ELECTRONIC SUPPLEMENTARY INFORMATION FOR:

TITLE: Thermodynamic assessment of (semi-)volatile hydrophobic organic chemicals in WWTP sludge – combining Solid Phase Microextraction with non-target GC/MS.

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Table ESI1: List of compounds from full scan HS-SPME-GC/MS on digested sludge data identified by ChemStation and the Spectral Library NIST. NIST Match is spectral similarity out of 1000. Grey shaded compounds are used in the further data analysis, whereas all the compounds are included in the kinetic analysis. These compounds were selected on the criteria of covering the full chromatogram range.

RT	Base peak m/z	m/z 2	m/z 3	Molecular ion	Tentative ID	NIST Match	Confirmed ID
18.913	68	93	67	136	Limonene	869	Citronella oil
19.712	107	108		108	p-Cresol	936	
20.304	57	71	85	156	Undecane	941	Diesel ref.+Standard
20.836	355	73	267		Decamethylcyclopentasiloxane, D5	932	Standard
22.358	57	71	85	170	Dodecane	924	Diesel ref.
24.045	57	71	85	240	2,6,10-trimethyltetradecane	796	
24.833	57	71	85	184	Tridecane	942	Diesel ref.
28.294	57	71	85	198	Tetradecane	931	Diesel ref.+ Standard
31.745	93	80	121	204	Humulene	816	
33.950	205			220	Butylated Hydroxytoluene	793	
33.540	57	71	85	212	Pentadecane	938	Diesel ref.
41.743	57	71	85	226	Hexadecane	896	Diesel ref.
44.239	91	161	105	232	Dodecan-6-ylbenzene	846	
47.337	191	57	192	206	1-Penten-3-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	768	
50.912	57	71	85	240	Heptadecane	917	Diesel ref.
57.081	193	69	109		1,5-Hexadien-3-ol, 3-methyl-6-(methylthio)-1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (E,E)-	710	
62.208	243	213		258	7-Acetyl-6-ethyl-1,1,4,4-tetramethyltetralin, versalide	852	

