LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062218\
Data File : BG035367.D
Acq On : 23 Jun 2018 14:11
Operator : JU/SJ
Sample : J3623-06
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 061918-DBRI-F-U-B

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	5.632	392	399	407	rBV	340365	566499	11.77%	2.950%
2	7.212	661	668	678	rBV	238542	461116	9.58%	2.401%
3	7.588	724	732	741	rVB	616452	1044786	21.71%	5.441%
4	8.053	805	811	819	rBV	177044	313398	6.51%	1.632%
5	8.376	858	866	878	rVB	849223	1506968	31.32%	7.848%
6	9.216	998	1009	1020	rBV	711520	1253653	26.05%	6.528%
7	10.855	1281	1288	1296	rBV	212602	387006	8.04%	2.015%
8	13.298	1697	1704	1713	rBV	1986181	3053215	63.45%	15.900%
9	14.121	1838	1844	1854	rBV	81209	119702	2.49%	0.623%
10	14.673	1931	1938	1946	rBV3	369261	602760	12.53%	3.139%
11	15.959	2153	2157	2161	rVB	83285	95167	1.98%	0.496%
12	16.159	2184	2191	2201	rBV	1063710	1609612	33.45%	8.382%
13	17.416	2397	2405	2413	rBV2	518564	769621	15.99%	4.008%
14	18.297	2549	2555	2561	rBV2	66180	93382	1.94%	0.486%
15	20.025	2843	2849	2855	rBV	3679957	4812023	100.00%	25.059%
16	20.818	2980	2984	2988	rBV3	45448	57763	1.20%	0.301%
17	21.329	3065	3071	3076	rBV2	87568	141452	2.94%	0.737%
18	21.681	3124	3131	3143	rVB2	567381	937284	19.48%	4.881%
19	21.875	3159	3164	3170	rBV2	63810	106018	2.20%	0.552%
20	22.486	3262	3268	3272	rBV2	61475	98558	2.05%	0.513%
21	23.179	3379	3386	3394	rBV3	58137	120223	2.50%	0.626%
22	23.978	3516	3522	3529	rBV4	48272	104051	2.16%	0.542%
23	24.900	3669	3679	3694	rBV2	314575	948583	19.71%	4.940%

Sum of corrected areas: 19202840

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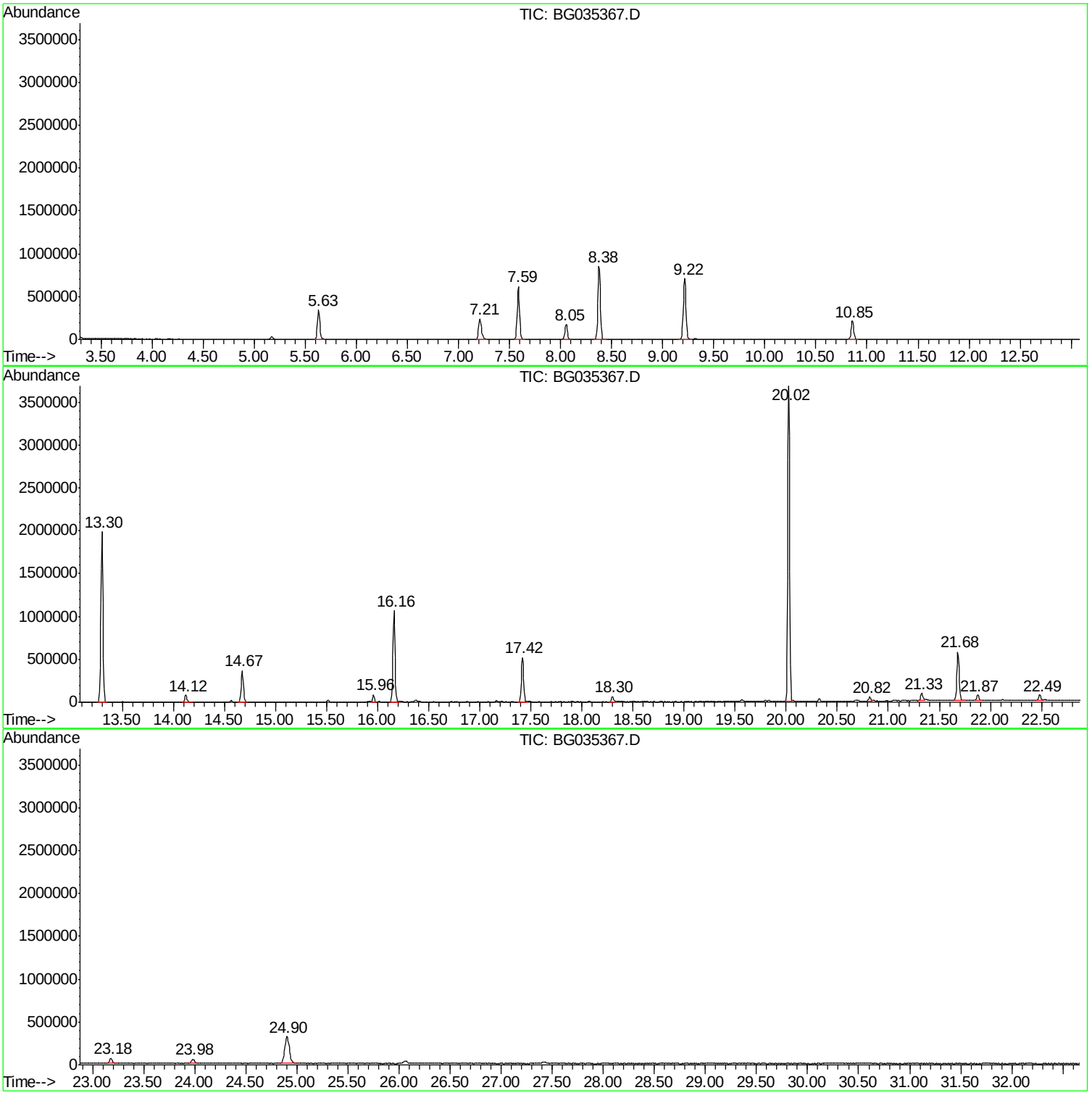
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
061918-DBRI-F-U-B

