LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112922\
Data File : BG055833.D
Acq On : 29 Nov 2022 18:05
Operator : CG/JU
Sample : N5795-04 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-12

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_G\Methods\8270-BG111622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055833.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.280	332	339	349	rBV	206362	326074	23.66%	2.498%
2	5.761	412	421	430	rBV	307416	520391	37.76%	3.987%
3	6.378	520	526	534	rVB	12145	20043	1.45%	0.154%
4	7.371	688	695	707	rBV	310105	553130	40.14%	4.237%
5	8.223	834	840	848	rVB	187556	313524	22.75%	2.402%
6	9.398	1029	1040	1049	rBV	187199	341116	24.75%	2.613%
7	10.803	1270	1279	1299	rBV	31449	98519	7.15%	0.755%
8	11.055	1314	1322	1328	rBV	252716	456933	33.16%	3.500%
9	11.102	1328	1330	1338	rVB	9898	14091	1.02%	0.108%
10	13.470	1725	1733	1742	rBV	540390	812995	58.99%	6.228%
11	13.723	1771	1776	1782	rVB2	14197	22281	1.62%	0.171%
12	14.575	1915	1921	1933	rBV	23123	46104	3.35%	0.353%
13	14.845	1960	1967	1974	rBV	422980	657948	47.74%	5.040%
14	15.239	2028	2034	2040	rVB3	9851	15103	1.10%	0.116%
15	15.891	2139	2145	2153	rBV3	12104	22365	1.62%	0.171%
16	16.184	2190	2195	2202	rVB2	17544	29171	2.12%	0.223%
17	16.331	2214	2220	2229	rBV	444251	676068	49.06%	5.179%
18	17.113	2345	2353	2356	rBV5	10172	18692	1.36%	0.143%
19	17.248	2370	2376	2379	rBV5	6936	14155	1.03%	0.108%
20	17.307	2382	2386	2394	rVV5	11727	19951	1.45%	0.153%
21	17.589	2428	2434	2438	rBV	541427	811192	58.86%	6.214%
22	17.630	2438	2441	2448	rVB	131770	191995	13.93%	1.471%
23	17.718	2451	2456	2461	rBV	69985	103171	7.49%	0.790%
24	17.994	2496	2503	2504	rBV	12374	21310	1.55%	0.163%
25	18.217	2537	2541	2545	rBV	14328	19286	1.40%	0.148%
26	18.458	2576	2582	2586	rBV2	58254	119219	8.65%	0.913%
27	18.505	2586	2590	2595	rVB	52533	80674	5.85%	0.618%
28	18.588	2600	2604	2610	rVV	24121	35767	2.60%	0.274%
29	18.658	2610	2616	2619	rVV2	47684	99555	7.22%	0.763%
30	18.687	2619	2621	2626	rVB	24655	30144	2.19%	0.231%
31	18.858	2646	2650	2654	rBV4	18175	22104	1.60%	0.169%
32	18.946	2661	2665	2669	rBV	27726	37722	2.74%	0.289%
33	18.993	2671	2673	2678	rVB5	10817	13982	1.01%	0.107%
34	19.281	2719	2722	2726	rBV2	12047	14849	1.08%	0.114%
35	19.375	2731	2738	2742	rBV4	41461	99203	7.20%	0.760%
36	19.504	2756	2760	2769	rBV4	37672	62147	4.51%	0.476%

LSC Area Percent Report

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Acq On : 29 Nov 2022 18:05
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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TP-12

