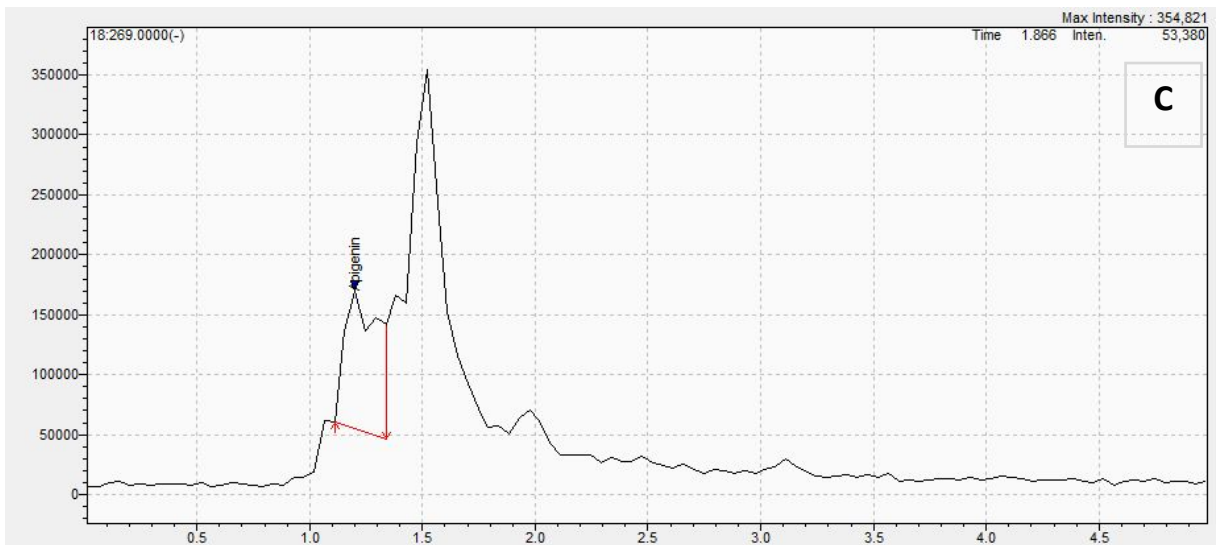
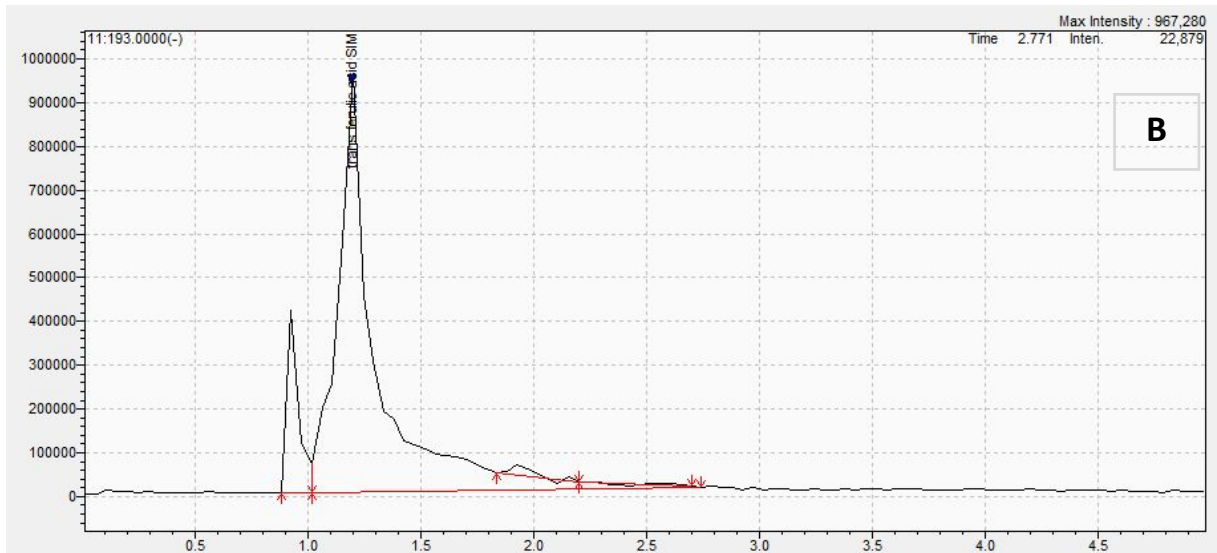
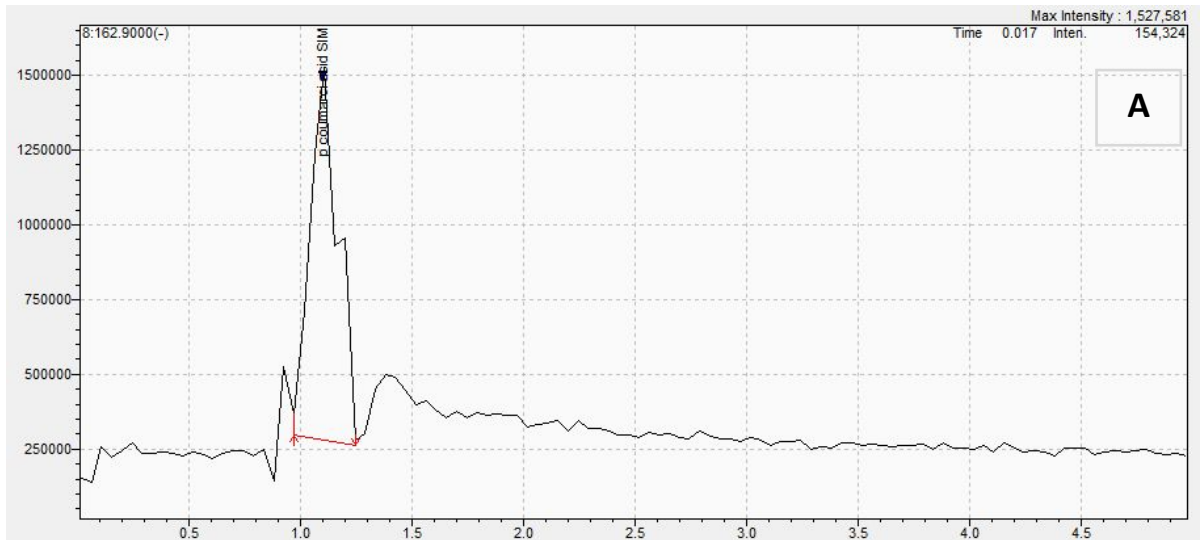
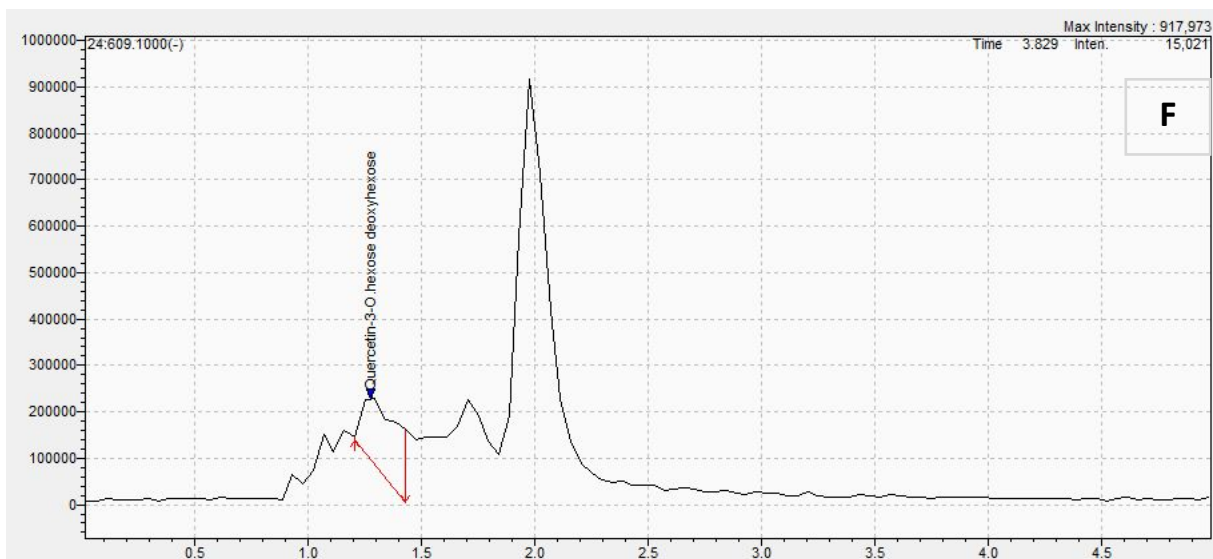
