

1 SUPPLEMENTAL INFORMATION

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3 DYNAMIC MULTIPLE REACTION MONITORING FOR HIGH THROUGHPUT
4 DETECTION AND QUANTITATION OF POLYCYCLIC AROMATIC COMPOUNDS

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23 **Table S11.** Concentration of calibration solutions for each analyte classes used in our study.

Analyte	Concentration (pg μL^{-1})		
	Low	Medium	High
PAHs	10.00	200.00	1000.00
APAHs	2.00	100.00	500.00
HPAHs	10.00	200.00	1000.00
HPACs	10.00	100.00	800.00
HHPACs	10.00	100.00	800.00

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25 **Table SI2.** Mass spectrometric properties of dMRM method.

Analyte	Quantitation Transition	Collision Energy (eV)	Delta Retention Time Window (min)	
			Left	Right
<u>PAHs</u>				
Nap	127.9→102.0	45	0.10	0.10
Ace	151.9→150.0	45	0.10	0.10
Acy	152.9→152.0	35	0.10	0.10
Fle	164.9→163.0	45	0.10	0.10
Phe	177.9→152.0	40	0.10	0.10
Ant	177.9→152.0	40	0.10	0.10
Flu	201.9→200.1	40	0.10	0.10
Pyr	201.9→200.1	40	0.10	0.10
BaA	227.9→226.1	40	0.10	0.10
Chr	227.9→226.1	40	0.10	0.10
BbF	251.9→250.1	35	0.10	0.10
BkF	251.9→250.1	35	0.10	0.10
BaP	251.9→250.1	40	0.10	0.10
Ind	275.9→275.9 ^a	15	0.10	0.10
DahA	277.9→277.9 ^a	15	0.10	0.10
BghiP	275.9→275.9 ^a	15	0.10	0.10
<u>APAHs</u>				
2-Methyl-Nap	141.8→141.1	15	0.20	0.20
1-Methyl-Nap	141.8→141.1	15	0.20	0.20
1,4-Dimethyl-Nap	155.8→141.1	15	0.40	0.33
2,3,5-Trimethyl-Nap	169.8→155.1; 169.8→141.1	15	0.75	0.44

1,4,6,7-Tetramethyl-Nap	183.8→169.1; 183.8→155.1; 183.8→141.1	15	0.67	1.00
1-Methyl-Phe	191.8→191.1	15	0.10	0.10
2-Methyl-Phe	191.8→191.1	15	0.10	0.10
3-Methyl-Phe	191.8→191.1	15	0.10	0.10
9-Methyl-Phe	191.8→191.1	15	0.10	0.10
1,7-Dimethyl-Phe	205.8→191.1	15	0.10	0.10
1,8-Dimethyl-Phe	205.8→191.1	15	0.10	0.10
2,6-Dimethyl-Phe	205.8→191.1	15	0.10	0.10
3,6-Dimethyl-Phe	205.8→191.1	15	0.10	0.10
1,3-Dimethyl-Phe	205.8→191.1	15	0.10	0.10
5-Methyl-Chr	241.8→239.1	15	0.70	0.87
6-Ethyl-Chr	255.8→241.1	15	0.50	2.45
6-n-Propyl-Chr	269.8→255.1; 269.8→241.1	15	0.75	2.92
1,2,6-Trimethyl-Phe	221.8→205.1; 221.8→191.1	15	1.80	0.10
Retene	219.0→204.1	15	0.10	0.10
1,2,6,9-Tetramethyl-Phe	233.8→219.1; 233.8→205.1; 233.8→191.1	15	1.22	1.92
1-Methyl-Fle	179.8→165.1	25	0.50	0.03
9-Ethyl-Fle	193.8→179.1	25	1.06	0.88
9-n-Propyl-Fle	207.8→193.1; 207.8→179.1	25	0.18	2.15
9-n-Butyl-Fle	222.1→193.1; 222.1→179.1; 222.1→165.1	15	0.10	2.50
1-Methyl-Pyr	215.8→215.1	15	1.17	0.46
1-Ethyl-Pyr	229.8→215.1	15	0.76	1.75
1-n-Propyl-Pyr	243.8→229.1; 243.8→215.1	15	0.36	2.53
1-n-Butyl-Pyr	257.8→243.1; 257.8→229.2; 257.8→215.1	15	0.12	2.97
6-Methyl-BaP	265.8→263.1	35	4.60	0.55

7,10-Dimethyl-BaP	279.8→265.1	35	3.43	0.46
<u>HPAHs</u>				
9-Cl-Fle	165.0→165.0 ^a	5	0.50	0.50
2-Cl-Fle	165.0→165.0 ^a	5	0.50	0.50
5-Br-Ana	234.1→153.1	25	0.10	0.10
9-Br-Fle	165.0→165.0 ^a	5	0.50	0.50
2-Br-Fle	165.0→165.0 ^a	5	0.50	0.50
1-Cl-Ant	212.0→176.0	25	0.50	0.50
2,7-Cl ₂ -Fle	234.0→199.1	15	0.10	0.10
1,2-Br ₂ -Any	310.0→149.9	25	0.10	0.10
3-Br-Phe	256.0→177.1	15	0.50	0.50
1-Br-Ant	256.0→177.1	15	0.50	0.50
1,4-Cl ₂ -Ant	246.0→176.1	25	0.50	0.50
5,6-Br ₂ -Ana	312.1→152.1	15	0.10	0.10
2,7-Br ₂ -Fle	324.0→243.0	15	0.10	0.10
3-Br-Flu	279.9→200.1	25	1.00	1.50
9,10-Br ₂ -Ant	335.9→176.0	25	0.75	0.75
4-Br-Pyr	279.9→200.1	25	1.00	1.50
9-Br-1,5-Cl ₂ -Ant	326.0→209.9	15	0.10	0.10
1,5,9,10-Cl ₄ -Ant	316.0→316.0 ^a	25	0.50	0.50
1,6-Br ₂ -Pyr	360.1→200.0	25	0.50	0.50
4-Br-BaA	308.0→225.9	25	0.50	0.50
2,3,9,10-Br ₄ -Ant	494.1→494.1 ^a	15	0.10	0.10
<u>HHPACs</u>				

Quinoline	129.1→102.0	25	0.10	0.10
Isoquinoline	129.1→102.1	25	0.10	0.10
Indole	117.1→89.0	35	0.10	0.10
2-Methylquinoline	143.0→115.0	25	0.10	0.10
4-Methylbenzothiophene	146.9→120.9	25	0.10	0.10
3-Methylisoquinoline	143.0→115.0	40	0.10	0.10
2,3-Dimethylbenzothiophene	147.0→103.0	25	0.10	0.10
2,5-Dimethyl-1-phenylpyrrole	171.0→170.0	15	0.10	0.10
4-Phenylpyridine	155.0→154.0	15	0.10	0.10
2,3-Dimethylindole	143.9→77.0	35	0.10	0.10
Dibenzofuran	168.0→139.0	25	0.10	0.10
2,3,4-Trimethylbenzothiophene	176.0→161.0	15	0.10	0.10
2-Methyldibenzofuran	181.0→152.0	35	0.10	0.10
Benzo[<i>h</i>]quinoline	179.0→178.0	25	0.10	0.10
1,2,3,4-Tetrahydrocarbazole	143.0→128.3	25	0.10	0.10
Acridine	179.1→178.0	25	0.10	0.10
9-Methylcarbazole	181.1→180.1	25	0.10	0.10
Carbazole	167.1→166.1	25	0.10	0.10
3-Methylbenzo[<i>f</i>]quinoline	193.0→165.0	35	0.10	0.10
2-Methylacridine	193.0→192.0	25	0.10	0.10
3,6-Dimethylcarbazole	180.1→179.0	25	0.10	0.10
Benzo[<i>b</i>]naphtho[2,3- <i>d</i>]furan	188.8→187.0	35	0.10	0.10
3-Tert-butyl-9H-carbazole	208.1→180.0	15	0.10	0.10
9-Phenylcarbazole	243.0→241.0	35	0.10	0.10
7,8,9,10-Tetrahydro-benzo[<i>b</i>]naphtho[2,3- <i>d</i>]thiophene	209.8→208.0	25	0.10	0.10
Benz[<i>c</i>]acridine	229.0→228.0	25	0.10	0.10
11H-Benzo[<i>a</i>]carbazole	217.1→216.0	30	0.10	0.10
7H-Benzo[<i>c</i>]carbazole	217.1→216.0	25	0.10	0.10

6-Methylbenzo[<i>b</i>]naphtho[2,1- <i>d</i>]thiophene	247.8→247.0	25	0.10	0.10
2-Phenyldibenzothiophene	259.7→257.0	40	0.10	0.10
Dinaphtho[1,2- <i>b</i> ;1',2'- <i>d</i>]furan	267.8→239.0	35	0.10	0.10
Dibenz[<i>c,h</i>]acridine	279.0→278.0	35	0.10	0.10
13(H)-Dibenzo[<i>a,i</i>]carbazole	267.0→266.0	35	0.10	0.10
Dibenzothiophene	183.8→139.1	45	0.10	0.10
2-Methyldibenzothiophene	197.8→197.1	15	0.10	0.42
1,2-Dimethyldibenzothiophene	211.8→197.1	15	1.06	0.16
4- <i>n</i> -Propyldibenzothiophene	225.8→211.1; 225.8→197.1	15	1.35	0.73
4,6-Diethyldibenzothiophene	239.8→225.1; 239.8→211.1; 239.8→197.1	15	0.23	2.92
Benzo[<i>b</i>]naphtho[1,2- <i>d</i>]thiophene	234.0→202.0	35	0.10	0.10
Benzo[<i>b</i>]naphtho[2,3- <i>d</i>]thiophene	234.0→202.0	35	0.10	0.10
<u>HHPACs</u>				
2,3-Br ₂ -thiophene	241.8→161.0	15	0.10	0.10
2-Cl-quinoline	162.9→128.0	15	0.10	0.10
2-Br-benzothiophene	213.8→133.0	25	0.10	0.10
2,3-Cl ₂ -benzothiophene	201.8→166.9	15	0.10	0.10
2-Br-quinoline	127.9→101.0	15	0.10	0.10
5-Cl-indole	150.9→89.0	15	0.10	0.10
3-Br-isoquinoline	127.9→101.0	15	0.10	0.10
5-Br-indole	116.0→89.0	15	0.10	0.10
2,3-Br ₂ -benzothiophene	131.9→92.9	25	0.10	0.10
9-Cl-acridine	212.9→178.0	15	0.10	0.10
2-Br-dibenzothiophene	263.7→183.0	25	0.10	0.10
9-Br-acridine	177.9→151.1	15	0.10	0.10