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_G\Methods\8270-BG111622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.628	2775	2781	2787	rBV	490320	687355	49.88%	5.266%
38	19.722	2793	2797	2801	rVB6	19832	30212	2.19%	0.231%
39	19.774	2804	2806	2810	rVB	22027	23775	1.73%	0.182%
40	19.951	2832	2836	2839	rBV2	70078	107550	7.80%	0.824%
41	19.992	2839	2843	2850	rVB	390392	544257	39.49%	4.169%
42	20.174	2868	2874	2879	rBV	930196	1211258	87.89%	9.279%
43	20.474	2922	2925	2930	rVB	87447	126600	9.19%	0.970%
44	20.573	2939	2942	2946	rVB2	52494	57471	4.17%	0.440%
45	21.249	3054	3057	3065	rVB	61207	106538	7.73%	0.816%
46	21.878	3156	3164	3169	rBV2	569420	1378126	100.00%	10.557%
47	21.925	3169	3172	3184	rVB	228390	398466	28.91%	3.053%
48	24.187	3551	3557	3564	rBV2	148099	456429	33.12%	3.497%
49	25.109	3708	3714	3723	rVB2	152644	417506	30.30%	3.198%
50	25.274	3734	3742	3751	rVB2	274703	767186	55.67%	5.877%

