Drug Metabolism and Disposition : Supplementary Information

Metabolism of anethole dithiolethione by rat and human liver microsomes: formation of various products deriving from its O-demethylation and S-oxidation. Involvement of cytochromes P450 and flavin monooxygenases in these pathways.

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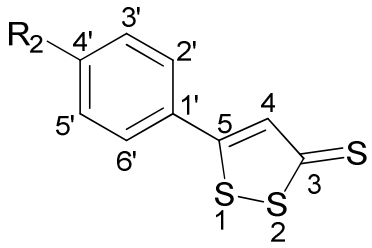
^{1}H NMR, UV-visible and high resolution mass spectra of ADT and metabolites.

- ^{1}H NMR data



Compounds	**$H_{2'}$ / $H_{6'}$**	**$H_{3'}$ / $H_{5'}$**	**R_2**	**H_4**
ADT	7.86, d, 2H, *J* = 8.5	7.11, d, 2H, *J* = 8.5	3.91, s, 3H	7.53, s, 1H
ADTSO	7.70, d, 2H, *J* = 8.5	7.08, d, 2H, *J* = 8.5	3.89, s, 3H	7.72, s, 1H
ADO	7.80, d, 2H, *J* = 8.5	7.10, d, 2H, *J* = 8.5	3.90, s, 3H	7.00, s, 1H
dmADT	7.79, d, 2H, *J* = 8.5	7.00, d, 2H, *J* = 8.5	9.45, s, 1H	7.50, s, 1H
dmADTSO	7.62, d, 2H, *J* = 8.5	6.97, d, 2H, *J* = 8.5	9.27, s, 1H	7.67, s, 1H
dmADO	7.71, d, 2H, *J* = 8.5	7.00, d, 2H, *J* = 8.5	9.33, s, 1H	6.95, s, 1H

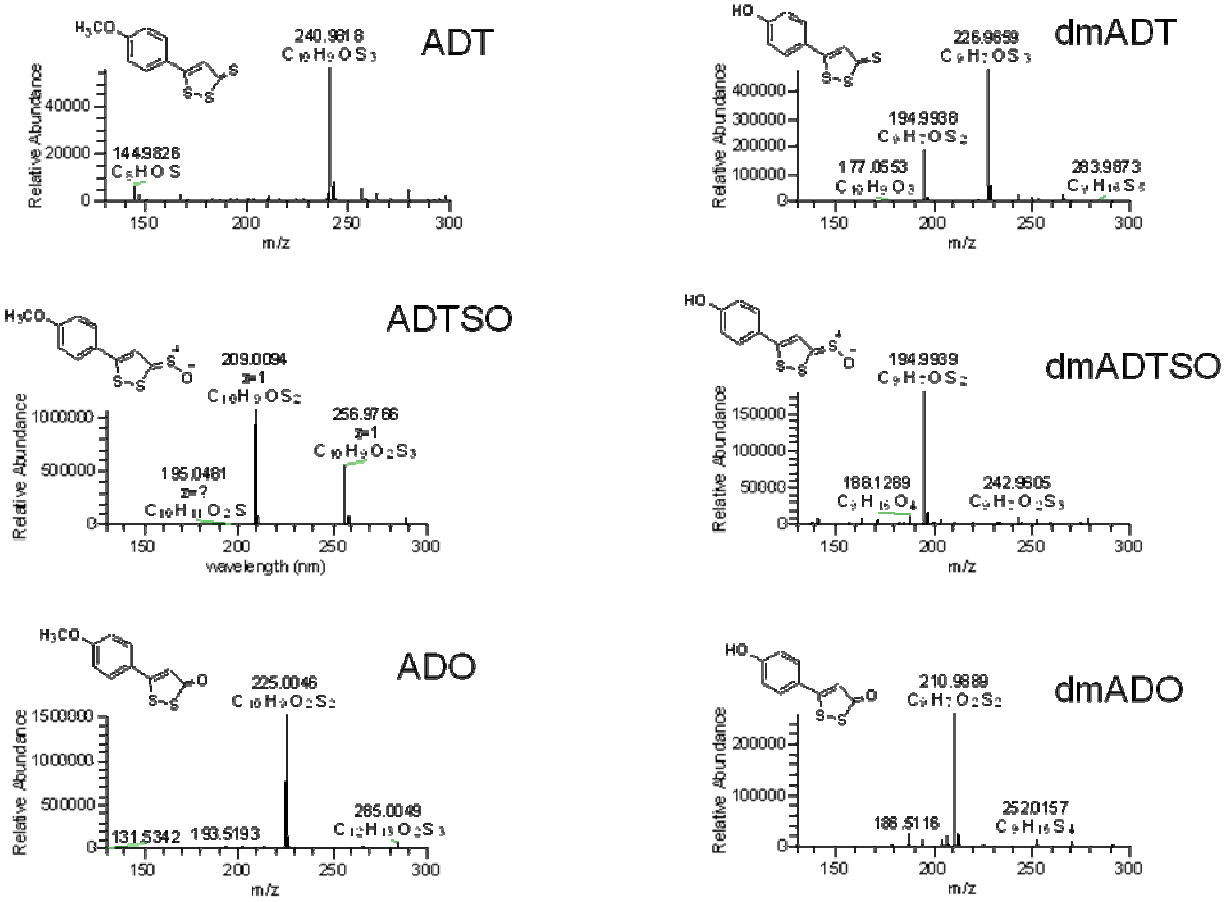
^{1}H NMR spectra were recorded on a 500 MHz Avance II Bruker NMR spectrometer (Wissembourg, France) in d_6 acetone. Chemical shifts are reported in parts per million (δ) relative to tetramethylsilane with peak multiplicities abbreviated as follows: singlet, s; doublet, d; coupling constants, *J*, are reported in Hz.

- UV/Visible data

Compounds	λ_{max} (nm)	**ε (M^{-1}/cm^{-1})**
ADT	420	19000
	360	17000
ADTSO	450	22600
	345	20100
ADO	322	22800
dmADT	426	17600
	360	13800
dmADTSO	456	18600
	345	16800
dmADO	322	22200

UV/Visible spectra were recorded in 0.1 M phosphate buffer pH 7.4 on an UVIKON 941 spectrophotometer in 1-cm path-length quartz cuvettes.

- High Resolution Mass Spectra



High Resolution Mass Spectra were recorded on an Exactive mass spectrometer (Thermo, Les Ulis, France) and analyzed with Excalibur software.