Supporting Information

Anticholinesterase Activity of Budmunchiamine Alkaloids Revealed by Comparative Chemical Profiling of Two *Albizia* spp., Molecular Docking and Dynamic Studies

Mai E. Hussein [1,*,†], Osama G. Mohamed [1,2,†], Ahlam M. El-Fishawy [1], Hesham I. El-Askary [1], Ahmed A. Hamed [3], Marwa M. Abdel-Aziz [4], Radwan Alnajjar [5,6,7], Amany Belal [8], Ahmed M. Naglah [9,10], Abdulrahman A. Almehizia [9], Ahmed A. Al-Karmalawy [11], Ashootosh Tripathi [2,12] and Amira S. El Senousy [1]

[1] Pharmacognosy Department, Faculty of Pharmacy, Cairo University, Kasr el Aini St., Cairo 11562, Egypt
[2] Natural Products Discovery Core, Life Sciences Institute, University of Michigan, Ann Arbor, MI 48109, USA
[3] Microbial Chemistry Department, National Research Centre, 33 El-Buhouth Street, Dokki, Giza 12622, Egypt
[4] Regional Center for Mycology and Biotechnology (RCMB), Al-Azhar University, Cairo 11651, Egypt
[5] Department of Chemistry, Faculty of Science, University of Benghazi, Benghazi, Libya
[6] PharmD, Faculty of Pharmacy, Libyan International Medical University, Benghazi, Libya
[7] Department of Chemistry, University of Cape Town, Rondebosch 7701, South Africa
[8] Medicinal Chemistry Department, Faculty of Pharmacy, Beni-Suef University, Beni-Suef 62514, Egypt
[9] Drug Exploration and Development Chair (DEDC), Department of Pharmaceutical Chemistry, College of Pharmacy, King Saud University, Riyadh 11451, Saudi Arabia
[10] Peptide Chemistry Department, National Research Centre, Dokki, Cairo 12622, Egypt
[11] Pharmaceutical Chemistry Department, Faculty of Pharmacy, Ahram Canadian University, 6th of October City, Giza 12566, Egypt
[12] Department of Medicinal Chemistry, College of Pharmacy, University of Michigan, Ann Arbor, MI 48109, USA
* Correspondence: mai.husein@pharma.cu.edu.eg
† These authors contributed equally to this work.

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Table S1: Identified metabolites in the negative ion mode of ethanolic extracts of *A. lucidior* and *A. procera* leaves using UHPLC-MS/MS

No.	R_t (min)	Name	Ion m/z ppm	Molecular Formula	MS/MS fragmentation product ions	Ref	Al	Ap
1	0.41	Dicaffeoylhexaric acid	533.1718	$C_{23}H_{33}O_{14}^-$	209.0653; 191.0561 85.0300	[1]	√	-
2	0.42	Quinic acid	191.0563	$C_7H_{11}O_6^-$	173.0447; 127.0396 93.0344; 85.0293	[2]	√	√
3	0.43	Xylonic acid	165.0403	$C_5H_9O_6^-$	147.0275; 135.0269 105.0185; 87.0084 75.0086	[2]	√	√
4	0.49	Gallic acid glucoside	331.0686	$C_{13}H_{15}O_{10}^-$	211.0237; 169.0147 151.0026; 125.0241	[1]	-	√
5	0.55	Gallic acid	169.0143	$C_7H_5O_5^-$	125.0258; 107.0153 97.0309; 79.0207	[3]	-	√
6	0.76	Protocatechuic acid	153.0190	$C_7H_5O_4^-$	109.0293	[4]	√	√
7	0.77	Vanillic acid-*O*-glucoside	329.0885	$C_{14}H_{17}O_9^-$	209.0452; 167.0345 125.0246; 123.0449	[1]	-	√
8	0.80	Catechol	109.0287	$C_6H_5O_2^-$	108.0217; 91.0191 81.0335; 66.0361	[5]	√	-
9	0.88	Gentisic acid-5-*O*-xyloside	285.0619	$C_{12}H_{13}O_8^-$	152.0114; 108.0216	[6]	√	-
10	0.91	Digalloyl-glucose	483.0779	$C_{20}H_{19}O_{14}^-$	313.0553; 271.0455 169.0137	[7]	-	√
11	0.99	Caffeic acid glucuronide	355.0685	$C_{15}H_{15}O_{10}^-$	209.0272;191.0545 161.0240; 85.0292	[2]	√	-
12	1.05	Methyl gallate	183.0301	$C_8H_7O_5^-$	168.0046; 124.0164	[3]	-	√
13	1.06	*p*-coumaric acid-4-*O*-glucoside	325.0936	$C_{15}H_{17}O_8^-$	163.0395; 119.0499	[8]	√	√
14	1.07	Aesculin	339.0731	$C_{15}H_{15}O_9^-$	177.0195	[8]	√	-
15	1.22	Ferulic acid glucoside	355.1033	$C_{16}H_{19}O_9^-$	309.0453; 193.0499 178.0266; 134.0374	[9]	-	√
16	1.34	Shikimic acid	173.0452	$C_7H_9O_5^-$	136.9332; 111.0452 93.0360; 85.0303 83.0133	[10]	√	√
17	1.36	Caffeoylquinic acid	353.0880	$C_{16}H_{17}O_9^-$	191.0556; 173.0445 135.0446; 85.0297	[8]	√	√
18	1.36	Umbelliferone	161.0241	$C_9H_5O_3^-$	133.0288	[11]	√	-
19	1.37	Caffeic acid	179.0352	$C_9H_7O_4^-$	135.0459; 89.0028	[1]	√	√
20	1.46	Esculetin	177.0193	$C_9H_5O_4^-$	149.0253; 133.0296 105.0347; 89.0399	[3]	√	√

