LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111319\
Data File : BG043627.D
Acq On : 14 Nov 2019 00:32
Operator : JU
Sample : K5804-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-MW-QA-2

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	3.158	8	12	27	rVB	357153	564595	21.27%	5.027%
2	4.709	268	276	286	rBV	86437	145169	5.47%	1.293%
3	5.596	420	427	437	rBV	182320	331651	12.49%	2.953%
4	7.200	690	700	712	rBV2	121666	273381	10.30%	2.434%
5	7.541	751	758	773	rBV	299558	560048	21.10%	4.987%
6	7.993	829	835	843	rBV	83708	152244	5.74%	1.356%
7	8.322	883	891	900	rBV	355527	642872	24.22%	5.724%
8	9.162	1026	1034	1047	rBV	236374	479988	18.08%	4.274%
9	10.807	1305	1314	1325	rBV	82977	185241	6.98%	1.649%
10	13.252	1720	1730	1743	rBV	846634	1390349	52.38%	12.380%
11	14.080	1865	1871	1883	rBV	24359	48692	1.83%	0.434%
12	14.626	1958	1964	1978	rBV2	184034	313697	11.82%	2.793%
13	16.119	2211	2218	2232	rBV	466889	857918	32.32%	7.639%
14	17.376	2424	2432	2449	rBV	235023	426347	16.06%	3.796%
15	18.269	2578	2584	2592	rBV2	61057	99123	3.73%	0.883%
16	19.985	2869	2876	2889	rBV	1947576	2654348	100.00%	23.635%
17	21.283	3091	3097	3112	rBV6	42309	144856	5.46%	1.290%
18	21.636	3150	3157	3166	rBV	303175	543846	20.49%	4.843%
19	21.818	3183	3188	3193	rBV3	25142	47960	1.81%	0.427%
20	22.417	3284	3290	3294	rBV2	39661	64898	2.44%	0.578%
21	23.099	3399	3406	3412	rBV	57132	104420	3.93%	0.930%
22	23.287	3431	3438	3446	rBV	107786	200687	7.56%	1.787%
23	23.886	3534	3540	3547	rVB	59629	120901	4.55%	1.077%
24	24.820	3686	3699	3712	rBV2	238122	712157	26.83%	6.341%
25	25.919	3877	3886	3895	rVB5	34333	112411	4.23%	1.001%
26	27.253	4108	4113	4121	rVB7	19961	52572	1.98%	0.468%

Sum of corrected areas: 11230371

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111319\
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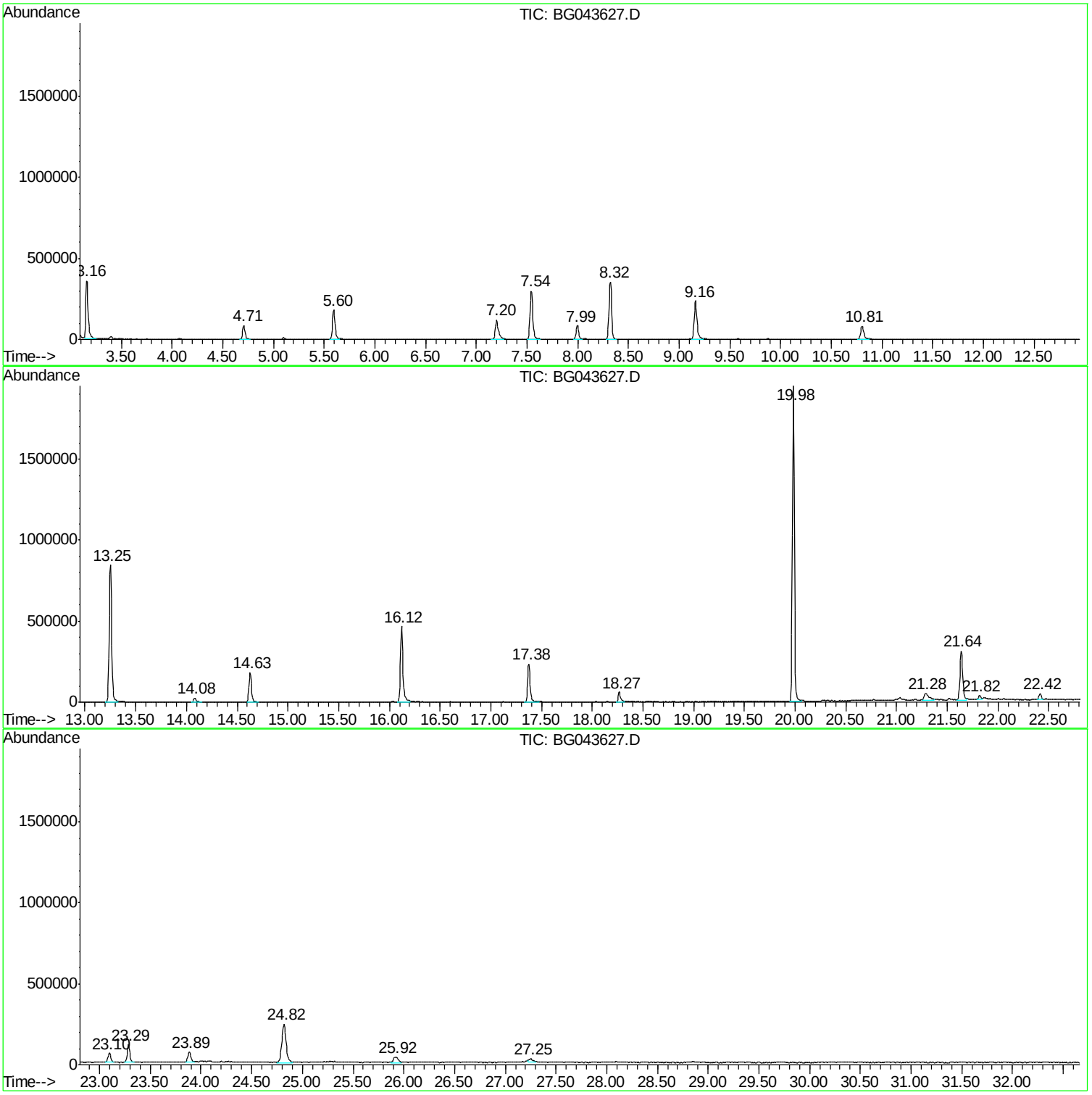
Sample : K5804-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TE-MW-QA-2