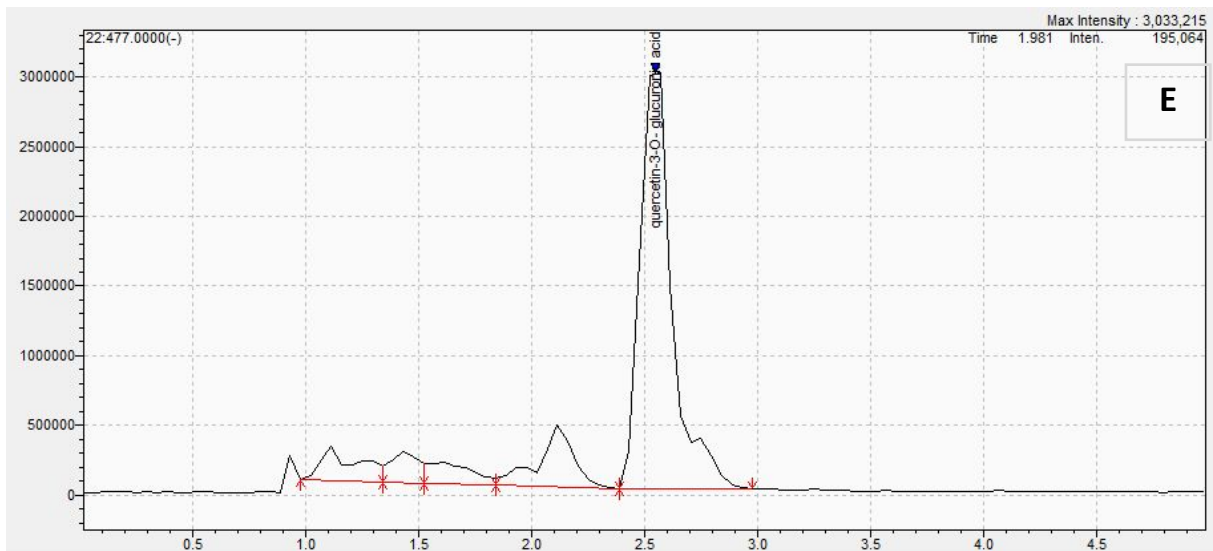
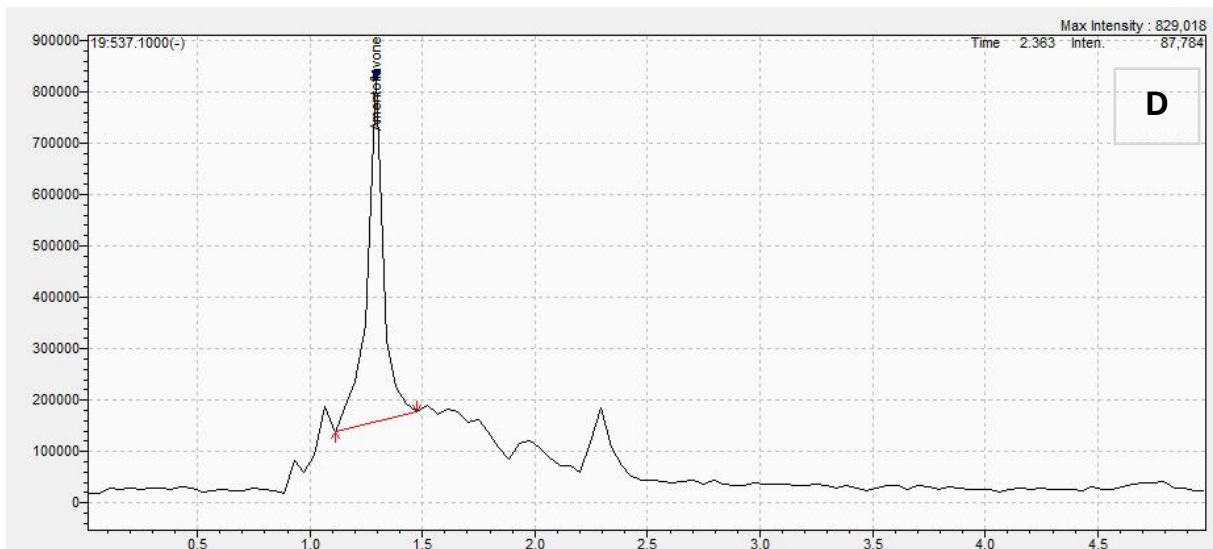


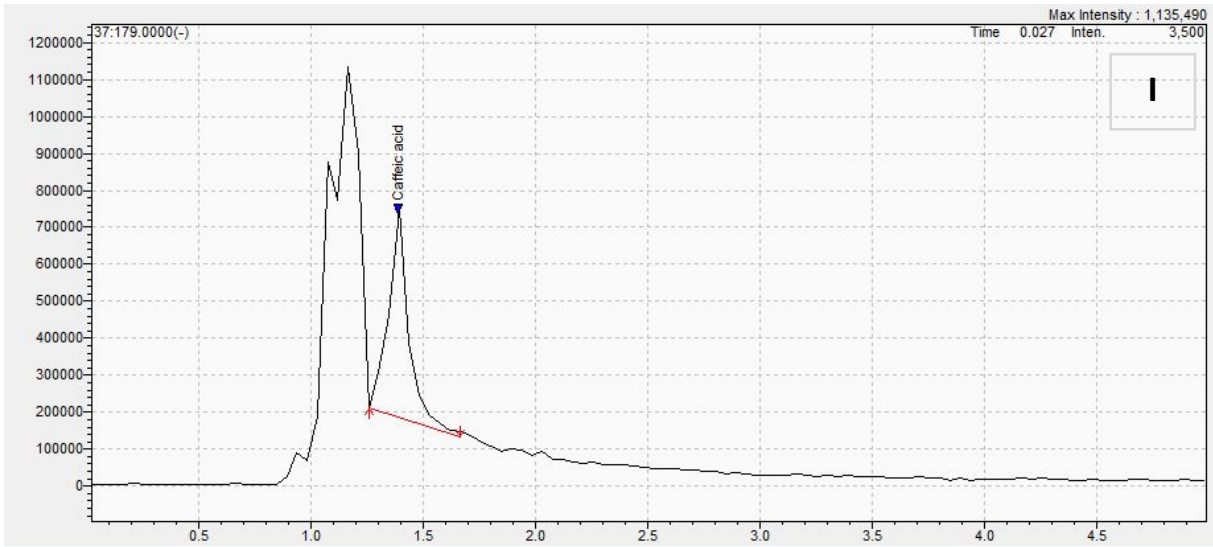
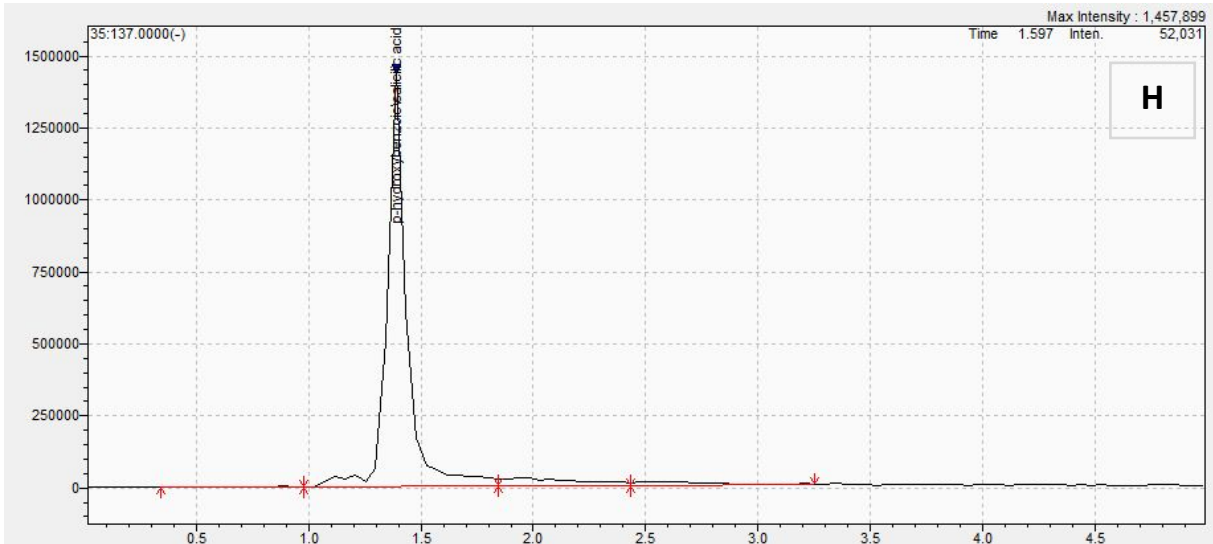
