Supporting Information

Medium-chain Chlorinated Paraffins (CPs) dominate in Australian sewage sludge

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Materials

The following eight commercial available CP standard mixtures were used for the deconvolution of the SCCP, MCCP and LCCP pattern in the 15 sewage sludge samples;

- Chlorinated paraffin C10-C13 51.5%Cl (SCCP 51.5%Cl)
- Chlorinated paraffin C10-C13 55.5%Cl (SCCP 55.5%Cl)
- Chlorinated paraffin C10-C13 63% Cl (SCCP 63%Cl)
- Chlorinated paraffin C14-C17 42% Cl (MCCP 42%Cl)
- Chlorinated paraffin C14-C17 52% Cl (MCCP 52%Cl)
- Chlorinated paraffin C14-C17 57% Cl (MCCP 57%Cl)
- Chlorinated paraffin C18-C20 36% Cl (LCCP 36%Cl)
- Chlorinated paraffin C18-C20 49% Cl (LCCP 49%Cl)

The concentration of the eight commercial CP standard mixtures was 100 ng/µL and purchased from Dr. Ehrenstorfer GmbH (Augsburg, Germany). All solvents and chemicals used were HPLC analysis grade. N-hexane, acetonitrile (ACN), acetone and dichloromethane (DCM) were used for extraction cleanup and analysis. Mass labeled (13C6) pentachlorophenol was used as injection standard and was purchased from Sigma Aldrich (Sunnyvale, CA, USA). Silicagel (63-200 µm) was also purchased from Sigma Aldrich (Sunnyvale, CA, USA), aluminum oxide (MP EcoChromTM Alumina B-Super I from MP Biomedical (Seven Hills, NSW, Australia) and Chem tube-hydromatrix was purchased from Agilent Technologies.

Sampling collection

Sewage sludge sampling occurred from the 4th March – 1st May 2014. Local sewage sludge samples were collected by Entox and samples from interstate were collected by WWTP employees. Samples were collected following the final dewatering step (typically the belt press or centrifuge) to represent the final sewage sludge product that is removed from each WWTP. Eight sub samples were collected at one time point from most sites. Sites S10 and S15 collected subsamples over longer time periods (representing several days to approximately one month) to obtain the most representative sample of a production batch. The sample from Site S11 was collected in a sludge lagoon that represented approximately a year of sludge accumulation. At one site located in South Australia (S9), samples were also collected from a stockpile dating from December 2012 (S12). Samples were collected in glass jars that were pre-rinsed with acetone and *n*-hexane and were refrigerated or frozen and couriered on an overnight service to Entox. Sewage sludge sub-samples from each site were mixed vigorously whilst wet and freeze-dried. Freeze-dried sub-samples were then manually ground into a fine powder and pooled equally to make one pooled sample per site.

Deconvolution and quantification

The CP pattern measured in each sample was reconstructed into a linear combination of patterns of CPs of the technical mixtures using a deconvolution algorithm. First, the m/z values of CP congener groups in the analysed sample (S) and in the technical CP mixtures (Y) were extracted from the full scan spectra and peak areas were integrated. After correcting for the injection standard ($^{13}C_6$-PCP), the peak area of each CP congener group (e.g. $C_{10}Cl_4$, $C_{10}Cl_5$, $C_{10}Cl_6$ etc.) was divided by the total sum of the peak areas of all congeners within each CP category (SCCPs, MCCPs or LCCPs). The sum of all CP congeners group within the corresponding CP category represents the relative contribution of each congener group to their CP category, which is also referred to as the congener group pattern (see Figure 2A for an example for SCCPs in sewage sludge sample S2). Also for the SCCP, MCCP, and LCCP technical formulations with known concentrations, their congener group patterns were calculated by the normalization procedure. The basic principle of the deconvolution procedure consists in assuming that for each CP category, its congener group pattern can be decomposed into a linear combination of the congener group patterns of the technical formulations of the corresponding CP category. Thus, the following system of linear equations is obtained: S = Y1 • X1 + Y2 • X2 + Y3 • X3 whereby, the known S=[⋮] and Y=[⋮ ⋮ ⋮] are the normalized CP congener group patterns of the sample and technical CP formulations, respectively (S/Y are vector/matrices with 34 lines corresponding to the 34 CP congener groups monitored here for the SCCPs). X1, X2, X3 are three unknowns of the overdetermined equation system and represent the contribution of each of the three technical formulations (51.5%, 55%, 63% Cl for the SCCPs) used to reconstruct (deconvolve) the CP congener pattern of the sample (see Figure 2B for an example of the reconstructed CP pattern in sewage sludge sample S2). The overdetermined equation system could be solved (i.e. X1, X2, and X3 estimated), following a least-squares approximation procedure in MATLAB with the following function X=lsqnonneg(Y,S). This function allows no negative values for X1, X2 and X3. The X1, X2 and X3 values were normalized to 1 in MATLAB using the following function (X=X/norm(X,1). The reconstructed CP pattern (i.e. the pattern recomposed with the estimated values of X1 , X2 and X3), was compared to the initial CP pattern of the analysed sample to determine the goodness of fit (R^2). Quantification was performed by external calibration standards, considering the known concentration of the technical CP mixtures and the instrumental response corrected for the contribution of the estimated X1 , X2 and X3 values of each of the three technical mixtures calculated for each sewage sludge sample.

Table S1. Details of the participating WWTPs

WWTP	Region	Connected population	Population Equivalents	Inflow volume (ML/d)	Biosolid Production (dry t/yr)	Source	Sludge treatment	Sampling point/s
S1	South-East Queensland	30,000	34,000	6	688	R; T	Activated sludge	Belt press
S2	South-East Queensland	455,000*	807,000	130	9198	R; T	Anaerobic digestors	Centrifuge
S3	North Queensland	25,000	31,000	6	475	R	Aerobic digestors	Belt press
S4	Northern Australia	32,100		18	3103	66% R; 33% C; 1% I	Flocculation, chemically assisted sludge treatment	Centrifuge
S5	South-East Queensland		200,000	45	4508	R, I, T	Activated sludge	Belt press
S6	South-East Queensland	30,000		5	566	R; I; T	Activated sludge	Centrifuge
S14	North Queensland	55,000	72,000	20	964	90% R; 8% I; 2% T	Aerobic digestors	Belt press
S16	North Queensland	27,000	25,000	5	1091	R	Activated sludge / bioreactor	Belt press
S7	Central New South Wales		115,000	27	1183	R; I; T	Aerobic disgestors	Centrifuge
S9	Southern Australia	>600,000	850,000	145	22995	90% R; 8-10% T,I	Anaerobic digestors	Centrifuge
S10	South-East Queensland	285,000	325,000	50	4198	85% R; 15% T	Thermal hydrolysis then anaerobic disgestors	Centrifuge
S11	Central New South Wales		32,000	7	423	R; I; T	Activated sludge	Mobile centrifuge at sludge lagoon
S13	Western Australia	>500,000		135	7884	Primarily R	Anaerobic digestors	Centrifuge
S15	North Queensland	51,000	68,600	24	1752	70% R; 30% I (40% infiltration currently)	Aerobic digestors	Belt press
S12	Southern Australia	>600,000	850,000	145		90% R; 8-10% T,I	Anaerobic digestors	Stockpile 2012

*Population estimate obtained from O'Brien et al. 2014; R=residential, I=industrial; T=trade waste, C=commercial; ML/d = megalitres per day; t/d = tonnes per day

Table S2. Calculated chlorination degree for the eight technical CP mixtures.

	calculated Cl-degree
SCCP (51.5%)	55.9% Cl
SCCP (55.5%)	58.2% Cl
SCCP (63%)	63.7% Cl
MCCP (42%)	49.4% Cl
MCCP (52%)	54.2% Cl
MCCP (57%)	57.5% Cl
LCCP (36%)	41.5% Cl
LCCP (49%)	49.0% Cl

Table S3. The results of a triplicate recovery experiments containing the three technical SCCP formulations which were extracted, cleaned and analysed in conjunction with the sewage sludge samples. The recoveries were only corrected by the injection standard ($^{13}C_6$-PCP). Results for the MCCPs and LCCPs are given in the Supplementary Table S2 and S4.

