LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110119\
Data File : BG043478.D
Acq On : 1 Nov 2019 23:06
Operator : JU
Sample : K5541-17 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 18-48-(0-2.5)

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-BG102119.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	3.193	13	18	28	rVB3	20729	51800	6.40%	0.842%
2	5.126	341	347	354	rBV2	18989	32947	4.07%	0.535%
3	5.607	423	429	441	rBV	82525	162460	20.09%	2.639%
4	7.206	694	701	716	rBV	73420	177274	21.92%	2.880%
5	7.558	755	761	775	rBV2	95829	190611	23.57%	3.097%
6	8.016	832	839	850	rBV	166872	311585	38.53%	5.062%
7	8.340	888	894	904	rBV	83686	151825	18.77%	2.466%
8	9.180	1028	1037	1051	rBV2	40543	106735	13.20%	1.734%
9	10.825	1307	1317	1337	rBV	201705	421461	52.11%	6.847%
10	13.269	1726	1733	1749	rBV	132884	251937	31.15%	4.093%
11	14.098	1864	1874	1881	rBV2	17725	32536	4.02%	0.529%
12	14.644	1960	1967	1975	rBV2	357063	592711	73.28%	9.629%
13	16.083	2206	2212	2215	rBV2	5717	9898	1.22%	0.161%
14	16.136	2215	2221	2230	rVV	110896	211188	26.11%	3.431%
15	16.383	2258	2263	2267	rVB	17046	22558	2.79%	0.366%
16	16.471	2273	2278	2283	rBV	37371	55586	6.87%	0.903%
17	16.530	2283	2288	2294	rVV3	39688	74709	9.24%	1.214%
18	16.589	2294	2298	2303	rVV2	38745	58362	7.22%	0.948%
19	16.630	2303	2305	2310	rVB2	22331	29779	3.68%	0.484%
20	16.683	2310	2314	2317	rBV3	12500	18134	2.24%	0.295%
21	16.736	2321	2323	2327	rVB4	12887	14979	1.85%	0.243%
22	16.788	2327	2332	2339	rBV4	28125	56845	7.03%	0.923%
23	16.853	2339	2343	2347	rBV	35507	47749	5.90%	0.776%
24	16.929	2352	2356	2362	rVB3	22981	34848	4.31%	0.566%
25	17.388	2427	2434	2440	rBV	425315	692099	85.57%	11.244%
26	17.817	2498	2507	2510	rBV	6215	16686	2.06%	0.271%
27	18.269	2581	2584	2588	rBV4	15698	26266	3.25%	0.427%
28	18.316	2588	2592	2596	rVV6	8498	17482	2.16%	0.284%
29	18.457	2611	2616	2621	rBV7	15675	33613	4.16%	0.546%
30	19.186	2735	2740	2741	rBV4	16524	23959	2.96%	0.389%
31	19.438	2779	2783	2789	rBV	94460	138085	17.07%	2.243%
32	19.803	2841	2845	2851	rVB2	100523	176423	21.81%	2.866%
33	19.996	2873	2878	2885	rBV	264840	361131	44.65%	5.867%
34	21.653	3155	3160	3166	rBV2	432910	742466	91.80%	12.062%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110119\
Data File : BG043478.D
Acq On : 1 Nov 2019 23:06
Operator : JU
Sample : K5541-17 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 18-48-(0-2.5)

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-BG102119.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	24.861	3698	3706	3715	rVB2	297469	808779	100.00%	13.139%

