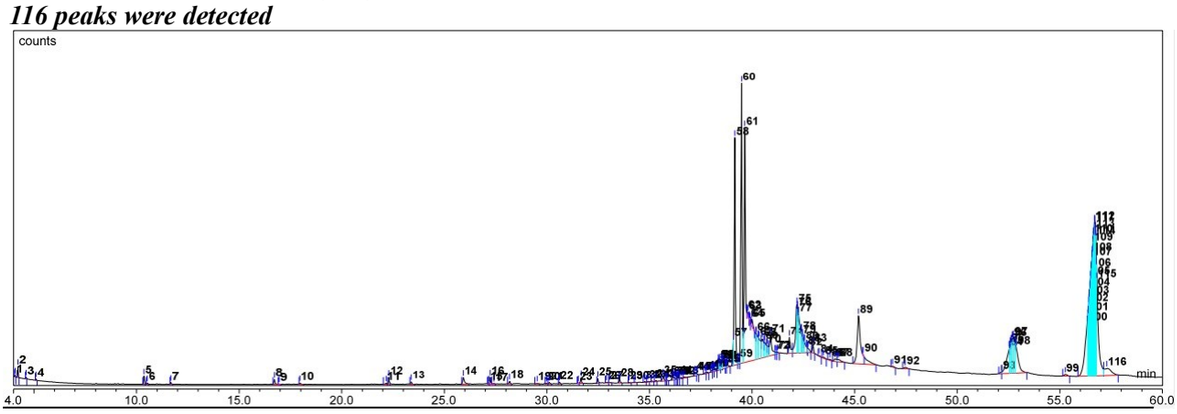
GC-MS

Chromatograms

A. Root Chloroform (RC)

116 peaks were detected



----------Identified pytochemical compounds

No	RT (min)	Chemical formula	Organic compounds	Relative area (%)	Bioactivities	Classifications
1	10.36	$C_{11}H_{24}$	undecane	0.14	*x*	hydrocarbons acyclic; alkanes [MeSH]
2	11.67	$C_{10}H_{22}$	decane	0.03	*x*	hydrocarbons acyclic; alkanes [MeSH]
3	16.71	$C_{15}H_{32}$	2,7,10-trimethyldodecane	0.14	*x*	hydrocarbons; alkanes [ChEBI]
4	16.95	$C_{19}H_{40}$	6-methyloctadecane	0.01	*x*	hydrocarbons; alkanes [ChEBI]
5	17.96	$C_{17}H_{36}$	2,6,10-trimethyltetradecane	0.05	*v* Zhao *et al*., 2019; Talbaoui *et al*., 2020	fatty acids; hydrocarbons [LOTUS]
6	22.29	$C_{16}H_{34}$	hexadecane	0.13	*ox*; *bx* Mou *et al*., 2013	hydrocarbons acyclic; alkanes [MeSH]
7	25.92	$C_{13}H_{14}O_4$	1’-acetoxychavicol acetate	0.31	*v* Kubota *et al*., 2001; Mahae & Chaiseri, 2009; Kojima-Yuasa & Matsui-Yuasa, 2020; Zhang *et al*., 2021	alcohols; benzyl alcohols [MeSH] carbonyl compound; carboxylic ester [ChEBI] phenylpropanoids; monolignols [KEGG: phytochemical compounds]
8	27.16	$C_{26}H_{54}$	3-ethyl-5-(2-ethylbutyl) octadecane	0.01	*ox*; *bx* Al-Marzoqi *et al*., 2015; Wang *et al*., 2018	hydrocarbons; alkanes [ChEBI] fatty acids; hydrocarbons [LOTUS]
9	27.23	$C_{21}H_{44}$	2,6,10,15-tetramethylheptadecane	0.16	*x*	prenol lipids; sesquiterpenoids [HMDB0062787]
10	27.42	$C_{17}H_{32}O_2$	7-methyl-z-tetradecen-1-ol acetate	0.02	*cx* El-Naggar *et al*., 2023; Sobhy *et al*., 2023	carbonyl compounds; carboxylic esters [ChEBI] fatty acids; wax monoesters [LOTUS]
11	29.53	$C_{17}H_{32}O$	13-heptadecyn-1-ol	0.04	*v* El Mokni *et al*., 2016; Al-Gara,awi *et al*., 2019	organic hydroxy compounds; alcohols; fatty alcohols [ChEBI]
12	30.11	$C_{17}H_{36}O$	2-methyl-1-hexadecanol	0.05	*v* Hussein *et al*., 2015; El-fayoumy *et al*., 2021	fatty acids; fatty alcohols [LOTUS]
13	31.54	$C_{25}H_{44}N_2O_5S$	2-myristynoyl pantetheine	0.01	*x*	organic chemicals;

