LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062218\
Data File : BG035356.D
Acq On : 23 Jun 2018 7:06
Operator : JU/SJ
Sample : J3587-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 061818-DBRI-E-U-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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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	5.631	392	399	409	rBV	282193	464482	10.69%	2.693%
2	7.211	661	668	681	rVB	185205	338408	7.79%	1.962%
3	7.587	724	732	740	rBV	507206	879508	20.24%	5.099%
4	8.057	805	812	820	rVB2	157393	270065	6.22%	1.566%
5	8.375	859	866	874	rBV	736504	1314007	30.24%	7.619%
6	9.215	1000	1009	1020	rBV	610307	1072340	24.68%	6.218%
7	10.859	1281	1289	1297	rBV	183443	336405	7.74%	1.951%
8	13.297	1697	1704	1714	rBV	1677584	2643426	60.83%	15.327%
9	14.120	1838	1844	1850	rBV	69216	105313	2.42%	0.611%
10	14.672	1929	1938	1947	rBV2	319607	536008	12.34%	3.108%
11	15.958	2153	2157	2162	rVB	63335	83308	1.92%	0.483%
12	16.158	2181	2191	2200	rBV	924844	1412480	32.51%	8.190%
13	17.415	2397	2405	2412	rBV	466963	707121	16.27%	4.100%
14	18.296	2547	2555	2564	rBV2	69436	106112	2.44%	0.615%
15	19.565	2767	2771	2781	rBV3	45463	66389	1.53%	0.385%
16	20.024	2843	2849	2856	rBV	3340655	4345268	100.00%	25.194%
17	21.328	3066	3071	3079	rBV8	25394	59116	1.36%	0.343%
18	21.680	3125	3131	3139	rBV2	530405	876882	20.18%	5.084%
19	22.479	3262	3267	3272	rBV3	44440	67463	1.55%	0.391%
20	23.172	3380	3385	3395	rVB3	79036	143778	3.31%	0.834%
21	23.977	3513	3522	3532	rVB3	89681	206250	4.75%	1.196%
22	24.905	3669	3680	3695	rVB2	299804	1005754	23.15%	5.831%
23	26.057	3868	3876	3885	rBV4	59710	158641	3.65%	0.920%
24	27.408	4097	4106	4107	rBV6	26571	48577	1.12%	0.282%