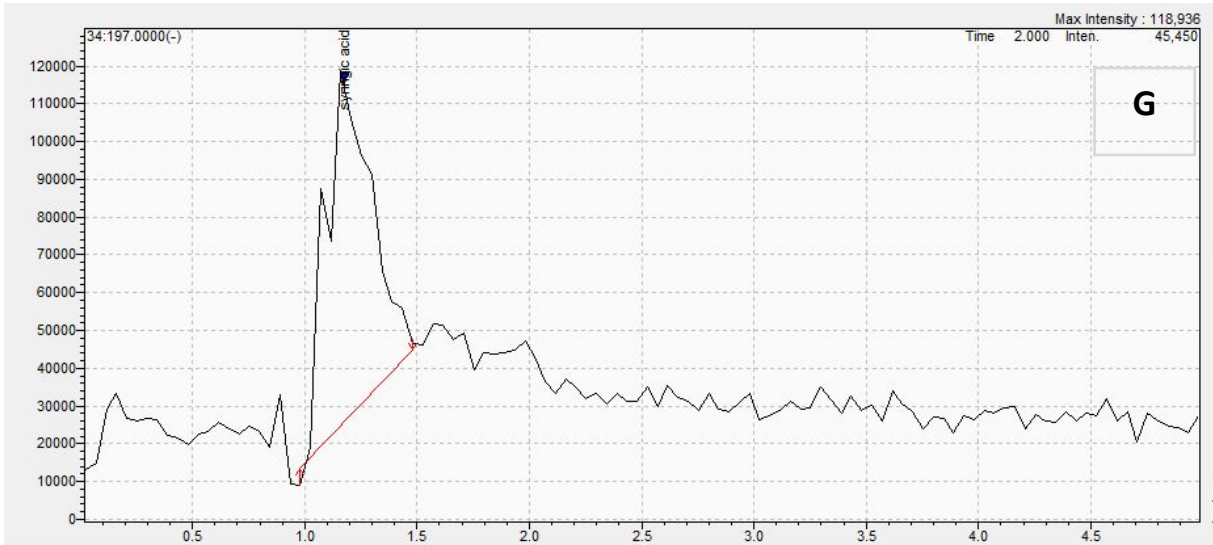
Phytochemical, Antioxidant Activity and Toxicity of Wild Medicinal Plant of *Melilotus Albus* Extracts, *In-vitro* and *In-Silico* Approaches

