LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111119\
Data File : BG043598.D
Acq On : 12 Nov 2019 00:30
Operator : JU
Sample : K5760-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-50

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-BG102119.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	3.164	8	13	26	rVB	356030	665867	35.04%	5.249%
2	5.103	337	343	352	rBV	40975	64079	3.37%	0.505%
3	5.597	420	427	439	rBV	282954	517174	27.21%	4.077%
4	7.201	691	700	717	rBV2	193855	437338	23.01%	3.447%
5	7.548	751	759	775	rBV	519637	953560	50.18%	7.516%
6	8.000	827	836	843	rBV	114644	198974	10.47%	1.568%
7	8.323	883	891	901	rBV	387916	705483	37.12%	5.561%
8	9.163	1027	1034	1052	rBV	295945	608911	32.04%	4.800%
9	10.808	1306	1314	1332	rBV	130007	270088	14.21%	2.129%
10	13.253	1723	1730	1744	rBV	923793	1516823	79.81%	11.956%
11	14.081	1864	1871	1882	rBV	127446	211766	11.14%	1.669%
12	14.633	1957	1965	1977	rBV	260689	455356	23.96%	3.589%
13	16.126	2212	2219	2233	rBV	812764	1401790	73.76%	11.050%
14	17.377	2425	2432	2446	rBV	328152	549710	28.93%	4.333%
15	18.270	2578	2584	2599	rBV3	75006	139926	7.36%	1.103%
16	19.539	2796	2800	2807	rBV4	12567	19321	1.02%	0.152%
17	19.986	2870	2876	2886	rBV	1413947	1900439	100.00%	14.980%
18	21.284	3091	3097	3108	rBV2	124765	254392	13.39%	2.005%
19	21.643	3149	3158	3172	rBV	285715	553975	29.15%	4.367%
20	21.825	3184	3189	3196	rVB	31868	46426	2.44%	0.366%
21	22.424	3285	3291	3296	rBV	47783	85774	4.51%	0.676%
22	23.106	3401	3407	3414	rBV3	57127	111514	5.87%	0.879%
23	23.893	3535	3541	3551	rVB2	61101	128077	6.74%	1.010%
24	24.827	3690	3700	3718	rVB2	247768	719457	37.86%	5.671%
25	25.932	3879	3888	3898	rBV5	38045	115818	6.09%	0.913%
26	27.260	4109	4114	4124	rVB6	18380	54283	2.86%	0.428%

Sum of corrected areas: 12686321

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111119\
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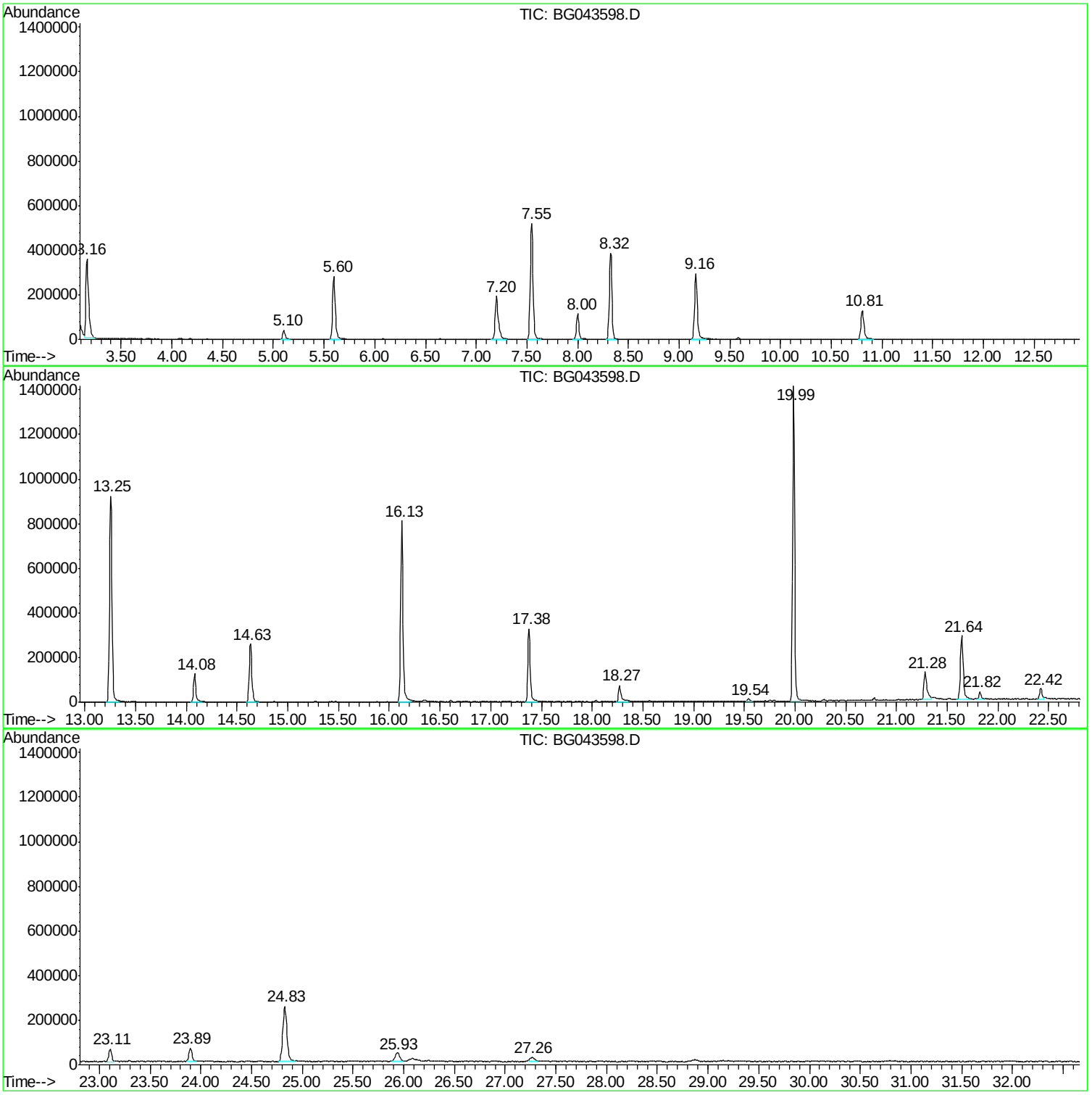
Sample : K5760-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR-50