Sum of corrected areas: 17247101

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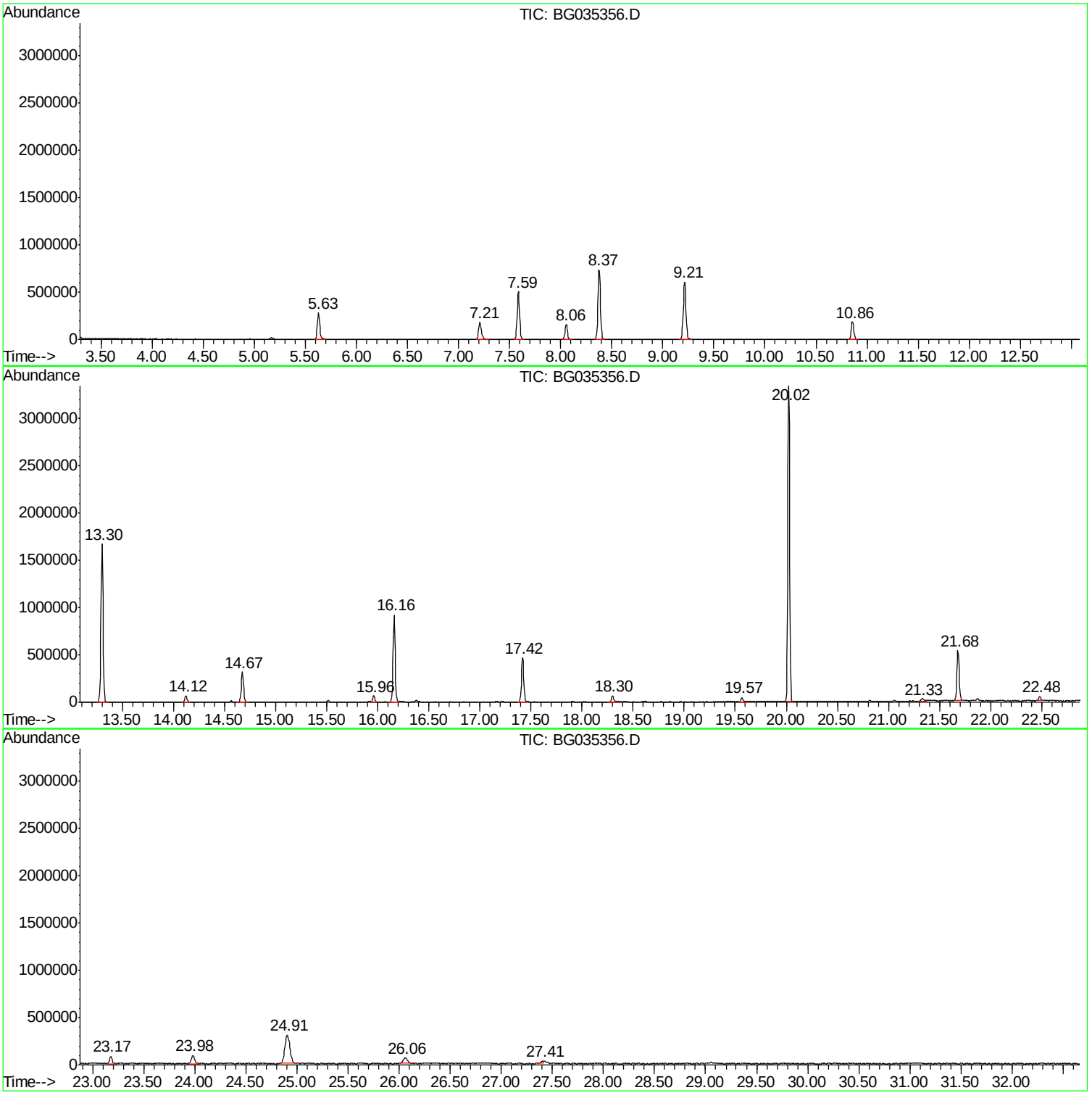
Instrument :
BNA_G
ClientSampleId :
061818-DBRI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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\BG062218\
Data File : BG035356.D
