LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG040518\
Data File : BG033622.D
Acq On : 6 Apr 2018 9:59
Operator : SJ/JU
Sample : J2239-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1-COMP

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:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.476	26	32	43	rBV2	72467	146417	4.16%	0.553%
2	3.564	43	47	56	rVB	43434	67461	1.92%	0.255%
3	5.773	415	423	430	rBV	49925	88281	2.51%	0.333%
4	6.284	504	510	535	rBV	877940	1740315	49.47%	6.569%
5	7.976	791	798	818	rBV	965094	2081228	59.16%	7.856%
6	8.376	858	866	888	rBV	879899	1867959	53.10%	7.051%
7	8.863	941	949	961	rBV	103632	256961	7.30%	0.970%
8	9.192	998	1005	1017	rBV	646019	1294047	36.78%	4.885%
9	10.062	1145	1153	1175	rBV	528456	1252246	35.60%	4.727%
10	11.742	1432	1439	1457	rBV	199616	439981	12.51%	1.661%
11	14.104	1834	1841	1861	rBV	1586585	2656008	75.50%	10.026%
12	14.897	1968	1976	1982	rBV	127865	196901	5.60%	0.743%
13	15.479	2068	2075	2083	rBV2	388733	693244	19.71%	2.617%
14	16.243	2201	2205	2212	rVB	45066	54895	1.56%	0.207%
15	16.948	2319	2325	2341	rBV	1310386	2294427	65.22%	8.661%
16	17.095	2346	2350	2358	rVB2	41828	74401	2.11%	0.281%
17	17.882	2478	2484	2489	rBV2	26039	36673	1.04%	0.138%
18	18.205	2531	2539	2544	rBV	468419	834225	23.71%	3.149%
19	18.246	2544	2546	2554	rVB	113689	184577	5.25%	0.697%
20	19.004	2669	2675	2681	rBV3	92671	145059	4.12%	0.548%
21	19.104	2689	2692	2697	rVB3	24391	38283	1.09%	0.145%
22	19.251	2711	2717	2720	rBV4	18924	38811	1.10%	0.147%
23	19.939	2829	2834	2839	rBV2	21937	40271	1.14%	0.152%
24	20.203	2874	2879	2884	rBV	247759	389241	11.06%	1.469%
25	20.379	2904	2909	2913	rBV4	28275	38774	1.10%	0.146%
26	20.526	2929	2934	2936	rBV4	38021	58925	1.67%	0.222%
27	20.561	2936	2940	2946	rVV	259619	371561	10.56%	1.403%
28	20.620	2946	2950	2957	rVB5	23611	35312	1.00%	0.133%
29	20.726	2960	2968	2979	rBV	2462246	3518009	100.00%	13.280%
30	20.873	2989	2993	3000	rVB4	26003	49711	1.41%	0.188%
31	21.043	3019	3022	3029	rVB3	37645	60993	1.73%	0.230%
32	21.149	3035	3040	3043	rBV2	24610	40949	1.16%	0.155%
33	21.208	3046	3050	3061	rVB2	50633	103381	2.94%	0.390%
34	21.355	3070	3075	3079	rBV	47292	78580	2.23%	0.297%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG040518\
Data File : BG033622.D
Acq On : 6 Apr 2018 9:59
Operator : SJ/JU
Sample : J2239-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1-COMP

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:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	21.413	3081	3085	3094	rVB6	49627	120530	3.43%	0.455%
36	21.866	3158	3162	3170	rVB3	38427	78058	2.22%	0.295%
37	21.971	3176	3180	3186	rVB2	39308	61688	1.75%	0.233%
38	22.042	3187	3192	3193	rBV2	41833	55706	1.58%	0.210%
39	22.077	3193	3198	3204	rVB4	78188	171005	4.86%	0.646%
40	22.189	3212	3217	3223	rBV3	37214	83316	2.37%	0.315%
41	22.254	3225	3228	3235	rVB4	29516	65339	1.86%	0.247%
42	22.553	3269	3279	3285	rBV3	510255	1301942	37.01%	4.915%
43	22.606	3285	3288	3299	rVB	153760	292230	8.31%	1.103%
44	22.700	3299	3304	3313	rVB5	36821	86291	2.45%	0.326%
45	22.788	3313	3319	3322	rBV4	23447	47674	1.36%	0.180%
46	23.029	3355	3360	3366	rVB7	33746	61687	1.75%	0.233%
47	23.352	3409	3415	3416	rBV3	39623	59741	1.70%	0.226%
48	23.387	3418	3421	3429	rVV2	80751	153479	4.36%	0.579%
49	23.470	3430	3435	3443	rVB2	50236	106333	3.02%	0.401%
50	23.705	3471	3475	3480	rBV6	25566	51802	1.47%	0.196%
51	23.858	3495	3501	3504	rBV8	25919	56861	1.62%	0.215%
52	24.228	3559	3564	3569	rVB5	25693	54523	1.55%	0.206%
53	24.375	3584	3589	3593	rBV3	29296	63008	1.79%	0.238%
54	25.115	3706	3715	3725	rBV2	107455	448141	12.74%	1.692%
55	25.967	3849	3860	3874	rBV2	86129	311986	8.87%	1.178%
56	26.137	3881	3889	3904	rVB2	105063	347873	9.89%	1.313%
57	26.319	3909	3920	3932	rBV	249877	823437	23.41%	3.108%
58	30.697	4654	4665	4674	rBV3	35487	162374	4.62%	0.613%
59	32.060	4890	4897	4915	rVB5	36107	157851	4.49%	0.596%