No.	R_t (min)	Name	Ion m/z ppm	Molecular Formula	MS/MS fragmentation product ions	Ref	Al	Ap
21	1.92	Rosmarinic acid-*O*-glucoside	521.2047	$C_{24}H_{25}O_{13}^-$	359.1511; 344.1271	[12]	-	√
22	2.03	Syringic acid	197.0457	$C_9H_9O_5^-$	169.0142; 124.0168	[7]	-	√
23	2.09	Feruloyl quinic acid	367.1042	$C_{17}H_{19}O_9^-$	193.0521;173.0454	[13]	-	√
24	2.10	*p*-coumaroyl quinic acid	337.0934	$C_{16}H_{17}O_8^-$	191.0556; 163.0394 119.0491; 93.0342	[12]	√	√
25	2.35	*p*-coumaric acid	163.0401	$C_9H_7O_3^-$	119.0510; 93.0350 91.0568	[1]	√	√
26	2.45	Myricetin-3-*O*-rutinoside	625.1415	$C_{27}H_{29}O_{17}^-$	317.0293; 316.0234 287.0917; 271.0252 178.9991; 151.0043	[14]	-	√
27	2.45	Coumaroyl-*O*-galloyl glucose	477.1040	$C_{22}H_{21}O_{12}^-$	313.0558; 169.0151	[7]	-	√
28	2.48	Hexosylrutin	771.1992	$C_{33}H_{39}O_{21}^-$	609.1453; 463.0886 301.0346; 300.0273	[9]	-	√
29	2.49	Methyl caffeoyl quinate	367.1033	$C_{17}H_{19}O_9^-$	191.0564; 179.0349 161.0249; 135.0452	[13]	√	√
30	2.51	Quercetin rhamnosyl-rutinoside	755.2053	$C_{33}H_{39}O_{20}^-$	609.1423; 301.0342 300.0280	[9]	√	-
31	2.51	Myricetin-3-*O*-glucoside	479.0837	$C_{21}H_{19}O_{13}^-$	317.0287; 316.0281 271.0235; 178.9972 151.0023	[1]	-	√
32	2.51	Myricetin-3-*O*-glucuronide	493.0630	$C_{21}H_{17}O_{14}^-$	317.0297; 299.0184 271.0262; 178.9974 151.0025	[15]	-	√
33	2.54	Naringenin-7-*O*-glucoside	433.1151	$C_{21}H_{21}O_{10}^-$	313.0707; 271.0618 193.0381; 119.0493	[10]	-	√
34	2.62	Myricetin-3-*O*-arabinoside	449.0760	$C_{20}H_{17}O_{12}^-$	317.0326; 316.0229 287.0182; 271.0238 178.9977	[14]	-	√
35	2.62	Kaempferol-rhamnosyl-galactoside-rhamnoside	739.2108	$C_{33}H_{39}O_{19}^-$	593.1507; 285.0403 284.0334; 255.0299	[9]	√	√
36	2.65	Quercetin-3-*O*-sambubioside	595.1318	$C_{26}H_{27}O_{16}^-$	301.0348; 300.0287 271.0252; 255.0304 178.9990; 151.0041	[16]	√	√
37	2.69	Kaempferol-3-(2G-xylosylrutinoside)	725.1944	$C_{32}H_{37}O_{19}^-$	575.1360; 285.0391 284.0327; 255.0304 227.0334; 151.0034	[9]	√	√
38	2.69	Rutin	609.1468	$C_{27}H_{29}O_{16}^-$	445.0696; 343.0456 301.0351; 300.0275 271.0242; 255.0297 178.9975; 151.0029	[2]	√	√

