LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033262.D
Acq On : 20 Mar 2018 5:08
Operator : SJ/JU
Sample : J1954-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031518-JETT-F-D-S

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	3.498	30	36	47	rBV2	152696	319457	7.72%	1.900%
2	3.587	47	51	61	rVB	95429	159329	3.85%	0.948%
3	6.313	509	515	533	rBV	144697	335287	8.11%	1.994%
4	7.999	796	802	817	rBV2	81902	240001	5.80%	1.427%
5	8.404	864	871	888	rBV	325511	740533	17.90%	4.404%
6	8.892	947	954	967	rBV	106462	245208	5.93%	1.458%
7	9.227	1001	1011	1032	rBV	476303	989825	23.93%	5.887%
8	10.091	1151	1158	1178	rBV	411463	977651	23.64%	5.814%
9	11.777	1436	1445	1464	rBV	163032	367454	8.88%	2.185%
10	14.139	1839	1847	1863	rBV	1340310	2283856	55.21%	13.582%
11	14.926	1973	1981	1990	rBV	71142	119949	2.90%	0.713%
12	15.332	2046	2050	2057	rBV	31617	44595	1.08%	0.265%
13	15.508	2074	2080	2092	rVB2	329995	578277	13.98%	3.439%
14	16.272	2207	2210	2215	rVB	52139	71751	1.73%	0.427%
15	16.671	2271	2278	2283	rBV3	24328	45538	1.10%	0.271%
16	16.983	2324	2331	2346	rBV	934823	1549081	37.45%	9.213%
17	17.130	2351	2356	2358	rBV	50216	69542	1.68%	0.414%
18	17.917	2485	2490	2495	rBV2	34783	49267	1.19%	0.293%
19	18.240	2538	2545	2558	rBV	493283	850535	20.56%	5.058%
20	19.039	2676	2681	2693	rBV	175073	287891	6.96%	1.712%
21	20.267	2886	2890	2896	rBV5	43994	67642	1.64%	0.402%
22	20.761	2967	2974	2984	rBV	3079935	4136437	100.00%	24.600%
23	22.106	3197	3203	3210	rBV	154304	267505	6.47%	1.591%
24	22.594	3279	3286	3295	rBV2	489106	950612	22.98%	5.653%
25	24.486	3600	3608	3617	rVB4	65738	154017	3.72%	0.916%
26	26.389	3921	3932	3948	rVB2	262999	913542	22.09%	5.433%