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 : BG035367.D
Acq On : 23 Jun 2018 14:11
Operator : JU/SJ
Sample : J3623-06
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 061918-DBRI-F-U-B

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

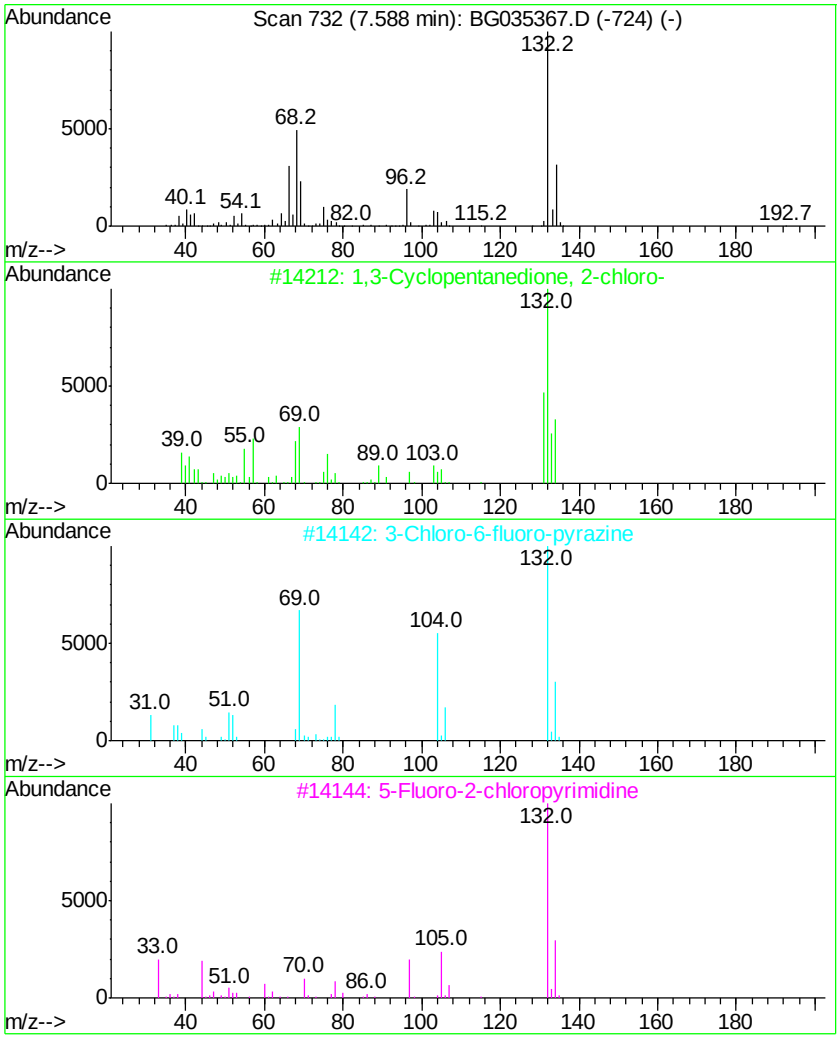
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

