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Efficient Oil Spill Identification Utilizing Hydrophobic Sampling Paper and Gas Chromatography/Mass Spectrometry

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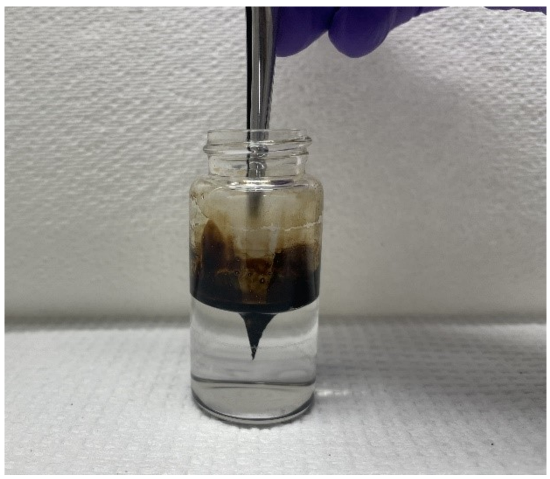


Supplementary Information:

Figure S1: Collection of an oil slick sample with hydrophobic paper

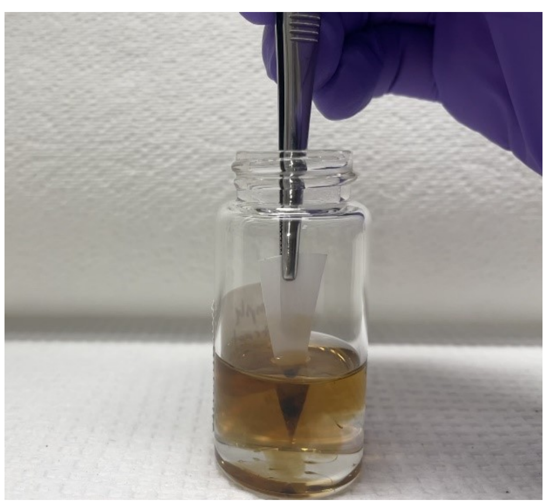


Figure S2: Extraction of an oiled hydrophobic paper sample into binary solvent (2DCM:3HEX)

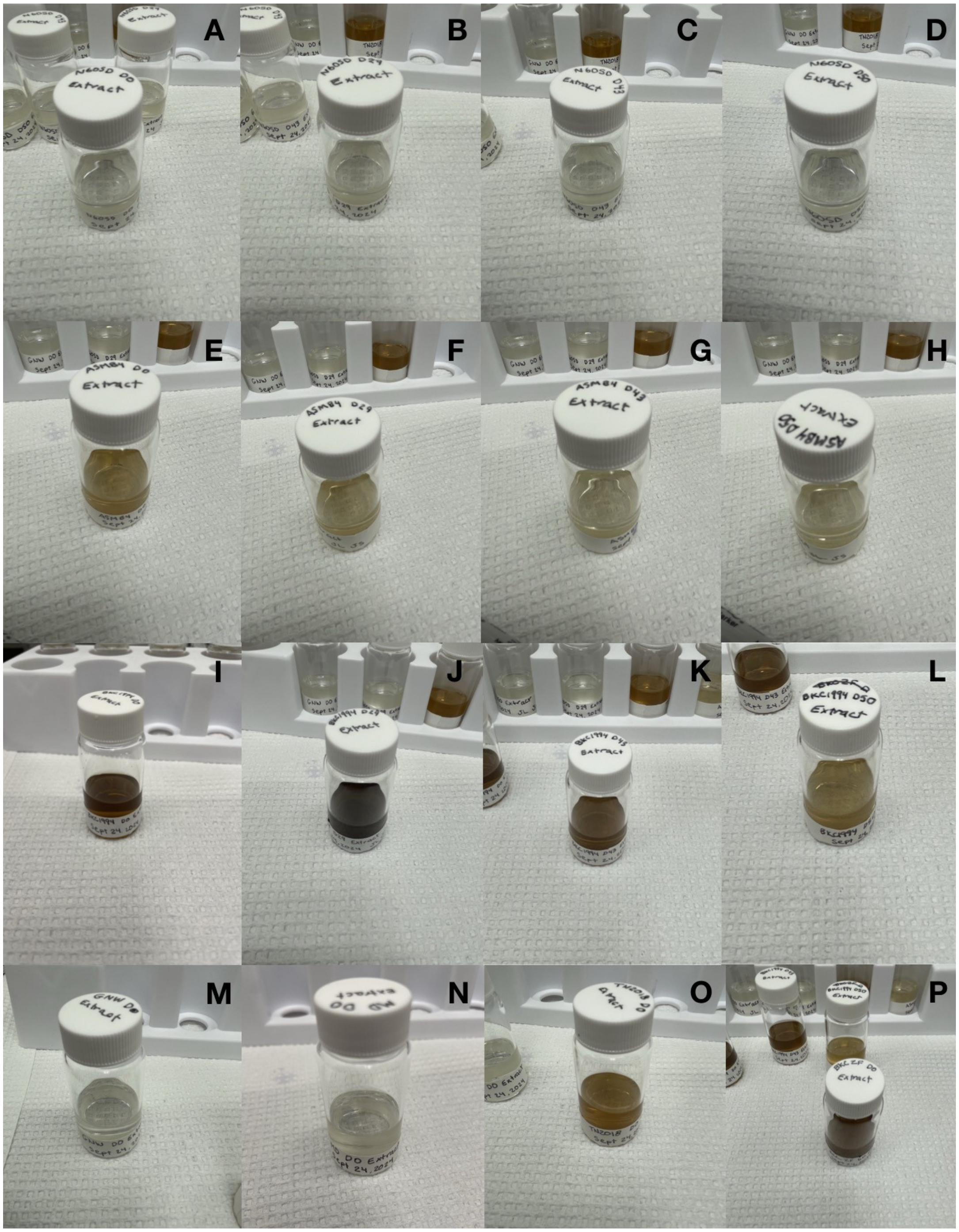


Figure S3: Oiled hydrophobic paper extracts including N60SD D0(S3A), N60SD D29(S3B), N60SD D43(S3C), N60SD D50(S3D), AMSB4 D0(S3E), ASMB4 D29(S3F), ASMB4 D43(S3G), ASMB4 D50(S3H), BKC1994 D0(S3I), BKC 1994 D29(S3J), BKC 1994 D43(S3K), BKC 1994 D50(S3L), GNW D0(S3M), MD D0(S3N), TN2018 D0(S3O), BKC ZF D0(S3P).

Table S1: Storage method of each weathered oil sample using the dipped hydrophobic paper method prior to extraction, where glass refers to glass vial with Teflon lined lid and plastic refers to retained in sealed plastic bag.

Timepoint for Sample	MD	N60SD	GNW	ASMB4	TN2018	BKC 1994	BKC ZF
Day 0	Not stored, analyzed on day						
Day 29	na	Glass	na	Glass	na	Glass	na
Day 43	na	Plastic	na	Plastic	na	Plastic	na
Day 50	na	Plastic	na	Plastic	na	Plastic	na

S1: GC/MS Analysis Standard Details

Sintef (ID: 2005-0439): An oil blend prepared by SINTEF Marine Environmental Technology (Trondheim, Norway) with a 2:3:1:4 ratio of heavy fuel oil (IFO 180): Russian crude oil (Kyrtael): Sicilian crude oil (Presioso): Aspheltenic oil from the North Sea (Grane).[1]

Table S2: Summary of flagged diagnostic ratios of different non weathered environmental samples compared to source oils using different solvents for extraction from the hydrophobic paper.

Source Oil	MD	MD	MD	Crude	Crude (a)	Crude (b)	Crude	BKC	BKC	BKC
Solvent	DCM	2DCM:3HEX	HEX	DCM	2DCM:3HEX	2DCM:3HEX	HEX	DCM	2DCM:3HEX	HEX
MD	20	19	20	60	56	58	59	46	46	46
Crude	54	53	54	18	19	18	16	51	53	50
BKC	57	55	56	55	53	54	53	23	17	20

S2: Solvent determination

1ml of each source was diluted with 10ml of binary solvent made of 40% DCM and 60% hexanes (HEX) (2DCM:3HEX) before being pitted onto 350ml of seawater in a 600ml beaker to form a slick. The slick was allowed to sit for 30 minutes so the binary solvent (2DCM:3HEX) could evaporate. 10ml of each solvent, DCM, binary (2DCM:3HEX), and HEX, was transferred into labelled 20ml vials for each source. Hydrophobic dipping papers were used to collect oil, as described in the methods section, before extraction. Marine diesels were extracted for 5seconds, crude oils were extracted for 10 seconds, and heavy fuel oils (BKC) were extracted for 20 seconds.

S3: Optimizing the concentration of oil extracts.

Table S3: Summary of the number of flagged diagnostic ratios at three different concentrations of ASMB4 D0 when compared to source samples. Probable matches are highlighted in green.

Preparation method detail		**Sources**							**95% confidence Interval**
ASMB4 D0 Final Blowdown Vol. (mL)	Liquid-liquid concentration factor (LCF)	MD	N60SD	GNW	ASMB 4	TN2018	BKC 1994	BKC ZF	Lower Limit
10	1	66	62	61	22	59	55	51	55
5	2	67	63	61	15	58	55	49	54
1	10	64	66	62	13	60	54	49	54

Nitrogen blowdown was performed to determine if the concentration of extracted study samples can improve the results of analysis. Three levels of concentration were investigated including a liquid-to-liquid concentration factor (LCF) of 1, where samples were taken from the original 10 mL extract, secondly a sample of 2 LCF taken after nitrogen blow down to 5 mL, and finally an LCF of 10 (10 LCF) taken after nitrogen blow down to 1 mL (SI Table S3). For weathered samples, the content of biomarkers is known to deplete over time, therefore increasing the concentration of the sample may improve the analysis by increasing the response from the low biomarker content.[6,16,26] Alternatively, extending blowdown could result in biomarker losses and resulting increased concentration could overwhelm the detector, thus impeding the analysis. Ultimately, it was found that the 1 mL study samples, with 10 LCF, produced the lowest number of flagged biomarker ratios for correct source to sample comparisons, as demonstrated across ASMB4 D0 samples in Table S3. Greater response from the concentrated biomarkers likely allowed for increased consistency of integration during data analysis. Generally, the number of flagged ratios only decreased for the correct assignments as concentration increased while no discernible trend was observed for incorrect comparisons (SI Table S3, SI Table S4). It is likely that the increased consistency of integration will have a larger impact on the number of flagged diagnostic ratios for the correct assignment, as these samples should present relative differences of less than 14%.[25] It is recognized that at low concentrations, inconsistencies in integration of peaks may exaggerate the relative percent difference consequentially increasing the number of flagged ratios. For mismatched comparisons, biomarker ratio comparisons between study samples and alternative sources are already expected to exceed the 14% relative error threshold. Therefore, exaggeration of the relative percent difference due to inconsistencies in integration would have little effect on the number of flagged ratios produced by an incorrect comparison. Further data for comparison of concentration results can be found in supplemental information (SI Table S4). Based on current study results, it was logical to conclude that 10 times concentration of sample extracts was optimal, and this procedure was incorporated into the current study for environmental spill assessments.

