LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020520\
Data File : BG044310.D
Acq On : 5 Feb 2020 18:45
Operator : CG/JU
Sample : L1390-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-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-BG013020.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	3.126	4	6	16	rVB	31201	48576	1.03%	0.190%
2	5.494	402	409	421	rBV	1041088	1726318	36.67%	6.768%
3	7.086	672	680	699	rBV	1105333	1975832	41.97%	7.746%
4	7.915	814	821	828	rBV	266098	446161	9.48%	1.749%
5	8.238	868	876	886	rBV	876157	1496360	31.79%	5.866%
6	9.072	1007	1018	1028	rBV	638690	1204335	25.58%	4.721%
7	10.717	1290	1298	1308	rBV	351099	654036	13.89%	2.564%
8	13.173	1709	1716	1732	rBV	1853990	2948416	62.63%	11.559%
9	14.008	1852	1858	1868	rBV	109174	180496	3.83%	0.708%
10	14.554	1943	1951	1962	rBV	646675	1027942	21.84%	4.030%
11	16.041	2197	2204	2217	rBV	1596589	2496937	53.04%	9.789%
12	17.298	2410	2418	2430	rBV	837425	1306488	27.75%	5.122%
13	17.686	2478	2484	2498	rBV	61397	103286	2.19%	0.405%
14	18.626	2637	2644	2648	rBV	106136	128412	2.73%	0.503%
15	19.912	2857	2863	2875	rBV	3547779	4707313	100.00%	18.455%
16	21.211	3079	3084	3094	rBV	310519	507496	10.78%	1.990%
17	21.540	3133	3140	3151	rBV2	811685	1429011	30.36%	5.602%
18	21.752	3171	3176	3184	rBV	77969	111158	2.36%	0.436%
19	22.345	3270	3277	3289	rBV3	109736	209101	4.44%	0.820%
20	23.009	3384	3390	3401	rVB	115980	222388	4.72%	0.872%
21	23.191	3414	3421	3430	rVB	259501	495510	10.53%	1.943%
22	23.784	3515	3522	3529	rBV	100385	216055	4.59%	0.847%
23	24.642	3657	3668	3686	rBV2	488599	1640062	34.84%	6.430%
