

TrainingResponses

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Predicting olfactory receptor neuron responses from odorant structure – additional file 2

index	substance name	ab1D	ab2A	ab2B	ab3A	ab3B	ab5B	ab6A
1	(E)2-hexen-1-ol	-3	-3	56	2	16	0	123
2	(E)2-hexenal	1	-1	2	3	(24)	2	85
3	(E)2-hexenyl acetate	-3	8	0	114	-11	22	78
4	(E)2-octenal	1	-3	3	(20)	8	3	71
5	(R)-(+)-limonene	-2	-7	1	-4	-6	-8	-8
6	1,4-cineole	-4	-2	1	-1	3	0	-6
7	1,4-diaminobutane	-1	-11	-1	-1	19	(13)	3
8	1-octen-3-ol	0	-3	(14)	49	39	(13)	175
9	1-propanethiol	3	-11	2	5	(22)	7	-1
10	2,3-butanedione	2	102	1	(21)	46	-5	42
11	2-heptanone	0	5	1	33	122	70	48
12	2-isobutyl-3-methoxy-pyrazine	6	-4	-1	-6	2	-4	-3
13	3-(methylthio)-1-propanol	9	-7	4	2	10	152	14
14	3-octanol	2	-2	7	57	112	27	162
15	4-isopropylbenzaldehyde	13	-2	1	-7	16	-1	-14
16	4-methylcyclohexanol	7	0	3	(13)	4	-2	-15
17	4-methylphenol	(22)	-3	0	-1	(31)	1	-12
18	Acetophenone	157	-8	2	-7	1	1	-15
19	alpha-pinene	-4	-8	0	-3	13	-5	12
20	Ammonia	5	-10	-1	-1	17	5	-10
21	beta-citronellol	-6	-7	3	-5	12	4	53
22	Benzaldehyde	49	-8	1	-5	3	-1	-13
23	Butanoic acid	1	-2	1	(20)	2	-4	82
24	Butanol	0	13	2	(11)	11	-5	-16
25	Carbon dioxide	0	5	1	4	14	1	10
26	cis-vaccenyl acetate	5	-6	1	(13)	-12	-1	-16
27	Cyclohexanone	-8	-2	-1	3	-1	-2	-15
28	Dipropyldisulphide	6	-10	-2	2	8	5	4
29	Ethanolamine	0	-9	5	4	9	8	-6
30	Ethyl 2-methylbutanoate	6	14	23	141	-7	2	2

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31	Ethyl acetate	4	156	1	(14)	9	8	9
32	Ethyl butanoate	4	(23)	73	145	5	3	-2
33	Ethyl propionate	-1	69	(20)	60	-10	8	-12
34	Eugenol methyl ether	11	-1	1	-7	11	-1	-15
35	Geranyl acetate	2	5	0	1	(29)	-5	(26)
36	gamma-valerolactone	32	-2	23	32	-2	-2	47
37	Hexanol	3	8	67	(20)	87	5	134
38	Indole	4	0	1	-1	10	-3	5
39	Iso-amyl acetate	50	7	9	104	8	45	(24)
40	Iso-amyl alcohol	1	1	4	(14)	6	1	-10
41	Linalool	-2	-7	-4	-1	14	-1	(36)
42	Methyl salicylate	187	-2	3	4	3	-3	5
43	Nonanal	1	-5	-1	-4	6	-4	-9
44	Pentyl acetate	5	(23)	2	111	(25)	198	69
45	Phenylacetaldehyde	76	-6	0	-3	12	-5	-19
46	Propanone	-3	88	1	1	2	1	(35)
47	Pyrrolidine	2	-5	6	-4	(24)	-1	(28)
lower threshold		20	20	10	10	20	10	20
upper threshold		30	30	20	30	35	20	40
number of actives		6	4	6	10	5	6	13
number of inactives		40	41	40	28	36	39	29