LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102618\
Data File : BG037590.D
Acq On : 26 Oct 2018 21:07
Operator : JU/SJ
Sample : J5662-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 102318-DBRI-F-D-B

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-BG101818.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	5.639	393	400	410	rBV	294683	492765	11.78%	2.612%
2	7.243	665	673	687	rBV2	206430	542033	12.96%	2.873%
3	7.625	730	738	747	rBV	541504	957578	22.89%	5.075%
4	8.101	811	819	833	rBV	190985	329090	7.87%	1.744%
5	8.424	866	874	884	rVB	700280	1268161	30.32%	6.721%
6	9.282	1011	1020	1032	rBV	632192	1170238	27.98%	6.202%
7	10.921	1292	1299	1308	rBV	258834	484022	11.57%	2.565%
8	13.359	1702	1714	1721	rBV	1765825	2844245	68.00%	15.075%
9	14.176	1848	1853	1859	rBV	61359	93133	2.23%	0.494%
10	14.734	1940	1948	1959	rBV2	465525	752829	18.00%	3.990%
11	16.221	2194	2201	2215	rBV	926241	1441142	34.45%	7.638%
12	17.484	2409	2416	2426	rBV	608577	964686	23.06%	5.113%
13	18.336	2556	2561	2572	rBV	72624	119697	2.86%	0.634%
14	19.605	2773	2777	2781	rBV2	33141	45735	1.09%	0.242%
15	20.081	2852	2858	2866	rBV	3020787	4182976	100.00%	22.170%
16	21.373	3073	3078	3089	rBV	78812	181245	4.33%	0.961%
17	21.767	3137	3145	3159	rBV	540791	999827	23.90%	5.299%
18	21.920	3167	3171	3179	rVB3	35810	53689	1.28%	0.285%
19	22.543	3271	3277	3284	rBV2	61012	104496	2.50%	0.554%
20	23.253	3391	3398	3407	rBV2	84154	170851	4.08%	0.906%
21	24.082	3532	3539	3550	rBV2	91896	218498	5.22%	1.158%
22	25.098	3697	3712	3726	rBV3	305018	1166605	27.89%	6.183%
23	26.238	3897	3906	3915	rVB3	60789	183374	4.38%	0.972%
24	27.637	4137	4144	4156	rVB6	29986	100818	2.41%	0.534%

