LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043367.D
Acq On : 29 Oct 2019 2:00
Operator : JU
Sample : K5503-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 171-06-(0-1.9)

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	3.191	13	17	25	rVB	52918	74681	2.25%	0.418%
2	5.130	339	347	356	rBV	50664	82592	2.49%	0.463%
3	5.611	422	429	444	rBV	682242	1181687	35.65%	6.618%
4	7.215	692	702	714	rBV	718272	1372737	41.42%	7.688%
5	7.568	754	762	774	rBV	731736	1328970	40.10%	7.443%
6	8.026	831	840	849	rBV	146594	266507	8.04%	1.493%
7	8.349	886	895	906	rBV	544989	960314	28.97%	5.378%
8	9.184	1029	1037	1054	rBV	371867	788484	23.79%	4.416%
9	10.829	1309	1317	1337	rBV	170855	349442	10.54%	1.957%
10	13.273	1726	1733	1748	rBV	1167544	1921908	57.99%	10.763%
11	14.101	1868	1874	1886	rBV	69666	131930	3.98%	0.739%
12	14.648	1960	1967	1980	rBV	320619	544381	16.43%	3.049%
13	16.140	2214	2221	2236	rBV	1162327	1936446	58.43%	10.845%
14	17.398	2427	2435	2452	rBV2	394192	703651	21.23%	3.941%
15	18.285	2577	2586	2597	rBV2	97080	184098	5.55%	1.031%
16	20.006	2872	2879	2896	rBV	2331255	3314339	100.00%	18.561%
17	21.311	3096	3101	3115	rBV6	58040	167392	5.05%	0.937%
18	21.663	3153	3161	3178	rVB	458100	894825	27.00%	5.011%
19	21.845	3187	3192	3198	rBV2	38567	59804	1.80%	0.335%
20	22.451	3289	3295	3301	rBV3	53525	93273	2.81%	0.522%
21	23.132	3405	3411	3419	rVB3	52104	102398	3.09%	0.573%
22	23.326	3438	3444	3453	rVB2	120237	233668	7.05%	1.309%
23	23.937	3542	3548	3553	rVB3	45027	84313	2.54%	0.472%
24	24.859	3695	3705	3722	rVB	339056	1025882	30.95%	5.745%
25	25.988	3890	3897	3903	rVB5	21353	52633	1.59%	0.295%

Sum of corrected areas: 17856355

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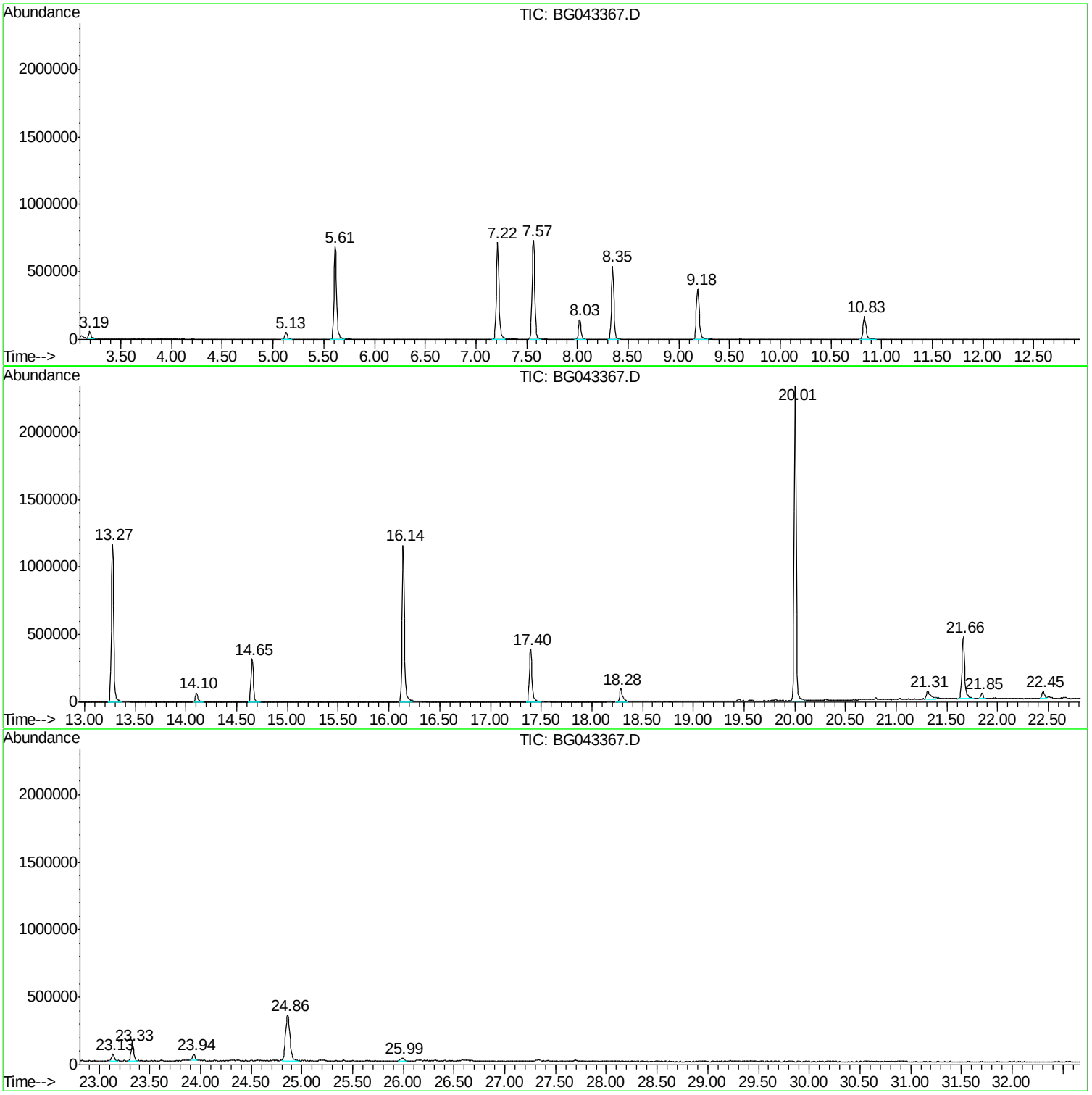
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
171-06-(0-1.9)

