LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100418\
Data File : BF109587.D
Acq On : 4 Oct 2018 15:30
Operator : JU/SJ
Sample : J5221-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100118-JETT-E-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_F\METHODS\8270-BF092218.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	4.887	473	476	484	rBV	73612	87547	2.90%	0.465%
2	5.316	545	549	567	rBV	664583	760153	25.16%	4.041%
3	6.340	720	723	742	rBV	376163	542741	17.96%	2.885%
4	6.475	742	746	769	rVV	1621148	1555680	51.49%	8.270%
5	6.704	781	785	794	rBV	530990	512764	16.97%	2.726%
6	6.863	808	812	815	rBV	2248875	2028279	67.13%	10.783%
7	7.269	876	881	907	rBV	1596516	1805107	59.75%	9.596%
8	7.987	999	1003	1023	rBV	651554	669971	22.18%	3.562%
9	9.063	1181	1186	1189	rBV	3285002	3021237	100.00%	16.061%
10	9.451	1249	1252	1257	rBV	41339	34964	1.16%	0.186%
11	9.734	1296	1300	1315	rVB	815732	717240	23.74%	3.813%
12	10.522	1430	1434	1448	rBV	1022864	1061306	35.13%	5.642%
13	11.210	1548	1551	1564	rBV	560190	591525	19.58%	3.145%
14	11.745	1640	1642	1646	rBV	33721	37441	1.24%	0.199%
15	12.798	1816	1821	1824	rBV	2066424	2115459	70.02%	11.246%
16	13.374	1917	1919	1929	rVB2	45295	78424	2.60%	0.417%
17	13.704	1972	1975	1983	rVB4	53558	85729	2.84%	0.456%
18	13.839	1994	1998	2009	rBV	598608	619491	20.50%	3.293%
19	14.016	2025	2028	2031	rBV	60109	64174	2.12%	0.341%
20	14.321	2077	2080	2083	rVB	124807	124758	4.13%	0.663%
21	14.610	2126	2129	2133	rBV	252375	252614	8.36%	1.343%
22	14.927	2179	2183	2187	rVB	370248	438433	14.51%	2.331%
23	15.245	2233	2237	2240	rBV	426822	530933	17.57%	2.822%
24	15.280	2240	2243	2248	rVB	384566	445812	14.76%	2.370%
25	15.680	2306	2311	2316	rVB	265053	400019	13.24%	2.127%
26	16.139	2384	2389	2397	rVB	133815	229012	7.58%	1.217%

