LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
Data File : BG040959.D
Acq On : 30 May 2019 20:49
Operator : HP/JU
Sample : K3084-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEST-PIT-8

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-BG052919.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	3.123	3	6	16	rVB	123741	244783	5.17%	0.857%
2	3.206	16	20	33	rVB	397874	610314	12.89%	2.138%
3	5.656	430	437	451	rBV	1226484	2008452	42.41%	7.035%
4	7.266	703	711	721	rBV	1312176	2273834	48.02%	7.964%
5	7.647	769	776	788	rBV	1281115	2169392	45.81%	7.598%
6	8.123	849	857	868	rBV	239977	414213	8.75%	1.451%
7	8.446	904	912	921	rBV	899132	1543590	32.60%	5.406%
8	9.298	1046	1057	1067	rBV	787526	1432289	30.24%	5.017%
9	10.944	1329	1337	1346	rBV	305708	529230	11.18%	1.854%
10	13.376	1740	1751	1761	rBV	1873175	2870321	60.61%	10.053%
11	14.193	1884	1890	1896	rBV	291416	418044	8.83%	1.464%
12	14.751	1978	1985	1993	rBV2	500371	797511	16.84%	2.793%
13	16.237	2231	2238	2252	rBV	1944606	2920527	61.67%	10.229%
14	17.495	2445	2452	2463	rVB2	759536	1097854	23.18%	3.845%
15	18.352	2591	2598	2612	rBV	307658	489550	10.34%	1.715%
16	19.610	2808	2812	2826	rBV	136267	232636	4.91%	0.815%
17	20.092	2887	2894	2903	rBV	3595990	4735624	100.00%	16.587%
18	21.372	3107	3112	3124	rBV	113873	202626	4.28%	0.710%
19	21.772	3174	3180	3188	rBV2	739774	1286599	27.17%	4.506%
20	21.925	3201	3206	3212	rBV2	63932	93172	1.97%	0.326%
21	22.548	3306	3312	3319	rBV2	84372	143283	3.03%	0.502%
22	23.259	3427	3433	3442	rBV2	94936	185208	3.91%	0.649%
23	23.458	3458	3467	3476	rBV	79155	169201	3.57%	0.593%
24	24.087	3568	3574	3582	rBV2	84290	169906	3.59%	0.595%
25	25.115	3734	3749	3762	rVB2	411248	1385014	29.25%	4.851%
26	26.237	3931	3940	3949	rBV5	43618	127564	2.69%	0.447%

Sum of corrected areas: 28550737

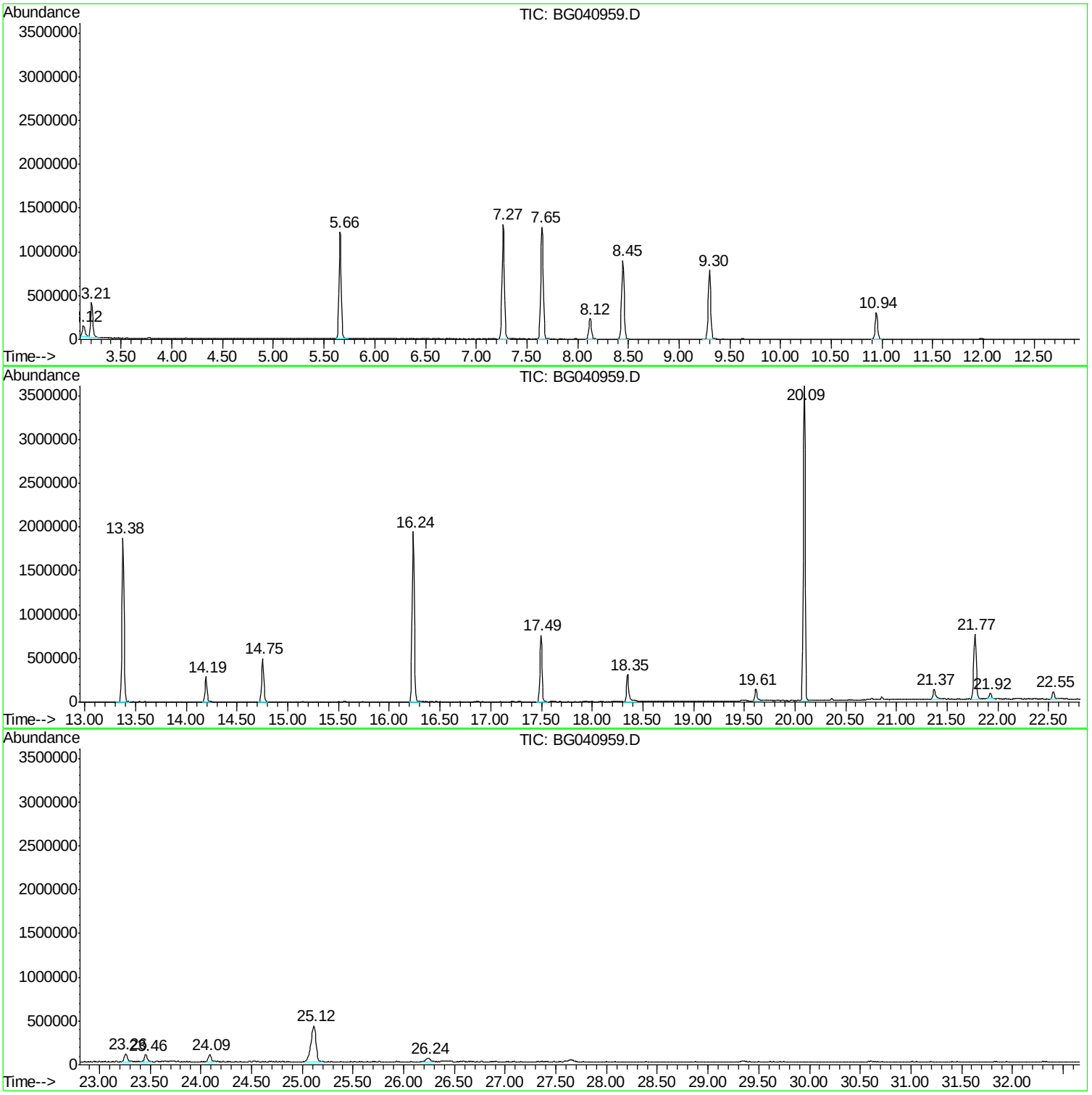
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
Data File : BG040959.D
Acq On : 30 May 2019 20:49
Operator : HP/JU
Sample : K3084-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEST-PIT-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.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\BG053019\
Data File : BG040959.D
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Operator : HP/JU
Sample : K3084-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEST-PIT-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