Sum of corrected areas: 16814782

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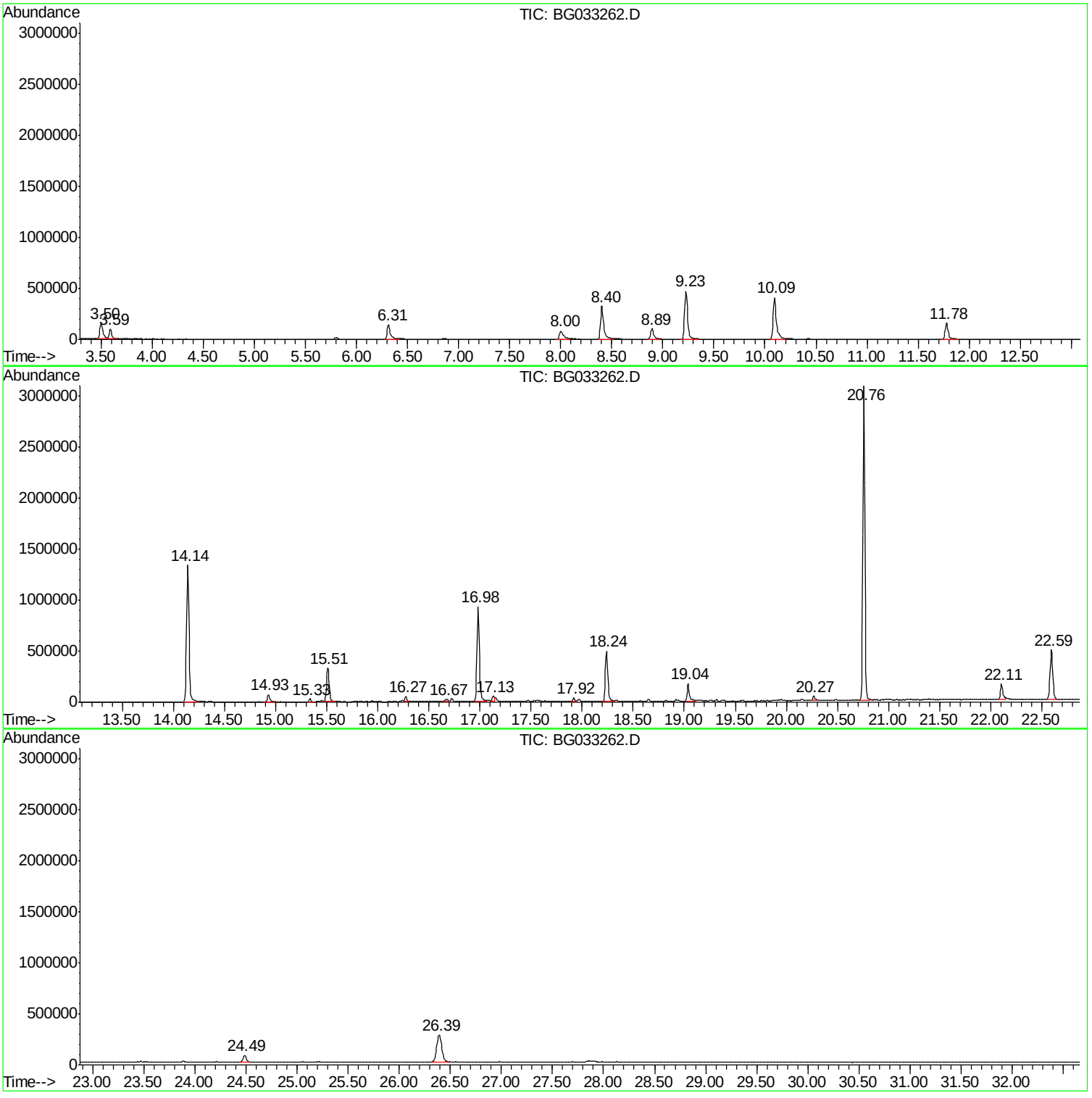
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031518-JETT-F-D-S

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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Data File : BG033262.D
Acq On : 20 Mar 2018 5:08
Operator : SJ/JU
Sample : J1954-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031518-JETT-F-D-S

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

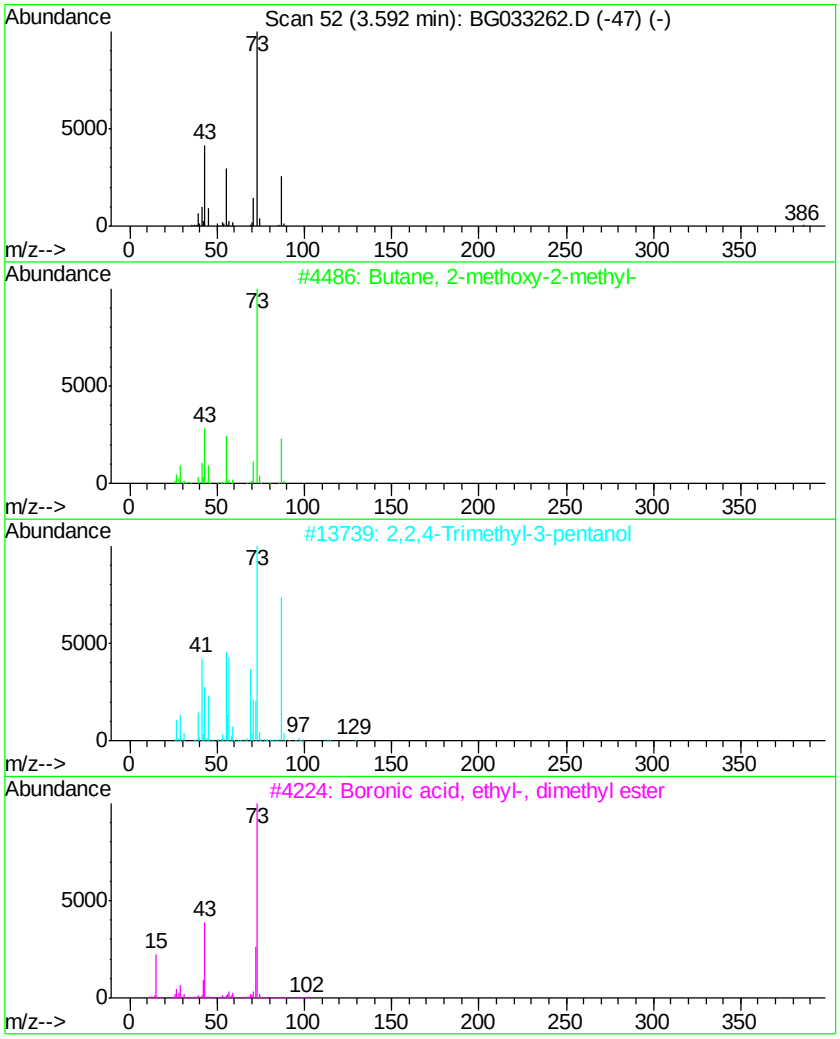
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

