LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033251.D
Acq On : 19 Mar 2018 22:13
Operator : SJ/JU
Sample : J1953-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-TIDO-F-D-S

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:\HPCHEM1\BNA_G\METHODS\8270-BG031918.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	3.501	30	36	46	rBV	148978	296075	7.65%	1.815%
2	3.589	46	51	62	rVB	89564	145982	3.77%	0.895%
3	6.315	508	515	529	rBV	133962	319204	8.25%	1.957%
4	6.850	599	606	623	rBV	67536	170802	4.42%	1.047%
5	8.002	796	802	828	rBV	77792	267565	6.92%	1.640%
6	8.401	862	870	890	rBV	312527	737762	19.07%	4.523%
7	8.895	942	954	971	rBV2	95060	236257	6.11%	1.448%
8	9.229	1003	1011	1027	rBV	485038	1012181	26.16%	6.205%
9	10.093	1150	1158	1173	rBV	397547	911320	23.56%	5.587%
10	11.779	1437	1445	1465	rBV	145634	340106	8.79%	2.085%
11	14.135	1836	1846	1859	rBV	1307025	2302982	59.53%	14.118%
12	14.929	1972	1981	1989	rBV2	50241	91792	2.37%	0.563%
13	15.334	2044	2050	2055	rBV	32194	45237	1.17%	0.277%
14	15.510	2073	2080	2091	rVB2	304943	538734	13.93%	3.303%
15	16.274	2205	2210	2216	rVB2	52423	74555	1.93%	0.457%
16	16.721	2282	2286	2291	rVB	37372	52013	1.34%	0.319%
17	16.979	2322	2330	2347	rBV	888166	1481201	38.29%	9.080%
18	17.126	2351	2355	2365	rVB	54303	91154	2.36%	0.559%
19	18.237	2537	2544	2556	rBV2	456295	820721	21.22%	5.031%
20	19.036	2675	2680	2690	rBV2	148463	226679	5.86%	1.390%
21	20.757	2967	2973	2985	rBV	2829253	3868491	100.00%	23.714%
22	22.108	3198	3203	3214	rBV	175960	332535	8.60%	2.038%
23	22.596	3278	3286	3296	rBV2	478351	926250	23.94%	5.678%
24	24.476	3598	3606	3615	rBV2	65365	158630	4.10%	0.972%
25	26.386	3919	3931	3948	rBV	244932	864547	22.35%	5.300%

Sum of corrected areas: 16312775

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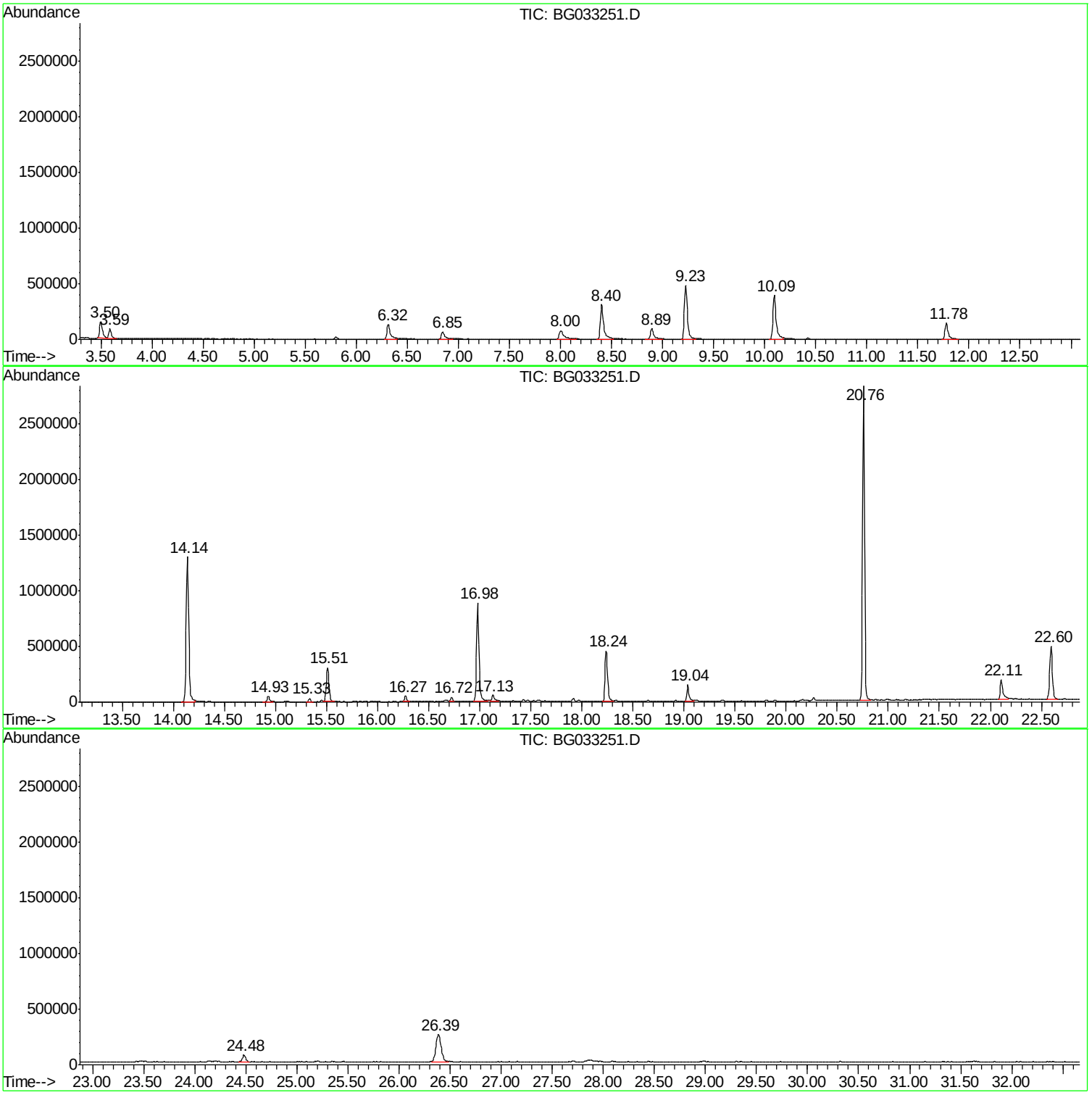
Instrument :
BNA_G
ClientSampleId :
031418-TIDO-F-D-S