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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\BG111119\
Data File : BG043598.D
Acq On : 12 Nov 2019 00:30
Operator : JU
Sample : K5760-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-50

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

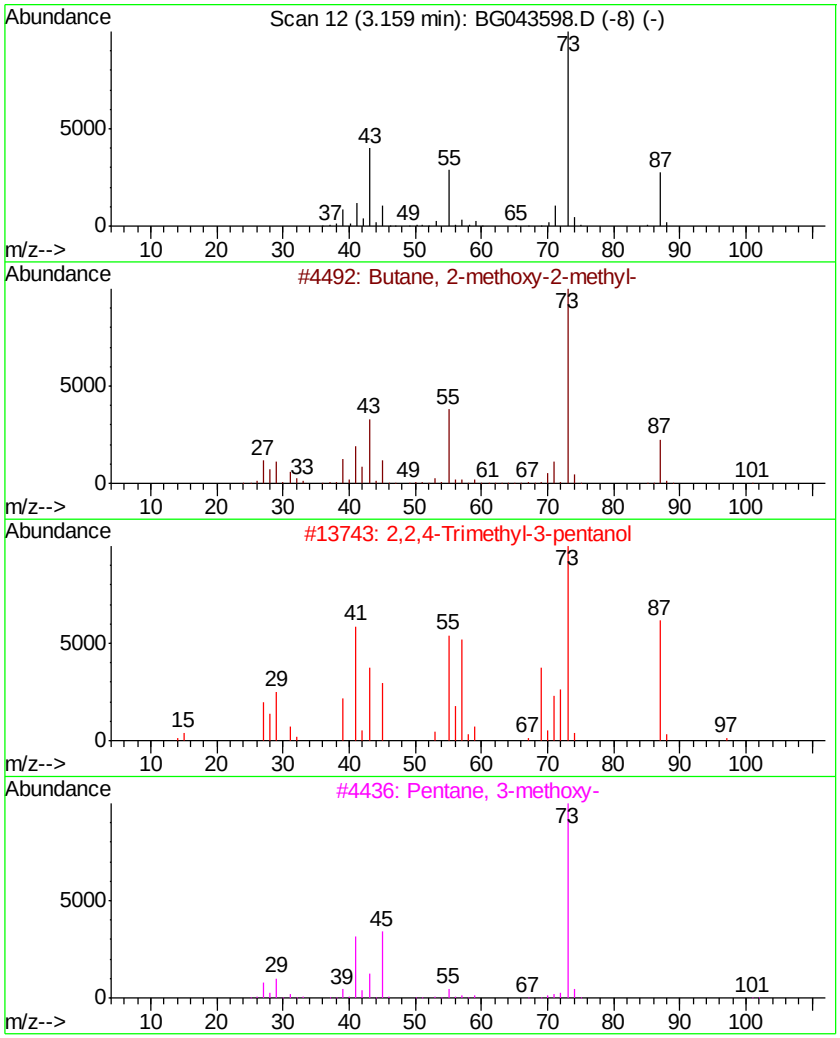
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

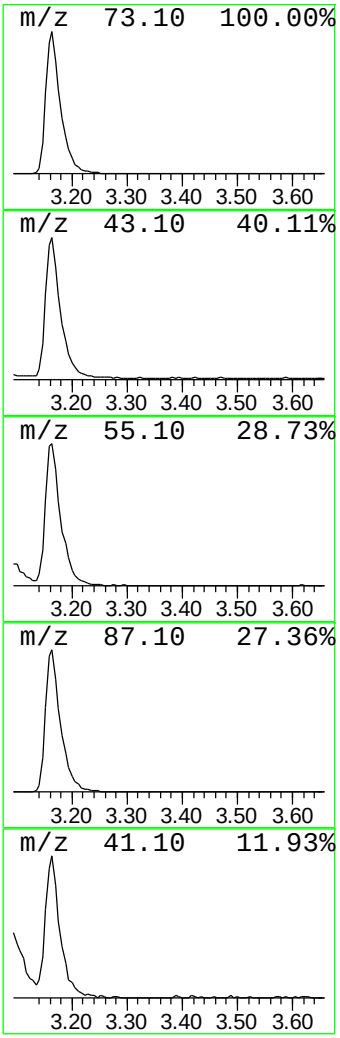
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.16	66.93 ng	665867	1,4-Dichlorobenzene-d4	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	50
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111119\
Data File : BG043598.D
Acq On : 12 Nov 2019 00:30
Operator : JU
Sample : K5760-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-50

