

Supplementary Information

Machine Learning Models for Predicting Bioavailability of Traditional and Emerging Aromatic Contaminants in Plant Roots

**Siyuan Li, Yuting Shen, Meng Gao, Huatai, Song, Zhanpeng Ge,
Qiuyue Zhang, Jiaping Xu, Yu Wang*, Hongwen Sun***

MOE Key Laboratory of Pollution Processes and Environmental Criteria, College of
Environmental Science and Engineering, Nankai University, Tianjin 300350, China

Corresponding Authors:

*Nankai University, 38 Tongyan Road, Jinnan District, Tianjin 300350, China. Tel.:
+86 22 23509241.

E-mail: yu.wang@nankai.edu.cn (Y. Wang); sunhongwen@nankai.edu.cn (H. Sun)

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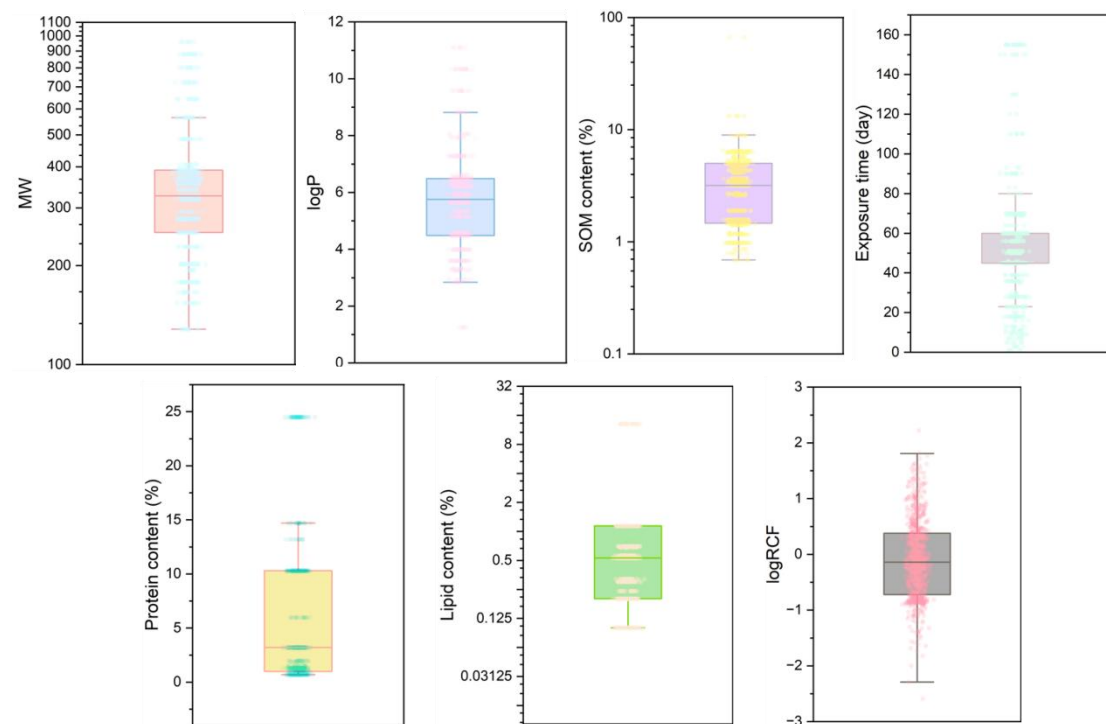


Figure S1 Variable distribution of RCF dataset

Table S1 The dataset of absorption behaviors of aromatic contaminants in plant root