Sum of corrected areas: 18867733

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102618\
Data File : BG037590.D
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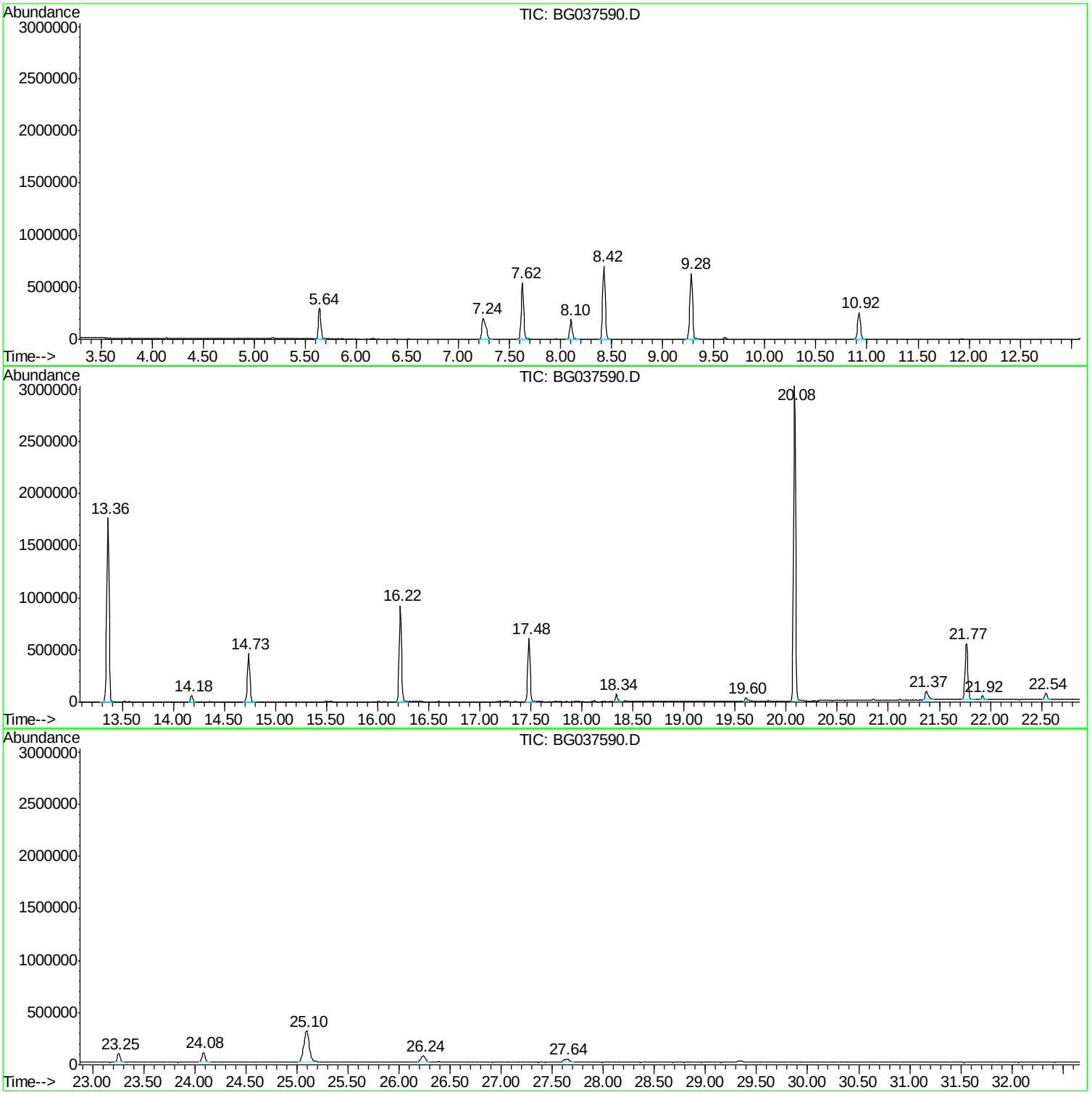
Operator : JU/SJ
Sample : J5662-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 102318-DBRI-F-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.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\BG102618\
Data File : BG037590.D
Acq On : 26 Oct 2018 21:07
Operator : JU/SJ
Sample : J5662-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 102318-DBRI-F-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.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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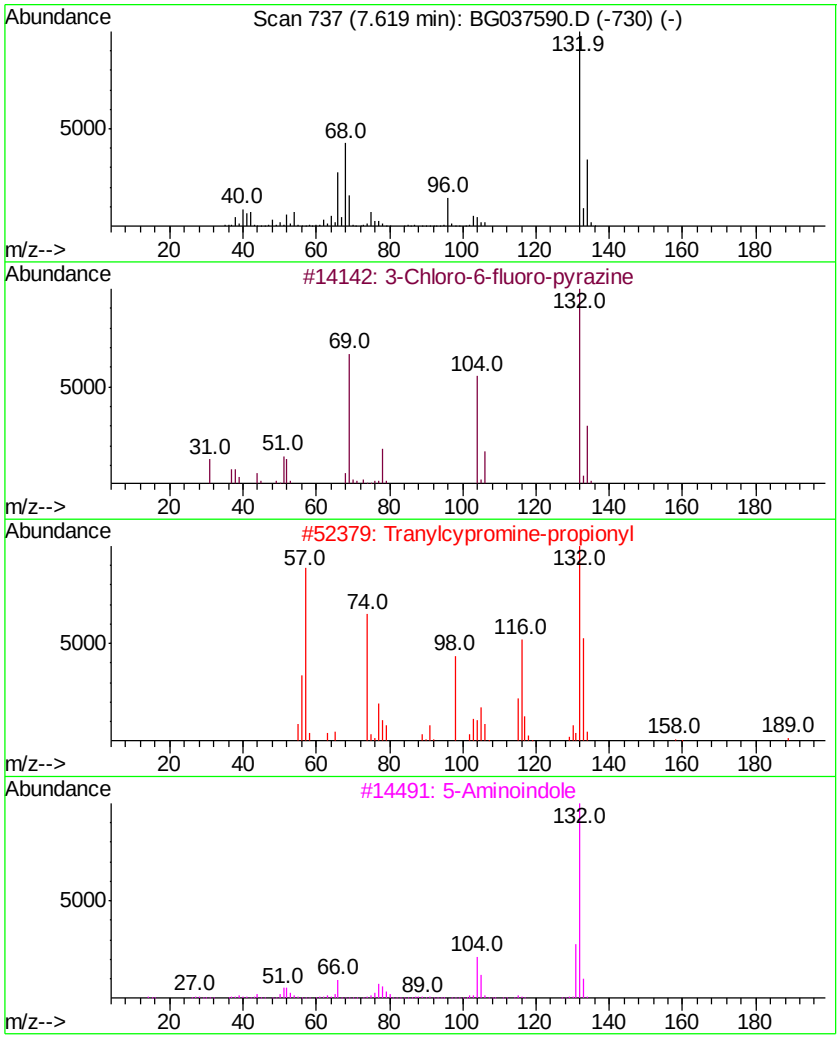
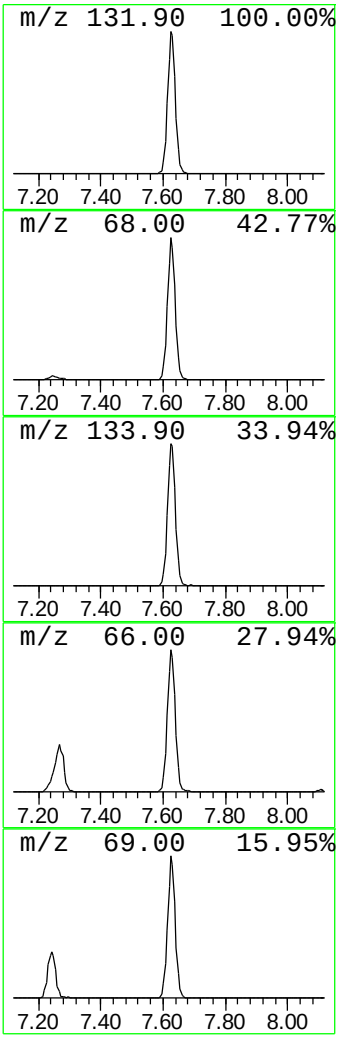