Sum of corrected areas: 18810813

LSC Report - Integrated Chromatogram

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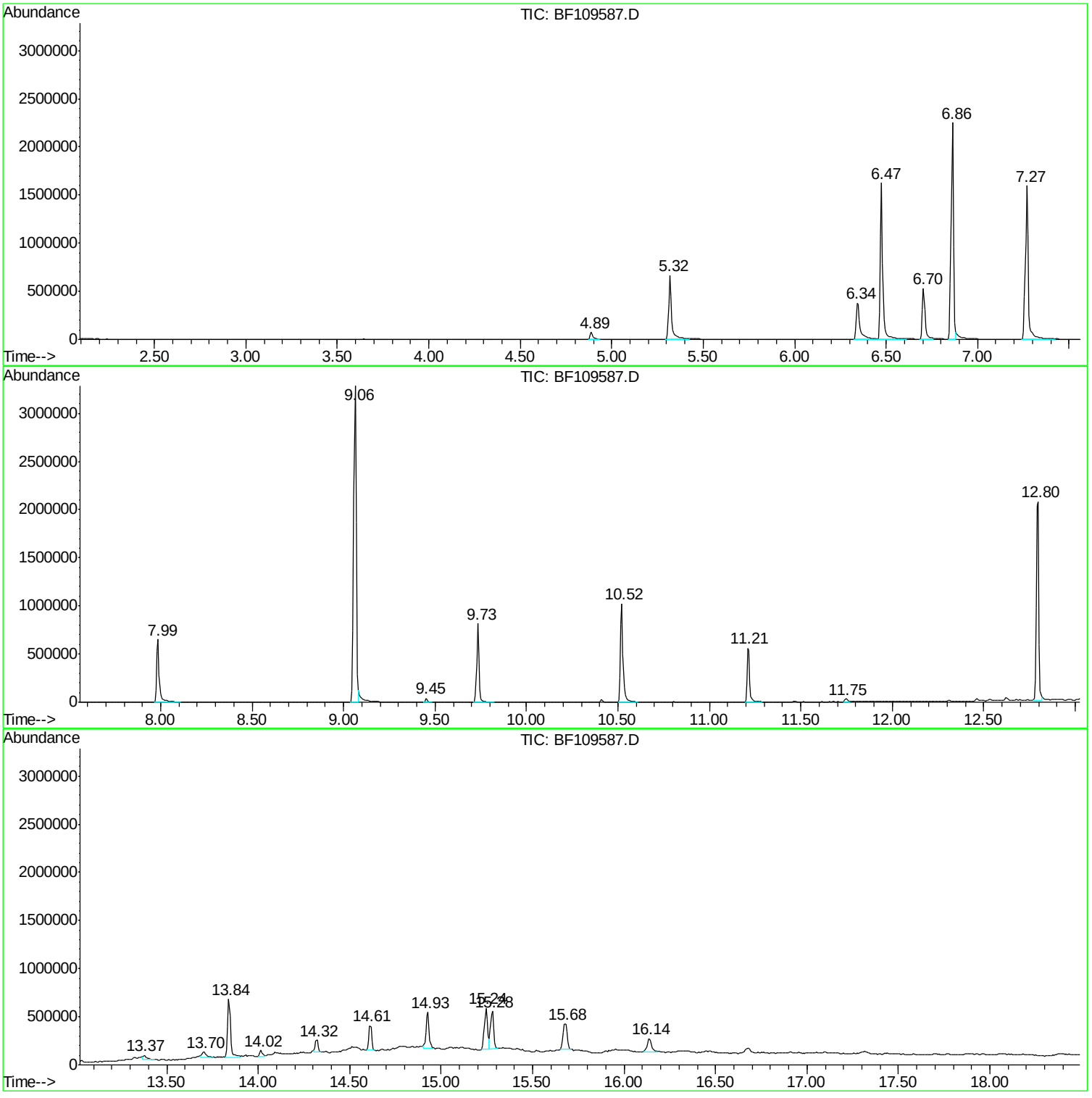
Operator : JU/SJ
Sample : J5221-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100118-JETT-E-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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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ClientSampleId : 100118-JETT-E-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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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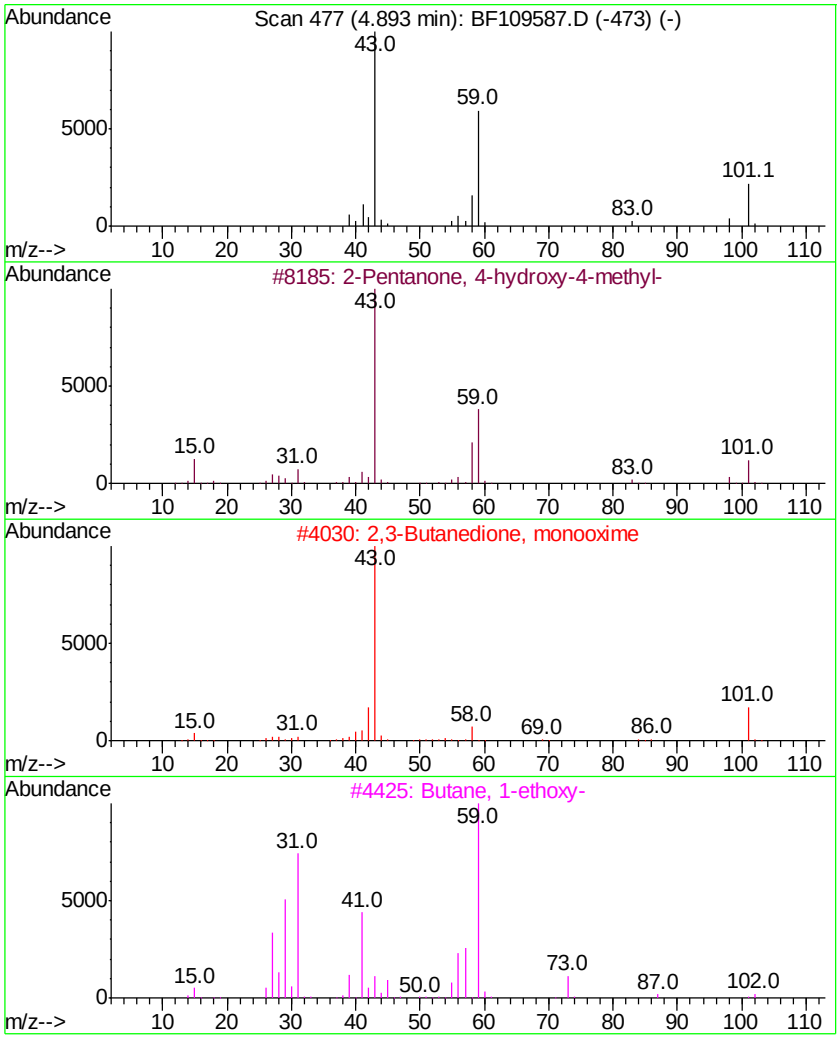
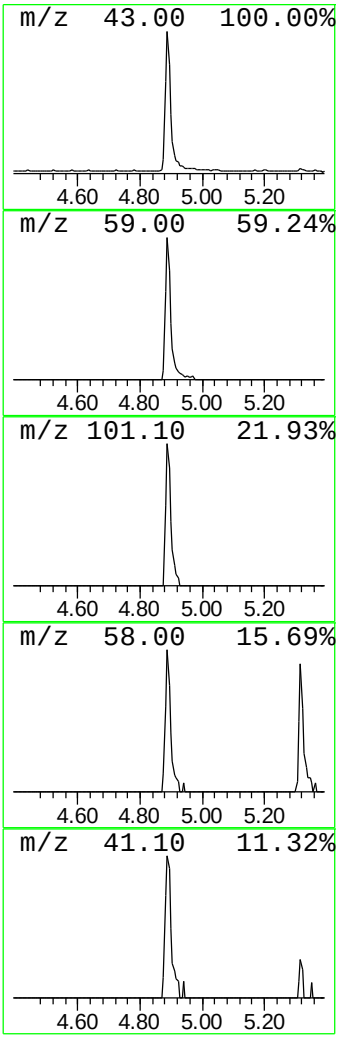
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	3.41 ng	87547	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

