LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101417\
Data File : BF099496.D
Acq On : 15 Oct 2017 00:19
Operator : SJ/JU
Sample : I5853-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-BPM-02-003-ABCD

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_F\METHODS\8270-BF092317.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	5.087	507	510	525	rBV	339123	460349	16.56%	2.020%
2	5.487	573	578	581	rBV	2435418	2430965	87.42%	10.667%
3	6.493	744	749	767	rBV	2229611	2605826	93.71%	11.434%
4	6.628	767	772	775	rBV	2754693	2562061	92.14%	11.242%
5	6.851	807	810	818	rVB	682384	548713	19.73%	2.408%
6	7.010	833	837	840	rBV	2231642	2031809	73.07%	8.915%
7	7.422	902	907	910	rBV	1563199	1602430	57.63%	7.031%
8	8.134	1024	1028	1039	rBV	883550	748985	26.94%	3.286%
9	9.210	1205	1211	1214	rBV	2979835	2780633	100.00%	12.201%
10	9.604	1274	1278	1289	rBV	461531	439464	15.80%	1.928%
11	9.886	1322	1326	1338	rVB2	893920	804010	28.91%	3.528%
12	10.680	1457	1461	1470	rBV	1471570	1375037	49.45%	6.033%
13	11.375	1576	1579	1585	rBV	775022	727086	26.15%	3.190%
14	12.957	1844	1848	1852	rBV	2020238	1944077	69.91%	8.530%
15	13.839	1995	1998	2002	rBV2	84814	94963	3.42%	0.417%
16	14.016	2025	2028	2037	rVB	457077	491597	17.68%	2.157%
17	14.104	2040	2043	2047	rVB3	27553	29307	1.05%	0.129%
18	14.474	2102	2106	2115	rVB6	41133	89392	3.21%	0.392%
19	15.098	2209	2212	2216	rBV3	36122	54199	1.95%	0.238%
20	15.492	2274	2279	2292	rVB	365224	542128	19.50%	2.379%
21	15.680	2308	2311	2314	rBV4	31556	47310	1.70%	0.208%
22	15.910	2346	2350	2355	rVB2	47383	70361	2.53%	0.309%
23	16.404	2431	2434	2439	rVB2	36853	58771	2.11%	0.258%
24	16.992	2530	2534	2541	rBV3	30798	59891	2.15%	0.263%
25	18.315	2752	2759	2769	rBV8	65451	191264	6.88%	0.839%

Sum of corrected areas: 22790628

LSC Report - Integrated Chromatogram

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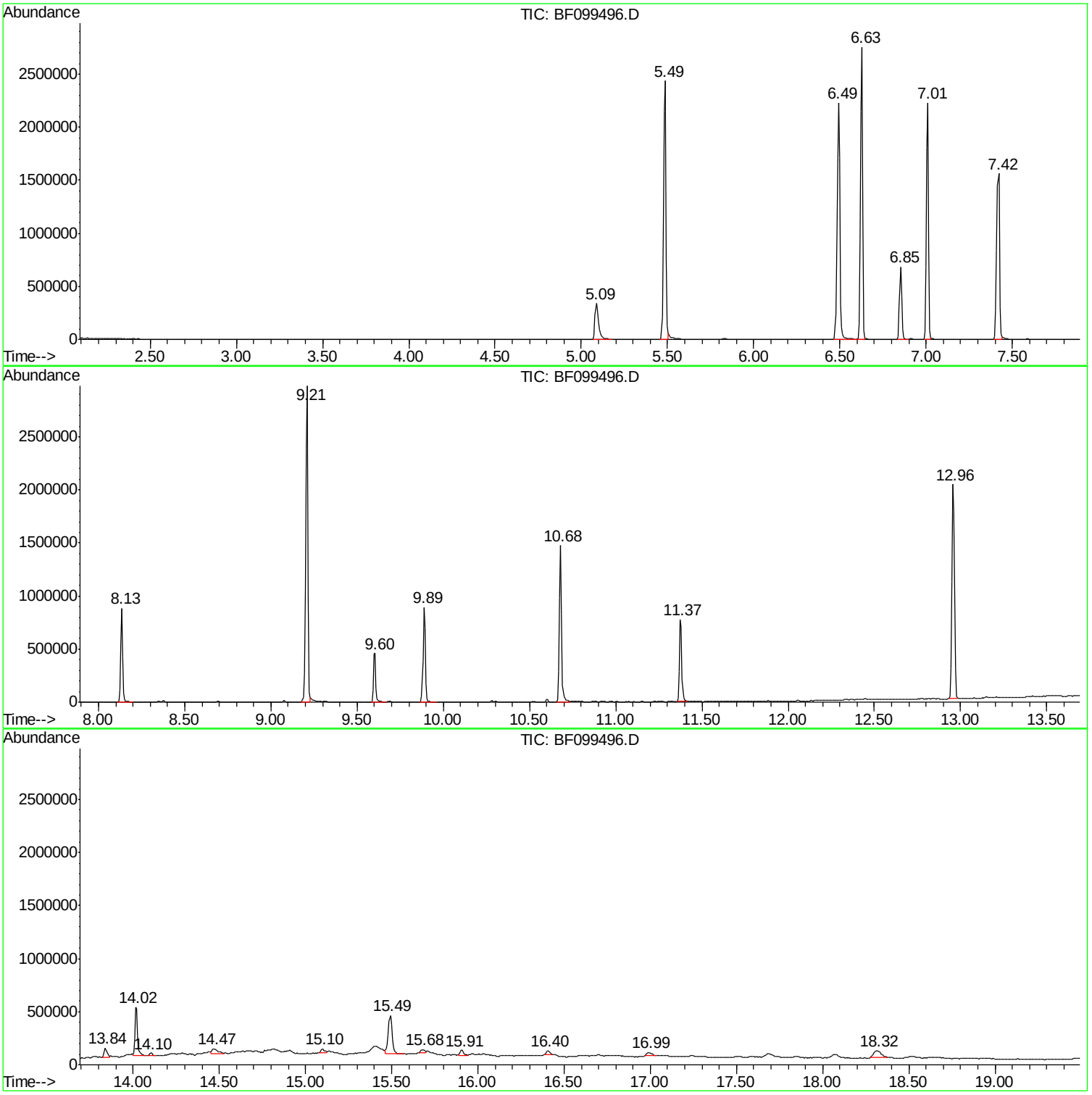
Instrument :
BNA_F
ClientSampleId :
FK-BPM-02-003-ABCD

