

Role of sulfur compounds in vegetable and mushroom aroma

Monika A. Marcinkowska, and Henryk H. Jeleń*

Faculty of Food Science and Nutrition, Poznań University of Life Sciences, Wojska

Polskiego 31, 60-624 Poznań, Poland; monika.marcinkowska@up.poznan.pl

* Correspondence: henrykj@up.poznan.pl; Tel.: +48-618-487-273

Supplementary file

Table S1. Variety of sulfur compounds in vegetables and mushrooms.

Class of Sulfur Compound	Name	Occurrence in vegetable (family)	Odor quality	Reference
Isothiocyanates	allyl isothiocyanate	Brassicaceae	pungent, onion-like	[1,2]
	3-but enyl isothiocyanate	Brassicaceae	pungent, garlic-like	[1,2]
	benzyl isothiocyanate	Brassicaceae	herb-like, sweaty, pungent	[1,2]
	1-isothiocyanato-4-(methylsulfanyl)butane	Brassicaceae	mushroom-like, broth-like	[1]
	(2-isothiocyanatoethyl)benzene	Brassicaceae	broth-like, vegetable-like	[1]
	isopropyl isothiocyanate	Brassicaceae	pungent, grassy	[3]
	sec-butyl isothiocyanate	Brassicaceae	radish-like, vegetative	[3]
	isobutyl isothiocyanate	Brassicaceae	cooked, pungent, sulphury	[3]
	butyl isothiocyanate	Brassicaceae	peppery, sulphurous, oniony	[3]
	isoamyl isothiocyanate	Brassicaceae	pungent, grassy	[3]
Nitriles and Epithionitriles	4-pentenyl isothiocyanate	Brassicaceae	pungent, peppery, sulphurous, musty	[3]
	pentyl isothiocyanate	Brassicaceae	cabbage, green, rotten	[3]
	octyl isothiocyanate	Brassicaceae	green, vegetative	[3]
	3-hydroxy-4-pentanenitrile	Brassicaceae	nf	[4]
	β-hydroxy-thiiranepropanenitrile	Brassicaceae	nf	[4]
	3-butenenitrile	Brassicaceae	grassy, pungent	[4]
	2-butenenitrile	Brassicaceae	pungent	[5]

	thiiraneacetonitrile	<i>Brassicaceae</i>	sweaty, onion-like, pungent	[2–4]
	4-pantanenitrile	<i>Brassicaceae</i>	nf	[4]
	3-pantanenitrile	<i>Brassicaceae</i>	pungent	[5]
	thiiranepropanenitrile	<i>Brassicaceae</i>	nf	[4]
	5-hexanenitrile	<i>Brassicaceae</i>	pungent	[4,5]
	thiiranebutanenitrile	<i>Brassicaceae</i>	nf	[4]
	phenyl-3-propanenitrile	<i>Brassicaceae</i>	nasturtium	[4,6]
	3-methyl-3-butenenitrile	<i>Brassicaceae</i>	nf	[5]
	5-(methanesulfinyl)pentanenitrile	<i>Brassicaceae</i>	broth-like, onion-like, sulfurous	[1]
	4-(methylsulfanyl)butanenitrile	<i>Brassicaceae</i>	broth-like, garlic-like, sulfurous	[1]
	5-(methylsulfanyl)pentanenitrile	<i>Brassicaceae</i>	broccoli-like, cabbage-like	[1]
	phenylacetonitrile	<i>Brassicaceae</i>	mushroom-like	[1]
	5-methylhexanenitrile	<i>Brassicaceae</i>	nf	[3]
	6-heptenenitrile	<i>Brassicaceae</i>	nf	[3]
	benzenepropanenitrile	<i>Brassicaceae</i>	herbal, green, floral	[3]
Sulfides and Polysulfides	hydrogen sulfide	<i>Brassicaceae,</i> <i>Caprifoliaceae,</i> <i>Amaranthaceae</i>	rotten eggs	[7,8]
	dimethyl sulfide	<i>Brassicaceae,</i> <i>Amaryllidaceae,</i> <i>Caprifoliaceae,</i> <i>Amaranthaceae,</i> <i>Asteraceae,</i> <i>Solanaceae,</i> <i>Tuberaceae</i>	cooked asparagus-like, putrid	[7–13]
	dimethyl disulfide	<i>Brassicaceae,</i> <i>Amaryllidaceae,</i> <i>Solanaceae,</i> <i>Tuberaceae</i>	cabbage-like, sulfuric	[1,7,11–14]
	dimethyl trisulfide	<i>Brassicaceae,</i> <i>Amaryllidaceae,</i> <i>Fabaceae,</i> <i>Solanaceae,</i> <i>Tuberaceae</i>	sulfuric, cabbage-like	[1,7,10,12–14]
	dimethyl tetrasulfide	<i>Amaranthaceae</i>	cabbage-like, rotten	[7,15]
	methyl 2-methyl-3-furyl disulfide	<i>Brassicaceae</i>	meat-like, cabbage-like	[1]
	methyl propyl disulfide	<i>Amaryllidaceae</i>	onion-like	[7,16]
	propyl allyl disulfide	<i>Amaryllidaceae</i>	onion-like	[16,17]
	dipropyl disulfide	<i>Amaryllidaceae</i>	onion-like	[7,16]
	methyl propyl trisulfide	<i>Amaryllidaceae</i>	onion-like, cabbage-like	[7,16]
	dipropyl trisulfide	<i>Amaryllidaceae</i>	onion-like, metallic	[7,16]