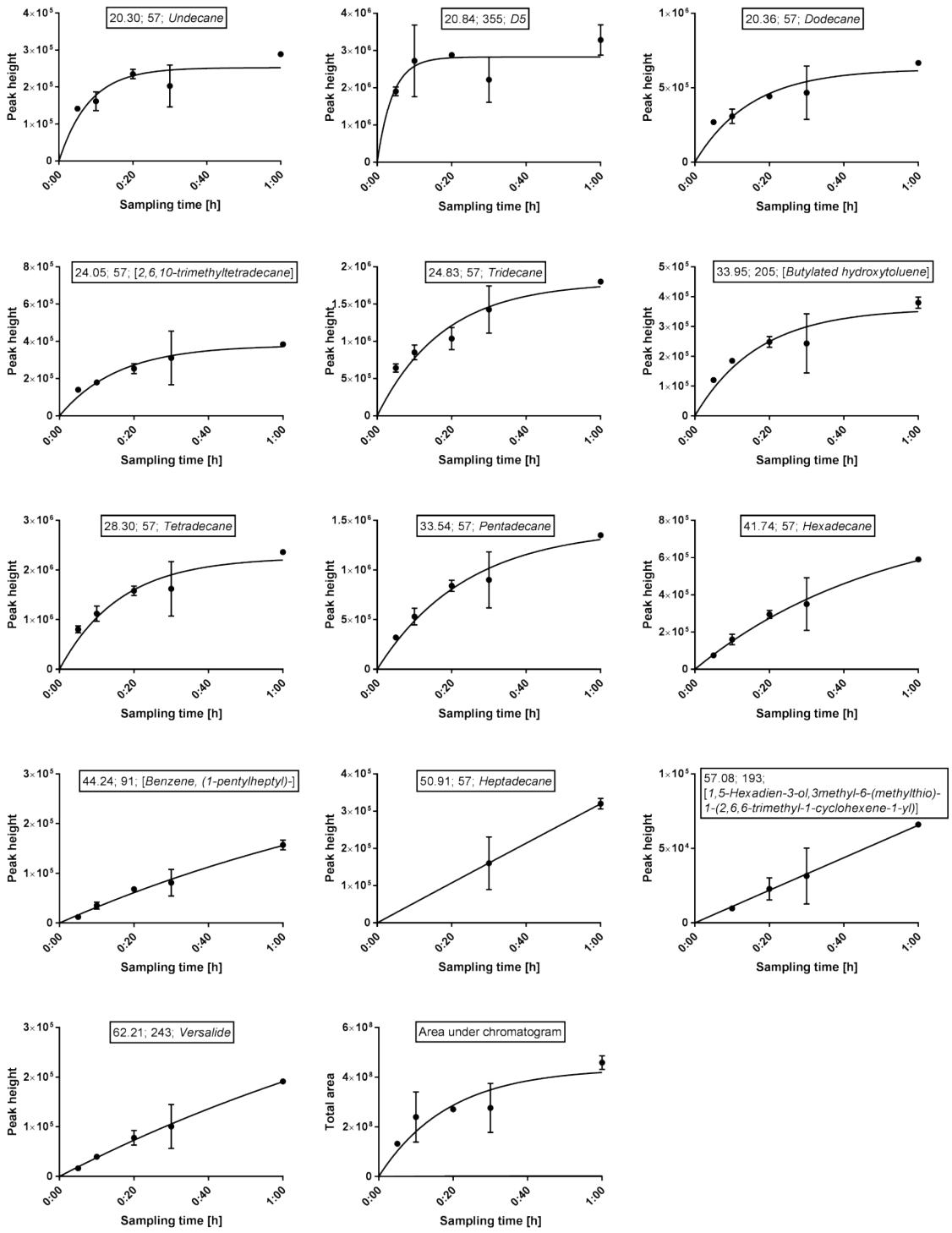


Figure ESI1: Base peak heights of selected molecular features at 5, 10, 20, 30 and 60 mins of sampling time. *n*=2. Curves are modeled by Y = Plateau*e^{-K*t}, where K is the rate constant, and t the time in minutes.

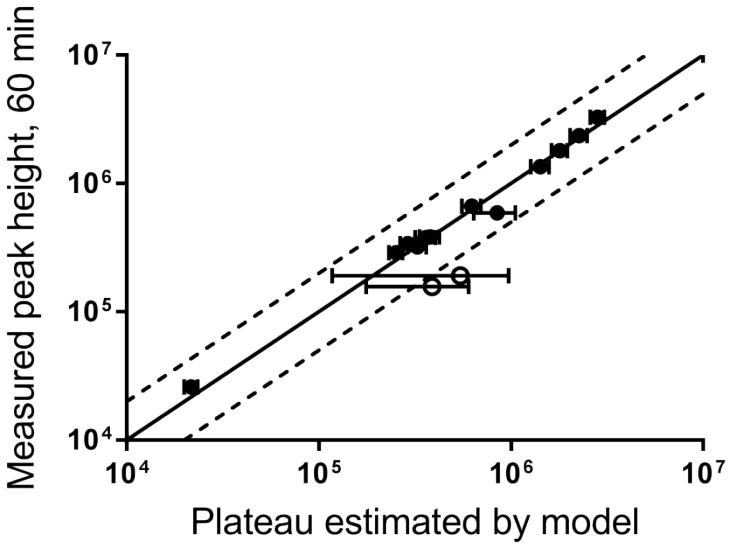


Figure ESI2: Measured base peak height of selected molecular features extracted by MassHunter at 60 mins of sampling time against the corresponding plateau values estimated by first order one phase association model (eq.1) used to model the uptake on the SPME fiber over time. Solid line is unity; dashed lines are a factor 2 deviation. Closed symbols are within a factor 2, whereas open symbols are less certain. The two open symbols are dodecan-6-ylbenzene and versalide. Error bars are SEM. Compounds included in this analysis are listed in Table ESI1.

