Supporting Information

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Isolation of amygdalin epimer at high diastereomeric purity and its structural characterization by spectroscopic and Q-TOF LC-MS methods

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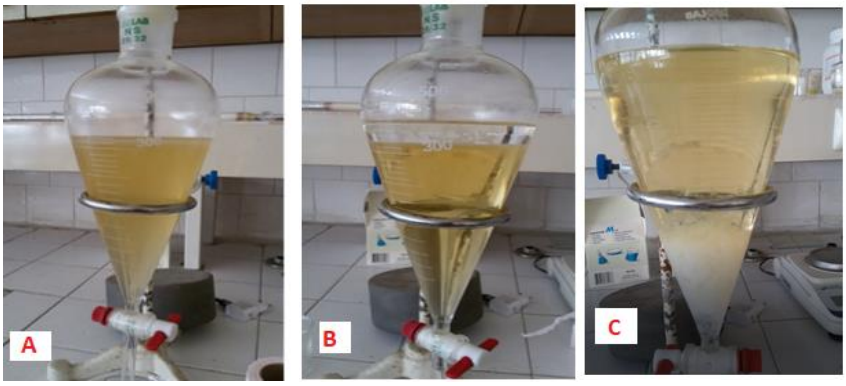


Figure S1: Liquid-Liquid Extractions (LLE); A = n-hexzane, B = petrelium ether, C = chloroform

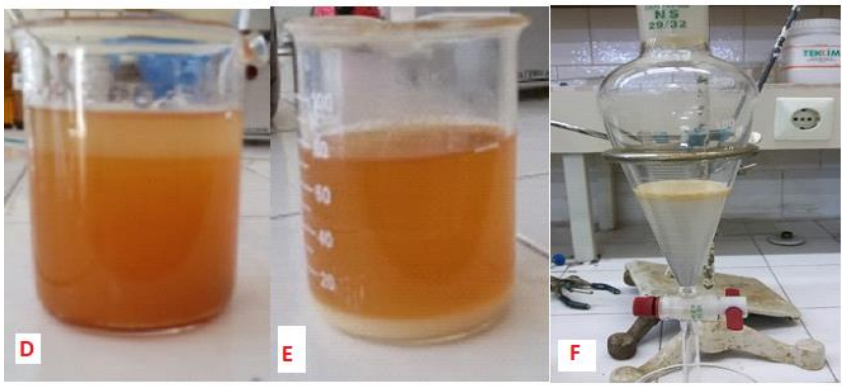


Figure S2: Decantation Methods; D = n-hexzane, E = petrelium ether, F = chloroform

