Table 1supp: List of compounds analysed and their abbreviations, also used in the text and figures.

Compound name	Abbreviation
Organochlorines	
2,4,4'-Trichlorobiphenyl	CB-28
2,4',5-Trichlorobiphenyl	CB-31
2,2',5,5'-Tetrachlorobiphenyl	CB-52
2,2',4,4',5-Pentachlorobiphenyl	CB-99
2,2',4,5,5'-Pentachlorobiphenyl	CB-101
2,3,3',4,4'-Pentachlorobiphenyl	CB-105
2,3,3',4',6-Pentachlorobiphenyl	CB-110
2,3',4,4',5-Pentachlorobiphenyl	CB-118
2,2',3,3',4,4'-Hexachlorobiphenyl	CB-128
2,2',3,4,4',5'-Hexachlorobiphenyl	CB-138
2,2',3,4',5',6-Hexachlorobiphenyl	CB-149
2,2',3,5,5',6-Hexachlorobiphenyl	CB-151
2,2',4,4',5,5-Hexachlorobiphenyl	CB-153
2,3,3',4,4',5-Hexachlorobiphenyl	CB-156
2,2',3,3'4,4',5-Heptachlorobiphenyl	CB-170
2,2',3,4,4',5,5'-Heptachlorobiphenyl	CB-180
2,2',3,4',5,5',6-Heptachlorobiphenyl	CB-187
2,2',3,4',5,6,6'-Heptachlorobiphenyl	CB-188
2,2',3,3',4,4',5,5'-Octachlorobiphenyl	CB-194
Decachlorobiphenyl	CB-209
α-Hexachlorocyclohexane	α-HCH

β-Hexachlorocyclohexane	β-HCH
γ-Hexachlorocyclohexane	γ-HCH
Hexachlorobenzene	HCB
Trans-nonachlor	TNC
p,p'-dichloro-diphenyl-trichloroethane	p,p'-DDT
p,p'-dichloro-diphenyl-dichloroethylene	p,p'-DDE
p,p'-dichloro-diphenyl-dichloroethane	p,p'-DDD
o,p'-dichloro-diphenyl-trichloroethane	o,p'-DDT
o,p'-dichloro-diphenyl-dichloroethylene	o,p'-DDE
PAHs	
Naphthalene	N
1-Methylnaphthalene	1-MN
2-Methylnaphthalene	2-MN
C2-Naphthalenes	C2N
C3-Naphthalenes	C3N
Acenaphthylene	Acy
Acenaphthene	Ace
Fluorene	F
Dibenzothiophene	DBT
C1-Dibenzothiophenes	C1DBT
C2-Dibenzothiophenes	C2DBT
Phenanthrene	P
2-Methylphenanthrene	2MP
C1-Phenanthrenes	C1P
C2-Phenanthrenes	C2P
C3-Phenanthrenes	C3P

