Supplementary Information

Isolation, *in vitro* and *in silico* Evaluation of Phenylethanoid Glycoside from *Arrabidaea brachypoda* as Lipoxygenase Inhibitor

Camila S. Bertanha,[a] Valéria M. M. Gimenez,[a] Ricardo A. Furtado,[a] Denise C. Tavares,[a] Wilson R. Cunha,[a] Márcio L. Andrade e Silva, [a] Ana H. Januario, [a] Alexandre Borges,[b] Daniel F. Kawano,[b] Renato L. T. Parreira [a] and Patrícia M. Pauletti *,[a]

[a]Núcleo de Pesquisa em Ciências Exatas e Tecnológicas, Universidade de Franca (UNIFRAN), Av. Dr. Armando Salles Oliveira, 201, 14404-600 Franca-SP, Brazil

[b]Faculdade de Ciências Farmacêuticas, Universidade Estadual de Campinas (Unicamp), Rua Cândido Portinari 200, 13083-871 Campinas-SP, Brazil

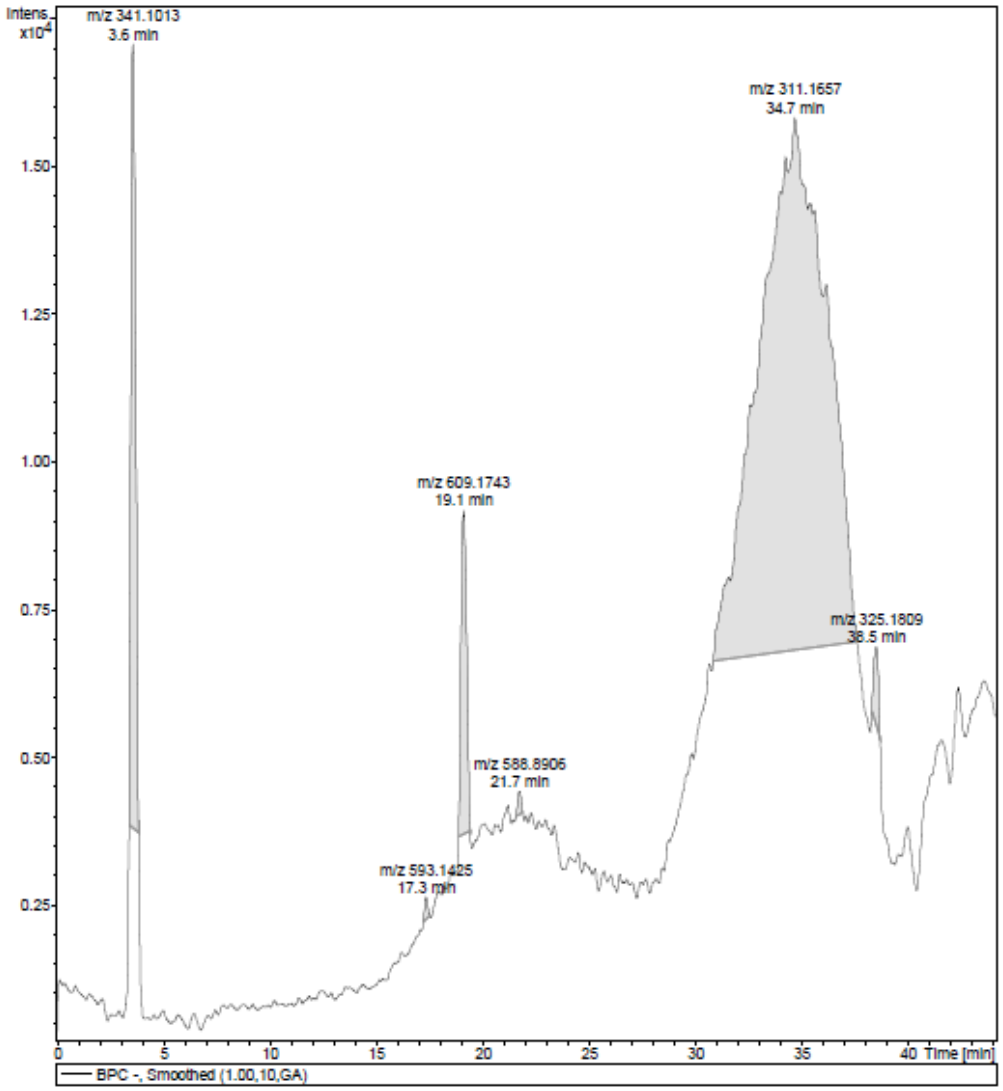


Figure S1. HPLC-HRMS chromatogram of *Arrabidaea brachypoda* ethanol extract (negative mode).

