Supporting information

Ecotoxicity risk assessment of amines used in 'switchable water' and CO_2-capturing processes

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Values of the mean effective concentration (EC_{50}, mg L^{-1}) of the amines with CI 95% values

A confidence interval (CI) is the mean of the estimate plus and minus the variation of the estimate. 95% CI gives 95% certainty that the expected values of the experiment will be within this interval. The 95% CI is calculated by a standard formula:

$$\bar{x} \pm 1.96\frac{s}{\sqrt{n}}$$

Where: $\bar{x}$ – the mean value

s – standard deviation

n – sample size

The EC_{50} values were determined at the 50% level on the X-axis of the dose–response curves.

Table S1. Values of the mean effective concentration (EC , mg L^{-1}) of amines tested with CI 95% values.

Compound	Short name	*A. fischeri*	*S. polyrhiza*	*D. magna*
		EC50, mg/l (CI 95%)	EC50, mg/l (CI 95%)	EC50, mg/l (CI 95%)
Monoethanolamine	MEA	227 (150; 304)	358.5 (262.4; 454.6)	260.3 (203.1; 317.5)
Diethanolamine	DEA	468 (280; 656)	549.5 (479.6; 619.4)	368 (288.5; 447.5)
Triethanolamine	TEA	1033 (896; 1169)	>1000	>1000
Dimethylethanolamine	DMEA	437 (293; 581)	228.7 (269.5; 379.7)	223 (213; 234)
2-amino-2methylpropanol	AMP	475 (279; 671)	310 (240.3; 379.7)	327 (287; 367)
N,N,N′,N′-tetramethylethane-1,2-diamine	TMEDA	167 (149; 186)	348 (308.1; 387.9)	247 (192; 302)
N,N,N′,N‘-tetramethyl-1,3-propanediamine	TMPDA	145 (117; 172)	61 (40.9; 81.1)	73 (69; 77)

Statistical analysis by one-way ANOVA

Table S2. One-way ANOVA and post hoc pairwise comparison (Tukey test) between EC_{50} values of studied amines p values are adjusted for multiple testing.

	AMP	**DEA**	**DMEA**	**MEA**	**TEA**	**TMEDA**	**TMPDA**
AMP	NA	NA	NA	NA	NA	NA	NA
DEA	$p = 0.178$	NA	NA	NA	NA	NA	NA
DMEA	$p = 0.398$	$p = 0.0006$	NA	NA	NA	NA	NA
MEA	$p = 0.1989$	$p = 0.0001$	$p = 0.9996$	NA	NA	NA	NA
TEA	$p < 0.0001$	$p < 0.0001$	$p < 0.0001$	$p < 0.0001$	NA	NA	NA
TMEDA	$p = 0.0331$	$p < 0.0001$	$p = 0.9022$	$p = 0.987$	$p < 0.0001$	NA	NA
TMPDA	$p < 0.0001$	$p < 0.0000$	$p < 0.0001$	$p = 0.0001$	$p < 0.0001$	$p = 0.0008$	NA

Amine stability after incubation under test conditions

Two amines (TMPDA and TMEDA) with a concentration of 4000 mgL^{-1} were incubated for 15 min in 2% NaCl aqueous solution and 72h in standard freshwater, in both cases without organisms. After incubation, the amines were extracted from the water-based media with $CHCl_2$. Next, the solvent was removed on the rotary evaporator, and the resulting residue was analyzed by ^{1}H and ^{13}C NMR. The obtained spectra were compared with the spectra of pure TMPDA and TMEDA. No changes in NMR spectra were detected except for a small $CHCl_2$ signal. Thus, it can be concluded that the incubation conditions and media do not cause the decomposition of these substances.

