Supplementary information

Quercetin hybrids – synthesis, spectral characterization and antioxidant activity

D. Kirkova[1, 2], Y. Stremski[1*], S. Statkova-Abeghe[1], M. Docheva[2]

[1] Department of Organic Chemistry, Faculty of Chemistry, University of Plovdiv "Paisii Hilendarski", Tzar Assen Str. 24, BG 4000 Plovdiv, Bulgaria

[2] Chemistry of Tobacco and Tobacco Smoke, Tobacco and Tobacco Products Institute BG 4108 Markovo, Plovdiv, Bulgaria

**Correspondence: stremski@uni-plovdiv.net (Y.S.); tel.: +359-32-261-346*

Table of Contents

^{1}H-NMR and ^{13}C-NMR data for **Quercetin** **Page 1 – 2**

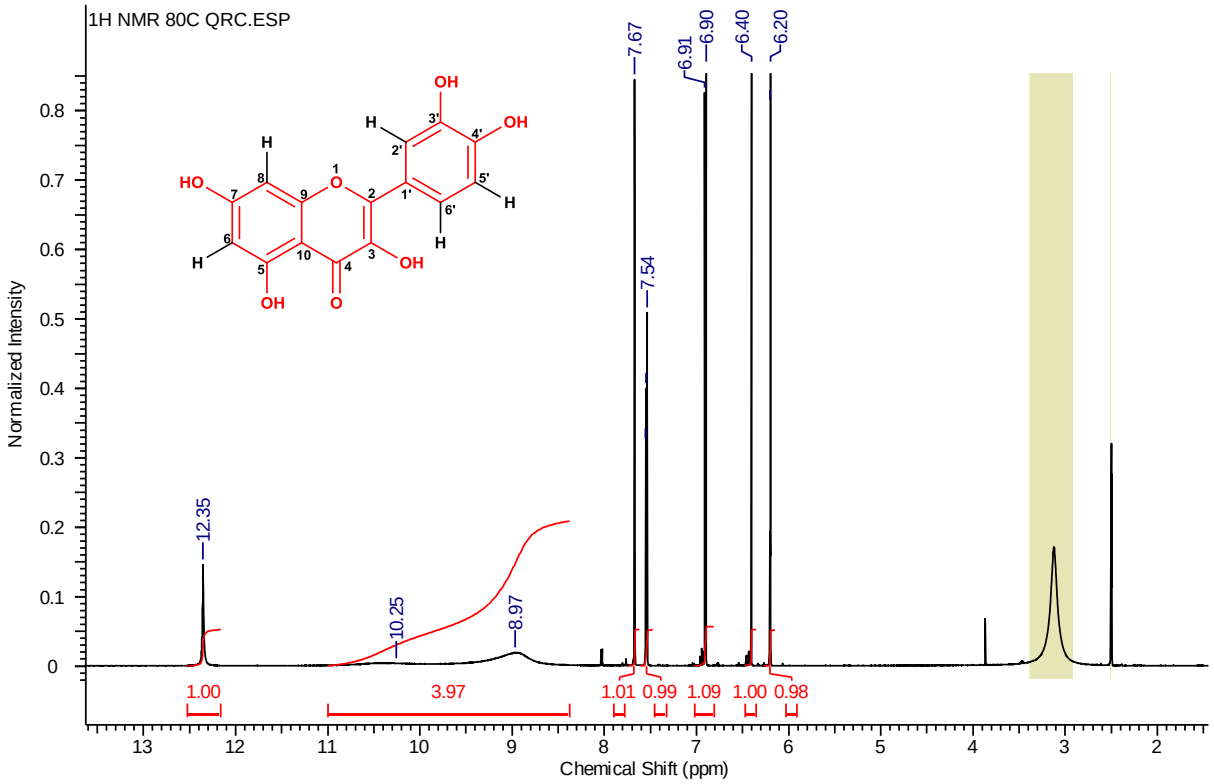
^{1}H-NMR, ^{13}C-NMR, IR and MS data for compound **6a** **Page 3 – 5**

^{1}H-NMR, ^{13}C-NMR and IR data for compound **6b** **Page 6 – 7**

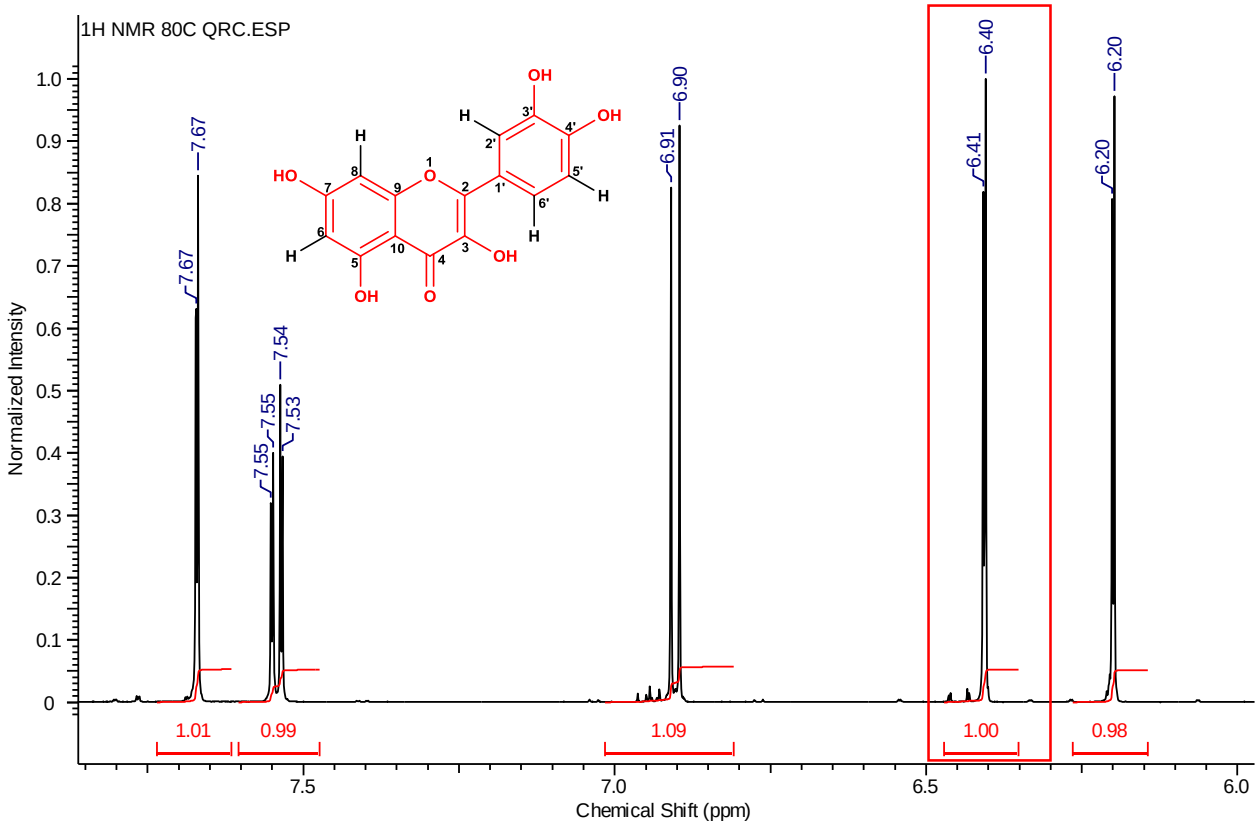
^{1}H-NMR, ^{13}C-NMR, IR and MS data for compound **7a** **Page 8 – 10**

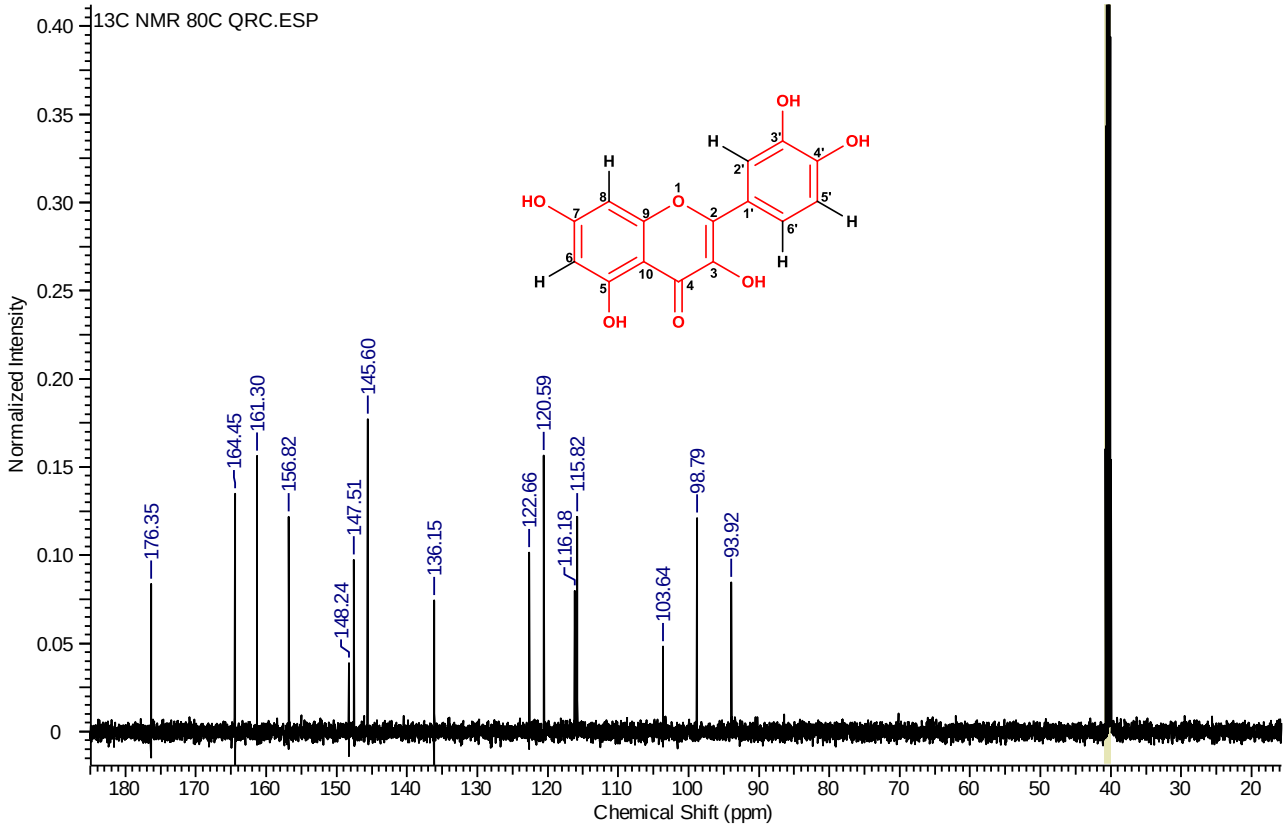
^{1}H-NMR, ^{13}C-NMR and IR data for compound **8a** **Page 11 – 12**

