

Article

Metabolic Profiling by GC-MS, *In Vitro* Biological Potential, and *In Silico* Molecular Docking Studies of *Verbena officinalis*

Rabia Nisar ^{1,2}, Saeed Ahmad ¹, Kashif-ur-Rehman Khan ^{1,*}, Asmaa E. Sherif ^{3,4}, Fawaz Alasmari ⁵, Afaf F. Almuqati ⁶, Chitchamai Ovatlarnporn ⁷, Mohsin Abbas Khan ¹, Muhammad Umair ^{8,*}, Huma Rao ¹, Bilal Ahmad Ghalloo ¹, Umair Khurshid ¹, Rizwana Dilshad ¹, Khaled S. Nassar ⁹ and Sameh A. Korma ^{10,11}

¹ Department of Pharmaceutical Chemistry, Faculty of Pharmacy, The Islamia University of Bahawalpur, Bahawalpur 63100, Pakistan

² Department of Chemistry and Physics, College of Sciences and Mathematics, Arkansas State University, Jonesboro, AR 72404, USA

³ Department of Pharmacognosy, College of Pharmacy, Prince Sattam bin Abdul Aziz University, Alkharj 11942, Saudi Arabia

⁴ Department of Pharmacognosy, Faculty of Pharmacy, Mansoura University, Mansoura 35516, Egypt

⁵ Department of Pharmacology and Toxicology, College of Pharmacy, King Saud University, Riyadh 11451, Saudi Arabia

⁶ Department of Pharmaceutical Chemistry, College of Pharmacy, University of Hafr Al-Batin, Hafr Al-Batin 31991, Saudi Arabia

⁷ Department of Pharmaceutical Chemistry, Faculty of Pharmaceutical Sciences, Prince of Songkla University, Hat Yai 90110, Thailand

⁸ Department of Food Science and Engineering, College of Chemistry and Engineering, Shenzhen University, Shenzhen 518060, China

⁹ Department of Food, Dairy Science and Technology, Faculty of Agriculture, Damanhour University, Damanhour 22516, Egypt

¹⁰ Department of Food Science, Faculty of Agriculture, Zagazig University, Zagazig 44519, Egypt

¹¹ School of Food Science and Engineering, South China University of Technology, 510641 Guangzhou, China

* Correspondence: kashifur.rahman@iub.edu.pk (K.-u.-R.K.); umair_uaf@hotmail.com (M.U.); Tel.: +92-3366708638 (K.-u.-R.K.); +86-17712915202 (M.U.)

Table S1. GC-MS study of a methanolic extract (CRVO), *n*-hexane extract (NHVO), ethyl acetate extract (EAVO) and *n*-butanol extract (NBVO) of *Verbena officinalis*.

No.	RT (min)	Peak Area (%)	Name of Compound	Molecular Formula	Molecular Weight (g/mol)
The compounds identified in methanolic extract (CRVO) of <i>V. officinalis</i>					
1	6.125	0.43	Benzyl alcohol	C ₇ H ₈ O	108
2	6.839	1.07	Benzoic acid, methyl ester	C ₈ H ₈ O ₂	136
3	7.526	0.47	3-Octyne, 7-methyl-	C ₉ H ₁₆	124
4	8.058	0.54	1,4:3,6-Dianhydro- α -d-glucopyranose	C ₆ H ₈ O ₄	144
5	8.685	0.36	3,5-Heptadienal, 2-ethylidene-6-methyl-	C ₁₀ H ₁₄ O	150
6	8.834	0.36	Phenol, 2-methyl-5-(1-methylethyl)-	C ₁₀ H ₁₄ O	150
7	8.920	0.46	Indole	C ₈ H ₇ N	117
8	10.881	0.59	Undecanoic acid, 10-methyl-, methyl ester	C ₁₃ H ₂₆ O ₂	214
9	11.111	0.64	2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (R)-	C ₁₁ H ₁₆ O ₂	180
10	11.825	0.24	Megastigmatrienone	C ₁₃ H ₁₈ O	190
11	12.483	2.57	Methyl tetradecanoate	C ₁₅ H ₃₀ O ₂	242

