LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG092718\
Data File : BG037051.D
Acq On : 28 Sep 2018 15:22
Operator : JU/SJ
Sample : J5099-01
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 7211975

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-BG092018.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	5.150	312	317	327	rVB	27038	45200	1.75%	0.238%
2	5.615	390	396	420	rBV	598786	1115182	43.30%	5.863%
3	7.201	659	666	685	rBV	597164	1221154	47.41%	6.420%
4	7.571	722	729	750	rBV	589769	1152748	44.76%	6.061%
5	8.041	802	809	822	rBV	122436	257197	9.99%	1.352%
6	8.358	856	863	881	rBV	443668	865110	33.59%	4.549%
7	9.199	999	1006	1032	rBV	345395	780647	30.31%	4.104%
8	10.844	1276	1286	1301	rBV	167042	349898	13.59%	1.840%
9	13.288	1693	1702	1719	rBV	873036	1519260	58.99%	7.988%
10	14.111	1835	1842	1851	rBV	91046	156022	6.06%	0.820%
11	14.663	1922	1936	1951	rBV2	282534	504074	19.57%	2.650%
12	16.149	2183	2189	2206	rBV	781556	1370027	53.19%	7.203%
13	17.413	2397	2404	2415	rBV	389055	676268	26.26%	3.556%
14	18.294	2549	2554	2561	rBV2	55478	96511	3.75%	0.507%
15	20.015	2841	2847	2861	rBV	1909587	2575503	100.00%	13.541%
16	21.314	3063	3068	3080	rBV	90127	164956	6.40%	0.867%
17	21.678	3123	3130	3143	rBV2	448905	807847	31.37%	4.247%
18	21.860	3156	3161	3169	rVB	125290	168854	6.56%	0.888%
19	22.465	3257	3264	3276	rBV	223477	395383	15.35%	2.079%
20	23.153	3374	3381	3391	rVB	352212	680367	26.42%	3.577%
21	23.952	3508	3517	3527	rBV	395922	872438	33.87%	4.587%
22	24.886	3664	3676	3694	rBV3	590977	1724025	66.94%	9.064%
23	26.008	3855	3867	3882	rBV2	259726	793349	30.80%	4.171%
24	27.348	4082	4095	4108	rBV	140190	487528	18.93%	2.563%
25	28.970	4360	4371	4387	rVB3	46660	191750	7.45%	1.008%
26	30.914	4690	4702	4704	rBV3	15734	48372	1.88%	0.254%

Sum of corrected areas: 19019670

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG092718\
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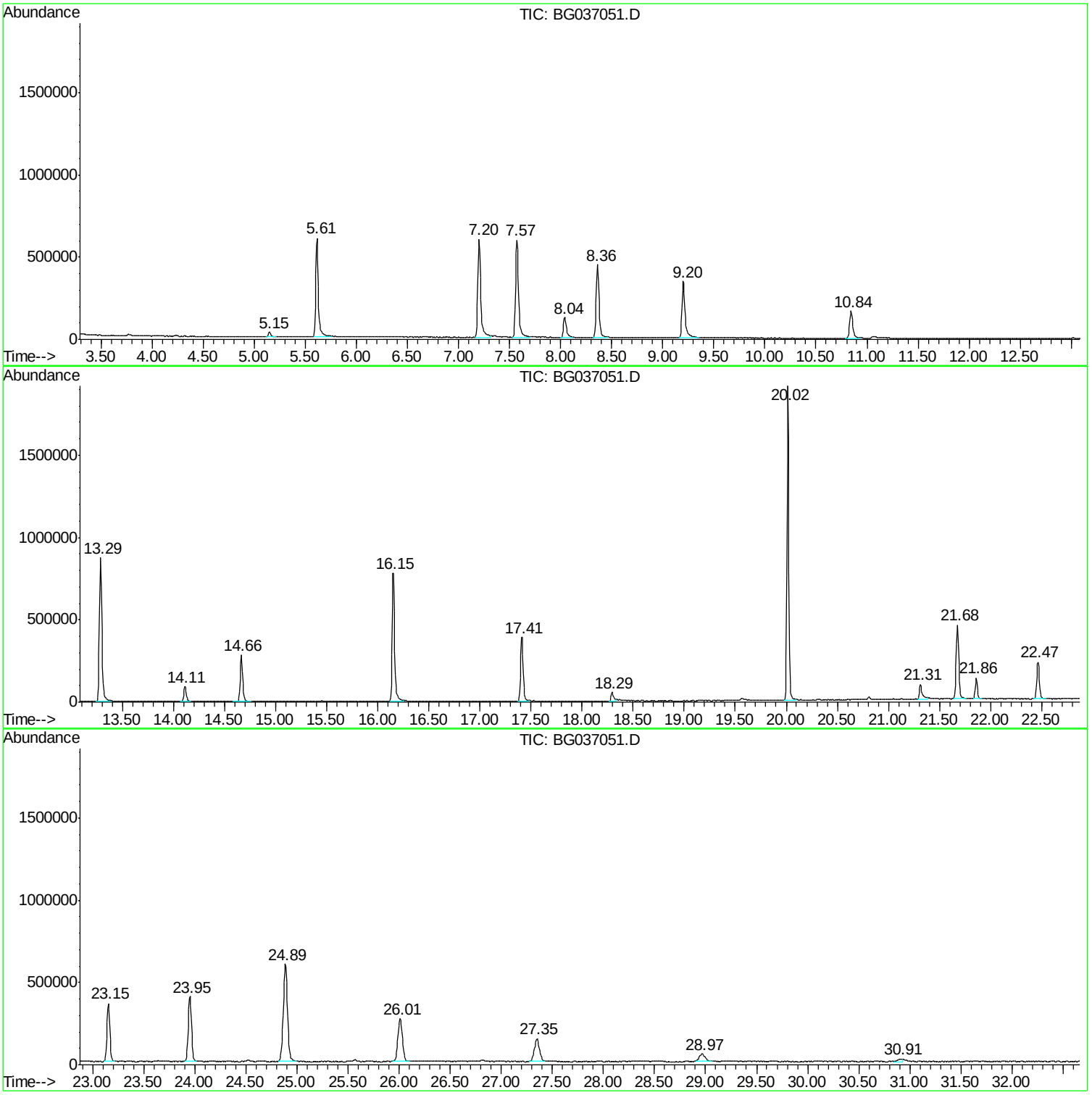
Sample : J5099-01
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
7211975

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.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\BG092718\
Data File : BG037051.D
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Operator : JU/SJ
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Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 7211975

