LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082124\
Data File : BM047303.D
Acq On : 21 Aug 2024 18:25
Operator : RC/JU
Sample : P3617-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VCPS-B4-081424-0-10

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047303.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.258	60	63	76	rBV	149196	223025	3.41%	0.404%
2	4.563	280	285	296	rVB	120966	176211	2.69%	0.319%
3	5.010	355	361	378	rBV	1888193	2774306	42.41%	5.022%
4	6.569	619	626	641	rBV	1833796	2947498	45.06%	5.336%
5	6.987	694	697	707	rBV	45381	87009	1.33%	0.158%
6	7.351	752	759	769	rBV	821935	1275219	19.50%	2.308%
7	8.498	947	954	964	rBV	1191673	1962343	30.00%	3.552%
8	10.110	1220	1228	1244	rBV	1005227	1728024	26.42%	3.128%
9	10.875	1351	1358	1371	rBV	142445	314399	4.81%	0.569%
10	12.616	1648	1654	1672	rBV	2880051	4385550	67.05%	7.939%
11	13.733	1839	1844	1853	rVB	77407	128525	1.96%	0.233%
12	14.016	1885	1892	1900	rBV	1572655	2345346	35.86%	4.246%
13	14.245	1926	1931	1933	rBV2	121446	168645	2.58%	0.305%
14	14.269	1933	1935	1941	rVB	138101	156726	2.40%	0.284%
15	15.521	2141	2148	2160	rBV	2606076	3948323	60.36%	7.147%
16	16.774	2356	2361	2366	rBV	1927806	2870272	43.88%	5.196%
17	16.821	2366	2369	2373	rVB	403875	520043	7.95%	0.941%
18	16.910	2380	2384	2390	rVB	87704	125859	1.92%	0.228%
19	17.198	2424	2433	2436	rBV2	41375	91405	1.40%	0.165%
20	17.486	2479	2482	2489	rVB2	49980	74600	1.14%	0.135%
21	17.657	2506	2511	2515	rBV	77348	118785	1.82%	0.215%
22	17.715	2515	2521	2529	rBV2	590587	916208	14.01%	1.659%
23	17.851	2539	2544	2547	rBV2	83239	141945	2.17%	0.257%
24	17.886	2548	2550	2557	rVB	58328	77363	1.18%	0.140%
25	18.127	2587	2591	2594	rBV	67596	91306	1.40%	0.165%
26	18.168	2594	2598	2602	rVV	68574	95643	1.46%	0.173%
27	18.215	2602	2606	2611	rVB	68762	92845	1.42%	0.168%
28	18.592	2666	2670	2674	rBV	54185	79544	1.22%	0.144%
29	18.657	2677	2681	2683	rBV2	50299	65639	1.00%	0.119%
30	18.733	2690	2694	2699	rBV2	65186	110714	1.69%	0.200%
31	18.857	2709	2715	2720	rBV	1420765	1949526	29.81%	3.529%
32	19.015	2737	2742	2747	rBV2	266383	404071	6.18%	0.731%
33	19.151	2762	2765	2769	rBV	146130	181580	2.78%	0.329%
34	19.221	2769	2777	2786	rVV2	1127800	1795874	27.46%	3.251%
35	19.298	2787	2790	2797	rVB2	63697	107436	1.64%	0.194%
36	19.409	2806	2809	2810	rBV	91267	91329	1.40%	0.165%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082124\
Data File : BM047303.D
Acq On : 21 Aug 2024 18:25
Operator : RC/JU
Sample : P3617-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VCPS-B4-081424-0-10

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.445	2810	2815	2820	rVV	5456526	6540862	100.00%	11.840%
38	19.562	2829	2835	2841	rBV2	101507	250606	3.83%	0.454%
39	19.692	2853	2857	2860	rBV3	94579	165640	2.53%	0.300%
40	19.733	2861	2864	2869	rVB	147115	194478	2.97%	0.352%
41	19.833	2878	2881	2885	rBV2	80567	92663	1.42%	0.168%
42	19.886	2886	2890	2895	rVB2	152111	225909	3.45%	0.409%
43	20.074	2919	2922	2925	rBV	54593	80534	1.23%	0.146%
44	20.486	2989	2992	2997	rVB	195481	246002	3.76%	0.445%
45	20.651	3016	3020	3024	rBV2	168684	245241	3.75%	0.444%
46	20.692	3024	3027	3030	rBV	132492	181783	2.78%	0.329%
47	20.756	3034	3038	3041	rVV3	257513	325054	4.97%	0.588%
48	21.015	3075	3082	3086	rBV2	2704394	4611239	70.50%	8.347%
49	21.056	3086	3089	3100	rVB	949977	1308130	20.00%	2.368%
50	22.303	3297	3301	3309	rVB4	237462	417299	6.38%	0.755%
51	22.609	3350	3353	3359	rVB	274750	414519	6.34%	0.750%
52	22.868	3392	3397	3404	rBV	612376	1583377	24.21%	2.866%
53	23.045	3422	3427	3441	rVB2	359071	1158495	17.71%	2.097%
54	23.462	3494	3498	3508	rVB	325248	701955	10.73%	1.271%
55	23.586	3514	3519	3530	rVB2	458006	992826	15.18%	1.797%
56	23.709	3533	3540	3548	rBV	1282729	2883354	44.08%	5.219%