S4: 95% confidence Intervals

The 95% confidence intervals were calculated using a one tailed t-distribution by the formula $\bar{x}-t*S/\sqrt{n}$ where $\bar{x}$ is the mean number of flags produced from incorrect source to environmental sample comparisons for a particular environmental sample, t is the critical t value, S is the standard deviation, and n is the number of observations. To determine the critical t value a significance level of 0.05 was chosen. As there were 6 incorrect sources to sample comparisons for each environmental sample, there were 5 degrees of freedom by the formula n-1. The test was considered a one tailed test as only values which were significantly lower than the mean number of flags yielded from incorrect source to environmental samples were of interest to the study. Therefore, this calculation used a critical t value of 2.02 based on the standardized table for critical t values.

Table S4: Summary of number of flagged ratios for each comparison as well as the mean, standard deviation, and the 95% confidence interval of incorrect comparisons for each environmental sample. Positive matches are highlighted in green while inconclusive matches are highlighted in orange.

Sample Oil	Final Vol.	Weathering	N60SD	MD	GN W	ASMB 4	TN201 8	BKC199 4	BKC ZF	Mean False Match	Std Dev	Lower conf. limit (95%)
N60SD	10 mL	D50	61	50	48	68	68	62	67	61	9	53
N60SD	10 mL	D43	52	49	49	67	66	67	64	60	9	53
N60SD	10 mL	D29	48	51	49	66	66	66	68	61	9	54
N60SD	10 mL	D0	26	41	51	63	62	65	66	58	10	50
N60SD	5 mL	D50	56	48	48	66	66	61	66	59	9	52
N60SD	5 mL	D43	47	45	52	64	65	65	64	59	9	52
N60SD	5 mL	D29	51	48	47	65	67	68	67	60	10	52
N60SD	5 mL	D0	25	41	53	63	64	64	65	58	10	50
N60SD	1 mL	D50	56	51	46	69	59	60	64	58	8	51
N60SD	1 mL	D43	46	53	52	65	63	65	65	61	6	55
N60SD	1 mL	D29	46	50	51	63	64	60	67	59	7	53
N60SD	1 mL	D0	14	50	61	63	64	65	66	62	6	57
MD	10 mL	D0	55	30	48	66	67	66	66	61	8	55
MD	5 mL	D0	56	25	49	65	65	66	65	61	7	55
MD	1 mL	D0	51	22	51	64	67	63	62	60	7	54
GNW	10 mL	D0	54	47	25	61	64	54	65	58	7	52
GNW	5 mL	D0	59	47	23	60	63	54	60	57	6	52
GNW	1 mL	D0	54	49	21	64	61	56	60	57	5	53
ASMB4	10 mL	D50	69	64	59	53	60	61	66	63	4	60
ASMB4	10 mL	D43	69	68	63	46	64	63	60	65	3	62
ASMB4	10	D29	69	67	65	58	65	65	63	66	2	64

	mL											
ASMB4	10 mL	D0	62	66	61	22	59	55	51	59	5	55
ASMB4	5 mL	D50	66	67	62	49	62	55	58	62	5	58
ASMB4	5 mL	D43	66	66	65	39	61	61	61	63	3	61
ASMB4	5 mL	D29	69	65	67	52	63	62	57	64	4	60
ASMB4	5 mL	D0	63	67	61	15	58	55	49	59	6	54
ASMB4	1 mL	D50	67	65	66	52	53	54	62	61	6	56
ASMB4	1 mL	D43	66	66	66	41	59	59	59	63	4	59
ASMB4	1 mL	D29	64	63	67	45	61	61	59	63	3	60
ASMB4	1 mL	D0	66	64	62	13	60	54	49	59	6	54
TN2018	10 mL	D0	63	69	64	61	13	61	65	64	3	61
TN2018	5 mL	D0	64	69	65	61	12	61	63	64	3	61
TN2018	1 mL	D0	63	70	61	58	15	59	62	62	4	59
BKC1994	10 mL	D50	59	53	50	66	66	59	65	60	7	54
BKC1994	10 mL	D43	60	59	61	62	68	55	63	62	3	60
BKC1994	10 mL	D29	65	67	64	61	64	46	58	63	3	61
BKC1994	10 mL	D0	63	59	58	58	64	21	57	60	3	57
BKC1994	5 mL	D50	60	58	55	63	64	56	64	61	4	58
BKC1994	5 mL	D43	63	60	63	56	65	49	62	62	3	59
BKC1994	5 mL	D29	66	68	63	59	62	43	58	63	4	59
BKC1994	5 mL	D0	65	60	60	53	62	18	56	59	4	56
BKC1994	1 mL	D50	63	63	65	62	62	49	59	62	2	61
BKC1994	1 mL	D43	64	62	66	59	65	40	61	63	3	61

BKC1994	1 mL	D29	65	68	65	61	59	37	60	63	4	60
BKC1994	1 mL	D0	64	61	59	55	61	9	55	59	4	56
BKCZF	10 mL	D0	68	66	63	57	64	56	22	62	5	58
BKCZF	5 mL	D0	66	67	65	58	60	57	15	62	4	59
BKCZF	1 mL	D0	65	67	64	57	62	55	15	62	5	58

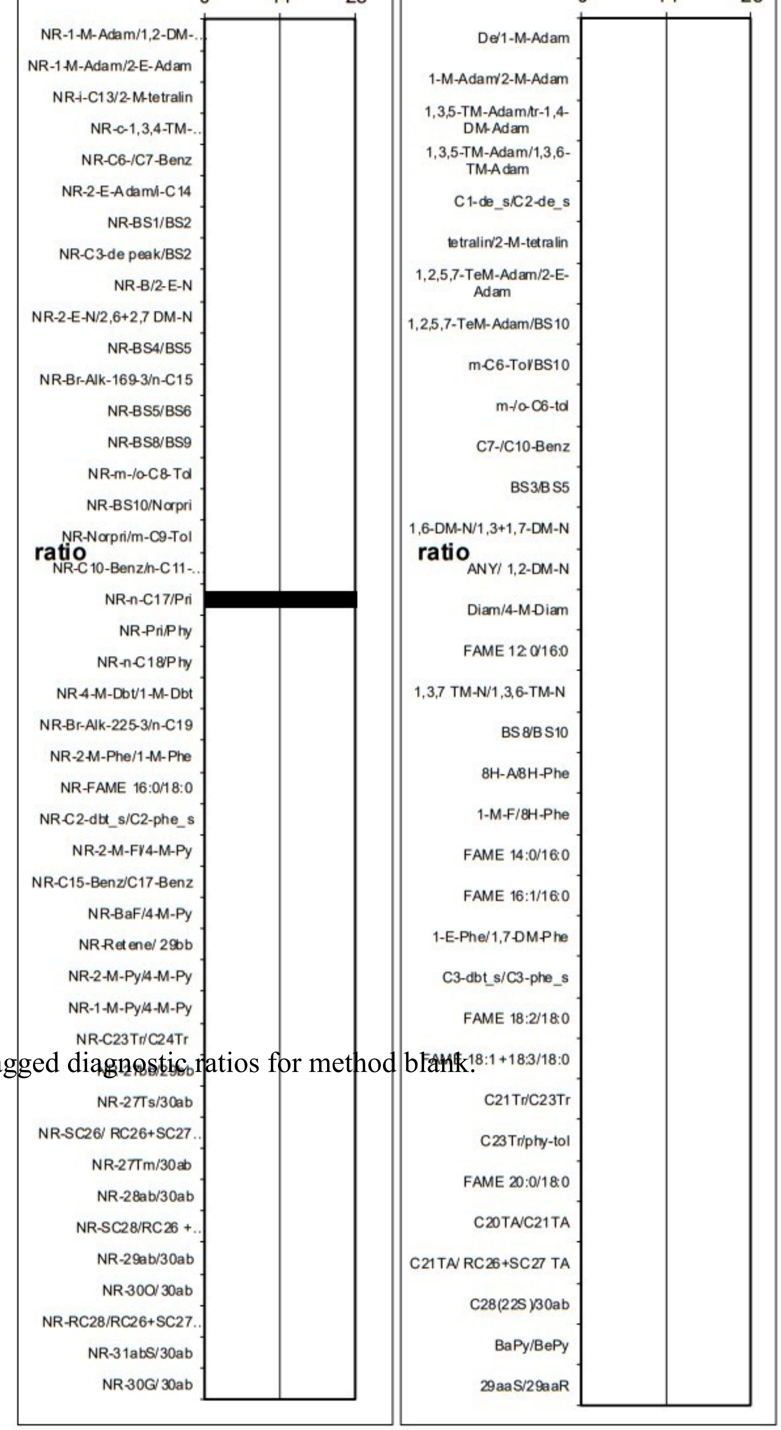


Figure S4: Visual summary of flagged diagnostic ratios for method blank.