3,6-Cl ₂ -9H-carbazole	234.8→200.0	25	0.10	0.10
2,8-Br ₂ -dibenzothiophene	181.8→138.0	15	0.10	0.10
3,6-Br ₂ -carbazole	324.8→243.9	15	0.10	0.10

26 ^apseudo-transition

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28 **Table SI3.** Some mass spectrometric properties for the developed dMRM and previously reported MRM method.^{1-4, a}

Compounds	dMRM					MRM				
	Dwell time (ms) ^b	Cycle time (ms/cycle) ^e	Duty cycle (%)	# of measurements of ion transitions (n) ^c	(n) ^{1/2 d}	Dwell time (ms)	Cycle time (ms/cycle)	Duty cycle (%)	# of measurements of ion transitions (n)	(n) ^{1/2 d}
<u>PAHs</u>										
Nap	64.0	333.3	19.2	18.0	4.2	45	229.3	19.6	26.2	5.1
Ace	26.4	333.3	7.9	18.0	4.2	30	354.1	8.5	16.9	4.1
Acy	27.6	333.3	8.3	18.0	4.2	45	229.3	19.6	26.2	5.1
Fle	26.1	333.3	7.8	18.0	4.2	30	354.1	8.5	16.9	4.1
Phe	19.9	333.3	6.0	18.0	4.2	45	320.8	14.0	18.7	4.3
Ant	19.9	333.3	6.0	18.0	4.2	45	320.8	14.0	18.7	4.3
Flu	19.4	333.3	5.8	18.0	4.2	40	326.8	12.2	18.4	4.3
Pyr	19.4	333.3	5.8	18.0	4.2	40	326.8	12.2	18.4	4.3
BaA	22.0	333.3	6.6	18.0	4.2	30	339.1	8.8	17.7	4.2
Chr	22.0	333.3	6.6	18.0	4.2	30	339.1	8.8	17.7	4.2
BbF	22.6	333.3	6.8	18.0	4.2	30	339.3	8.8	17.7	4.2
BkF	22.6	333.3	6.8	18.0	4.2	30	339.3	8.8	17.7	4.2
BaP	30.7	333.3	9.2	18.0	4.2	30	339.3	8.8	17.7	4.2
Ind	36.3	333.3	10.9	18.0	4.2	30	247.4	12.1	24.3	4.9
DahA	35.6	333.3	10.7	18.0	4.2	30	247.4	12.1	24.3	4.9
BghiP	73.3	333.3	22.0	18.0	4.2	50	204.0	24.5	29.4	5.4
<u>APAHs</u>										
2-Methyl-Nap	53.2	333.3	16.0	18.0	4.2	45	229.3	19.6	26.2	5.1
1-Methyl-Nap	53.2	333.3	16.0	18.0	4.2	45	229.3	19.6	26.2	5.1

1,4-Dimethyl-Nap	35.4	333.3	10.6	18.0	4.2	45	229.3	19.6	26.2	5.1
2,3,5-Trimethyl-Nap	32.0	333.3	9.6	18.0	4.2	30	354.1	8.5	16.9	4.1
1,4,6,7-Tetramethyl-Nap	28.0	333.3	8.4	18.0	4.2	45	320.8	14.0	18.7	4.3
1-Methyl-Phe	27.9	333.3	8.4	18.0	4.2	300	301.2	99.6	19.9	4.5
2-Methyl-Phe	27.9	333.3	8.4	18.0	4.2	300	301.2	99.6	19.9	4.5
3-Methyl-Phe	27.9	333.3	8.4	18.0	4.2	300	301.2	99.6	19.9	4.5
9-Methyl-Phe	27.9	333.3	8.4	18.0	4.2	300	301.2	99.6	19.9	4.5
1,7-Dimethyl-Phe	18.7	333.3	5.6	18.0	4.2	40	326.8	12.2	18.4	4.3
1,8-Dimethyl-Phe	18.7	333.3	5.6	18.0	4.2	40	326.8	12.2	18.4	4.3
2,6-Dimethyl-Phe	18.7	333.3	5.6	18.0	4.2	40	326.8	12.2	18.4	4.3
3,6-Dimethyl-Phe	18.7	333.3	5.6	18.0	4.2	40	326.8	12.2	18.4	4.3
1,3-Dimethyl-Phe	18.7	333.3	5.6	18.0	4.2	40	326.8	12.2	18.4	4.3
5-Methyl-Chr	45.2	333.3	13.6	18.0	4.2	30	339.3	8.8	17.7	4.2
6-Ethyl-Chr	25.4	333.3	7.6	18.0	4.2	30	339.3	8.8	17.7	4.2
6-n-Propyl-Chr	28.1	333.3	8.4	18.0	4.2	30	339.3	8.8	17.7	4.2
1,2,6-Trimethyl-Phe	23.0	333.3	6.9	18.0	4.2	40	326.8	12.2	18.4	4.3
Retene	37.2	333.3	11.2	18.0	4.2	40	326.8	12.2	18.4	4.3
1,2,6,9-Tetramethyl-Phe	24.7	333.3	7.4	18.0	4.2	30	339.1	8.8	17.7	4.2
1-Methyl-Fle	46.4	333.3	13.9	18.0	4.2	30	308.6	9.7	19.4	4.4
9-Ethyl-Fle	31.1	333.3	9.3	18.0	4.2	30	308.6	9.7	19.4	4.4
9-n-Propyl-Fle	22.6	333.3	6.8	18.0	4.2	30	308.6	9.7	19.4	4.4
9-n-Butyl-Fle	23.0	333.3	6.9	18.0	4.2	30	308.6	9.7	19.4	4.4
1-Methyl-Pyr	32.1	333.3	9.6	18.0	4.2	25	284.3	8.8	21.1	4.6
1-Ethyl-Pyr	23.8	333.3	7.1	18.0	4.2	25	284.3	8.8	21.1	4.6
1-n-Propyl-Pyr	34.7	333.3	10.4	18.0	4.2	25	284.3	8.8	21.1	4.6
1-n-Butyl-Pyr	43.1	333.3	12.9	18.0	4.2	50	335.2	14.9	17.9	4.2
6-Methyl-BaP	60.7	333.3	18.2	18.0	4.2	50	153.1	32.7	39.2	6.3

7,10-Dimethyl-BaP	65.4	333.3	19.6	18.0	4.2	50	153.1	32.7	39.2	6.3
<u>HPAHs</u>										
9-Cl-Fle	20.1	333.3	6.0	18.0	4.2	30	216.5	13.9	27.7	5.3
2-Cl-Fle	20.1	333.3	6.0	18.0	4.2	30	216.5	13.9	27.7	5.3
5-Br-Ana	15.8	333.3	4.7	18.0	4.2	30	216.5	13.9	27.7	5.3
9-Br-Fle	24.3	333.3	7.3	18.0	4.2	30	216.5	13.9	27.7	5.3
2-Br-Fle	24.3	333.3	7.3	18.0	4.2	30	216.5	13.9	27.7	5.3
1-Cl-Ant	20.9	333.3	6.3	18.0	4.2	30	185.6	16.2	32.3	5.7
2,7-Cl ₂ -Fle	18.4	333.3	5.5	18.0	4.2	30	185.6	16.2	32.3	5.7
1,2-Br ₂ -Any	17.0	333.3	5.1	18.0	4.2	30	185.6	16.2	32.3	5.7
3-Br-Phe	22.6	333.3	6.8	18.0	4.2	80	323.7	24.7	18.5	4.3
1-Br-Ant	22.6	333.3	6.8	18.0	4.2	80	323.7	24.7	18.5	4.3
1,4-Cl ₂ -Ant	33.2	333.3	10.0	18.0	4.2	30	185.7	16.2	32.3	5.7
5,6-Br ₂ -Ana	28.9	333.3	8.7	18.0	4.2	30	185.7	16.2	32.3	5.7
2,7-Br ₂ -Fle	25.2	333.3	7.6	18.0	4.2	30	185.7	16.2	32.3	5.7
3-Br-Flu	25.9	333.3	7.8	18.0	4.2	30	185.5	16.2	32.3	5.7
9,10-Br ₂ -Ant	24.3	333.3	7.3	18.0	4.2	25	258.9	9.7	23.2	4.8
4-Br-Pyr	25.9	333.3	7.8	18.0	4.2	25	258.9	9.7	23.2	4.8
9-Br-1,5-Cl ₂ -Ant	30.7	333.3	9.2	18.0	4.2	40	204.7	19.5	29.3	5.4
1,5,9,10-Cl ₄ -Ant	21.2	333.3	6.4	18.0	4.2	20	250.7	8.0	23.9	4.9
1,6-Br ₂ -Pyr	22.6	333.3	6.8	18.0	4.2	20	250.7	8.0	23.9	4.9
4-Br-BaA	30.2	333.3	9.1	18.0	4.2	20	250.7	8.0	23.9	4.9
2,3,9,10-Br ₄ -Ant	41.4	333.3	12.4	18.0	4.2	30	248.1	12.1	24.2	4.9
<u>HPACs</u>										
Quinoline	66.6	333.3	20.0	18.0	4.2	30	348.9	8.6	17.2	4.1
Isoquinoline	66.6	333.3	20.0	18.0	4.2	30	348.9	8.6	17.2	4.1