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.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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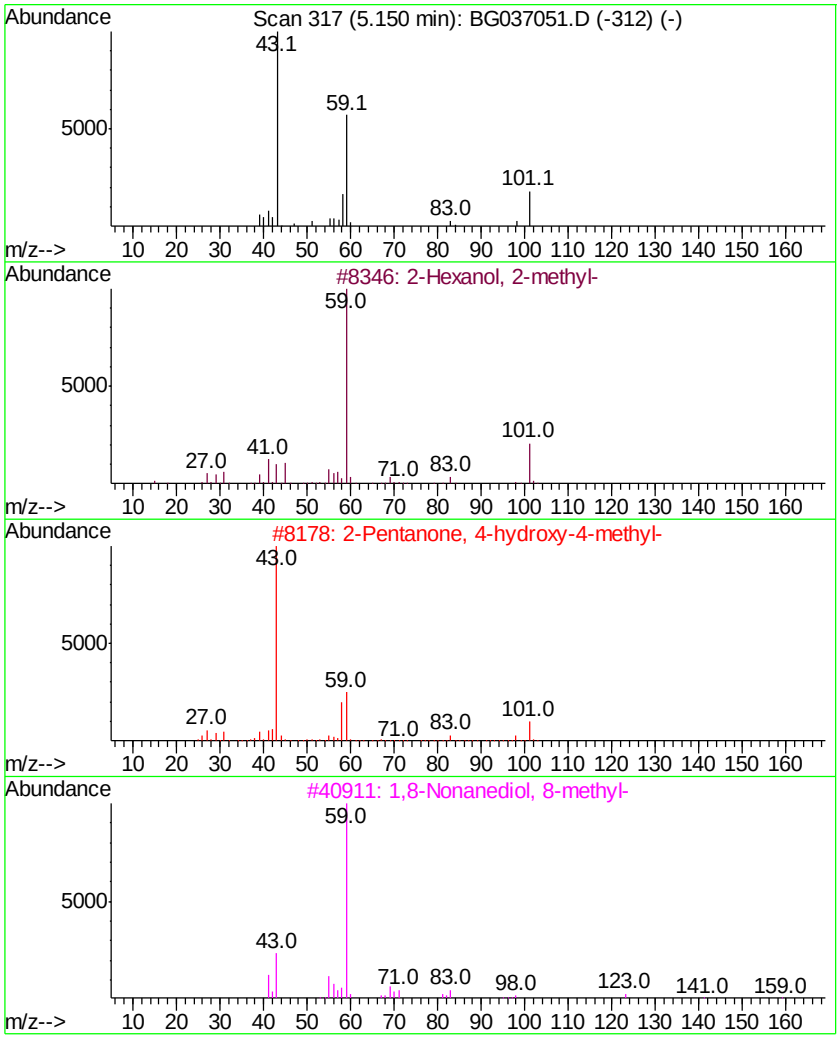
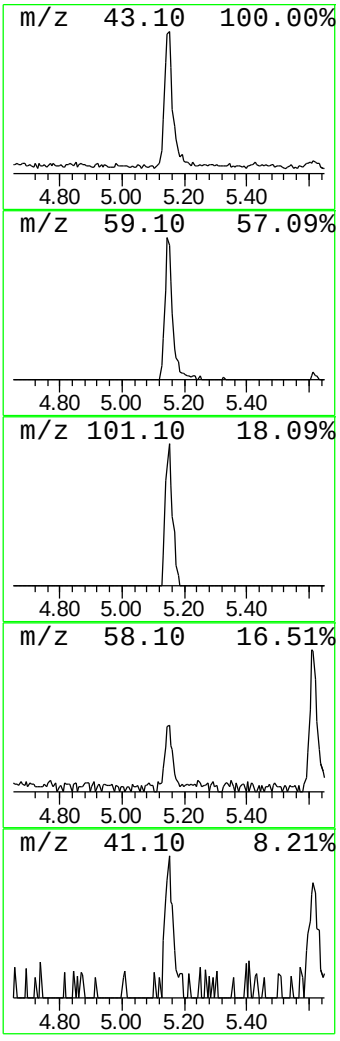
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	3.51 ng	45200	1,4-Dichlorobenzene-d4	8.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	50
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9





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Data File : BG037051.D
Acq On : 28 Sep 2018 15:22
Operator : JU/SJ
Sample : J5099-01
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 7211975

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

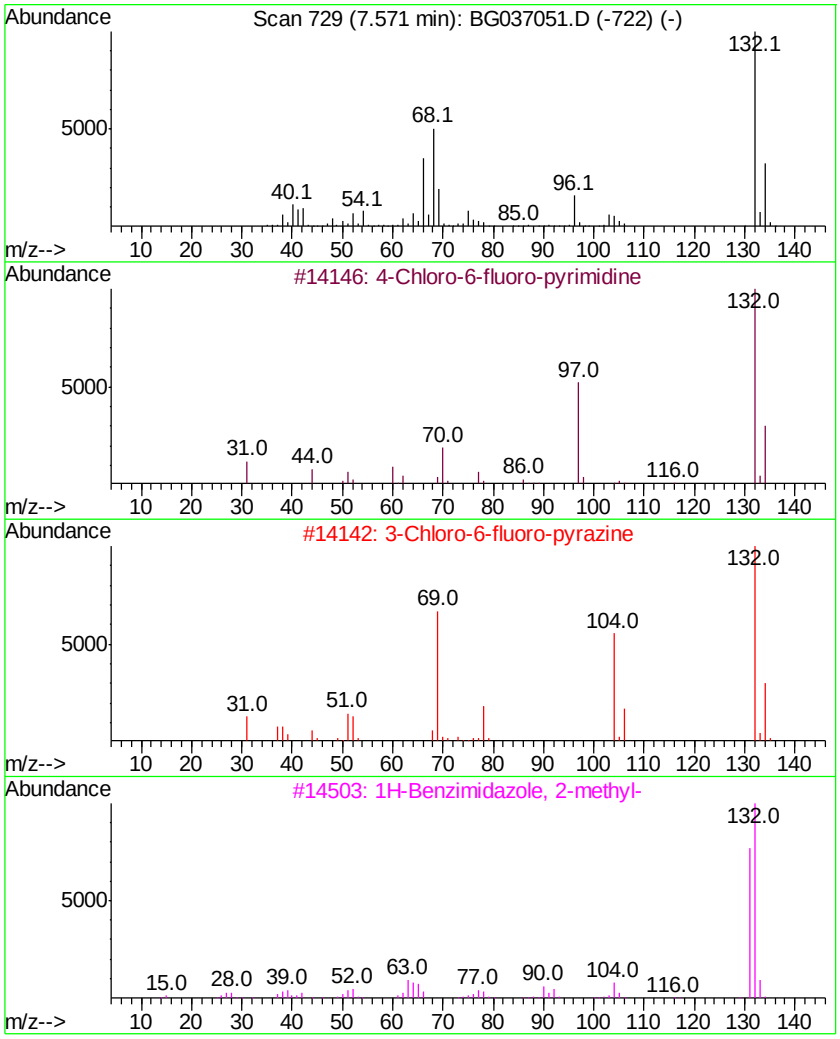
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

