

Erratum to: Mass spectrometric screening and identification of acidic metabolites in fulvic acid fractions of contaminated groundwater

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The authors would like to call the reader's attention to the following:

The second paragraph in the section “Elucidation of unknown structures” should read:

“A query for the chemical formula of peak 3 ($C_8H_8O_3$) in PubChem resulted in 633 hits. The fragmentation pattern of peak 3 reveals the loss of CO_2 typical for aromatic or heterocyclic acids (Fig. 5a)”.

In Table 3 two words were misspelled. They should correctly read: “Dihydrocarboxybenzothiophene” and “Benzofuranmethylsuccinic acid”.

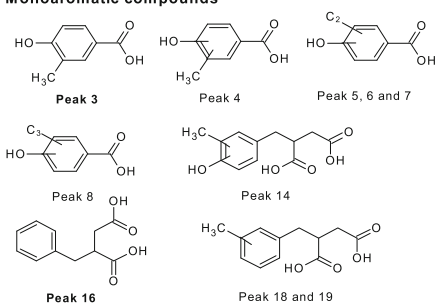
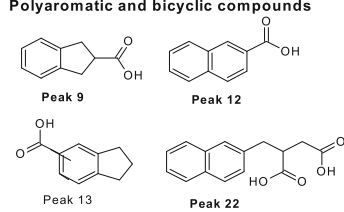
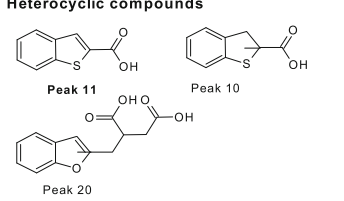
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Table 4 was unfortunately reproduced incorrectly. Below please find the corrected version:

Table 4 Identified (*bold*) and tentatively identified metabolites in the FA-fraction of the contaminated region (B22 FA). Additionally structural proposals (*grey*) for metabolites are listed

	Formula	Metabolites	Chemical structures
1	C ₉ H ₈ O ₃ S	-	<p>Monoaromatic compounds</p>  <p>Polyaromatic and bicyclic compounds</p>  <p>Heterocyclic compounds</p> 
2	C ₉ H ₈ O ₄	Methyldicarboxybenzene	
3	C ₈ H ₈ O ₃	4-hydroxy-3-methylbenzoic acid	
4	C ₈ H ₈ O ₃	Hydroxymethylbenzoic acid	
5	C ₉ H ₁₀ O ₃	C ₂ -hydroxybenzoic acid	
6	C ₉ H ₁₀ O ₃	C ₂ -hydroxybenzoic acid	
7	C ₉ H ₁₀ O ₃	C ₂ -hydroxybenzoic acid	
8	C ₁₀ H ₁₂ O ₃	C ₃ -hydroxybenzoic acid	
9	C ₁₀ H ₁₀ O ₂	2-carboxyindane	
10	C ₉ H ₈ O ₂ S	Dihydrocarboxybenzothiophene	
11	C ₉ H ₆ O ₂ S	2-carboxybenzothiophene	
12	C ₁₁ H ₈ O ₂	2-naphthoic acid	
13	C ₁₀ H ₁₀ O ₂	Carboxyindane	
14	C ₁₂ H ₁₄ O ₅	Hydroxymethylbenzylsuccinic acid	
15	-	-	
16	C ₁₁ H ₁₂ O ₄	Benzylsuccinic acid	
17	C ₁₁ H ₁₂ O ₄	-	
18	C ₁₂ H ₁₄ O ₄	Methylbenzylsuccinic acid	
19	C ₁₂ H ₁₄ O ₄	Methylbenzylsuccinic acid	
20	C ₁₃ H ₁₂ O ₅	Benzofuranmethylsuccinic acid	
21	C ₁₃ H ₁₄ O ₄	Indanesuccinic acid	
22	C ₁₅ H ₁₄ O ₄	Naphthyl-2-methylsuccinic acid	

In the “Electronic Supplementary Material” the legend to Figure S2 should correctly read:

“Figure S2. (Part 3): LC-ESI-QTOF-MS fragmentation spectra (exemplarily at a collision energy of CE=10 eV) of the most intensive peaks derived from the NLS $\Delta m/z=44$. For peak 15 no fragmentation spectra could be obtained”.

In the “Electronic Supplementary Material” Table S1 was unfortunately reproduced incorrectly. Below please find the corrected version:

Table S1: Results of a literature search for acidic metabolites of monoaromatic, polycyclic aromatic, bicyclic and heterocyclic compounds found in batch experiments (b) and/or in the field (f)