Indole	58.7	333.3	17.6	18.0	4.2	30	348.9	8.6	17.2	4.1
2-Methylquinoline	77.1	333.3	23.1	18.0	4.2	30	348.9	8.6	17.2	4.1
4-Methylbenzothiophene	65.1	333.3	19.5	18.0	4.2	30	348.9	8.6	17.2	4.1
3-Methylisoquinoline	77.1	333.3	23.1	18.0	4.2	30	348.9	8.6	17.2	4.1
2,3-Dimethylbenzothiophene	39.5	333.3	11.9	18.0	4.2	40	326.7	12.2	18.4	4.3
2,5-Dimethyl-1-phenylpyrrole	61.4	333.3	18.4	18.0	4.2	40	326.7	12.2	18.4	4.3
4-Phenylpyridine	62.5	333.3	18.8	18.0	4.2	40	326.7	12.2	18.4	4.3
2,3-Dimethylindole	25.6	333.3	7.7	18.0	4.2	40	326.7	12.2	18.4	4.3
Dibenzofuran	31.4	333.3	9.4	18.0	4.2	40	326.5	12.3	18.4	4.3
2,3,4-Trimethylbenzothiophene	27.4	333.3	8.2	18.0	4.2	40	326.5	12.3	18.4	4.3
2-Methyldibenzofuran	33.0	333.3	9.9	18.0	4.2	40	326.5	12.3	18.4	4.3
Benzo[<i>h</i>]quinoline	15.1	333.3	4.5	18.0	4.2	25	309.9	8.1	19.4	4.4
1,2,3,4-Tetrahydrocarbazole	14.8	333.3	4.4	18.0	4.2	25	309.9	8.1	19.4	4.4
Acridine	14.9	333.3	4.5	18.0	4.2	25	309.9	8.1	19.4	4.4
9-Methylcarbazole	19.1	333.3	5.7	18.0	4.2	25	309.9	8.1	19.4	4.4
Carbazole	22.0	333.3	6.6	18.0	4.2	25	309.9	8.1	19.4	4.4
3-Methylbenzo[<i>f</i>]quinoline	25.2	333.3	7.6	18.0	4.2	40	326.6	12.2	18.4	4.3
2-Methylacridine	25.2	333.3	7.6	18.0	4.2	40	326.6	12.2	18.4	4.3
3,6-Dimethylcarbazole	16.5	333.3	5.0	18.0	4.2	40	408.4	9.8	14.7	3.8
Benzo[<i>b</i>]naphtho[2,3- <i>d</i>]furan	29.1	333.3	8.7	18.0	4.2	40	408.4	9.8	14.7	3.8
3-Tert-butyl-9H-	29.6	333.3	8.9	18.0	4.2	40	408.4	9.8	14.7	3.8

carbazole										
9-Phenylcarbazole	28.7	333.3	8.6	18.0	4.2	50	305.3	16.4	19.7	4.4
7,8,9,10-Tetrahydrobenzo[<i>b</i>]naphtho[2,3- <i>d</i>]thiophene	21.0	333.3	6.3	18.0	4.2	50	305.3	16.4	19.7	4.4
Benz[<i>c</i>]acridine	21.5	333.3	6.5	18.0	4.2	50	305.3	16.4	19.7	4.4
11H-Benzo[<i>a</i>]carbazole	19.5	333.3	5.9	18.0	4.2	50	305.2	16.4	19.7	4.4
7H-Benzo[<i>c</i>]carbazole	42.2	333.3	12.7	18.0	4.2	50	305.2	16.4	19.7	4.4
6-Methylbenzo[<i>b</i>]naphtho[2,1- <i>d</i>]thiophene	43.9	333.3	13.2	18.0	4.2	50	305.2	16.4	19.7	4.4
2-Phenyldibenzothiophene	38.8	333.3	11.6	18.0	4.2	50	305.2	16.4	19.7	4.4
Dinaphtho[1,2- <i>b</i> ;1',2'- <i>d</i>]furan	26.7	333.3	8.0	18.0	4.2	50	305.2	16.4	19.7	4.4
Dibenz[<i>c,h</i>]acridine	68.6	333.3	20.6	18.0	4.2	40	254.4	15.7	23.6	4.9
13(H)-Dibenzo[<i>a,i</i>]carbazole	48.8	333.3	14.6	18.0	4.2	40	254.4	15.7	23.6	4.9
Dibenzothiophene	21.0	333.3	6.3	18.0	4.2	30	308.6	9.7	19.4	4.4
2-Methyldibenzothiophene	27.7	333.3	8.3	18.0	4.2	30	308.6	9.7	19.4	4.4
1,2-Dimethyldibenzothiophene	20.5	333.3	6.2	18.0	4.2	30	308.5	9.7	19.4	4.4
4-n-Propyldibenzothiophene	21.1	333.3	6.3	18.0	4.2	30	308.5	9.7	19.4	4.4
4,6-Diethyldibenzothiophene	30.1	333.3	9.0	18.0	4.2	30	308.5	9.7	19.4	4.4

ne											
Benzo[<i>b</i>]naphtho[1,2- <i>d</i>]thiophene	21.9	333.3	6.6	18.0	4.2	30	339.1	8.8	17.7	4.2	
Benzo[<i>b</i>]naphtho[2,3- <i>d</i>]thiophene	21.9	333.3	6.6	18.0	4.2	30	339.1	8.8	17.7	4.2	
HHPACs											
2,3-Br ₂ -thiophene	68.6	333.3	20.6	18.0	4.2	40	408.5	9.8	14.7	3.8	
2-Cl-quinoline	48.8	333.3	14.6	18.0	4.2	40	408.5	9.8	14.7	3.8	
2-Br-benzothiophene	29.0	333.3	8.7	18.0	4.2	40	408.5	9.8	14.7	3.8	
2,3-Cl ₂ -benzothiophene	28.5	333.3	8.6	18.0	4.2	40	408.5	9.8	14.7	3.8	
2-Br-quinoline	40.6	333.3	12.2	18.0	4.2	35	296.8	11.8	20.2	4.5	
5-Cl-indole	38.9	333.3	11.7	18.0	4.2	35	296.8	11.8	20.2	4.5	
3-Br-isoquinoline	28.1	333.3	8.4	18.0	4.2	35	296.8	11.8	20.2	4.5	
5-Br-indole	39.1	333.3	11.7	18.0	4.2	40	326.9	12.2	18.4	4.3	
2,3-Br ₂ -benzothiophene	33.5	333.3	10.1	18.0	4.2	40	326.9	12.2	18.4	4.3	
9-Cl-acridine	24.5	333.3	7.4	18.0	4.2	40	326.9	12.2	18.4	4.3	
2-Br-dibenzothiophene	17.0	333.3	5.1	18.0	4.2	50	305.3	16.4	19.7	4.4	
9-Br-acridine	17.1	333.3	5.1	18.0	4.2	50	305.3	16.4	19.7	4.4	
3,6-Cl ₂ -9H-carbazole	27.2	333.3	8.2	18.0	4.2	30	225.3	13.3	26.6	5.2	
2,8-Br ₂ -dibenzothiophene	20.7	333.3	6.2	18.0	4.2	30	225.3	13.3	26.6	5.2	
3,6-Br ₂ -carbazole	33.4	333.3	10.0	18.0	4.2	100	403.8	24.8	14.9	3.9	

29 ^aColors indicates which analytes were monitored during the same GC-MS/MS run using our conventional MRM method. Details of the time-segments used in
30 the convention MRM method can be found in the references; ^bDuty cycle calculated as dwell time/cycle time × 100%; ^cnumber of measurements is calculated by
31 dividing the typical width of a GC-peak (i.e., 6s) by the cycle time; ^dthis gives an approximation of the signal to noise ratio

32 **Table SI4.** Method performance characteristics of dMRM and MRM methods for the analysis of PACs in calibration solutions.

Analyte	Internal standard	dMRM								MRM									
		Calibration solution level								LO D (pg/ μ L)	LO Q (pg/ μ L)	Calibration solution level						LO D (pg/ μ L)	LO Q (pg/ μ L)
		Low		Medium		High		Low				Medium		High					
		Bias (%)	Precision (RSD %)	Bias (%)	Precision (RSD %)	Bias (%)	Precision (RSD %)	Bias (%)	Precision (RSD %)			Bias (%)	Precision (RSD %)	Bias (%)	Precision (RSD %)				
PAHs																			
Nap	d ₈ -Nap	-3.6	3.7	0.7	0.9	-0.6	0.4	0.5	1.7	-1.6	0.8	-3.6	0.9	3.7	1.2	0.1	0.4		
Ace	d ₁₀ -Ace	-5.2	2.4	-3.6	0.9	3.8	1.0	0.3	1.1	-7.7	1.5	-5.4	1.0	5.7	1.8	0.2	0.7		
Acy	d ₈ -Acy	-6.7	4.1	-4.9	1.5	5.2	1.0	0.5	1.8	-5.3	1.2	-3.7	0.5	3.8	1.0	0.2	0.5		
Fle	d ₁₀ -Fle	4.6	3.5	-6.4	1.2	6.8	0.3	0.5	1.6	7.9	3.5	-4.1	1.9	4.2	1.2	0.5	1.6		
Phe	d ₁₀ -Phe	-6.3	2.6	-5.5	1.8	5.8	1.1	0.3	1.2	-7.3	2.0	-6.4	0.7	6.8	1.0	0.3	0.9		
Ant	d ₁₀ -Phe	-3.5	3.9	-8.9	3.2	9.8	1.4	0.5	1.7	-7.7	4.4	-7.3	0.5	7.9	1.5	0.6	2.0		
Flu	d ₁₀ -Flu	-3.3	3.6	-3.3	1.7	3.4	0.6	0.5	1.6	-3.0	2.2	-4.3	0.4	4.5	1.2	0.3	1.0		
Pyr	d ₁₀ -Pyr	-8.8	3.1	-6.2	0.7	6.6	1.0	0.4	1.4	-6.1	1.2	-6.9	1.3	7.5	0.9	0.2	0.5		
BaA	d ₁₂ -BaA	-13.3	4.0	-9.0	1.3	9.9	0.3	0.5	1.8	-6.7	2.2	-10.8	1.2	12.1	1.1	0.3	1.0		
Chr	d ₁₂ -Chr	-6.9	2.4	-0.5	4.0	0.5	5.5	0.3	1.1	-6.2	2.5	-0.8	3.1	0.8	0.6	0.3	1.1		
BbF	d ₁₂ -BbF	-4.7	8.5	-19.7	6.1	20.4	1.7	1.1	3.8	-10.6	5.5	-14.3	1.9	16.7	1.6	0.7	2.5		
BkF	d ₁₂ -BkF	-6.0	3.6	1.6	2.8	-1.6	1.9	0.5	1.6	-3.7	4.3	2.1	1.4	-2.1	0.6	0.6	1.9		
BaP	d ₁₂ -BaP	-15.0	9.5	-17.1	2.3	20.6	2.4	1.3	4.3	-15.3	3.5	-13.9	1.0	16.1	1.6	0.5	1.6		
Ind	d ₁₂ -Ind	-17.5	3.6	-18.2	3.8	22.2	3.4	0.5	1.6	-10.3	4.8	-16.2	5.2	19.4	5.3	0.6	2.2		
DahA	d ₁₄ -DahA	-10.0	5.7	-13.0	1.6	14.9	1.5	0.8	2.6	-8.9	2.0	-11.4	1.3	12.9	2.6	0.3	0.9		