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Misc :
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Instrument : BNA_G
ClientSampleId : 061818-DBRI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

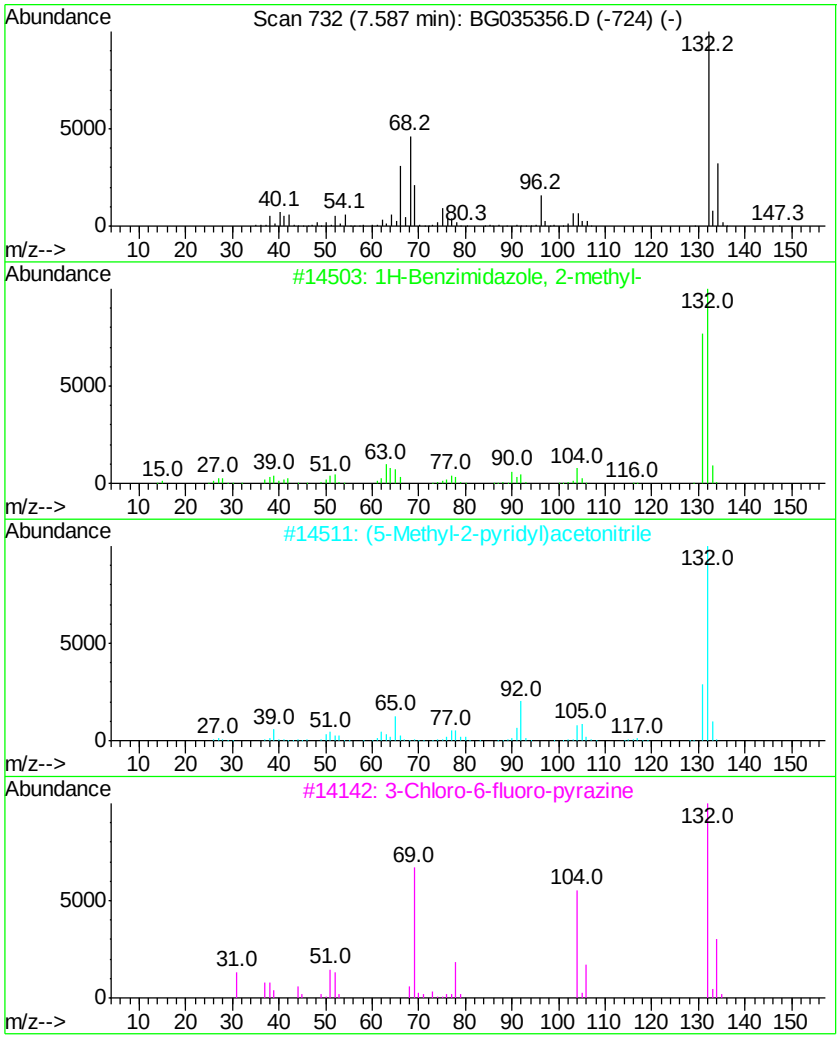
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