No.	R_t (min)	Name	Ion m/z ppm	Molecular Formula	MS/MS fragmentation product ions	Ref	Al	Ap
39	2.71	Quercetin-*O*-galloyl-glucoside	615.0990	$C_{28}H_{23}O_{16}^-$	463.0890; 313.0557 301.0354; 300.0281 271.0246; 255.0286 169.0143	[2]	√	-
40	2.76	Myricetin-3-*O*-rhamnoside (myricitrin)	463.0894	$C_{21}H_{19}O_{12}^-$	317.0298; 316.0232 287.0202; 271.0248 178.9984	[3]	√	√
41	2.79	Quercetin-3-*O*-glucuronide	477.0684	$C_{21}H_{17}O_{13}^-$	301.0354; 255.0295 178.9984; 151.0033	[15]	-	√
42	2.80	Kaempferol-3-*O*-rutinoside	593.1522	$C_{27}H_{29}O_{15}^-$	285.0403; 284.0323 255.0299; 227.0345 151.0033	[2]	√	√
43	2.85	Quercetin pentose deoxy-hexose	579.1375	$C_{26}H_{27}O_{15}^-$	447.0832; 301.0326 300.0288; 255.0314	[9]	√	-
44	2.85	*p*-Hydroxybenzoic acid	137.0245	$C_7H_5O_3^-$	93.0354; 65.0397	[13]	√	-
45	2.85	Azelaic acid	187.0975	$C_9H_{15}O_4^-$	169.0863; 125.0980 123.0825; 97.0669	[17]	√	-
46	2.93	Kaempferol-3-*O*-sambubioside	579.2086	$C_{26}H_{27}O_{15}^-$	417.1552; 285.0408	[18]	√	-
47	2.94	Quercetin-3-*O*-arabinoside (Avicularin)	433.0789	$C_{20}H_{17}O_{11}^-$	301.0344; 300.0275 271.0241; 255.0301 151.0043	[9]	√	√
48	2.96	Myrciacitrin	477.1030	$C_{23}H_{25}O_{11}^-$	317.0247; 316.0231 287.0188; 178.9986 151.0023	[9]	-	√
49	2.98	Kaempferol-3-*O*-glucuronide	461.0736	$C_{21}H_{17}O_{12}^-$	285.0406; 257.0453 229.0506	[14]	-	√
50	3.00	Quercetin 3-*O*-rhamnoside (Quercitrin)	447.0950	$C_{21}H_{19}O_{11}^-$	301.0356; 300.0281 271.0249; 255.0301 178.9987; 151.0043	[3]	√	√
51	3.06	Ferulic acid	193.0508	$C_{10}H_9O_4^-$	161.0247; 134.0374 133.0298	[1]	√	√
52	3.10	Phloridzin	435.1304	$C_{21}H_{23}O_{10}^-$	273.0775; 167.0353	[3]	-	√
53	3.18	Quercetin benzoyl-glucoside	583.4803	$C_{28}H_{23}O_{14}^-$	463.0891; 301.0322 300.0269; 271.0229 255.0282; 152.0106	[7]	√	-