24	25.782	3853	3862	3871	rBV3	50993	154070	3.27%	0.604%
25	27.075	4077	4082	4091	rVB3	26314	71812	1.53%	0.282%

Sum of corrected areas: 25507571

LSC Report - Integrated Chromatogram

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Misc :
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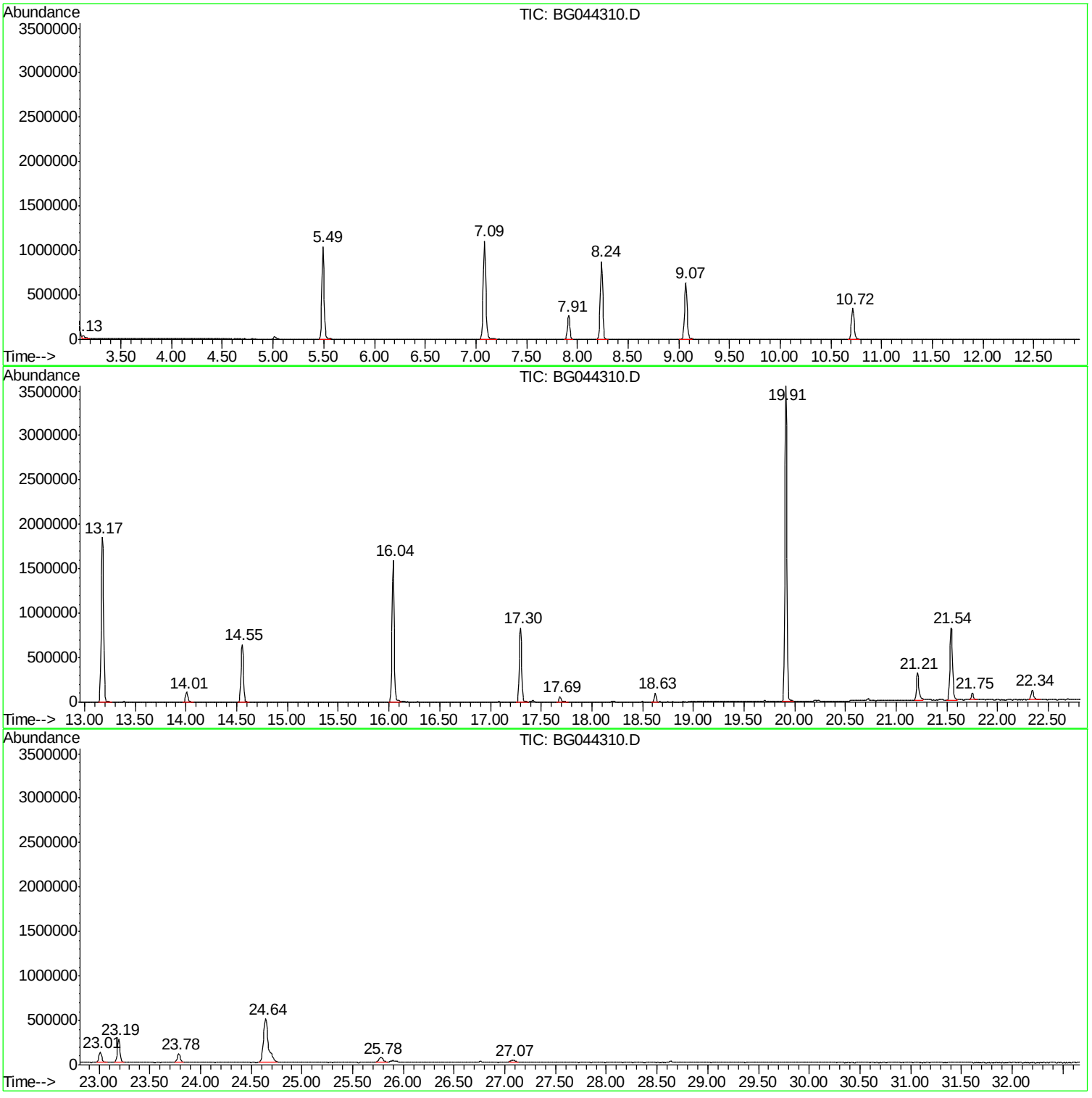
Instrument : BNA_G
ClientSampleId : SB-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.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 : BG044310.D
Acq On : 5 Feb 2020 18:45
Operator : CG/JU
Sample : L1390-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.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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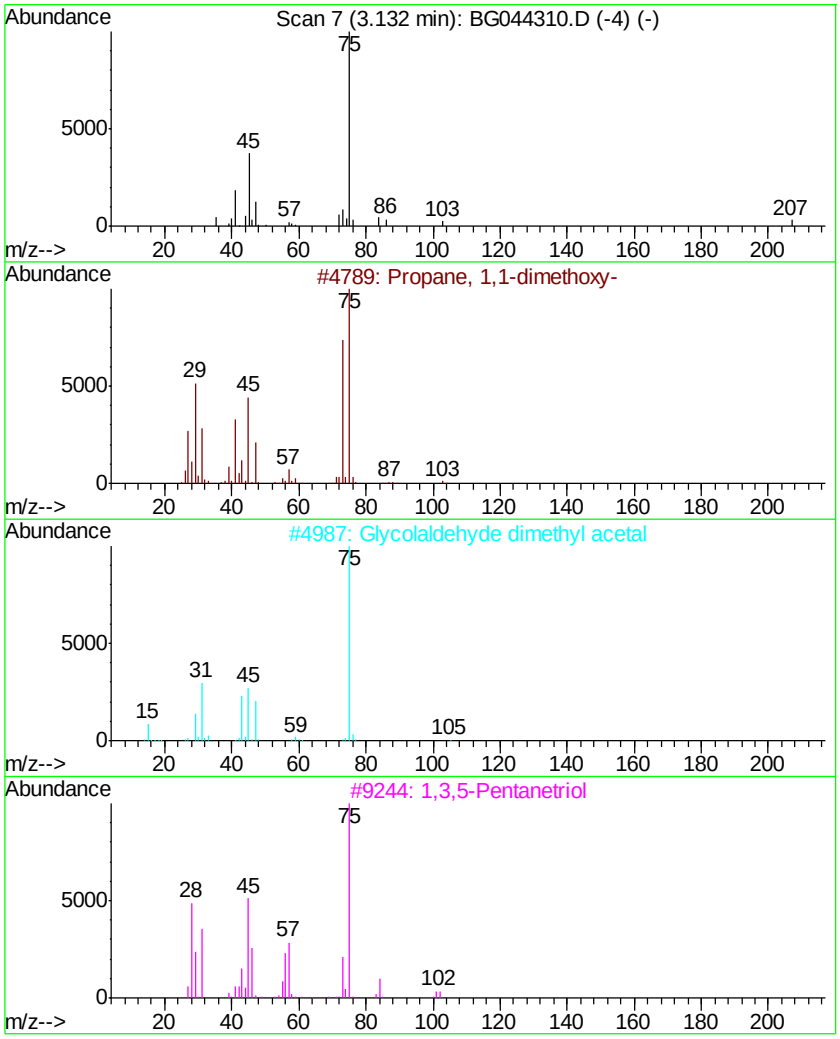
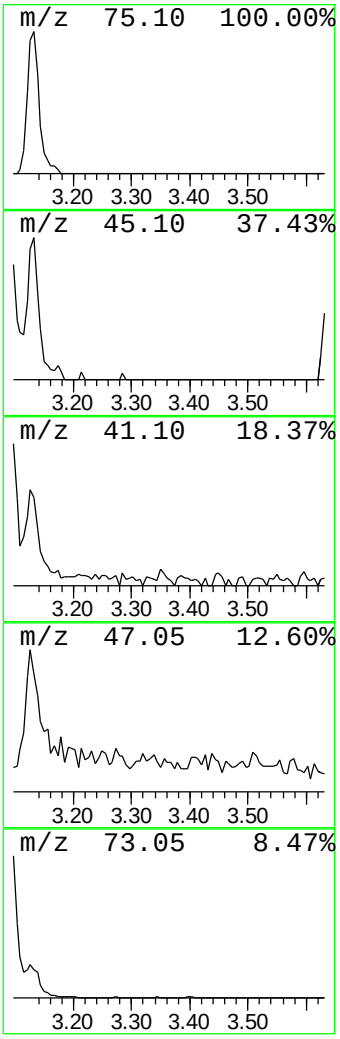
