Electronic Supplementary Information

Irreversible electron attachment - a key to DNA damage by solvated electrons in aqueous solution

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Scheme S1 Digestion of a TXT trimer by Micrococcal (MC) or P1 nuclease (P1).

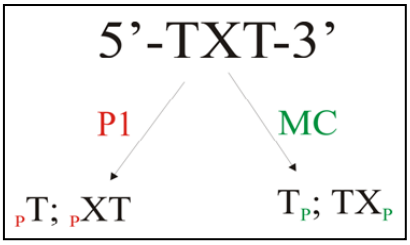

Table S1 Retention times (for HPLC conditions see the *Chromatography* section) for dimers (pXT/TXp) and monomers (pT/Tp) obtained by enzymatic digestion with Micrococcal Nuclease (A) and P1 nuclease (B)

A

	Retention time [min.]	
Name	**$_{HO}T_{P}$**	**$_{HO}TX_{P}$**
TAT	7,3-9,3	10,8-11,4
TCT	-	10,3-10,9
TTT	7,2-7,8	11,7-12,3
TUT	-	11,4-12,1
TGT	-	9,4-10,0

B

	Retention time [min.]	
Name	**$_{P}T_{OH}$**	**$_{P}XT_{OH}$**
TAT	5,0-5,8	-
TCT	4,9-5,5	-
TTT	5,1-5,8	-
TUT	5,1-5,8	9,8-11,2
TGT	-	-

Table S2 Stable fragments obtained after gamma irradiation of modified trimmers in 30 mM Tris

	dT=O	$_{HO}T_{OH}$	$_{P}T_{OH}$	$_{HO}T_{P}$	$_{HO}TX{=}O$	$_{HO}TX_{P}$	$_{HO}XT_{OH}$/ $_{HO}TX_{OH}$	$_{P}XT_{OH}$	$T_{HO}XT$	$T_{OXO}XT$	abasic site	TXT	TYT
TBrUT	+	+	+	+	+	+	+	+	+	-	+	+	+
TBrCT	+	+	+	+	+	+	+	+	+	-	+	+	+
TBrAT	-	+	+	+	-	+	+	+	-	-	-	+	+
TBrGT	-	+	+	+	-	+	+	+	-	+	-	+	+

Table S3 Molar absorption coefficients[1]

TYT	TXT	dihydro-TXT	$_{P}XT_{OH}$	$_{HO}XT_{OH}$/ $_{HO}TX_{OH}$	$_{P}T_{OH}$/ $_{HO}T_{P}$	$_{HO}T_{OH}$	$_{HO}TX{=}O$	dT=O	Abasic site	$T_{HO}XT$	$T_{OXO}XT$
					TBrAT						
30200	30800	28400	22800	23400	8700	8700	23400	8700	16800	n/a	26500
					TBrCT						
19300	23600	21200	15200	16200	8700	8700	16200	8700	16800	19600	n/a
					TBrUT						
21300	26432	24032	18332	18332	8700	8700	18332	8700	16800	21100	n/a
					TBrGT						
27300	27500	25100	20000	19000	8700	8700	19000	8700	16800	n/a	21900
					TTT						
n/a	24800	22400	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a

[1]absorption coefficient, ε_{TXT}, calculated using the nearest neighbor model (*Biophys. Chem.* **2008**, *133*, 66–70; http://biophysics.idtdna.com/UVSpectrum.html);

Absorption coefficient, ε_{Y}, taken from http://www.glenresearch.com/Technical/Extinctions.html;