12	12.576	0.34	2,6-Diisopropyl-naphthalene	C ₁₆ H ₂₀	212
13	12.643	0.26	1,4-Di-iso-propyl-naphthalene	C ₁₆ H ₂₀	212
14	12.795	0.22	Caparratriene	C ₁₅ H ₂₆	206
15	13.056	0.57	Methyl 13-methyl tetradecanoate	C ₁₆ H ₃₂ O ₂	256
16	13.180	1.59	6-Octadecenoic acid, methyl ester, (Z)-	C ₁₉ H ₃₆ O ₂	296
17	13.275	0.59	9-Octadecenoic acid (Z)-, methyl ester	C ₁₉ H ₃₆ O ₂	296
18	13.360	0.26	11,13-Dimethyl-12-tetradecen-1-ol acetate	C ₁₈ H ₃₄ O ₂	282
19	13.590	0.40	Neophytadiene	C ₂₀ H ₃₈	278
20	13.669	0.90	2-Pentadecanone, 6,10,14-trimethyl	C ₁₈ H ₃₆ O	268
21	13.869	0.26	8,10-Dodecadien-1-ol, (E,E)-	C ₁₂ H ₂₂ O	182
22	14.164	0.36	Pentadecanoic acid, 14-methyl-, methyl ester	C ₁₇ H ₃₄ O ₂	270
23	14.391	0.54	Methyl hexadec-9-enoate	C ₁₇ H ₃₂ O ₂	268
24	14.653	39.93	Hexadecanoic acid, methyl ester	C ₁₇ H ₃₄ O ₂	270

The compounds identified in *n*-hexane extract (NHVO) of *V. officinalis*

No.	RT (min)	Peak Area (%)	Name of Compound	Molecular For- mula	Molecular Weight (g/mol)
1	8.017	0.71	Benzoic acid, methyl ester	C ₈ H ₈ O ₂	136
2	8.447	0.30	Octanoic acid, methyl ester	C ₉ H ₁₈ O ₂	158
3	9.466	0.09	Cyclododecane	C ₁₂ H ₂₄	168
4	9.505	0.09	2-Decanone	C ₁₀ H ₂₀ O	156
5	9.962	0.06	Nonanoic acid, methyl ester	C ₁₀ H ₂₀ O ₂	172
6	10.294	0.13	Hexanedioic acid, dimethyl ester	C ₈ H ₁₄ O ₄	174
7	10.941	0.52	Thymol	C ₁₀ H ₁₄ O	150
8	13.192	0.10	Dimethyl phthalate	C ₁₀ H ₁₀ O ₄	194
9	13.291	0.20	n-hexadecyl methyl imine	C ₁₇ H ₃₅ N	253
10	13.778	0.08	1,4-Benzenedicarboxylic acid, dimethyl ester	C ₁₀ H ₁₀ O ₄	194
11	13.844	1.90	2,4-Di-tert-butylphenol	C ₁₄ H ₂₂ O	206
12	13.975	0.56	Dodecanoic acid, methyl ester	C ₁₃ H ₂₆ O ₂	214
13	14.218	0.10	2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (R)-	C ₁₁ H ₁₆ O ₂	180
14	14.788	0.25	2-Tetradecene, (E)-	C ₁₄ H ₂₈	196
15	14.872	0.39	Hexadecane	C ₁₆ H ₃₄	226
16	15.166	0.14	Heptadecanoic acid, methyl ester	C ₁₈ H ₃₆ O ₂	284
17	15.329	0.24	Benzene, (1-butylheptyl)-	C ₁₇ H ₂₈	232
18	15.632	0.09	1-Nonadecene	C ₁₉ H ₃₈	266
19	15.724	1.31	αR-Turmerone	C ₁₅ H ₂₀ O	216
20	16.019	0.17	Heptadecane	C ₁₇ H ₃₆	240
21	16.108	0.22	Benzene, (1-methyldecyl)-	C ₁₇ H ₂₈	232
22	16.150	0.28	Curlone	C ₁₅ H ₂₂	218
23	16.308	0.56	Methyl tetradecanoate	C ₁₅ H ₃₀ O ₂	242