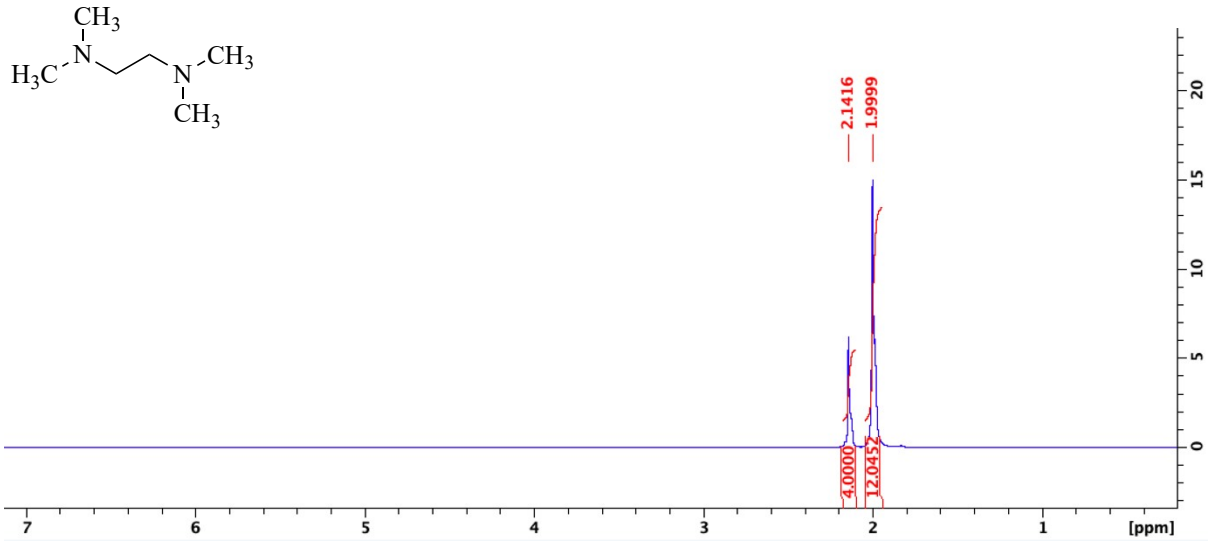


Fig. S1. ^{1}H 400 MHz NMR spectrum of TMEDA without incubation

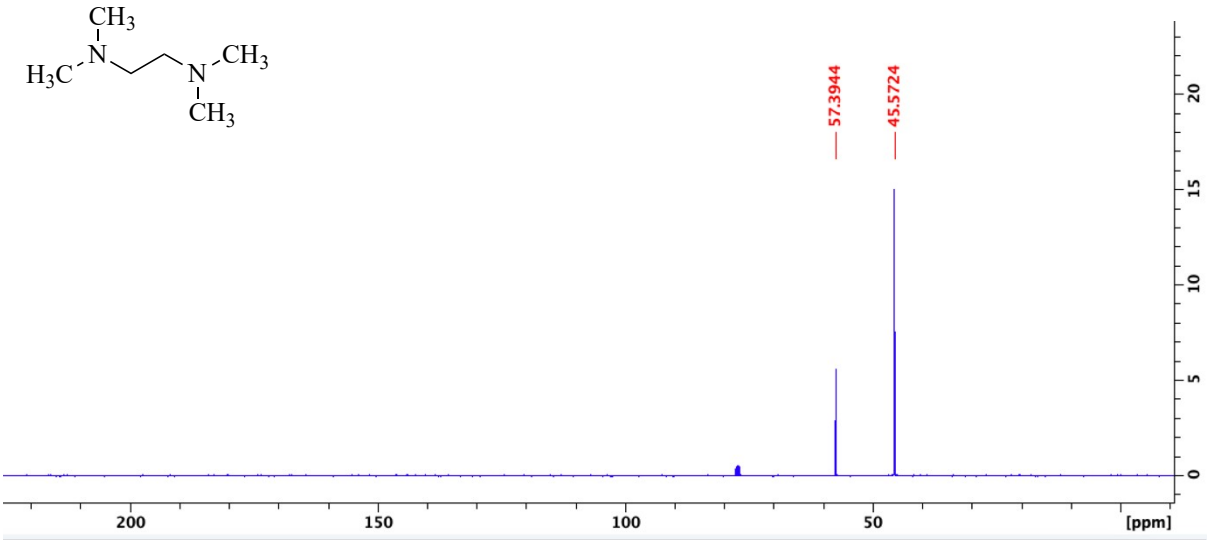


Fig. S2. ^{13}C 400 MHz NMR spectrum of TMEDA without incubation

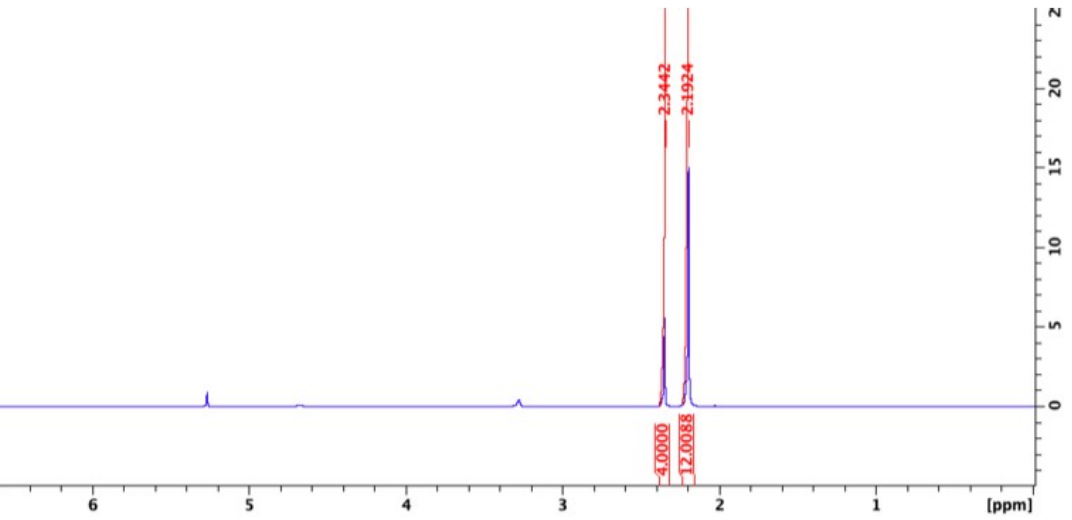