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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:\HPCHEM1\BNA_F\DATA\BF101417\
Data File : BF099496.D
Acq On : 15 Oct 2017 00:19
Operator : SJ/JU
Sample : I5853-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-BPM-02-003-ABCD

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

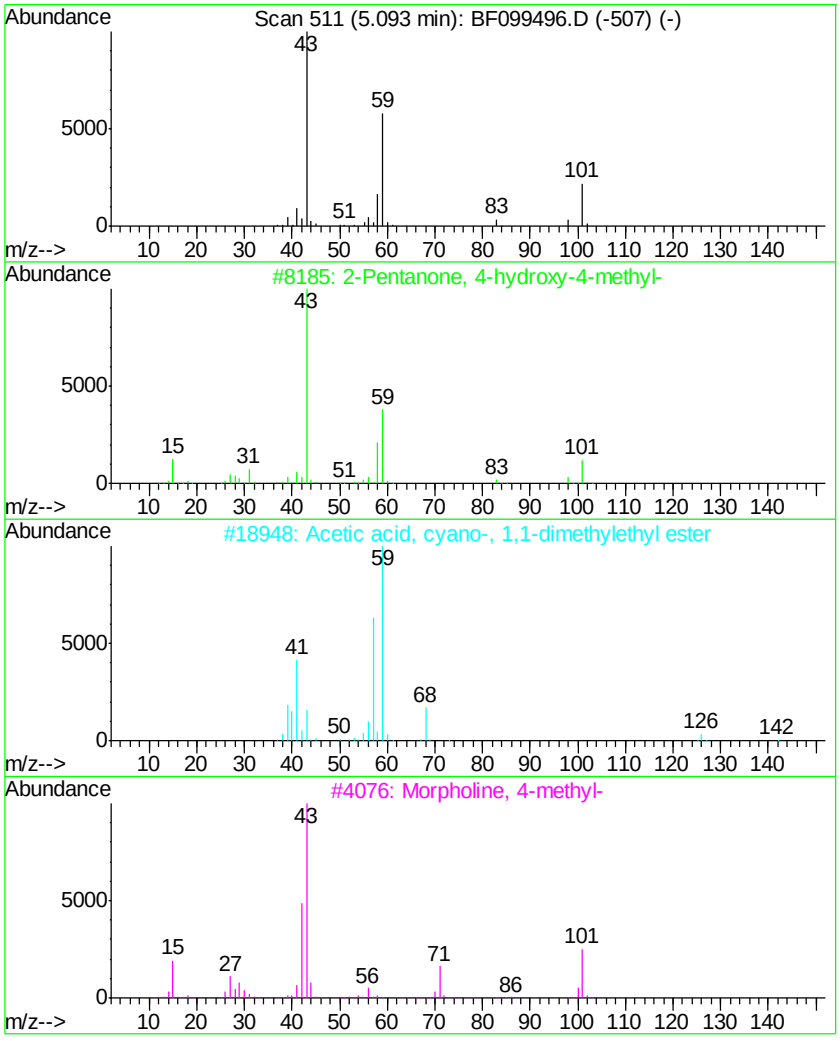
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

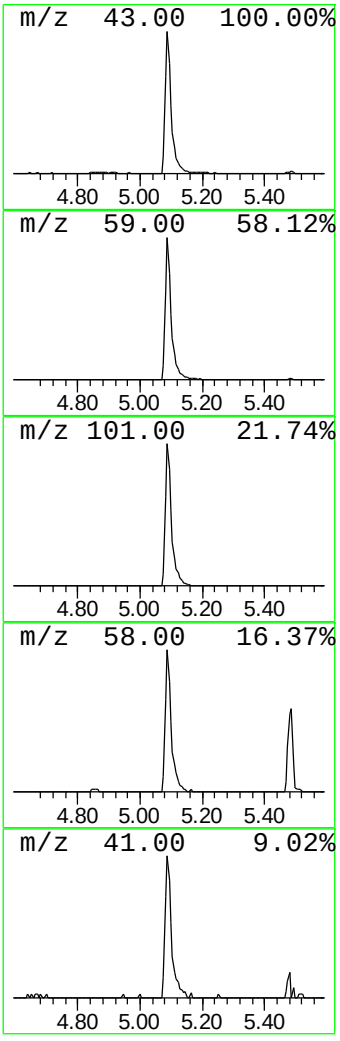
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	16.78 ng	460349	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Allyl acetate	100	C5H8O2	000591-87-7	9
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9