BghiP	d ₁₂ -BghiP	-8.5	2.7	-9.6	2.3	10.6	2.0	0.4	1.2	-9.6	6.7	-8.6	1.0	9.5	1.0	0.9	3.0
APAHs																	
2-Methyl-Nap	d ₈ -Acy	-8.5	6.8	-5.7	3.9	6.1	1.9	0.9	3.0	1.5	2.2	-5.1	1.5	5.4	1.3	0.3	1.0
1-Methyl-Nap	d ₈ -Acy	3.9	6.4	-3.9	3.1	4.1	2.2	0.9	2.9	15.7	2.5	-3.9	1.8	4.1	0.8	0.3	1.1
1,4-Dimethyl-Nap	d ₈ -Acy	0.4	4.2	-5.1	1.8	5.4	1.7	0.6	1.9	7.2	3.4	-4.5	1.4	4.7	1.8	0.5	1.5
2,3,5-Trimethyl-Nap	d ₈ -Acy	3.7	3.4	-10.3	3.1	11.5	1.9	0.5	1.5	11.0	7.8	-7.8	1.2	8.5	0.9	1.0	3.5
1,4,6,7-Tetramethyl-Nap	d ₁₀ -Phe	18.1	5.2	-7.4	2.2	8.0	1.6	0.7	2.3	27.4	3.6	-5.6	2.3	5.9	2.0	0.5	1.6
1-Methyl-Phe	d ₁₀ -Phe	4.7	3.1	-12.2	4.0	13.9	2.8	0.4	1.4	4.0	4.2	-12.1	1.7	13.7	3.6	0.6	1.9
2-Methyl-Phe	d ₁₀ -Phe	-0.6	5.7	-15.9	0.8	19.0	1.4	0.8	2.5	-4.8	2.3	-9.4	0.8	10.4	2.4	0.3	1.0
3-Methyl-Phe	d ₁₀ -Phe	-21.2	5.4	-11.8	0.6	13.3	1.3	0.7	2.4	-13.0	2.0	-10.5	1.2	11.8	2.6	0.3	0.9
9-Methyl-Phe	d ₁₀ -Phe	-7.3	5.4	-13.8	1.2	16.0	2.6	0.7	2.4	-9.8	2.4	-9.4	2.0	10.3	3.4	0.3	1.1
1,7-Dimethyl-Phe	d ₁₀ -Flu	13.6	7.4	-12.9	2.1	14.9	1.3	1.0	3.3	9.7	6.8	-11.8	1.0	13.4	1.8	0.9	3.1
1,8-Dimethyl-Phe	d ₁₀ -Flu	9.6	7.6	-9.6	2.8	10.7	0.7	1.0	3.4	6.8	1.2	-9.9	1.1	10.9	1.5	0.2	0.5
2,6-Dimethyl-	d ₁₀ -Flu	-2.3	4.1	-15.3	3.9	18.1	1.2	0.5	1.8	-2.1	2.0	-7.6	0.9	8.2	2.7	0.3	0.9

Phe																	
3,6-Dimethyl-Phe	d ₁₀ -Flu	-5.8	6.2	-8.8	1.5	9.6	1.0	0.8	2.8	-7.0	3.3	-4.1	0.3	4.3	2.4	0.4	1.5
1,3-Dimethyl-Phe	d ₁₀ -Flu	5.2	2.6	-12.0	1.9	13.7	0.9	0.4	1.2	6.7	6.8	-8.3	1.1	9.1	2.4	0.9	3.1
5-Methyl-Chr	d ₁₂ -Chr	-10.9	7.6	0.5	8.0	-0.5	6.9	1.0	3.4	-6.6	9.1	9.7	3.9	-8.9	1.0	1.2	4.1
6-Ethyl-Chr	d ₁₂ -Chr	1.5	7.7	2.5	7.8	-2.4	7.2	1.0	3.4	5.9	7.1	10.7	4.1	-9.7	1.0	1.0	3.2
6-n-Propyl-Chr	d ₁₂ -BaP	12.2	5.5	-14.7	2.1	17.2	2.8	0.7	2.5	13.8	6.7	-3.6	1.2	3.7	3.6	0.9	3.0
1,2,6-Trimethyl-Phe	d ₁₀ -Pyr	-8.9	3.3	-10.6	1.0	11.8	2.1	0.4	1.5	-0.6	4.4	-5.7	1.9	6.0	1.1	0.6	2.0
Retene	d ₁₀ -Pyr	-5.3	2.9	-14.8	1.6	17.3	2.0	0.4	1.3	5.0	3.8	-10.1	2.3	11.2	1.3	0.5	1.7
1,2,6,9-Tetramethyl-Phe	d ₁₀ -Pyr	8.9	6.3	-15.2	1.2	17.9	9.5	0.8	2.8	12.2	9.5	11.3	4.8	-10.2	2.0	1.3	4.3
1-Methyl-Fle	d ₈ -Acy	-33.0	4.4	6.0	2.6	-5.7	2.2	0.6	2.0	-21.0	7.1	5.1	2.6	-4.8	1.6	1.0	3.2
9-Ethyl-Fle	d ₁₀ -Phe	8.0	8.0	23.8	3.4	-19.2	2.3	1.1	3.6	-8.7	6.5	20.9	5.0	-17.3	3.9	0.9	2.9
9-n-Propyl-Fle	d ₁₀ -Phe	-17.2	9.2	19.2	2.2	-16.1	2.1	1.2	4.1	-10.3	6.9	18.4	1.5	-15.6	1.0	0.9	3.1
9-n-Butyl-Fle	d ₁₀ -Phe	-18.9	9.6	21.2	1.3	-17.5	1.9	1.3	4.3	-14.0	7.4	18.5	2.9	-15.6	1.2	1.0	3.3
1-Methyl-Pyr	d ₁₀ -Pyr	-23.8	5.3	7.4	2.5	-6.9	2.1	0.7	2.4	-22.6	6.8	5.2	1.9	-4.9	3.6	0.9	3.0
1-Ethyl-	d ₁₂ -Chr	-34.3	6.7	19.4	7.6	-16.2	8.4	0.9	3.0	-28.8	8.7	12.1	2.9	-10.8	4.8	1.2	3.9

Pyr																	
1-n-Propyl-Pyr	d ₁₀ -Pyr	-12.6	8.6	2.8	3.5	-2.7	2.4	1.2	3.9	-10.9	7.1	2.2	1.3	-2.2	1.1	1.0	3.2
1-n-Butyl-Pyr	d ₁₀ -Pyr	-17.6	9.0	-1.2	5.0	1.2	1.9	1.2	4.0	-9.8	9.9	-2.3	1.0	2.3	0.7	1.3	4.4
6-Methyl-BaP	d ₁₂ -BaP	-25.8	9.0	-12.6	9.3	14.5	8.8	1.2	4.0	-25.6	4.3	-1.9	3.8	1.9	2.7	0.6	1.9
7,10-Dimethyl-BaP	d ₁₂ -BaP	-20.3	9.6	4.9	6.8	-4.7	7.5	1.3	4.3	-0.2	8.6	4.2	3.1	-4.0	1.6	1.2	3.9
HPAHs																	
9-Cl-Fle	d ₁₀ -Phe	2.0	7.8	0.0	3.9	0.0	8.1	1.1	3.5	1.5	5.3	3.2	5.0	-3.1	5.4	0.7	2.4
2-Cl-Fle	d ₁₀ -Phe	-5.6	3.9	-7.7	2.3	8.3	0.7	0.5	1.8	-4.2	2.3	-0.8	2.2	0.8	1.8	0.3	1.0
5-Br-Ana	d ₁₀ -Phe	-3.9	6.6	-8.0	2.7	8.6	1.3	0.9	3.0	-0.3	3.1	2.3	5.2	-2.3	4.1	0.4	1.4
9-Br-Fle	d ₁₀ -Phe	-5.6	3.9	-7.7	2.3	8.3	0.7	0.5	1.8	-17.8	8.8	-4.9	3.4	5.1	7.8	1.2	4.0
2-Br-Fle	d ₁₀ -Phe	-14.1	3.0	-12.0	2.1	13.7	1.2	0.4	1.3	-6.5	6.0	1.4	7.6	-1.4	7.1	0.8	2.7
1-Cl-Ant	d ₁₀ -Flu	-6.2	8.1	-8.8	2.1	9.6	1.2	1.1	3.6	7.1	4.5	-5.6	2.9	5.9	1.6	0.6	2.0
2,7-Cl ₂ -Fle	d ₁₀ -Flu	-2.6	9.0	-12.9	3.5	14.8	3.8	1.2	4.0	1.0	5.3	-8.3	2.9	9.0	1.6	0.7	2.4
1,2-Br ₂ -Any	d ₁₀ -Flu	-10.8	9.2	-13.7	5.5	15.9	6.5	1.2	4.1	4.6	3.6	-7.4	2.8	8.0	2.2	0.5	1.6
3-Br-Phe	d ₁₀ -Flu	-13.6	3.8	-4.2	2.2	4.3	1.2	0.5	1.7	4.3	5.1	-7.5	2.6	8.1	2.0	0.7	2.3
1-Br-Ant	d ₁₀ -Pyr	-4.8	5.6	-10.0	3.0	11.1	1.5	0.7	2.5	4.7	3.4	-4.5	3.2	4.7	3.5	0.5	1.5
1,4-Cl ₂ -Ant	d ₁₀ -Pyr	-9.1	4.0	-7.4	1.4	8.0	0.8	0.5	1.8	1.1	3.8	-5.3	5.8	5.6	6.0	0.5	1.7
5,6-Br ₂ -Ana	d ₁₀ -Pyr	2.4	4.8	-14.5	6.4	17.0	8.5	0.6	2.1	4.2	6.7	-4.6	3.5	4.8	7.1	0.9	3.0
2,7-Br ₂ -	d ₁₀ -Pyr	-3.8	9.7	-12.3	3.9	14.1	7.5	1.3	4.3	-0.4	6.4	-5.1	1.9	5.4	6.6	0.9	2.9