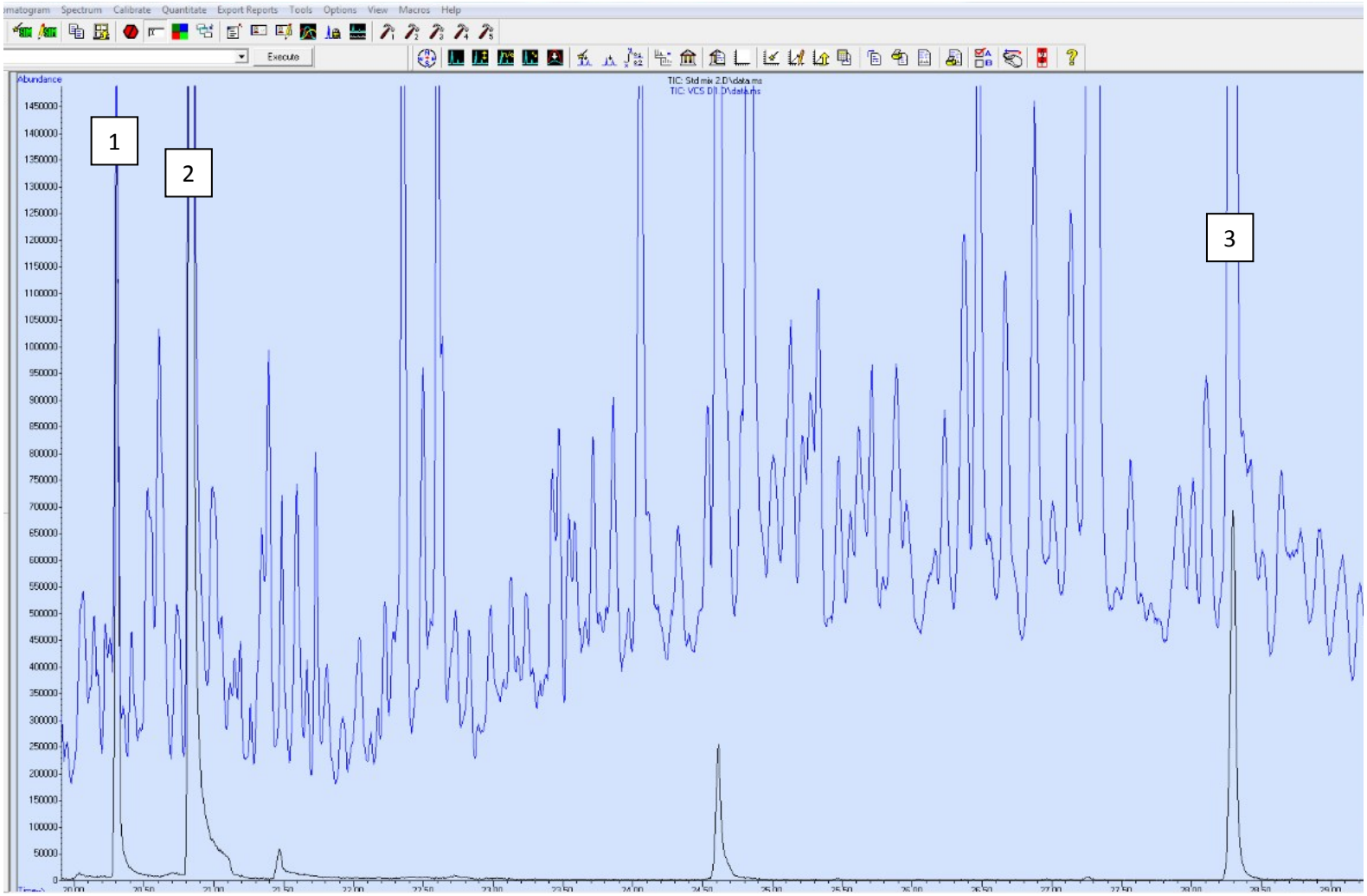
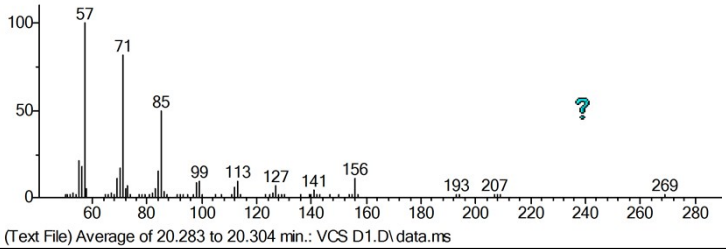
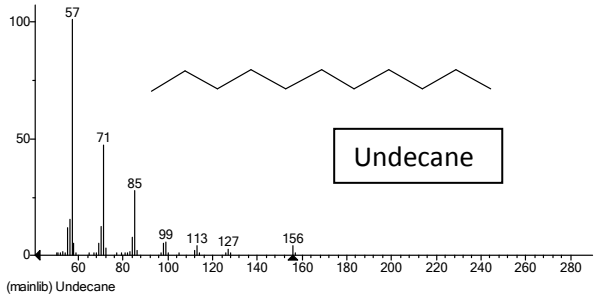
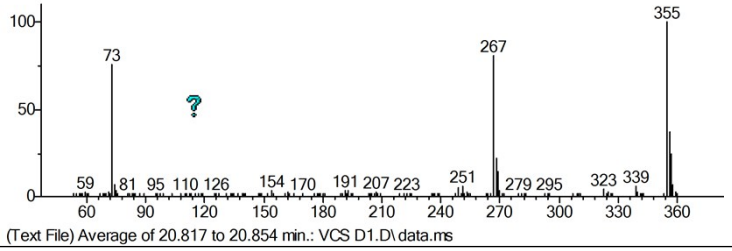
