1 **Electronic Supplementary Information**

2 **Table ES-1** Chemical information on 41 musks with ready biodegradation and/or *Daphnia* acute data[f]

Name	SMILES	Musk class	Log K_{OW}[a] [ref]	Log K_{OW}[b]	Log K_{OA}[b]	% Deg in ready test; (method 301B, C,D,F)[a]	RB test ref[c]	Log BAF lower trophic[b]	Log BAF upper trophic[b]	Log 48h *Daphnia* EC_{50}[a,c] [ref]
Helvetolide	CCC(=O)OCC(C)(C)OC(C)C1CC(C)(C)CCC1	Alicyclic		5.51	8.34	17 (D)	74	2.78	2.37	0.519 [74]
Romandolide	CCC(=O)OCC(=O)OC(C)C1CC(C)(C)CCC1	Alicyclic		4.45	7.49	68 (D)	75	1.38	1.20	>0.500 [75]
	confidential	Macrocyclic		5.37	6.33	82(B)	P	3.17	2.76	
	confidential	Macrocyclic		4.41	6.76	80 (D)	P	2.41	2.26	
	confidential	Macrocyclic		4.81	5.89	84 (F)	P	2.80	2.58	
	CCOC(=O)CC(=O)OC(C)C1CC(C)(C)CCC1	Alicyclic		4.45	8.34	89 (B)	P	1.38	1.20	0.544, P
	CC1CC(=O)CCCCCCCCC=CC1	Macrocyclic		5.26	6.89	70 (F)	76	3.74	3.65	-0.237 [76]
	confidential	Alicyclic		5.37	8.60	19 (B)	P	2.72	2.37	
Serenolide	C1CC1C(=O)OCC(C)(C)OC(C)C2CC(C)(C)CCC2	Alicyclic	5.6 [37]	5.82	8.66	12 (C)	37	2.73	2.30	>0.173 [37]
Sylkolide	CC(C)C=C(C)C(C)OC(C)(C)COC(=O)C1CC1	Alicyclic		4.9	7.84	67 (D)	P	2.45	2.23	>0.301, P
3-Methylcyclopentadecenone	O=C1CC(C)=CCCCCCCCCCC1	Macrocyclic		5.88	7.31	70 (B,B,D,F)	76	4.48	4.04	-0.409 [76]

Z-4-Cyclopentadecen-1-one	O=C(CCC=CCCCCCCCC1)C1	Macrocyclic		5.33	6.96	84 (B)	76	3.74	3.35	
5-Cyclohexadecen-1-one	O=C1CCCC=CCCCCCCCCC1	Macrocyclic		5.82	7.33	72 (B,B,C,C,C,F)	76	4.35	3.87	
Ethylene brassylate	O=C1CCCCCCCCCCCC(=O)OCCO1	Macrocyclic		4.71	8.60	78 (B,B,C,D,F,F,F,F,)	76	1.77	1.58	
Omega-pentadecalactone	O=C(OCCCCCCCCCCCCCC1)C1	Macrocyclic		6.15	7.17	84 (B,B,D,F)	76	3.83	2.95	
Ethylene dodecanedioate	C1CCCCCC(=O)OCCOC(=O)CCCC1	Macrocyclic	3.65 [76]	4.22	7.67	83 (B,B,B,C)	76	1.35	1.19	
Oxacyclohexadecen-2-one	O=C1/C=C/CCCCCCCCCCCCO1	Macrocyclic		4.88	6.23	91 (B,C,F)	76	2.78	2.55	-0.319 [76]
Oxacycloheptadec-10-ene-2-one	O=C(OCCCCCCCC=CCCCCCC1)C1	Macrocyclic		5.37	6.33	84 (F)	76	3.17	2.76	
Celestolide	O=C(c(c(c(cc1C(C)(C)C)C(C2)(C)C)C2)c1)C	Polycyclic	5.4,6.6 [21,77]	5.93	8.89	0 (not stated)	10	3.92	3.13	
Phantolide	O=C(c(c(cc(c1C(C2C)(C)C)C2(C)C)C)c1)C	Polycyclic	5.8,6.7 [21,77]	5.85	9.14	0 (D)	10	4.40	3.64	-0.481 [78]
Galaxolide	CC1(C)C(C)C(C)(C)C2C=C3C(C)COCC3=CC=21	Polycyclic	5.9 [29]	5.9	8.17	0 (B)	19,26	3.97	3.26	-0.0458 [79]
Tonalide	O=C(c(c(cc(c1C(CC2C)(C)C)C2(C)C)C)c1)C	Polycyclic	5.7,5.8 [29,21]	5.7	7.95	0 (not stated)	19,26	4.40	4.06	-0.0969 [79]
Musk ketone	O=C(c(c(c(N(=O)=O)c(c1N(=O)=O)C(C)(C)C)C)c1C)C	Nitro	4.3 [77]	4.3	12.01	0 (not stated)	19,26	2.02	1.86	
Musk xylene	N(=O)(=O)c(c(c(N(=O)(=O))c(c	Nitro	4.9 [77]	4.45	12.27	2 (C)	19,26	2.17	1.95	