Sum of corrected areas: 26490982

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Data File : BG033622.D
Acq On : 6 Apr 2018 9:59
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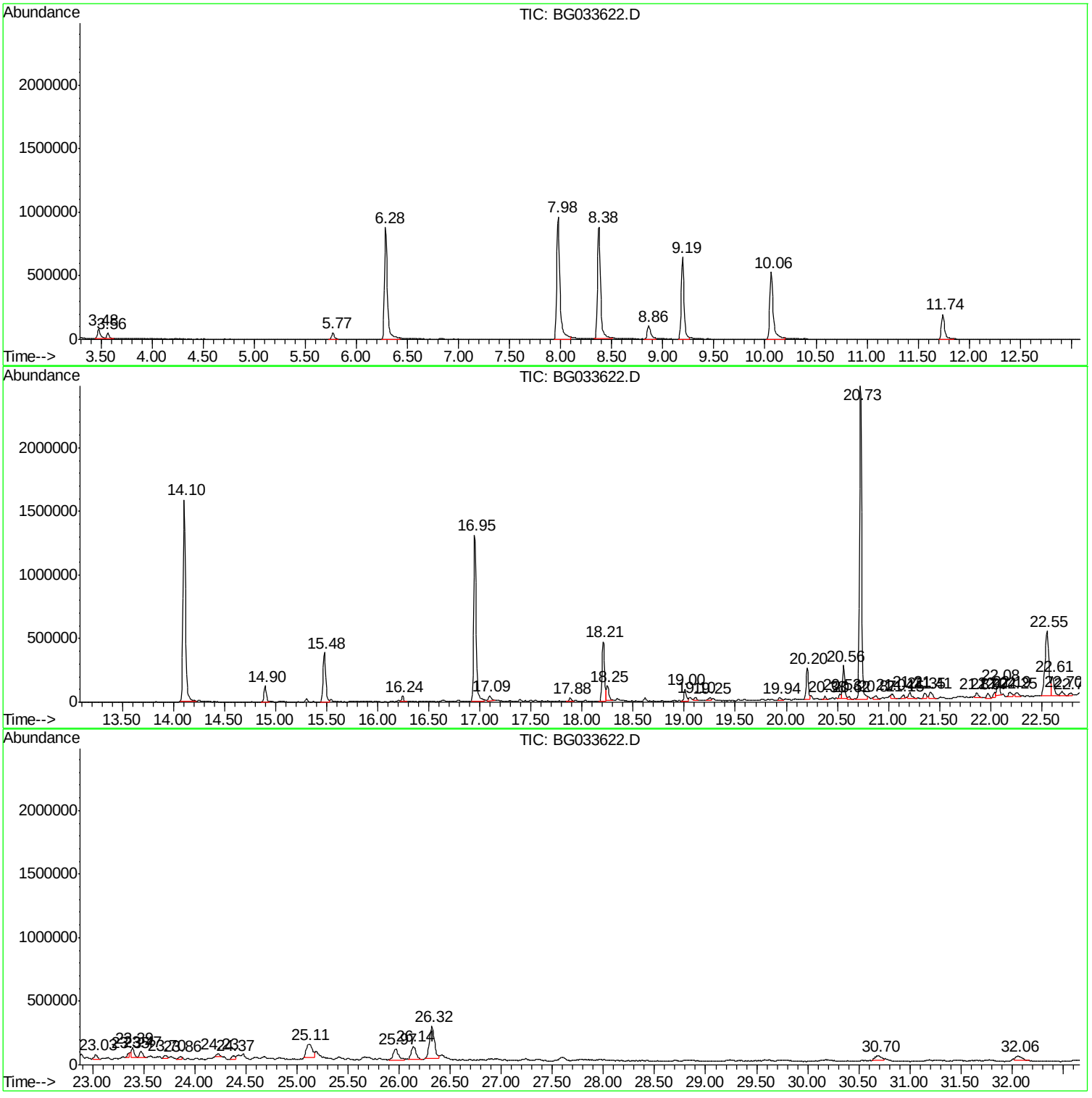
Sample : J2239-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S-1-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA G\DATA\BG040518\
Data File : BG033622.D
Acq On : 6 Apr 2018 9:59
Operator : SJ/JU
Sample : J2239-01
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ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