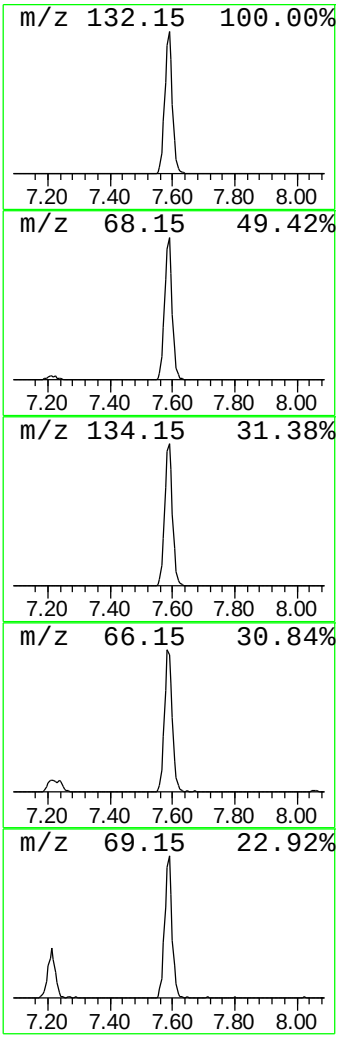
****

Peak Number 1 unknown7.59 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	66.67 ng	1044790	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





Library Search Compound Report

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Data File : BG035367.D
Acq On : 23 Jun 2018 14:11
Operator : JU/SJ
Sample : J3623-06
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 061918-DBRI-F-U-B

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

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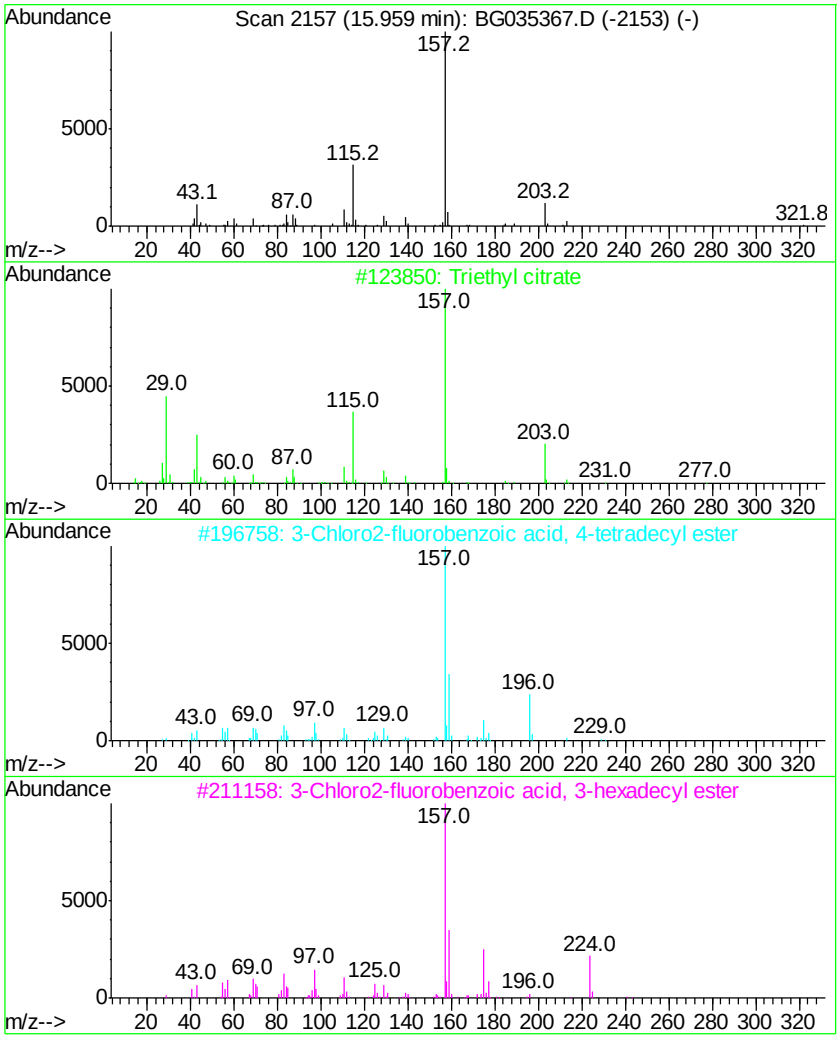
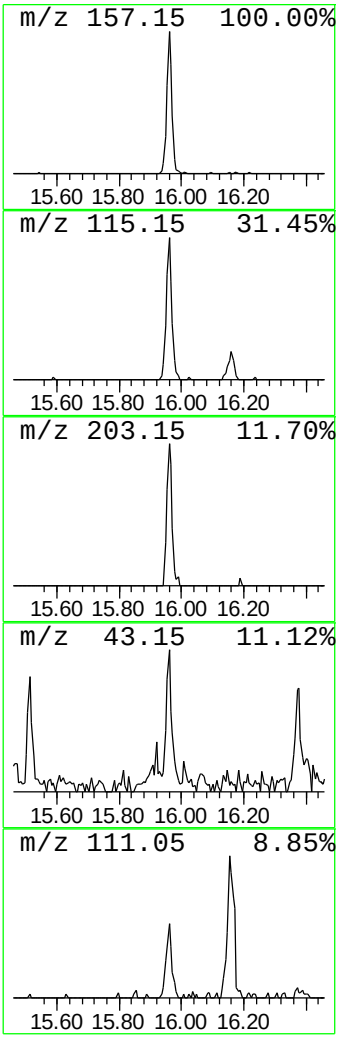
Peak Number 3 Triethyl citrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.96	3.16 ng	95167	Acenaphthene-d10	14.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	78
2	3-Chloro2-fluorobenzoic acid, 4-...	370	C21H32ClFO2	1000338-64-7	33
3	3-Chloro2-fluorobenzoic acid, 3-...	398	C23H36ClFO2	1000338-65-4	33
4	3-Chloro2-fluorobenzoic acid, 5-...	384	C22H34ClFO2	1000338-65-2	33
5	3-Chloro2-fluorobenzoic acid, 4-...	356	C20H30ClFO2	1000338-64-4	33