$\varepsilon_{TYT} = \varepsilon_{TXT} - \varepsilon_{X} + \varepsilon_{Y}$; $\varepsilon_{pXT_{OH}} = \varepsilon_{_{OH}XT_{OH}} = \varepsilon_{XT}$; $\varepsilon_{_{OH}Tp} = \varepsilon_{pT_{OH}} = \varepsilon_{_{OH}T_{OH}} = \varepsilon_{T}$;
$\varepsilon_{O=XT_{OH}} = \varepsilon_{TX}$; $\varepsilon_{dT=O} = \varepsilon_{T}$; $\varepsilon_{abasic\ site} = \varepsilon_{TXT} - \varepsilon_{X}$; $\varepsilon_{T_{HO}XT} = \varepsilon_{TXT} - \varepsilon_{X} + \varepsilon_{_{HO}X}$,
$\varepsilon_{T_{oxo}XT} = \varepsilon_{TXT} - \varepsilon_{X} + \varepsilon_{_{oxo}X}$; $\varepsilon_{dihydro-TXT} = \varepsilon_{TXT} - \varepsilon_{T} + \varepsilon_{dihydro-T}$

Table S4 Molar contribution (in %) of individual products generated by irradiation of 3 x 10^{-5} M TBrAT solution containing various amount of Tris with 140 Gy (for individual molar absorption coefficients see Table S3 and for product symbols see Fig. 2).

Product	0[a]	60[a]	200[a]
$_{P}T_{OH}$	1.19	0.27	0.19
$_{HO}T_{OH}/_{HO}T_{P}$	1.65	0.55	0.52
$_{HO}TA_{OH}/$ $_{HO}AT_{OH}$	8.75	2.65	2.52
$_{P}AT_{OH}$	7.67	1.60	1.49
$T_{OXO}AT$	1.03	-	-
TAT	29.83	11.94	14.2