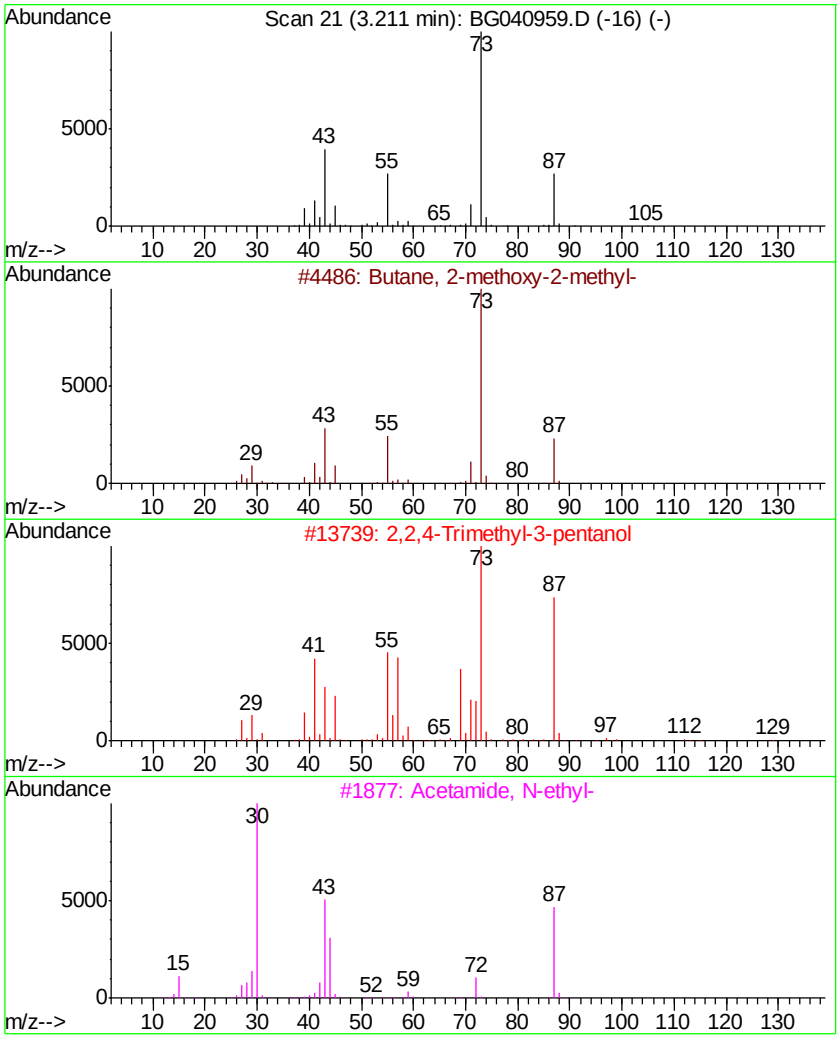
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

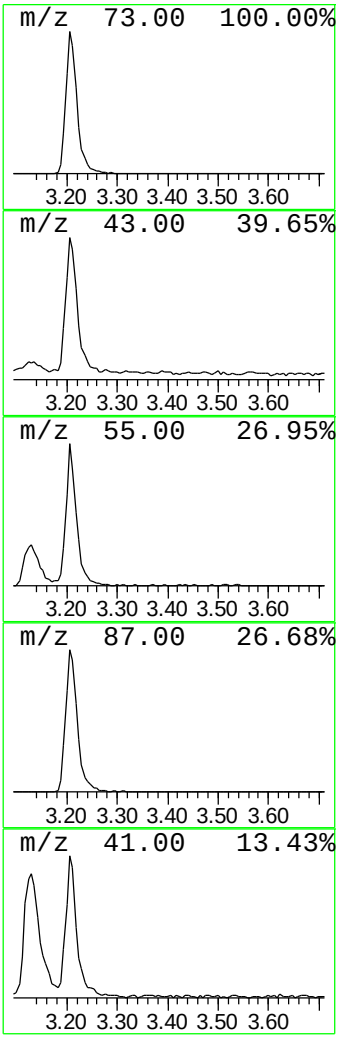
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.21	29.47 ng	610314	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Library Search Compound Report

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Data File : BG040959.D
Acq On : 30 May 2019 20:49
Operator : HP/JU
Sample : K3084-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEST-PIT-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