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\BG111319\
Data File : BG043627.D
Acq On : 14 Nov 2019 00:32
Operator : JU
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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-MW-QA-2

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

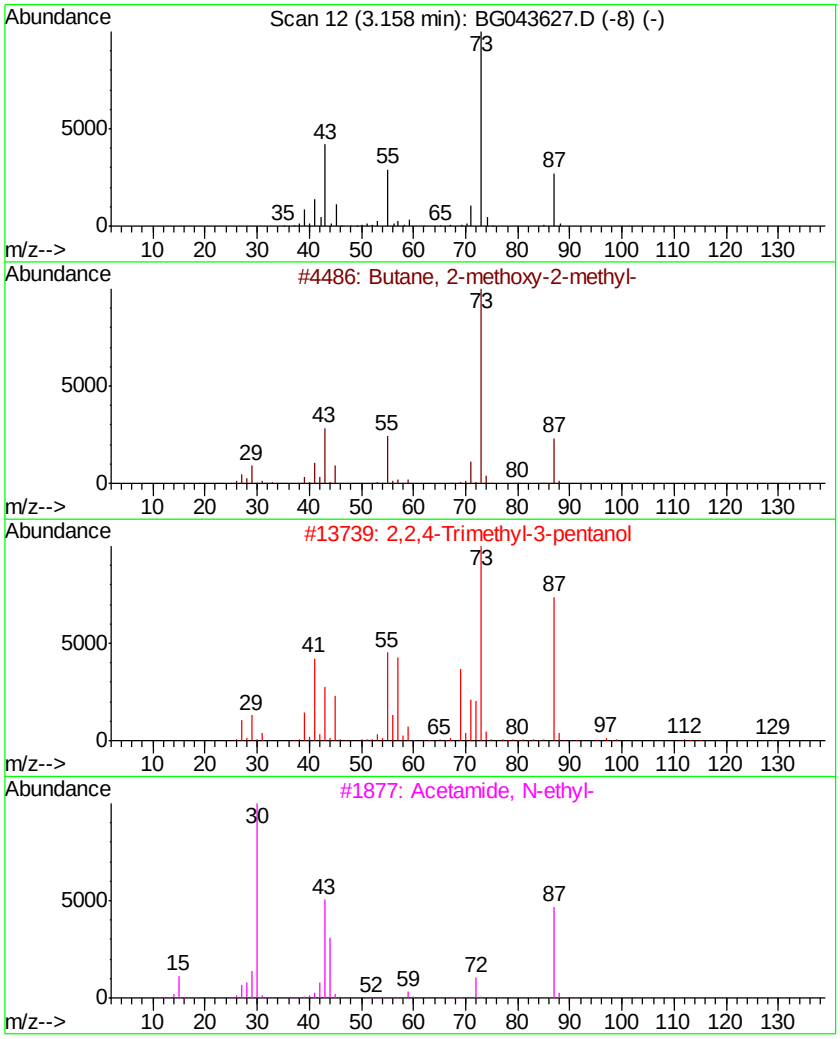
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

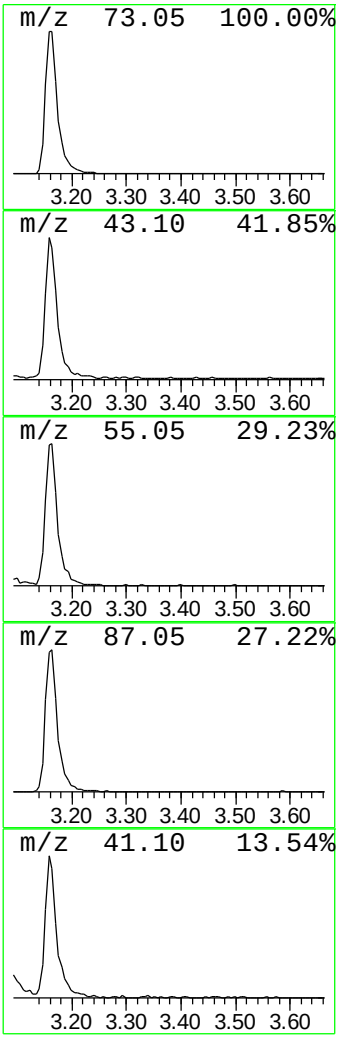
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.16	74.17 ng	564595	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	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	35
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111319\
Data File : BG043627.D
Acq On : 14 Nov 2019 00:32
Operator : JU
Sample : K5804-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-MW-QA-2