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062218\
Data File : BG035367.D
Acq On : 23 Jun 2018 14:11
Operator : JU/SJ
Sample : J3623-06
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 061918-DBRI-F-U-B

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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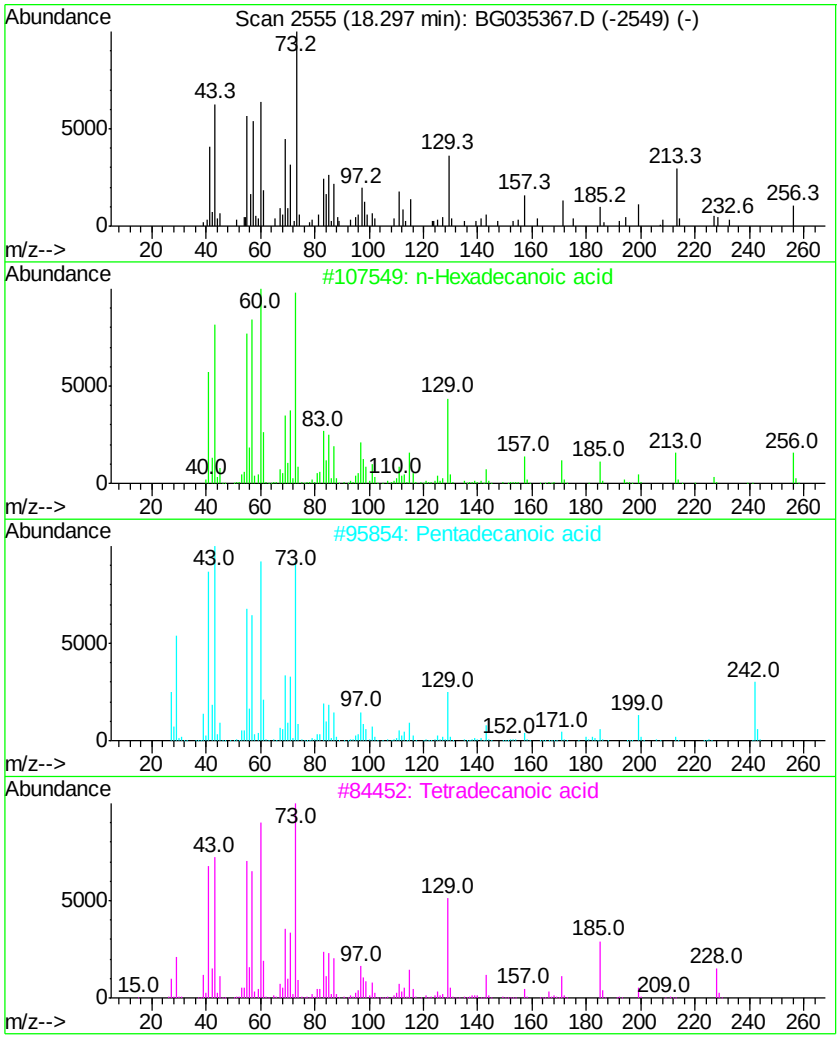
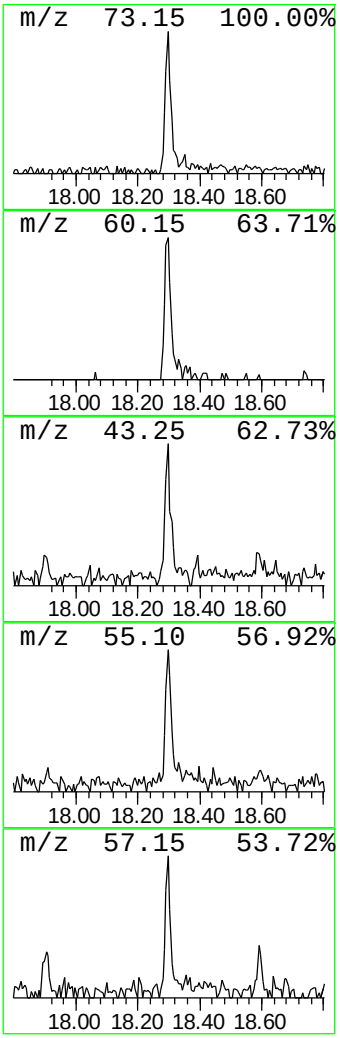
Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	2.43 ng	93382	Phenanthrene-d10	17.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	59
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
4	n-Decanoic acid	172	C10H20O2	000334-48-5	43
5	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	35