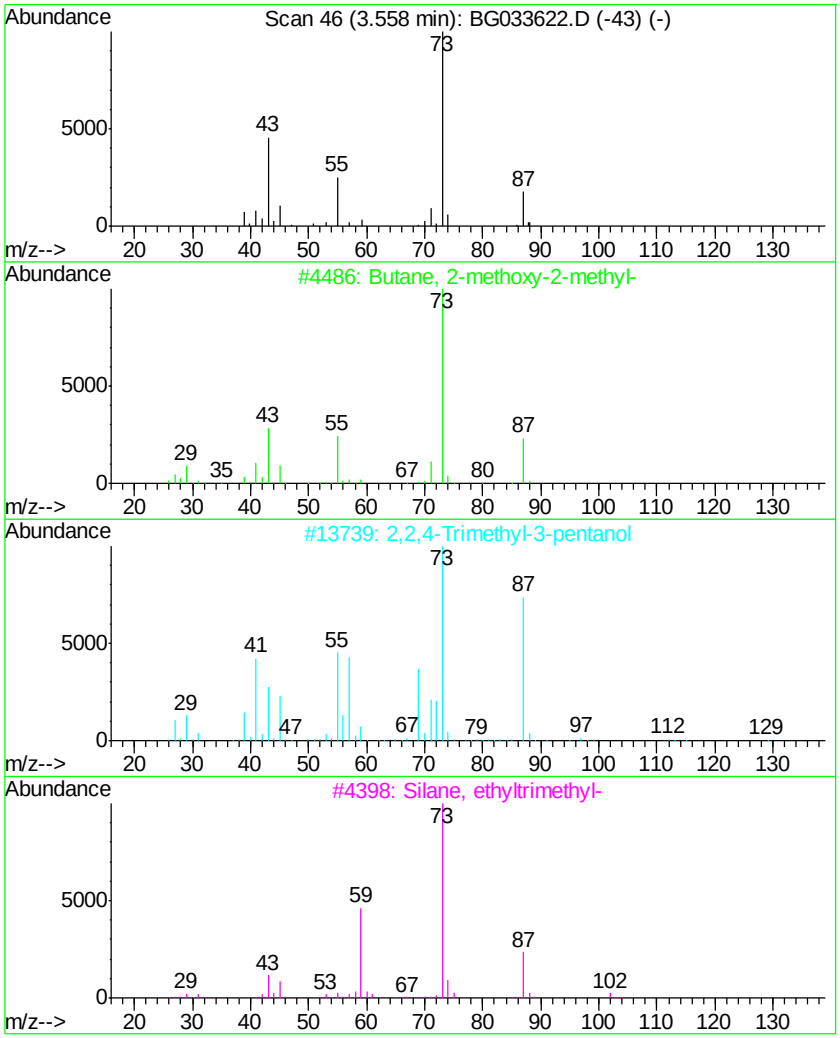
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

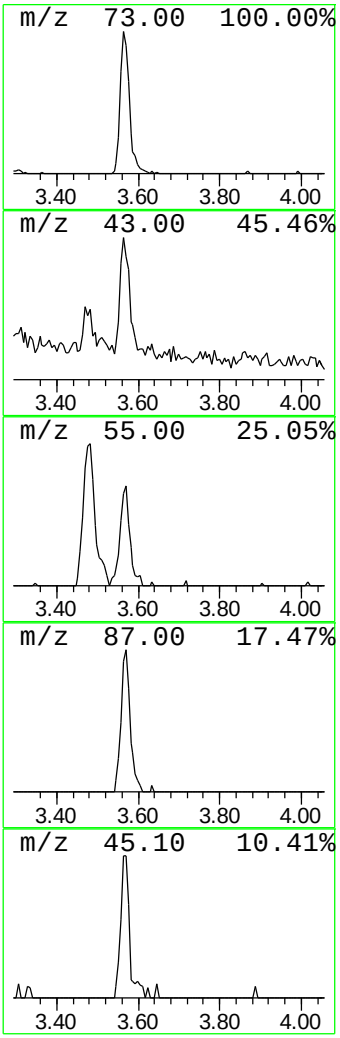
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.56	5.25 ng	67461	1,4-Dichlorobenzene-d4	8.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	33
4	Disilane, ethylpentamethyl-	160	C7H20Si2	015063-64-6	33
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	12





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG040518\
Data File : BG033622.D
Acq On : 6 Apr 2018 9:59
Operator : SJ/JU
Sample : J2239-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

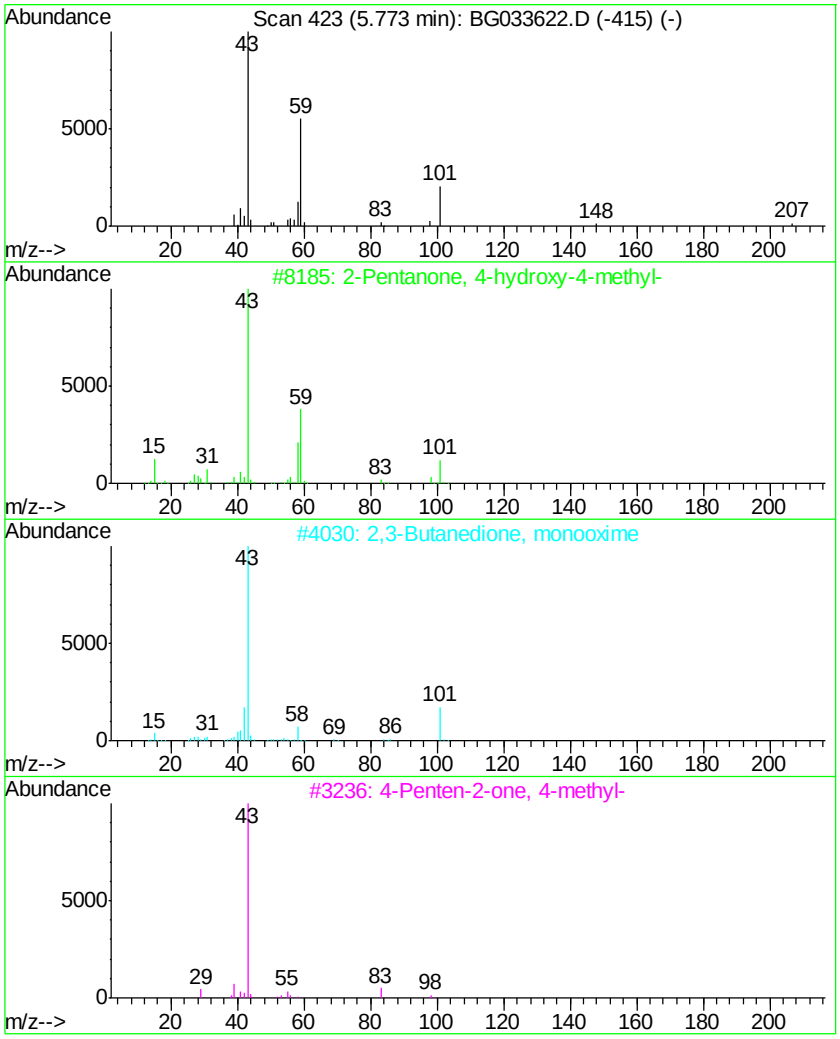
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