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043367.D
Acq On : 29 Oct 2019 2:00
Operator : JU
Sample : K5503-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 171-06-(0-1.9)

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

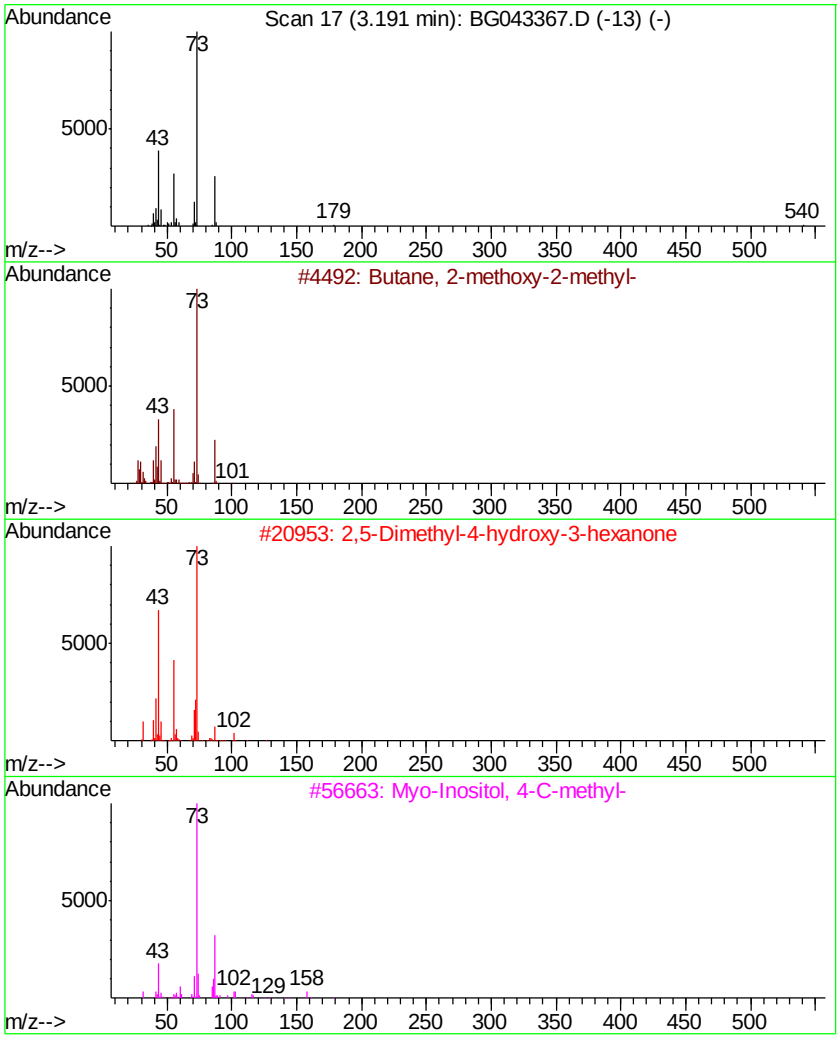
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

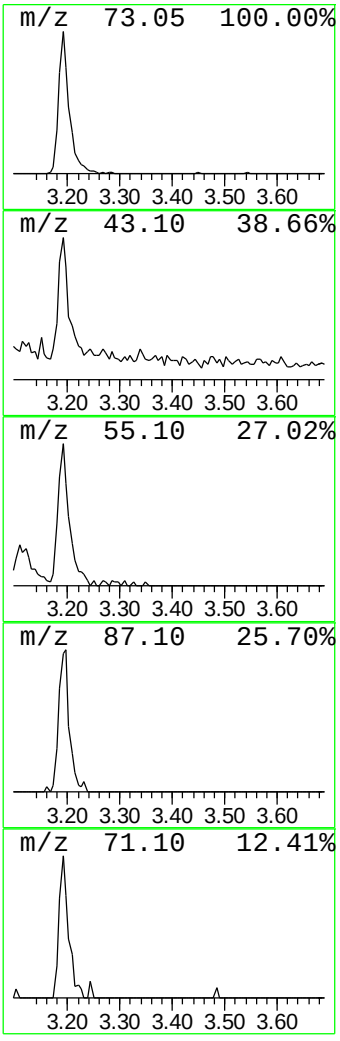
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.19	5.60 ng	74681	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	50
2	2,5-Dimethyl-4-hydroxy-3-hexanone	144	C8H16O2	000815-77-0	43
3	Myo-Inositol, 4-C-methyl-	194	C7H14O6	000472-95-7	38
4	Myo-Inositol, 2-C-methyl-	194	C7H14O6	000472-96-8	38
5	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38





