molecules

MDPI

Suplementary material

Rutamarin: Efficient liquid-liquid chromatographic isolation from Ruta graveolens L. and evaluation of its in vitro and in silico MAO-B inhibitory activity

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Supplementary File Content

Figure S1. Chromatograms of CCC separations rutamarin from a crude dichloromethane extract of *Ruta graveolens* L.

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Figure S7. HMBC NMR spectrum of **rutamarin** in CD_3OD

Figure S8. ROESY NMR spectrum of **rutamarin** in CD_3OD

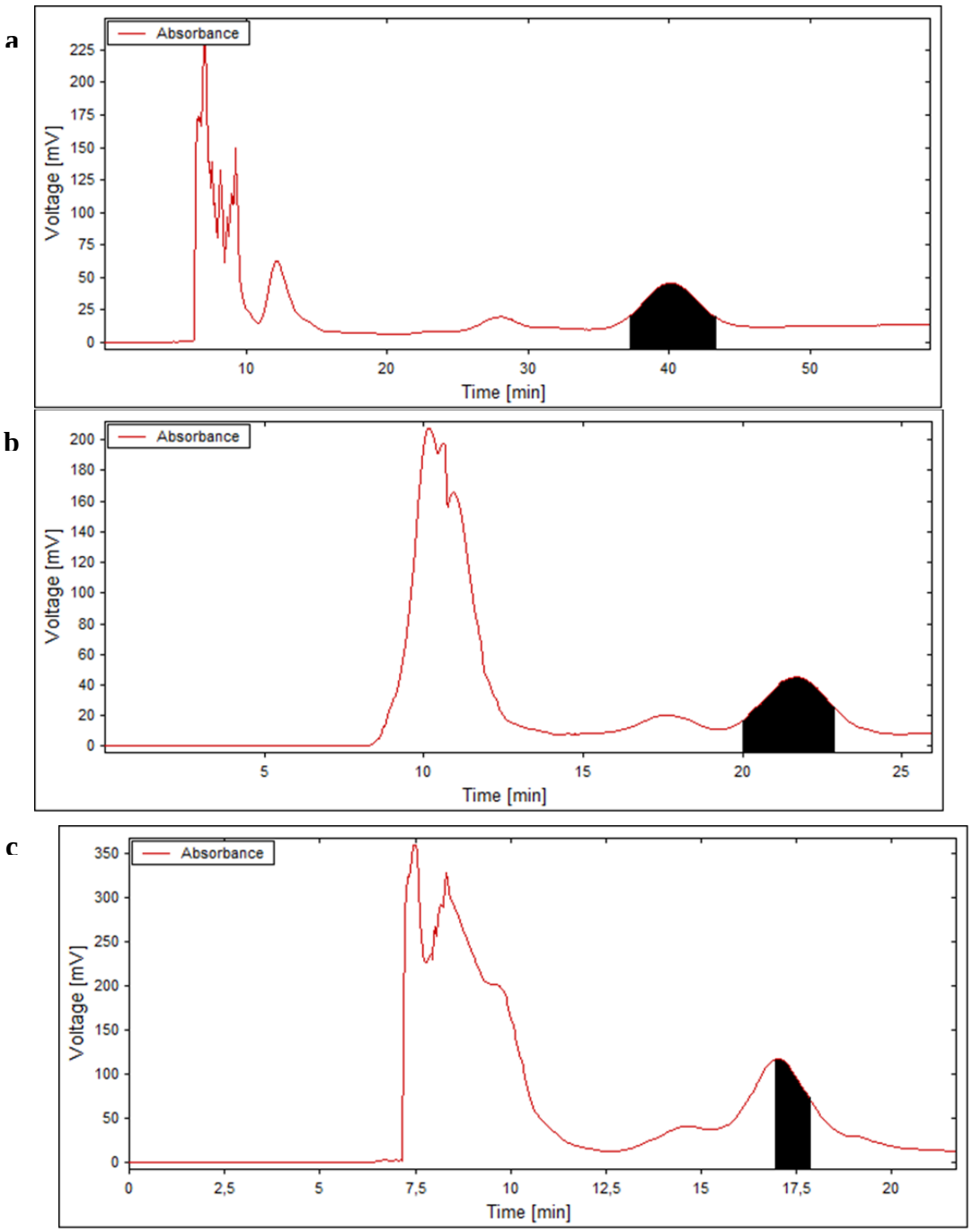