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Instrument : BNA_F
ClientSampleId : FK-BPM-02-003-ABCD

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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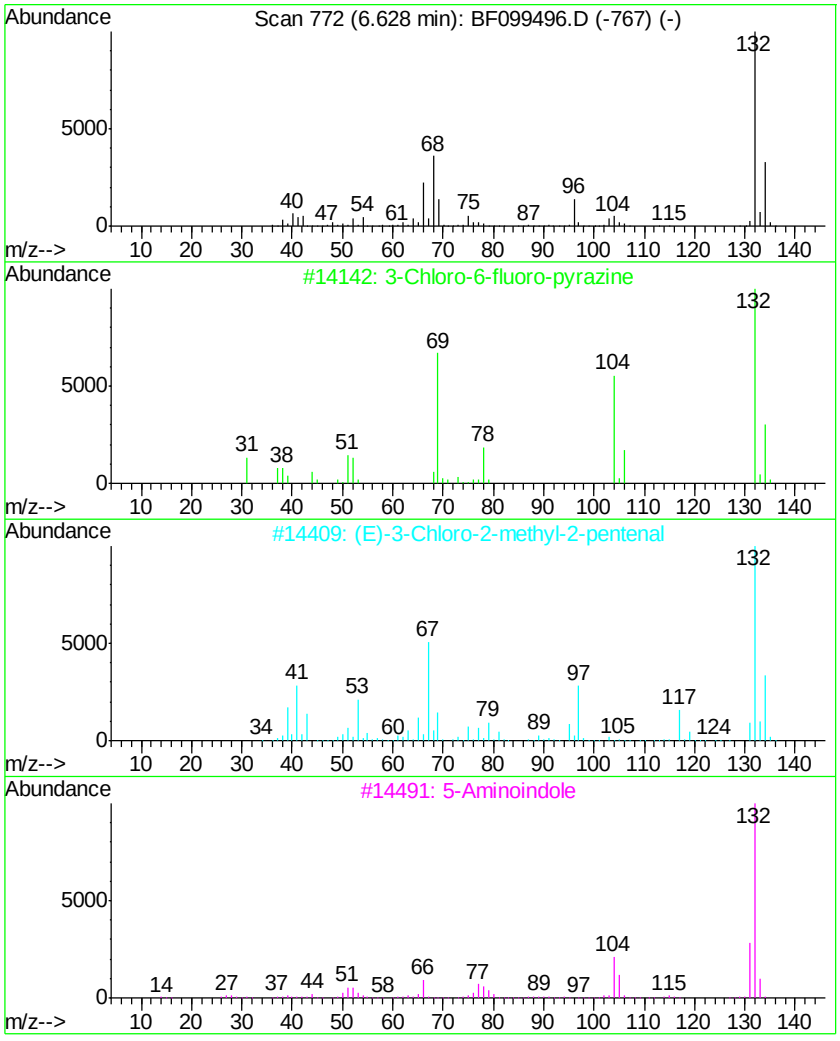
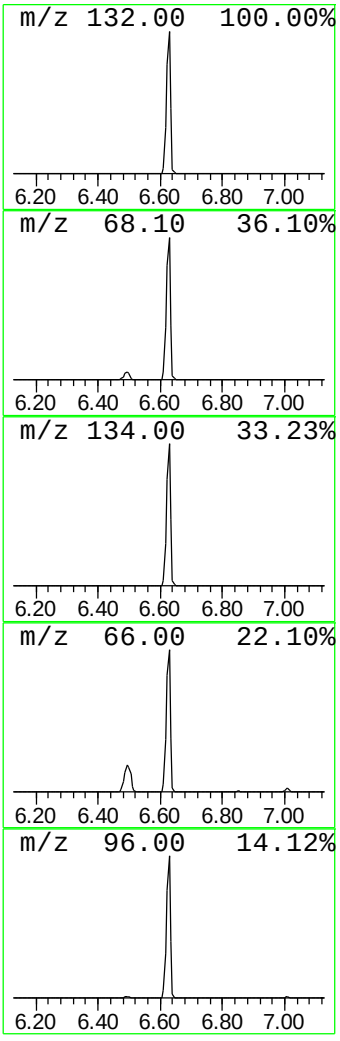
Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	93.38 ng	2562060	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Xenon	132	Xe	007440-63-3	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





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Sample : I5853-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-BPM-02-003-ABCD

