

## POTENTIAL BIOACTIVE PHYTOCONSTITUENTS IN *CARTHAMUS OXYCANTHA* M. BIEB. ROOT

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### ABSTRACT

*Carthamus oxycantha* M.Bieb. roots were extracted in methanol and GC-MS analysis showed presence of 130 natural compounds in the extract. The predominant compound was (R\*,S\*)-2,3-Dihydroxybutanoic acid, tris(trimethylsilyl) deriv. (73.28%) Followed by l-Isoleucine, N-trifluoro acetyl- (10.93%), 2,5-Dimethyl-4-hydroxy-3(2H)-furanone (0.66%), Pimelic acid, 2TMS derivative (0.59%), Silane, dimethyl(4-(2-phenylprop-2-yl)phenoxy) tridecyloxy- (0.13%), 9-Hexadecenoic acid, methyl ester, (Z)- (0.12%) and 2-Keto-l-gluconic acid, Penta (O-trimethylsilyl)- (0.11%). Peak areas of remaining 123 compounds were below 0.11%. Among the compounds identified in the present study, many are known to possess antibacterial, antifungal, antioxidant, anticancer, hemolytic, anti-androgenic, hypocholesterolemic and nematocidal activities.

**Keywords:** Bioactive compounds, *Carthamus oxycantha*, GC-MS analysis, Methanolic extract, Root,

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### INTRODUCTION

Asteraceae is a large dicotyledonous family of angiosperms that includes more than 32,913 accepted plant species distributed around the world (Kew, 2018). Mostly, it includes herbs or shrubs but rarely trees or climbers (Salem *et al.*, 2014). Many plants in this family possess allelopathy and show herbicidal, antimicrobial and other bioactivities (Bashir *et al.*, 2012; Banaras *et al.*, 2017). *Carthamus oxycantha* M. Bieb, a weed, belongs to this family is found in open places and in barren lands mostly in Afghanistan, Iran, Pakistan, and Tajikistan. It is a medium sized herb with orange yellow flowers (Ravikumar *et al.*, 2007). This plant has a wide range of medicinal applications and its flowers are used to treat cerebral thrombosis, rheumatism, male infertility and bronchitis (Zick *et al.*, 2008).

*C. oxycantha* is being used in pharmaceutical industry to prepare medicines for the treatment of ulcer, itching and as a pain relief agent especially in case of swelling trauma. The medicines obtained from other species of genus *Carthamus* are traditionally used for many health problems (Hassan *et al.*, 2010). The other member of genus such as *C. tinctorius* is used as anti-pyretic, purgative and for treatment of abdominal colic, asthma, bronchitis, jaundice, rheumatism (Bukhari 2013). *C. lanatus* is used to reduce stress and as anti-tumour agent. Some species of this genus have pharmacological properties like *C. oxycantha* for cholinomimetic, and *C. tinctorius* for antihypertensive, antioxidant, calcium antagonistic and anti-cancer activities. *C. lanatus* have been reported effective antibacterial, antifungal, analgesic, anti-inflammatory as well as a cytotoxic agent (Raza *et al.*, 2015).

The chemical analysis of different parts of *C. oxycantha* i.e. leave, stem, and flowers have uncovered the presence of several bioactive compounds belonging to tinctormine, quinochalcone, and phenols (Arslan and Tarikahya, 2018). Recently, important glycosides and flavonoids have been reported which have vital biological importance (Zhou *et al.*, 2008; Jiang *et al.*, 2010). The seeds of the *C. oxycantha* are also being used for liver diseases and as antioxidant (Ellahi *et al.*, 2014; Khalil and Alahmed, 2017). Keeping in view the importance of this weed species, the current study was conducted to find out the potential bioactive compounds present in roots of *C. oxycantha* through GC-MS.

### MATERIALS AND METHODS

During June 2017, plants of *C. oxycantha* were collected from Lahore Pakistan. Roots were separated, cut into small pieces, dried and crushed thoroughly. Five grams of crushed roots were soaked in 100 mL methanol for two weeks. The material was passed through filter paper and stored in a glass vial for performing GC-MS.

Analysis of GC-MS was done by following the Rafiq *et al.* (2017) procedure. Then, this extract was dried for a night in a speed Vac system as it was shifted into GC vials. Extract was passed through methoxylation with methoxyamine hydrochloride for the duration of 90 minutes at 30 °C. Afterwards, the sample was passed through the process of silylation with BSTFA/TCMS (sigma) at the temperature of 60 °C for 30 minutes. It was exposed to

gas chromatography-mass spectrometry (GC-MS) on an Agilent 7890C gas chromatograph in tandem with a 5975C MSD. Program of GC oven initiated at 80 °C and it was done for 1 minute, then temperature was increased 15 °C per minute. Identification and quantification was done by using AMDIS by the manually curated retention indexed GC-MS Library and additional identification was carried out by using the NIST17 and Wiley 11 GC-MS spectral libraries.

