LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111819\
Data File : BG043682.D
Acq On : 18 Nov 2019 20:52
Operator : JU
Sample : K5904-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 11-(2-4)

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	3.158	6	12	21	rVB	71704	121854	4.32%	0.977%
2	5.097	336	342	354	rBV	97801	154201	5.47%	1.237%
3	5.590	418	426	438	rBV	444999	786941	27.93%	6.312%
4	7.188	688	698	714	rBV	481231	940423	33.37%	7.543%
5	7.535	750	757	768	rBV	486258	893706	31.71%	7.168%
6	7.993	826	835	844	rBV	95407	167160	5.93%	1.341%
7	8.316	882	890	900	rBV	378772	673867	23.91%	5.405%
8	9.156	1025	1033	1044	rBV	254882	511516	18.15%	4.103%
9	10.802	1305	1313	1323	rBV	94385	205411	7.29%	1.648%
10	13.246	1722	1729	1745	rBV	813515	1392228	49.40%	11.167%
11	14.074	1864	1870	1881	rBV	64760	127734	4.53%	1.025%
12	14.627	1956	1964	1979	rBV	186447	330904	11.74%	2.654%
13	16.113	2211	2217	2231	rBV	684197	1248768	44.31%	10.016%
14	17.370	2425	2431	2441	rBV	240118	423845	15.04%	3.400%
15	19.979	2869	2875	2886	rVB	2027255	2817993	100.00%	22.603%
16	21.283	3092	3097	3113	rVB4	53664	160496	5.70%	1.287%
17	21.636	3150	3157	3166	rBV2	316963	597863	21.22%	4.795%
18	21.859	3191	3195	3204	rVB3	22591	37716	1.34%	0.303%
19	21.953	3207	3211	3215	rVV2	23923	39124	1.39%	0.314%
20	21.994	3215	3218	3224	rVB	22528	35738	1.27%	0.287%
21	22.271	3261	3265	3270	rBV3	20677	29657	1.05%	0.238%
22	22.406	3283	3288	3292	rBV8	18545	34801	1.23%	0.279%
23	22.611	3318	3323	3327	rBV4	23295	41859	1.49%	0.336%
24	23.875	3534	3538	3545	rVB6	19652	37387	1.33%	0.300%
25	24.815	3688	3698	3710	rBV2	211122	626051	22.22%	5.021%
26	25.925	3880	3887	3894	rVB9	11697	30344	1.08%	0.243%