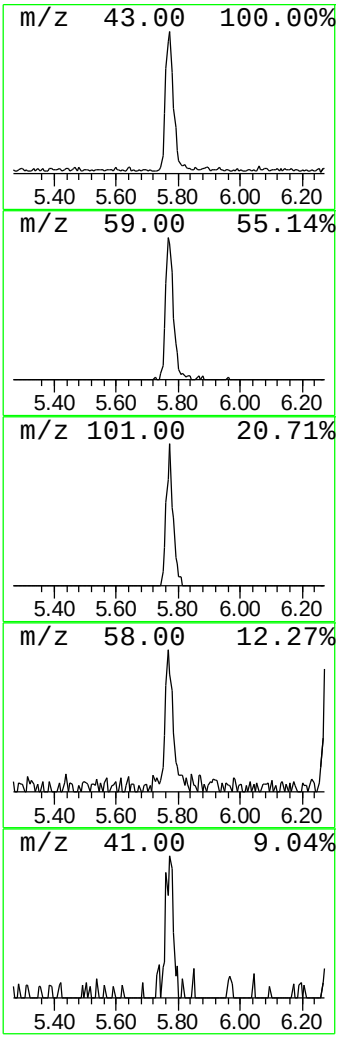
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.77	6.87 ng	88281	1,4-Dichlorobenzene-d4	8.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9
5	.alpha.-D-Galactopyranoside, met...	249	C10H19NO6	017296-07-0	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG040518\
Data File : BG033622.D
Acq On : 6 Apr 2018 9:59
Operator : SJ/JU
Sample : J2239-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

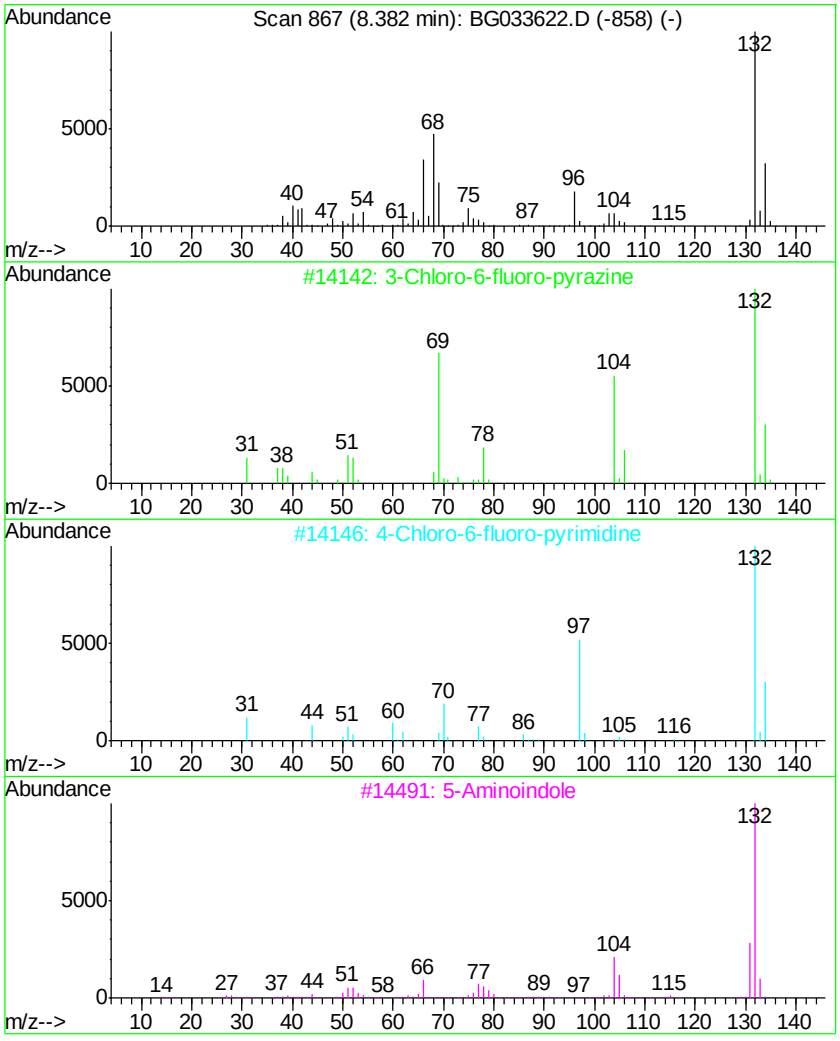
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

