

Supporting Information

Quantification of Phytochelatins in *Chlamydomonas reinhardtii*

5 using ferrocene-based derivatization

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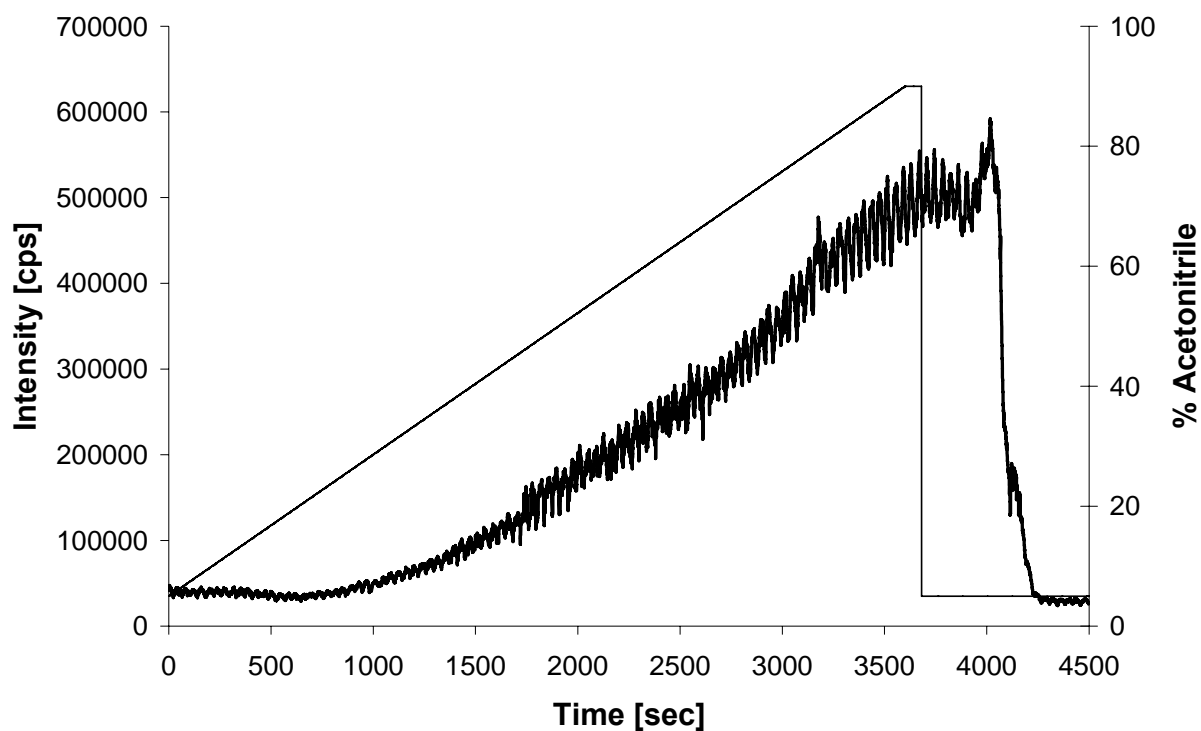


Figure S-1 ICP-MS signal of ⁵⁶Fe (bold line) fed continually via sheath flow (366 ppm, 0.66 mL/h), injection of 10 μ L solvent A; 2nd axis shows the LC gradient course (fine line).

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Thiol	Retention time [min]	<i>m/z</i> calculated	<i>m/z</i> measured	Δ ppm	Number of FMEA-tags	charge
TCEP-FMEA	13.74	603.116	603.1189	-4.70	1	[M+H] ⁺
Cysteine	13.99	474.0762	474.0781	-4.04	1	[M+H] ⁺
GSH	15.10	660.1420	660.1427	-0.94	1	[M+H] ⁺
PC ₃ desGly/ CysPC ₂ Glu	18.21	886.1624	886.1673	-5.54	3	[M+2H] ²⁺
CysPC ₂ desGly	18.97	821.6460	n. d.			[M+2H] ²⁺
CysGSHGlu/ PC ₂ desGly	21.79	1187.2149	1187.2239	-7.63	2	[M+H] ⁺
CysGsH	21.95	1115.1942	1115.2023	-7.30	2	[M+H] ⁺
CysGSHdesGly	22.55	1058.1809	1058.1814	-0.45	2	[M+H] ⁺
PC ₂	23.45	1244.2348	1244.2455	-8.50	2	[M+H] ⁺
CysPC ₂	26.36	850.1476	850.1567	-10.80	3	[M+2H] ²⁺
PC ₃	27.77	914.1786	914.1741	+4.93	3	[M+2H] ²⁺
CysPC ₃	29.19	1142.2097	1142.2081	+1.35	4	[M+2H] ²⁺
PC ₂ Ala	29.29	1258.2627	1258.2611	+1.31	2	[M+H] ⁺
PC ₄	30.69	1206.724	1206.7294	-4.38	4	[M+2H] ²⁺
CysPC ₄	31.56	1434.2483	1434.2595	-7.80	5	[M+2H] ²⁺

Table S-1: Measured and calculated exact masses of phytochelatins via LC/ESI-ToF-MS in a *C. reinhardtii* sample incubated 48 h with Cd.

Element	c [$\mu\text{g/L}$]	SD [$\mu\text{g/L}$]	RSD [%]
Fe	264.24	0.55	0.21
Cu	488.35	1.23	0.25
Zn	5.93	0.04	0.75

5 **Table S-2:** Concentrations of Fe, Cu and Zn in the TAP culture medium determined by ICP-OES. Standard deviation (SD) and Relative Standard Deviation (RSD) are calculated of three individual measurements ($n = 3$).