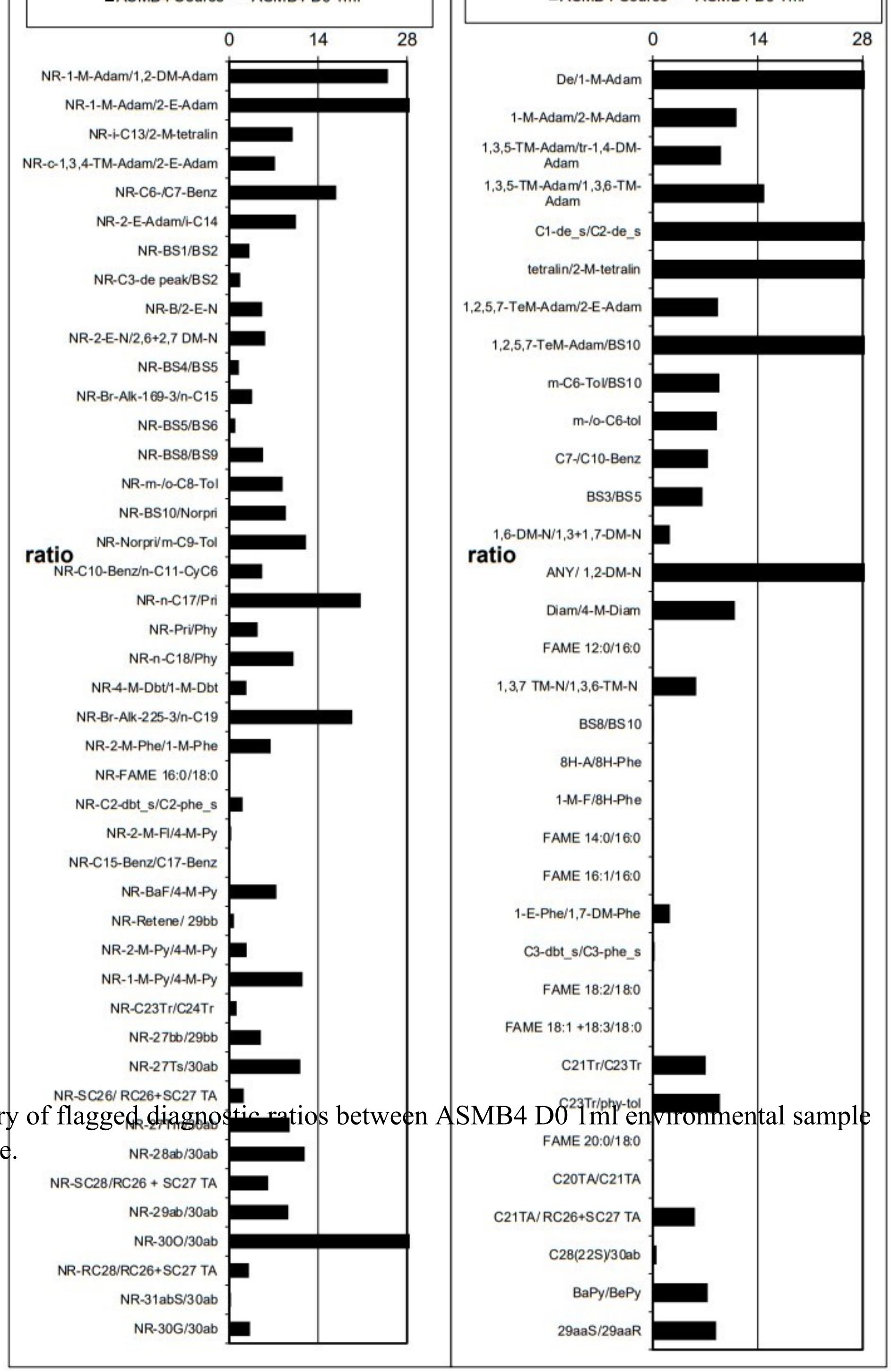
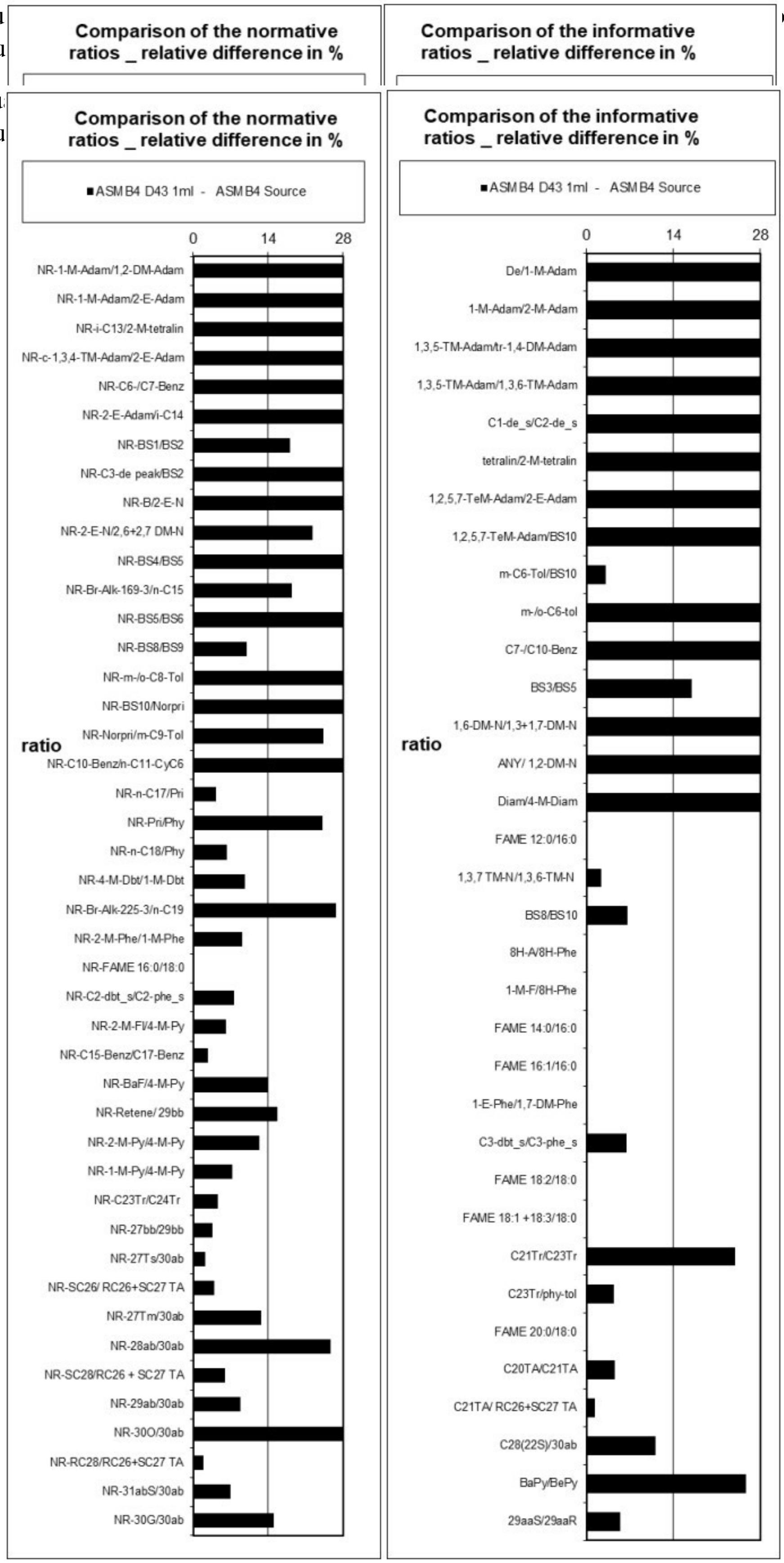


Figure S5: Visual summary of flagged diagnostic ratios between ASMB4 D0 1ml environmental sample and ASMB4 source sample.

Figure S6: Visu ... nmental sample and ASMB4 sou

Figure S7: Visu ... nmental sample and ASMB4 sou



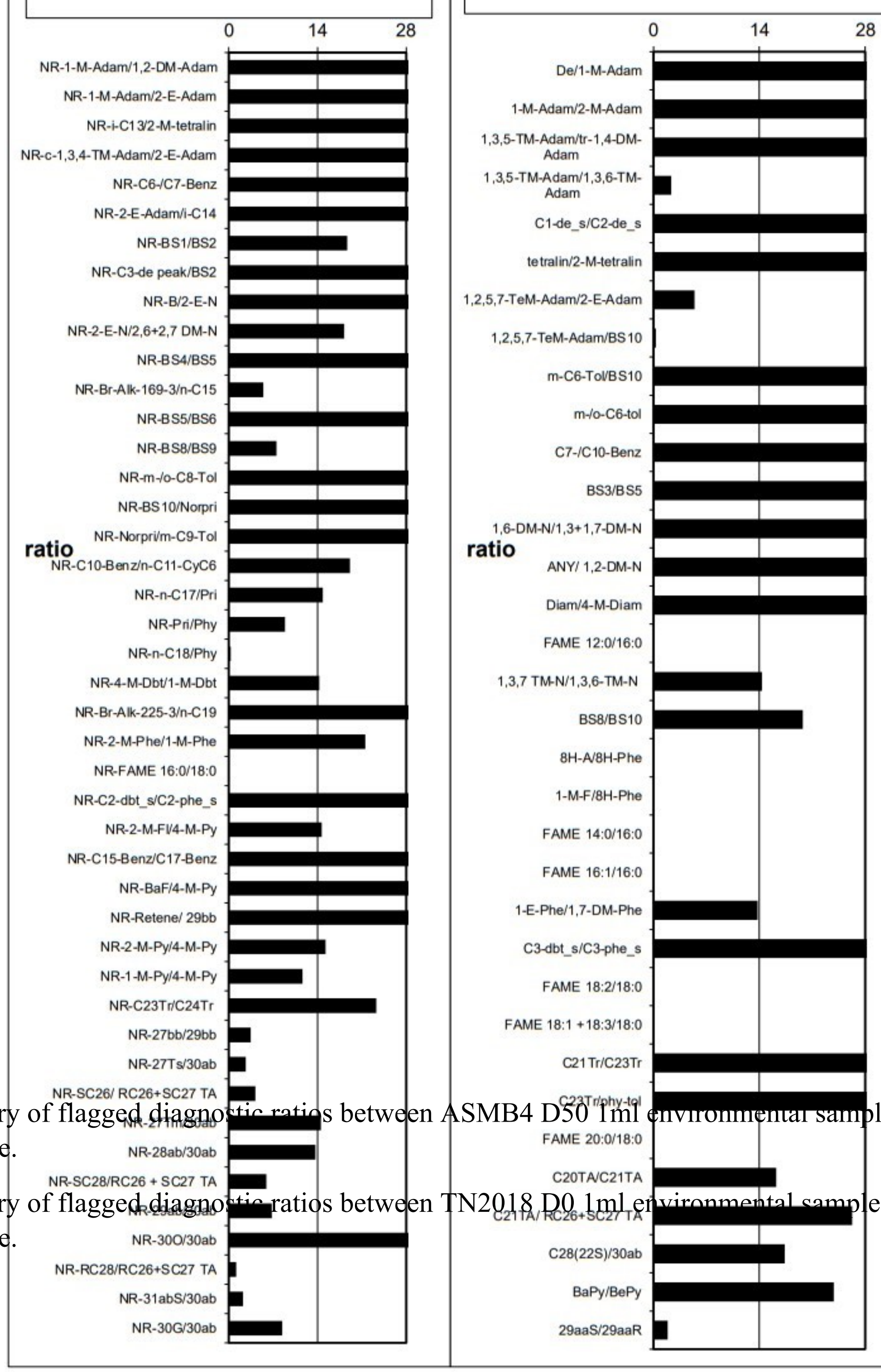


Figure S8: Visual summary of flagged diagnostic ratios between ASMB4 D50 1ml environmental sample and ASMB4 source sample.

Figure S9: Visual summary of flagged diagnostic ratios between TN2018 D0 1ml environmental sample and TN2018 source sample.