Sample	CPs	measured conc. (ng abs)	spiked conc. (ng abs)	recovery (%)	R^2 of deconvolution
1	SCCP 63%Cl	123	141	87%	
	SCCP 55.5%Cl	150	141	106%	
	SCCP 51.5%Cl	101	141	72%	
	Total SCCPs	374	424	88%	0.95
2	SCCP 63%Cl	106	141	75%	
	SCCP 55.5%Cl	154	141	109%	
	SCCP 51.5%Cl	79	141	56%	
	Total SCCPs	339	424	80%	0.95
3	SCCP 63%Cl	93	141	66%	
	SCCP 55.5%Cl	112	141	79%	
	SCCP 51.5%Cl	83	141	59%	
	Total SCCPs	288	424	68%	0.94

Table S4. The results of a triplicate spike experiments with three technical SCCP formulations for four different sewage sludge samples. The recovery was calculated by subtracting the values observed in the samples from the spiked samples. The values were only corrected by the injection standard (^{13}C-PCP). Results for the MCCPs and LCCPs are given in the Supplementary Table S3 and S5.

Sample	CPs	measured conc. (ng abs)	spiked conc. (ng abs)	recovery (%)	R^2 of deconvolution
1	SCCP 63%Cl	114	121	94%	
	SCCP 55.5%Cl	141	121	116%	
	SCCP 51.5%Cl	51	121	42%	
	Total SCCPs	305	363	84%	0.97
2	SCCP 63%Cl	115	121	95%	
	SCCP 55.5%Cl	182	121	150%	
	SCCP 51.5%Cl	46	121	38%	
	Total SCCPs	343	363	94%	0.97
3	SCCP 63%Cl	129	121	106%	
	SCCP 55.5%Cl	143	121	118%	
	SCCP 51.5%Cl	83	121	69%	
	Total SCCPs	355	363	98%	0.94
4	SCCP 63%Cl	131	121	108%	
	SCCP 55.5%Cl	139	121	115%	
	SCCP 51.5%Cl	88	121	73%	
	Total SCCPs	358	363	99%	0.97

Table S5. The results of a triplicate recovery experiment containing the three technical MCCP formulations which were extracted, cleaned and analysed in conjunction with the sewage sludge samples. The recoveries were only corrected by the injection standard (^{13}C-PCP).

Sample	CPs	measured conc. (ng abs)	spiked conc. (ng abs)	recovery (%)	R^2 of deconvolution
1	MCCP 42%Cl	73	159	46%	
	MCCP 52%Cl	177	159	111%	
	MCCP 57%Cl	168	159	105%	
	Total MCCPs	417	478	87%	0.93
2	MCCP 42%Cl	72	159	45%	
	MCCP 52%Cl	179	159	113%	
	MCCP 57%Cl	167	159	105%	
	Total MCCPs	419	478	88%	0.94
3	MCCP 42%Cl	67	159	42%	
	MCCP 52%Cl	122	159	76%	
	MCCP 57%Cl	131	159	82%	
	Total MCCPs	320	478	67%	0.93

Table S6. The results of a triplicate spike experiment with the three technical MCCP formulations on four different sewage sludge samples. The recovery was calculated by subtracting the values measured in the samples from the spiked samples. The values were only corrected by the injection standard (^{13}C-PCP).

Sample	CPs	measured conc. (ng abs)	spiked conc. (ng abs)	recovery (%)	R^2 of deconvolution
1	MCCP 42%Cl	48	121	39%	
	MCCP 52%Cl	129	121	107%	
	MCCP 57%Cl	175	121	144%	
	Total MCCPs	352	410	86%	0.97
2	MCCP 42%Cl	0	121	0%	
	MCCP 52%Cl	235	121	194%	
	MCCP 57%Cl	231	121	191%	
	Total MCCPs	465	410	113%	0.97
3	MCCP 42%Cl	50	121	41%	
	MCCP 52%Cl	147	121	121%	
	MCCP 57%Cl	203	121	168%	
	Total MCCPs	400	410	98%	0.94
4	MCCP 42%Cl	64	121	53%	
	MCCP 52%Cl	156	121	129%	
	MCCP 57%Cl	202	121	167%	
	Total MCCPs	421	410	103%	0.97

Table S7. The results of a triplicate recovery experiment containing the three technical LCCP formulations which were extracted, cleaned and analysed in conjunction with the sewage sludge samples. The recovery was only corrected by the injection standard (13C-PCP).

Sample	CPs	measured conc. (ng abs)	spiked conc. (ng abs)	recovery (%)	R^2 of deconvolution
1	LCCP 36%Cl	125	144	87%	
	LCCP 49%Cl	164	144	113%	
	Total LCCPs	289	289	100%	1.00
2	LCCP 36%Cl	112	144	77%	
	LCCP 49%Cl	158	144	110%	
	Total LCCPs	270	289	94%	1.00
3	LCCP 36%Cl	90	144	63%	
	LCCP 49%Cl	144	144	100%	
	Total LCCPs	234	289	81%	1.00

Table S8. The results of a triplicate spike experiment with the three technical MCCP formulations on four different sewage sludge samples. The recovery was calculated by subtracting the values measured in the samples from the spiked samples. The values were only corrected by the injection standard (13C-PCP).

Sample	CPs	measured conc. (ng abs)	spiked conc. (ng abs)	recovery (%)	R^2 of deconvolution
1	LCCP 36%Cl	89	121	73%	
	LCCP 49%Cl	156	121	129%	
	Total LCCPs	245	247	99%	1.00
2	LCCP 36%Cl	99	121	82%	
	LCCP 49%Cl	203	121	168%	
	Total LCCPs	302	247	122%	0.54
3	LCCP 36%Cl	103	121	85%	
	LCCP 49%Cl	186	121	153%	
	Total LCCPs	288	247	117%	1.00
4	LCCP 36%Cl	114	121	94%	
	LCCP 49%Cl	191	121	158%	
	Total LCCPs	304	247	123%	1.00

Table S9. Average peak area of the SCCPs and MCCPS of an 8-fold measurement of sewage sludge sample S9.

