LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101819\
Data File : BG043282.D
Acq On : 18 Oct 2019 19:23
Operator : JU
Sample : K5406-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3

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-BG092519.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	3.129	3	7	15	rVV2	125604	240659	6.54%	1.194%
2	3.206	15	20	36	rVB	765167	1227516	33.36%	6.090%
3	5.621	423	431	449	rBV	482922	876292	23.82%	4.347%
4	7.213	694	702	725	rBV	352370	733910	19.95%	3.641%
5	7.577	754	764	786	rBV	756808	1394869	37.91%	6.920%
6	8.036	835	842	850	rBV	154165	274151	7.45%	1.360%
7	8.359	890	897	907	rBV	521679	946745	25.73%	4.697%
8	9.199	1028	1040	1057	rBV	417364	858587	23.34%	4.260%
9	10.844	1312	1320	1330	rBV	166497	342632	9.31%	1.700%
10	13.288	1727	1736	1749	rBV	1217128	2075301	56.41%	10.296%
11	14.111	1870	1876	1892	rBV	134149	228984	6.22%	1.136%
12	14.663	1961	1970	1981	rBV2	322386	547232	14.87%	2.715%
13	16.150	2216	2223	2239	rBV	1182887	2021630	54.95%	10.029%
14	17.407	2431	2437	2449	rBV	383430	664340	18.06%	3.296%
15	18.300	2584	2589	2605	rBV2	238942	399601	10.86%	1.982%
16	19.569	2800	2805	2813	rBV2	82891	146082	3.97%	0.725%
17	20.016	2876	2881	2894	rBV	2641898	3679206	100.00%	18.253%
18	21.320	3098	3103	3111	rBV2	190965	322491	8.77%	1.600%
19	21.678	3158	3164	3174	rBV2	439273	808618	21.98%	4.012%
20	21.866	3192	3196	3202	rVB	67792	96442	2.62%	0.478%
21	22.472	3294	3299	3304	rBV	109180	164923	4.48%	0.818%
22	23.165	3410	3417	3424	rBV	140499	263645	7.17%	1.308%
23	23.964	3546	3553	3560	rVB2	133472	284826	7.74%	1.413%
24	24.892	3701	3711	3723	rBV3	375562	1180376	32.08%	5.856%
25	26.032	3897	3905	3914	rVB3	86532	252247	6.86%	1.251%
26	27.378	4126	4134	4144	rBV5	39485	125553	3.41%	0.623%

Sum of corrected areas: 20156858

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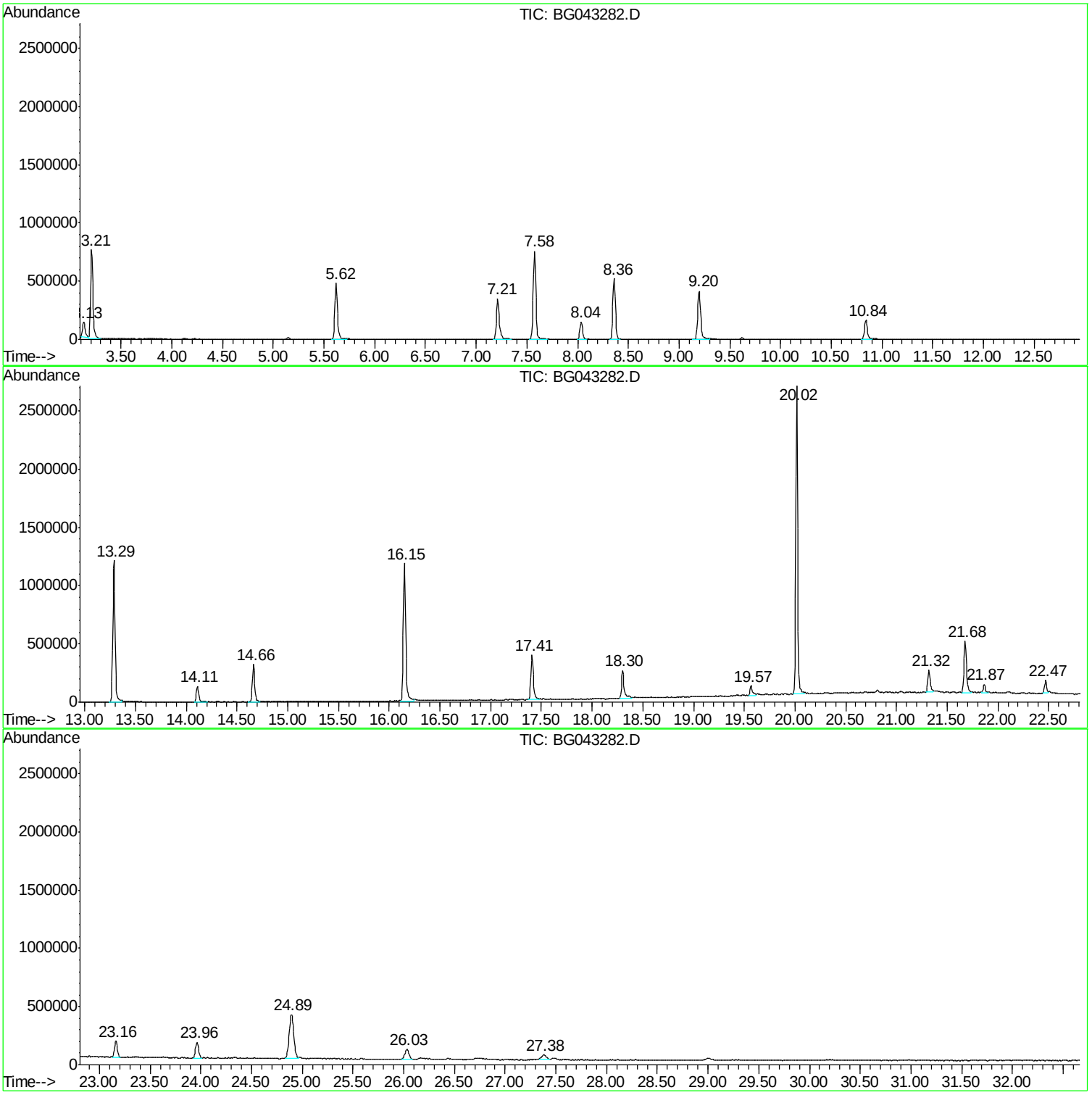
Sample : K5406-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.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\BG101819\
Data File : BG043282.D
Acq On : 18 Oct 2019 19:23
Operator : JU
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ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