Library Search Compound Report

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Data File : BG043367.D
Acq On : 29 Oct 2019 2:00
Operator : JU
Sample : K5503-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 171-06-(0-1.9)

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

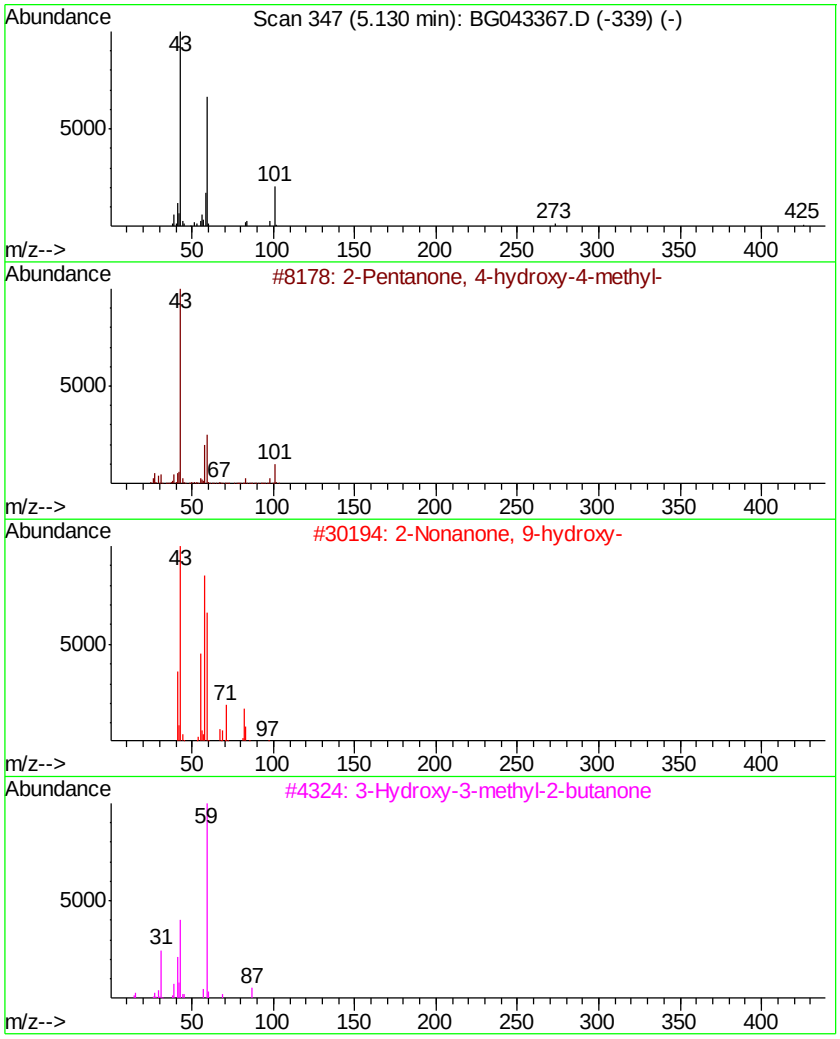
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

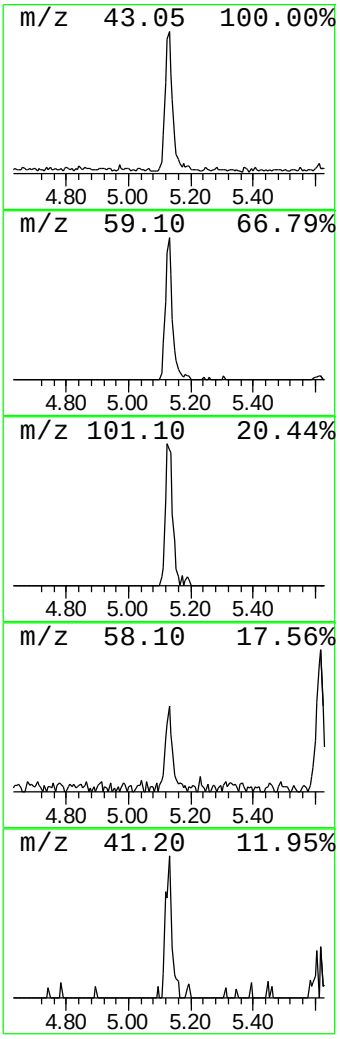
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	6.20 ng	82592	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	28
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Acetone	58	C3H6O	000067-64-1	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043367.D
Acq On : 29 Oct 2019 2:00
Operator : JU
Sample : K5503-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 171-06-(0-1.9)