SCCPs	average peak area	std	rel std (%)	
C10Cl4				
C10Cl5	207	94	45%	
C10Cl6	6762	1135	17%	
C10Cl7	1541	284	18%	
C10Cl8	475	222	47%	
C10Cl9				
C10Cl10				
Total C10 RSD(%)				**32%**
C11Cl4				
C11Cl5				
C11Cl6	5119	565	11%	
C11Cl7	5538	440	8%	
C11Cl8	2217	322	15%	
C11Cl9	1001	283	28%	
C11Cl10				
C11Cl11				
Total C11 RSD(%)				**15%**
C12Cl4				
C12Cl5	650	264	41%	
C12Cl6	7719	787	10%	
C12Cl7	10495	837	8%	
C12Cl8	4538	244	5%	
C12Cl9	963	301	31%	
C12Cl10				
C12Cl11				
C12Cl12				
Total C10 RSD(%)				**19%**
C13Cl4				
C13Cl5	2025	567	28%	
C13Cl6	17022	592	3%	
C13Cl7	22099	1137	5%	
C13Cl8	10307	831	8%	
C13Cl9	1951	319	16%	
C13Cl10	504	145	29%	
C13Cl11				
C13Cl12				
C13Cl13				
Total C10 RSD(%)				**15%**
overall RSD			20%	

MCCPs	average peak area	std	rel std (%)	
C14Cl4	259	71	27%	
C14Cl5	36194	1846	5%	
C14Cl6	158432	4039	3%	
C14Cl7	182620	4305	2%	
C14Cl8	82817	4211	5%	
C14Cl9	24836	1670	7%	
C14Cl10	4936	654	13%	
C14Cl11				
C14Cl12				
C14Cl13				
C14Cl14				
Total C14 RSD (%)				**9%**
C15Cl4	195	69	35%	
C15Cl5	25884	2272	9%	
C15Cl6	112266	6551	6%	
C15Cl7	151734	2519	2%	
C15Cl8	73103	2173	3%	
C15Cl9	26543	731	3%	
C15Cl10	4873	1041	21%	
C15Cl11	686	236	34%	
C15Cl12				
C15Cl13				
C15Cl14				
C15Cl15				
Total C15 RSD (%)				**14%**
C16Cl4	113	14	12%	
C16Cl5	3385	475	14%	
C16Cl6	40224	1957	5%	
C16Cl7	56293	1689	3%	
C16Cl8	35680	769	2%	
C16Cl9	14072	605	4%	
C16Cl10	2751	264	10%	
C16Cl11				
C16Cl12				
C16Cl13				
C16Cl14				
C16Cl15				
C16Cl16				
Total C16 RSD (%)				**7%**
C17Cl4	167	37	22%	
C17Cl5	4212	641	15%	
C17Cl6	18980	1625	9%	
C17Cl7	25902	3158	12%	
C17Cl8	20418	1045	5%	
C17Cl9	10159	512	5%	
C17Cl10	2340	260	11%	
C17Cl11	249	99	40%	
C17Cl12				
C17Cl13				
C17Cl14				
C17Cl15				
C17Cl16				
C17Cl17				
Total C17 RSD (%)				**15%**
overall RSD			11%	

Table S10. list of m/z ratios considered for CPs.

SCCP congener	m/z of $[M+Cl]^-$	MCCP congener	m/z of $[M+Cl]^-$	MCCP congener	m/z of $[M+Cl]^-$
C10Cl4	314.9817	C14Cl4	371.0448	C16Cl15	776.6415
C10Cl4	316.9792	C14Cl4	373.0418	C16Cl15	778.6385
C10Cl5	348.9432	C14Cl5	405.0058	C16Cl16	810.6025
C10Cl5	350.9403	C14Cl5	407.0029	C16Cl16	812.5996
C10Cl6	382.9042	C14Cl6	438.9668	C17Cl4	413.0917
C10Cl6	384.9013	C14Cl6	440.9639	C17Cl4	415.0888
C10Cl7	416.8653	C14Cl7	472.9279	C17Cl5	447.0528
C10Cl7	418.8623	C14Cl7	474.9249	C17Cl5	449.0498
C10Cl8	450.8263	C14Cl8	506.8889	C17Cl6	481.0138
C10Cl8	452.8233	C14Cl8	508.8859	C17Cl6	483.0108
C10Cl9	486.7844	C14Cl9	542.8470	C17Cl7	514.9748
C10Cl9	488.7814	C14Cl9	544.8440	C17Cl7	516.9719
C10Cl10	520.7454	C14Cl10	576.8080	C17Cl8	548.9358
C10Cl10	522.7424	C14Cl10	578.8050	C17Cl8	550.9329
C11Cl4	328.9978	C14Cl11	610.7690	C17Cl9	584.8939
C11Cl4	330.9949	C14Cl11	612.7661	C17Cl9	586.8910
C11Cl5	362.9589	C14Cl12	644.7300	C17Cl10	618.8549
C11Cl5	364.9559	C14Cl12	646.7271	C17Cl10	620.8520
C11Cl6	396.9199	C14Cl13	680.6881	C17Cl11	654.8130
C11Cl6	398.9169	C14Cl13	682.6852	C17Cl11	652.8160
C11Cl7	430.8809	C14Cl14	714.6492	C17Cl12	686.7770
C11Cl7	432.8780	C14Cl14	716.6462	C17Cl12	688.7740
C11Cl8	464.8419	C15Cl4	385.0604	C17Cl13	722.7351
C11Cl8	466.8390	C15Cl4	387.0575	C17Cl13	724.7321
C11Cl9	500.8000	C15Cl5	419.0215	C17Cl14	756.6961
C11Cl9	502.7971	C15Cl5	421.0185	C17Cl14	758.6932
C11Cl10	534.7610	C15Cl6	452.9825	C17Cl15	790.6571
C11Cl10	536.7581	C15Cl6	454.9795	C17Cl15	792.6542
C11Cl11	568.7221	C15Cl7	486.9435	C17Cl16	824.6182
C11Cl11	570.7191	C15Cl7	488.9406	C17Cl16	826.6152
C12Cl4	343.0135	C15Cl8	520.9045	C17Cl17	860.5762
C12Cl4	345.0105	C15Cl8	522.9016	C17Cl17	862.5733
C12Cl5	376.9745	C15Cl9	556.8626		
C12Cl5	378.9716	C15Cl9	558.8597		
C12Cl6	410.9355	C15Cl10	590.8236		
C12Cl6	412.9326	C15Cl10	592.8207		
C12Cl7	444.8966	C15Cl11	624.7847		
C12Cl7	446.8936	C15Cl11	626.7817		
C12Cl8	478.8576	C15Cl12	658.7457		
C12Cl8	480.8546	C15Cl12	660.7427		
C12Cl9	514.8157	C15Cl13	694.7038		
C12Cl9	516.8127	C15Cl13	696.7008		
C12Cl10	548.7767	C15Cl14	728.6648		
C12Cl10	550.7737	C15Cl14	730.6619		
C12Cl11	582.7377	C15Cl15	762.6258		
C12Cl11	584.7348	C15Cl15	764.6229		
C12Cl12	618.6958	C16Cl4	399.0761		
C12Cl12	620.6928	C16Cl4	401.0731		
C13Cl4	357.0291	C16Cl5	433.0371		
C13Cl4	359.0262	C16Cl5	435.0342		
C13Cl5	390.9902	C16Cl6	466.9981		
C13Cl5	392.9872	C16Cl6	468.9952		
C13Cl6	424.9512	C16Cl7	500.9592		
C13Cl6	426.9482	C16Cl7	502.9562		
C13Cl7	458.9122	C16Cl8	534.9202		
C13Cl7	460.9093	C16Cl8	536.9172		
C13Cl8	492.8732	C16Cl9	570.8783		
C13Cl8	494.8703	C16Cl9	572.8753		
C13Cl9	528.8313	C16Cl10	604.8393		
C13Cl9	530.8284	C16Cl10	606.8363		
C13Cl10	562.7923	C16Cl11	638.8003		
C13Cl10	564.7894	C16Cl11	640.7974		
C13Cl11	596.7534	C16Cl12	672.7613		
C13Cl11	598.7504	C16Cl12	674.7584		
C13Cl12	630.7144	C16Cl13	708.7194		
C13Cl12	632.7114	C16Cl13	710.7165		
C13Cl13	666.6725	C16Cl14	742.6805		
C13Cl13	668.6695	C16Cl14	744.6775		