## RESULTS AND DISCUSSION

A total of 130 phytoconstituents were identified in methanolic root extract of *C. oxycantha* belonging to diverse groups of natural compounds. GC-MS chromatogram of the extract is shown in Fig. 1. Names of identified compounds along with their names, retention time (RT), molecular mass, molecular formula and peak area percentage are presented in Table 1. The predominant compound was (R\*, S\*)-2,3-Dihydroxybutanoic acid, tris(trimethylsilyl) derivative (**1**) with 73.28% peak area. The second most abundant constituent was l-Isoleucine, N-trifluoro acetyl- (**2**) showing 10.93% peak area. Compounds **3** to **7** namely 2,5-Dimethyl-4-hydroxy-3(2H)-furanone (**3**), Pimelic acid, 2TMS derivative (**4**), Silane, dimethyl(4-(2-phenylprop-2-yl)phenoxy)tridecyloxy- (**5**), 9-Hexadecenoic acid, methyl ester, (Z)- (**6**), and 2-Keto-l-gluconic acid, Penta (O-trimethylsilyl)- (**7**) were less abundant with peak areas ranging from 0.11 to 0.66. Compound **3** is also known as furaneol. For the first time, it was identified in pineapple as an aroma component. Later on, it was also identified in a number of other fruits including grape, strawberry, kiwi, raspberry, mango and tomato (Buttery *et al.*, 1995; Lavid *et al.*, 2002; Schwab, 2013). This compound is known to exhibit a number of biological activities including antioxidant (Sasaki *et al.*, 1998), antifungal and antibacterial (Sung *et al.*, 2006).

Table 1. Compounds identified from methanolic root extract of *Carthamus oxycantha* through GC-MS analysis.

	Names of compounds	Formula	Weight	Retention time (min)	Peak area (%)
<b>1</b>	(R*,S*)-2,3-Dihydroxybutanoic acid, tris(trimethylsilyl) deriv.	C <sub>13</sub> H <sub>32</sub> O <sub>4</sub> Si <sub>3</sub>	336.16	7.00	73.28
<b>2</b>	l-Isoleucine, N-trifluoro acetyl-	C <sub>8</sub> H <sub>12</sub> F <sub>3</sub> NO <sub>3</sub>	227.07	6.48	10.93
<b>3</b>	2,5-Dimethyl-4-hydroxy-3(2H)-furanone	C <sub>6</sub> H <sub>8</sub> O <sub>3</sub>	128.04	4.30	0.66
<b>4</b>	Pimelic acid, 2TMS derivative	C <sub>13</sub> H <sub>28</sub> O <sub>4</sub> Si <sub>2</sub>	304.15	9.09	0.59
<b>5</b>	Silane, dimethyl(4-(2-phenylprop-2-yl)phenoxy) tridecyloxy-	C <sub>30</sub> H <sub>48</sub> O <sub>2</sub> Si	468.34	17.37	0.13
<b>6</b>	9-Hexadecenoic acid, methyl ester, (Z)-	C <sub>17</sub> H <sub>32</sub> O <sub>2</sub>	268.24	11.27	0.12
<b>7</b>	2-Keto-l-gluconic acid, penta(O-trimethylsilyl)-	C <sub>21</sub> H <sub>50</sub> O <sub>7</sub> Si <sub>5</sub>	554.24	10.55	0.11
<b>8</b>	Heptadecanoic acid	C <sub>17</sub> H <sub>34</sub> O <sub>2</sub>	270.26	12.28	0.10
<b>9</b>	Levogluconone	C <sub>6</sub> H <sub>6</sub> O <sub>3</sub>	126.03	4.87	0.10
<b>10</b>	Bis(2-ethylhexyl) phthalate	C <sub>24</sub> H <sub>38</sub> O <sub>4</sub>	390.27	15.11	0.10
<b>11</b>	4-Hydroxy-2,2',4',6'-tetrachlorobiphenyl, trimethylsilyl ether	C <sub>15</sub> H <sub>14</sub> Cl <sub>4</sub> O <sub>2</sub> Si	377.95	16.11	0.10
<b>12</b>	Benzoic acid, 4-hydroxy-3-methoxy-, methyl ester	C <sub>10</sub> H <sub>12</sub> O <sub>4</sub>	196.07	8.47	0.10
<b>13</b>	Pyridine, 2-pentyl-	C <sub>13</sub> H <sub>13</sub> N	183.10	5.64	0.10
<b>14</b>	2-methylidene-6,10,14-trimethylpen2-methylidene-6,10,14-trimethylpentadecanoic acid silyated	C <sub>22</sub> H <sub>44</sub> O <sub>2</sub> Si	368.31	11.72	0.10
<b>15</b>	5-Amino-8-hydroxyquinoline, N,O-bis(trimethylsilyl)-	C <sub>15</sub> H <sub>24</sub> N <sub>2</sub> O <sub>2</sub> Si <sub>2</sub>	304.14	16.35	0.10
<b>16</b>	3-Vanilpropanol, bis(trimethylsilyl)-	C <sub>16</sub> H <sub>30</sub> O <sub>3</sub> Si <sub>2</sub>	326.17	10.74	0.10
<b>17</b>	Pentadecanoic acid	C <sub>15</sub> H <sub>30</sub> O <sub>2</sub>	242.22	10.94	0.10
<b>18</b>	Azelaic acid	C <sub>9</sub> H <sub>16</sub> O <sub>4</sub>	188.10	9.34	0.10
<b>19</b>	9-Octadecenamide, (Z)-	C <sub>18</sub> H <sub>35</sub> NO	281.27	14.10	0.10
<b>20</b>	N,N-Bis(2-hydroxyethyl)-p-toluidine	C <sub>11</sub> H <sub>17</sub> NO <sub>2</sub>	195.12	14.38	0.10
<b>21</b>	9-Octadecenoic acid, (E)-, TMS derivative	C <sub>21</sub> H <sub>42</sub> O <sub>2</sub> Si	354.29	13.26	0.10
<b>22</b>	2,3-Butanediol, 2TMS derivative	C <sub>10</sub> H <sub>26</sub> O <sub>2</sub> Si <sub>2</sub>	234.14	4.08	0.10
<b>23</b>	DL-Glyceraldehyde, tris(trimethylsilyl) ether	C <sub>12</sub> H <sub>30</sub> O <sub>3</sub> Si <sub>3</sub>	306.15	9.71	0.10