Fig. S3. ^{1}H 400 MHz NMR spectrum of TMEDA after 15-minute incubation in NaCl

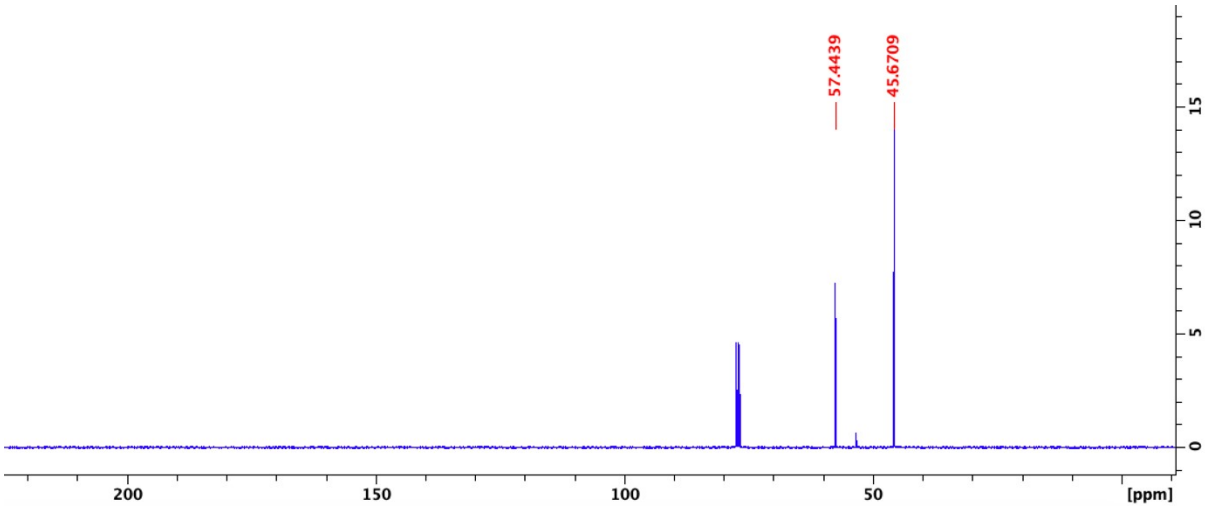


Fig. S4. ^{13}C 400 MHz NMR spectrum of TMEDA after 15-minute incubation in NaCl

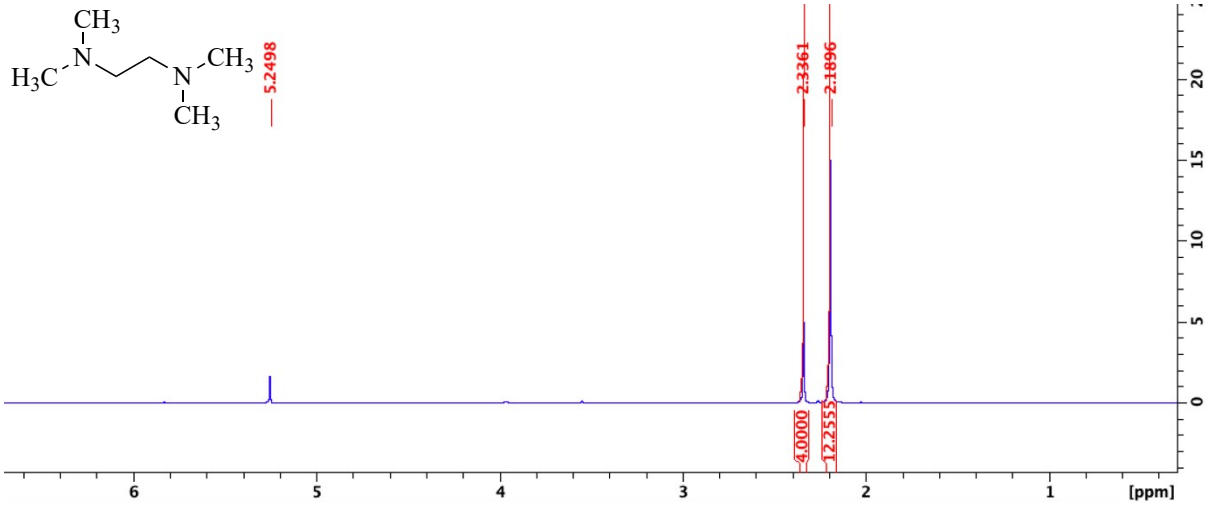


Fig. S5. ^{1}H 400 MHz NMR spectrum of TMEDA after 72h incubation in freshwater media

