

Table S1. Chemical structures obtained in Methanolic extract of *C. crassa*.

No.	Name of the Chemical Compound	Structures	Kovats Index (iu) in Present Study	Active Phase	Kovats Index Value from the Previous Study	Reference
1.	Tritriacontane, 13-decyl-13-heptyl-		4907	DB-5MS	500.99	[1]
2.	Hexadecane		1612	DB-5MS	268.29	[2]
				DB-5MS	272.02	[2]
3.	Hydroperoxide, 1-methylhexyl		1013	-	-	-
4.	Oxalic acid, isobutyl nonyl ester		1783	-	-	-
5.	Dodecanoic acid, 1,2,3-propanetriyl ester		4336	-	-	-
6.	Phthalic acid, 6-ethyl-3-octyl butyl ester		2505	5% Phenyl methyl siloxane	2209	[3]

(iu: index unit).

Table S2. Details of Phytochemicals identified through GC-MS Analysis of Methanolic Extract.

No.	Name of the Chemical Compound	Structures	Kovats Index (iu) in Present Study	Active Phase	Kovats Index Value from the Previous Study	Reference
1.	n-Hexadecanoic acid		1968	BP-1	1961.	[4]
				HP-5MS	1964	[5]
				DB-5	1972	[6]
				SE-30	1940	[7]
				HP-5	1970	[8]
				RTX-1	1942	[9]
2.			1702	HP-5 MS	1708	[10]

	Oxiran e, tetradecyl-		TR-5 MS	1676	[11]	
3.	Oleic Acid		HP-5 HP-5MS <u>DB-5</u> <u>DB-Wax</u>	2144 2141 2161 3184	[12] [13] [14] [15]	
4.	9,12- Octadecadi enoic acid [Z]-, phenylmeth yl ester		2766	HP-5MS	2764.5	[16]
5.	5- Methyl-Z-5- docosene		2292	-	-	-
6.	Ergost- 5-en-3-ol, acetate, [3β,24R]-		2771	OV-1 OV-1	3323 3278	[17] [17]
7.	Stigma stan-6,22- dien, 3,5- dedihydro-		2437	-	-	-
8.	6,9,12- Octadecatri enoic acid, phenylmeth yl ester, [Z,Z,Z]-		2774	HP-5	2702	[18]
9.	Trideca noidal		1690	HP-5	2229	[19]
10.	9,10- Secocholest a-5,7,10[19]- triene- 3,24,25- triol, [3β,5Z,7E]-		3124	-	-	-
11.	Stigma stan-3,5- diene		2525	OV-101	3040	[20]
12.	6- Octadeceno ic acid, methyl ester, [Z]-		2085	VF-5MS	2104.5	[21]
13.	9- Octadeceno ic acid [Z]-,		2758	OV-101 CP Sil 5 CB DB-1	2074.7 2072 2085	[22] [23] [24]

phenylmeth yl ester		SE-30	2081	[25]
		DB-5	2085	[26]
14. Z-8- Methyl-9- tetradeceno ic acid		1813	-	-
15. E-11- Tetradecen ol, trimethylsil yl ether		1705	-	-

(iu: index unit).

