# 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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TABLE OF CONTENTS

LIST OF FIGURES

Figure Page

# 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-diepoxybutane) |
| 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 |
| $t_1$ | evolution period |
| $\tau_m$ | mixing time |
| TOCSY | total correlation spectroscopy |
| TPPI | time-proportional phase increment |