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

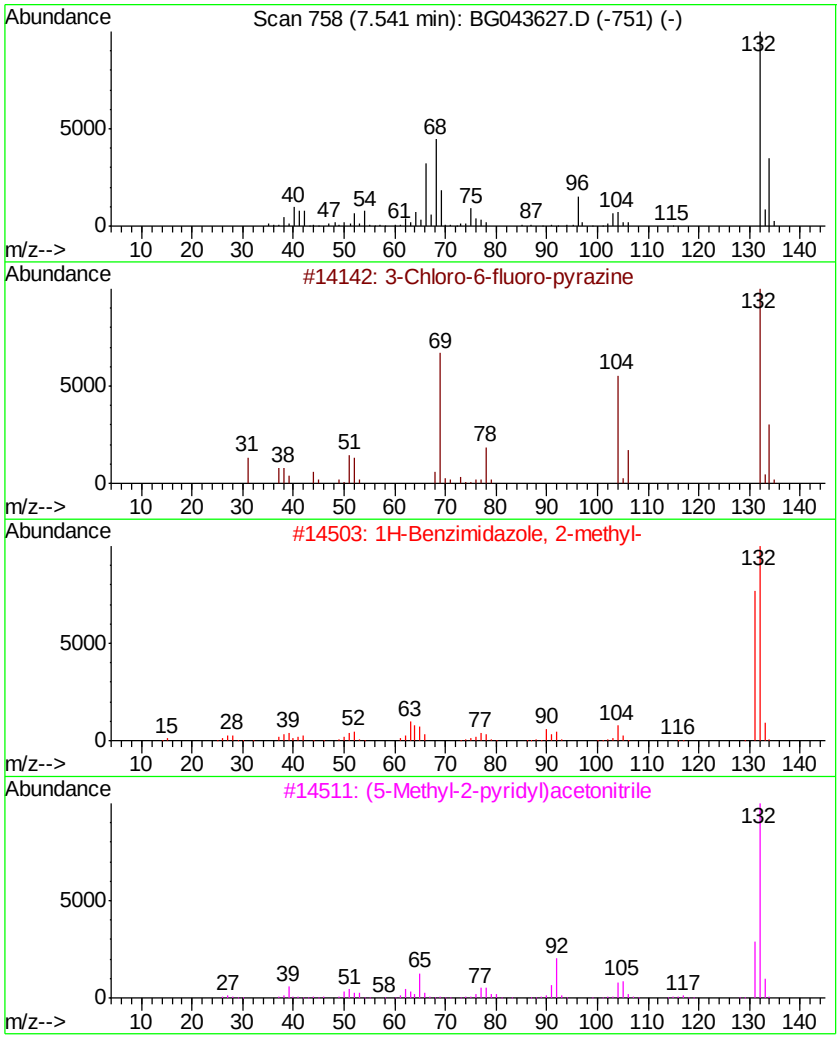
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

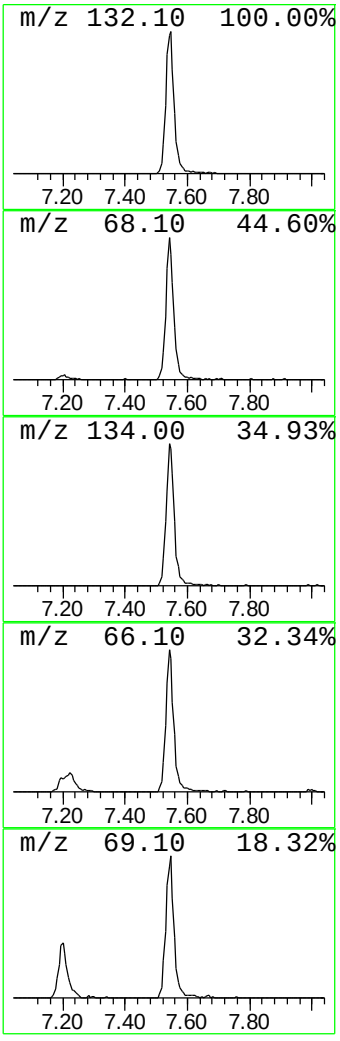
****

Peak Number 3 unknown7.54 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.54	73.57 ng	560048	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	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	22
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
5	5-Aminoindole	132	C8H8N2	005192-03-0	22





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Data File : BG043627.D
Acq On : 14 Nov 2019 00:32
Operator : JU
Sample : K5804-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-MW-QA-2

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

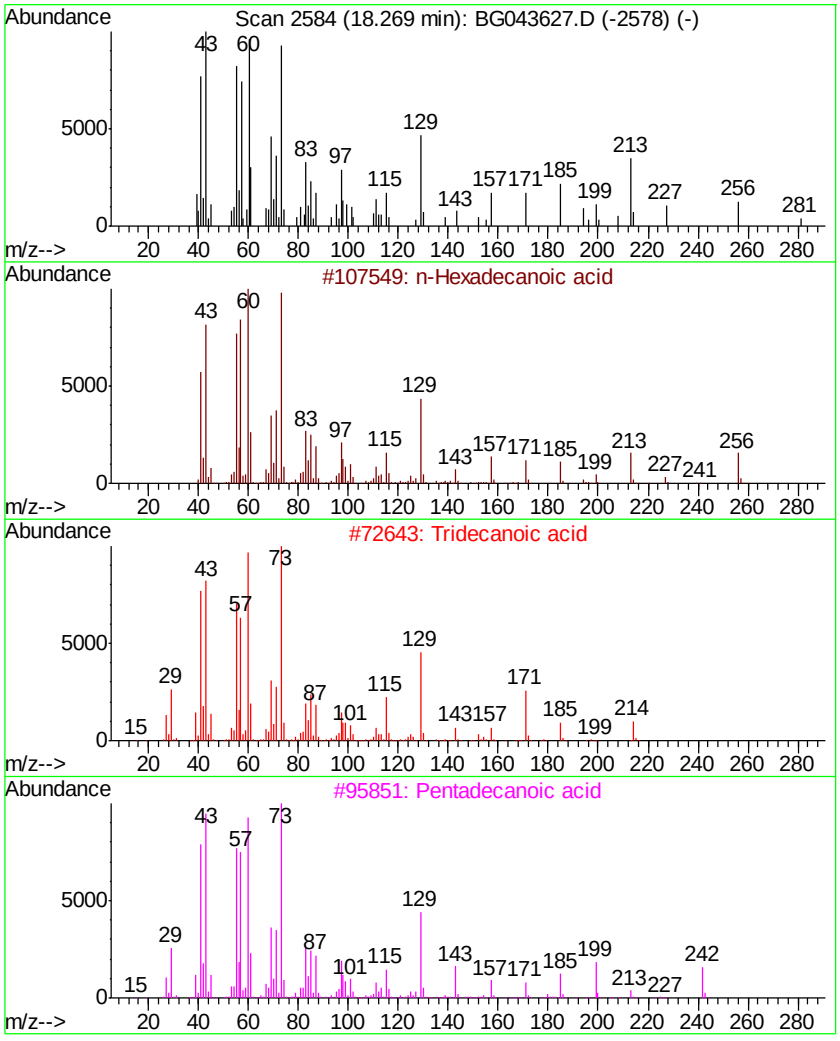
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