[a] Tris concentration in mM

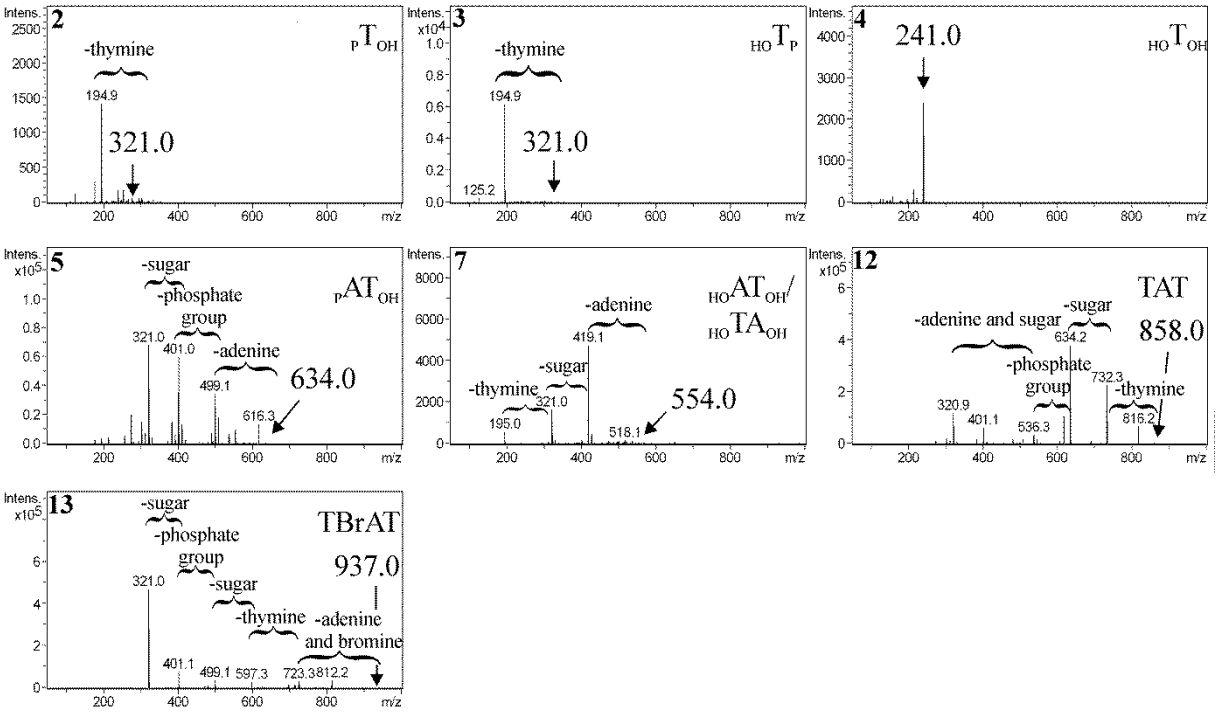

Fig. S1 MS/MS (in the negative ionization mode) spectra of gamma irradiated aqueous solution of TBrAT (the arrows indicate the mass of pseudomolecular anions; for species symbols see Fig. 2).