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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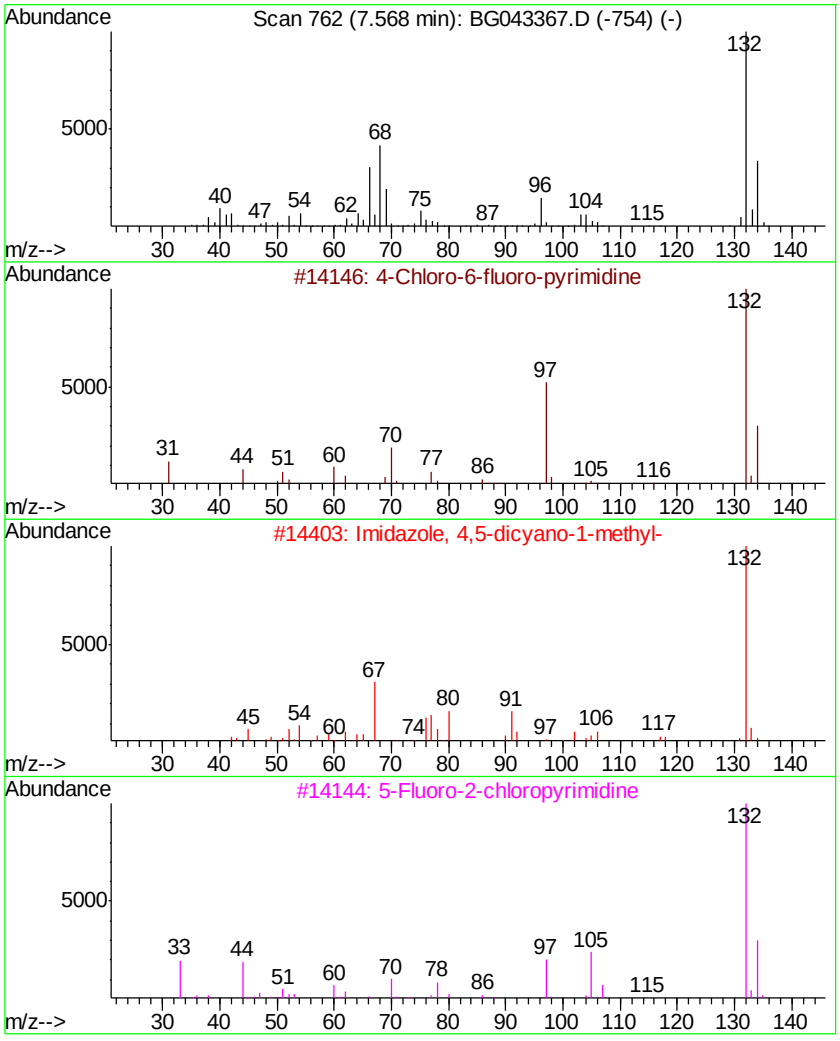
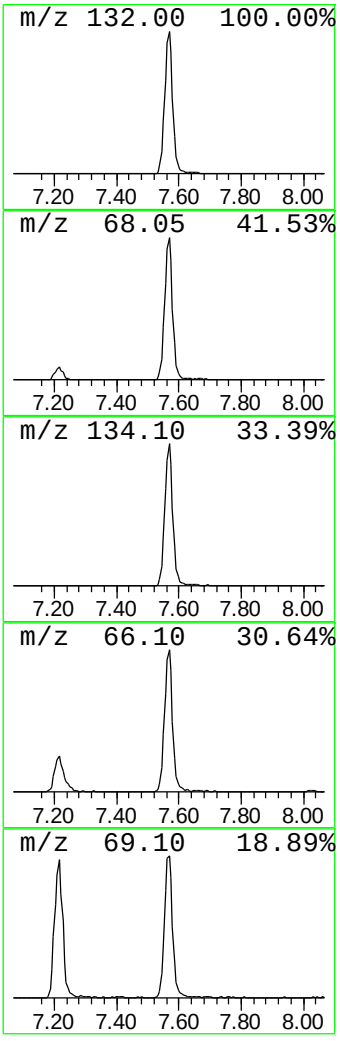
****

Peak Number 3 unknown7.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.57	99.73 ng	1328970	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043367.D
Acq On : 29 Oct 2019 2:00
Operator : JU
Sample : K5503-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 171-06-(0-1.9)