^{1}H-NMR, ^{13}C-NMR, IR and HSQC data for compound **8b** **Page 13 – 15**

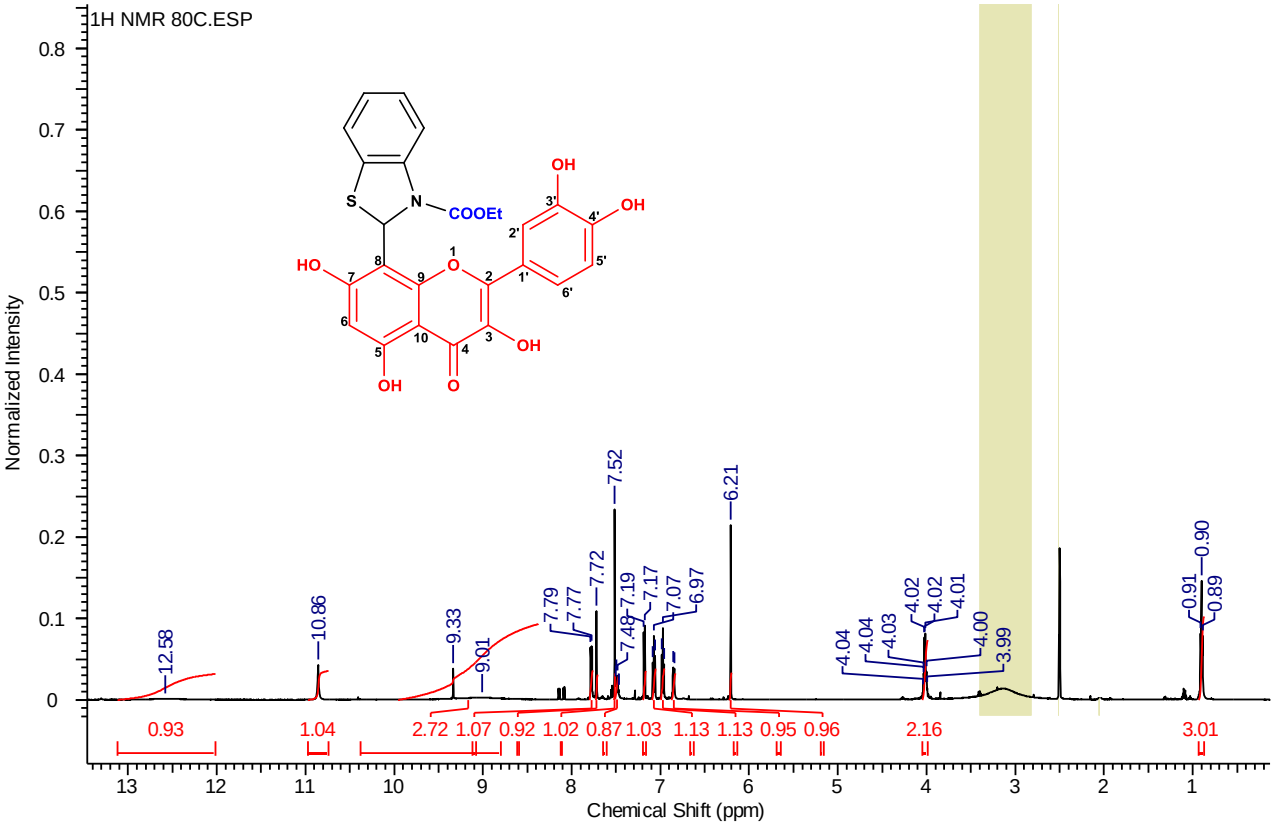


Quercetin - ^{1}H-NMR spectra - DMSO-d_6, 80 °C, 600 MHz

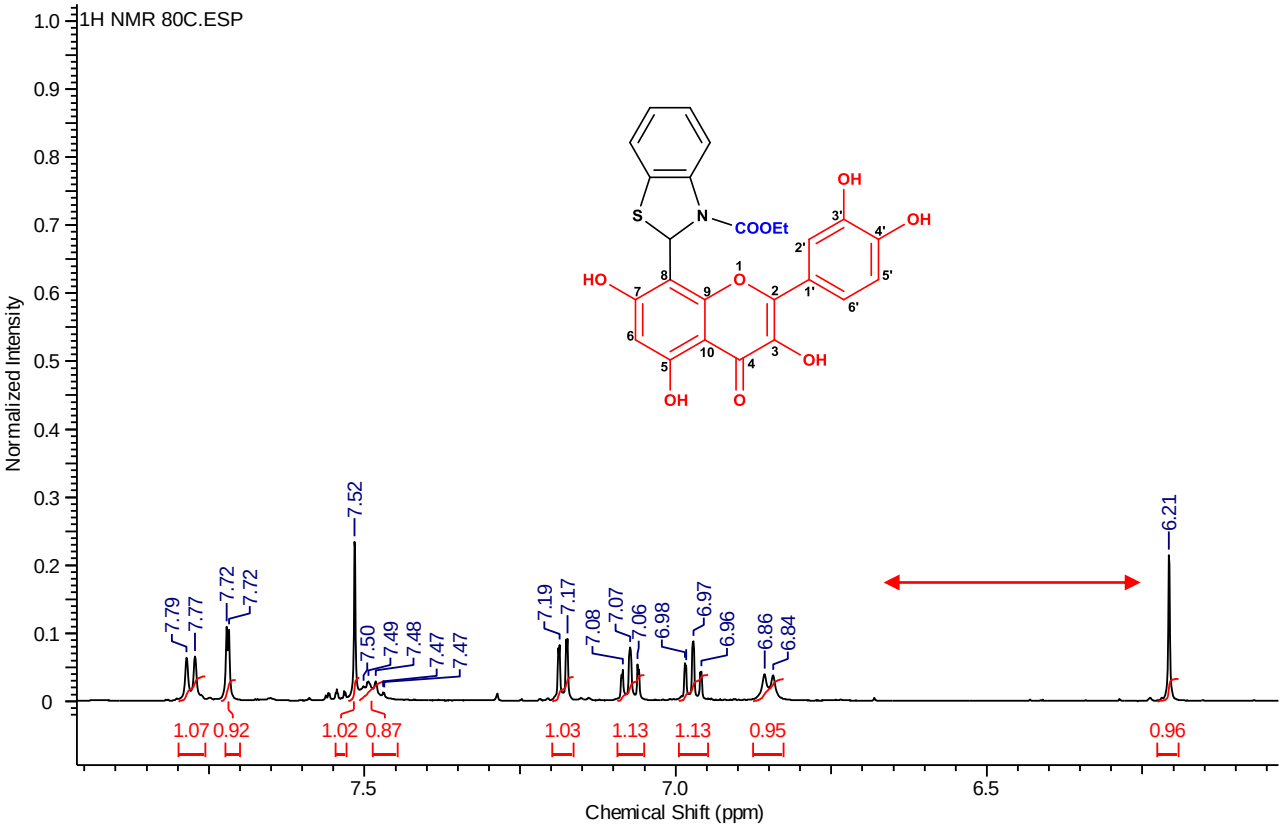


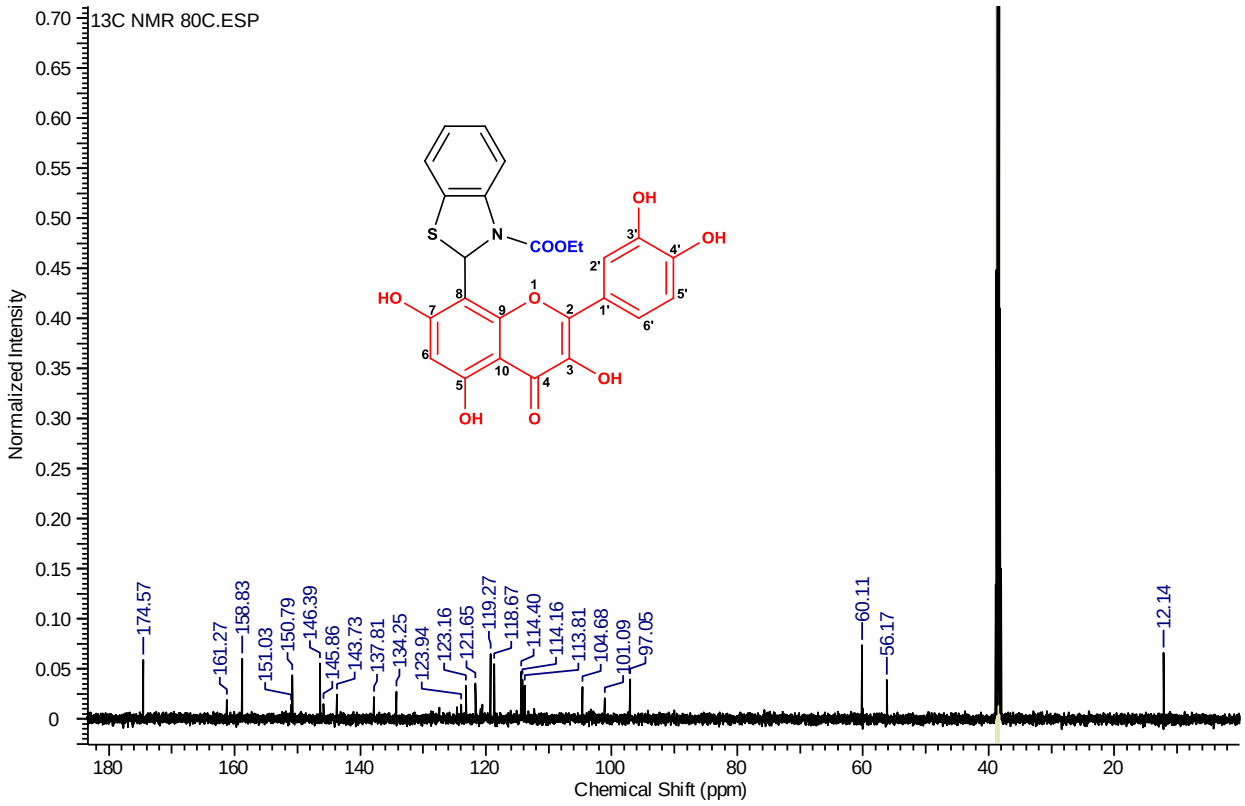


Quercetin - ^{13}C-NMR spectra - DMSO-d_6, 80 ^{o}C, 150 MHz

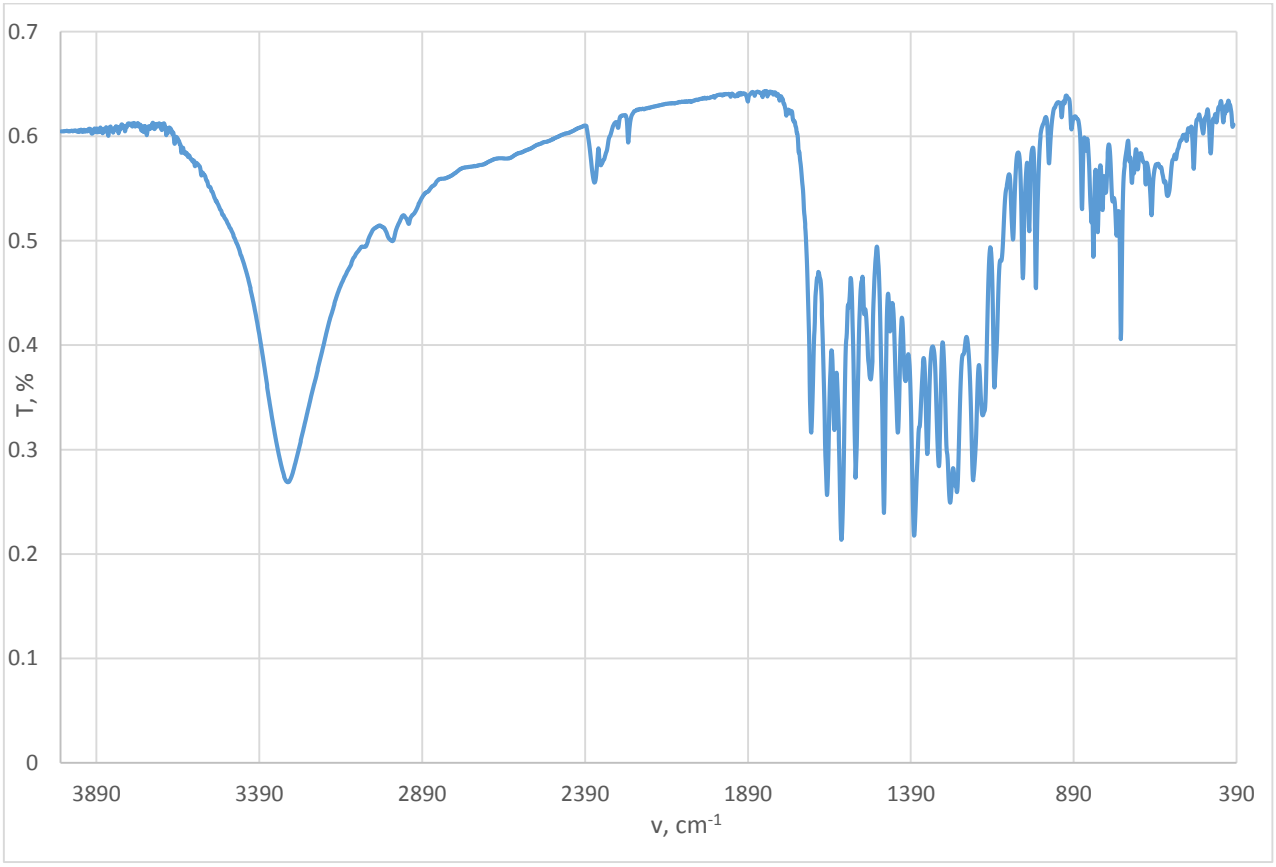


Compound **6a** - ^{1}H-NMR spectra - DMSO-d_6, 80 ^{o}C, 600 MHz





Compound **6a** - ^{13}C-NMR spectra - DMSO-d_6, 80 °C, 150 MHz