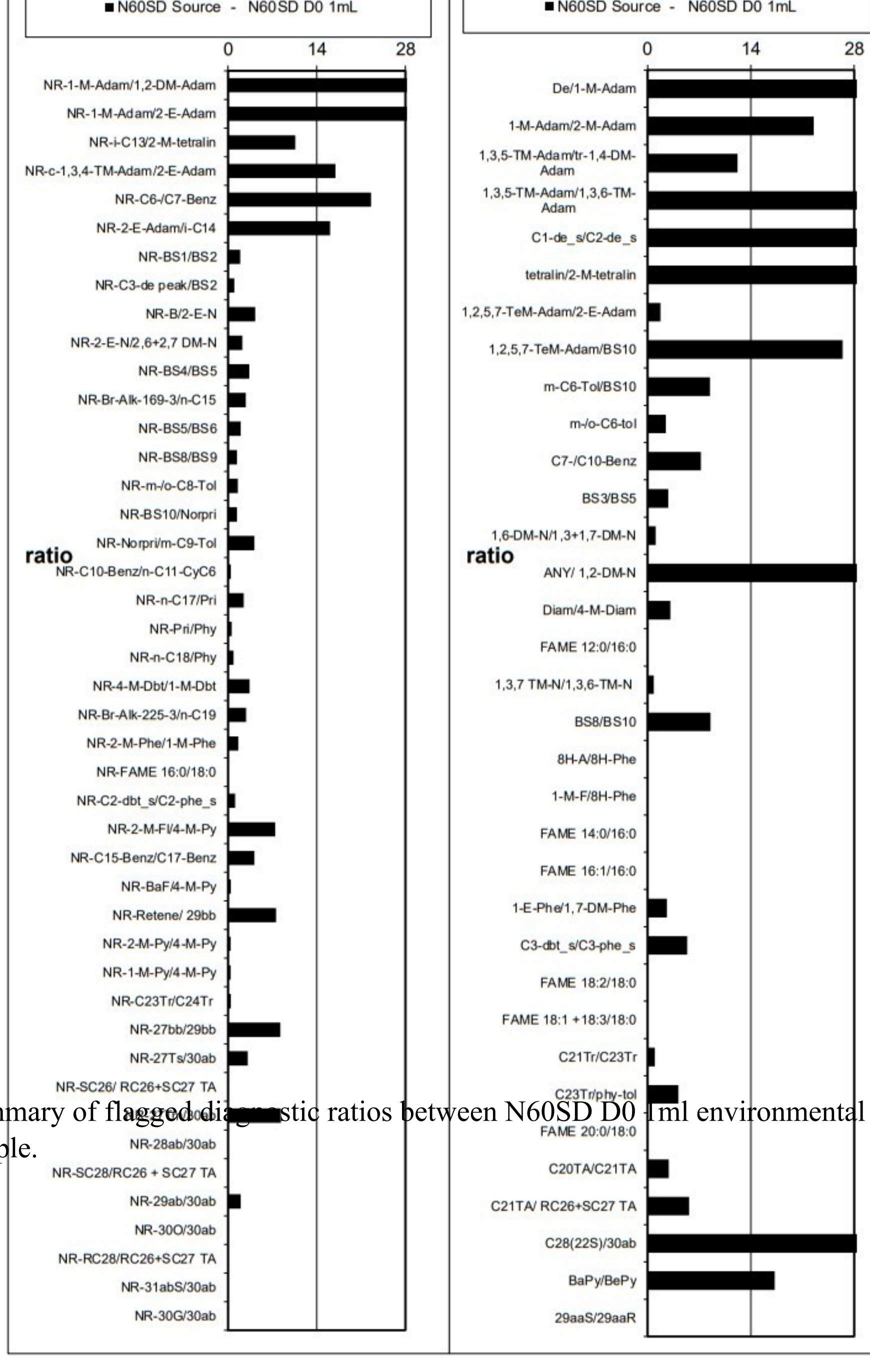


Figure S10: Visual summary of flagged diagnostic ratios between N60SD D0 1ml environmental sample and N60SD source sample.

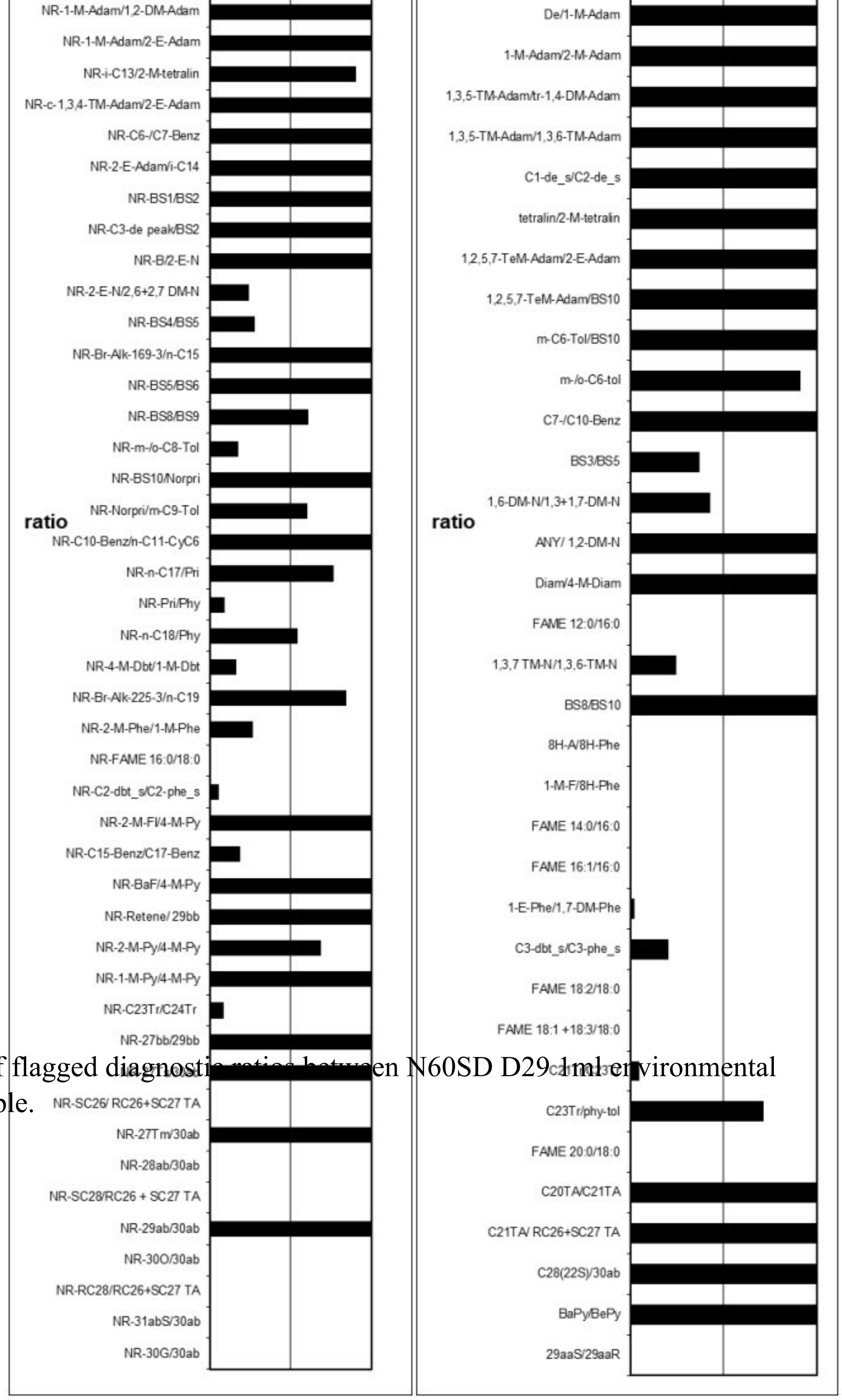


Figure S11: Visual summary of flagged diagnostic ratios between N60SD D29 1ml environmental sample and N60SD source sample.

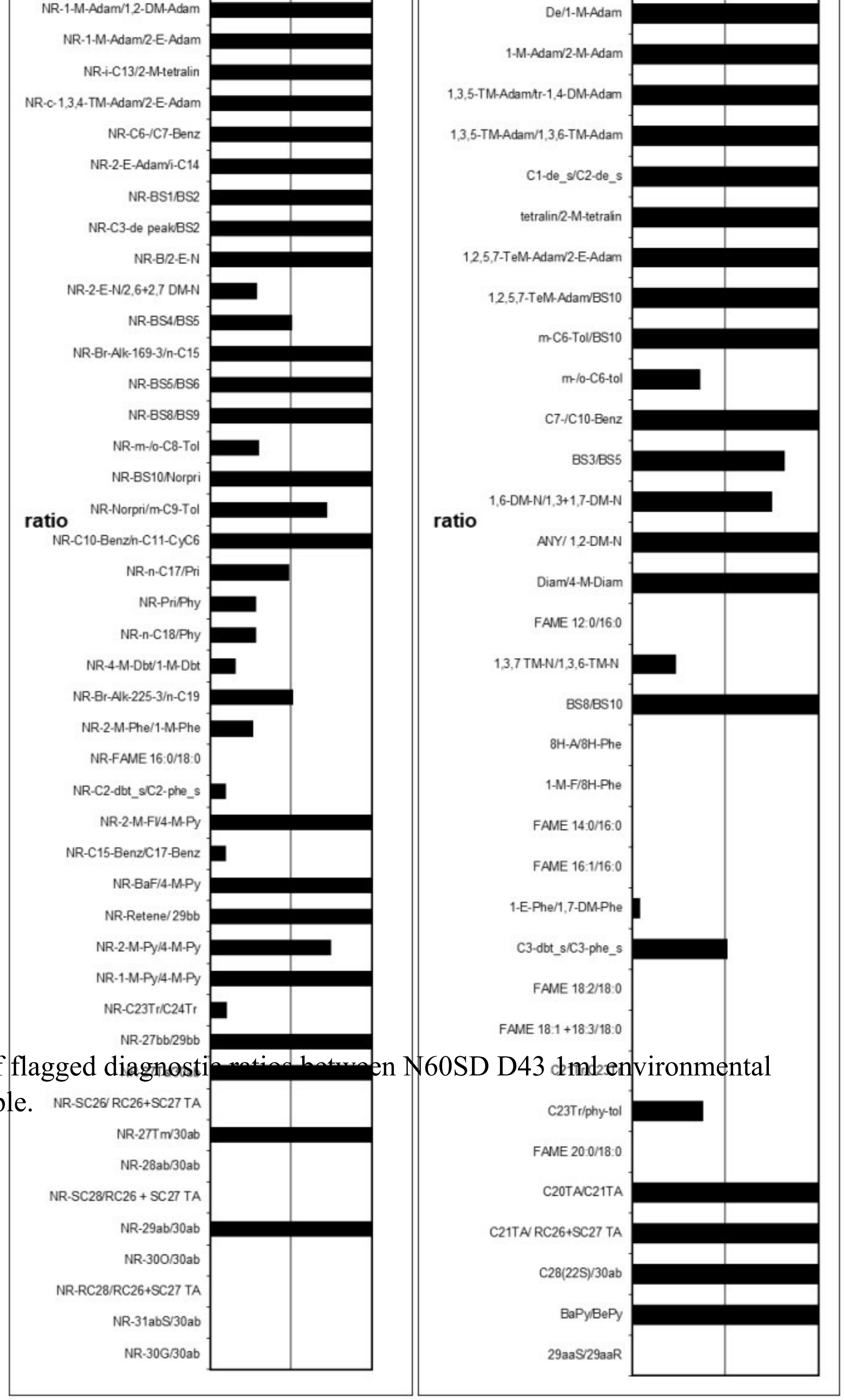


Figure S12: Visual summary of flagged diagnostic ratios between N60SD D43 1ml environmental sample and N60SD source sample.