LCCP congener	m/z of [M+Cl]$^-$	LCCP congener	m/z of [M+Cl]$^-$	LCCP congener	m/z of [M+Cl]$^-$	LCCP congener	m/z of [M+Cl]$^-$	LCCP congener	m/z of [M+Cl]$^-$	LCCP congener	m/z of [M+Cl]$^-$
C18Cl4	427.1074	C20Cl7	557.0217	C22Cl6	551.0920	C23Cl21	1082.5113	C25Cl14	868.8213	C26Cl26	1296.3604
C18Cl4	429.1044	C20Cl7	559.0188	C22Cl6	553.0891	C23Cl21	1084.5084	C25Cl14	870.8184	C26Cl26	1298.3575
C18Cl5	461.0684	C20Cl8	590.9828	C22Cl7	585.0531	C23Cl22	1116.4723	C25Cl15	902.7823	C27Cl4	553.2482
C18Cl5	463.0654	C20Cl8	592.9798	C22Cl7	587.0501	C23Cl22	1118.4694	C25Cl15	904.7794	C27Cl4	555.2453
C18Cl6	495.0294	C20Cl9	626.9409	C22Cl8	619.0141	C23Cl23	1150.4334	C25Cl16	936.7434	C27Cl5	587.2093
C18Cl6	497.0265	C20Cl9	628.9379	C22Cl8	621.0111	C23Cl23	1152.4304	C25Cl16	938.7404	C27Cl5	589.2063
C18Cl7	528.9905	C20Cl10	660.9019	C22Cl9	654.9722	C24Cl4	511.2013	C25Cl17	972.7014	C27Cl6	621.1703
C18Cl7	530.9875	C20Cl10	662.8989	C22Cl9	656.9692	C24Cl4	513.1983	C25Cl17	974.6985	C27Cl6	623.1673
C18Cl8	562.9515	C20Cl11	694.8629	C22Cl10	688.9332	C24Cl5	545.1623	C25Cl18	1006.6625	C27Cl7	655.1313
C18Cl8	564.9485	C20Cl11	696.8600	C22Cl10	690.9302	C24Cl5	547.1594	C25Cl18	1008.6595	C27Cl7	657.1284
C18Cl9	598.9096	C20Cl12	728.8239	C22Cl11	722.8942	C24Cl6	579.1233	C25Cl19	1040.6235	C27Cl8	689.0923
C18Cl9	600.9066	C20Cl12	730.8210	C22Cl11	724.8913	C24Cl6	581.1204	C25Cl19	1042.6205	C27Cl8	691.0894
C18Cl10	632.8706	C20Cl13	764.7820	C22Cl12	756.8552	C24Cl7	613.0844	C25Cl20	1074.5845	C27Cl9	725.0504
C18Cl10	634.8676	C20Cl13	766.7791	C22Cl12	758.8523	C24Cl7	615.0814	C25Cl20	1076.5816	C27Cl9	727.0475
C18Cl11	666.8316	C20Cl14	798.7431	C22Cl13	792.8133	C24Cl8	647.0454	C25Cl21	1110.5426	C27Cl10	759.0114
C18Cl11	668.8287	C20Cl14	800.7401	C22Cl13	794.8104	C24Cl8	649.0424	C25Cl21	1112.5397	C27Cl10	761.0085
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C18Cl12	702.7897	C20Cl15	834.7011	C22Cl14	828.7714	C24Cl9	685.0005	C25Cl22	1146.5007	C27Cl11	794.9695
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C18Cl14	772.7088	C20Cl17	904.6202	C22Cl16	896.6935	C24Cl11	752.9226	C25Cl24	1214.4227	C27Cl13	864.8886
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C18Cl16	840.6309	C20Cl19	972.5423	C22Cl18	966.6126	C24Cl13	822.8417	C26Cl4	527.2140	C27Cl15	932.8107
C18Cl17	874.5919	C20Cl20	1004.5063	C22Cl19	998.5765	C24Cl14	854.8057	C26Cl5	573.1936	C27Cl16	964.7747
C18Cl17	876.5889	C20Cl20	1006.5033	C22Cl19	1000.5736	C24Cl14	856.8027	C26Cl5	575.1907	C27Cl16	966.7717
C18Cl18	908.5529	C21Cl4	469.1543	C22Cl20	1032.5376	C24Cl15	888.7667	C26Cl6	607.1546	C27Cl17	1000.7327
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C19Cl7	545.0031	C21Cl8	608.9925	C23Cl5	533.1437	C24Cl19	1028.6049	C26Cl10	746.9928	C27Cl21	1140.5709
C19Cl8	576.9671	C21Cl9	640.9565	C23Cl6	565.1077	C24Cl20	1060.5689	C26Cl11	778.9568	C27Cl22	1172.5349
C19Cl8	578.9642	C21Cl9	642.9536	C23Cl6	567.1047	C24Cl20	1062.5659	C26Cl11	780.9539	C27Cl22	1174.5320
C19Cl9	612.9252	C21Cl10	674.9175	C23Cl7	599.0687	C24Cl21	1096.5270	C26Cl12	812.9178	C27Cl23	1206.4959
C19Cl9	614.9223	C21Cl10	676.9146	C23Cl7	601.0658	C24Cl21	1098.5240	C26Cl12	814.9149	C27Cl23	1208.4930
C19Cl10	646.8862	C21Cl11	708.8786	C23Cl8	635.0268	C24Cl22	1130.4880	C26Cl13	848.8759	C27Cl24	1240.4570
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C19Cl11	680.8473	C21Cl12	742.8396	C23Cl9	668.9878	C24Cl23	1164.4490	C26Cl14	882.8370	C27Cl25	1276.4151
C19Cl11	682.8443	C21Cl12	744.8366	C23Cl9	670.9849	C24Cl23	1166.4461	C26Cl14	884.8340	C27Cl25	1278.4121
C19Cl12	714.8083	C21Cl13	778.7977	C23Cl10	702.9488	C24Cl24	1198.4100	C26Cl15	916.7980	C27Cl26	1310.3761
C19Cl12	716.8053	C21Cl13	780.7947	C23Cl10	704.9459	C24Cl24	1200.4071	C26Cl15	918.7950	C27Cl26	1312.3731
C19Cl13	750.7664	C21Cl14	812.7587	C23Cl11	736.9099	C25Cl4	525.2169	C26Cl16	950.7590	C27Cl27	1416.2719
C19Cl13	752.7634	C21Cl14	814.7558	C23Cl11	738.9069	C25Cl4	527.2140	C26Cl16	952.7561	C27Cl27	1418.2689
C19Cl14	784.7274	C21Cl15	846.7197	C23Cl12	770.8709	C25Cl5	559.1780	C26Cl17	986.7171		
C19Cl14	786.7245	C21Cl15	848.7168	C23Cl12	772.8679	C25Cl5	561.1750	C26Cl17	988.7141		
C19Cl15	818.6884	C21Cl16	880.6808	C23Cl13	806.8290	C25Cl6	593.1390	C26Cl18	1020.6781		
C19Cl15	820.6855	C21Cl16	882.6778	C23Cl13	808.8260	C25Cl6	595.1360	C26Cl18	1022.6752		
C19Cl16	852.6495	C21Cl17	916.6388	C23Cl14	840.7900	C25Cl7	627.1000	C26Cl19	1054.6391		
C19Cl16	854.6465	C21Cl17	918.6359	C23Cl14	842.7871	C25Cl7	629.0971	C26Cl19	1056.6362		
C19Cl17	888.6075	C21Cl18	950.5999	C23Cl15	874.7510	C25Cl8	661.0610	C26Cl20	1088.6002		
C19Cl17	890.6046	C21Cl18	952.5969	C23Cl15	876.7481	C25Cl8	663.0581	C26Cl20	1090.5972		
C19Cl18	922.5686	C21Cl19	984.5609	C23Cl16	908.7121	C25Cl9	697.0191	C26Cl21	1124.5582		
C19Cl18	924.5656	C21Cl19	986.5579	C23Cl16	910.7091	C25Cl9	699.0162	C26Cl21	1126.5553		
C19Cl19	956.5296	C21Cl20	1018.5219	C23Cl17	944.6701	C25Cl10	730.9801	C26Cl22	1158.5193		
C19Cl19	958.5266	C21Cl20	1020.5190	C23Cl17	946.6672	C25Cl10	732.9772	C26Cl22	1160.5163		
C20Cl4	455.1387	C21Cl21	1054.4800	C23Cl18	978.6312	C25Cl11	764.9412	C26Cl23	1192.4803		
C20Cl4	457.1357	C21Cl21	1056.4771	C23Cl18	980.6282	C25Cl11	766.9382	C26Cl23	1194.4774		
C20Cl5	489.0997	C22Cl4	483.1700	C23Cl19	1012.5922	C25Cl12	798.9022	C26Cl24	1226.4413		
C20Cl5	491.0967	C22Cl4	485.1670	C23Cl19	1014.5892	C25Cl12	800.8992	C26Cl24	1228.4384		
C20Cl6	523.0607	C22Cl5	517.1310	C23Cl20	1046.5532	C25Cl13	834.8603	C26Cl25	1262.3994		
C20Cl6	525.0578	C22Cl5	519.1281	C23Cl20	1048.5503	C25Cl13	836.8573	C26Cl25	1264.3965		