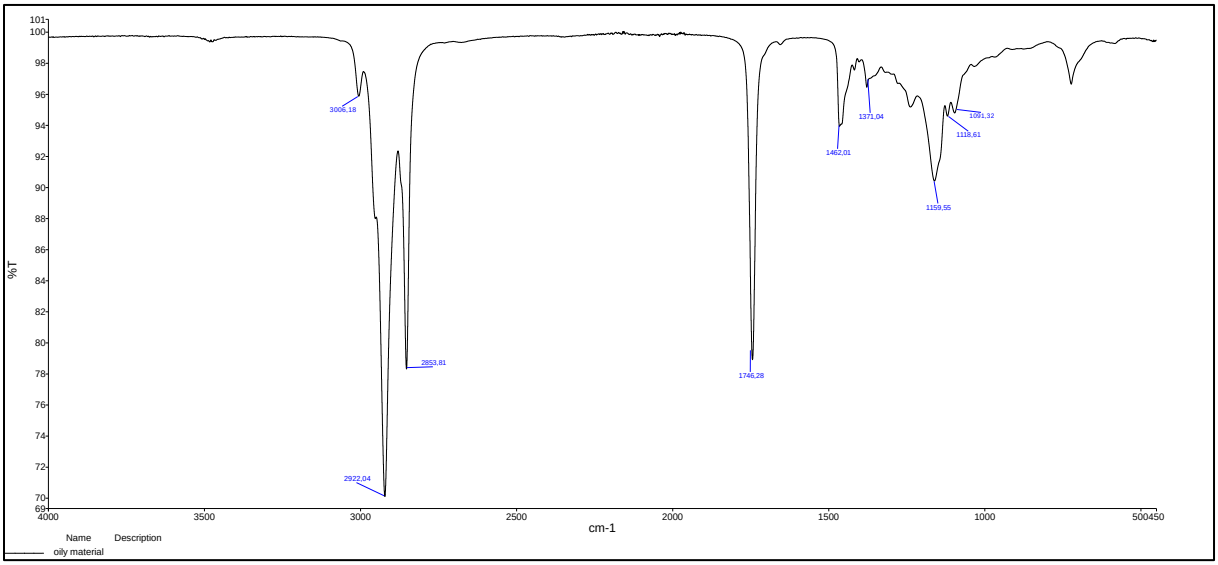


Figure S3: ATR-IR spectrum of the amygdalin-free component of the extract

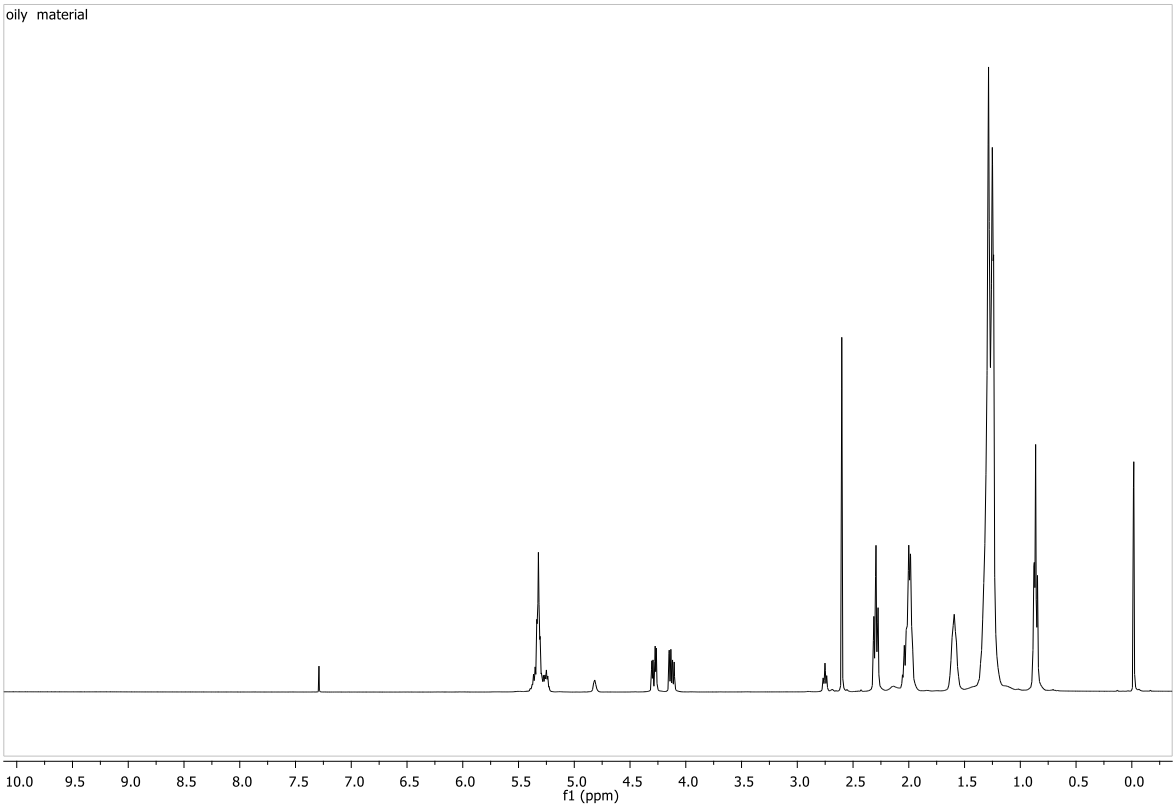


Figure S4: ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of the amygdalin-free component of the extract

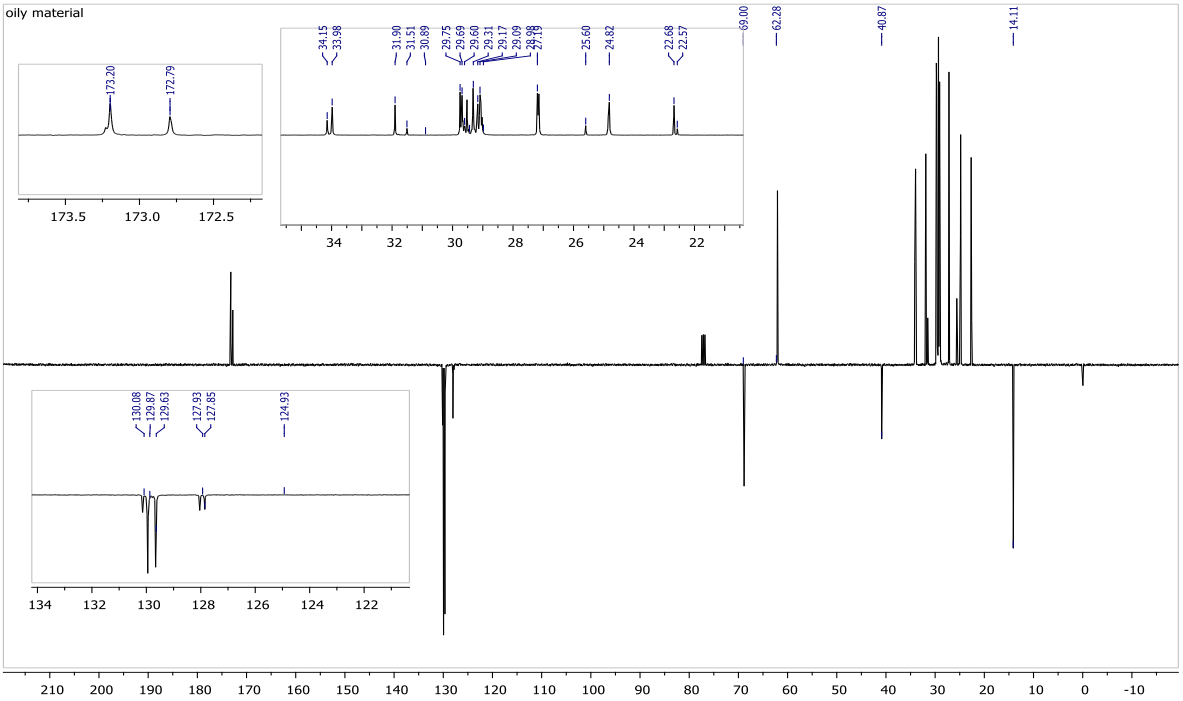


Figure S5: ^{13}C-NMR (400 MHz, $CDCl_3$) spectrum of the amygdalin-free component of the extract