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Data File : BG035367.D
Acq On : 23 Jun 2018 14:11
Operator : JU/SJ
Sample : J3623-06
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 061918-DBRI-F-U-B

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

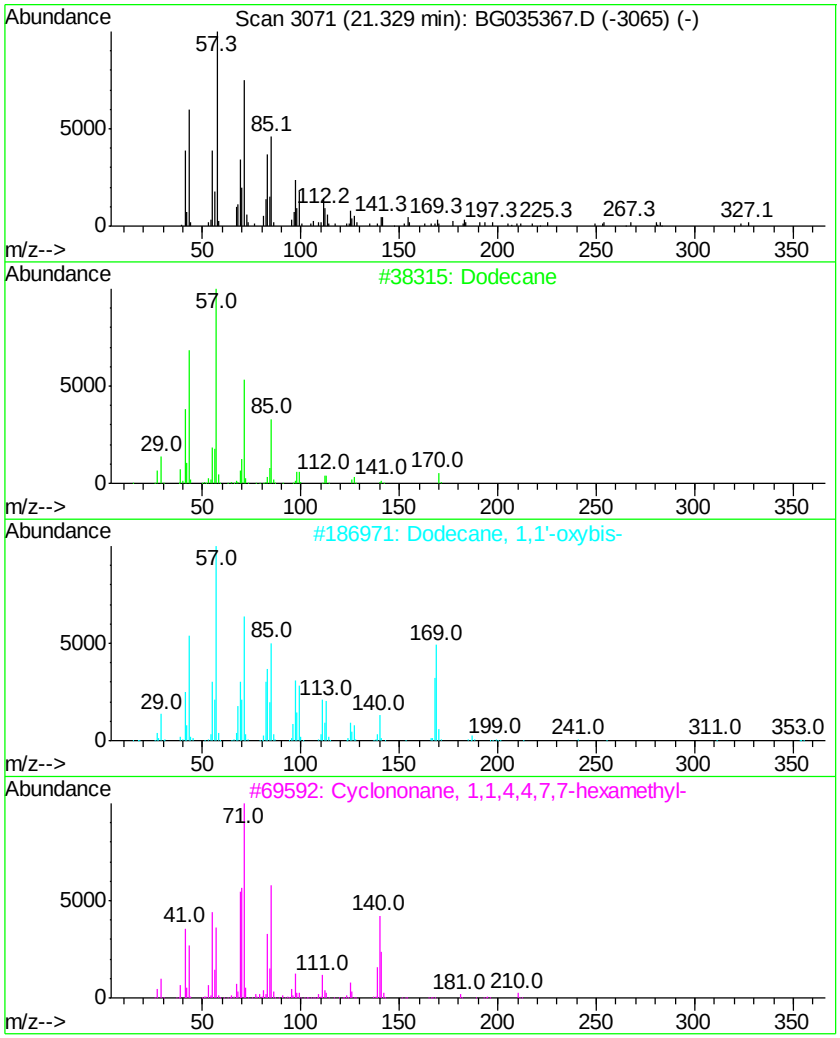
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

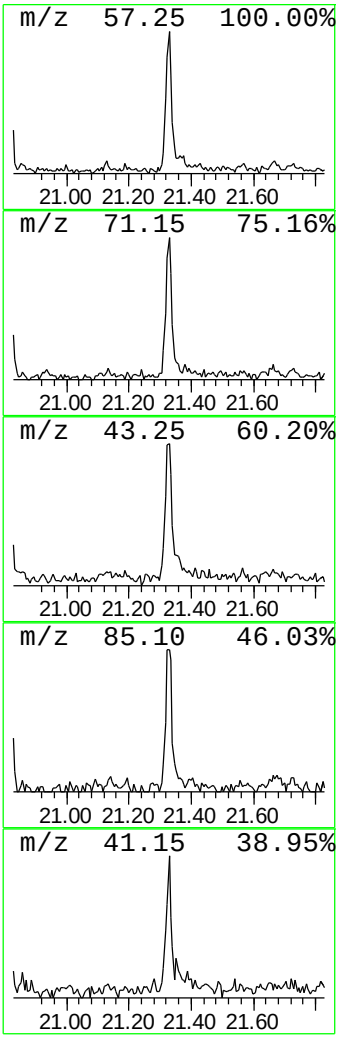
****

Peak Number 5 Dodecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.33	3.02 ng	141452	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	95
2	Dodecane, 1,1'-oxybis-	354	C24H50O	004542-57-8	91
3	Cyclononane, 1,1,4,4,7,7-hexamet...	210	C15H30	149331-19-1	62
4	Eicosane	282	C20H42	000112-95-8	60
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	58