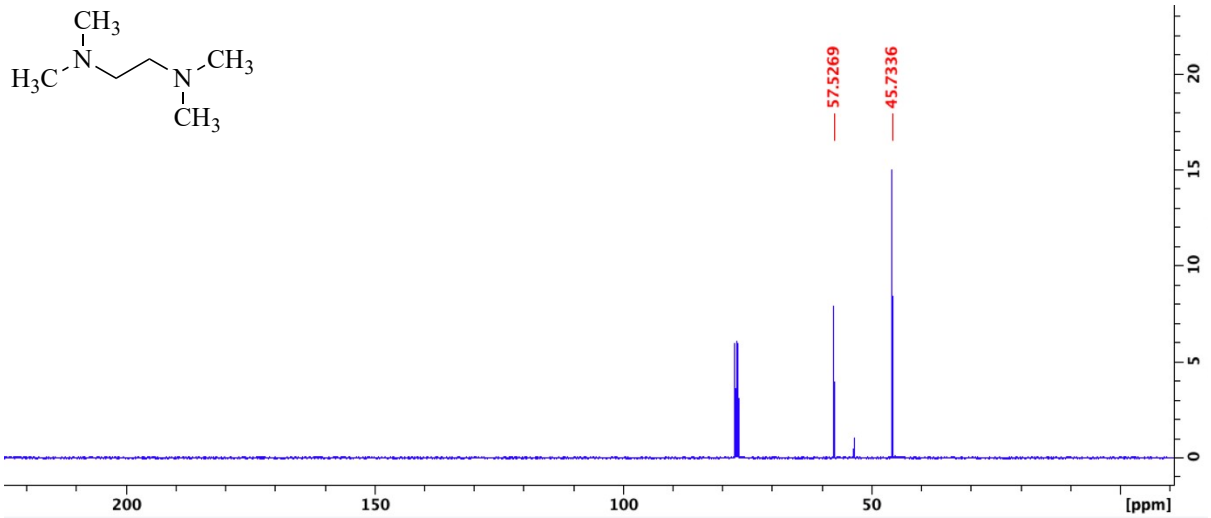
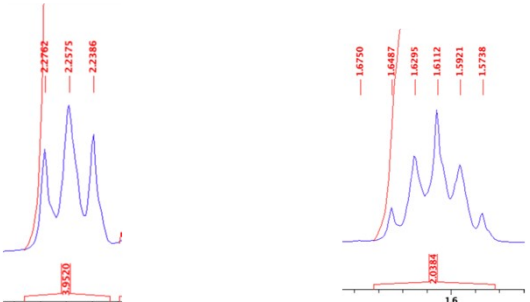


Fig. S6. ^{13}C 400 MHz NMR spectrum of TMEDA after 72h incubation in freshwater media



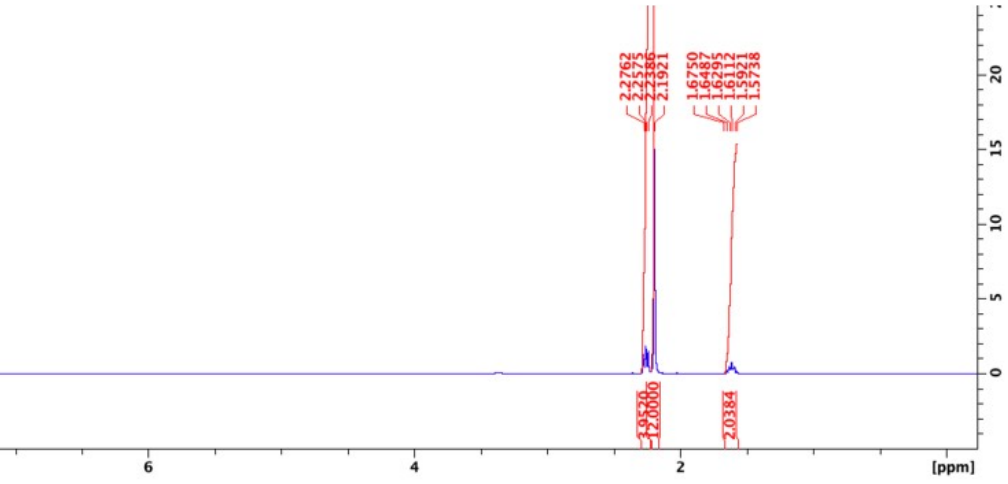
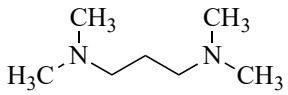