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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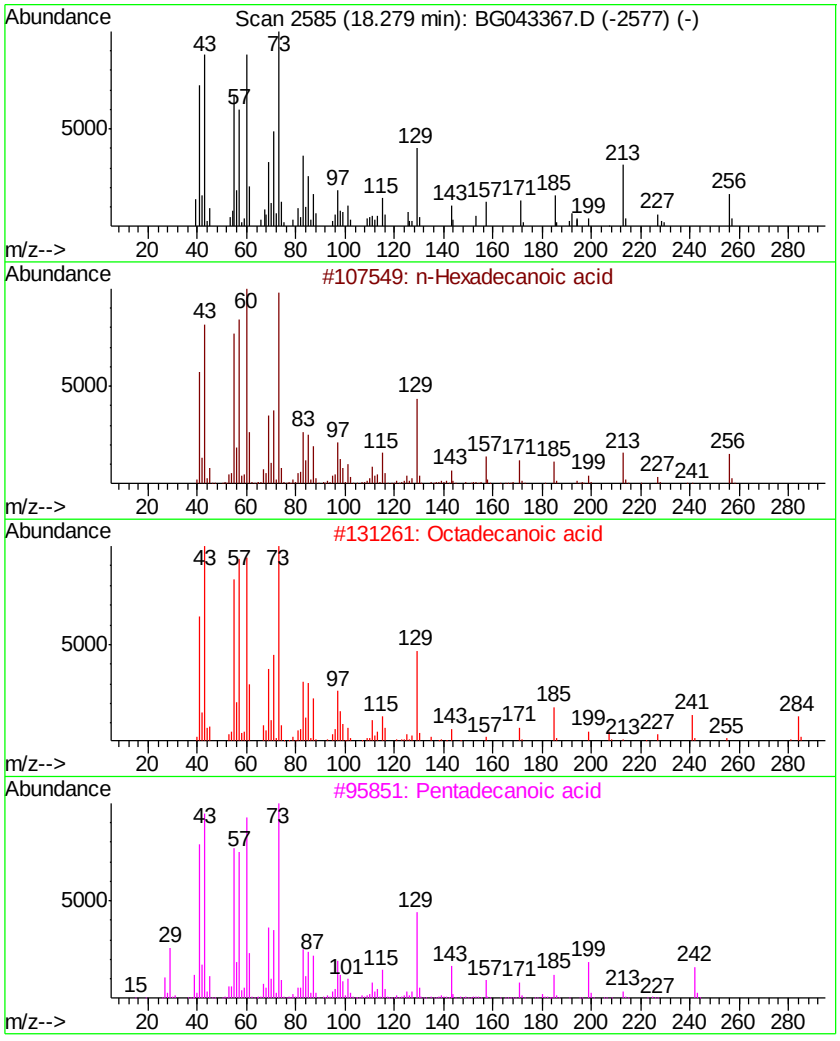
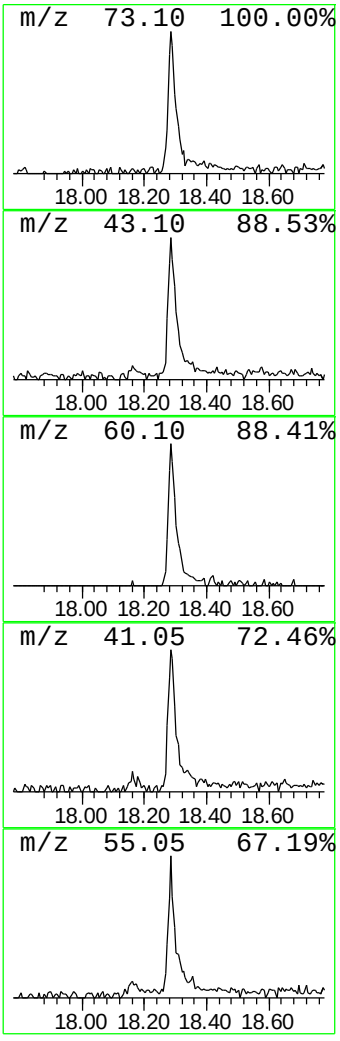
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.28	5.23 ng	184098	Phenanthrene-d10	17.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Octadecanoic acid	284	C18H36O2	000057-11-4	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Tridecanoic acid	214	C13H26O2	000638-53-9	80





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043367.D
Acq On : 29 Oct 2019 2:00
Operator : JU
Sample : K5503-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 171-06-(0-1.9)

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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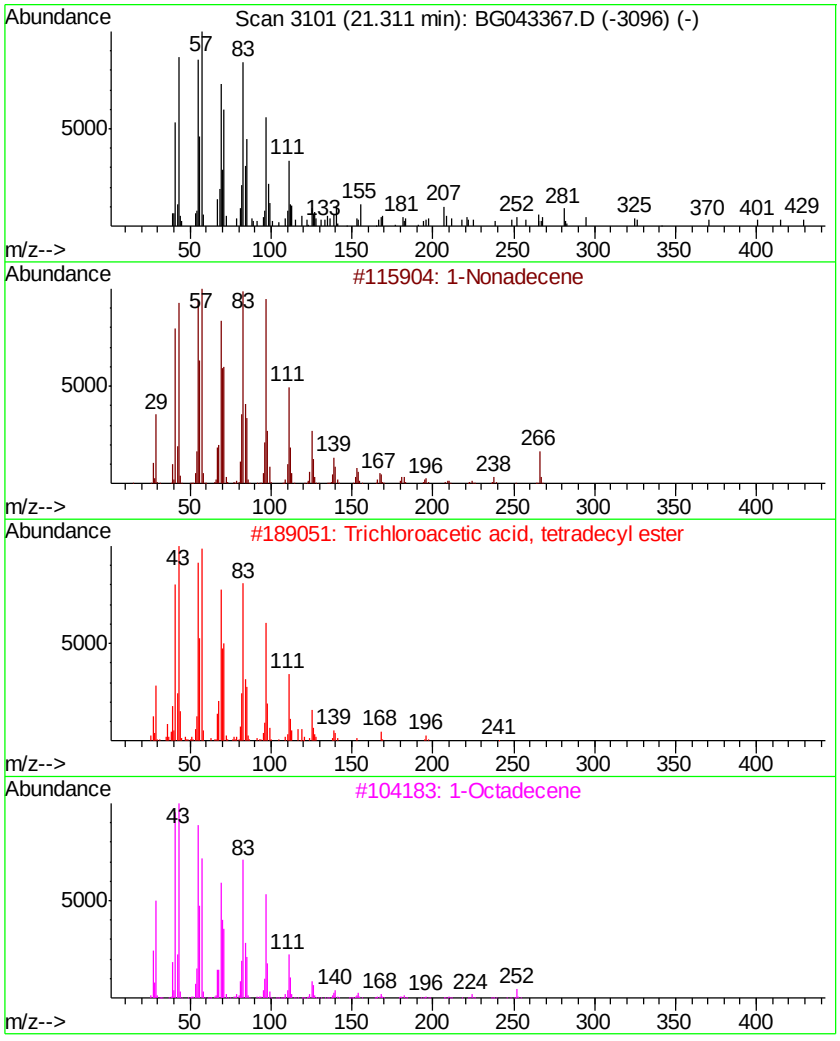
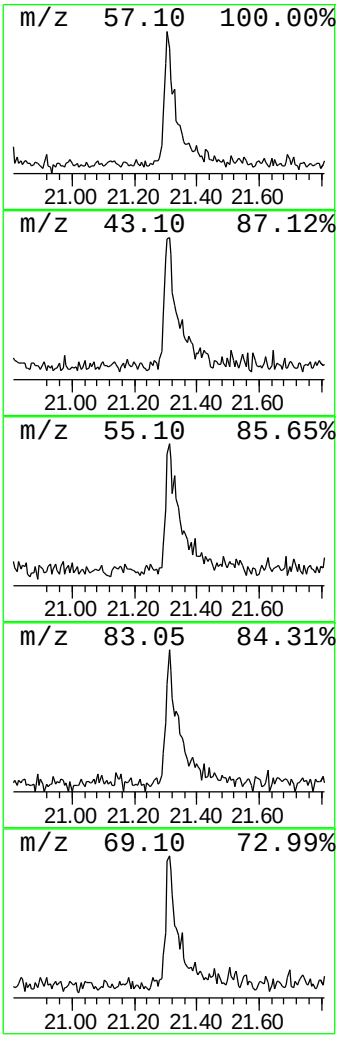
****

