Supplementary Material

Striking difference in reactivity of trienes and oximes derived from glucose and xylose

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Calculations of molecular orbitals (MO) were performed by the Gaussian 09 program suite, at the B3LYP/6-311G(2d,p) theory level, using B3LYP/6-31G(2d,p) optimized compound structures. Conformations of compounds were selected arbitrarily. Numbering plan of orbitals, as well as their energy (a.u.), was given as provided by the Gaussian software.
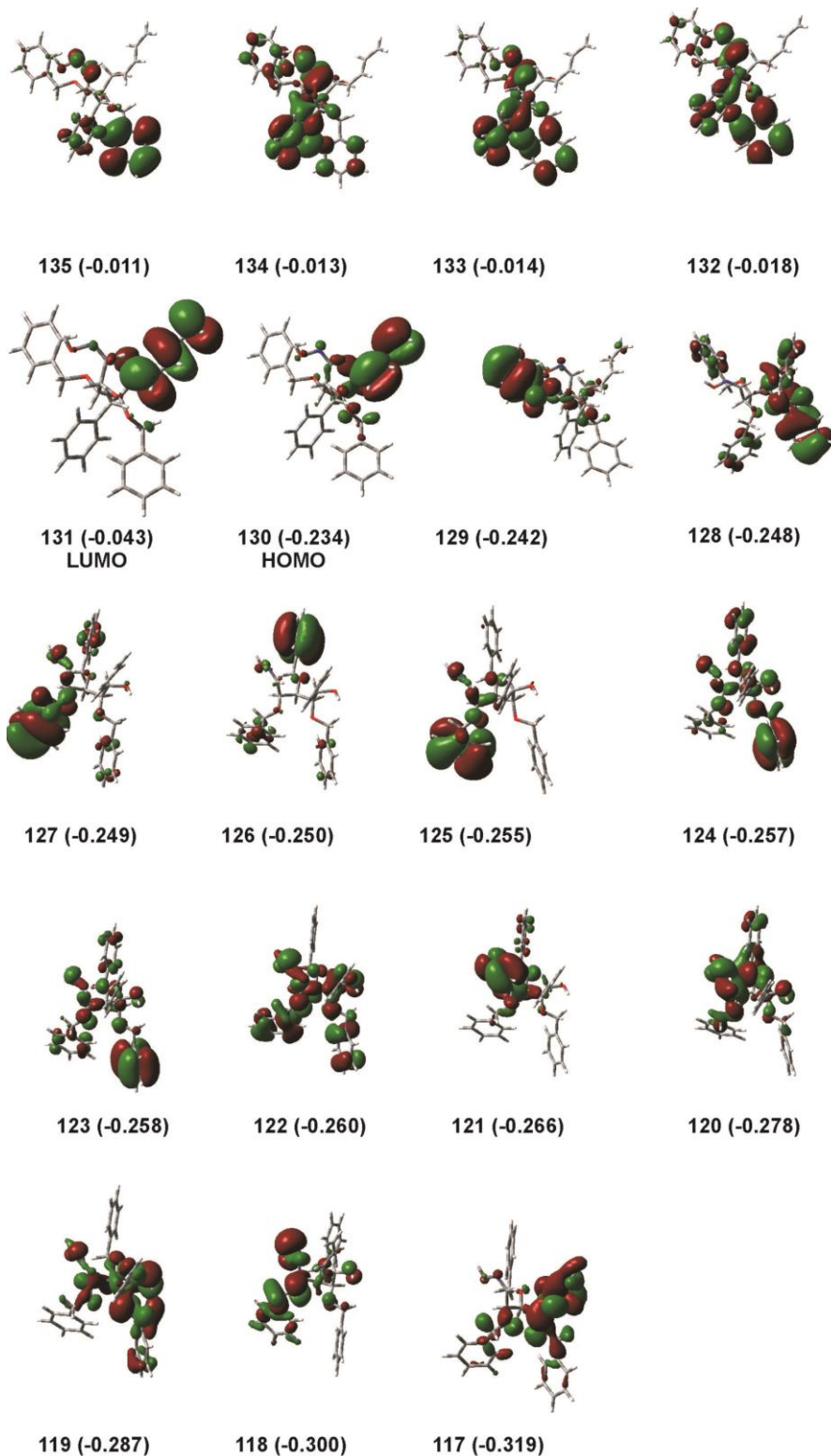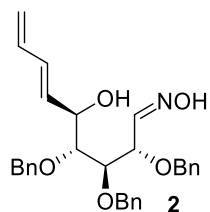
135 (-0.011)   134 (-0.013)   133 (-0.014)   132 (-0.018)

131 (-0.043)
LUMO

130 (-0.234)
HOMO

129 (-0.242)

128 (-0.248)

127 (-0.249)   126 (-0.250)   125 (-0.255)   124 (-0.257)

123 (-0.258)   122 (-0.260)   121 (-0.266)   120 (-0.278)

119 (-0.287)   118 (-0.300)   117 (-0.319)

Figure 1S. Selected MO for **2**.