Figure S1. Chromatograms of CCC separations rutamarin from a crude dichloromethane extract of *Ruta graveolens* L. with (**a**) *n*-hexane/ethyl acetate/methanol/water (5/2/5/2, *v*/*v*/*v*/*v*) (**b**) *n*-hexane/ethyl acetate/methanol/water (3/1/3/1, *v*/*v*/*v*/*v*) and (**c**) *n*-hexane/ethyl acetate/methanol/water (4/1/4/1, *v*/*v*/*v*/*v*); upper phase as stationary phases (reversed-phase, head-to-tail mode, descending mode); flow-rate: 6 mL/min; V_{inj} = 6 mL; C_{inj} = 16.67 mg/mL; ω = 1900 rpm, S_F = 80%; UV 335 nm.

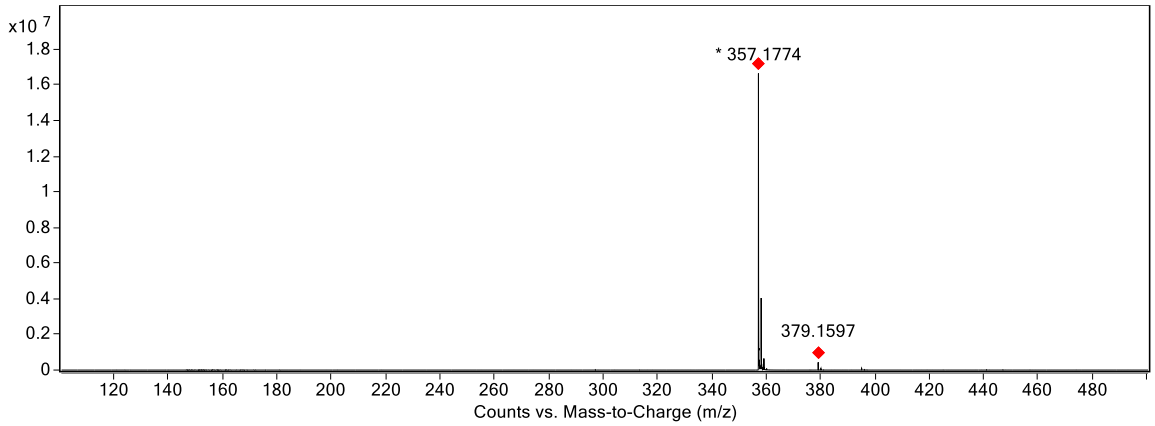

Figure S2a. HRESIMS spectrum of rutamarin.