Figure S1. Composition profile of the SCCPs, MCCPS and LCCPs congeners in the 15 sewage sludge samples and the 2 blanks.

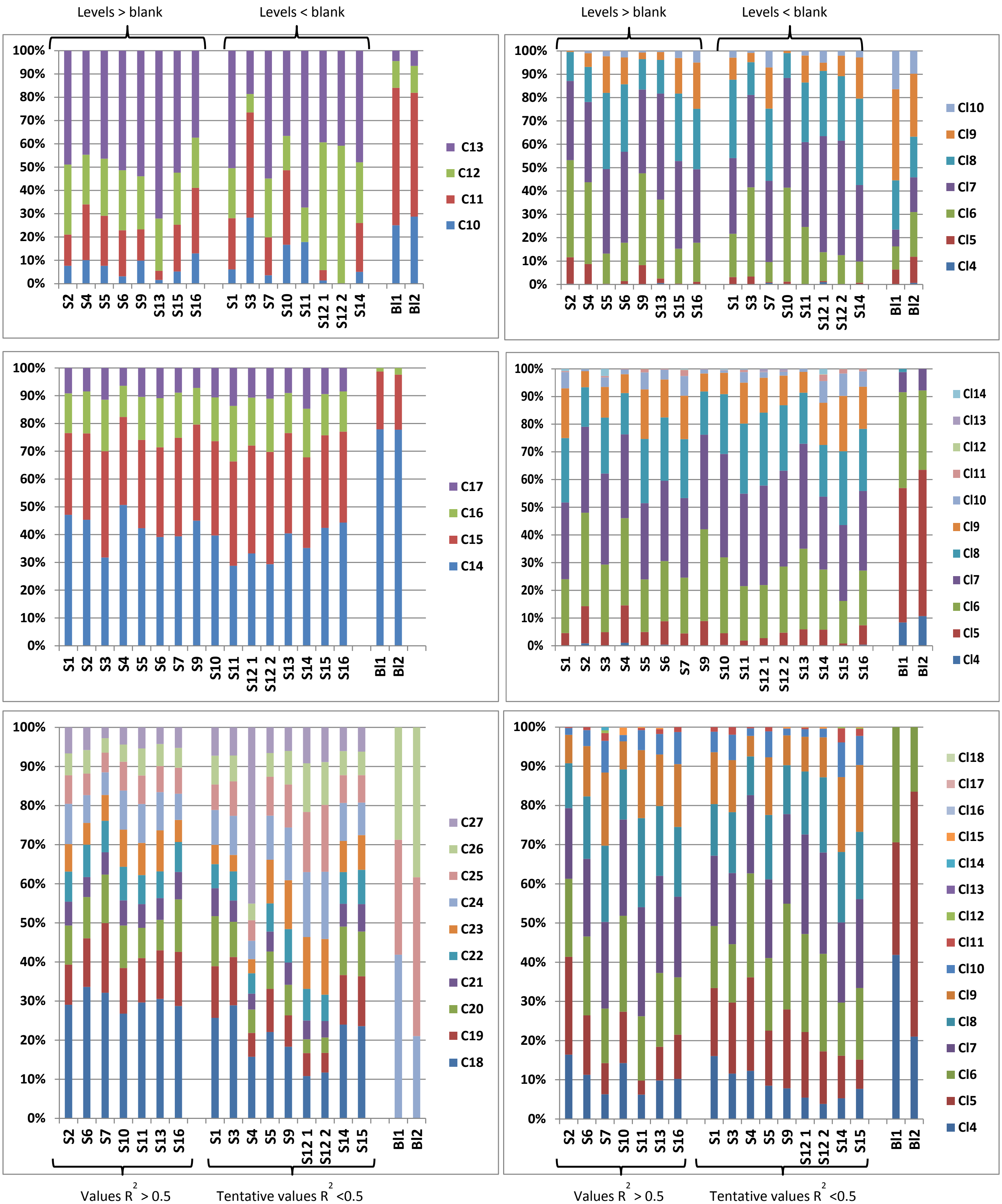


Figure S2. Congener pattern of the three SCCPs technical mixtures.