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Acq On : 23 Jun 2018 14:11
Operator : JU/SJ
Sample : J3623-06
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ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 061918-DBRI-F-U-B

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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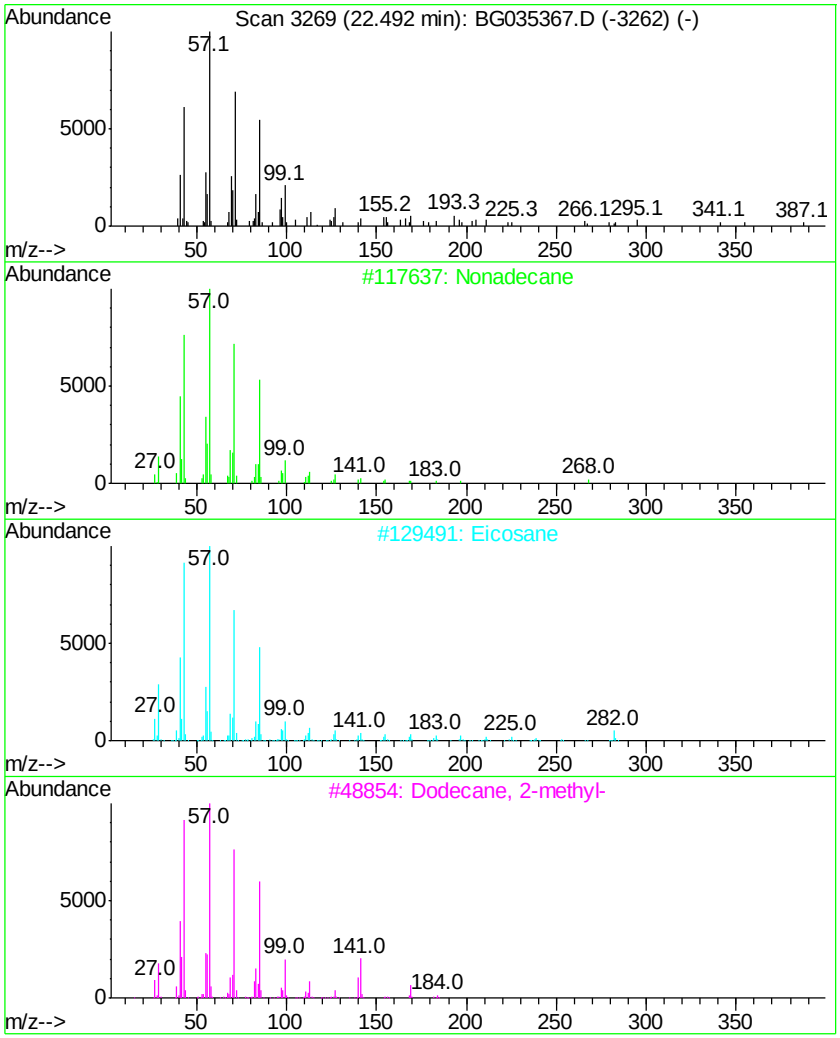
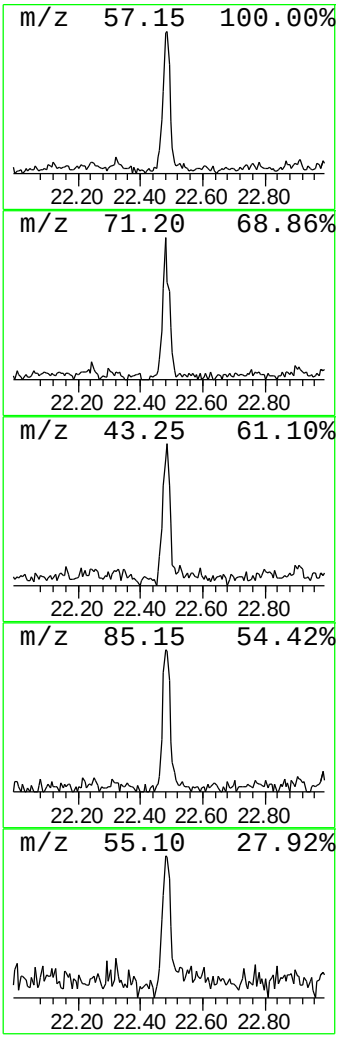
****