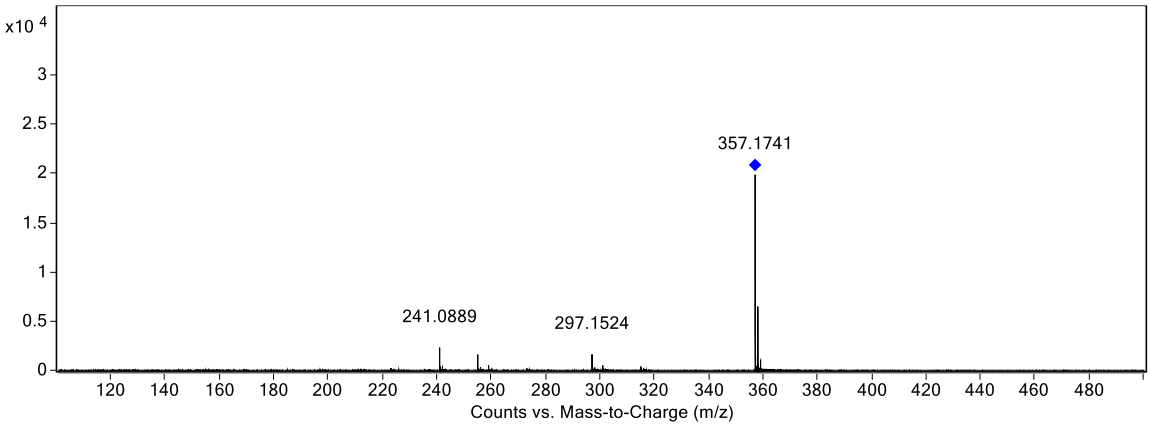

Figure S2b. MS/MS spectrum of rutamarin.