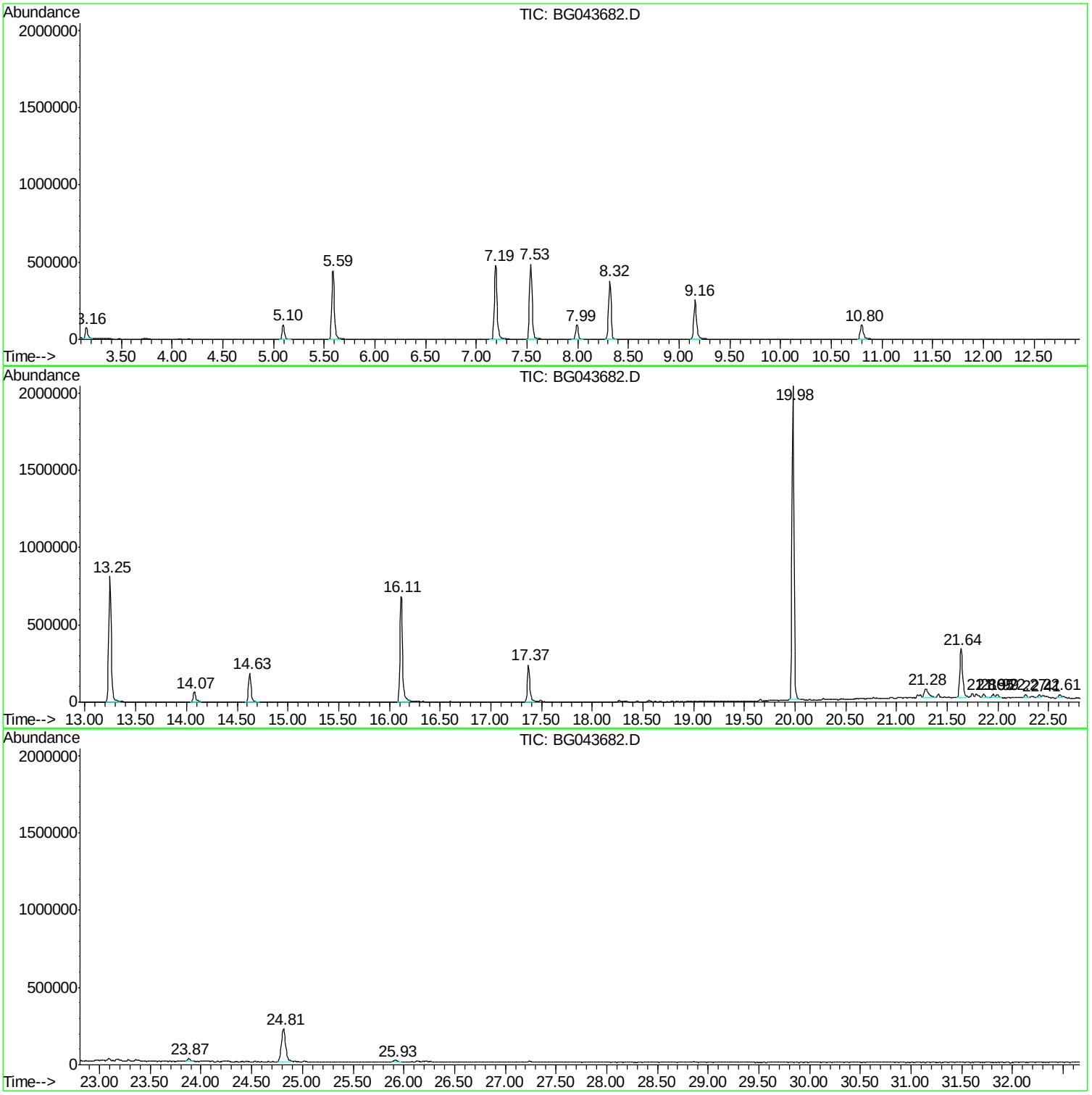
Sum of corrected areas: 12467587

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111819\
Data File : BG043682.D
Acq On : 18 Nov 2019 20:52
Operator : JU
Sample : K5904-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
11-(2-4)

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\BG111819\
Data File : BG043682.D
Acq On : 18 Nov 2019 20:52
Operator : JU
Sample : K5904-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 11-(2-4)

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

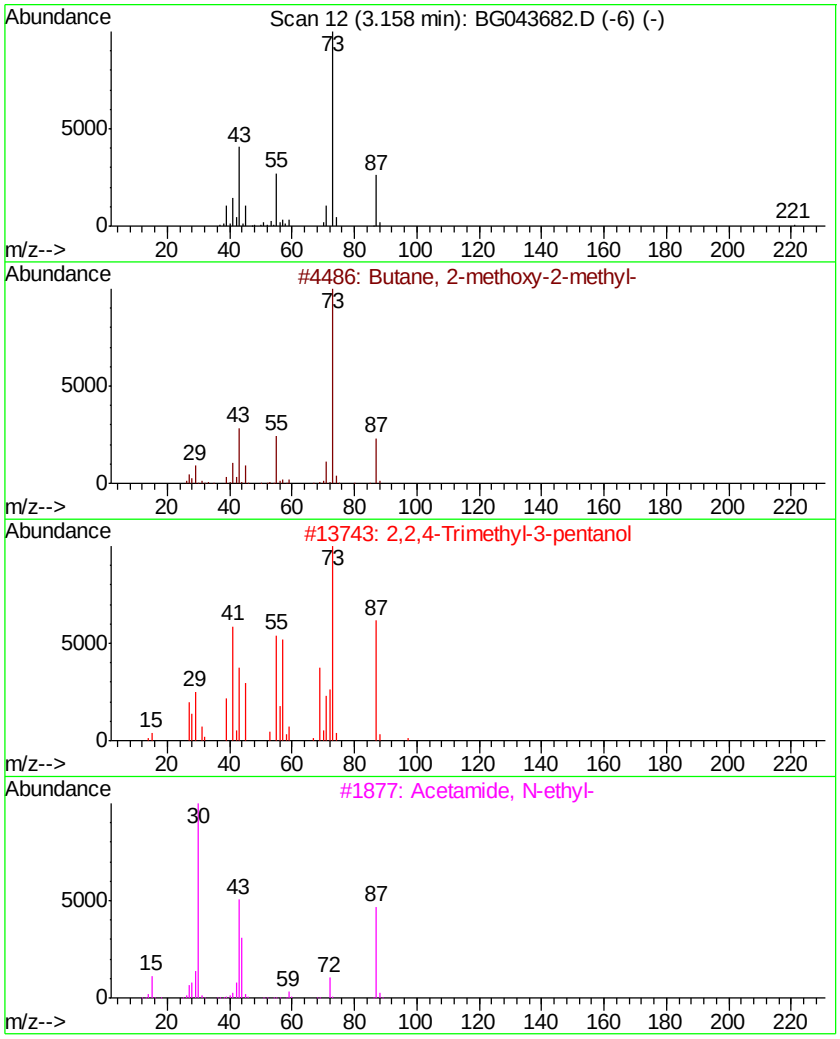
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