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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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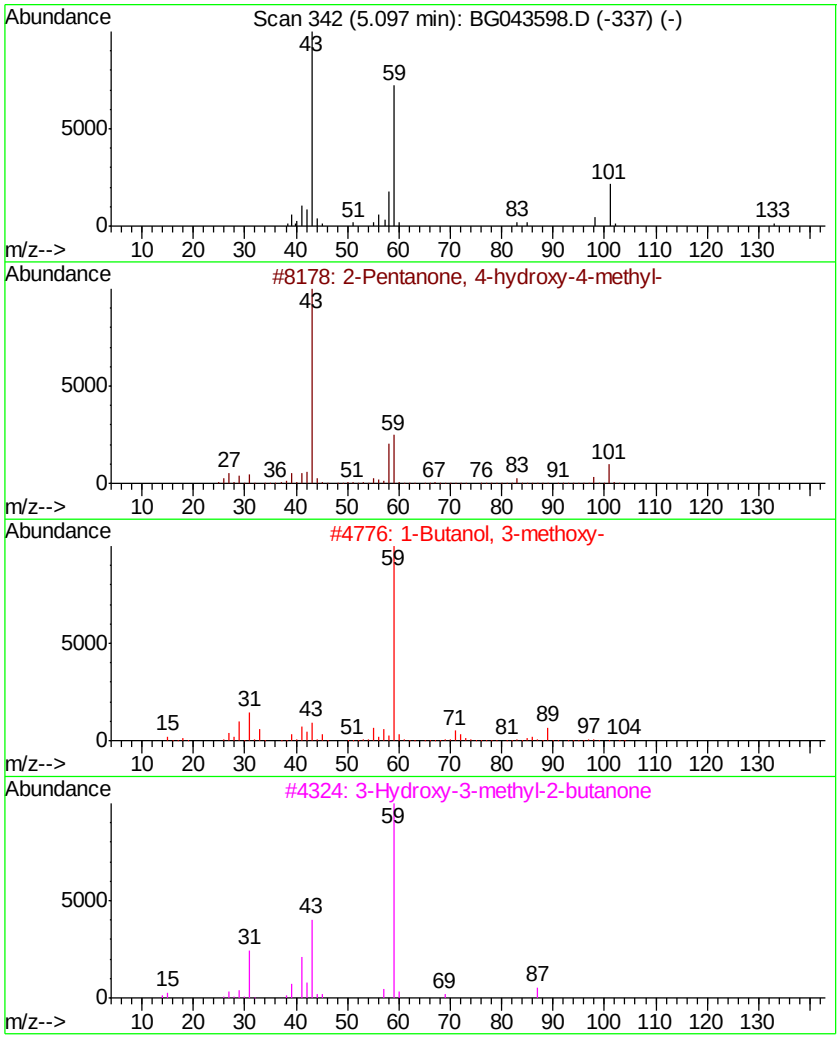
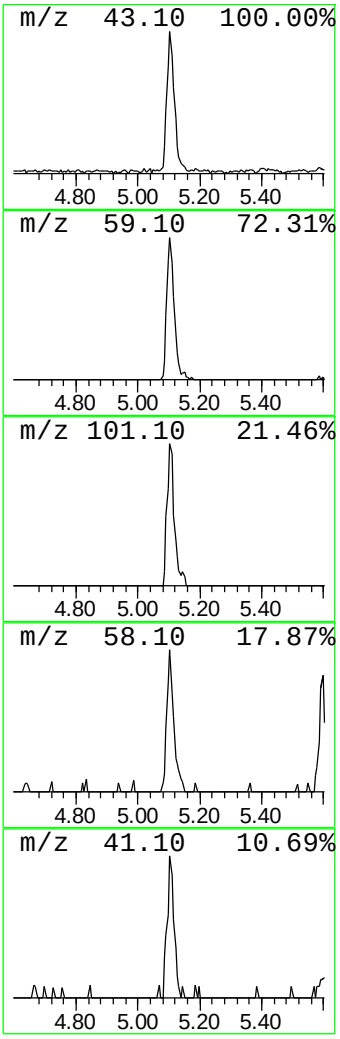
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	6.44 ng	64079	1,4-Dichlorobenzene-d4	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	32
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
5	Pentanal, oxime	101	C5H11NO	000628-79-5	17





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Data File : BG043598.D
Acq On : 12 Nov 2019 00:30
Operator : JU
Sample : K5760-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-50

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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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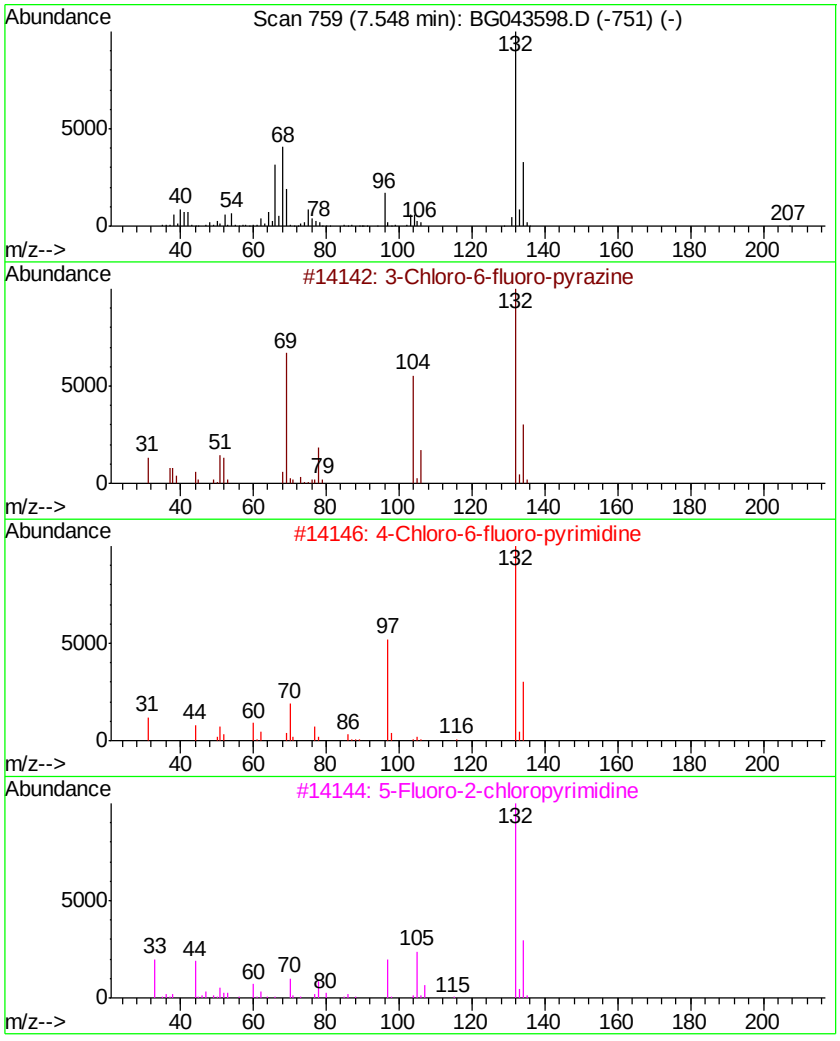
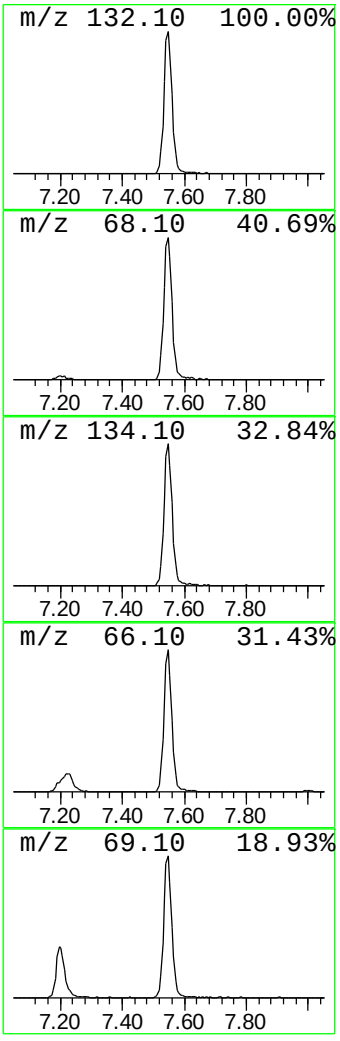
Peak Number 3 unknown7.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.55	95.85 ng	953560	1,4-Dichlorobenzene-d4	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	22
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111119\
Data File : BG043598.D
Acq On : 12 Nov 2019 00:30
Operator : JU
Sample : K5760-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-50