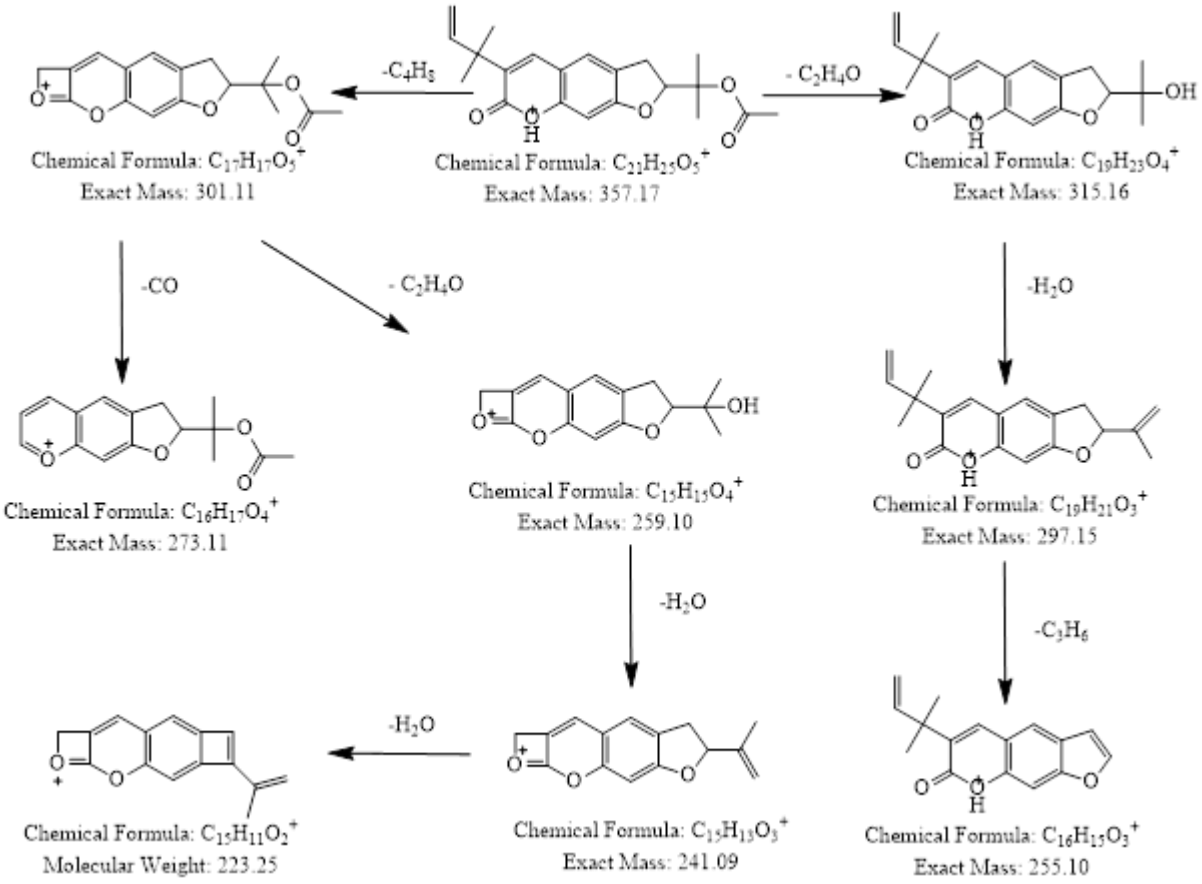

Figure S2c. MS/MS fragmentation patterns proposed for **rutamarin.**

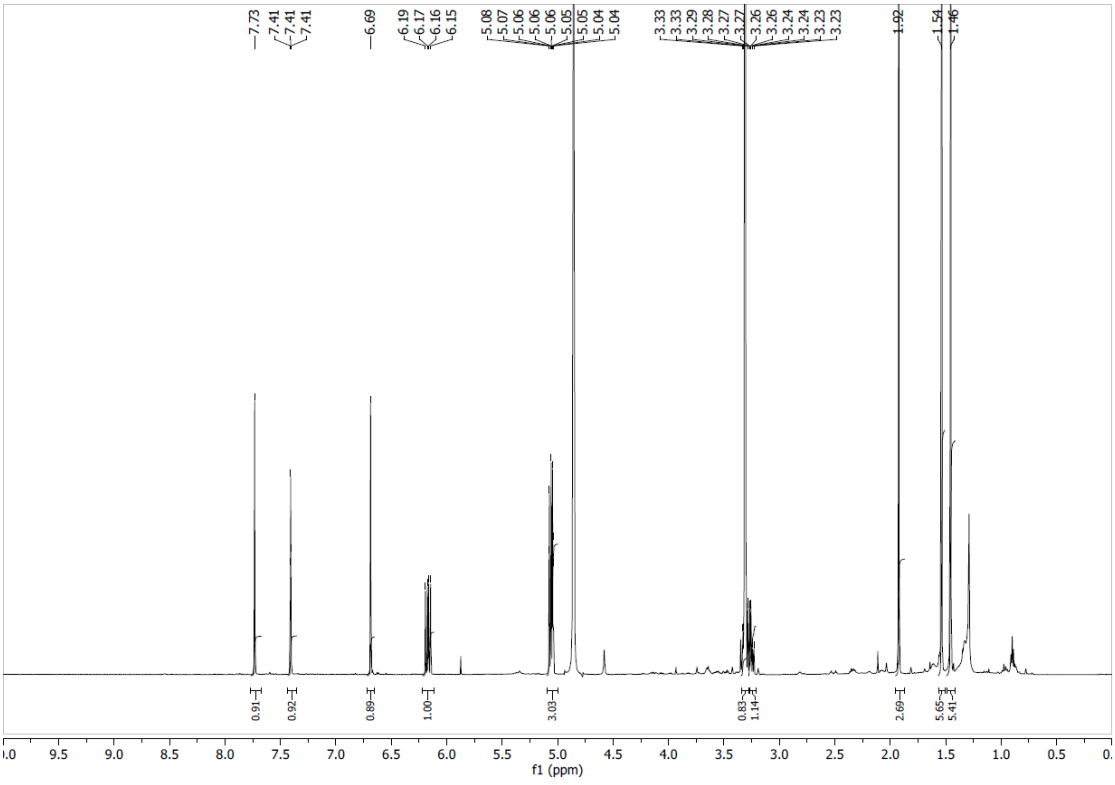

Figure S3. ^{1}H-NMR spectrum of **rutamarin** in CD_3OD.