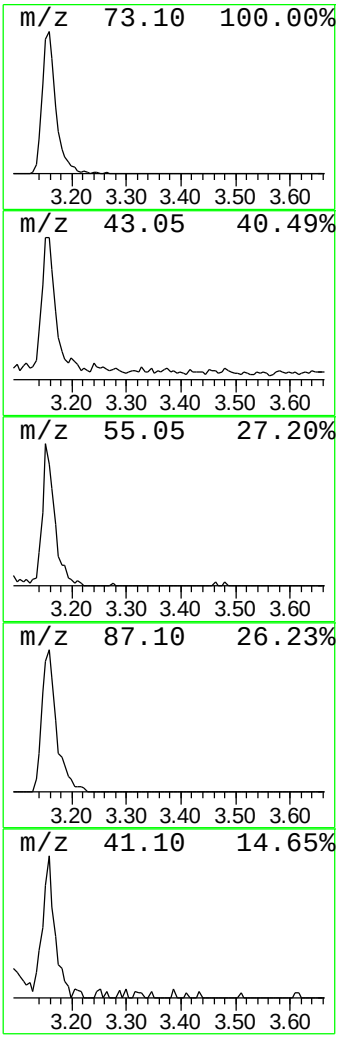
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.16	14.58 ng	121854	1,4-Dichlorobenzene-d4	7.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10
4	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111819\
Data File : BG043682.D
Acq On : 18 Nov 2019 20:52
Operator : JU
Sample : K5904-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 11-(2-4)