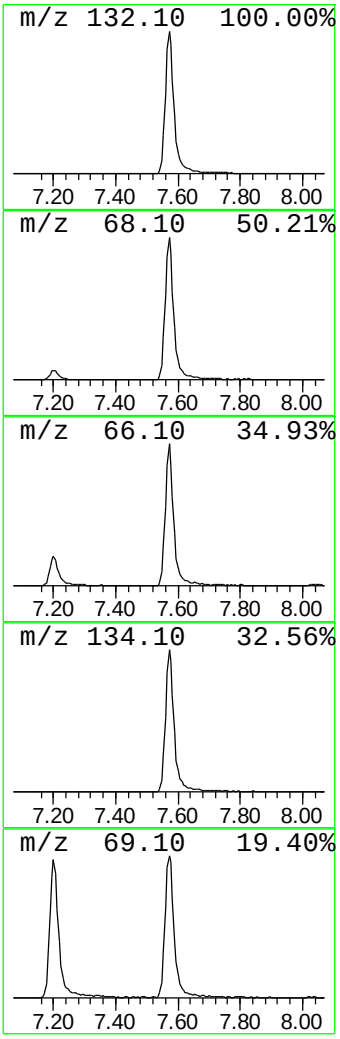
****

Peak Number 2 unknown7.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.57	89.64 ng	1152750	1,4-Dichlorobenzene-d4	8.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	13





Library Search Compound Report

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Data File : BG037051.D
Acq On : 28 Sep 2018 15:22
Operator : JU/SJ
Sample : J5099-01
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 7211975

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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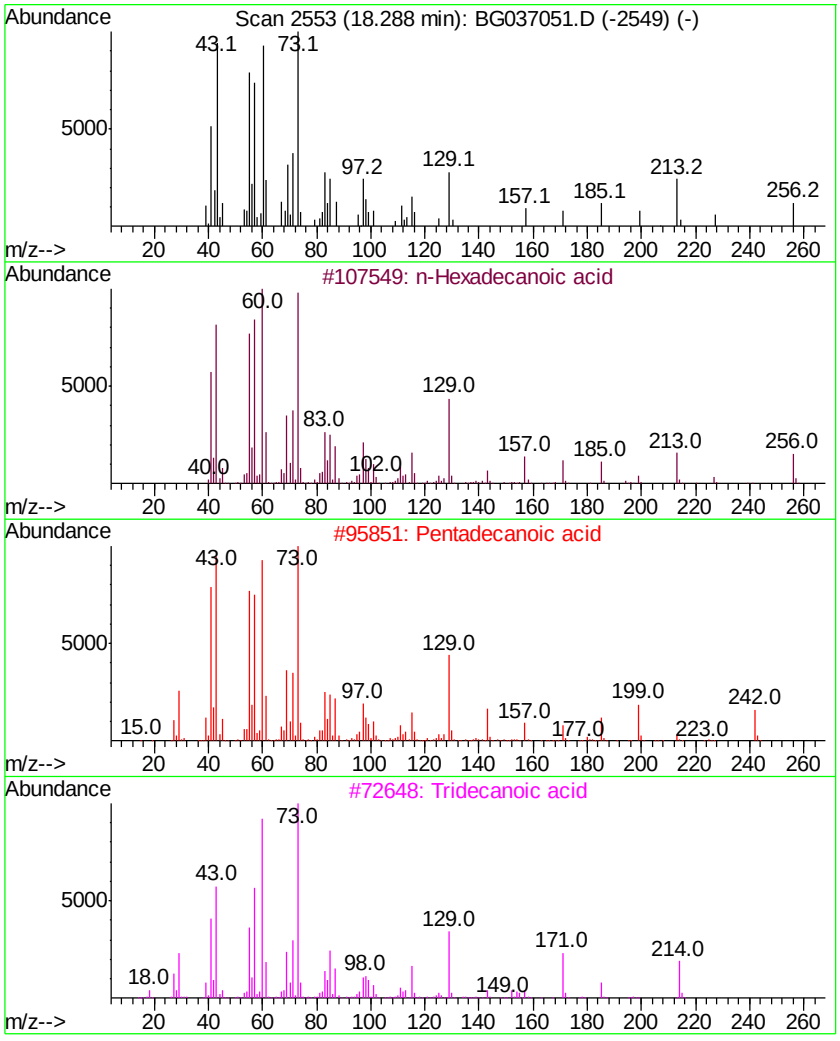
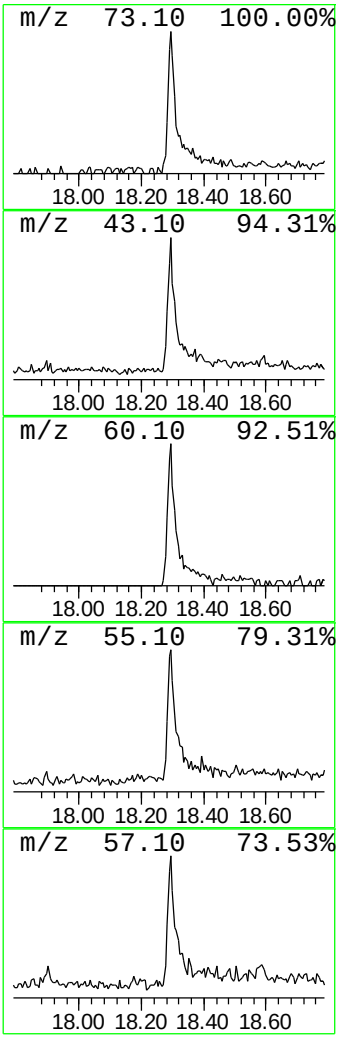
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.29	2.85 ng	96511	Phenanthrene-d10	17.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	53





Library Search Compound Report

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Data File : BG037051.D
Acq On : 28 Sep 2018 15:22
Operator : JU/SJ
Sample : J5099-01
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 7211975