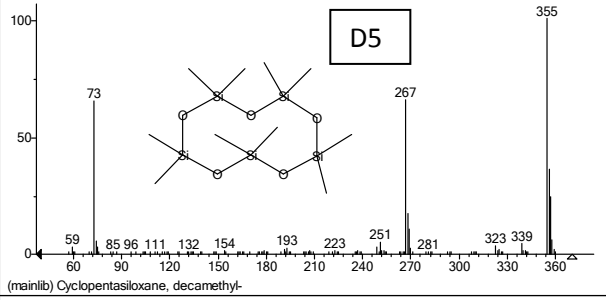
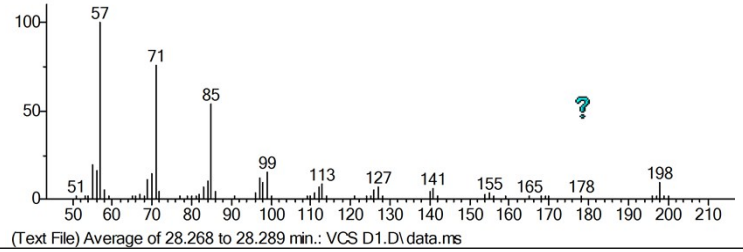
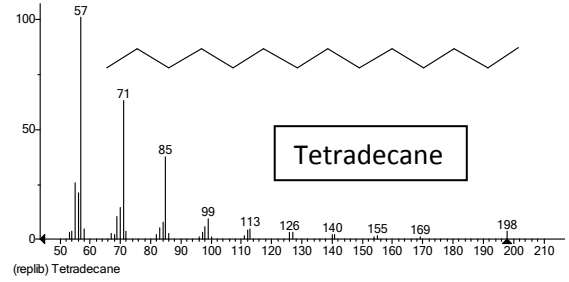