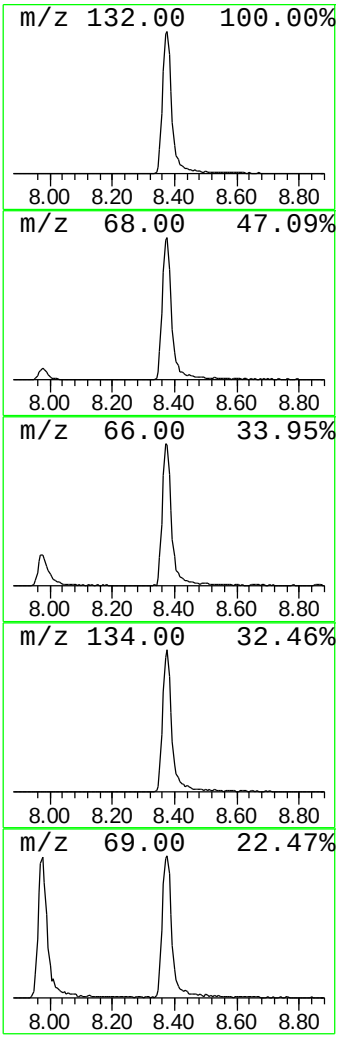
****

Peak Number 4 unknown8.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.38	145.39 ng	1867960	1,4-Dichlorobenzene-d4	8.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	5-Aminoindole	132	C8H8N2	005192-03-0	22
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





Data Path : Z:\HPCHEM1\BNA G\DATA\BG040518\
Data File : BG033622.D
Acq On : 6 Apr 2018 9:59
Operator : SJ/JU
Sample : J2239-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

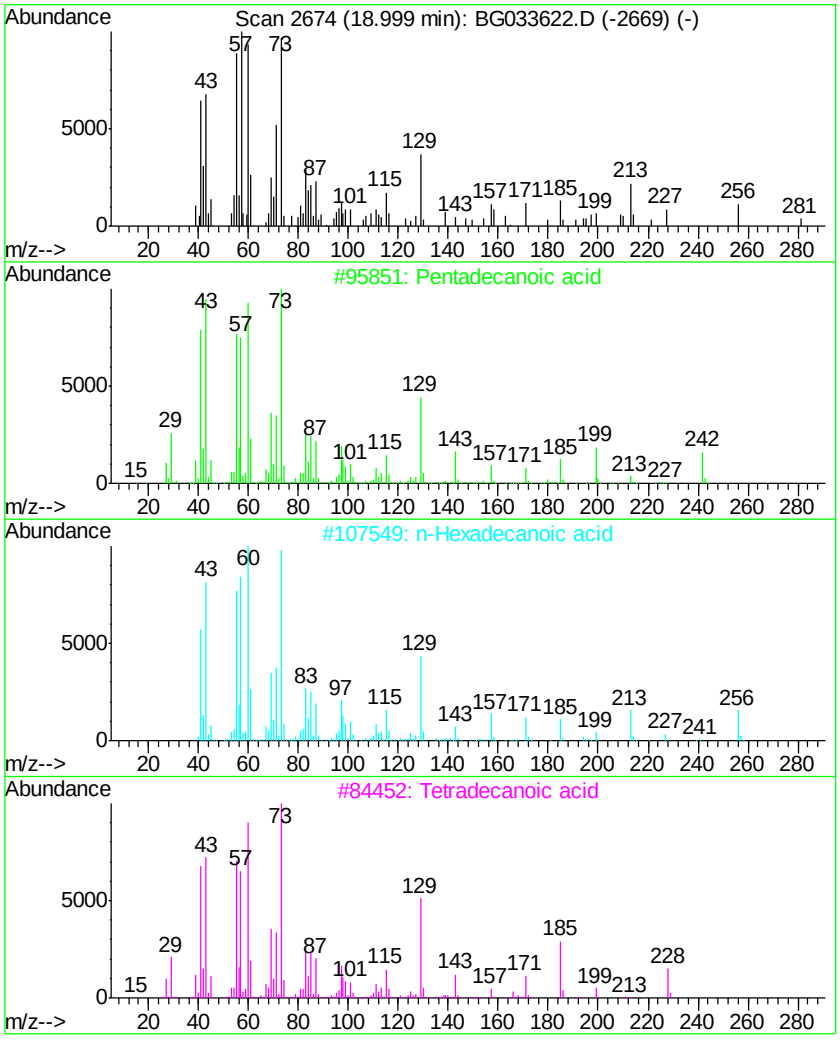
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