Peak Number 1 unknown7.62 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.62	58.20 ng	957578	1,4-Dichlorobenzene-d4	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	5-Aminoindole	132	C8H8N2	005192-03-0	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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Data File : BG037590.D
Acq On : 26 Oct 2018 21:07
Operator : JU/SJ
Sample : J5662-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 102318-DBRI-F-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.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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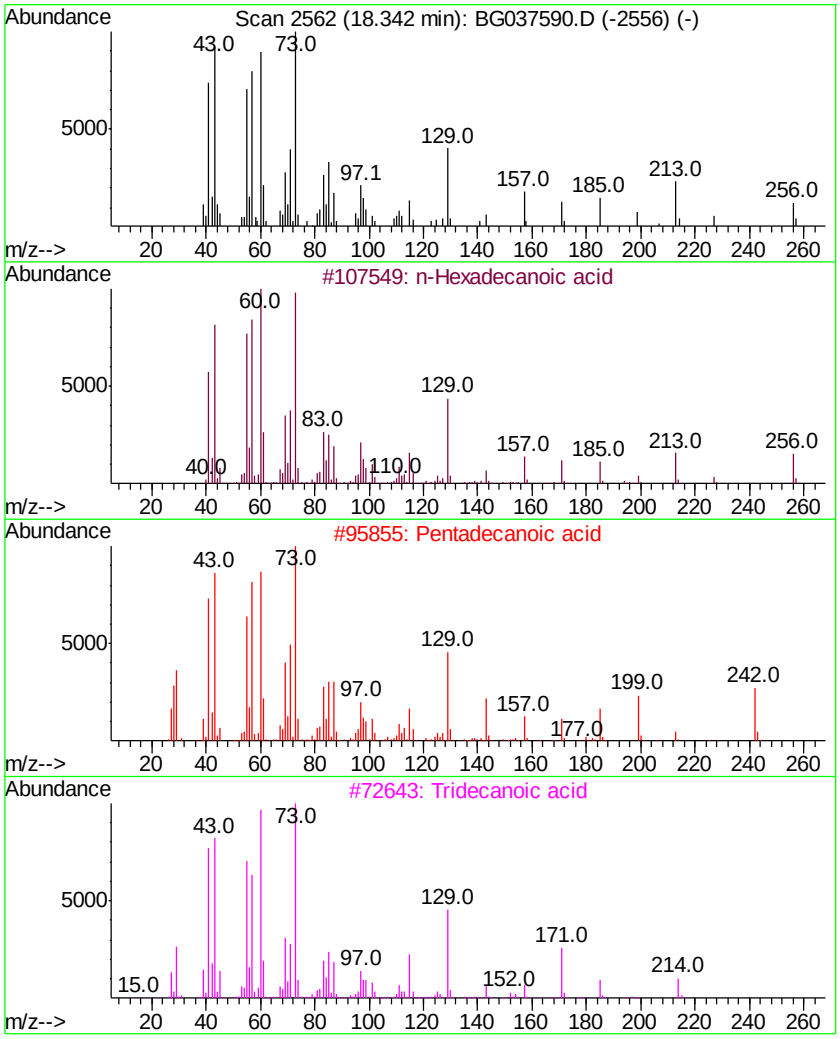
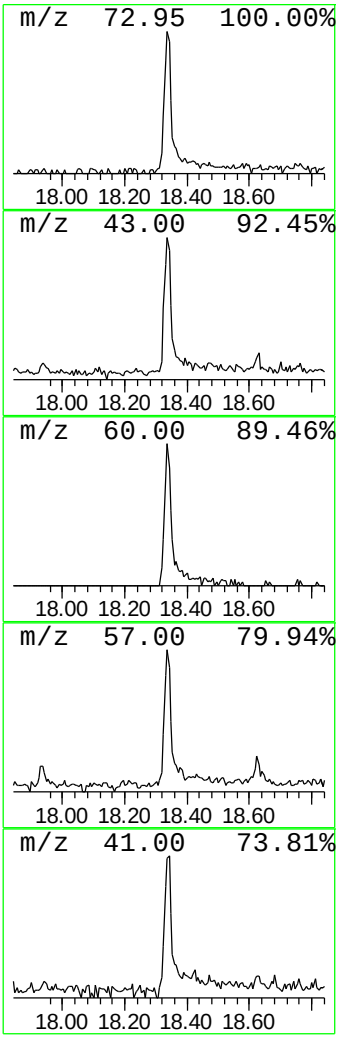
Peak Number 3 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.34	2.48 ng	119697	Phenanthrene-d10	17.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3	Tridecanoic acid	214	C13H26O2	000638-53-9	70
4	n-Decanoic acid	172	C10H20O2	000334-48-5	47
5	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	30