24	16.388	0.32	Benzene, (1-pentylheptyl)-	C ₁₈ H ₃₀	246
25	16.443	0.33	Benzene, (1-butyloctyl)-	C ₁₈ H ₃₀	246
26	16.579	0.28	Benzene, (1-propylnonyl)-	C ₁₈ H ₃₀	246
27	16.717	0.11	Cyclotetradecane	C ₁₄ H ₂₈	196
28	16.817	0.21	Benzene, (1-ethyldecyl)-	C ₁₈ H ₃₀	246
29	17.037	0.85	1-Octadecene	C ₁₈ H ₃₆	252
30	17.160	3.26	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	C ₁₉ H ₃₄ O ₂	294
31	17.318	12.07	7,10,13-Hexadecatrienoic acid, methyl ester	C ₁₇ H ₂₈ O ₂	264
32	17.442	1.47	6-Octadecenoic acid, methyl ester, (Z)-	C ₁₉ H ₃₆ O ₂	296
33	17.532	1.75	Neophytadiene	C ₂₀ H ₃₈	278
34	17.602	1.92	2-Pentadecanone, 6,10,14-trimethyl	C ₂₀ H ₃₈	278
35	17.791	0.51	Phytol	C ₂₀ H ₄₀ O	296
36	17.896	2.36	Heptadecanoic acid, 16-methyl-, methyl ester	C ₁₉ H ₃₈ O ₂	298
37	18.415	12.11	Hexadecanoic acid, methyl ester	C ₁₇ H ₃₄ O ₂	270
38	18.647	0.48	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester	C ₁₈ H ₂₈ O ₃	292
39	18.864	0.42	1-Chloroeicosane	C ₂₀ H ₄₁ Cl	316
40	19.077	1.19	5-Eicosene, (E)-	C ₂₀ H ₄₀	280
41	19.133	0.69	Eicosane	C ₂₀ H ₄₂	282
42	19.275	0.28	Henicos-1-ene	C ₂₁ H ₄₂	294
43	19.399	0.41	Methyl 10-methyl-hexadecanoate	C ₁₈ H ₃₆ O ₂	284
44	19.528	0.36	Cyclohexane, 1-(1,5-dimethylhexyl)-4-(4-methylpentyl)-	C ₂₀ H ₄₀	280
45	19.975	0.50	Nonacos-1-ene	C ₂₉ H ₅₈	406
46	20.064	4.92	11,14-Octadecadienoic acid, methyl ester	C ₁₉ H ₃₄ O ₂	294
47	20.124	17.87	9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)-	C ₁₉ H ₃₂ O ₂	292
48	20.342	2.14	Methyl stearate	C ₁₉ H ₃₈ O ₂	298
49	20.514	0.86	Pentadecafluorooctanoic acid, octadecyl ester	C ₂₆ H ₃₇ F ₁₅ O ₂	666
50	20.676	0.45	1-Docosene	C ₂₂ H ₄₄	308
51	20.939	1.63	Octacosyl acetate	C ₃₀ H ₆₀ O ₂	452
52	21.060	0.54	Pentadec-7-ene, 7-bromomethyl-	C ₁₆ H ₃₁ Br	302
53	21.485	0.41	3-Eicosene, (E)-	C ₂₀ H ₄₀	280
54	21.903	0.76	1-Hexacosene	C ₂₆ H ₅₂	364
55	22.033	0.56	9-Tricosene, (Z)-	C ₂₃ H ₄₆	322
56	22.701	0.94	Triacetyl acetate	C ₃₂ H ₆₄ O ₂	480

The compounds identified in ethyl acetate extract (EAVO) of *V. officinalis*

No.	RT (min)	Peak Area (%)	Name of Compound	Molecular Formula	Molecular Weight (g/mol)
1	5.372	3.07	2-Cyclopenten-1-one, 3-methyl-	C ₆ H ₈ O	96
2	6.027	4.44	1-Hexanol, 2-ethyl-	C ₈ H ₁₈ O	130