Figure ESI3: Chromatographic data supporting identification of undecane (1), D5 (2), and tetradecane (3). Retention time match in full scan run of digested sludge sample (blue) and composed standard mix consisting of 0.01‰ undecane, D5 and tetradecane in Miglyol oil (black). The corresponding mass spectra are shown in Table ESI2.

Table ESI2: Spectral data supporting identification of undecane, D5, and tetradecane. Mass spectra corresponding to the peaks 1, 2 and 3 in the sludge sample (Figure ESI3) compared with the best match from the NIST library. Compound number # labelled with Rt (retention time) and m/z (mass to charge ratio); spectra from full scan of sludge sample (the question mark indicates it is a spectrum from a sample); ID (identity) and corresponding spectra from NIST library.

Compound no.	Full scan of sludge sample	ID and spectrum from NIST library
1 [Rt: 20.31; m/z 57]		
2 [Rt: 20.84; m/z 355]		
3 [Rt: 28.29; m/z 57]		

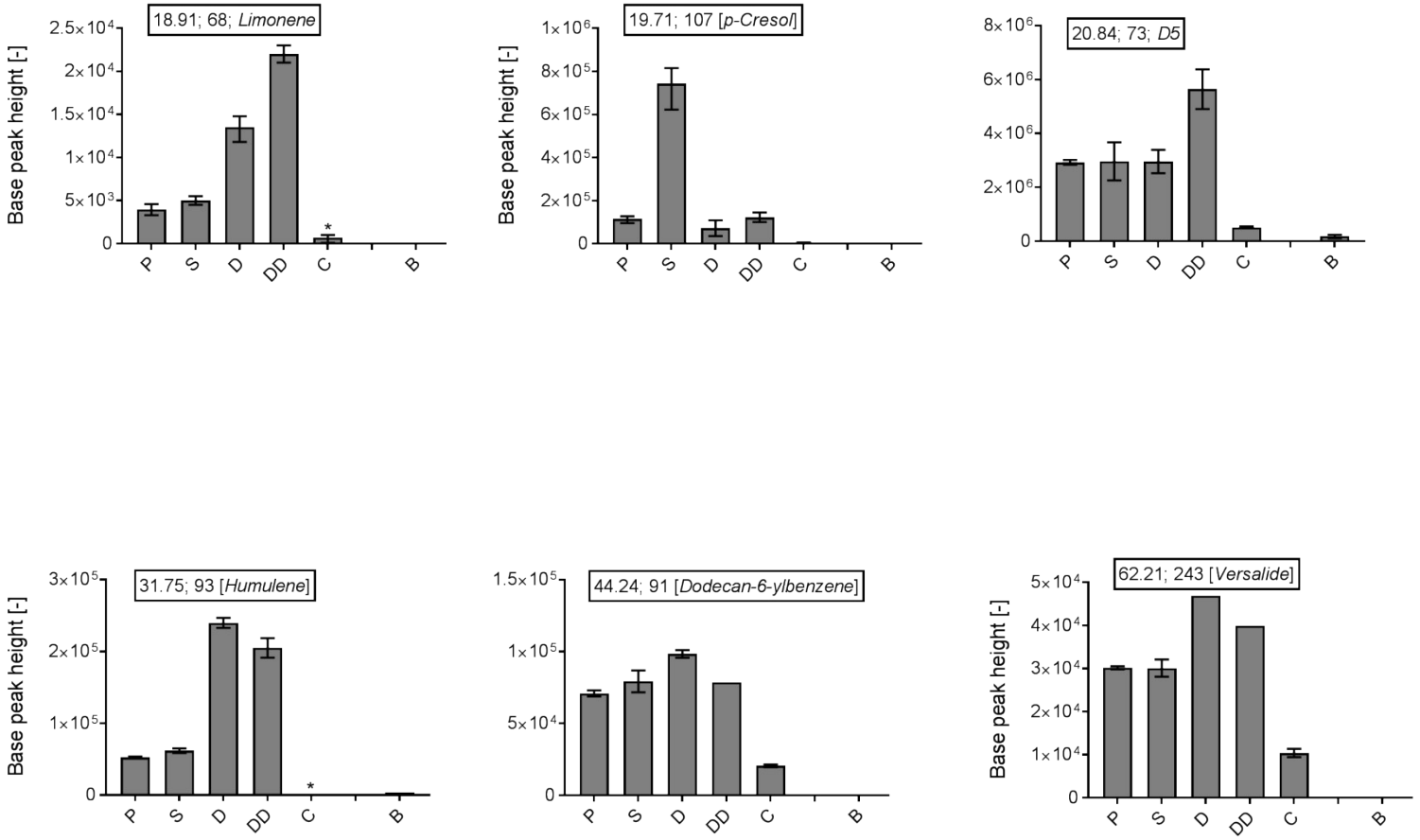


Figure ESI4: Base peak height of selected single molecular features of which some are included in Fig. 3 measured in each of the five sludge stages and in a blank sample. ID of molecular features is: retention time; m/z of base peak ion [*tentative id from NIST*]. P: Primary; S: Secondary; D: Digested; DD: Digested and Dewatered and C: Composted sludge; B: Blank. Values below data processing threshold limit (peak height <5000) were manually checked and marked with a * if present in the chromatogram and data manually extracted in ChemStation.