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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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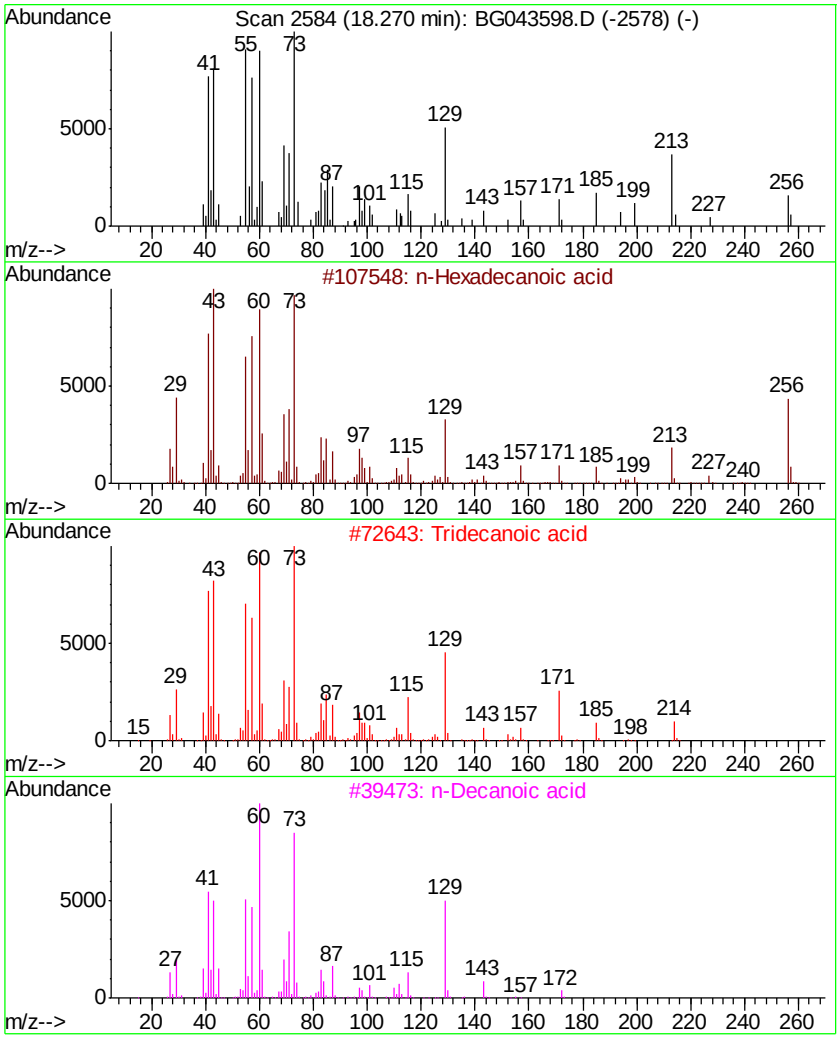
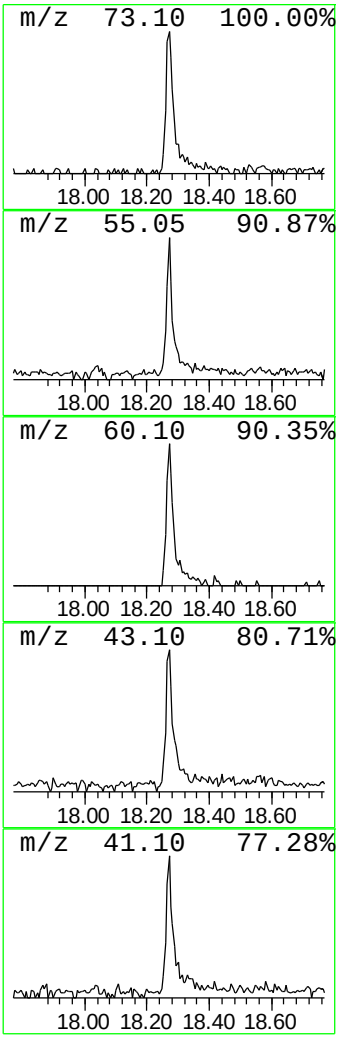
Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.27	5.09 ng	139926	Phenanthrene-d10	17.38