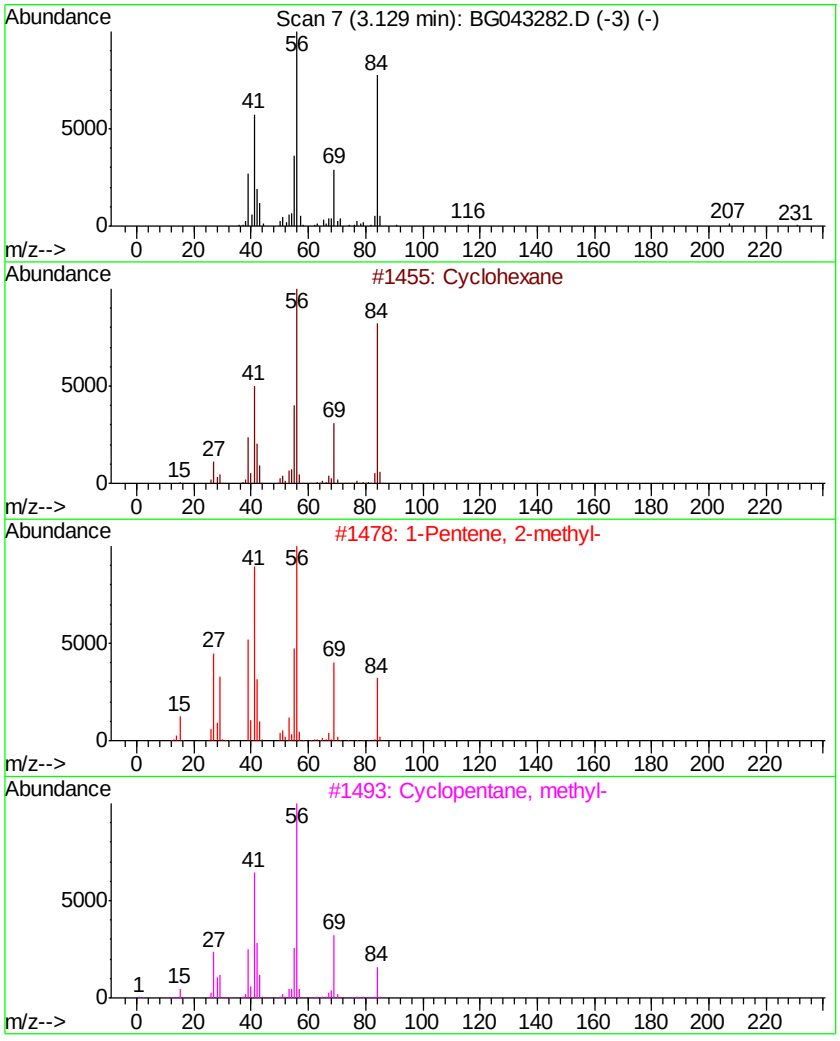
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

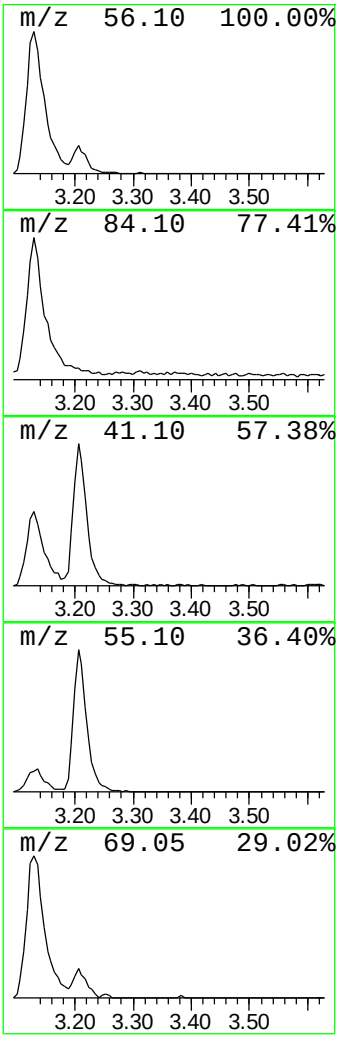
****

Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	17.56 ng	240659	1,4-Dichlorobenzene-d4	8.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	93
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	72
3	Cyclopentane, methyl-	84	C6H12	000096-37-7	50
4	1-Hexene	84	C6H12	000592-41-6	50
5	4H-1,2,4-Triazol-4-amine	84	C2H4N4	000584-13-4	43





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101819\
Data File : BG043282.D
Acq On : 18 Oct 2019 19:23
Operator : JU
Sample : K5406-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

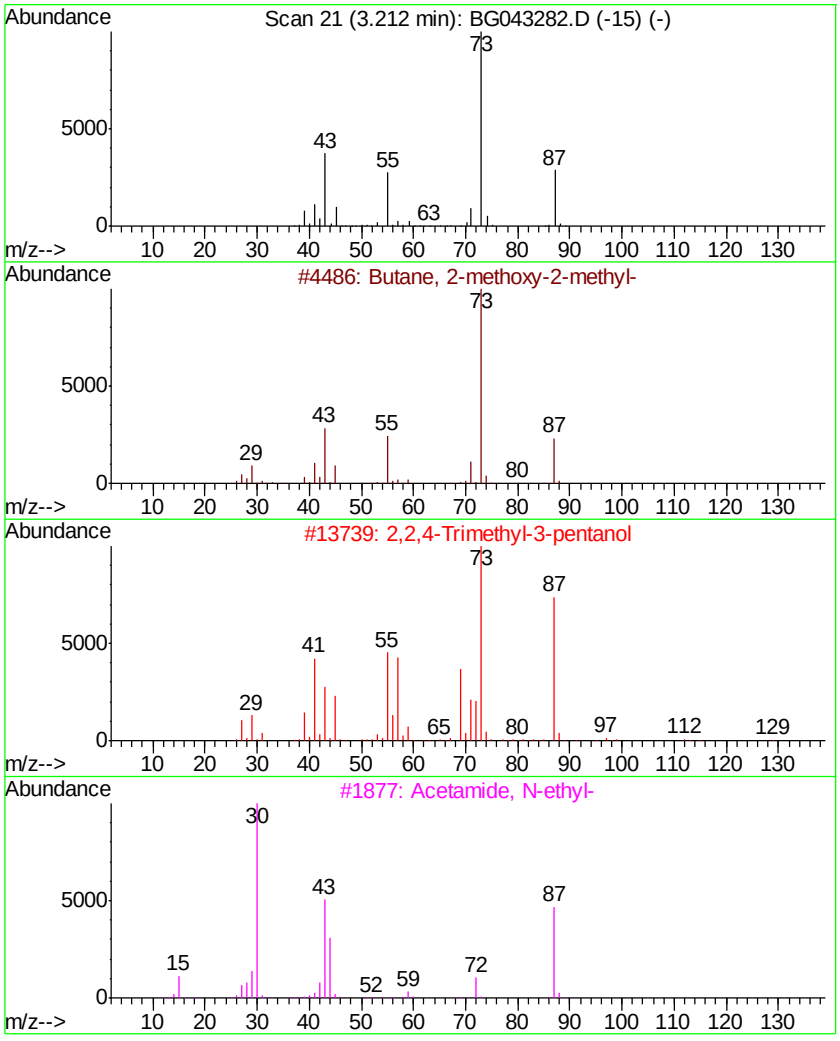
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

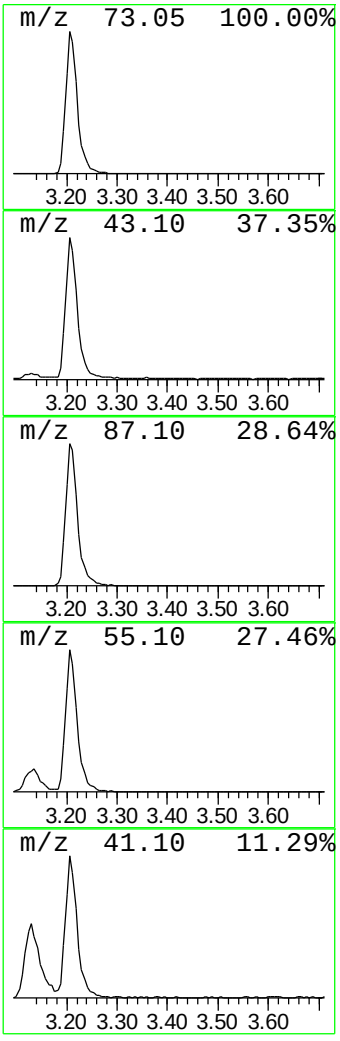
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.21	89.55 ng	1227520	1,4-Dichlorobenzene-d4	8.04