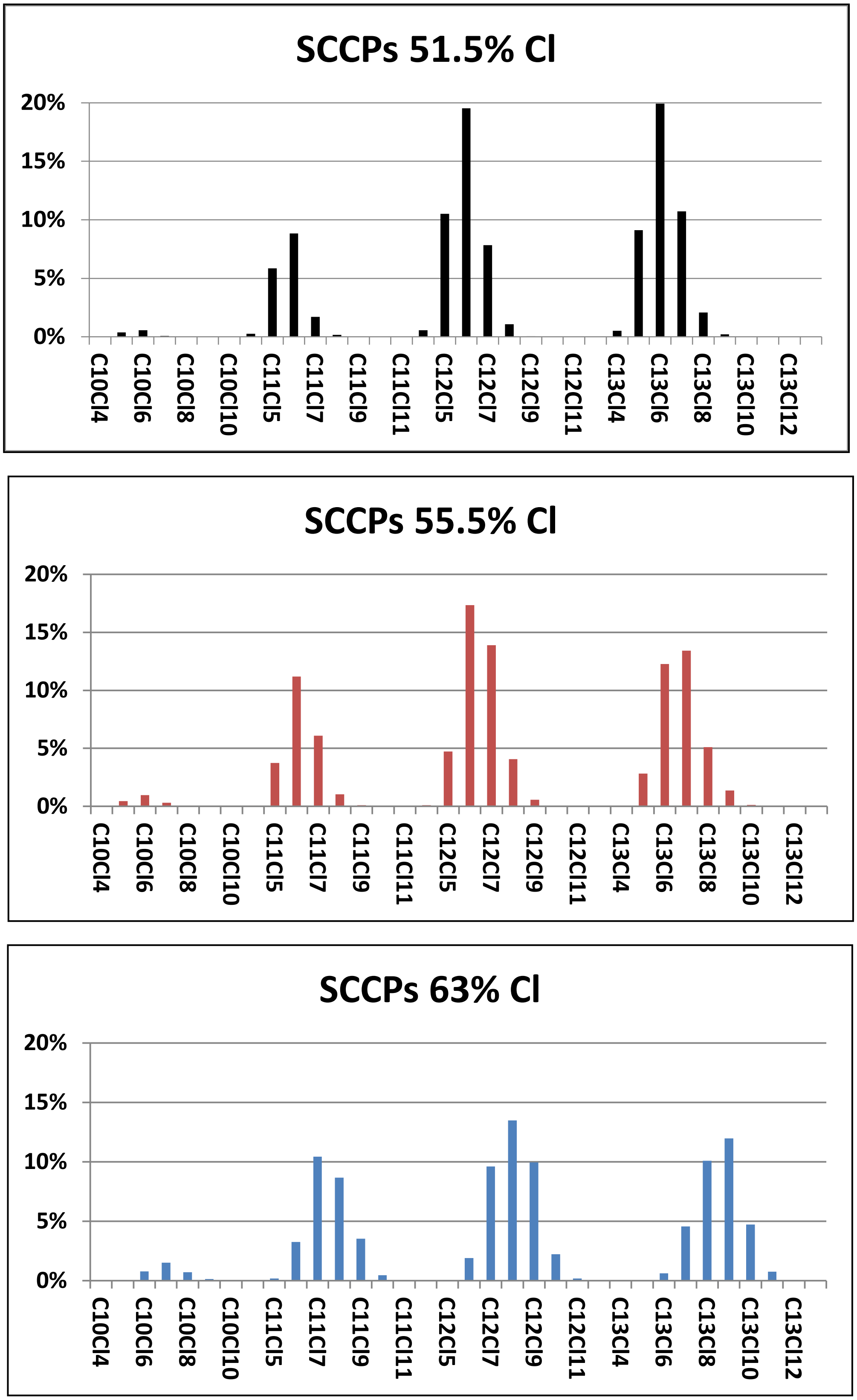


Figure S3. Congener pattern of the three MCCPs technical mixtures.

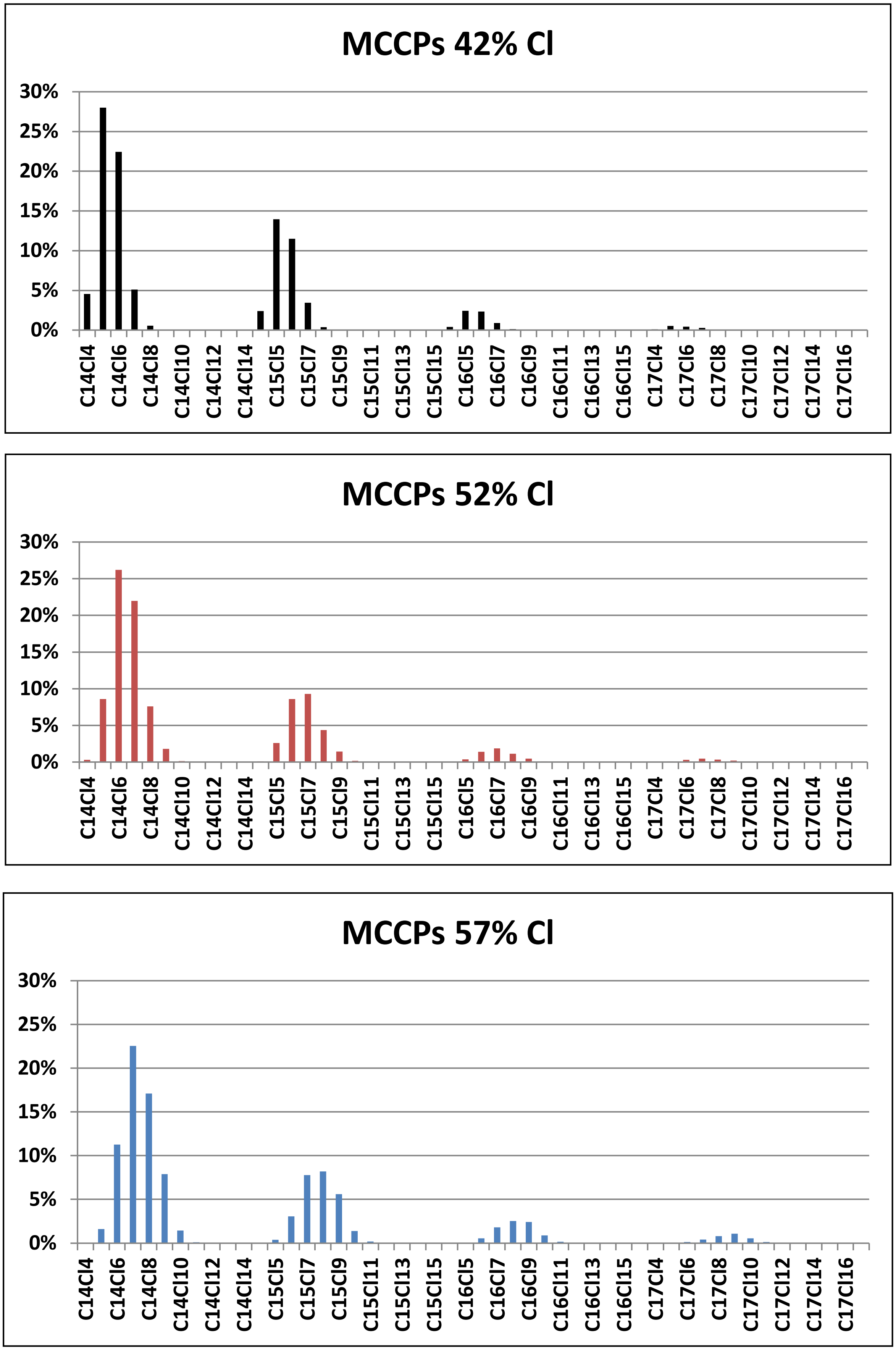


Figure S4. Congener pattern of the two LCCPs technical mixtures.