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	91
3	n-Decanoic acid	172	C10H20O2	000334-48-5	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111119\
Data File : BG043598.D
Acq On : 12 Nov 2019 00:30
Operator : JU
Sample : K5760-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-50

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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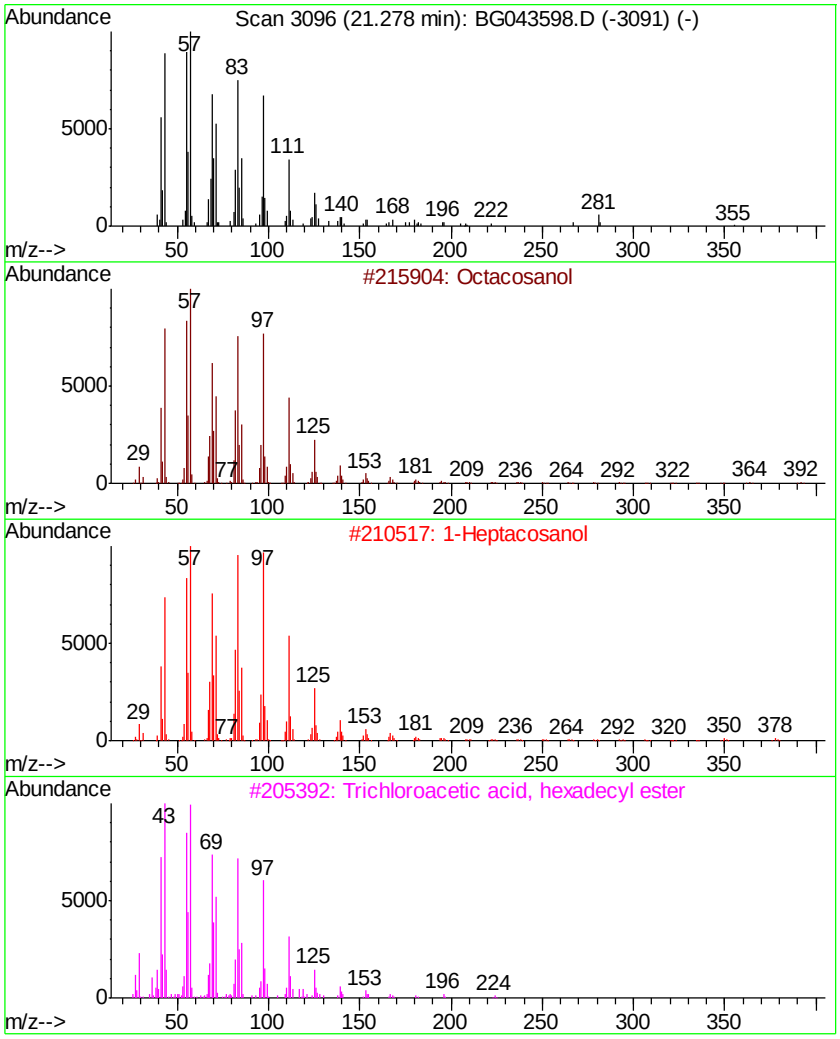
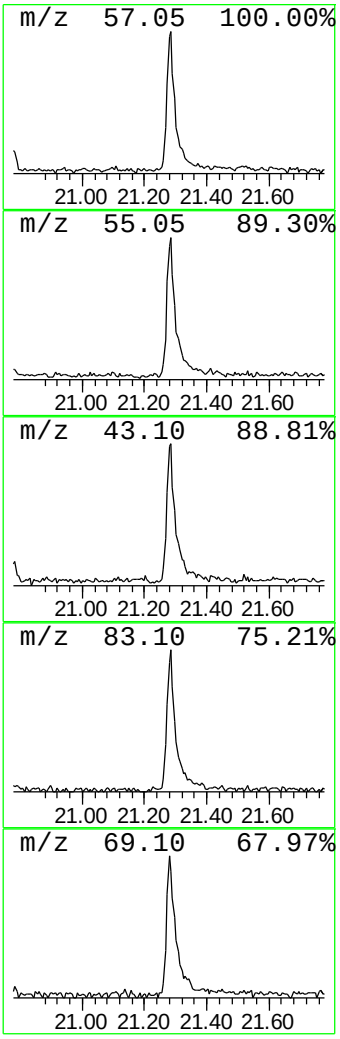
****

Peak Number 6 Octacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.28	9.18 ng	254392	Chrysene-d12	21.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	95
2	1-Heptacosanol	396	C27H56O	002004-39-9	95
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5	Cycloeicosane	280	C20H40	000296-56-0	93





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111119\
Data File : BG043598.D
Acq On : 12 Nov 2019 00:30
Operator : JU
Sample : K5760-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-50

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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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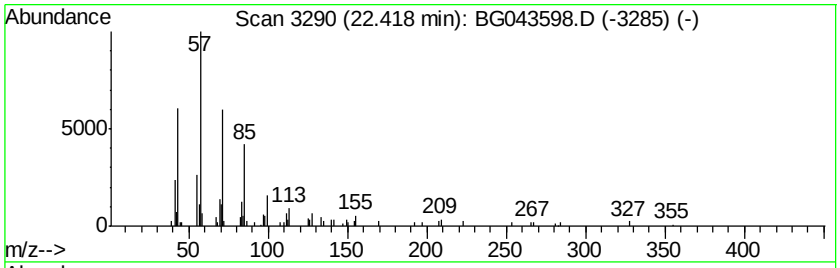
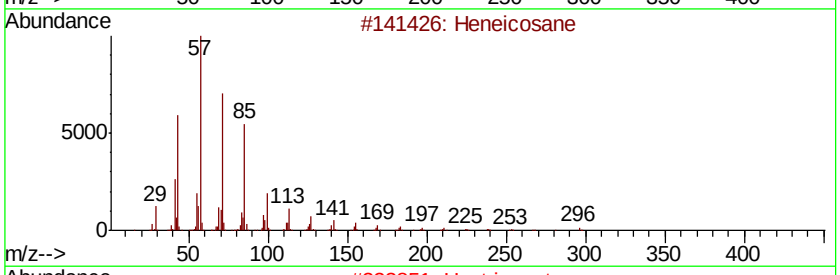
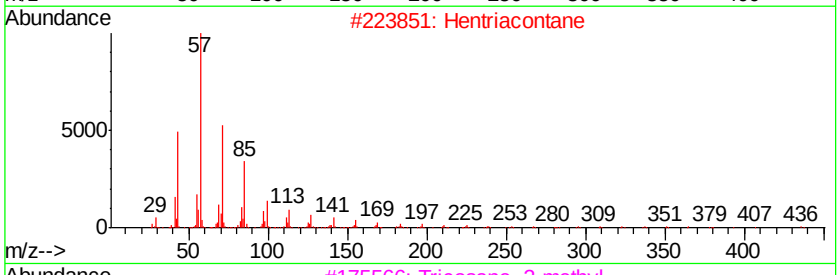
Peak Number 7 Heneicosane Concentration Rank 10