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

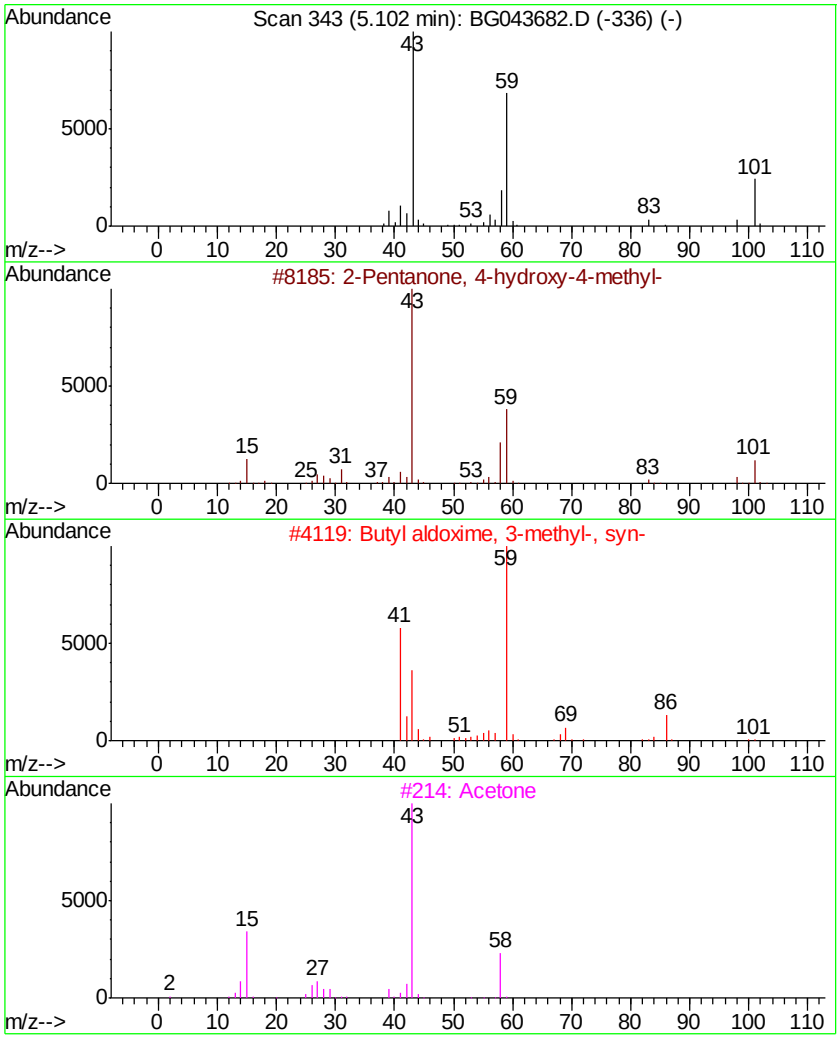
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

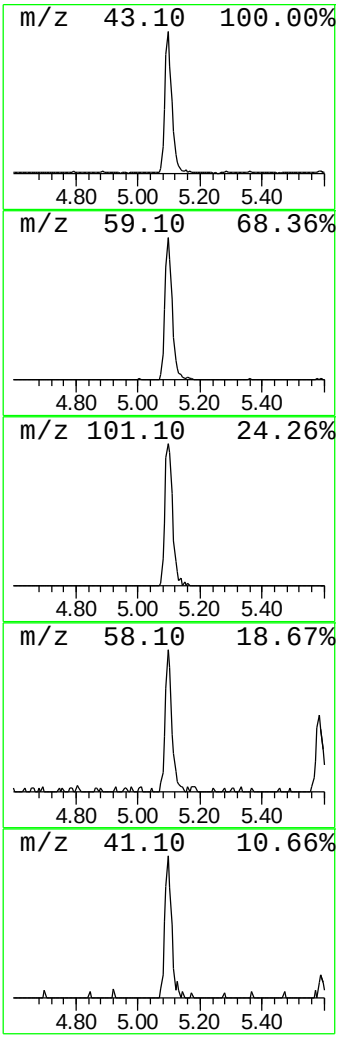
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	18.45 ng	154201	1,4-Dichlorobenzene-d4	7.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
3	Acetone	58	C3H6O	000067-64-1	10
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111819\
Data File : BG043682.D
Acq On : 18 Nov 2019 20:52
Operator : JU
Sample : K5904-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 11-(2-4)