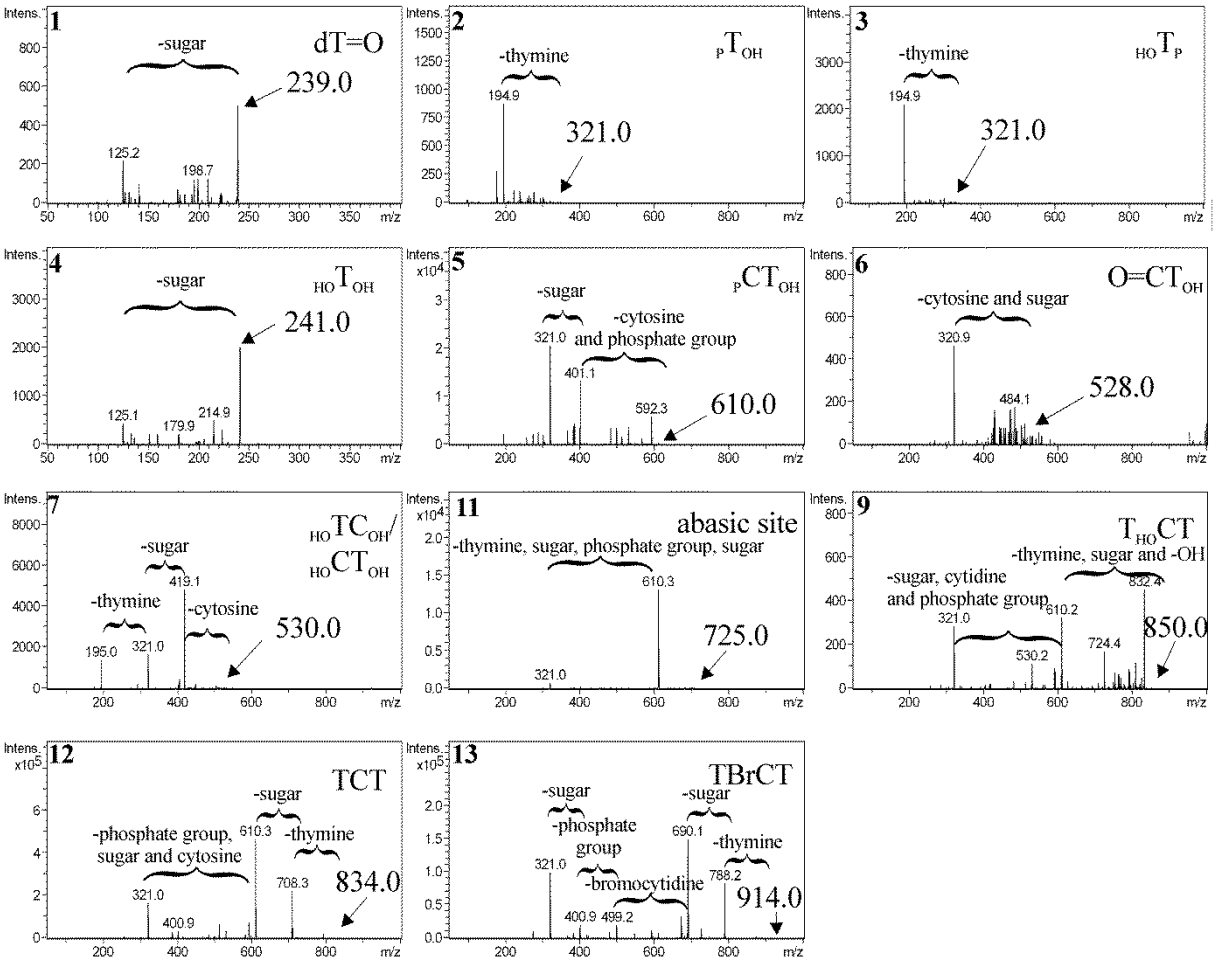

Fig. S2 MS/MS (in the negative ionization mode) spectra of gamma irradiated aqueous solution of TBrCT (the arrows indicate the mass of pseudomolecular anions; for species symbols see Fig. 2).

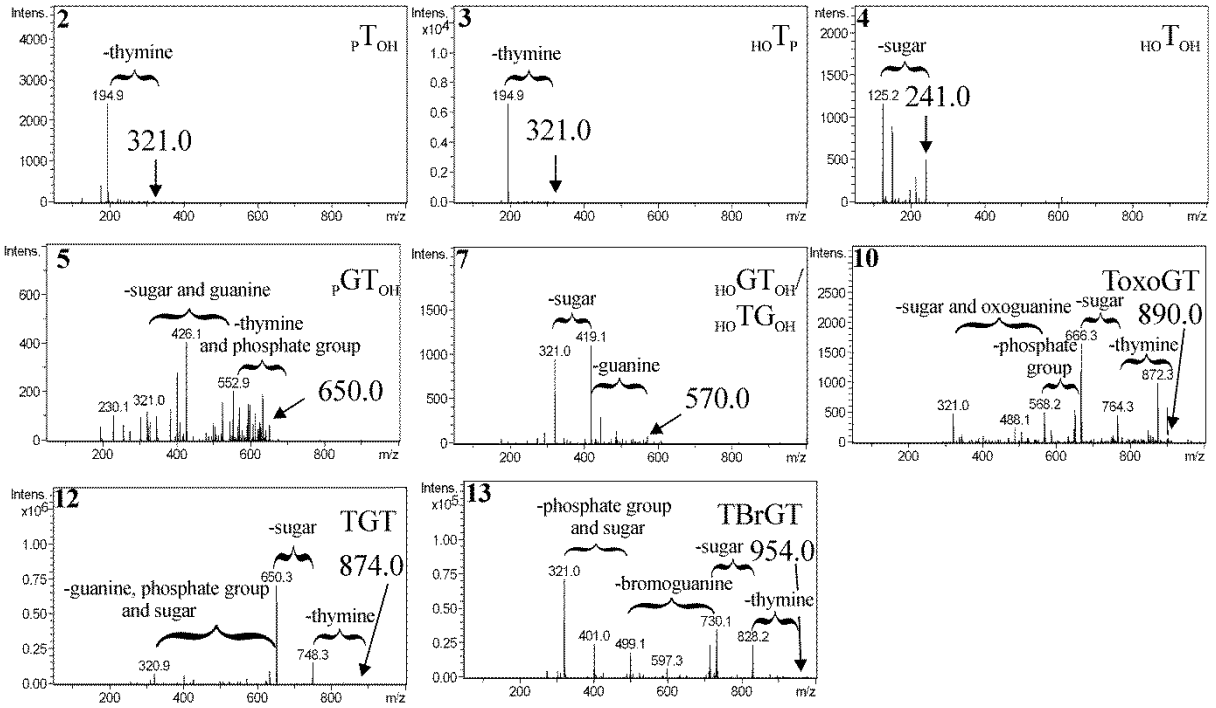

Fig. S3 MS/MS (in the negative ionization mode) analysis of gamma irradiated aqueous solution of TBrGT (the arrows indicate the mass of pseudomolecular anions; for species symbols see Fig. 2).