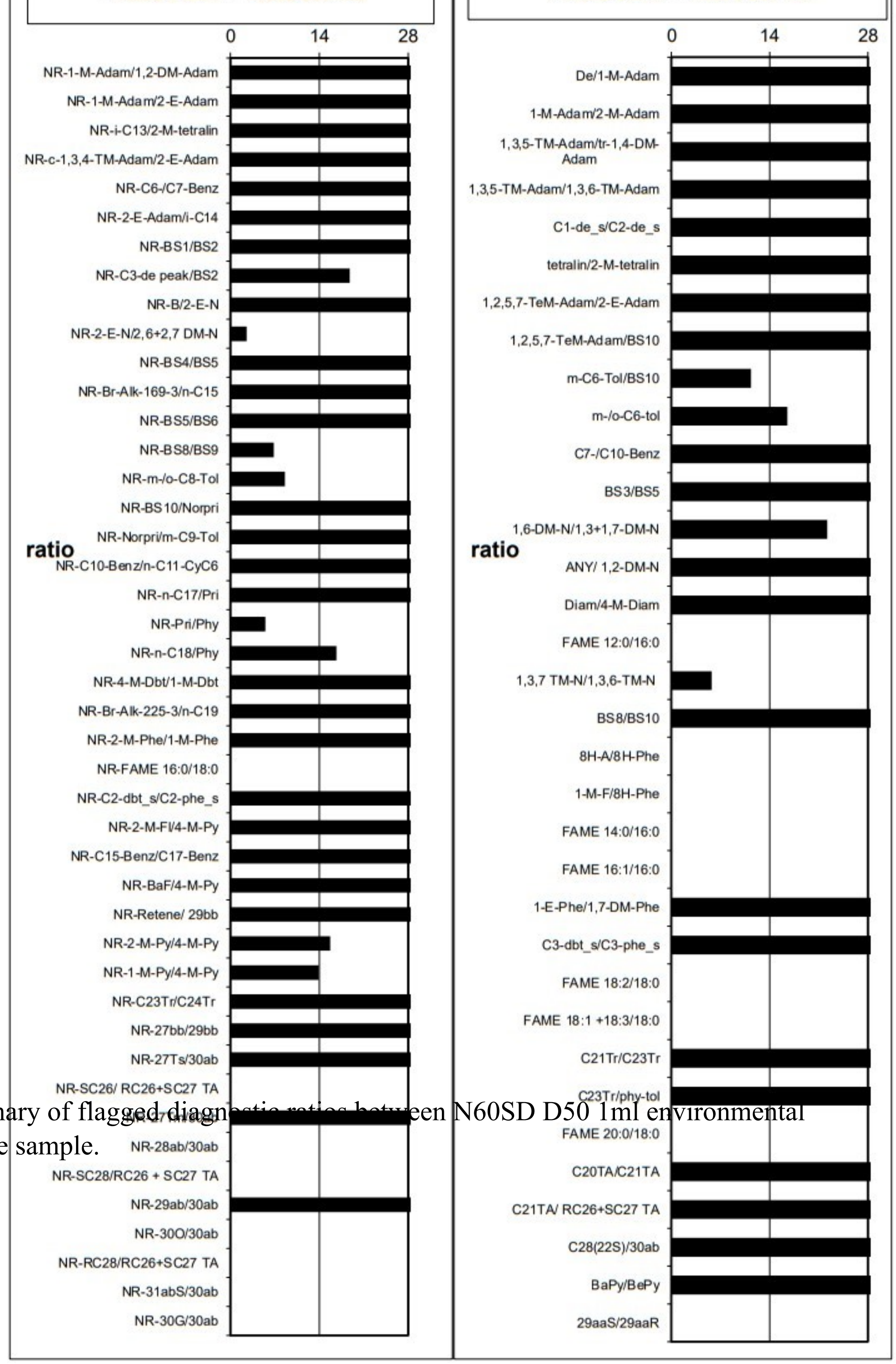


Figure S13: Visual summary of flagged diagnostic ratios between N60SD D50 1ml environmental sample and N60SD source sample.

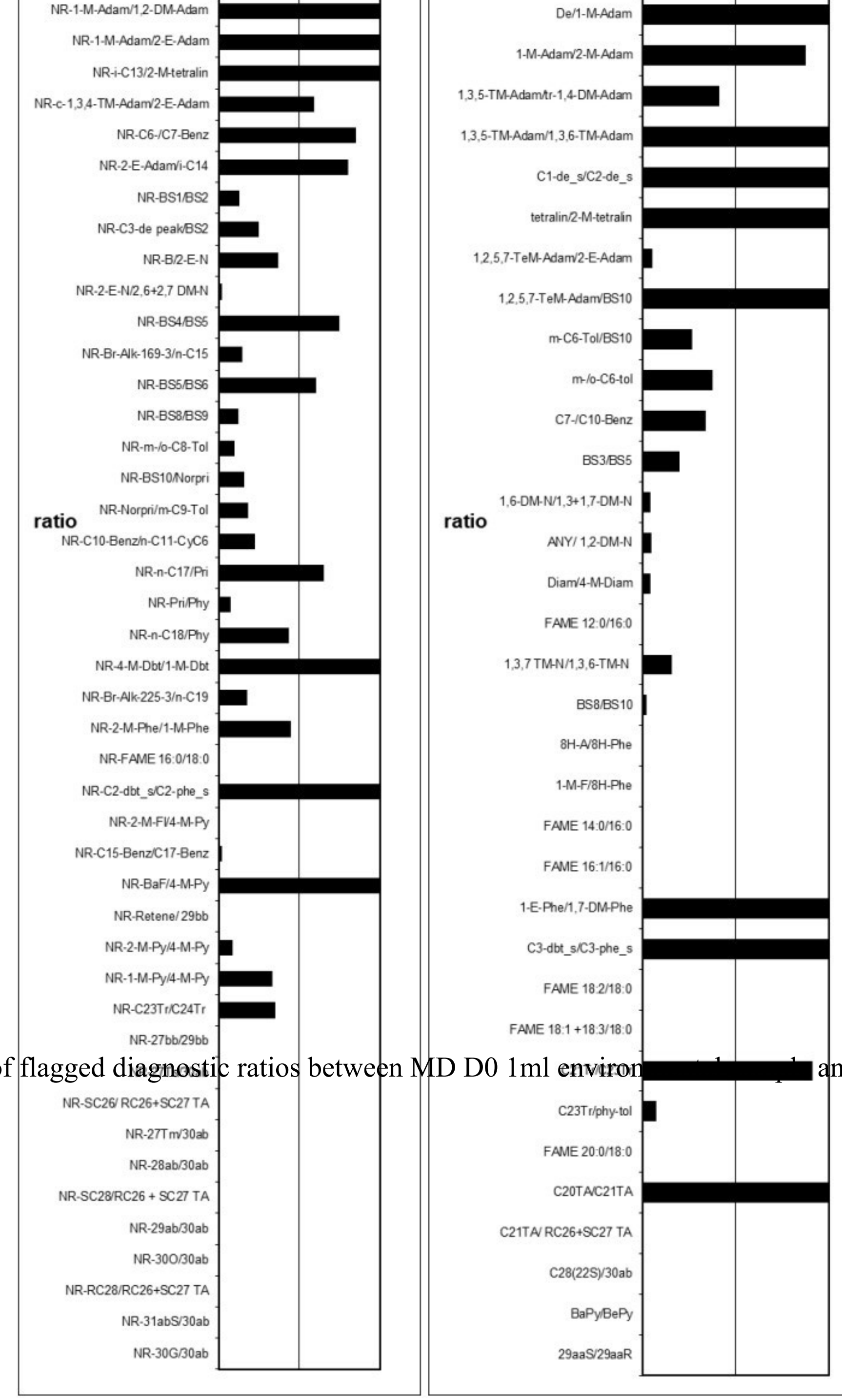


Figure S14: Visual summary of flagged diagnostic ratios between MD D0 1ml environmental sample and MD source sample.

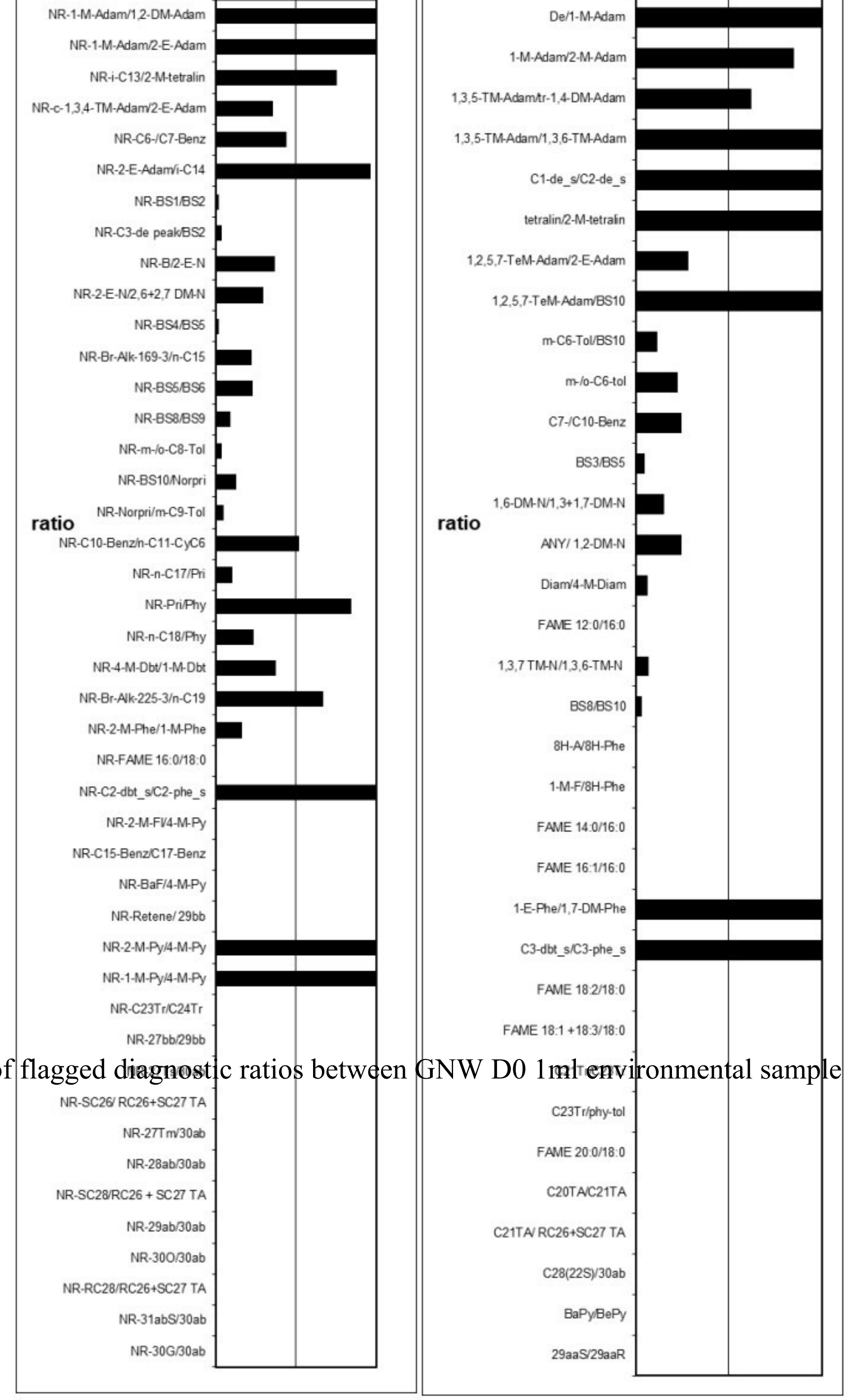


Figure S15: Visual summary of flagged diagnostic ratios between GNW D0 1ml environmental sample and GNW source sample.