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

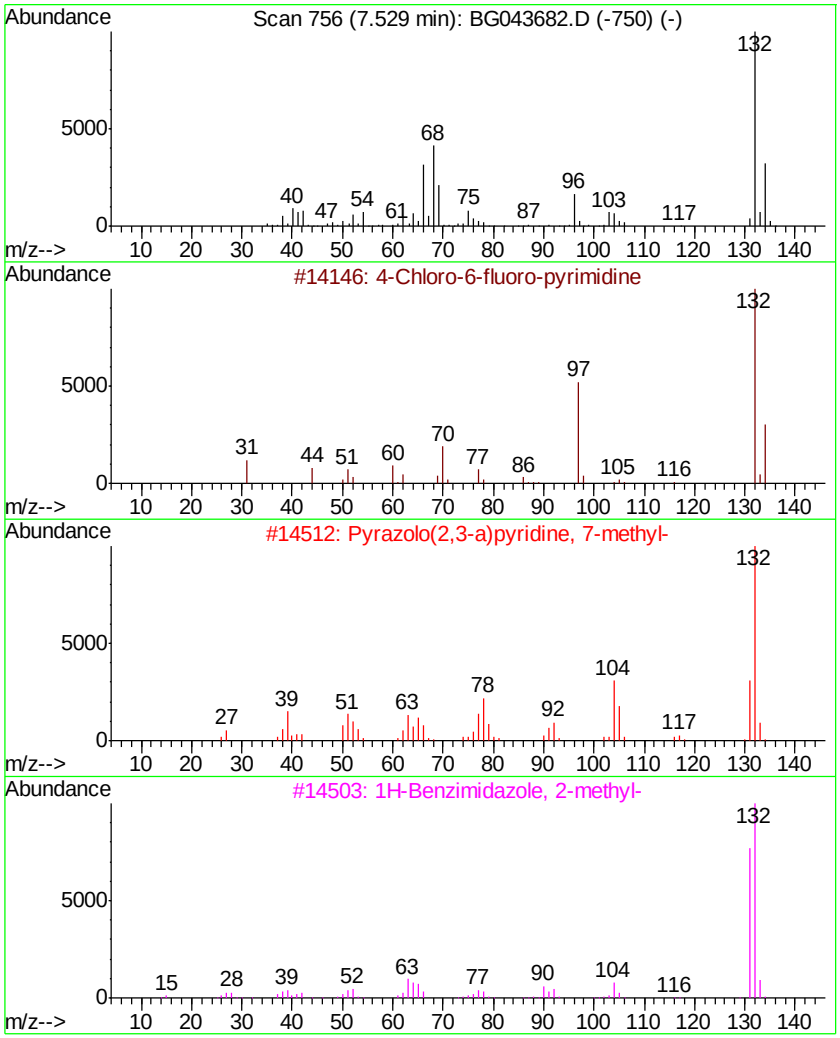
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

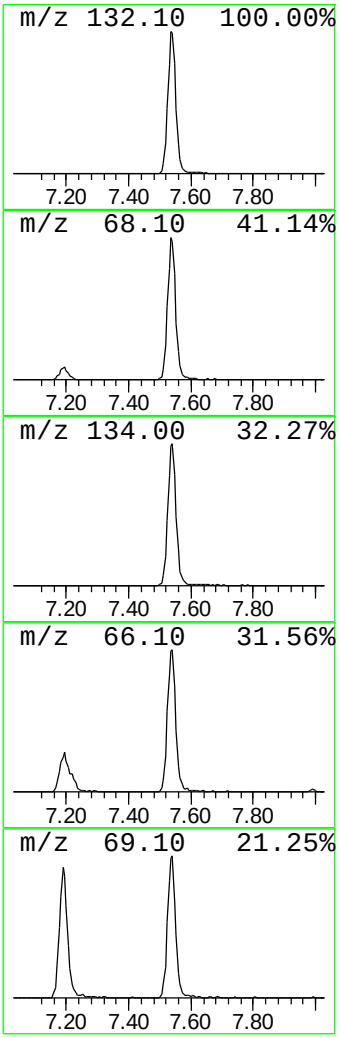
****

Peak Number 3 unknown7.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.53	106.93 ng	893706	1,4-Dichlorobenzene-d4	7.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	22
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	22
5	5-Aminoindole	132	C8H8N2	005192-03-0	22





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111819\
Data File : BG043682.D
Acq On : 18 Nov 2019 20:52
Operator : JU
Sample : K5904-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 11-(2-4)