Sum of corrected areas: 6155506

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110119\
Data File : BG043478.D
Acq On : 1 Nov 2019 23:06
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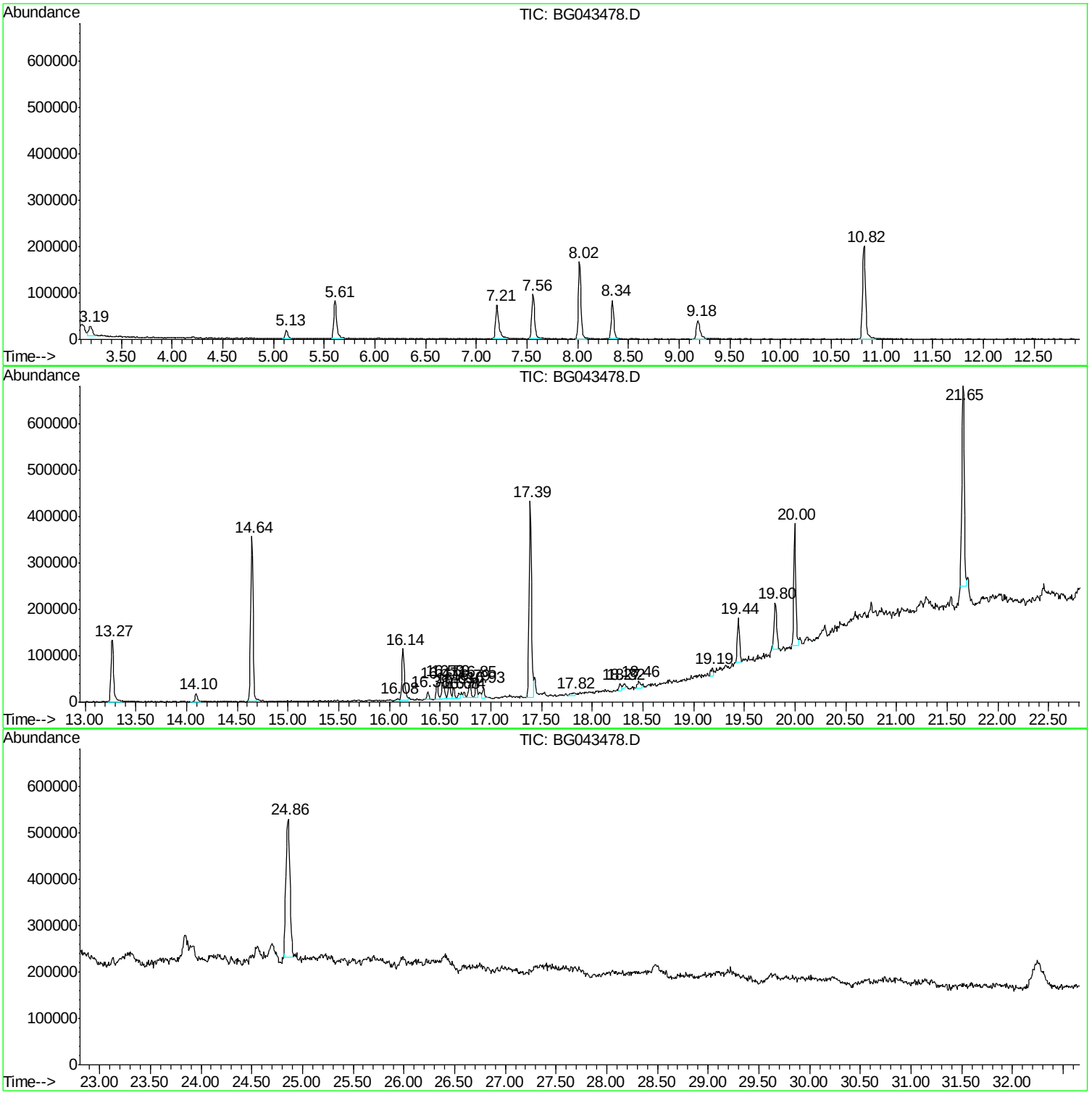
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
18-48-(0-2.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110119\
Data File : BG043478.D
Acq On : 1 Nov 2019 23:06
Operator : JU
Sample : K5541-17 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 18-48-(0-2.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