Metabolites	Elemental formulae	(Possible) parent compound	Batch (b)/ Field(f)	Literature (examples)
of monoaromatic compounds (e.g. BTEX)				
Benzoic acid	C ₇ H ₆ O ₂	BTEX	(b), (f)	[1-5]
Benzylsuccinic acid	C ₁₁ H ₁₂ O ₄	Toluene	(b), (f)	[3, 5-10]
Benzylfumaric acid	C ₁₁ H ₁₀ O ₄	Toluene	(b), (f)	[7]
Methylbenzylsuccinic acid	C ₁₂ H ₁₄ O ₄	Xylene	(b), (f)	[3, 5-7, 11, 12]
Methylbenzylfumaric acid	C ₁₂ H ₁₂ O ₄	Xylene	(f)	[7]
Methylbenzoic acid	C ₈ H ₈ O ₂	Xylene	(f)	[3-5, 13]
Dimethylbenzoic acid	C ₉ H ₁₀ O ₂	Trimethylbenzene	(b), (f)	[2, 14]
Phthalic acid	C ₈ H ₆ O ₄	Xylene	(f)	[3]
Trimethylbenzoic acid	C ₁₀ H ₁₂ O ₂	Tetramethylbenzene	(f)	[13-15]
C ₄ - to C ₆ -benzoic acid	C ₁₁ H ₁₄ O ₂ ... C ₁₃ H ₁₈ O ₂	C ₅ - to C ₇ -benzene	(f)	[13]
C ₂ - to C ₅ -benzylsuccinic acid	C ₁₃ H ₁₆ O ₄ ... C ₁₆ H ₂₂ O ₄	C ₃ - to C ₆ -benzene	(f)	[13, 16]
Methylphenylacetic acid	C ₉ H ₁₀ O ₂		(f)	[14]
of polycyclic aromatic hydrocarbons (PAH) and bicyclic compounds				
Naphthyl-2-methylsuccinic acid	C ₁₅ H ₁₄ O ₄	Naphthalene, 2-methylnaphthalene	(b), (f)	[4-6, 17-19]
Naphthoic acid	C ₁₁ H ₈ O ₂	Naphthalene, Methylnaphthalene	(b), (f)	[5, 6, 17, 18, 20, 21]
Naphthyl-2-methylenesuccinic acid	C ₁₅ H ₁₂ O ₄	Naphthalene, 2-methylnaphthalene	(b), (f)	[17, 19, 22]
Tetra-, hexa-, octa- and decahydronaphthoic acid	C ₁₁ H ₁₂ O ₂ ... C ₁₁ H ₁₈ O ₂	Naphthalene, 2-Methylnaphthalene	(b), (f)	[4, 5, 17, 23, 24]
Carboxycyclohexylacetic acid	C ₉ H ₁₄ O ₄	Naphthalene, 2-methylnaphthalene	(b)	[25]
Methylnaphthoic acid	C ₁₂ H ₁₀ O ₂	2-methylnaphthalene	(b), (f)	[4-6, 24, 26, 27]
1-methylnaphthyl-2-methylsuccinic acid	C ₁₆ H ₁₆ O ₄	1-methylnaphthalene	(b)	[5, 6, 22]
Naphthylacetic acid	C ₁₂ H ₁₀ O ₂	Naphthalene	(f)	[18]
Hydroxynaphthoic acid	C ₁₁ H ₈ O ₃	Naphthalene	(f)	[18]
Dimethylnaphthoic acid	C ₁₃ H ₁₂ O ₂		(b)	[28]
Acenaphthoic acid	C ₁₃ H ₁₀ O ₂	Acenaphthene	(b)	[5, 6, 22]
Acenaphthylmethylsuccinic acid	C ₁₇ H ₁₆ O ₄	Acenaphthene	(b)	[5]
Acenaphthyleneic acid	C ₁₃ H ₈ O ₂	Acenaphthylene	(b)	[22]
Phenanthrene carboxylic acid	C ₁₅ H ₁₀ O ₂	Phenanthrene	(b)	[20]
Fluorenoic acid	C ₁₄ H ₁₀ O ₂	Fluorene	(f)	[5]
Carboxyindane	C ₁₀ H ₁₀ O ₂	Indane	(b), (f)	[5, 22]
Carboxyindene	C ₁₀ H ₈ O ₂	Indene	(b), (f)	[5, 22]
of heterocyclic compounds				
Carboxybenzothiophene	C ₉ H ₆ O ₂ S	Benzothiophene	(b), (f)	[4-6, 22, 29]
Methylcarboxybenzothiophene	C ₁₀ H ₈ O ₂ S	Methylbenzothiophene	(f)	[6]
Dihydrocarboxybenzothiophene	C ₉ H ₈ O ₂ S	Benzothiophene	(f)	[4, 6, 29]
Benzothiophenemethylsuccinic acid	C ₁₃ H ₁₂ O ₄ S	Benzothiophene	(b), (f)	[6, 22]
Benzothiophenemethylenesuccinic acid	C ₁₃ H ₁₀ O ₄ S	Benzothiophene	(b)	[22]
Carboxybenzofuran	C ₉ H ₆ O ₃	Benzo-furan	(b), (f)	[5, 6, 22]
Benzo-furanmethylsuccinic acid	C ₁₃ H ₁₂ O ₅	Benzo-furan	(b)	[6, 22]
Benzo-furanmethylenesuccinic acid	C ₁₃ H ₁₀ O ₅	Benzo-furan	(b)	[22]
Indolic acid	C ₉ H ₇ O ₂	Indole	(b)	[22]