

LC-ESI-MS/MS Analysis of *Echium asperrimum* from the Algerian Aurès Region: Antioxidant, Antimicrobial, Cholinesterase Inhibitory, and Antiproliferative Activities

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Table S1. LC-ESI-MS/MS parameters and fragmentation data of phenolic compounds identified in *Echium asperrimum* extracts.

Compound Name	Precursor Ion	Product Ion	Dwell	Frag (V)	CE (V)	Polarity
Isoquercitrin	464.9	302.8	9	95	8	Positive
Polydatin	391	229	9	80	8	Positive
Epigallocatechin	307	139	9	99	8	Positive
Catechin	291	165	9	80	12	Positive
Catechin	291	139	9	80	12	Positive
Catechin	291	123	9	80	12	Positive
Sinapic acid	224.9	206.9	9	90	3	Positive
Sinapic acid	224.9	174.8	9	90	3	Positive
Syringic acid	199	154.9	9	85	6	Positive
Syringic acid	199	140.2	9	85	6	Positive
<i>trans</i> -Ferulic acid	195.1	176.9	9	75	10	Positive
<i>trans</i> -Ferulic acid	195.1	144.7	9	75	10	Positive

Vanillin	152.9	124.9	9	65	13	Positive
Vanillin	152.9	93.1	9	65	13	Positive
Vanillin	152.9	65.2	9	65	13	Positive
Rutin	609.1	300.2	9	185	40	Negative
Chlorogenic acid	353	191	9	110	12	Negative
Taxifolin	303	284.8	9	144	6	Negative
Taxifolin	303	124.7	9	144	6	Negative
Catechin	288.9	245.1	9	140	12	Negative
<i>trans</i> -Ferulic acid	193.1	133.9	9	95	14	Negative
Caffeic Acid	178.9	135	9	80	16	Negative
Gallic acid	168.9	124.9	9	100	12	Negative
Vanillic acid	167.1	152	9	96	12	Negative
Vanillic acid	167.1	123.1	9	96	12	Negative
Vanillic acid	167.1	107.7	9	96	12	Negative
<i>p</i> -coumaric acid	163.1	119.2	9	85	12	Negative
Gentisic acid	152.8	108.9	9	100	13	Negative
Gentisic acid	152.8	108	9	100	13	Negative
Hydroxybenzaldehyde	121	92	9	110	24	Negative
Baicalin	447	270.9	38	130	16	Positive
Baicalin	447	112.5	38	130	16	Positive
Protocatechuic acid	154.9	136.4	38	118	11	Positive
Protocatechuic acid	154.9	111	38	118	11	Positive
Protocatechuic acid	154.9	93.1	38	118	11	Positive
Protocatehuic ethyl ester	181	152.9	38	110	20	Negative
Protocatehuic ethyl ester	181	107.9	38	110	20	Negative
<i>o</i> -Coumaric acid	162.8	119	38	66	13	Negative
Protocatechuic acid	152.9	108.9	38	150	14	Negative
Salicylic Acid	137	93.1	38	85	18	Negative
Morin	302.9	136.8	18	145	32	Positive
Morin	302.8	153	18	145	30	Positive
Quercetin	302.8	152.9	18	125	34	Positive
Quercetin	302.8	136.9	18	125	34	Positive
Kaempferol	287	212.9	18	120	34	Positive
Kaempferol	287	164.7	18	120	34	Positive
Kaempferol	287	152.7	18	120	34	Positive
Kaempferol	287	120.9	18	120	34	Positive
7-Hydroxyflavone	238.9	137.1	18	170	30	Positive
Resveratrol	229	135	18	105	14	Positive
<i>trans</i> -cinnamic acid	149.1	131.1	18	90	6	Positive
<i>trans</i> -cinnamic acid	149	131.1	18	75	6	Positive
<i>trans</i> -cinnamic acid	149	103	18	75	10	Positive
Quercetin	300.8	179	18	130	20	Negative

Quercetin	300.7	150.9	18	130	22	Negative
Naringenin	270.9	150.8	18	130	26	Negative
Naringenin	270.9	119.1	18	115	24	Negative
Resveratrol	227	184.9	18	130	22	Negative
Resveratrol	227	143	18	130	22	Negative
<i>trans</i> -cinnamic acid	147.1	103.1	18	70	8	Negative
Diosgenin	415.3	271.1	48	110	16	Positive
Diosgenin	415.3	253	48	110	16	Positive
Luteolin	285	133.1	48	132	36	Positive
Biochanin A	284.9	151.9	48	170	28	Positive
Chrysin	255	102.9	48	155	30	Positive
Chrysin	254.9	153	48	160	32	Positive
5-Hydroxyflavone	238.9	165	48	170	36	Positive
Biochanin A	283	267.9	48	110	19	Negative

Compound identification was based on accurate mass measurements and MS/MS fragmentation patterns and should be considered putative, as no compound isolation or structural elucidation was performed.