Fig. S7. ^{1}H 400 MHz NMR spectrum of TMPDA without incubation



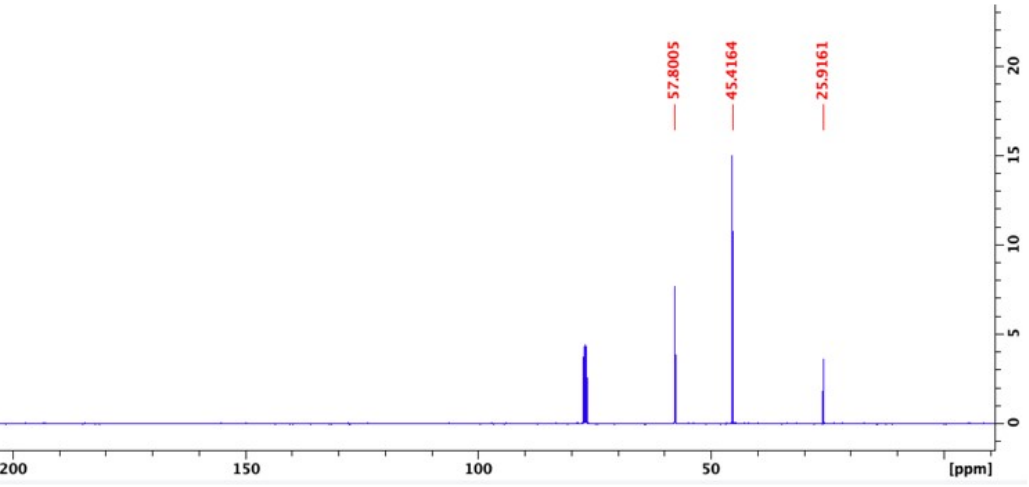


Fig. S8. ^{13}C 400 MHz NMR spectrum of TMPDA without incubation

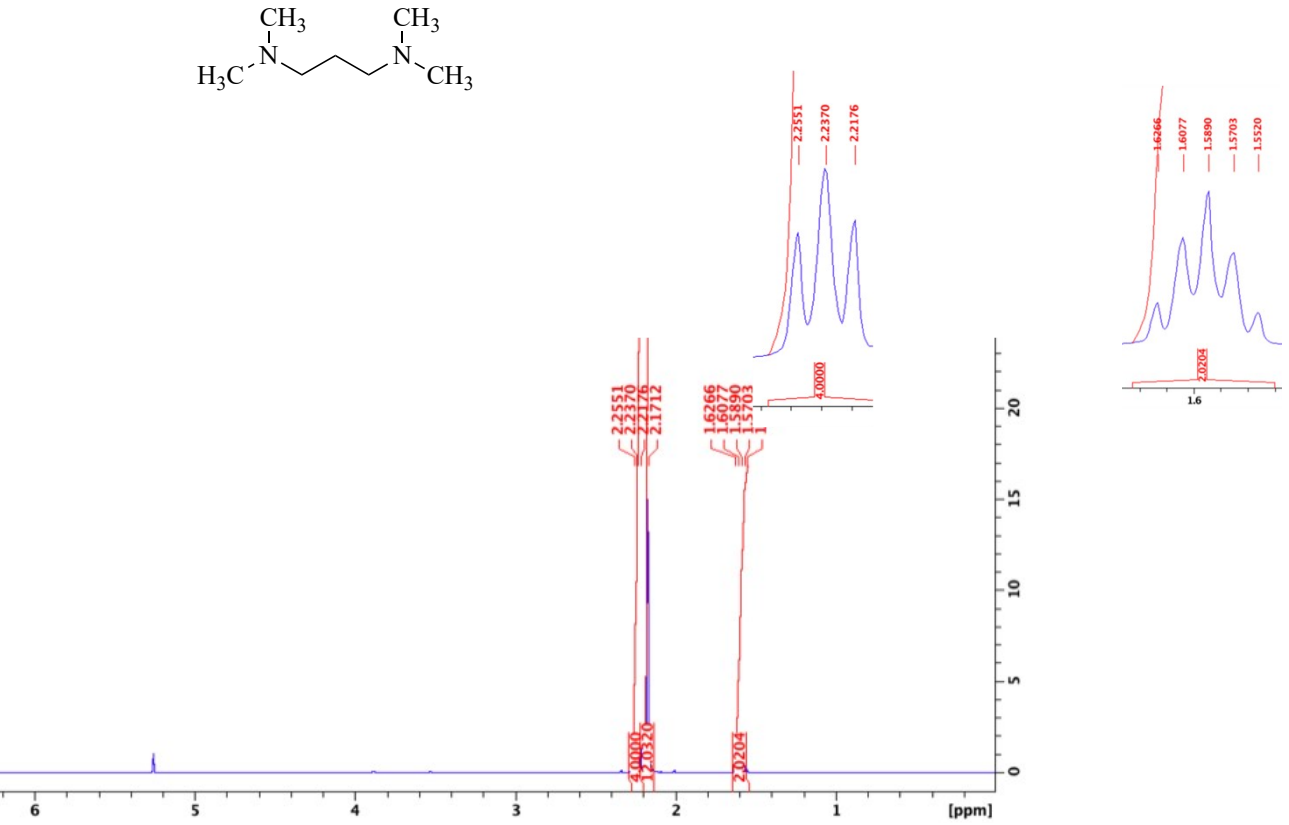
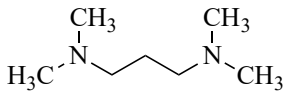