	2-propenyl propyl trisulfide	<i>Amaryllidaceae</i>	onion-like	[16,17]
	ethyl methyl disulfide	<i>Amaryllidaceae, Solanaceae</i>	white truffles-like	[11,14,18]
	diallyl sulfide	<i>Amaryllidaceae</i>	garlic-like	[7,14]
	allyl methyl disulfide	<i>Amaryllidaceae</i>	garlic-like	[7,14]
			sulphurous,	
	ethyl propyl disulfide	<i>Amaryllidaceae</i>	green, vegetable-like	[6,14]
	butyl methyl disulfide	<i>Amaryllidaceae</i>	nf	[14]
	ethyl methyl trisulfide	<i>Amaryllidaceae</i>	garlic-like, green, onion-like	[6,14]
	diallyl disulfide	<i>Amaryllidaceae</i>	garlic-like	[7,14]
	dipropyl disulfide	<i>Amaryllidaceae</i>	onion-like	[7,14]
	allyl methyl trisulfide	<i>Amaryllidaceae</i>	garlic-like	[7,14]
	methyl propyl trisulfide	<i>Amaryllidaceae</i>	onion-like, cabbage-like	[7,14]
	dimethyl tetrasulfide	<i>Amaryllidaceae</i>	sulfurous	[6,14]
	butyl methyl trisulfide	<i>Amaryllidaceae</i>	nf	[14]
	diallyl trisulfide	<i>Amaryllidaceae</i>	garlic-like	[7,14]
	dipropyl trisulfide	<i>Amaryllidaceae</i>	onion-like, metallic	[7,14]
	methyl pentyl tetrasulfide	<i>Amaryllidaceae</i>	nf	[14]
	dipropyl tetrasulfide	<i>Amaryllidaceae</i>	cooked onion-like	[7,14]
	allyl propyl tetrasulfide	<i>Amaryllidaceae</i>	nf	[14]
	propyl methyl pentasulfide	<i>Amaryllidaceae</i>	nf	[14]
	bis(methylthio)methane	<i>Tuberaceae</i>	white truffle-like	[12,13]
	pentane-1-thiol	<i>Brassicaceae</i>	burned, rubber-like	[1]
	(1S)-1-phenylethane-1-thiol	<i>Brassicaceae</i>	burned	[1]
	2-phenylethane-1-thiol	<i>Brassicaceae</i>	rubber-like	[1]
	1-propanethiol	<i>Amaryllidaceae</i>	leek-like, onion-like	[17]
	2-propene-1-thiol	<i>Amaryllidaceae</i>	garlic-like	[10]
Thiols	methanethiol	<i>Brassicaceae, Caprifoliaceae, Amaranthaceae, Solanaceae, Tuberaceae</i>	sulfurous, gasoline-like, garlic-like	[8,11,13,19]
	ethanethiol	<i>Solanaceae</i>	rotten, onion-like	[7,11]
	butanethiol	<i>Solanaceae</i>	garlic-like, burned, rubber-like	[7,11]
	1-menthen-8-thiol	<i>Brassicaceae</i>	grape-like, resinous, woody	[20]
		<i>Brassicaceae, Liliaceae, Tuberaceae</i>	cooked potato-like	[1,21,22]
Miscellaneous	methionol	<i>Brassicaceae, Amaryllidaceae</i>	cooked potato-like	[7,12,13,23–25]
	methional			