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033251.D
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Operator : SJ/JU
Sample : J1953-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-TIDO-F-D-S

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

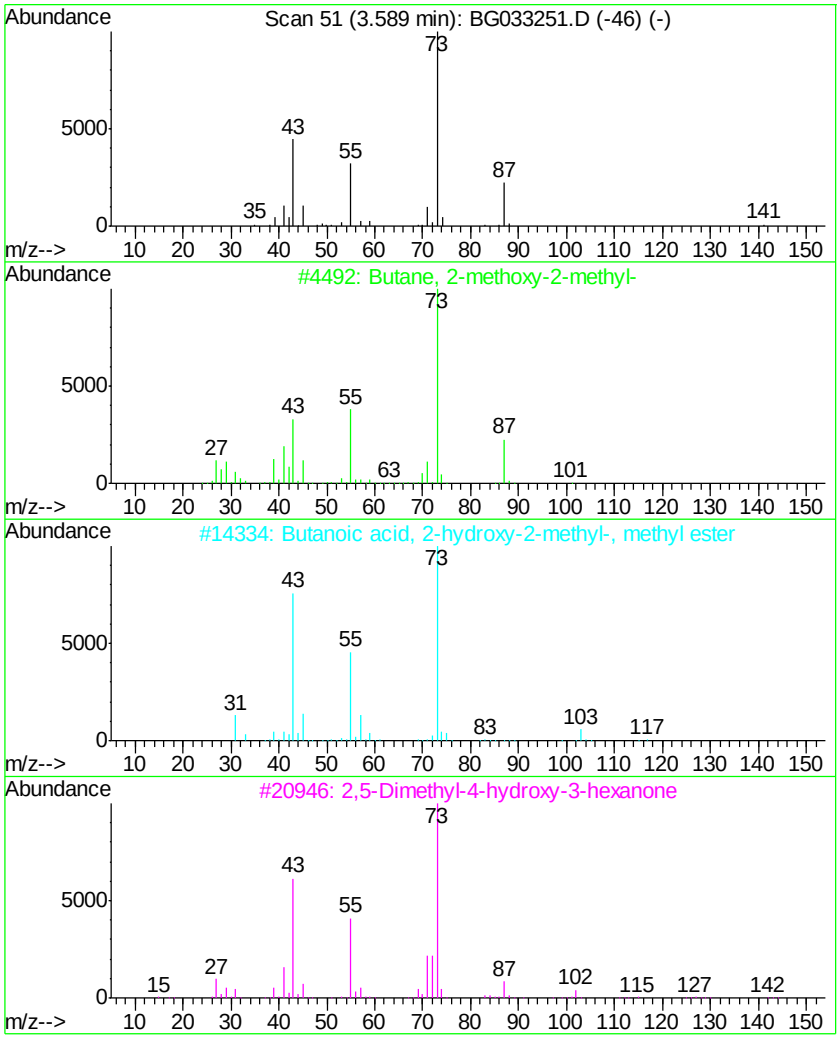
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

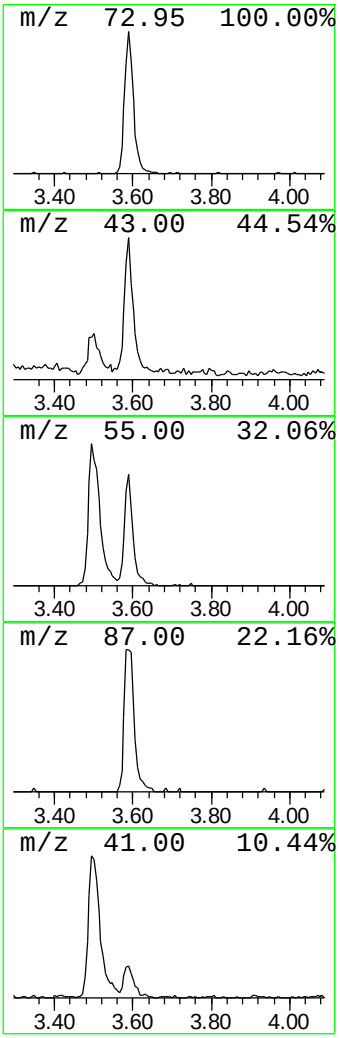
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.59	12.36 ng	145982	1,4-Dichlorobenzene-d4	8.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	Butanoic acid, 2-hydroxy-2-methy...	132	C6H12O3	032793-34-3	25
3	2,5-Dimethyl-4-hydroxy-3-hexanone	144	C8H16O2	000815-77-0	25
4	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	17
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	17