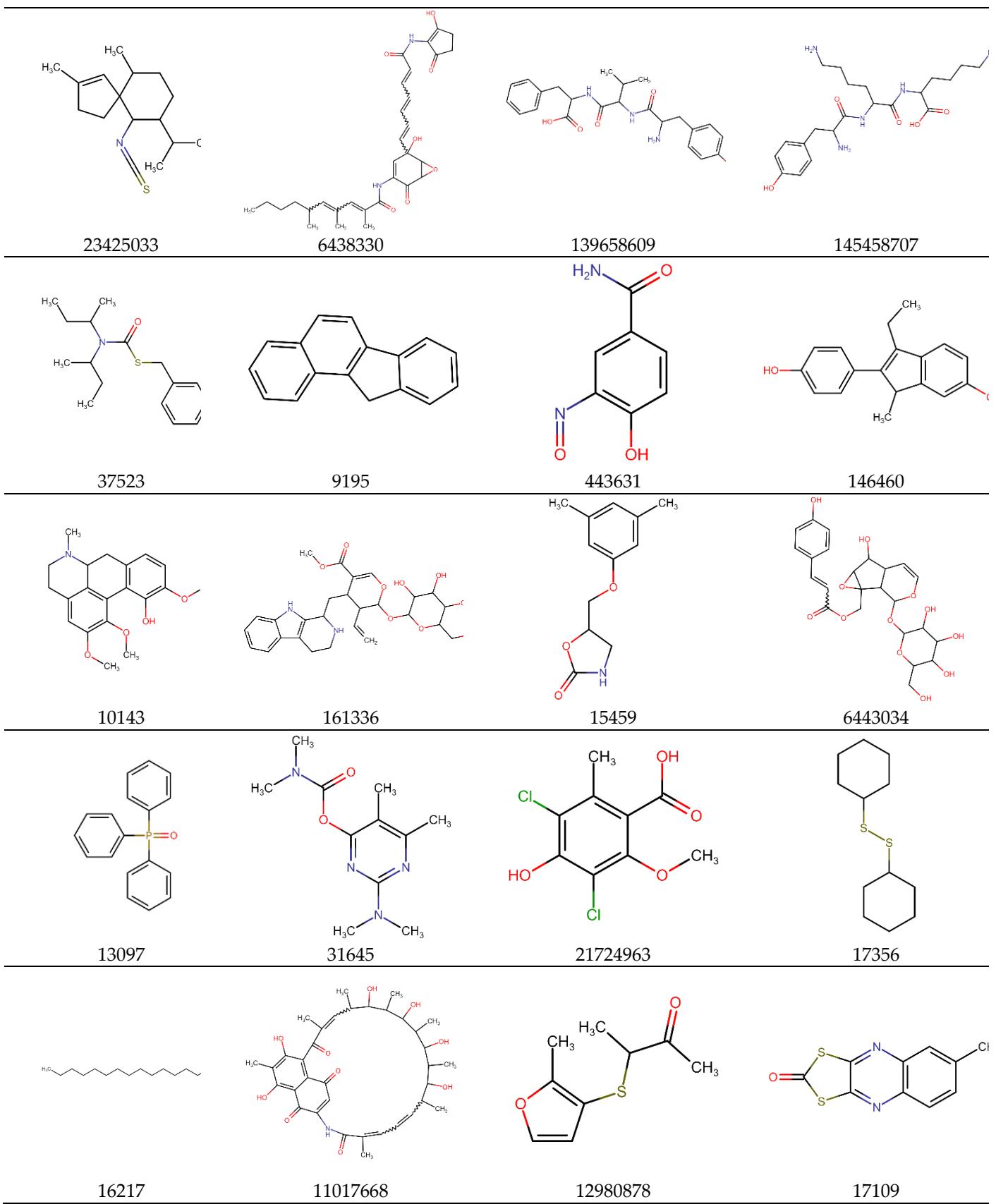
Table S3. Chemical structures of carbohydrate derivatives obtained by HRLCMS-QTOF in *C. crassa*.

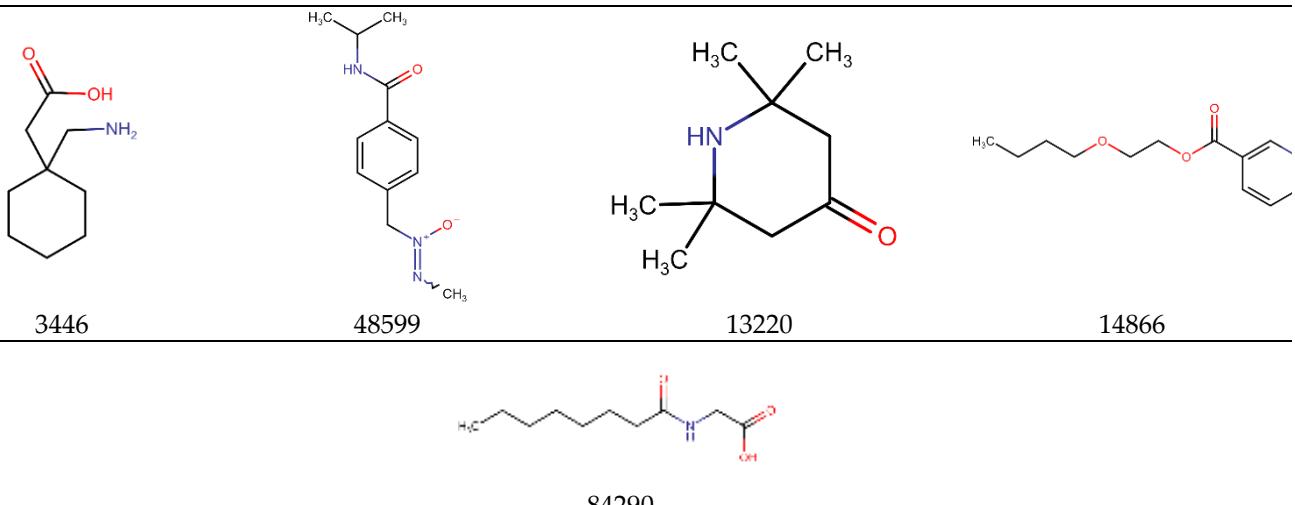
10753054	198272	16069998	156269
102331585	23622616	54676871	

(Each obtained chemical structure labeled with its PubChem ID; PubChem ID tabulated in Table 6).