thiophene-2-carbaldehyde	<i>Solanaceae,</i> <i>Tuberaceae</i>		
4-methyl-5-thiazoleethanol	<i>Brassicaceae</i>	roasty	[1]
dimethyl sulfone	<i>Brassicaceae</i>	broth-like, sulfurous, nutty	[1]
dimethyl sulfoxide	<i>Brassicaceae</i> , <i>Asteraceae,</i> <i>Tuberaceae</i>	sulfurous garlic-like, mushroom-like	[19],[9,19,22]
1,3-thiazole	<i>Brassicaceae</i>	roasty	[5]
5-methyl-1,3-thiazole	<i>Brassicaceae</i>	roasty, meat-like	[5]
5-ethyl-1,3-thiazole	<i>Brassicaceae</i>	roasty	[5]
2-methyl-3-furanthiol	<i>Brassicaceae,</i> <i>Tuberaceae</i>	meat-like, onion-like	[5,12]
S-methyl thioacetate	<i>Liliaceae</i>	warm, cooked-like	[21]
2,4-dimethylthiophene	<i>Amaryllidaceae</i>	nf	[16]
2,5-dimethylthiophene	<i>Amaryllidaceae</i>	nutty, sulfurous	[6,16]
3,4- or 2,4-dimethyl thiophen	<i>Amaryllidaceae</i>	wood, dry smell, green, bookstore	[17]
2-acetylthiazole	<i>Brassicaceae,</i> <i>Solanaceae</i>	roasty, popcorn-like	[1,7,11]
benzothiazole	<i>Brassicaceae,</i> <i>Asteraceae,</i> <i>Solanaceae</i>	rubber-like, cabbage-like	[1,9,11]
cycloalliin	<i>Amaryllidaceae</i>	nf	[26]
S-methyl-L-cysteine sulfoxide (methiin)	<i>Brassicaceae,</i> <i>Amaryllidaceae</i>	odourless	[26–28]
S-propyl-L-cysteine sulfoxide (propiin)	<i>Amaryllidaceae</i>	odourless	[26,27]
S-allyl-L-cysteine sulfoxides (alliine)	<i>Amaryllidaceae</i>	odourless	[26,27]
S-propenyl-1-L-cysteine sulfoxides (isoalliin)	<i>Amaryllidaceae</i>	odourless	[26,27]
2-propenyl sulfenic acid	<i>Amaryllidaceae</i>	nf	[29]
(E)-1-propenyl sulfenic acid	<i>Amaryllidaceae</i>	nf	[29]
diallyl thiosulfinate (allicin)	<i>Amaryllidaceae</i>	freshly crushed garlic-like	[30]
methylmethanethiosulfinate	<i>Brassicaceae,</i> <i>Amaryllidaceae</i>	freshly cut onion-like	[27,31]
1-propenyl thiosulfinates	<i>Amaryllidaceae</i>	freshly cut onion-like	[27,31]
3-vinyl-4H-1,2-dithiin	<i>Amaryllidaceae</i>	garlic-like	[23]
2-vinyl-4H-1,3-dithiin	<i>Amaryllidaceae</i>	pungent, garlic-like	[23]
5-methyl-2-thiophenecarboxaldehyde	<i>Amaryllidaceae</i>	aniseed-like	[23]
1,2,4-trithiolane	<i>Omphalotaceae</i>	sulfury, onion-like	[7,32]
1,2,4,5-tetrathiane	<i>Omphalotaceae</i>	sulfury, burned	[7,32]

lenthionine	<i>Omphalotaceae</i>	sulfury, burned	[32,33]
hexathiepane	<i>Omphalotaceae</i>	nf	[32]
cyclic octaatomiac sulfur	<i>Omphalotaceae</i>	nf	[32]
2-methyl-4,5-dihydrothiophene	<i>Tuberaceae</i>	aged cheese-like, rubber-like	[12,13]
3-methyl-4,5-dihydrothiophene	<i>Tuberaceae</i>	onion-like, truffle-like	[12]

nf, not found.