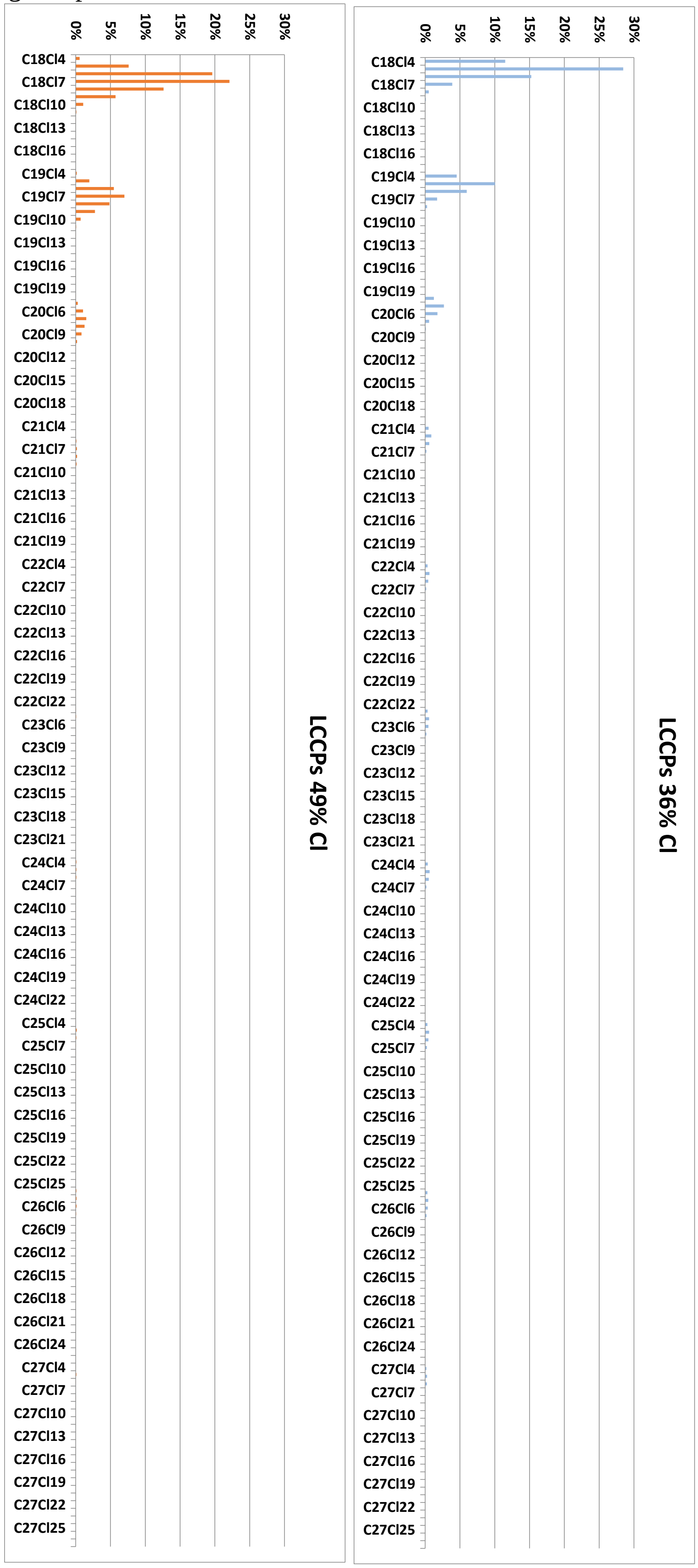


Figure S5. Example of the measured and deconvoluted congener pattern of SCCPs in the sewage sludge sample S1.

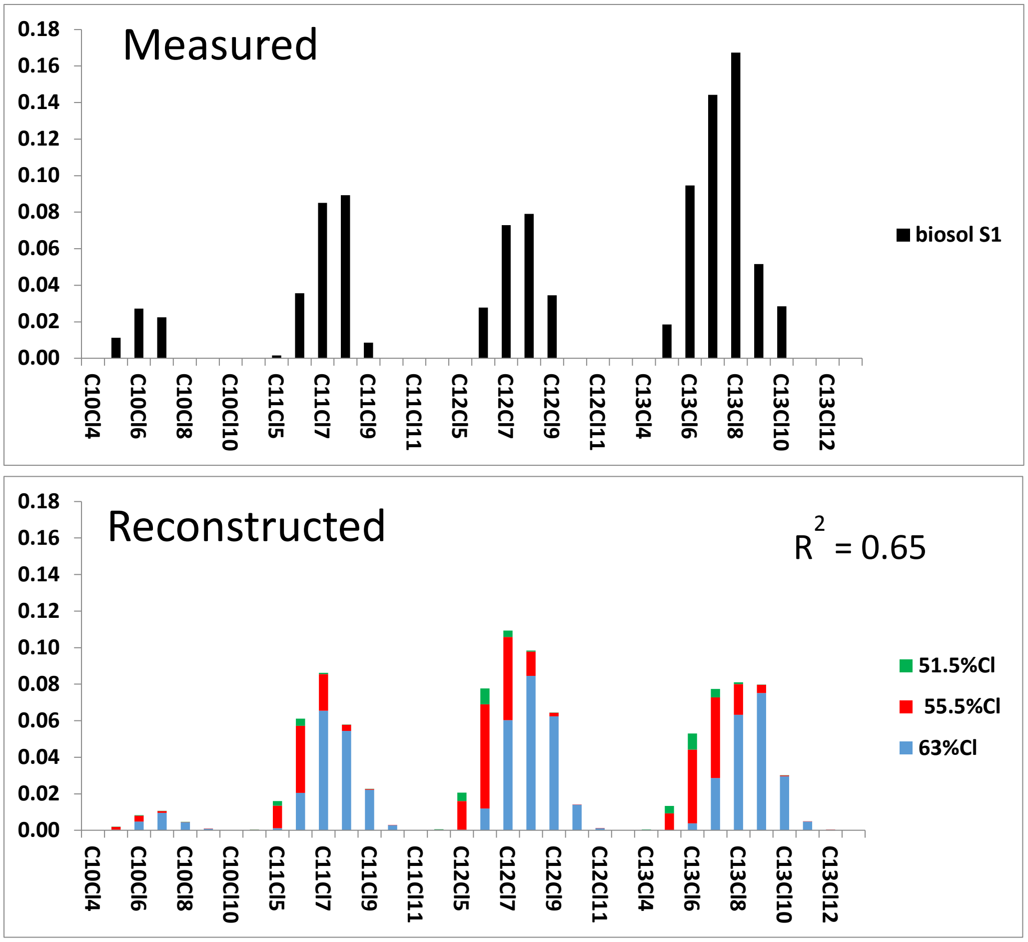


Figure S6. Example of the measured and deconvoluted congener pattern of MCCPs in the sewage sludge sample S3.

