

Comparison of different solid phase extraction sorbents for the qualitative assessment of dissolved organic nitrogen in freshwater samples using FT-ICR-MS

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Tab. S1. Conditions for the compound classification after Santl-Temkiv *et al.* (2013).

Compound class	H/C ratio	O/C ratio	Aromaticity index	# nitrogen atoms
Black carbon	-	-	>0.666	0
Polyphenols	-	-	$0.5 \leq AI_{\text{mod}} \leq 0.666$	-
Highly unsaturated	<1.5	<0.9	<0.5	-
Unsaturated aliphatics	$1.5 \leq \text{H/C} \leq 2$	<0.9	-	0
Saturated fatty acids	>2	<0.9	-	0
Sugars	-	>0.9	-	0
Peptides	$1.5 \leq \text{H/C} \leq 2$	<0.9	-	>0

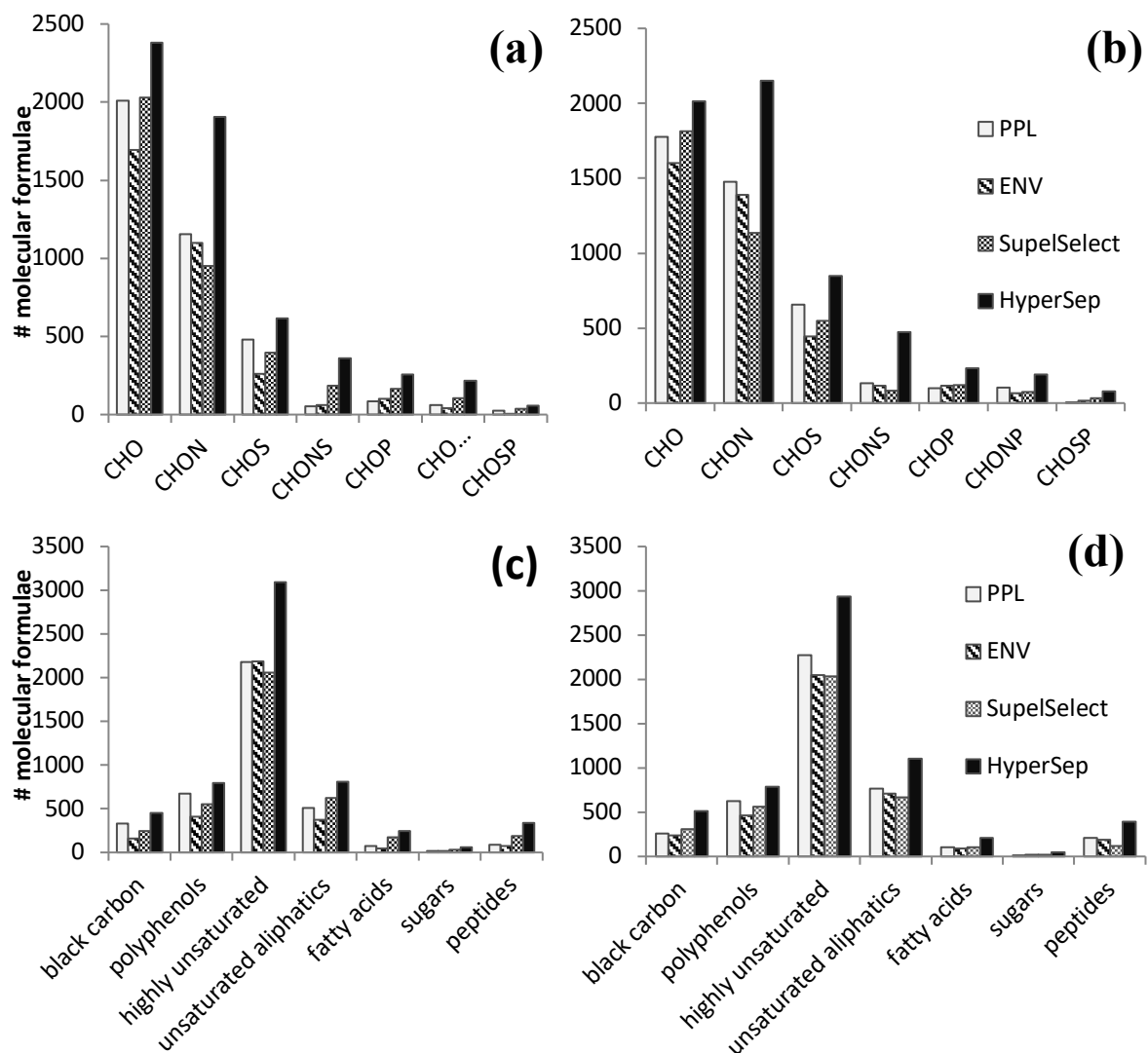


Fig. S1. Number of identified molecular formulae for each cartridge for (a) Lake Lucerne (average value of the duplicates) and (b) Lake Rotsee and number of identified compound classes for (c) Lake Lucerne and (d) Lake Rotsee.