Peak Number 1 unknown3.13 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	2.18 ng	48576	1,4-Dichlorobenzene-d4	7.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	36
2	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	9
3	1,3,5-Pentanetriol	120	C5H12O3	004328-94-3	9
4	N-Formylglycine	103	C3H5NO3	002491-15-8	5
5	1-Butanamine, 4-methoxy-	103	C5H13NO	034039-36-6	5





Library Search Compound Report

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Data File : BG044310.D
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Operator : CG/JU
Sample : L1390-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.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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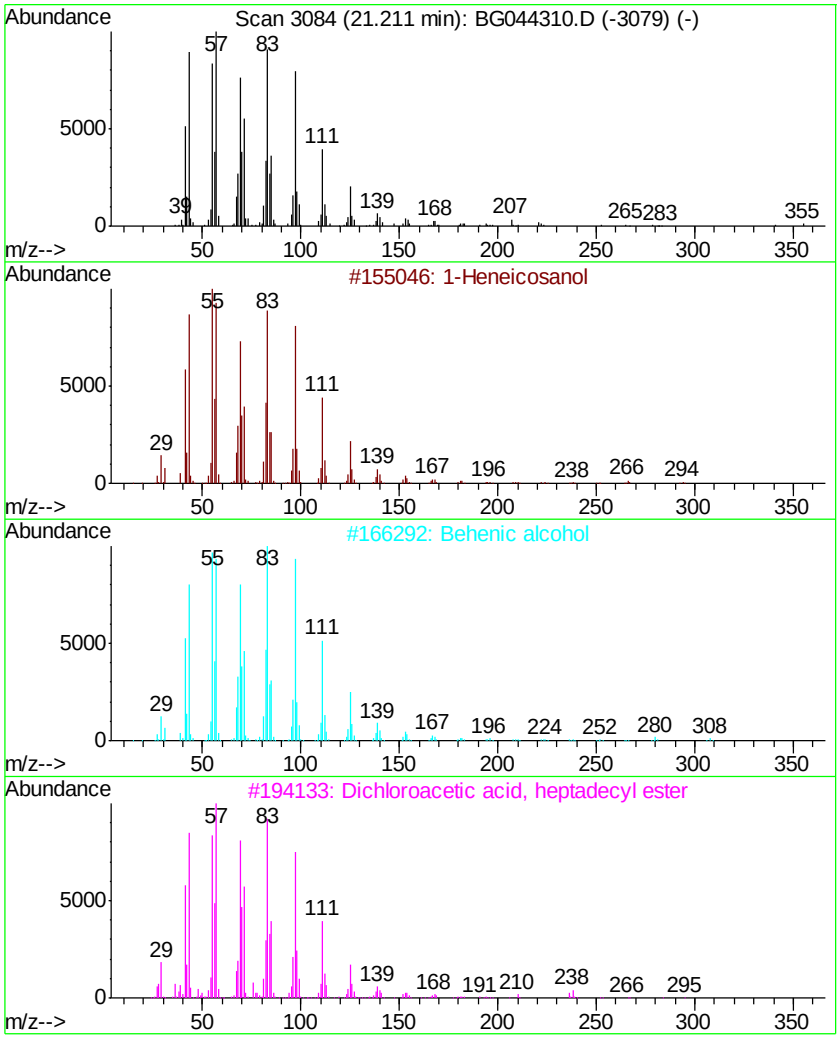
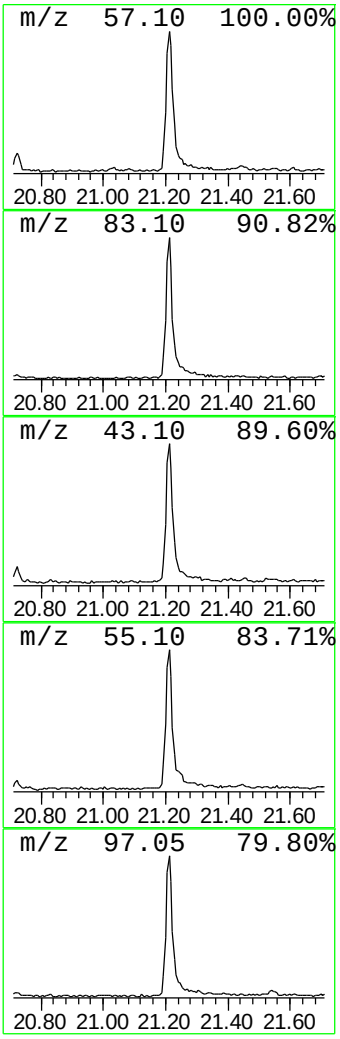