						sulfur compounds [MeSH] organonitrogen compounds; carboxamide; pantothenic acids [ChEBI] fatty acids; n-acyl amines [LOTUS] carboxylic acids; amino acids [CPD-511]
14	32.91	$C_{18}H_{24}O_2$	methyl 5,8,11-heptadecatriynoate	0.03	*x*	fatty acids; methyl esters [CAS reg. number: 56554-57-5] fatty acids; palmitic acids [MeSH]
15	33.05	$C_{18}H_{36}O_2$	ethyl palmitate	0.04	*ox* Bu, *et al*., 2012; Alghamdi *et al*., 2018	lipids; fatty acid derivatives; fatty acid esters [ChEBI] fatty acyls; short fatty esters [LIPID MAPS]
16	33.55	$C_{20}H_{40}O_2$	ethanol, 2-(9-octadecenyloxy)-, (z)-	0.03	*cx* Altameme *et al*., 2015	dialkyl ethers [CAS reg. number: 5353-25-3]
17	36.42	$C_{26}H_{54}$	3-ethyl-5-(2-ethylbutyl) octadecane	0.06	*ox*; *bx* Al-Marzoqi *et al*., 2015; Wang *et al*., 2018	hydrocarbons; alkanes [ChEBI] fatty acids; hydrocarbons [LOTUS]
18	37.23	$C_{37}H_{76}O$	1-heptatriacontanol	0.11	*v* Hadi *et al*., 2016; Ganesh & Mohankumar, 2017; Diab *et al*., 2021; Addai *et al*., 2022; Abdullah *et al*., 2022	fatty acids; fatty alcohols [LOTUS]
19	38.36	$C_{16}H_{30}O_2$	9-hexadecenoic acid	0.20	*v* Rahman *et al*., 2014; Reza *et al*., 2021	fatty acids; unsaturated fatty acids; monounsaturated fatty acids; palmitoleic acids [MeSH] lipids; fatty acids; palmitelaidic acids [ChEBI] fatty acyls; unsaturated fatty acids [LIPID]
20	39.09	$C_{20}H_{30}O_2$	podocarpa-8,11,13-triene-7ß,13-diol, 14-isopropyl-	0.47	*cx*; *bx* Tada *et al*., 2010; Yu *et al*., 2018; Forzato & Nitti, 2022	terpenoids; podocarpane diterpenoids [LOTUS] hydrocarbons; terpenes; diterpenes; abietanes [MeSH]
21	39.16	$C_{20}H_{30}O$	ferruginol	6.72	*v* Topçu & Gören, 2007; Espinoza *et al*., 2008; Tsujimura *et al*., 2019; González-Cardenete *et al*., 2021	terpenoids; diterpenoids (C20) [KEGG: phytochemical compounds]