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	38
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	35
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101819\
Data File : BG043282.D
Acq On : 18 Oct 2019 19:23
Operator : JU
Sample : K5406-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

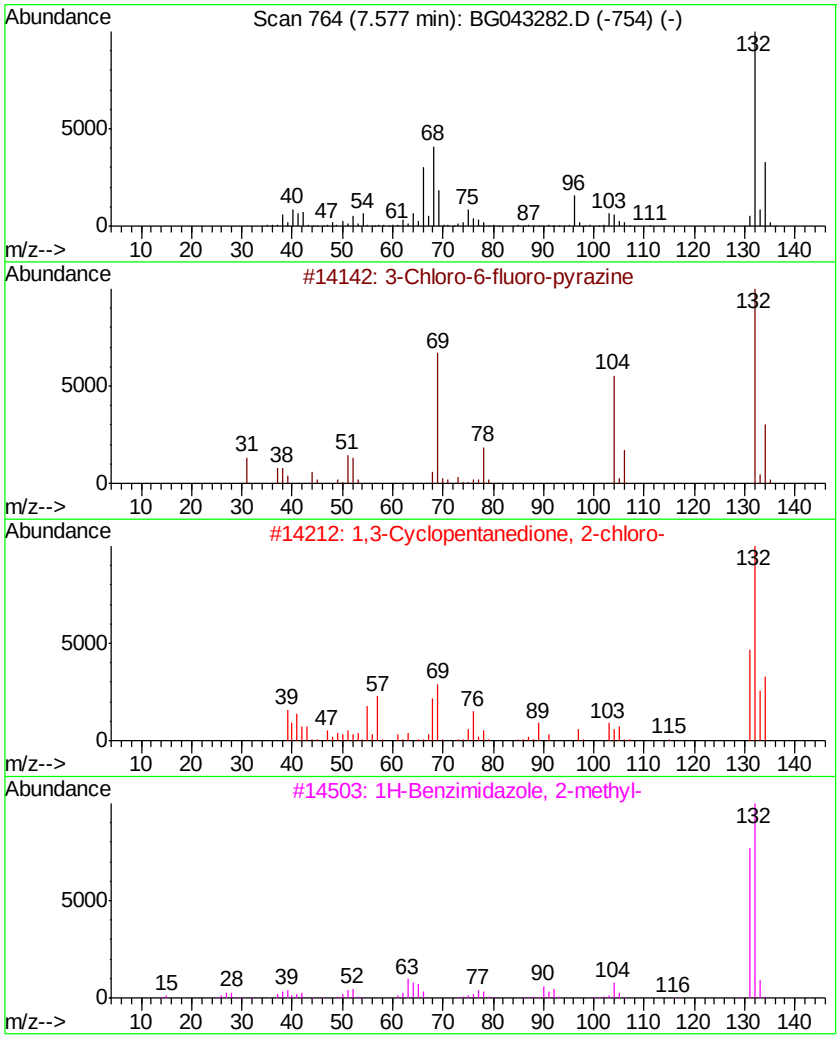
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

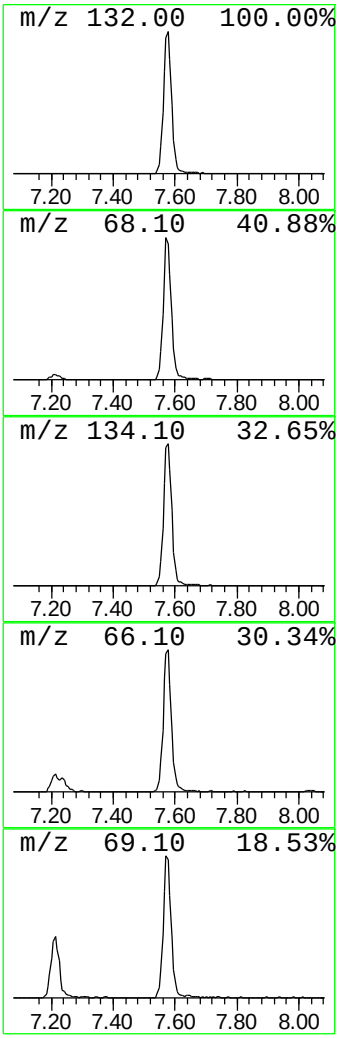
****

Peak Number 3 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	101.76 ng	1394870	1,4-Dichlorobenzene-d4	8.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





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Acq On : 18 Oct 2019 19:23
Operator : JU
Sample : K5406-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

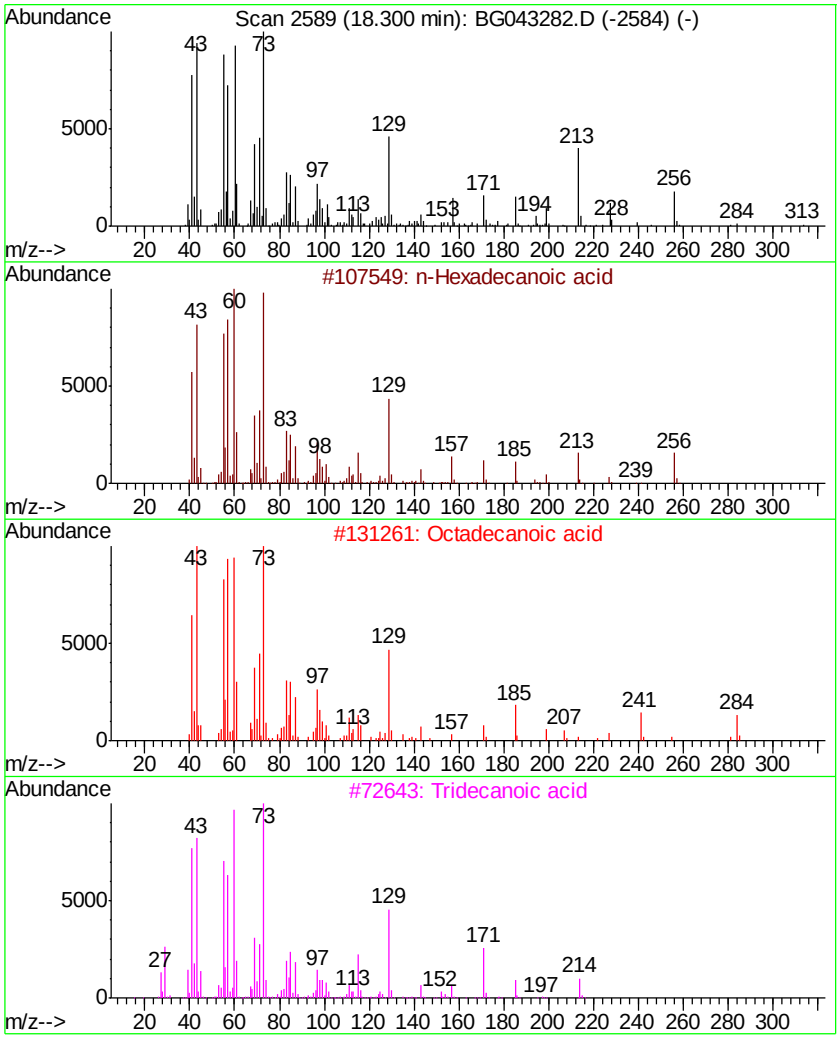
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