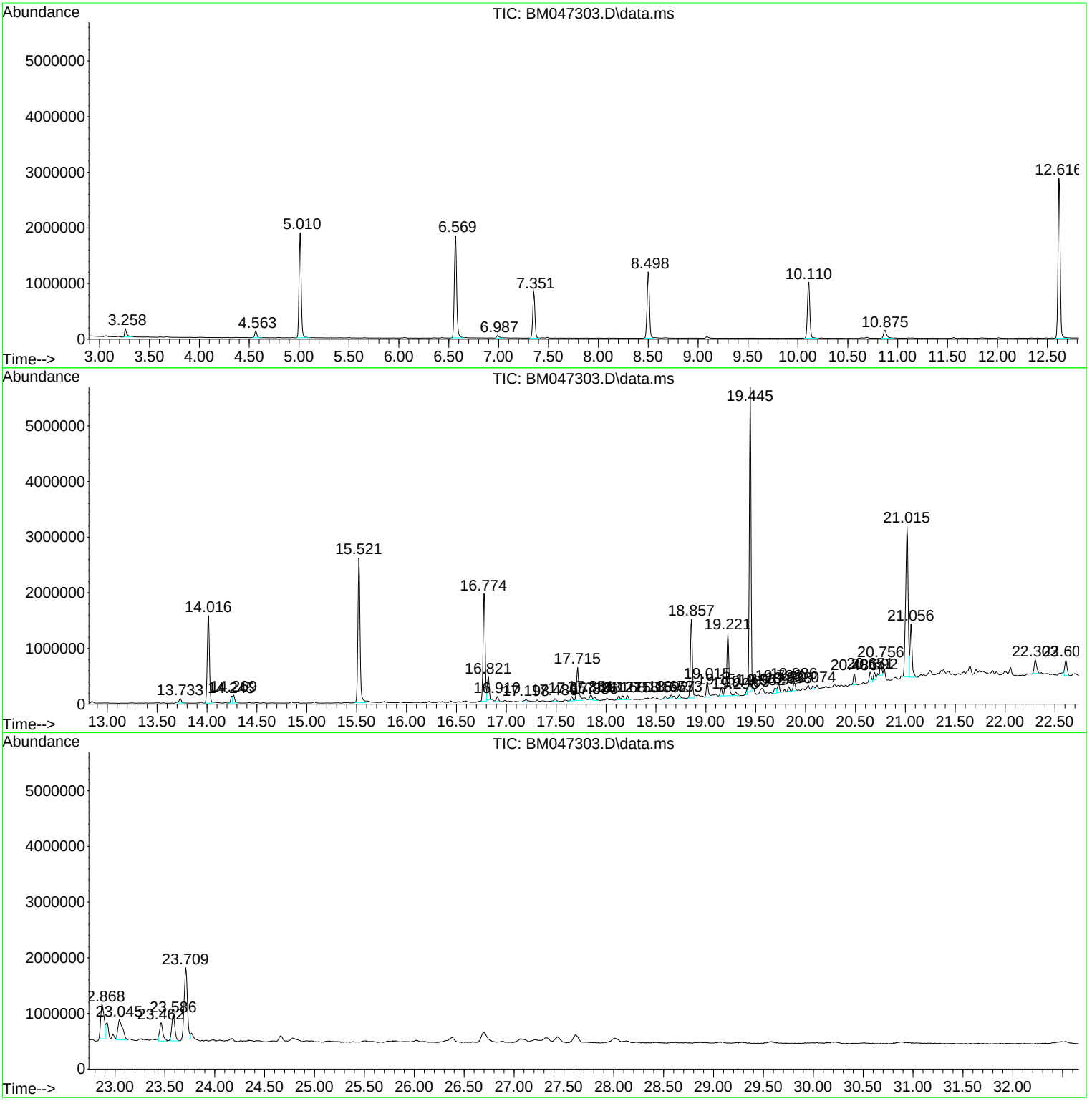
Sum of corrected areas: 55243102

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082124\
Data File : BM047303.D
Acq On : 21 Aug 2024 18:25
Operator : RC/JU
Sample : P3617-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VCPS-B4-081424-0-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082124\
Data File : BM047303.D
Acq On : 21 Aug 2024 18:25
Operator : RC/JU
Sample : P3617-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VCPS-B4-081424-0-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