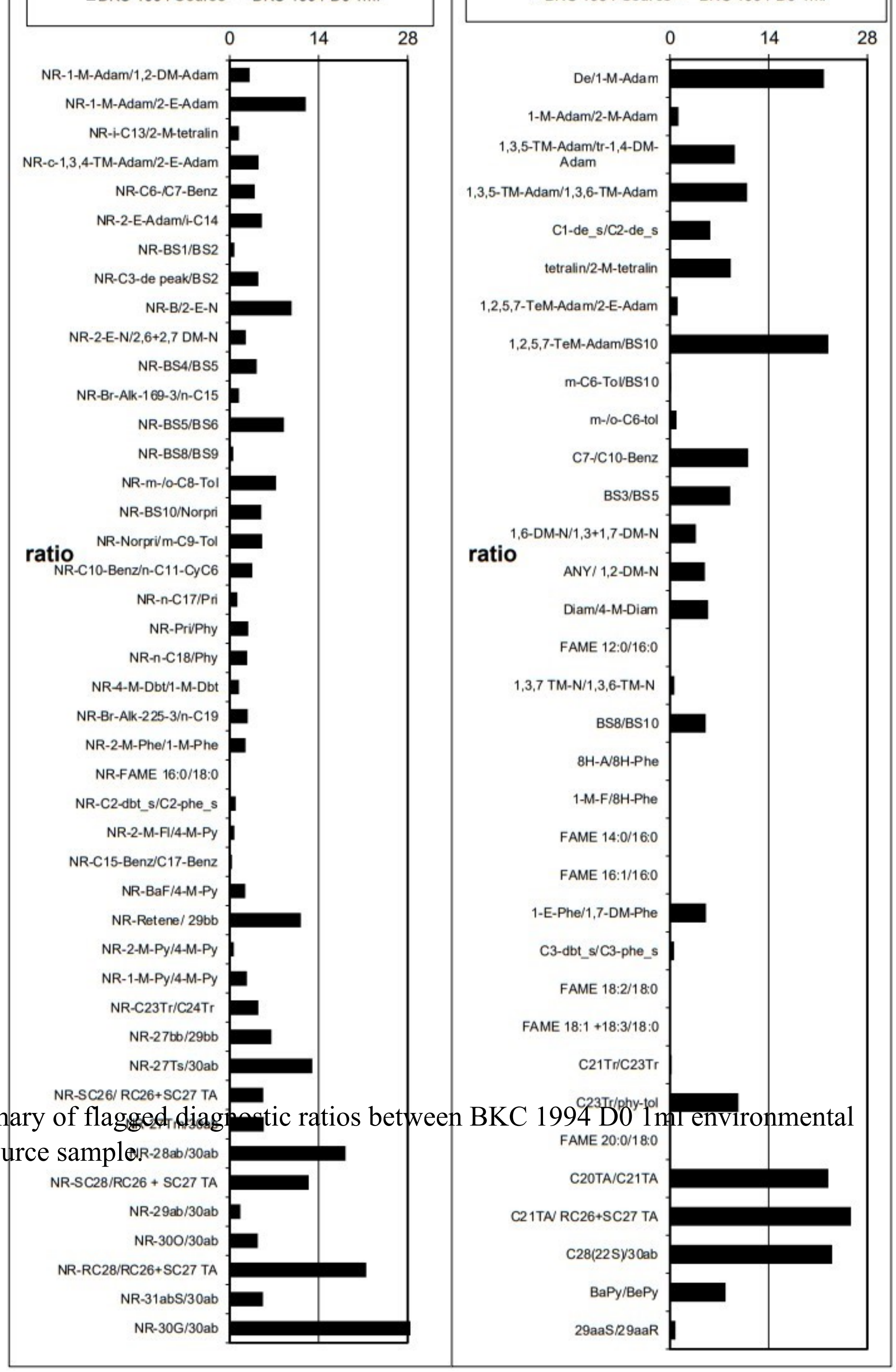


Figure S16: Visual summary of flagged diagnostic ratios between BKC 1994 D0 1ml environmental sample and BKC 1994 source sample.

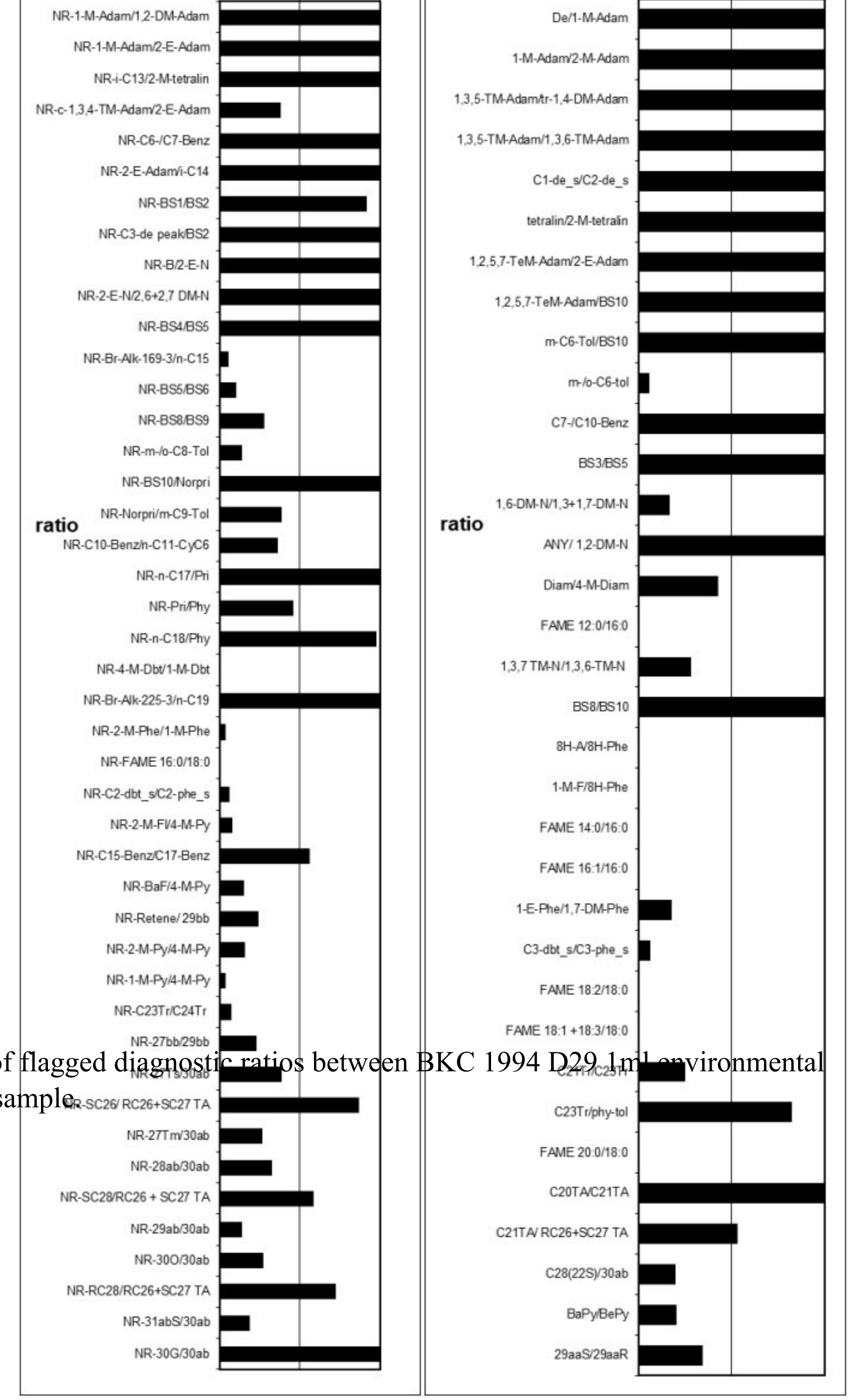


Figure S17: Visual summary of flagged diagnostic ratios between BKC 1994 D29 1ml environmental sample and BKC 1994 source sample.