	1N(=O)(=O))C(C)(C)C)c1C									
Musk tibetene	N(=O)(=O)c(c(c(N(=O)(=O))c(c1C)C)C(C)(C)C)c1C	Nitro		5.18	10.11	0 (C)[d]	78	2.50	2.22	
Musk moskene	N(=O)(=O)c(c(c(N(=O)(=O))c(c1C(C2)(C)C)C2(C)C)C)c1	Nitro		5.39	10.47	0 (C)[d]	78	2.79	2.42	
Versalide(1a)	CC1(C)c2cc(C(C)=O)c(CC)cc2C(C)(C)CC1	Polycyclic	5.7 [38]	6.42	8.46	0 (F)	38	4.22	3.75	
Versalide(1b)	CSi1(C)c2cc(C(C)=O)c(CC)cc2Si(C)(C)CC1	Polycyclic sila	6.5[e] [38]	7.24	9.28	0 (F)	38	5.61	5.78	
Versalide(2a)	CC1(C)c2cc(C(C)=O)c(C)cc2C(C)(C)CC1	Polycyclic	4.8 [38]	5.93	7.69	0 (F)	38	3.33	3.17	
Versalide(2b)	CSi1(C)c2cc(C(C)=O)c(C)cc2Si(C)(C)CC1	Polycyclic sila	6 [38]	6.75	8.90	0 (F)	38	5.12	5.23	
Versalide(3a)	CC1(C)c2cc(C(C)=O)ccc2C(C)(C)CC1	Polycyclic	4.8 [38]	5.38	7.73	0 (F)	38	3.46	3.35	
Versalide(3b)	CSi1(C)c2cc(C(C)=O)ccc2Si(C)(C)CC1	Polycyclic sila	5.5 [38]	6.2	8.45	0 (F)	38	4.62	4.84	
cyclohexadecanone	O=C1CCCCCCCCCCCCCCC1	Macrocyclic		6.04	7.489	43 (B)	76	4.59	4.11	
muscone	O=C1CC(C)CCCCCCCCCCC1	Macrocyclic		5.96	7.409	80 (F)	76	4.58	4.16	
3-methyl-5-cyclopentadecen-1-one	O=C1CC(C)CC=CCCCCCCCCC1	Macrocyclic	6.57 [76]	5.75	8.075	80 (F)	76	5.21	4.96	
10-oxahexadecanolide	O=C(OCCCCCCCCCCCCCC1)C1	Macrocyclic		4.90	7.979	100 (B)	76	2.71	2.48	
11-	O=C(OCCCCCO	Macrocyclic		4.90	7.979	80 (B)	76	2.71	2.48	

oxahexadecanolide	CCCCCCCC1)C1									
Cervolide	O=C(OCCCCOCCCCCCCC1)C1	Macrocyclic		4.90	7.979	97 (B)	76	2.71	2.48	
oxacyclohexadecane-2,13-dione	O=C1OCCCC(=O)CCCCCCCCC1	Macrocyclic		4.10	8.542	83 (B)	76	2.12	1.98	1.326 [76]
Traseolide	CC(C)C1c2cc(C(C)=O)c(C)cc2C(C)(C)C(C)1	Polycyclic		6.31	9.073	No data		4.17	3.258	-0.377 [78]
Musk ambrette	c1(C(C)(C)C)c(OC)c(N(=O)=O)c(C)c(N(=O)=O)c1	Nitro		4.17	10.41	No data		2.27	2.142	-0.208 [80]

[a] Measured.