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.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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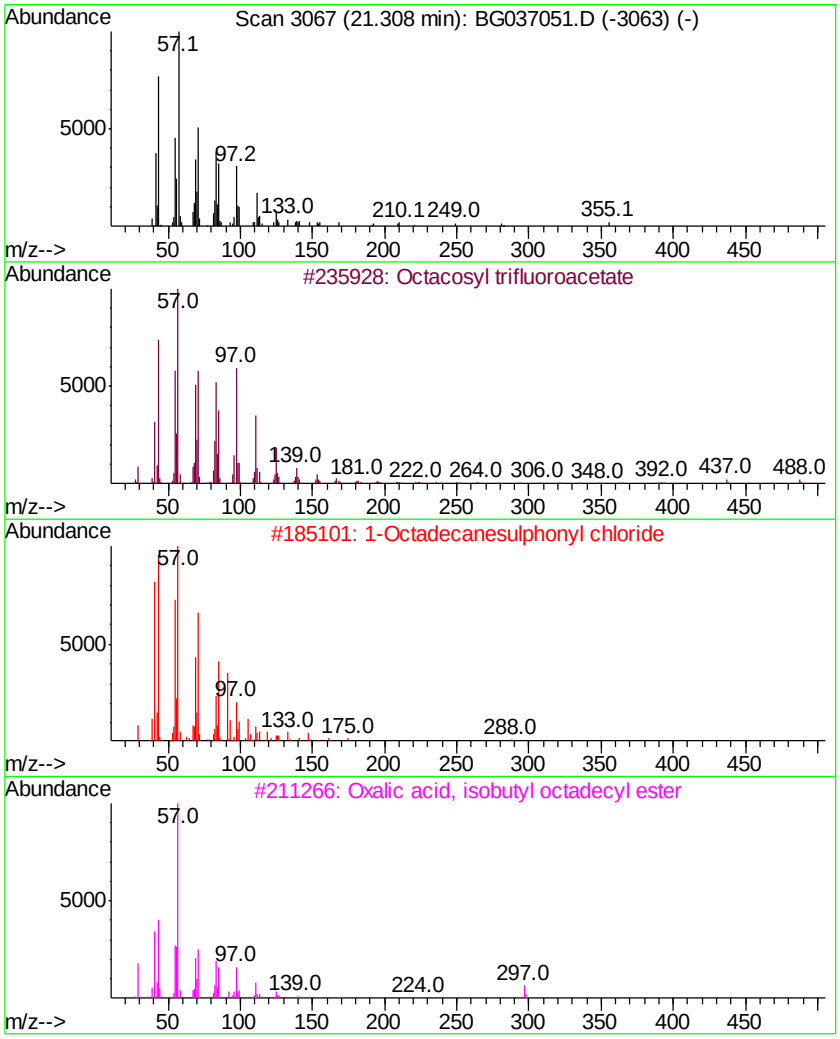
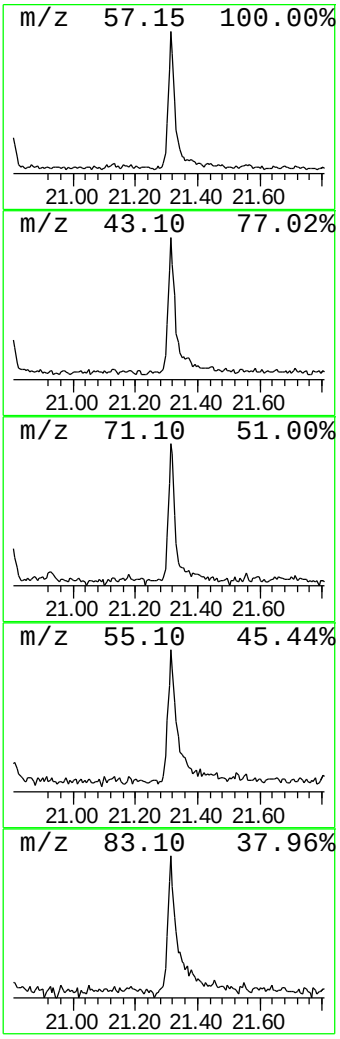
Peak Number 5 Octacosyl trifluoroacetate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.31	4.08 ng	164956	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	90
2	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	80
3	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	68
4	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	68
5	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	68





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG092718\
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Acq On : 28 Sep 2018 15:22
Operator : JU/SJ
Sample : J5099-01
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 7211975

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.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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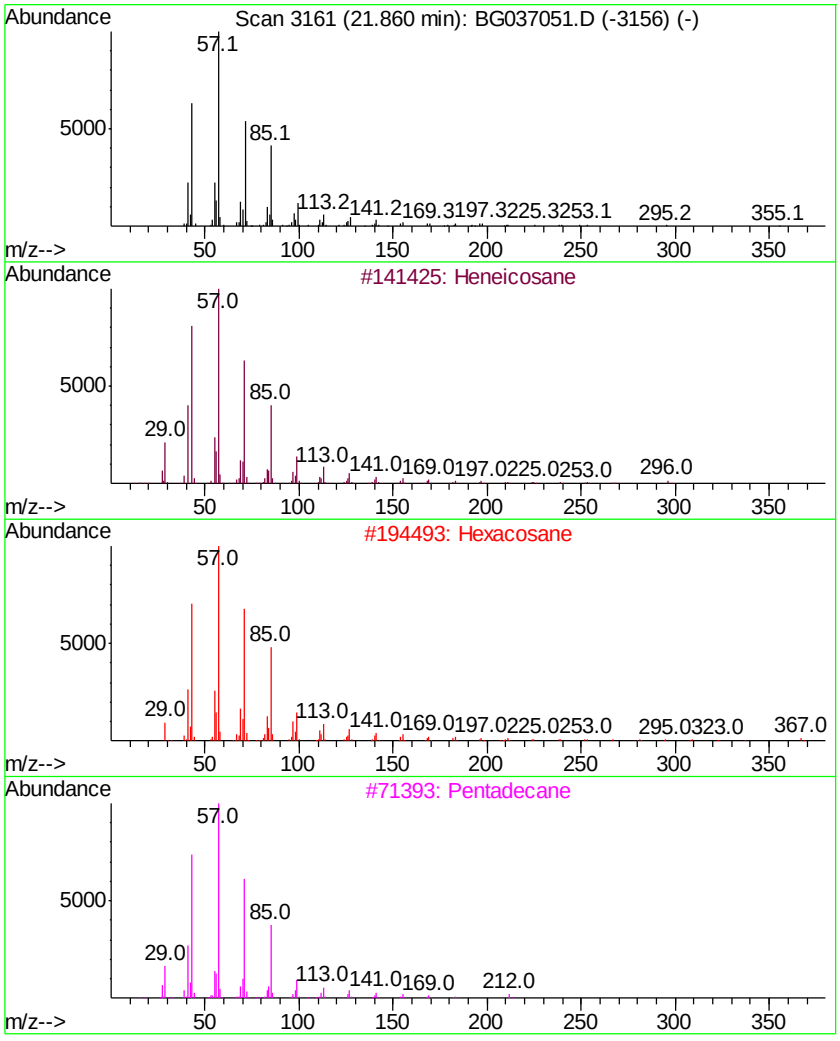
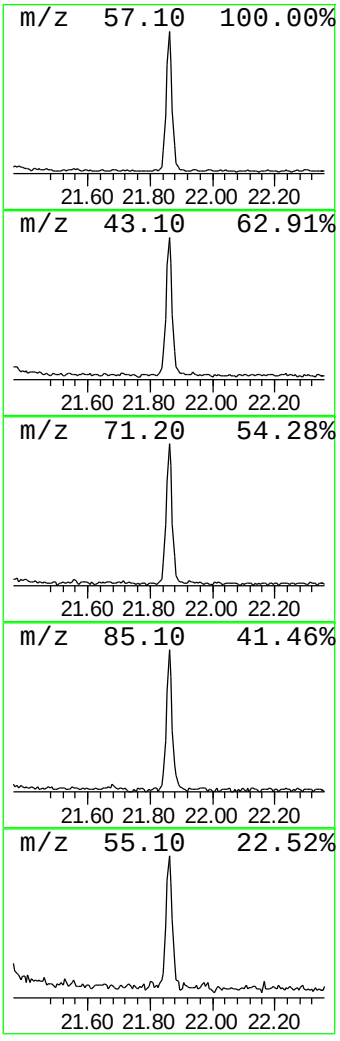
Peak Number 6 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.86	4.18 ng	168854	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	90
3	Pentadecane	212	C15H32	000629-62-9	87
4	Hexadecane	226	C16H34	000544-76-3	87
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG092718\
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Acq On : 28 Sep 2018 15:22
Operator : JU/SJ
Sample : J5099-01
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 7211975