22	39.49	$C_{21}H_{30}O_2$	methyl retinoate	8.78	*v* Vilhais-Neto & Pourquié, 2008; Bittencourt *et al*., 2015	vitamins; vitamin A [MeSH] prenol lipids; retinoids; retinoid esters [HMDB0254612] hormones; adrenal cortex hormones [MeSH]
23	39.65	$C_{21}H_{32}O_2$	pregn-5-en-20-one, 3-hydroxy-, (3ß,17a)-	16.21	*v* Iqbal & Siddiqui, 2021	alcohols; secondary alcohols; 3beta-hydroxy steroids; pregnenolone [ChEBI]
24	39.79	$C_{20}H_{28}O_3$	16-hydroxymethyleneandrost-5-en-3-ol-17-one	0.06	*cx* Vosooghi *et al*., 2013	alcohols; secondary alcohols; 3beta-hydroxy steroids; dehydroepiandrosterone [ChEBI] terpenoids; androstane steroids [LOTUS]
25	41.82	$C_{20}H_{38}O_2$	paullinic acid	0.71	*x*	lipids; fatty acids; long-chain fatty acids; (z)-icos-13-enoic acid [ChEBI] fatty acyls; unsaturated fatty acids [LIPID]
26	42.97	$C_{69}H_{134}O_6$	tribehenin	0.25	*x*	lipids; fatty acids; glyceryl behenate [MeSH] glycerolipids; triacylglycerols [LIPID]
27	45.41	$C_{22}H_{28}O_6$	quassin	5.16	*x*	hydrocarbons; terpenes; triterpenes; quassins; quassin [MeSH]
28	52.16	$C_{26}H_{44}O_5$	ethyl iso-allocholate	0.07	*v* Malathi *et al*., 2016; Ojo *et al*., 2022; Ibrahim *et al*., 2022	terpenoids; cholane steroids [LOTUS]
29	52.69	$C_{28}H_{48}O$	campesterol	1.31	*ox*; *cx* Choi *et al*., 2007; Miras-Moreno *et al*., 2016; Prommaban *et al*., 2020	phytochemicals; phytosterols [MeSH] alcohols; secondary alcohols; 3beta-hydroxy steroids [ChEBI] terpenoids; steroids [KEGG: phytochemical compounds]
30	56.75	$C_{29}H_{48}O$	stigmasterol	2.75	*v* Alawode *et al*., 2021; Ashraf & Bhatti, 2021; Bakrim *et al*., 2022	alcohols; secondary alcohols; 3beta-

						hydroxy steroids [ChEBI] terpenoids; steroids [KEGG: phytochemical compounds]

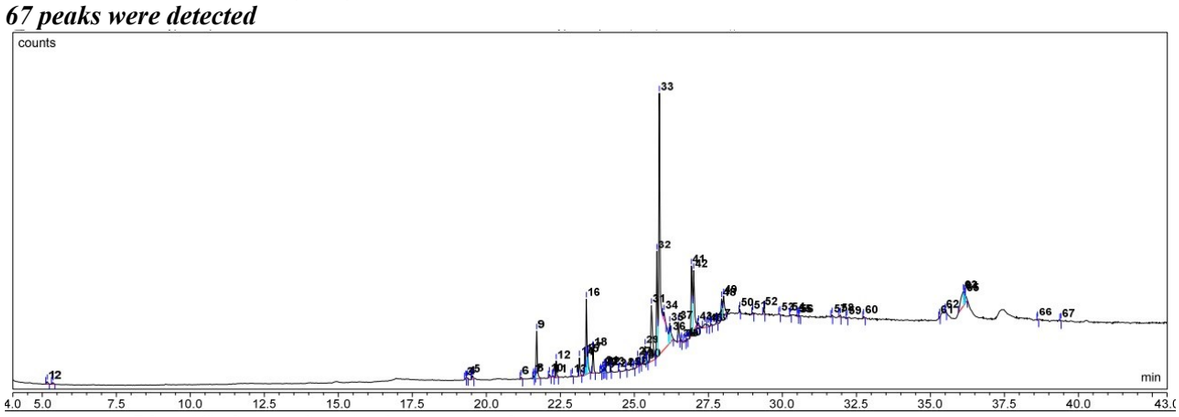
RT = retention time; ox = antioxidants/radical scavenging activity; bx = antibacterial/antimicrobial; cx = cytotoxicity/anticancer/antiproliferative/anticarcinogenic; x = no activity reported related to ox, bx, and cx; v = ox, bx, and cx activities reported.