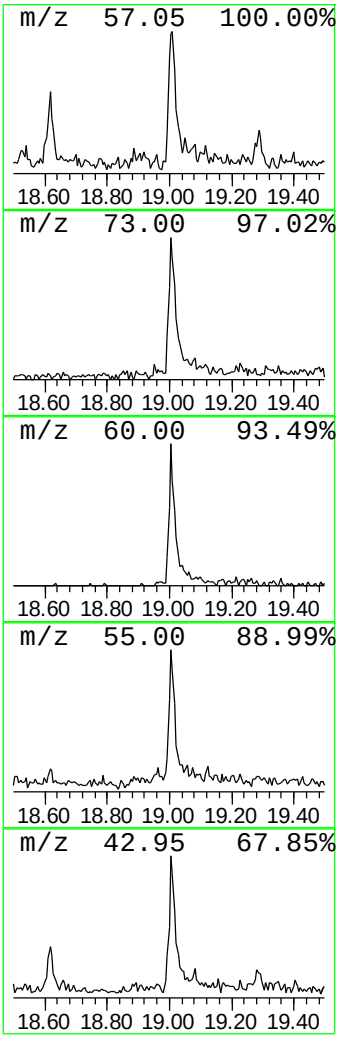
****

Peak Number 6 Pentadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.00	3.48 ng	145059	Phenanthrene-d10	18.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Tridecanoic acid	214	C13H26O2	000638-53-9	50
5	Dodecanoic acid	200	C12H24O2	000143-07-7	50





Data Path : Z:\HPCHEM1\BNA G\DATA\BG040518\
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Acq On : 6 Apr 2018 9:59
Operator : SJ/JU
Sample : J2239-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

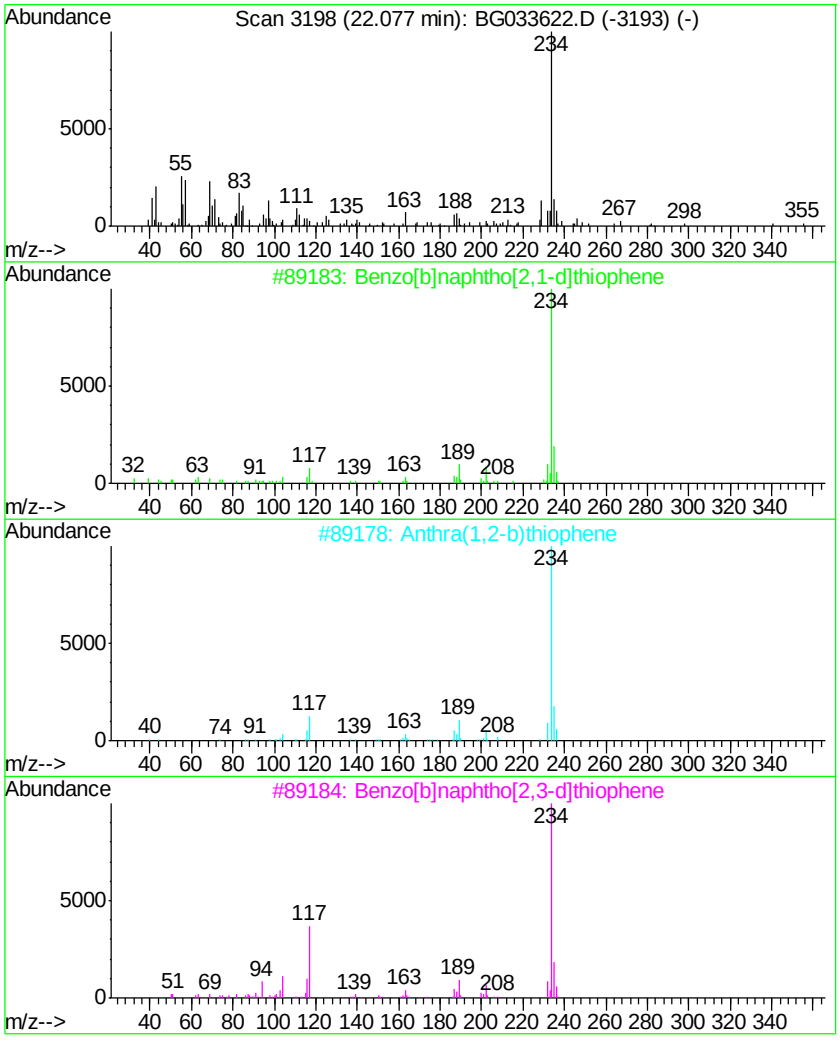
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

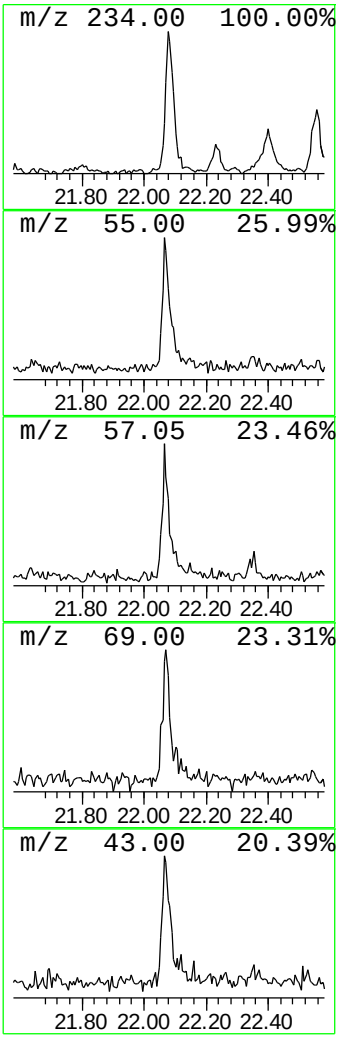
****

Peak Number 7 Benzo[b]naphtho[2,1-d]thiop... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.08	2.63 ng	171005	Chrysene-d12	22.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]naphtho[2,1-d]thiophene	234	C16H10S	000239-35-0	64
2	Anthra(1,2-b)thiophene	234	C16H10S	000227-86-1	62
3	Benzo[b]naphtho[2,3-d]thiophene	234	C16H10S	000243-46-9	59
4	Thiazol-2-amine, 4-(1-adamantyl)-	234	C13H18N2S	019735-74-1	59
5	Phenanthro(2,1-b)thiophene	234	C16H10S	000219-25-0	58