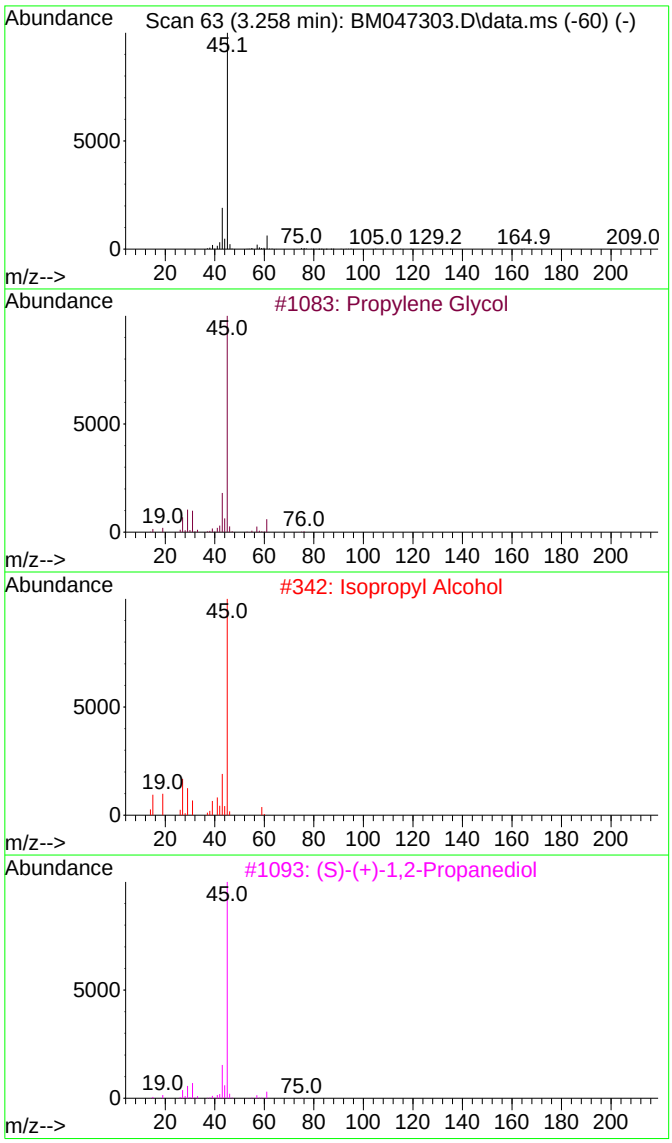
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

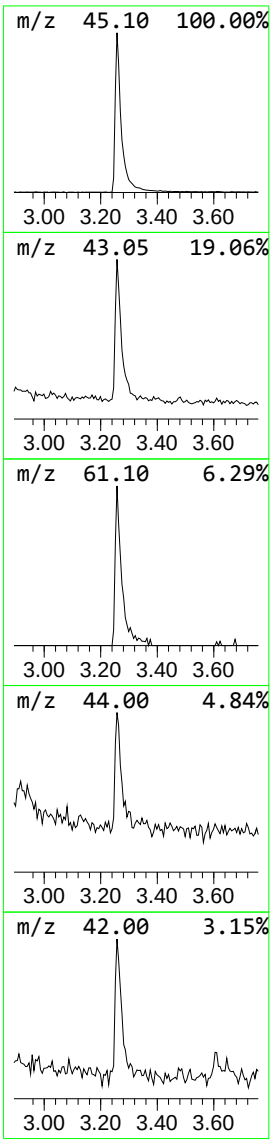
****

Peak Number 1 Propylene Glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.258	3.50 ng	223025	1,4-Dichlorobenzene-d4	7.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	78
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	40
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
4	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082124\
Data File : BM047303.D
Acq On : 21 Aug 2024 18:25
Operator : RC/JU
Sample : P3617-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VCPS-B4-081424-0-10