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

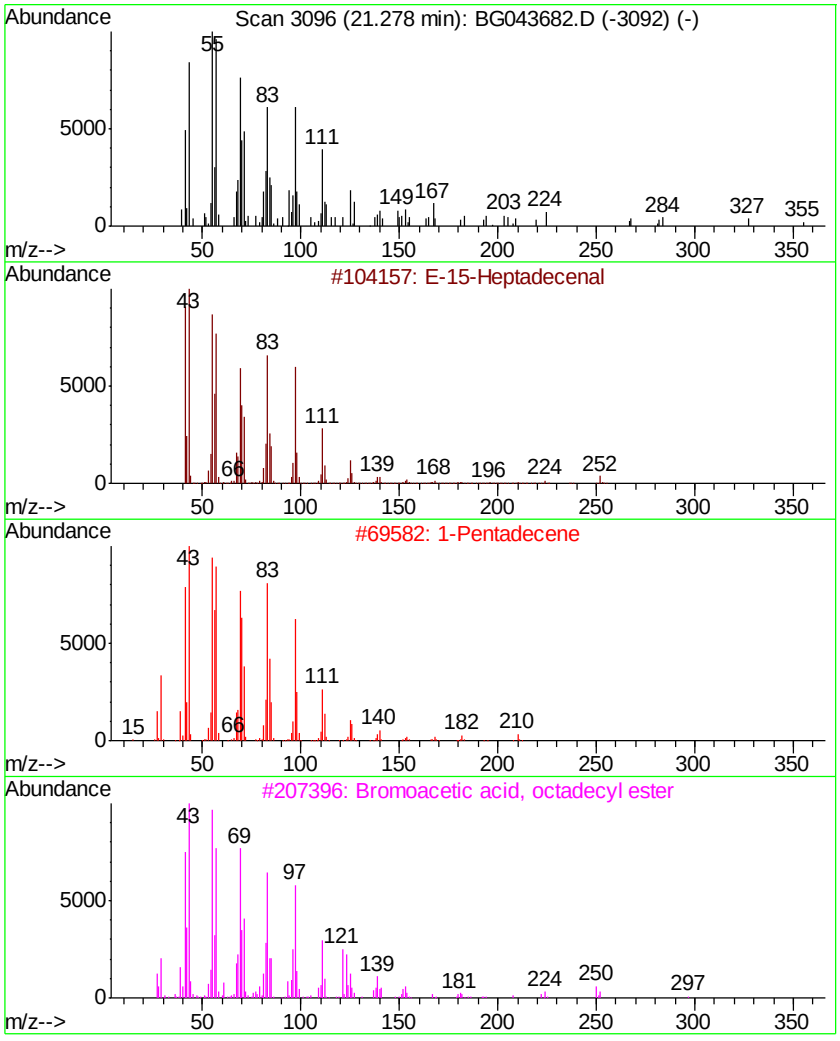
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

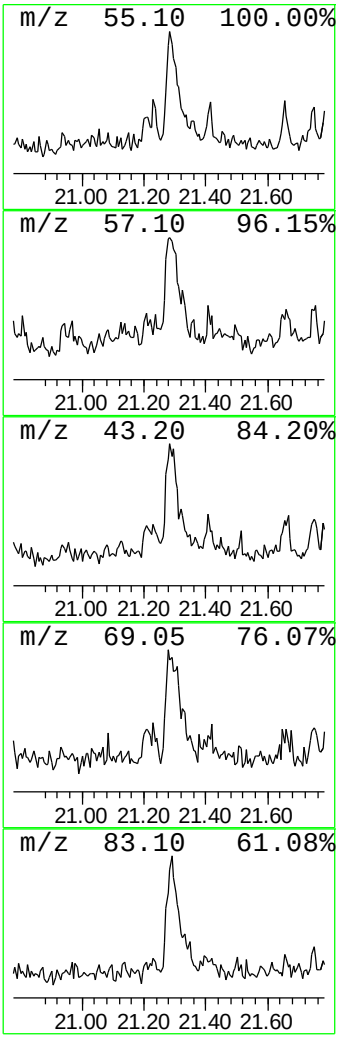
****

Peak Number 5 E-15-Heptadecenal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.28	5.37 ng	160496	Chrysene-d12	21.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	58
2	1-Pentadecene	210	C15H30	013360-61-7	55
3	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	52
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	49
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG111819\
Data File : BG043682.D
Acq On : 18 Nov 2019 20:52
Operator : JU
Sample : K5904-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 11-(2-4)

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
Butane, 2-methoxy...	3.16	14.6	ng	121854	1	7.99	167160	20.0
2-Pentanone, 4-hy...	5.10	18.4	ng	154201	1	7.99	167160	20.0
unknown7.53	7.53	106.9	ng	893706	1	7.99	167160	20.0
E-15-Heptadecenal	21.28	5.4	ng	160496	5	21.64	597863	20.0