No.	R_t (min)	Name	Ion m/z ppm	Molecular Formula	MS/MS fragmentation product ions	Ref	Al	Ap
54	3.18	Kaempferol-3-*O*-rhamnoside	431.0988	$C_{21}H_{19}O_{10}^-$	285.0416; 284.0340 255.0310; 227.0360 151.0036	[2]	√	√
55	3.19	Myricetin	317.0309	$C_{15}H_9O_8^-$	178.9998; 151.0448 137.0250	[9]	-	√
56	3.21	Quercetin-3-*O*-glucosyl-6″-acetate	505.1002	$C_{23}H_{21}O_{13}^-$	329.0664; 301.0343 300.0280; 271.0241 255.0290; 151.0023	[10]	-	√
57	3.21	Myricetin-*O*-(*O*-galloyl)-3-rhamnoside	615.1002	$C_{28}H_{23}O_{16}^-$	463.0895; 317.0315 178.9998;169.0148 151.0047	[3]	-	√
58	3.21	Quercetin-di-*O*-glucoside	625.1202	$C_{27}H_{29}O_{17}^-$	463.0891; 301.0359 300.0284; 255.0315	[1]	√	-
59	3.21	Chrysoeriol-*O*-glucoside	461.1084	$C_{22}H_{21}O_{11}^-$	299.0200	[19]	-	√
60	3.41	Quercetin galloyl rhamnoside	599.1051	$C_{28}H_{23}O_{15}^-$	447.0920; 383.1042 301.0368; 273.0402 178.9991; 151.0041	[2]	-	√
61	3.41	Kaempferol acetyl glycoside	489.1044	$C_{23}H_{21}O_{12}^-$	285.0409; 284.0335 255.0306; 227.0359	[1]	-	√
62	3.43	Quercetin coumaroyl glucoside	609.1263	$C_{30}H_{25}O_{14}^-$	463.0872; 301.0352 300.0276; 271.0238 178.9977; 151.0031	[1]	√	-
63	3.46	Quercetin feruloyl glucoside	639.1359	$C_{31}H_{27}O_{15}^-$	463.0881; 301.0350 300.0276; 271.0248 255.0291; 151.0025	[7]	√	-
64	3.48	Ethyl caffeate	207.0665	$C_{11}H_{11}O_4^-$	179.0352; 161.0250 135.0453; 134.0376	[13]	√	√
65	3.52	*p*-methoxycinnamic acid	177.0563	$C_{10}H_9O_3^-$	162.0317; 145.0296 133.0061;118.0427	[20]	-	√
66	3.55	Quercetin	301.0345	$C_{15}H_9O_7^-$	178.9993; 151.0045 121.0296;107.0147	[1]	√	√
67	3.55	Kaempferol	285.0396	$C_{15}H_9O_6^-$	243.0301; 217.0505 199.0403; 175.0397	[1]	√	√
68	3.60	Trihydroxyoctadienoic acid	327.2182	$C_{18}H_{31}O_5^-$	291.1969; 229.1449 211.1349; 171.1033	[2]	√	√
69	3.77	Trihydroxyoctadecenoic acid	329.2336	$C_{18}H_{33}O_5^-$	229.1452; 211.1348 171.1031	[2]	√	√
70	3.85	Naringenin	271.0623	$C_{15}H_{11}O_5^-$	151.0039; 119.0509 65.0045	[1]	-	√
71	3.85	Dihydroxy palmitic acid	287.2233	$C_{16}H_{31}O_4^-$	269.2144; 241.2189 223.2067	[2]	√	√