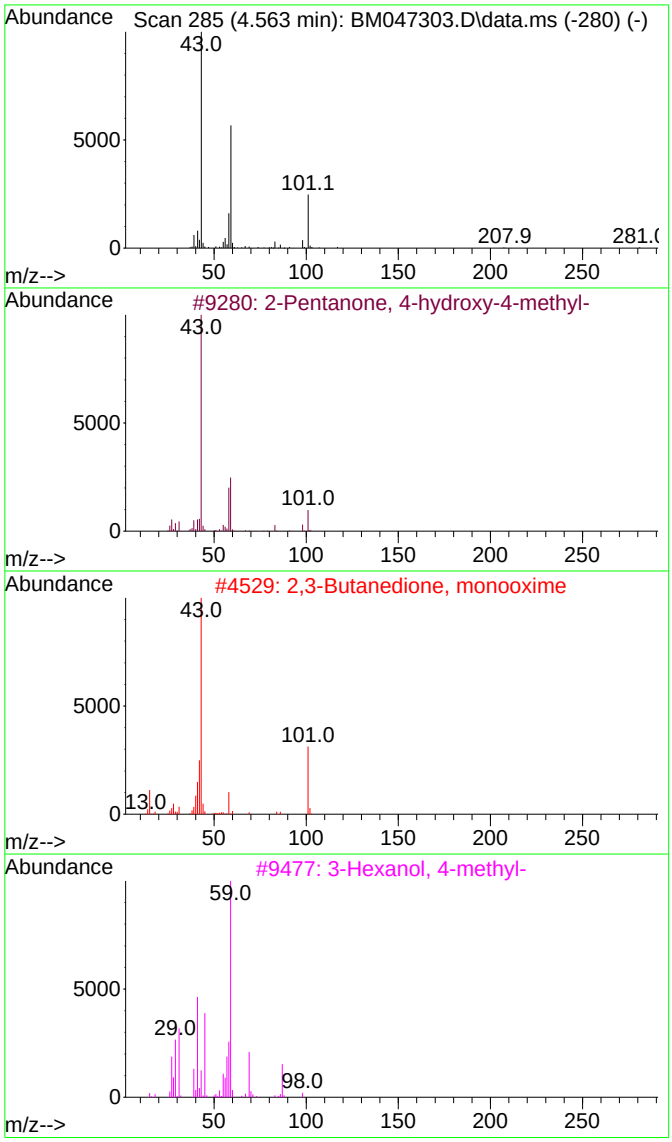
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

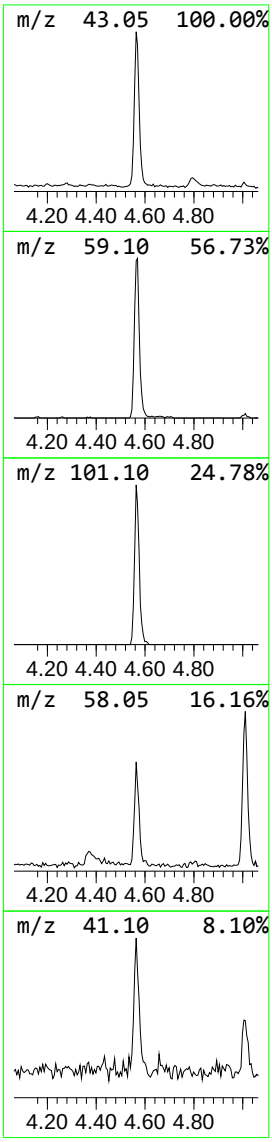
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.563	2.76 ng	176211	1,4-Dichlorobenzene-d4	7.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082124\
Data File : BM047303.D
Acq On : 21 Aug 2024 18:25
Operator : RC/JU
Sample : P3617-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VCPS-B4-081424-0-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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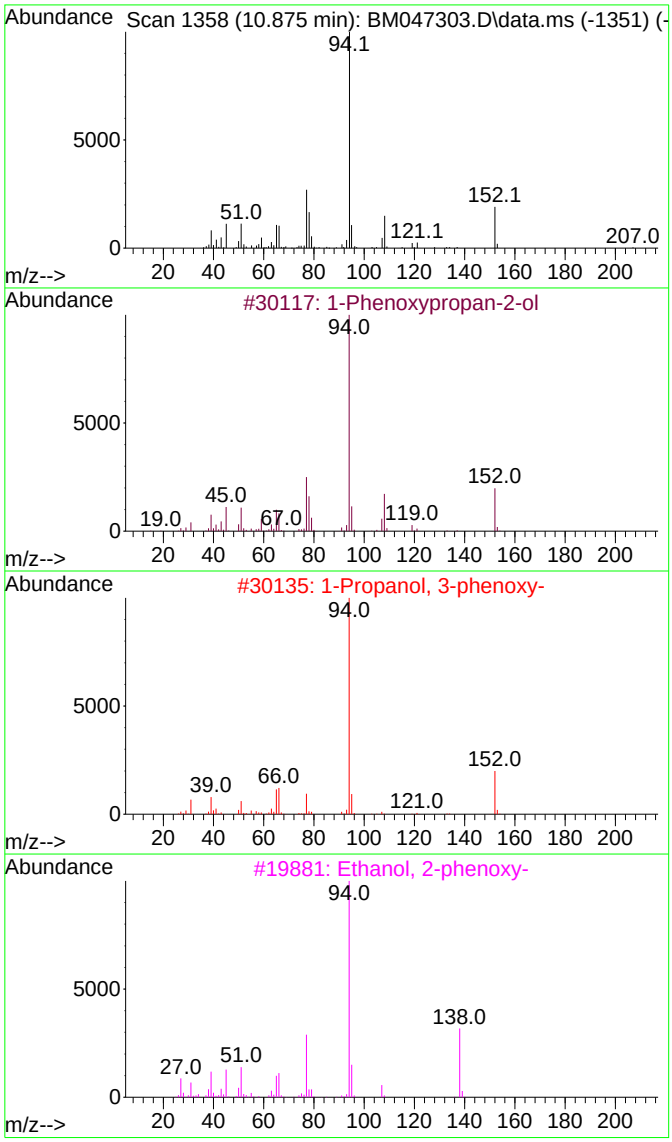
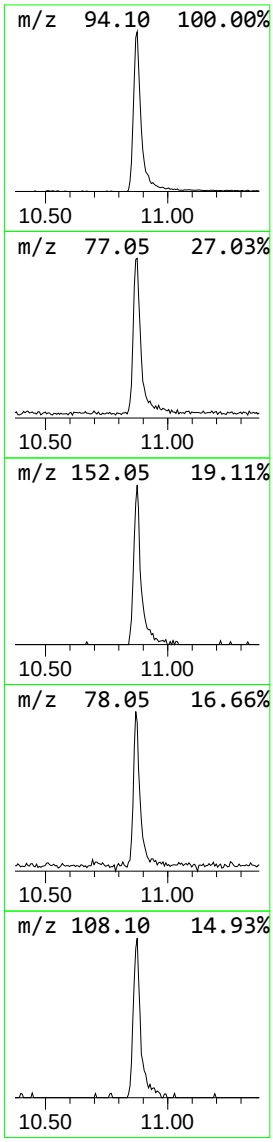
Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.875	3.64 ng	314399	Naphthalene-d8	10.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	76
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	59
4	Benzene, (4-chlorobutoxy)-	184	C10H13ClO	002651-46-9	53
5	3-Phenoxypropionic acid	166	C9H10O3	007170-38-9	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082124\
Data File : BM047303.D
Acq On : 21 Aug 2024 18:25
Operator : RC/JU
Sample : P3617-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VCPS-B4-081424-0-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