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Acq On : 6 Apr 2018 9:59
Operator : SJ/JU
Sample : J2239-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

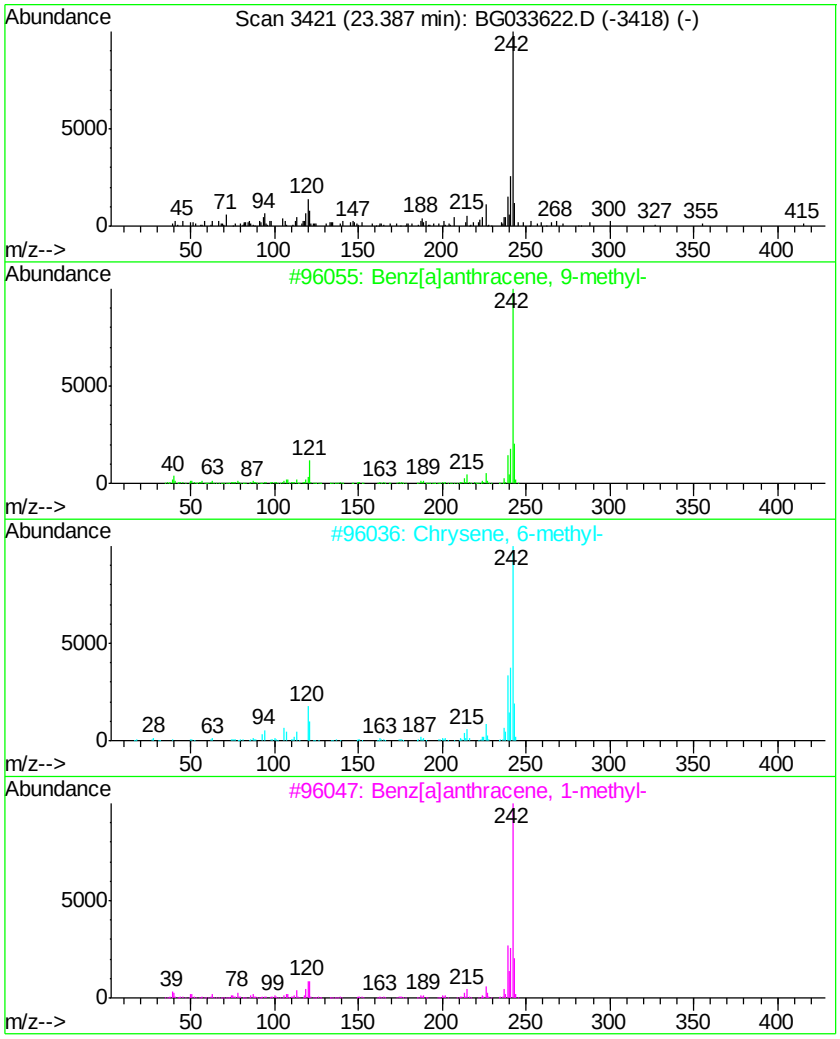
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

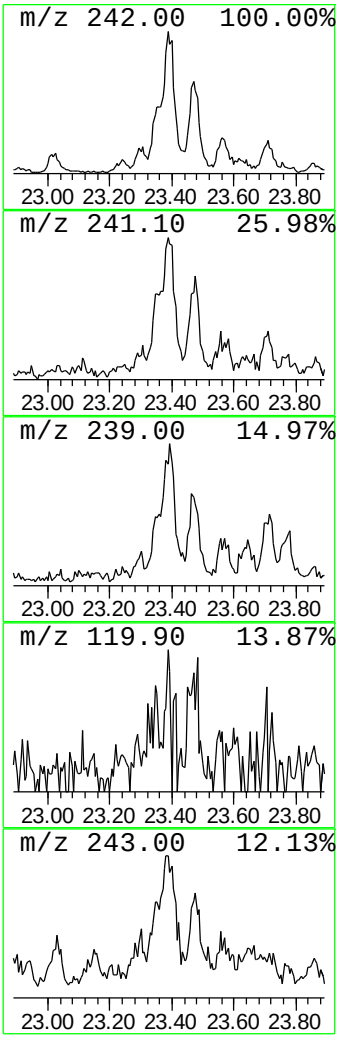
****

Peak Number 8 Benz[a]anthracene, 9-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.39	2.36 ng	153479	Chrysene-d12	22.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benz[a]anthracene, 9-methyl-	242	C19H14	002381-16-0	72
2	Chrysene, 6-methyl-	242	C19H14	001705-85-7	68
3	Benz[a]anthracene, 1-methyl-	242	C19H14	002498-77-3	68
4	Triphenylene, 2-methyl-	242	C19H14	001705-84-6	64
5	Chrysene, 1-methyl-	242	C19H14	003351-28-8	64