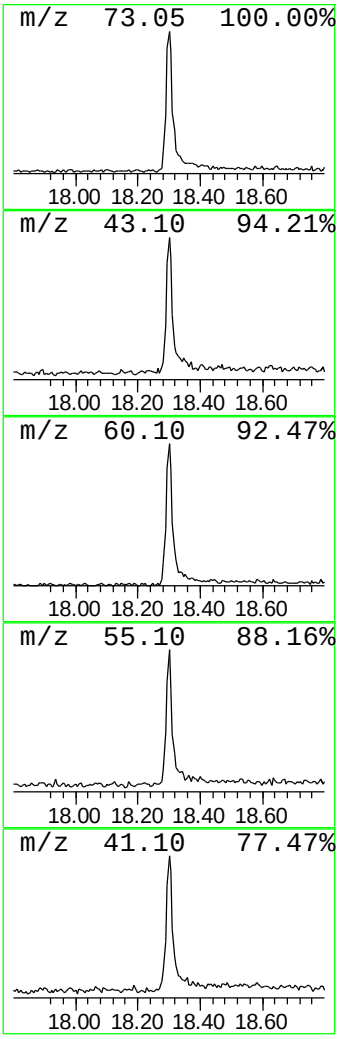
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	12.03 ng	399601	Phenanthrene-d10	17.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	76





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101819\
Data File : BG043282.D
Acq On : 18 Oct 2019 19:23
Operator : JU
Sample : K5406-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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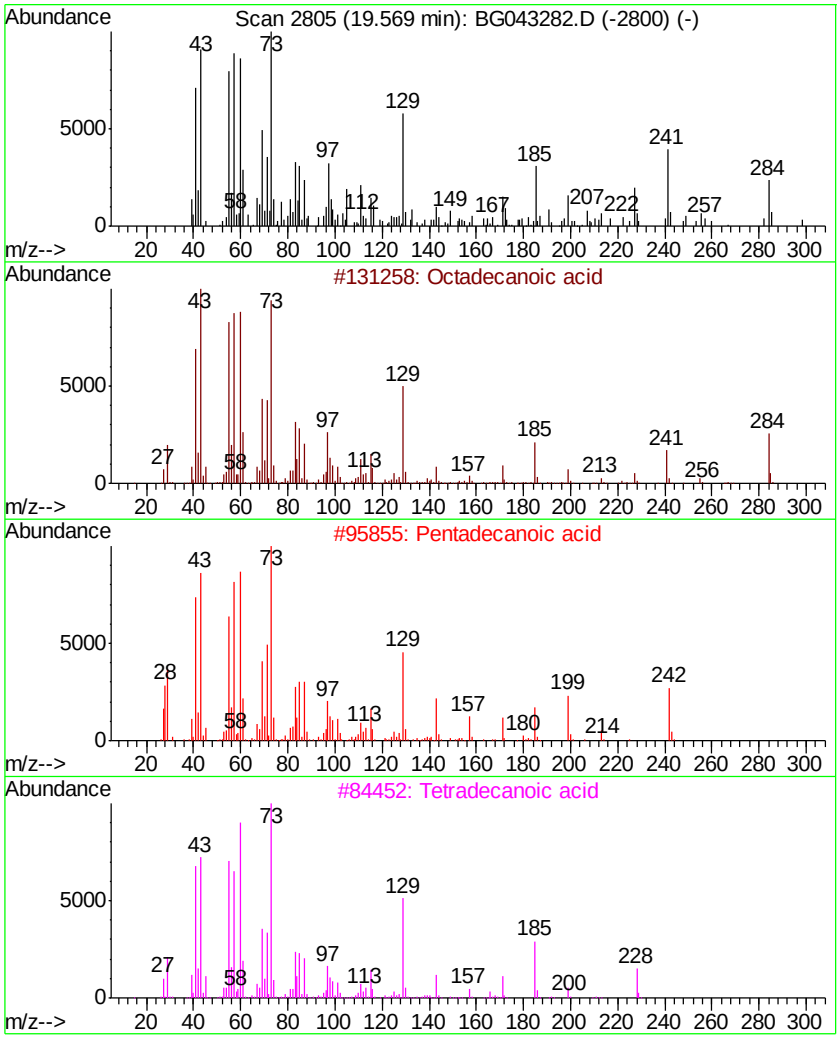
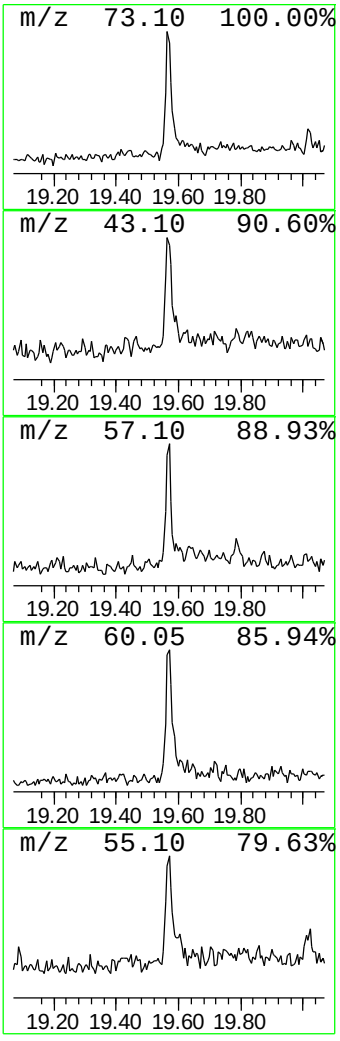
****

Peak Number 6 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.57	3.61 ng	146082	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
4	n-Decanoic acid	172	C10H20O2	000334-48-5	45
5	Undecanoic acid	186	C11H22O2	000112-37-8	41





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101819\
Data File : BG043282.D
Acq On : 18 Oct 2019 19:23
Operator : JU
Sample : K5406-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

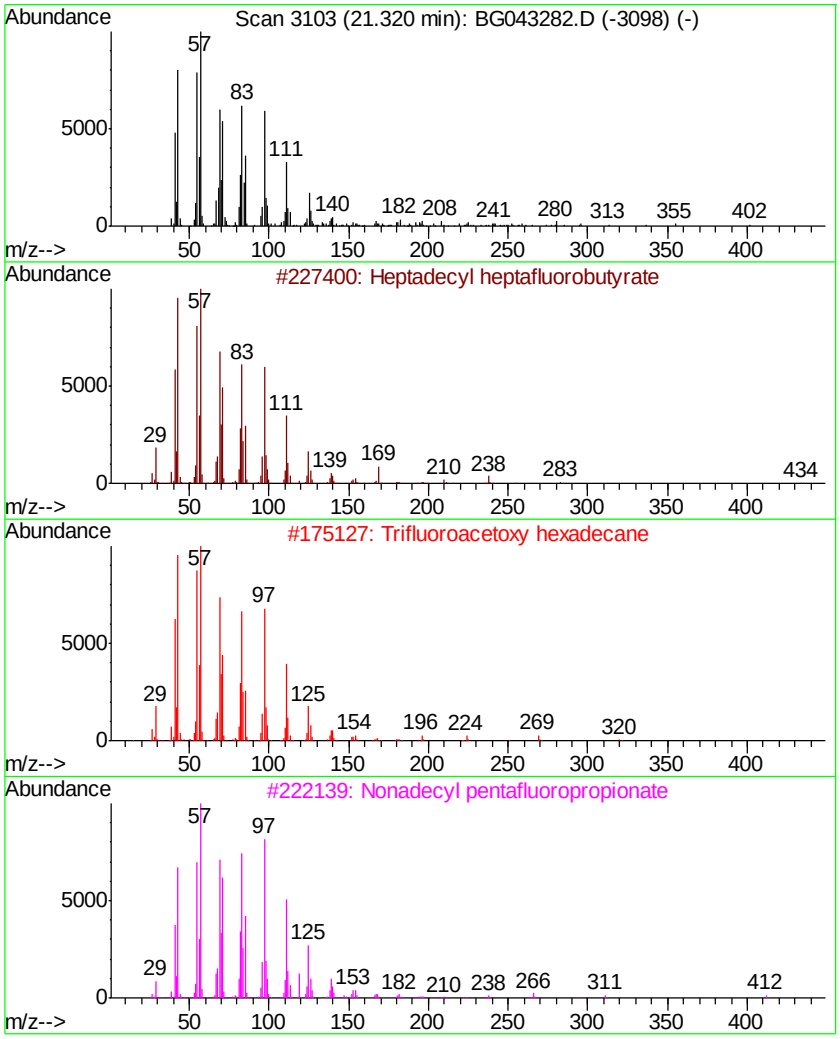
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