Fig. S9. ^{1}H 400 MHz NMR spectrum of TMPDA after 15-minute incubation in NaCl



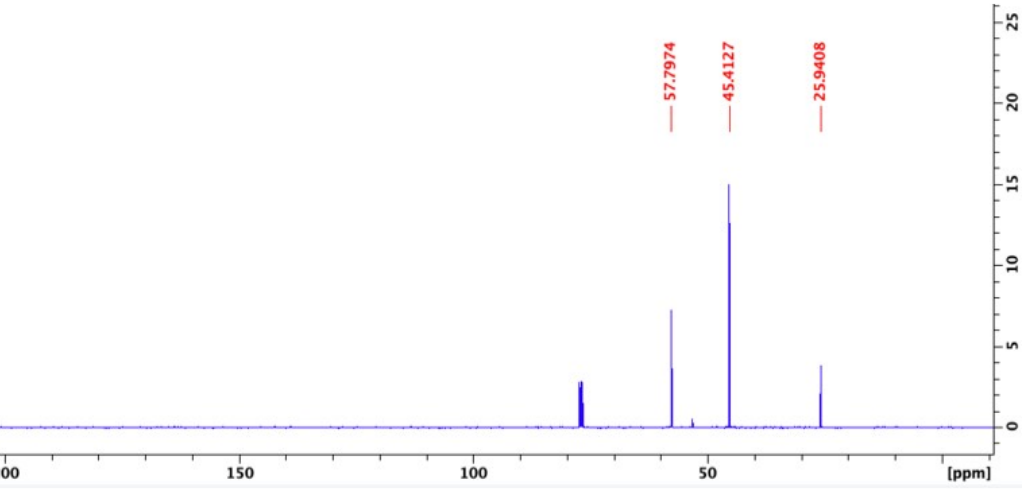
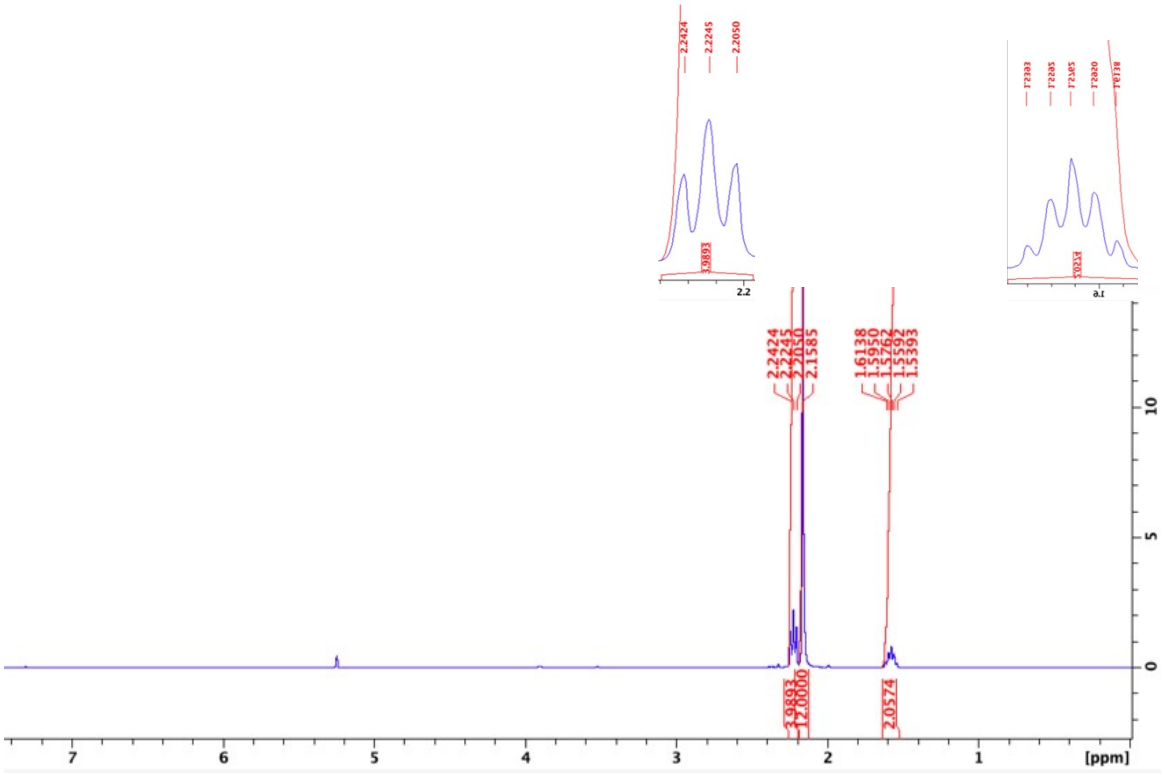