Fle																	
3-Br-Flu	d ₁₂ -BaA	-13.1	7.6	-7.8	4.6	8.5	2.9	1.0	3.4	-13.1	4.0	-2.9	3.8	3.0	5.7	0.5	1.8
9,10-Br ₂ -Ant	d ₁₂ -BaA	-13.9	4.2	-9.5	5.7	10.5	2.9	0.6	1.9	-1.5	3.8	-1.5	2.4	1.6	1.6	0.5	1.7
4-Br-Pyr	d ₁₂ -Chr	-14.9	8.8	-10.5	3.0	11.7	8.3	1.2	3.9	-1.6	6.2	-6.9	3.9	7.4	4.7	0.8	2.8
9-Br-1,5-Cl ₂ -Ant	d ₁₂ -BbF	-22.9	9.9	-14.6	3.5	7.7	3.0	1.3	4.4	-18.2	9.6	-11.8	2.9	13.4	3.4	1.3	4.3
1,5,9,10-Cl ₄ -Ant	d ₁₂ -BbF	-13.8	3.0	-12.5	3.2	14.4	6.1	0.4	1.3	-10.7	1.9	-16.0	5.3	19.1	3.7	0.3	0.9
1,6-Br ₂ -Pyr	d ₁₂ -BaP	-6.9	8.3	-20.6	1.5	25.9	4.5	1.1	3.7	-10.3	7.7	-9.6	5.2	10.6	3.4	1.0	3.4
4-Br-BaA	d ₁₂ -BaP	-15.1	3.4	-22.7	3.5	29.4	4.9	0.4	1.5	-12.6	4.3	-12.6	3.0	14.5	1.7	0.6	1.9
2,3,9,10-Br ₄ -Ant	d ₁₂ -Ind	-36.8	2.2	-13.2	3.3	15.2	3.5	0.3	1.0	-27.3	5.6	-11.7	4.2	13.3	9.0	0.8	2.5
HHPACs																	
Quinoline	d ₈ -Nap	-21.9	2.3	1.1	6.0	-1.1	7.6	0.3	1.0	-37.7	5.3	2.2	8.8	-2.1	7.7	0.7	2.4
Isoquinoline	d ₈ -Nap	-34.6	9.7	-14.2	4.9	16.6	7.2	1.3	4.4	-32.2	6.8	-8.9	4.5	9.8	8.2	0.9	3.0
Indole	d ₈ -Nap	-10.9	5.6	-7.8	2.0	8.5	5.0	0.7	2.5	-11.8	2.1	-7.6	2.0	8.2	2.4	0.3	1.0
2-Methylquinoline	d ₈ -Nap	-15.1	1.1	-4.1	10.6	4.2	7.6	0.1	0.5	-36.8	3.9	3.9	5.4	-3.7	9.3	0.5	1.7
4-Methylbenzothioephene	d ₈ -Nap	-0.2	6.4	-4.5	2.6	4.8	6.3	0.9	2.9	-6.6	7.3	-0.8	2.7	0.8	2.0	1.0	3.3
3-Methylisoquinoline	d ₈ -Nap	-18.5	8.0	-8.1	9.9	8.9	4.9	1.1	3.6	-37.4	8.5	-9.6	9.8	10.6	7.1	1.1	3.8

2,3-Dimethylbenzothioephene	d ₈ -Nap	-1.0	4.1	-4.4	1.7	4.7	3.5	0.5	1.8	-8.0	3.5	-2.8	2.8	2.9	4.6	0.5	1.6
2,5-Dimethyl-1-phenylpyrrole	d ₈ -Nap	14.5	3.3	3.7	4.8	-3.6	2.7	0.4	1.5	4.4	5.0	5.6	5.2	-5.3	2.3	0.7	2.2
4-Phenylpyridine	d ₈ -Nap	13.4	7.4	6.3	4.2	-6.0	1.8	1.0	3.3	11.3	7.3	8.3	3.7	-7.6	3.7	1.0	3.2
2,3-Dimethylindole	d ₈ -Nap	-7.2	6.3	-13.5	2.3	15.6	6.0	0.9	2.8	-13.8	8.5	-8.4	5.8	9.2	4.1	1.1	3.8
Dibenzofuran	d ₈ -Nap	-8.3	1.7	-11.6	4.8	13.2	3.5	0.2	0.8	-11.8	4.2	-4.6	5.6	4.8	2.9	0.6	1.9
2,3,4-Trimethylbenzothioephene	d ₁₀ -Fle	-3.3	2.7	-1.0	2.1	1.0	0.5	0.4	1.2	0.6	4.3	0.5	3.1	-0.5	1.5	0.6	1.9
2-Methyldibenzofuran	d ₁₀ -Fle	-3.1	3.8	-10.2	3.8	11.3	0.9	0.5	1.7	-12.7	5.5	5.2	5.7	-4.9	2.0	0.7	2.4
Benzo[<i>h</i>]quinoline	d ₁₀ -Phe	-13.2	2.1	-3.4	9.1	3.5	5.2	0.3	0.9	-14.6	5.3	6.5	3.6	-6.1	4.5	0.7	2.4
1,2,3,4-Tetrahydrocarbazole	d ₁₀ -Phe	-6.0	7.0	3.2	5.7	-3.1	7.4	0.9	3.1	5.7	7.9	4.2	3.6	-4.0	4.7	1.1	3.5
Acridine	d ₁₀ -Phe	-10.9	4.7	2.4	5.7	-2.4	5.9	0.6	2.1	-39.2	10.0	9.3	9.2	-8.5	8.8	1.3	4.5
9-Methylcarbazole	d ₁₀ -Phe	-5.8	8.3	0.2	1.3	-0.2	2.3	1.1	3.7	1.8	5.9	0.0	3.4	0.0	2.7	0.8	2.6

Carbazole	d ₁₀ -Phe	-9.1	7.9	1.8	3.2	-1.8	6.0	1.1	3.5	-24.2	9.2	3.1	2.4	-3.1	2.2	1.2	4.1
3-Methylbenzo[<i>f</i>]quinoline	d ₁₀ -Phe	-3.6	3.7	0.7	0.9	24.2	0.4	0.5	1.7	-1.6	0.8	-3.6	0.9	29.7	1.2	0.1	0.4
2-Methylacridine	d ₁₀ -Phe	-26.6	9.7	-9.4	8.6	10.4	7.8	1.3	4.3	-33.3	8.8	-1.1	9.6	0.7	9.0	1.2	3.9
3,6-Dimethylcarbazole	d ₁₀ -Phe	-16.6	8.1	-3.8	4.3	4.0	6.2	1.1	3.6	-24.7	8.8	-6.2	6.6	6.6	4.9	1.2	3.9
Benzo[<i>b</i>]naphtho[2,3- <i>d</i>]furan	d ₁₀ -Phe	-19.9	10.0	-2.9	3.8	16.7	5.3	1.3	4.5	-16.8	9.7	4.6	4.9	-4.4	6.5	1.3	4.3
3-Tert-butyl-9H-carbazole	d ₁₀ -Pyr	-13.2	5.7	-6.4	2.6	6.8	0.6	0.8	2.6	-7.9	4.4	-1.6	6.2	1.6	4.2	0.6	2.0
9-Phenylcarbazole	d ₁₀ -Pyr	-5.8	4.7	-2.3	5.0	2.3	0.8	0.6	2.1	-4.7	7.4	3.6	7.0	-3.5	4.6	1.0	3.3
7,8,9,10-Tetrahydrobenzo[<i>b</i>]naphtho[2,3- <i>d</i>]thiophene	d ₁₀ -Pyr	-9.2	6.6	-9.8	5.1	10.8	3.0	0.9	2.9	-6.6	7.5	-4.2	4.9	4.4	2.7	1.0	3.4
Benz[<i>c</i>]acridine	d ₁₀ -Pyr	-13.2	8.1	-12.9	6.5	14.9	3.9	1.1	3.6	-14.7	5.2	-10.2	3.6	11.4	3.4	0.7	2.3
11H-Benzo[<i>a</i>]carbazole	d ₁₂ -Chr	-24.7	9.1	-8.9	5.0	14.3	6.8	1.2	4.1	-28.0	6.6	-3.3	6.2	3.4	1.3	0.9	3.0

7H- Benzo[<i>c</i>]c arbazole	d ₁₂ -Chr	-36.4	9.6	-3.7	5.9	14.8	7.1	1.3	4.3	-25.8	4.9	7.4	6.9	-6.9	2.1	0.7	2.2
6- Methylben zo[<i>b</i>]napht ho[2,1- <i>d</i>]thiophen e	d ₁₂ -BaA	-9.6	4.4	-6.9	1.5	7.4	2.8	0.6	2.0	-10.4	7.8	-4.3	2.8	4.5	2.2	1.0	3.5
2- Phenyldib enzothiop hene	d ₁₂ -BbF	-20.7	8.4	-16.1	2.8	19.1	6.1	1.1	3.8	-11.5	6.9	-11.9	1.9	13.5	4.3	0.9	3.1
Dinaphtho [1,2- <i>b</i> ;1',2'- <i>d</i>]furan	d ₁₂ -BkF	-9.8	6.9	-16.8	7.0	20.2	5.7	0.9	3.1	-11.7	9.9	-13.2	3.1	15.2	5.1	1.3	4.4
Dibenz[<i>c,h</i>]acridine	d ₁₂ - BghiP	-10.0	3.4	-18.1	6.9	21.4	1.6	0.5	1.5	-12.7	2.2	-14.5	1.5	17.0	1.8	0.3	1.0
13(H)- Dibenzo[<i>a</i> <i>i</i>]carbazol e	d ₁₂ - BghiP	-36.4	8.8	-21.2	4.2	26.9	3.3	1.2	4.0	-34.2	5.0	-14.5	5.0	16.9	4.5	0.7	2.2
Dibenzoth iophene	d ₁₀ -Phe	-16.9	4.9	14.8	0.5	-12.9	1.5	0.7	2.2	-16.5	5.7	14.9	1.3	-12.9	1.0	0.8	2.5
2- Methyldib enzothiop hene	d ₁₀ -Phe	-19.3	8.2	11.4	1.3	-10.3	2.6	1.1	3.7	-16.9	3.7	9.6	1.0	-8.8	1.9	0.5	1.7
1,2- Dimethyld ibenzothio phene	d ₁₀ -Pyr	-25.9	4.6	8.7	2.2	-8.0	1.2	0.6	2.1	-20.2	4.1	6.7	1.7	-6.3	2.4	0.6	1.8