*e-mail: patricia.pauletti@unifran.edu.br

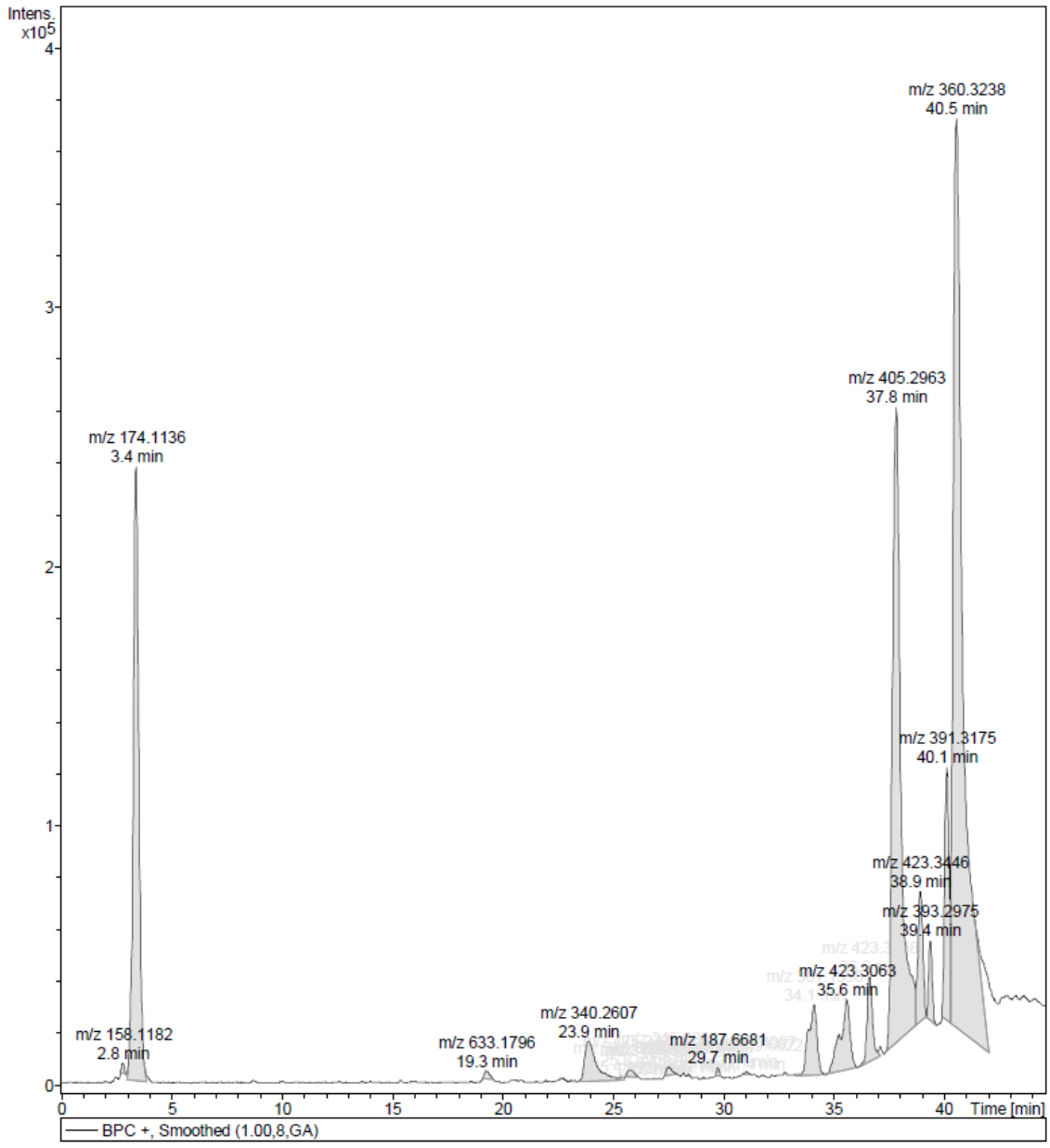


Figure S2. HPLC-HRMS chromatogram of *Arrabidaea brachypoda* ethanol extract (positive mode).