No.	R_t (min)	Name	Ion m/z ppm	Molecular Formula	MS/MS fragmentation product ions	Ref	Al	Ap
72	4.42	Dihydroxyoctadecadienoic acid	311.2223	$C_{18}H_{31}O_4^-$	311.2208; 293.2096 275.2005; 223.1705	[19]	√	√
73	4.51	Epoxy-hydroxyoctadeca-dienoic acid	309.2073	$C_{18}H_{29}O_4^-$	291.1959; 273.1980 221.1541	[19]	√	√
74	4.56	Pinocembrin	255.0665	$C_{15}H_{11}O_4^-$	213.0556; 171.0443 151.0031; 107.0134 83.0136; 65.0037	[1]	-	√
75	4.58	Dihydroxyoctadecenoic acid	313.2386	$C_{18}H_{33}O_4^-$	295.2300; 277.2174 183.1392	[19]	-	√
76	4.98	Sphingolipid conjugate II	564.3315	$C_{27}H_{51}O_9NP^-$	279.2329	[19]	√	-
77	5.00	13-keto-octadeca-9,11-dienoic acid	293.2126	$C_{18}H_{29}O_3^-$	275.2027; 223.1346 195.1396; 179.1463	[5]	√	√
78	5.13	Hydroxyoctadecenoic acid	297.1535	$C_{18}H_{33}O_3^-$	279.9880; 183.0120	[19]	√	√
79	5.17	9-hydroxy-10,12-octadecadienoic acid	295.2276	$C_{18}H_{31}O_3^-$	277.2178; 195.1393 171.1029	[5]	√	√
80	5.20	Sphingolipid conjugate III	566.3478	$C_{27}H_{53}O_9NP^-$	281.2497	[19]	√	-
81	5.76	Hydroxy palmitic acid	271.2275	$C_{16}H_{31}O_3^-$	253.2167; 225.2220	[19]	√	√
82	5.93	Linolenic acid	277.2171	$C_{18}H_{29}O_2^-$	259.2068; 234.1868	[5]	√	√
83	5.96	Yohimbic acid	339.1999	$C_{20}H_{23}N_2O_3^-$	183.0117	[10]	√	√
84	6.15	Linoleic acid	279.2326	$C_{18}H_{31}O_2^-$	261.2199; 59.0138	[5]	√	√
85	6.32	Palmitic acid	255.2328	$C_{16}H_{31}O_2^-$	234.9956; 206.9872 166.9912	[19]	√	√
86	6.44	Oleic acid	281.2486	$C_{18}H_{33}O_2^-$	260.9945; 240.9874	[5]	√	√
87	6.74	Stearic acid	283.2632	$C_{18}H_{35}O_2^-$	242.9835;179.0094	[19]	√	√