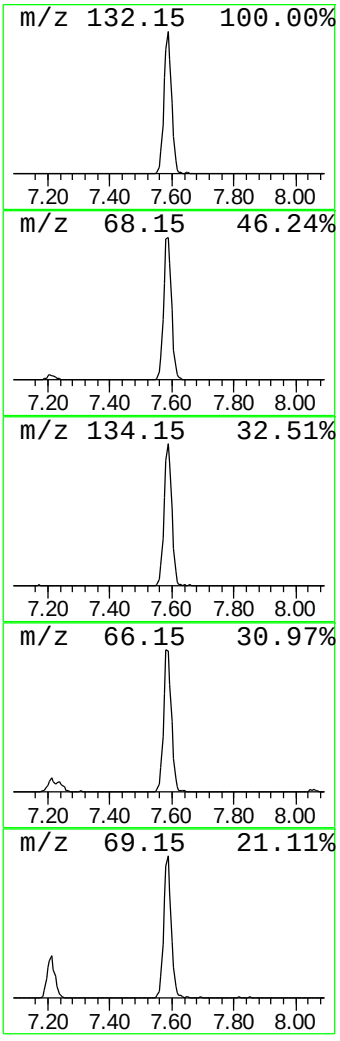
****

Peak Number 1 unknown7.59 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	65.13 ng	879508	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
2	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	22
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	5-Aminoindole	132	C8H8N2	005192-03-0	12





Library Search Compound Report

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Misc :
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Instrument : BNA_G
ClientSampleId : 061818-DBRI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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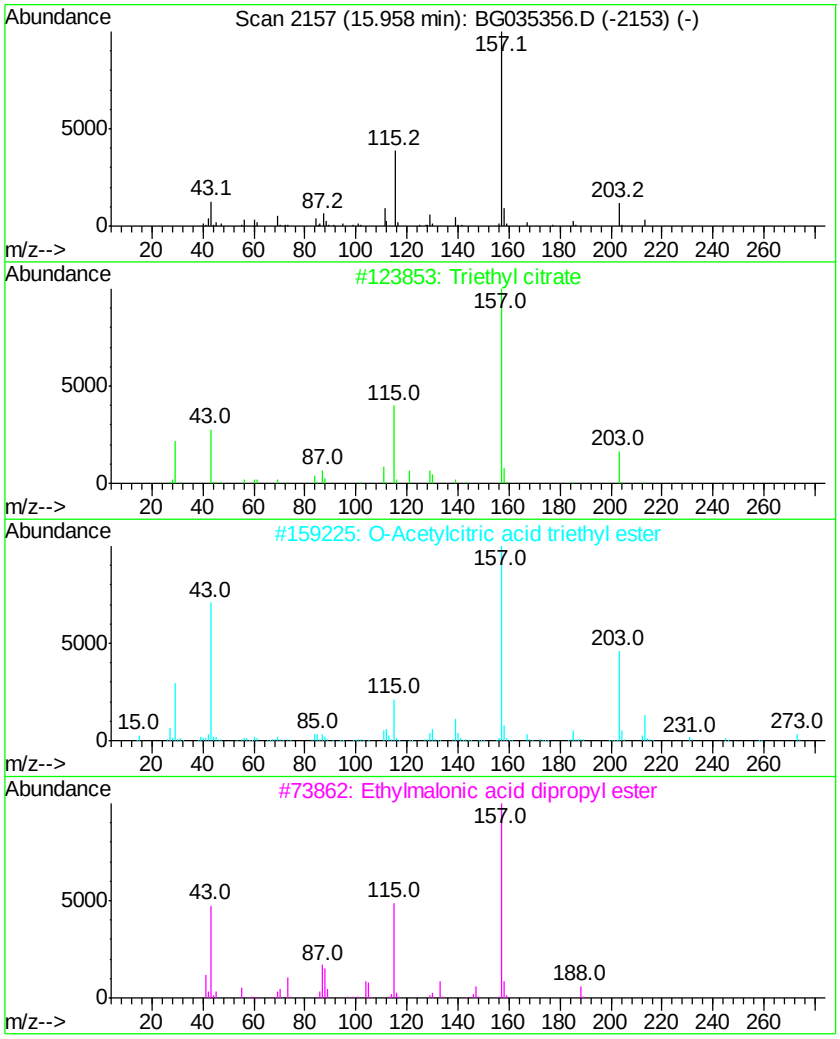
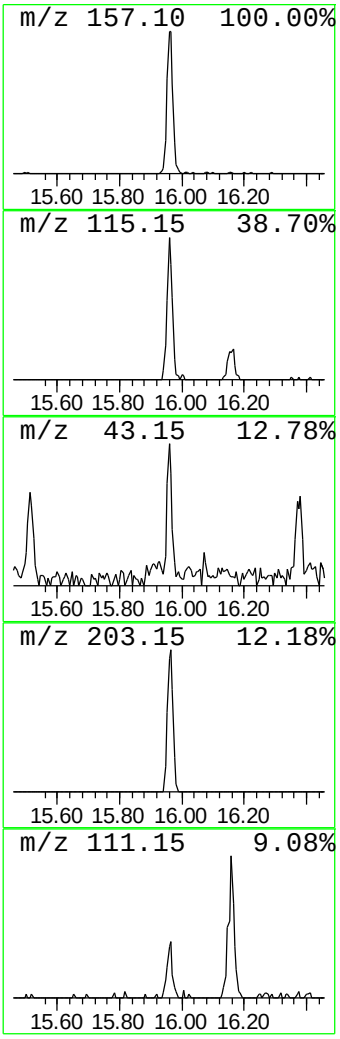
****