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
Phenanthrene	178.23	0.79	Radish	0	64	0.7	0.1	-0.55	[96]
Fluorene	166.22	0.79	Radish	0	64	0.7	0.1	-0.10	[96]
Fluoranthene	202.25	0.79	Radish	0	64	0.7	0.1	0.58	[96]
Anthracene	178.23	0.79	Radish	0	64	0.7	0.1	-0.55	[96]
Dibutyl phthalate	390.6	0.79	Radish	0	64	0.7	0.1	-0.32	[96]
bis (2-ethylhexyl)phthalate	390.6	0.79	Radish	0	64	0.7	0.1	-1.52	[96]
Phenanthrene	178.23	1.45	Amaranth	0	45	13.2	0.32	-0.21	[97]
Phenanthrene	178.23	1.45	Amaranth	0	45	13.2	0.32	-0.57	[97]
Phenanthrene	178.23	1.45	Amaranth	0	45	13.2	0.32	-0.83	[97]
Phenanthrene	178.23	1.45	Amaranth	0	45	13.2	0.32	-0.86	[97]
Phenanthrene	178.23	1.45	Amaranth	0	45	13.2	0.32	-0.93	[97]
Phenanthrene	178.23	1.45	Amaranth	0	45	13.2	0.32	-0.87	[97]
Phenanthrene	178.23	1.45	Amaranth	0	45	13.2	0.32	-0.96	[97]
Pyrene	202.25	1.45	Amaranth	0	45	13.2	0.32	-0.83	[97]
Pyrene	202.25	1.45	Amaranth	0	45	13.2	0.32	-0.87	[97]
Pyrene	202.25	1.45	Amaranth	0	45	13.2	0.32	-0.99	[97]
Pyrene	202.25	1.45	Amaranth	0	45	13.2	0.32	-1.06	[97]
Pyrene	202.25	1.45	Amaranth	0	45	13.2	0.32	-1.09	[97]
Pyrene	202.25	1.45	Amaranth	0	45	13.2	0.32	-1.03	[97]
Pyrene	202.25	1.45	Amaranth	0	45	13.2	0.32	-1.08	[97]
Phenanthrene	178.23	1.45	Chinese cabbage	0	45	1.2	0.68	-0.57	[97]
Phenanthrene	178.23	1.45	Chinese cabbage	0	45	1.2	0.68	-0.54	[97]
Phenanthrene	178.23	1.45	Chinese	0	45	1.2	0.68	-0.55	[97]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
			cabbage						
Phenanthrene	178.23	1.45	Chinese cabbage	0	45	1.2	0.68	-0.85	[97]
Phenanthrene	178.23	1.45	Chinese cabbage	0	45	1.2	0.68	-0.88	[97]
Phenanthrene	178.23	1.45	Chinese cabbage	0	45	1.2	0.68	-0.88	[97]
Phenanthrene	178.23	1.45	Chinese cabbage	0	45	1.2	0.68	-0.92	[97]
Phenanthrene	178.23	1.45	Chinese cabbage	0	45	1.2	0.68	-1.03	[97]
Pyrene	202.25	1.45	Chinese cabbage	0	45	1.2	0.68	-0.26	[97]
Pyrene	202.25	1.45	Chinese cabbage	0	45	1.2	0.68	-0.13	[97]
Pyrene	202.25	1.45	Chinese cabbage	0	45	1.2	0.68	-0.25	[97]
Pyrene	202.25	1.45	Chinese cabbage	0	45	1.2	0.68	-0.24	[97]
Pyrene	202.25	1.45	Chinese cabbage	0	45	1.2	0.68	-0.24	[97]
Pyrene	202.25	1.45	Chinese cabbage	0	45	1.2	0.68	-0.25	[97]
Pyrene	202.25	1.45	Chinese cabbage	0	45	1.2	0.68	-0.33	[97]
Pyrene	202.25	1.45	Chinese cabbage	0	45	1.2	0.68	-0.38	[97]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
Phenanthrene	178.23	1.45	Ryegrass	0	45	24.5	0.32	-0.67	[97]
Phenanthrene	178.23	1.45	Ryegrass	0	45	24.5	0.32	-0.66	[97]
Phenanthrene	178.23	1.45	Ryegrass	0	45	24.5	0.32	-0.77	[97]
Phenanthrene	178.23	1.45	Ryegrass	0	45	24.5	0.32	-0.81	[97]
Phenanthrene	178.23	1.45	Ryegrass	0	45	24.5	0.32	-0.85	[97]
Phenanthrene	178.23	1.45	Ryegrass	0	45	24.5	0.32	-0.86	[97]
Phenanthrene	178.23	1.45	Ryegrass	0	45	24.5	0.32	-0.83	[97]
Phenanthrene	178.23	1.45	Ryegrass	0	45	24.5	0.32	-0.97	[97]
Pyrene	202.25	1.45	Ryegrass	0	45	24.5	0.32	-0.28	[97]
Pyrene	202.25	1.45	Ryegrass	0	45	24.5	0.32	-0.39	[97]
Pyrene	202.25	1.45	Ryegrass	0	45	24.5	0.32	-0.38	[97]
Pyrene	202.25	1.45	Ryegrass	0	45	24.5	0.32	-0.45	[97]
Pyrene	202.25	1.45	Ryegrass	0	45	24.5	0.32	-0.45	[97]
Pyrene	202.25	1.45	Ryegrass	0	45	24.5	0.32	-0.43	[97]
Pyrene	202.25	1.45	Ryegrass	0	45	24.5	0.32	-0.53	[97]
Pyrene	202.25	1.45	Ryegrass	0	45	24.5	0.32	-0.81	[97]
Acenaphthene	154.21	5.31	Wheat	0	45	10.3	1.14	0.56	[98]
Acenaphthene	154.21	1.41	Wheat	0	45	10.3	1.14	2.22	[98]
Acenaphthene	154.21	4.33	Wheat	0	45	10.3	1.14	0.89	[98]
Acenaphthene	154.21	2.70	Wheat	0	45	10.3	1.14	0.98	[98]
Acenaphthene	154.21	5.70	Wheat	0	45	10.3	1.14	0.32	[98]
Acenaphthene	154.21	2.60	Wheat	0	45	10.3	1.14	0.92	[98]
Acenaphthene	154.21	3.47	Wheat	0	45	10.3	1.14	0.48	[98]
Acenaphthene	154.21	5.30	Wheat	0	45	10.3	1.14	0.62	[98]
Acenaphthene	154.21	3.47	Wheat	0	45	10.3	1.14	0.54	[98]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
Acenaphthene	154.21	6.22	Wheat	0	45	10.3	1.14	0.32	[98]
Acenaphthene	154.21	4.80	Wheat	0	45	10.3	1.14	0.69	[98]
Acenaphthene	154.21	3.47	Wheat	0	45	10.3	1.14	0.54	[98]
Acenaphthene	154.21	2.67	Wheat	0	45	10.3	1.14	0.83	[98]
Acenaphthene	154.21	4.74	Wheat	0	45	10.3	1.14	0.75	[98]
Acenaphthene	154.21	4.15	Wheat	0	45	10.3	1.14	0.61	[98]
Anthracene	178.23	5.31	Wheat	0	45	10.3	1.14	0.13	[98]
Anthracene	178.23	1.41	Wheat	0	45	10.3	1.14	0.78	[98]
Anthracene	178.23	4.33	Wheat	0	45	10.3	1.14	1.14	[98]
Anthracene	178.23	2.70	Wheat	0	45	10.3	1.14	0.76	[98]
Anthracene	178.23	5.70	Wheat	0	45	10.3	1.14	0.30	[98]
Anthracene	178.23	2.60	Wheat	0	45	10.3	1.14	0.50	[98]
Anthracene	178.23	3.47	Wheat	0	45	10.3	1.14	0.67	[98]
Anthracene	178.23	5.30	Wheat	0	45	10.3	1.14	0.61	[98]
Anthracene	178.23	3.47	Wheat	0	45	10.3	1.14	0.05	[98]
Anthracene	178.23	6.22	Wheat	0	45	10.3	1.14	0.34	[98]
Anthracene	178.23	4.80	Wheat	0	45	10.3	1.14	0.71	[98]
Anthracene	178.23	3.47	Wheat	0	45	10.3	1.14	0.05	[98]
Anthracene	178.23	2.67	Wheat	0	45	10.3	1.14	1.03	[98]
Anthracene	178.23	4.74	Wheat	0	45	10.3	1.14	0.65	[98]
Anthracene	178.23	4.15	Wheat	0	45	10.3	1.14	0.71	[98]
Fluoranthene	202.25	5.31	Wheat	0	45	10.3	1.14	0.30	[98]
Fluoranthene	202.25	1.41	Wheat	0	45	10.3	1.14	1.01	[98]
Fluoranthene	202.25	4.33	Wheat	0	45	10.3	1.14	0.57	[98]
Fluoranthene	202.25	2.70	Wheat	0	45	10.3	1.14	1.00	[98]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
Fluoranthene	202.25	5.70	Wheat	0	45	10.3	1.14	0.55	[98]
Fluoranthene	202.25	2.60	Wheat	0	45	10.3	1.14	1.20	[98]
Fluoranthene	202.25	3.47	Wheat	0	45	10.3	1.14	0.74	[98]
Fluoranthene	202.25	5.30	Wheat	0	45	10.3	1.14	0.55	[98]
Fluoranthene	202.25	3.47	Wheat	0	45	10.3	1.14	0.50	[98]
Fluoranthene	202.25	6.22	Wheat	0	45	10.3	1.14	0.94	[98]
Fluoranthene	202.25	4.80	Wheat	0	45	10.3	1.14	1.30	[98]
Fluoranthene	202.25	3.47	Wheat	0	45	10.3	1.14	0.50	[98]
Fluoranthene	202.25	2.67	Wheat	0	45	10.3	1.14	1.04	[98]
Fluoranthene	202.25	4.74	Wheat	0	45	10.3	1.14	1.45	[98]
Fluoranthene	202.25	4.15	Wheat	0	45	10.3	1.14	1.51	[98]
Fluorene	166.22	5.31	Wheat	0	45	10.3	1.14	0.62	[98]
Fluorene	166.22	1.41	Wheat	0	45	10.3	1.14	0.96	[98]
Fluorene	166.22	4.33	Wheat	0	45	10.3	1.14	0.72	[98]
Fluorene	166.22	2.70	Wheat	0	45	10.3	1.14	1.14	[98]
Fluorene	166.22	5.70	Wheat	0	45	10.3	1.14	0.45	[98]
Fluorene	166.22	2.60	Wheat	0	45	10.3	1.14	1.11	[98]
Fluorene	166.22	3.47	Wheat	0	45	10.3	1.14	0.65	[98]
Fluorene	166.22	5.30	Wheat	0	45	10.3	1.14	0.60	[98]
Fluorene	166.22	3.47	Wheat	0	45	10.3	1.14	0.52	[98]
Fluorene	166.22	6.22	Wheat	0	45	10.3	1.14	0.34	[98]
Fluorene	166.22	4.80	Wheat	0	45	10.3	1.14	0.80	[98]
Fluorene	166.22	3.47	Wheat	0	45	10.3	1.14	0.52	[98]
Fluorene	166.22	2.67	Wheat	0	45	10.3	1.14	0.88	[98]
Fluorene	166.22	4.74	Wheat	0	45	10.3	1.14	-0.21	[98]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
Fluorene	166.22	4.15	Wheat	0	45	10.3	1.14	0.70	[98]
Naphthalene	128.17	5.31	Wheat	0	45	10.3	1.14	0.58	[98]
Naphthalene	128.17	1.41	Wheat	0	45	10.3	1.14	0.99	[98]
Naphthalene	128.17	4.33	Wheat	0	45	10.3	1.14	0.84	[98]
Naphthalene	128.17	2.70	Wheat	0	45	10.3	1.14	1.17	[98]
Naphthalene	128.17	5.70	Wheat	0	45	10.3	1.14	0.39	[98]
Naphthalene	128.17	2.60	Wheat	0	45	10.3	1.14	0.98	[98]
Naphthalene	128.17	3.47	Wheat	0	45	10.3	1.14	0.34	[98]
Naphthalene	128.17	5.30	Wheat	0	45	10.3	1.14	0.63	[98]
Naphthalene	128.17	3.47	Wheat	0	45	10.3	1.14	0.35	[98]
Naphthalene	128.17	6.22	Wheat	0	45	10.3	1.14	0.18	[98]
Naphthalene	128.17	4.80	Wheat	0	45	10.3	1.14	0.56	[98]
Naphthalene	128.17	3.47	Wheat	0	45	10.3	1.14	0.35	[98]
Naphthalene	128.17	2.67	Wheat	0	45	10.3	1.14	0.83	[98]
Naphthalene	128.17	4.74	Wheat	0	45	10.3	1.14	0.83	[98]
Naphthalene	128.17	4.15	Wheat	0	45	10.3	1.14	0.90	[98]
Phenanthrene	178.23	5.31	Wheat	0	45	10.3	1.14	0.27	[98]
Phenanthrene	178.23	1.41	Wheat	0	45	10.3	1.14	0.84	[98]
Phenanthrene	178.23	4.33	Wheat	0	45	10.3	1.14	0.73	[98]
Phenanthrene	178.23	2.70	Wheat	0	45	10.3	1.14	0.86	[98]
Phenanthrene	178.23	5.70	Wheat	0	45	10.3	1.14	0.20	[98]
Phenanthrene	178.23	2.60	Wheat	0	45	10.3	1.14	0.86	[98]
Phenanthrene	178.23	3.47	Wheat	0	45	10.3	1.14	0.46	[98]
Phenanthrene	178.23	5.30	Wheat	0	45	10.3	1.14	0.44	[98]
Phenanthrene	178.23	3.47	Wheat	0	45	10.3	1.14	0.05	[98]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
Phenanthrene	178.23	6.22	Wheat	0	45	10.3	1.14	0.28	[98]
Phenanthrene	178.23	4.80	Wheat	0	45	10.3	1.14	0.64	[98]
Phenanthrene	178.23	3.47	Wheat	0	45	10.3	1.14	0.05	[98]
Phenanthrene	178.23	2.67	Wheat	0	45	10.3	1.14	0.79	[98]
Phenanthrene	178.23	4.74	Wheat	0	45	10.3	1.14	0.53	[98]
Phenanthrene	178.23	4.15	Wheat	0	45	10.3	1.14	0.59	[98]
Pyrene	202.25	5.31	Wheat	0	45	10.3	1.14	-0.01	[98]
Pyrene	202.25	1.41	Wheat	0	45	10.3	1.14	0.87	[98]
Pyrene	202.25	4.33	Wheat	0	45	10.3	1.14	0.50	[98]
Pyrene	202.25	2.70	Wheat	0	45	10.3	1.14	1.06	[98]
Pyrene	202.25	5.70	Wheat	0	45	10.3	1.14	0.47	[98]
Pyrene	202.25	2.60	Wheat	0	45	10.3	1.14	1.14	[98]
Pyrene	202.25	3.47	Wheat	0	45	10.3	1.14	0.72	[98]
Pyrene	202.25	5.30	Wheat	0	45	10.3	1.14	0.40	[98]
Pyrene	202.25	3.47	Wheat	0	45	10.3	1.14	0.40	[98]
Pyrene	202.25	6.22	Wheat	0	45	10.3	1.14	0.47	[98]
Pyrene	202.25	4.80	Wheat	0	45	10.3	1.14	0.98	[98]
Pyrene	202.25	3.47	Wheat	0	45	10.3	1.14	0.40	[98]
Pyrene	202.25	2.67	Wheat	0	45	10.3	1.14	1.07	[98]
Pyrene	202.25	4.74	Wheat	0	45	10.3	1.14	0.70	[98]
Pyrene	202.25	4.15	Wheat	0	45	10.3	1.14	0.90	[98]
Benzo[a]anthracene	228.3	5.31	Wheat	0	45	10.3	1.14	-0.40	[98]
Benzo[a]anthracene	228.3	1.41	Wheat	0	45	10.3	1.14	1.11	[98]
Benzo[a]anthracene	228.3	4.33	Wheat	0	45	10.3	1.14	0.56	[98]
Benzo[a]anthracene	228.3	2.70	Wheat	0	45	10.3	1.14	1.03	[98]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
Benzo[a]anthracene	228.3	5.70	Wheat	0	45	10.3	1.14	0.56	[98]
Benzo[a]anthracene	228.3	2.60	Wheat	0	45	10.3	1.14	0.96	[98]
Benzo[a]anthracene	228.3	3.47	Wheat	0	45	10.3	1.14	0.82	[98]
Benzo[a]anthracene	228.3	5.30	Wheat	0	45	10.3	1.14	0.28	[98]
Benzo[a]anthracene	228.3	3.47	Wheat	0	45	10.3	1.14	0.65	[98]
Benzo[a]anthracene	228.3	6.22	Wheat	0	45	10.3	1.14	0.76	[98]
Benzo[a]anthracene	228.3	4.80	Wheat	0	45	10.3	1.14	1.02	[98]
Benzo[a]anthracene	228.3	3.47	Wheat	0	45	10.3	1.14	0.65	[98]
Benzo[a]anthracene	228.3	2.67	Wheat	0	45	10.3	1.14	1.62	[98]
Benzo[a]anthracene	228.3	4.74	Wheat	0	45	10.3	1.14	0.99	[98]
Benzo[a]anthracene	228.3	4.15	Wheat	0	45	10.3	1.14	1.12	[98]
Benzo[a]pyrene	252.3	5.31	Wheat	0	45	10.3	1.14	-0.23	[98]
Benzo[a]pyrene	252.3	1.41	Wheat	0	45	10.3	1.14	1.08	[98]
Benzo[a]pyrene	252.3	4.33	Wheat	0	45	10.3	1.14	0.88	[98]
Benzo[a]pyrene	252.3	2.70	Wheat	0	45	10.3	1.14	1.05	[98]
Benzo[a]pyrene	252.3	5.70	Wheat	0	45	10.3	1.14	0.48	[98]
Benzo[a]pyrene	252.3	2.60	Wheat	0	45	10.3	1.14	1.34	[98]
Benzo[a]pyrene	252.3	3.47	Wheat	0	45	10.3	1.14	0.79	[98]
Benzo[a]pyrene	252.3	5.30	Wheat	0	45	10.3	1.14	0.52	[98]
Benzo[a]pyrene	252.3	3.47	Wheat	0	45	10.3	1.14	0.67	[98]
Benzo[a]pyrene	252.3	6.22	Wheat	0	45	10.3	1.14	0.80	[98]
Benzo[a]pyrene	252.3	4.80	Wheat	0	45	10.3	1.14	1.23	[98]
Benzo[a]pyrene	252.3	3.47	Wheat	0	45	10.3	1.14	0.67	[98]
Benzo[a]pyrene	252.3	2.67	Wheat	0	45	10.3	1.14	1.37	[98]
Benzo[a]pyrene	252.3	4.74	Wheat	0	45	10.3	1.14	0.82	[98]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
Benzo[a]pyrene	252.3	4.15	Wheat	0	45	10.3	1.14	1.18	[98]
Benzo[b]fluoranthene	252.3	5.31	Wheat	0	45	10.3	1.14	-0.88	[98]
Benzo[b]fluoranthene	252.3	1.41	Wheat	0	45	10.3	1.14	0.46	[98]
Benzo[b]fluoranthene	252.3	4.33	Wheat	0	45	10.3	1.14	-0.16	[98]
Benzo[b]fluoranthene	252.3	2.70	Wheat	0	45	10.3	1.14	-0.10	[98]
Benzo[b]fluoranthene	252.3	5.70	Wheat	0	45	10.3	1.14	-0.50	[98]
Benzo[b]fluoranthene	252.3	2.60	Wheat	0	45	10.3	1.14	0.18	[98]
Benzo[b]fluoranthene	252.3	3.47	Wheat	0	45	10.3	1.14	0.19	[98]
Benzo[b]fluoranthene	252.3	5.30	Wheat	0	45	10.3	1.14	-0.25	[98]
Benzo[b]fluoranthene	252.3	3.47	Wheat	0	45	10.3	1.14	-0.29	[98]
Benzo[b]fluoranthene	252.3	6.22	Wheat	0	45	10.3	1.14	0.03	[98]
Benzo[b]fluoranthene	252.3	4.80	Wheat	0	45	10.3	1.14	0.24	[98]
Benzo[b]fluoranthene	252.3	3.47	Wheat	0	45	10.3	1.14	-0.29	[98]
Benzo[b]fluoranthene	252.3	2.67	Wheat	0	45	10.3	1.14	0.80	[98]
Benzo[b]fluoranthene	252.3	4.74	Wheat	0	45	10.3	1.14	-0.35	[98]
Benzo[b]fluoranthene	252.3	4.15	Wheat	0	45	10.3	1.14	0.34	[98]
Benzo[g,i,h]perylene	276.3	5.31	Wheat	0	45	10.3	1.14	-1.11	[98]
Benzo[g,i,h]perylene	276.3	1.41	Wheat	0	45	10.3	1.14	-0.31	[98]
Benzo[g,i,h]perylene	276.3	4.33	Wheat	0	45	10.3	1.14	-0.39	[98]
Benzo[g,i,h]perylene	276.3	2.70	Wheat	0	45	10.3	1.14	0.29	[98]
Benzo[g,i,h]perylene	276.3	5.70	Wheat	0	45	10.3	1.14	-0.04	[98]
Benzo[g,i,h]perylene	276.3	2.60	Wheat	0	45	10.3	1.14	0.70	[98]
Benzo[g,i,h]perylene	276.3	3.47	Wheat	0	45	10.3	1.14	0.00	[98]
Benzo[g,i,h]perylene	276.3	5.30	Wheat	0	45	10.3	1.14	-0.33	[98]
Benzo[g,i,h]perylene	276.3	3.47	Wheat	0	45	10.3	1.14	0.18	[98]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
Benzo[g,i,h]perylene	276.3	6.22	Wheat	0	45	10.3	1.14	-0.23	[98]
Benzo[g,i,h]perylene	276.3	4.80	Wheat	0	45	10.3	1.14	0.47	[98]
Benzo[g,i,h]perylene	276.3	3.47	Wheat	0	45	10.3	1.14	0.18	[98]
Benzo[g,i,h]perylene	276.3	2.67	Wheat	0	45	10.3	1.14	0.58	[98]
Benzo[g,i,h]perylene	276.3	4.74	Wheat	0	45	10.3	1.14	-0.05	[98]
Benzo[g,i,h]perylene	276.3	4.15	Wheat	0	45	10.3	1.14	0.40	[98]
Benzo[k]fluoranthene	252.3	5.31	Wheat	0	45	10.3	1.14	-0.58	[98]
Benzo[k]fluoranthene	252.3	1.41	Wheat	0	45	10.3	1.14	-0.55	[98]
Benzo[k]fluoranthene	252.3	4.33	Wheat	0	45	10.3	1.14	-0.51	[98]
Benzo[k]fluoranthene	252.3	2.70	Wheat	0	45	10.3	1.14	0.85	[98]
Benzo[k]fluoranthene	252.3	5.70	Wheat	0	45	10.3	1.14	-0.25	[98]
Benzo[k]fluoranthene	252.3	2.60	Wheat	0	45	10.3	1.14	0.88	[98]
Benzo[k]fluoranthene	252.3	3.47	Wheat	0	45	10.3	1.14	0.03	[98]
Benzo[k]fluoranthene	252.3	5.30	Wheat	0	45	10.3	1.14	0.53	[98]
Benzo[k]fluoranthene	252.3	3.47	Wheat	0	45	10.3	1.14	-0.04	[98]
Benzo[k]fluoranthene	252.3	6.22	Wheat	0	45	10.3	1.14	-0.04	[98]
Benzo[k]fluoranthene	252.3	4.80	Wheat	0	45	10.3	1.14	0.79	[98]
Benzo[k]fluoranthene	252.3	3.47	Wheat	0	45	10.3	1.14	-0.04	[98]
Benzo[k]fluoranthene	252.3	2.67	Wheat	0	45	10.3	1.14	0.57	[98]
Benzo[k]fluoranthene	252.3	4.74	Wheat	0	45	10.3	1.14	1.05	[98]
Benzo[k]fluoranthene	252.3	4.15	Wheat	0	45	10.3	1.14	1.36	[98]
Chrysene	228.3	5.31	Wheat	0	45	10.3	1.14	-0.81	[98]
Chrysene	228.3	1.41	Wheat	0	45	10.3	1.14	-0.82	[98]
Chrysene	228.3	4.33	Wheat	0	45	10.3	1.14	-0.49	[98]
Chrysene	228.3	2.70	Wheat	0	45	10.3	1.14	-0.17	[98]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
Chrysene	228.3	5.70	Wheat	0	45	10.3	1.14	-0.20	[98]
Chrysene	228.3	2.60	Wheat	0	45	10.3	1.14	-0.39	[98]
Chrysene	228.3	3.47	Wheat	0	45	10.3	1.14	-0.22	[98]
Chrysene	228.3	5.30	Wheat	0	45	10.3	1.14	-0.54	[98]
Chrysene	228.3	3.47	Wheat	0	45	10.3	1.14	-0.10	[98]
Chrysene	228.3	6.22	Wheat	0	45	10.3	1.14	-0.25	[98]
Chrysene	228.3	4.80	Wheat	0	45	10.3	1.14	0.09	[98]
Chrysene	228.3	3.47	Wheat	0	45	10.3	1.14	-0.10	[98]
Chrysene	228.3	2.67	Wheat	0	45	10.3	1.14	0.51	[98]