Table S4. Chemical structures obtained by HRLCMS-QTOF in *C. crassa*.

14866	107982	122121	5312303





(Each obtained chemical structure labeled with its PubChem ID; PubChem ID tabulated in Table 7).

Reference

- Chen, P.H.; Keeran, W.S.; Van Ausdale, W.A.; Schindler, D.R.; Roberts, D.W. Application of Lee retention indices to the confirmation of tentatively identified compounds from GC/MS analysis of environmental samples. In Proceedings of the Ninth Annual Waste Testing and Quality Assurance Symposium, Washington, DC, USA, July 12-16, 1993.
- Chen, P.H.; Keeran, W.S.; Van-Ausdale, W.A.; Schindler, D.R.; Roberts, D.W. Technical paper, Analytical Services Division; Environmental Science and Engineering, Inc., PO Box 1703, Gainesville, FL 32602, 11(2002).
- Zaikin, V.G. Chromatography-mass spectrometry. *J. Anal. Chem.* **2011**, *66*, 1090–1094.
- Raina, V.K.; Verma, S.C.; Dhawan, S.; Khan, M.; Ramesh, S.; Singh, S.C.; Yadav, A.; Srivastava, S.K. Essential oil composition of *Murraya exotica* from the plains of northern India. *Flavour Fragr. J.* **2006**, *21*, 140–142. <https://doi.org/10.1002/ffj.1547>.
- Asuming, W.A.; Beauchamp, P.S.; Descalzo, J.T.; Dev, B.C.; Dev, V.; Frost, S.; Ma, C.W. Essential oil composition of four *Lomatium Raf.* species and their chemotaxonomy. *Biochem. Syst. Ecol.* **2005**, *33*, 17–26. <https://doi.org/10.1016/j.bse.2004.06.005>.
- Morteza-Semnani, K.; Azadbakht, M.; Goodarzi, A. The essential oils composition of *Phlomis herba-venti* L. leaves and flowers of Iranian origin. *Flavour Fragr. J.* **2004**, *19*, 29–31.
- Jantan, I.; Ahmad, A.S.; Ahmad, A.R.; Ali, N.A.M.; Ayop, N. Chemical Composition of Some Citrus Oils from Malaysia. *J. Essent. Oil Res.* **1996**, *8*, 627–632. <https://doi.org/10.1080/10412905.1996.9701030>.
- Stojanovic, G.; Palic, R.; Alagic, S.; Zeković, Z. Chemical composition and antimicrobial activity of the essential oil and CO₂ extracts of semi-oriental tobacco, Otlja. *Flavour Fragr. J.* **2000**, *15*, 335–338. [https://doi.org/10.1002/1099-1026\(200009/10\)15:5;3.co;2-n](https://doi.org/10.1002/1099-1026(200009/10)15:5;3.co;2-n).
- Paolini, J.; Muselli, A.; Bernardini, A.-F.; Bighelli, A.; Casanova, J.; Costa, J. Thymol derivatives from essential oil of *Doronicum corsicum* L. *Flavour Fragr. J.* **2007**, *22*, 479–487. <https://doi.org/10.1002/ffj.1824>.
- Xu, L.-L.; Han, T.; Wu, J.-Z.; Zhang, Q.-Y.; Zhang, H.; Huang, B.-K.; Rahman, K.; Qin, L.-P. Comparative research of chemical constituents, antifungal and antitumor properties of ether extracts of *Panax ginseng* and its endophytic fungus. *Phytomedicine* **2009**, *16*, 609–616. <https://doi.org/10.1016/j.phymed.2009.03.014>.
- Kurashov, E.A.; Mitrukova, G.G.; Krylova, Y.V. Dynamics of essential oil composition in *Ceratophyllum demersum* (Ceratophyllaceae) during vegetation. *Rastit. Resur.* **2014**, *50*, 132–144.
- Leffingwell, J.C.; Alford, E.D. Volatile constituents of perique tobacco. *Electron. J. Environ. Agric. Food Chem.* **2005**, *4*, 899–915.
- Pino, J.A.; Mesa, J.; Muñoz, Y.; Martí, M.P.; Marbot, R. Volatile Components from Mango (*Mangifera indica* L.) Cultivars. *J. Agric. Food Chem.* **2005**, *53*, 2213–2223. <https://doi.org/10.1021/jf0402633>.
- A Priestap, H.; van Baren, C.M.; Lira, P.D.L.; Coussio, J.; Bandoni, A.L. Volatile constituents of *Aristolochia argentina*. *Phytochemistry* **2003**, *63*, 221–225. [https://doi.org/10.1016/s0031-9422\(02\)00751-3](https://doi.org/10.1016/s0031-9422(02)00751-3).
- Chung, T.Y.; Eiserich, J.P.; Shibamoto, T. Volatile compounds produced from peanut oil heated with different amounts of cysteine. *J. Agric. Food Chem.* **1994**, *42*, 1743–1746. <https://doi.org/10.1021/jf00044a032>.
- Andriamaharavo, N.R. 2014, Retention data. NIST Mass Spectrometry Data Center. Available online: <https://webbook.nist.gov/cgi/inchi?ID=C60045274&Mask=2000> (accessed on November 16, 2021).
- Itoh, T.; Tani, H.; Fukushima, K.; Tamura, T.; Matsumoto, T. Structure-retention relationship of sterols and triterpene alcohols in gas chromatography on a glass capillary column. *J. Chromatogr. A* **1982**, *234*, 65–76. [https://doi.org/10.1016/s0021-9673\(00\)81781-1](https://doi.org/10.1016/s0021-9673(00)81781-1).