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102618\
Data File : BG037590.D
Acq On : 26 Oct 2018 21:07
Operator : JU/SJ
Sample : J5662-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 102318-DBRI-F-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.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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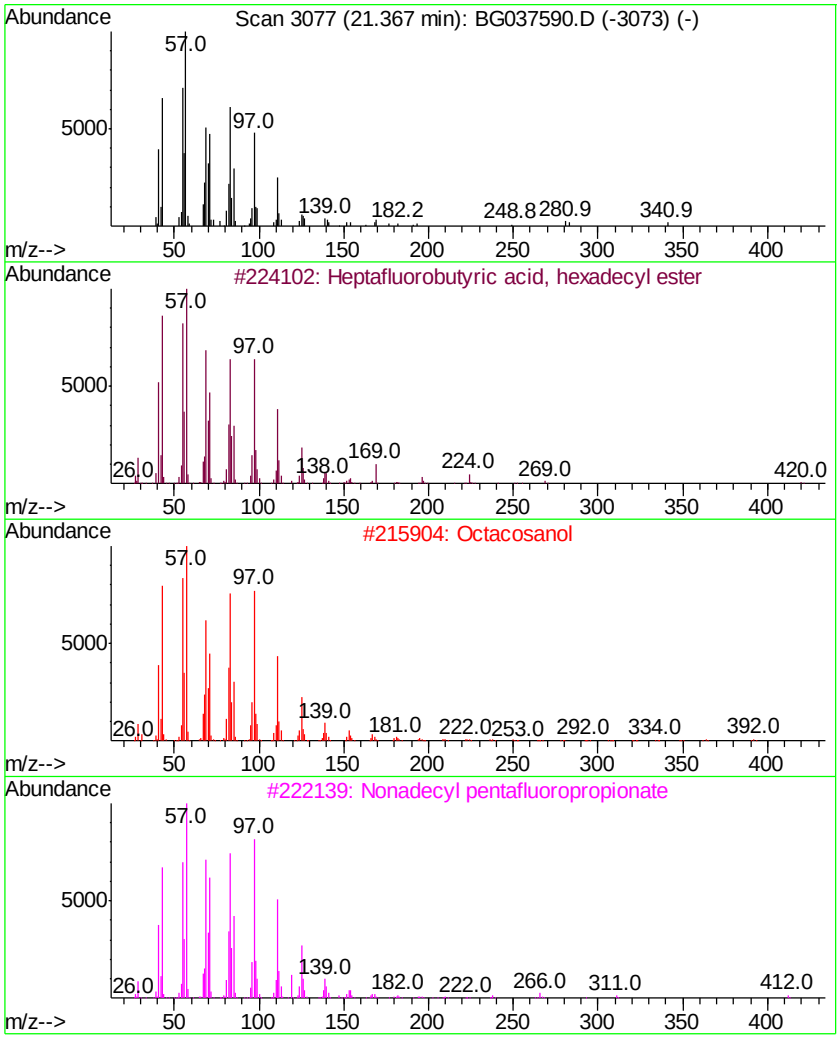
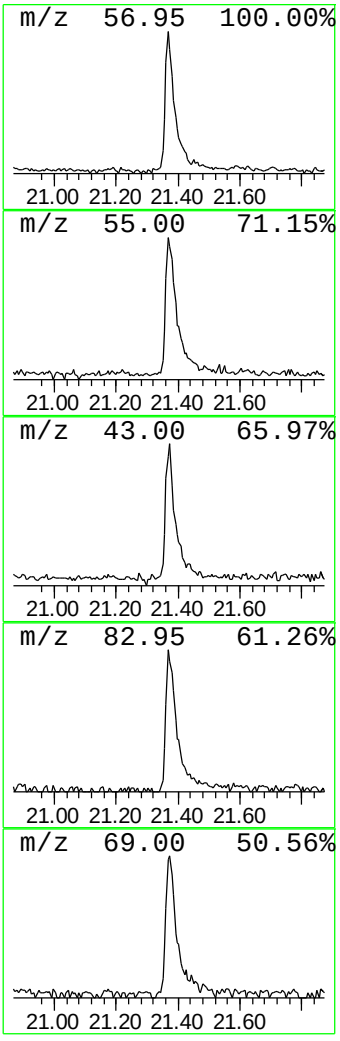
Peak Number 4 Heptafluorobutyric acid, he... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.37	3.63 ng	181245	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
2	Octacosanol	410	C28H58O	000557-61-9	91
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4	1-Heptacosanol	396	C27H56O	002004-39-9	91
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102618\
Data File : BG037590.D
Acq On : 26 Oct 2018 21:07
Operator : JU/SJ
Sample : J5662-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 102318-DBRI-F-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.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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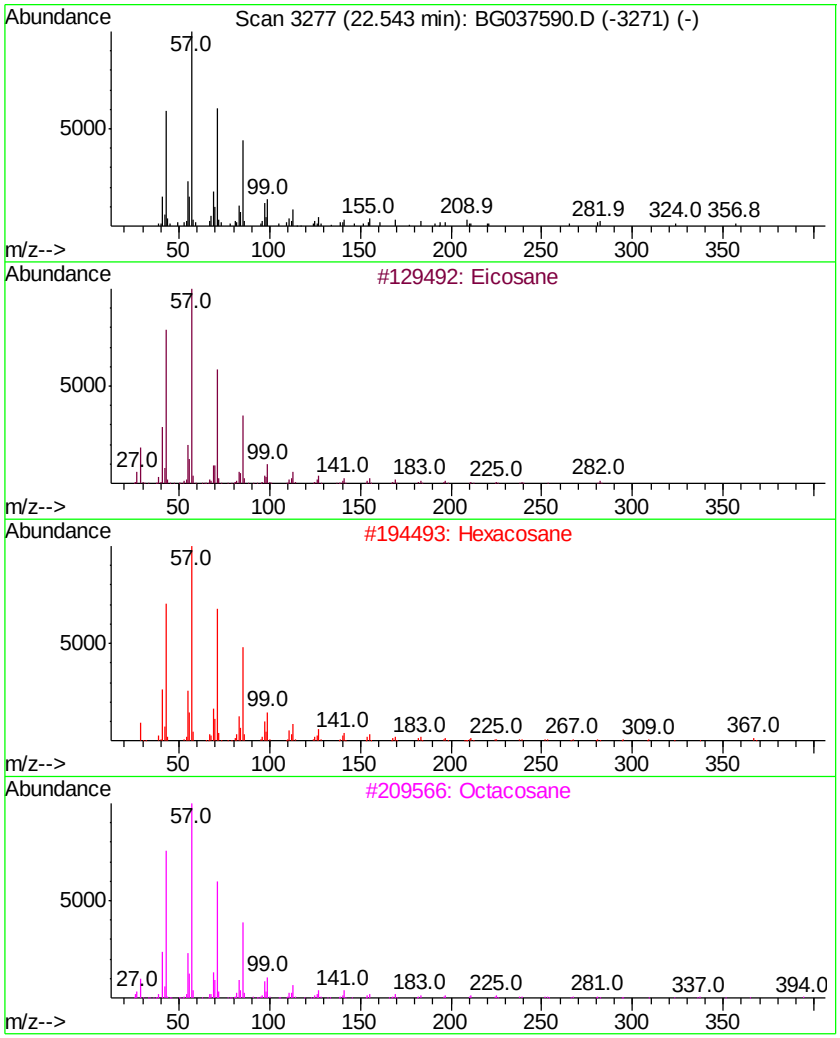
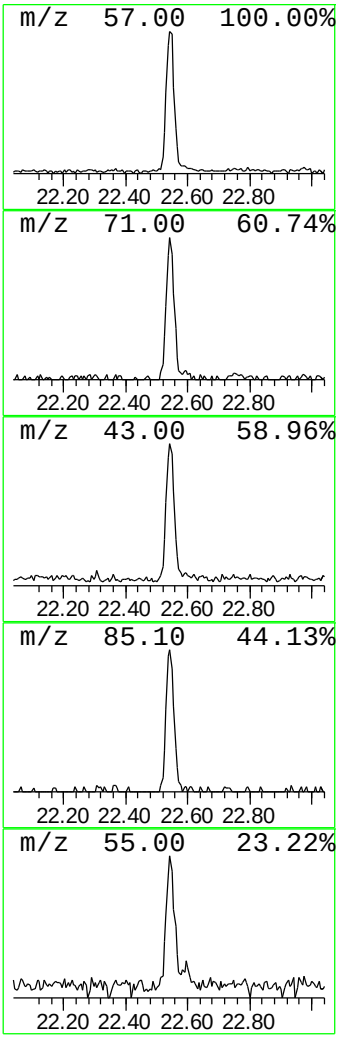
Peak Number 5 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.54	2.09 ng	104496	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Hexacosane	366	C26H54	000630-01-3	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Tricosane	324	C23H48	000638-67-5	87
5	Tetracosane	338	C24H50	000646-31-1	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102618\
Data File : BG037590.D
Acq On : 26 Oct 2018 21:07
Operator : JU/SJ
Sample : J5662-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 102318-DBRI-F-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