Chrysene	228.3	4.74	Wheat	0	45	10.3	1.14	0.24	[98]
Chrysene	228.3	4.15	Wheat	0	45	10.3	1.14	0.16	[98]
Dibenzo[a,h]anthracene	278.3	5.31	Wheat	0	45	10.3	1.14	-1.20	[98]
Dibenzo[a,h]anthracene	278.3	1.41	Wheat	0	45	10.3	1.14	-0.22	[98]
Dibenzo[a,h]anthracene	278.3	4.33	Wheat	0	45	10.3	1.14	0.88	[98]
Dibenzo[a,h]anthracene	278.3	2.70	Wheat	0	45	10.3	1.14	0.01	[98]
Dibenzo[a,h]anthracene	278.3	5.70	Wheat	0	45	10.3	1.14	-0.25	[98]
Dibenzo[a,h]anthracene	278.3	2.60	Wheat	0	45	10.3	1.14	-0.36	[98]
Dibenzo[a,h]anthracene	278.3	3.47	Wheat	0	45	10.3	1.14	0.10	[98]
Dibenzo[a,h]anthracene	278.3	5.30	Wheat	0	45	10.3	1.14	-0.65	[98]
Dibenzo[a,h]anthracene	278.3	3.47	Wheat	0	45	10.3	1.14	0.01	[98]
Dibenzo[a,h]anthracene	278.3	6.22	Wheat	0	45	10.3	1.14	-0.26	[98]
Dibenzo[a,h]anthracene	278.3	4.80	Wheat	0	45	10.3	1.14	0.40	[98]
Dibenzo[a,h]anthracene	278.3	3.47	Wheat	0	45	10.3	1.14	0.01	[98]
Dibenzo[a,h]anthracene	278.3	2.67	Wheat	0	45	10.3	1.14	0.64	[98]
Dibenzo[a,h]anthracene	278.3	4.74	Wheat	0	45	10.3	1.14	-0.14	[98]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
Dibenzo[a,h]anthracene	278.3	4.15	Wheat	0	45	10.3	1.14	0.43	[98]
Phenanthrene	178.23	1.1-2.0	Carrot	1	45	0.9	0.24	0.50	[99]
Fluoranthene	202.25	1.1-2.0	Carrot	1	45	0.9	0.24	0.05	[99]
benzo[b]fluoranthene	252.3	1.1-2.0	Carrot	1	45	0.9	0.24	-0.92	[99]
benzo[k]fluoranthene	252.3	1.1-2.0	Carrot	1	45	0.9	0.24	-0.85	[99]
Anthracene	178.23	1.1-2.0	Carrot	1	45	0.9	0.24	0.15	[99]
Benzo[a]anthracene	228.3	1.1-2.0	Carrot	1	45	0.9	0.24	-0.77	[99]
Chrysene	228.3	1.1-2.0	Carrot	1	45	0.9	0.24	-1.64	[99]
Pyrene	202.25	1.1-2.0	Carrot	1	45	0.9	0.24	0.15	[99]
Benzo[a]pyrene	252.3	1.1-2.0	Carrot	1	45	0.9	0.24	-0.72	[99]
Benzo[e]pyrene	252.3	1.1-2.0	Carrot	1	45	0.9	0.24	-0.74	[99]
Indeno[1,2,3-cd]pyrene	276.3	1.1-2.0	Carrot	1	45	0.9	0.24	-0.80	[99]
Benz[phi]perylene	276.3	1.1-2.0	Carrot	1	45	0.9	0.24	-0.89	[99]
2,2',4,4',6-pentabromodiphenyl ether	564.7	3.19	Maize	0	60	3.2	0.53	-0.73	[100]
2,2',4,4',6-pentabromodiphenyl ether	564.7	1.90	Maize	0	60	3.2	0.53	-0.28	[100]
2,2',4,4',6-pentabromodiphenyl ether	564.7	0.98	Maize	0	60	3.2	0.53	-0.13	[100]
2,2',4,4',5,5'-Hexabromodiphenyl ether	643.6	1.90	Maize	0	60	3.2	0.53	-0.32	[100]
2,2',4,4',5,5'-Hexabromodiphenyl ether	643.6	0.98	Maize	0	60	3.2	0.53	-0.08	[100]
2,2',4,4',5,6'-Hexabromodiphenyl ether	643.6	3.19	Maize	0	60	3.2	0.53	-0.28	[100]
2,2',4,4',5,6'-Hexabromodiphenyl ether	643.6	1.90	Maize	0	60	3.2	0.53	-0.41	[100]
2,2',4,4',5,6'-Hexabromodiphenyl ether	643.6	0.98	Maize	0	60	3.2	0.53	-0.13	[100]
2,2',4-tribromodiphenyl ether	406.89	3.19	Maize	0	60	3.2	0.53	-0.15	[100]
2,2',4-tribromodiphenyl ether	406.89	1.90	Maize	0	60	3.2	0.53	-0.10	[100]
2,2',3,4,4',5',6-heptabromodiphenyl ether	722.5	3.19	Maize	0	60	3.2	0.53	-0.66	[100]
2,2',3,4,4',5',6-heptabromodiphenyl ether	722.5	1.90	Maize	0	60	3.2	0.53	-0.03	[100]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
2,2',3,4,4',5',6-heptabromodiphenyl ether	722.5	0.98	Maize	0	60	3.2	0.53	-0.59	[100]
2,3,3',4,4',5',6-Heptabromodiphenyl ether	722.5	3.19	Maize	0	60	3.2	0.53	0.11	[100]
2,3,3',4,4',5',6-Heptabromodiphenyl ether	722.5	1.90	Maize	0	60	3.2	0.53	0.08	[100]
2,3,3',4,4',5',6-Heptabromodiphenyl ether	722.5	0.98	Maize	0	60	3.2	0.53	-0.11	[100]
2,2',3,3',4,4',5,6'-Octabromodiphenyl ether	801.4	3.19	Maize	0	60	3.2	0.53	-0.21	[100]
2,2',3,3',4,4',5,6'-Octabromodiphenyl ether	801.4	1.90	Maize	0	60	3.2	0.53	-0.43	[100]
2,2',3,3',4,4',5,6'-Octabromodiphenyl ether	801.4	0.98	Maize	0	60	3.2	0.53	-0.84	[100]
2,2',3,3',4,4',6,6'-Octabromodiphenyl ether	801.4	3.19	Maize	0	60	3.2	0.53	-0.45	[100]
2,2',3,3',4,4',6,6'-Octabromodiphenyl ether	801.4	1.90	Maize	0	60	3.2	0.53	-0.25	[100]
2,2',3,3',4,4',6,6'-Octabromodiphenyl ether	801.4	0.98	Maize	0	60	3.2	0.53	-0.49	[100]
Nonabromodiphenyl ether	880.3	3.19	Maize	0	60	3.2	0.53	-0.03	[100]
Nonabromodiphenyl ether	880.3	1.90	Maize	0	60	3.2	0.53	-1.15	[100]
Nonabromodiphenyl ether	880.3	0.98	Maize	0	60	3.2	0.53	-0.58	[100]
2,2',3,3',4,4',5,6,6'-nonabromodiphenyl ether	880.3	3.19	Maize	0	60	3.2	0.53	-0.56	[100]
2,2',3,3',4,4',5,6,6'-nonabromodiphenyl ether	880.3	1.90	Maize	0	60	3.2	0.53	-1.22	[100]
2,2',3,3',4,4',5,6,6'-nonabromodiphenyl ether	880.3	0.98	Maize	0	60	3.2	0.53	-0.81	[100]
1,2,3,4,5-Pentabromo-6-(2,3,5,6-tetrabromophenoxy)benzene	880.3	1.90	Maize	0	60	3.2	0.53	-1.20	[100]
1,2,3,4,5-Pentabromo-6-(2,3,5,6-tetrabromophenoxy)benzene	880.3	0.98	Maize	0	60	3.2	0.53	-1.37	[100]
Decabromodiphenyl ether	959.2	3.19	Maize	0	60	3.2	0.53	-0.55	[100]
Decabromodiphenyl ether	959.2	1.90	Maize	0	60	3.2	0.53	-0.61	[100]
Decabromodiphenyl ether	959.2	0.98	Maize	0	60	3.2	0.53	-0.77	[100]
2,4,4'-tribromodiphenyl ether	406.89	3.19	Maize	0	60	3.2	0.53	-0.20	[100]
2,4,4'-tribromodiphenyl ether	406.89	1.90	Maize	0	60	3.2	0.53	0.00	[100]
2,4,4'-tribromodiphenyl ether	406.89	0.98	Maize	0	60	3.2	0.53	-0.32	[100]
2,2',4,4'-Tetrabromodiphenyl ether	485.79	3.19	Maize	0	60	3.2	0.53	0.05	[100]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
2,2',4,4'-Tetrabromodiphenyl ether	485.79	1.90	Maize	0	60	3.2	0.53	0.18	[100]
2,2',4,4'-Tetrabromodiphenyl ether	485.79	0.98	Maize	0	60	3.2	0.53	-0.12	[100]
2,2',4,5'-Tetrabromodiphenyl ether	485.79	3.19	Maize	0	60	3.2	0.53	-0.05	[100]
2,3',4,4'-tetrabromodiphenyl ether	485.79	3.19	Maize	0	60	3.2	0.53	0.09	[100]
2,3',4,4'-tetrabromodiphenyl ether	485.79	1.90	Maize	0	60	3.2	0.53	-0.35	[100]
2,3',4,4'-tetrabromodiphenyl ether	485.79	0.98	Maize	0	60	3.2	0.53	-0.84	[100]
2,2',3,4,4'-Pentabromodiphenyl ether	564.7	3.19	Maize	0	60	3.2	0.53	-0.08	[100]
2,2',3,4,4'-Pentabromodiphenyl ether	564.7	1.90	Maize	0	60	3.2	0.53	-0.47	[100]
2,2',3,4,4'-Pentabromodiphenyl ether	564.7	0.98	Maize	0	60	3.2	0.53	-0.17	[100]
2,2',4,4',5-Pentabromodiphenyl ether	564.7	3.19	Maize	0	60	3.2	0.53	-0.15	[100]
2,2',4,4',5-Pentabromodiphenyl ether	564.7	1.90	Maize	0	60	3.2	0.53	-0.13	[100]
2,2',4,4',5-Pentabromodiphenyl ether	564.7	0.98	Maize	0	60	3.2	0.53	-0.12	[100]
2,2',4,4',6-pentabromodiphenyl ether	564.7	3.19	Pumpkin	0	60	1	0.7	-0.47	[100]
2,2',4,4',6-pentabromodiphenyl ether	564.7	1.90	Pumpkin	0	60	1	0.7	-0.19	[100]
2,2',4,4',6-pentabromodiphenyl ether	564.7	0.98	Pumpkin	0	60	1	0.7	-0.09	[100]
2,2',4,4',5,5'-Hexabromodiphenyl ether	643.6	3.19	Pumpkin	0	60	1	0.7	-0.94	[100]
2,2',4,4',5,5'-Hexabromodiphenyl ether	643.6	1.90	Pumpkin	0	60	1	0.7	-0.47	[100]
2,2',4,4',5,5'-Hexabromodiphenyl ether	643.6	0.98	Pumpkin	0	60	1	0.7	-0.07	[100]
2,2',4,4',5,6'-Hexabromodiphenyl ether	643.6	3.19	Pumpkin	0	60	1	0.7	-0.30	[100]
2,2',4,4',5,6'-Hexabromodiphenyl ether	643.6	1.90	Pumpkin	0	60	1	0.7	-0.25	[100]
2,2',4,4',5,6'-Hexabromodiphenyl ether	643.6	0.98	Pumpkin	0	60	1	0.7	-0.17	[100]
2,2',4-tribromodiphenyl ether	406.89	3.19	Pumpkin	0	60	1	0.7	-0.11	[100]
2,2',4-tribromodiphenyl ether	406.89	1.90	Pumpkin	0	60	1	0.7	-0.12	[100]
2,2',4-tribromodiphenyl ether	406.89	0.98	Pumpkin	0	60	1	0.7	0.18	[100]
2,2',3,4,4',5',6-heptabromodiphenyl ether	722.5	3.19	Pumpkin	0	60	1	0.7	-0.57	[100]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
2,2',3,4,4',5',6-heptabromodiphenyl ether	722.5	1.90	Pumpkin	0	60	1	0.7	-0.19	[100]
2,2',3,4,4',5',6-heptabromodiphenyl ether	722.5	0.98	Pumpkin	0	60	1	0.7	-0.72	[100]
2,3,3',4,4',5',6-Heptabromodiphenyl ether	722.5	3.19	Pumpkin	0	60	1	0.7	-0.07	[100]
2,3,3',4,4',5',6-Heptabromodiphenyl ether	722.5	1.90	Pumpkin	0	60	1	0.7	0.15	[100]
2,3,3',4,4',5',6-Heptabromodiphenyl ether	722.5	0.98	Pumpkin	0	60	1	0.7	-0.46	[100]
2,2',3,3',4,4',5,6'-Octabromodiphenyl ether	801.4	3.19	Pumpkin	0	60	1	0.7	0.21	[100]
2,2',3,3',4,4',5,6'-Octabromodiphenyl ether	801.4	1.90	Pumpkin	0	60	1	0.7	-0.09	[100]
2,2',3,3',4,4',6,6'-Octabromodiphenyl ether	801.4	3.19	Pumpkin	0	60	1	0.7	-0.45	[100]
2,2',3,3',4,4',6,6'-Octabromodiphenyl ether	801.4	1.90	Pumpkin	0	60	1	0.7	-0.10	[100]
2,2',3,3',4,4',6,6'-Octabromodiphenyl ether	801.4	0.98	Pumpkin	0	60	1	0.7	-0.34	[100]
Nonabromodiphenyl ether	880.3	3.19	Pumpkin	0	60	1	0.7	-0.14	[100]
Nonabromodiphenyl ether	880.3	1.90	Pumpkin	0	60	1	0.7	-1.39	[100]
Nonabromodiphenyl ether	880.3	0.98	Pumpkin	0	60	1	0.7	-0.76	[100]
2,2',3,3',4,4',5,6,6'-nonabromodiphenyl ether	880.3	3.19	Pumpkin	0	60	1	0.7	-0.28	[100]
2,2',3,3',4,4',5,6,6'-nonabromodiphenyl ether	880.3	1.90	Pumpkin	0	60	1	0.7	-1.62	[100]
2,2',3,3',4,4',5,6,6'-nonabromodiphenyl ether	880.3	0.98	Pumpkin	0	60	1	0.7	-1.03	[100]
1,2,3,4,5-Pentabromo-6-(2,3,5,6-tetrabromophenoxy)benzene	880.3	3.19	Pumpkin	0	60	1	0.7	-1.04	[100]
1,2,3,4,5-Pentabromo-6-(2,3,5,6-tetrabromophenoxy)benzene	880.3	1.90	Pumpkin	0	60	1	0.7	-1.18	[100]
1,2,3,4,5-Pentabromo-6-(2,3,5,6-tetrabromophenoxy)benzene	880.3	0.98	Pumpkin	0	60	1	0.7	-1.32	[100]
Decabromodiphenyl ether	959.2	3.19	Pumpkin	0	60	1	0.7	-0.30	[100]
Decabromodiphenyl ether	959.2	1.90	Pumpkin	0	60	1	0.7	-0.52	[100]
Decabromodiphenyl ether	959.2	0.98	Pumpkin	0	60	1	0.7	-0.68	[100]
2,4,4'-tribromodiphenyl ether	406.89	1.90	Pumpkin	0	60	1	0.7	-0.24	[100]
2,2',4,4'-Tetrabromodiphenyl ether	485.79	3.19	Pumpkin	0	60	1	0.7	0.18	[100]
2,2',4,4'-Tetrabromodiphenyl ether	485.79	1.90	Pumpkin	0	60	1	0.7	0.34	[100]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
2,2',4,4'-Tetrabromodiphenyl ether	485.79	0.98	Pumpkin	0	60	1	0.7	0.06	[100]
2,2',4,5'-Tetrabromodiphenyl ether	485.79	3.19	Pumpkin	0	60	1	0.7	0.14	[100]
2,2',4,5'-Tetrabromodiphenyl ether	485.79	0.98	Pumpkin	0	60	1	0.7	-1.58	[100]
2,3',4,4'-tetrabromodiphenyl ether	485.79	3.19	Pumpkin	0	60	1	0.7	0.05	[100]
2,3',4,4'-tetrabromodiphenyl ether	485.79	1.90	Pumpkin	0	60	1	0.7	-0.21	[100]
2,3',4,4'-tetrabromodiphenyl ether	485.79	0.98	Pumpkin	0	60	1	0.7	-1.10	[100]
2,2',3,4,4'-Pentabromodiphenyl ether	564.7	3.19	Pumpkin	0	60	1	0.7	-0.19	[100]
2,2',3,4,4'-Pentabromodiphenyl ether	564.7	1.90	Pumpkin	0	60	1	0.7	-0.45	[100]
2,2',3,4,4'-Pentabromodiphenyl ether	564.7	0.98	Pumpkin	0	60	1	0.7	-0.16	[100]
2,2',4,4',5-Pentabromodiphenyl ether	564.7	3.19	Pumpkin	0	60	1	0.7	-0.10	[100]
2,2',4,4',5-Pentabromodiphenyl ether	564.7	1.90	Pumpkin	0	60	1	0.7	0.07	[100]
2,2',4,4',5-Pentabromodiphenyl ether	564.7	0.98	Pumpkin	0	60	1	0.7	0.00	[100]
2,2',4,4',6-pentabromodiphenyl ether	564.7	3.19	Ryegrass	0	60	24.5	0.56	-0.55	[100]
2,2',4,4',6-pentabromodiphenyl ether	564.7	1.90	Ryegrass	0	60	24.5	0.56	-0.42	[100]
2,2',4,4',6-pentabromodiphenyl ether	564.7	0.98	Ryegrass	0	60	24.5	0.56	0.03	[100]
2,2',4,4',5,5'-Hexabromodiphenyl ether	643.6	3.19	Ryegrass	0	60	24.5	0.56	-0.27	[100]
2,2',4,4',5,5'-Hexabromodiphenyl ether	643.6	1.90	Ryegrass	0	60	24.5	0.56	-0.32	[100]
2,2',4,4',5,5'-Hexabromodiphenyl ether	643.6	0.98	Ryegrass	0	60	24.5	0.56	-0.26	[100]
2,2',4,4',5,6'-Hexabromodiphenyl ether	643.6	1.90	Ryegrass	0	60	24.5	0.56	-0.45	[100]
2,2',4,4',5,6'-Hexabromodiphenyl ether	643.6	0.98	Ryegrass	0	60	24.5	0.56	-0.19	[100]
2,2',4-tribromodiphenyl ether	406.89	3.19	Ryegrass	0	60	24.5	0.56	-0.28	[100]
2,2',4-tribromodiphenyl ether	406.89	1.90	Ryegrass	0	60	24.5	0.56	-0.13	[100]
2,2',4-tribromodiphenyl ether	406.89	0.98	Ryegrass	0	60	24.5	0.56	-0.26	[100]
2,2',3,4,4',5',6-heptabromodiphenyl ether	722.5	3.19	Ryegrass	0	60	24.5	0.56	-0.41	[100]
2,2',3,4,4',5',6-heptabromodiphenyl ether	722.5	1.90	Ryegrass	0	60	24.5	0.56	-0.07	[100]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
2,2',3,4,4',5',6-heptabromodiphenyl ether	722.5	0.98	Ryegrass	0	60	24.5	0.56	-0.54	[100]
2,3,3',4,4',5',6-Heptabromodiphenyl ether	722.5	3.19	Ryegrass	0	60	24.5	0.56	0.04	[100]
2,3,3',4,4',5',6-Heptabromodiphenyl ether	722.5	1.90	Ryegrass	0	60	24.5	0.56	-0.10	[100]
2,3,3',4,4',5',6-Heptabromodiphenyl ether	722.5	0.98	Ryegrass	0	60	24.5	0.56	-0.24	[100]
2,2',3,3',4,4',5,6'-Octabromodiphenyl ether	801.4	3.19	Ryegrass	0	60	24.5	0.56	0.14	[100]
2,2',3,3',4,4',5,6'-Octabromodiphenyl ether	801.4	1.90	Ryegrass	0	60	24.5	0.56	-0.66	[100]
2,2',3,3',4,4',5,6'-Octabromodiphenyl ether	801.4	0.98	Ryegrass	0	60	24.5	0.56	-0.87	[100]
2,2',3,3',4,4',6,6'-Octabromodiphenyl ether	801.4	3.19	Ryegrass	0	60	24.5	0.56	-0.24	[100]
2,2',3,3',4,4',6,6'-Octabromodiphenyl ether	801.4	1.90	Ryegrass	0	60	24.5	0.56	-0.54	[100]
2,2',3,3',4,4',6,6'-Octabromodiphenyl ether	801.4	0.98	Ryegrass	0	60	24.5	0.56	-0.72	[100]
Nonabromodiphenyl ether	880.3	3.19	Ryegrass	0	60	24.5	0.56	-0.64	[100]
Nonabromodiphenyl ether	880.3	1.90	Ryegrass	0	60	24.5	0.56	-1.82	[100]
Nonabromodiphenyl ether	880.3	0.98	Ryegrass	0	60	24.5	0.56	-0.74	[100]
2,2',3,3',4,4',5,6,6'-nonabromodiphenyl ether	880.3	3.19	Ryegrass	0	60	24.5	0.56	-0.64	[100]
2,2',3,3',4,4',5,6,6'-nonabromodiphenyl ether	880.3	1.90	Ryegrass	0	60	24.5	0.56	-1.49	[100]
2,2',3,3',4,4',5,6,6'-nonabromodiphenyl ether	880.3	0.98	Ryegrass	0	60	24.5	0.56	-0.97	[100]
1,2,3,4,5-Pentabromo-6-(2,3,5,6-tetrabromophenoxy)benzene	880.3	1.90	Ryegrass	0	60	24.5	0.56	-1.38	[100]
1,2,3,4,5-Pentabromo-6-(2,3,5,6-tetrabromophenoxy)benzene	880.3	0.98	Ryegrass	0	60	24.5	0.56	-1.45	[100]
Decabromodiphenyl ether	959.2	3.19	Ryegrass	0	60	24.5	0.56	-0.42	[100]
Decabromodiphenyl ether	959.2	1.90	Ryegrass	0	60	24.5	0.56	-0.69	[100]
Decabromodiphenyl ether	959.2	0.98	Ryegrass	0	60	24.5	0.56	-0.91	[100]
2,4,4'-tribromodiphenyl ether	406.89	1.90	Ryegrass	0	60	24.5	0.56	0.16	[100]
2,4,4'-tribromodiphenyl ether	406.89	0.98	Ryegrass	0	60	24.5	0.56	0.04	[100]
2,2',4,4'-Tetrabromodiphenyl ether	485.79	3.19	Ryegrass	0	60	24.5	0.56	0.07	[100]
2,2',4,4'-Tetrabromodiphenyl ether	485.79	1.90	Ryegrass	0	60	24.5	0.56	0.22	[100]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
2,2',4,4'-Tetrabromodiphenyl ether	485.79	0.98	Ryegrass	0	60	24.5	0.56	-0.32	[100]
2,2',4,5'-Tetrabromodiphenyl ether	485.79	1.90	Ryegrass	0	60	24.5	0.56	-0.21	[100]
2,3',4,4'-tetrabromodiphenyl ether	485.79	3.19	Ryegrass	0	60	24.5	0.56	0.01	[100]
2,3',4,4'-tetrabromodiphenyl ether	485.79	1.90	Ryegrass	0	60	24.5	0.56	-0.28	[100]
2,3',4,4'-tetrabromodiphenyl ether	485.79	0.98	Ryegrass	0	60	24.5	0.56	-0.76	[100]
2,2',3,4,4'-Pentabromodiphenyl ether	564.7	3.19	Ryegrass	0	60	24.5	0.56	-0.29	[100]
2,2',3,4,4'-Pentabromodiphenyl ether	564.7	1.90	Ryegrass	0	60	24.5	0.56	-0.38	[100]
2,2',3,4,4'-Pentabromodiphenyl ether	564.7	0.98	Ryegrass	0	60	24.5	0.56	-0.10	[100]
2,2',4,4',5-Pentabromodiphenyl ether	564.7	3.19	Ryegrass	0	60	24.5	0.56	-0.16	[100]
2,2',4,4',5-Pentabromodiphenyl ether	564.7	1.90	Ryegrass	0	60	24.5	0.56	-0.31	[100]
2,2',4,4',5-Pentabromodiphenyl ether	564.7	0.98	Ryegrass	0	60	24.5	0.56	0.07	[100]
Diieldrin	380.9	1.40	Carrot	1	93	0.9	0.24	-0.60	[101]
Diieldrin	380.9	3.60	Carrot	1	93	0.9	0.24	-0.99	[101]
Diieldrin	380.9	66.50	Carrot	1	93	0.9	0.24	-2.29	[101]
Diieldrin	380.9	1.40	Onions	1	83	1.1	0.1	-1.68	[101]
Diieldrin	380.9	3.60	Onions	1	83	1.1	0.1	-1.73	[101]
Diieldrin	380.9	1.40	Radish	1	35	0.7	0.1	-1.38	[101]
Diieldrin	380.9	3.60	Radish	1	35	0.7	0.1	-1.33	[101]