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Data File : BG033251.D
Acq On : 19 Mar 2018 22:13
Operator : SJ/JU
Sample : J1953-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-TIDO-F-D-S

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

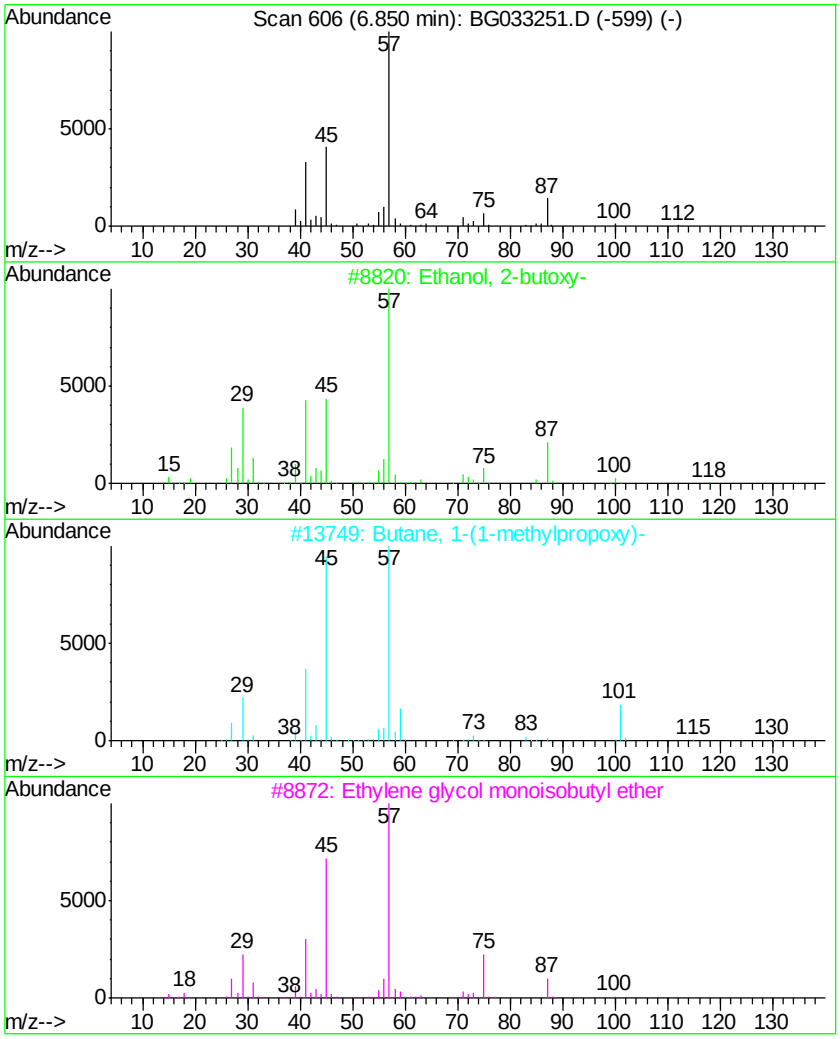
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

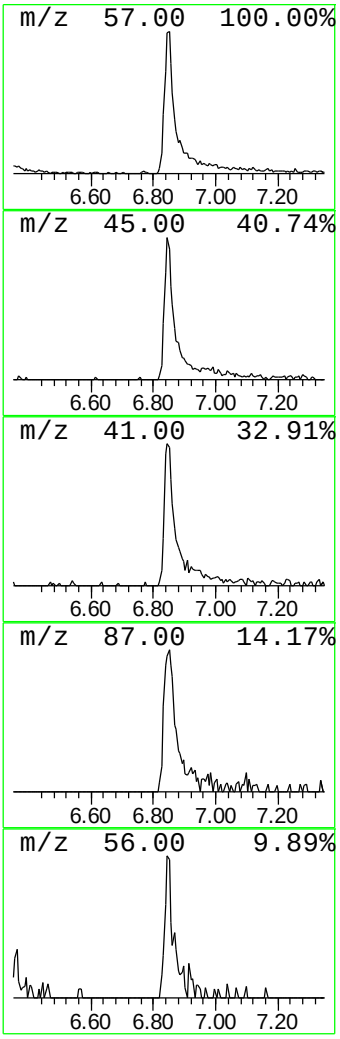
****

Peak Number 3 Ethanol, 2-butoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.85	14.46 ng	170802	1,4-Dichlorobenzene-d4	8.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	83
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	64
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
4	3-Ethyl-5-hexen-3-ol	128	C8H16O	001907-46-6	45
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	40





Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033251.D
Acq On : 19 Mar 2018 22:13
Operator : SJ/JU
Sample : J1953-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-TIDO-F-D-S