Peak Number 7 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.49	2.10 ng	98558	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	96
2	Eicosane	282	C20H42	000112-95-8	96
3	Dodecane, 2-methyl-	184	C13H28	001560-97-0	93
4	Hexacosane	366	C26H54	000630-01-3	90
5	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	87





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Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 061918-DBRI-F-U-B

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

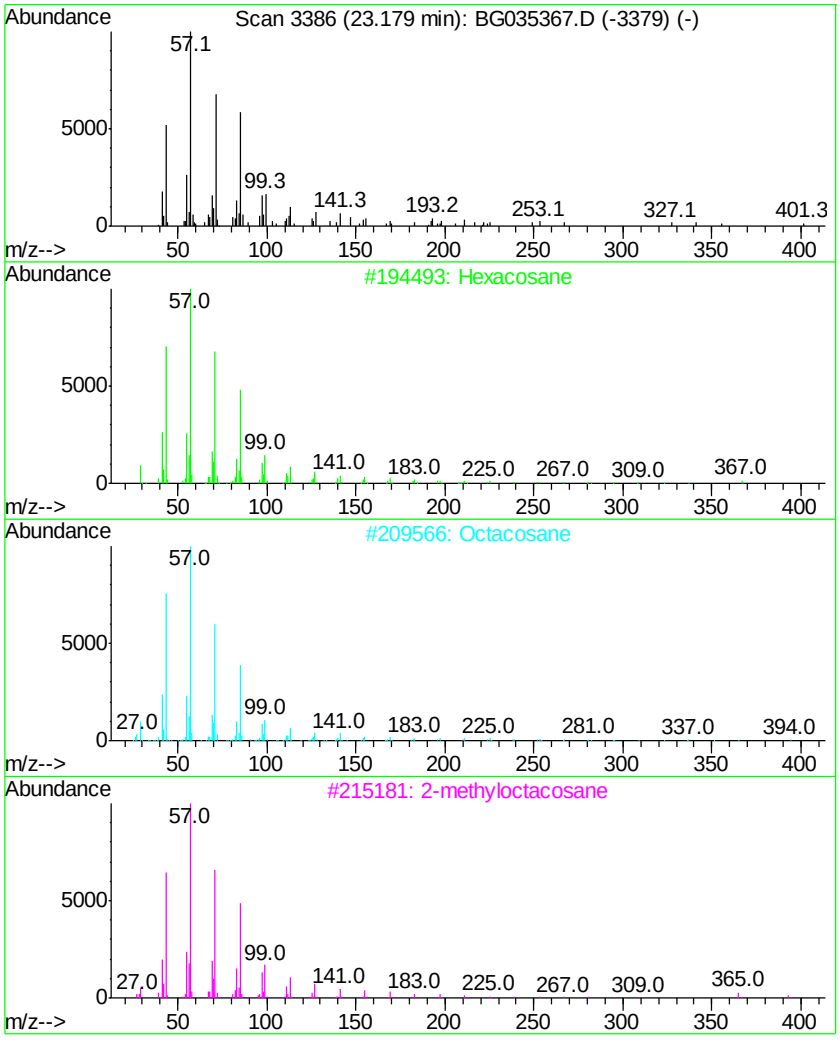
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

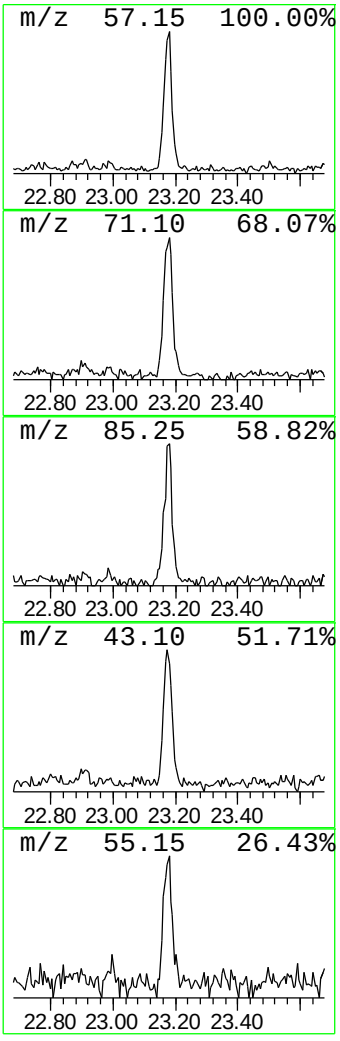
****

Peak Number 8 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.18	2.57 ng	120223	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Octacosane	394	C28H58	000630-02-4	87
3	2-methyloctacosane	408	C29H60	1000376-72-8	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Eicosane	282	C20H42	000112-95-8	86





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ClientSampleId : 061918-DBRI-F-U-B

