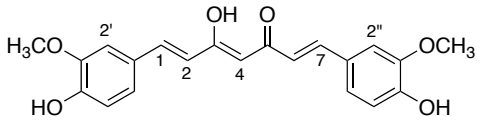
SUPPLEMENTAL DATA

Griesser et al., Autoxidative and COX-2 catalyzed transformation of the dietary chemopreventive agent curcumin

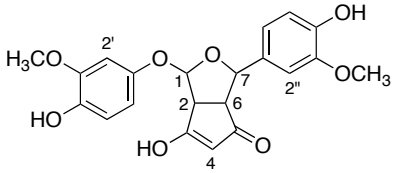
Supplemental Fig. S1.
Nomenclature and carbon numbering of curcumin and its main oxygenated metabolite (**1**).

Supplemental Fig. S2.
MS2 spectra of the main oxygenated metabolite **1** of curcumin formed in unlabeled (MS2 of *m/z* 399, top) and ^{18}O-labeled buffer (MS2 of *m/z* 401, below).

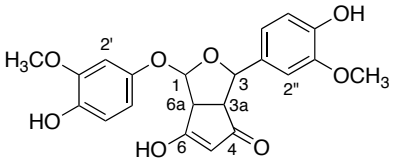
Supplemental Fig. S3.
Predicted product formation by autoxidative and COX-2 catalyzed transformation of 4'-methoxycurcumin. MS2 spectra of the main oxygenated metabolite **1** of 4'-methoxycurcumin formed in unlabeled (MS2 of *m/z* 413, middle) and ^{18}O-labeled buffer (MS2 of *m/z* 415, below).



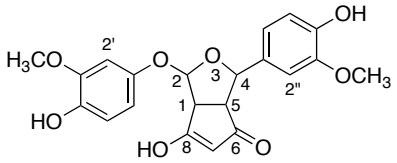
curcumin
(1*E*,4*Z*,6*E*)-5-hydroxy-1,7-*bis*(4-hydroxy-
3-methoxyphenyl)hepta-1,4,6-trien-3-one



bicyclopentadione
(showing the curcumin-based numbering of carbons)