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.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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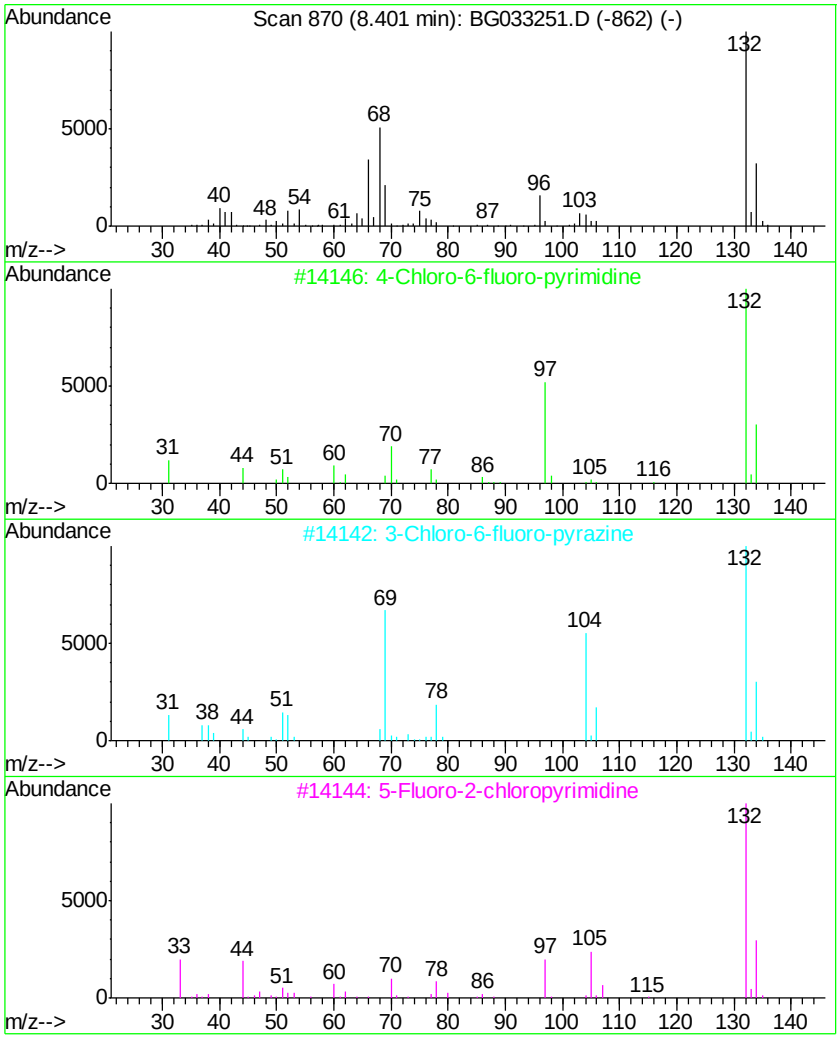
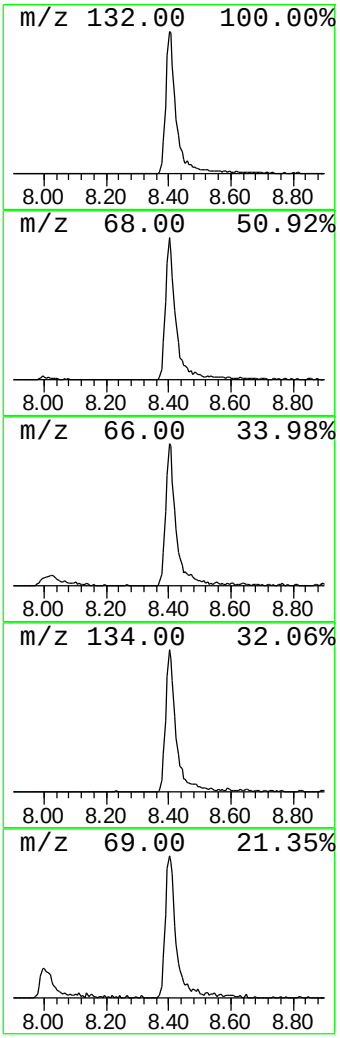
Peak Number 4 unknown8.40 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.40	62.45 ng	737762	1,4-Dichlorobenzene-d4	8.89

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	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
4	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	12
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	10





Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033251.D
Acq On : 19 Mar 2018 22:13
Operator : SJ/JU
Sample : J1953-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-TIDO-F-D-S