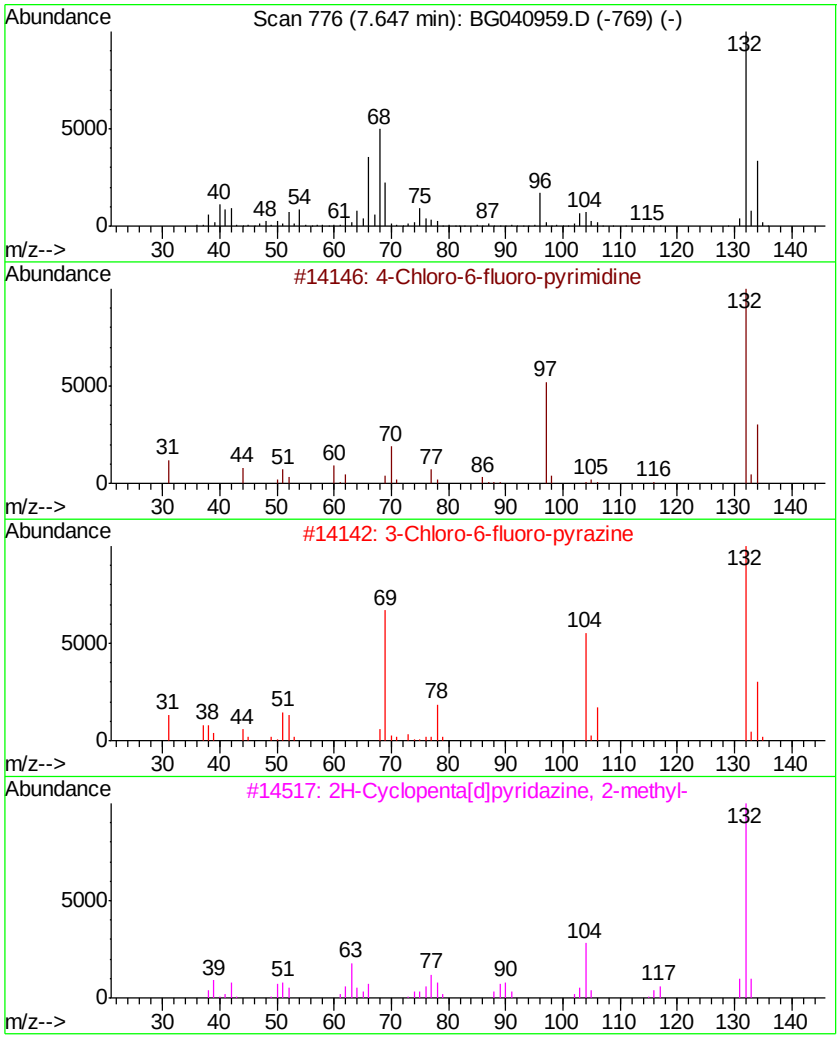
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

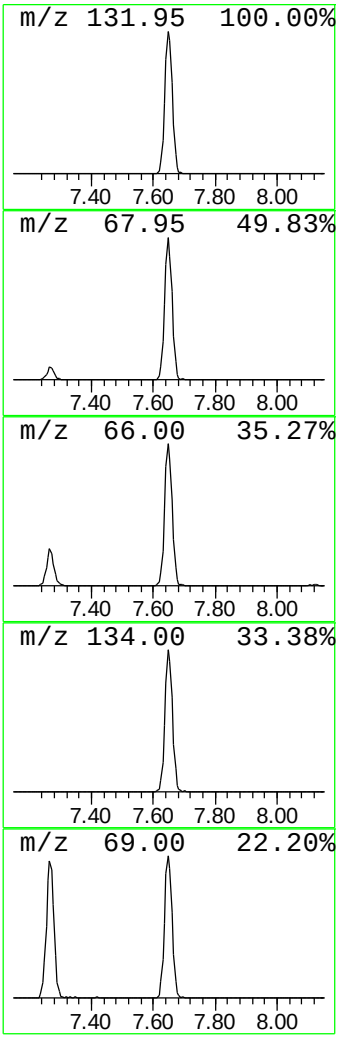
****

Peak Number 3 unknown7.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	104.75 ng	2169390	1,4-Dichlorobenzene-d4	8.12

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	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	22
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
Data File : BG040959.D
Acq On : 30 May 2019 20:49
Operator : HP/JU
Sample : K3084-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEST-PIT-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

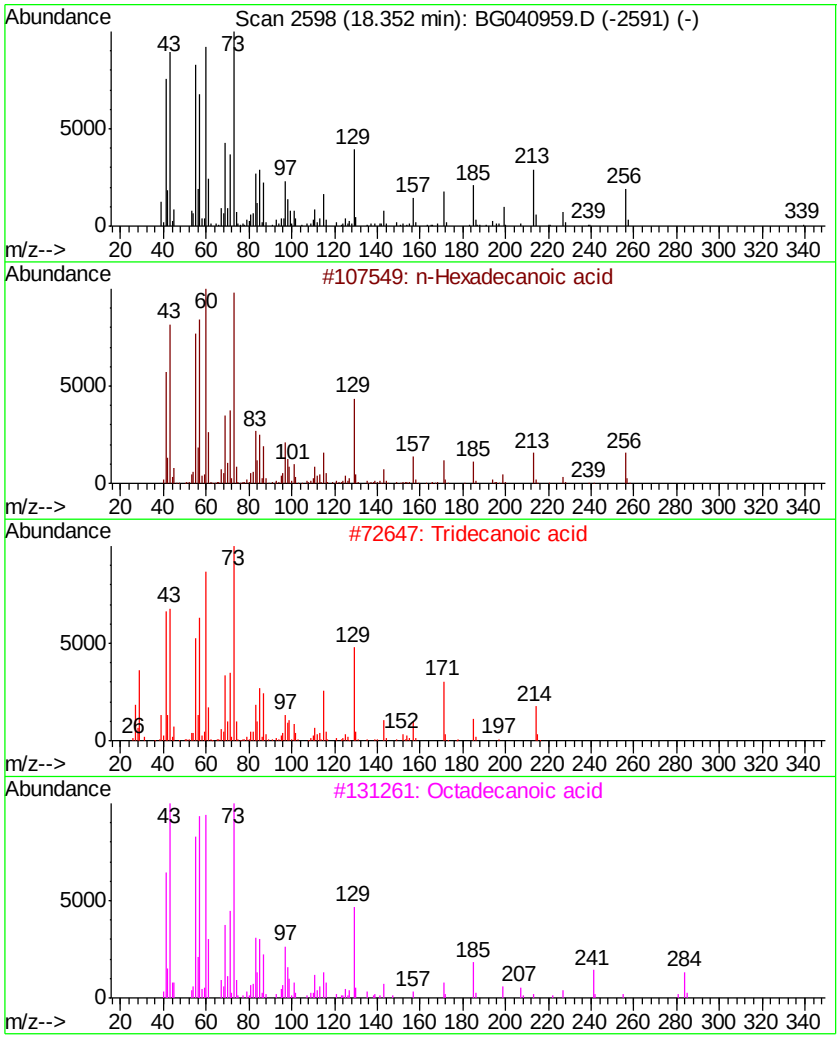
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