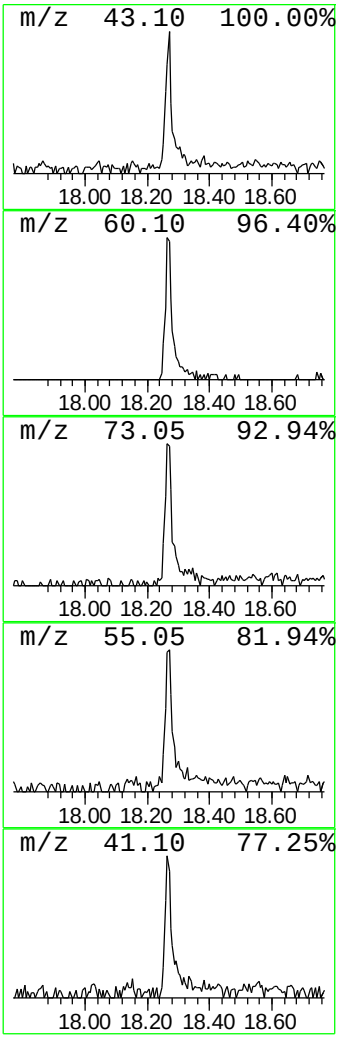
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.27	4.65 ng	99123	Phenanthrene-d10	17.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	60





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111319\
Data File : BG043627.D
Acq On : 14 Nov 2019 00:32
Operator : JU
Sample : K5804-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-MW-QA-2

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

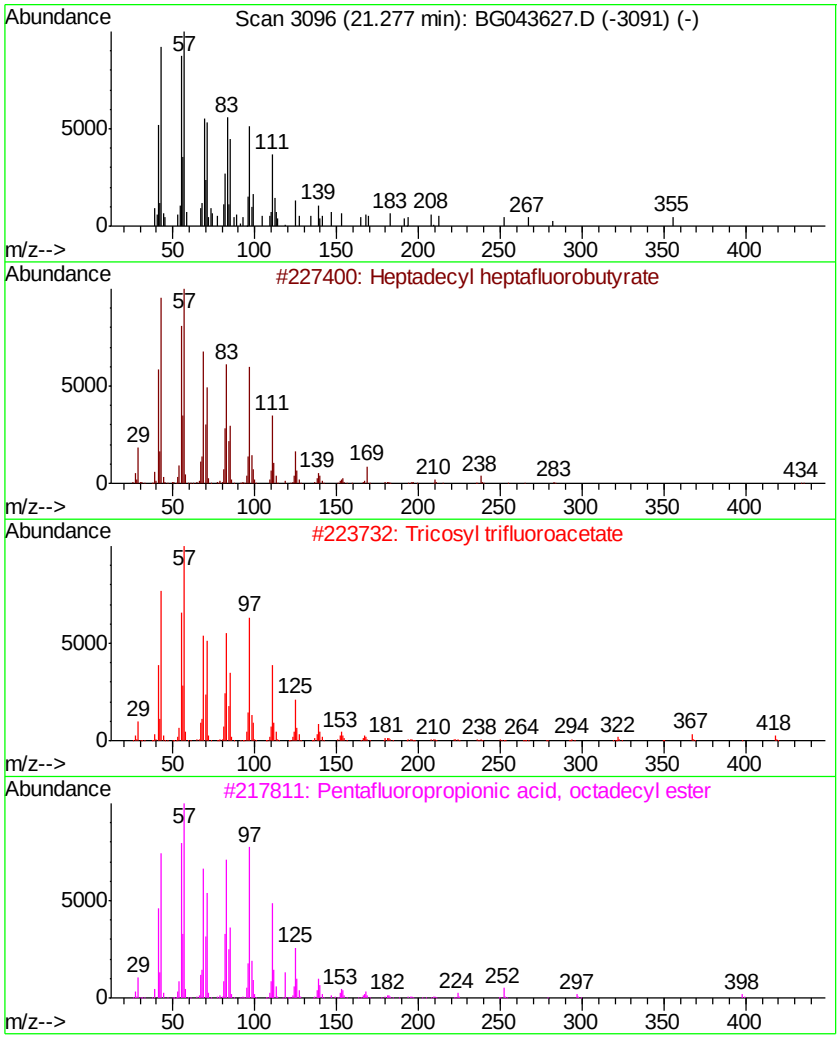
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

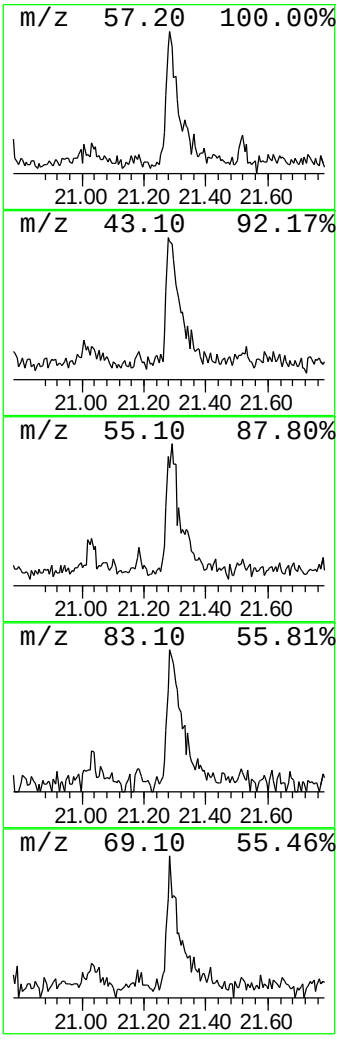
****

Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.28	5.33 ng	144856	Chrysene-d12	21.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
2	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	87
3	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	87
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	87
5	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	83