Sum of corrected areas: 13053703

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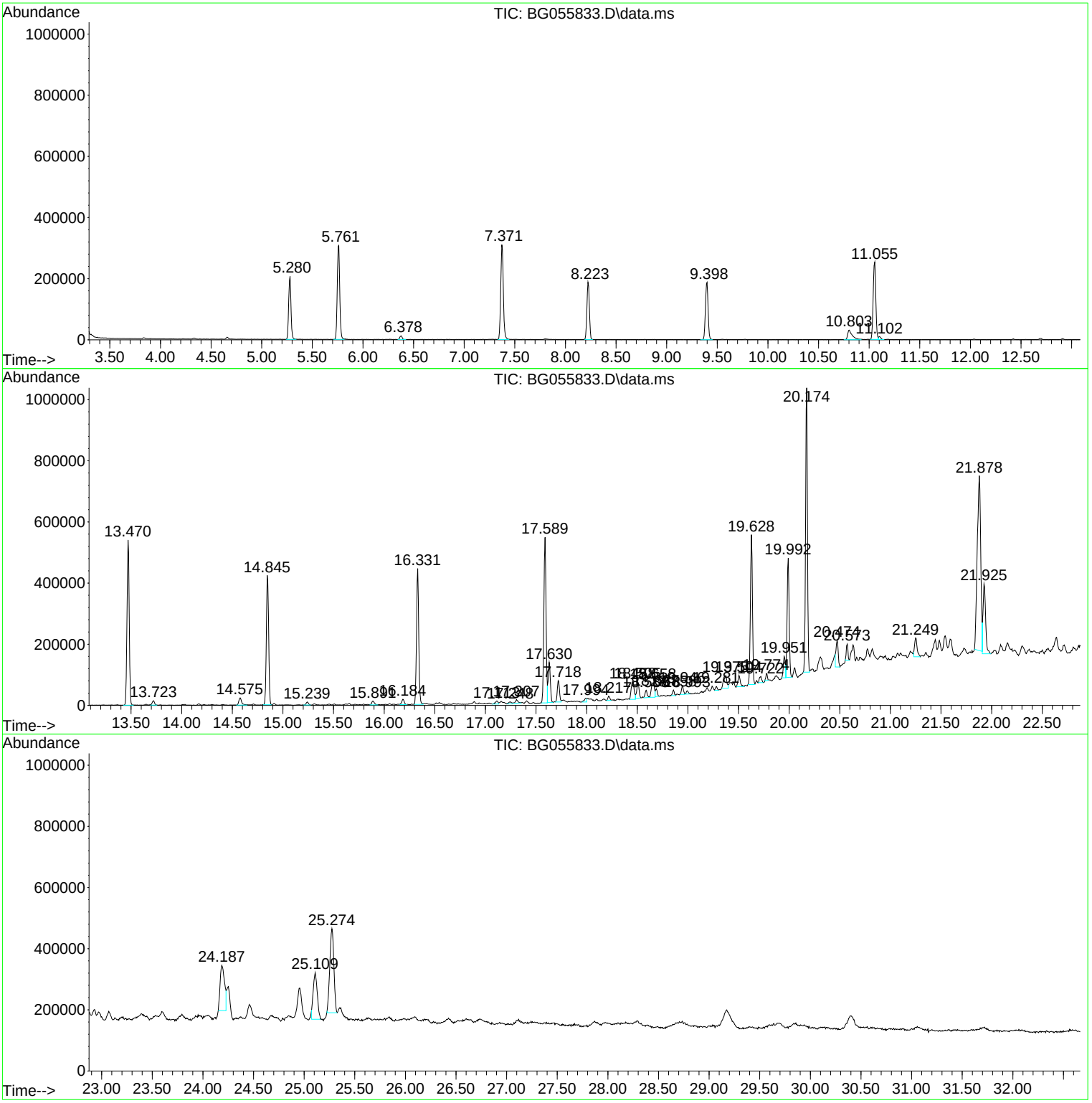
Instrument :
BNA_G
ClientSampleId :
TP-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.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_G\Data\BG112922\
Data File : BG055833.D
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Operator : CG/JU
Sample : N5795-04 2X
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Instrument :
BNA_G
ClientSampleId :
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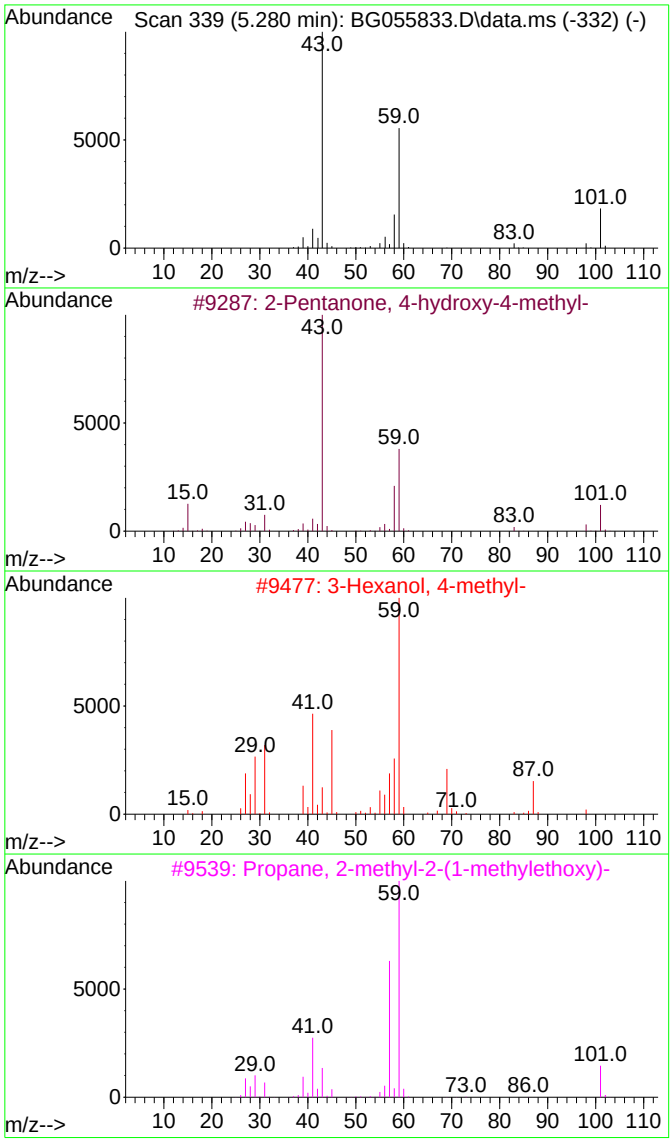
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

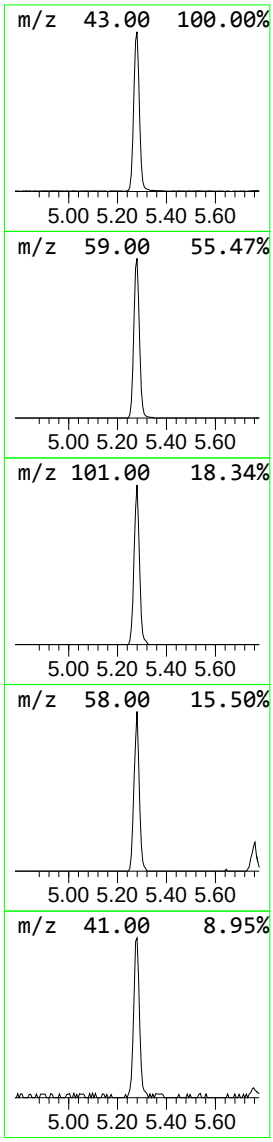
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.280	20.80 ng	326074	1,4-Dichlorobenzene-d4	8.223