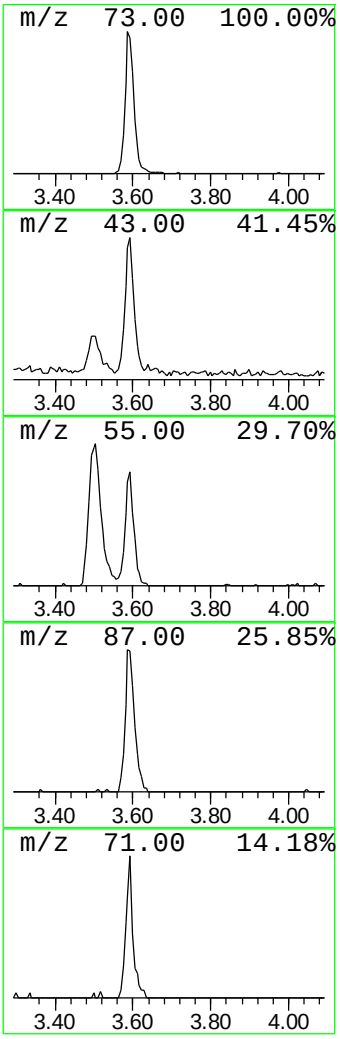
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.59	13.00 ng	159329	1,4-Dichlorobenzene-d4	8.90

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	39
3	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	17
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

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Data File : BG033262.D
Acq On : 20 Mar 2018 5:08
Operator : SJ/JU
Sample : J1954-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031518-JETT-F-D-S

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

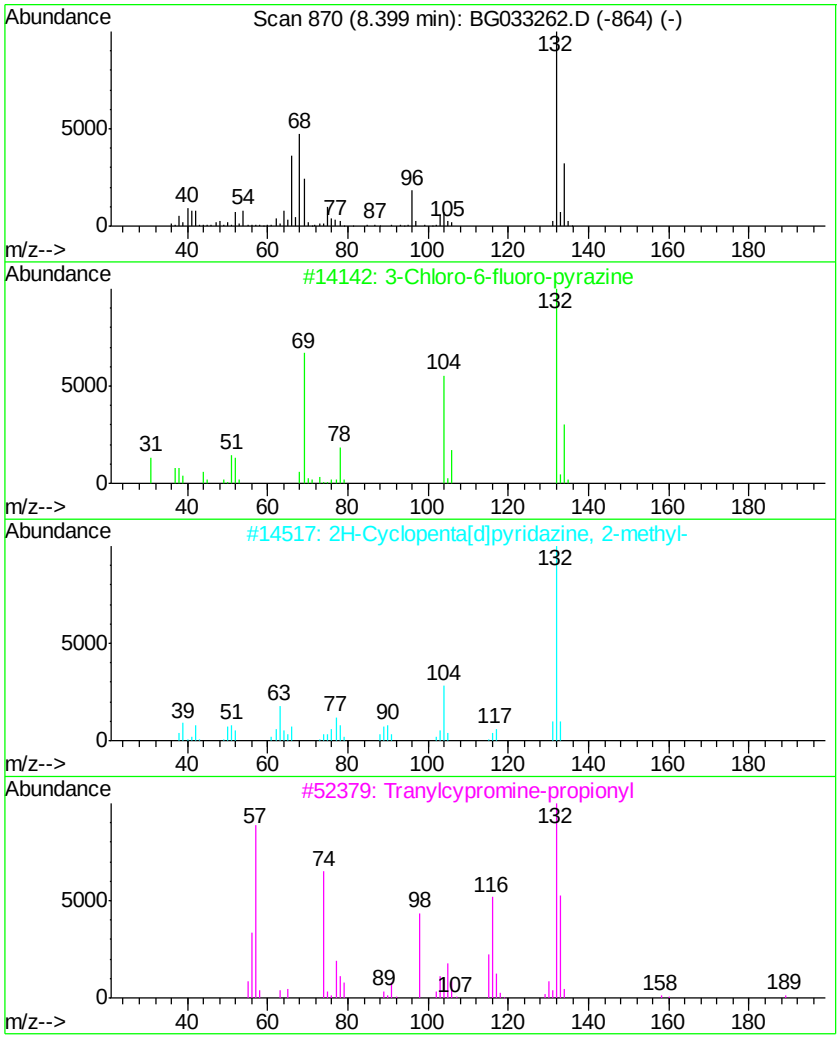
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