Compound **6a** - FT-IR spectra, KBr tablet, cm^{-1}

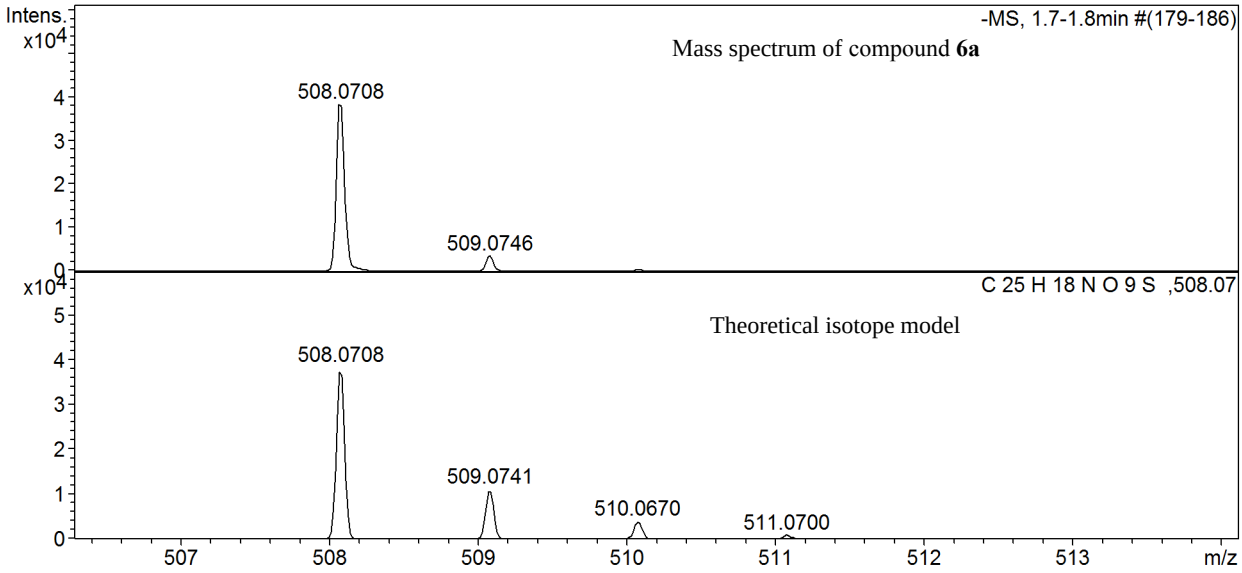
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	\\Utof\data\Jan\ESI38453nb_10_01_2291.d		
Method	2.5min_cal_sample_neg_naf_24-01-11.m	Operator	Mass Spec
Sample Name	ESI38453nb	Instrument / Ser#	micrOTOF 92
Comment			

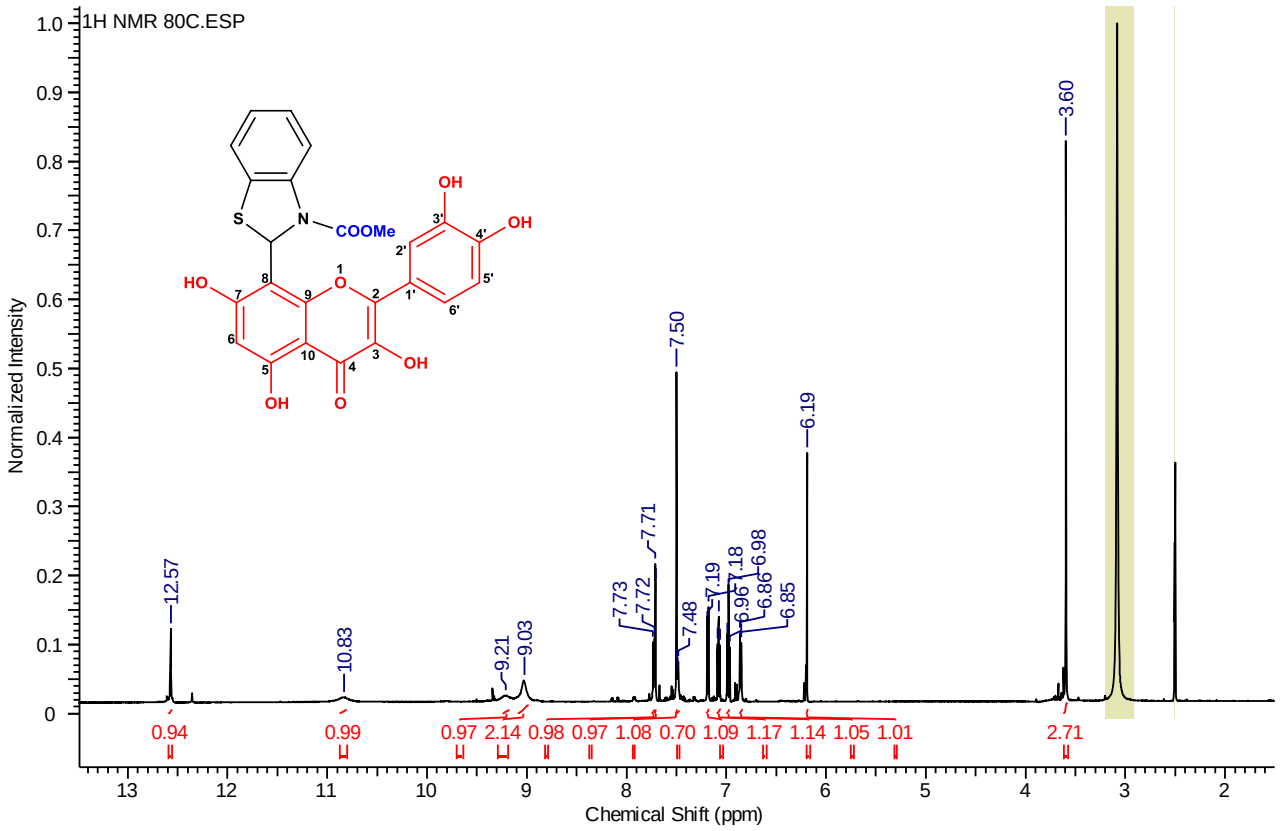
Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	2.0 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	10.0 l/min
Scan End	1200 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