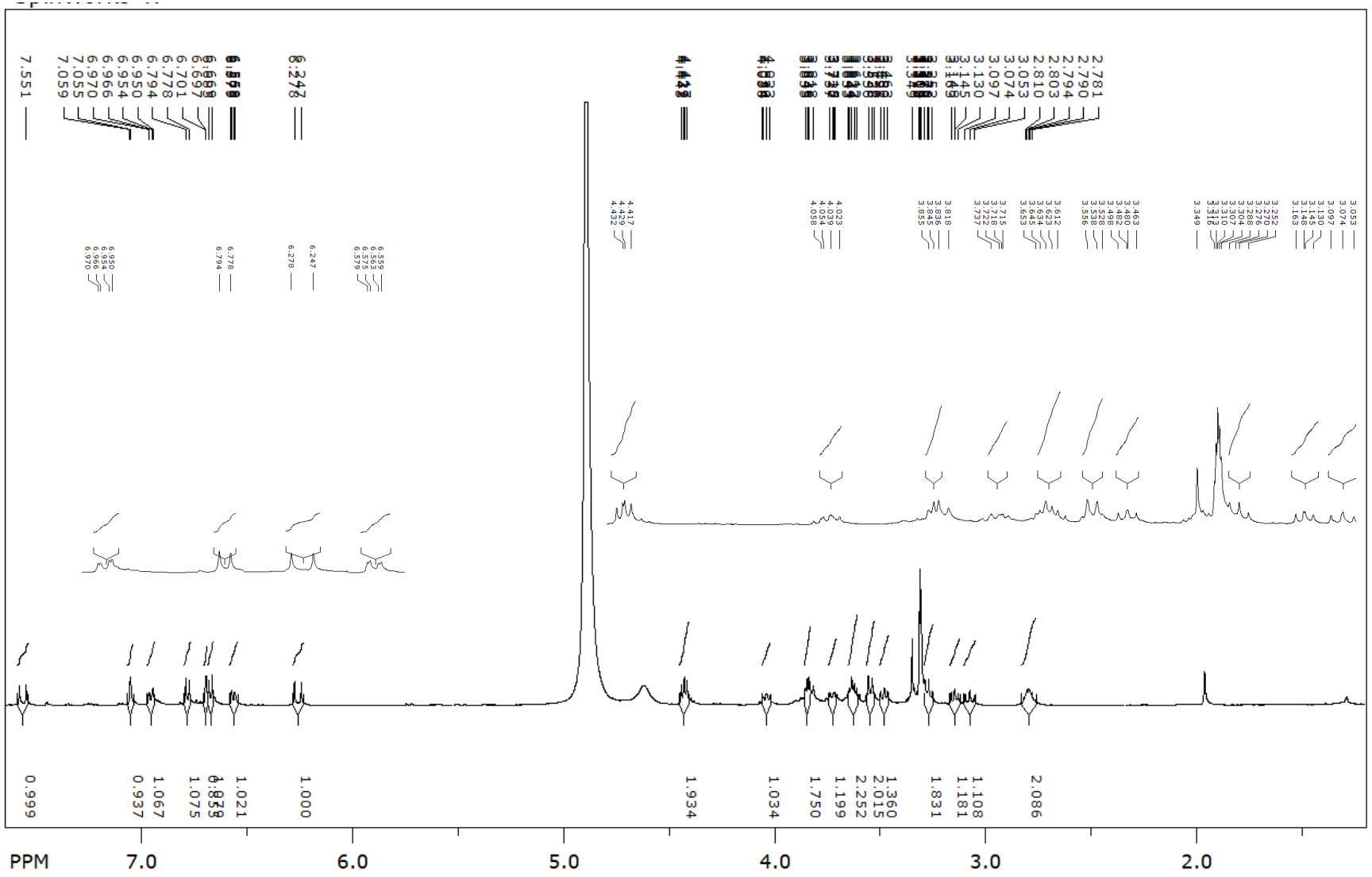


Figure S3. ^{1}H NMR (500 MHz, CD_3OD) spectrum of the compound **1**.