4-n-Propyldibenzothio- phene	d ₁₀ -Pyr	-32.8	4.4	12.3	2.3	-11.0	1.5	0.6	2.0	-18.3	9.4	7.4	1.4	-6.9	2.6	1.3	4.2
4,6-Diethyldibenzothio- phene	d ₁₀ -Pyr	-24.9	4.8	10.1	2.2	-9.2	0.7	0.6	2.2	-26.7	4.2	8.9	0.7	-8.1	2.3	0.6	1.9
Benzo[<i>b</i>]naphtho[1,2- <i>d</i>]thiophene	d ₁₀ -Pyr	-9.9	9.6	-7.9	0.9	8.6	1.2	1.3	4.3	-7.2	9.8	-6.3	1.8	6.7	1.4	1.3	4.4
Benzo[<i>b</i>]naphtho[2,3- <i>d</i>]thiophene	d ₁₀ -Pyr	-18.1	7.2	-18.0	3.8	21.9	3.3	1.0	3.2	-14.6	7.7	-10.7	3.7	12.0	2.2	1.0	3.5
HHPACs																	
2,3-Br ₂ -thiophene	d ₁₀ -Fle	-10.3	6.0	2.2	2.1	-2.2	3.5	0.8	2.7	2.3	2.1	3.8	4.3	-3.7	2.6	0.3	0.9
2-Cl-quinoline	d ₁₀ -Fle	-12.9	4.8	-7.4	2.4	8.0	3.5	0.6	2.1	-4.5	5.9	-6.3	3.4	6.7	1.9	0.8	2.6
2-Br-benzothio- phene	d ₁₀ -Fle	-16.0	6.0	1.9	4.3	-1.9	5.1	0.8	2.7	-6.1	5.1	-5.0	3.6	5.3	3.9	0.7	2.3
2,3-Cl ₂ -benzothio- phene	d ₁₀ -Fle	-13.2	5.2	0.7	1.4	-0.7	2.7	0.7	2.3	2.9	4.6	-3.3	3.0	3.4	3.7	0.6	2.0
2-Br-quinoline	d ₁₀ -Fle	-16.8	3.7	-5.3	1.3	5.6	4.1	0.5	1.6	-7.3	9.7	-9.3	5.0	10.2	2.7	1.3	4.4

5-Cl-indole	d ₁₀ -Fle	-18.2	6.1	-15.4	0.9	18.1	4.2	0.8	2.7	-9.2	6.6	-13.0	6.2	14.9	2.1	0.9	3.0
3-Br-isoquinoline	d ₈ -Nap	17.4	7.5	-13.1	3.3	15.0	5.3	1.0	3.4	15.7	4.0	-11.3	4.3	12.7	2.1	0.5	1.8
5-Br-indole	d ₈ -Nap	-8.3	8.7	-20.4	7.9	25.7	5.5	1.2	3.9	-2.6	3.5	-17.9	3.1	21.8	1.7	0.5	1.6
2,3-Br ₂ -benzothio- phene	d ₁₀ -Phe	-15.7	6.8	0.3	3.6	-0.3	2.5	0.9	3.0	-13.6	8.0	-3.3	3.2	3.4	2.3	1.1	3.6
9-Cl-acridine	d ₁₀ -Phe	6.8	6.6	-13.1	3.9	15.1	4.5	0.9	2.9	6.1	5.6	-2.2	7.3	2.3	4.3	0.8	2.5
2-Br-dibenzothi- ophene	d ₁₀ -Phe	7.5	9.3	-15.0	5.6	17.6	4.9	1.2	4.2	27.2	9.5	-10.1	2.1	11.2	3.6	1.3	4.3
9-Br-acridine	d ₁₀ -Phe	-4.4	4.6	-19.8	5.5	24.6	7.2	0.6	2.0	-1.5	9.4	-10.0	6.7	11.1	3.8	1.3	4.2
3,6-Cl ₂ - 9H-carbazole	d ₁₀ -Pyr	-26.2	3.8	-20.4	6.1	25.6	4.5	0.5	1.7	-26.2	5.1	-14.1	3.5	16.5	3.7	0.7	2.3
2,8-Br ₂ - dibenzothi- ophene	d ₁₀ -Pyr	-3.6	3.7	0.7	0.9	24.2	0.4	0.5	1.7	-1.6	0.8	-3.6	0.9	29.7	1.2	0.1	0.4
3,6-Br ₂ - carbazole	d ₁₂ -Chr	-30.4	8.9	-16.0	4.6	19.0	4.9	1.2	4.0	-19.6	8.4	-16.0	4.6	19.0	4.9	1.1	3.7

34 **Table SI5.** Statistical result of dMRM and MRM methods for the analysis of PACs in calibration solutions.

Analyte	Internal standard	<i>p</i> value ^a
<u>PAHs</u>		
Nap	d ₈ -Nap	0.13
Ace	d ₁₀ -Ace	0.04
Acy	d ₈ -Acy	0.25
Fle	d ₁₀ -Fle	0.11
Phe	d ₁₀ -Phe	0.16
Ant	d ₁₀ -Phe	0.11
Flu	d ₁₀ -Flu	0.45
Pyr	d ₁₀ -Pyr	0.07
BaA	d ₁₂ -BaA	0.00
Chr	d ₁₂ -Chr	0.25
BbF	d ₁₂ -BbF	0.19
BkF	d ₁₂ -BkF	0.23
BaP	d ₁₂ -BaP	0.47
Ind	d ₁₂ -Ind	0.02
DahA	d ₁₄ -DahA	0.34
BghiP	d ₁₂ -BghiP	0.34
<u>APAHs</u>		
2-Methyl-Nap	d ₈ -Acy	0.01

1-Methyl-Nap	d ₈ -Acy	0.11
1,4-Dimethyl-Nap	d ₈ -Acy	0.03
2,3,5-Trimethyl-Nap	d ₈ -Acy	0.08
1,4,6,7-Tetramethyl-Nap	d ₁₀ -Phe	0.06
1-Methyl-Phe	d ₁₀ -Phe	0.35
2-Methyl-Phe	d ₁₀ -Phe	0.05
3-Methyl-Phe	d ₁₀ -Phe	0.11
9-Methyl-Phe	d ₁₀ -Phe	0.17
1,7-Dimethyl-Phe	d ₁₀ -Flu	0.11
1,8-Dimethyl-Phe	d ₁₀ -Flu	0.11
2,6-Dimethyl-Phe	d ₁₀ -Flu	0.11
3,6-Dimethyl-Phe	d ₁₀ -Flu	0.32
1,3-Dimethyl-Phe	d ₁₀ -Flu	0.46
5-Methyl-Chr	d ₁₂ -Chr	0.14
6-Ethyl-Chr	d ₁₂ -Chr	0.19
6-n-Propyl-Chr	d ₁₂ -BaP	0.33
1,2,6-Trimethyl-Phe	d ₁₀ -Pyr	0.02
Retene	d ₁₀ -Pyr	0.01
1,2,6,9-Tetramethyl-Phe	d ₁₀ -Pyr	0.16
1-Methyl-Fle	d ₈ -Acy	0.01
9-Ethyl-Fle	d ₁₀ -Phe	0.01
9-n-Propyl-Fle	d ₁₀ -Phe	0.11
9-n-Butyl-Fle	d ₁₀ -Phe	0.11
1-Methyl-Pyr	d ₁₀ -Pyr	0.39

1-Ethyl-Pyr	d ₁₂ -Chr	0.08
1-n-Propyl-Pyr	d ₁₀ -Pyr	0.48
1-n-Butyl-Pyr	d ₁₀ -Pyr	0.09
6-Methyl-BaP	d ₁₂ -BaP	0.31
7,10-Dimethyl-BaP	d ₁₂ -BaP	0.02
<u>HPAHs</u>		
9-Cl-Fle	d ₁₀ -Phe	0.42
2-Cl-Fle	d ₁₀ -Phe	0.18
5-Br-Ana	d ₁₀ -Phe	0.13
9-Br-Fle	d ₁₀ -Phe	0.004
2-Br-Fle	d ₁₀ -Phe	0.04
1-Cl-Ant	d ₁₀ -Flu	0.02
2,7-Cl ₂ -Fle	d ₁₀ -Flu	0.28
1,2-Br ₂ -Any	d ₁₀ -Flu	0.01
3-Br-Phe	d ₁₀ -Flu	0.003
1-Br-Ant	d ₁₀ -Pyr	0.01
1,4-Cl ₂ -Ant	d ₁₀ -Pyr	0.004
5,6-Br ₂ -Ana	d ₁₀ -Pyr	0.11
2,7-Br ₂ -Fle	d ₁₀ -Pyr	0.30
3-Br-Flu	d ₁₂ -BaA	0.11
9,10-Br ₂ -Ant	d ₁₂ -BaA	0.11
4-Br-Pyr	d ₁₂ -Chr	0.001
9-Br-1,5-Cl ₂ -Ant	d ₁₂ -BbF	0.11

1,5,9,10-Cl ₄ -Ant	d ₁₂ -BbF	0.09
1,6-Br ₂ -Pyr	d ₁₂ -BaP	0.29
4-Br-BaA	d ₁₂ -BaP	0.21
2,3,9,10-Br ₄ -Ant	d ₁₂ -Ind	0.01
<u>HHPACs</u>		
Quinoline	d ₈ -Nap	0.0001
Isoquinoline	d ₈ -Nap	0.11
Indole	d ₈ -Nap	0.38
2-Methylquinoline	d ₈ -Nap	0.00001
4-Methylbenzothiophene	d ₈ -Nap	0.00001
3-Methylisoquinoline	d ₈ -Nap	0.01
2,3-Dimethylbenzothiophene	d ₈ -Nap	0.01
2,5-Dimethyl-1-phenylpyrrole	d ₈ -Nap	0.02
4-Phenylpyridine	d ₈ -Nap	0.35
2,3-Dimethylindole	d ₈ -Nap	0.14
Dibenzofuran	d ₈ -Nap	0.05
2,3,4-Trimethylbenzothiophene	d ₁₀ -Fle	0.08
2-Methyldibenzofuran	d ₁₀ -Fle	0.01
Benzo[<i>h</i>]quinoline	d ₁₀ -Phe	0.30
1,2,3,4-Tetrahydrocarbazole	d ₁₀ -Phe	0.12
Acridine	d ₁₀ -Phe	0.001
9-Methylcarbazole	d ₁₀ -Phe	0.14
Carbazole	d ₁₀ -Phe	0.03