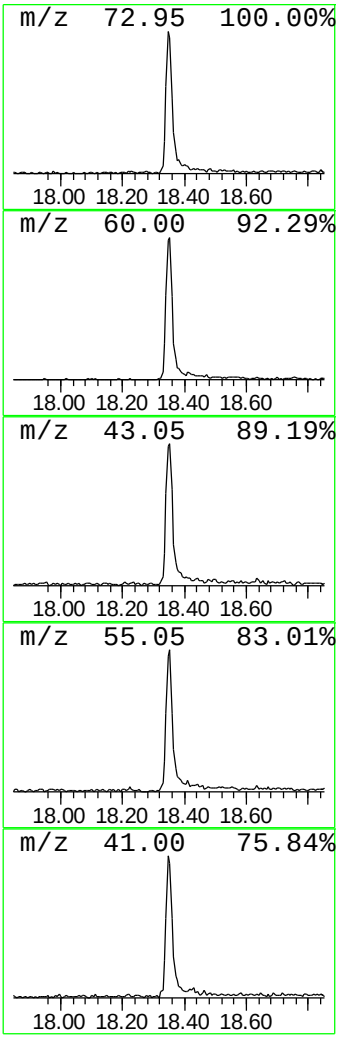
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.35	8.92 ng	489550	Phenanthrene-d10	17.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	97
3	Octadecanoic acid	284	C18H36O2	000057-11-4	81
4	Undecanoic acid	186	C11H22O2	000112-37-8	70
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	68





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
Data File : BG040959.D
Acq On : 30 May 2019 20:49
Operator : HP/JU
Sample : K3084-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEST-PIT-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

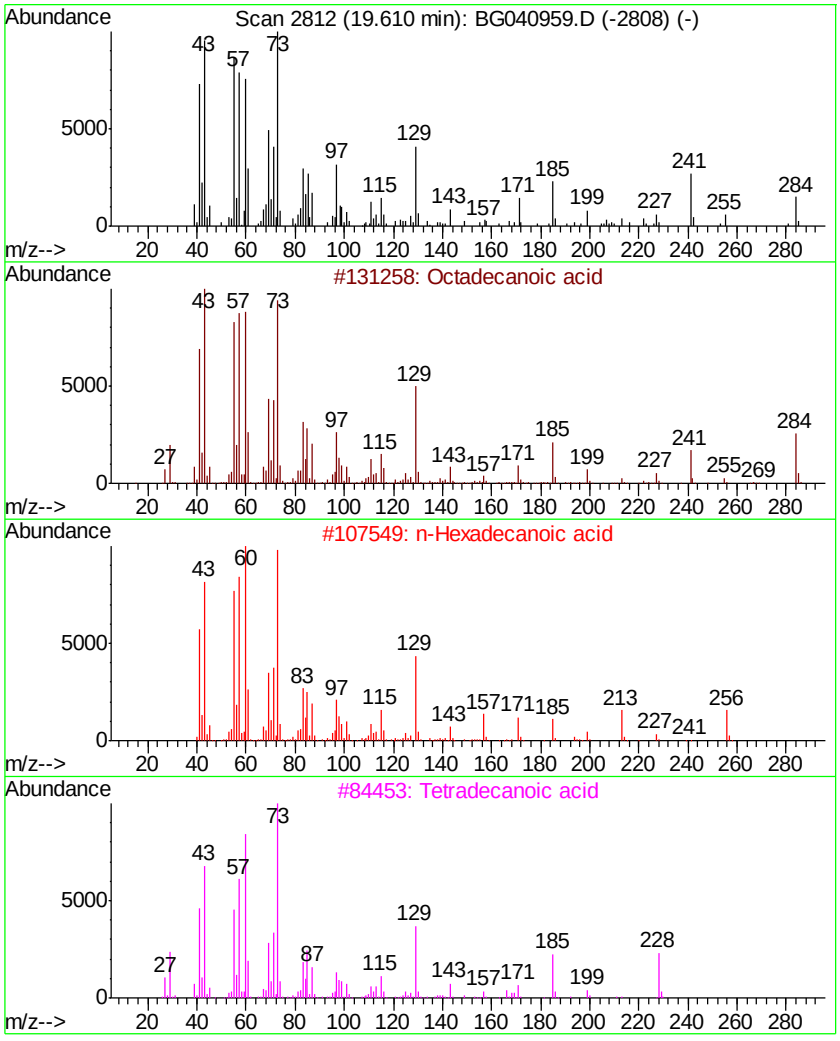
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

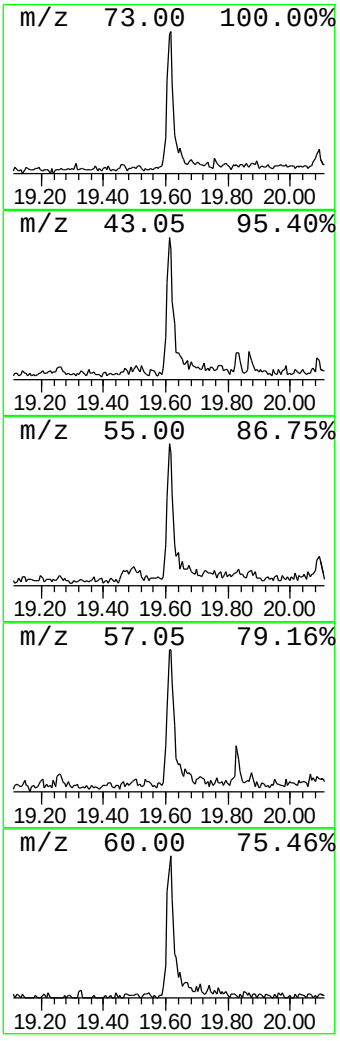
****

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.61	4.24 ng	232636	Phenanthrene-d10	17.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
Data File : BG040959.D
Acq On : 30 May 2019 20:49
Operator : HP/JU
Sample : K3084-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEST-PIT-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