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Instrument :
BNA_G
ClientSampleId :
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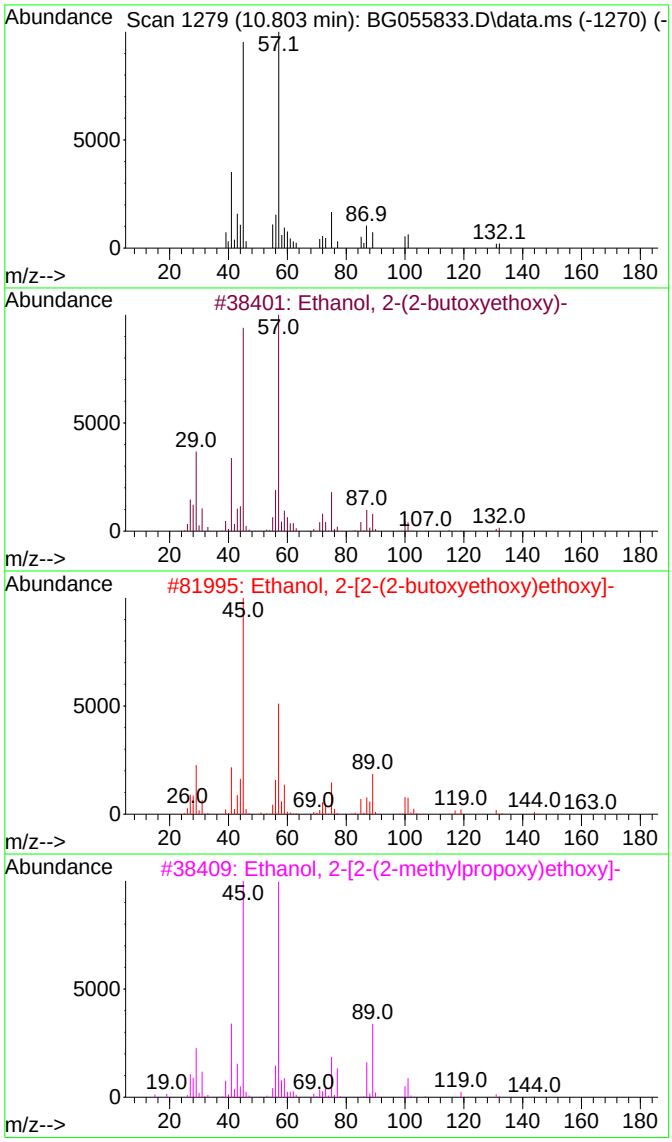
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

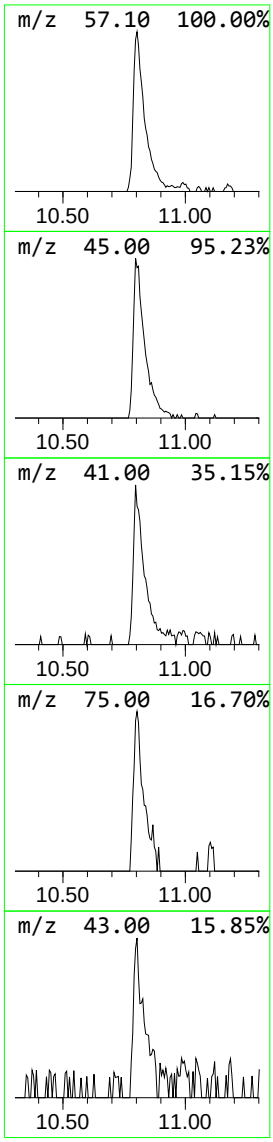
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.803	4.31 ng	98519	Naphthalene-d8	11.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	72
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
5	Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	50