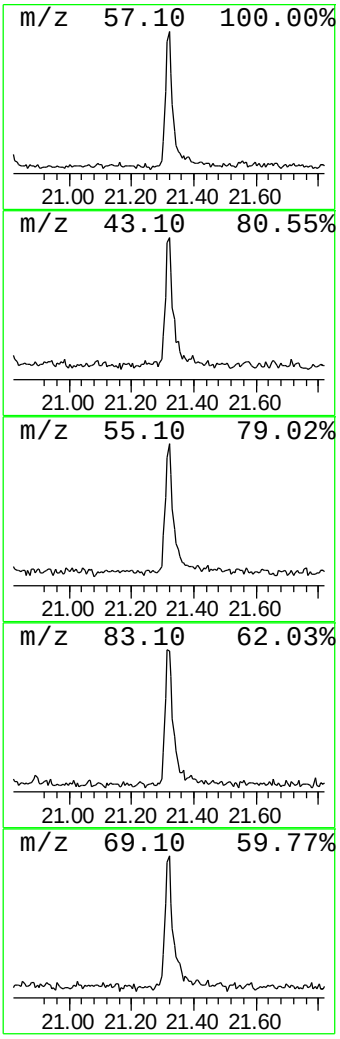
****

Peak Number 7 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.32	7.98 ng	322491	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
5	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91





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Sample : K5406-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

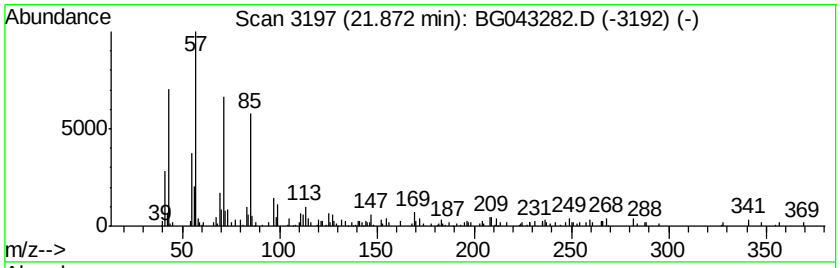
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

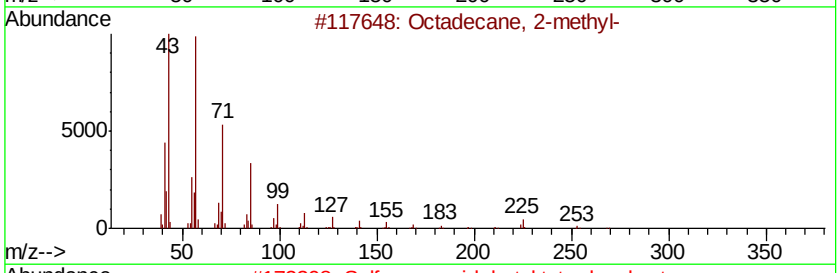
****

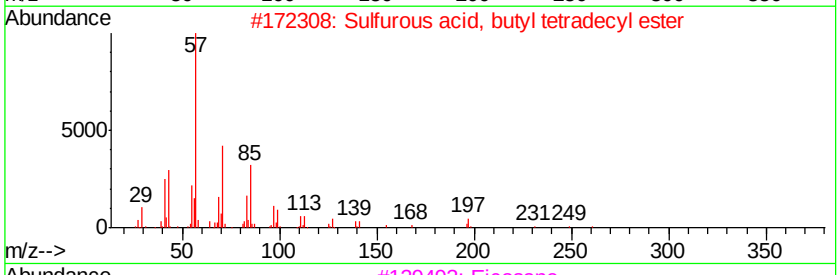
Peak Number 8 Octadecane, 2-methyl- Concentration Rank 12

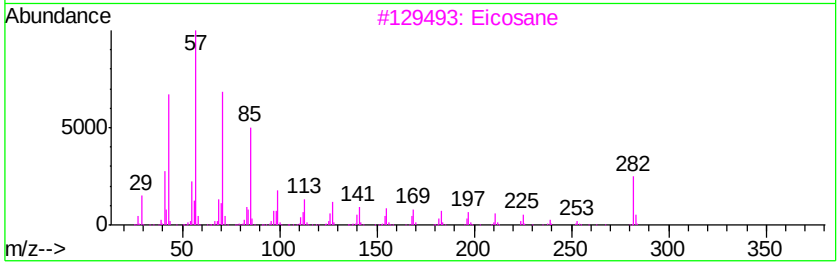
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.87	2.39 ng	96442	Chrysene-d12	21.68

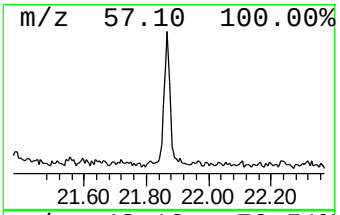
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
2	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	90
3	Eicosane	282	C20H42	000112-95-8	87
4	Behenyl chloride	344	C22H45Cl	042217-03-8	87
5	Hentriacontane	437	C31H64	000630-04-6	86