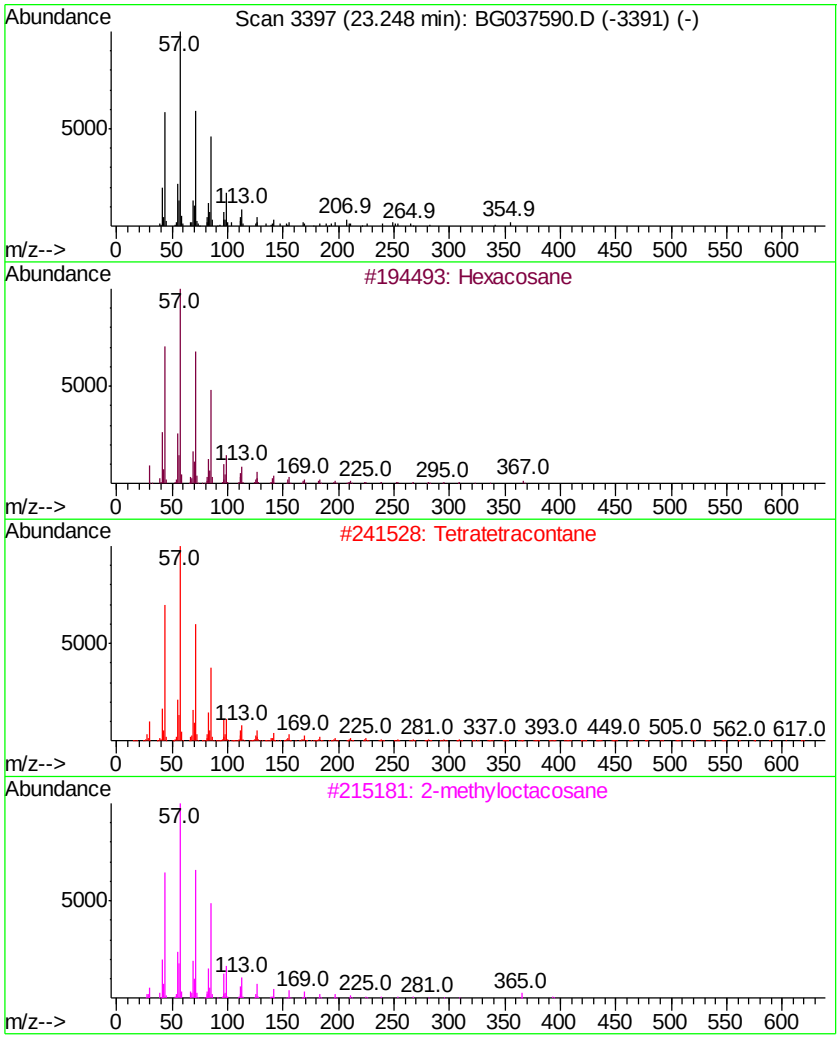
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