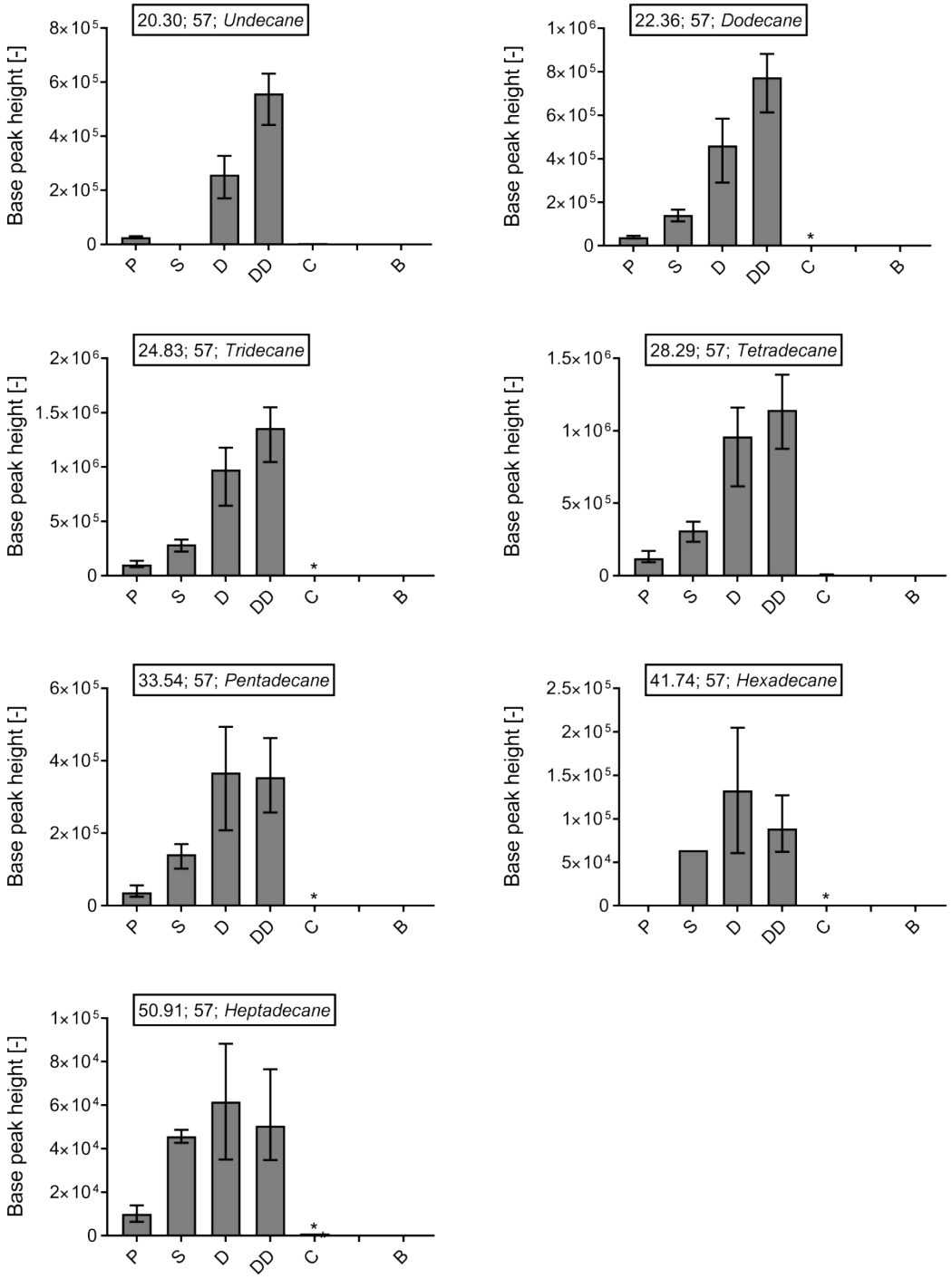


Figure ESI5: Base peak heights from MassHunter deconvolution on digested sludge for alkanes included in Fig. 3. Values below data processing threshold limit (peak height <5000) were manually checked and marked with a * if present in the chromatogram and data manually extracted in ChemStation.

