

Supplementary Information

Anti-inflammatory effects of cinnamon extract and identification of active compounds influencing the TLR2 and TLR4 signaling pathways

Anne Schink^{a,*}, Katerina Naumoska^{a,b,*}, Zoran Kitanovski^a, Christopher Johannes Kampf^{a,c}, Janine Fröhlich-Nowoisky^a, Eckhard Thines^{d,e}, Ulrich Pöschl^a, Detlef Schuppan^{f,g,§} and Kurt Lucas^{a,§,#}

^aMultiphase Chemistry Department, Max Planck Institute for Chemistry, Hahn-Meitner-Weg 1, 55128 Mainz, Germany

^bDepartment of Food Chemistry, National Institute of Chemistry, Hajdrihova 19, 1001, Ljubljana, Slovenia

^cInstitute of Organic Chemistry, Johannes Gutenberg University Mainz, Duesbergweg 10-14, 55128 Mainz, Germany

^dInstitut für Biotechnologie und Wirkstoff Forschung gGmbH, Erwin-Schrödinger-Straße 56, Kaiserslautern, Germany

^eInstitute of Molecular Physiology, Johannes Gutenberg University Mainz, Johannes-von-Müller-Weg 6 Mainz, Germany

^fInstitute of Translational Immunology, University Medical Center of the Johannes Gutenberg University, Langenbeckstraße 1, 55131 Mainz, Germany

^gDivision of Gastroenterology, Beth Israel Deaconess Medical Center, Harvard Medical School, 330 Brookline Ave, Boston, MA 02215, USA

**Both authors contributed equally to this work.*

§ equal senior authorship

corresponding author:

Dr. Kurt Lucas, Max Planck Institute for Chemistry, Multiphase Chemistry Department, Hahn-Meitner-Weg 1, 55128 Mainz, Germany. Tel.: +49 6131 305 7703; E-mail address: k.lucas@mpic.de