126 (-0.011)   125 (-0.012)   124 (-0.016)   123 (-0.038)
                                                                    LUMO

122 (-0.235)   121 (-0.247)   120 (-0.248)   119 (-0.249)
HOMO

118 (-0.249)   117 (-0.255)   116 (-0.255)   115 (-0.258)

114 (-0.265)   113 (-0.272)   112 (-0.282)   111 (-0.289)
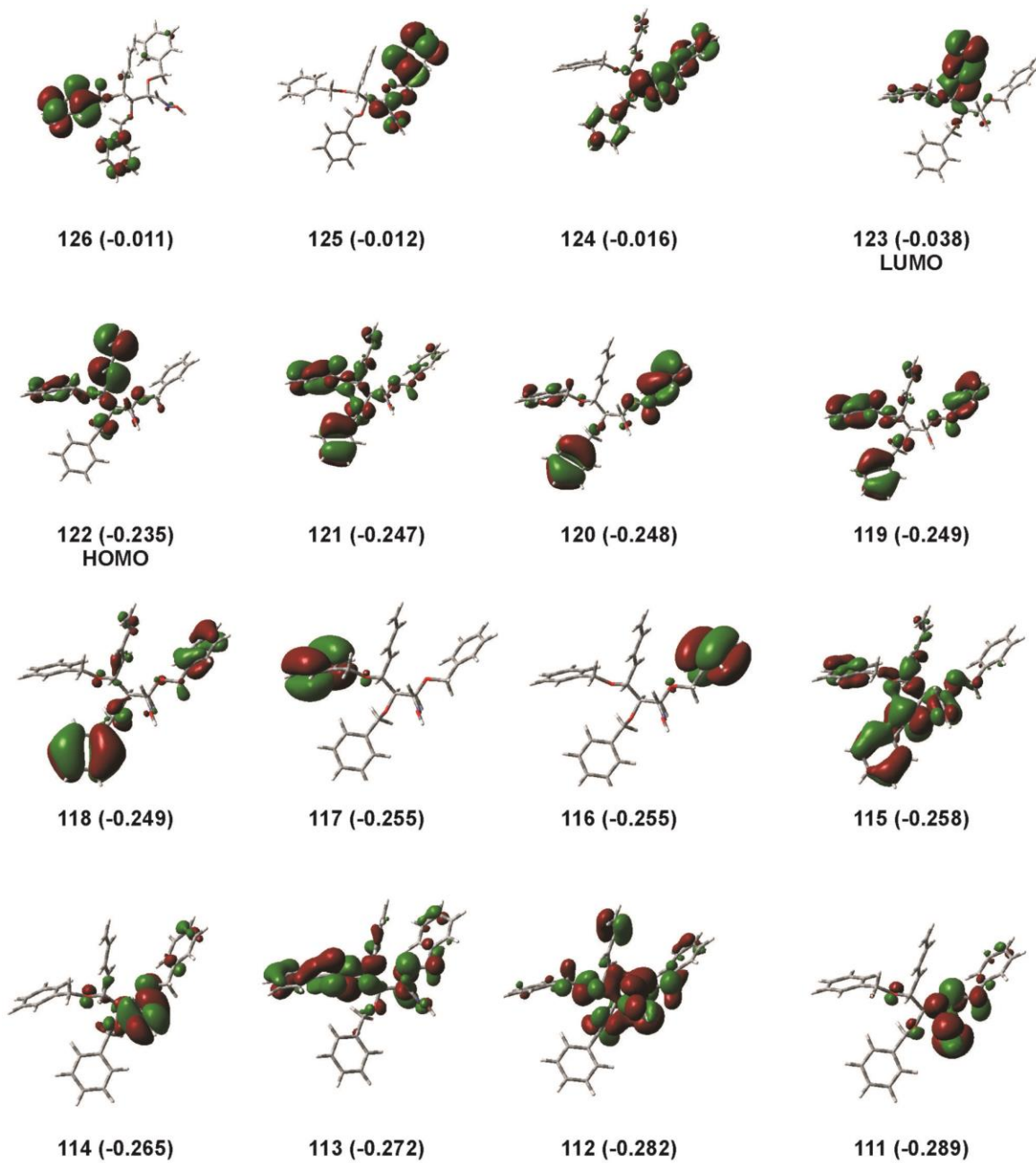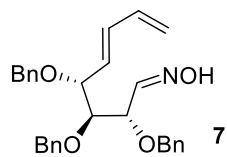
Figure 2S. Selected MO for **7**.