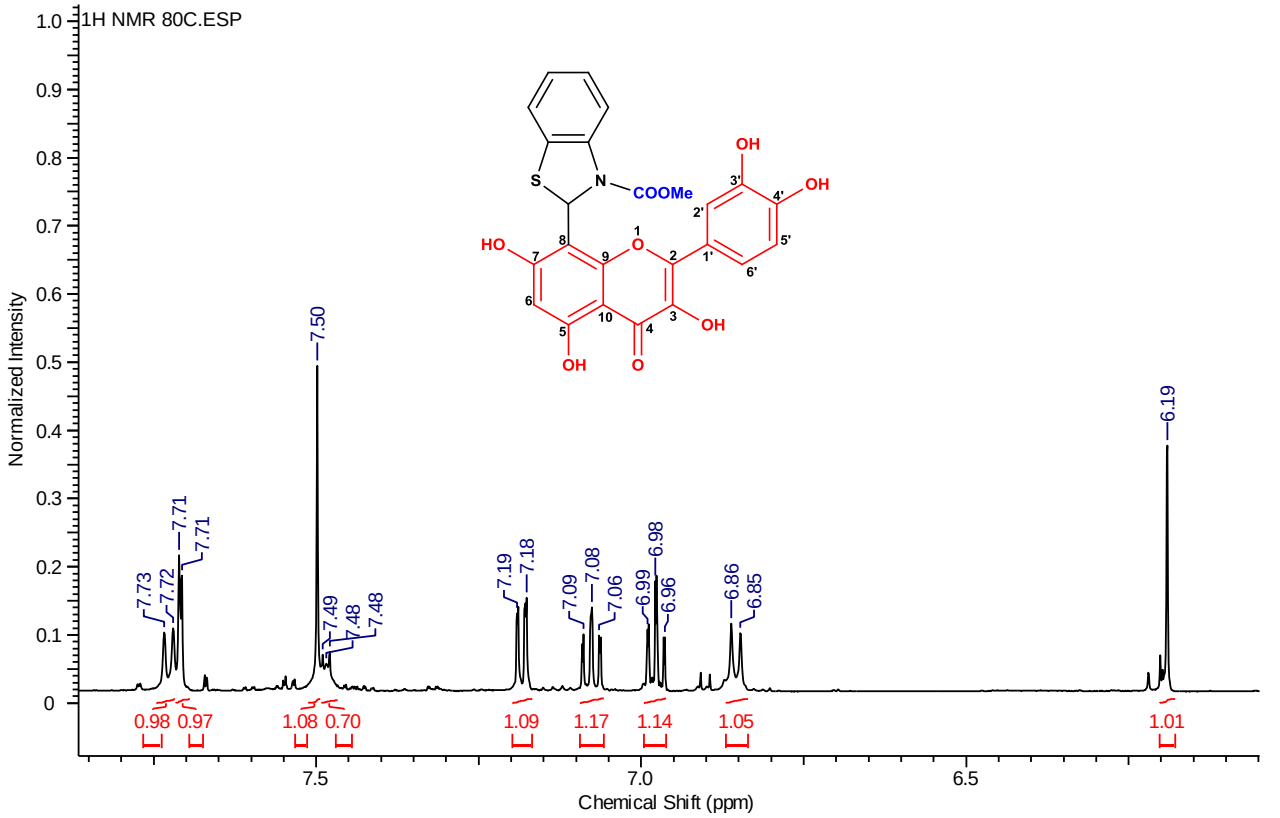


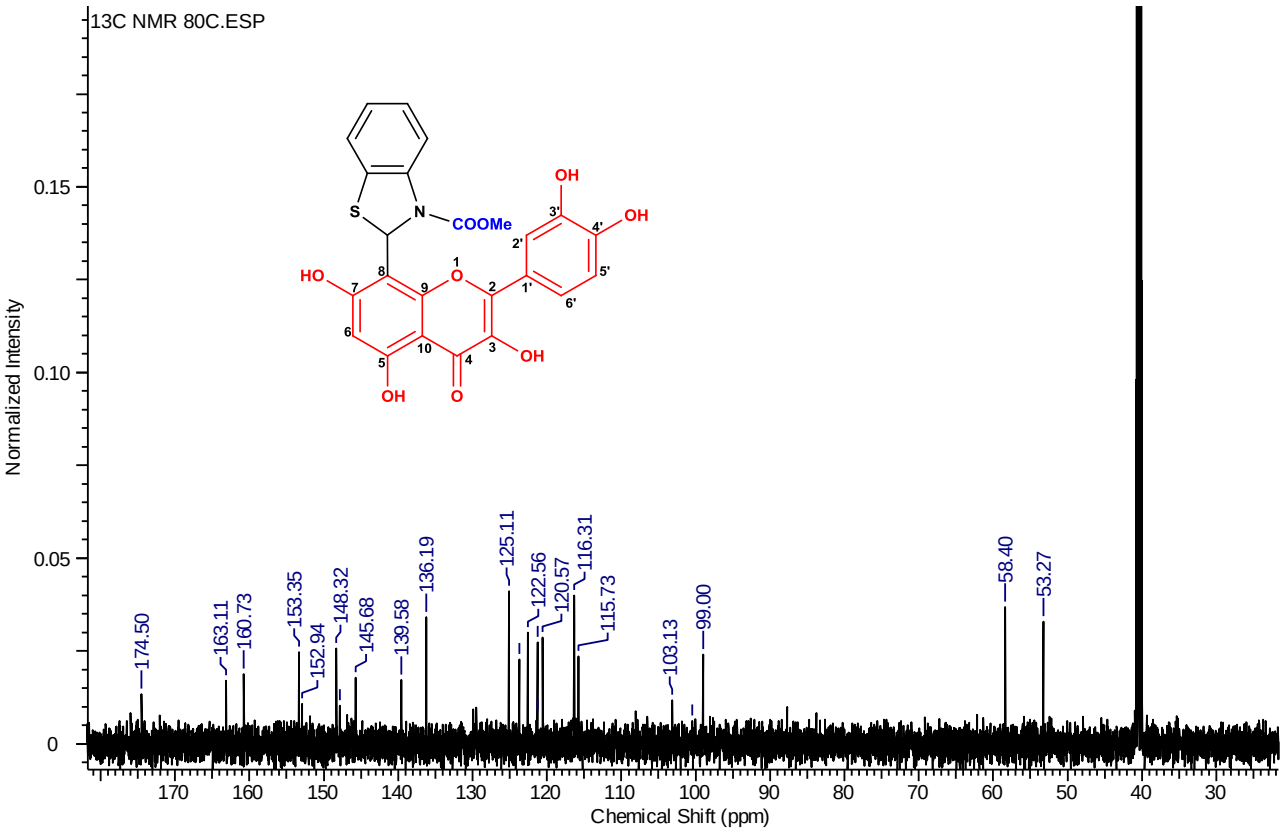
Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma
508.0708									
	1	C 25 H 18 N O 9 S	508.0708	0.0	-0.1	17.5	ok	even	107.27