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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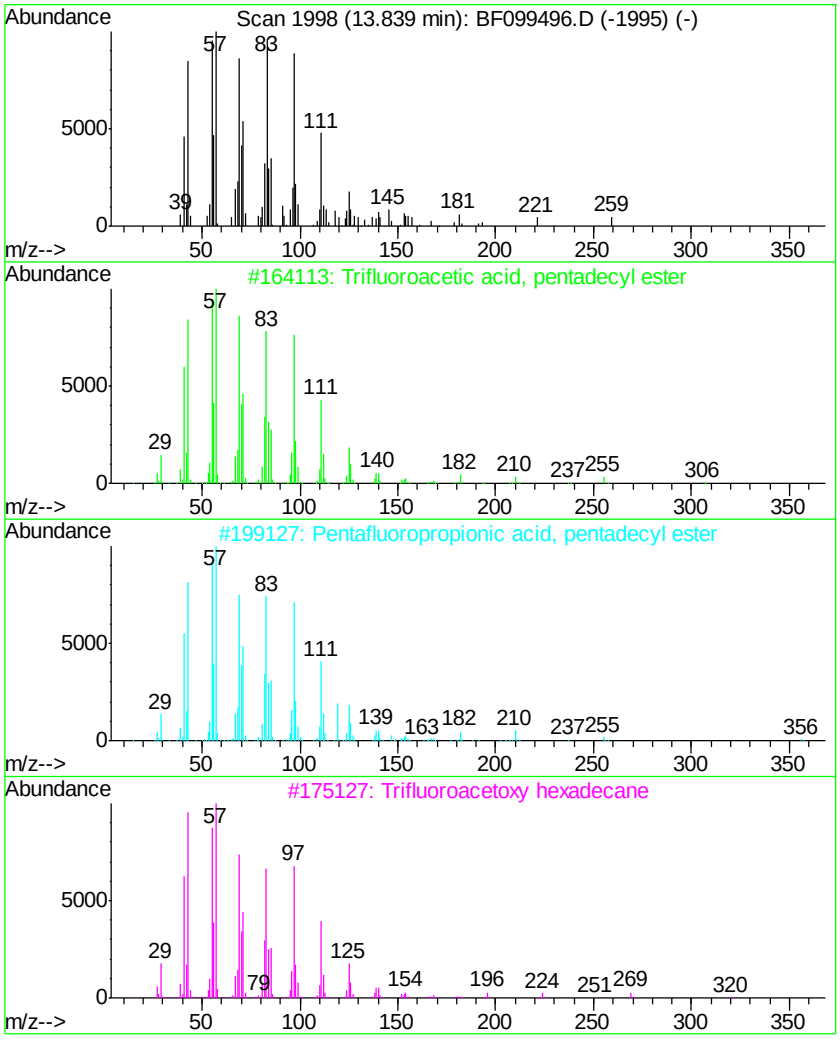
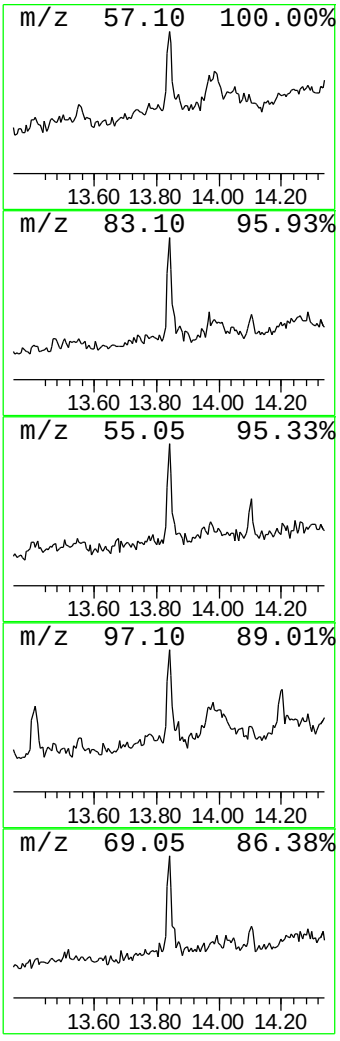
Peak Number 4 Trifluoroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	3.86 ng	94963	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94





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Sample : I5853-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-BPM-02-003-ABCD