Library Search Compound Report

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Data File : BG043627.D
Acq On : 14 Nov 2019 00:32
Operator : JU
Sample : K5804-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-MW-QA-2

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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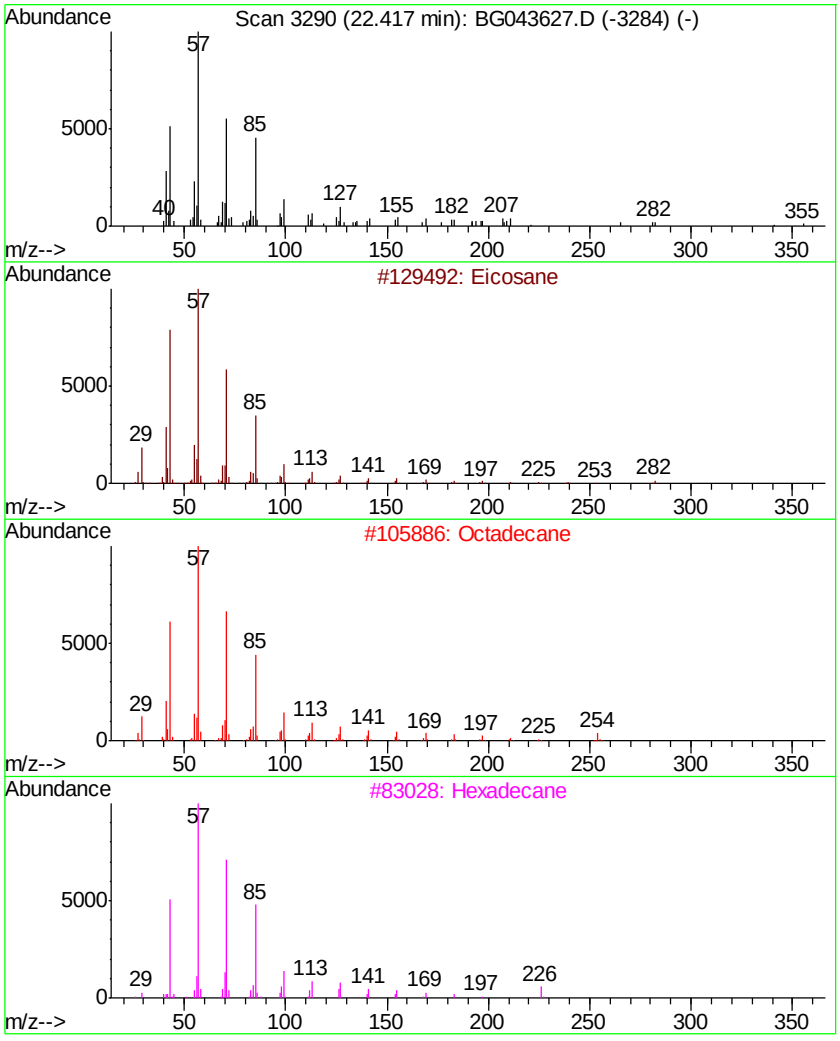
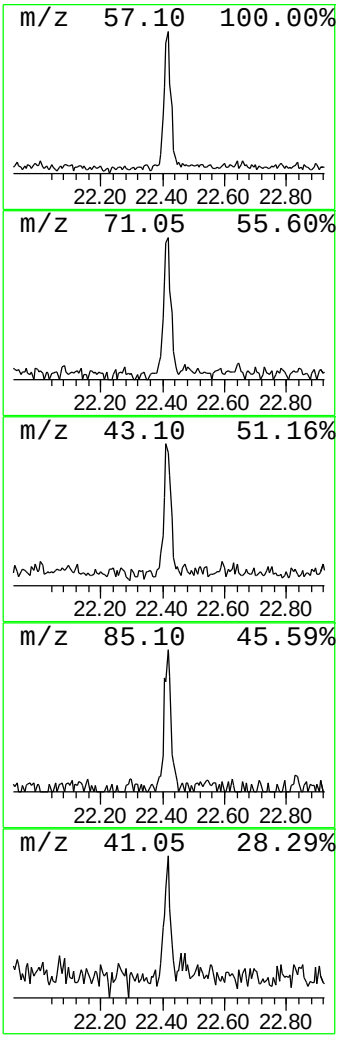
Peak Number 7 Octadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.42	2.39 ng	64898	Chrysene-d12	21.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Octadecane	254	C18H38	000593-45-3	87
3	Hexadecane	226	C16H34	000544-76-3	83
4	Docosane	310	C22H46	000629-97-0	83
5	Nonadecane	268	C19H40	000629-92-5	83





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111319\
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Operator : JU
Sample : K5804-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-MW-QA-2