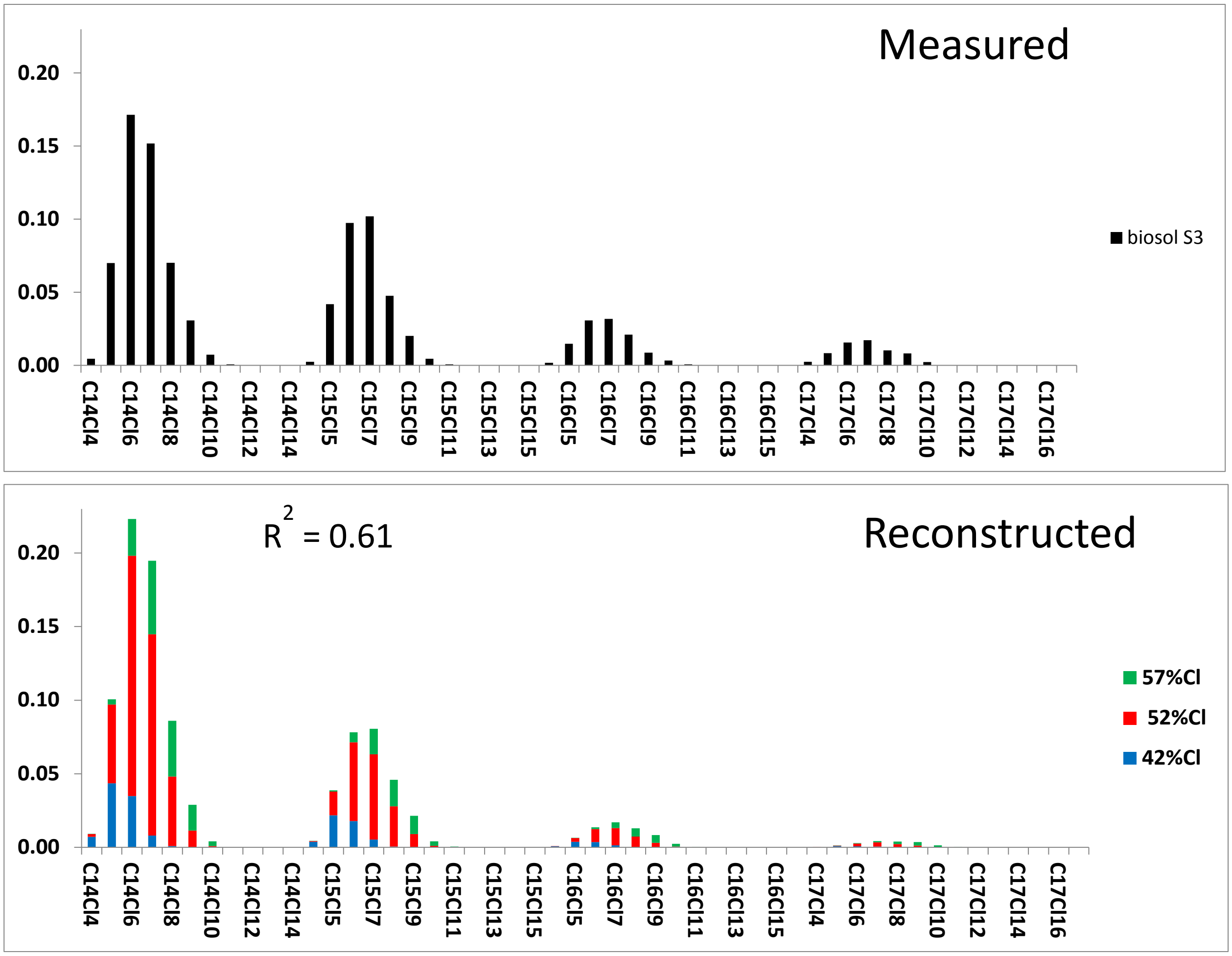
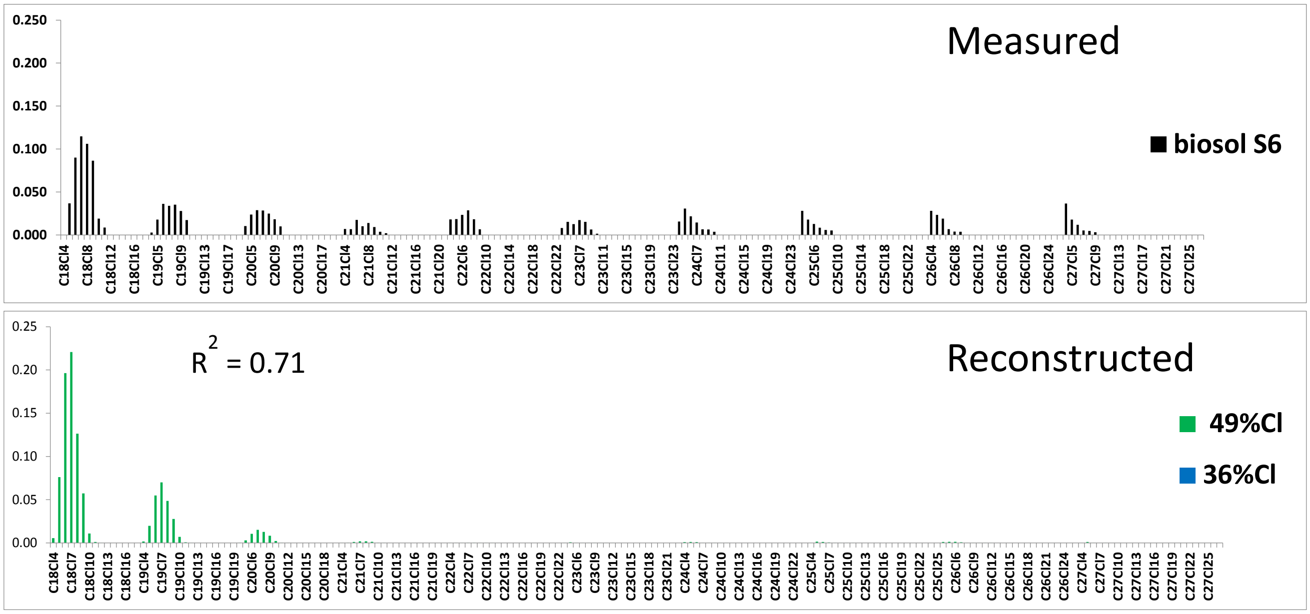


Figure S7. Example of the measured and deconvoluted congener pattern of LCCPs in the sewage sludge sample S6.



Reference

O'Brien, J.W., Thai, P.K., Eaglesham, G., Ort, C., Scheidegger, A., Carter, S., Yin Lai, F., Mueller, J.F., 2014. A Model to Estimate the Population Contributing to the Wastewater Using Samples Collected on Census Day. Environ. Sci. Technol., 48, 517-525.