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.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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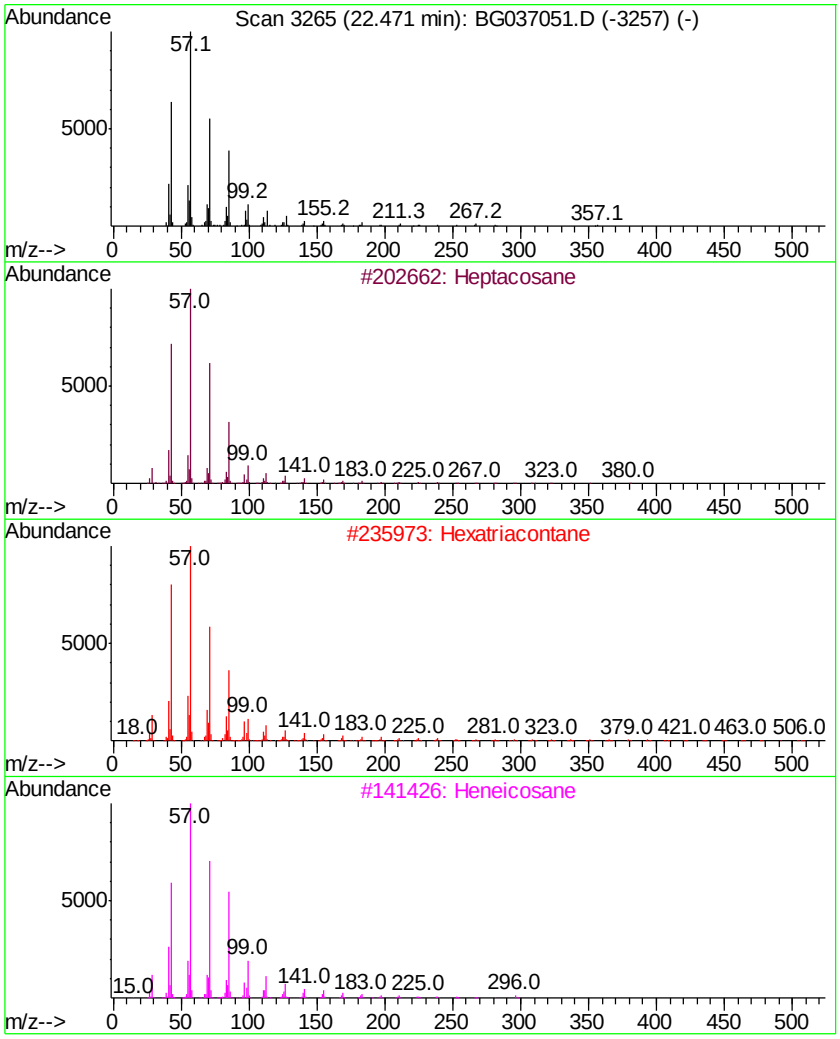
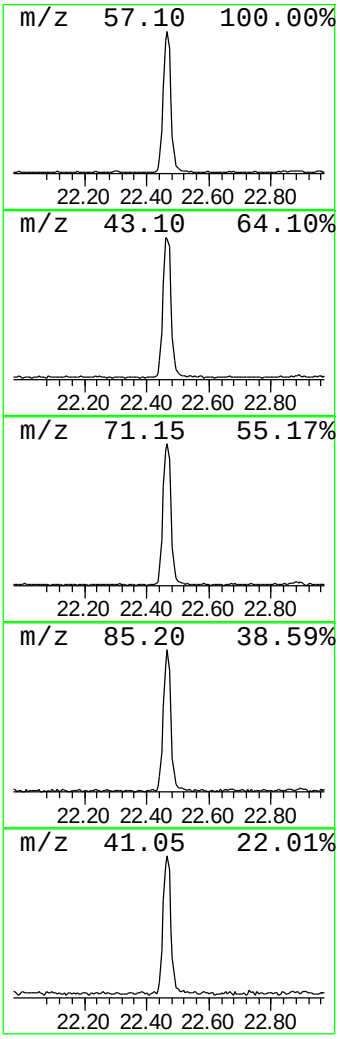
Peak Number 7 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.47	9.79 ng	395383	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Hexatriacontane	507	C36H74	000630-06-8	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	Tetracosane	338	C24H50	000646-31-1	90





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Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 7211975

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.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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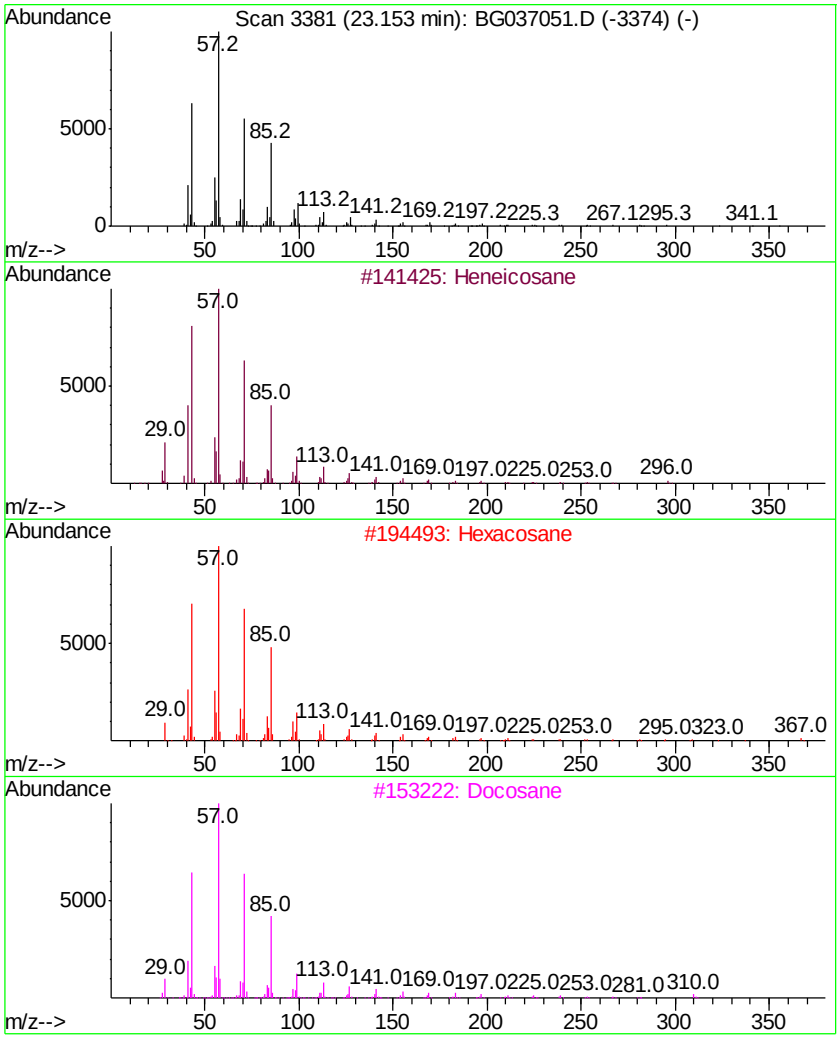
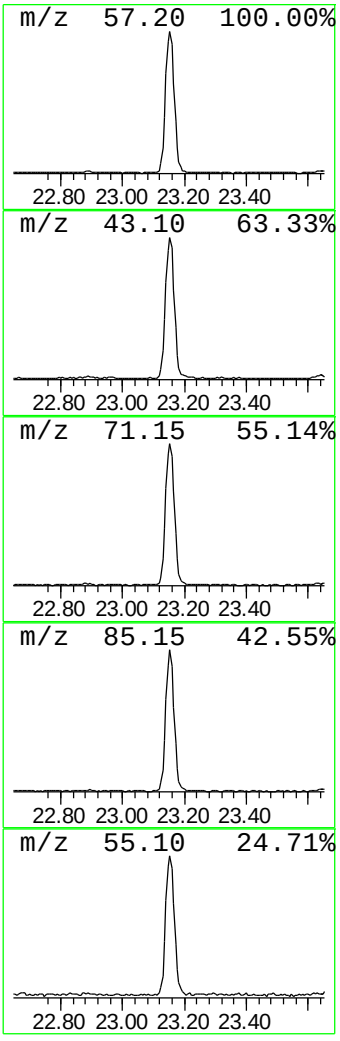
Peak Number 8 Docosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.15	16.84 ng	680367	Chrysene-d12	21.68