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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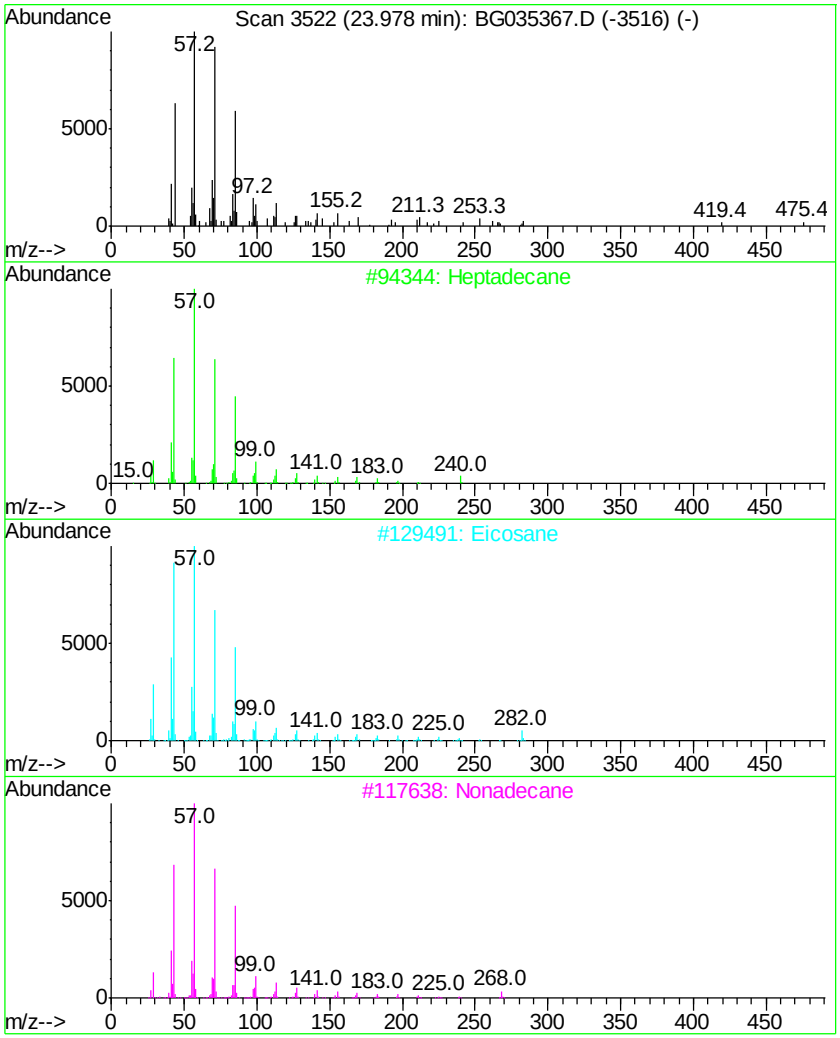
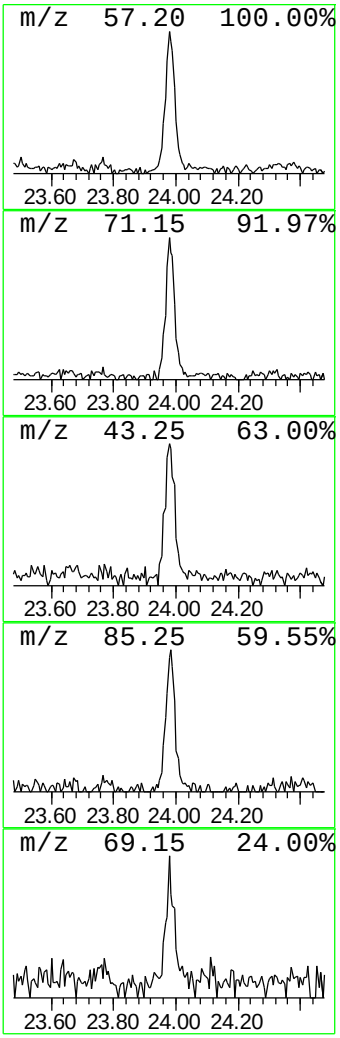
Peak Number 9 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.98	2.19 ng	104051	Perylene-d12	24.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	87
2	Eicosane	282	C20H42	000112-95-8	86
3	Nonadecane	268	C19H40	000629-92-5	86
4	Heneicosane	296	C21H44	000629-94-7	83
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	80





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown7.59	7.59	66.7	ng	1044790	1	8.06	313398	20.0
Triethyl citrate	15.96	3.2	ng	95167	3	14.67	602760	20.0
n-Hexadecanoic acid	18.30	2.4	ng	93382	4	17.42	769621	20.0
Dodecane	21.33	3.0	ng	141452	5	21.68	937284	20.0
Nonadecane	22.49	2.1	ng	98558	5	21.68	937284	20.0
Hexacosane	23.18	2.6	ng	120223	5	21.68	937284	20.0
Heptadecane	23.98	2.2	ng	104051	6	24.90	948583	20.0