Fig. S10. ^{13}C 400 MHz NMR spectrum of TMPDA after 15-minute incubation in NaCl



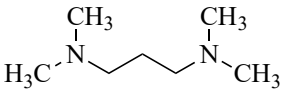
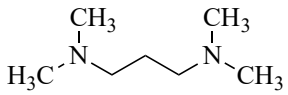


Fig. S11. ^{1}H 400 MHz NMR spectrum of TMPDA after 72h incubation in freshwater media



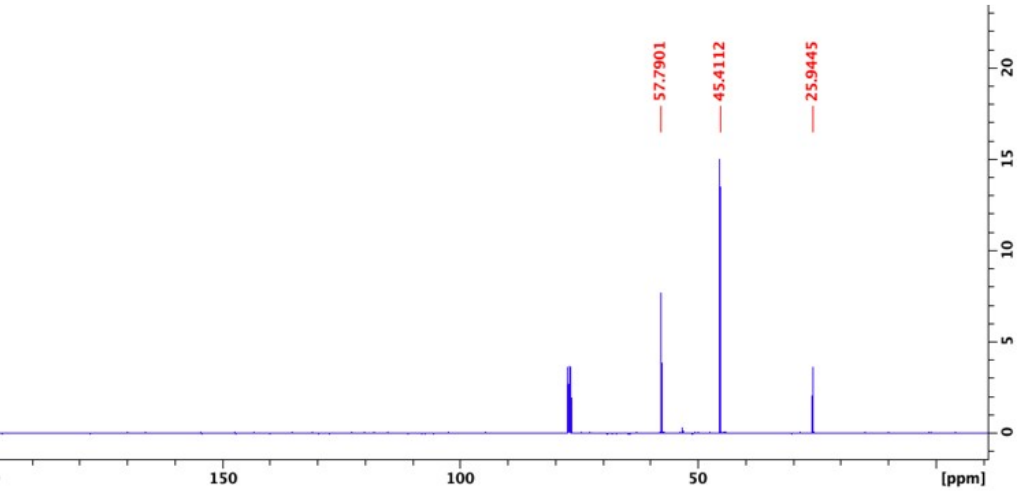


Fig. S12. ^{13}C 400 MHz NMR spectrum of TMPDA after 72h incubation in freshwater media