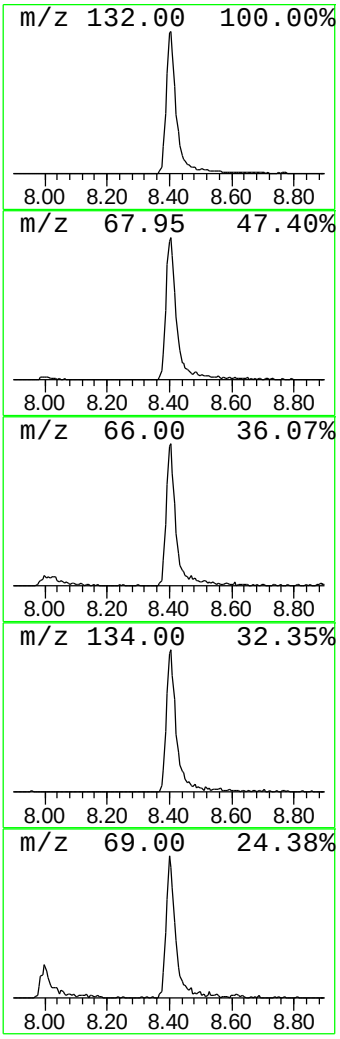
****

Peak Number 3 unknown8.40 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.40	60.40 ng	740533	1,4-Dichlorobenzene-d4	8.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	22
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	12





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033262.D
Acq On : 20 Mar 2018 5:08
Operator : SJ/JU
Sample : J1954-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031518-JETT-F-D-S

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

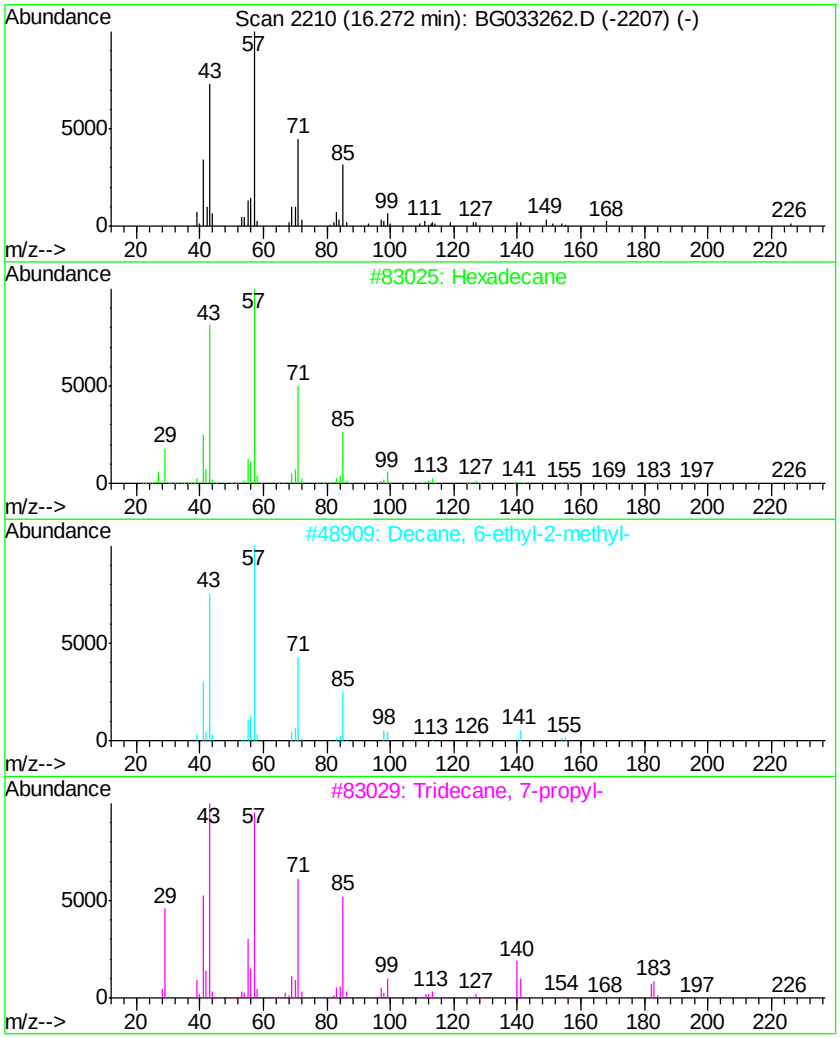
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