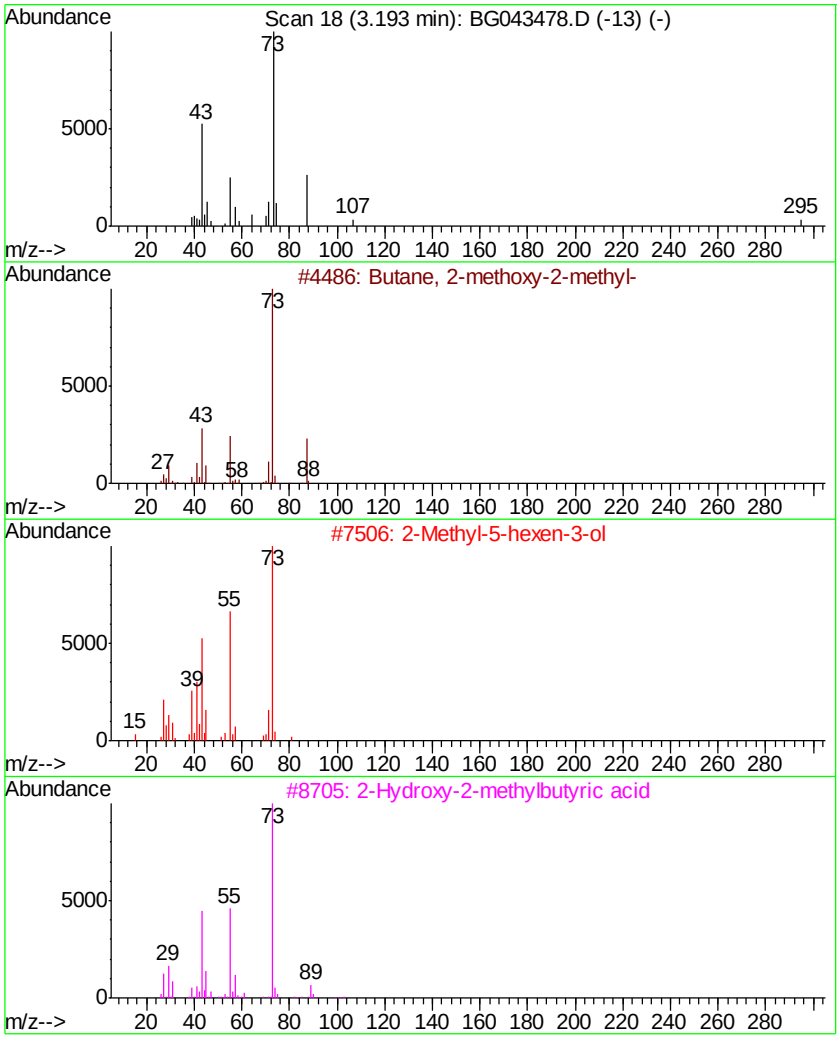
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

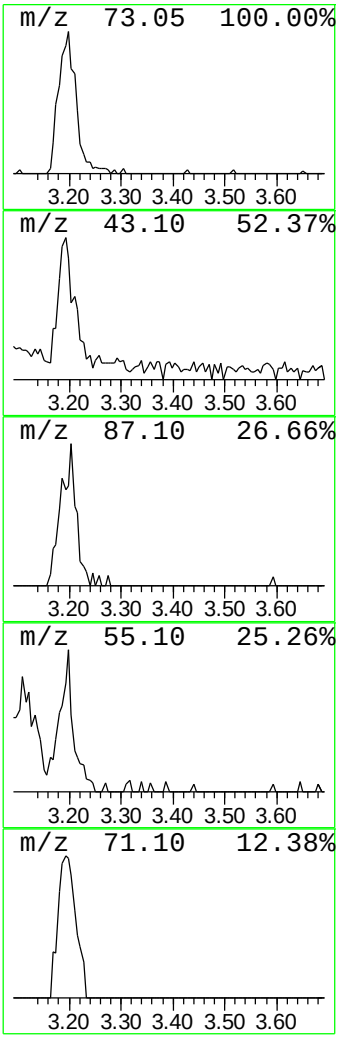
****

Peak Number 1 unknown3.19 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.19	3.32 ng	51800	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	42
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
3	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	23
4	Acetamide, N-acetyl-N-methyl-	115	C5H9NO2	001113-68-4	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110119\
Data File : BG043478.D
Acq On : 1 Nov 2019 23:06
Operator : JU
Sample : K5541-17 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 18-48-(0-2.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