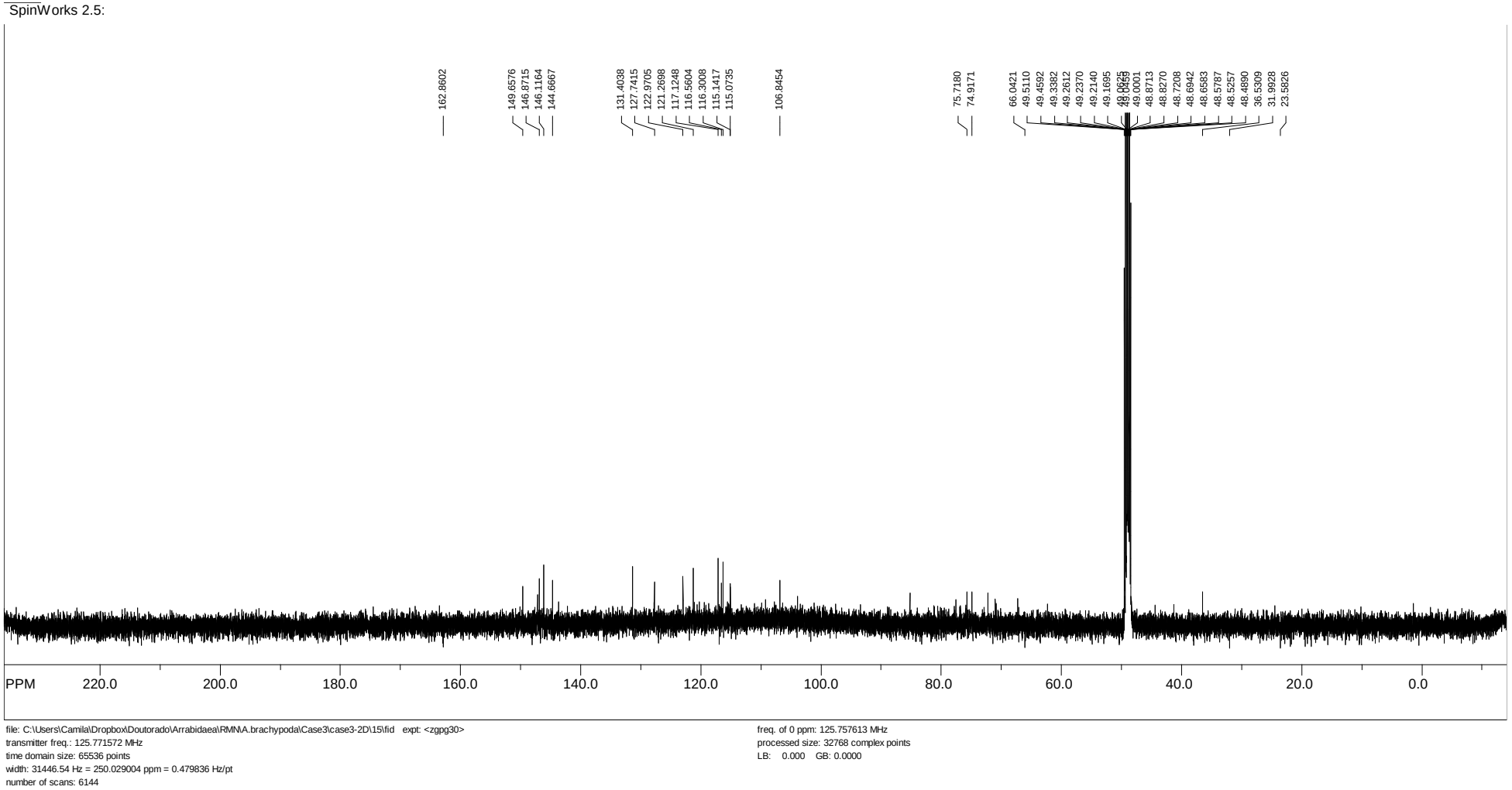


Figure S4. ^{13}C NMR (125 MHz, CD_3OD) spectrum of the compound **1**.