Diieldrin	380.9	66.50	Radish	1	35	0.7	0.1	-2.59	[101]
Diieldrin	380.9	1.40	Turnips	1	120	0.9	0.1	-1.38	[101]
Diieldrin	380.9	3.60	Turnips	1	120	0.9	0.1	-1.56	[101]
Diieldrin	380.9	13.28	Maize	0	39	3.2	0.53	0.19	[102]
Diieldrin	380.9	0.86	Maize	0	39	3.2	0.53	1.47	[102]
Diieldrin	380.9	6.55	Maize	0	39	3.2	0.53	0.43	[102]
Diieldrin	380.9	1.20	Maize	0	39	3.2	0.53	1.29	[102]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
Dieldrin	380.9	8.96	Maize	0	39	3.2	0.53	0.30	[102]
Dieldrin	380.9	0.69	Maize	0	39	3.2	0.53	1.52	[102]
Dieldrin	380.9	13.28	Maize	0	69	3.2	0.53	0.47	[102]
Dieldrin	380.9	0.86	Maize	0	69	3.2	0.53	1.38	[102]
Dieldrin	380.9	6.55	Maize	0	69	3.2	0.53	0.42	[102]
Dieldrin	380.9	1.20	Maize	0	69	3.2	0.53	1.30	[102]
Dieldrin	380.9	8.96	Maize	0	69	3.2	0.53	0.40	[102]
Dieldrin	380.9	0.69	Maize	0	69	3.2	0.53	1.55	[102]
Dieldrin	380.9	13.28	Maize	0	90	3.2	0.53	0.33	[102]
Dieldrin	380.9	0.86	Maize	0	90	3.2	0.53	1.35	[102]
Dieldrin	380.9	6.55	Maize	0	90	3.2	0.53	0.27	[102]
Dieldrin	380.9	1.20	Maize	0	90	3.2	0.53	1.40	[102]
Dieldrin	380.9	8.96	Maize	0	90	3.2	0.53	0.18	[102]
Dieldrin	380.9	0.69	Maize	0	90	3.2	0.53	1.33	[102]
Dieldrin	380.9	13.28	Maize	0	39	3.2	0.53	0.18	[102]
Dieldrin	380.9	0.86	Maize	0	39	3.2	0.53	1.63	[102]
Dieldrin	380.9	6.55	Maize	0	39	3.2	0.53	0.46	[102]
Dieldrin	380.9	1.20	Maize	0	39	3.2	0.53	1.22	[102]
Dieldrin	380.9	8.96	Maize	0	39	3.2	0.53	0.19	[102]
Dieldrin	380.9	0.69	Maize	0	39	3.2	0.53	1.62	[102]
Dieldrin	380.9	13.28	Maize	0	69	3.2	0.53	0.30	[102]
Dieldrin	380.9	0.86	Maize	0	69	3.2	0.53	1.46	[102]
Dieldrin	380.9	6.55	Maize	0	69	3.2	0.53	0.37	[102]
Dieldrin	380.9	1.20	Maize	0	69	3.2	0.53	1.24	[102]
Dieldrin	380.9	8.96	Maize	0	69	3.2	0.53	0.38	[102]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
Dieldrin	380.9	0.69	Maize	0	69	3.2	0.53	1.28	[102]
Dieldrin	380.9	13.28	Maize	0	90	3.2	0.53	0.03	[102]
Dieldrin	380.9	0.86	Maize	0	90	3.2	0.53	1.59	[102]
Dieldrin	380.9	6.55	Maize	0	90	3.2	0.53	0.30	[102]
Dieldrin	380.9	1.20	Maize	0	90	3.2	0.53	1.22	[102]
Dieldrin	380.9	8.96	Maize	0	90	3.2	0.53	0.36	[102]
Dieldrin	380.9	0.69	Maize	0	90	3.2	0.53	1.48	[102]
Dieldrin	380.9	8.80	leek	0	39	1.5	0.1	-0.66	[103]
Dieldrin	380.9	8.80	leek	0	39	1.5	0.1	-0.89	[103]
Dieldrin	380.9	8.80	leek	0	39	1.5	0.1	-0.73	[103]
Mitotane	320	5.02	Radish	1	18	0.7	0.1	0.30	[53]
Mitotane	320	5.02	Radish	1	28	0.7	0.1	0.45	[53]
Mitotane	320	5.02	Radish	1	56	0.7	0.1	-0.08	[53]
Mitotane	320	5.02	Radish	1	23	0.7	0.1	0.02	[53]
Mitotane	320	5.02	Radish	1	36	0.7	0.1	-0.05	[53]
Mitotane	320	5.02	Radish	1	51	0.7	0.1	-0.14	[53]
Mitotane	320	5.02	Radish	1	70	0.7	0.1	0.45	[53]
Mitotane	320	6.36	Radish	1	18	0.7	0.1	-0.33	[53]
Mitotane	320	6.36	Radish	1	28	0.7	0.1	-0.26	[53]
Mitotane	320	6.36	Radish	1	56	0.7	0.1	-0.79	[53]
Mitotane	320	6.36	Radish	1	23	0.7	0.1	-0.70	[53]
Mitotane	320	6.36	Radish	1	36	0.7	0.1	-0.80	[53]
Mitotane	320	6.36	Radish	1	51	0.7	0.1	-0.46	[53]
Mitotane	320	6.36	Radish	1	70	0.7	0.1	-0.25	[53]
2,2-(2-Chlorophenyl-4'-chlorophenyl)-1,1-dichloroethene	318	5.02	Radish	1	18	0.7	0.1	0.02	[53]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
2,2-(2-Chlorophenyl-4'-chlorophenyl)-1,1-dichloroethene	318	5.02	Radish	1	28	0.7	0.1	0.28	[53]
2,2-(2-Chlorophenyl-4'-chlorophenyl)-1,1-dichloroethene	318	5.02	Radish	1	56	0.7	0.1	-0.19	[53]
2,2-(2-Chlorophenyl-4'-chlorophenyl)-1,1-dichloroethene	318	5.02	Radish	1	23	0.7	0.1	-0.15	[53]
2,2-(2-Chlorophenyl-4'-chlorophenyl)-1,1-dichloroethene	318	5.02	Radish	1	36	0.7	0.1	-0.17	[53]
2,2-(2-Chlorophenyl-4'-chlorophenyl)-1,1-dichloroethene	318	5.02	Radish	1	51	0.7	0.1	-0.09	[53]
2,2-(2-Chlorophenyl-4'-chlorophenyl)-1,1-dichloroethene	318	5.02	Radish	1	70	0.7	0.1	0.42	[53]
2,2-(2-Chlorophenyl-4'-chlorophenyl)-1,1-dichloroethene	318	6.36	Radish	1	18	0.7	0.1	-0.37	[53]
2,2-(2-Chlorophenyl-4'-chlorophenyl)-1,1-dichloroethene	318	6.36	Radish	1	28	0.7	0.1	-0.31	[53]
2,2-(2-Chlorophenyl-4'-chlorophenyl)-1,1-dichloroethene	318	6.36	Radish	1	56	0.7	0.1	-0.77	[53]
2,2-(2-Chlorophenyl-4'-chlorophenyl)-1,1-dichloroethene	318	6.36	Radish	1	23	0.7	0.1	-0.53	[53]
2,2-(2-Chlorophenyl-4'-chlorophenyl)-1,1-dichloroethene	318	6.36	Radish	1	36	0.7	0.1	-1.00	[53]
2,2-(2-Chlorophenyl-4'-chlorophenyl)-1,1-dichloroethene	318	6.36	Radish	1	51	0.7	0.1	-0.62	[53]
2,2-(2-Chlorophenyl-4'-chlorophenyl)-1,1-dichloroethene	318	6.36	Radish	1	70	0.7	0.1	-0.49	[53]
1,1,1-trichloro-2-(2-chlorophenyl)-2-(4-chlorophenyl)ethane	354.5	5.02	Radish	1	18	0.7	0.1	-0.02	[53]
1,1,1-trichloro-2-(2-chlorophenyl)-2-(4-chlorophenyl)ethane	354.5	5.02	Radish	1	28	0.7	0.1	0.31	[53]
1,1,1-trichloro-2-(2-chlorophenyl)-2-(4-chlorophenyl)ethane	354.5	5.02	Radish	1	56	0.7	0.1	-0.25	[53]
1,1,1-trichloro-2-(2-chlorophenyl)-2-(4-chlorophenyl)ethane	354.5	5.02	Radish	1	23	0.7	0.1	-0.01	[53]
1,1,1-trichloro-2-(2-chlorophenyl)-2-(4-chlorophenyl)ethane	354.5	5.02	Radish	1	36	0.7	0.1	-0.21	[53]
1,1,1-trichloro-2-(2-chlorophenyl)-2-(4-chlorophenyl)ethane	354.5	5.02	Radish	1	51	0.7	0.1	-0.14	[53]
1,1,1-trichloro-2-(2-chlorophenyl)-2-(4-chlorophenyl)ethane	354.5	5.02	Radish	1	70	0.7	0.1	0.34	[53]
1,1,1-trichloro-2-(2-chlorophenyl)-2-(4-chlorophenyl)ethane	354.5	6.36	Radish	1	18	0.7	0.1	-0.22	[53]
1,1,1-trichloro-2-(2-chlorophenyl)-2-(4-chlorophenyl)ethane	354.5	6.36	Radish	1	28	0.7	0.1	-0.33	[53]
1,1,1-trichloro-2-(2-chlorophenyl)-2-(4-chlorophenyl)ethane	354.5	6.36	Radish	1	56	0.7	0.1	-0.79	[53]
1,1,1-trichloro-2-(2-chlorophenyl)-2-(4-chlorophenyl)ethane	354.5	6.36	Radish	1	23	0.7	0.1	-0.62	[53]
1,1,1-trichloro-2-(2-chlorophenyl)-2-(4-chlorophenyl)ethane	354.5	6.36	Radish	1	36	0.7	0.1	-0.84	[53]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
1,1,1-trichloro-2-(2-chlorophenyl)-2-(4-chlorophenyl)ethane	354.5	6.36	Radish	1	51	0.7	0.1	-0.46	[53]
1,1,1-trichloro-2-(2-chlorophenyl)-2-(4-chlorophenyl)ethane	354.5	6.36	Radish	1	70	0.7	0.1	-0.30	[53]
Dichlorodiphenyldichloroethane	320	5.02	Radish	1	18	0.7	0.1	-0.23	[53]
Dichlorodiphenyldichloroethane	320	5.02	Radish	1	28	0.7	0.1	0.26	[53]
Dichlorodiphenyldichloroethane	320	5.02	Radish	1	56	0.7	0.1	0.00	[53]
Dichlorodiphenyldichloroethane	320	5.02	Radish	1	23	0.7	0.1	-0.09	[53]
Dichlorodiphenyldichloroethane	320	5.02	Radish	1	36	0.7	0.1	0.04	[53]
Dichlorodiphenyldichloroethane	320	5.02	Radish	1	51	0.7	0.1	0.14	[53]
Dichlorodiphenyldichloroethane	320	5.02	Radish	1	70	0.7	0.1	0.50	[53]
Dichlorodiphenyldichloroethane	320	6.36	Radish	1	18	0.7	0.1	-0.37	[53]
Dichlorodiphenyldichloroethane	320	6.36	Radish	1	28	0.7	0.1	-0.33	[53]
Dichlorodiphenyldichloroethane	320	6.36	Radish	1	56	0.7	0.1	-0.69	[53]
Dichlorodiphenyldichloroethane	320	6.36	Radish	1	23	0.7	0.1	-0.70	[53]
Dichlorodiphenyldichloroethane	320	6.36	Radish	1	36	0.7	0.1	-0.65	[53]
Dichlorodiphenyldichloroethane	320	6.36	Radish	1	51	0.7	0.1	-0.43	[53]
Dichlorodiphenyldichloroethane	320	6.36	Radish	1	70	0.7	0.1	-0.05	[53]
1,1-Dichloro-2,2-bis(4-chlorophenyl)ethene	318	5.02	Radish	1	18	0.7	0.1	-0.12	[53]
1,1-Dichloro-2,2-bis(4-chlorophenyl)ethene	318	5.02	Radish	1	28	0.7	0.1	0.25	[53]
1,1-Dichloro-2,2-bis(4-chlorophenyl)ethene	318	5.02	Radish	1	56	0.7	0.1	-0.16	[53]
1,1-Dichloro-2,2-bis(4-chlorophenyl)ethene	318	5.02	Radish	1	23	0.7	0.1	-0.09	[53]
1,1-Dichloro-2,2-bis(4-chlorophenyl)ethene	318	5.02	Radish	1	36	0.7	0.1	-0.21	[53]
1,1-Dichloro-2,2-bis(4-chlorophenyl)ethene	318	5.02	Radish	1	51	0.7	0.1	-0.05	[53]
1,1-Dichloro-2,2-bis(4-chlorophenyl)ethene	318	5.02	Radish	1	70	0.7	0.1	0.34	[53]
1,1-Dichloro-2,2-bis(4-chlorophenyl)ethene	318	6.36	Radish	1	18	0.7	0.1	-0.19	[53]
1,1-Dichloro-2,2-bis(4-chlorophenyl)ethene	318	6.36	Radish	1	28	0.7	0.1	-0.13	[53]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
1,1-Dichloro-2,2-bis(4-chlorophenyl)ethene	318	6.36	Radish	1	56	0.7	0.1	-0.63	[53]
1,1-Dichloro-2,2-bis(4-chlorophenyl)ethene	318	6.36	Radish	1	23	0.7	0.1	-0.55	[53]
1,1-Dichloro-2,2-bis(4-chlorophenyl)ethene	318	6.36	Radish	1	36	0.7	0.1	-0.75	[53]
1,1-Dichloro-2,2-bis(4-chlorophenyl)ethene	318	6.36	Radish	1	51	0.7	0.1	-0.39	[53]
1,1-Dichloro-2,2-bis(4-chlorophenyl)ethene	318	6.36	Radish	1	70	0.7	0.1	-0.24	[53]
Chlorophenothane	354.5	5.02	Radish	1	18	0.7	0.1	-0.11	[53]
Chlorophenothane	354.5	5.02	Radish	1	28	0.7	0.1	0.16	[53]
Chlorophenothane	354.5	5.02	Radish	1	56	0.7	0.1	-0.38	[53]
Chlorophenothane	354.5	5.02	Radish	1	23	0.7	0.1	-0.08	[53]
Chlorophenothane	354.5	5.02	Radish	1	36	0.7	0.1	-0.15	[53]
Chlorophenothane	354.5	5.02	Radish	1	51	0.7	0.1	-0.09	[53]
Chlorophenothane	354.5	5.02	Radish	1	70	0.7	0.1	0.33	[53]
Chlorophenothane	354.5	6.36	Radish	1	18	0.7	0.1	-0.22	[53]
Chlorophenothane	354.5	6.36	Radish	1	28	0.7	0.1	-0.10	[53]
Chlorophenothane	354.5	6.36	Radish	1	56	0.7	0.1	-0.74	[53]
Chlorophenothane	354.5	6.36	Radish	1	23	0.7	0.1	-0.48	[53]
Chlorophenothane	354.5	6.36	Radish	1	36	0.7	0.1	-0.85	[53]
Chlorophenothane	354.5	6.36	Radish	1	51	0.7	0.1	-0.40	[53]
Chlorophenothane	354.5	6.36	Radish	1	70	0.7	0.1	-0.27	[53]
2,2',4,5,5'-Pentachlorobiphenyl	326.4	5.02	Radish	1	18	0.7	0.1	0.81	[53]
2,4,5,2',5'-Pentachlorobiphenyl	326.4	5.02	Radish	1	28	0.7	0.1	0.49	[53]
2,2',4,5,5'-Pentachlorobiphenyl	326.4	5.02	Radish	1	56	0.7	0.1	0.30	[53]
2,4,5,2',5'-Pentachlorobiphenyl	326.4	5.02	Radish	1	23	0.7	0.1	-0.08	[53]
2,2',4,5,5'-Pentachlorobiphenyl	326.4	5.02	Radish	1	36	0.7	0.1	0.25	[53]
2,2',4,5,5'-Pentachlorobiphenyl	326.4	5.02	Radish	1	51	0.7	0.1	-0.07	[53]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
2,2',4,5,5'-Pentachlorobiphenyl	326.4	5.02	Radish	1	70	0.7	0.1	0.79	[53]
2,4,5,2',5'-Pentachlorobiphenyl	326.4	6.36	Radish	1	18	0.7	0.1	-0.41	[53]
2,2',4,5,5'-Pentachlorobiphenyl	326.4	6.36	Radish	1	28	0.7	0.1	-0.49	[53]
2,2',4,5,5'-Pentachlorobiphenyl	326.4	6.36	Radish	1	56	0.7	0.1	-0.89	[53]
2,4,5,2',5'-Pentachlorobiphenyl	326.4	6.36	Radish	1	23	0.7	0.1	-0.73	[53]
2,2',4,5,5'-Pentachlorobiphenyl	326.4	6.36	Radish	1	36	0.7	0.1	-1.13	[53]
2,2',4,5,5'-Pentachlorobiphenyl	326.4	6.36	Radish	1	51	0.7	0.1	-0.88	[53]
2,2',4,5,5'-Pentachlorobiphenyl	326.4	6.36	Radish	1	70	0.7	0.1	-0.72	[53]
2,2',3,4,4',5'-Hexachlorobiphenyl	360.9	5.02	Radish	1	18	0.7	0.1	0.39	[53]
2,2',3,4,4',5'-Hexachlorobiphenyl	360.9	5.02	Radish	1	28	0.7	0.1	0.27	[53]
2,2',3,4,4',5'-Hexachlorobiphenyl	360.9	5.02	Radish	1	56	0.7	0.1	-0.13	[53]
2,2',3,4,4',5'-Hexachlorobiphenyl	360.9	5.02	Radish	1	23	0.7	0.1	-0.16	[53]
2,2',3,4,4',5'-Hexachlorobiphenyl	360.9	5.02	Radish	1	36	0.7	0.1	0.13	[53]
2,2',3,4,4',5'-Hexachlorobiphenyl	360.9	5.02	Radish	1	51	0.7	0.1	-0.38	[53]
2,2',3,4,4',5'-Hexachlorobiphenyl	360.9	5.02	Radish	1	70	0.7	0.1	0.29	[53]
2,2',3,4,4',5'-Hexachlorobiphenyl	360.9	6.36	Radish	1	18	0.7	0.1	-0.47	[53]
2,2',3,4,4',5'-Hexachlorobiphenyl	360.9	6.36	Radish	1	28	0.7	0.1	-0.49	[53]
2,2',3,4,4',5'-Hexachlorobiphenyl	360.9	6.36	Radish	1	56	0.7	0.1	-1.09	[53]
2,2',3,4,4',5'-Hexachlorobiphenyl	360.9	6.36	Radish	1	23	0.7	0.1	-0.70	[53]
2,2',3,4,4',5'-Hexachlorobiphenyl	360.9	6.36	Radish	1	36	0.7	0.1	-1.01	[53]
2,2',3,4,4',5'-Hexachlorobiphenyl	360.9	6.36	Radish	1	51	0.7	0.1	-0.79	[53]
2,2',3,4,4',5'-Hexachlorobiphenyl	360.9	6.36	Radish	1	70	0.7	0.1	-0.43	[53]
2,2',4,4',5,5'-Hexachlorobiphenyl	360.9	5.02	Radish	1	18	0.7	0.1	0.55	[53]
2,2',4,4',5,5'-Hexachlorobiphenyl	360.9	5.02	Radish	1	28	0.7	0.1	0.25	[53]
2,2',4,4',5,5'-Hexachlorobiphenyl	360.9	5.02	Radish	1	56	0.7	0.1	0.06	[53]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
2,2',4,4',5,5'-Hexachlorbiphenyl	360.9	5.02	Radish	1	23	0.7	0.1	-0.11	[53]
2,2',4,4',5,5'-Hexachlorbiphenyl	360.9	5.02	Radish	1	36	0.7	0.1	0.12	[53]
2,2',4,4',5,5'-Hexachlorbiphenyl	360.9	5.02	Radish	1	51	0.7	0.1	-0.33	[53]
2,2',4,4',5,5'-Hexachlorbiphenyl	360.9	5.02	Radish	1	70	0.7	0.1	0.51	[53]
2,2',4,4',5,5'-Hexachlorbiphenyl	360.9	6.36	Radish	1	18	0.7	0.1	-0.52	[53]
2,2',4,4',5,5'-Hexachlorbiphenyl	360.9	6.36	Radish	1	28	0.7	0.1	-0.57	[53]
2,2',4,4',5,5'-Hexachlorbiphenyl	360.9	6.36	Radish	1	56	0.7	0.1	-1.03	[53]
2,2',4,4',5,5'-Hexachlorbiphenyl	360.9	6.36	Radish	1	23	0.7	0.1	-0.77	[53]
2,2',4,4',5,5'-Hexachlorbiphenyl	360.9	6.36	Radish	1	36	0.7	0.1	-1.12	[53]
2,2',4,4',5,5'-Hexachlorbiphenyl	360.9	6.36	Radish	1	51	0.7	0.1	-0.80	[53]
2,2',4,4',5,5'-Hexachlorbiphenyl	360.9	6.36	Radish	1	70	0.7	0.1	-0.50	[53]
2,2',3,4,4',5,5'-Heptachlorbiphenyl	395.3	5.02	Radish	1	18	0.7	0.1	0.30	[53]
2,2',3,4,4',5,5'-Heptachlorbiphenyl	395.3	5.02	Radish	1	28	0.7	0.1	0.05	[53]
2,2',3,4,4',5,5'-Heptachlorbiphenyl	395.3	5.02	Radish	1	56	0.7	0.1	-0.12	[53]
2,2',3,4,4',5,5'-Heptachlorbiphenyl	395.3	5.02	Radish	1	23	0.7	0.1	-0.16	[53]
2,2',3,4,4',5,5'-Heptachlorbiphenyl	395.3	5.02	Radish	1	36	0.7	0.1	0.15	[53]
2,2',3,4,4',5,5'-Heptachlorbiphenyl	395.3	5.02	Radish	1	51	0.7	0.1	-0.36	[53]
2,2',3,4,4',5,5'-Heptachlorbiphenyl	395.3	5.02	Radish	1	70	0.7	0.1	0.23	[53]
2,2',3,4,4',5,5'-Heptachlorbiphenyl	395.3	6.36	Radish	1	18	0.7	0.1	-0.54	[53]
2,2',3,4,4',5,5'-Heptachlorbiphenyl	395.3	6.36	Radish	1	28	0.7	0.1	-0.60	[53]
2,2',3,4,4',5,5'-Heptachlorbiphenyl	395.3	6.36	Radish	1	56	0.7	0.1	-1.07	[53]
2,2',3,4,4',5,5'-Heptachlorbiphenyl	395.3	6.36	Radish	1	23	0.7	0.1	-0.74	[53]
2,2',3,4,4',5,5'-Heptachlorbiphenyl	395.3	6.36	Radish	1	36	0.7	0.1	-1.11	[53]
2,2',3,4,4',5,5'-Heptachlorbiphenyl	395.3	6.36	Radish	1	51	0.7	0.1	-0.80	[53]
2,2',3,4,4',5,5'-Heptachlorbiphenyl	395.3	6.36	Radish	1	70	0.7	0.1	-0.49	[53]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
2,2',5,5'-Tetrachlorbiphenyl	292	5.02	Radish	1	18	0.7	0.1	1.59	[53]
2,2',5,5'-Tetrachlorbiphenyl	292	5.02	Radish	1	28	0.7	0.1	1.26	[53]
2,2',5,5'-Tetrachlorbiphenyl	292	5.02	Radish	1	56	0.7	0.1	0.83	[53]
2,2',5,5'-Tetrachlorbiphenyl	292	5.02	Radish	1	23	0.7	0.1	0.72	[53]
2,2',5,5'-Tetrachlorbiphenyl	292	5.02	Radish	1	36	0.7	0.1	0.78	[53]
2,2',5,5'-Tetrachlorbiphenyl	292	5.02	Radish	1	51	0.7	0.1	0.66	[53]
2,2',5,5'-Tetrachlorbiphenyl	292	5.02	Radish	1	70	0.7	0.1	0.76	[53]
2,2',5,5'-Tetrachlorbiphenyl	292	6.36	Radish	1	18	0.7	0.1	0.07	[53]
2,2',5,5'-Tetrachlorbiphenyl	292	6.36	Radish	1	28	0.7	0.1	-0.19	[53]
2,2',5,5'-Tetrachlorbiphenyl	292	6.36	Radish	1	56	0.7	0.1	0.04	[53]
2,2',5,5'-Tetrachlorbiphenyl	292	6.36	Radish	1	23	0.7	0.1	-0.31	[53]
2,2',5,5'-Tetrachlorbiphenyl	292	6.36	Radish	1	36	0.7	0.1	-0.14	[53]
2,2',5,5'-Tetrachlorbiphenyl	292	6.36	Radish	1	51	0.7	0.1	-0.74	[53]
2,2',5,5'-Tetrachlorbiphenyl	292	6.36	Radish	1	70	0.7	0.1	-0.22	[53]
Triphenylphosphate	326.3	4.33	Rice	1	10	14.7	0.3	-0.44	[104-108]
Triphenylphosphate	326.3	4.33	Rice	1	16	14.7	0.3	0.37	[104-108]
Triphenylphosphate	326.3	4.33	Rice	1	46	14.7	0.3	0.22	[104-108]
Triphenylphosphate	326.3	4.33	Rice	1	58	14.7	0.3	0.70	[104-108]
Triphenylphosphate	326.3	4.33	Rice	1	110	14.7	0.3	0.00	[104-108]
Triphenylphosphate	326.3	4.33	Rice	1	130	14.7	0.3	-1.00	[104-108]
Triphenylphosphate	326.3	4.33	Rice	1	150	14.7	0.3	-0.28	[104-108]
