MeTEDGA_opt_MBO	1.32	1.01	0.97	0.21	-	0.65	0.58	0.60	0.59
MeTEDGA_conf_MBO	1.94	0.91	0.91	0.93	-	0.93	0.93	0.93	0.93
MeTEDGA_opt_NBO	1.64	0.97`	0.95	0.92	-	1.02	1.02	1.02	1.02
MeTEDGA_conf_NBO	1.68	0.97	0.97	1.01	-	1.03	1.02	1.02	1.02
Me2TEDGA_opt_MBO	1.20	0.88	1.00	0.19	0.31	0.54	0.66	0.44	0.59
Me2TEDGA_conf_MBO	1.96	0.92	0.93	0.89	0.90	0.93	0.93	0.93	0.92
Me2TEDGA_opt_NBO	1.63	0.95	0.96	1.02	1.01	1.02	1.02	1.02	1.02
Me2TEDGA_conf_NBO	1.70	0.97	0.97	1.00	1.00	1.02	1.02	1.02	1.02

Table S3. Dose constants for the investigated molecules and CRD value (0.85 quantile of CDD×SASA_k).

DGA molecule	Dose constant, 10 ⁻³ kGy	0.85 quantile of CDD×SASA _{k (conf)} absolute value
TMDGA	14.9 ± 1.2	5.58
TEDGA	11.1 ± 0.9	1.75
Me-TEDGA	7.8 ± 0.7	1.19
Me ₂ -TEDGA	7.3 ± 2.1	0.75