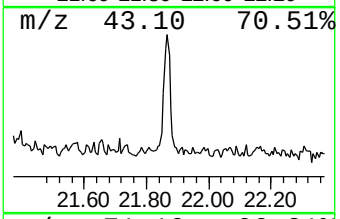


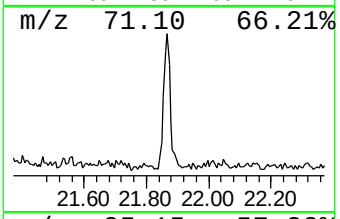


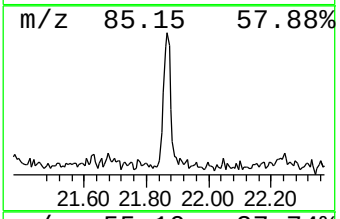


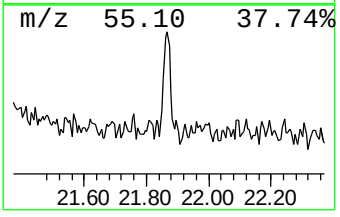












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Acq On : 18 Oct 2019 19:23
Operator : JU
Sample : K5406-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.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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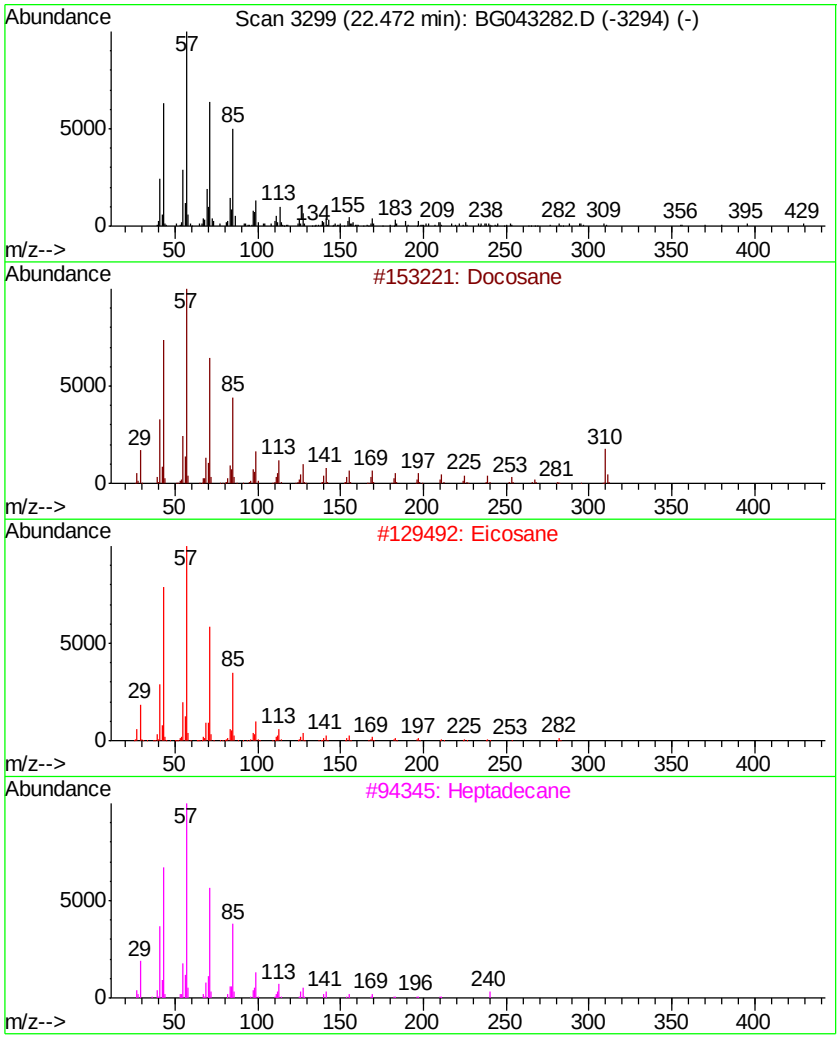
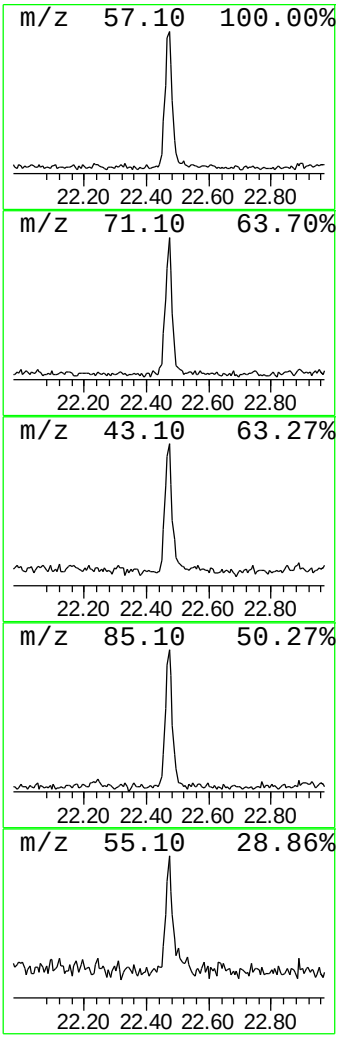
Peak Number 9 Docosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.47	4.08 ng	164923	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	95
2	Eicosane	282	C20H42	000112-95-8	93
3	Heptadecane	240	C17H36	000629-78-7	93
4	Tetracosane	338	C24H50	000646-31-1	90
5	Hexacosane	366	C26H54	000630-01-3	90





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Sample : K5406-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3

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TIC Integration Parameters: LSCINT.P