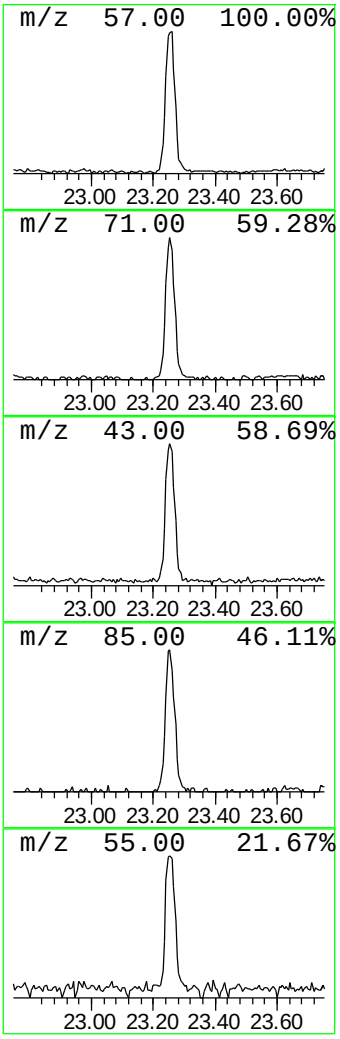
****

Peak Number 6 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.25	3.42 ng	170851	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Tetratetracontane	619	C44H90	007098-22-8	90
3	2-methyloctacosane	408	C29H60	1000376-72-8	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Octacosane	394	C28H58	000630-02-4	90





Library Search Compound Report

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Sample : J5662-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 102318-DBRI-F-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