Peak Number 3 Triethyl citrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.96	3.11 ng	83308	Acenaphthene-d10	14.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	83
2	O-Acetylcitric acid triethyl ester	318	C14H22O8	000077-89-4	78
3	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	39
4	3-Chloro2-fluorobenzoic acid, 6-...	370	C21H32ClFO2	1000338-64-9	33
5	3-Chloro2-fluorobenzoic acid, 4-...	370	C21H32ClFO2	1000338-64-7	33





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062218\
Data File : BG035356.D
Acq On : 23 Jun 2018 7:06
Operator : JU/SJ
Sample : J3587-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 061818-DBRI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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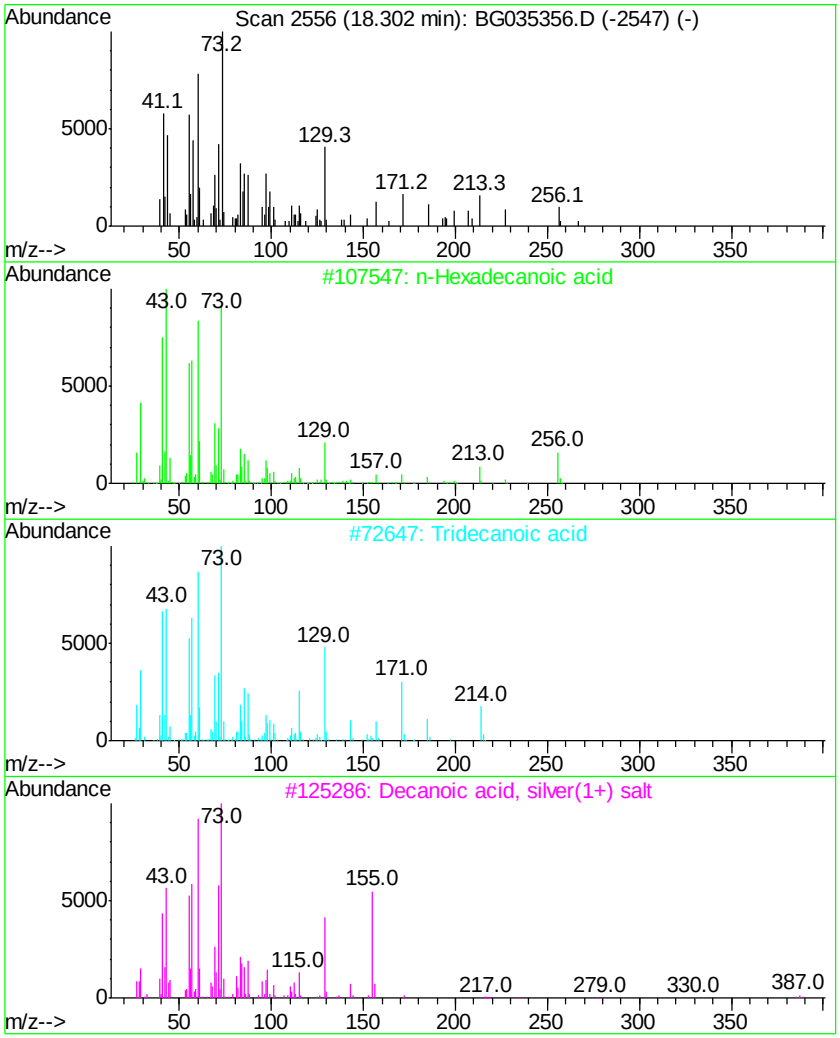
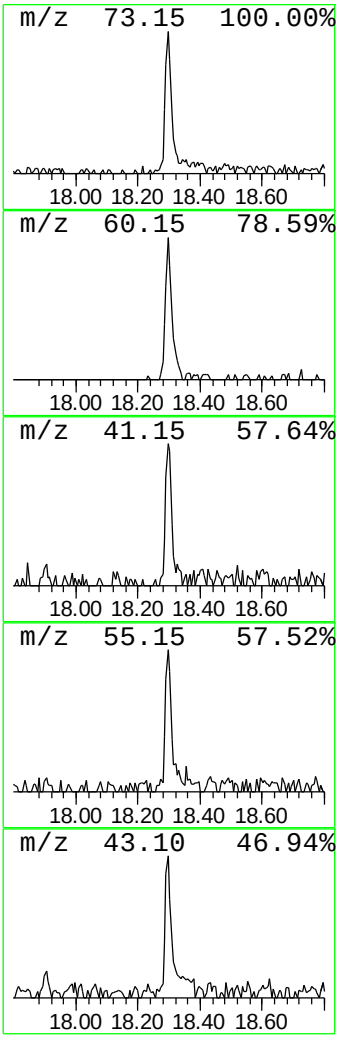
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	3.00 ng	106112	Phenanthrene-d10	17.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	86
3	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	59
4	Undecanoic acid	186	C11H22O2	000112-37-8	53
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	53