24	Benzoic acid, 3,4-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester	$C_{14}H_{24}O_4Si_2$	312.12	10.76	0.10
25	Decanedioic acid, dibutyl ester	$C_{18}H_{34}O_4$	314.24	12.95	0.10
26	D-Ribofuranose, 2,3,5-tris-O-(trimethylsilyl)-, bis(trimethylsilyl) phosphate	$C_{20}H_{51}O_8PSi_5$	590.21	14.69	0.10
27	Dodecanoic acid	$C_{12}H_{24}O_2$	200.17	8.72	0.10
28	2-Furoic acid, TMS derivative	$C_8H_{12}O_3Si$	184.05	4.95	0.10
29	Malic acid 1-ethyl ester, 2TMS	$C_{12}H_{26}O_5Si_2$	306.13	8.214	0.10
30	Hexanoic acid, 3-trimethylsilyloxy, trimethylsilyl ester	$C_{12}H_{28}O_3Si_2$	276.15	6.59	0.10
31	Phytol	$C_{20}H_{40}O$	296.31	12.65	0.10
32	Octadecanoic acid, butyl ester	$C_{22}H_{44}O_2$	340.33	14.20	0.10
33	13-Docosenoic acid, methyl ester, (Z)-	$C_{23}H_{44}O_2$	352.33	14.84	0.10
34	Octadecane	$C_{18}H_{38}$	254.30	10.52	0.10
35	L-Valine, 2TMS derivative	$C_{11}H_{27}NO_2Si_2$	261.15	5.75	0.10
36	$\alpha$ -Linolenic acid, TMS derivative	$C_{21}H_{38}O_2Si$	350.26	13.27	0.10
37	Salicylic acid, 2TMS derivative	$C_{13}H_{22}O_3Si_2$	282.11	8.42	0.10
38	Methyl 3-(3,4-bis(tert. - butyldimethylsilyl)oxyphenyl) prop-2-enoate	$C_{22}H_{38}O_4Si_2$	422.23	13.80	0.10
39	Methyl stearate	$C_{19}H_{38}O_2$	298.29	12.69	0.10
40	Butane, 1,1-dibutoxy-	$C_{12}H_{26}O_2$	202.19	6.06	0.10
42	Hexadecanoic acid, 4-[(trimethylsilyl)oxy] butyl ester	$C_{23}H_{48}O_3Si$	400.33	15.87	0.10
43	Vanillyl alcohol, 2TMS derivative	$C_{14}H_{26}O_3Si_2$	298.14	9.41	0.10
44	Benzoic acid, 4-[(trimethylsilyl)oxy]-, trimethylsilyl ester	$C_{13}H_{23}NO_2Si_2$	281.12	9.31	0.10
45	Salicylic acid	$C_7H_6O_3$	138.03	6.61	0.10
46	Isopropyl myristate	$C_{17}H_{34}O_2$	270.26	10.71	0.10
47	Androst-4-ene-3,17-dione, 15-hydroxy-, (15 $\alpha$ )-	$C_{19}H_{26}O_3$	302.18	14.55	0.10
48	Butanoic acid, 3,4-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester	$C_{13}H_{32}O_4Si_3$	336.16	7.72	0.10
49	Octahydro-1H-cyclopenta[b]pyridin-4-ol	$C_8H_{15}NO$	141.12	4.26	0.10
50	Eicosane	$C_{20}H_{42}$	282.33	11.88	0.10
51	Hexadecanoic acid, ethyl ester	$C_{18}H_{34}O_2$	282.26	11.85	0.10
52	Acetoacetic acid, bis(trimethylsilyl)- deriv.	$C_{10}H_{22}O_3Si_2$	246.11	6.18	0.10
53	1H-Pyrrole-2,5-dione, 3-ethyl-4-methyl-	$C_7H_7NO_2$	137.05	5.90	0.10
54	L-Proline, 5-oxo-1-(trimethylsilyl)-, trimethylsilyl ester	$C_{11}H_{23}NO_3Si_2$	273.12	8.51	0.10
55	2-Trimethylsilyloxyheptanoic acid, trimethylsilyl ester	$C_{13}H_{30}O_3Si_2$	290.17	7.11	0.10
56	Dodecane	$C_{12}H_{26}$	170.20	5.55	0.10
57	Cyclononasiloxane, octadecamethyl-	$C_{18}H_{54}O_9Si_9$	666.16	10.71	0.10
59	Fructofuranoside, methyl 1,3,4,6-tetrakis-O-(trimethylsilyl)-, $\alpha$ .-D-	$C_{19}H_{46}O_6Si_4$	482.23	10.55	0.10
59	3-Trimethylsilyloxyoctanoic acid, trimethylsilyl ester	$C_{14}H_{32}O_3Si_2$	304.18	8.05	0.10
60	2-Aminoethanol, N-acetyl-, O-TMS	$C_7H_{17}NO_2Si$	175.10	5.64	0.10
61	1-Hexacosene	$C_{26}H_{52}$	364.41	13.09	0.10
62	Chondrillasterol	$C_{29}H_{48}O$	412.37	19.41	0.10
63	Galactopyranose, 5TMS derivative	$C_{21}H_{52}O_6Si_5$	540.26	17.97	0.10
64	9-Octadecenoic acid, methyl ester, (E)-	$C_{19}H_{36}O_2$	296.27	12.55	0.10
65	2-Methylpentacosane	$C_{26}H_{54}$	366.42	14.31	0.10
66	2-Ethylhexanol, TMS derivative	$C_{11}H_{26}OSi$	202.17	4.66	0.10
67	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	$C_{17}H_{24}O_3$	276.17	11.47	0.10
68	9-Octadecenoic acid (Z)-, 2,3-bis[(trimethylsilyl)oxy]propyl ester	$C_{27}H_{56}O_4Si_2$	500.37	16.14	0.10
69	1-Monopalmitin, 2TMS derivative	$C_{25}H_{54}O_4Si_2$	474.35	15.29	0.10