Bruker Compass DataAnalysis 4.0

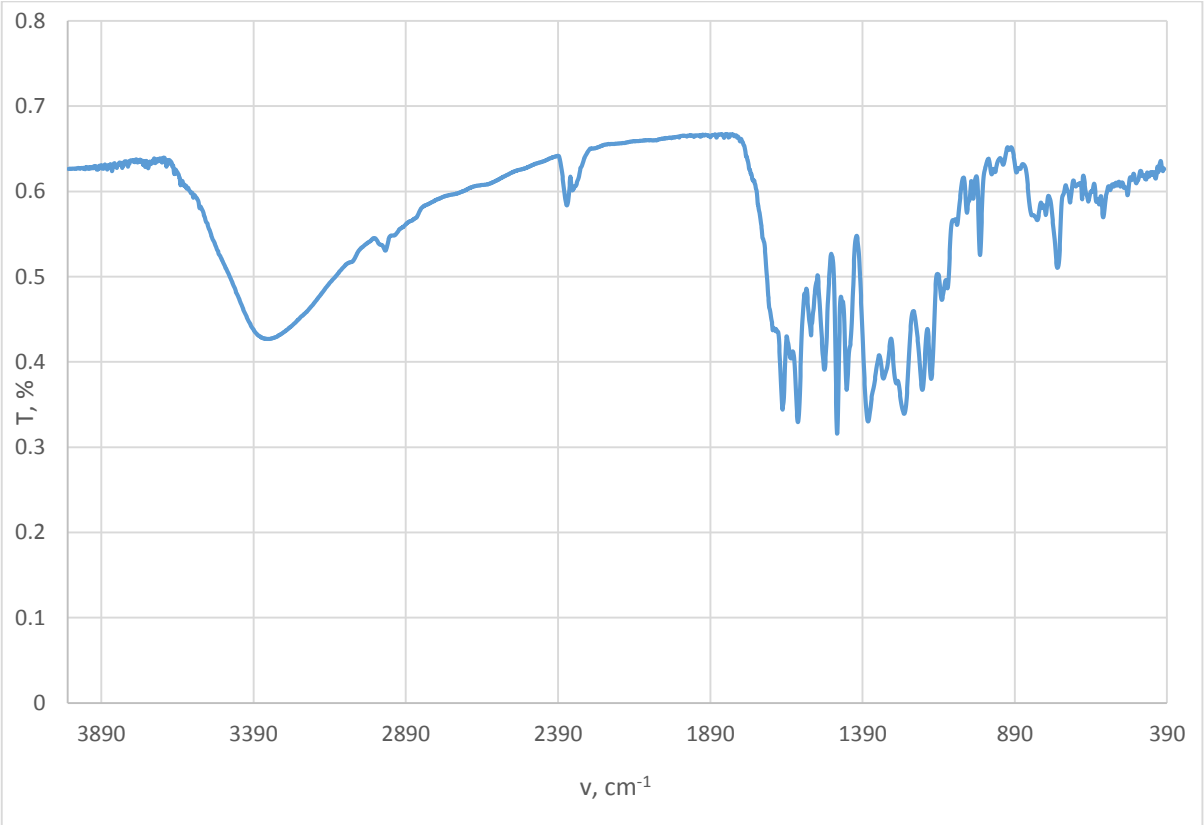


Compound **6b** - ^{1}H-NMR spectra - DMSO-d_6, 80 ^{o}C, 600 MHz

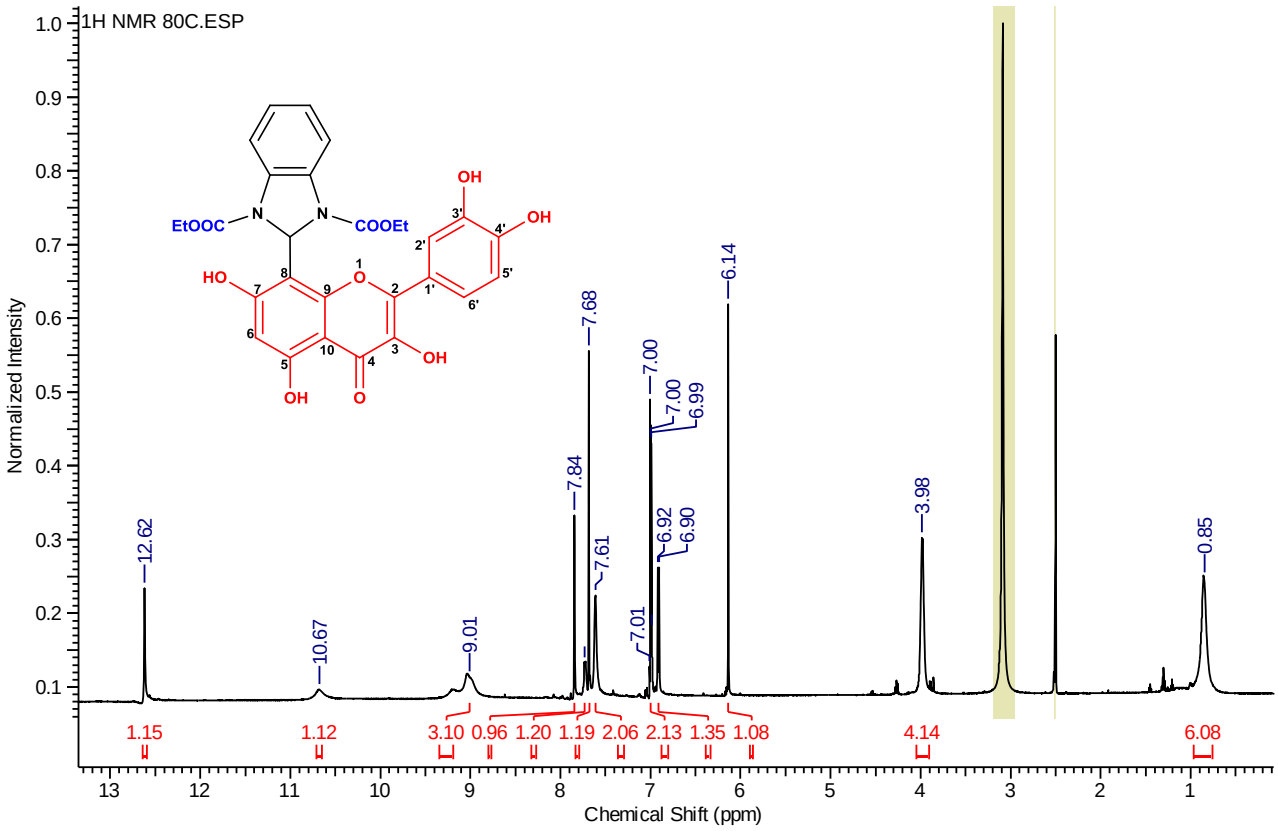




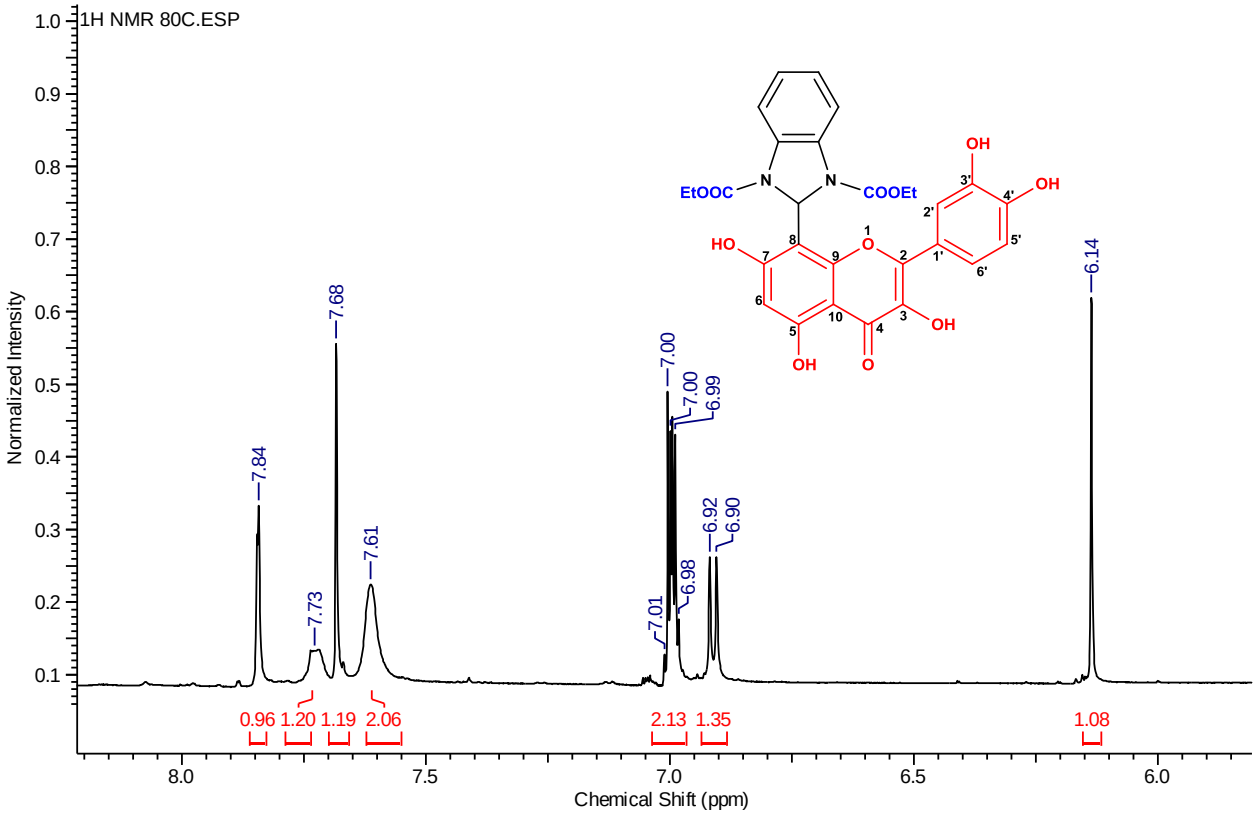
Compound **6b** - ^{13}C-NMR spectra - DMSO-d_6, 80 °C, 150 MHz