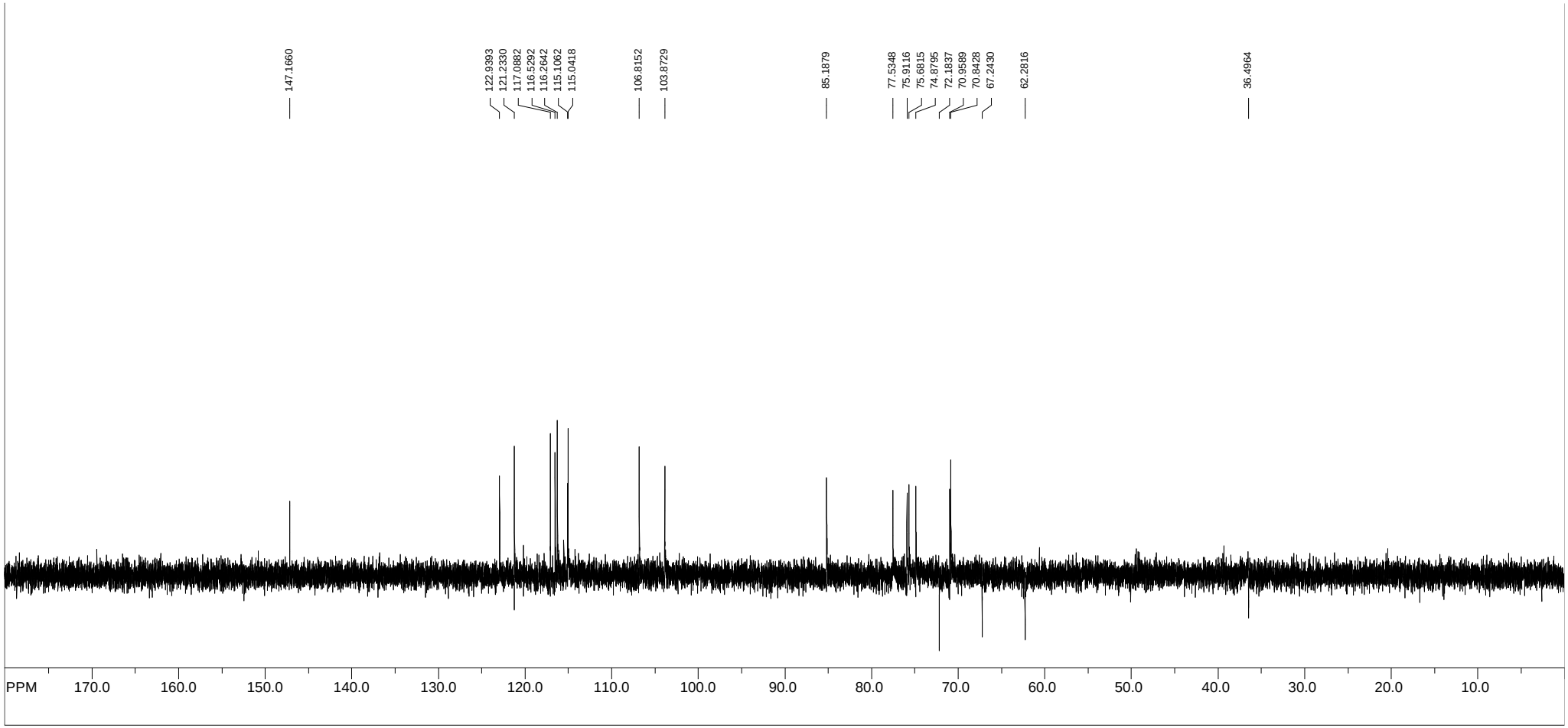


Figure S5. DEPT NMR (125 MHz, CD_3OD) spectrum of the compound **1**.