3-Methylbenzo[<i>f</i>]quinoline	d ₁₀ -Phe	0.13
2-Methylacridine	d ₁₀ -Phe	0.12
3,6-Dimethylcarbazole	d ₁₀ -Phe	0.09
Benzo[<i>b</i>]naphtho[2,3- <i>d</i>]furan	d ₁₀ -Phe	0.29
3-Tert-butyl-9H-carbazole	d ₁₀ -Pyr	0.04
9-Phenylcarbazole	d ₁₀ -Pyr	0.31
7,8,9,10-Tetrahydro-benzo[<i>b</i>]naphtho[2,3- <i>d</i>]thiophene	d ₁₀ -Pyr	0.26
Benz[<i>c</i>]acridine	d ₁₀ -Pyr	0.37
11H-Benzo[<i>a</i>]carbazole	d ₁₂ -Chr	0.09
7H-Benzo[<i>c</i>]carbazole	d ₁₂ -Chr	0.03
6-Methylbenzo[<i>b</i>]naphtho[2,1- <i>d</i>]thiophene	d ₁₂ -BaA	0.39
2-Phenyldibenzothiophene	d ₁₂ -BbF	0.01
Dinaphtho[1,2- <i>b</i> ;1',2'- <i>d</i>]furan	d ₁₂ -BkF	0.20
Dibenz[<i>c,h</i>]acridine	d ₁₂ -BghiP	0.11
13(H)-Dibenzo[<i>a,i</i>]carbazole	d ₁₂ -BghiP	0.39
Dibenzothiophene	d ₁₀ -Phe	0.45
2-Methyldibenzothiophene	d ₁₀ -Phe	0.25
1,2-Dimethyldibenzothiophene	d ₁₀ -Pyr	0.02
4-n-Propyldibenzothiophene	d ₁₀ -Pyr	0.01
4,6-Diethyldibenzothiophene	d ₁₀ -Pyr	0.15
Benzo[<i>b</i>]naphtho[1,2- <i>d</i>]thiophene	d ₁₀ -Pyr	0.12
HHPACs		

2,3-Br ₂ -thiophene	d ₁₀ -Fle	0.002
2-Cl-quinoline	d ₁₀ -Fle	0.02
2-Br-benzothiophene	d ₁₀ -Fle	0.01
2,3-Cl ₂ -benzothiophene	d ₁₀ -Fle	0.004
2-Br-quinoline	d ₁₀ -Fle	0.07
5-Cl-indole	d ₁₀ -Fle	0.02
3-Br-isoquinoline	d ₈ -Nap	0.36
5-Br-indole	d ₈ -Nap	0.12
2,3-Br ₂ -benzothiophene	d ₁₀ -Phe	0.29
9-Cl-acridine	d ₁₀ -Phe	0.44
2-Br-dibenzothiophene	d ₁₀ -Phe	0.03
9-Br-acridine	d ₁₀ -Phe	0.29
3,6-Cl ₂ -9H-carbazole	d ₁₀ -Pyr	0.49
2,8-Br ₂ -dibenzothiophene	d ₁₀ -Pyr	0.13
3,6-Br ₂ -carbazole	d ₁₂ -Chr	0.002

35 ^aStudent *t*-test results (one-tailed, paired) for concentration of analytes by dMRM and MRM method at low concentration level.
36

37 **Table SI6.** Statistical result of dMRM and MRM methods for the analysis of PACs in standard reference materials.

Analyte ^a	<i>p</i> value ^b
<u>SRM-1944</u>	
Ace	0.481
Acy	n.a.
Ant	0.031
BaA*	0.024
BaP*	0.176
BbF*	0.101
BghiP*	0.084
BkF*	0.070
Chr*	0.059
DahA*	0.426
Flu*	0.003
Fle	0.179
Ind*	0.068
Nap	0.148
Phe*	0.420
Pyr*	0.438
1,7-Dimethyl-Phe	0.125
1,8-Dimethyl-Phe	0.298

1-Methyl-Nap	0.042
1-Methyl-Phe	0.007
2,6-Dimethyl-Phe	0.122
2-Methyl-Nap	0.200
2-Methyl-Phe	0.001
3-Methyl-Phe	0.001
<u>BS-317</u>	
Ace	0.019
Acy	0.016
Ant	0.139
BaA*	0.006
BaP*	0.099
BbF*	0.258
BghiP*	0.051
BkF*	0.167
Chr*	0.016
DahA	0.021
Flu*	0.023
Fle	0.041
Ind	0.204
Nap	0.033
Phe*	0.407

Pyr*	0.007
1-Methyl-Nap	0.013
1-Methyl-Phe*	0.017
2-Methyl-Nap	0.010
2-Methyl-Phe*	0.001
C2-Phe*	0.001
<u>In-House RM</u>	
Ace	0.003
Acy	0.216
Ant	0.288
BaA	0.047
BaP	0.290
BbF	0.455
BghiP	0.185
BkF	0.180
Chr	0.043
DahA	0.043
Flu	0.066
Fle	0.400
Ind	0.469
Nap	0.420
Phe	0.365

Pyr	0.103
1,7-Dimethyl-Phe	0.108
1,8-Dimethyl-Phe	0.219
1-Methyl-Nap	0.013
1-Methyl-Phe	0.400
2,6-Dimethyl-Phe	0.041
2-Methyl-Nap	0.019
2-Methyl-Phe	0.060
3,6-Dimethyl-Phe	0.018
3-Methyl-Phe	0.136
9-Methyl-Phe	0.025
5-Methyl-Chr	0.377
6-Ethyl-Chr	0.058
1,4-Dimethyl-Nap	0.226
1,3-Dimethyl-Phe	0.143
6-n-Propyl-Chr	0.438
2,3,5-Trimethyl-Nap	0.332
1,2,6-Trimethyl-Phe	0.254
6-n-Propyl-Chr	0.189
1,4,6,7-Tetramethyl-Nap	0.035
1,2,6,9-Tetramethyl-Phe	0.088
Retene	0.276

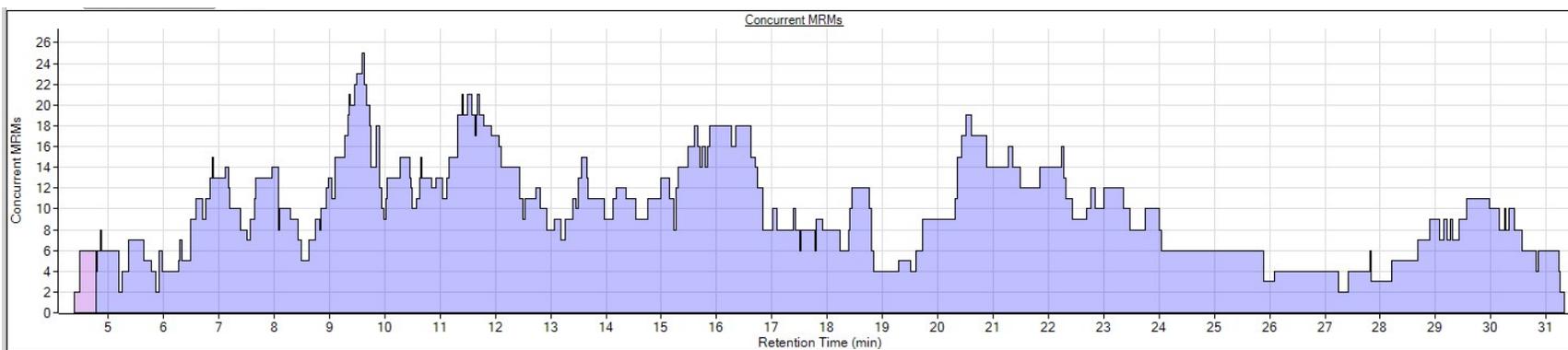
6-Methyl-Bap	0.055
1-Methyl-Fle	0.491
1-Methyl-Pyr	0.357
7,10-Dimethyl-Bap	0.487
9-Ethyl-Fle	0.029
1-Ethyl-Pyr	0.145
9-n-Propyl-Fle	0.128
1-n-Propyl-Pyr	0.313
9-n-Butyl-Fle	0.079
1-n-Butyl-Pyr	0.486
Dibenzothiophene	0.118
2-Methyldibenzothiophene	0.258
1,2-Dimethyldibenzothiophene	0.360
4-n-Propyldibenzothiophene	0.390
4,6-Diethyldibenzothiophene	0.007
Benzo[<i>b</i>]naphtho[1,2- <i>d</i>]thiophene	0.379
Benzo[<i>b</i>]naphtho[2,3- <i>d</i>]thiophene	0.391

38 ^aCertified analytes are in bold and denoted by *.