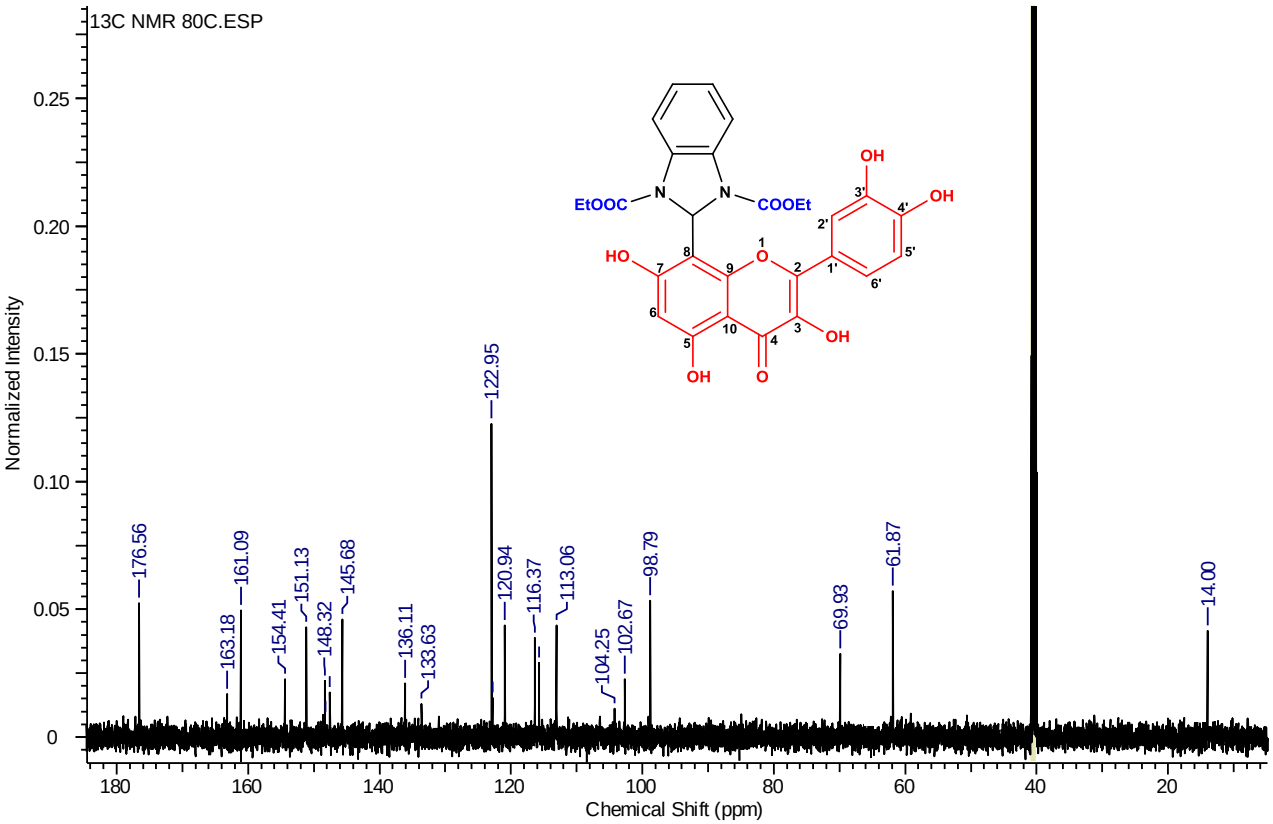


Compound **6b** - FT-IR spectra, KBr tablet, cm^{-1}

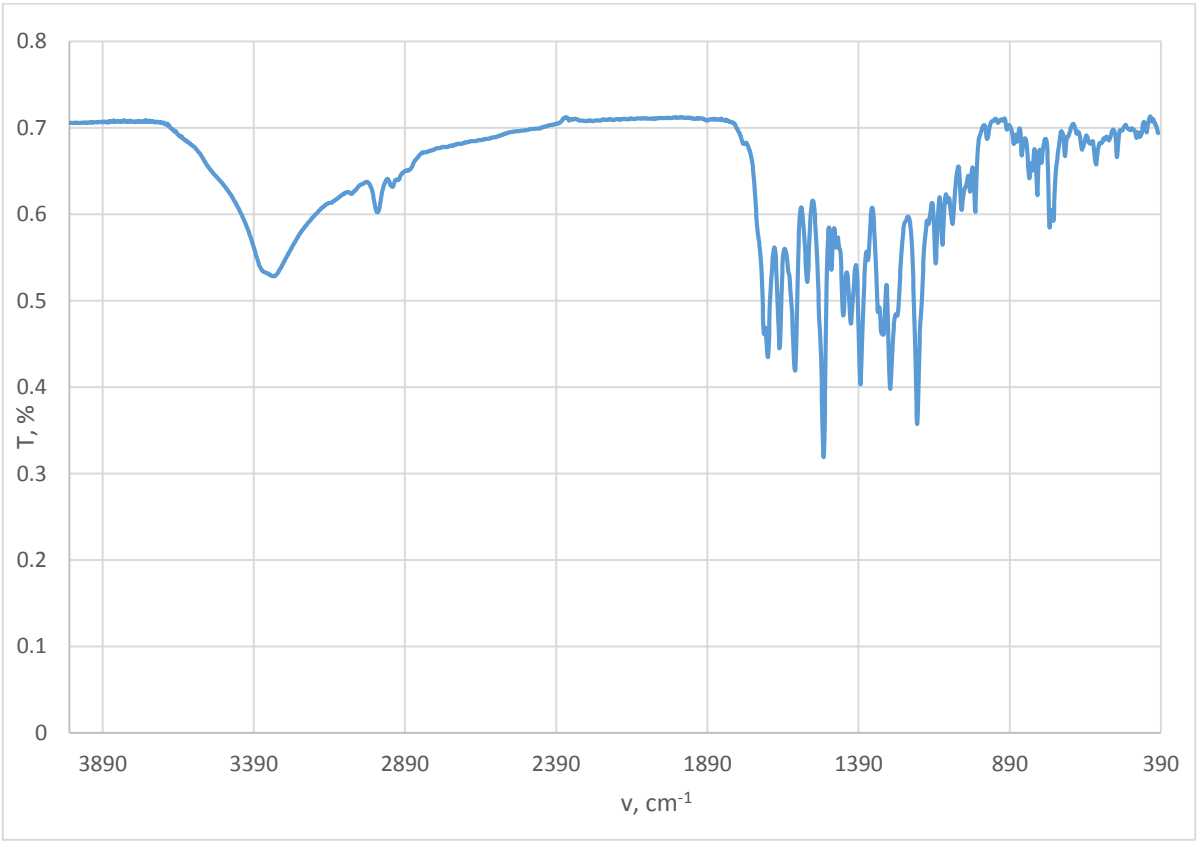


Compound **7a** - ^{1}H-NMR spectra - DMSO-d_6, 80 ^{o}C, 600 MHz





Compound **7a** - ^{13}C-NMR spectra - DMSO-d_6, 80 ^{o}C, 150 MHz



Compound **7a** - FT-IR spectra, KBr tablet, cm^{-1}

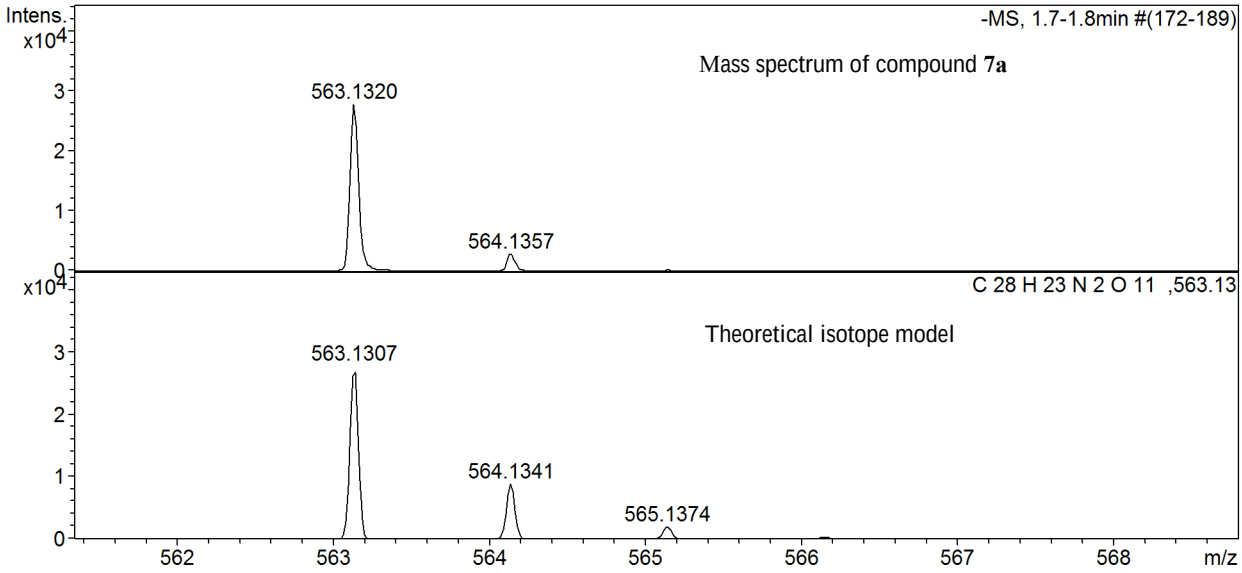
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	\\Utof\data\Jan\ESI38452nb_9_01_2290.d		
Method	2.5min_cal_sample_neg_naf_24-01-11.m	Operator	Mass Spec
Sample Name	ESI38452nb	Instrument / Ser#	micrOTOF 92
Comment			

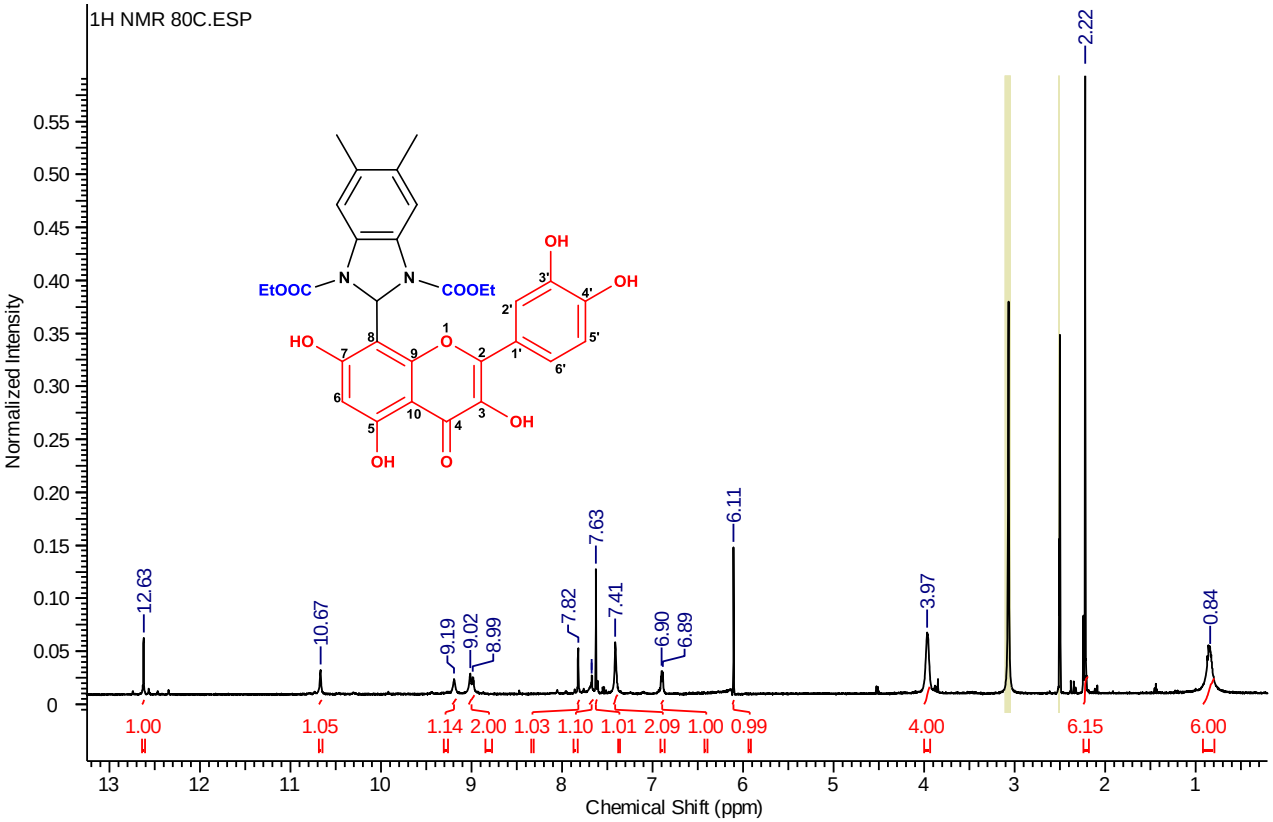
Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	2.0 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	10.0 l/min
Scan End	1200 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