1. Marcinkowska, M.; Frank, S.; Steinhaus, M.; Jelení, H.H. Key Odorants of Raw and Cooked Green Kohlrabi (*Brassica oleracea* var. *gongylodes* L.). *J. Agric. Food Chem.* **2021**, *69*, 12270–12277, doi:10.1021/acs.jafc.1c04339.
2. Kroener, E.M.; Buettner, A. Sensory-analytical comparison of the aroma of different horseradish varieties (*Armoracia rusticana*). *Front. Chem.* **2018**, *6*, 1–11, doi:10.3389/fchem.2018.00149.
3. Bell, L.; Kitsopanou, E.; Oloyede, O.O.; Lignou, S. Important odorants of four brassicaceae species, and discrepancies between glucosinolate profiles and observed hydrolysis products. *Foods* **2021**, *10*, doi:10.3390/foods10051055.
4. Collett, M.G.; Stegelmeier, B.L.; Tapper, B.A. Could nitrile derivatives of turnip (*Brassica rapa*) glucosinolates be hepato- or cholangiotoxic in cattle? *J. Agric. Food Chem.* **2014**, *62*, 7370–7375, doi:10.1021/jf500526u.
5. Jia, X.; Wang, L.; Zheng, C.; Yang, Y.; Wang, X.; Hui, J.; Zhou, Q. Key Odorant Differences in Fragrant *Brassica napus* and *Brassica juncea* Oils Revealed by Gas Chromatography–Olfactometry, Odor Activity Values, and Aroma Recombination. *J. Agric. Food Chem.* **2020**, *68*, 14950–14960, doi:10.1021/acs.jafc.0c05944.
6. Nursten, H.E. *The Maillard Reaction*; The Royal Society of Chemistry, 2005; ISBN 978-0-85404-964-6.
7. Kreissl, J.; Mall, V.; Steinhaus, P.; Steinhaus, M. Leibniz-LSB@TUM Odorant Database, Version 1.0. Leibniz-Institute for Food Systems Biology at the Technical University of Munich: Freising, Germany Available online: <https://www.leibniz-lsb.de/en/databases/leibniz-lsb-tum-odorant-database> (accessed on May 18, 2021).
8. Dryahina, K.; Som, S.; Smith, D.; Španěl, P. Characterization of spoilage-related volatile organic compounds in packaged leaf salads. *Flavour Fragr. J.* **2020**, *35*, 24–33, doi:10.1002/ffj.3535.
9. Deza-Durand, K.M.; Petersen, M.A. Volatile compounds of modified atmosphere packaged cut iceberg lettuce: Effect of extremely low O₂, season, cultivar and storage time. *Food Res. Int.* **2014**, *62*, 254–261, doi:10.1016/j.foodres.2014.02.017.
10. Van Ruth, S.M.; Roozen, J.P.; Cozijnsen, J.L.; Posthumus, M.A. Volatile compounds of rehydrated French beans, bell peppers and leeks. Part II. Gas chromatography/sniffing port analysis and sensory evaluation. *Food Chem.* **1995**, *54*, 1–7, doi:10.1016/0308-8146(95)92655-4.

11. Dresow, J.F.; Böhm, H. The influence of volatile compounds of the flavour of raw, boiled and baked potatoes: Impact of agricultural measures on the volatile components. *Landbauforsch. Volkenrode* **2009**, *59*, 309–337.
12. Vahdatzadeh, M.; Deveau, A.; Splivallo, R. The role of the microbiome of truffles in aroma formation: A meta-analysis approach. *Appl. Environ. Microbiol.* **2015**, *81*, 6946–6952, doi:10.1128/AEM.01098-15.
13. Splivallo, R.; Ottonello, S.; Mello, A.; Karlovsky, P. Truffle volatiles: From chemical ecology to aroma biosynthesis. *New Phytol.* **2011**, *189*, 688–699, doi:10.1111/j.1469-8137.2010.03523.x.
14. Pino, J.A.; Fuentes, V.; Correa, M.T. Volatile constituents of Chinese chive (*Allium tuberosum* Rottl. ex Sprengel) and rakkkyo (*Allium chinense* G. Don). *J. Agric. Food Chem.* **2001**, *49*, 1328–1330, doi:10.1021/jf9907034.
15. Masanetz, C.; Guth, H.; Grosch, W. Fishy and hay-like off-flavours of dry spinach. *Eur. Food Res. Technol.* **1998**, *206*, 108–113.
16. Chung, M.S. Volatile compounds of the cultivated dumebuchu (*Allium senescens* L. var. *senescens*). *Food Sci. Biotechnol.* **2010**, *19*, 1679–1682, doi:10.1007/s10068-010-0238-0.
17. Nielsen, G.S.; Poll, L. Determination of Odor Active Aroma Compounds in Freshly Cut Leek (*Allium ampeloprasum* Var. Bulga) and in Long-Term Stored Frozen Unblanched and Blanched Leek Slices by Gas Chromatography Olfactometry Analysis. *J. Agric. Food Chem.* **2004**, *52*, 1642–1646, doi:10.1021/jf030682k.
18. Chemical Book. Available online: <https://www.chemicalbook.com/> (accessed on 18th January 2022).
19. Zhou, Q.; Tang, H.; Jia, X.; Zheng, C.; Huang, F.; Zhang, M. Distribution of glucosinolate and pungent odors in rapeseed oils from raw and microwaved seeds. *Int. J. Food Prop.* **2018**, *21*, 2296–2308, doi:10.1080/10942912.2018.1514632.
20. Hong, S.J.; Boo, C.G.; Lee, J.; Hur, S.W.; Jo, S.M.; Jeong, H.; Yoon, S.; Lee, Y.; Park, S.S.; Shin, E.C. Chemosensory approach supported-analysis of wintering radishes produced in Jeju island by different processing methods. *Food Sci. Biotechnol.* **2021**, *30*, 1033–1049, doi:10.1007/s10068-021-00948-2.
21. Ulrich, D.; Hoberg, E.; Bittner, T.; Engewald, W.; Meilchen, K. Contribution of volatile compounds to the flavor of cooked asparagus. *Eur. Food Res. Technol.* **2001**, *213*, 200–204, doi:10.1007/s002170100349.
22. Mustafa, A.M.; Angeloni, S.; Nzekoue, F.K.; Abouelenein, D.; Sagratini, G.; Caprioli, G.; Torregiani, E. An overview on truffle aroma and main volatile compounds. *Molecules* **2020**, *25*, 1–27, doi:10.3390/molecules25245948.
23. Abe, K.; Hori, Y.; Myoda, T. Characterization of key aroma compounds in aged garlic extract. *Food Chem.* **2020**, *312*, 126081, doi:10.1016/j.foodchem.2019.126081.
24. Jia, X.; Wang, L.; Zheng, C.; Yang, Y.; Wang, X.; Hui, J.; Zhou, Q. Key Odorant Differences in Fragrant *Brassica napus* and *Brassica juncea* Oils Revealed by Gas Chromatography-Olfactometry, Odor Activity Values, and Aroma Recombination. *J.*