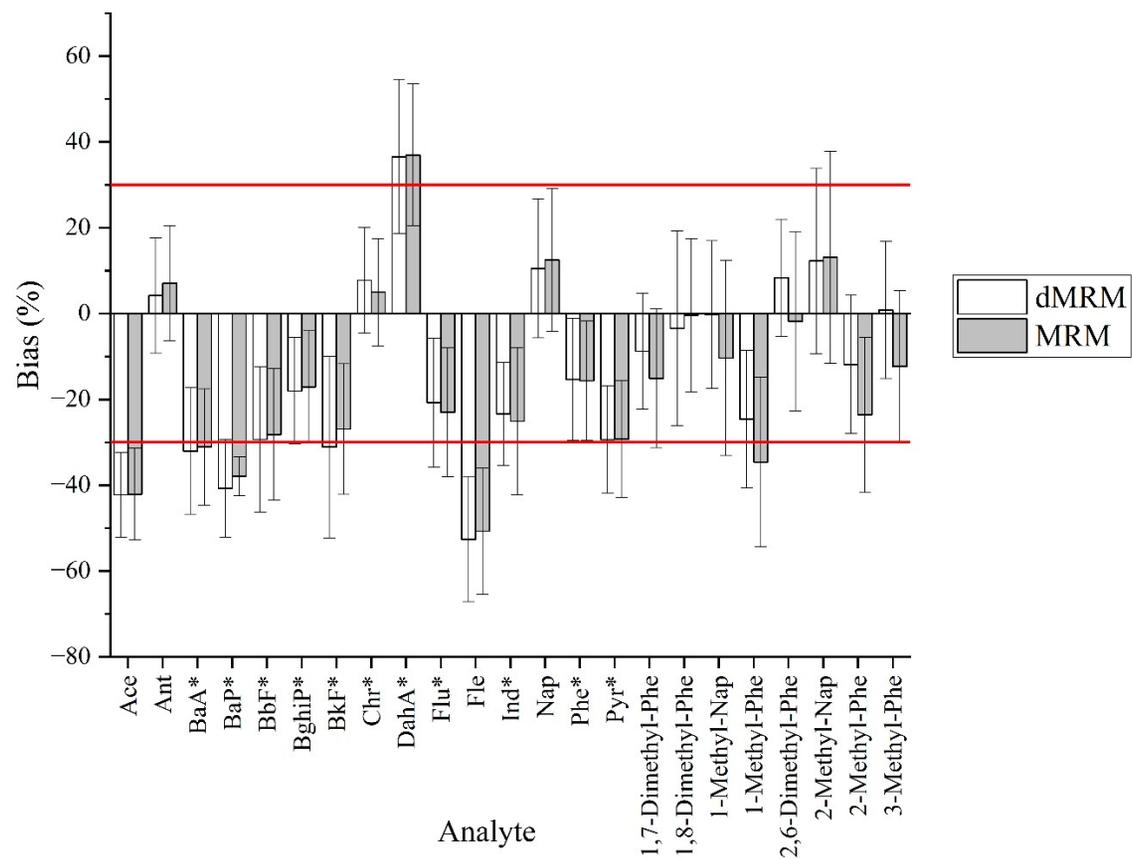
39 ^bStudent *t*-test results (one-tailed, paired) for recoveries of analytes by dMRM and MRM method.

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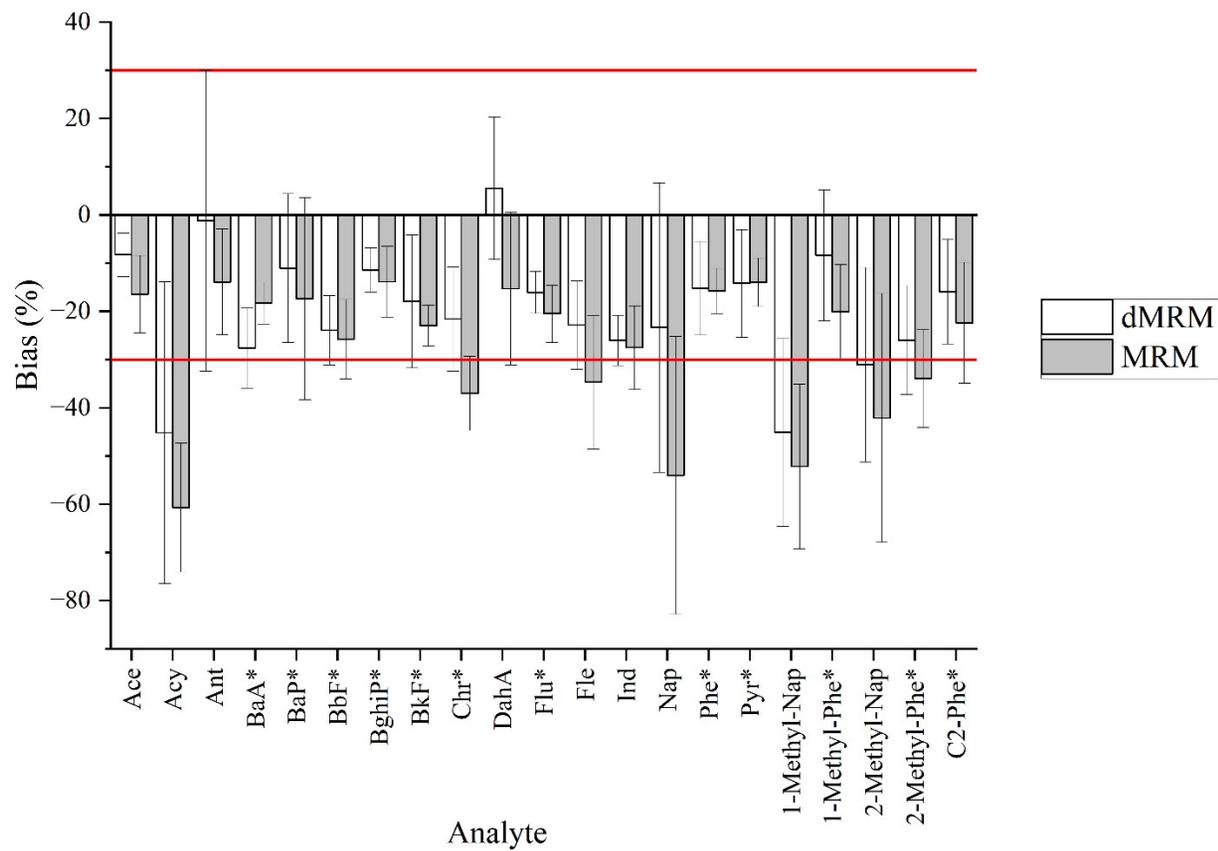
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43 **Figure S11.** Transition concurrency across GC gradient of dMRM method (generated by MassHunter GC/MS Acquisition).
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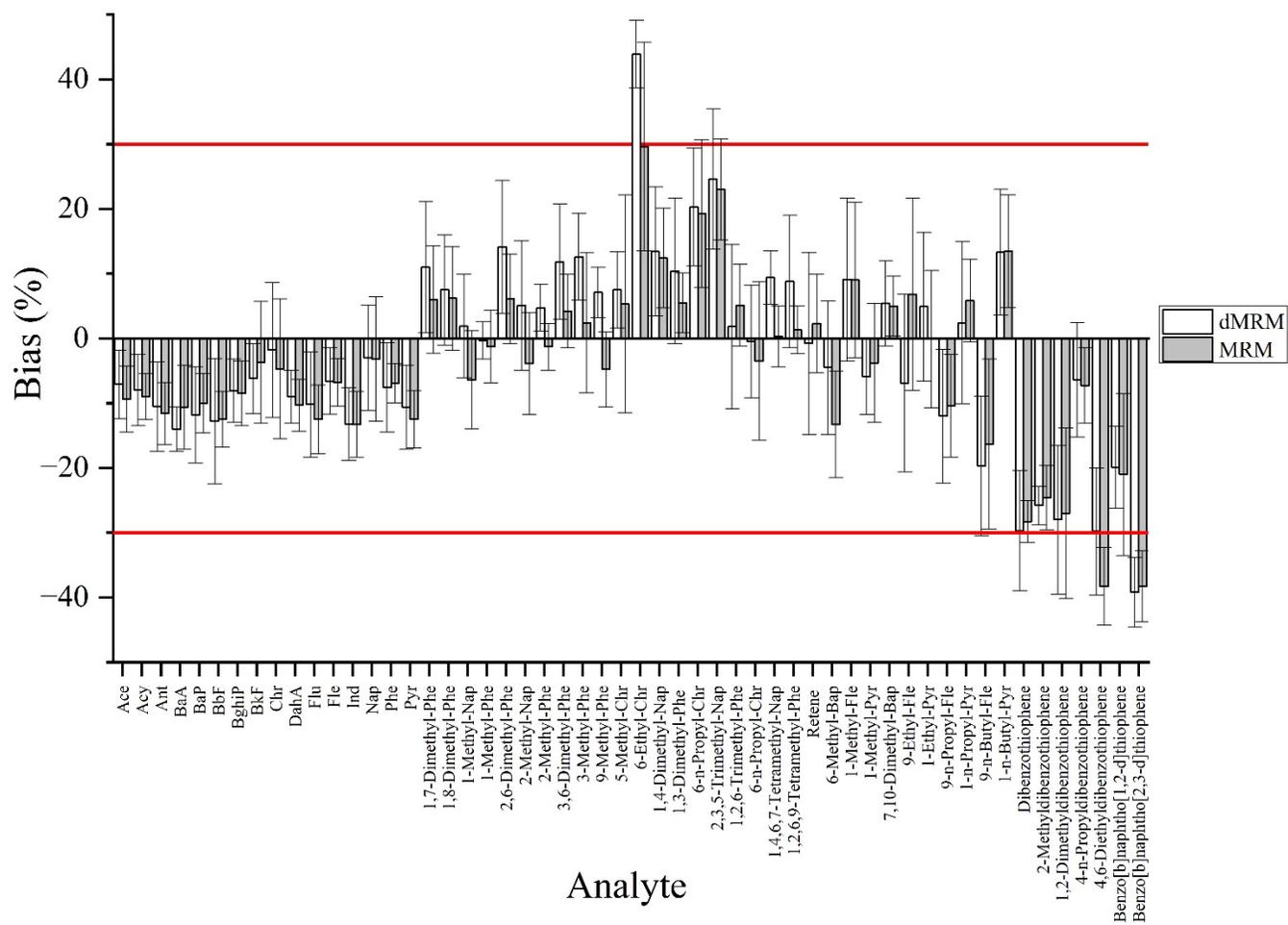
46 **Figure SI2.** Percent bias (average \pm SD, $n=5$) for PACs in SRM 1944 determined using dMRM and conventional MRM with the
 47 acceptable limits ($\pm 30\%$, certified value was denoted by *).

48



49

50 **Figure SI3.** Percent bias (average \pm SD, $n=5$) for PACs in BS-317 determining using dMRM and conventional MRM with the
 51 acceptable limits ($\pm 30\%$, certified value was denoted by *).



52

53 **Figure SI4.** Percent bias (average \pm SD, $n=5$) for PACs in our in-house egg reference material determined using dMRM and

54 convention MRM with acceptable limits ($\pm 30\%$).

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