Peak Number 6 1-Nonadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.31	3.74 ng	167392	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	90
2	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	90
3	1-Octadecene	252	C18H36	000112-88-9	89
4	5-Octadecene, (E)-	252	C18H36	007206-21-5	89
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87





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Instrument : BNA_G
ClientSampleId : 171-06-(0-1.9)

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

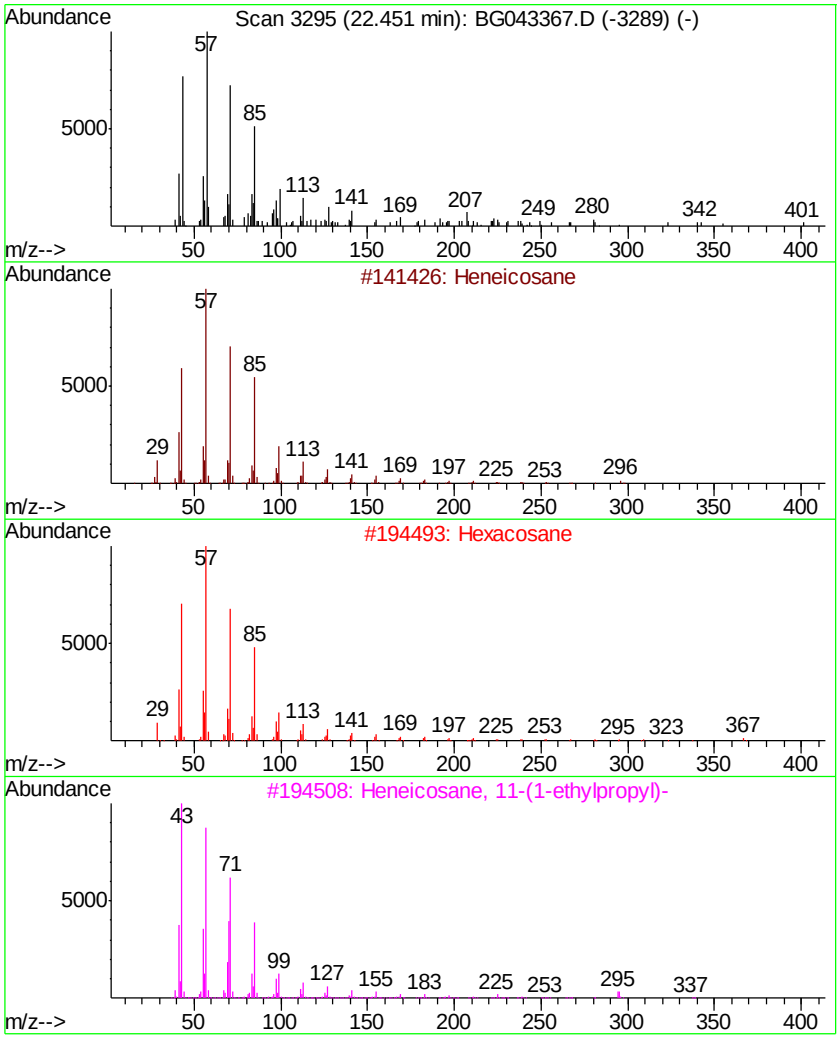
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