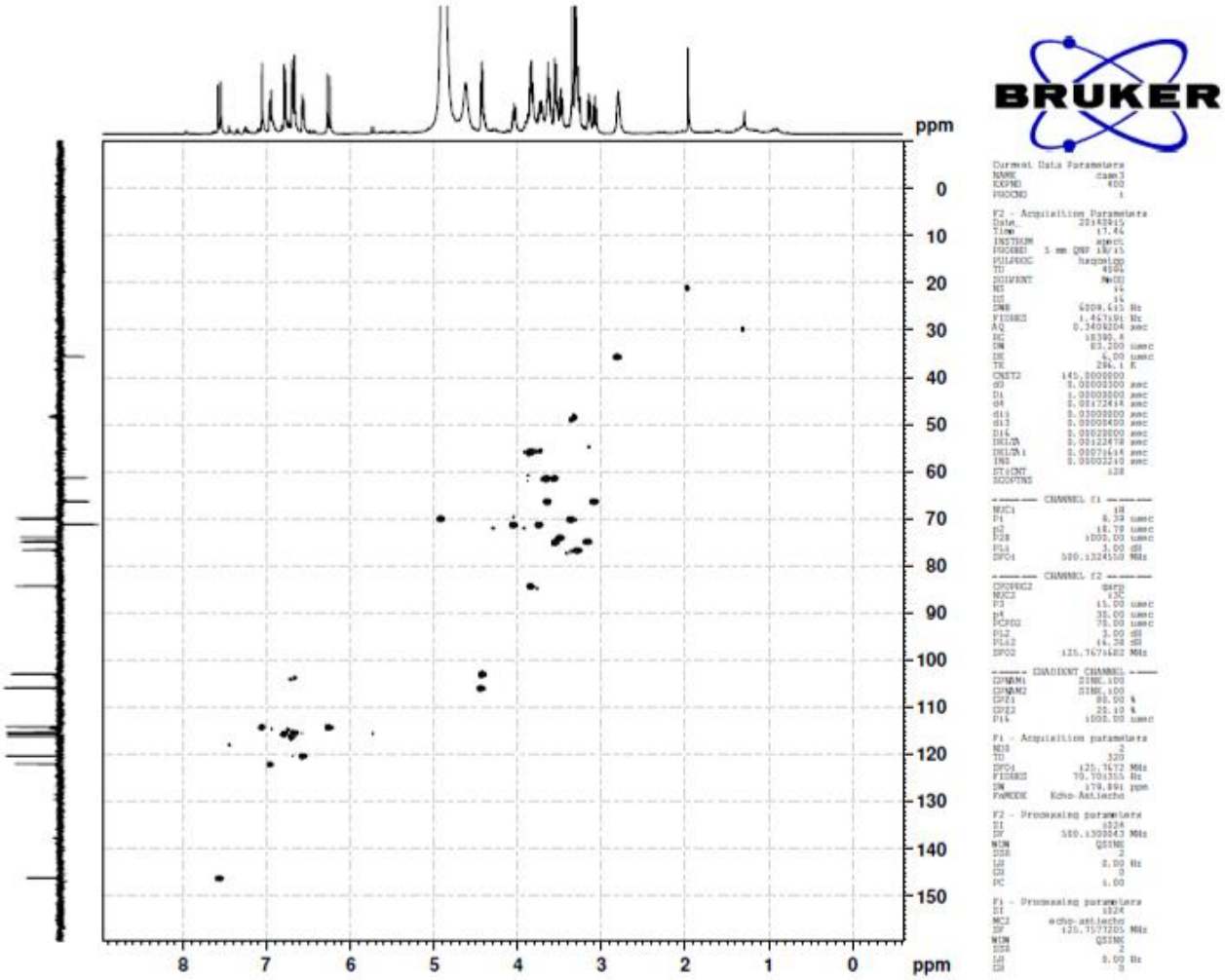


Figure S6. HSQC spectrum of the compound **1** (CD_3OD).