| Anthracene	Ant
Benzo[a]fluorene	BaF
Fluoranthene	Fl
Pyrene	Pyr
1-Methylpyrene	1MPyr
Benzo[a]anthracene	BaAnt
Chrysene/Triphenylene	Chr/Trp
Benzo[b+j+k]fluoranthene	BbjkFl
Benzo[e]pyrene	BePyr
Benzo[a]pyrene	BaPyr
Perylene	Per
Indeno[1,2,3-cd]pyrene	Ipyr
Benzo[g,h,i]perylene	BghiPer
Dibenzo[ah]anthracene	DBahAnt
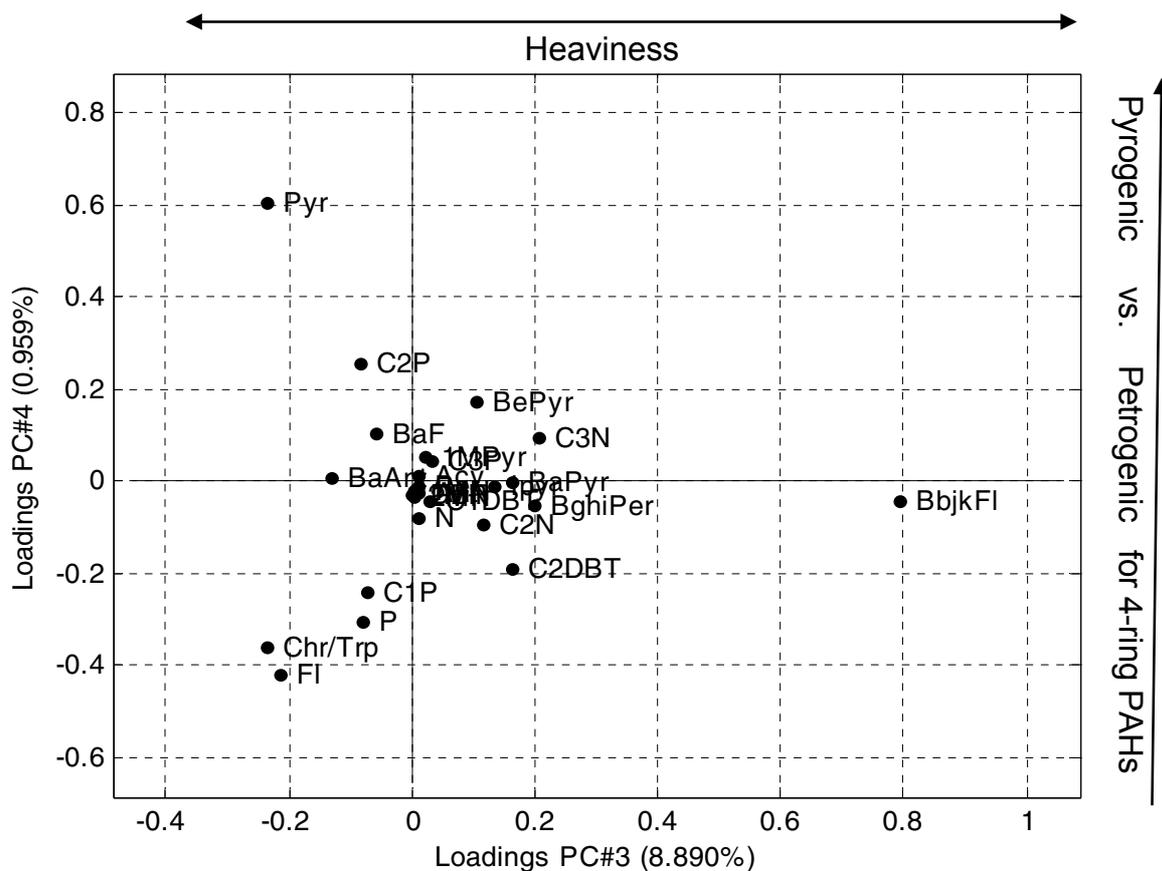
Figure 1supp: Loading plot of PC3 vs. PC4 for the PCA model based on the mean-centred training set consisting of 40 samples and 27 PAH concentrations.
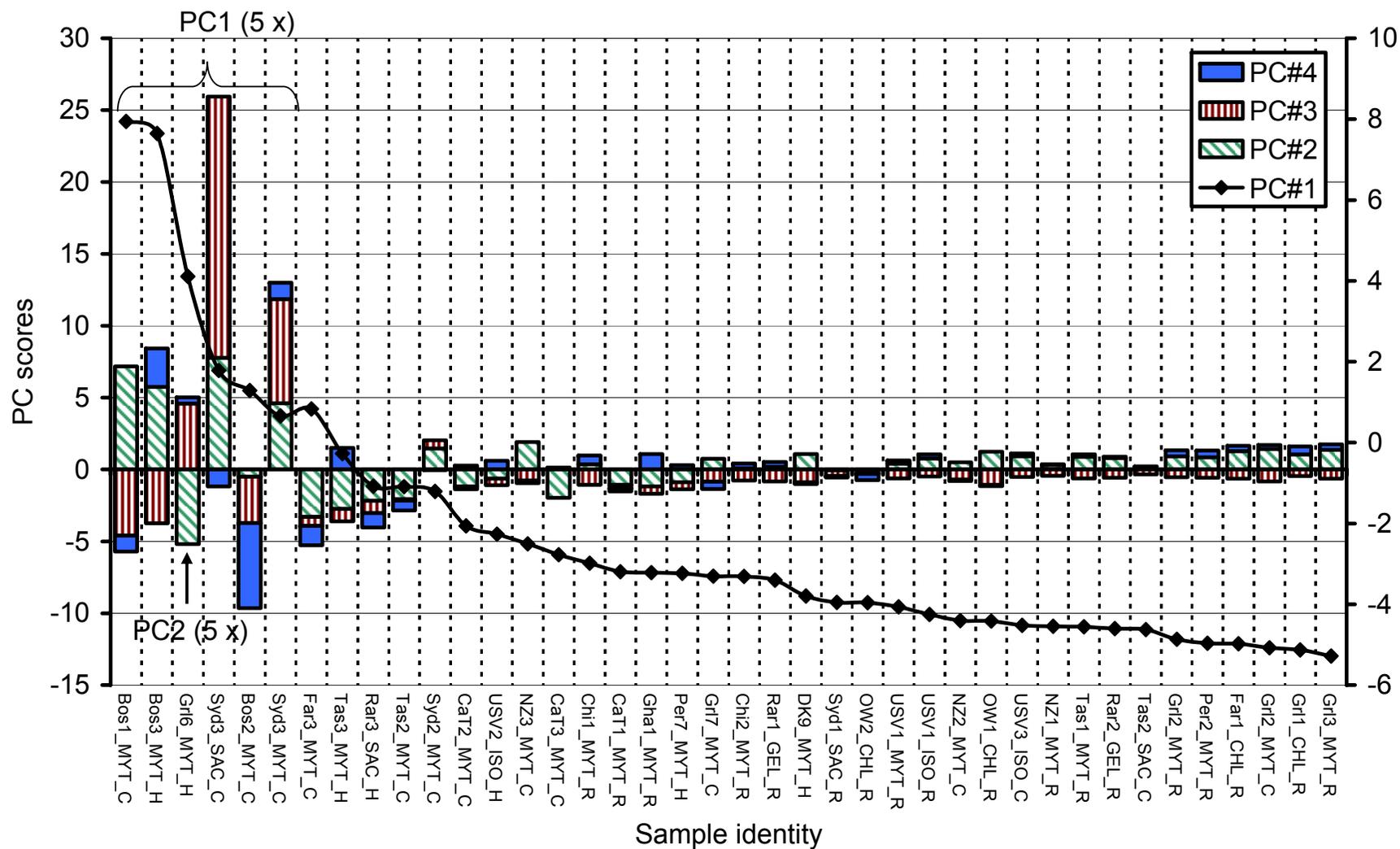
Figure 2supp: Score plots of PC1 (line with markers) and PC2 to PC4 (cumulative bar plot) for the PCA model based on the mean-centred training set consisting of 40 samples and 27 PAH concentrations. The PC1 scores for the six samples with large $\sum PAH_{27}$ have been scaled down with a factor of five, while the PC2 scores for Grl6_MYT_H have been scaled up with 5.