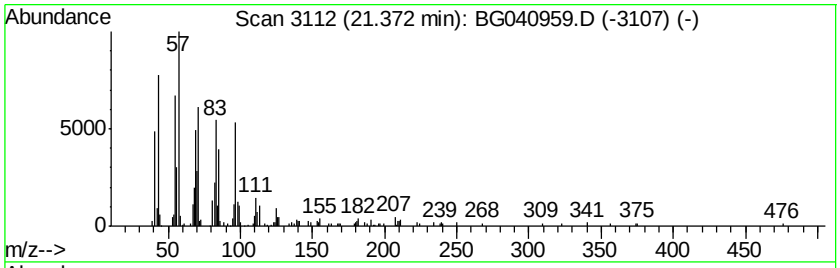
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

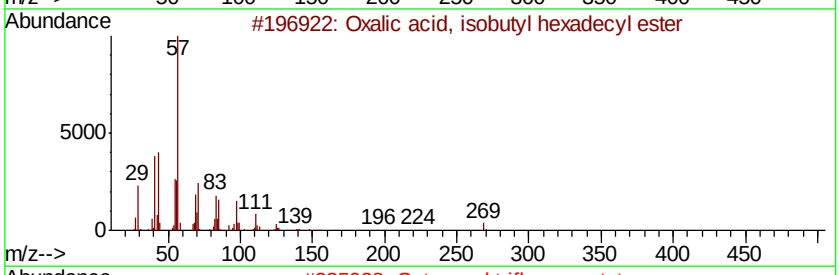
****

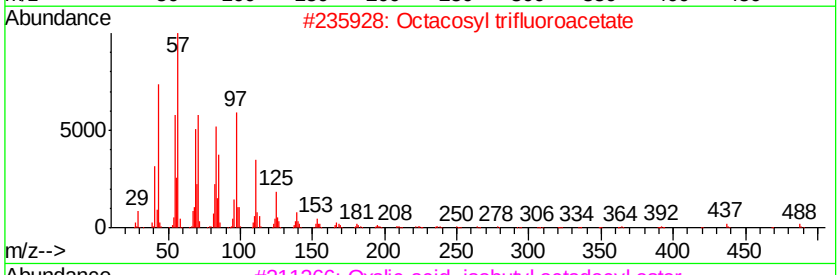
Peak Number 7 Oxalic acid, isobutyl hexad... Concentration Rank 7

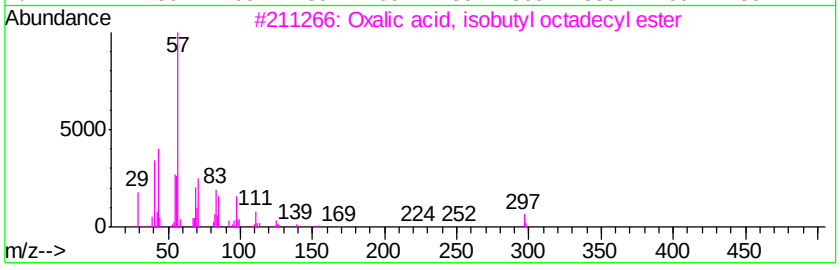
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.37	3.15 ng	202626	Chrysene-d12	21.77

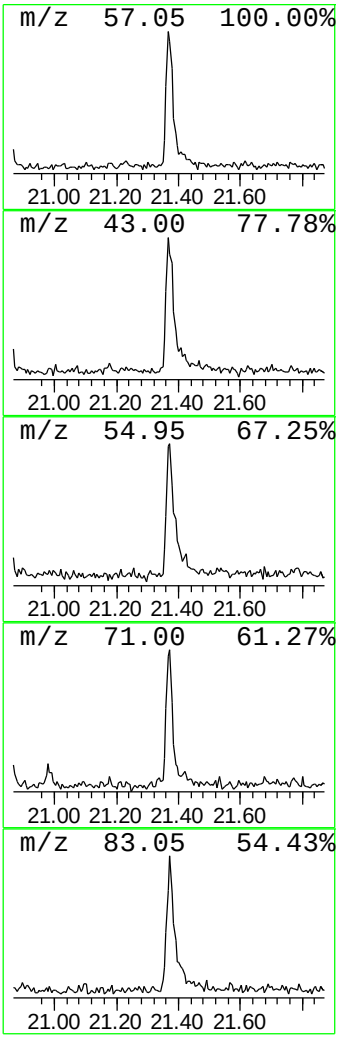
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
2	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	90
3	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	90
4	17-Pentatriacontene	491	C35H70	006971-40-0	68
5	1-Heptadecene	238	C17H34	006765-39-5	55











Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
Data File : BG040959.D
Acq On : 30 May 2019 20:49
Operator : HP/JU
Sample : K3084-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEST-PIT-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