70	Squalene	C <sub>30</sub> H <sub>50</sub>	410.39	16.48	0.10
71	1H-Indole-2-carboxylic acid, 1-(trimethylsilyl)-5-[(trimethylsilyl)oxy]-, trimethylsilyl ester	C <sub>18</sub> H <sub>31</sub> NO <sub>3</sub> Si <sub>3</sub>	393.16	11.54	0.10
72	Bohlmann k2631	C <sub>15</sub> H <sub>20</sub> O <sub>2</sub>	232.14	11.92	0.10
73	Hydracrylic acid, 2TMS derivative	C <sub>9</sub> H <sub>22</sub> O <sub>3</sub> Si <sub>2</sub>	234.11	5.02	0.10
74	cis-13-Eicosenoic acid, methyl ester	C <sub>21</sub> H <sub>40</sub> O <sub>2</sub>	324.30	13.75	0.10
75	Pentadecanoic acid, methyl ester	C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>	256.24	10.71	0.10
76	cis-12-Octadecenoic acid methyl ester	C <sub>19</sub> H <sub>36</sub> O <sub>2</sub>	296.27	12.55	0.10
77	1-Hexadecene	C <sub>16</sub> H <sub>32</sub>	224.25	8.98	0.10
78	Traumatic acid, (E)-, 2TMS derivative	C <sub>18</sub> H <sub>36</sub> O <sub>4</sub> Si <sub>2</sub>	372.21	12.39	0.10
79	4-Methoxybenzyl alcohol, TMS derivative	C <sub>11</sub> H <sub>18</sub> O <sub>2</sub> Si	210.10	7.42	0.10
80	D-Fructose, 5TMS derivative	C <sub>21</sub> H <sub>52</sub> O <sub>6</sub> Si <sub>5</sub>	540.26	6.71	0.10
81	5-O-Coumaroyl-D-quinic acid, 5TMS	C <sub>31</sub> H <sub>58</sub> O <sub>8</sub> Si <sub>5</sub>	698.29	17.32	0.10
82	1H-Indole, 1-(trimethylsilyl)-2,5-bis[(trimethylsilyl)oxy]-	C <sub>17</sub> H <sub>31</sub> NO <sub>2</sub> Si <sub>3</sub>	365.16	10.94	0.10
83	Tetradecanoic acid	C <sub>14</sub> H <sub>28</sub> O <sub>2</sub>	228.21	10.24	0.10
84	3-(1-ethoxyethoxy)-1-phenyl-6-heptene	C <sub>19</sub> H <sub>32</sub> O <sub>3</sub>	308.24	6.00	0.10
85	1,2,3,4,5,6-Hexa-O-trimethylsilyl-myoinositol	C <sub>24</sub> H <sub>60</sub> O <sub>6</sub> Si <sub>6</sub>	612.30	11.83	0.10
86	8a-Methyl-3,5-dimethylenedecahydronaphtho[2,3-b]furan-2(3H)-one	C <sub>15</sub> H <sub>20</sub> O <sub>2</sub>	232.14	11.79	0.10
87	n-Tetracosanol-1	C <sub>24</sub> H <sub>50</sub> O	354.38	14.23	0.10
88	Phenylethyl Alcohol, TMS derivative	C <sub>11</sub> H <sub>18</sub> OSi	194.11	5.87	0.10
89	Eicosanoic acid, methyl ester	C <sub>21</sub> H <sub>42</sub> O <sub>2</sub>	326.31	13.86	0.10
90	Monomethyl succinate, trimethylsilyl ester	C <sub>8</sub> H <sub>16</sub> O <sub>4</sub> Si	204.08	5.35	0.10
91	3-Hydroxy-2,3-dihydromaltol, 2-O-TMS	C <sub>12</sub> H <sub>24</sub> O <sub>4</sub> Si <sub>2</sub>	288.12	7.89	0.10
92	Phosphoric acid, dioctadecyl ester	C <sub>18</sub> H <sub>39</sub> O <sub>4</sub> P	350.26	13.01	0.10
93	cis-13-Octadecenoic acid	C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>	282.26	12.78	0.10
94	5-Hydroxymethylfurfural	C <sub>6</sub> H <sub>6</sub> O <sub>3</sub>	126.03	5.96	0.10
95	Benzeneacetamide, TMS derivative	C <sub>11</sub> H <sub>17</sub> NOSi	207.10	7.95	0.10
96	Xylonic acid, 2,3,4-tris-O-(trimethylsilyl)-, δ-lactone, D-	C <sub>14</sub> H <sub>32</sub> O <sub>5</sub> Si <sub>3</sub>	364.15	9.42	0.10
97	Vitispirane	C <sub>13</sub> H <sub>20</sub> O	192.15	6.40	0.10
98	Hexacosane	C <sub>26</sub> H <sub>54</sub>	366.42	13.76	0.10
99	Glycerol, 1,2-di (TMS)-	C <sub>9</sub> H <sub>24</sub> O <sub>3</sub> Si <sub>2</sub>	236.12	5.55	0.10
100	Phosphoric acid, bis(trimethylsilyl)monomethyl ester	C <sub>7</sub> H <sub>21</sub> O <sub>4</sub> PSi <sub>2</sub>	256.07	5.42	0.10
101	5-Propyl-10,11-dihydro-5H-dibenzo [a, d] cyclohepten-5,10-imine hydrochloride	C <sub>18</sub> H <sub>19</sub> N	249.15	12.85	0.10
102	Picoxystrobin	C <sub>18</sub> H <sub>16</sub> F <sub>3</sub> NO <sub>4</sub>	367.10	12.96	0.10
103	Methyl tetradecanoate	C <sub>15</sub> H <sub>30</sub> O <sub>2</sub>	242.22	9.99	0.10
104	Hexadecanoic acid, butyl ester	C <sub>20</sub> H <sub>40</sub> O <sub>2</sub>	312.30	13.05	0.10
105	Hexadecanoic acid, methyl ester	C <sub>17</sub> H <sub>34</sub> O <sub>2</sub>	270.26	11.40	0.10
106	Oleic acid, butyl ester	C <sub>22</sub> H <sub>42</sub> O <sub>2</sub>	338.31	13.83	0.10
107	Pantothenic acid tritms	C <sub>18</sub> H <sub>41</sub> NO <sub>5</sub> Si <sub>3</sub>	435.22	11.97	0.10
108	Heptadecane, 3-methyl-	C <sub>18</sub> H <sub>38</sub>	254.30	10.32	0.10
109	L-Valine, TMS derivative	C <sub>8</sub> H <sub>19</sub> NO <sub>2</sub> Si	189.11	4.53	0.10
110	Benzeneacetic acid	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>	136.05	6.07	0.10
111	Heneicosanoic acid, methyl ester	C <sub>22</sub> H <sub>44</sub> O <sub>2</sub>	340.33	14.41	0.10
112	D-Glucose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-, O-methylloxime	C <sub>22</sub> H <sub>55</sub> NO <sub>6</sub> Si <sub>5</sub>	569.28	11.42	0.10
113	Piperine	C <sub>17</sub> H <sub>19</sub> NO <sub>3</sub>	285.14	16.99	0.10
114	2,4-Thiazolidinedione	C <sub>3</sub> H <sub>3</sub> NO <sub>2</sub> S	116.99	5.06	0.10
115	2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)-	C <sub>14</sub> H <sub>20</sub> O <sub>2</sub>	196.07	8.08	0.10
116	Phloretic acid, 2TMS derivative	C <sub>15</sub> H <sub>26</sub> O <sub>3</sub> Si <sub>2</sub>	310.14	10.32	0.10