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Data File : BG055833.D
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Misc :
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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

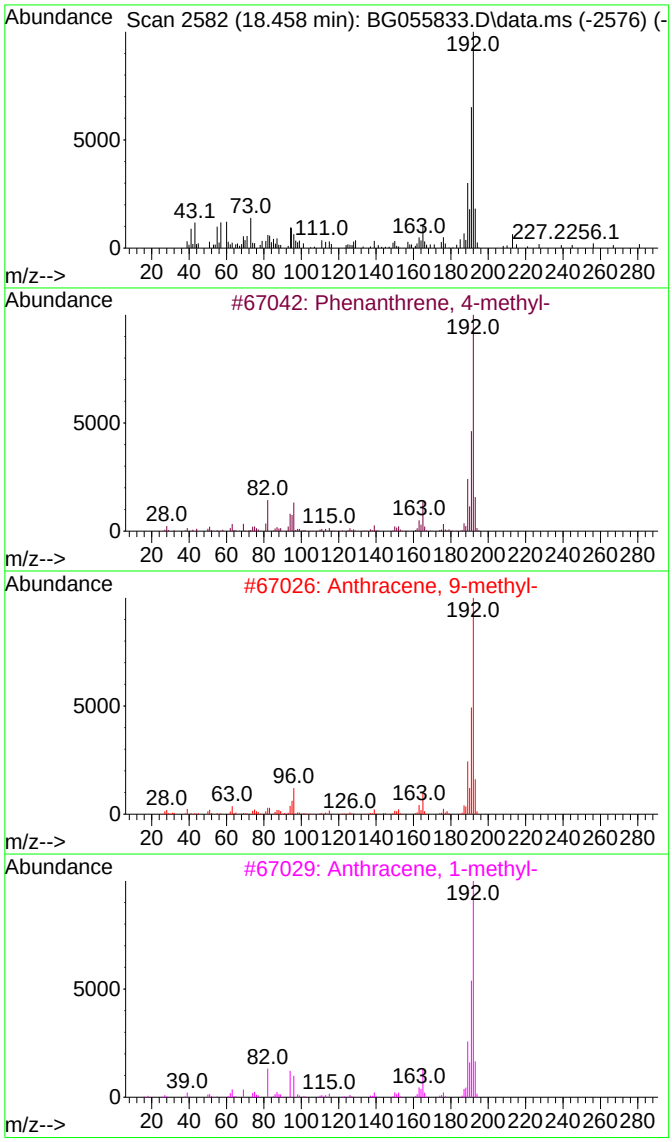
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

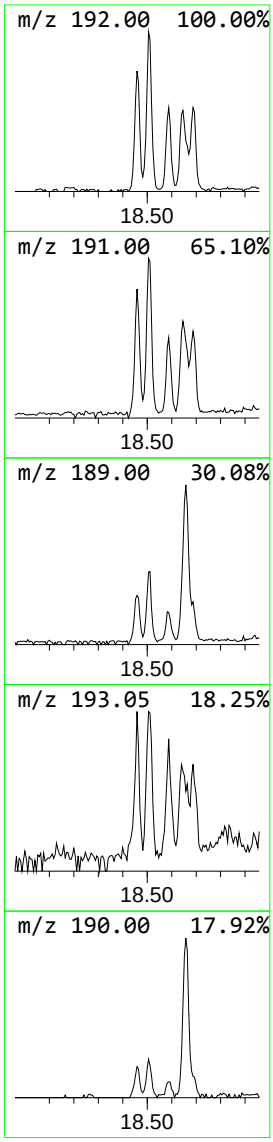
****

Peak Number 3 Phenanthrene, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.458	2.94 ng	119219	Phenanthrene-d10	17.589

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	90
2	Anthracene, 9-methyl-	192	C15H12	000779-02-2	90
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	89
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	89
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	89





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112922\
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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-12