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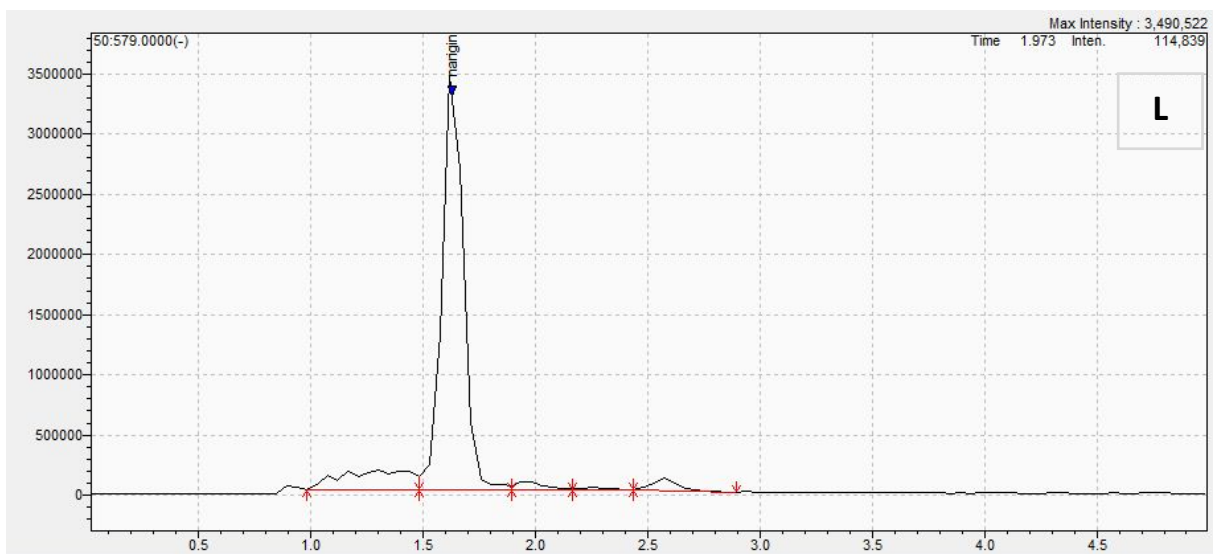
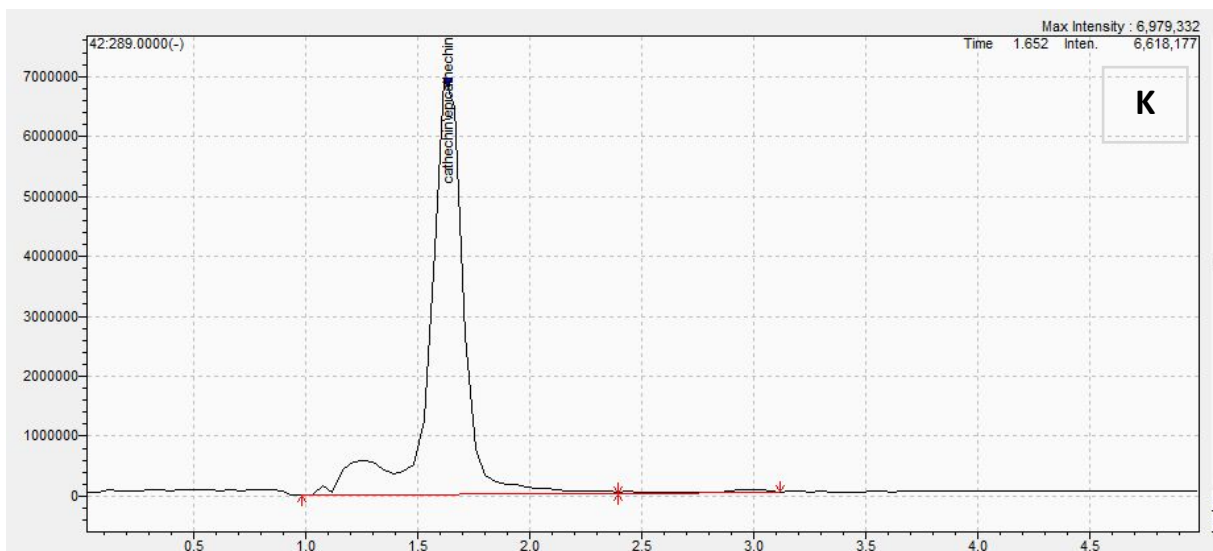
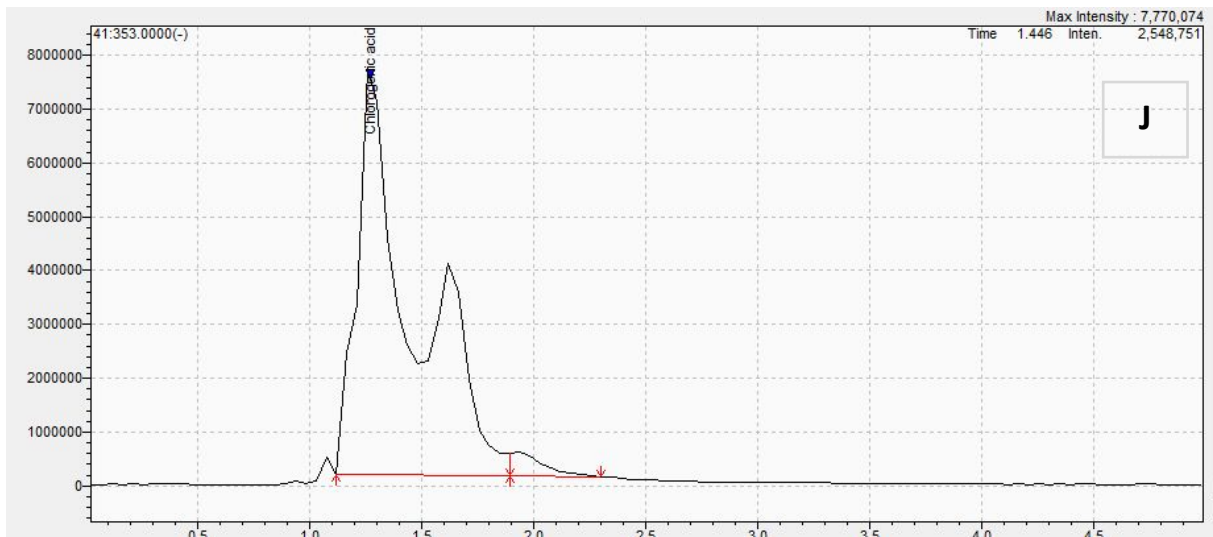


Figure S1: LC-MS/MS analysis graphs of the *M. albus* extract. A. p-coumaric acid; B. trans ferulic acid; C. Apigenin; D. Amentoflavone; E. quercetin-3-O- glucuronic acid; F. Quercetin-

3-O. hexose deoxyhexose; G. syringic acid; H. p-hydroxybenzoic\salicylic acid; I. Caffeic acid; J. Chlorogenic acid; K. catechin\epicatechin; L. Narigin.