117	Piperidine, 1-[5-(1,3-benzodioxol-5-yl)-1-oxo-2,4-pentadienyl]-, (Z, Z)-	C <sub>17</sub> H <sub>19</sub> NO <sub>3</sub>	285.13	16.19	0.10
118	Octadecanoic acid	C <sub>18</sub> H <sub>36</sub> O <sub>2</sub>	284.27	12.90	0.10
119	2,2'-Bipyridine	C <sub>10</sub> H <sub>8</sub> N <sub>2</sub>	156.07	7.89	0.10
120	n-Hexadecanoic acid	C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>	256.24	11.65	0.10
121	Benzoic acid, 3,4,5-tris (trimethylsiloxy)-, trimethylsilyl ester	C <sub>19</sub> H <sub>38</sub> O <sub>5</sub> Si <sub>4</sub>	458.17	11.73	0.10
122	Docosanoic acid, methyl ester	C <sub>23</sub> H <sub>46</sub> O <sub>2</sub>	354.35	14.95	0.10
123	Xylitol, 5TMS derivative	C <sub>20</sub> H <sub>52</sub> O <sub>5</sub> Si <sub>5</sub>	512.26	10.07	0.10
124	Phenol, 4-ethenyl-2,6-dimethoxy-	C <sub>10</sub> H <sub>12</sub> O <sub>3</sub>	180.08	8.85	0.10
125	Octacosane	C <sub>28</sub> H <sub>58</sub>	394.45	16.28	0.10
126	2-O-Glycerol-.alpha.-d-galactopyranoside, hexa-TMS	C <sub>27</sub> H <sub>66</sub> O <sub>8</sub> Si <sub>6</sub>	686.33	13.99	0.10
127	Benzene, [(3-butynyloxy) methyl]-	C <sub>11</sub> H <sub>12</sub> O	160.09	17.08	0.10
128	γ-Sitosterol	C <sub>29</sub> H <sub>50</sub> O	414.39	19.41	0.10
129	Triethylene glycol, 2TMS derivative	C <sub>12</sub> H <sub>30</sub> O <sub>4</sub> Si <sub>2</sub>	294.16	8.30	0.10
130	Benzyl alcohol, TMS derivative	C <sub>10</sub> H <sub>16</sub> OSi	180.10	5.17	0.10