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

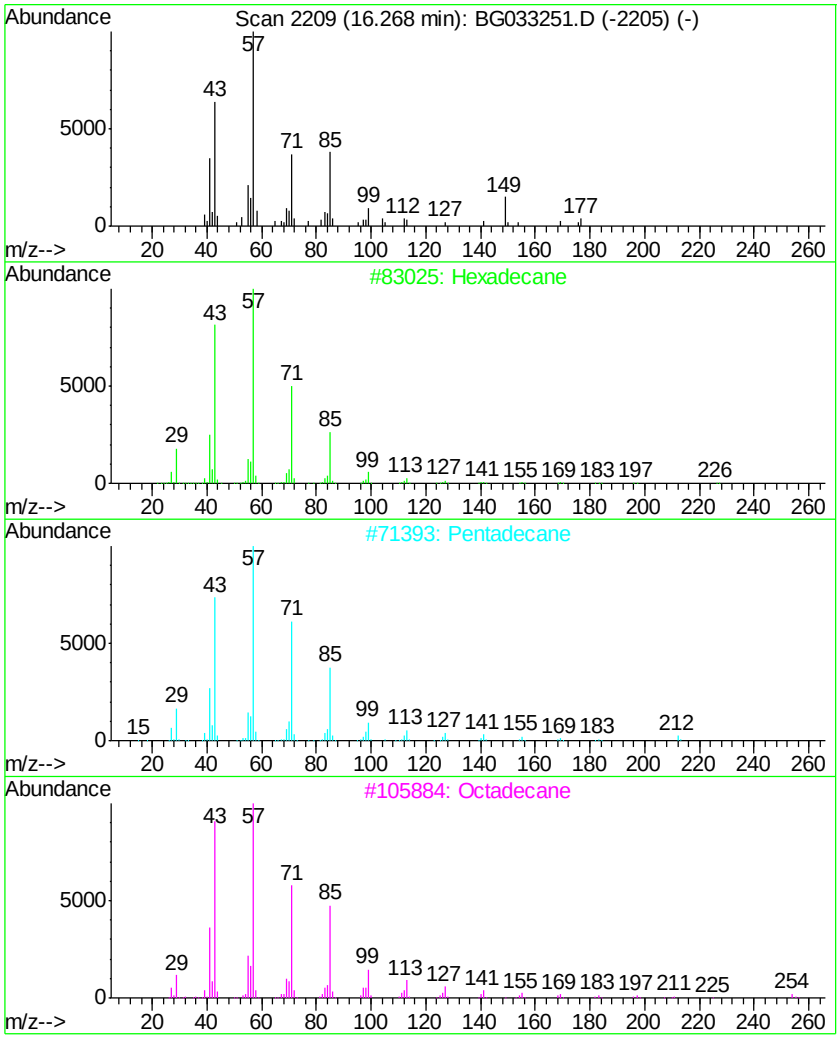
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

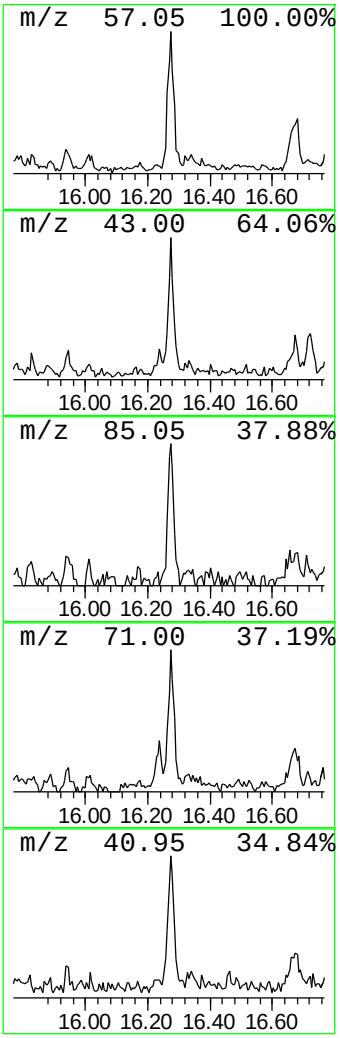
****

Peak Number 6 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.27	2.77 ng	74555	Acenaphthene-d10	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	80
2	Pentadecane	212	C15H32	000629-62-9	72
3	Octadecane	254	C18H38	000593-45-3	64
4	Eicosane	282	C20H42	000112-95-8	64
5	Tetradecane	198	C14H30	000629-59-4	64





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033251.D
Acq On : 19 Mar 2018 22:13
Operator : SJ/JU
Sample : J1953-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-TIDO-F-D-S

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

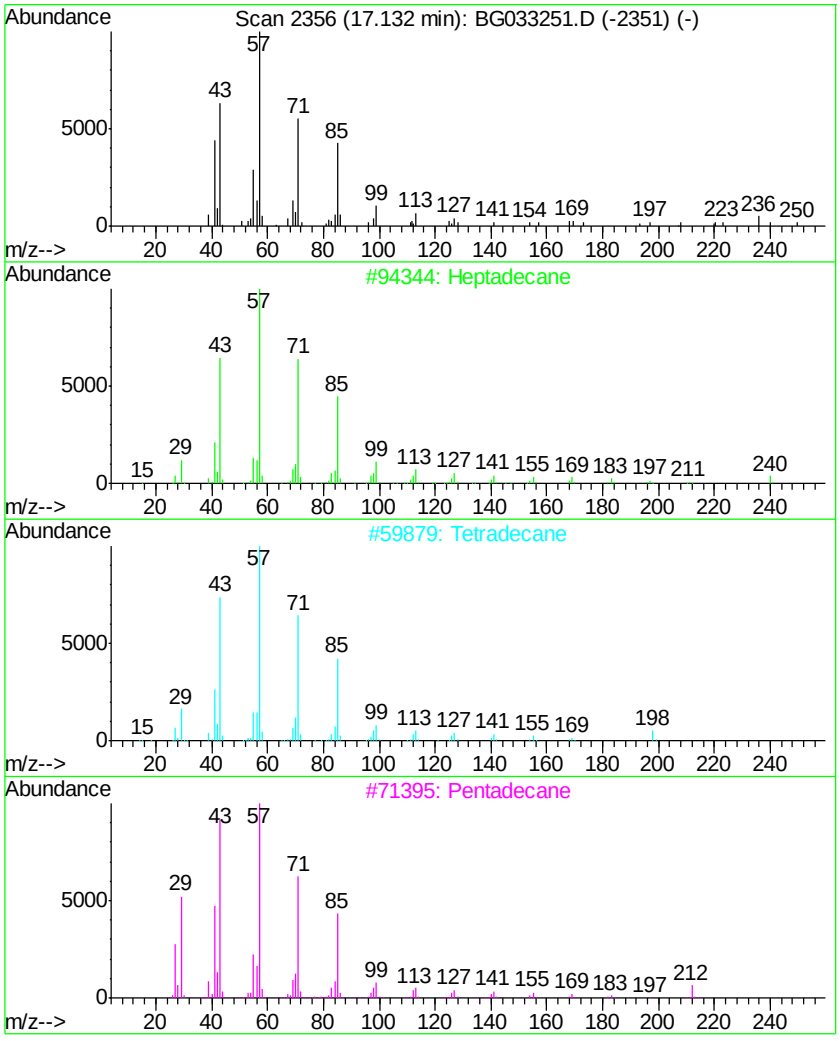
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