2-Ethylhexyl diphenyl phosphate	362.4	4.33	Rice	1	10	14.7	0.3	-0.02	[104-108]
2-Ethylhexyl diphenyl phosphate	362.4	4.33	Rice	1	16	14.7	0.3	-1.10	[104-108]
2-Ethylhexyl diphenyl phosphate	362.4	4.33	Rice	1	46	14.7	0.3	0.16	[104-108]
2-Ethylhexyl diphenyl phosphate	362.4	4.33	Rice	1	58	14.7	0.3	0.46	[104-108]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
2-Ethylhexyl diphenyl phosphate	362.4	4.33	Rice	1	110	14.7	0.3	-0.38	[104-108]
2-Ethylhexyl diphenyl phosphate	362.4	4.33	Rice	1	130	14.7	0.3	0.42	[104-108]
2-Ethylhexyl diphenyl phosphate	362.4	4.33	Rice	1	150	14.7	0.3	0.29	[104-108]
Triphenyl phosphine oxide	278.3	4.33	Rice	1	10	14.7	0.3	-0.85	[104-108]
Triphenyl phosphine oxide	278.3	4.33	Rice	1	16	14.7	0.3	-1.22	[104-108]
Triphenyl phosphine oxide	278.3	4.33	Rice	1	46	14.7	0.3	-1.30	[104-108]
Triphenyl phosphine oxide	278.3	4.33	Rice	1	58	14.7	0.3	-0.18	[104-108]
Triphenyl phosphine oxide	278.3	4.33	Rice	1	110	14.7	0.3	-0.54	[104-108]
Triphenyl phosphine oxide	278.3	4.33	Rice	1	130	14.7	0.3	-0.59	[104-108]
Triphenyl phosphine oxide	278.3	4.33	Rice	1	150	14.7	0.3	-1.40	[104-108]
Tricresyl phosphate	368.4	4.33	Rice	1	10	14.7	0.3	-0.16	[104-108]
Tricresyl phosphate	368.4	4.33	Rice	1	16	14.7	0.3	-0.03	[104-108]
Tricresyl phosphate	368.4	4.33	Rice	1	46	14.7	0.3	-0.06	[104-108]
Tricresyl phosphate	368.4	4.33	Rice	1	58	14.7	0.3	-0.08	[104-108]
Tricresyl phosphate	368.4	4.33	Rice	1	110	14.7	0.3	0.13	[104-108]
Tricresyl phosphate	368.4	4.33	Rice	1	130	14.7	0.3	0.29	[104-108]
Tricresyl phosphate	368.4	4.33	Rice	1	150	14.7	0.3	-0.15	[104-108]
Triphenyl phosphate	326.3	3.69	Maize	1	20	3.2	0.53	0.01	[104-108]
Triphenyl phosphate	326.3	3.69	Maize	1	30	3.2	0.53	0.03	[104-108]
Triphenyl phosphate	326.3	3.69	Maize	1	50	3.2	0.53	-0.08	[104-108]
Triphenyl phosphate	326.3	3.69	Maize	1	80	3.2	0.53	-0.13	[104-108]
Triphenyl phosphate	326.3	3.69	Maize	1	110	3.2	0.53	1.36	[104-108]
Triphenyl phosphate	326.3	3.69	Maize	1	150	3.2	0.53	0.45	[104-108]
2-Ethylhexyl diphenyl phosphate	362.4	3.69	Maize	1	20	3.2	0.53	-0.54	[104-108]
2-Ethylhexyl diphenyl phosphate	362.4	3.69	Maize	1	30	3.2	0.53	-0.08	[104-108]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
2-Ethylhexyl diphenyl phosphate	362.4	3.69	Maize	1	50	3.2	0.53	-0.55	[104-108]
2-Ethylhexyl diphenyl phosphate	362.4	3.69	Maize	1	80	3.2	0.53	-0.51	[104-108]
2-Ethylhexyl diphenyl phosphate	362.4	3.69	Maize	1	110	3.2	0.53	-0.77	[104-108]
2-Ethylhexyl diphenyl phosphate	362.4	3.69	Maize	1	150	3.2	0.53	0.15	[104-108]
Triphenyl-phosphine oxide	278.3	3.69	Maize	1	20	3.2	0.53	-0.51	[104-108]
Triphenyl-phosphine oxide	278.3	3.69	Maize	1	30	3.2	0.53	-0.55	[104-108]
Triphenyl-phosphine oxide	278.3	3.69	Maize	1	50	3.2	0.53	-0.48	[104-108]
Triphenyl-phosphine oxide	278.3	3.69	Maize	1	80	3.2	0.53	-2.00	[104-108]
Triphenyl-phosphine oxide	278.3	3.69	Maize	1	110	3.2	0.53	-0.60	[104-108]
Triphenyl-phosphine oxide	278.3	3.69	Maize	1	150	3.2	0.53	-0.02	[104-108]
Tricresyl phosphate	368.4	3.69	Maize	1	20	3.2	0.53	-0.72	[104-108]
Tricresyl phosphate	368.4	3.69	Maize	1	30	3.2	0.53	0.41	[104-108]
Tricresyl phosphate	368.4	3.69	Maize	1	50	3.2	0.53	-0.12	[104-108]
Tricresyl phosphate	368.4	3.69	Maize	1	80	3.2	0.53	-0.59	[104-108]
Tricresyl phosphate	368.4	3.69	Maize	1	110	3.2	0.53	-0.31	[104-108]
Tricresyl phosphate	368.4	3.69	Maize	1	150	3.2	0.53	-0.64	[104-108]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.80	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.80	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.80	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.79	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.83	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.78	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.87	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.77	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.85	[109]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.82	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.82	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.84	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.84	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.83	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.83	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.82	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.85	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.85	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.84	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.83	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.88	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.84	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.86	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.83	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.87	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.86	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.85	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.79	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.85	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.82	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.88	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.77	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.84	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.84	[109]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.84	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.81	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.89	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.83	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.88	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.83	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.90	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.82	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.88	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.84	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.87	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.81	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.83	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.84	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.87	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.79	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.91	[109]
Di-n-butyl phthalate	278.3	1.57	cabbage	0	45	1.3	0.2	-0.84	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.85	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.88	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.83	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.85	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.84	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.84	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.86	[109]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.82	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.84	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.84	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.83	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.86	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.84	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.85	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.84	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.90	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.83	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.86	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.82	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.85	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.80	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.81	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.78	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.82	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.77	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.84	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.83	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.82	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.79	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.85	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.77	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.83	[109]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.77	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.79	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.77	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.84	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.79	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.87	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.80	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.89	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.78	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.80	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.82	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.79	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.83	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.89	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.79	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.83	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.80	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.84	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.83	[109]
Di-(2-ethylhexyl) phthalate	390.6	1.57	cabbage	0	45	1.3	0.2	-0.90	[109]
Di-n-butyl phthalate	278.3	1.17	Maize	1	155	3.2	0.53	0.18	[110]
Di-n-butyl phthalate	278.3	1.17	Maize	1	155	3.2	0.53	0.06	[110]
Di-n-butyl phthalate	278.3	1.17	Maize	1	155	3.2	0.53	0.31	[110]
Di-n-butyl phthalate	278.3	1.17	Maize	1	155	3.2	0.53	0.26	[110]
Di-(2-ethylhexyl) phthalate	390.6	1.17	Maize	1	155	3.2	0.53	0.19	[110]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
Di-(2-ethylhexyl) phthalate	390.6	1.17	Maize	1	155	3.2	0.53	0.14	[110]
Di-(2-ethylhexyl) phthalate	390.6	1.17	Maize	1	155	3.2	0.53	0.30	[110]
Di-(2-ethylhexyl) phthalate	390.6	1.17	Maize	1	155	3.2	0.53	0.32	[110]
Diisobutyl phthalate	278.34	1.17	Maize	1	155	3.2	0.53	0.32	[110]
Diisobutyl phthalate	278.34	1.17	Maize	1	155	3.2	0.53	0.22	[110]
Diisobutyl phthalate	278.34	1.17	Maize	1	155	3.2	0.53	0.48	[110]
Diisobutyl phthalate	278.34	1.17	Maize	1	155	3.2	0.53	0.40	[110]
Dimethyl phthalate	194.18	1.17	Maize	1	155	3.2	0.53	0.18	[110]
Dimethyl phthalate	194.18	1.17	Maize	1	155	3.2	0.53	0.27	[110]
Dimethyl phthalate	194.18	1.17	Maize	1	155	3.2	0.53	0.29	[110]
Dimethyl phthalate	194.18	1.17	Maize	1	155	3.2	0.53	0.34	[110]
Di-n-butyl phthalate	278.3	1.17	Potato	1	155	2	0.1	-0.31	[110]
Di-n-butyl phthalate	278.3	1.17	Potato	1	155	2	0.1	-0.25	[110]
Di-n-butyl phthalate	278.3	1.17	Potato	1	155	2	0.1	-0.09	[110]
Di-n-butyl phthalate	278.3	1.17	Potato	1	155	2	0.1	-0.25	[110]
Di(2-Ethylhexyl) phthalate	390.6	1.17	Potato	1	155	2	0.1	0.08	[110]
Di(2-Ethylhexyl) phthalate	390.6	1.17	Potato	1	155	2	0.1	0.07	[110]
Di(2-Ethylhexyl) phthalate	390.6	1.17	Potato	1	155	2	0.1	-0.06	[110]
Di(2-Ethylhexyl) phthalate	390.6	1.17	Potato	1	155	2	0.1	0.09	[110]
Diisobutyl phthalate	278.34	1.17	Potato	1	155	2	0.1	-0.06	[110]
Diisobutyl phthalate	278.34	1.17	Potato	1	155	2	0.1	-0.17	[110]
Diisobutyl phthalate	278.34	1.17	Potato	1	155	2	0.1	-0.03	[110]
Diisobutyl phthalate	278.34	1.17	Potato	1	155	2	0.1	-0.09	[110]
Dimethyl phthalate	194.18	1.17	Potato	1	155	2	0.1	0.34	[110]
Dimethyl phthalate	194.18	1.17	Potato	1	155	2	0.1	0.38	[110]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
Dimethyl phthalate	194.18	1.17	Potato	1	155	2	0.1	0.33	[110]
Dimethyl phthalate	194.18	1.17	Potato	1	155	2	0.1	0.23	[110]
Di-n-butyl phthalate	278.3	3.47	Cabbage	0	50	1.3	0.2	-0.24	[54]
Di-n-butyl phthalate	278.3	3.47	Cabbage	0	50	1.3	0.2	-0.23	[54]
Di-n-butyl phthalate	278.3	3.47	Cabbage	0	50	1.3	0.2	-0.72	[54]
Di-n-butyl phthalate	278.3	3.47	Cabbage	0	50	1.3	0.2	-0.76	[54]
Di-n-butyl phthalate	278.3	3.47	Cabbage	0	50	1.3	0.2	-0.78	[54]
Di-n-butyl phthalate	278.3	3.47	Cabbage	0	50	1.3	0.2	-0.73	[54]
Di(2-Ethylhexyl) phthalate	390.6	3.47	Cabbage	0	50	1.3	0.2	-0.15	[54]
Di(2-Ethylhexyl) phthalate	390.6	3.47	Cabbage	0	50	1.3	0.2	-0.38	[54]
Di(2-Ethylhexyl) phthalate	390.6	3.47	Cabbage	0	50	1.3	0.2	-0.73	[54]
Di(2-Ethylhexyl) phthalate	390.6	3.47	Cabbage	0	50	1.3	0.2	-0.69	[54]
Di(2-Ethylhexyl) phthalate	390.6	3.47	Cabbage	0	50	1.3	0.2	-0.58	[54]
Di(2-Ethylhexyl) phthalate	390.6	3.47	Cabbage	0	50	1.3	0.2	-0.60	[54]
Cresyl diphenyl phosphate	340.3	1.47	Clove	0	1	5.97	13	0.31	[111]
Cresyl diphenyl phosphate	340.3	1.47	Clove	0	3	5.97	13	0.90	[111]
Cresyl diphenyl phosphate	340.3	1.47	Clove	0	5	5.97	13	0.71	[111]
Cresyl diphenyl phosphate	340.3	1.47	Clove	0	7	5.97	13	0.35	[111]
Cresyl diphenyl phosphate	340.3	1.47	Clove	0	9	5.97	13	0.23	[111]
Cresyl diphenyl phosphate	340.3	1.47	Clove	0	11	5.97	13	0.87	[111]
Cresyl diphenyl phosphate	340.3	1.47	Clove	0	13	5.97	13	1.28	[111]
Triphenyl phosphate	326.3	1.47	Clove	0	1	5.97	13	0.13	[111]
Triphenyl phosphate	326.3	1.47	Clove	0	3	5.97	13	0.33	[111]
Triphenyl phosphate	326.3	1.47	Clove	0	5	5.97	13	0.61	[111]
Triphenyl phosphate	326.3	1.47	Clove	0	7	5.97	13	-0.20	[111]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
Triphenyl phosphate	326.3	1.47	Clove	0	9	5.97	13	-0.12	[111]
Triphenyl phosphate	326.3	1.47	Clove	0	11	5.97	13	0.39	[111]
Triphenyl phosphate	326.3	1.47	Clove	0	13	5.97	13	0.59	[111]
Tricresyl phosphate	368.4	1.47	Clove	0	7	5.97	13	-0.05	[111]
Tricresyl phosphate	368.4	1.47	Clove	0	9	5.97	13	0.01	[111]
Tricresyl phosphate	368.4	1.47	Clove	0	11	5.97	13	1.25	[111]
Tricresyl phosphate	368.4	1.47	Clove	0	13	5.97	13	1.35	[111]
Cresyl diphenyl phosphate	340.3	1.47	Lemon	0	1	1.5	0.3	0.38	[111]
Cresyl diphenyl phosphate	340.3	1.47	Lemon	0	3	1.5	0.3	0.40	[111]
Cresyl diphenyl phosphate	340.3	1.47	Lemon	0	5	1.5	0.3	0.72	[111]
Cresyl diphenyl phosphate	340.3	1.47	Lemon	0	7	1.5	0.3	1.26	[111]
Cresyl diphenyl phosphate	340.3	1.47	Lemon	0	9	1.5	0.3	0.78	[111]
Cresyl diphenyl phosphate	340.3	1.47	Lemon	0	11	1.5	0.3	1.01	[111]
Cresyl diphenyl phosphate	340.3	1.47	Lemon	0	13	1.5	0.3	1.01	[111]
Triphenyl phosphate	326.3	1.47	Lemon	0	1	1.5	0.3	1.54	[111]
Triphenyl phosphate	326.3	1.47	Lemon	0	3	1.5	0.3	1.81	[111]
Triphenyl phosphate	326.3	1.47	Lemon	0	5	1.5	0.3	0.72	[111]
Triphenyl phosphate	326.3	1.47	Lemon	0	7	1.5	0.3	0.88	[111]
Triphenyl phosphate	326.3	1.47	Lemon	0	9	1.5	0.3	0.28	[111]
Triphenyl phosphate	326.3	1.47	Lemon	0	11	1.5	0.3	1.11	[111]
Triphenyl phosphate	326.3	1.47	Lemon	0	13	1.5	0.3	1.02	[111]
Tricresyl phosphate	368.4	1.47	Lemon	0	7	1.5	0.3	0.65	[111]
Tricresyl phosphate	368.4	1.47	Lemon	0	9	1.5	0.3	-0.07	[111]
Tricresyl phosphate	368.4	1.47	Lemon	0	11	1.5	0.3	0.14	[111]
Tricresyl phosphate	368.4	1.47	Lemon	0	13	1.5	0.3	-0.26	[111]