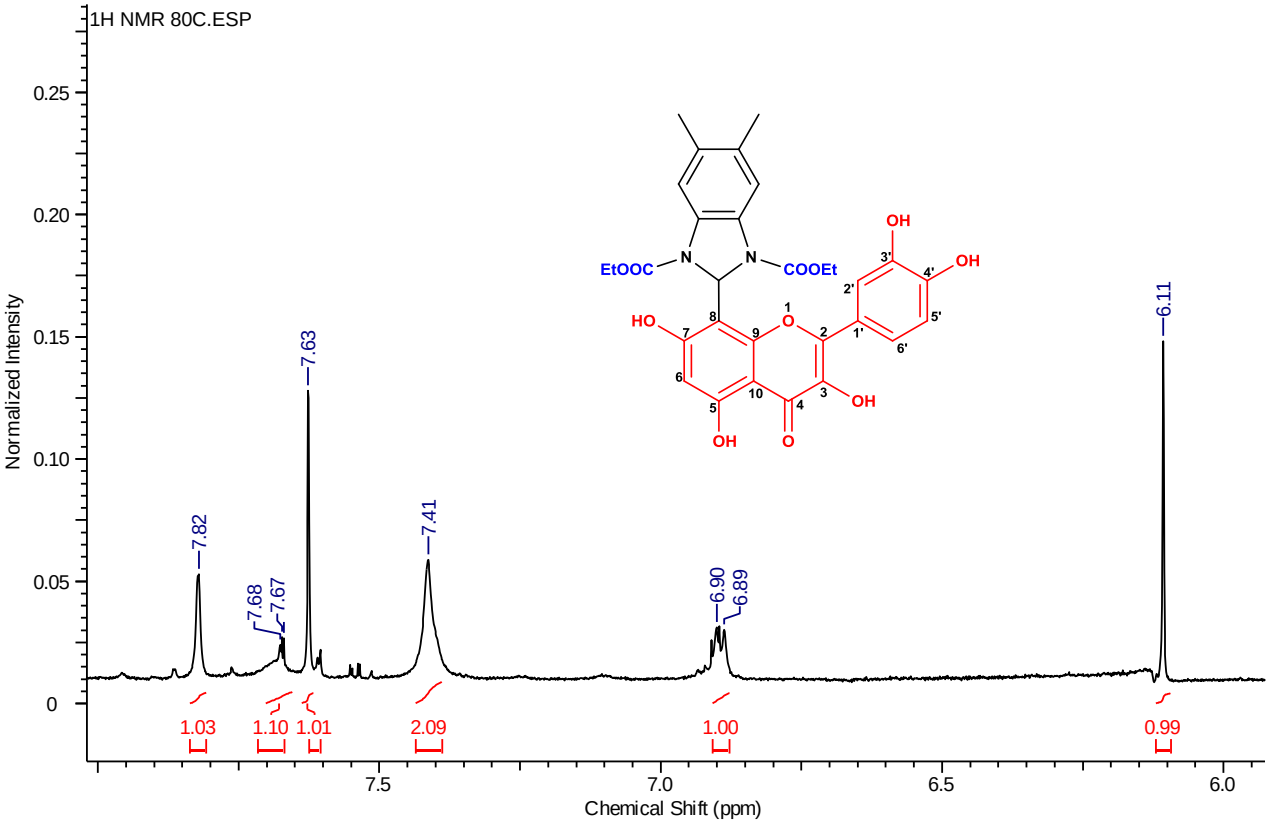


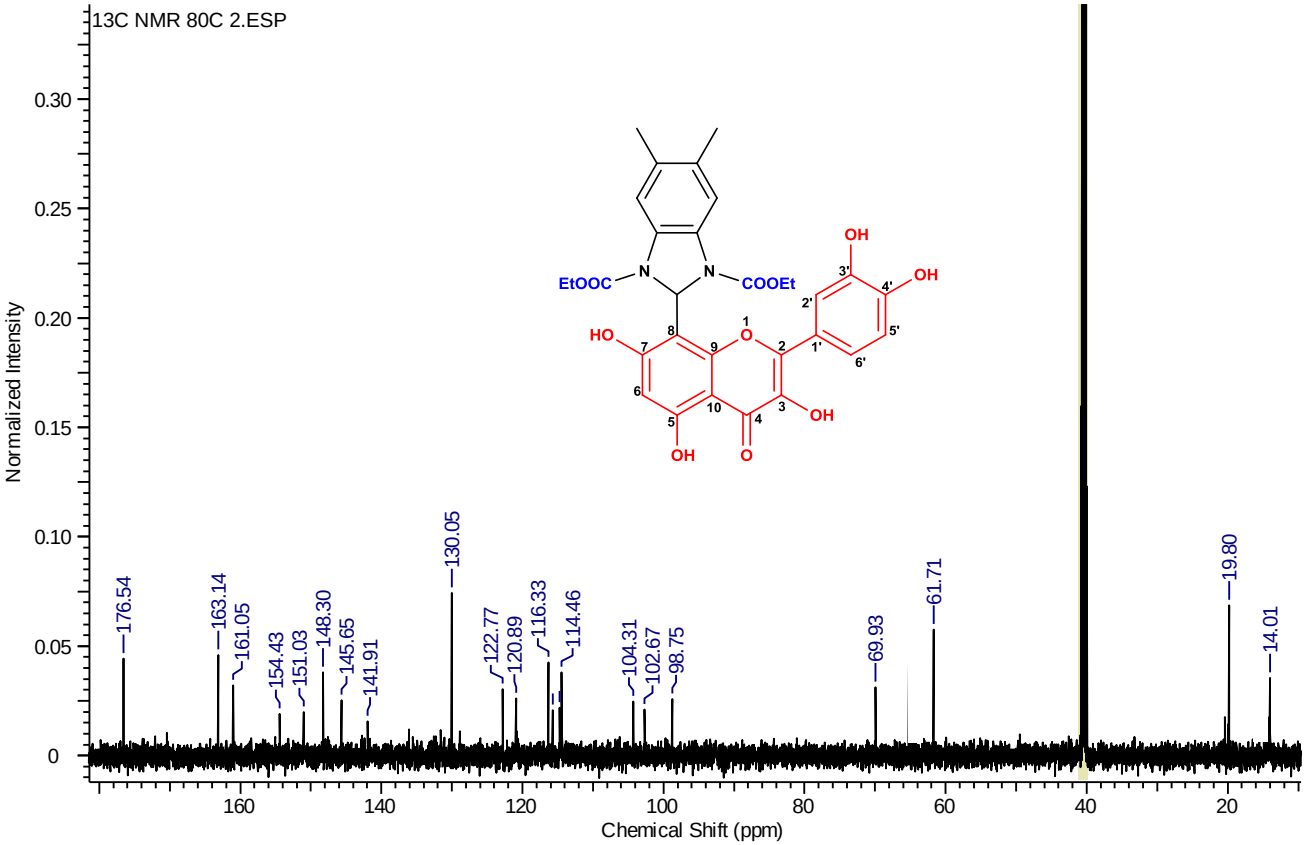
Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e¯ Conf	mSigma
563.1320									
	1	C 28 H 23 N 2 O 11	563.1307	-2.2	-2.3	18.5	ok	even	112.56