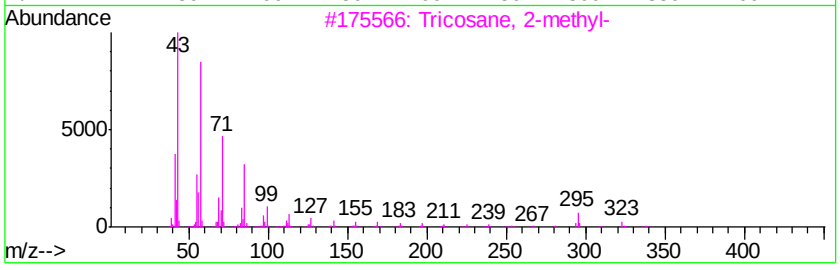
R.T.	EstConc	Area	Relative to ISTD	R.T.
22.42	3.10 ng	85774	Chrysene-d12	21.64

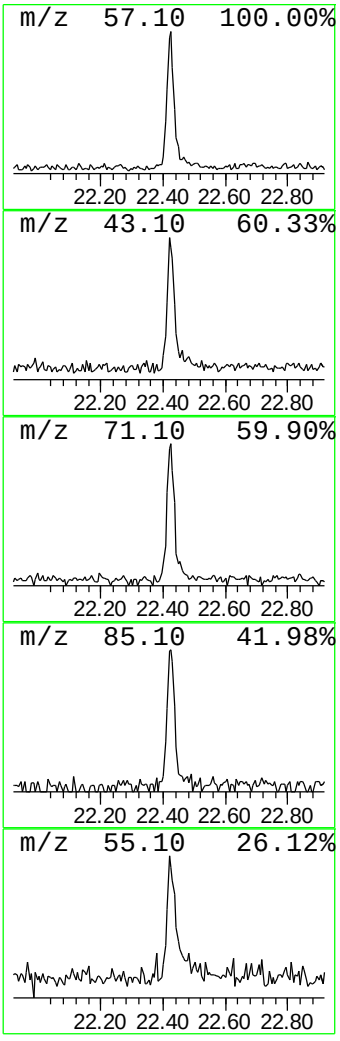
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	96
2	Hentriacontane	437	C31H64	000630-04-6	87
3	Tricosane, 2-methyl-	338	C24H50	001928-30-9	86
4	Tetratetracontane	619	C44H90	007098-22-8	86
5	Docosane	310	C22H46	000629-97-0	83











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Misc :
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Instrument : BNA_G
ClientSampleId : RBR-50

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

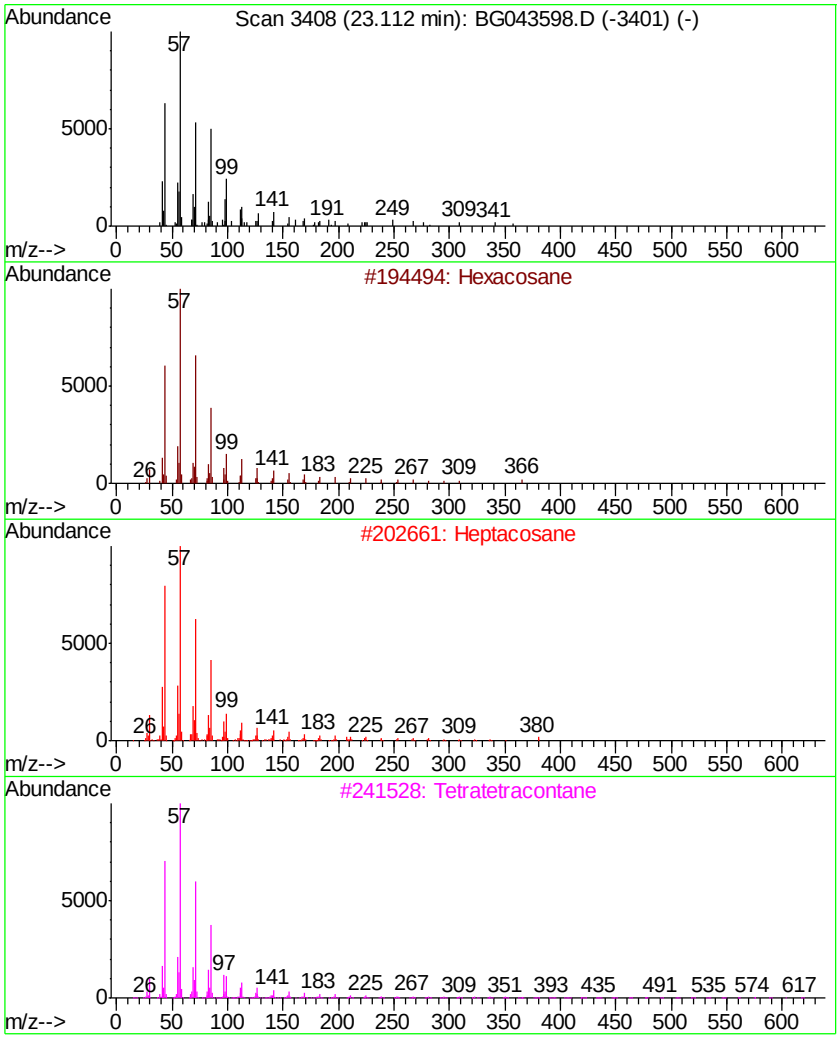
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