Compounds	Molecular Weight	SOM content/%	Plants	Cultivate mode	Exposure time (day)	Protein content (%)	Lipid content (%)	Log RCF	References
Cresyl diphenyl phosphate	340.3	1.47	Cape	0	1	1.9	0.7	1.04	[111]
Cresyl diphenyl phosphate	340.3	1.47	Cape	0	3	1.9	0.7	0.92	[111]
Cresyl diphenyl phosphate	340.3	1.47	Cape	0	5	1.9	0.7	1.04	[111]
Cresyl diphenyl phosphate	340.3	1.47	Cape	0	7	1.9	0.7	0.90	[111]
Cresyl diphenyl phosphate	340.3	1.47	Cape	0	9	1.9	0.7	1.72	[111]
Cresyl diphenyl phosphate	340.3	1.47	Cape	0	11	1.9	0.7	1.29	[111]
Cresyl diphenyl phosphate	340.3	1.47	Cape	0	13	1.9	0.7	1.53	[111]
Triphenyl phosphate	326.3	1.47	Cape	0	1	1.9	0.7	0.38	[111]
Triphenyl phosphate	326.3	1.47	Cape	0	3	1.9	0.7	0.59	[111]
Triphenyl phosphate	326.3	1.47	Cape	0	5	1.9	0.7	0.75	[111]
Triphenyl phosphate	326.3	1.47	Cape	0	7	1.9	0.7	0.83	[111]
Triphenyl phosphate	326.3	1.47	Cape	0	9	1.9	0.7	0.99	[111]
Triphenyl phosphate	326.3	1.47	Cape	0	11	1.9	0.7	0.52	[111]
Triphenyl phosphate	326.3	1.47	Cape	0	13	1.9	0.7	0.51	[111]
Tricresyl phosphate	368.4	1.47	Cape	0	9	1.9	0.7	1.77	[111]
Tricresyl phosphate	368.4	1.47	Cape	0	11	1.9	0.7	1.02	[111]
Tricresyl phosphate	368.4	1.47	Cape	0	13	1.9	0.7	0.15	[111]

