

STRUCTURAL INVESTIGATIONS OF STEREOISOMERIC N3-(2-HYDROXY-3-
BUTEN-1-YL)-2'-DEOXYURIDINE DNA ADDUCTS

By

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To my loving husband,

Ryan Benjamin Musser

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LIST OF ABBREVIATIONS

1D	one dimensional
2D	two dimensional
BD	1,3-butadiene
BDE	3,4-epoxy-1,2-butanediol
BDO	butadiene monoepoxide (1,2-epoxy-3-butene)
BDO ₂	butadiene diepoxide (1,2:3,4-diepoxbutane)
CORMA	complete relaxation matrix analysis
COSY	correlation spectroscopy
dA	deoxyadenosine
dC	deoxycytidine
dG	deoxyguanosine
dT	deoxythymidine
DNA	deoxyribonucleic acid
DQF-COSY	double-quantum filtered correlation spectroscopy
EDTA	ethylenediamine tetraacetic acid
HPLC	high performance liquid chromatography
MD	molecular dynamics
NMR	nuclear magnetic resonance
NOE	nuclear Overhauser effect
NOESY	two dimensional nuclear Overhauser effect spectroscopy
PEM	potential energy minimization
ppm	parts per million
R-BD-N3-dU	R-N3-(2-hydroxy-3-butene-1-yl)-2'-deoxyuridine adduct
R ₁ ^x	sixth root residual index
rMD	restrained molecular dynamics
rmsd	root mean square deviation
S-BD-N3-dU	S-N3-(2-hydroxy-3-butene-1-yl)-2'-deoxyuridine adduct
<i>t</i> ₁	evolution period
τ_m	mixing time
TOCSY	total correlation spectroscopy
TPPI	time-proportional phase increment