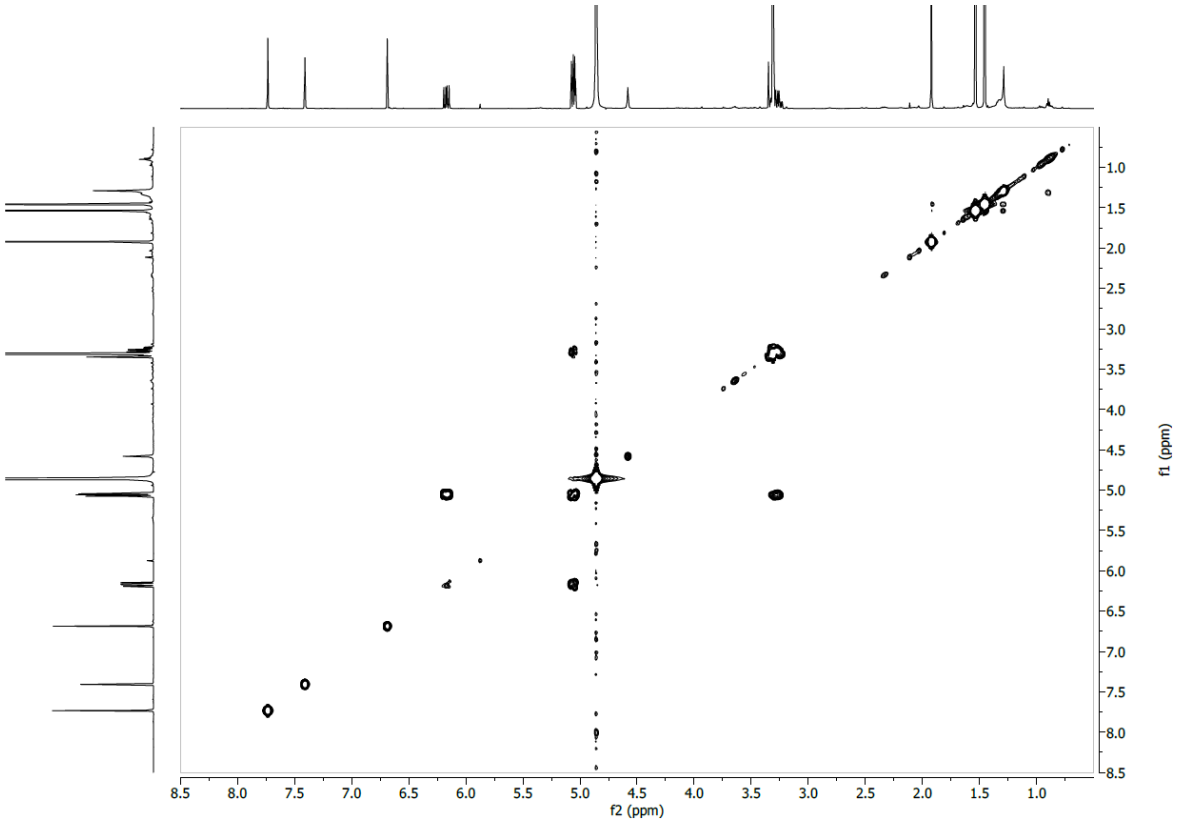

Figure S4. COSY NMR spectrum of **rutamarin** in CD_3OD.