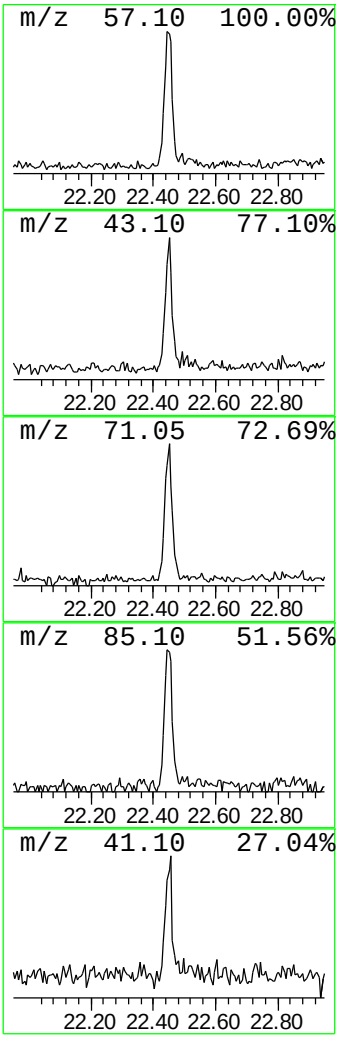
****

Peak Number 7 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.45	2.08 ng	93273	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
4	Heptacosane	380	C27H56	000593-49-7	90
5	Pentacosane	352	C25H52	000629-99-2	90





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Misc :
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Instrument : BNA_G
ClientSampleId : 171-06-(0-1.9)

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

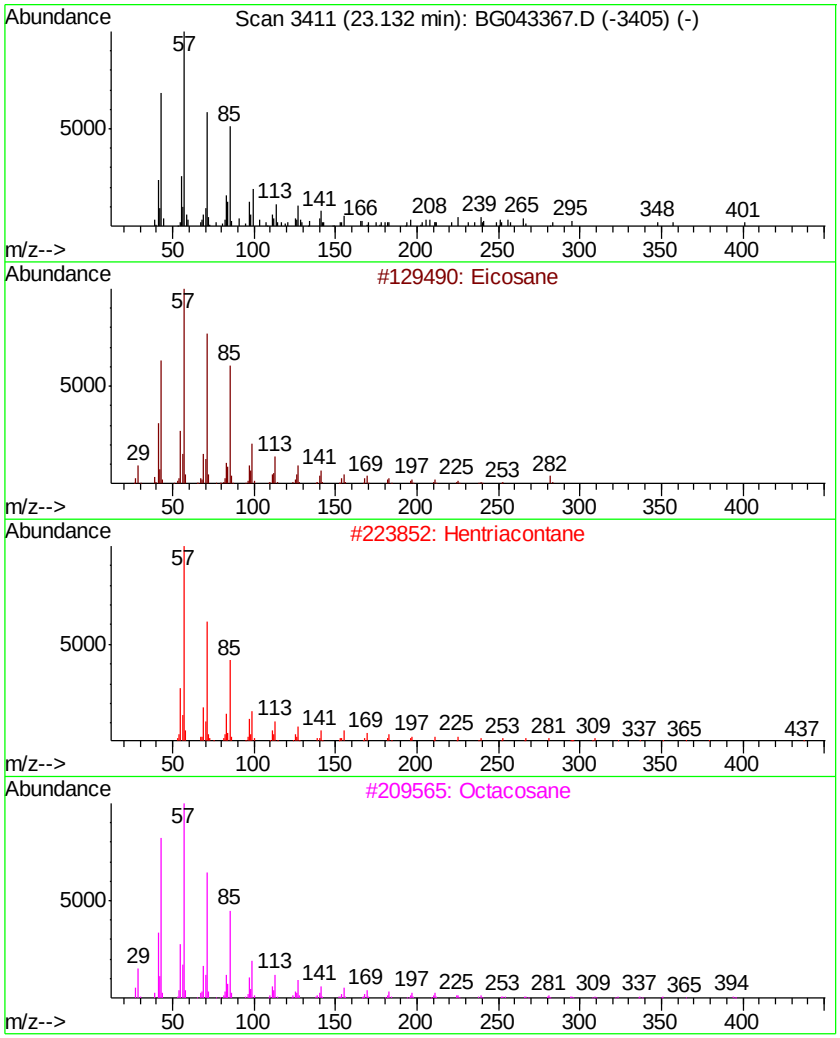
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

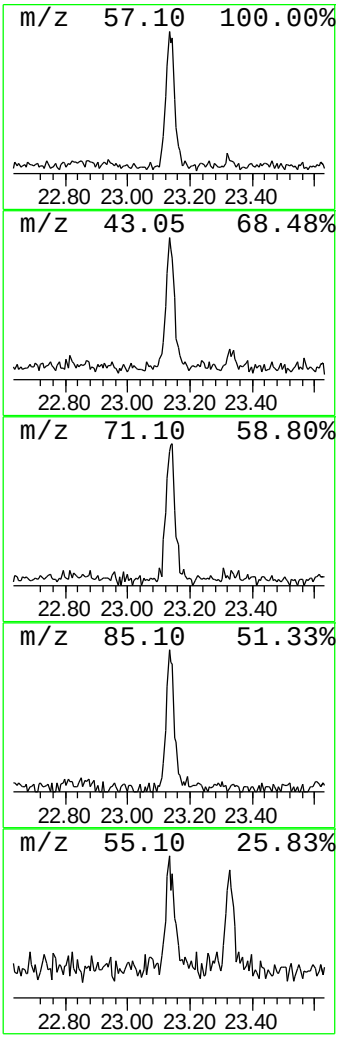
****

Peak Number 8 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.13	2.29 ng	102398	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Hentriacontane	437	C31H64	000630-04-6	87
3	Octacosane	394	C28H58	000630-02-4	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	86