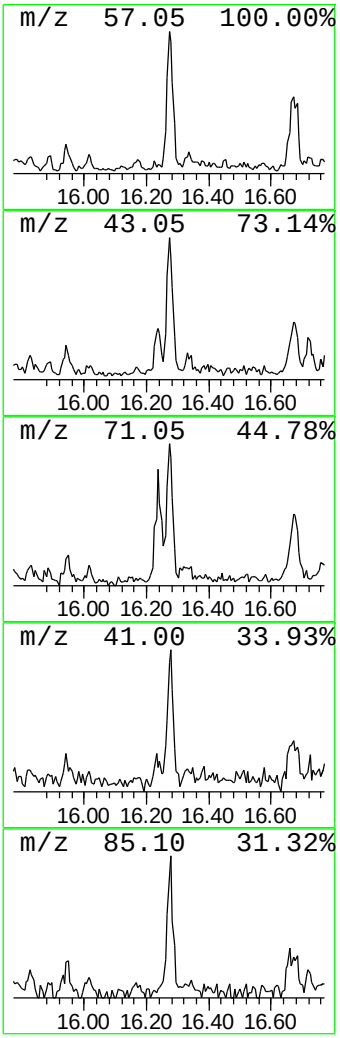
****

Peak Number 5 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.27	2.48 ng	71751	Acenaphthene-d10	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	83
3	Tridecane, 7-propyl-	226	C16H34	055045-09-5	80
4	Dodecane	170	C12H26	000112-40-3	72
5	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	72





Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033262.D
Acq On : 20 Mar 2018 5:08
Operator : SJ/JU
Sample : J1954-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031518-JETT-F-D-S