Linear trends for log(1/EC_{50}) versus logK_{ow} according to test organisms

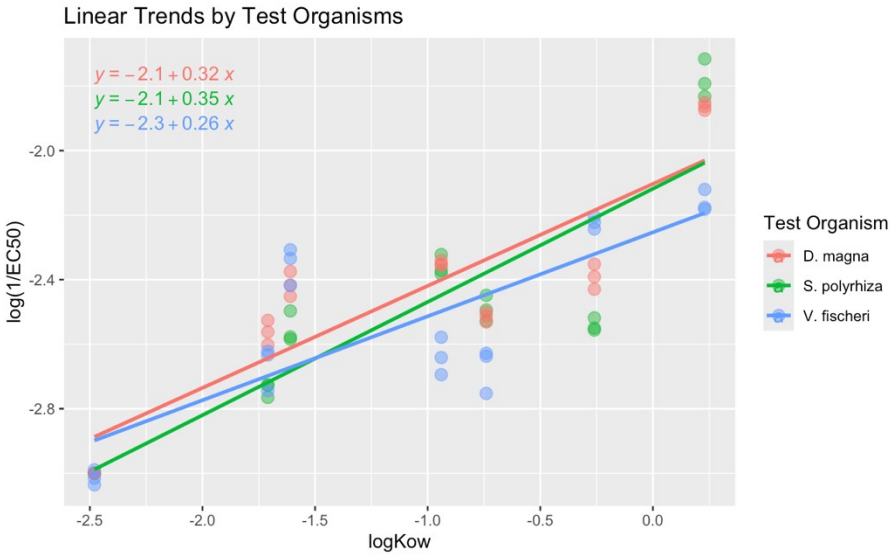


Fig. 13. Plot of log(1/EC50) against logKow for tested compounds

```
Call:
lm(formula = log ~ logKow * test, data = amine_stat)

Residuals:
     Min       1Q   Median       3Q      Max
-0.34672 -0.12701  0.01172  0.11129  0.36475

Coefficients:
                 Estimate Std. Error t value Pr(>|t|)
(Intercept)      -2.10323    0.06189 -33.983  < 2e-16 ***
logKow            0.31610    0.04504   7.018 2.97e-09 ***
testS_pol        -0.01514    0.08753  -0.173   0.8632
testV_fish       -0.15017    0.08753  -1.716   0.0916 .
logKow:testS_pol  0.03470    0.06369   0.545   0.5880
logKow:testV_fish -0.05594    0.06369  -0.878   0.3835
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.1772 on 57 degrees of freedom
Multiple R-squared:  0.7193,    Adjusted R-squared:  0.6946
F-statistic: 29.21 on 5 and 57 DF,  p-value: 1.436e-14
```

Fig. 14. Summary output of a linear regression model

Eq1 and eq2 were taken from the literature.[1]

eq1(inert compounds): log(1/EC50) = 0.824 * logKow + 1.58

eq2 (less inert compoundes): log(1/EC50) = 0.571 * logKow + 2.78

eq3 (tested amines): log(1/EC50) = 0.32 * logKow - 2.

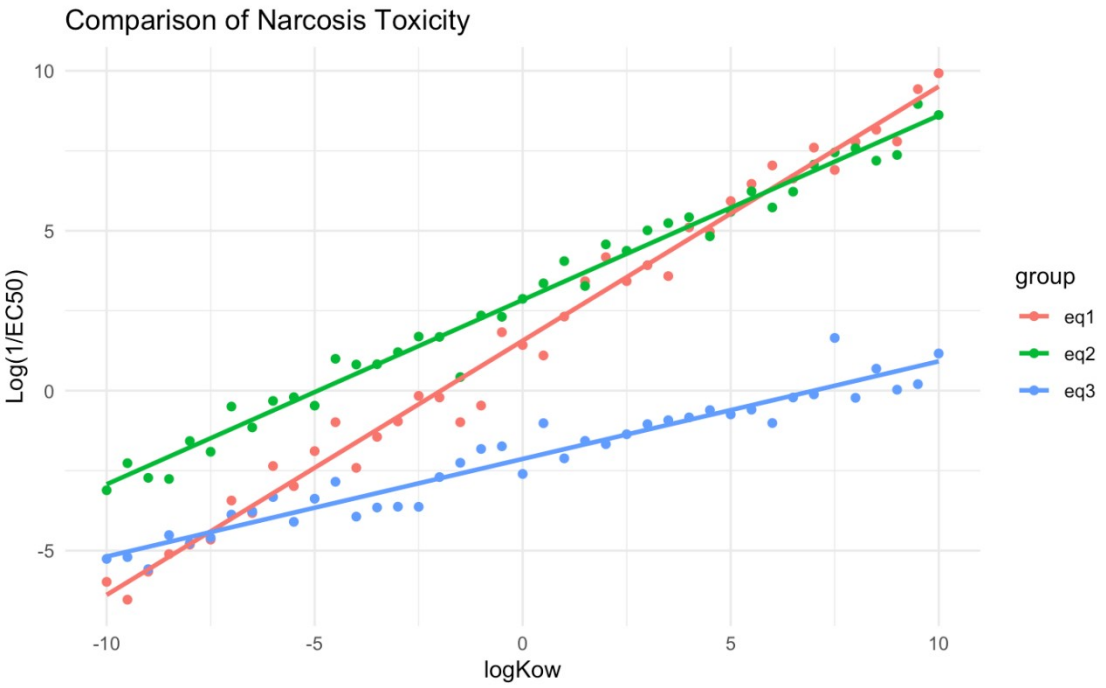


Fig 15. Comparison of narcosis toxicity to *D. magna*

References:

1 X. Zhang, W. Qin, J. He, Y. Wen, L. Su, L. Sheng and Y. Zhao, Discrimination of excess toxicity from narcotic effect: Comparison of toxicity of class-based organic chemicals to daphnia magna and tetrahymena pyriformis, *Chemosphere*, 2013, **93**, 397–407.