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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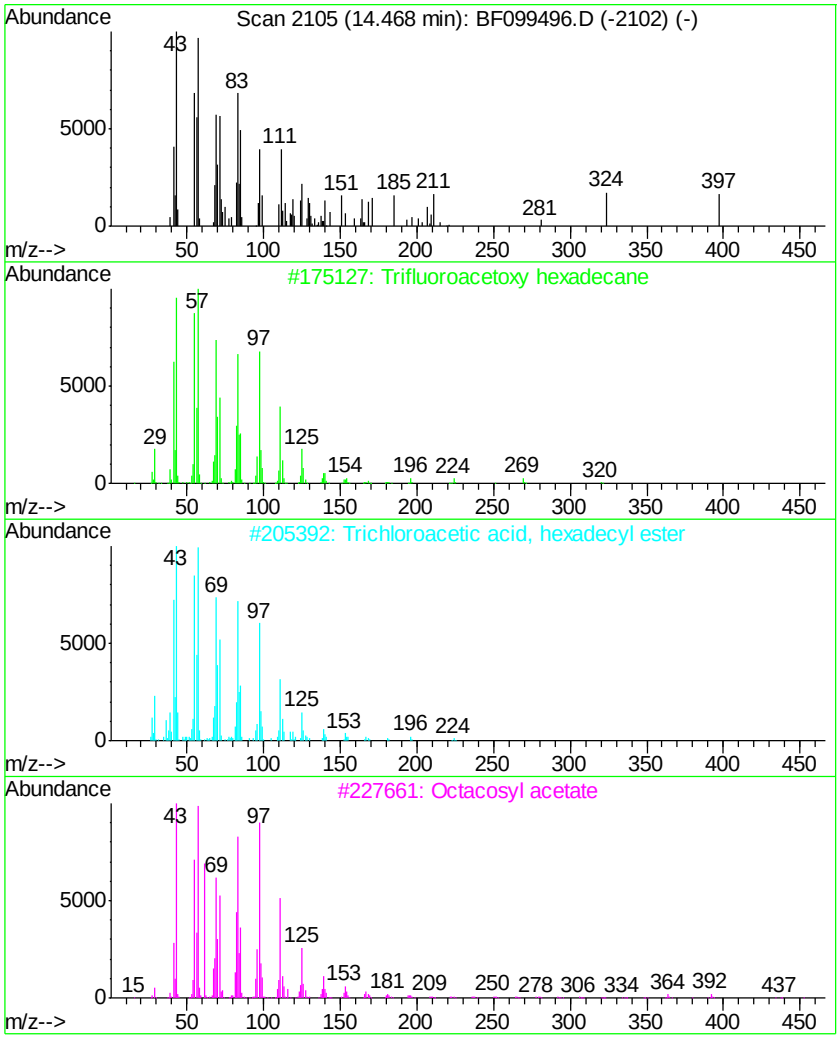
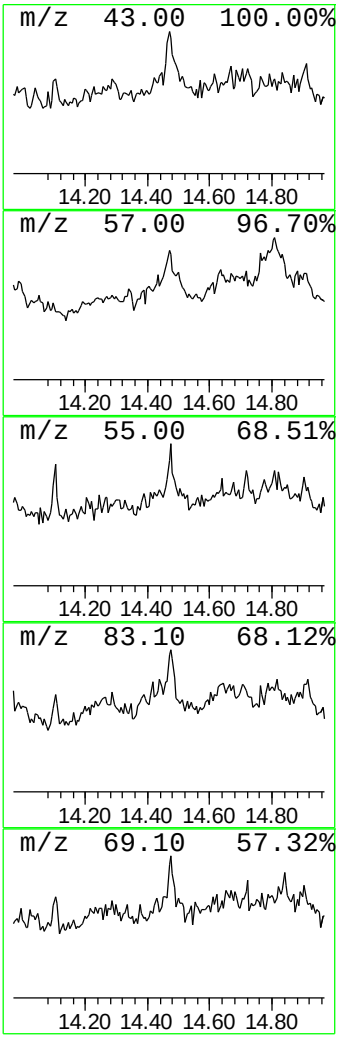
Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	3.64 ng	89392	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	76
3	Octacosyl acetate	452	C30H60O2	018206-97-8	74
4	Behenic alcohol	326	C22H46O	000661-19-8	74
5	Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	74





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Data File : BF099496.D
Acq On : 15 Oct 2017 00:19
Operator : SJ/JU
Sample : I5853-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-BPM-02-003-ABCD

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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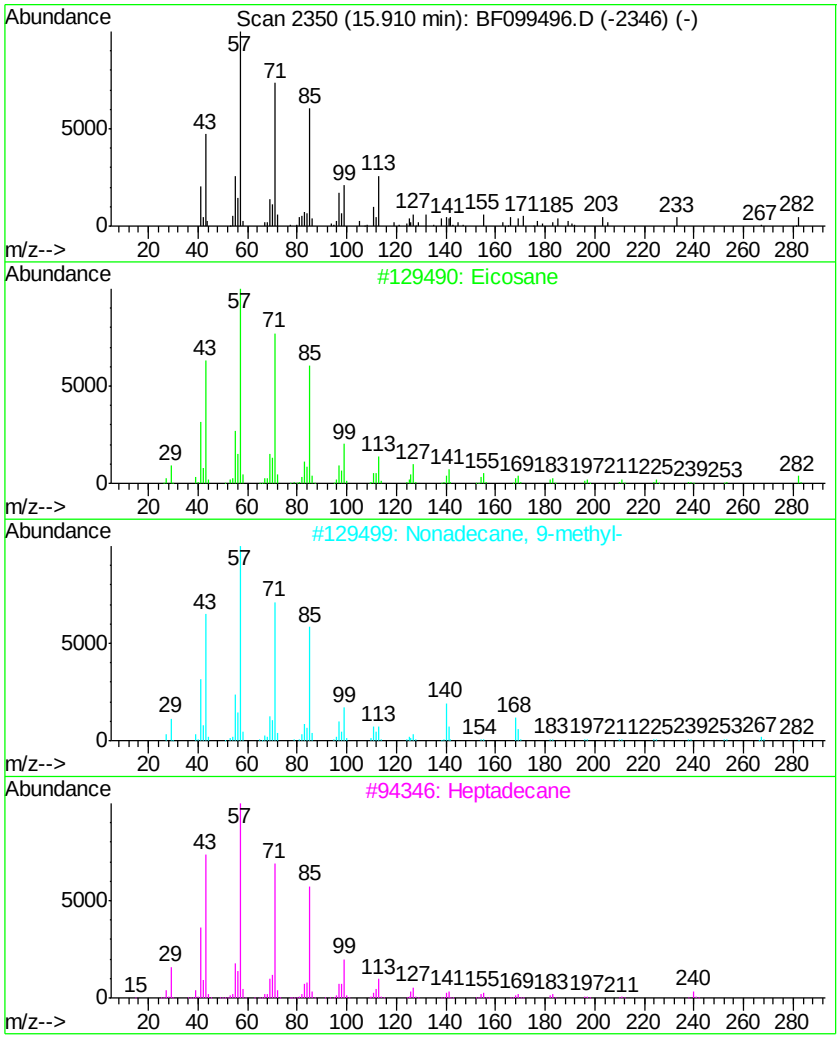
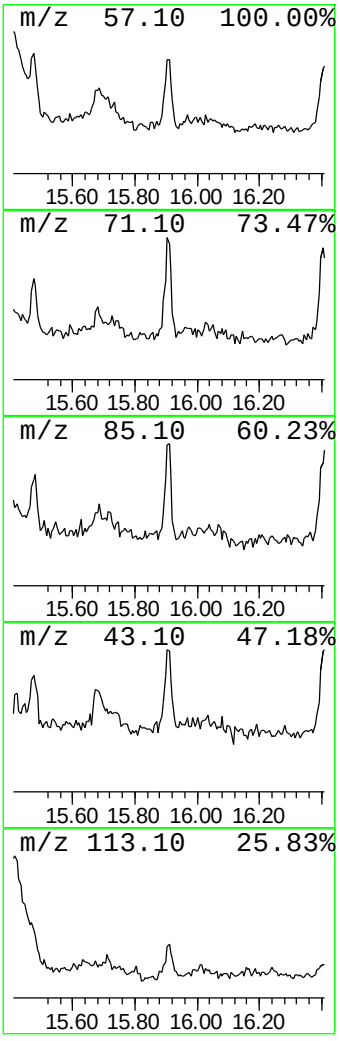
Peak Number 6 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.91	2.60 ng	70361	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	80
3	Heptadecane	240	C17H36	000629-78-7	74
4	Heneicosane	296	C21H44	000629-94-7	72
5	Hexacosane	366	C26H54	000630-01-3	72