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

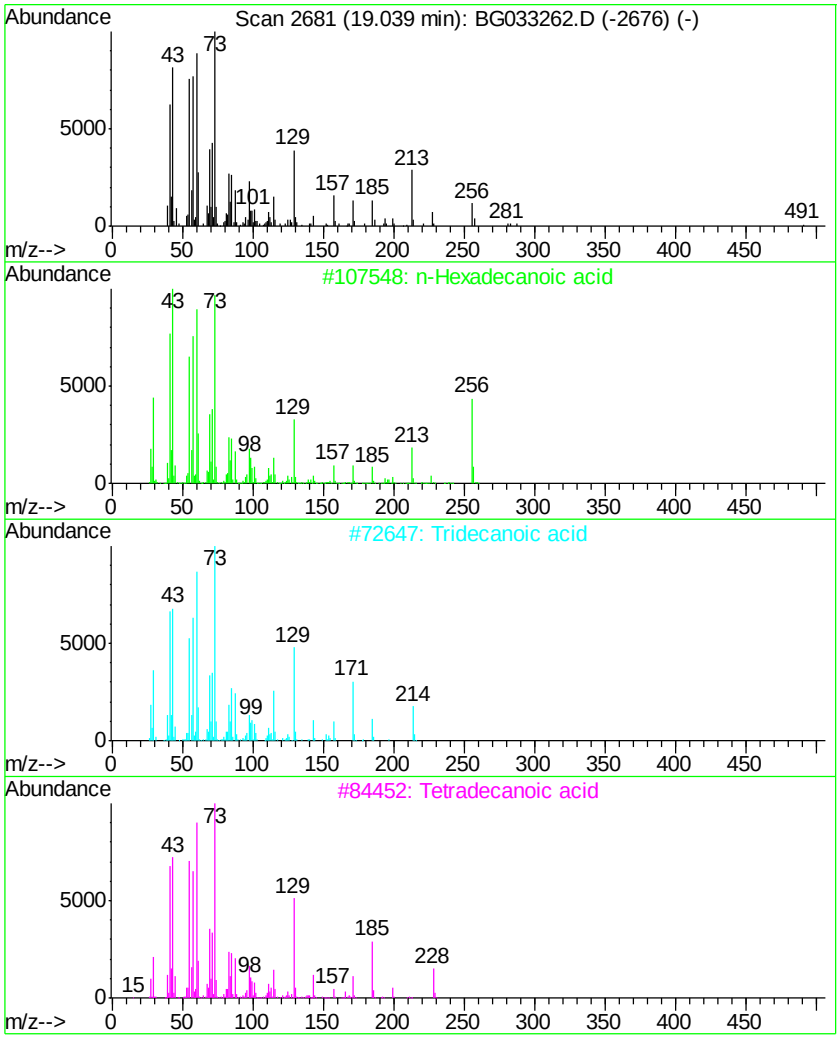
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

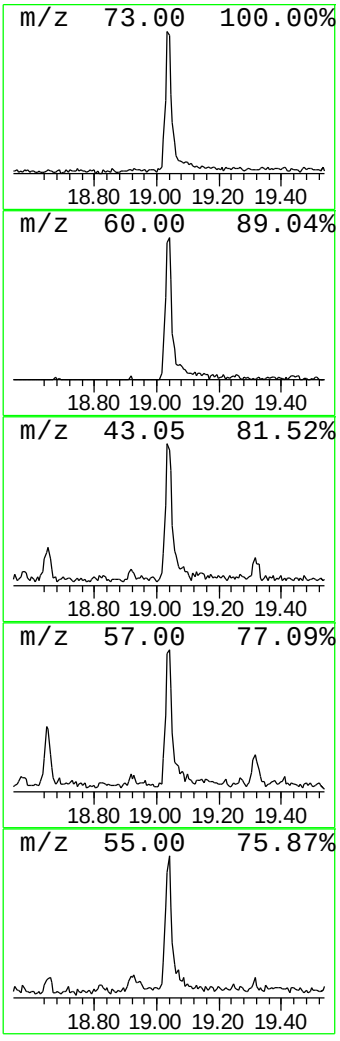
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.04	6.77 ng	287891	Phenanthrene-d10	18.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
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	83





Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
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Acq On : 20 Mar 2018 5:08
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Sample : J1954-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031518-JETT-F-D-S

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

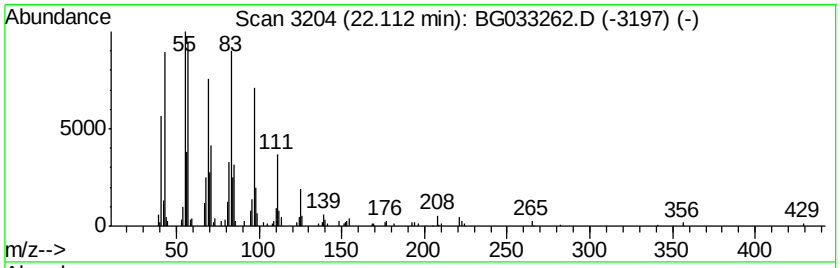
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