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	Docosane	310	C22H46	000629-97-0	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	3,5-Dimethyldodecane	198	C14H30	107770-99-0	87





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Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 7211975

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

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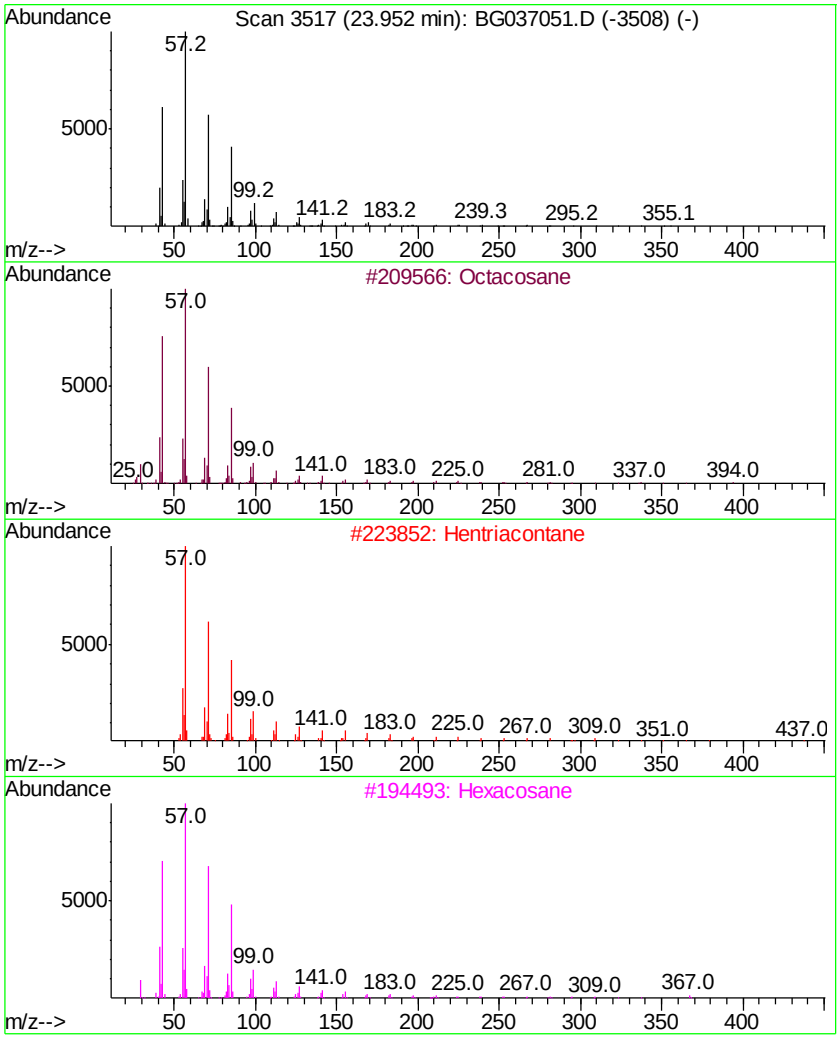
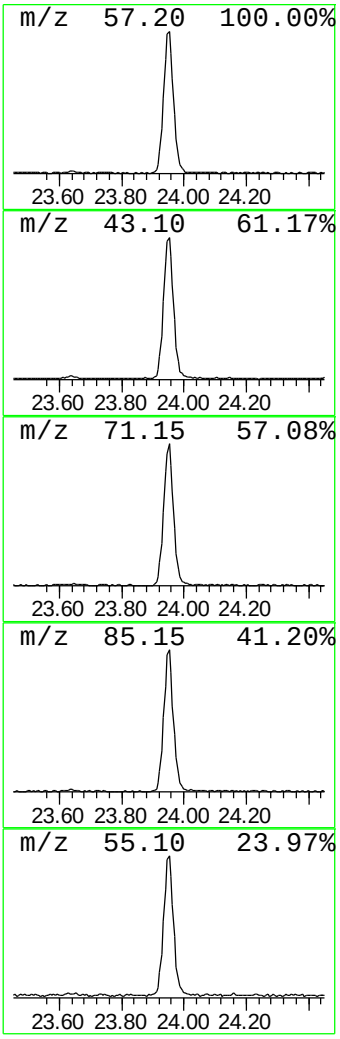
Peak Number 9 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.95	10.12 ng	872438	Perylene-d12	24.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hentriacontane	437	C31H64	000630-04-6	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Heneicosane	296	C21H44	000629-94-7	91





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Instrument : BNA_G
ClientSampleId : 7211975