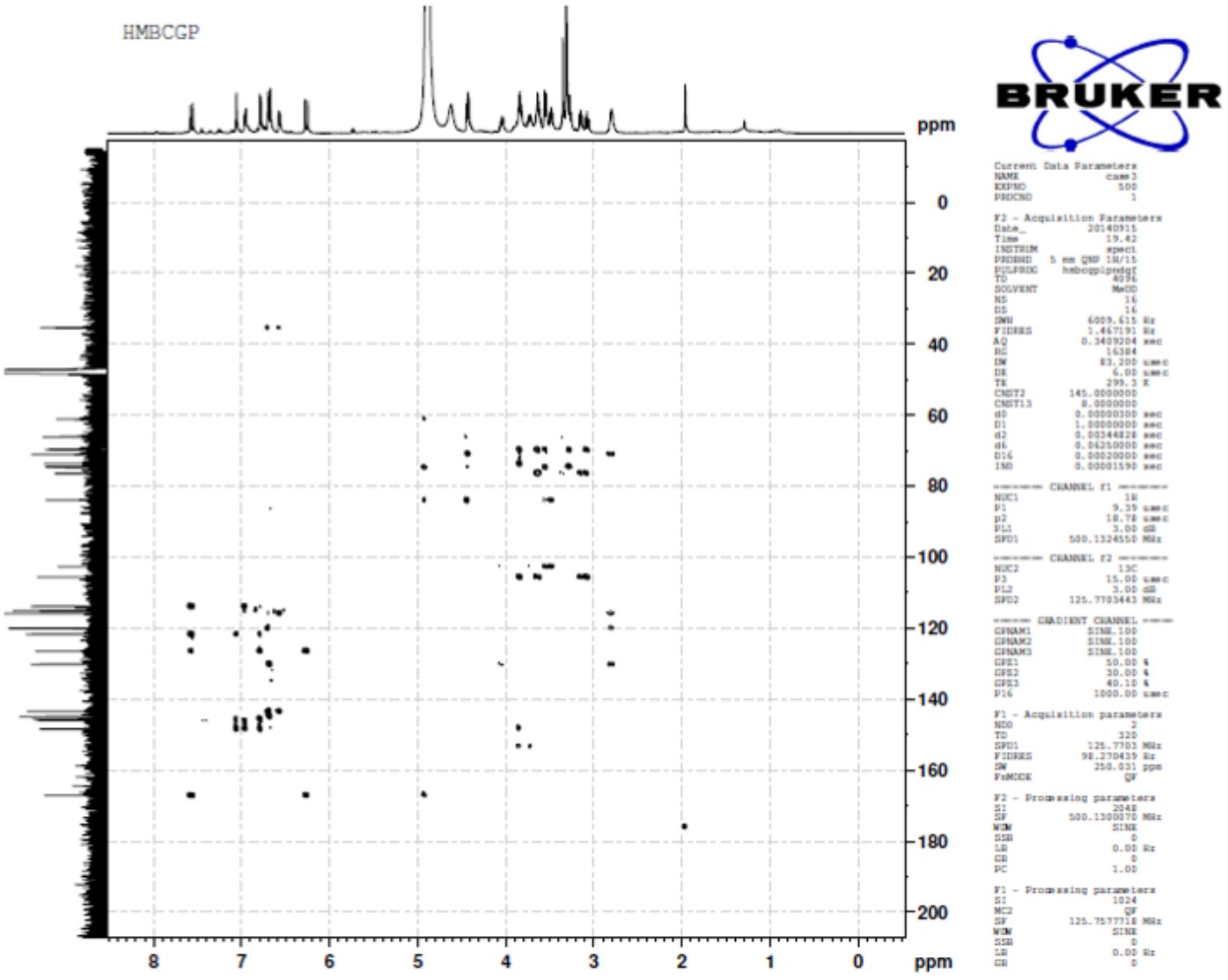


Figure S7. HMBC spectrum of the compound **1** (CD_3OD).