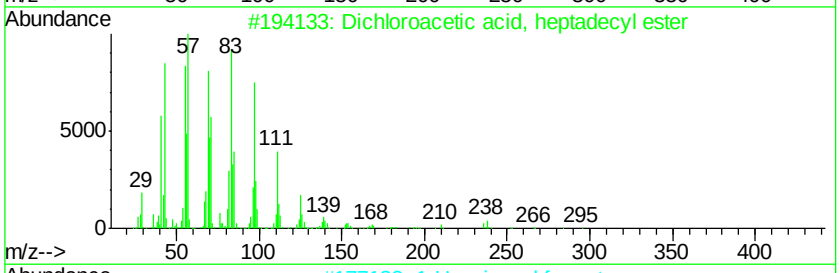
****

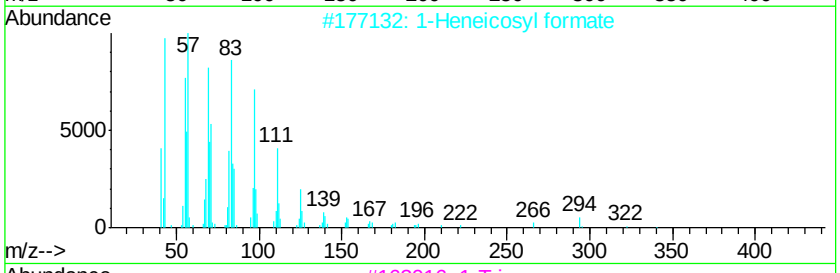
Peak Number 7 Dichloroacetic acid, heptad... Concentration Rank 6

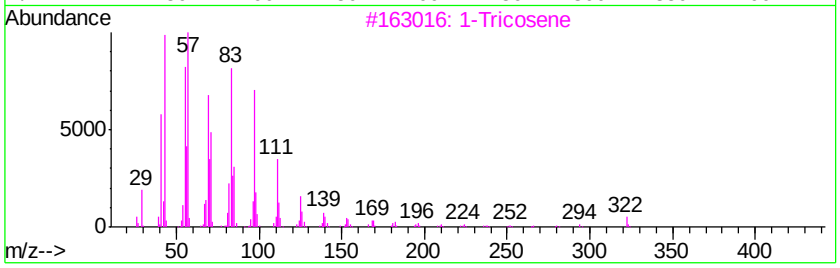
R.T.	EstConc	Area	Relative to ISTD	R.T.
22.11	5.63 ng	267505	Chrysene-d12	22.59

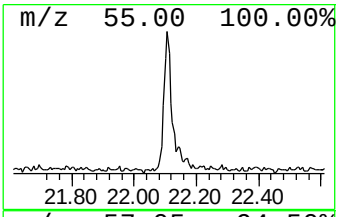
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3	1-Tricosene	322	C23H46	018835-32-0	94
4	1-Docosene	308	C22H44	001599-67-3	94
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94

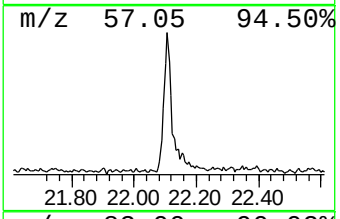


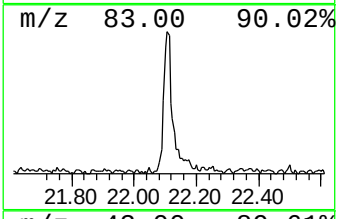


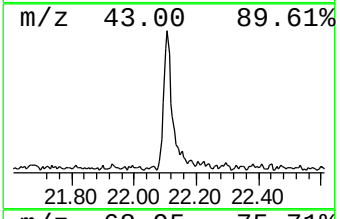


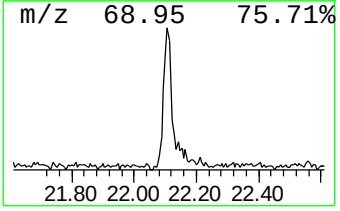












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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