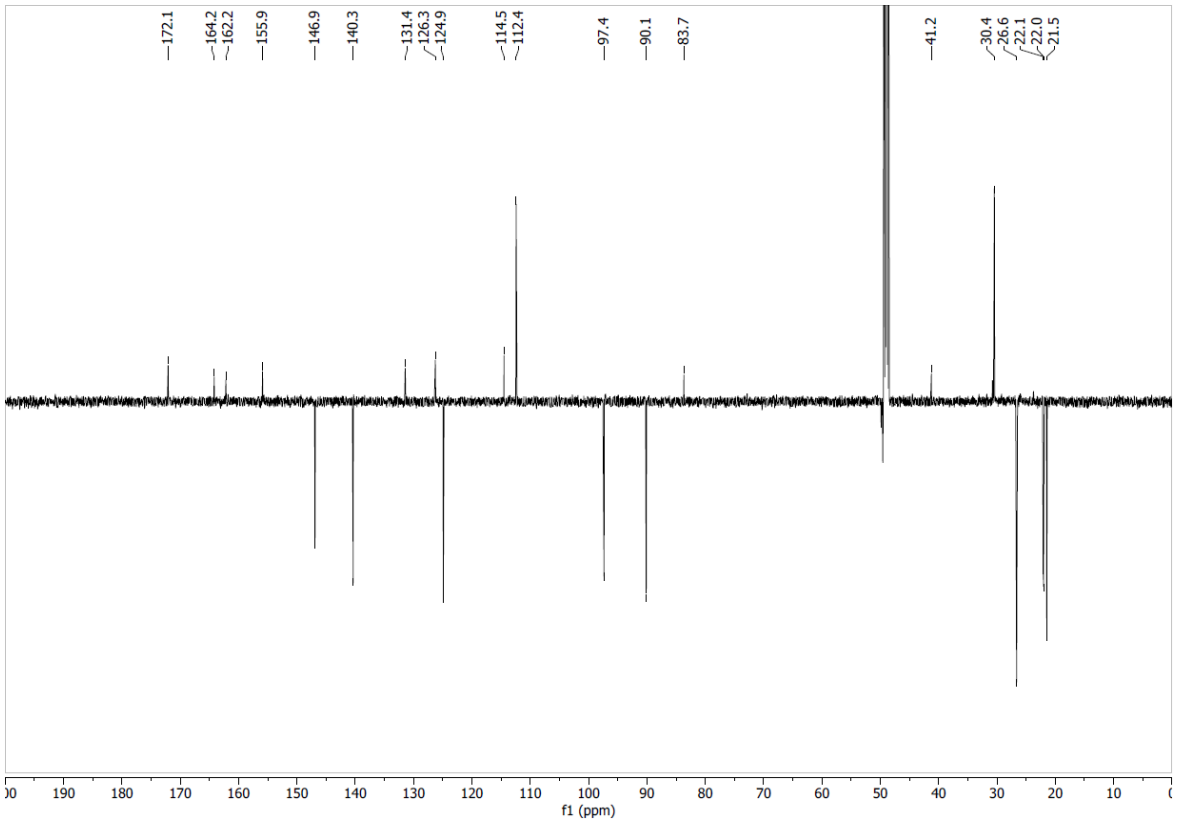

Figure S5. ^{13}C-DEPTQ NMR spectrum of **rutamarin** in CD_3OD at 151 MHz.