Peak Number 3 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.21	7.10 ng	507496	Chrysene-d12	21.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
5	1-Heptacosanol	396	C27H56O	002004-39-9	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020520\
Data File : BG044310.D
Acq On : 5 Feb 2020 18:45
Operator : CG/JU
Sample : L1390-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.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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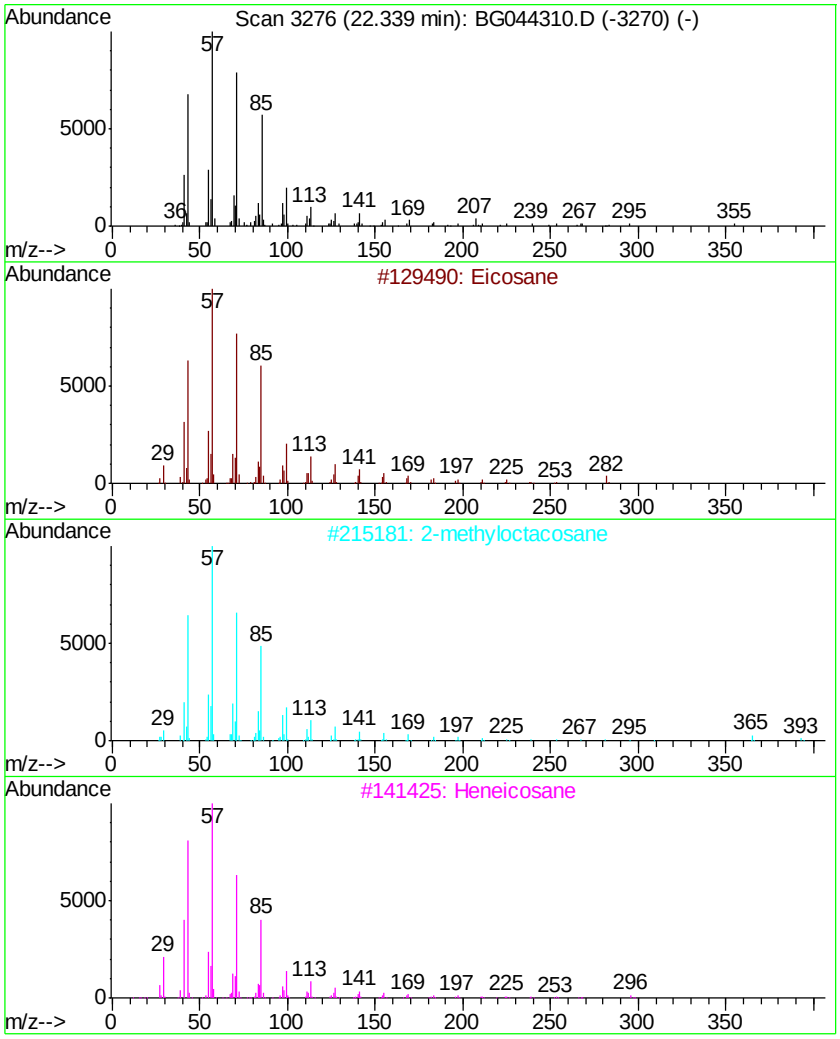
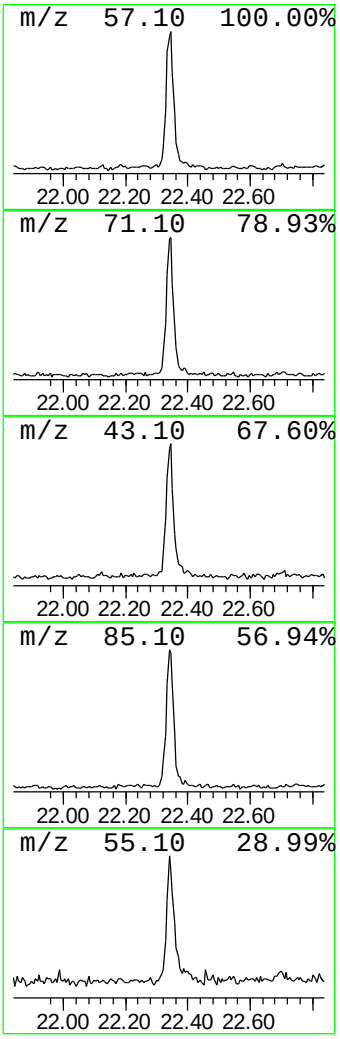
Peak Number 4 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.34	2.93 ng	209101	Chrysene-d12	21.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	97
2	2-methyloctacosane	408	C29H60	1000376-72-8	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	Octadecane	254	C18H38	000593-45-3	90