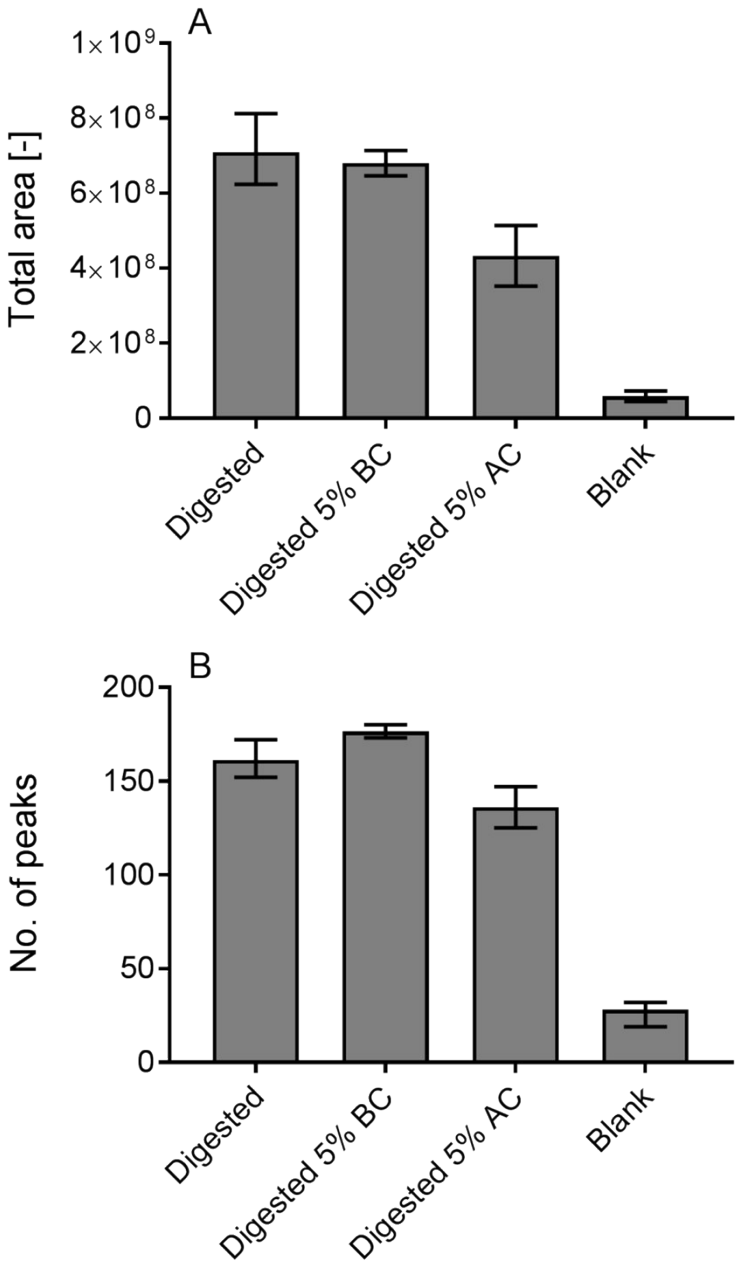
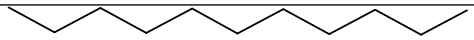
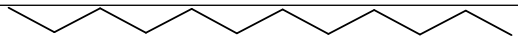
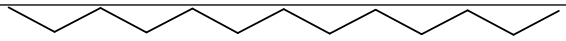
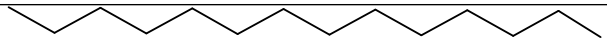
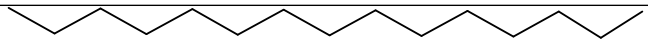
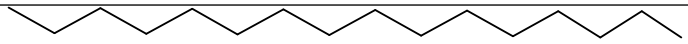
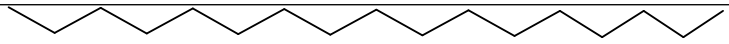
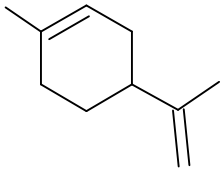
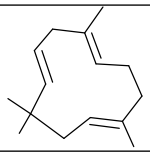
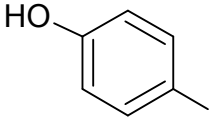
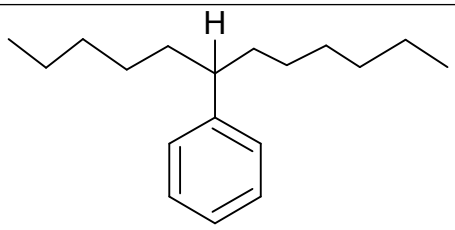
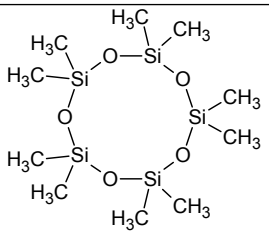
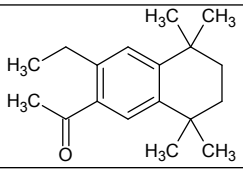


Figure ESI6: Sum of peak areas (A) and number of peaks (B) of molecular features extracted by MassHunter from 15 to 60 min retention time, measured in non-treated digested sludge, digested sludge with 5% amendment of activated carbon (AC) and digested sludge with 5% amendment of biochar (BC) and in a blank sample.

Table ESI3: Physical-chemical properties for studied compounds

Compound	**CAS no.**	**Structure**	**K_H** [atm-m3/mole]	**LogK_{ow}**
Undecane	001120-21-4		1.93E+00	5.74
Dodecane	000112-40-3		8.18E+00	6.10
Tridecane	000629-50-5		2.88E+00	6.73
Tetradecane	000629-59-4		9.20E+00	7.20
Pentadecane	000629-62-9		1.26E+01	7.71
Hexadecane	000544-76-3		4.73E-01	8.20
Heptadecane	000629-78-7		7.56E+01*	8.69
Limonene	000138-86-3		3.19E-02	4.57
Humulene	006753-98-6		1.63E+00**	6.95
p-Cresol	000106-44-5		1.00E-06	1.94
Dodecan-6-ylbenzene	4537-14-8		1.94E-01	7.59
D5	000541-02-6		3.06E-01	8.03
Versalide	000088-29-9		9.96E-06	6.42*

Values from EpiSuite v.41. (US Environmental Protection Agency); *Estimated by group method; **Estimated by bond method