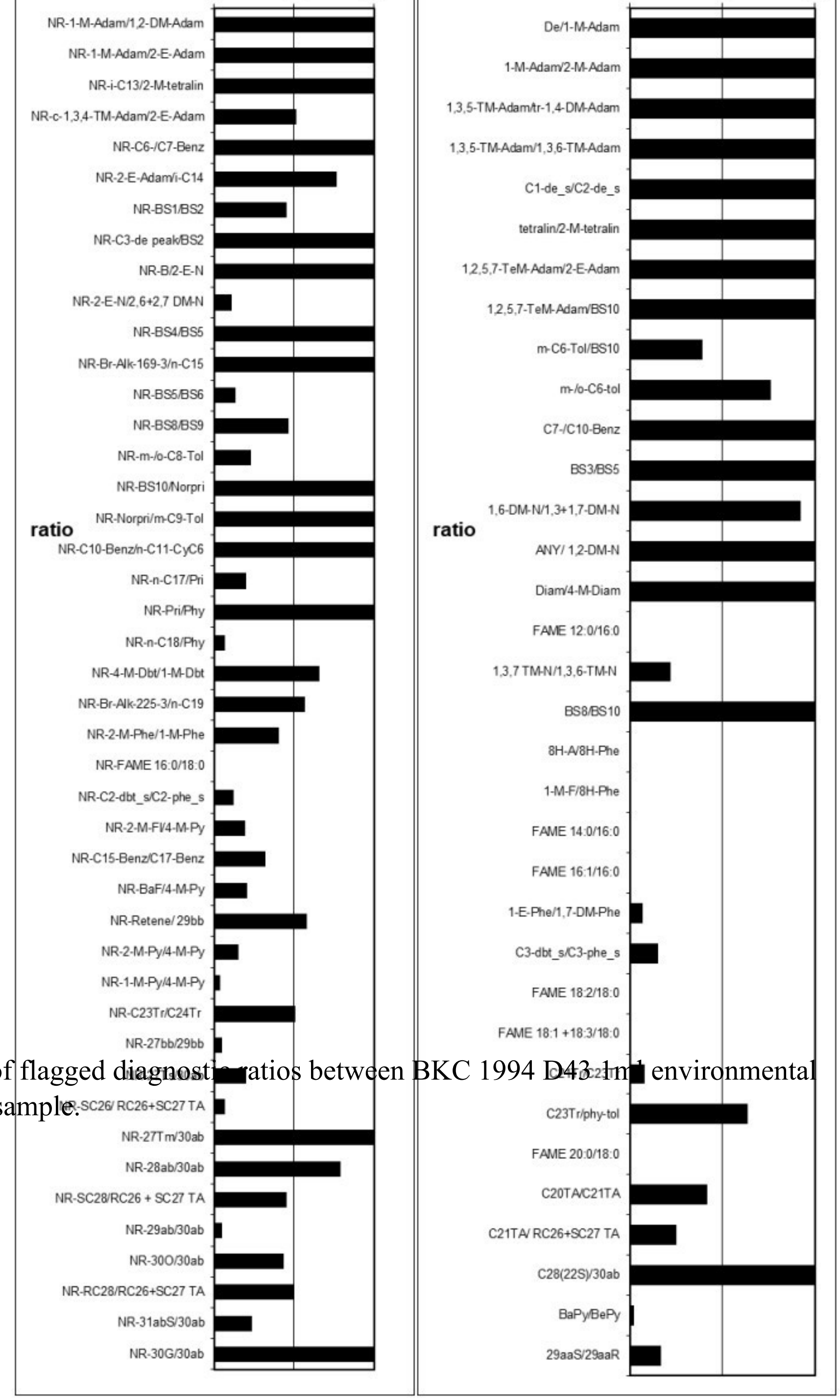


Figure S18: Visual summary of flagged diagnostic ratios between BKC 1994 D43-1ml environmental sample and BKC 1994 source sample.

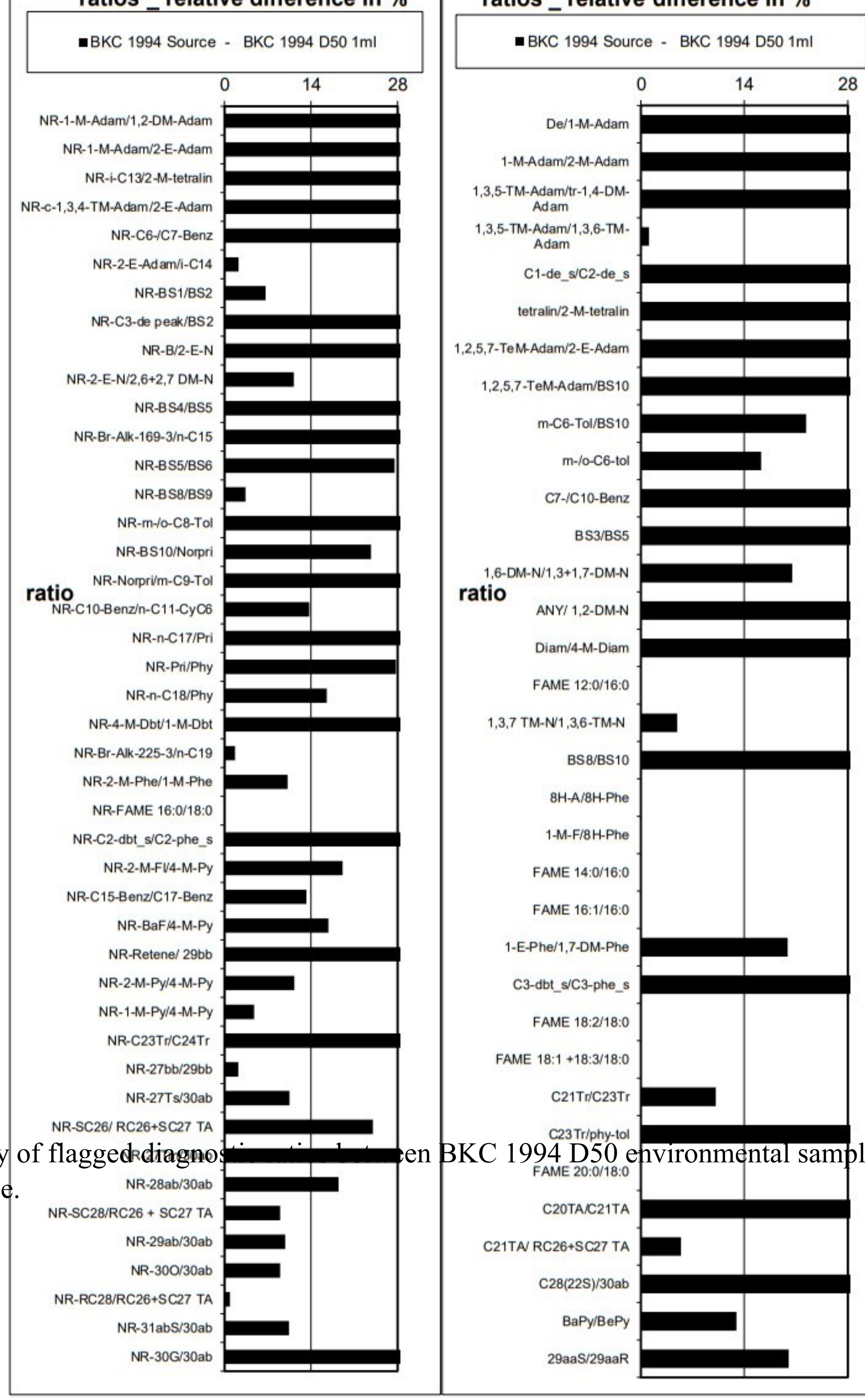


Figure S19: Visual summary of flagged diagnostic ratios between BKC 1994 D50 environmental sample and BKC 1994 source sample.

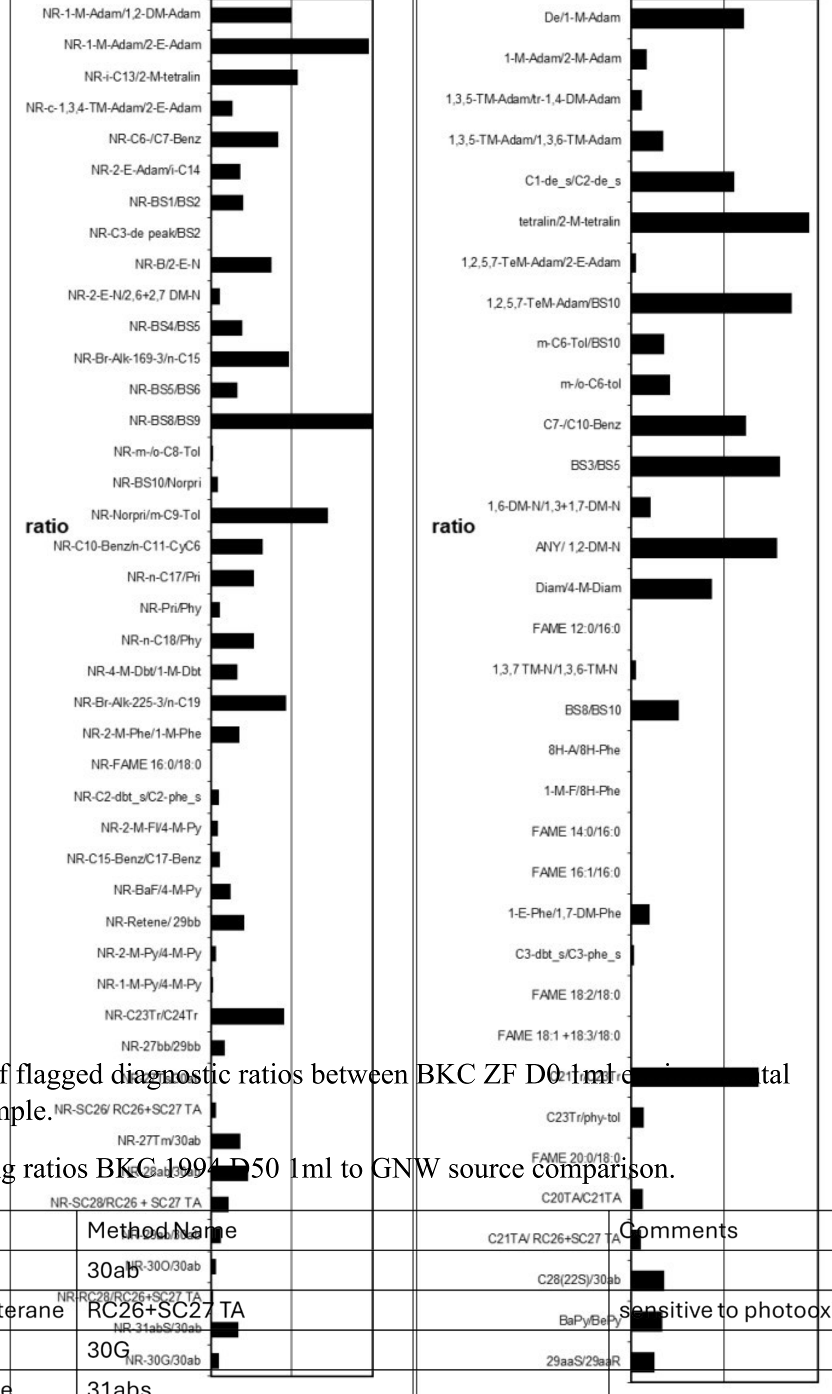


Figure S20: Visual summary of flagged diagnostic ratios between BKC ZF D0 1ml environmental sample and BKC ZF source sample.

Table S5: Biomarkers in missing ratios BKC 1994 D50 1ml to GNW source comparison.