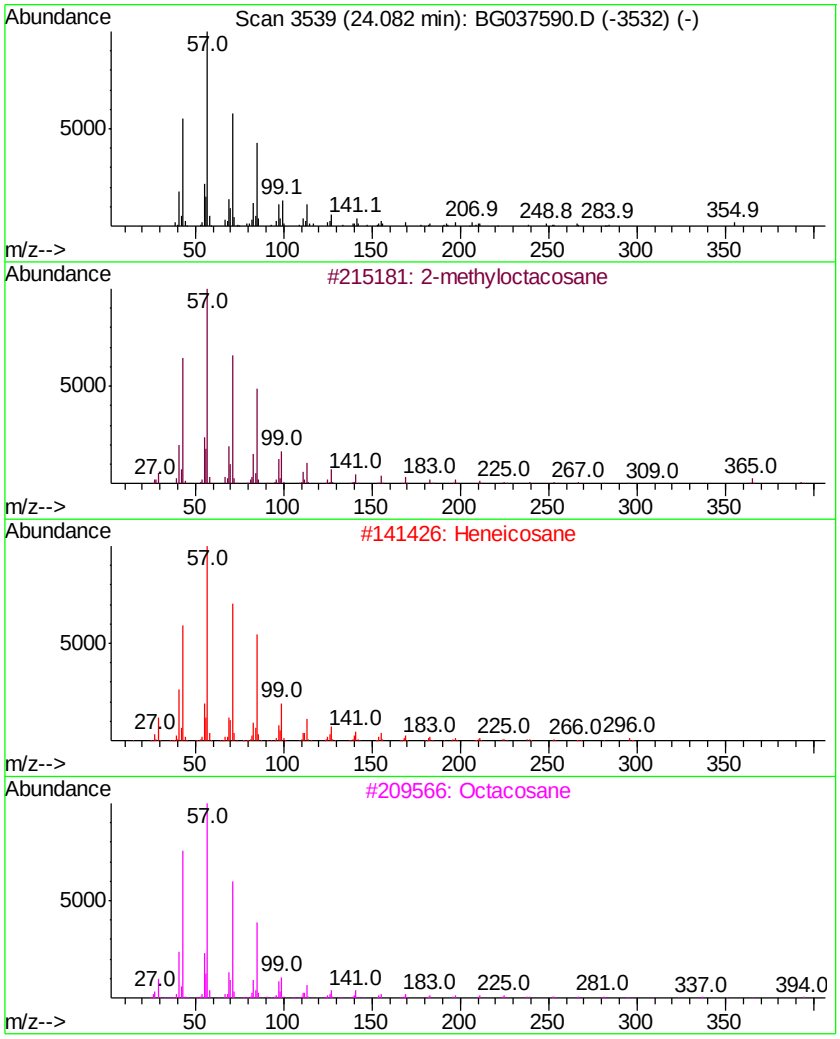
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

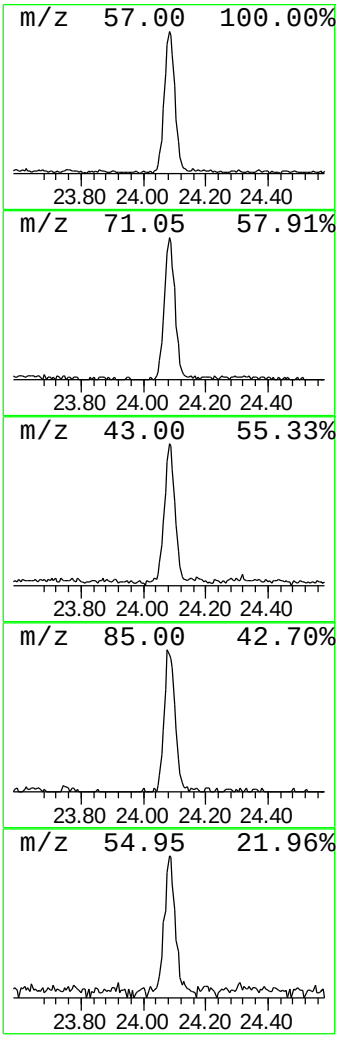
****

Peak Number 7 2-methyloctacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.08	3.75 ng	218498	Perylene-d12	25.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	90
2	Heneicosane	296	C21H44	000629-94-7	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	Heptacosane	380	C27H56	000593-49-7	87





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Instrument : BNA_G
ClientSampleId : 102318-DBRI-F-D-B

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

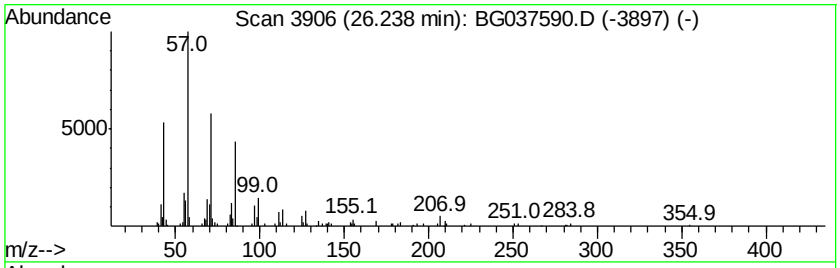
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