Table S2 The optimal hyperparameter values for three different model

Machine learning model	The optimal hyperparameter values
GBRT	learning rate: 0.1133, max depth: 23, max features: 45, min samples leaf: 7, min samples spilt: 4, n estimators: 57
RF	max depth: 18, max features: 47, min samples leaf: 2, min samples spilt: 6, n estimators: 69
SVR	C: 5.0024, gamma: auto, kernel: rbf

Table S3 Predicted logRCF values from different models

Actual logRCF	GBRT_Predicted logRCF	RF_Predicted logRCF	SVR_Predicted logRCF	Lasso LR Predicted logRCF
-0.17	-0.351721975	-0.330010239	-0.266332433	-0.324505451
-1.2	-0.289880162	-0.101261768	-0.360962712	0.091057861
0.32	0.108389572	-0.011296608	-0.296675525	0.12592239
-0.84	-0.633755447	-0.453114431	-0.216319803	0.008597265
-0.05	0.070959261	0.066607974	0.12492506	0.124118022
-0.79	-0.828939597	-0.830494053	-0.769583745	-0.827859644
0.06	-0.040415885	0.083590917	-0.280344995	-0.375027748
0.03	0.23125008	0.317326652	0.039702414	0.363114236
-0.23	-0.74892435	-0.719227599	-0.679806153	-0.590059134
-0.81	-0.79625528	-0.793199786	-0.760063755	-0.436053871
-1.38	-1.493891987	-1.335013144	-0.186676457	0.587766955
-0.83	-0.846236188	-0.84547546	-0.810147335	-0.809931357
0.52	0.789537665	0.77994784	0.705078254	0.900058411
-0.07	-0.574554561	-0.577821459	-0.818244857	-0.315675395
1.59	0.964160002	0.735032495	0.809306868	-0.003339433
-0.85	-0.742644051	-0.719272154	-0.669983795	-0.490917631
-0.25	-0.160026544	-0.079539543	-0.125792757	-0.175069479
-0.29	0.009086372	0.057880843	0.08974573	0.443816427
-0.21	0.707345359	0.689487138	0.607544337	0.692094301
-0.84	-0.846236188	-0.84547546	-0.810147335	-0.809931357
-0.12	-0.171218403	-0.24224881	-0.46328657	-0.050659887
-1.73	-1.46894102	-1.36387607	-1.576902944	-1.520690031
0.19	0.240171121	0.160169977	0.07108195	-0.054149064
0.61	0.67589409	0.682503451	0.635926156	0.762053185
-0.28	-0.512818614	-0.538332936	-0.490349916	-0.425780236
-0.77	-0.828939597	-0.830494053	-0.769583745	-0.827859644
-0.89	-0.838630157	-0.839449163	-0.800296213	-0.829251799
0.34	0.332869383	0.382153813	0.39737276	0.305748193
-0.8	-0.846236188	-0.84547546	-0.810147335	-0.809931357
0.13	0.284657852	0.388940735	0.491302091	0.349370058
-0.25	-0.307874091	-0.311886358	-0.339891801	-0.480643996
0.48	0.115248488	0.10749239	0.086017864	0.053830085
0.55	0.808543649	0.729337474	0.656340524	0.630760082
0.19	-0.063142461	0.039828145	-0.074324813	0.185709336
-0.74	-0.127307459	-0.153897807	-0.198191284	-0.160680731
-0.59	-0.332137867	-0.32942738	-0.103277042	-0.249917709
-0.56	-0.791397779	-0.752043583	-0.786095869	-0.70042374
0.76	0.951058836	0.828791076	0.754457115	0.47448332

Actual logRCF	GBRT_Predicted logRCF	RF_Predicted logRCF	SVR_Predicted logRCF	Lasso LR Predicted logRCF
-0.09	-0.10657409	-0.046004203	-0.067255172	-0.01937091
-0.7	-0.471897945	-0.366048414	-0.262420837	-0.23348397
-0.09	-0.152815051	0.006871722	-0.127650178	-0.280819043
0.35	0.457698595	0.586998735	0.798135413	0.761341518
-0.12	-0.222251009	-0.246753549	-0.047313049	-0.100421203
0.88	0.863945343	0.83018696	0.813214538	0.654939078
0.64	0.598429334	0.471246377	0.412462182	0.370982159
0.79	0.887407958	0.794601008	0.64667615	0.473086085
0.5	0.956416487	0.852837257	0.764304802	0.479276932
0.27	0.132776616	-0.066006464	-0.264192196	-0.377470728
-0.58	-0.968339348	-0.829817228	-0.548705609	-0.380875614
-0.23	0.107842562	0.066666379	-0.115481703	-0.171584813
-0.16	-0.129540782	-0.056352361	-0.079672884	-0.265406474
-0.33	-0.32688686	-0.441631815	-0.316864668	-0.252381205
-0.6	-0.513489736	-0.538686367	-0.613085354	-0.445028286
0.78	0.600166945	0.426224223	0.162251598	0.111644759
0.9	1.14651973	1.145509578	1.182415675	0.892418175
-0.02	0.285578128	0.034205607	-0.146313022	-0.192817286
0.18	0.280347395	0.419658213	0.625194992	0.431858409
0.51	0.291703588	0.212932405	-0.287814877	-0.368489083
0.29	0.287502317	0.105038998	0.32914417	-0.383584682
-0.47	-0.32441891	-0.222069228	-0.227327433	-0.098762957
0.38	0.200331963	0.181899359	0.130110324	0.058338693
-0.54	-0.76015587	-0.736926014	-0.923933107	-0.514290107
-0.77	-0.615626735	-0.510916006	-0.643398577	-0.614301831
1.28	0.708603509	0.461075655	0.33764729	0.475023881
0.13	0.022642774	-0.044228723	0.028680115	-0.252866957
1.51	1.149402379	1.011953892	0.803293086	0.705061061
-0.16	-0.143422575	-0.09372351	-0.259721377	-0.379805966
1.48	1.509279133	1.412373309	1.346791423	0.966629932
0.28	1.004677832	1.057076236	0.98342593	0.771451711
-0.77	-0.821654113	-0.821573249	-0.789862022	-0.675068248
0.33	0.200331963	0.181899359	0.130110324	0.058338693
-0.8	-0.980197167	-0.863907284	-0.601648614	-0.385808088
0.18	0.173786515	0.233720696	0.207074619	0.184996889
-0.19	-0.110832283	-0.012422986	-0.078471177	-0.120675916
-0.05	-0.133839147	-0.065595518	-0.087671309	-0.267741712
0.65	1.13643511	0.985371167	0.58858637	0.73263563
-1.56	-1.4580621	-1.402191888	-0.354044344	0.4823075
0.51	-0.169104171	-0.227845063	-0.054346765	0.219596716
-0.77	-0.846236188	-0.84547546	-0.810147335	-0.809931357

Actual logRCF	GBRT_Predicted logRCF	RF_Predicted logRCF	SVR_Predicted logRCF	Lasso LR Predicted logRCF
-0.83	-0.846236188	-0.84547546	-0.810147335	-0.809931357
-0.48	-0.52503234	-0.402861775	-0.450497466	-0.254916499
-0.19	-0.378799193	-0.360537853	-0.339368136	-0.377117592
1.22	1.303775384	1.28561687	1.343614732	0.918363089
0.03	-0.199966416	-0.143252123	-0.192921703	0.311992109
-0.08	-0.440352096	-0.406601876	-0.532558587	-0.085636248
-0.43	-0.689059414	-0.708809071	-0.423201076	-0.400874655
0.29	0.22390118	0.017066989	-0.287713951	-0.357854732
-0.64	-1.02177224	-0.951070934	-0.964031902	-0.825445573
1.04	1.090451351	1.043145649	1.178324426	0.89148408
-0.6	-1.416333025	-1.360789574	-0.767801426	0.475934427
1.53	1.256067949	1.189695914	1.194166582	0.89522046
-0.11	-0.180925847	-0.187261005	-0.153071146	-0.238286616
1.25	1.056264629	0.60794686	1.250812967	0.200163426
0.09	0.024910142	-0.309138979	-0.298522815	-0.097341551
0.65	0.755604701	0.852510399	0.919702252	0.705424446
-0.47	-0.647177846	-0.510290963	-0.827202925	-0.359776621
-0.8	-0.811940347	-0.810261361	-0.749981513	-0.829043932
0.14	-0.349571659	-0.498378009	-0.633687462	-0.712731965
1.36	0.028255626	0.074056791	0.210253628	0.209364663
-0.59	-0.811282271	-0.738888954	-0.906935614	-0.504949156
0.54	0.539952936	0.599774834	0.703646987	0.794649744
0.39	0.154058425	-0.041373269	-0.254925888	-0.382141204
0.28	0.247803949	0.324606604	0.253144786	0.302912874
-0.14	-0.867810748	-0.86155207	-0.8188497	-0.630667809
0.75	0.63481601	0.677296411	0.576696044	0.733770877
-0.84	-0.445572268	-0.294484002	-0.081775868	-0.278105915
-0.7	-0.503433353	-0.349868054	-0.229272132	-0.163174305
-0.84	-0.846236188	-0.84547546	-0.810147335	-0.809931357
0.05	0.373265675	0.577745992	0.677986552	0.437572511
0.18	0.325185665	0.101865214	0.0903925	0.073601361
-0.13	-0.263038699	-0.336698086	-0.274645314	-0.327437168
-0.52	-0.467736125	-0.529413159	-0.422186551	-0.45700995
-0.85	-0.662471435	-0.488504209	-0.432060903	-0.248844881
-1.2	-1.307578526	-1.128617285	-1.152405956	-0.762148592
-0.63	-0.514547044	-0.440305085	-0.235848333	-0.329640869
-0.32	0.186968032	0.093882523	0.131182952	-0.163947058
-0.26	-0.216033506	-0.182646345	-0.190622371	-0.327125565
0.14	-0.003596634	0.017758109	-0.060389267	-0.156172244
-0.79	-0.706773026	-0.669318331	-0.391598956	-0.598910246
0.18	0.646605614	0.3266183	0.177839869	0.485520847