√, found; -, not found; Al, *A. lucidior*; Ap, *A. procera*

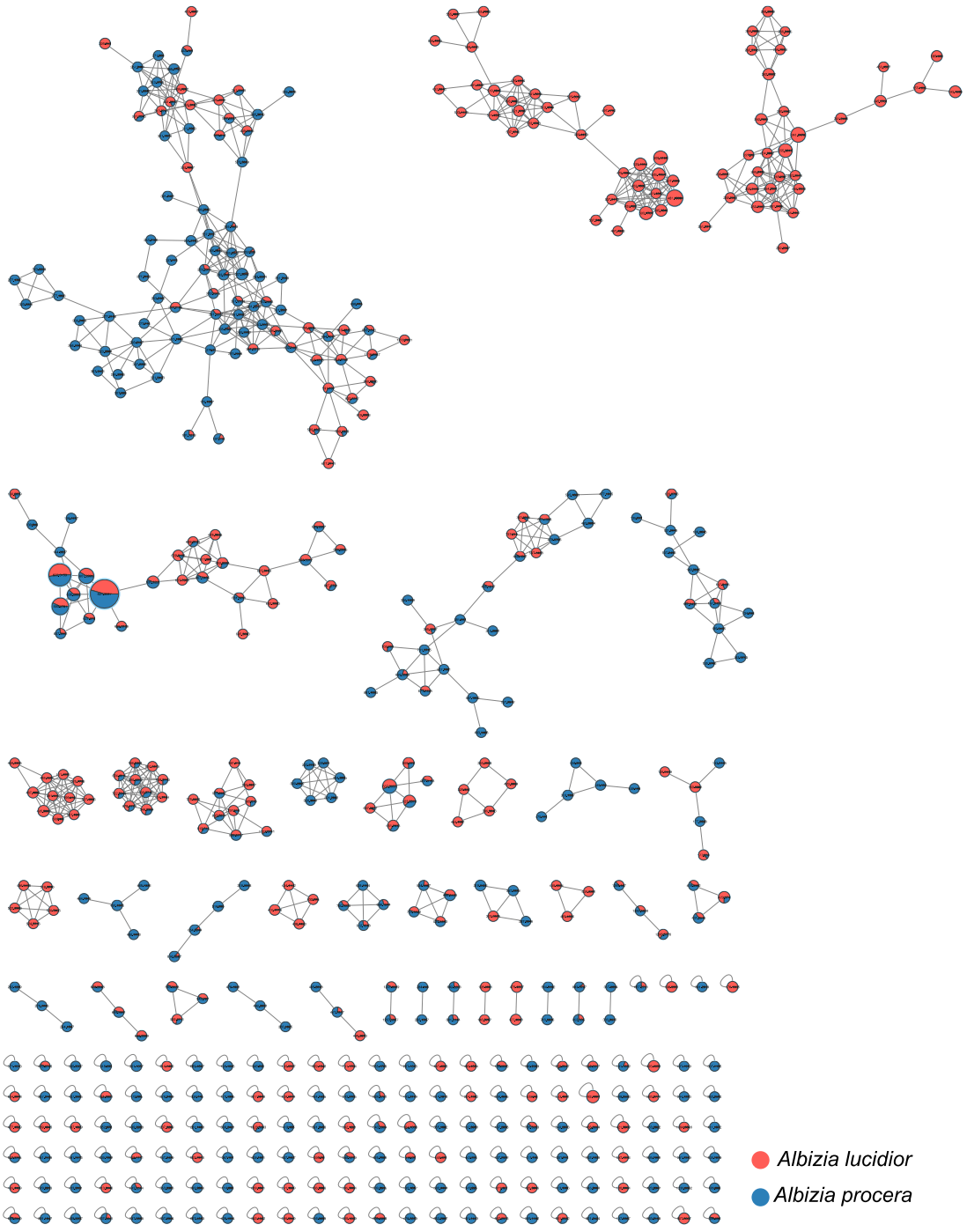

Figure S1. GNPS molecular network of two *Albizia* spp. ethanolic extracts in the positive ion mode. Each node is displayed as pie chart representing relative abundance of the metabolite with red and blue colors in the ethanolic extracts of *A. lucidior* and *A. procera*, respectively. The node label represents precursor mass (*m*/*z*). The node size represents the sum of precursor ion intensity.