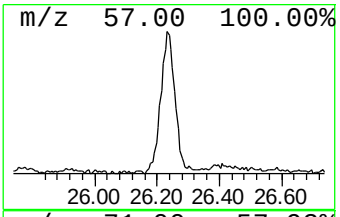
****

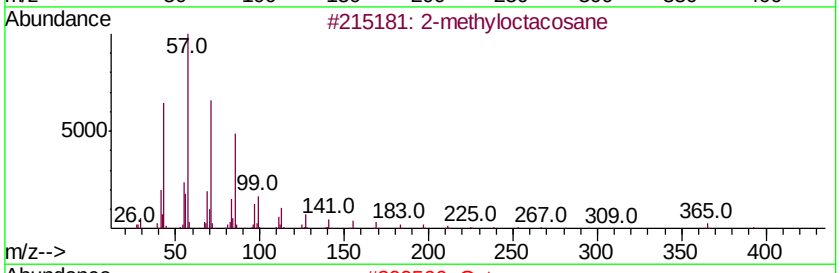
Peak Number 8 Octacosane Concentration Rank 6

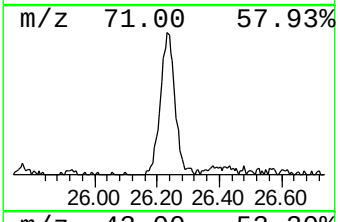
R.T.	EstConc	Area	Relative to ISTD	R.T.
26.24	3.14 ng	183374	Perylene-d12	25.10

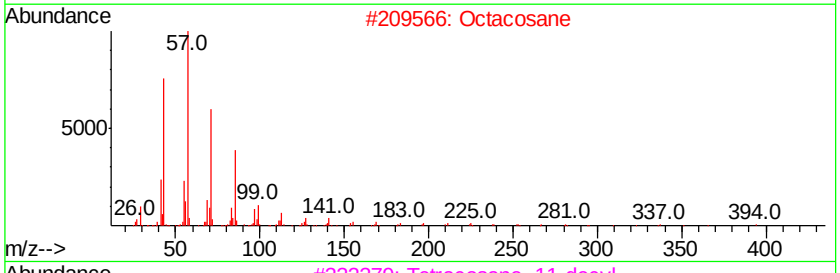
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	90
2	Octacosane	394	C28H58	000630-02-4	90
3	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	87
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5	Docosane, 11-decyl-	451	C32H66	055401-55-3	87

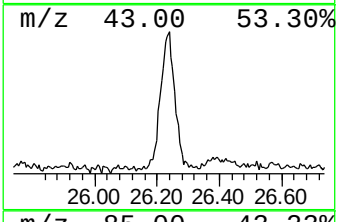


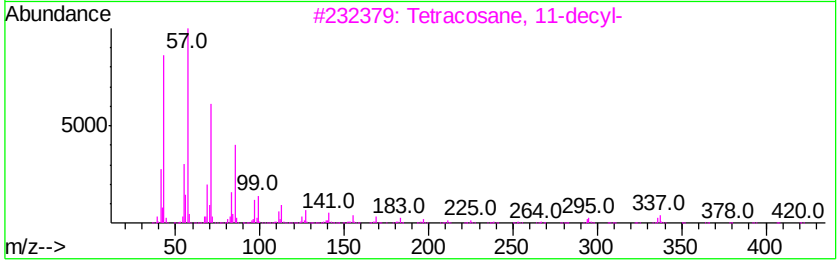


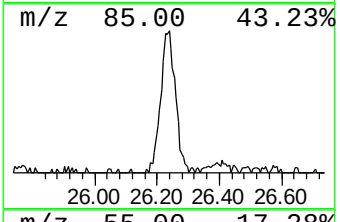


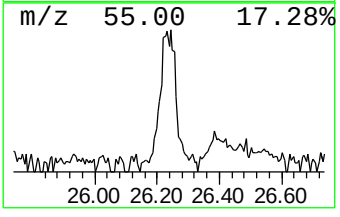












Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG102618\
Data File : BG037590.D
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Operator : JU/SJ
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Instrument : BNA_G
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.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
unknown7.62	7.62	58.2	ng	957578	1	8.10	329090	20.0
n-Hexadecanoic acid	18.34	2.5	ng	119697	4	17.48	964686	20.0
Heptafluorobutyri...	21.37	3.6	ng	181245	5	21.77	999827	20.0
Eicosane	22.54	2.1	ng	104496	5	21.77	999827	20.0
Hexacosane	23.25	3.4	ng	170851	5	21.77	999827	20.0
2-methyloctacosane	24.08	3.8	ng	218498	6	25.10	1166610	20.0
Octacosane	26.24	3.1	ng	183374	6	25.10	1166610	20.0