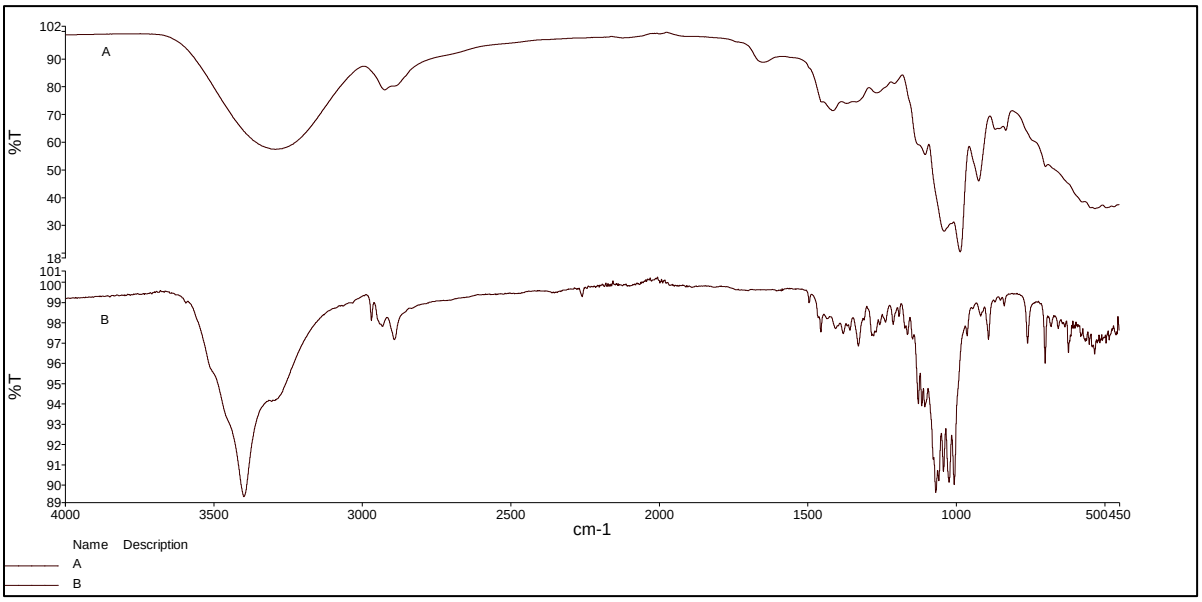


Figure S6 :(A) ATR-FTIR spectrum of the extract obtained without any purification operations; (B) ATR-FTIR spectrum of the isolated amygdalin at high diastereomeric purity