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

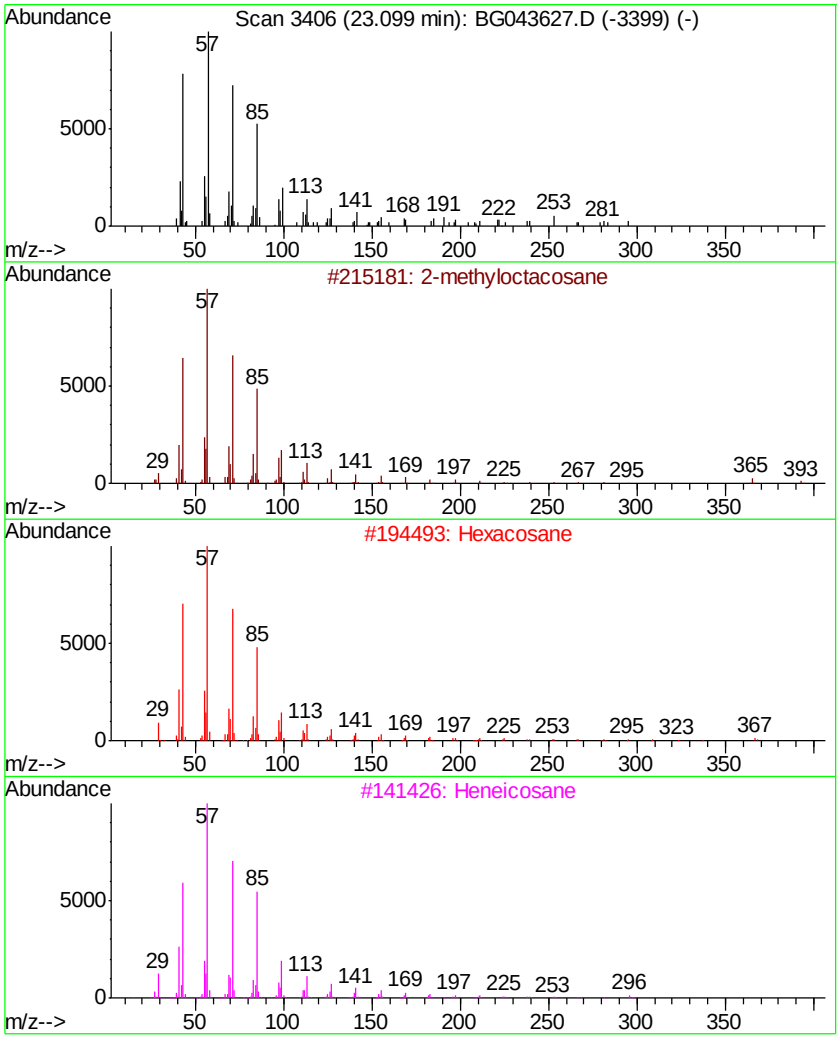
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

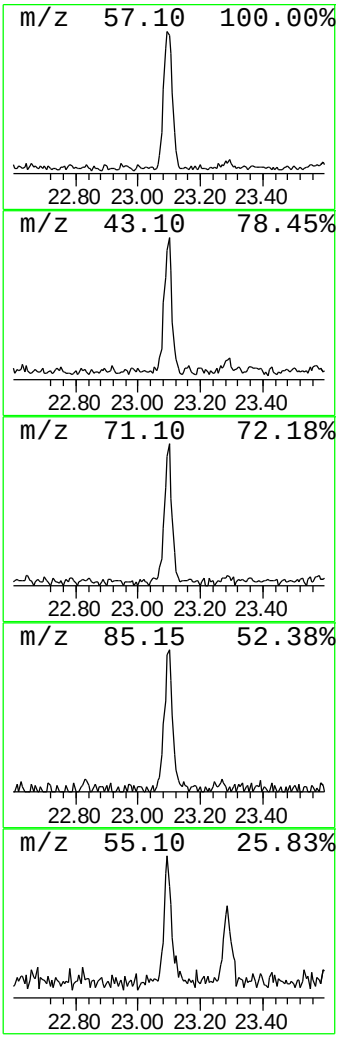
****

Peak Number 8 2-methyloctacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.10	3.84 ng	104420	Chrysene-d12	21.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Eicosane	282	C20H42	000112-95-8	91
5	Heptacosane	380	C27H56	000593-49-7	91





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Sample : K5804-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-MW-QA-2

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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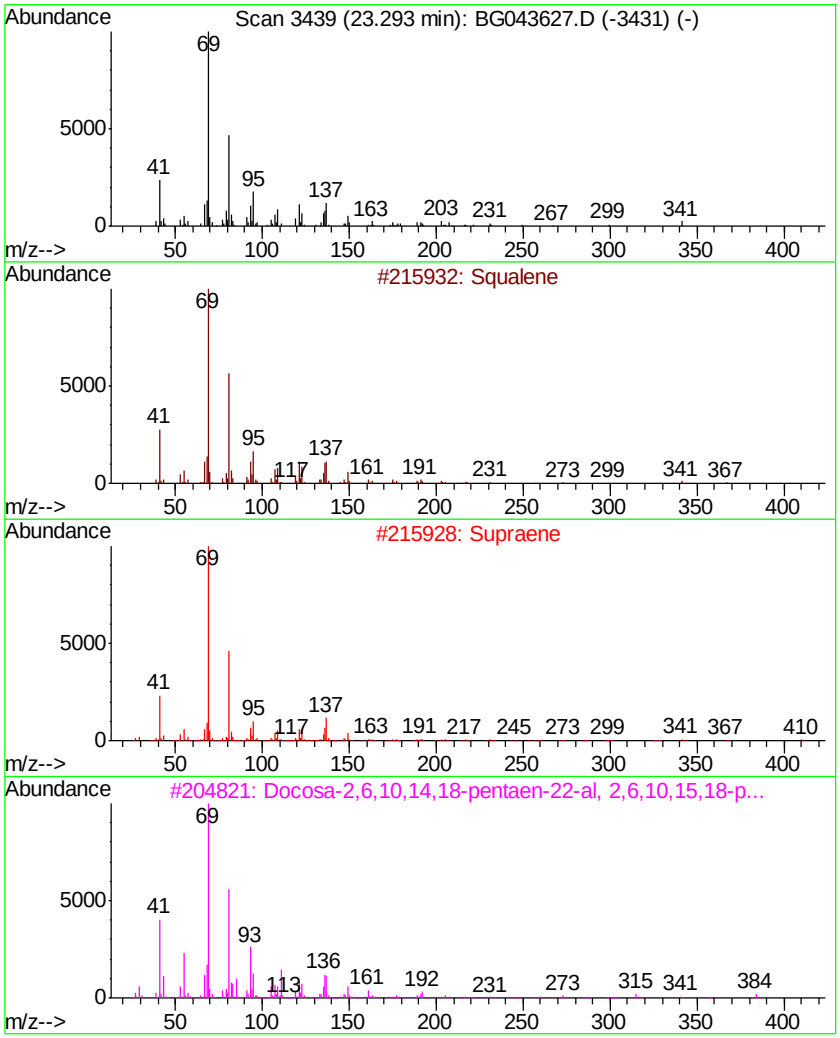
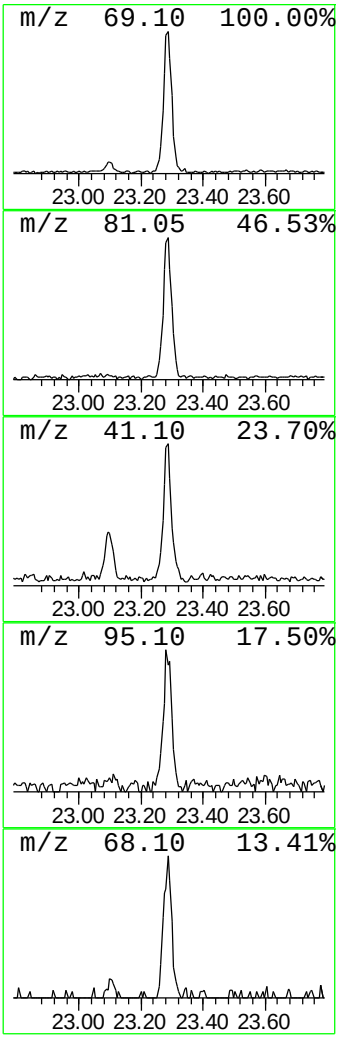
Peak Number 9 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.29	5.64 ng	200687	Perylene-d12	24.82