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

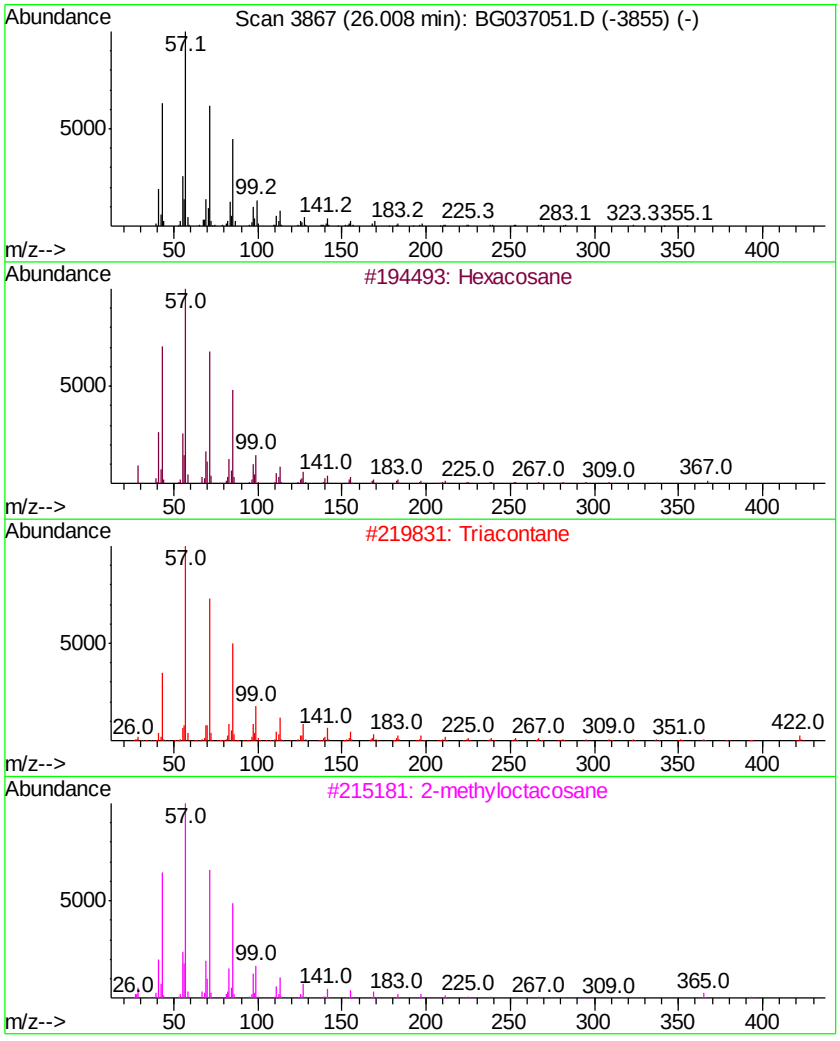
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

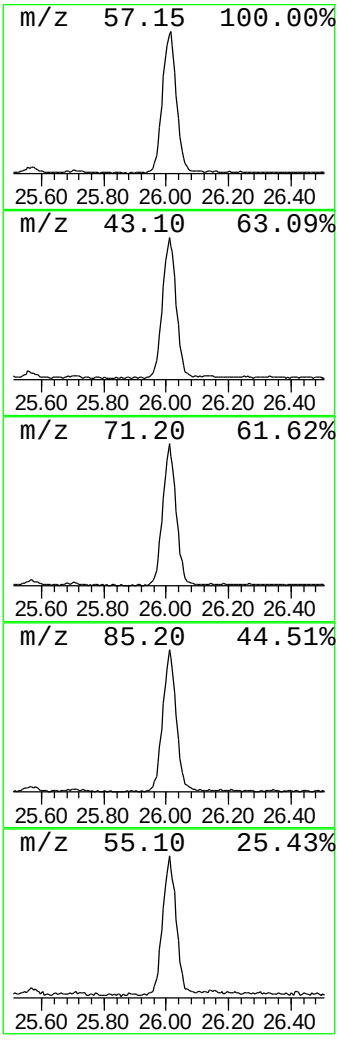
****

Peak Number 10 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.01	9.20 ng	793349	Perylene-d12	24.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	94
2	Triacontane	422	C30H62	000638-68-6	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Tetratetracontane	619	C44H90	007098-22-8	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG092718\
Data File : BG037051.D
Acq On : 28 Sep 2018 15:22
Operator : JU/SJ
Sample : J5099-01
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 7211975

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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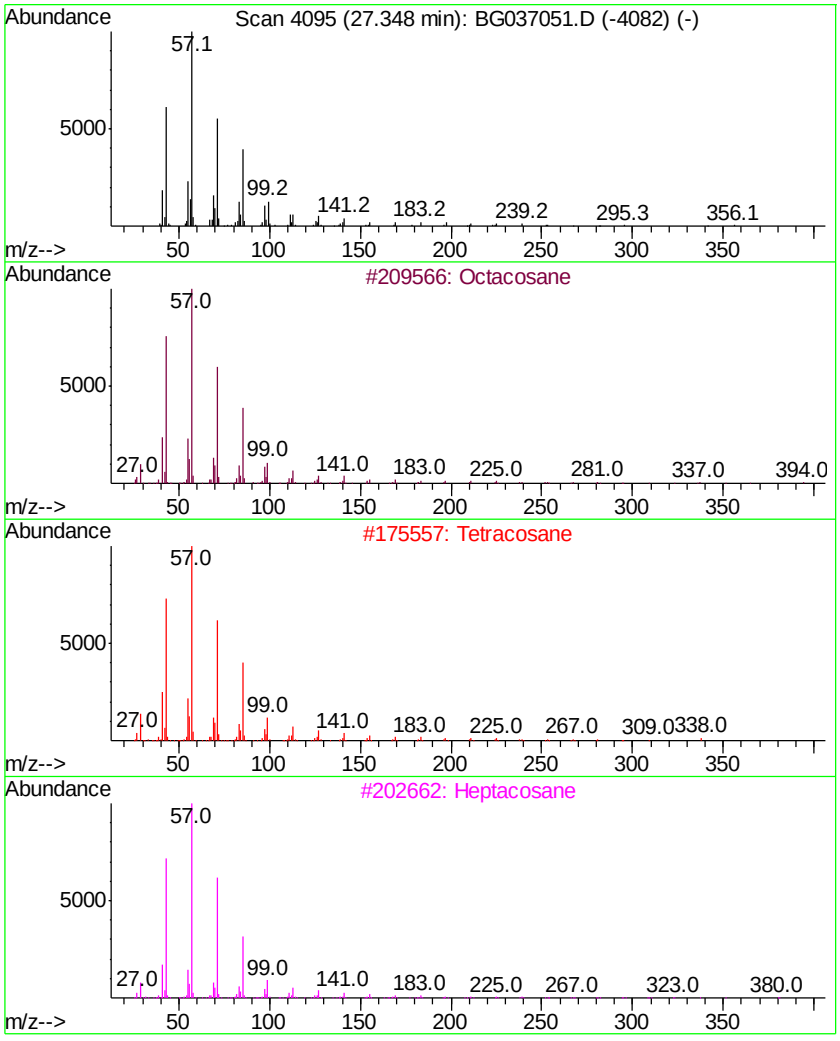
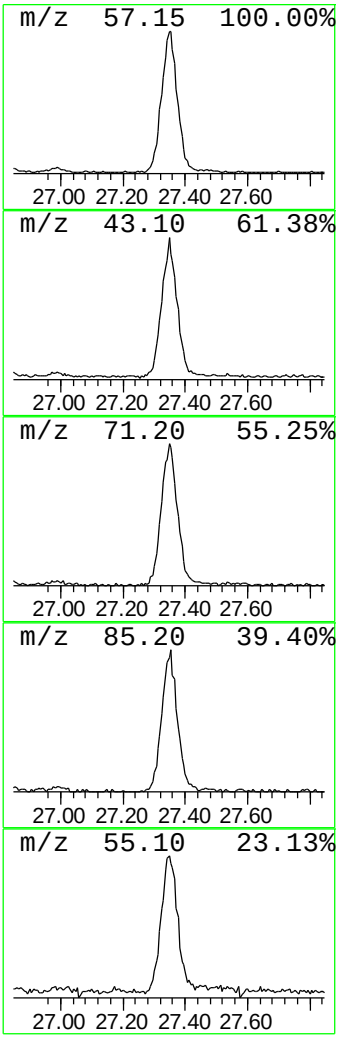
****

