Supporting Information

Toluene dioxygenase-mediated oxidation of halogen-substituted benzoate esters

Vladislav Semak, a Thomas A. Metcalf, a Mary Ann A. Endoma-Arias, a Pavel Mach, b and Tomas Hudlicky a *

a Department of Chemistry, Brock University, 500 Glenridge Ave, St. Catharines, On, Canada, L2S 3A1
*Corresponding author. Tel.: +1-905-688-5550x4956; fax: +1-905-984-4841; e-mail address:
thudlicky@brocku.ca

b Department of Nuclear Physics and Biophysics, Faculty of Mathematics, Physics and Informatics,
Comenius University, Mlynská dolina, 842 15 Bratislava, Slovakia

[To whom correspondence regarding calculations should be addressed]

Table of Contents

| Copies of ¹H and ¹³C spectra | S2-S25 |

S1
1d carbon with proton decoupling
In carbon with proton decoupling
In carbon with proton decoupling