Table 2. Potential bioactive phytoconstituents in methanolic root extract of *Carthamus oxycantha*.

Compound No.	Names of compounds	Property	Reference
3	2,5-Dimethyl-4-hydroxy-3(2H)-furanone	Antioxidant, antifungal, antibacterial	Sasaki <i>et al.</i> (1998), Sung <i>et al.</i> (2006)
10	Bis(2-ethylhexyl) phthalate	Antimicrobial	Habib and Karim (2009)
27	Dodecanoic acid	Antifungal, antibacterial	McGraw <i>et al.</i> (2002)
31	Phytol	Antibacterial, antifungal, anticancer, anti-inflammatory	Hema <i>et al.</i> (2011), Tyagi and Agarwal (2017)
50	Eicosane	Antifungal	Ahsan <i>et al.</i> (2017)
51	Hexadecanoic acid, ethyl ester	Antioxidant, Hemolytic, Anti-androgenic, Hypocholesterolemic, Nematicide	Tyagi and Agarwal (2017)
75	Pentadecanoic acid, methyl ester	Antibacterial, antifungal	Chandrasekaran <i>et al.</i> (2011)
77	1-Hexadecene	Antibacterial, antifungal, antioxidant	Hsouna <i>et al.</i> (2011), Yogeswari <i>et al.</i> (2012), Mou <i>et al.</i> (2013)
83	Tetradecanoic acid	Antifungal, antibacterial, larvicidal	McGraw <i>et al.</i> (2002), Sivakumar <i>et al.</i> (2011)
98	Hexacosane	Antimicrobial	Rukaiyat <i>et al.</i> (2015)
104	Hexadecanoic acid, butyl ester	Antimicrobial, antioxidant	Prakash <i>et al.</i> (2011), Sujatha <i>et al.</i> (2014)
105	Hexadecanoic acid, methyl ester	Antibacterial, antifungal, antioxidant, anti-inflammatory	Chandrasekaran <i>et al.</i> (2011), Hema <i>et al.</i> (2011)
114	2,4-Thiazolidinedione	Antimicrobial	Alagawadi and Alegaon (2011)
118	Octadecanoic acid	Antifungal, antibacterial	Rahuman <i>et al.</i> (2000), McGraw <i>et al.</i> (2002)
120	n-Hexadecanoic acid	Antifungal, antibacterial, mosquito larvicide, Anti-inflammatory, antioxidant, nematicide, pesticide.	Rahuman <i>et al.</i> (2000), McGraw <i>et al.</i> (2002), Kumar <i>et al.</i> (2010), Aparna <i>et al.</i> (2012)
128	γ-Sitosterol	Antimicrobial	Karthikeyan <i>et al.</i> (2014)