[b] Estimated; see text for details.

[c] P=Measured, US Premanufacture Notice data.

[d] Stated to be not inherently biodegradable in MITI-II (OECD 302C) test; therefore, assigned 0% for ready biodegradability in the MITI-I (301C) test.

[e] Given as >6.0; extrapolated to 6.5 based on differences among estimated values for the non-Si analogs (i.e. Versalide 1a, 2a, 3a).

[f] Additional references not cited in text:

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Table ES-2 Forty-eight musks described in research reports and lacking published biodegradation data[a]

ID	Source chem. no.	SMILES	Odor profile	Musk class	Reference	Ready biodeg prediction
1	12	CC1(C)CC(C(C)(C)OC(=O)COC(=O)CC)CCC1	Strongly musky, woody, ambery	Alicyclic Romandolide	44	RB
2	13	CC1(C)CC(C(C)(C)OC(=O)COC(=O)C)CCC1	Musky, erogenous, animalic	Alicyclic Romandolide	44	RB
3	14	CC1CC(C(C)(C)OC(=O)COC(=O)CC)CCC1	Musky, ambery, animalic	Alicyclic Romandolide	44	RB
4	15	CC1C(C(C)(C)OC(=O)COC(=O)CC)CCCC1	Fruity, sweet, slightly musky	Alicyclic Romandolide	44	RB
5	17	CC1(C)CC(C(C)(C)OC(C)COC(=O)CC)CCC1	Slightly musky, sweet	Alicyclic Helvetolide	44	NRB
6	18	C1CC(C(C)OC(C)(C)COC(=O)CC)CCC1	Musky, erogenous, floral	Alicyclic Helvetolide	44	RB
7	19	CC1CC(C(C)OC(C)(C)COC(=O)CC)CCC1	Strongly musky, floral	Alicyclic Helvetolide	44	NRB
8	20	C1C(C)C(C(C)OC(C)(C)COC(=O)CC)CCC1	Musky, natural, like muscone	Alicyclic Helvetolide	44	NRB
9	24	CC1CC(C(C)OC(=O)COC(=O)CC)CCC1	Musky, erogenous, floral	Alicyclic Romandolide	44	RB
10	22	C1(=O)CC2CC(CCC(C)CO1)CCCCC2	Musky, powerful, fresh, anisic, ambery, fruity	Macrobicyclic lactone	39	RB
11	27b	C1(=O)C2OC(CCCCCCCCCC1)CCC2	Strong musk odor	Macrobicyclic ketone	41	NRB
12	27c	C1(=O)C2OC(CCCCCCCCC1)CC(C)C2	Strong musk odor	Macrobicyclic ketone	41	NRB
13	241	C1C2OC(=O)CCCCCCCCCCCCC2CC1	Slightly musky, aldehydric, fatty, woody	Macrobicyclic lactone	60	RB