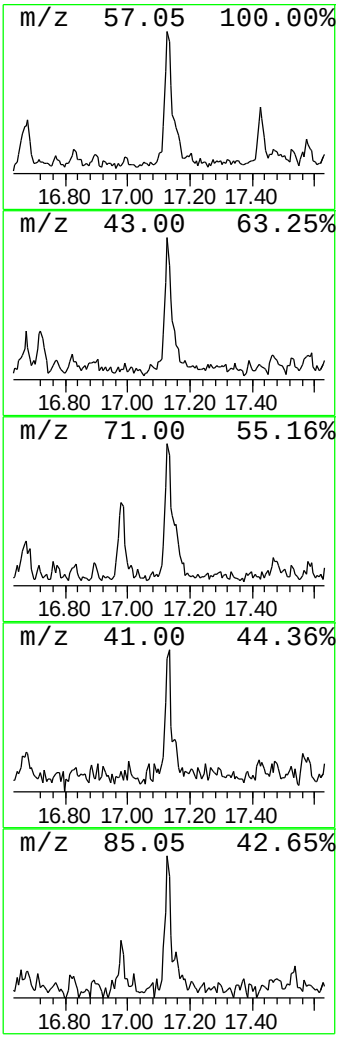
****

Peak Number 7 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.13	2.22 ng	91154	Phenanthrene-d10	18.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	87
2	Tetradecane	198	C14H30	000629-59-4	80
3	Pentadecane	212	C15H32	000629-62-9	72
4	Heptacosane	380	C27H56	000593-49-7	58
5	Octacosane	394	C28H58	000630-02-4	58





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Sample : J1953-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-TIDO-F-D-S

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.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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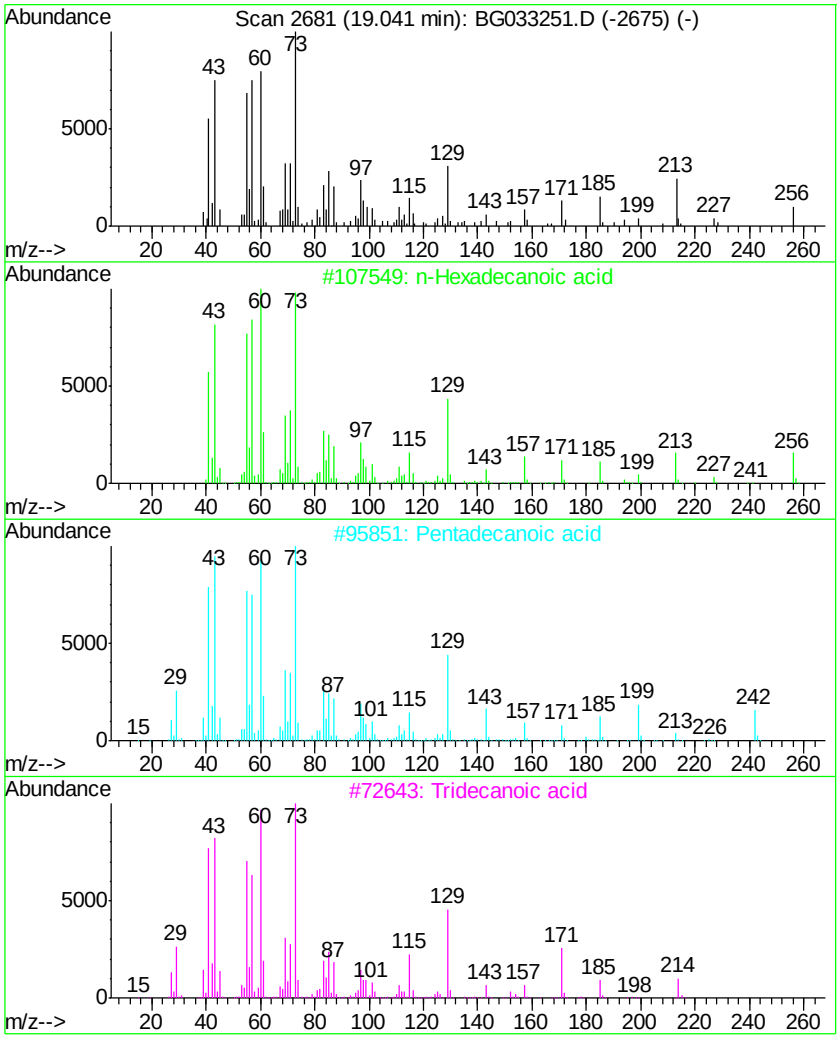
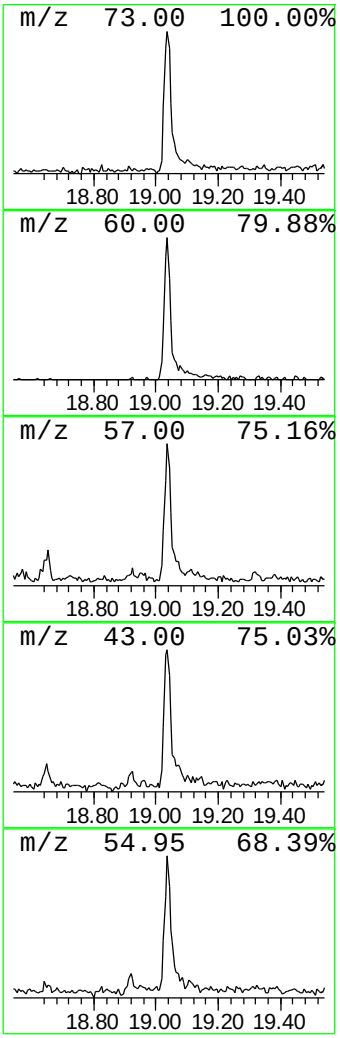
Peak Number 8 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.04	5.52 ng	226679	Phenanthrene-d10	18.24