3	6.119	0.76	Benzyl alcohol	C ₇ H ₈ O	108
4	7.048	0.65	Levoglucosenone	C ₆ H ₆ O ₃	126
5	7.112	1.29	Octanoic acid, methyl ester	C ₉ H ₁₈ O ₂	158
6	7.835	0.79	Benzene, 1-methyl-3-(1-methylethyl)-	C ₁₀ H ₁₄	134
7	8.681	1.37	Bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-trimethyl-, (1S)-	C ₁₀ H ₁₄ O	150
8	8.919	0.85	Benzyl nitrile	C ₈ H ₇ N	117
9	9.120	1.06	Decanoic acid, methyl ester	C ₁₁ H ₂₂ O ₂	186
10	10.365	1.60	Dimethyl phthalate	C ₁₀ H ₁₀ O ₄	194
11	10.455	1.09	Cyclododecane	C ₁₂ H ₂₄	168
12	10.620	1.34	4-(2,6,6-Trimethylcyclohexa-1,3-dienyl)but-3-en-2-one	C ₁₃ H ₁₈ O	190
13	10.766	0.47	2-(2-Propenyl)-m-anisidine	C ₁₀ H ₁₃ NO	163
14	10.878	0.95	Dodecanoic acid, methyl ester	C ₁₃ H ₂₆ O ₂	214
15	11.300	0.61	3-Pyrazolidinone, 4,4-dimethyl-1-phenyl-	C ₁₁ H ₁₄ N ₂ O ₃	222
16	11.436	0.93	Megastigmatrienone	C ₁₃ H ₁₈ O	190
17	11.610	0.44	Naphthalene, decahydro-4a-methyl-1-methylene-7-(1-methylethylidene)-, (4aR-trans)-	C ₁₅ H ₂₄	204
18	11.821	0.49	1-N-Methyl-4-(trifluoromethyl)benzene-1,2-diamine	C ₈ H ₉ F ₃ N ₂	190
19	12.315	0.85	2,4,4-Trimethyl-3-(3-oxobutyl)cyclohex-2-enone	C ₁₃ H ₂₀ O ₂	208
20	12.478	2.21	Methyl tetradecanoate	C ₁₅ H ₃₀ O ₂	242
21	13.047	3.96	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	C ₁₉ H ₃₄ O ₂	294
22	13.202	15.38	9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)-	C ₁₉ H ₃₂ O ₂	292
23	13.665	0.83	2-Pentadecanone, 6,10,14-trimethyl	C ₁₈ H ₃₆ O	268
24	13.899	0.84	Heptadecanoic acid, 14-methyl-, methyl ester	C ₁₉ H ₃₈ O ₂	298
25	14.647	4.12	Hexadecanoic acid, methyl ester	C ₁₇ H ₃₄ O ₂	270

The compounds identified in *n*-butanol extract (NBVO) of *V. officinalis*

No.	RT (min)	Peak Area (%)	Name of Compound	Molecular Formula	Molecular Weight (g/mol)
1	6.028	3.85	2-Cyclopenten-1-one, 3-methyl-	C ₆ H ₈ O	96
2	6.108	1.28	3-Heptyne	C ₇ H ₁₂	96
3	6.146	1.75	2,4-Dimethylfuran	C ₆ H ₈ O	96
4	7.187	3.56	Phenol, 3-methyl-	C ₇ H ₈ O	108
5	8.473	5.95	Octanoic acid, methyl ester	C ₉ H ₁₈ O ₂	158
6	10.778	0.69	Hexadecane, 2,6,10,14-tetramethyl-	C ₂₀ H ₄₂	282
7	13.863	1.27	2,4-Di-tert-butylphenol	C ₁₄ H ₂₂ O	206
8	18.158	0.58	Eicosane	C ₂₀ H ₄₂	282
9	18.434	2.90	Hexadecanoic acid, methyl ester	C ₁₇ H ₃₄ O ₂	270