Library Search Compound Report

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Acq On : 5 Feb 2020 18:45
Operator : CG/JU
Sample : L1390-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.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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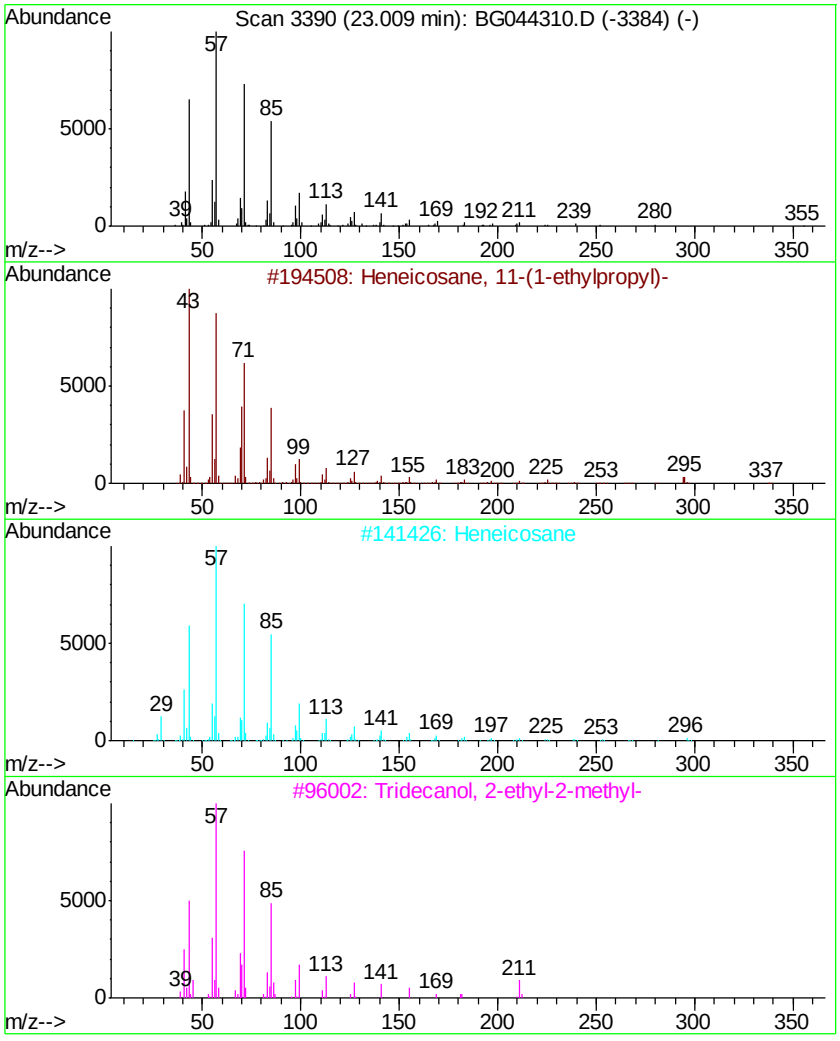
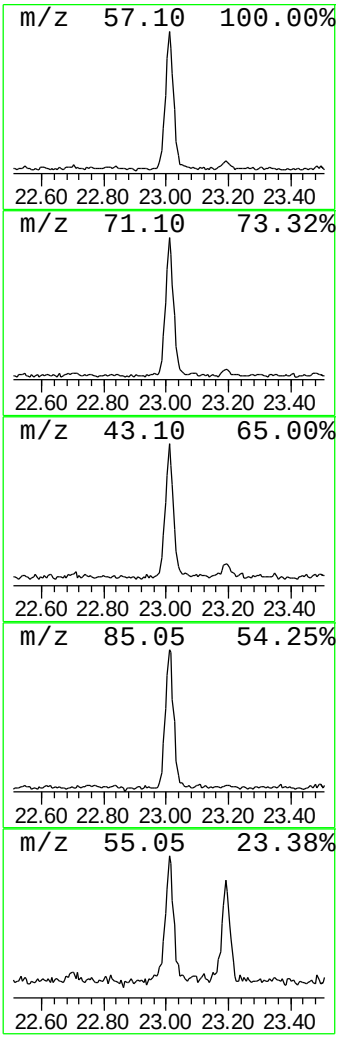
Peak Number 5 Heneicosane, 11-(1-ethylpro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.01	3.11 ng	222388	Chrysene-d12	21.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Docosane	310	C22H46	000629-97-0	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020520\
Data File : BG044310.D
Acq On : 5 Feb 2020 18:45
Operator : CG/JU