Compounds 8 to 130 were least abundant with peak areas less than 0.11%. Among these, many compounds are known to exhibit various biological activities including antibacterial, antifungal, anticancer, anti-inflammatory, nematicidal, hemolytic, anti-androgenic and hypocholesterolemic activities. Compounds namely Heptadecanoic acid (8), Pentadecanoic acid (17), Dodecanoic acid (27), Tetradecanoic acid (83), Octadecanoic acid (118) and n-Hexadecanoic acid (120) belong to fatty acid group. Many fatty acids including Tetradecanoic acid, n-

Hexadecanoic acid, Octadecanoic acid and Dodecanoic acid are also known to show antifungal and antibacterial activities (McGraw *et al.*, 2002). *n*-Hexadecanoic acid is a compound with a variety of bioactivities including hypocholesterolemic, antioxidant, nematicide, pesticide, hemolytic (Kumar *et al.*, 2010), anti-inflammatory (Aparna *et al.*, 2012), and mosquito larvicide (Rahuman *et al.*, 2000). Lipids kill bacteria and fungi by disrupting their cellular member (Lampe *et al.*, 1998). Lipids can enter in extensive network of peptidoglycane in cell wall and reach bacterial membrane leading to its disintegration (Ismail *et al.*, 2014). Likewise, antifungal fatty acids increase fluidity of fungal membrane resulting in leakage of cellular components and death of fungal cell (Pohl *et al.*, 2011).

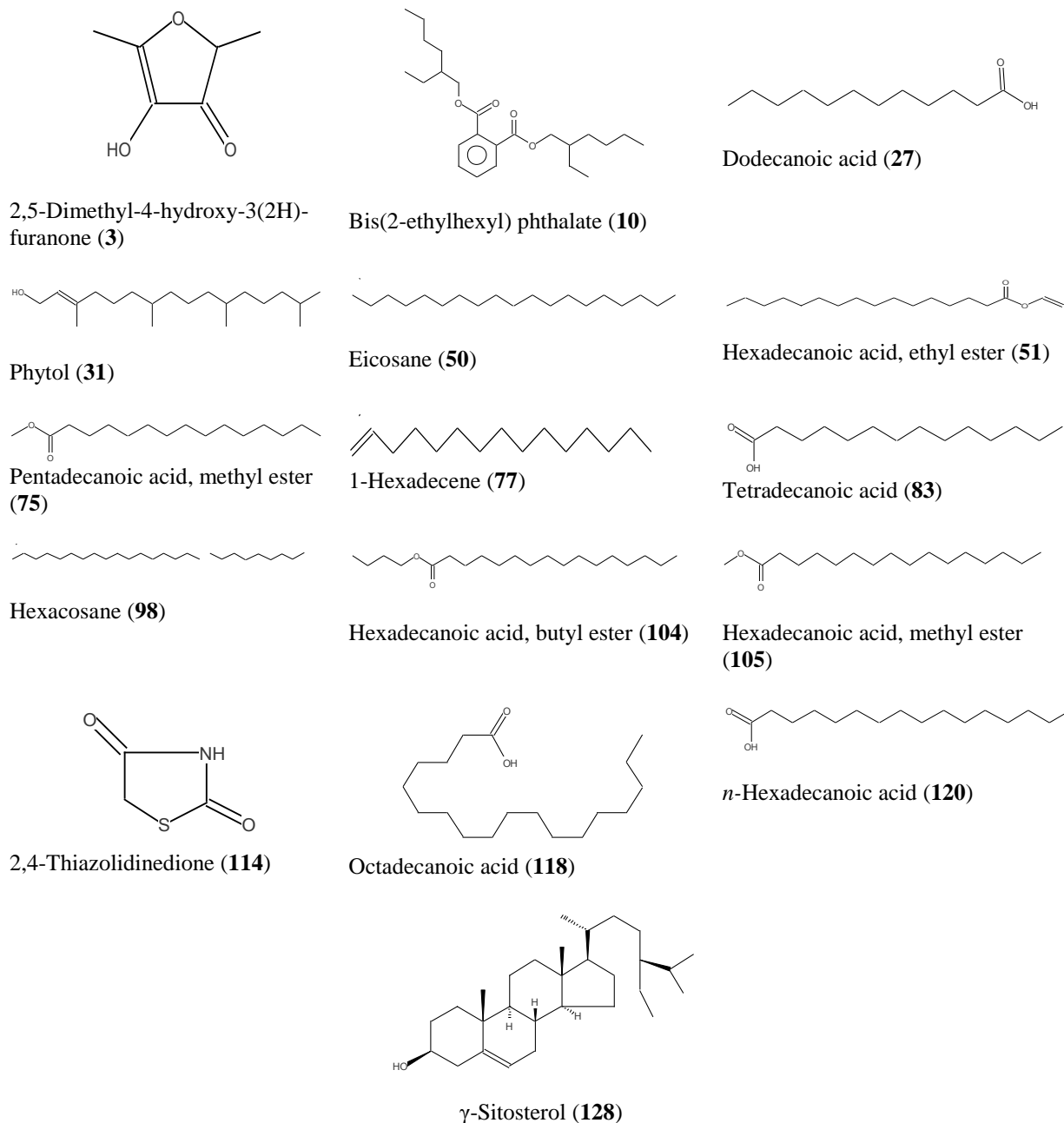


Fig. 2. Structures of bioactive compounds in methanolic root extract of *Carthamus oxycantha*.