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Instrument : BNA_G
ClientSampleId : 171-06-(0-1.9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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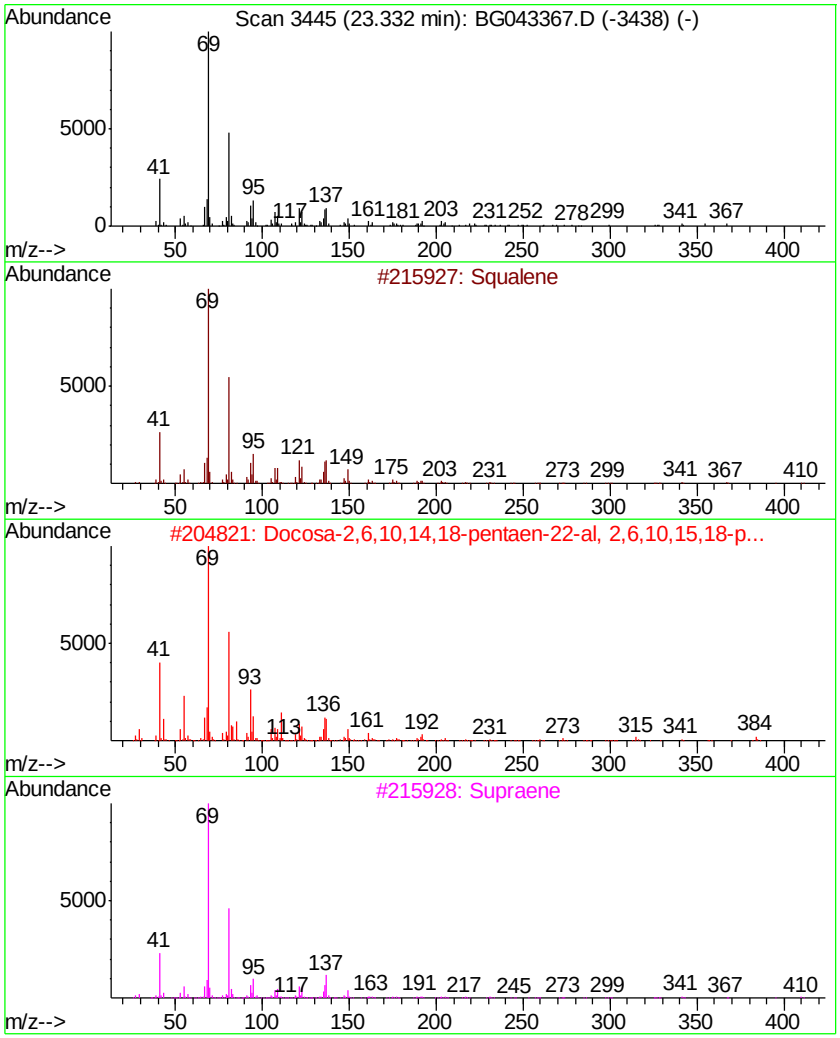
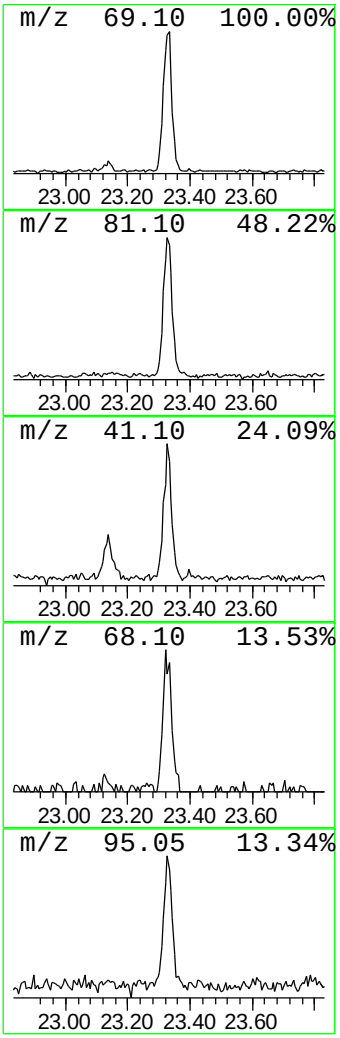
Peak Number 9 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.33	4.56 ng	233668	Perylene-d12	24.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	78
3	Supraene	410	C30H50	007683-64-9	72
4	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	68
5	trans-Farnesol	222	C15H26O	000106-28-5	64





Tentatively Identified Compound (LSC) summary

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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...	3.19	5.6	ng	74681	1	8.02	266507	20.0
2-Pentanone, 4-hy...	5.13	6.2	ng	82592	1	8.02	266507	20.0
unknown7.57	7.57	99.7	ng	1328970	1	8.02	266507	20.0
n-Hexadecanoic acid	18.28	5.2	ng	184098	4	17.40	703651	20.0
1-Nonadecene	21.31	3.7	ng	167392	5	21.66	894825	20.0
Heneicosane	22.45	2.1	ng	93273	5	21.66	894825	20.0
Eicosane	23.13	2.3	ng	102398	5	21.66	894825	20.0
Squalene	23.33	4.6	ng	233668	6	24.85	1025880	20.0