GC-MS

Chromatograms

B. Root Methanol (RM)

67 peaks were detected



----------Identified pytochemical compounds

No	RT (min)	Chemical formula	Organic compounds	Relative area (%)	Bioactivities	Classifications
1	5.17	$C_{27}H_{44}O_3$	1,25-dihydroxyvitamin D3	0.29	*cx*; *bx* Wang *et al*., 2004; Evans *et al*., 2006	vitamins; cholecalciferols; hydroxycholecalciferols; calcitriol [MeSH]
2	21.70	$C_{17}H_{34}O_2$	methyl palmitate	3.35	*ox*; *bx* Pinto *et al*., 2017; Hamed *et al*., 2020; Astiti & Ramona, 2021; Fajrih *et al*., 2022	lipids; fatty acids; palmitic acids; palmitates [MeSH]
3	22.36	$C_{18}H_{36}O_2$	ethyl palmitate	0.93	*ox* Bu *et al*., 2012; Alghamdi *et al*., 2018	fatty acids; palmitic acids [MeSH]
4	23.15	$C_{20}H_{30}$	7-isopropyl-1,1,4a-trimethyl-1,2,3,4,4a,9,10,10a-octahydrophenanthrene	1.22	*x*	lipids; fatty acid derivatives; fatty acid esters [ChEBI]
5	23.33	$C_{19}H_{34}O_2$	7,10-octadecadienoic acid, methyl ester	1.14	*x*	fatty acyls; short fatty esters [LIPID MAPS]
6	23.38	$C_{19}H_{36}O_2$	cis-13-octadecenoic acid, methyl ester	4.65	*cx* Abdullah *et al*., 2020	terpenoids; abietane diterpenoids [LOTUS]
7	23.43	$C_{19}H_{36}O_2$	10-octadecenoic acid, methyl ester	1.55	*ox*; *bx* Alqahtani *et al*., 2019; Abdel-Rahman *et al*., 2020	lineolic acids and derivatives [CAS reg. number: 56554-24-6]
8	23.60	$C_{19}H_{38}O_2$	methyl isostearate	1.5	*x*	lipids; fatty acids; unsaturated fatty acids; monounsaturated fatty acids; oleic acids [MeSH]
9	23.93	$C_{26}H_{44}O_5$	ethyl iso-allocholate	0.18	*v* Malathi *et al*., 2016; Ojo *et al*., 2022; Ibrahim *et al*., 2022	fatty acids; wax monoesters [LOTUS]
10	25.11	$C_{35}H_{68}O_5$	1,2-dipalmitoyl-rac-glycerol	0.54	*x*	fatty acids; wax monoesters [LOTUS]
11	25.36	$C_{24}H_{36}O_6$	8,14-seco-3,19-epoxyandrostane-8,14-	1.17	*cx* Gupta & Gupta, 2017	terpenoids; cholane steroids [LOTUS]
						lipids; glycerolipids; glycerides; diglycerides [ChEBI]
						ketals [PubChem CID 550132]

			dione, 17-acetoxy-3ß-methoxy-4,4-dimethyl-			
12	25.57	$C_{20}H_{30}O$	ferruginol	7.21	*v* Topçu & Gören, 2007; Espinoza *et al*., 2008; Tsujimura *et al*., 2019; González-Cardenete *et al*., 2021	hydrocarbons; terpenes; diterpenes; abietanes [MeSH] terpenoids; diterpenoids (C20) [KEGG: phytochemical compounds]
13	25.76	$C_{20}H_{26}O_5$	gibberellin A44 (GA44)	7.90	*x*	isoprenoids; terpenoids; diterpenoids; gibberellins [ChEBI]
14	26.00	$C_{20}H_{28}O_3$	16-hydroxymethyleneandrost-5-en-3-ol-17-one	0.73	*cx* Vosooghi *et al*., 2013	alcohols; secondary alcohols; 3beta-hydroxy steroids; dehydroepiandrosterone [ChEBI] terpenoids; androstane steroids [LOTUS]
15	26.20	$C_{32}H_{48}O_6$	dodecanoic acid, 1a,2,5,5a,6,9,10,10a-octahydro-5a-hydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-6,11-dioxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-5-yl ester, [1aR-(1aa,2a,5ß,5aß,8aa,9a,10aa)]-	1.71	*bx*; *ox* Chionis *et al*., 2016; Astiti & Ramona, 2021	lipids; fatty acids; lauric acids [MeSH] lipids; fatty acids; dodecanoid acid [ChEBI] fatty acid related compounds; fatty acids [KEGG: phytochemical compounds]
16	26.24	$C_{24}H_{34}O_6$	butanoic acid, 1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, [1aR-(1aa,2a,5ß,5aß,6ß,8aa,9a,10aa)]-	0.71	*cx*; *bx* Kennedy *et al*., 2019; Almodarresiyeh *et al*., 2022	carboxylic acids; acyclic acids; butyric acid [MeSH] lipids; fatty acids; straight-chain fatty acids [ChEBI] fatty acid related compounds; fatty acids [KEGG: phytochemical compounds]
17	26.59	$C_{32}H_{39}NO_{10}$	3-pyridinecarboxylic acid, 2,7,10-tris(acetyloxy)-1,1a,2,3,4,6,7,10,11,11a-decahydro-1,1,3,6,9-pentamethyl-4-oxo-4a,7a-epoxy-5H-cyclopenta[a]cyclopropa[f]cycloundecen-11-yl ester, [1aR-(1aR*,2R*,3S*,4aR*,6S*,7S*,7aS*,8E,10R*,11R*,11aS*)]-	0.07	*ox* Moussaoui *et al*., 2022	diterpenoids [CAS reg. number: 51906-00-4]
18	28.01	$C_{22}H_{28}O_6$	quassin	2.48	*x*	hydrocarbons; terpenes;

