

Table S3

Top twenty¹ scaled-score outputs obtained with Elastic-Net, Random Forest and Support-Vector Machine.

Elastic-net		Random forest		Support-vector machine	
Predictor compound	Scaled score				
2-Octen-1-ol, (E)-	100	Isoamyl cyanide	100	Dicyclohexyl phthalate	100
2-Hexenoic acid, 3,4,4-trimethyl-5-oxo-, (Z)-	92,06	Dodecanoic acid	99,96	Benzoic acid, 2-hydroxy-, pentyl ester	84,21
1H-Pyrazol-3-amine	90,8	2-Hexenoic acid, 3,4,4-trimethyl-5-oxo-, (Z)-	95,64	2-Octen-1-ol, (E)-	82,89
n-Decanoic acid	89,69	n-Decanoic acid	76,54	Tetracosane	78,95
2-Methylbutanoic anhydride	89,58	Formic acid, 2-propenyl ester	63,88	2-Piperidinone	78,95
Isothiazole	87,14	Oxalic acid, isobutyl pentyl ester	52,14	Undecane, 2,6-dimethyl-	77,63
2-Piperidinone	83,93	2-Octen-1-ol, (E)-	51,45	2,4-Nonadienal	77,63
Isoamyl cyanide	83,67	9-Hexadecenoic acid	50,77	Pentadecanoic acid	76,32
Dodecanoic acid	81,11	2-Methylbutanoic anhydride	49,8	Propanamide	73,68
Oxalic acid, isobutyl pentyl ester	71,95	Phthalic acid, 6-ethyl-3-octyl butyl ester	47,21	Benzene, (2-methylpropyl)-	73,68
1-Nonen-3-ol	64,84	Ethanone, 1-(2-methyl-1-cyclopenten-1-yl)-	45,82	Pyridine, 2,4-dimethyl-	71,05
Formic acid, 2-propenyl ester	64,21	2,4-Decadienal, (E,E)-	43,81	Butanamide, 3-methyl-	68,42
Propanoic acid, ethenyl ester	55,42	Pyridine, 3-ethyl-4-methyl-	43,32	Z-10-Pentadecen-1-ol	68,42
Ethanone, 1-(2-methyl-1-cyclopenten-1-yl)-	50,88	Isothiazole	43,13	6-Methyl-3,5-heptadiene-2-one	67,11
1,2-Ethanediamine, N,N-diethyl-	47,72	Indene	43	Cyclodecane	65,79
Naphthalene, 1,2,3,4-tetrahydro-1,4-dimethyl-	46,44	Butane, 2,2-dimethyl	42,02	Dimethyl ether	65,79
9-Hexadecenoic acid	44,74	2-Piperidinone	40,83	Isopropyl acetate	65,79
Cyclodecane	39,94	Pentadecane, 2,6,10,14-tetramethyl-	40,42	Naphthalene, 2,3,6-trimethyl-	63,16
				Cyclopentaneacetic acid, 3-oxo-2-pentyl-, methyl ester	61,84
3-Pentanol, 2,4-dimethyl,	39,75	Pyridine, 2,4-dimethyl-	39,39	Benzene, propyl-	60,53
Propanal	37,83	Pentadecanoic acid	38,68		

¹The full scaled-score outputs for the pre-processed set of 1131 variables are available upon request.