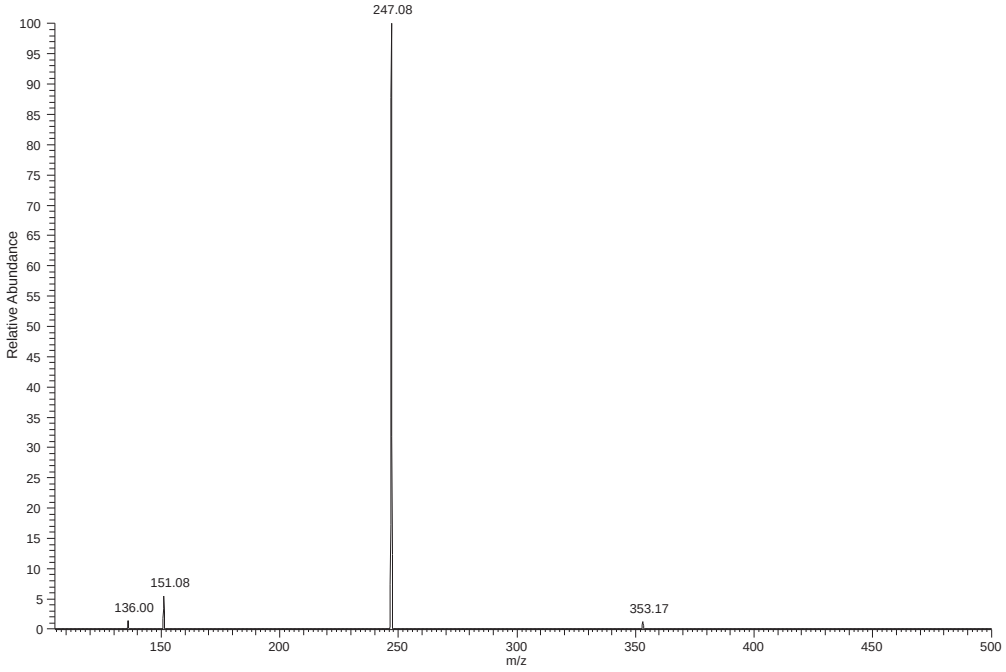


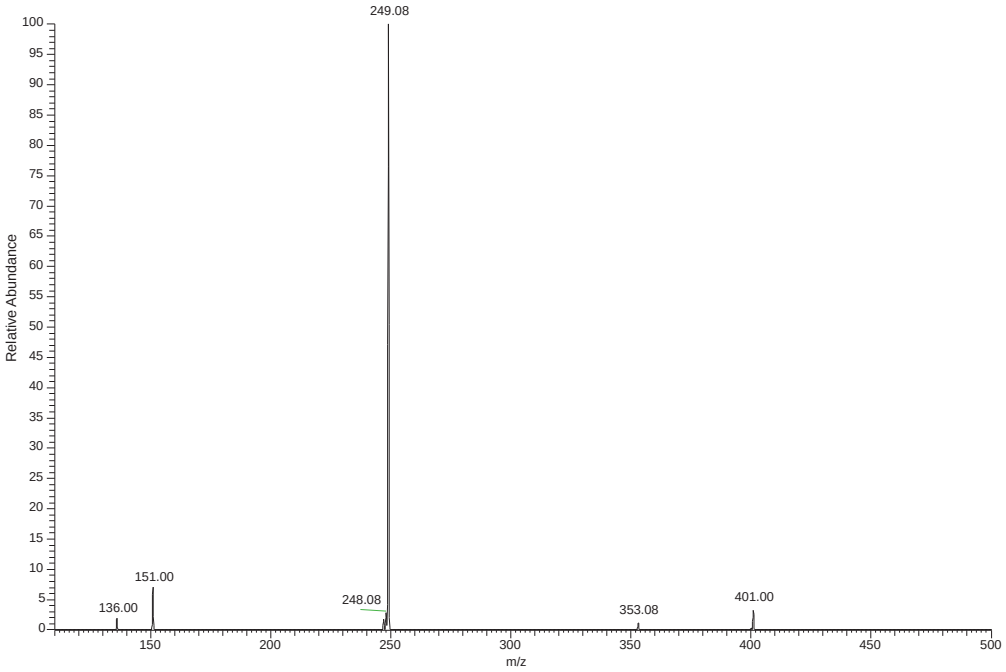
bicyclopentadione
(using chemically correct numbering of carbons)
6-hydroxy-1-(4'-hydroxy-3'-methoxyphenoxy)
-3-(4"-hydroxy-3"-methoxyphenyl)-3,3a-dihydro-
1*H*-cyclopenta[*c*]furan-4(6a*H*)-one



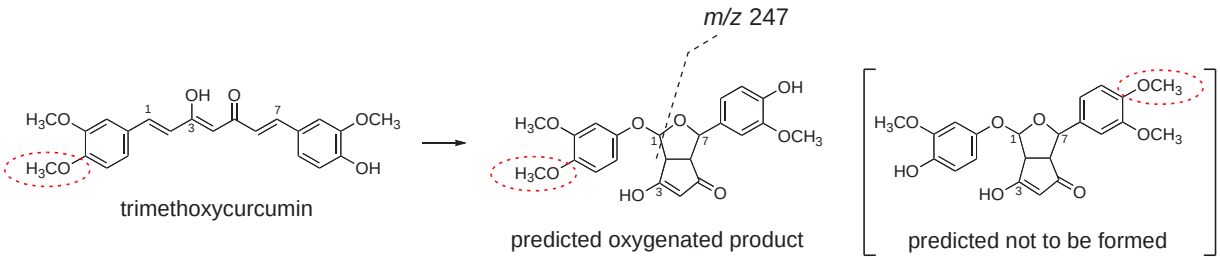
bicyclopentadione
(using alternative numbering of carbons, cf.
Schneider et al. J. Mol. Catal. B: Enzymatic, 4 (1998), 219)
2-(4'-hydroxy-3'-methoxyphenoxy)
-4-(4"-hydroxy-3"-methoxyphenyl)-8-hydroxy
-6-oxo-3-oxa-bicyclo[3.3.0]-7-octene