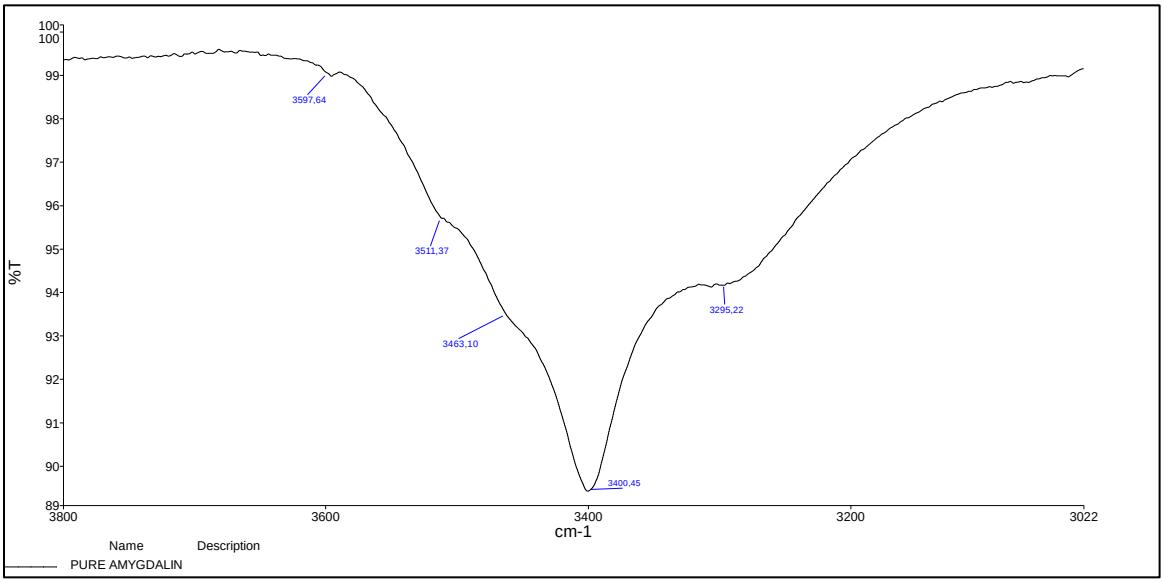


Figure S7: O-H bonds region of amygdalin

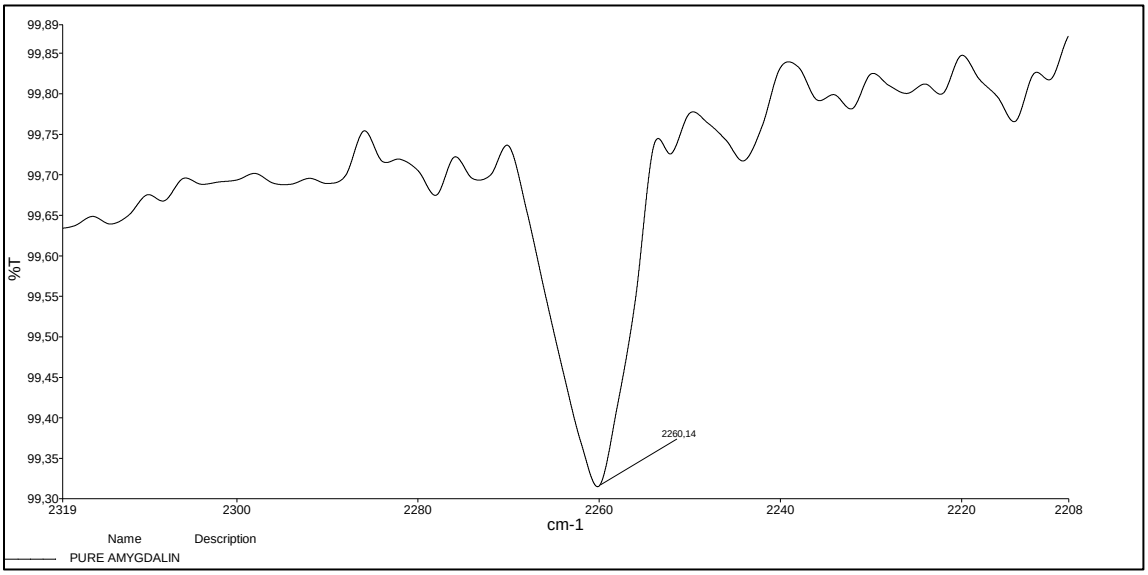


Figure S8: Nitrile region of amygdalin

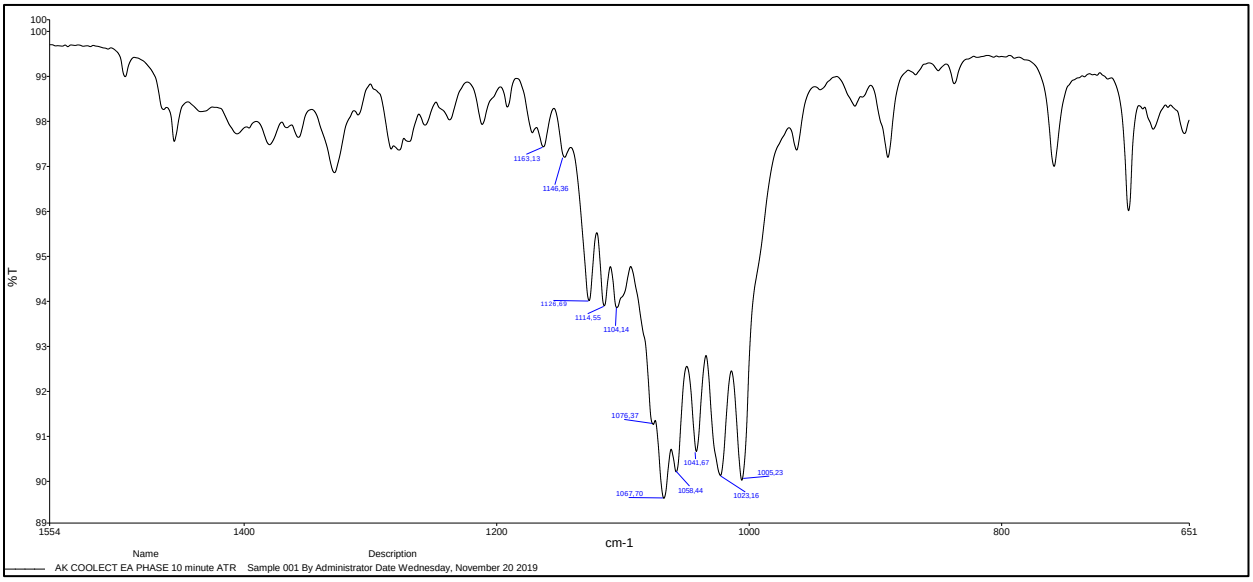


Figure S9: C-O-H and C-O-C bond region of amygdalin

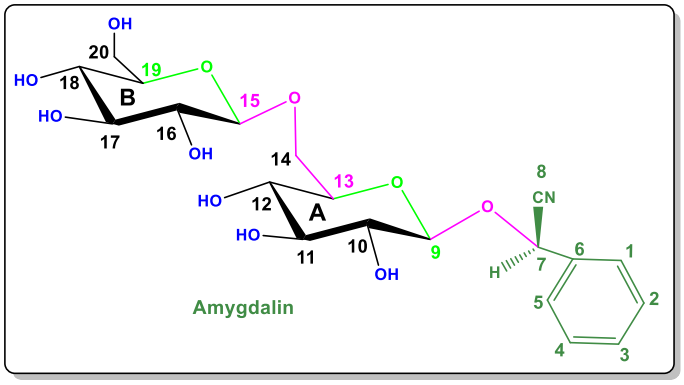


Figure S10: Numbering system used to evaluate NMR spectra of amygdalin. It is not related to the IUPAC numbering system

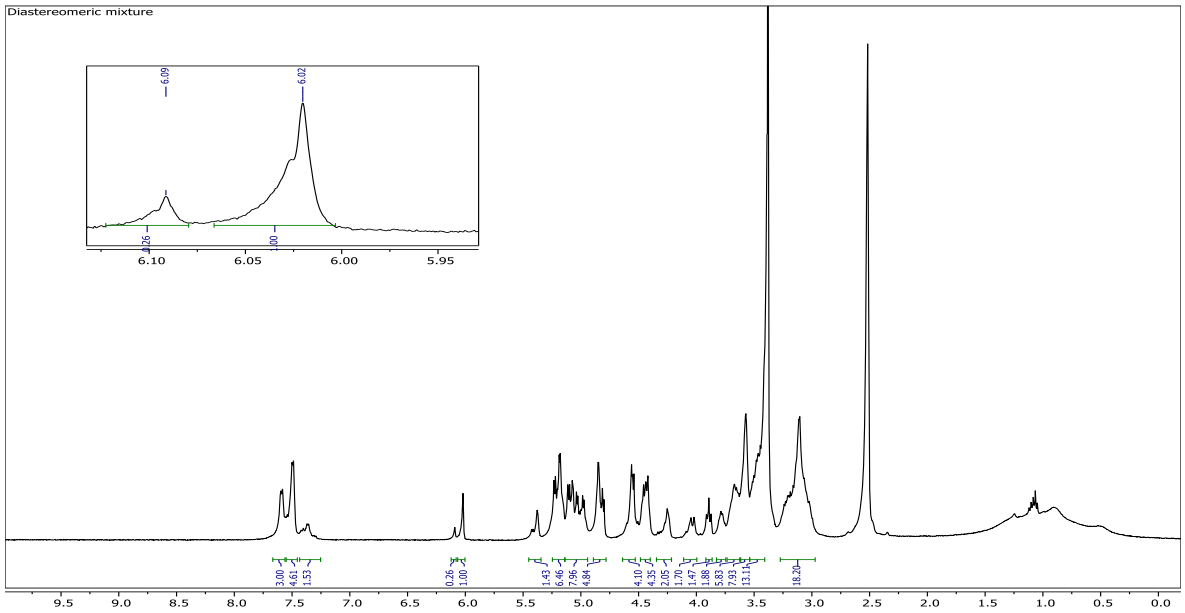


Figure S11: ^{1}H-NMR (400 MHz, DMSO-d_6) spectrum of the extract obtained after LLE