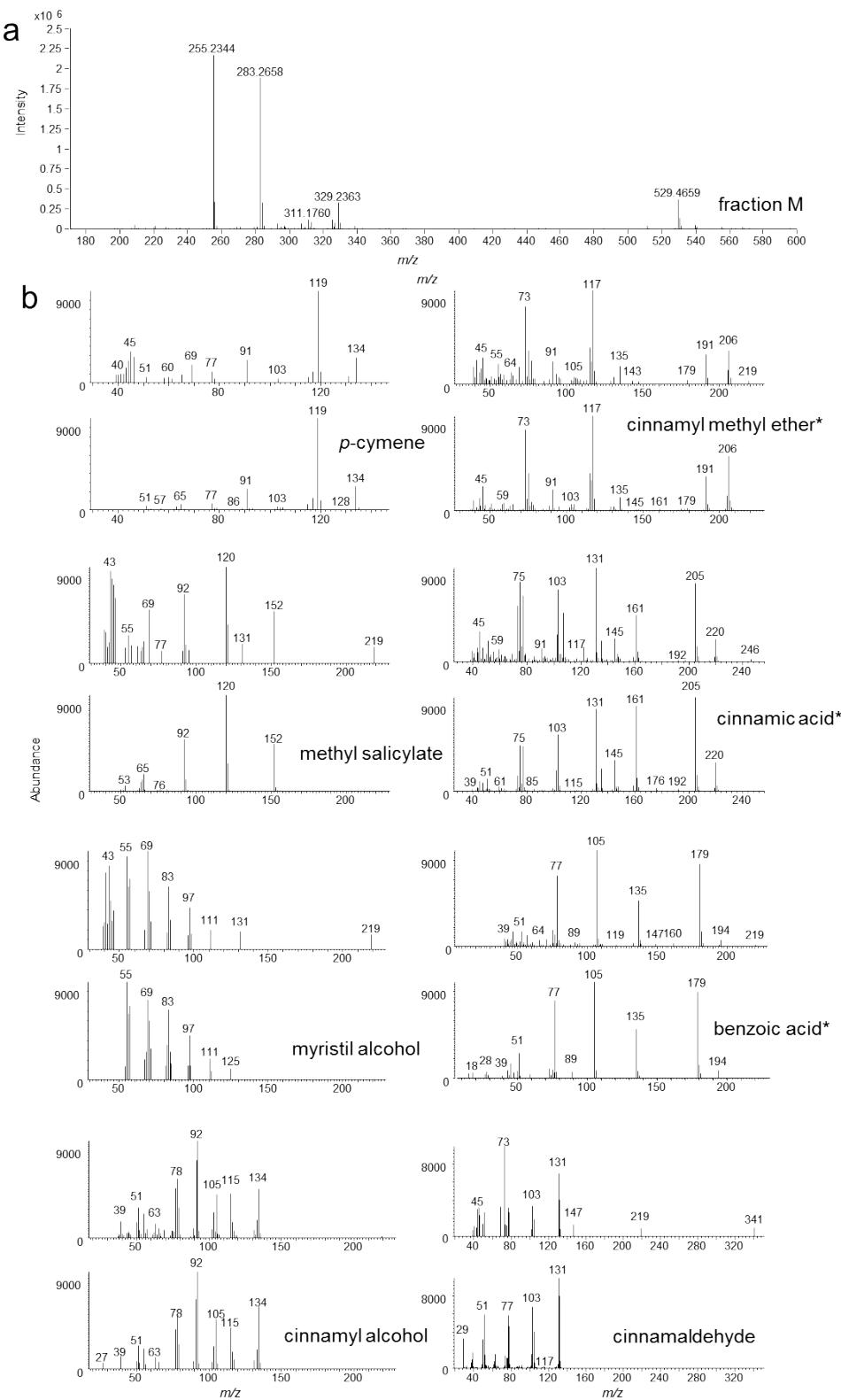


Figure S1: HRMS and GC-MS spectra of the fractions and compounds identified in 70% aqueous ethanolic cinnamon extract, respectively (Table S2).

a: (-)ESI-MS spectrum of fraction M. **b:** GC-EI-MS spectra of *p*-cymene and methyl salicylate (fraction B), 1-tetradecanol (myristyl alcohol) (fraction D), cinnamyl alcohol (fraction F) and cinnamaldehyde (fraction M), as well as trimethyl silyl esters(*) of

cinnamyl methyl ether, cinnamic and benzoic acid (derivatized fraction F). In each GC-MS spectral comparison, the upper spectrum belongs to the acquired spectrum for the compounds observed in the anti-inflammatory fractions, while the lower spectrum corresponds to compound spectrum contained in the NIST mass spectral library.

Tables

Table S1: Select cinnamon extract fractions and retention times.

Cinnamon extract was fractionated using HPLC-DAD (Conditions: C18 column and mobile phase composed of acetonitrile and 0.1% formic acid in water, gradient elution). Corresponding chromatogram is shown in **Fig. 3**.

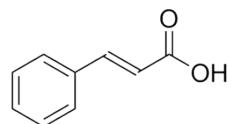
Fraction name	Retention time (min)
Fraction A	3.20 – 4.00
Fraction B	4.60 – 6.20
Fraction C	6.21 – 7.30
Fraction D	7.31 – 7.99
Fraction E	8.00 – 10.00
Fraction F	10.10 – 10.60
Fraction G	10.80 – 11.80
Fraction H	13.40 – 13.90
Fraction I	15.60 – 17.10
Fraction J	18.20 – 20.00
Fraction K	21.60 – 22.60
Fraction L	23.60 – 24.50
Fraction M	25.40 – 27.40
Fraction N	27.45 – 30.10
Fraction O	50.00 – 52.50

Table S2: Anti-inflammatory cinnamon extract fractions and identified compounds with corresponding structures.

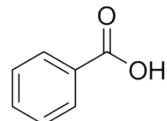
Using GC-MS¹ and HRMS², 12 compounds were identified in the anti-inflammatory fractions presented in **Figs. 3 and 4**.

Fraction name	Identified compound	Structure
Fraction B	<i>p</i> -Cymene ¹	
	Methyl salicylate ¹	
Fraction D	1-Tetradecanol (myristyl alcohol) ¹	
Fraction F	Cinnamyl alcohol ¹	
	Cinnamyl methyl ether ¹	

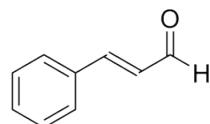
Cinnamic acid¹



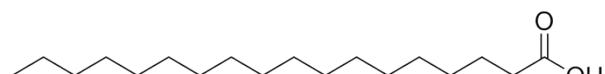
Benzoic acid¹



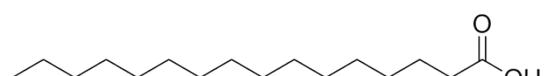
Fraction M Cinnamaldehyde¹



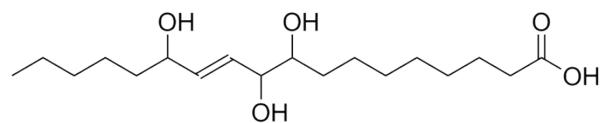
Stearic acid²



Palmitic acid²



9,10,13, TriHOME(11)²



Octadecyl
3,5-di-*tert*-butyl-4-
hydroxyhydrocinnamate²