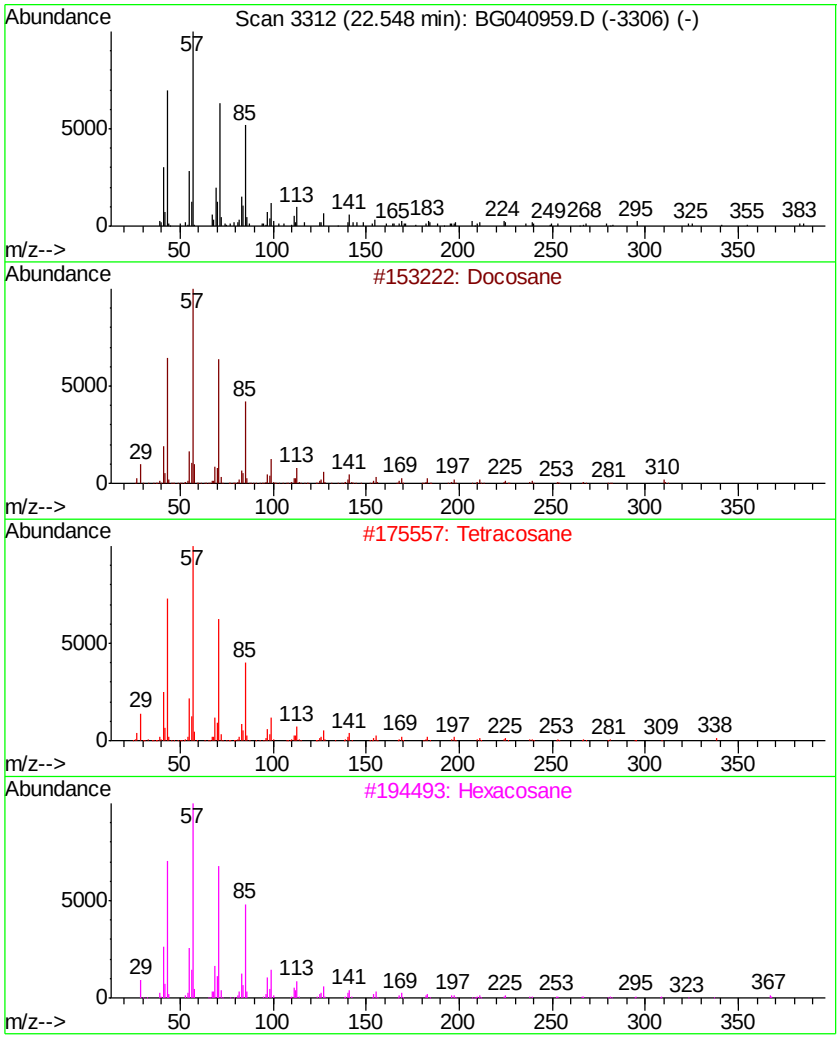
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

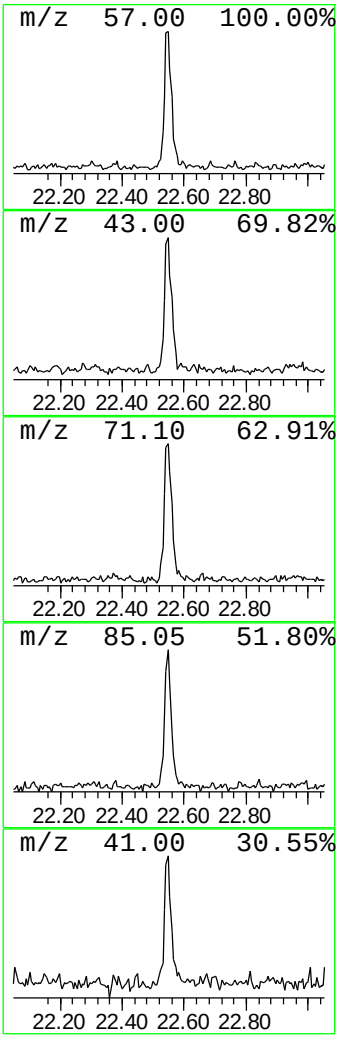
****

Peak Number 8 Docosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.55	2.23 ng	143283	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	90
2	Tetracosane	338	C24H50	000646-31-1	90
3	Hexacosane	366	C26H54	000630-01-3	87
4	Heptadecane	240	C17H36	000629-78-7	87
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86





Library Search Compound Report

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Data File : BG040959.D
Acq On : 30 May 2019 20:49
Operator : HP/JU
Sample : K3084-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEST-PIT-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
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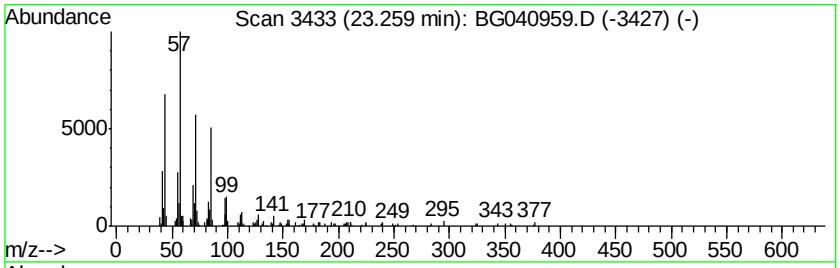
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

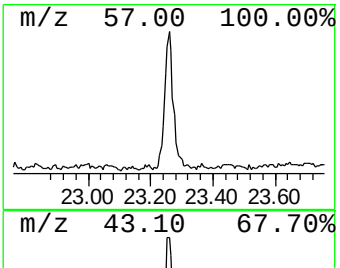
****

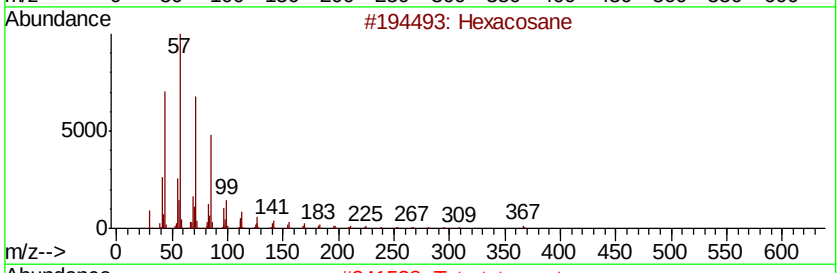
Peak Number 9 Hexacosane Concentration Rank 8

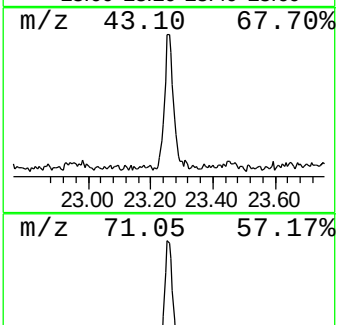
R.T.	EstConc	Area	Relative to ISTD	R.T.
23.26	2.88 ng	185208	Chrysene-d12	21.77