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Data File : BG033622.D
Acq On : 6 Apr 2018 9:59
Operator : SJ/JU
Sample : J2239-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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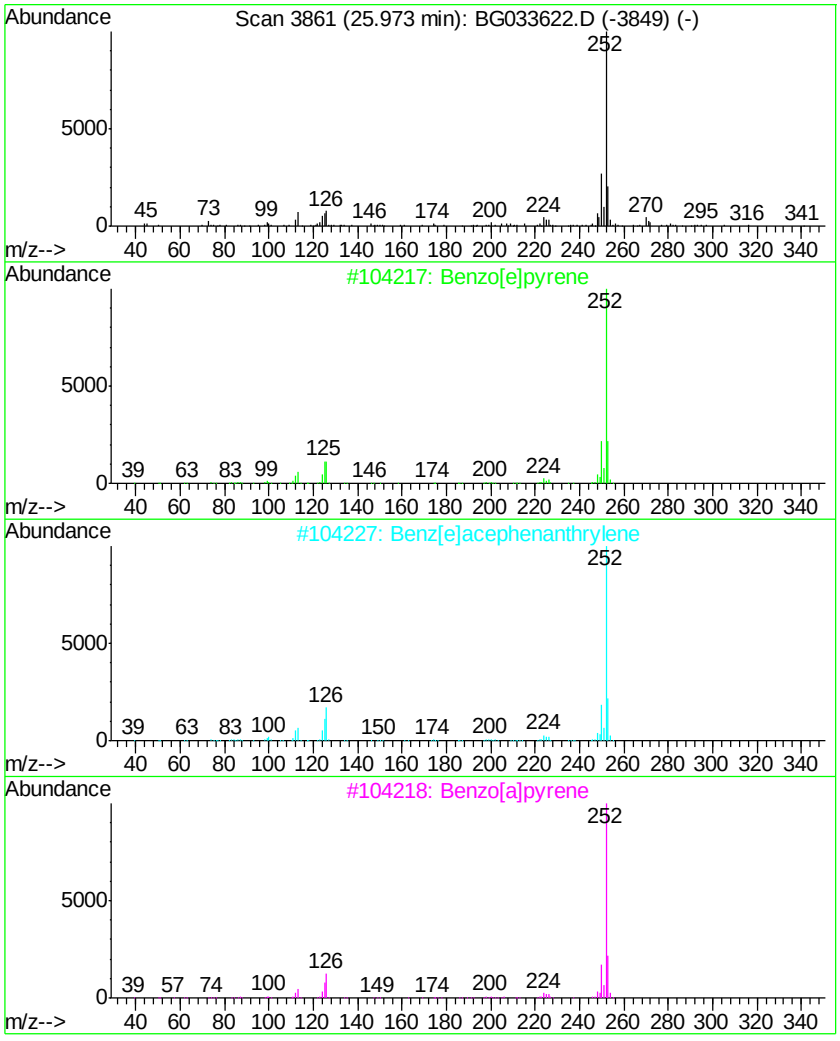
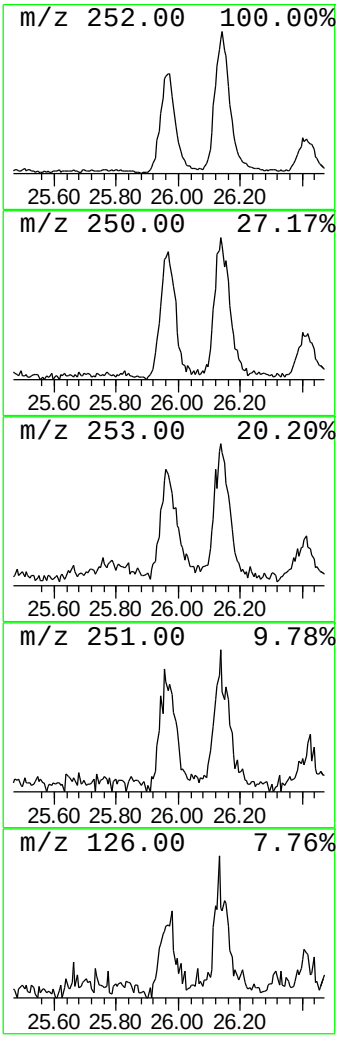
Peak Number 9 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.97	7.58 ng	311986	Perylene-d12	26.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
3	Benzo[a]pyrene	252	C20H12	000050-32-8	93
4	Perylene	252	C20H12	000198-55-0	90
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG040518\
Data File : BG033622.D
Acq On : 6 Apr 2018 9:59
Operator : SJ/JU
Sample : J2239-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-1-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	3.56	5.3	ng	67461	1	8.86	256961	20.0
2-Pentanone, 4-hy...	5.77	6.9	ng	88281	1	8.86	256961	20.0
unknown8.38	8.38	145.4	ng	1867960	1	8.86	256961	20.0
Pentadecanoic acid	19.00	3.5	ng	145059	4	18.21	834225	20.0
Benzo[b]naphtho[2...	22.08	2.6	ng	171005	5	22.55	1301940	20.0
Benz[a]anthracene...	23.39	2.4	ng	153479	5	22.55	1301940	20.0
Benzo[e]pyrene	25.97	7.6	ng	311986	6	26.32	823437	20.0