18. Zhao, Y.-P.; Wang, X.-Y.; Wang, Z.-C.; Lu, Y.; Fu, C.-X.; Chen, S.-Y. Essential oil of *Actinidia macrosperma*, a catnip response kiwi endemic to China. *J. Zhejiang Univ. Sci. B* **2006**, *7*, 708–712. <https://doi.org/10.1631/jzus.2006.b0708>.
19. Zeng, Q.Y.; Wu, J.; Lin, P.C. Chemical Composition and Antimicrobial Activity of the Essential Oil from *Epilobium angustifolium*. *Chem. Nat. Compd.* **2016**, *52*, 1113–1115. <https://doi.org/10.1007/s10600-016-1878-y>.
20. Velisek, J.; Davidek, J.; Kubelka, V. Formation of DELTA.3,5-diene and 3-chloro DELTA.5-ene analogs of sterols in protein hydrolysates. *J. Agric. Food Chem.* **1986**, *34*, 660–662. <https://doi.org/10.1021/jf00070a017>.
21. Tret'yakov, K.V. Retention Data NIST Mass Spectrometry Data Center. 2007. Available online: <http://webbook.nist.gov/cgilib/book.cgi> (accessed on November 18, 2021).
22. Kittiratanapiboon, K.; Jeyashoke, N.; Krisnangkura, K. The Relationship of Kováts Retention Indices and Equivalent Chain Lengths of Fatty Acid Methyl Esters on a Methyl Silicone Capillary Column. *J. Chromatogr. Sci.* **1998**, *36*, 361–364.
23. Hanai, T.; Hong, C. Structure-retention correlation in CGC. *J. High Resolut. Chromatogr.* **1989**, *12*, 327–332. <https://doi.org/10.1002/jhrc.1240120517>.
24. Golovnya, R.V.; Kuzmenko, T.E. Thermodynamic evaluation of the interaction of fatty acid methyl esters with polar and non-polar stationary phases, based on their retention indices. *Chromatographia* **1977**, *10*, 545–548. <https://doi.org/10.1007/bf02262915>.
25. Golovnya, R.; Uralets, V.; Kuzmenko, T. Characterization of fatty acid methyl esters by gas chromatography on siloxane liquid phases. *J. Chromatogr. A* **1976**, *121*, 118–121. [https://doi.org/10.1016/s0021-9673\(00\)82312-2](https://doi.org/10.1016/s0021-9673(00)82312-2).
26. Wu, S.; Zorn, H.; Krings, U.; Berger, R.G. Volatiles from submerged and surface-cultured beefsteak fungus, *Fistulina hepatica*. *Flavour Fragr. J.* **2007**, *22*, 53–60. <https://doi.org/10.1002/ffj.1758>.