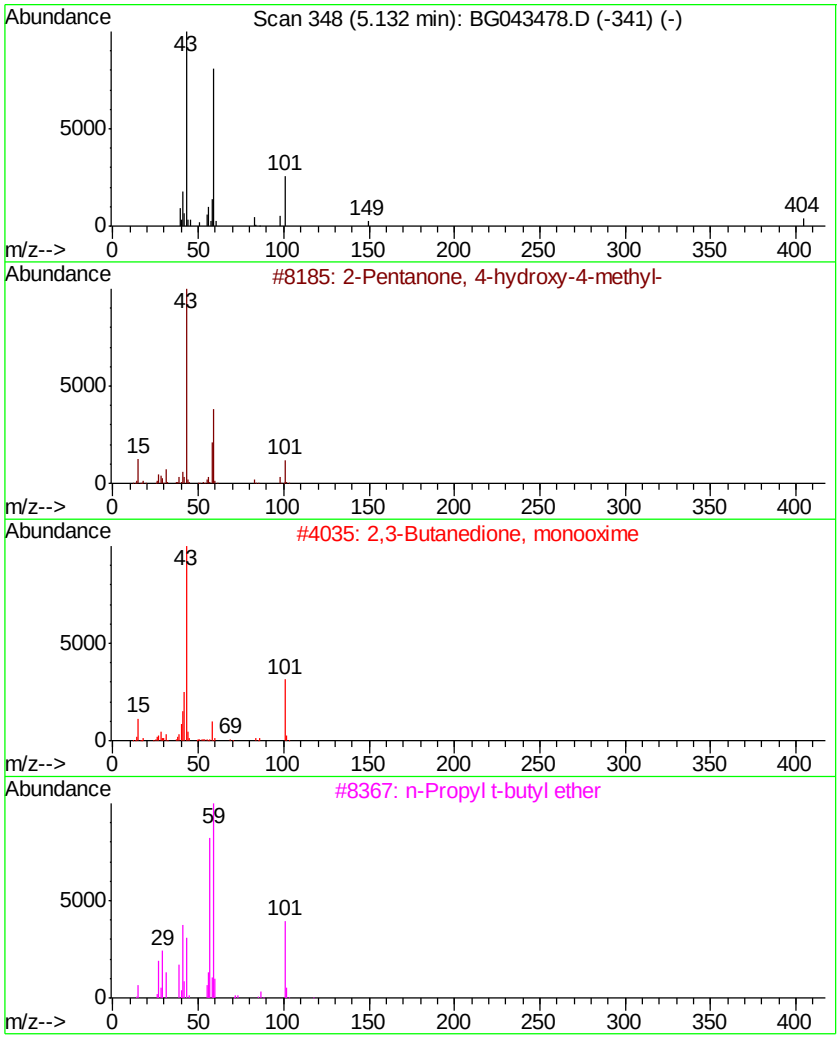
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

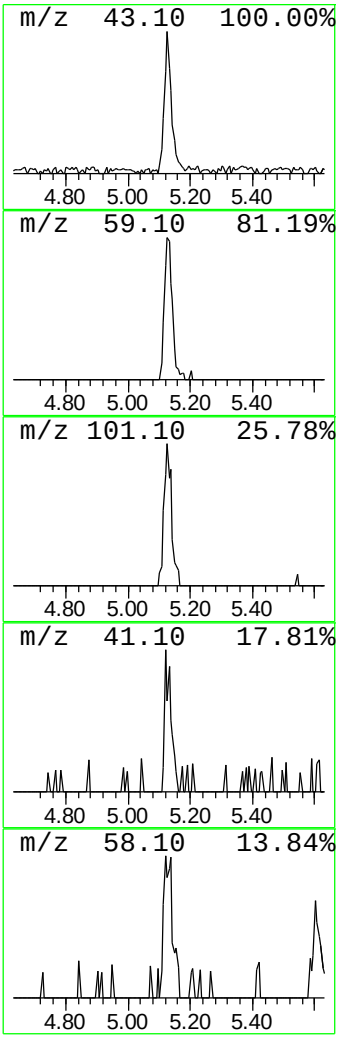
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	2.11 ng	32947	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
3	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butyl aldoxime, 3-methyl-, anti	101	C5H11NO	005775-74-6	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110119\
Data File : BG043478.D
Acq On : 1 Nov 2019 23:06
Operator : JU
Sample : K5541-17 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 18-48-(0-2.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