Table S1: The prediction of physicochemical properties of twelve chemical compounds based on the five rules of Lipinski.

Compounds Numbers	Physico-chemical properties						Lipinski rules
	Molecular weight (g/mol)	Molar Refractive Index	Log (Ethanol/wa ter)	P Hydrogen Bonds Acceptors	Hydrogen Donors	Bonds	Categorical (Yes/No)
Rule	≤ 500	$40 \leq MR \leq 130$	< 5	≤ 10	< 5		
C1	164.16	45.13	0.95	3	2		Yes
C2	194.18	51.63	1.62	4	2		Yes
C3	270.24	73.99	1.89	5	3		Yes
C4	<u>538.46</u>	<u>146.97</u>	3.06	10	<u>6</u>		<u>No</u>
C5	478.36	111.59	0.50	<u>13</u>	<u>8</u>		<u>No</u>
C6	<u>594.52</u>	<u>140.22</u>	2.60	<u>15</u>	<u>9</u>		<u>No</u>
C7	198.17	48.41	1.54	5	2		Yes
C8	138.12	35.42	1.13	3	2		Yes
C9	180.16	47.16	0.97	4	3		Yes
C10	354.31	83.50	0.87	9	6		Yes
C11	290.27	74.33	1.47	6	5		Yes
C12	<u>580.53</u>	<u>134.91</u>	2.07	<u>14</u>	<u>8</u>		<u>No</u>

Table S2: The prediction of ADMET in-silico pharmacokinetic properties of twelve chemical compounds.

Compound Numbers	Absorption		Distribution		Metabolism						Excretion	
	Intestinal Absorption (human)	BBB permeability	CNS permeability	Substrate			Inhibitor			Total Clearance	AMES toxicity	
				Cytochromes								
				2D6	3A4	1A2	2C19	2C9	2D6			3A4
Numeric Absorbed)	(% (Log BB)	Numeric (Log PS)	Categorical (Yes/No)						Numeric (Log ml/min/kg)			
C1	91.673	-0.239	-2.413	No	No	No	No	No	No	No	0.696	No
C2	95.598	-0.25	-2.569	No	No	No	No	No	No	No	0.641	No
C3	91.622	-0.968	-2.176	No	No	Yes	Yes	Yes	No	Yes	0.616	No
C4	83.84	-2.063	-3.599	No	No	No	No	No	No	No	0.807	No
C5	28.49	-2.241	-5.584	No	No	No	No	No	No	No	0.9	<u>Yes</u>
C6	40.45	-2.13	-5.594	No	No	No	No	No	No	No	-0.151	<u>Yes</u>
C7	82.412	0.067	-2.963	No	No	No	No	No	No	No	0.663	No
C8	77.71	-0.313	-2.909	No	No	No	No	No	No	No	0.655	No
C9	59.008	-0.816	-3.361	No	No	No	No	No	No	No	0.558	<u>Yes</u>
C10	17.157	-1.443	-4.034	No	No	No	No	No	No	No	0.373	No
C11	72.519	-1.066	-3.395	No	No	No	No	No	No	No	0.266	<u>Yes</u>
C12	22.117	-1.791	-5.058	No	No	No	No	No	No	No	0.496	<u>Yes</u>