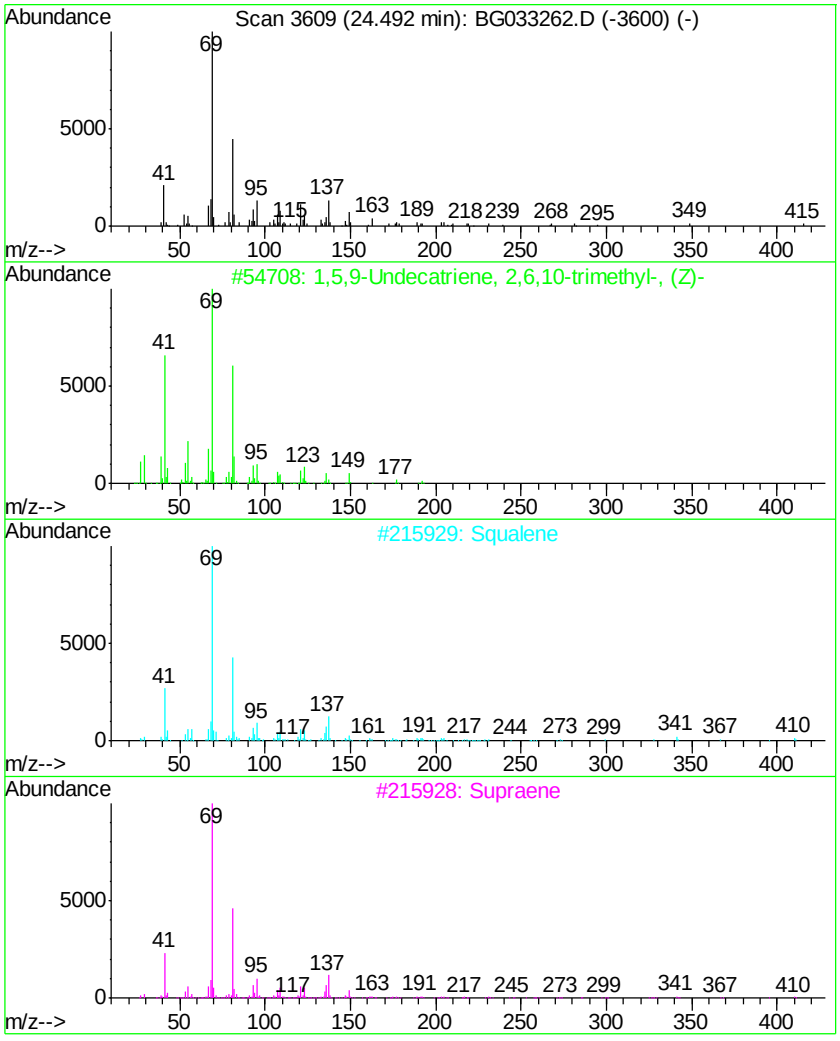
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

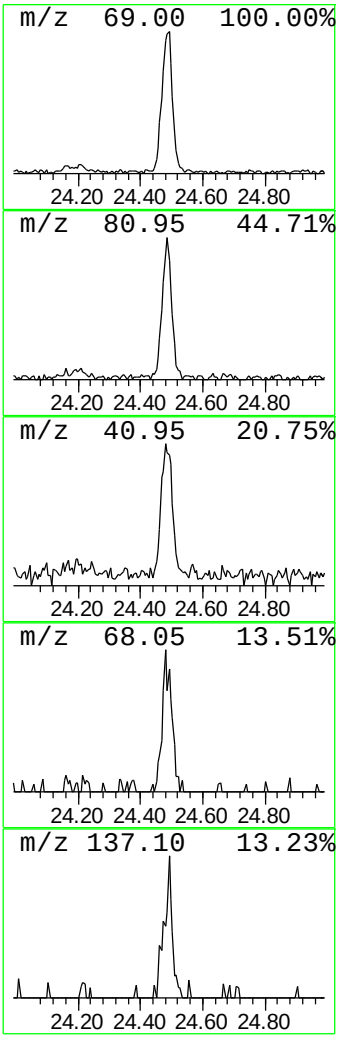
****

Peak Number 8 1,5,9-Undecatriene, 2,6,10-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.49	3.24 ng	154017	Chrysene-d12	22.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	83
2	Squalene	410	C30H50	000111-02-4	72
3	Supraene	410	C30H50	007683-64-9	64
4	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	59
5	1,5-Heptadiene, 3,3,5-trimethyl-	138	C10H18	074630-29-8	59





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	3.59	13.0	ng	159329	1	8.90	245208	20.0
unknown8.40	8.40	60.4	ng	740533	1	8.90	245208	20.0
Hexadecane	16.27	2.5	ng	71751	3	15.51	578277	20.0
n-Hexadecanoic acid	19.04	6.8	ng	287891	4	18.24	850535	20.0
Dichloroacetic ac...	22.11	5.6	ng	267505	5	22.59	950612	20.0
1,5,9-Undecatrien...	24.49	3.2	ng	154017	5	22.59	950612	20.0