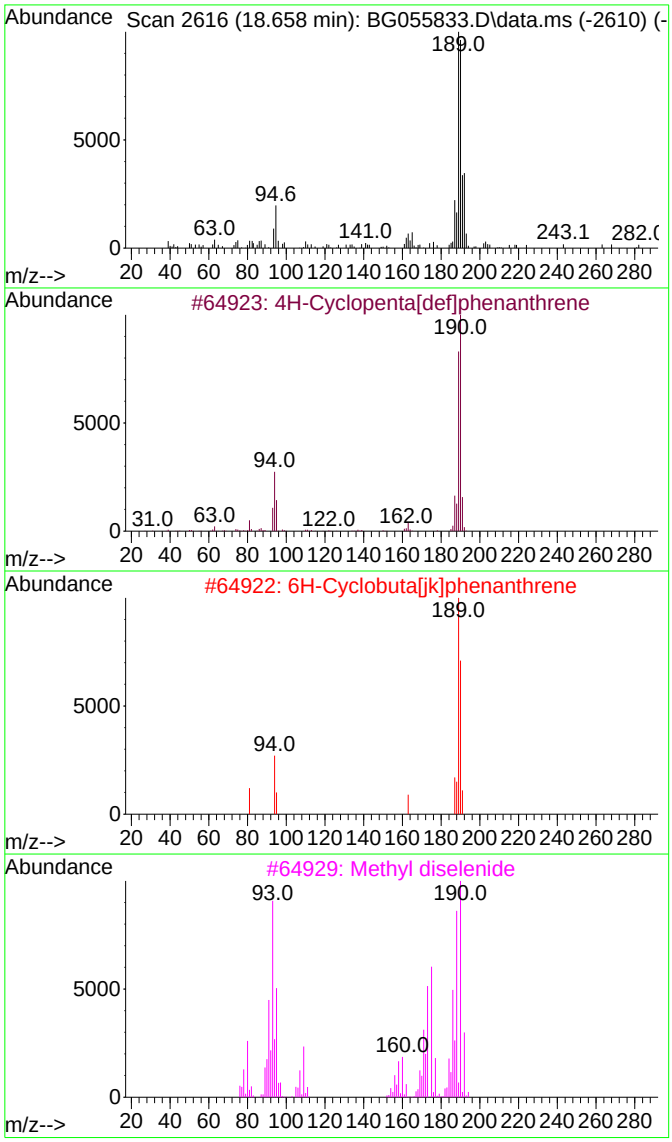
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

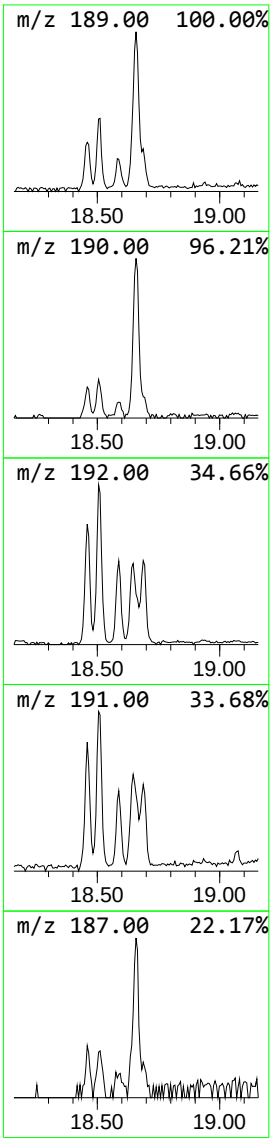
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.658	2.45 ng	99555	Phenanthrene-d10	17.589

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	72
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	64
3	Methyl diselenide	190	C2H6Se2	007101-31-7	46
4	1H-Pyrazole-4-carboxaldehyde, 1-...	190	C10H7FN2O	1000338-05-6	40
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38





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Misc :
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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