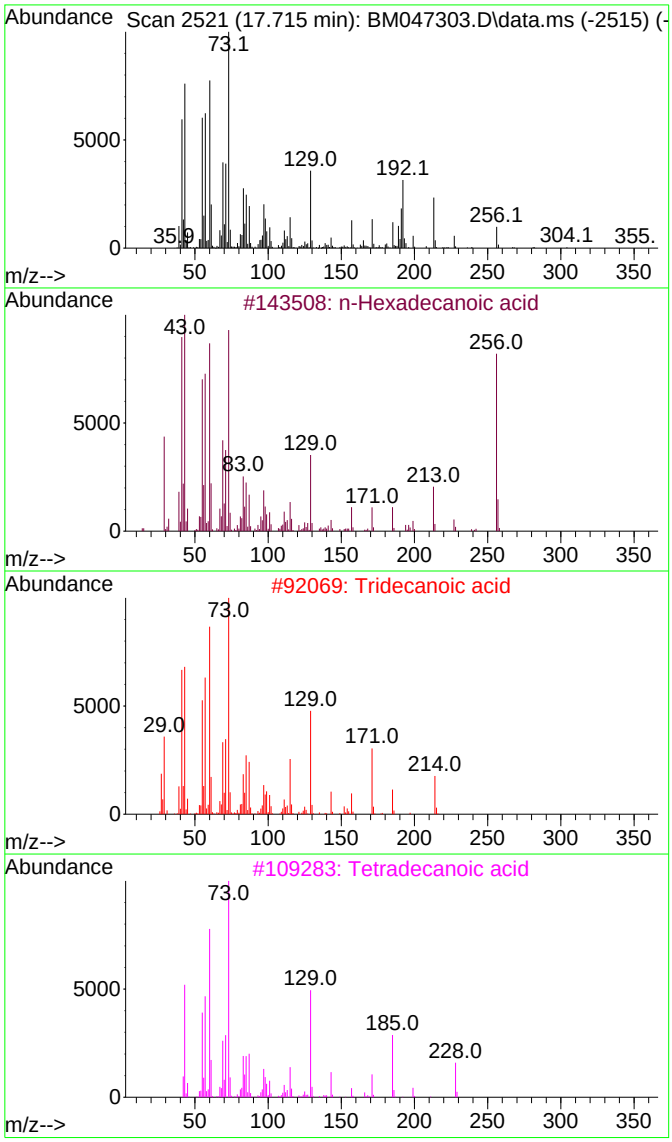
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