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062218\
Data File : BG035356.D
Acq On : 23 Jun 2018 7:06
Operator : JU/SJ
Sample : J3587-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 061818-DBRI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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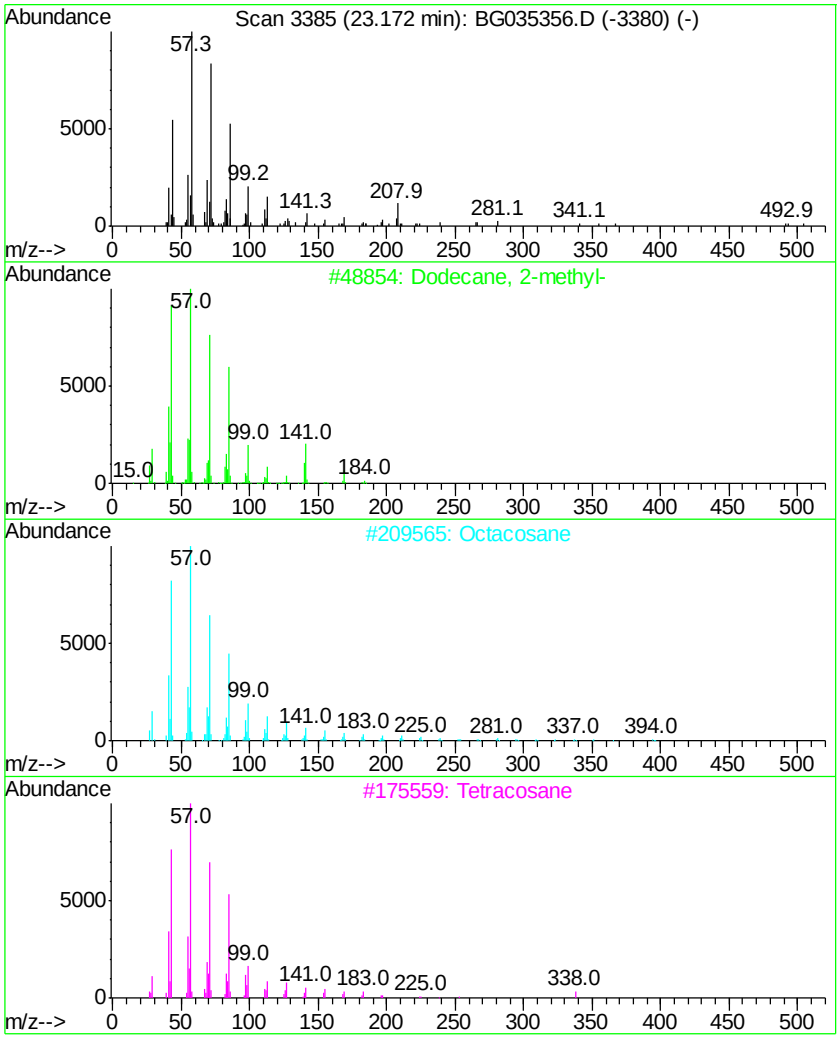
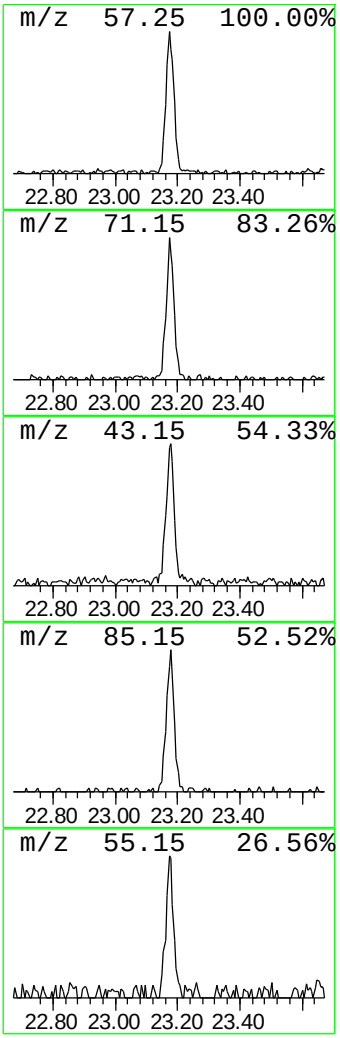
****

Peak Number 5 Dodecane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.17	3.28 ng	143778	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-	184	C13H28	001560-97-0	93
2	Octacosane	394	C28H58	000630-02-4	87
3	Tetracosane	338	C24H50	000646-31-1	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Pentacosane	352	C25H52	000629-99-2	86