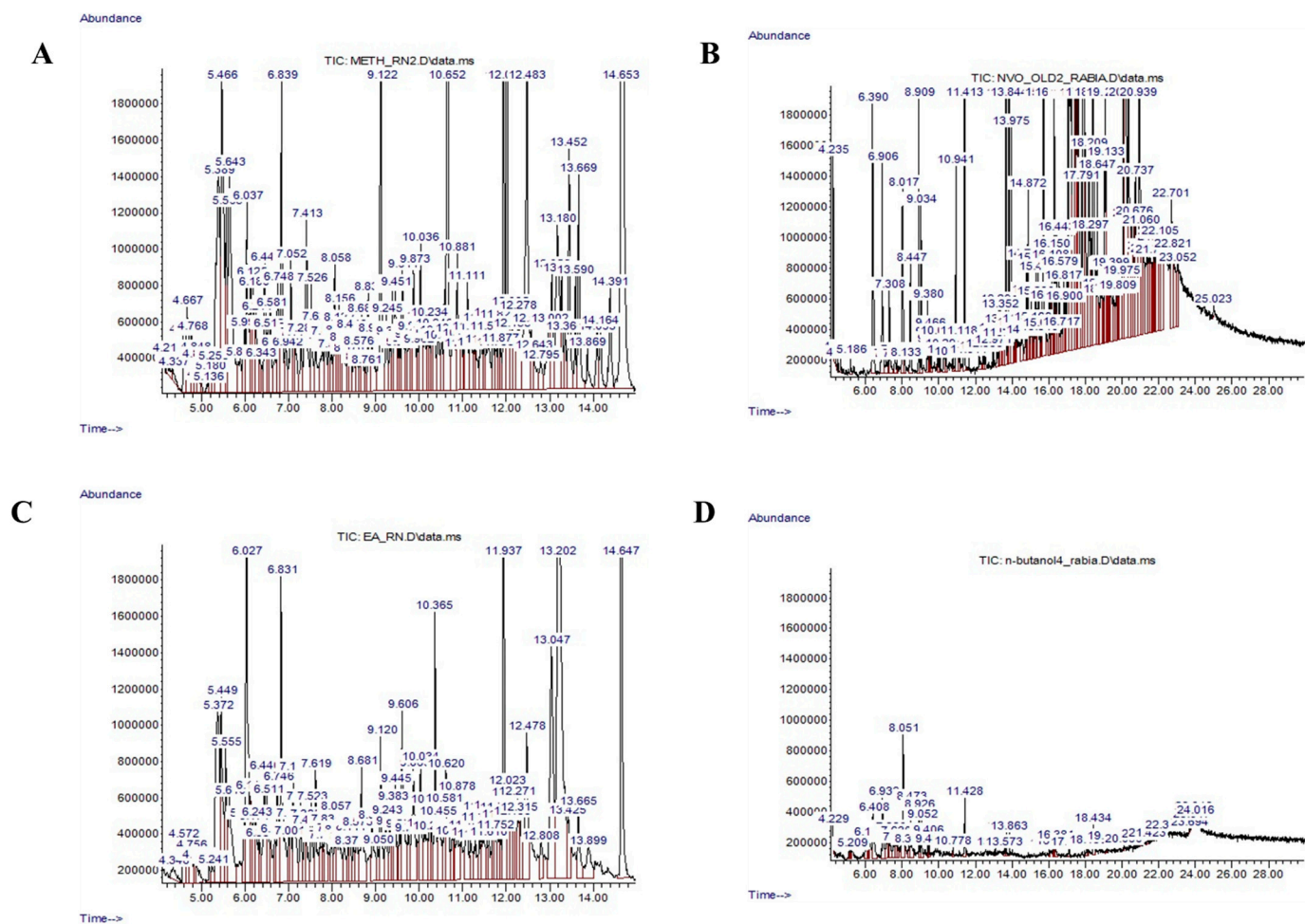


Figure S1. GC-MS chromatogram of (A) methanolic crude extract (CRVO), (B) *n*-hexane extract (NHVO), (C) ethyl acetate extract (EAVO) and (D) *n*-butanol extract (NBVO) of *Verbena officinalis*.