Actual logRCF	GBRT_Predicted logRCF	RF_Predicted logRCF	SVR_Predicted logRCF	Lasso LR Predicted logRCF
0.07	0.179155603	0.055622876	0.103358724	-0.269885873
-0.43	-0.512818614	-0.538332936	-0.490349916	-0.425780236
-0.19	-0.290977123	-0.316965409	-0.314202148	-0.259812234
-0.69	-0.513489736	-0.538686367	-0.613085354	-0.445028286
-0.33	-0.311142909	-0.206734331	0.088252423	0.097273797
-0.43	-0.232094816	-0.246810201	-0.11511643	-0.322207141
-0.47	-0.4800129	-0.54088216	-0.429450201	-0.446375599
-0.85	-0.828939597	-0.830494053	-0.769583745	-0.827859644
-0.33	-0.025303844	0.081941504	-0.276932445	-0.377362986
0.99	0.783659736	0.77973528	0.701495	0.899124316
0.7	-0.045972164	-0.105885738	-0.223829268	-0.236587902
-0.1	-0.426868123	-0.397371761	-0.365723154	-0.52281764
-0.25	-0.307874091	-0.311886358	-0.339891801	-0.480643996
-0.24	-0.307874091	-0.311886358	-0.339891801	-0.480643996
-0.83	-0.846236188	-0.84547546	-0.810147335	-0.809931357
-0.89	-0.846236188	-0.84547546	-0.810147335	-0.809931357
-0.62	-0.775777518	-0.603031631	-0.259303975	-0.187245549
-0.23	-0.257043988	-0.255222656	0.027533224	0.053172571
0.88	1.129353937	1.009838525	0.837272217	0.79132206
0.71	0.863855175	0.68027469	0.543530639	0.373817477
0.15	0.323311348	-0.017488844	0.500908388	-0.512173629
0.3	0.545505716	0.750268288	0.693599612	0.649455167
-0.61	-0.669457867	-0.516158265	-0.622232082	-0.658403058
0.04	-0.008410608	-0.034230747	0.147679469	-0.128395124
-0.36	-0.015348878	-0.085818095	-0.051259929	-0.444037628
0.16	-0.22994029	-0.072222001	0.219937851	-0.432157626
-0.25	-0.369724741	-0.414033238	-0.41751565	-0.574512446
0.14	-0.753625481	-0.636992755	-0.448088936	-0.364181771
-1.52	-0.331597157	-0.368600863	-0.419890913	-0.284042544
0.89	0.647703463	0.682503451	0.617899181	0.753424685
-0.9	-0.815949571	-0.803568146	-0.720314737	-0.814007054
-0.6	-0.158050935	-0.350020626	-0.183880121	-0.053718632
0.3	0.431001546	0.349624067	0.741015903	0.685724295
-0.87	-0.784210652	-0.779205394	-0.689977855	-0.790062002
0.62	0.25025689	0.4614062	0.543194886	0.664770715
-2	-0.177806642	-0.337281668	-0.28752881	-0.067730058
0.01	0.778696338	0.557177364	1.251315997	0.199229331
-0.38	-0.332834797	-0.252491109	-0.209844142	-0.13805711
-0.77	-0.804632715	-0.599613757	-0.256201636	-0.184910311
-0.88	-0.742644051	-0.719272154	-0.669983795	-0.490917631
0.57	1.125725494	1.011953892	0.786394173	0.69643256

Actual logRCF	GBRT_Predicted logRCF	RF_Predicted logRCF	SVR_Predicted logRCF	Lasso LR Predicted logRCF
-0.93	-0.723989298	-0.730587204	-0.770108001	-0.798109811
-0.15	-0.190199483	-0.081567173	-0.011300435	-0.205362449
-0.82	-0.838630157	-0.839449163	-0.800296213	-0.829251799
0	0.173786515	0.233720696	0.207074619	0.184996889
-0.51	-0.465757126	-0.337790639	-0.310260745	-0.062283871
0.34	0.457698595	0.586998735	0.798135413	0.761341518
-0.28	-0.49407365	-0.37007003	-0.279160469	-0.421781918
-1.22	-1.177957278	-0.858719263	-0.69139608	-0.539029779
-0.13	-0.307874091	-0.311886358	-0.339891801	-0.480643996
-0.38	-0.513489736	-0.538686367	-0.613085354	-0.445028286
-0.79	-0.963118347	-0.907628537	-0.415528689	-0.409748558
-0.54	-0.418738396	-0.367158387	-0.272825028	0.093524732
-0.46	-0.73048915	-0.510289264	-0.217114789	-0.150096974
-1.03	-1.007826504	-0.931185922	-0.568890505	-0.683072407
0.71	0.908181454	0.709980234	0.609584472	0.404975953

Text S1 Selected molecular descriptors

1. MATS Descriptors: MATSv5, MATSe5, MATSe6, MATSe8, MATSm5, MATSm6, MATSp4, MATS5m, MATS3e, MATS7e, MATS7i, MATS8i
2. GATS Descriptors: GATSe8, GATSv8, GATS3m, GATS4m, GATS5m, GATS7m, GATS7e, GATS8e, GATS5p, GATS8p, GATS2i, GATS8i, GATS1s, GATS7s
3. VSA and PEOE Descriptors: VSAEstate10, MRVSA9, MRVSA8, PEOEVSA10, PEOEVSA3, PEOEVSA7, PEOEVSA9, EstateVSA4, EstateVSA1
4. Topological and Connectivity Descriptors: dchi0, IC3, chiChain.7, autoCorrelationCharge.4, chiCluster.1, fmf, chiChain.3, carbonTypes.6, longestAliphaticChain, carbonTypes.7
5. Fragment-Based Descriptors: fr_C_O, fr_allylic_oxid, fr_aryl_methyl, fr_bicyclic, fr_unbrch_alkane
6. Miscellaneous Descriptors: nP.1, AATS6i, AATS1s, SpMax5_Bhp, C1SP3, C3SP3, SCH-6, VCH-5, SC-5, VR3_Dt, maxsBr, ETA_Shape_X, ETA_BetaP_s, CIC5.1, nAtomLAC, MDEC-33, LipinskiFailures, topoRadius, GGI10, JGI2, JGI5, VE3_D, VR2_D
7. ATSC and AATSC Descriptors: ATSC3c, ATSC6c, ATSC8c, ATSC6v, ATSC8e, ATSC2p, ATSC3p, ATSC5p, ATSC6i, ATSC3s, ATSC4s, ATSC5s, AATSC4m, AATSC0v, AATSC2v, AATSC3v, AATSC0p, AATSC2i, AATSC3i, AATSC4i, AATSC7s, AATSC8s
8. BCUT Descriptors: bcute10, bcutp5

Text S2 The code of machine learning

(1) t-SNE analysis

```
# Import necessary libraries
import pandas as pd
from sklearn.preprocessing import StandardScaler
from sklearn.manifold import TSNE
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
from matplotlib import rcParams

data = pd.read_excel('data.xlsx')

features = data.drop(columns=['logRCF'])
labels = data['logRCF']

scaler = StandardScaler()
features_scaled = scaler.fit_transform(features)

tsne = TSNE(n_components=3, perplexity=20, learning_rate=200, random_state=42)
tsne_results = tsne.fit_transform(features_scaled)
data['t-SNE-1'] = tsne_results[:, 0]
data['t-SNE-2'] = tsne_results[:, 1]
data['t-SNE-3'] = tsne_results[:, 2]
config = {
    "font.family": 'serif',
    "font.size": 12,
    "mathtext.fontset": 'stix',
    "font.serif": ['Times New Roman'],
    'axes.unicode_minus': False
}
rcParams.update(config)

cm = plt.cm.get_cmap('RdYlGn')
fig = plt.figure(figsize=(12, 10))
ax = fig.add_subplot(111, projection='3d') # Set the 3D plot projection
sc = ax.scatter(tsne_results[:, 0], tsne_results[:, 1], tsne_results[:, 2], c=labels,
               cmap=cm, s=50, alpha=0.75)
plt.colorbar(sc, label='logRCF')
ax.set_xlabel('t-SNE 1', fontsize=12)
ax.set_ylabel('t-SNE 2', fontsize=12)
ax.set_zlabel('t-SNE 3', fontsize=12)
plt.title('3D t-SNE')
plt.grid(True)
```

```
plt.show()
```

```
data.to_excel('tsne_results.xlsx', index=False)
```

(2) Model construction and interpretation

```
import pandas as pd
import numpy as np
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import train_test_split, cross_val_score
from hyperopt import fmin, tpe, hp
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.metrics import r2_score, mean_squared_error, mean_absolute_error
import matplotlib.pyplot as plt
import shap
from sklearn.inspection import partial_dependence
from mpl_toolkits.mplot3d import Axes3D
from matplotlib.gridspec import GridSpec
from matplotlib import rcParams

random_seed = 42

data = pd.read_excel("database.xlsx")
X = data.drop(columns=['logRCF'])
y = data['logRCF'].to_numpy()

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,
random_state=random_seed)

scaler = StandardScaler()
X_train = scaler.fit_transform(X_train)
X_test = scaler.transform(X_test)

best_scores = {
    'gradient_boosting': {'score': float('inf'), 'params': None},
}

def objective(params):
    param = params.pop('model')
    model_type = param.pop('type')

    if model_type == 'gradient_boosting':
        model = GradientBoostingRegressor(**param,
random_state=random_seed)
        score = cross_val_score(model, X_train, y_train, cv=5, scoring='r2').mean()
```

```

r2 = -score

if r2 < best_scores[model_type]['score']:
    best_scores[model_type]['score'] = r2
    best_scores[model_type]['params'] = param

return r2

search_space = {
    'model': hp.choice('model_type', [
        {
            'type': 'gradient_boosting',
            'n_estimators': hp.choice('n_estimators_gb', range(30,80)),
            'learning_rate': hp.uniform('learning_rate_gb', 0.1, 0.2),
            'max_depth': hp.choice('max_depth_gb', range(15, 25)),
            'min_samples_split': hp.choice('min_samples_split_gb', range(2, 20)),
            'min_samples_leaf': hp.choice('min_samples_leaf_gb', range(2, 20)),
            'max_features': hp.choice('max_features_gb', range(35, 50))
        },
    ])
}

best_params = fmin(fn=objective, space=search_space, algo=tpe.suggest,
max_evals=500, rstate=np.random.default_rng(random_seed))

for model_type, model_info in best_scores.items():
    print(f'Model: {model_type}, Best Score: {model_info['score']}, Best Params: {model_info['params']}")

print()
for model_type, model_info in best_scores.items():
    model_params = model_info['params'].copy()
    if model_type == 'gradient_boosting':
        model = GradientBoostingRegressor(**model_params,
random_state=random_seed)

    model.fit(X_train, y_train)
    y_pred = model.predict(X_test)

    r2 = r2_score(y_test, y_pred)
    mse = mean_squared_error(y_test, y_pred)
    mae = mean_absolute_error(y_test, y_pred)

    print(f'Model: {model_type:<20}\t R2: {r2:.6f}\t MSE: {mse:.6f}\t MAE:

```

```
{mae:.6f}")
```

PFI analysis

```
feature_importance = model.feature_importances_  
feature_importance_df = pd.DataFrame({'Feature': X.columns, 'Importance':  
feature_importance})  
feature_importance_df = feature_importance_df.sort_values(by='Importance',  
ascending=False)
```

```
top_15_features = feature_importance_df.head(15)
```

```
config = {  
    "font.family": 'Arial',  
    "font.size": 42,  
    "mathtext.fontset": 'stix',  
    "font.serif": ['Arial'],  
    'axes.unicode_minus': False,  
    'axes.labelweight': 'bold',
```

```
}  
rcParams.update(config)
```

```
plt.figure(figsize=(20, 10))  
plt.barh(top_15_features['Feature'], top_15_features['Importance'], color='#B54764')  
plt.xlabel('Permutaion Importance')  
plt.ylabel('Features')  
plt.title('The top 15 most important features')  
plt.xticks(fontsize=40, fontweight='bold')  
plt.yticks(fontsize=40, fontweight='bold')  
plt.gca().invert_yaxis()  
plt.savefig(f'PFI.png')
```

SHAP analysis

```
best_model =  
GradientBoostingRegressor(**best_scores['gradient_boosting']['params'],  
random_state=random_seed)  
best_model.fit(X_train, y_train)
```

```
explainer = shap.Explainer(best_model, X_train)  
shap_values = explainer.shap_values(X_test, check_additivity=False)
```

```
config = {  
    "font.family": 'Arial',  
    "font.size": 30,
```

```

    "mathtext.fontset": 'stix',
    "font.serif": ['Arial'],
    'axes.unicode_minus': False,
}
rcParams.update(config)

shap.summary_plot(shap_values, X_test, plot_type="dot", feature_names=X.columns,
show=False)
fig = plt.gcf()
fig.set_size_inches(12,8)
plt.xlabel('SHAP Value')
plt.ylabel('Feature')
plt.xticks(fontsize=22, fontweight='bold')
plt.yticks(fontsize=22, fontweight='bold')
plt.savefig(f'SHAP.png')

# ICE analysis
SOM_step_lst = np.arange(SOM_min, SOM_max, 0.01)

SOM_df = pd.DataFrame(index=np.arange(X_test.shape[0]),
columns=list(SOM_step_lst))

for jj in range(X_test.shape[0]):
    for ii, som_val in enumerate(SOM_step_lst):
        SOM_sample = X_test[jj, :].copy()
        SOM_sample[X.columns.get_loc('SOM')] = (som_val -
scaler.mean_[X.columns.get_loc('SOM')]) / scaler.scale_[X.columns.get_loc('SOM')]
        SOM_pred = best_model.predict(SOM_sample.reshape(1, -1))[0]
        SOM_df.iloc[jj, ii] = SOM_pred

config = {
    "font.family": 'Arial',
    "font.size": 16, #
    "mathtext.fontset": 'stix',
    "font.serif": ['Arial'],
    'axes.unicode_minus': False,
}
rcParams.update(config)

plt.figure(figsize=(10, 6))
for ii in range(SOM_df.shape[0]):
    plt.plot(SOM_step_lst, SOM_df.iloc[ii, :], alpha=0.12, c='#ED630A',
linewidth=0.4)

```

```
SOM_df_mean = SOM_df.mean(axis=0)
plt.plot(SOM_step_lst, SOM_df_mean, alpha=1, c='#ED630A', label="average")

plt.legend(loc=1, prop={'family': 'Arial'})
plt.xlabel('SOM (%)', fontsize=26, family='Arial')
plt.ylabel('Partial Dependence', fontsize=26, family='Arial')
plt.xticks(fontsize=22, fontweight='bold')
plt.yticks(fontsize=22, fontweight='bold')
plt.savefig(f'SOM-ICE.png')
```