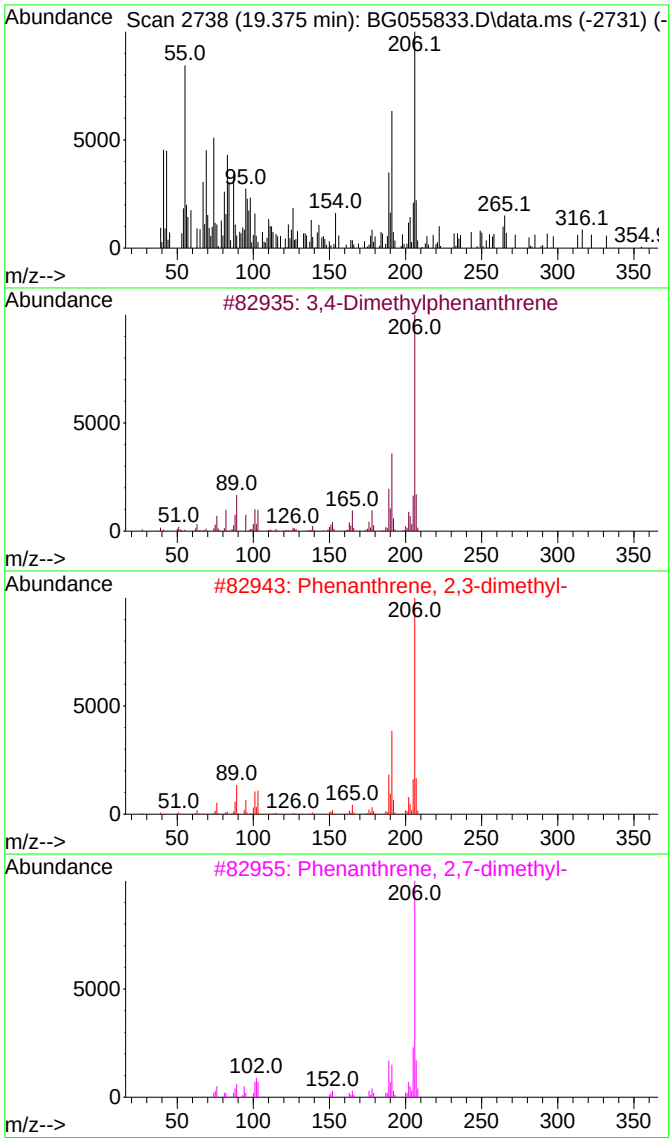
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

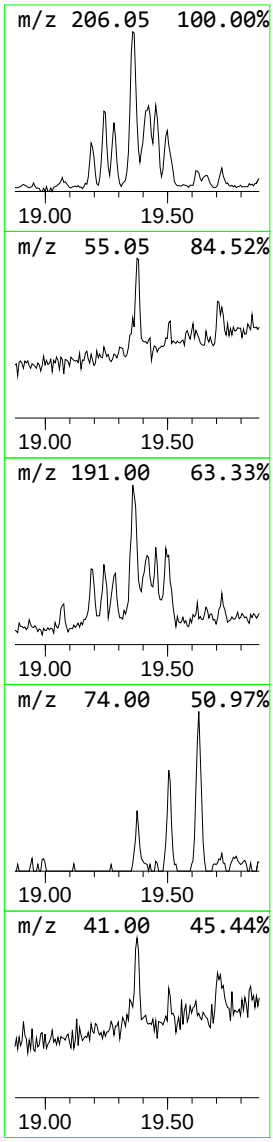
****

Peak Number 5 3,4-Dimethylphenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.375	2.45 ng	99203	Phenanthrene-d10	17.589

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	70
2	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	62
3	Phenanthrene, 2,7-dimethyl-	206	C16H14	001576-69-8	60
4	Phenanthrene, 4,5-dimethyl-	206	C16H14	003674-69-9	58
5	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112922\
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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
2-Pentanone, 4-...	5.280	20.8	ng	326074	1	8.223	313524	20.0
Ethanol, 2-(2-b...	10.803	4.3	ng	98519	2	11.055	456933	20.0
Phenanthrene, 4...	18.458	2.9	ng	119219	4	17.589	811192	20.0
4H-Cyclopenta[d...	18.658	2.5	ng	99555	4	17.589	811192	20.0
3,4-Dimethylphe...	19.375	2.5	ng	99203	4	17.589	811192	20.0