11a   **11b**

(a)

69 (-0.033)
LUMO+1

68 (-0.063)
LUMO

67 (-0.233)
HOMO

66 (-0.260)
HOMO-1

(b)

69 (-0.022)
LUMO+1

68 (-0.052)
LUMO

67 (-0.220)
HOMO

66 (-0.265)
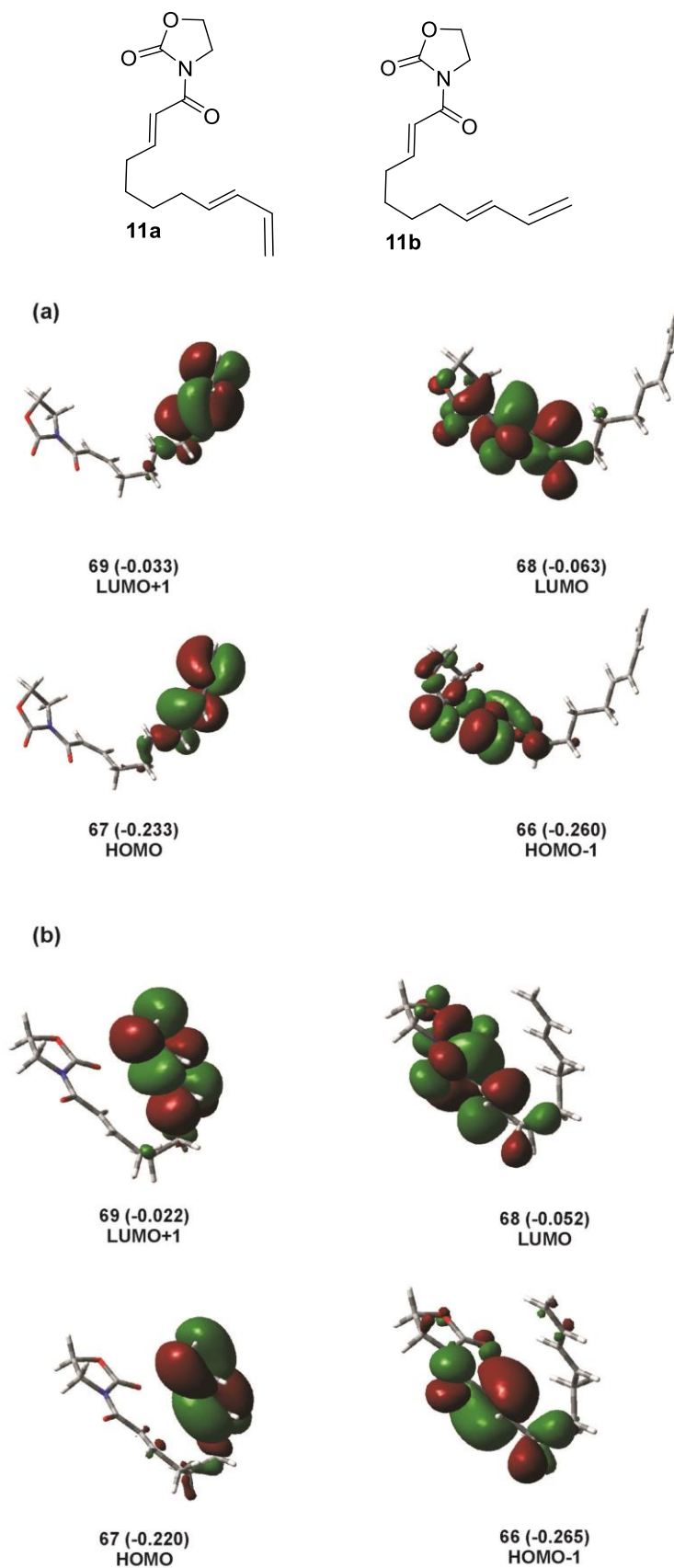HOMO-1

Figure 3S. Selected MO for two conformers of **11**, *s-cis* (a) and *s-trans* (b).