Peak Number 11 Sulfurous acid, butyl tetra... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.35	5.66 ng	487528	Perylene-d12	24.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	91
5	Hexacosane	366	C26H54	000630-01-3	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG092718\
Data File : BG037051.D
Acq On : 28 Sep 2018 15:22
Operator : JU/SJ
Sample : J5099-01
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 7211975

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

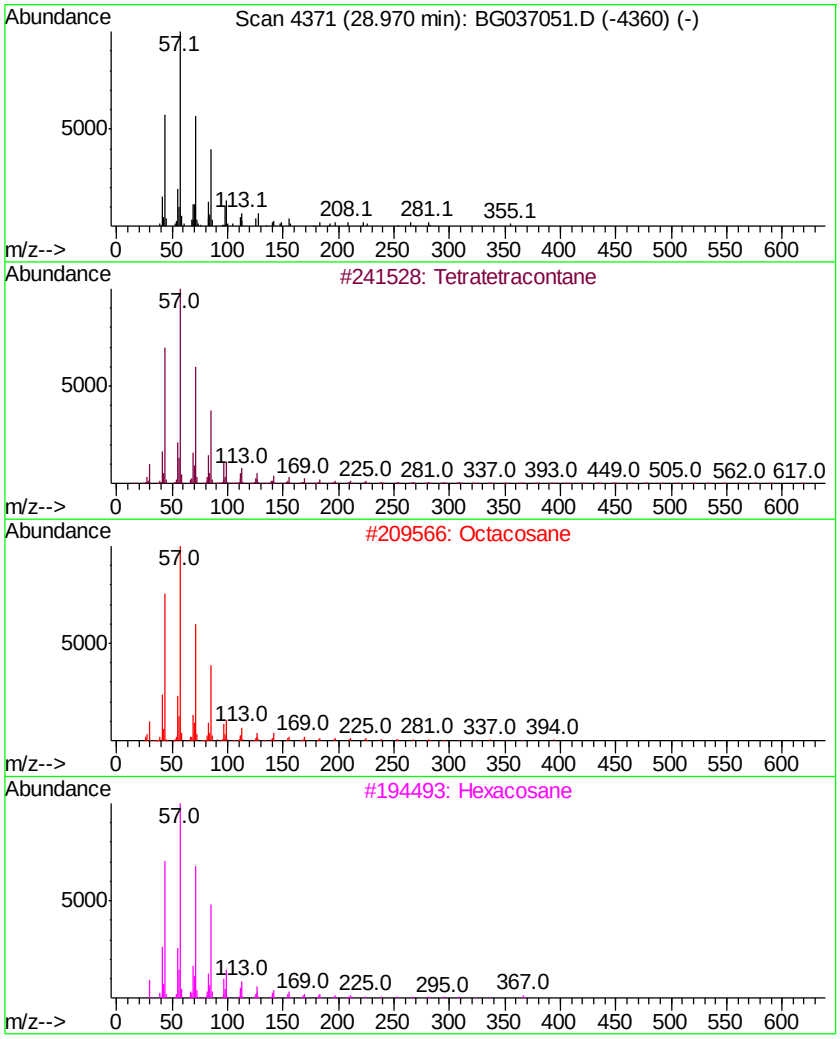
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

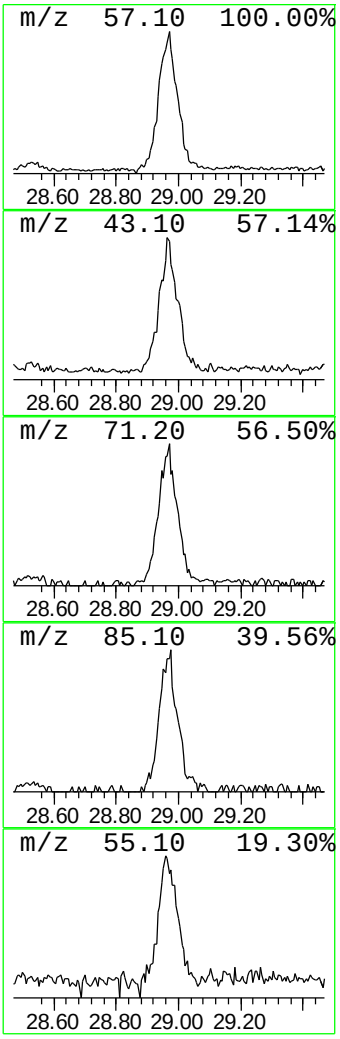
****

Peak Number 12 Tetratetracontane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.97	2.22 ng	191750	Perylene-d12	24.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	90
2	Octacosane	394	C28H58	000630-02-4	90
3	Hexacosane	366	C26H54	000630-01-3	90
4	Tetracosane	338	C24H50	000646-31-1	87
5	Heptadecane	240	C17H36	000629-78-7	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG092718\
Data File : BG037051.D
Acq On : 28 Sep 2018 15:22
Operator : JU/SJ
Sample : J5099-01
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 7211975

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.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
2-Pentanone, 4-hy...	5.15	3.5	ng	45200	1	8.04	257197	20.0
unknown7.57	7.57	89.6	ng	1152750	1	8.04	257197	20.0
n-Hexadecanoic acid	18.29	2.9	ng	96511	4	17.41	676268	20.0
Octacosyl trifluo...	21.31	4.1	ng	164956	5	21.68	807847	20.0
Heneicosane	21.86	4.2	ng	168854	5	21.68	807847	20.0
Heptacosane	22.47	9.8	ng	395383	5	21.68	807847	20.0
Docosane	23.15	16.8	ng	680367	5	21.68	807847	20.0
Octacosane	23.95	10.1	ng	872438	6	24.87	1724030	20.0
Hexacosane	26.01	9.2	ng	793349	6	24.87	1724030	20.0
Sulfurous acid, b...	27.35	5.7	ng	487528	6	24.87	1724030	20.0
Tetratetracontane	28.97	2.2	ng	191750	6	24.87	1724030	20.0