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	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





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Instrument : BNA_G
ClientSampleId : 031418-TIDO-F-D-S

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

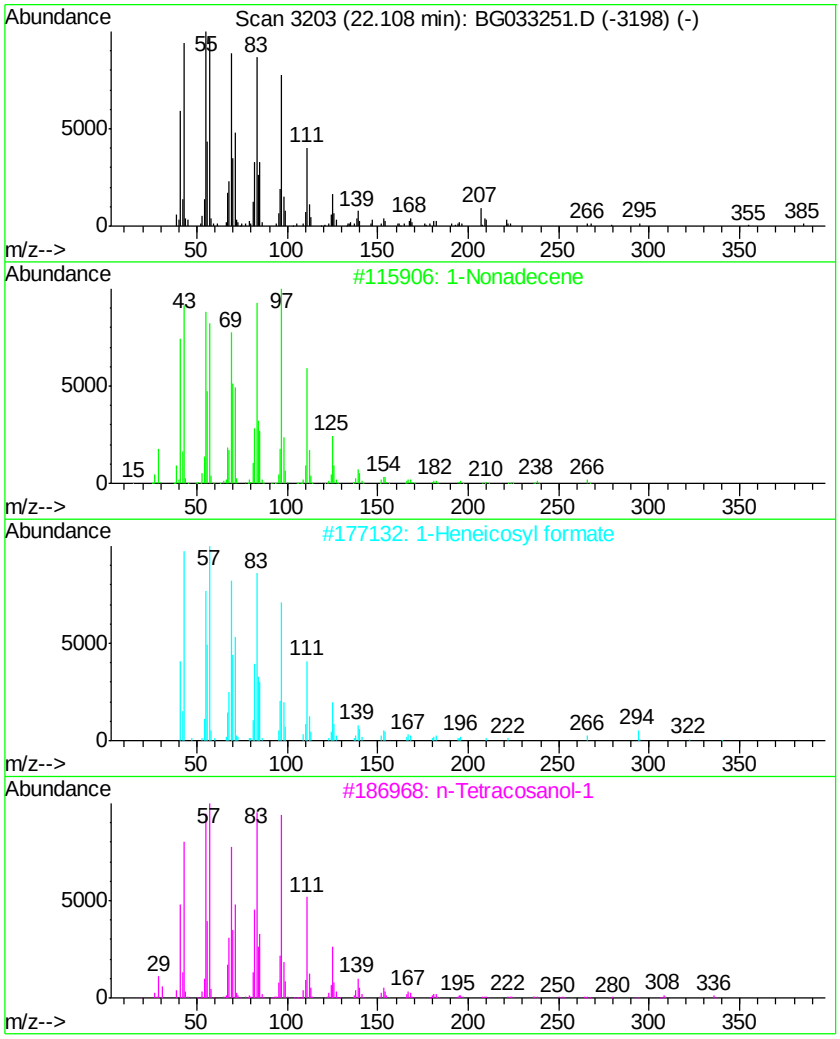
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

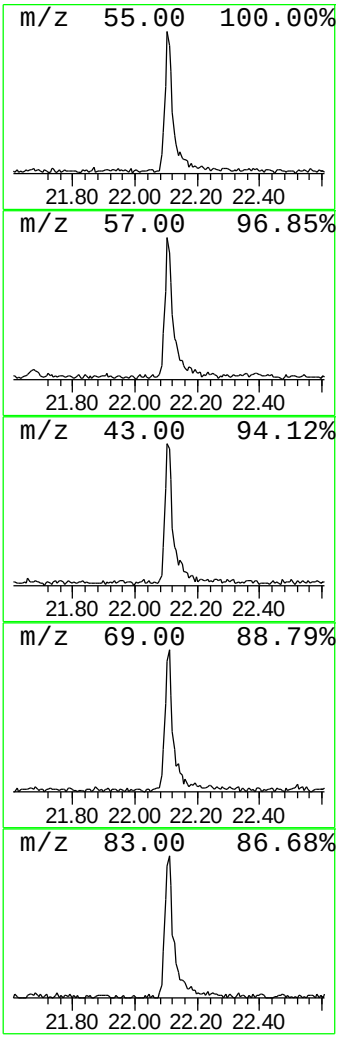
****

Peak Number 9 1-Nonadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.11	7.18 ng	332535	Chrysene-d12	22.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	98
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	90
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	89