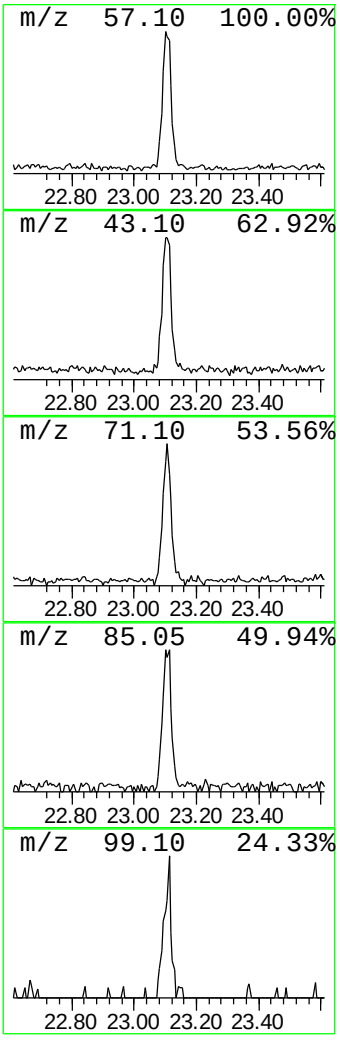
****

Peak Number 8 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.11	4.03 ng	111514	Chrysene-d12	21.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Tetratetracontane	619	C44H90	007098-22-8	90
4	2-methylhexacosane	380	C27H56	1000376-72-7	90
5	Pentacosane	352	C25H52	000629-99-2	90





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

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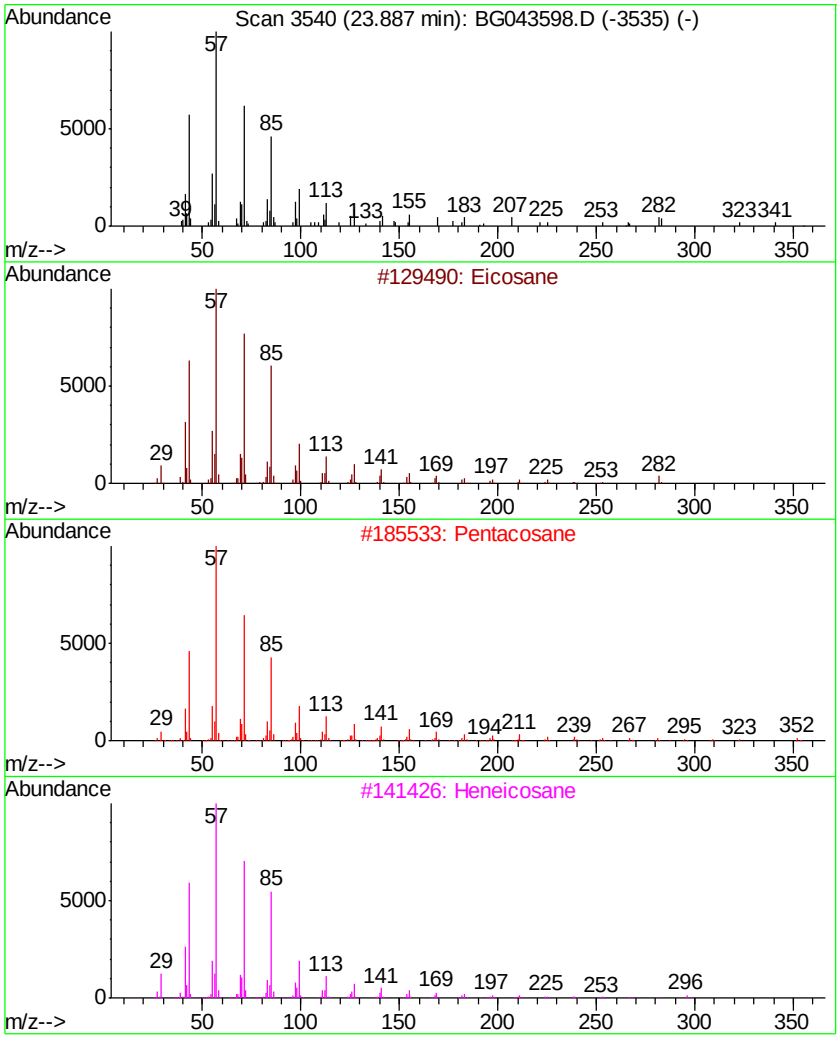
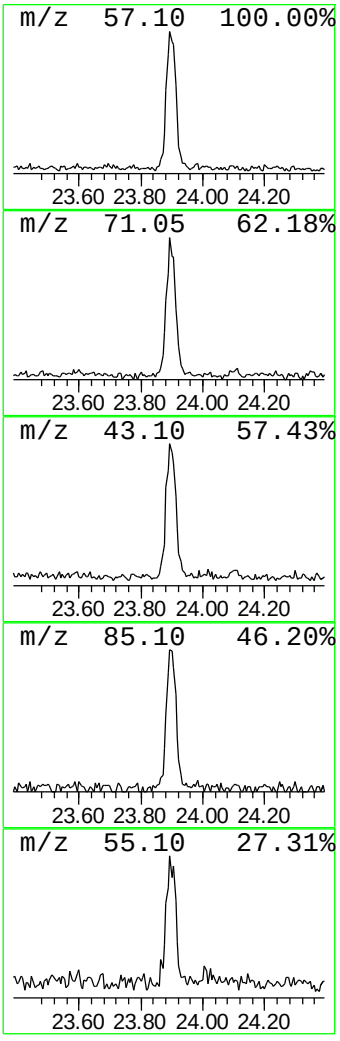
Peak Number 9 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.89	3.56 ng	128077	Perylene-d12	24.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Pentacosane	352	C25H52	000629-99-2	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Docosane	310	C22H46	000629-97-0	91
5	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	91