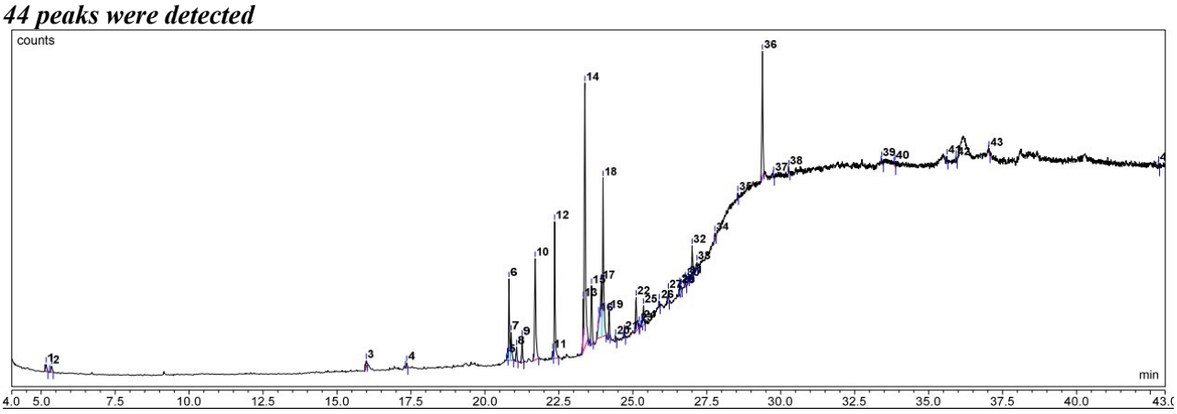
GC-MS
Chromatograms

19	28.56	$C_{36}H_{69}NO_6Si_3$	methyl glycocholate, 3TMS derivative	0.13	*ox* Mustanir *et al*., 2021; Mirzaei & Fazeli, 2022; Abdelsattar *et al*., 2022	triterpenes; quassins; quassin [MeSH] glycinated bile acids and derivatives [PubChem CID 22214169] alcohols; secondary alcohols; 3beta-hydroxy steroids [ChEBI] terpenoids; steroids [KEGG: phytochemical compounds]
20	36.11	$C_{29}H_{48}O$	stigmasterol	3.26	*v* Alawode *et al*., 2021; Ashraf & Bhatti, 2021; Bakrim *et al*., 2022	
21	38.62	$C_{16}H_{50}O_7Si_8$	1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyloctasiloxane	0.09	*x*	siloxanes [CAS reg. number: 19095-24-0]

RT = retention time; ox = antioxidants/radical scavenging activity; bx = antibacterial/antimicrobial; cx = cytotoxicity/anticancer/antiproliferative/anticarcinogenic; x = no activity reported related to ox, bx, and cx; v = ox, bx, and cx activities reported.