Bruker Compass DataAnalysis 4.0

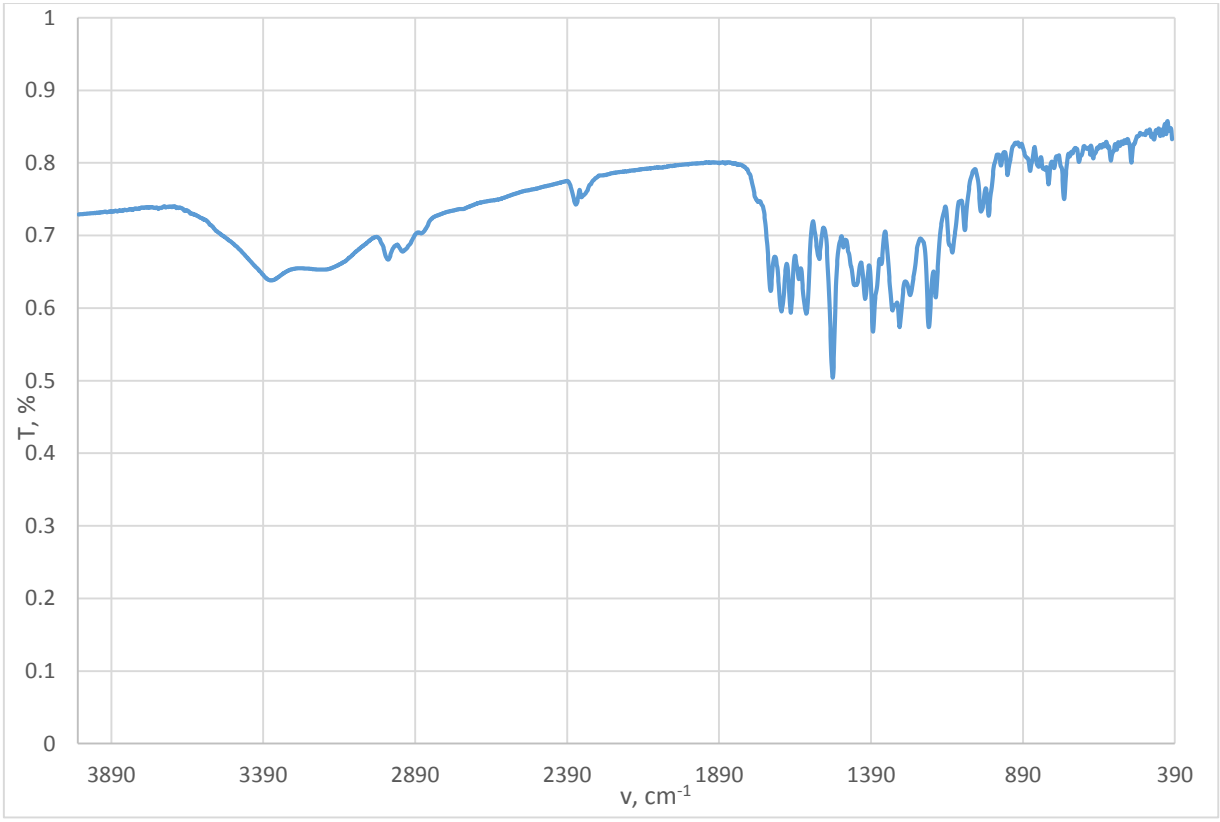


Compound **8a** - ^{1}H-NMR spectra - DMSO-d_6, 80 ^{o}C, 600 MHz

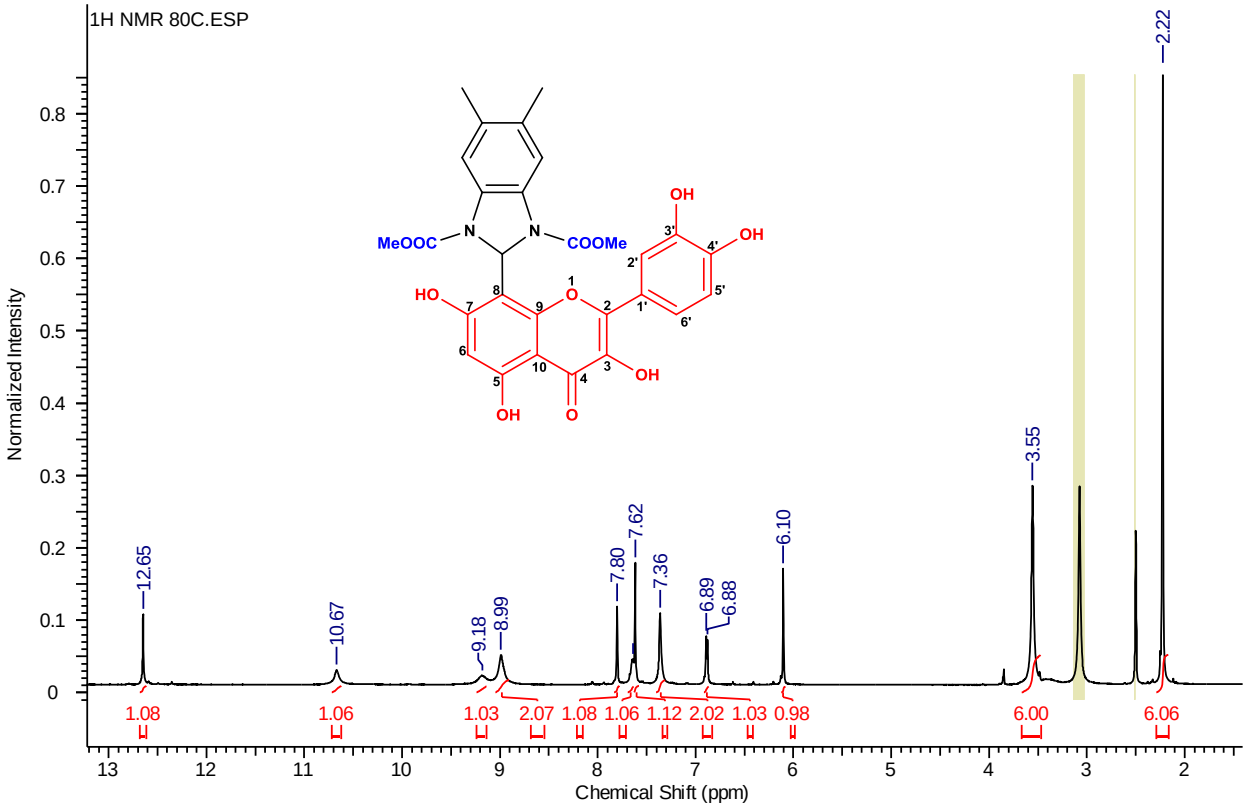




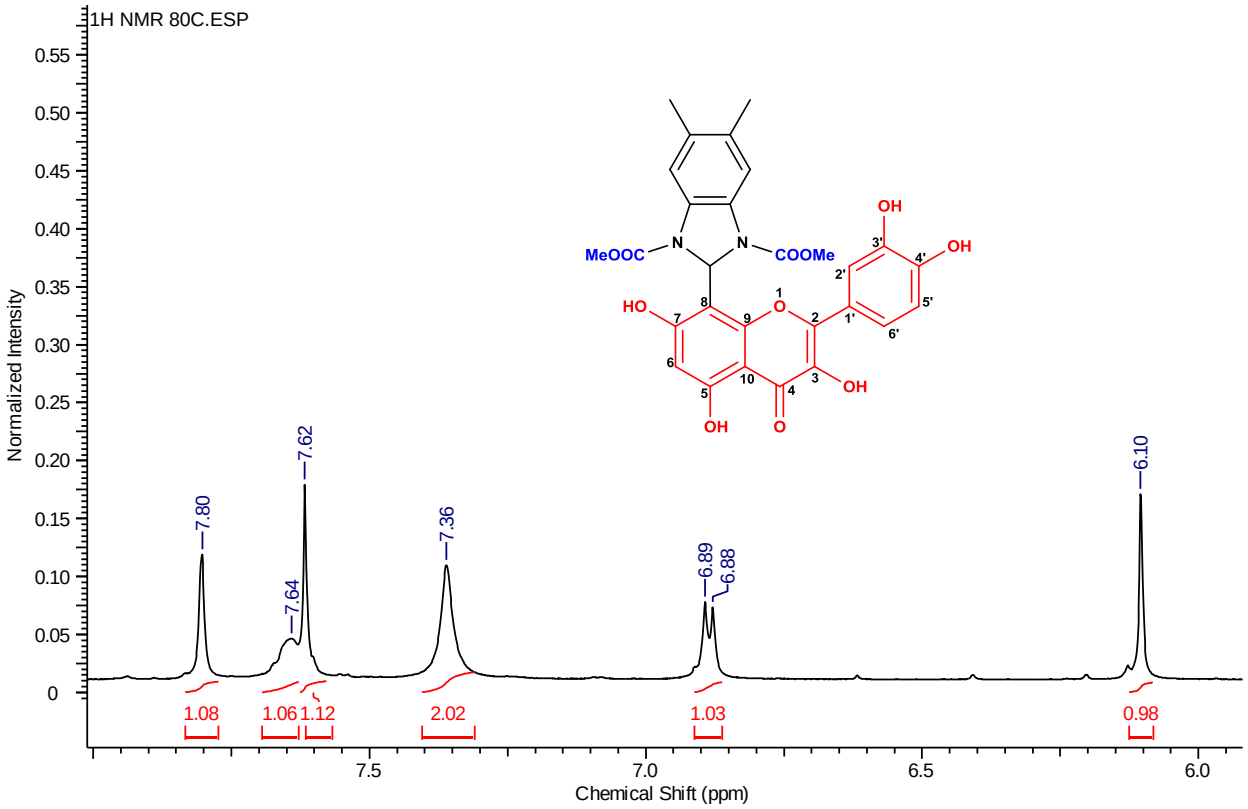
Compound **8a** - ^{13}C-NMR spectra - DMSO-d_6, 80 ^{o}C, 150 MHz

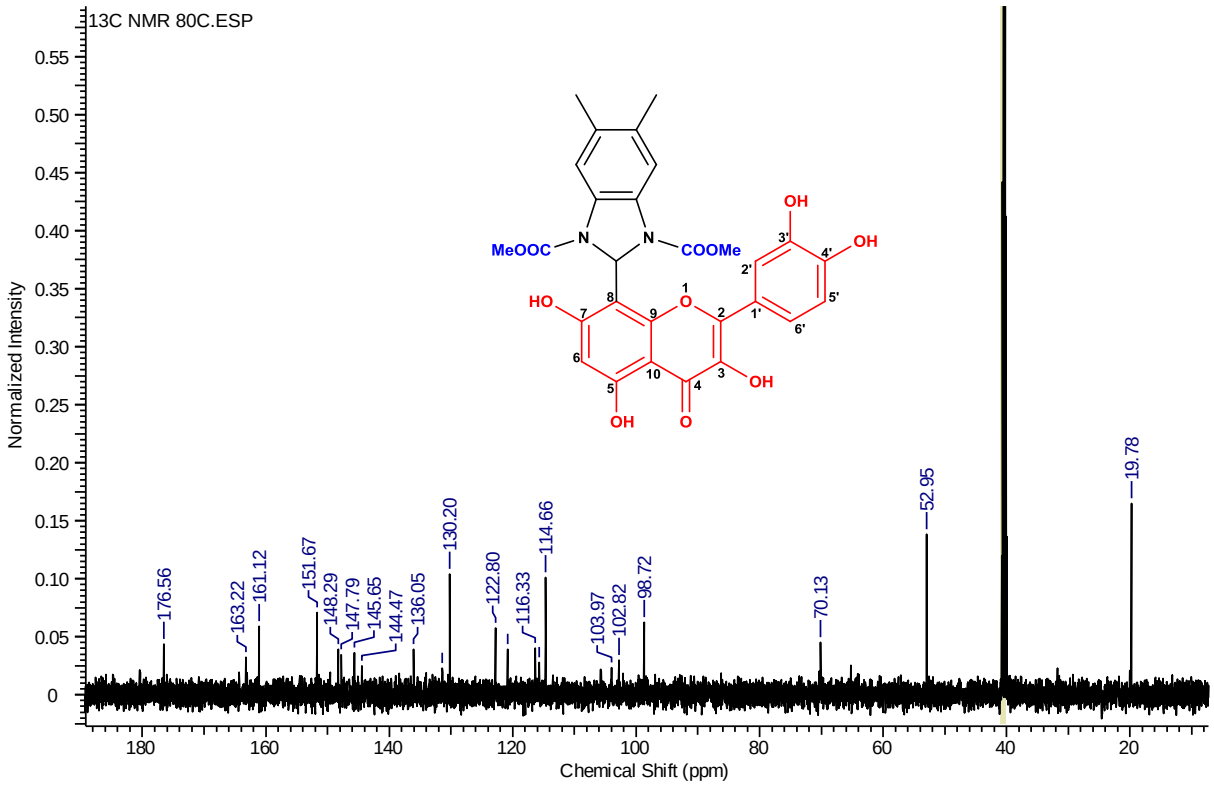


Compound **8a** - FT-IR spectra, KBr tablet, cm^{-1}

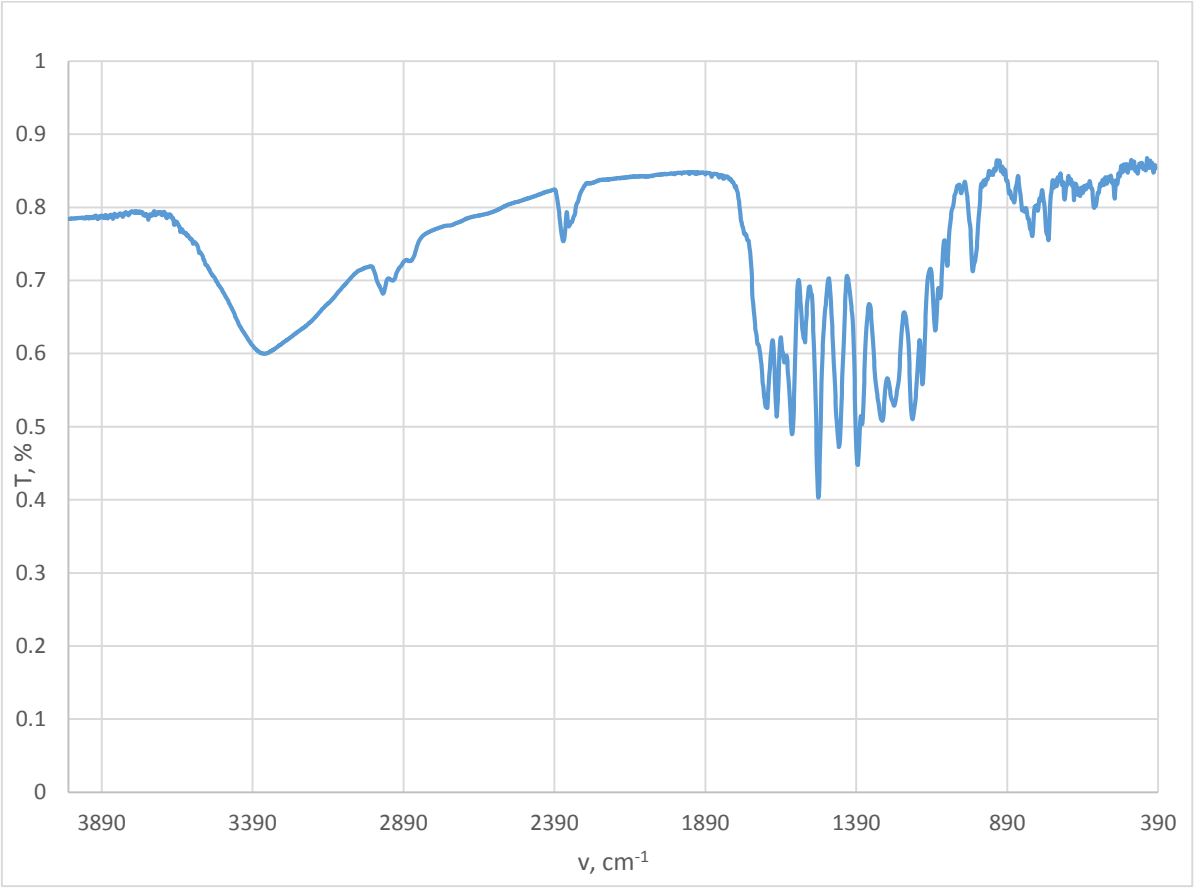


Compound **8b** - ^{1}H-NMR spectra - DMSO-d_6, 80 ^{o}C, 600 MHz





Compound **8b** - ^{13}C-NMR spectra - DMSO-d_6, 80 ^{o}C, 150 MHz



Compound **8b** - FT-IR spectra, KBr tablet, cm^{-1}