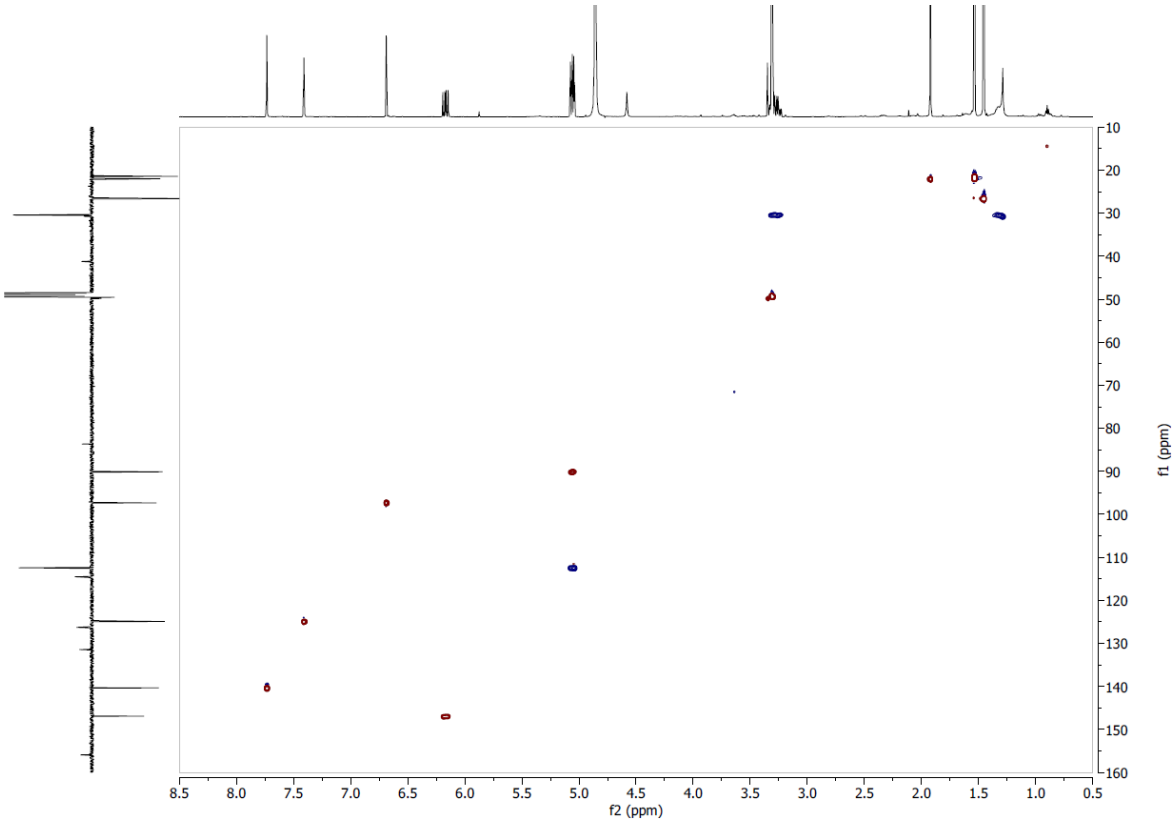

Figure S6. Edited-HSQC NMR spectrum of **rutamarin** in CD_3OD.