Sample : L1390-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.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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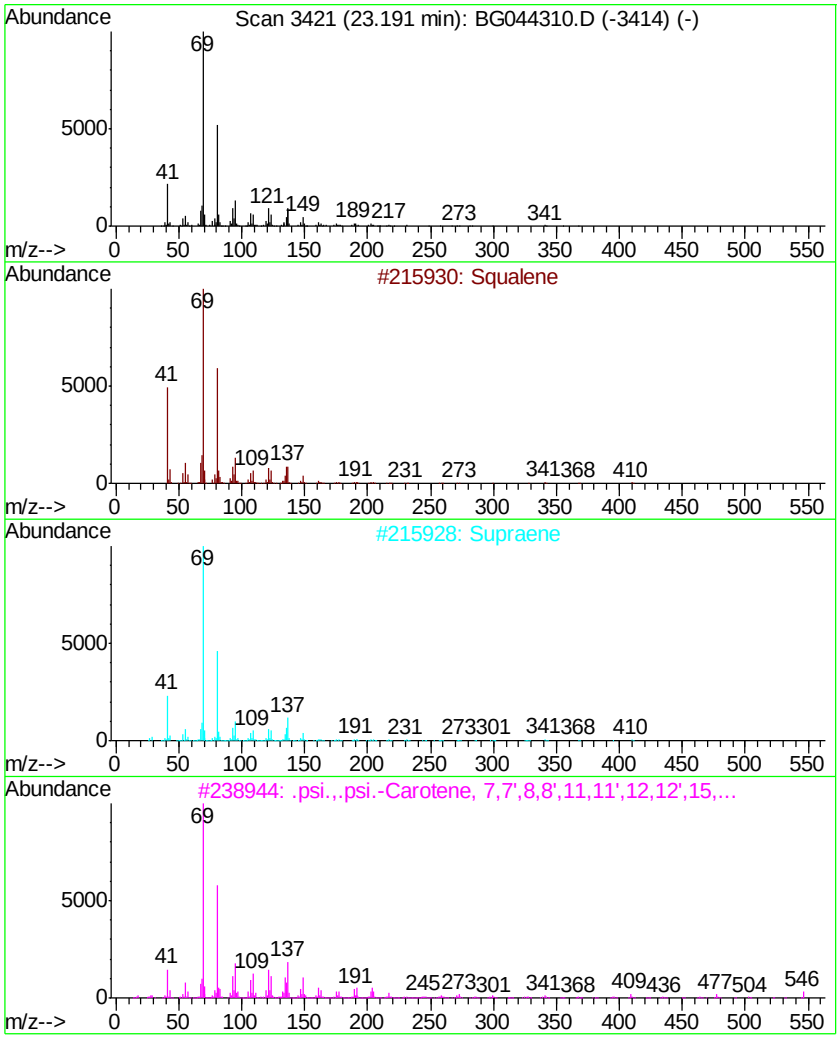
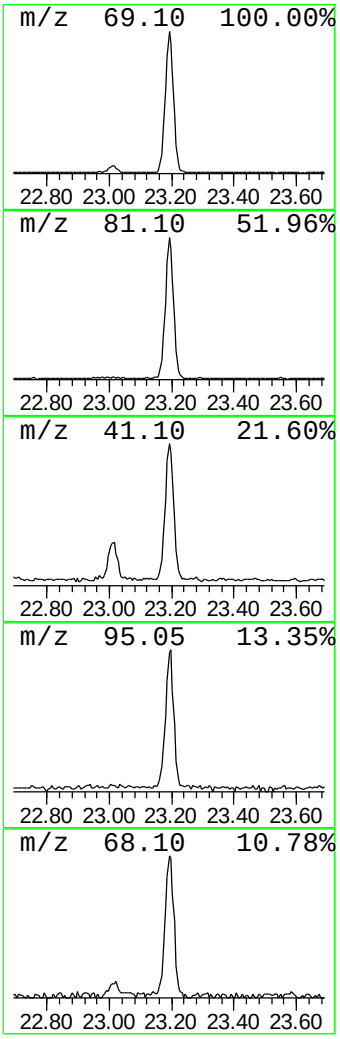
Peak Number 6 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.19	6.04 ng	495510	Perylene-d12	24.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
4	4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	50
5	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	50





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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.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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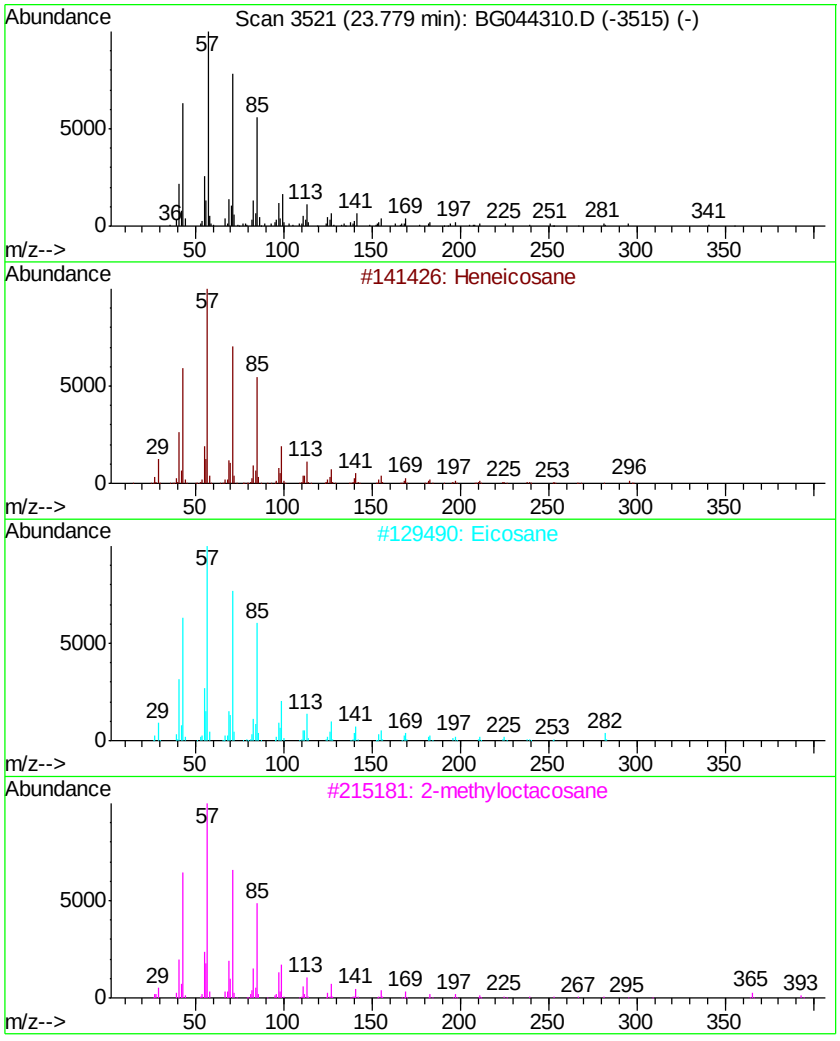
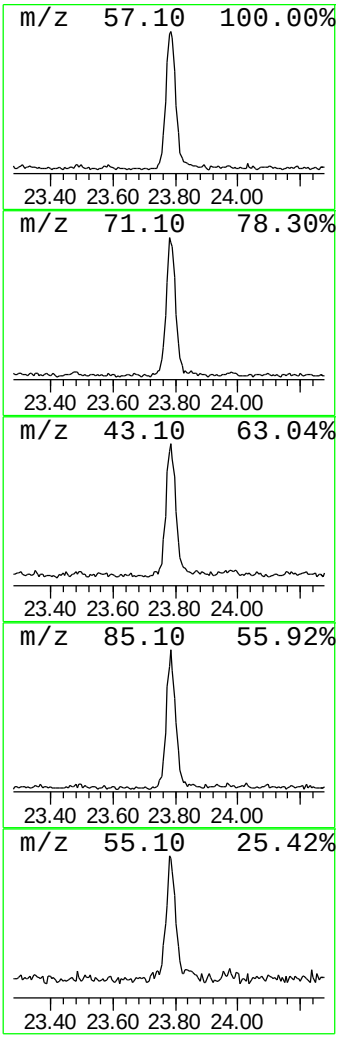
Peak Number 7 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.78	2.63 ng	216055	Perylene-d12	24.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Eicosane	282	C20H42	000112-95-8	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Pentacosane	352	C25H52	000629-99-2	90
5	Tetratetracontane	619	C44H90	007098-22-8	81





Tentatively Identified Compound (LSC) summary

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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
unknown3.13	3.13	2.2	ng	48576	1	7.91	446161	20.0
1-Heneicosanol	21.21	7.1	ng	507496	5	21.54	1429010	20.0
Eicosane	22.34	2.9	ng	209101	5	21.54	1429010	20.0
Heneicosane, 11-(...	23.01	3.1	ng	222388	5	21.54	1429010	20.0
Squalene	23.19	6.0	ng	495510	6	24.64	1640060	20.0
Heneicosane	23.78	2.6	ng	216055	6	24.64	1640060	20.0