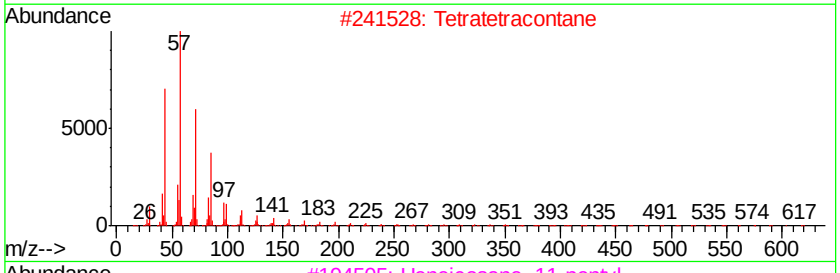
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Tetratetracontane	619	C44H90	007098-22-8	86
3	Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	86
4	Triacontane	422	C30H62	000638-68-6	83
5	Docosane	310	C22H46	000629-97-0	83

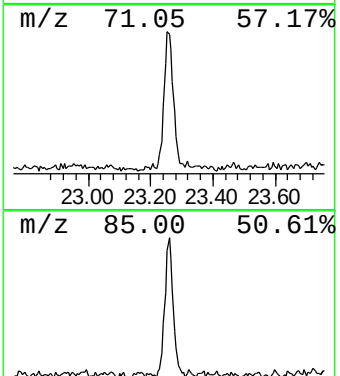


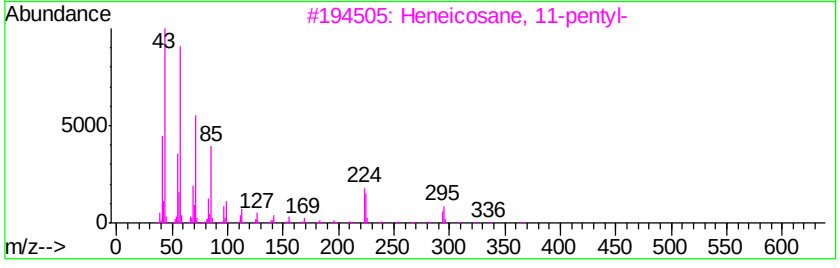


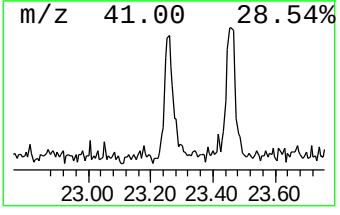












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Data File : BG040959.D
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Operator : HP/JU
Sample : K3084-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEST-PIT-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

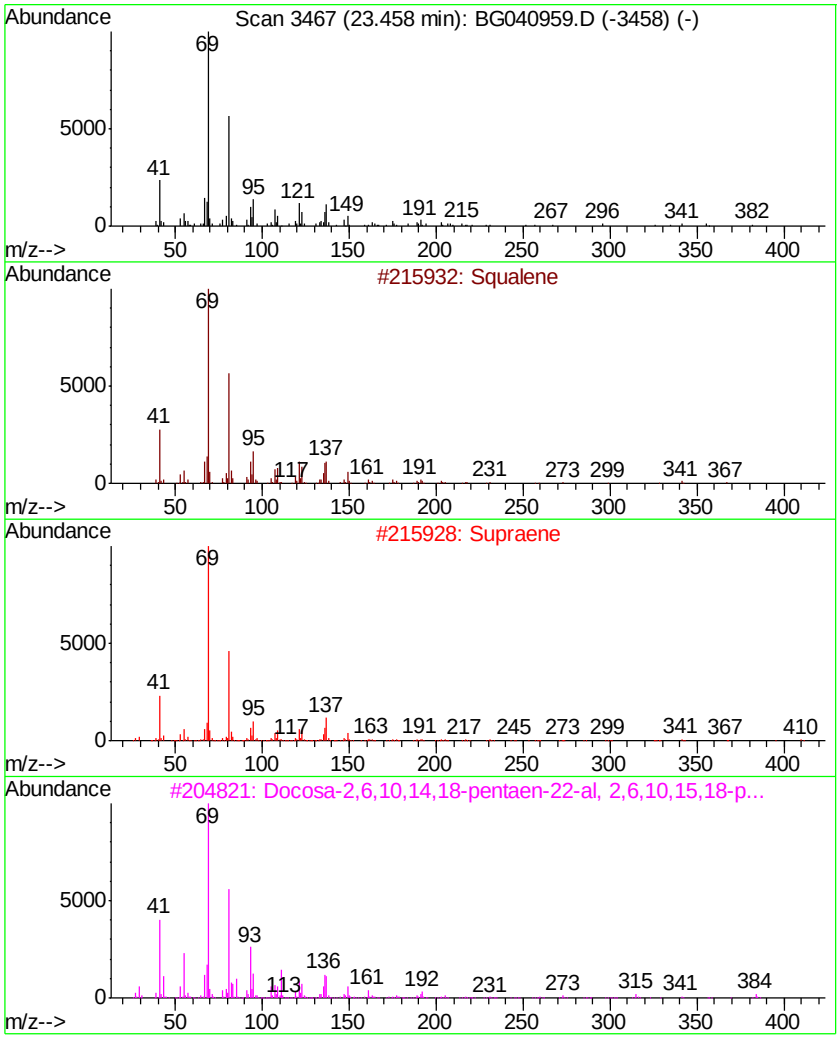
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

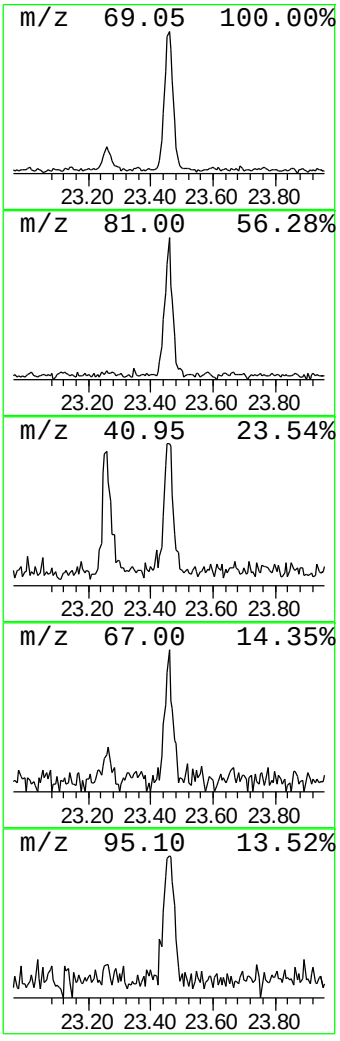
****

Peak Number 10 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.46	2.44 ng	169201	Perylene-d12	25.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	87
2	Supraene	410	C30H50	007683-64-9	83
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	72
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5	Geranyl bromide	216	C10H17Br	006138-90-5	53