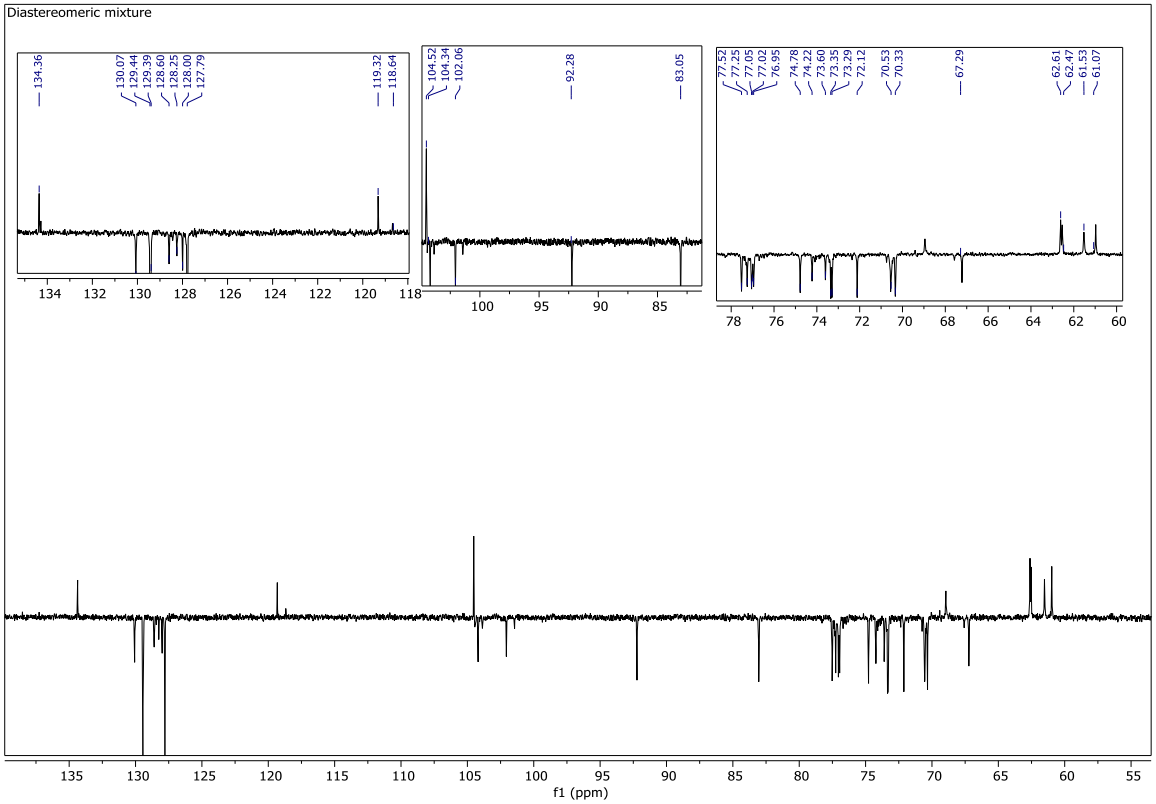


Figure S12: ^{13}C-NMR (100 MHz, DMSO-d_6) spectrum of the extract obtained after LLE

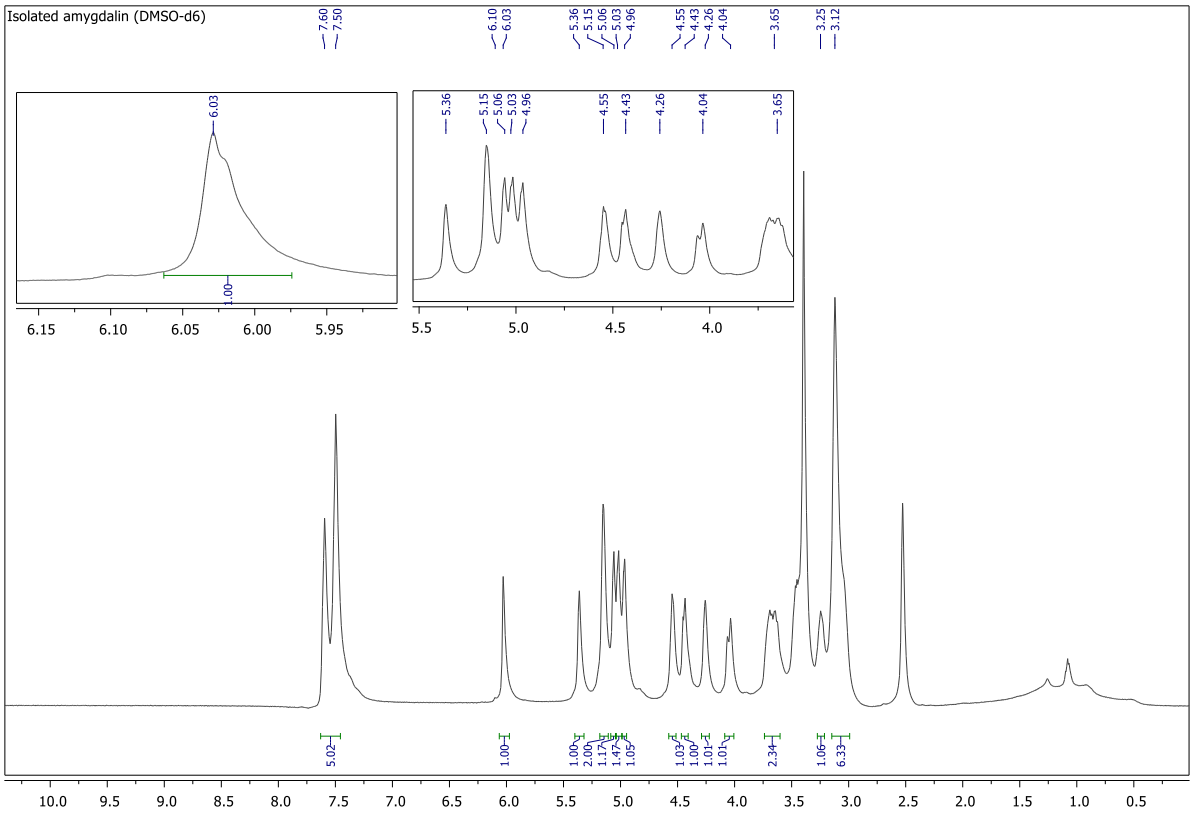


Figure S13: ^{1}H-NMR (400 MHz, DMSO-d_6) spectrum of the amygdalin isolated at high purity after column chromatography