Many other least abundant compounds namely Bis(2-ethylhexyl) phthalate (**10**), Phytol (**31**), Eicosane (**50**), Hexadecanoic acid, ethyl ester (**51**), 1-Hexadecene (**77**), Hexacosane (**98**), Hexadecanoic acid, butyl ester (**104**), 2,4-

Thiazolidinedione (**114**) and  $\gamma$ -Sitosterol (**128**) are known to possess various biological activities such as antifungal, antibacterial, anti-androgenic, hypocholesterolemic, nematocidal antioxidant, anticancer and anti-inflammatory as shown in Table 2 (Habib and Karim, 2009; Alagawadi and Alegaon, 2011; Hema *et al.*, 2011; Mou *et al.*, 2013; Karthikeyan *et al.*, 2014; Sujatha *et al.*, 2014; Rukaiyat *et al.*, 2015; Ahsan *et al.*, 2017; Tyagi and Agarwal, 2017).

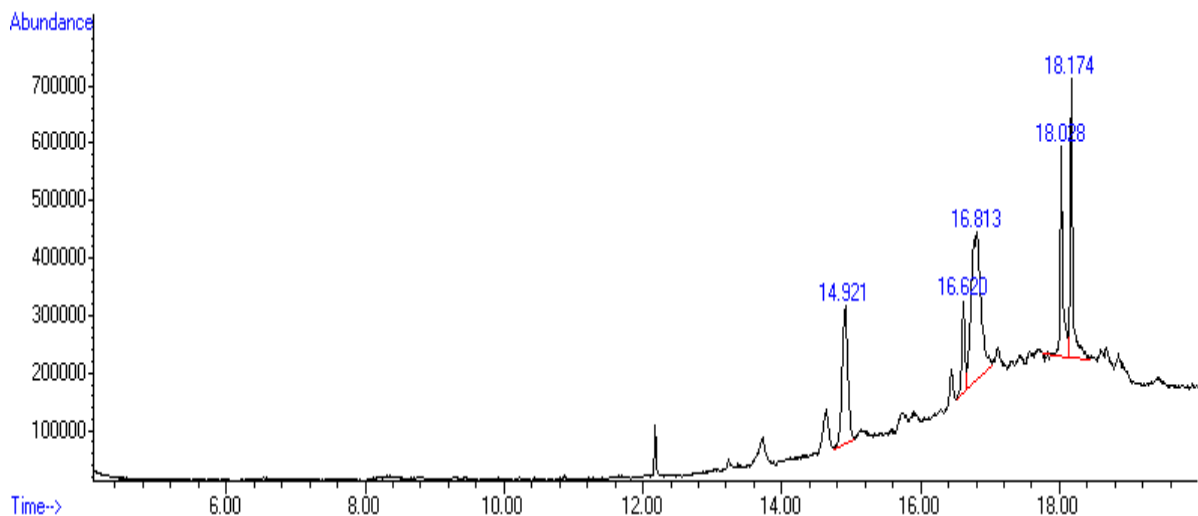


Fig. 1. GC-MS chromatograms of methanolic root extract of *Carthamus oxycantha*.

Various compounds namely 9-Hexadecenoic acid, methyl ester, (Z)- (**6**), 9-Octadecenoic acid, methyl ester, (E)- (**64**), cis-13-Eicosenoic acid, methyl ester (**74**), Pentadecanoic acid, methyl ester (**75**), cis-12-Octadecenoic acid methyl ester (**76**), Eicosanoic acid, methyl ester (**89**), Hexadecanoic acid, methyl ester (**105**), Heneicosanoic acid, methyl ester (**111**) and Docosanoic acid, methyl ester (**122**) belong to fatty acid methyl esters (FAME) group. Most of the fatty acid methyl esters are known to exhibit antifungal, antibacterial or both the properties (Chandrasekaran *et al.*, 2011; Hema *et al.*, 2011). FAME in sunflower and soybean oils showed remarkable antifungal activity against *Paracoccidioides brasiliensis* and *P. lutzii* (Pinto *et al.*, 2017). Agoramoorthy *et al.* (2007) stated that FAME extract of *Excoecaria agallocha* has the ability to control growth of different *Candida* and bacterial species. Similar effect of FAME extract of *Quercus leucotrichophora* was reported by Sati *et al.* (2017) against certain bacterial species. A mixture of FAME of sunflower and essential oil of *Mentha piperita* exhibited herbicidal activity against *Chenopodium album* (Synowiec *et al.*, 2017).

The present study concludes that root of *C. oxycantha* is a store house of potent bioactive compounds including fatty acids, fatty acid methyl esters, furaneol,  $\gamma$ -Sitosterol, phytol and others which possess antifungal, antibacterial, antioxidant, anticancer, anti-inflammatory and various other bioactive properties.

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