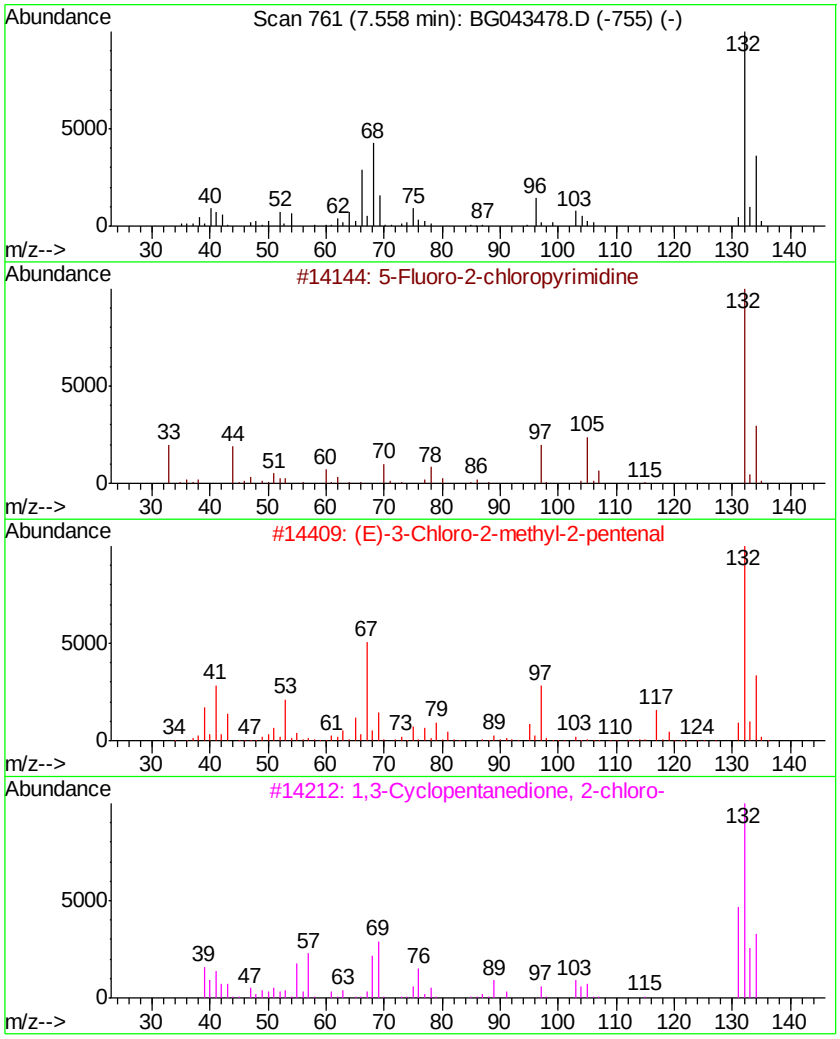
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

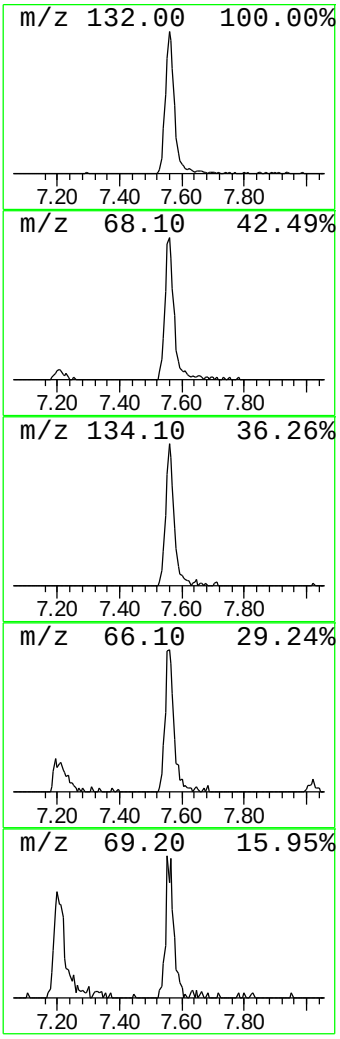
****

Peak Number 3 unknown7.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	12.23 ng	190611	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	13
4	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	12
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110119\
Data File : BG043478.D
Acq On : 1 Nov 2019 23:06
Operator : JU
Sample : K5541-17 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 18-48-(0-2.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

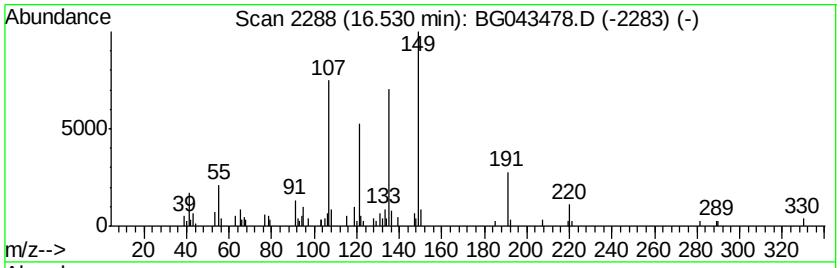
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