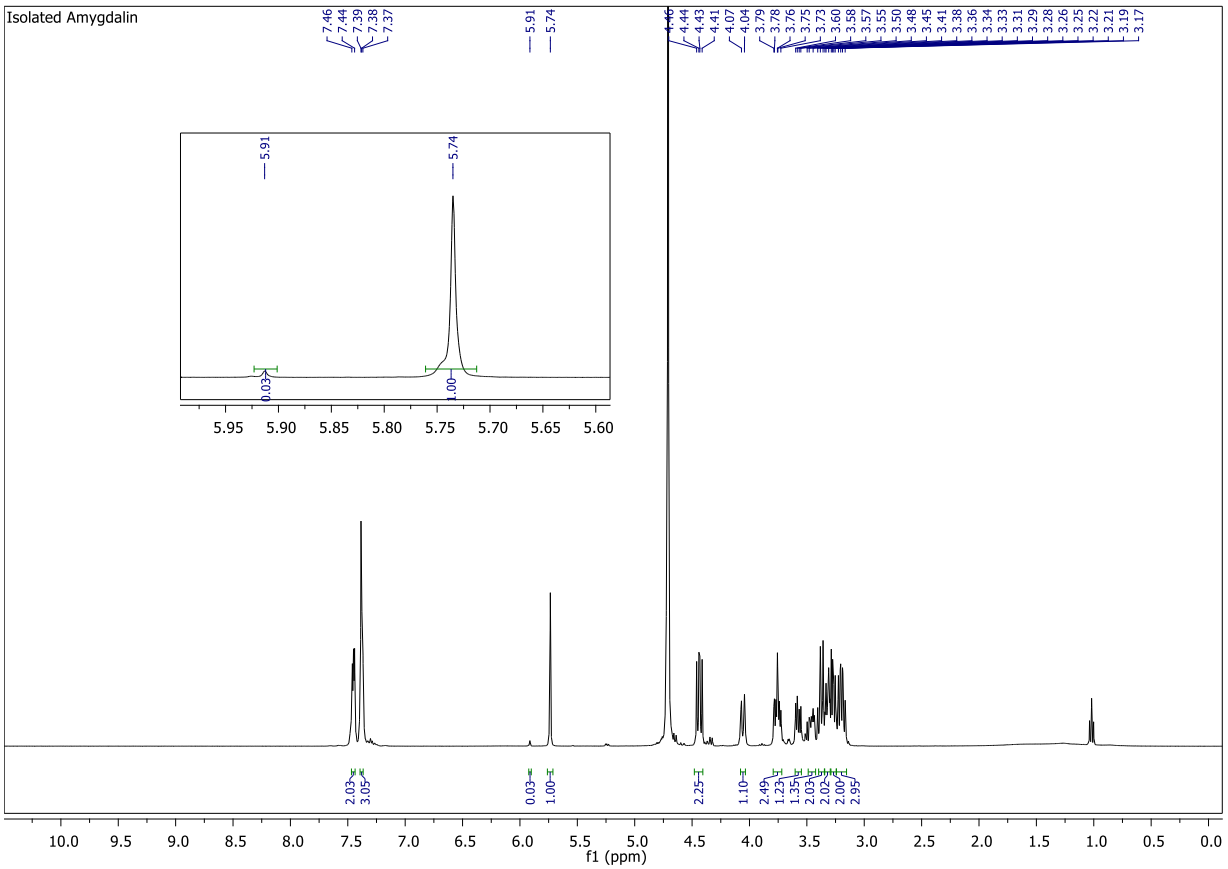


Figure S14: The ^{1}H-NMR (400 MHz, D_20) spectrum of the amygdalin after column chromatography

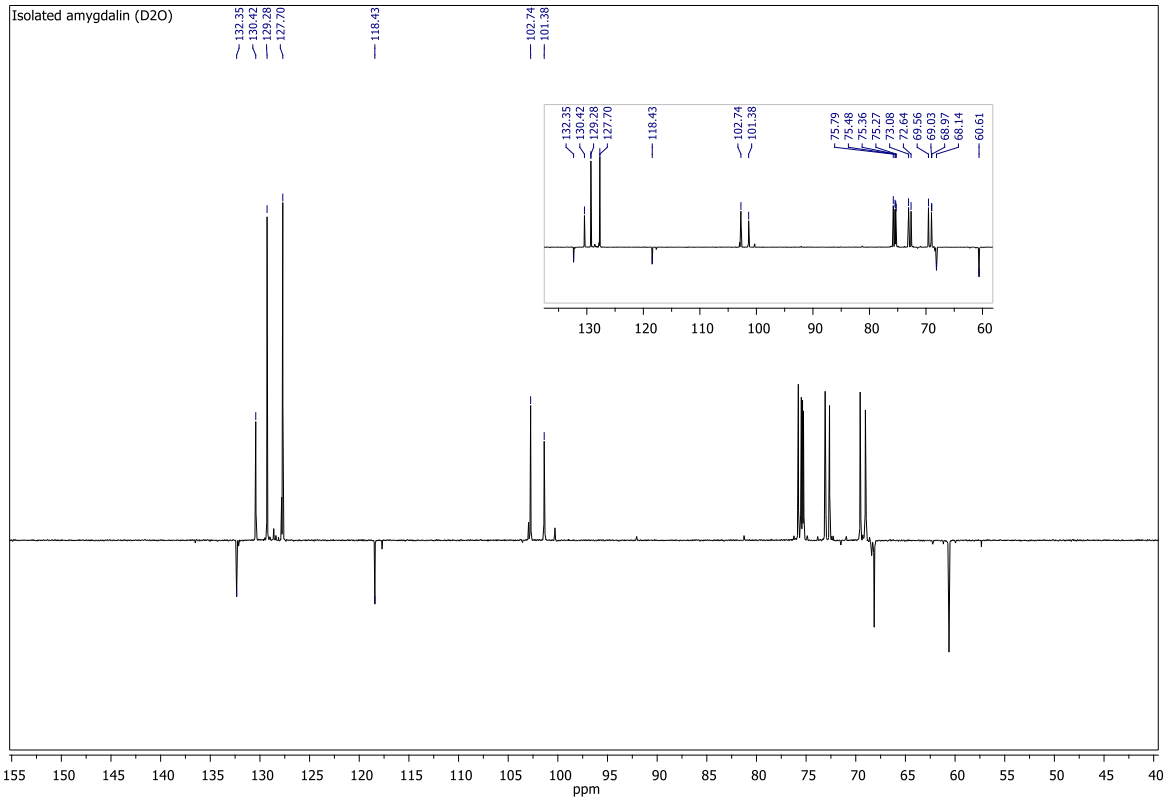


Figure S15: ^{13}C-NMR (100 MHz, D_2O) spectrum of the amygdalin isolated after column chromatography