14	17	C1(=O)CC2CC(CCCCCO1)CCCC2		Macrobicyclic lactone	40	RB
15	18	C1(=O)CC2CC(CCCCO1)CCCCC2		Macrobicyclic lactone	40	RB
16	58/5	O=C1OCCCCCCCCSCCCC1	Musky, sweet, green	Thiamacrolide	7	RB
17	58/11	O=C1OCCCCCCCCCCSCCC1	Musky, powdery, fruity	Thiamacrolide	7	RB
18	58/12	O=C1OCCCCCCCCCCSC(C)CC1	Musky, metallic, sweet	Thiamacrolide	7	RB
19	58/13	O=C1OCCCCCCCCCCSCCCC1	Musky, powdery, dry	Thiamacrolide	7	RB
20	61	O1CC=CCOCCCCCCCCCC1	Musky, pleasant, powdery, sweet	Macrocyclic (ether)	7	NRB
21	1b	O1CCCCOCCCCCCCCCC1	Musky, intense, animalic	Macrocyclic (ether)	47	NRB
22	59	O=C1CCCCCCCOCCC(C)CCO1		Macrocyclic	7	RB
23	62	C=C1CCCCCCOC(=O)CCCCCCC1	Intense, sweet, musky, animalic	Macrocyclic (methylene)	7	RB
24	63	O1C(=O)CC=CCCC=CCCCCCCC1	Strong erogenous, natural musk	Macrocyclic	7	RB
25	229	C=C1CCCCCOC(=O)CCCCCCCC1	Sweet, animalic, waxy undertone	Macrocyclic (methylene)	60	RB
26	237	O=C1CCCCCC=CCCCCCCCO1		Macrocyclic	60	RB
27	246	O=C1OCCC(C)CCOCCCCCCC1	Extremely powerful	Macrocyclic	60	RB
28	5	O=C1CCCCCCCC=CCCCCCCC1	Civetone	Macrocyclic	7	RB
29	6	O=C1CCCCCCCCCCCCCC1	Exaltone	Macrocyclic	7	RB
30	7	O=C1CCCC=CCCCCCCCC(C)C1		Macrocyclic	7	NRB
31	44	O=C1OCCC=CCCCCCCCCCC1	Habanolide (Globalide);	Macrocyclic	7	RB

			elegant, metallic			
32	1	O1C(=O)CCCCCCCCCCCCC(C)C1	Muscolide; musky, erogenous, animalic	Macrocyclic	81	RB
33	50	O=C1CCCCCCC=CCCCCCCC1	Globanone; aldehydic, waxy	Macrocyclic	7	RB
34	4	CC1Si(C)(C)c2cc(C(=O)C)c(C)cc2Si(C)(C)1	Round and refined musk note	Sila polycyclic	43	NRB
35	6	C=C1Si(C)(C)c2cc(C(=O)C)c(C)cc2Si(C)(C)1	Soft but distinct musk note, floral, green-fruity	Sila polycyclic	43	NRB
36	7	C=C1Si(C)(C)c2cc(C(=O)C)ccc2Si(C)(C)1	Musky, dry, lightly animalic	Sila polycyclic	43	NRB
37	12	C1CC12Si(C)(C)c3cc(C(=O)C)c(C)cc3Si(C)(C)2	Green, musky, ambrette seed	Sila polycyclic	43	NRB
38	13	C1CC12Si(C)(C)c3cc(C(=O)C)ccc3Si(C)(C)2	Distinct musk note, fruity-floral, rose	Sila polycyclic	43	NRB
39	37	CC(C)C=C(C)C(C)OC(C)(C)CCC(=O)CC	Musky, sweet, fruity	Noncyclic (Helvetolide like)	40	NRB
40	38	CC(C)CC(C)C(C)OC(C)(C)CCC(=O)CC	Musky, slightly fruity-floral	Noncyclic (Helvetolide like)	40	NRB
41	9	CC1(C)C=C(C(C)OC(C)(C)COC(=O)CC)CCC1		Alicyclic Helvetolide	44	NRB
42	1	CC(=C)C1C(CC(C)(C)COC(=O)CC)=C(C)CC1	Cyclomusk; fruity, strawberry-like	Alicyclic Helvetolide	44	RB
43	26	CC1(C)CC(C(C)OC(C)(C)COC(=O)C2CCCC2)CCC1		Alicyclic Helvetolide	40	NRB
44	27	CC1(C)C=C(C(C)OC(C)(C)COC(=O)CC)CCC1		Alicyclic Helvetolide	40	NRB
45	28	CC1(C)CC(C(C)OC(C)(C)COC(=O)CC)=CCC1		Alicyclic Helvetolide	40	NRB
46	29	CC1(C)C=C(C(C)OC(=O)COC(=O)CC)CCC1		Alicyclic Romandolide	40	RB

47	30	CC1(C)CC(C(C)OC(=O)COC(=O)CC)=CCC1		Alicyclic Romandolide	40	RB
48	42	CC1(C)CC(C(C)C(=O)OCC(=O)OCC)CCC1	Typical musk, fruity, rhubarb, rosy	Alicyclic Romandolide	40	RB

[a] Additional reference not cited in text:

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