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Sample : I5853-01
Misc :
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Instrument :
BNA_F
ClientSampleId :
FK-BPM-02-003-ABCD

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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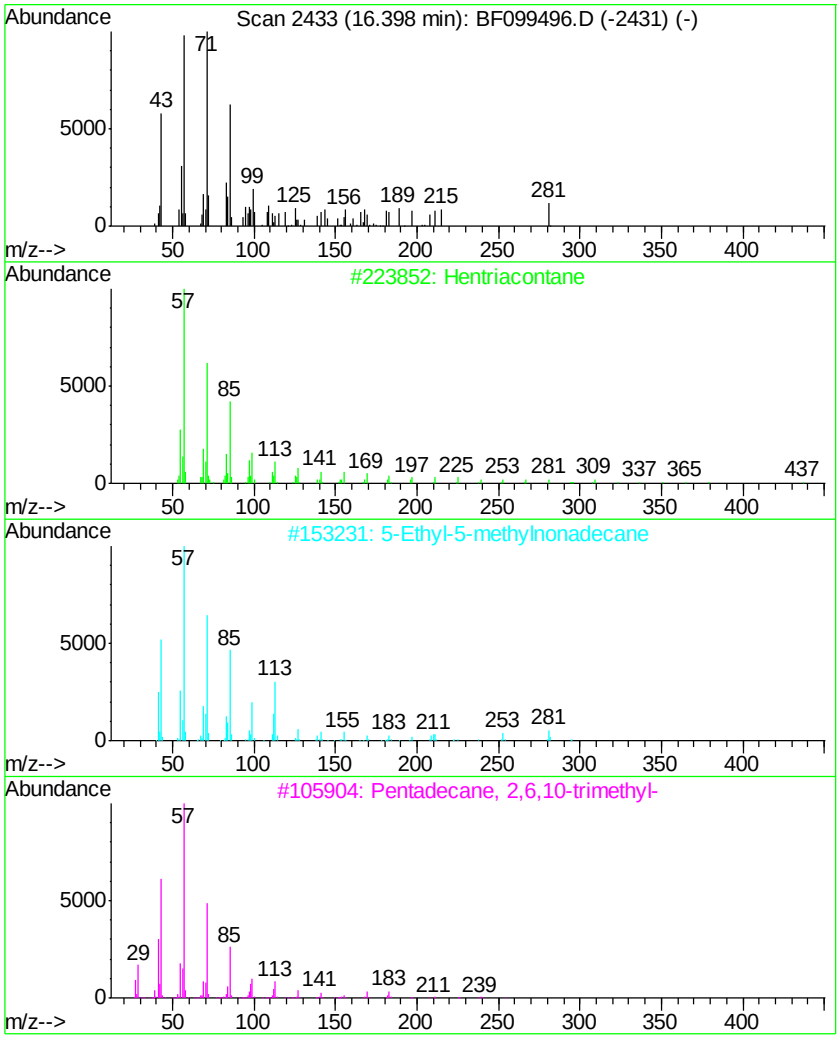
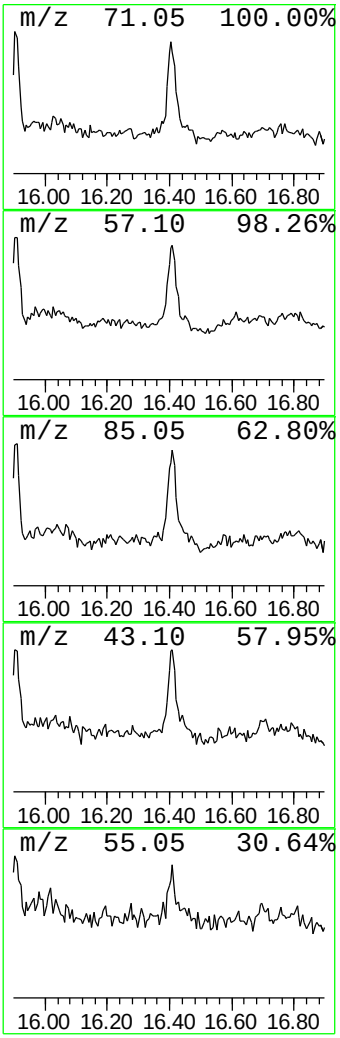
Peak Number 7 Hentriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.40	2.17 ng	58771	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	74
2	5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	72
3	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	72
4	Hexadecane	226	C16H34	000544-76-3	59
5	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	59