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	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
4	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
5	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	78





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ClientSampleId : TE-MW-QA-2

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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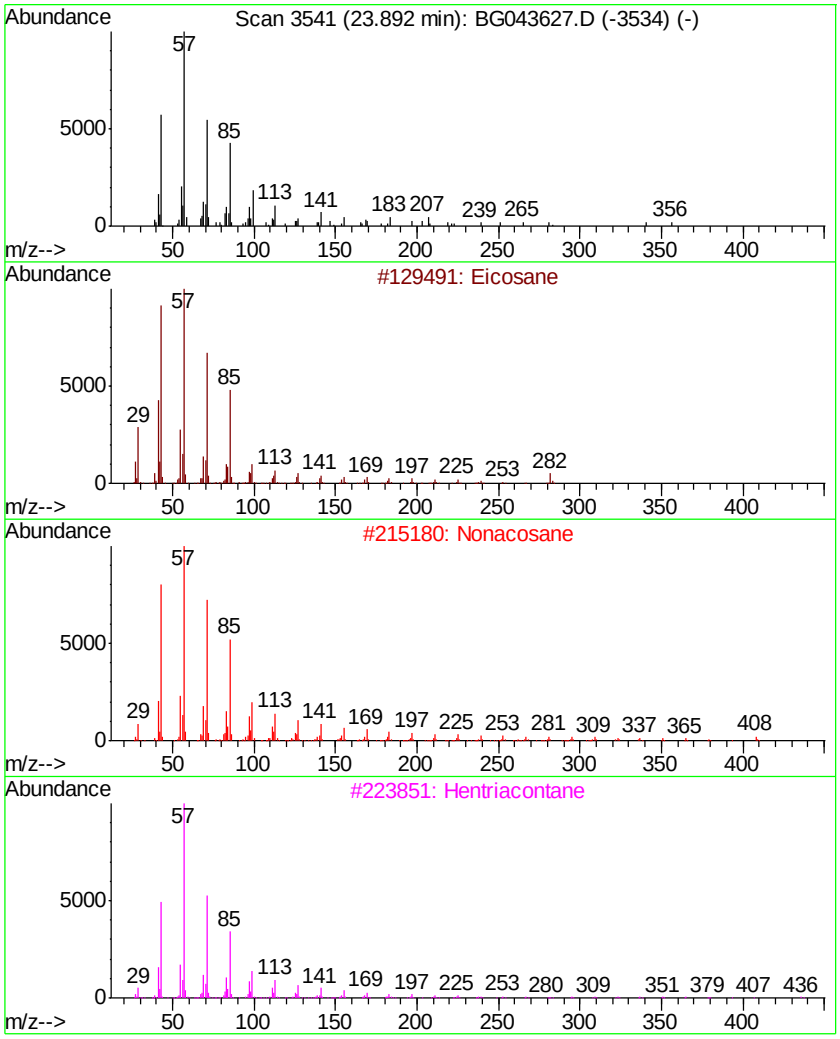
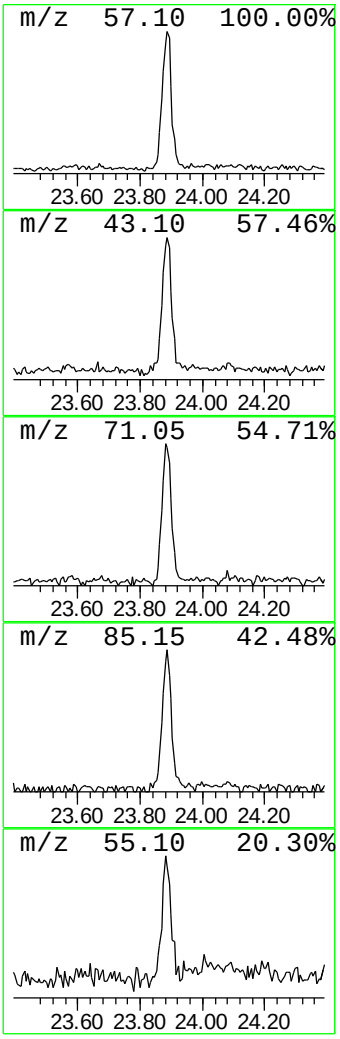
Peak Number 10 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.89	3.40 ng	120901	Perylene-d12	24.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Nonacosane	408	C29H60	000630-03-5	90
3	Hentriacontane	437	C31H64	000630-04-6	87
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
5	Triacontane	422	C30H62	000638-68-6	87