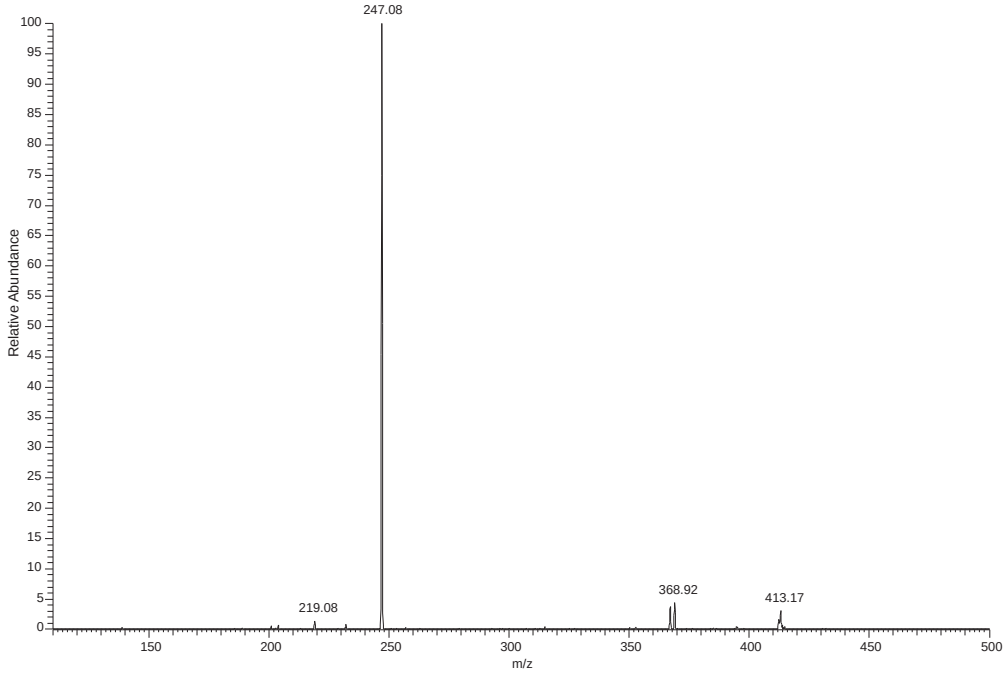
Supplemental Fig. S1, Griesser et al.

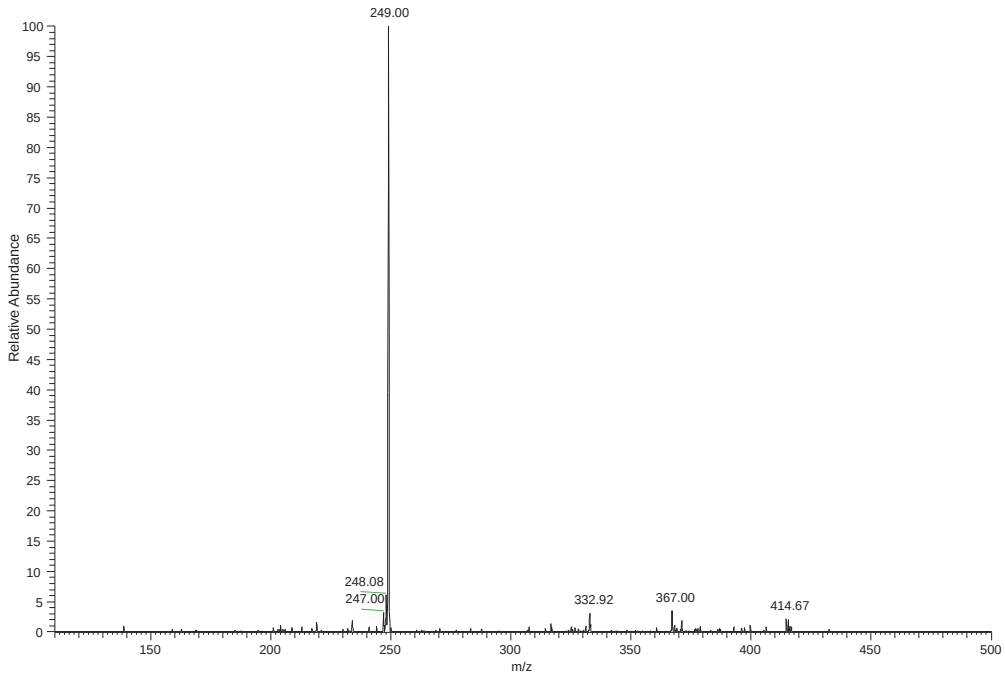




Supplemental Fig. S2, Griesser et al.







Supplemental Fig. S3, Griesser et al.