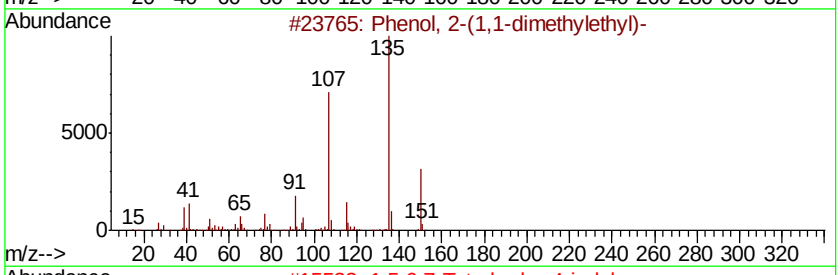
****

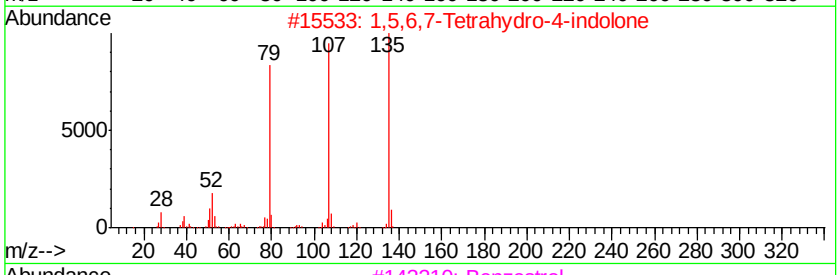
Peak Number 5 unknown16.53 Concentration Rank 4

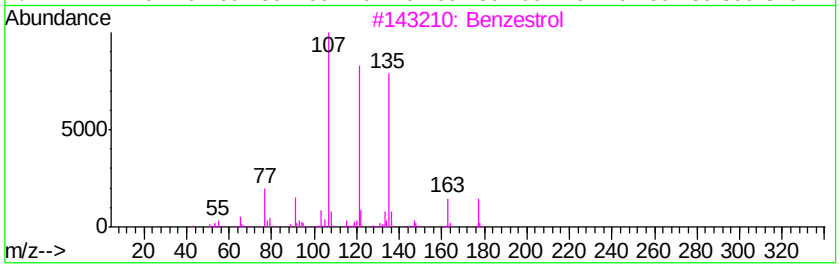
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	2.16 ng	74709	Phenanthrene-d10	17.39

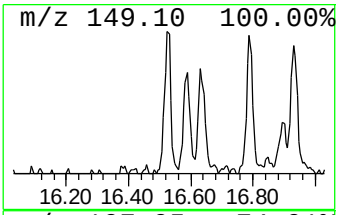
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	38
2	1,5,6,7-Tetrahydro-4-indolone	135	C8H9NO	013754-86-4	38
3	Benzestrol	298	C20H26O2	000085-95-0	38
4	Silane, chlorotripropyl-	192	C9H21ClSi	000995-25-5	38
5	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	35

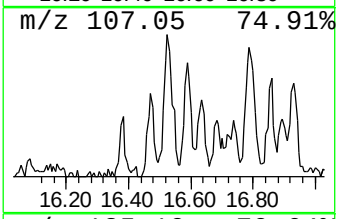


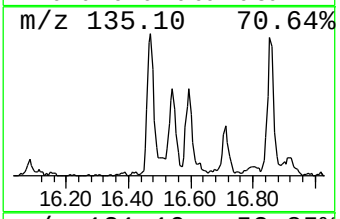


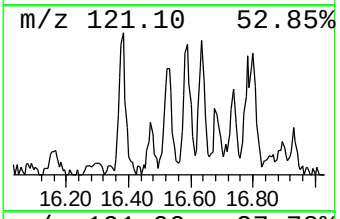


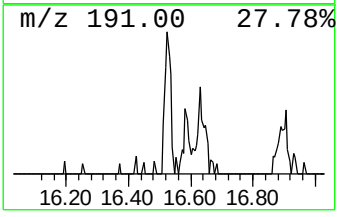












Tentatively Identified Compound (LSC) summary

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Data File : BG043478.D
Acq On : 1 Nov 2019 23:06
Operator : JU
Sample : K5541-17 5X
Misc :
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Instrument : BNA_G
ClientSampleId : 18-48-(0-2.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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
unknown3.19	3.19	3.3	ng	51800	1	8.02	311585	20.0
2-Pentanone, 4-hy...	5.13	2.1	ng	32947	1	8.02	311585	20.0
unknown7.56	7.56	12.2	ng	190611	1	8.02	311585	20.0
unknown16.53	16.53	2.2	ng	74709	4	17.39	692099	20.0