Agric. Food Chem. **2020**, *68*, 14950–14960, doi:10.1021/acs.jafc.0c05944.

25. Bough, R.A.; Holm, D.G.; Jayanty, S.S. Evaluation of Cooked Flavor for Fifteen Potato Genotypes and the Correlation of Sensory Analysis to Instrumental Methods. *Am. J. Potato Res.* **2020**, *97*, 63–77, doi:10.1007/s12230-019-09757-0.
26. Goncharov, N.; Orekhov, A.N.; Voitenko, N.; Ukolov, A.; Jenkins, R.; Avdonin, P. *Organosulfur Compounds as Nutraceuticals*; Elsevier Inc., 2016; ISBN 9780128021477.
27. Olech, Z.; Zaborska, W.; Kot, M. Jack bean urease inhibition by crude juices of Allium and Brassica plants. Determination of thiosulfinate. *Food Chem.* **2014**, *145*, 154–160, doi:10.1016/j.foodchem.2013.08.044.
28. Rose, P.; Moore, P.K.; Whiteman, M.; Zhu, Y.Z. An appraisal of developments in Allium sulfur chemistry: Expanding the pharmacopeia of garlic. *Molecules* **2019**, *24*, 1–17, doi:10.3390/molecules24214006.
29. Yoshimoto, N.; Saito, K. S-Alk(en)ylcysteine sulfoxides in the genus Allium: Proposed biosynthesis, chemical conversion, and bioactivities. *J. Exp. Bot.* **2019**, *70*, 4123–4137, doi:10.1093/jxb/erz243.
30. Borlinghaus, J.; Foerster, J.; Kappler, U.; Antelmann, H.; Noll, U.; Gruhlke, M.C.H.; Slusarenko, A.J. Allicin, the odor of freshly crushed garlic: A review of recent progress in understanding allicin's effects on cells. *Molecules* **2021**, *26*, doi:10.3390/molecules26061505.
31. Løkke, M.M.; Edelenbos, M.; Larsen, E.; Feilberg, A. Investigation of volatiles emitted from freshly cut onions (*Allium cepa* L.) by real time proton-transfer reaction-mass spectrometry (PTR-MS). *Sensors (Switzerland)* **2012**, *12*, 16060–16076, doi:10.3390/s121216060.
32. Li, S.; Wang, A.; Liu, L.; Tian, G.; Wei, S.; Xu, F. Evaluation of nutritional values of shiitake mushroom (*Lentinus edodes*) stipes. *J. Food Meas. Charact.* **2018**, *12*, 2012–2019, doi:10.1007/s11694-018-9816-2.
33. Wang, S.L.; Lin, S.Y.; Du, H.T.; Qin, L.; Lei, L.M.; Chen, D. An insight by molecular sensory science approaches to contributions and variations of the key odorants in shiitake mushrooms. *Foods* **2021**, *10*, doi:10.3390/foods10030622.