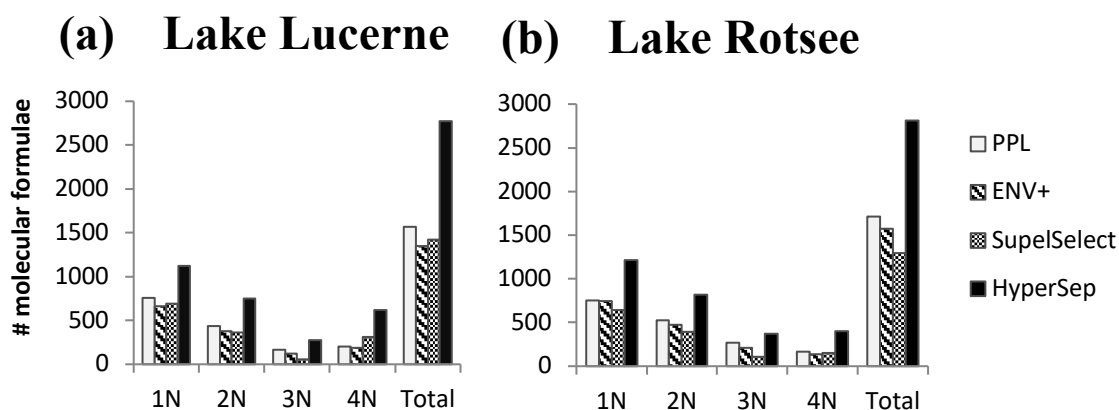


Fig. S2. Number of identified molecular formulae with one, two, three and four nitrogens. The duplicates of LL were combined for the comparison.

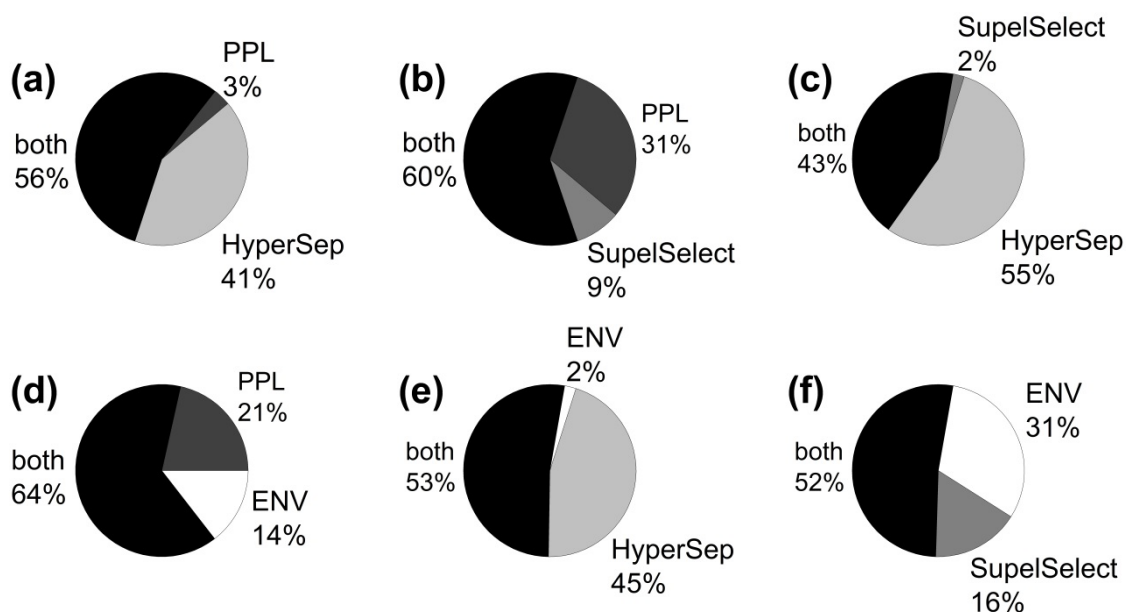


Fig. S3. Comparison of the nitrogen compounds extracted by different sorbent types for Lake Rotsee. The PPL sorbent was compared with the SupelSelect sorbent (a) and with the HyperSep sorbent (b). The SupelSelect sorbent was compared with the HyperSep sorbent (c). The ENV+ sorbent was compared with PPL (d), HyperSep (e) and SupelSelect (f).