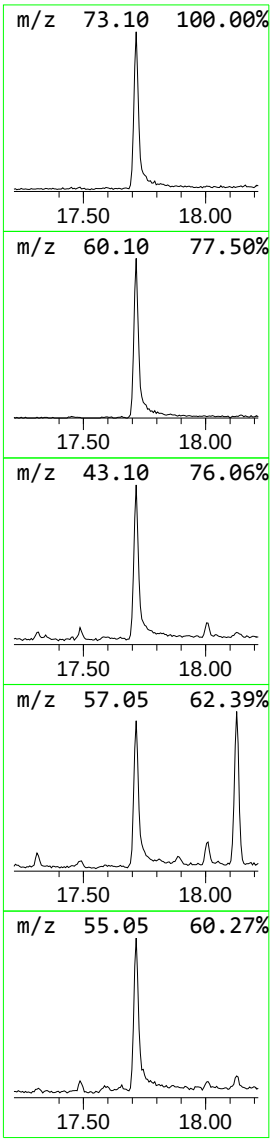
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.715	6.38 ng	916208	Phenanthrene-d10	16.780

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Octadecanoic acid	284	C18H36O2	000057-11-4	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082124\
Data File : BM047303.D
Acq On : 21 Aug 2024 18:25
Operator : RC/JU
Sample : P3617-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VCPS-B4-081424-0-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

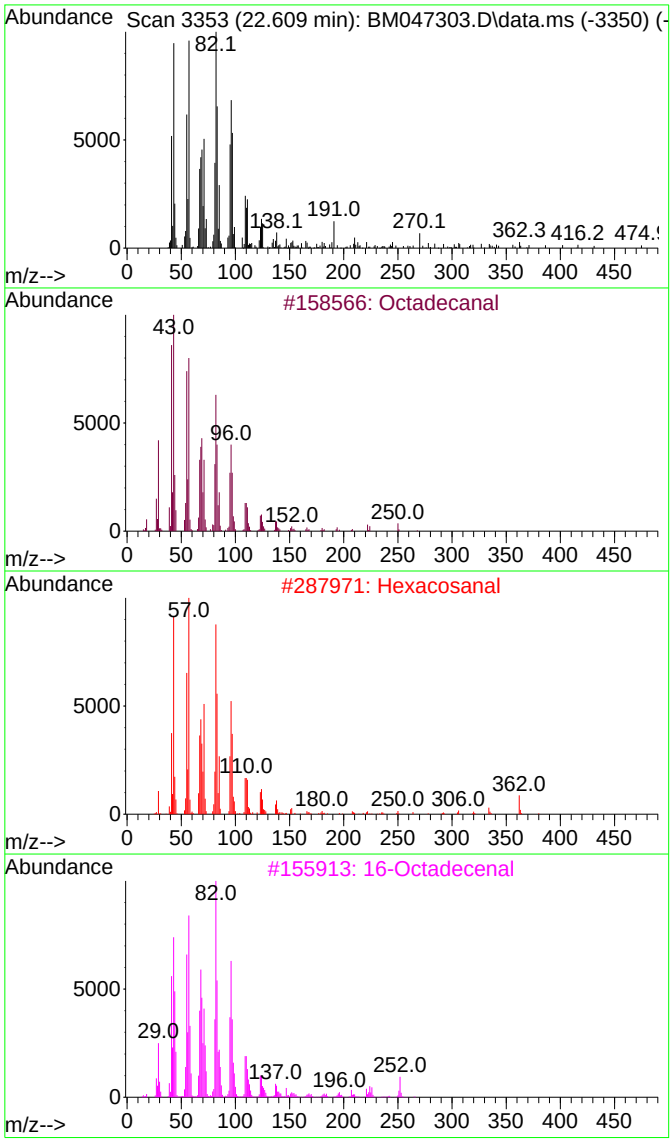
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

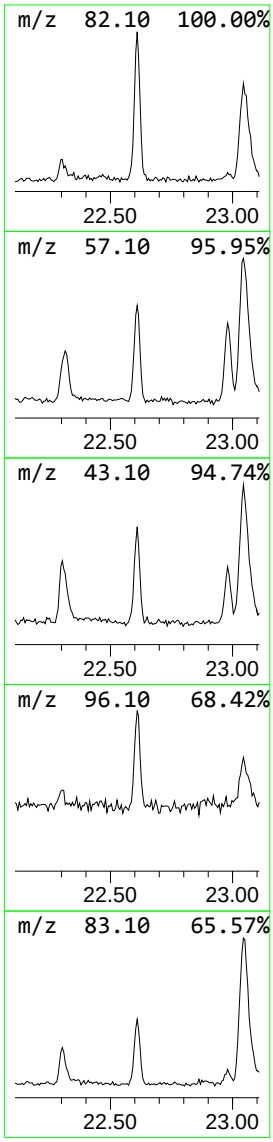
****

Peak Number 5 Octadecanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.609	2.88 ng	414519	Perylene-d12	23.709