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Instrument : BNA_F
ClientSampleId : FK-BPM-02-003-ABCD

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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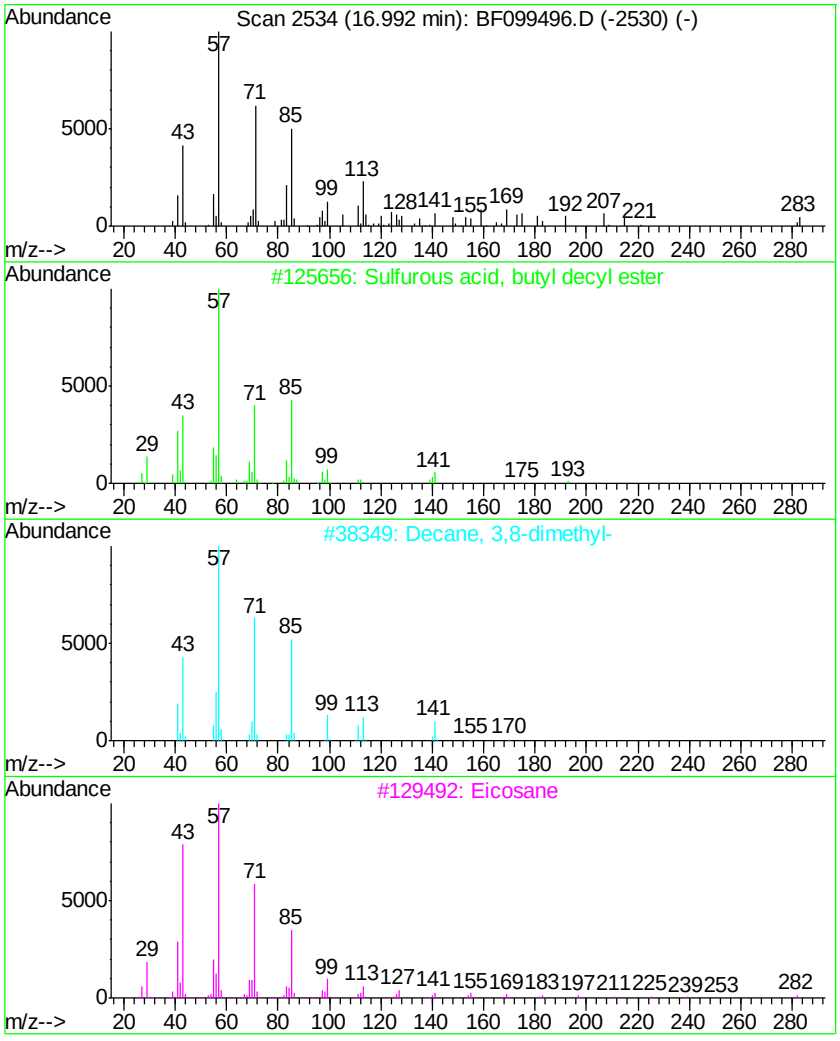
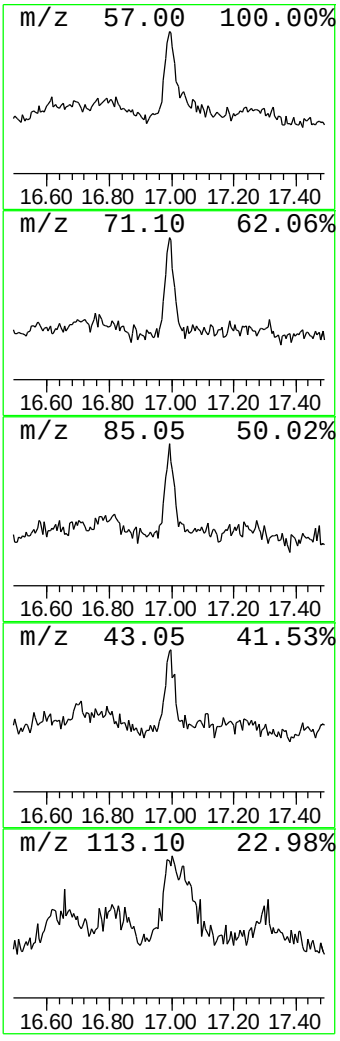
Peak Number 8 Sulfurous acid, butyl decyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.99	2.21 ng	59891	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	53
2	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	53
3	Eicosane	282	C20H42	000112-95-8	52
4	Undecane	156	C11H24	001120-21-4	50
5	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	50