C. Leaf Methanol (LM)

44 peaks were detected



----------Identified pytochemical compounds

No	RT (min)	Chemical formula	Organic compounds	Relative area (%)	Bioactivities	Classifications
1	17.36	$C_{30}H_{48}O_2$	ergosta-5,22-dien-3-ol, acetate, (3ß,22E)-(brassicasterol)	0.28	*cx*; *ox* Byju *et al*., 2014; Suleimen *et al*., 2021; Hazra *et al*., 2023	terpenoids; cholestane steroids [LOTUS]
2	20.82	$C_{20}H_{38}$	neophytadiene	4.48	*ox*; *bx* Venkata *et al*., 2012; Bawamenewi *et al*., 2016; Ceyhan-Güvensen & Keskin, 2016; Pratama *et al*., 2019; Bhardwaj *et al*., 2020; Ngobeni *et al*., 2020	hydrocarbons; olefins; acyclic olefins [ChEBI] terpenoids; phytane diterpenoids [LOTUS]
3	21.70	$C_{17}H_{34}O_2$	methyl palmitate	8.28	*ox*; *bx* Pinto *et al*., 2017; Hamed *et al*., 2020; Astiti & Ramona, 2021	lipids; fatty acids; palmitic acids; palmitates [MeSH] fatty acids; palmitic acids [MeSH] lipids; fatty acid derivatives;
4	22.36	$C_{18}H_{36}O_2$	ethyl palmitate	8.55	*ox* Bu *et al*., 2012; Alghamdi *et al*., 2018	

5	23.33	$C_{19}H_{34}O_2$	7,10-octadecadienoic acid, methyl ester	1.71	*x*	fatty acid esters [ChEBI] fatty acyls; short fatty esters [LIPID MAPS] lineolic acids and derivatives [CAS reg. number: 56554-24-6]
6	23.38	$C_{19}H_{36}O_2$	trans-13-octadecenoic acid, methyl ester	22.13	*cx* Krishnamoorthy & Subramaniam, 2014; Reddy *et al*., 2020	fatty acid methyl esters [CAS reg. number: 56554-47-3] fatty esters; fatty acid methyl esters [CAS reg. number: 5129-61-3] fatty acids; wax monoesters [LOTUS]
7	23.60	$C_{19}H_{38}O_2$	methyl isostearate	3.80	*x*	terpenoids; cholane steroids [LOTUS] lipids; fatty acids; unsaturated fatty acids; essential fatty acids; linoleic acids [MeSH] lipids; fatty acid derivatives; fatty acid esters; fatty acid ethyl esters [ChEBI] lipids; glycerolipids; glycerides; diglycerides; 1,2-diglycerides [ChEBI] fatty acids; diacylglycerols [LOTUS] lipids and lipid like molecules; fatty acyls; fatty acid esters; fatty acid methyl esters [HMDB0031018]
8	23.85	$C_{26}H_{44}O_5$	ethyl iso-allocholate	0.60	*v* Malathi *et al*., 2016; Ojo *et al*., 2022; Ibrahim *et al*., 2022	
9	24.00	$C_{20}H_{34}O_2$	ethyl linolenate	12.04	*x*	
10	25.11	$C_{35}H_{68}O_5$	1,2-dipalmitoyl-sn-glycerol	2.68	*x*	
11	25.36	$C_{24}H_{46}O_2$	methyl 12-(2-octylcyclopropyl) dodecanoate	1.29	*ox*; *bx* Al-Rubaye *et al*., 2017	
12	27.01	$C_{24}H_{36}O_6$	8,14-seco-3,19-epoxyandrostane-8,14-dione, 17-acetoxy-3ß-methoxy-4,4-dimethyl-	1.77	*cx* Gupta & Gupta, 2017	ketals [PubChem CID 550132]
13	27.17	$C_{27}H_{40}O_4$	spirost-8-en-11-one, 3-hydroxy-, (3ß,5a,14ß,20ß,22ß,25 R)-	0.43	*v* Altameme *et al*., 2015; Marhamati *et al*., 2021; Jalil *et al*., 2022	11-oxosteroids [CAS reg. number: 54965-96-7]

14	42.78	$C_{16}H_{50}O_7Si_8$	1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyloctasiloxane	0.26	*x*	siloxanes [CAS reg. number: 19095-24-0]

RT = retention time; ox = antioxidants/radical scavenging activity; bx = antibacterial/antimicrobial; cx = cytotoxicity/anticancer/antiproliferative/anticarcinogenic; x = no activity reported related to ox, bx, and cx; v = ox, bx, and cx activities reported.

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