Biomarker	Method Name	Comments
17α(H), 21β(H)-hopane	30ab	
C26,20R- + C27,20S-triaromatic sterane	RC26+SC27 TA	sensitive to photooxidation
gammacerane	30G	
17α(H), 21β(H), 22(S)-homohopane	31abs	
18α(H)-oleanane	30O	
18α(H)-22,29,30-trisnorneohopane	27Ts	
17α(H)-22,29,30-trisnorhopane	27Tm	
17α(H), 21β(H)-28,30-bisnorhopane	28ab	
17α(H), 21β(H)-30-norhopane	29ab	
17α(H), 21β(H), 22(S)-homohopane	31abS	
C28,20R-triaromatic sterane	RC28TA	sensitive to photooxidation
C28,20S-triaromatic sterane	SC28TA	sensitive to photooxidation
C26,20S-triaromatic sterane	SC26TA	sensitive to photooxidation
5α (H),14β(H),17β(H), 20(R+S)-cholestane.	27bbR+S	
29bbR+S	24-ethyl-5α(H),14β (H),17β(H), 20(R+S)-cholestane	

Table S6: SIM Ions m/z table

Ion Table									
Time Segment	1	2	3	4	5	6	7	8	9
Start Time	7.0	20.6	24.1	26.7	30.5	34.6	39.0	44.1	49.1
Dwell Time	50	20	15	18	14	14	16	20	20
Ions	83 85	83	74	74	74	74	74	85	
	85	85	83	83	83	83	83	92	92
	92	92	85	85	85	85	85	106	106
	104	104	92	92	92	92	92	177	177
	106	106	106	106	106	106	106	191	191
	113	113	113	113	113	192	191	205	205
	128	123	123	123	123	194	206	217	217
	134	128	128	152	170	198	212	218	218
	135	135	142	154	178	202	216	230	231
	138	142	152	156	180	206	219	231	242
	148	148	154	162	184	208	220	234	245
	149	152	156	166	186	212	226	242	252
	152	154	162	168	188	216	228	244	276
	163	156	168	170	192	219	230	245	278
	166	162	169	176	194	220	231	252	412
	177	166	170	180	198	226	234	256	
	180	169	176	184	206	234	242	276	
		177	179	186	208	290	244	412	
		179	187	187	212		256		
		180	188	188	225		290		
				193					

Table S7: List of biomarker ratios in the traditional CEN method included in the study.

Biomarker diagnostic ratios	Full compound names in ratio	Normative (N) or informative (I)	Included or excluded from study
NR-1-M-Adam/1,2-DM-Adam	1-methyl-adamantane/ 1,2-dimethyl-adamantane	N	Included
NR-1-M-Adam/2-E-Adam	1-methyl-adamantane/ 2-ethyl-adamantane	N	Included
NR-i-C13/2-M-tetralin	2,6-dimethylundecane/2-methyl-1,2,3,4-tetrahydronaphtalene	N	Included
NR-c-1,3,4-TM-Adam/2-E-Adam	cis-1,3,4-trimethyl-adamantane/2-ethyl-adamantane	N	Included
NR-C6-/C7-Benz	hexyl-benzene/heptyl-benzene	N	Included
NR-2-E-Adam/i-C14	2-ethyl-adamantane/2,6,10-trimethylundecane	N	Included
NR-BS1/BS2	bicyclic sesquiterpane 1/bicyclic sesquiterpane 2	N	Included
NR-C3-de peak/BS2	C3-decalin/ bicyclic sesquiterpane 2	N	Included
NR-B/2-E-N	biphenyl/2-ethyl-naphthalene	N	Included
NR-2-E-N/2,6+2,7 DM-N	2-ethyl-naphthalene/ 2,6+2,7-dimethyl-naphthalene	N	Included
NR-BS4/BS5	bicyclic sesquiterpane 4/bicyclic sesquiterpane 5	N	Included
NR-Br-alk-169-3/n-C15	Branched alkane m/z 169-3/ pentadecane	N	Included
NR-BS5/BS6	bicyclic sesquiterpane 5/bicyclic sesquiterpane 6	N	Included
NR-BS8/BS9	bicyclic sesquiterpane 8/bicyclic sesquiterpane 9	N	Included
NR-m-/o-C8-Tol	meta-octyl-toluene/ortho-octyl-toluene	N	Included
NR-BS10/Norpri	bicyclic sesquiterpane 10/ 2,6,10-trimethylpentadecane (Norpristan)	N	Included
NR-Norpri/m-C9-Tol	2,6,10-trimethylpentadecane (Norpristan)/ meta-nonyl-toluene	N	Included
NR-C10-Benz/n-C11-CyC6	decyl-benzene/ n-undecyl cyclohexane	N	Included
NR-n-C_{17}/Pri	heptadecane/2,6,10,14-tetramethylpentadecane (Pristane)	N	Included
NR-Pri/Phy	2,6,10,14-	N	Included

	tetramethylpentadecane (Pristane)/ 2,6,10,14 tetramethylhexadecane (Phystane)		
NR-n-C_{18}/Phy	octadecane/ 2,6,10,14 tetramethylhexadecane (Phystane)	N	Included
NR-4-M-Dbt/1-M-Dbt	4-methyl-dibenzothiophene/ 1-methyl-dibenzothiophene	N	Included
NR-Br-alk-225-3/n-C19	Branched alkane 225-3/ nonadecane	N	Included
NR-2-M-Phe/1-M-Phe	2-methyl-phenanthrene/ 1-methyl-phenanthrene	N	Included
NR-FAME 16:0/18:0	FAME 18.0/ FAME 16.0	N	Excluded
NR-C2-dbt_s/C2-phe_s	C2-dibenzothiophenes/ C2-phenanthrenes anthracenes	N	Included
NR-2-M-Fl/4-M-Py	2-methyl-fluoranthene/4-methyl-pyrene	N	Included
NR-C15-Benz/C17-Benz	pentadecyl-enzene/heptadecyl-benzene	N	Included
NR-BaF/4-M-Py	benzo(a)-fluorene/4-methyl-pyrene	N	Included
NR-Retene/ 29bb	1-methyl-7-isopropyl-phenantrene/24-ethyl-5α(H),14β (H),17β(H), 20(R+S)- cholestane	N	Included
NR-2-M-Py/4-M-Py	2-methyl-pyrene/4-methyl-pyrene	N	Included
NR-1-M-Py/4-M-Py	1-methyl-pyrene/4-methyl-pyrene	N	Included
NR-C23Tr/C24Tr	C23 tricyclic terpane/C24 tricyclic terpane	N	Included
NR-27bb/29bb	5α (H),14β(H),17β(H), 20(R+S)-cholestane /24-ethyl-5α(H),14β (H),17β(H), 20(R+S)-cholestane	N	Included
NR-27Ts/30ab	18α(H)-22,29,30-trisnorneohopane/17α(H), 21β(H)-hopane (hopane)	N	Included
NR-SC26/ RC26+SC27 TA	C26,20S-triaromatic sterane/ C26,20R- + C27,20S-triaromatic sterane	N	Included
NR-27Tm/30ab	17α(H)-22,29,30-trisnorhopane/17α(H), 21β(H)-hopane (hopane)	N	Included

NR-28ab/30ab	17α(H), 21β(H)-28,30-bisnorhopane/17α(H), 21β(H)-hopane (hopane)	N	Included
NR-SC28/RC26 + SC27 TA	C28,20S-triaromatic sterane/C26,20R- + C27,20S-triaromatic sterane	N	Included
NR-29ab/30ab	17α(H), 21β(H)-30-norhopane/17α(H), 21β(H)-hopane (hopane)	N	Included
NR-30O/30ab	18α(H)-oleanane/17α(H), 21β(H)-hopane (hopane)	N	Included
NR-RC28/RC26+SC27 TA	C28,20R-triaromatic sterane/C26,20R- + C27,20S-triaromatic sterane	N	Included
NR-31abS/30ab	17α(H), 21β(H), 22(S)-homohopane/17α(H), 21β(H)-hopane (hopane)	N	Included
NR-30G/30ab	gammacerane/17α(H), 21β(H)-hopane (hopane)	N	Included
De/1-M-Adam	Decalin/ 1-methyl-adamantane	I	Included
1-M-Adam/2-M-Adam	1-methyl-adamantane/2-methyl-adamantane	I	Included
1,3,5-TM-Adam/tr-1,4-DM-Adam	1,3,5-trimethyl adamantane/trans-1,4-dimethyl adamantane	I	Included
1,3,5-TM-Adam/1,3,6-TM-Adam	1,3,5-trimethyl adamantane/1,3,6-trimethyl adamantane	I	Included
C1-de_s/C2-de_s	C1-decalins/C2-decalins	I	Included
tetralin/2-M-tetralin	1,2,3,4 tetrahydronaphtalene/2-methyl-1,2,3,4-tetrahydronaphtalene	I	Included
1,2,5,7-TeM-Adam/2-E-Adam	1,2,5,7-tetramethyl-adamantane/2-ethyl-adamantane	I	Included
1,2,5,7-TeM-Adam/BS10	1,2,5,7-tetramethyl-adamantane/bicyclic sesquiterpane 10	I	Included
m-C6-Tol/BS10	meta-hexyl-toluene/ bicyclic sesquiterpane 10	I	Included
m-/o-C6-tol	meta-octyl-toluene/ortho-octyl-toluene	I	Included
C7-/C10-Benz	heptyl-benzene/decyl-benzene	I	Included
BS3/BS5	bicyclic sesquiterpane 3/bicyclic sesquiterpane 5	I	Included

1,6-DM-N/1,3+1,7-DM-N	1,6-dimethyl-naphthalene/1,3+1,7-dimethyl-naphthalene	I	Included
ANY/ 1,2-DM-N	acenaphthylene	I	Included
Diam/4-M-Diam	diamantane/4-methyl-diamantane	I	Included
FAME 12:0/16:0	FAME 12.0/ FAME 16.0	I	Excluded
1,3,7 TM-N/1,3,6-TM-N	1,3,7-trimethyl-naphthalene/1,3,6-trimethyl-naphthalene	I	Included
BS8/BS10	bicyclic sesquiterpane 8/bicyclic sesquiterpane 10	I	Included
8H-A/8H-Phe	1,2,3,4,5,6,7,8-octahydroanthracene /1,2,3,4,5,6,7,8-octahydrophenanthrene	I	Included
1-M-F/8H-Phe	1-methyl-fluorene /1,2,3,4,5,6,7,8-octahydrophenanthrene	I	Included
FAME 14:0/16:0	FAME 14.0/ FAME 16.0	I	Excluded
FAME 16:1/16:0	FAME 16.1/ FAME 16.0	I	Excluded
1-E-Phe/1,7-DM-Phe	1-ethyl-phenanthrene/ 1,7-dimethyl-phenanthrene	I	Included
C3-dbt_s/C3-phe_s	C3-dibenzothiophenes/C3-phenanthrenes anthracenes	I	Included
FAME 18:2/18:0	FAME 18.2/ FAME 18.0	I	Excluded
FAME 18:1 +18:3/18:0	FAME 18.0/ FAME 16.0	I	Excluded
C21Tr/C23Tr	C21 tricyclic terpane/C23 tricyclic terpane	I	Included
C23Tr/phy-tol	C23 tricyclic terpane/phytanyl-toluene (1-methyl-3-phytanylbenzene)	I	Included
FAME 20:0/18:0	FAME 20.0/ FAME 18.0	I	Excluded
C20TA/C21TA	C20-triaromatic sterane/C21-triaromatic sterane	I	Included
C21TA/ RC26+SC27 TA	/C26,20R- + C27,20S-triaromatic sterane	I	Included
C28(22S)/30ab	C28 tricyclic terpane/17α(H), 21β(H)-hopane (hopane)	I	Included
BaPy/BePy	benzo (a) pyrene /benzo (e) pyrene	I	Included
29aaS/29aaR	24-ethyl-5α(H),14α(H),17α(H),	I	Included

	20S- cholestane/ 24-ethyl-5α(H),14α(H),17α(H), 20R- cholestane		

NR=Normative ratio