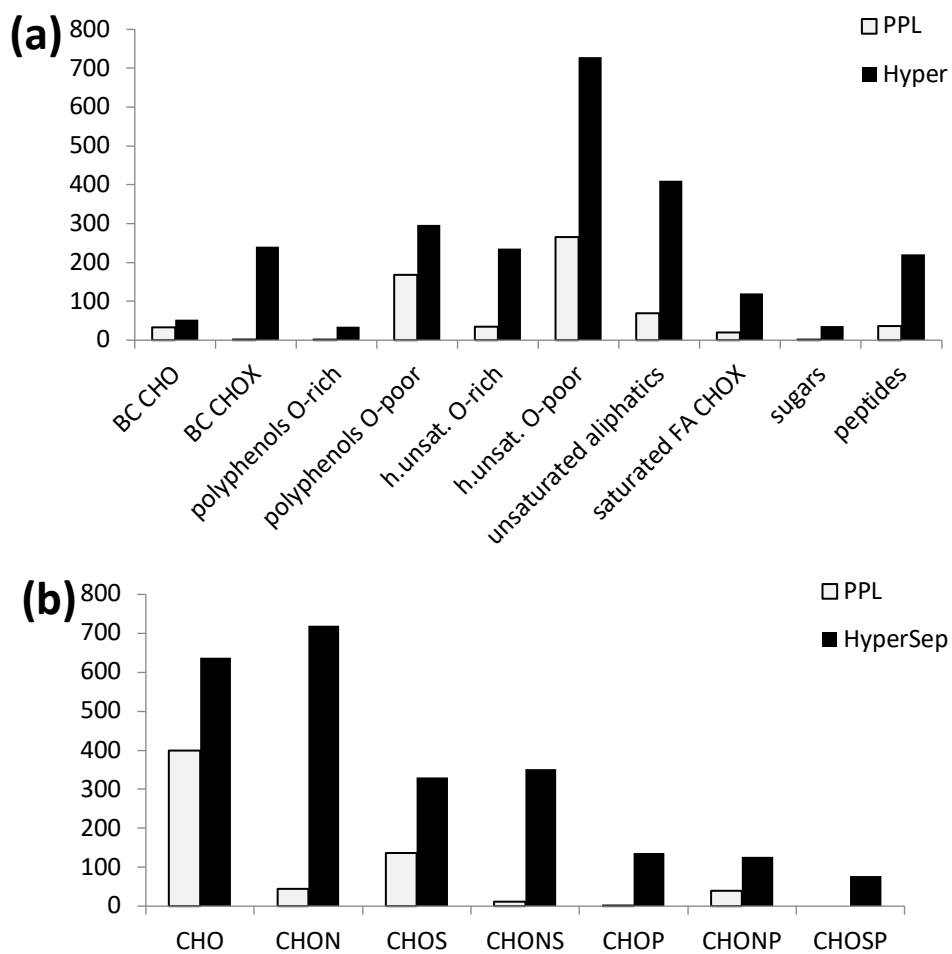


Fig. S4. Comparison of the PPL extract with the HyperSep extract. The compounds found in both sorbent types are not shown. The compounds were then classified after Santl-Temkiv (a) and according to their molecular formula (b).

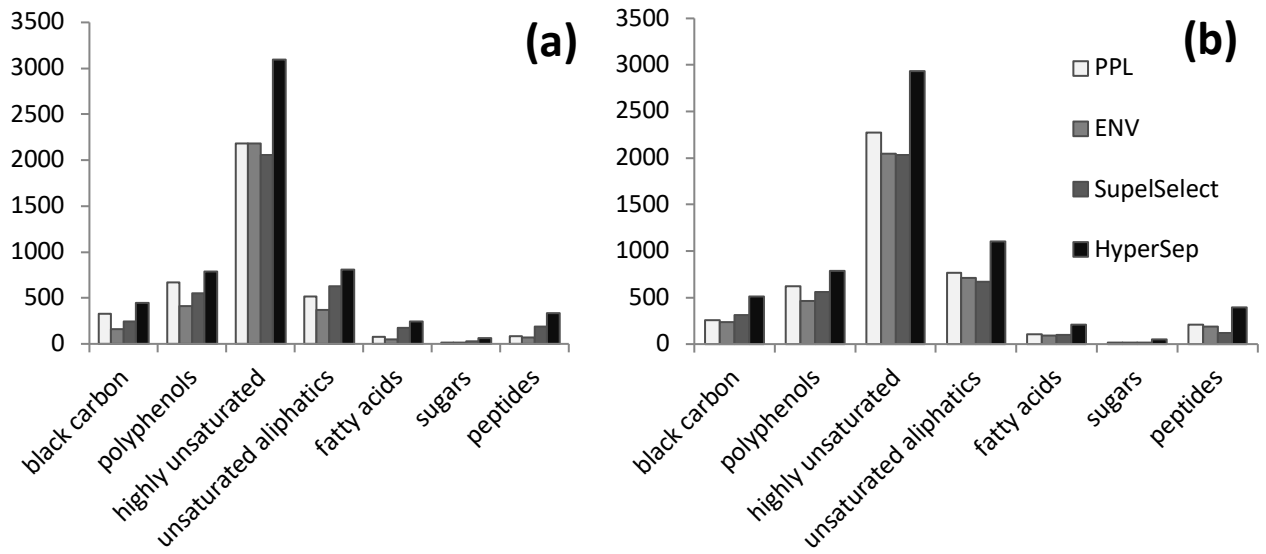


Fig. S5. Number of identified compound classes for (a) Lake Lucerne and (b) Lake Rotsee.