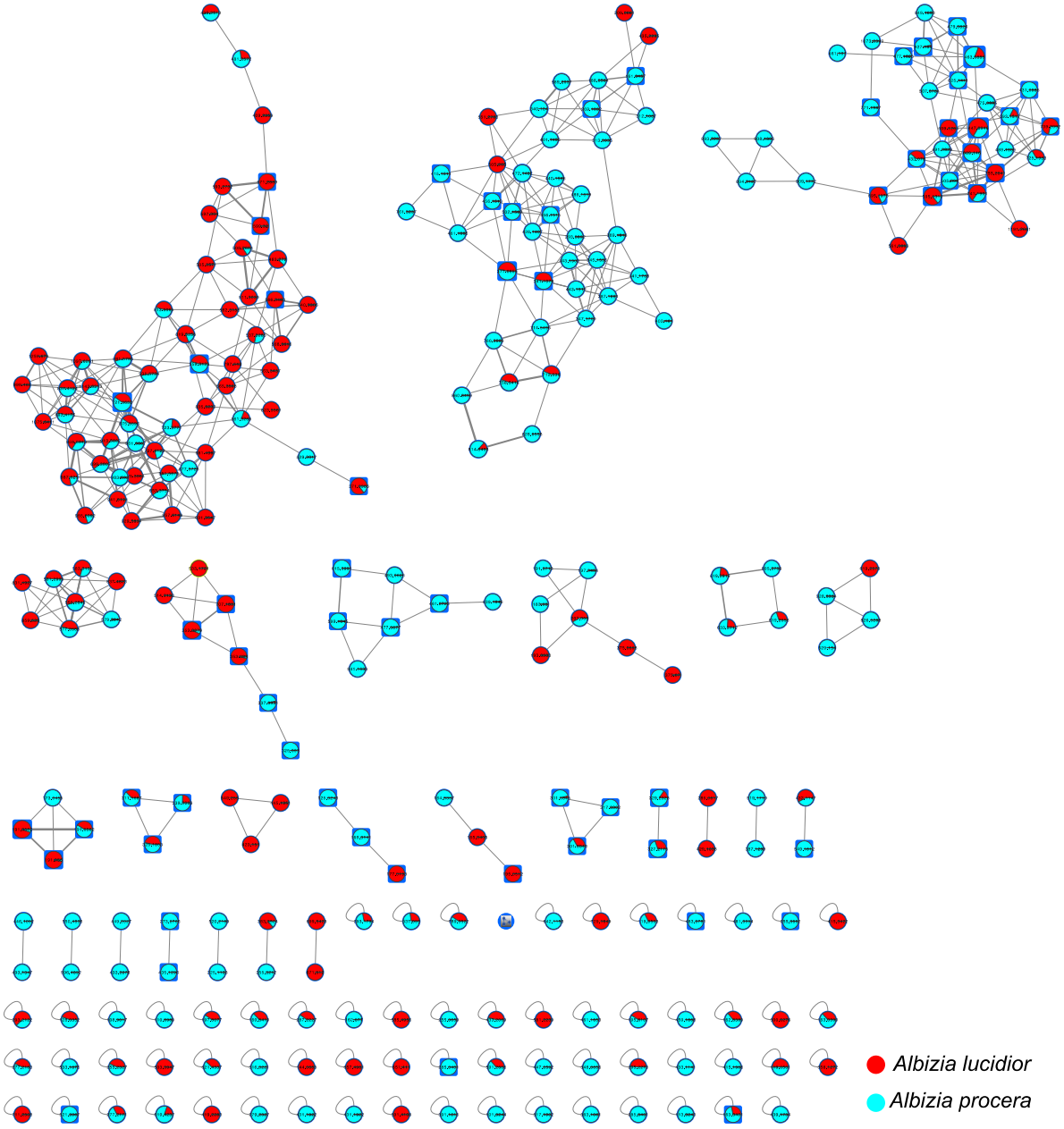

Figure S2. GNPS molecular network of two *Albizia* spp. ethanolic extracts in the negative ion mode. Each node is displayed as pie chart representing relative abundance of the metabolite with red and blue colors in the ethanolic extracts of *A. lucidior* and *A. procera*, respectively. The node label represents precursor mass (*m*/*z*). The node size represents the sum of precursor ion intensity.

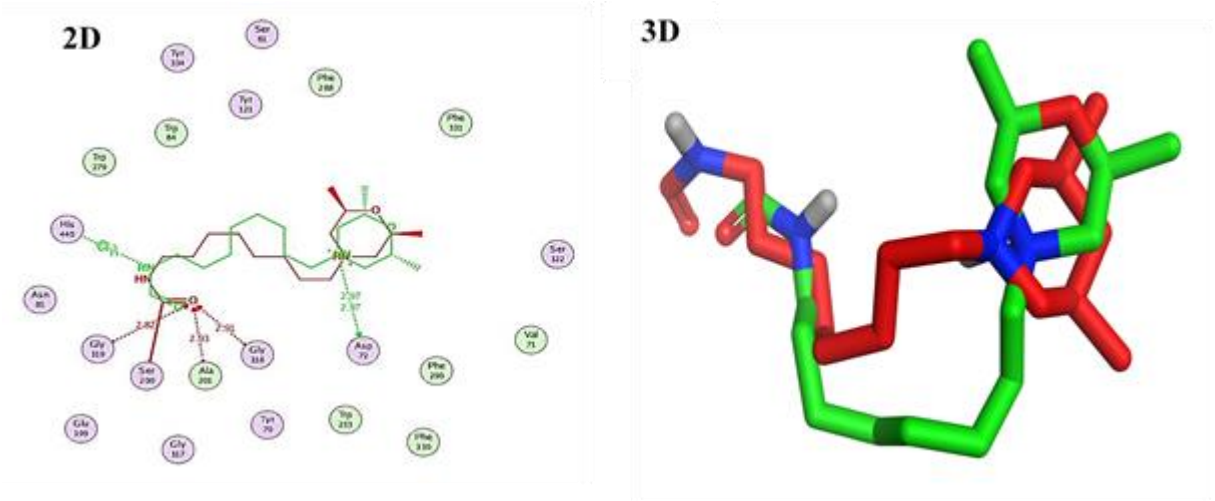

Figure S3. Superimposition of the redocked MF2 700 inhibitor (green) over its native one (red).

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