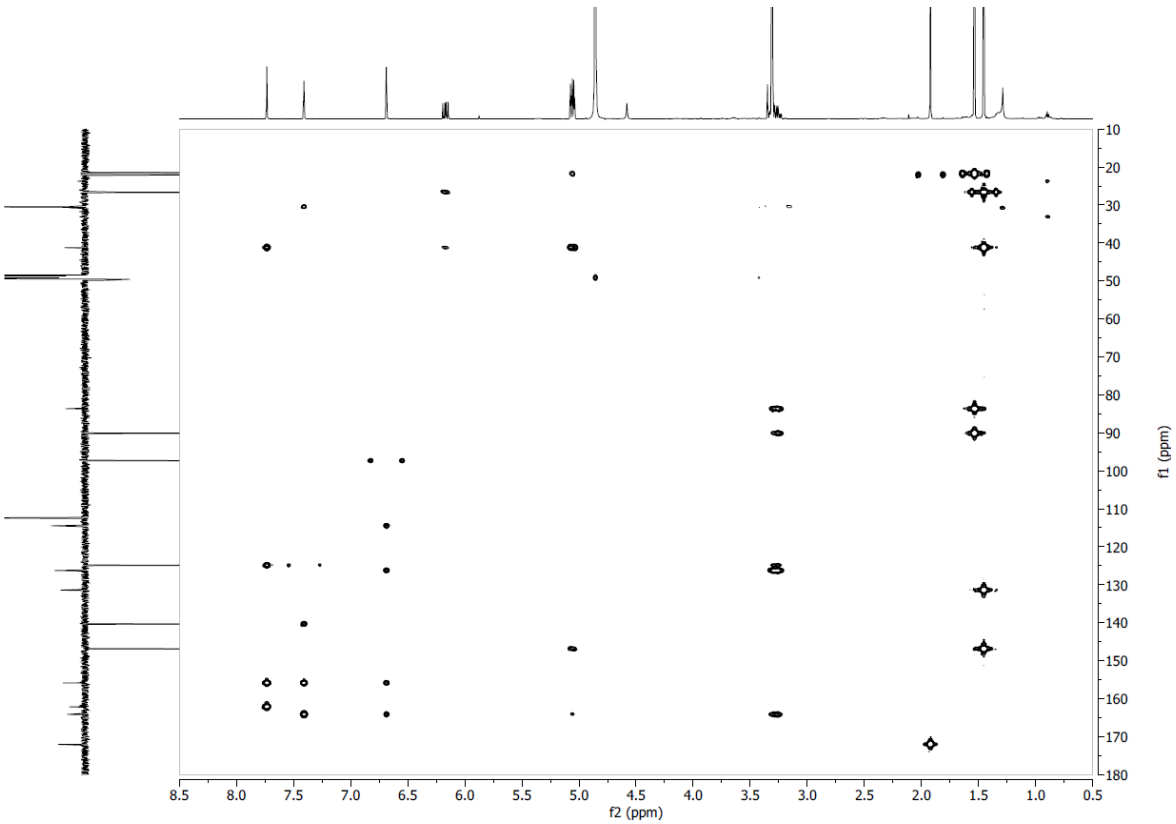

Figure S7. HMBC NMR spectrum of **rutamarin** in CD_3OD.

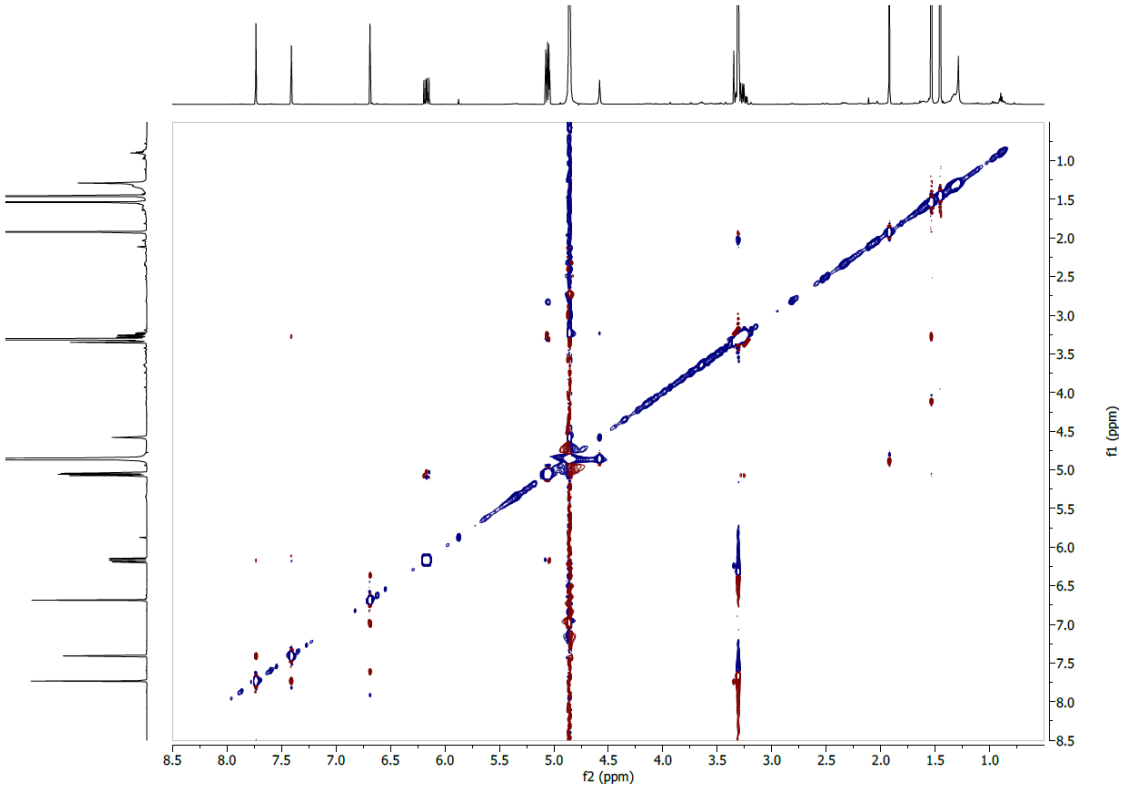

Figure S8. ROESY NMR spectrum of **rutamarin** in CD_3OD.