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	91
2	Hexacosanal	380	C26H52O	026627-85-0	87
3	16-Octadecenal	266	C18H34O	056554-87-1	74
4	1,19-Eicosadiene	278	C20H38	014811-95-1	74
5	17-Octadecenal	266	C18H34O	056554-86-0	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082124\
Data File : BM047303.D
Acq On : 21 Aug 2024 18:25
Operator : RC/JU
Sample : P3617-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VCPS-B4-081424-0-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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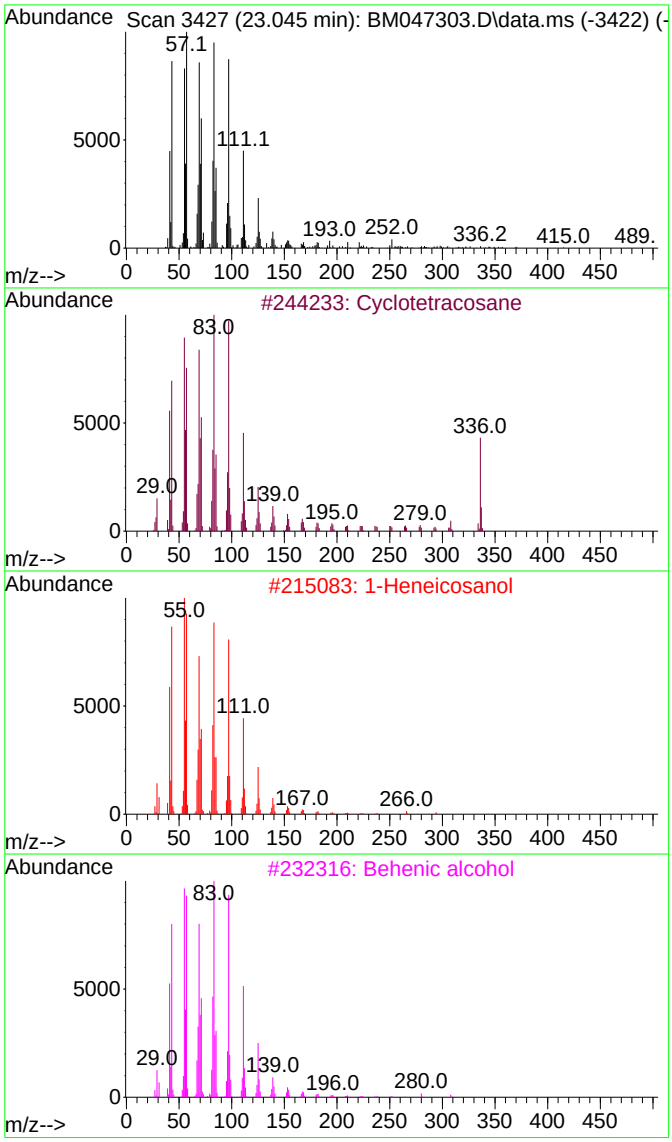
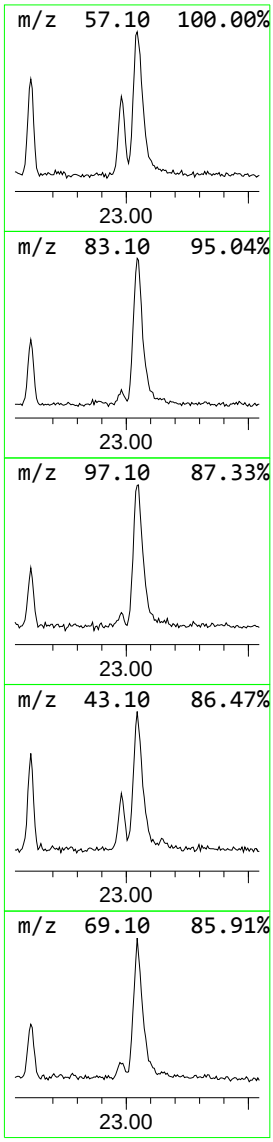
Peak Number 6 Cyclotetracosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.044	8.04 ng	1158500	Perylene-d12	23.709

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	98
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	1-Heptacosanol	396	C27H56O	002004-39-9	94
5	1-Hexacosene	364	C26H52	018835-33-1	93