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TIC Library : C:\Database\NIST11.L
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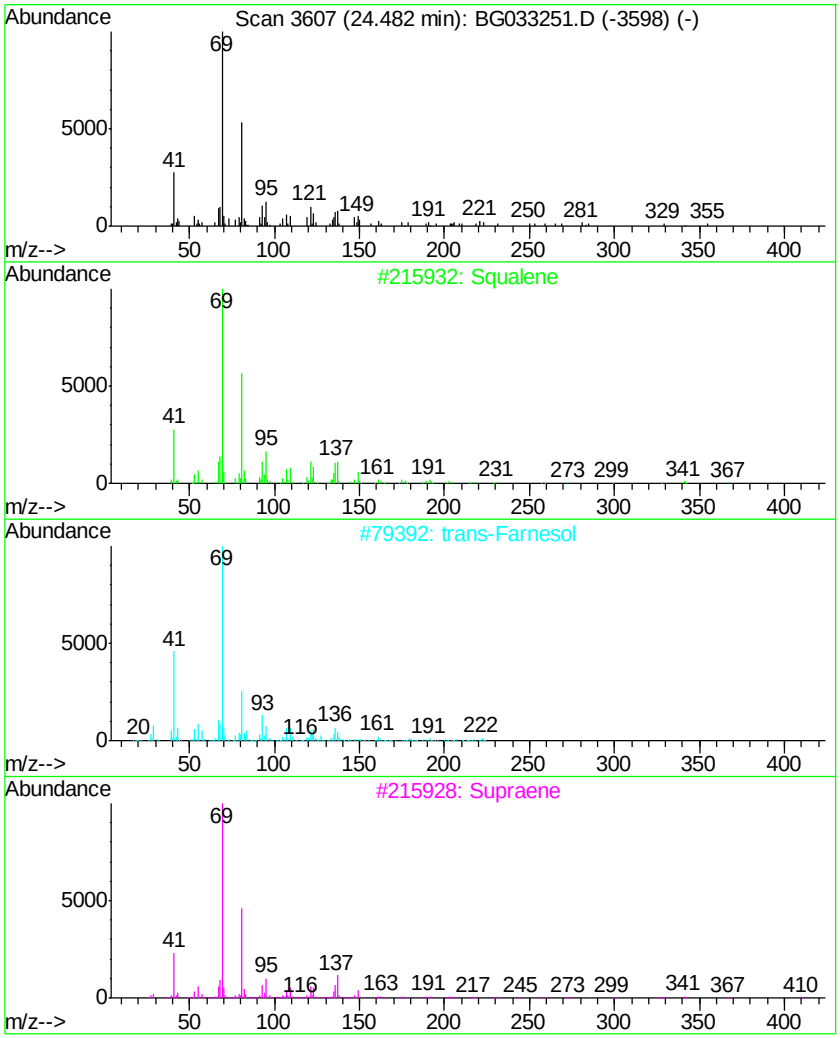
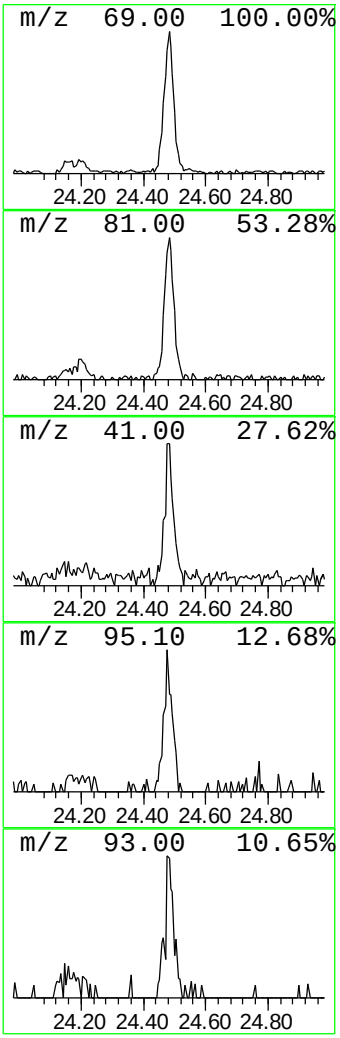
Peak Number 10 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.48	3.43 ng	158630	Chrysene-d12	22.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	80
2	trans-Farnesol	222	C15H26O	000106-28-5	70
3	Supraene	410	C30H50	007683-64-9	64
4	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	59
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	59





Tentatively Identified Compound (LSC) summary

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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...	3.59	12.4	ng	145982	1	8.89	236257	20.0
Ethanol, 2-butoxy-	6.85	14.5	ng	170802	1	8.89	236257	20.0
unknown8.40	8.40	62.5	ng	737762	1	8.89	236257	20.0
Hexadecane	16.27	2.8	ng	74555	3	15.51	538734	20.0
Heptadecane	17.13	2.2	ng	91154	4	18.24	820721	20.0
n-Hexadecanoic acid	19.04	5.5	ng	226679	4	18.24	820721	20.0
1-Nonadecene	22.11	7.2	ng	332535	5	22.59	926250	20.0
Squalene	24.48	3.4	ng	158630	5	22.59	926250	20.0