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Data File : BG040959.D
Acq On : 30 May 2019 20:49
Operator : HP/JU
Sample : K3084-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEST-PIT-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

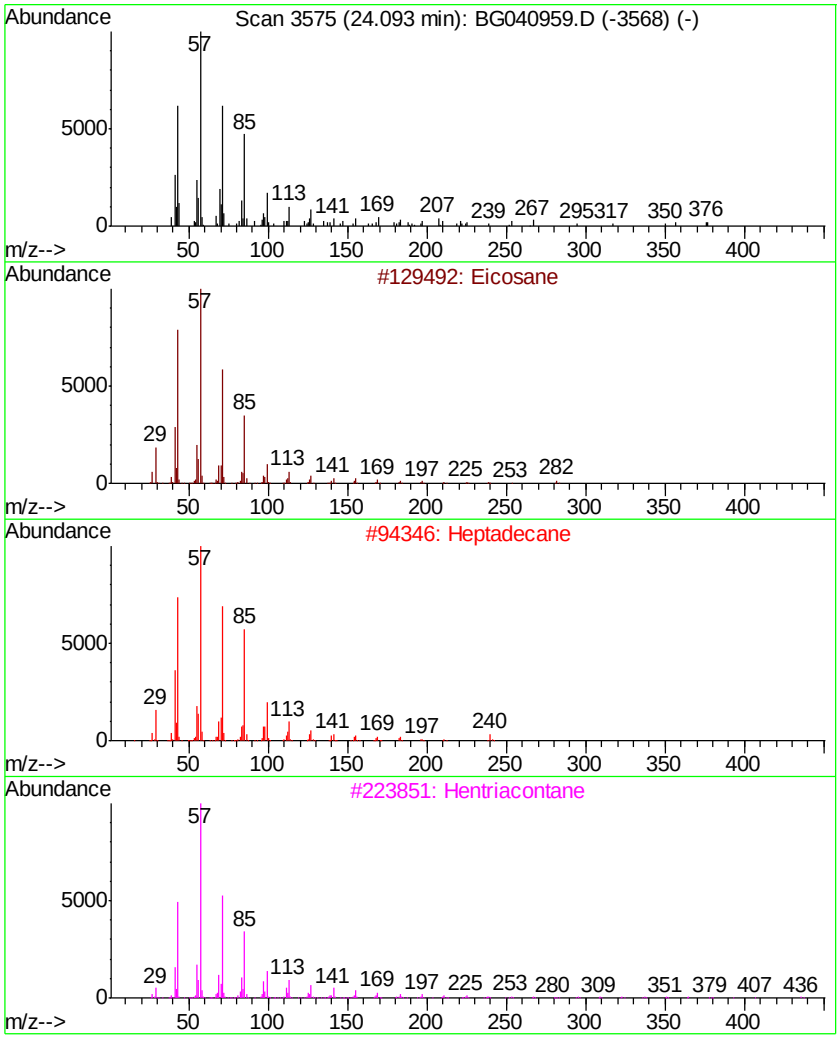
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

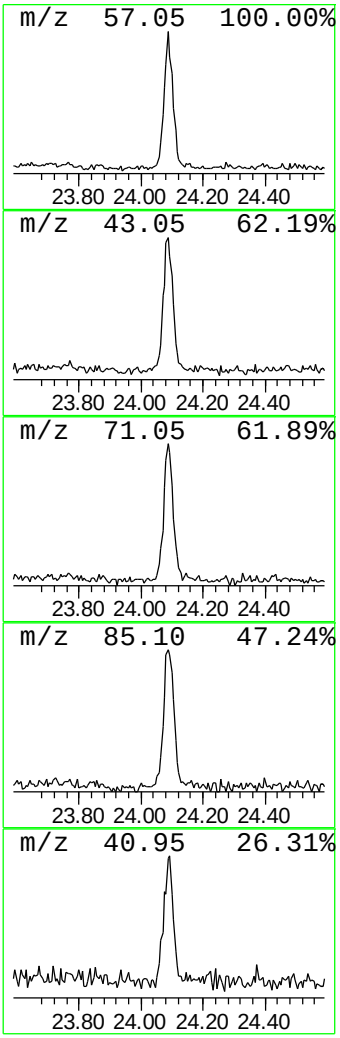
****

Peak Number 11 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.09	2.45 ng	169906	Perylene-d12	25.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Heptadecane	240	C17H36	000629-78-7	83
3	Hentriacontane	437	C31H64	000630-04-6	83
4	Tetracosane	338	C24H50	000646-31-1	83
5	Triacontane	422	C30H62	000638-68-6	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG053019\
Data File : BG040959.D
Acq On : 30 May 2019 20:49
Operator : HP/JU
Sample : K3084-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEST-PIT-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.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...	3.21	29.5	ng	610314	1	8.12	414213	20.0
unknown7.65	7.65	104.8	ng	2169390	1	8.12	414213	20.0
n-Hexadecanoic acid	18.35	8.9	ng	489550	4	17.49	1097850	20.0
Octadecanoic acid	19.61	4.2	ng	232636	4	17.49	1097850	20.0
Oxalic acid, isob...	21.37	3.1	ng	202626	5	21.77	1286600	20.0
Docosane	22.55	2.2	ng	143283	5	21.77	1286600	20.0
Hexacosane	23.26	2.9	ng	185208	5	21.77	1286600	20.0
Squalene	23.46	2.4	ng	169201	6	25.12	1385010	20.0
Eicosane	24.09	2.5	ng	169906	6	25.12	1385010	20.0