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Data File : BM047303.D
Acq On : 21 Aug 2024 18:25
Operator : RC/JU
Sample : P3617-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VCPS-B4-081424-0-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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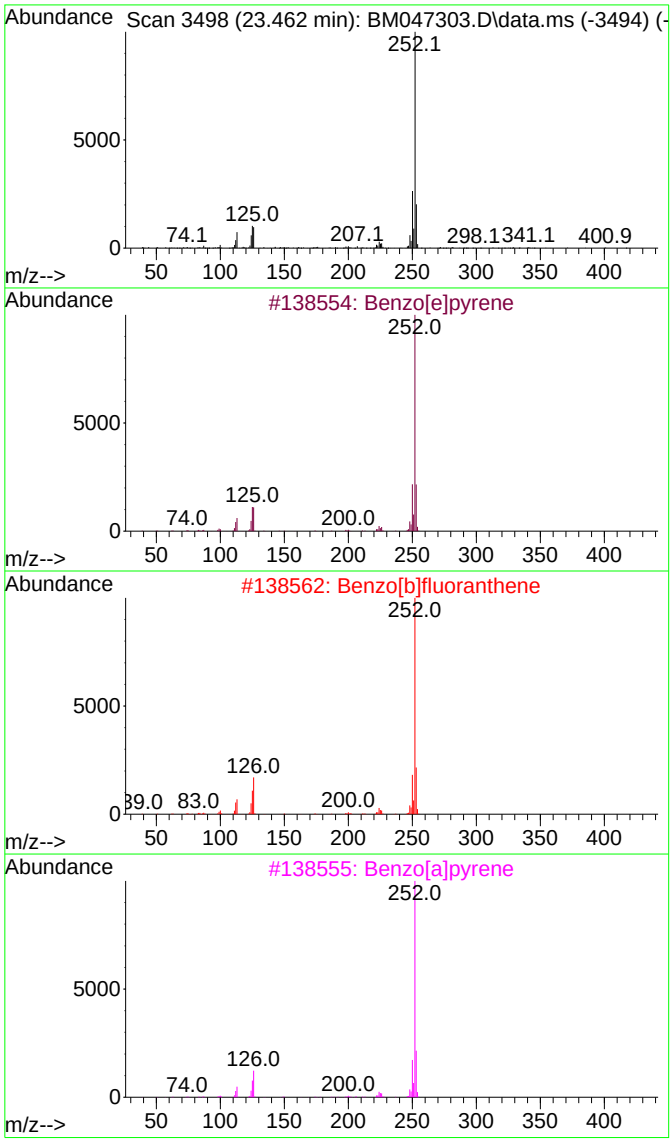
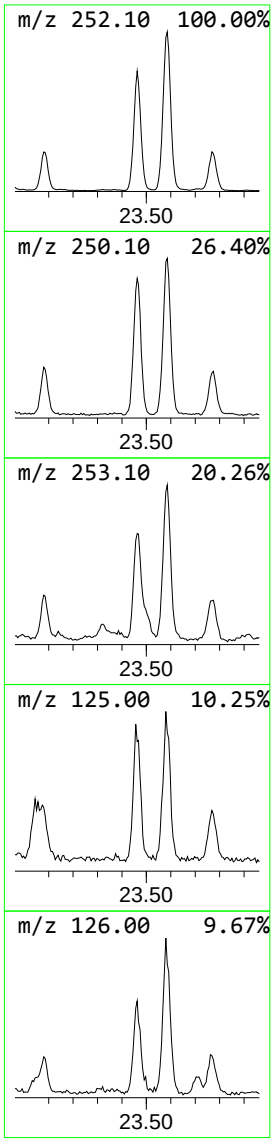
Peak Number 7 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.462	4.87 ng	701955	Perylene-d12	23.709

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
3	Benzo[a]pyrene	252	C20H12	000050-32-8	93
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	91
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082124\
Data File : BM047303.D
Acq On : 21 Aug 2024 18:25
Operator : RC/JU
Sample : P3617-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VCPS-B4-081424-0-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propylene Glycol	3.258	3.5	ng	223025	1	7.351	1275220	20.0
2-Pentanone, 4-...	4.563	2.8	ng	176211	1	7.351	1275220	20.0
1-Phenoxypropan...	10.875	3.6	ng	314399	2	10.110	1728020	20.0
n-Hexadecanoic ...	17.715	6.4	ng	916208	4	16.780	2870270	20.0
Octadecanal	22.609	2.9	ng	414519	6	23.709	2883350	20.0
Cyclotetracosane	23.044	8.0	ng	1158500	6	23.709	2883350	20.0
Benzo[e]pyrene	23.462	4.9	ng	701955	6	23.709	2883350	20.0