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ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-MW-QA-2

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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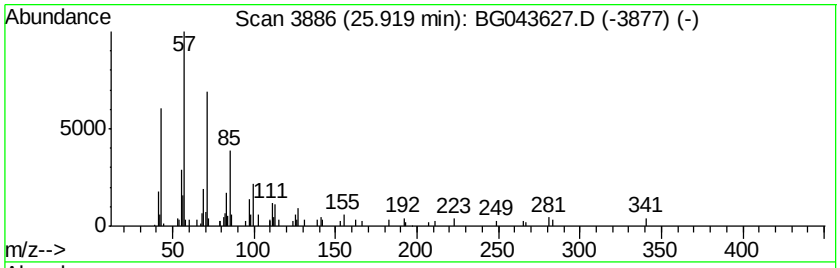
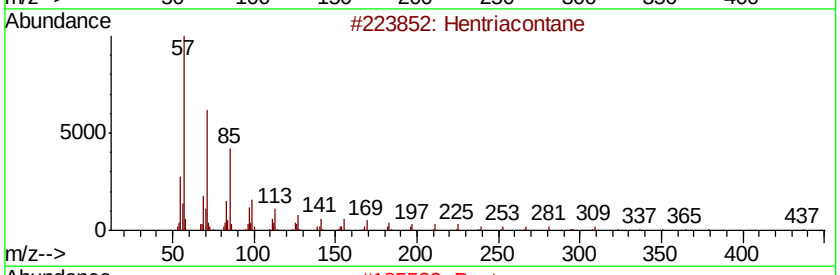
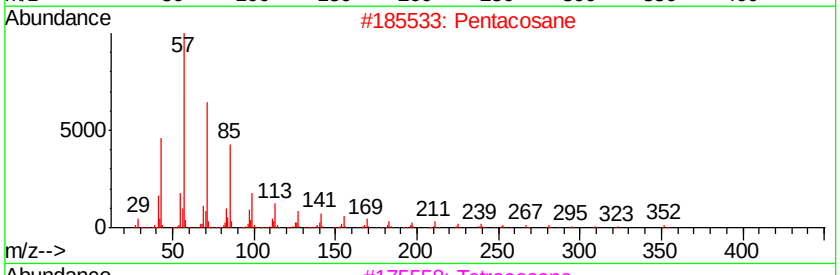
Peak Number 11 Hentriacontane Concentration Rank 10

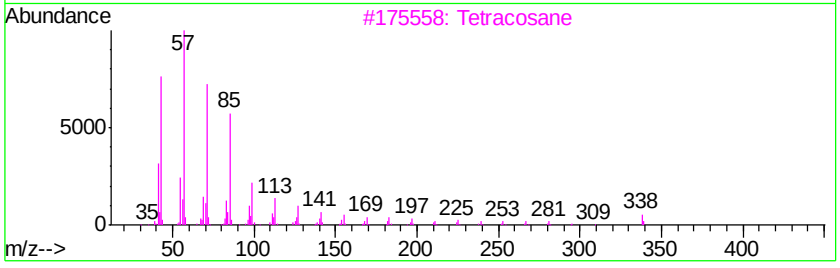
R.T.	EstConc	Area	Relative to ISTD	R.T.
25.92	3.16 ng	112411	Perylene-d12	24.82

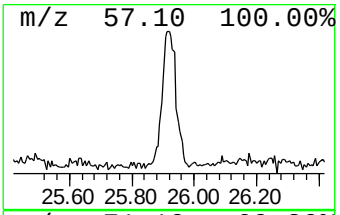
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	90
2	Pentacosane	352	C25H52	000629-99-2	80
3	Tetracosane	338	C24H50	000646-31-1	80
4	Tetratetracontane	619	C44H90	007098-22-8	74
5	2-methyloctacosane	408	C29H60	1000376-72-8	72

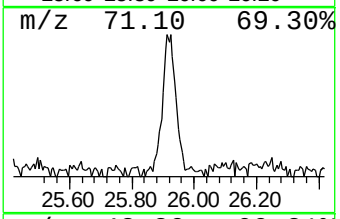


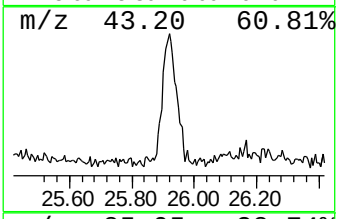


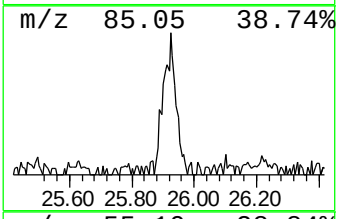


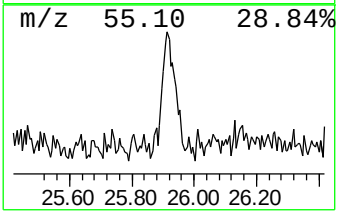












Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG111319\
Data File : BG043627.D
Acq On : 14 Nov 2019 00:32
Operator : JU
Sample : K5804-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-MW-QA-2

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	74.2	ng	564595	1	8.00	152244	20.0
unknown7.54	7.54	73.6	ng	560048	1	8.00	152244	20.0
n-Hexadecanoic acid	18.27	4.7	ng	99123	4	17.38	426347	20.0
Heptadecyl heptaf...	21.28	5.3	ng	144856	5	21.64	543846	20.0
Octadecane	22.42	2.4	ng	64898	5	21.64	543846	20.0
2-methyloctacosane	23.10	3.8	ng	104420	5	21.64	543846	20.0
Squalene	23.29	5.6	ng	200687	6	24.82	712157	20.0
Eicosane	23.89	3.4	ng	120901	6	24.82	712157	20.0
Hentriacontane	25.92	3.2	ng	112411	6	24.82	712157	20.0