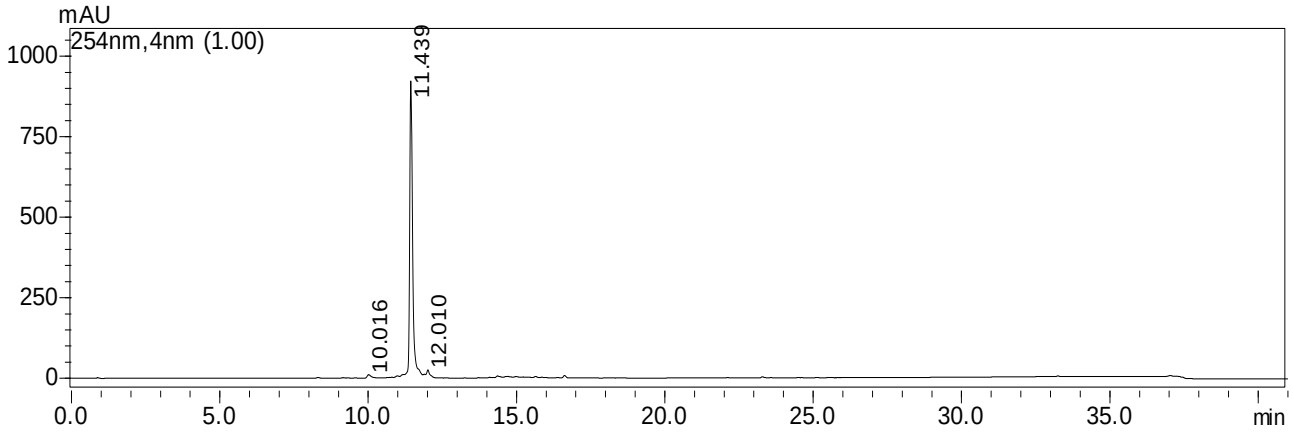
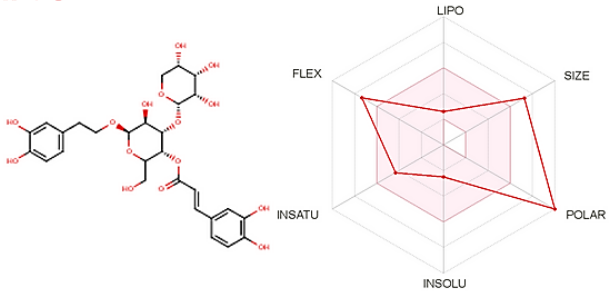


Figure S8. HPLC-UV of compound **1**.

Conandroside



SMILES OCC1O[C@@H](OCCc2ccc(c(c2)O)O)[C@H]([C@@H]([C@@H]1OC(=O)/C=C/c1ccc(c(c1)O)O)O[C@@H]1OC[C@@H]([C@@H]([C@@H]1O)O)O)O

Physicochemical Properties	
Formula	C28H34O15
Molecular weight	610.56 g/mol
Num. heavy atoms	43
Num. arom. heavy atoms	12
Fraction Csp3	0.46
Num. rotatable bonds	11
Num. H-bond acceptors	15
Num. H-bond donors	9
Molar Refractivity	143.62
TPSA	245.29 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	1.64
Log $P_{o/w}$ (XLOGP3)	-0.94
Log $P_{o/w}$ (WLOGP)	-1.51
Log $P_{o/w}$ (MLOGP)	-2.57
Log $P_{o/w}$ (SILICOS-IT)	-1.27
Consensus Log $P_{o/w}$	-0.93

Water Solubility	
Log *S* (ESOL)	-2.51
Solubility	1.87e+00 mg/ml ; 3.06e-03 mol/l
Class	Soluble
Log *S* (Ali)	-3.73
Solubility	1.15e-01 mg/ml ; 1.88e-04 mol/l
Class	Soluble
Log *S* (SILICOS-IT)	-0.08
Solubility	5.07e+02 mg/ml ; 8.30e-01 mol/l
Class	Soluble

Pharmacokinetics	
GI absorption	Low
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-10.69 cm/s

Druglikeness	
Lipinski	No; 3 violations: MW>500, NorO>10, NHorOH>5
Ghose	No; 4 violations: MW>480, WLOGP<-0.4, MR>130, #atoms>70
Veber	No; 2 violations: Rotors>10, TPSA>140
Egan	No; 1 violation: TPSA>131.6
Muegge	No; 4 violations: MW>600, TPSA>150, H-acc>10, H-don>5
Bioavailability Score	0.17

Medicinal Chemistry	
PAINS	1 alert: catechol_A
Brenk	2 alerts: catechol, michael_acceptor_1
Leadlikeness	No; 2 violations: MW>350, Rotors>7
Synthetic accessibility	6.18

Figure S9. Computed parameter values (bioavailability radar, physicochemical properties, lipophilicity, water-solubility, pharmacokinetics, drug-likeness, and medicinal chemistry) for conandroside. The parameters were obtained by using SwissADME web tool.[1]

Reference

1. http://www.swissadme.ch/index.php, accessed in October 2019.