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Data File : BG043598.D
Acq On : 12 Nov 2019 00:30
Operator : JU
Sample : K5760-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-50

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

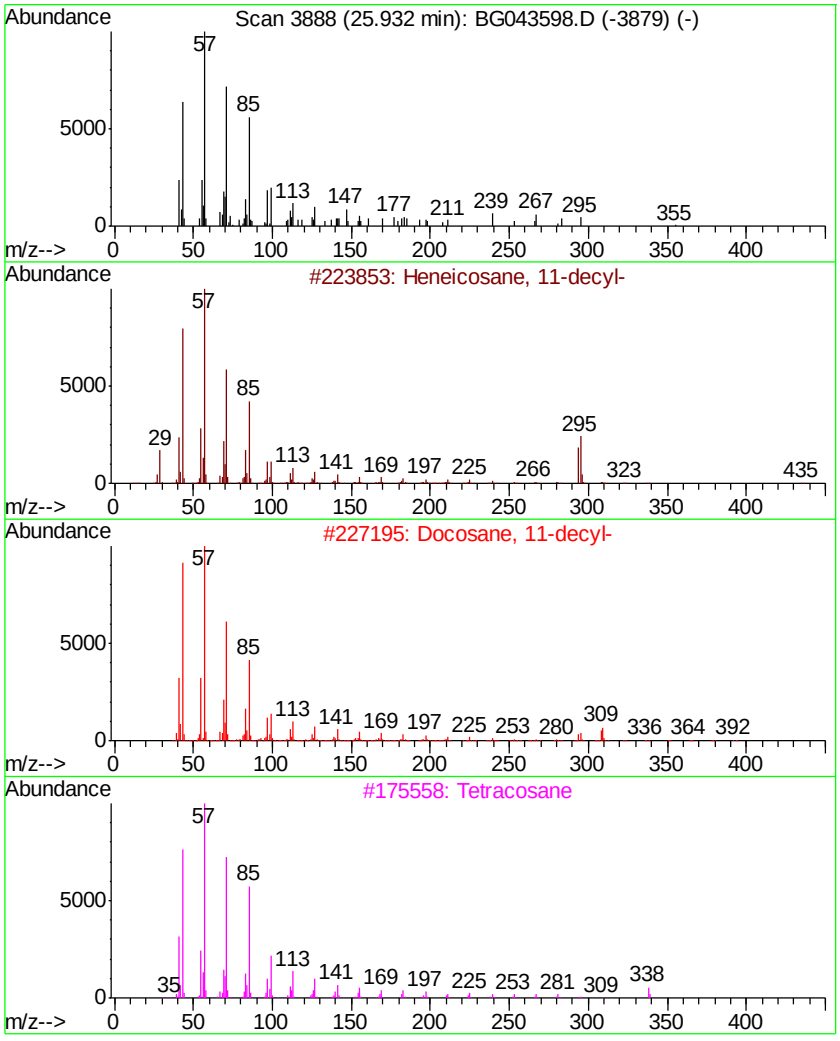
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

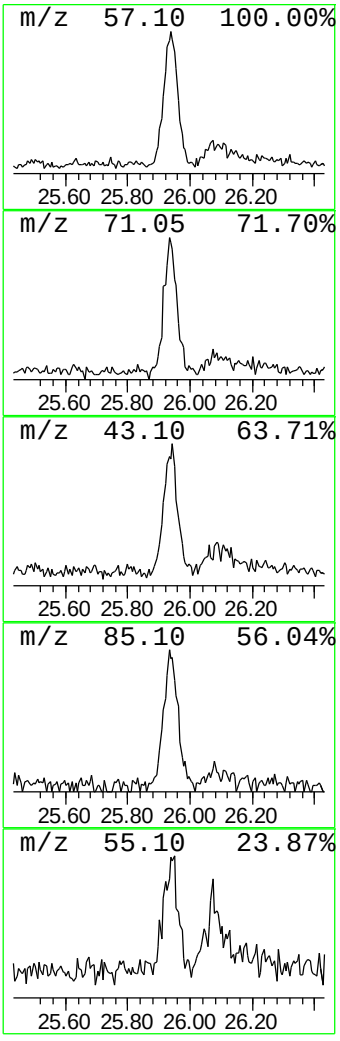
****

Peak Number 10 Heneicosane, 11-decyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.93	3.22 ng	115818	Perylene-d12	24.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	90
2	Docosane, 11-decyl-	451	C32H66	055401-55-3	90
3	Tetracosane	338	C24H50	000646-31-1	86
4	Tetratetracontane	619	C44H90	007098-22-8	86
5	Docosane	310	C22H46	000629-97-0	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG111119\
Data File : BG043598.D
Acq On : 12 Nov 2019 00:30
Operator : JU
Sample : K5760-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-50

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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
Butane, 2-methoxy...	3.16	66.9	ng	665867	1	8.00	198974	20.0
2-Pentanone, 4-hy...	5.10	6.4	ng	64079	1	8.00	198974	20.0
unknown7.55	7.55	95.8	ng	953560	1	8.00	198974	20.0
n-Hexadecanoic acid	18.27	5.1	ng	139926	4	17.38	549710	20.0
Octacosanol	21.28	9.2	ng	254392	5	21.64	553975	20.0
Heneicosane	22.42	3.1	ng	85774	5	21.64	553975	20.0
Hexacosane	23.11	4.0	ng	111514	5	21.64	553975	20.0
Eicosane	23.89	3.6	ng	128077	6	24.83	719457	20.0
Heneicosane, 11-d...	25.93	3.2	ng	115818	6	24.83	719457	20.0