Library Search Compound Report

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Operator : JU/SJ
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Misc :
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Instrument : BNA_G
ClientSampleId : 061818-DBRI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
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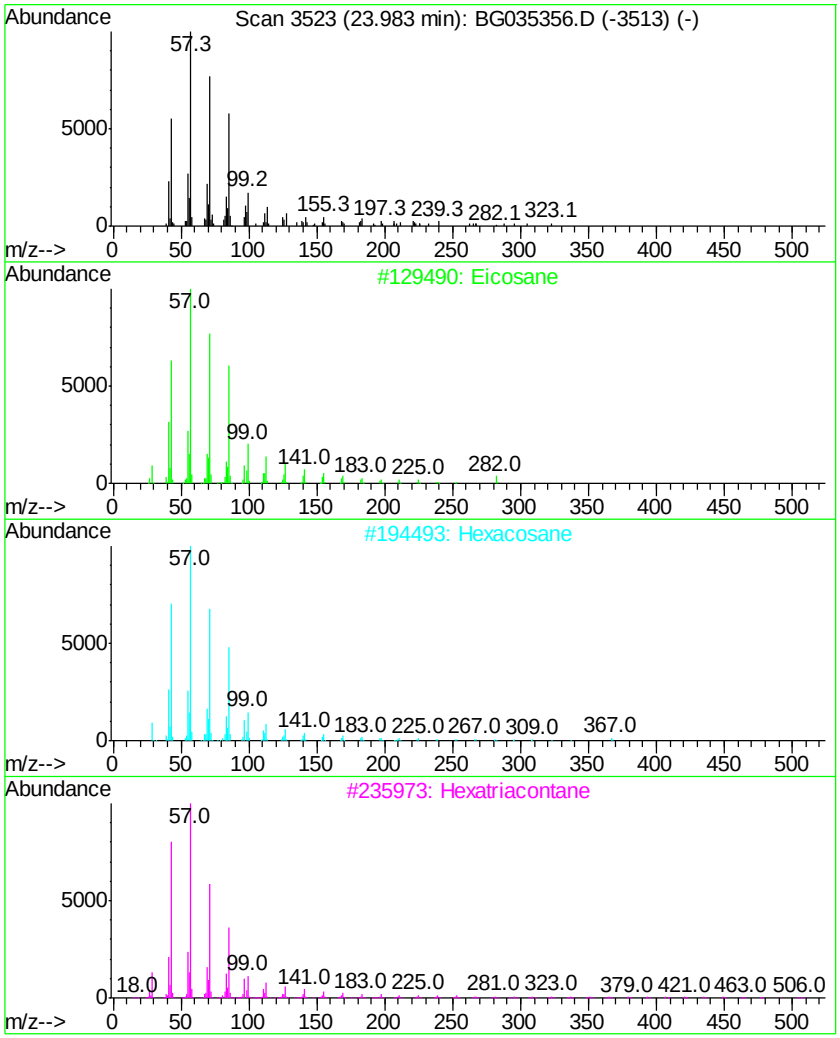
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

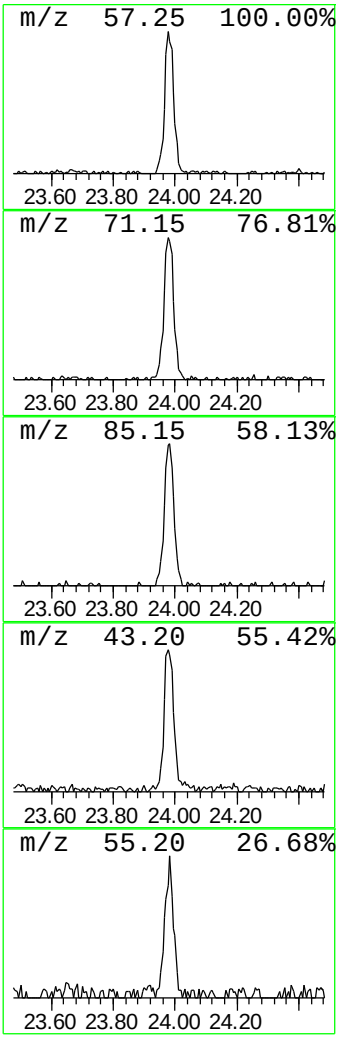
****

Peak Number 6 Eicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.98	4.10 ng	206250	Perylene-d12	24.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	97
2	Hexacosane	366	C26H54	000630-01-3	91
3	Hexatriacontane	507	C36H74	000630-06-8	91
4	Hentriacontane	437	C31H64	000630-04-6	91
5	Heneicosane	296	C21H44	000629-94-7	91





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Misc :
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Instrument : BNA_G
ClientSampleId : 061818-DBRI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

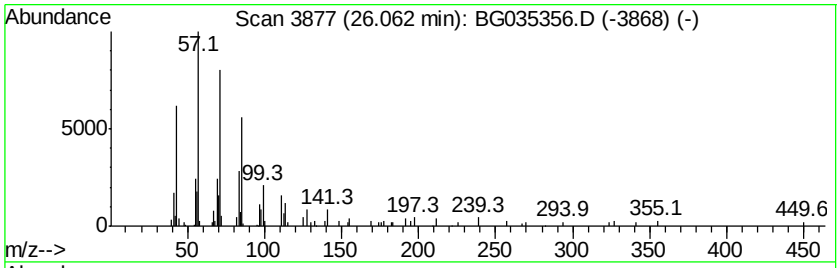
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