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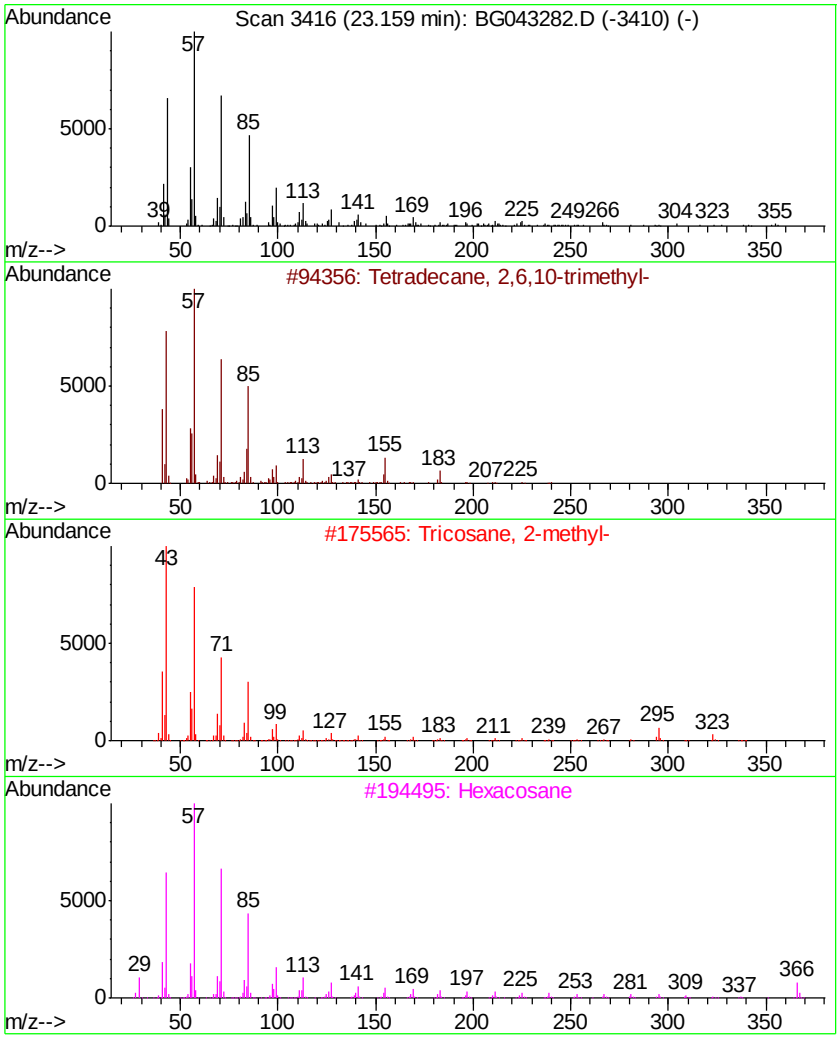
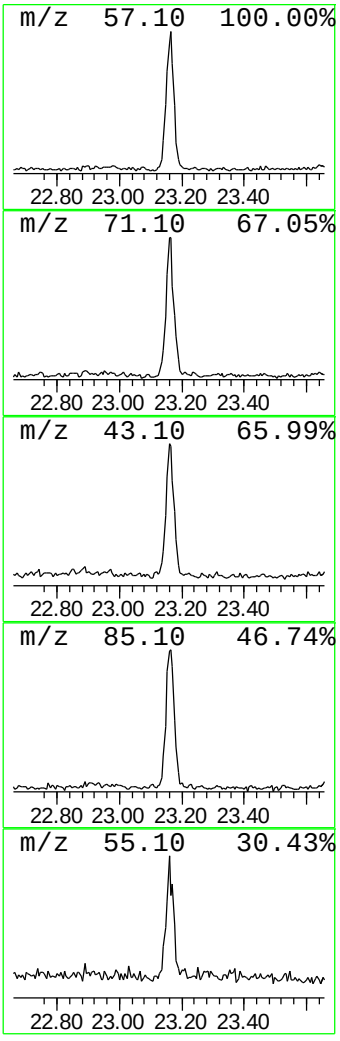
Peak Number 10 Tetradecane, 2,6,10-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.16	6.52 ng	263645	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	93
2	Tricosane, 2-methyl-	338	C24H50	001928-30-9	93
3	Hexacosane	366	C26H54	000630-01-3	91
4	Tetracosane	338	C24H50	000646-31-1	90
5	Tetratetracontane	619	C44H90	007098-22-8	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101819\
Data File : BG043282.D
Acq On : 18 Oct 2019 19:23
Operator : JU
Sample : K5406-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.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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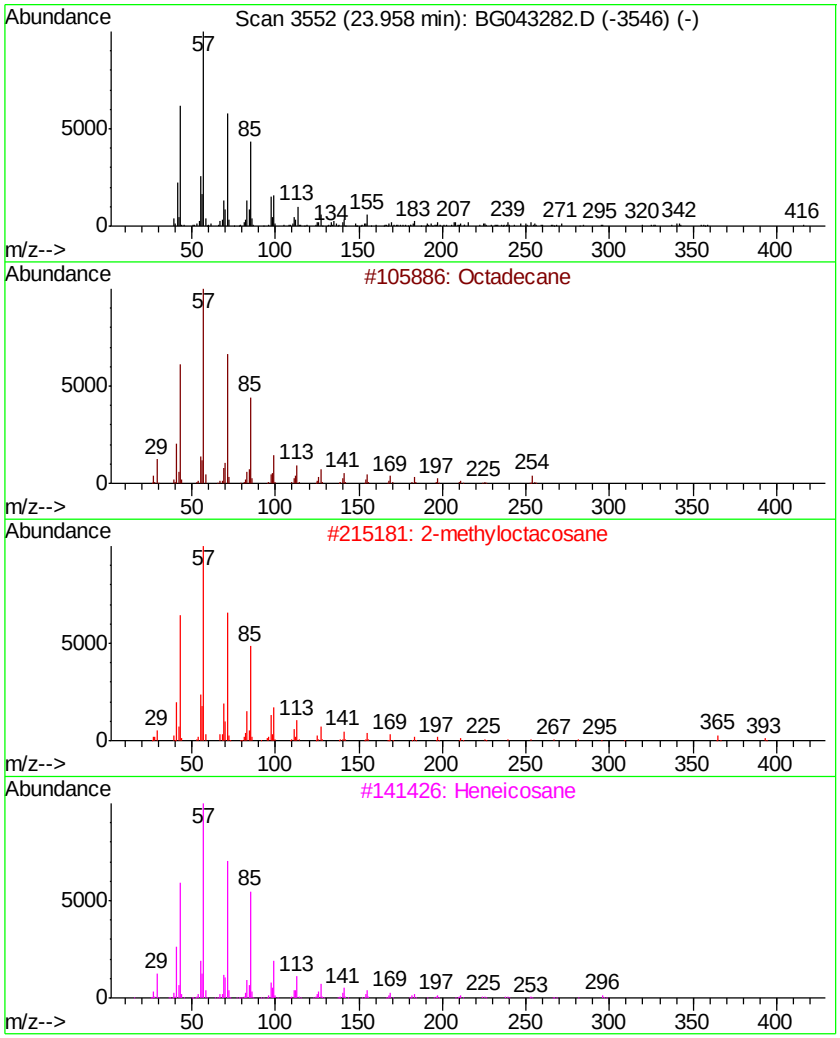
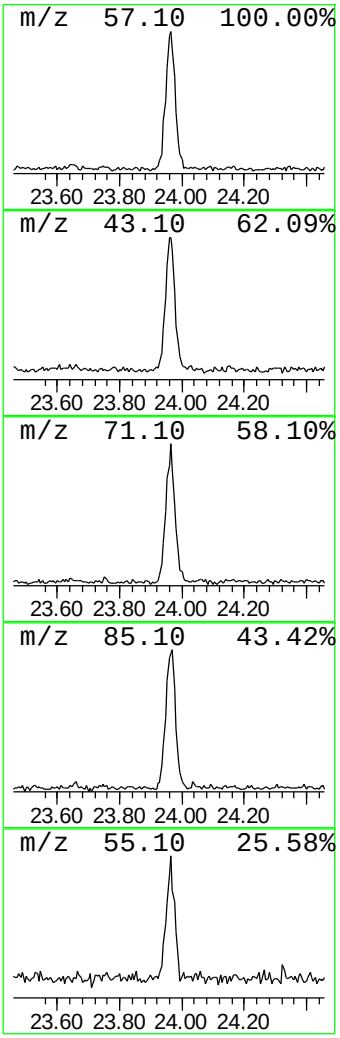
Peak Number 11 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.96	4.83 ng	284826	Perylene-d12	24.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	95
2	2-methyloctacosane	408	C29H60	1000376-72-8	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Nonadecane	268	C19H40	000629-92-5	90
5	Octacosane	394	C28H58	000630-02-4	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101819\
Data File : BG043282.D
Acq On : 18 Oct 2019 19:23
Operator : JU
Sample : K5406-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.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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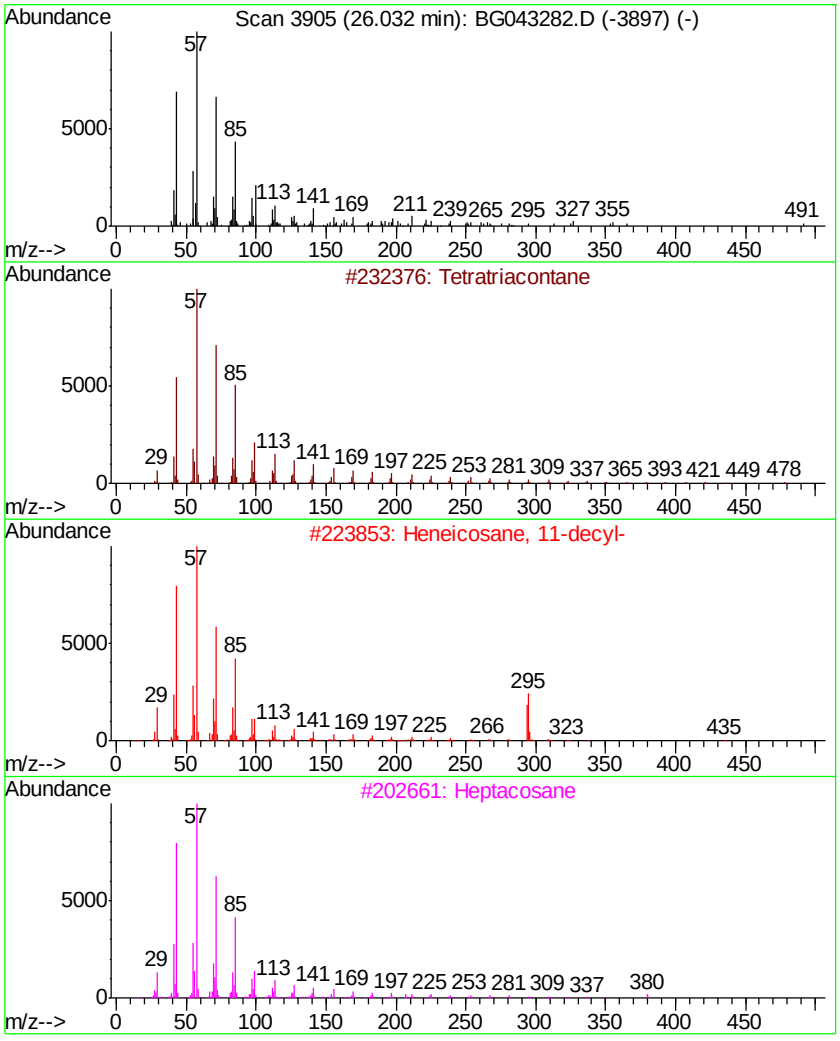
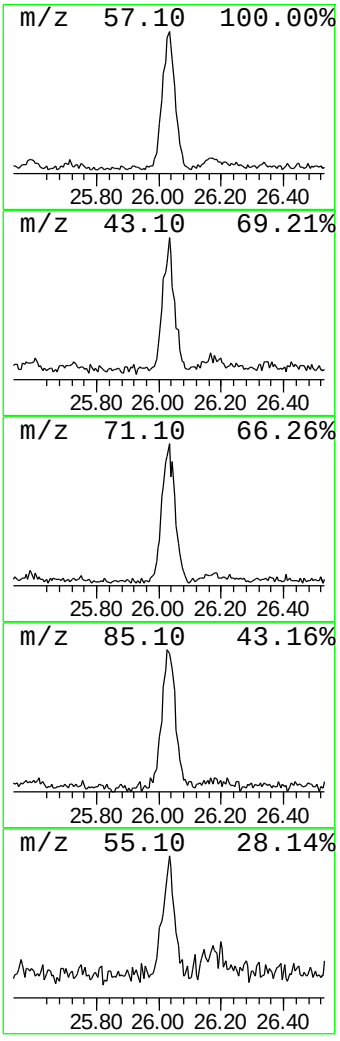
Peak Number 12 Tetratriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.03	4.27 ng	252247	Perylene-d12	24.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratriacontane	479	C34H70	014167-59-0	86
2	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	83
3	Heptacosane	380	C27H56	000593-49-7	83
4	Tetratetracontane	619	C44H90	007098-22-8	83
5	Hexacosane	366	C26H54	000630-01-3	83