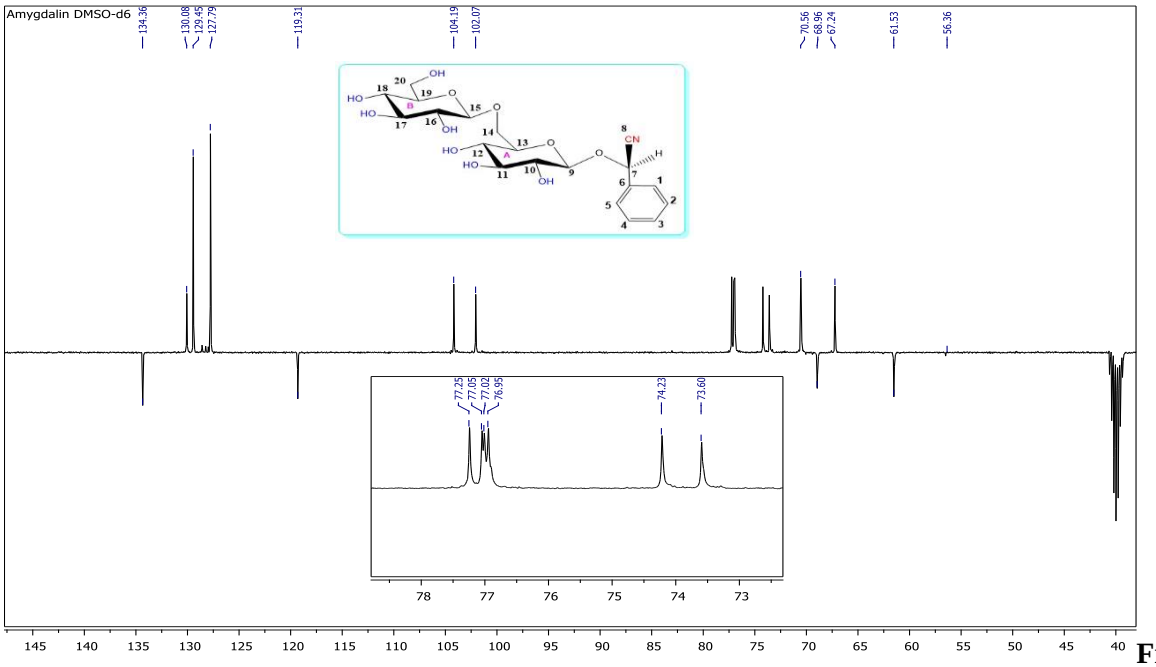


Figure S16: ^{13}C-NMR (100 MHz, DMSO-d_6) spectrum of the amygdalin isolated at high purity column chromatography

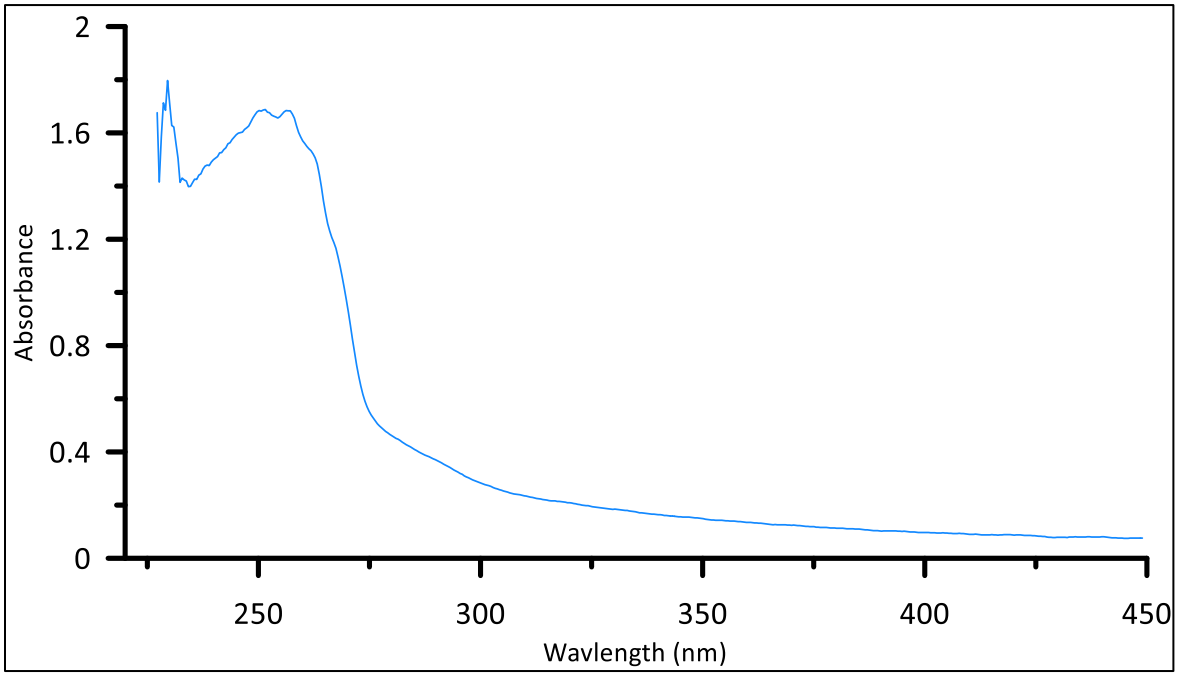


Figure S17: The UV-VIS spectrum of the isolated pure amygdalin.