177 (-0.036)

176 (-0.064)
LUMO

175 (-0.221)
HOMO

174 (-0.227)

173 (-0.243)

172 (-0.245)

171 (-0.249)

170 (-0.250)

169 (-0.250)

168 (-0.254)

167 (-0.255)

166 (-0.262)

165 (-0.272)

164 (-0.277)

163 (-0.282)

162 (-0.284)

161 (-0.289)

160 (-0.290)

159 (-0.306)

162 (-0.313)

Figure 4S. Some MO for **13**.

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149 (-0.041)   148 (-0.060)   147 (-0.234)   146 (-0.251)

LUMO   HOMO

145 (-0.254)   144 (-0.257)   143 (-0.258)   142 (-0.261)

141 (-0.262)   140 (-0.268)   139 (-0.273)   138 (-0.274)
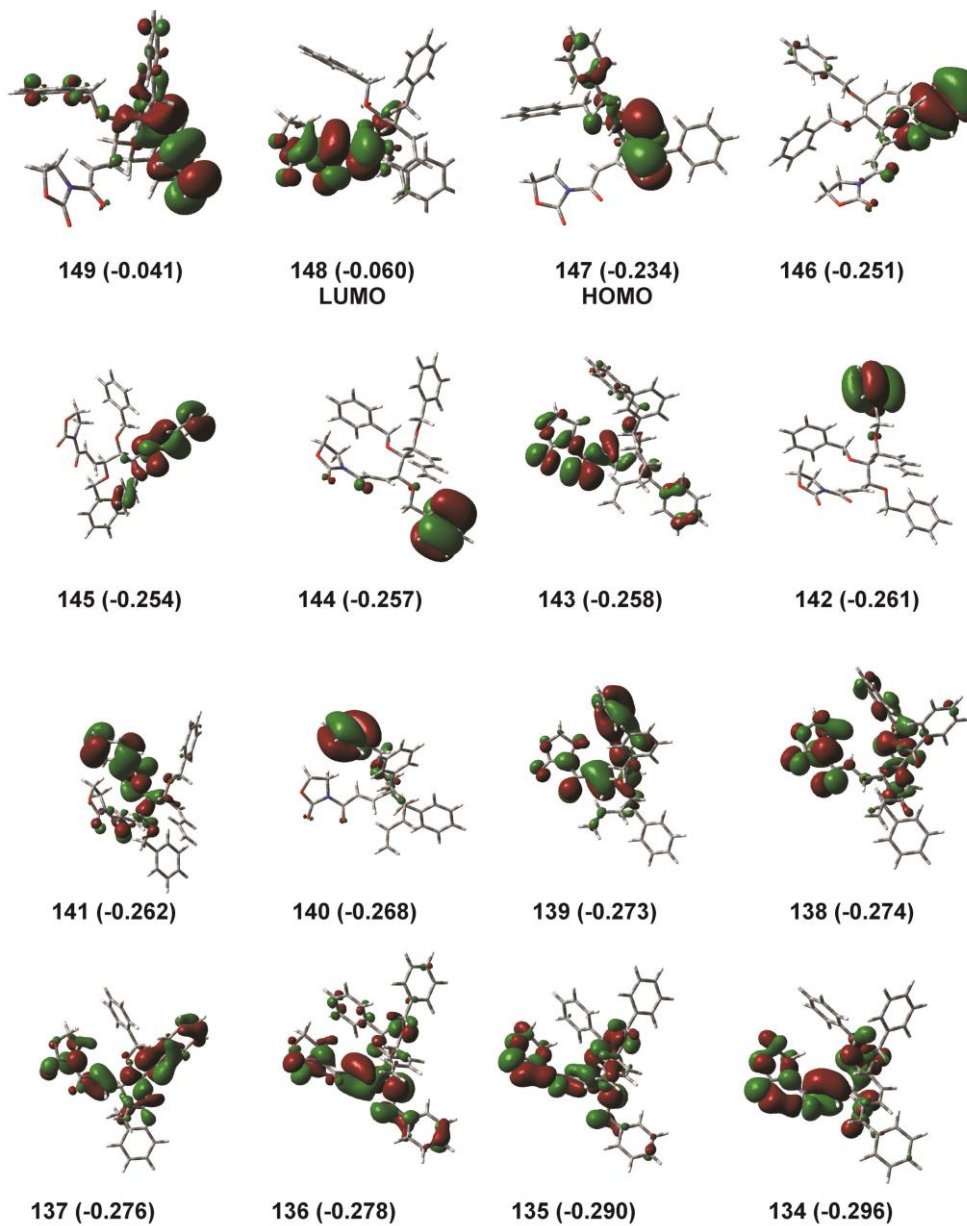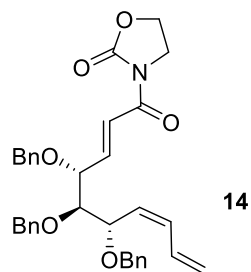
137 (-0.276)   136 (-0.278)   135 (-0.290)   134 (-0.296)
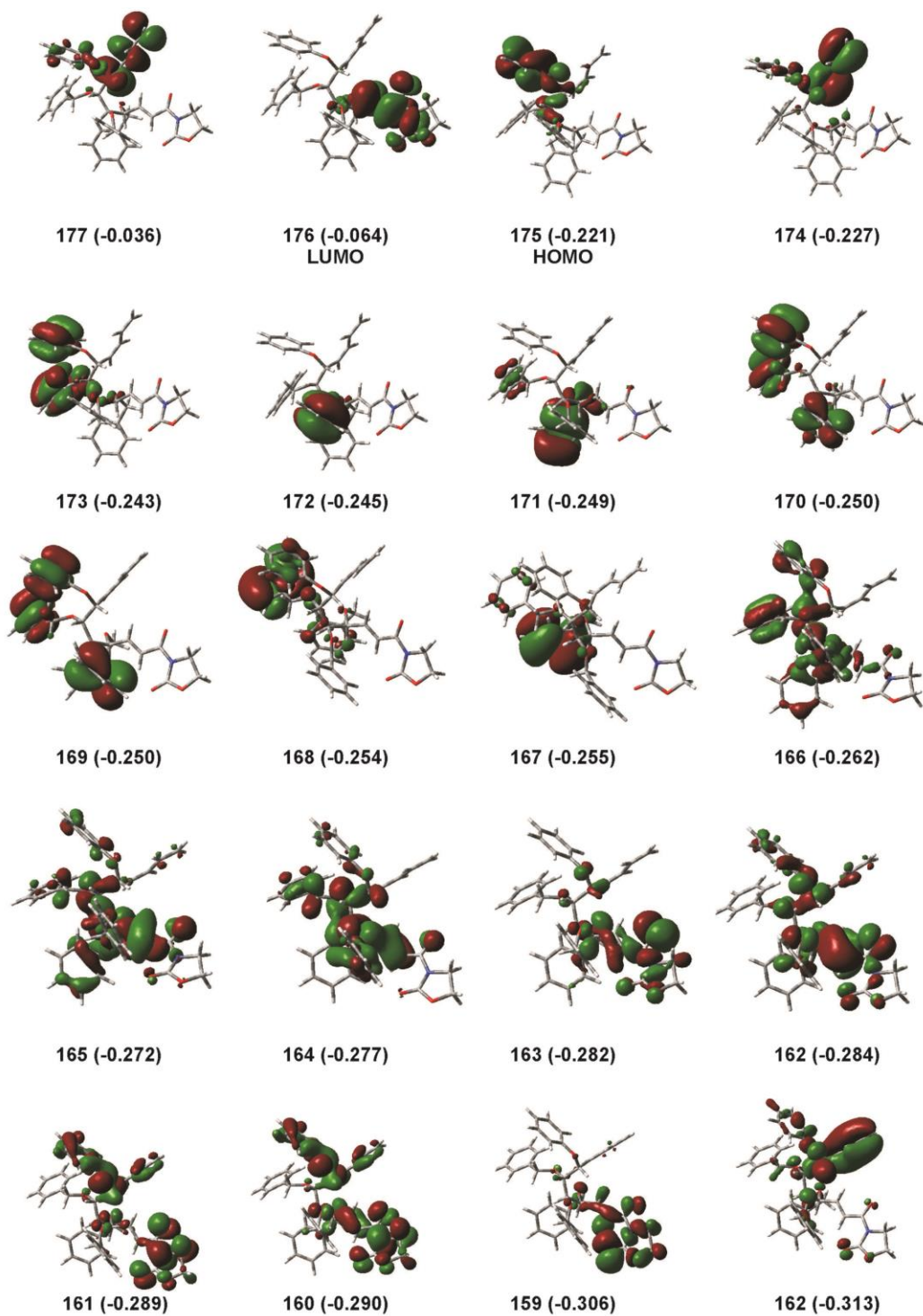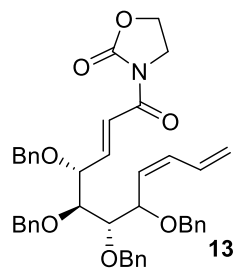
Figure 5S. Some molecular orbitals for **14.**