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101819\
Data File : BG043282.D
Acq On : 18 Oct 2019 19:23
Operator : JU
Sample : K5406-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.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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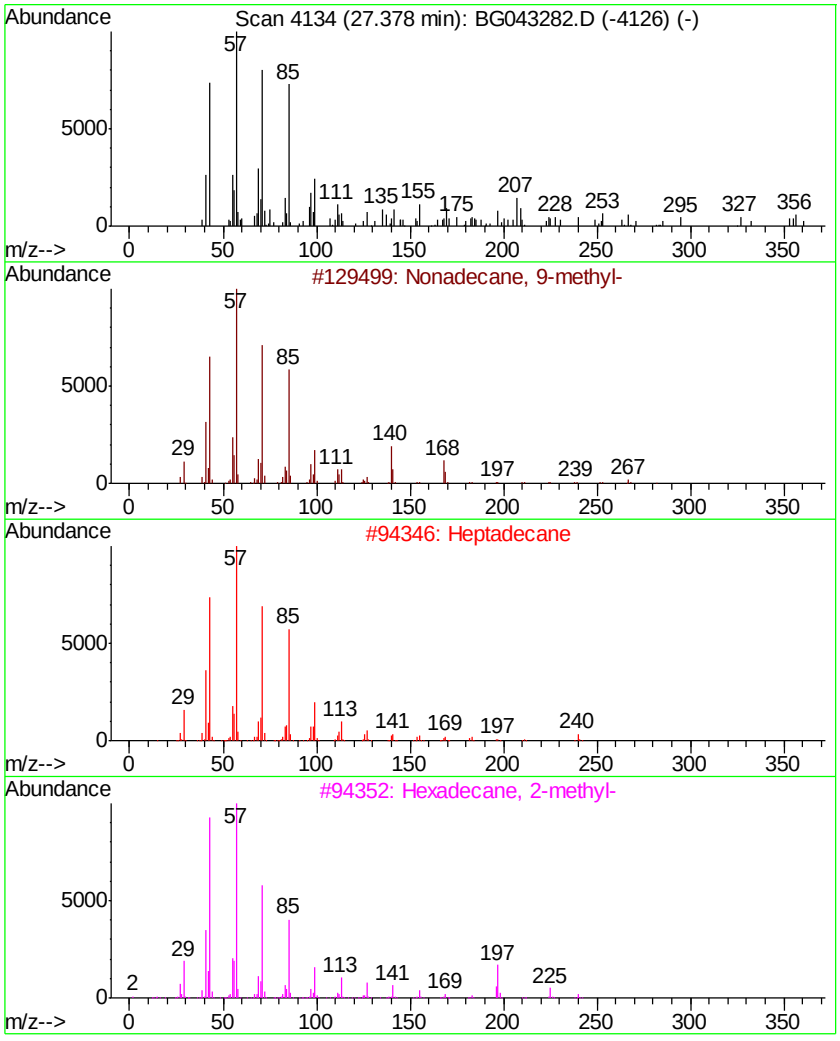
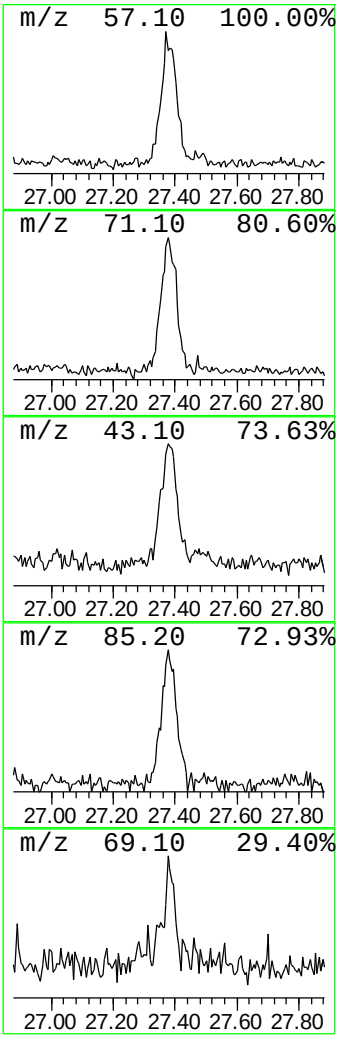
Peak Number 13 Nonadecane, 9-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.38	2.13 ng	125553	Perylene-d12	24.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	93
2	Heptadecane	240	C17H36	000629-78-7	81
3	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	72
4	Octacosane	394	C28H58	000630-02-4	72
5	Heptacosane	380	C27H56	000593-49-7	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG101819\
Data File : BG043282.D
Acq On : 18 Oct 2019 19:23
Operator : JU
Sample : K5406-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.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
1-Pentene, 2-methyl-	3.13	17.6	ng	240659	1	8.04	274151	20.0
Butane, 2-methoxy...	3.21	89.5	ng	1227520	1	8.04	274151	20.0
unknown7.58	7.58	101.8	ng	1394870	1	8.04	274151	20.0
n-Hexadecanoic acid	18.30	12.0	ng	399601	4	17.41	664340	20.0
Octadecanoic acid	19.57	3.6	ng	146082	5	21.68	808618	20.0
Heptadecyl heptaf...	21.32	8.0	ng	322491	5	21.68	808618	20.0
Octadecane, 2-met...	21.87	2.4	ng	96442	5	21.68	808618	20.0
Docosane	22.47	4.1	ng	164923	5	21.68	808618	20.0
Tetradecane, 2,6,...	23.16	6.5	ng	263645	5	21.68	808618	20.0
Octadecane	23.96	4.8	ng	284826	6	24.89	1180380	20.0
Tetratriacontane	26.03	4.3	ng	252247	6	24.89	1180380	20.0
Nonadecane, 9-met...	27.38	2.1	ng	125553	6	24.89	1180380	20.0