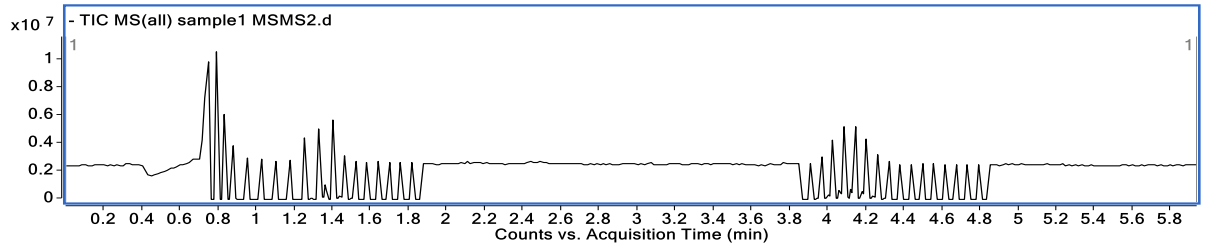


Figure S18: TIC of the sample in MS-MS mode

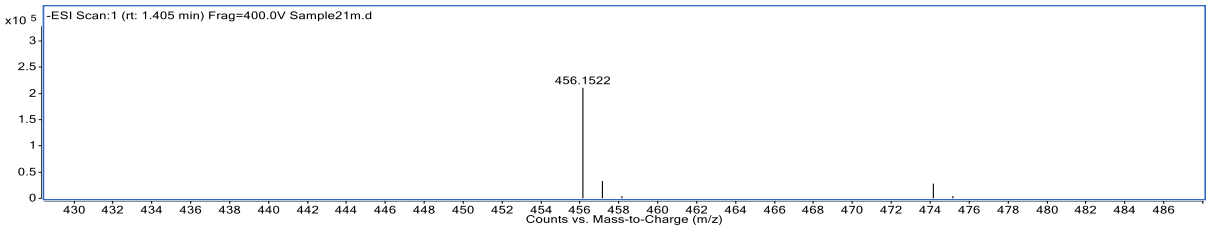
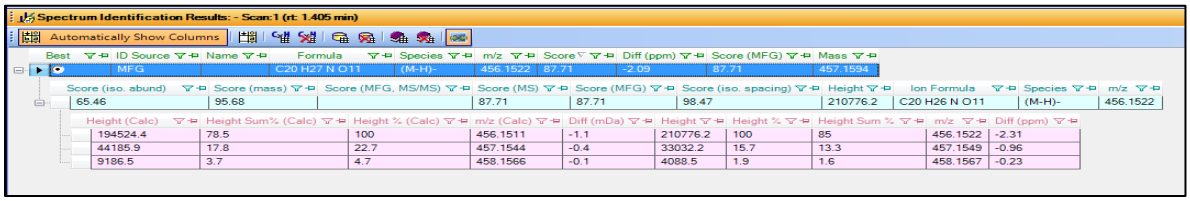


Figure S19: MS spectrum of peak at RT 1.41



Best	ID Source	Name	Formula	Species	m/z	Score	Diff (ppm)	Score (MFG)	Mass
	MFG		C20 H27 N O11	(M-H)-	456.1522	87.71	-2.09	87.71	457.1594

Score (iso. abund)	Score (mass)	Score (MFG, MS/MS)	Score (MS)	Score (MFG)	Score (iso. spacing)	Height	Ion Formula	Species	m/z
65.46	95.68		87.71	87.71	98.47	210776.2	C20 H26 N O11	(M-H)-	456.1522

Height (Calc)	Height Sum% (Calc)	Height % (Calc)	m/z (Calc)	Diff (mDa)	Height	Height %	Height Sum %	m/z	Diff (ppm)
194524.4	78.5	100	456.1511	-1.1	210776.2	100	85	456.1522	-2.31
44185.9	17.8	22.7	457.1544	-0.4	33032.2	15.7	13.3	457.1549	-0.96
9186.5	3.7	4.7	458.1566	-0.1	4088.5	1.9	1.6	458.1567	-0.23

Figure S20. Isotopic distribution of 456 ion at RT 1.42 showing experimental and calculated values

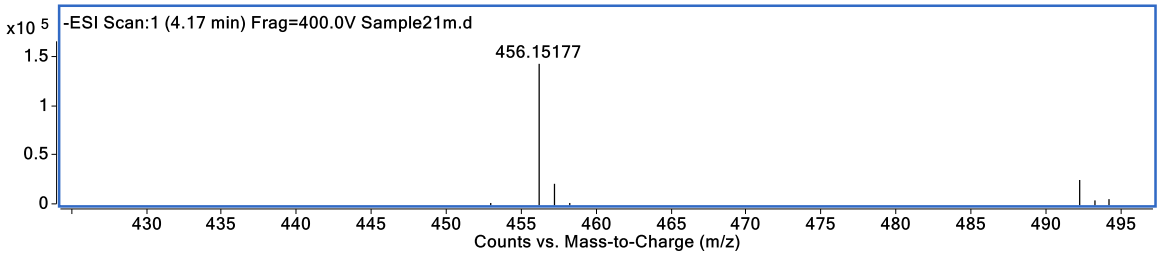


Figure S21: MS spectrum of peak at RT 4.17

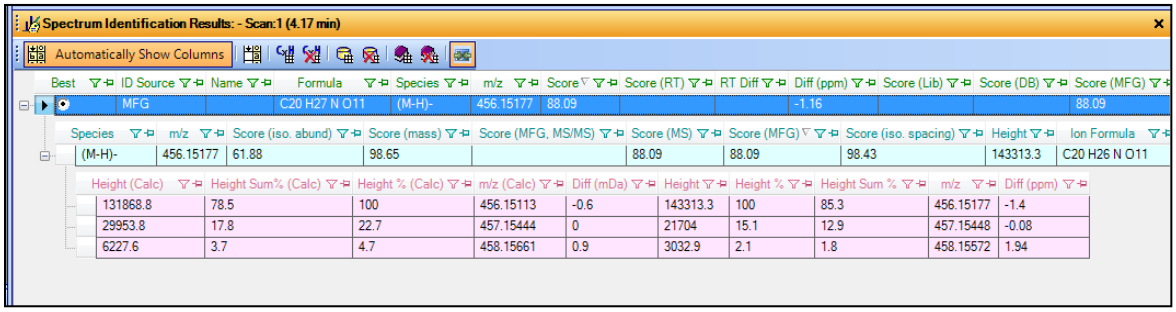


Figure S22: Isotopic distribution of 456 ion at RT 4.17