Short Note Bio-catalytic synthesis of Quercetin-3-oleate

Gabriele Carullo¹ and Francesca Aiello^{1,*}

- ¹ Department of Pharmacy, Health and Nutritional Sciences; University of Calabria, Edificio Polifunzionale, 87036, Arcavacata Rende (CS), Italy. E-mail <u>gabriele.carullo@unical.it</u>
- * Correspondence: <u>francesca.aiello@unical.it</u>; Tel.: +39-0984-493154

Purity by absolute qNMR

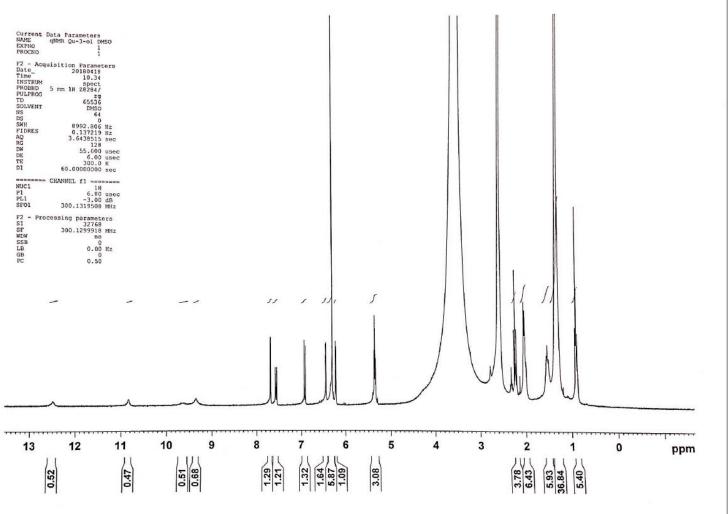
The purity was calculated using IC Method by Maleic acid Standard for quantitative NMR, TraceCERT®. The NMR tube was prepared adding to 0.180 mL of compound **2** Sample (5mg/mL) a solution of Maleic acid 0.095 mL (5mg/mL) as Internal Calibrant. Only the integral values of quercetin were considered significant, considering that the signals related to the oleic fragment overlapped with the DMSO.

 $m_s = 0.0009 \ m_t c = 0.000475$ $P_{tc} = \text{Standard for quantitative NMR 99.99\%}; Int_t = 5.87, n_t = 1; Int_t = 1.09, n_t c = 2; MW_t = 566.6818, n_t = 1.09, n_t c = 2; MW_t = 566.6818, n_t = 1.09, n_t c = 2; MW_t = 566.6818, n_t = 1.09, n_t c = 2; MW_t = 566.6818, n_t c = 1.09, n_t c = 2; MW_t = 566.6818, n_t c = 1.09, n_t c = 2; MW_t = 566.6818, n_t c = 1.09, n_t c = 2; MW_t = 566.6818, n_t c = 1.09, n_t c = 2; MW_t = 566.6818, n_t c = 1.09, n_t c = 2; MW_t = 566.6818, n_t c = 1.09, n_t c = 2; MW_t = 566.6818, n_t c = 1.09, n_t c = 2; MW_t = 566.6818, n_t c = 1.09, n_t c = 2; MW_t = 566.6818, n_t c = 1.09, n_t c = 2; MW_t = 566.6818, n_t c = 1.09, n_t c = 2; MW_t = 566.6818, n_t c = 1.09, n_t c = 2; MW_t = 566.6818, n_t c = 1.09, n_t c = 2; MW_t = 566.6818, n_t c = 1.09, n_t c = 2; MW_t = 566.6818, n_t c = 1.09, n_t c = 2; MW_t = 566.6818, n_t c = 1.09, n_t c = 2; MW_t = 566.6818, n_t c = 1.09, n_t c = 1.09, n_t c = 2; MW_t = 566.6818, n_t c = 1.09, n_t c = 1.0$

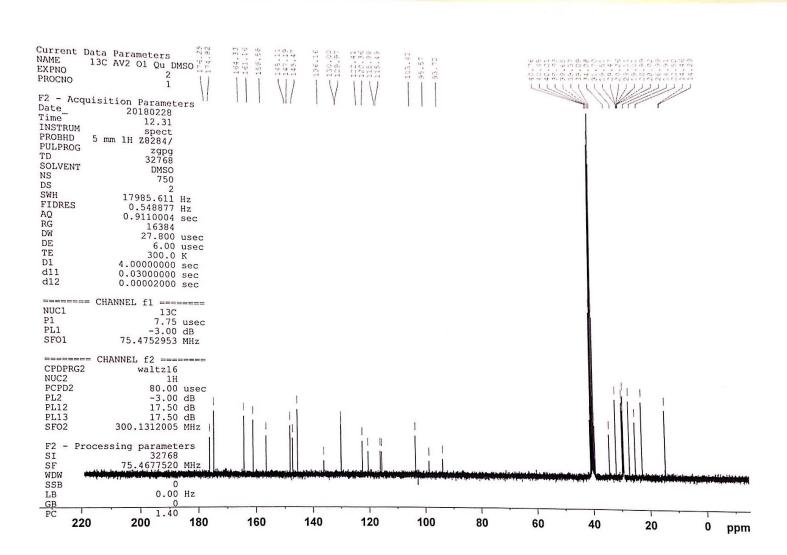
MW_{IC} = 116.0722

 $P[\%] = (n_{lC} \cdot Int_t \cdot MW_t \cdot m_{lC} / n_t \cdot Int_{lC} \cdot MW_{lC} \cdot m_t) \cdot P_{lC} = 94.73\%$

¹H-NMR for qNMR calculation



¹³C NMR of compound 2



IR spectrum

PerkinElmer Spectrum Versione 10.4.00 martedi 26 giugno 2018 13.06

Dettagli Report

Posizione Report Autore Report Data Report C:\pel_data\AIELLO\Campioni 1_14.pdf AIELLO FRANCESCA martedi 26 giugno 2018 13.06

Grafico Spettro