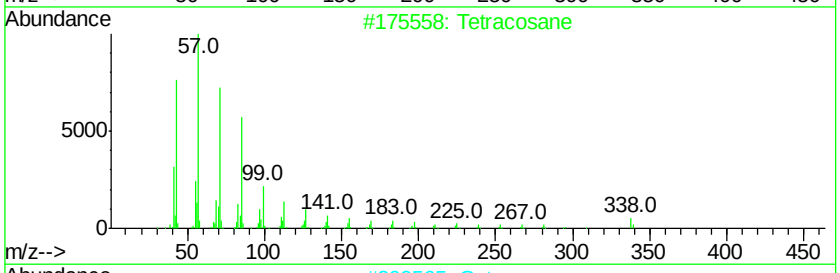
****

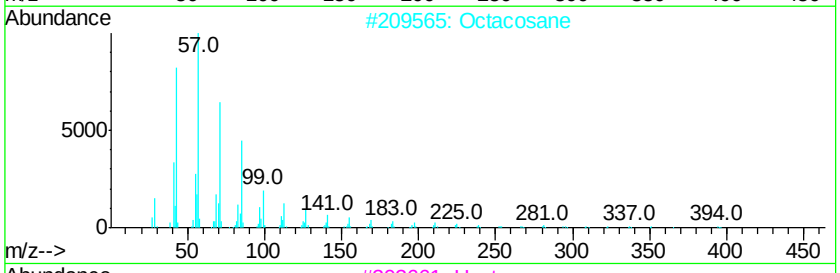
Peak Number 7 Tetracosane Concentration Rank 5

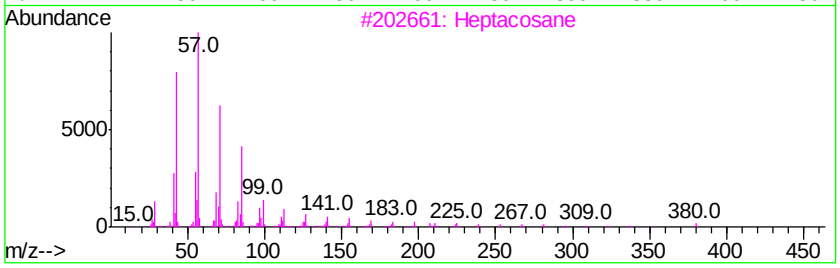
R.T.	EstConc	Area	Relative to ISTD	R.T.
26.06	3.15 ng	158641	Perylene-d12	24.90

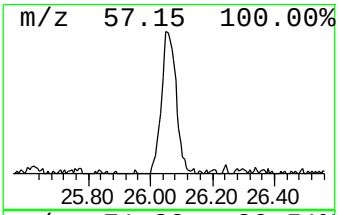
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	90
2	Octacosane	394	C28H58	000630-02-4	90
3	Heptacosane	380	C27H56	000593-49-7	87
4	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	87
5	Pentacosane	352	C25H52	000629-99-2	87

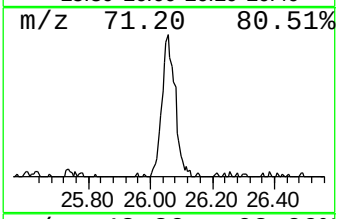


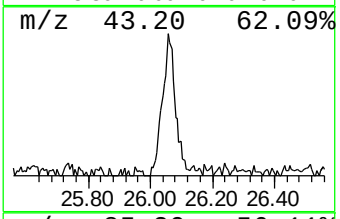


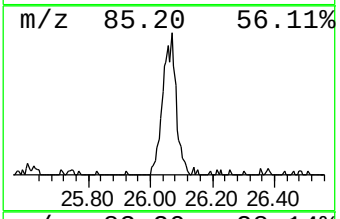


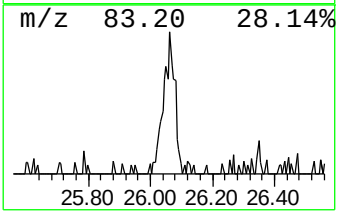












Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown7.59	7.59	65.1	ng	879508	1	8.06	270065	20.0
Triethyl citrate	15.96	3.1	ng	83308	3	14.67	536008	20.0
n-Hexadecanoic acid	18.30	3.0	ng	106112	4	17.42	707121	20.0
Dodecane, 2-methyl-	23.17	3.3	ng	143778	5	21.68	876882	20.0
Eicosane	23.98	4.1	ng	206250	6	24.90	1005750	20.0
Tetracosane	26.06	3.1	ng	158641	6	24.90	1005750	20.0