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TIC Library : C:\DATABASE\NIST11.L
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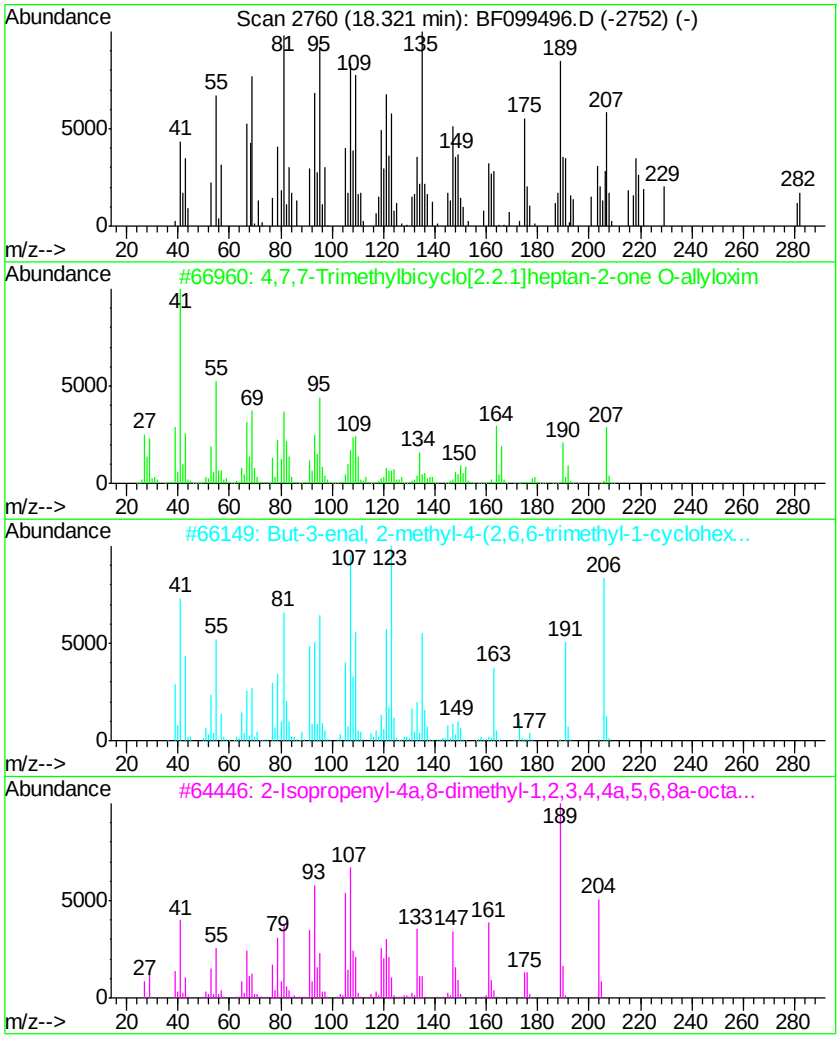
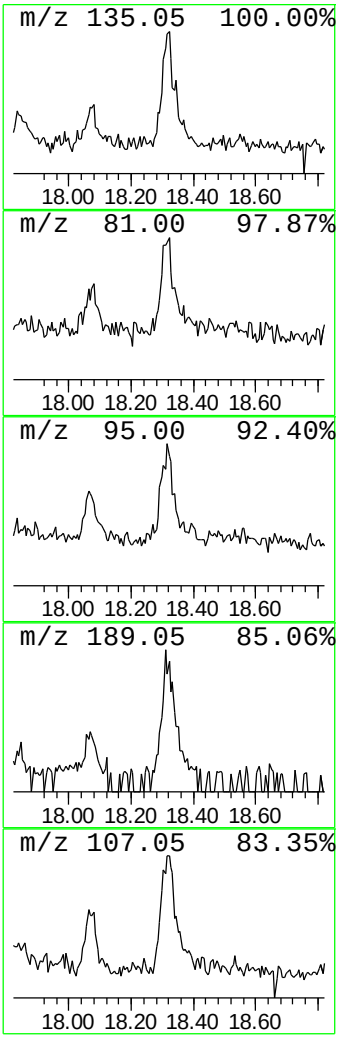
Peak Number 9 unknown18.32 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.32	7.06 ng	191264	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,7,7-Trimethylbicyclo[2.2.1]hep...	207	C13H21NO	1000210-89-8	38
2	But-3-enal, 2-methyl-4-(2,6,6-tr...	206	C14H22O	104900-59-6	38
3	2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000193-57-0	35
4	1,3-Cyclopentadiene, 2,3,4,5-tet...	190	C14H22	1000161-28-7	30
5	1,1,6-trimethyl-3-methylene-2-(3...	452	C33H56	1000373-94-5	27





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
2-Pentanone, 4-hy...	5.09	16.8	ng	460349	1	6.85	548713	20.0
unknown6.63	6.63	93.4	ng	2562060	1	6.85	548713	20.0
Trifluoroacetic a...	13.84	3.9	ng	94963	5	14.02	491597	20.0
Trifluoroacetoxy ...	14.47	3.6	ng	89392	5	14.02	491597	20.0
Eicosane	15.91	2.6	ng	70361	6	15.49	542128	20.0
Hentriacontane	16.40	2.2	ng	58771	6	15.49	542128	20.0
Sulfurous acid, b...	16.99	2.2	ng	59891	6	15.49	542128	20.0
unknown18.32	18.32	7.1	ng	191264	6	15.49	542128	20.0