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Data File : BF109587.D
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Operator : JU/SJ
Sample : J5221-01
Misc :
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Instrument : BNA_F
ClientSampleId : 100118-JETT-E-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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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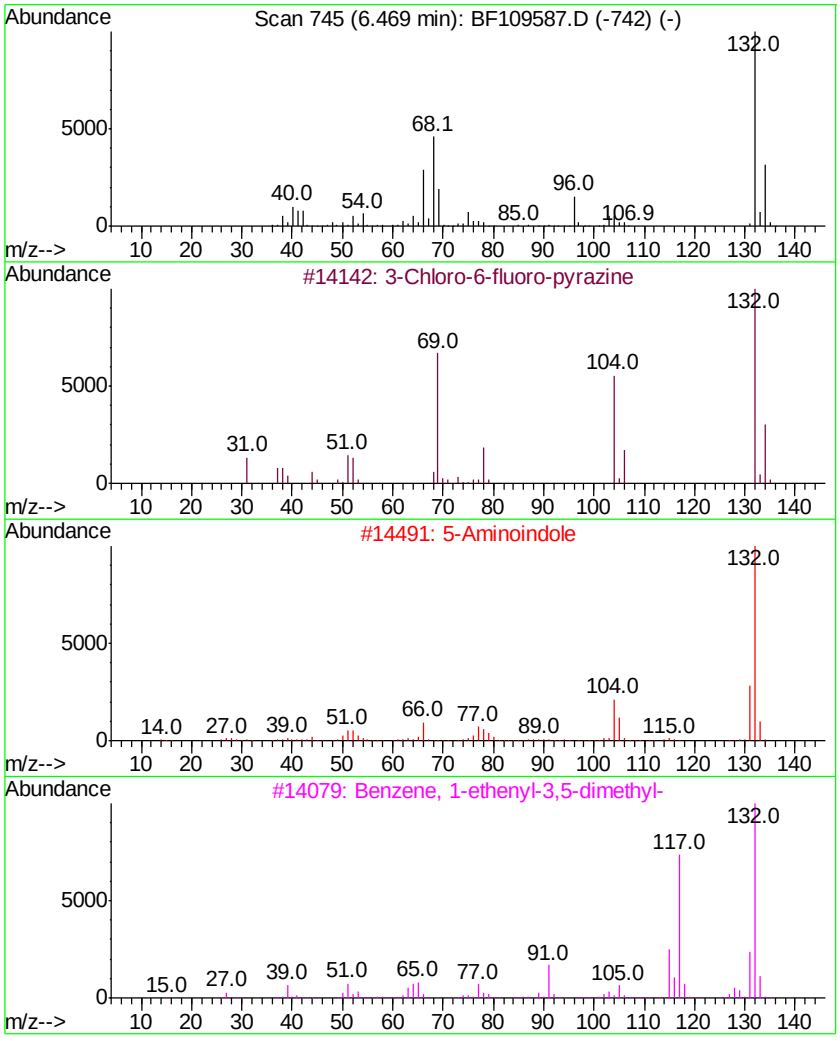
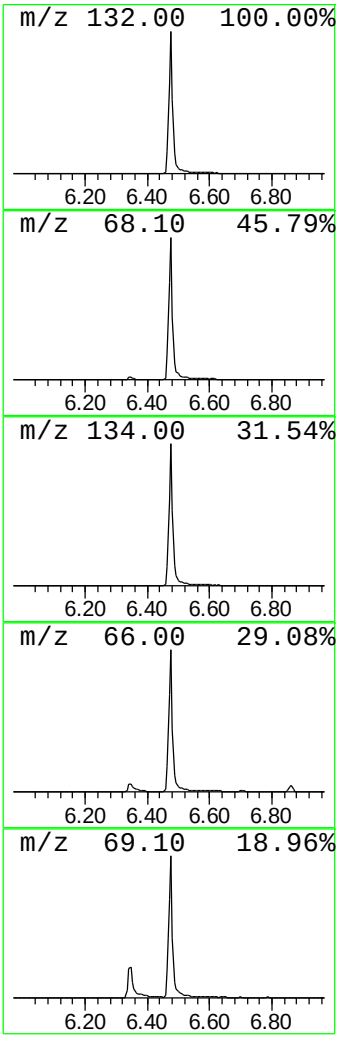
Peak Number 2 unknown6.47 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	60.68 ng	1555680	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

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Operator : JU/SJ
Sample : J5221-01
Misc :
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Instrument : BNA_F
ClientSampleId : 100118-JETT-E-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
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TIC Library : C:\DATABASE\NIST11.L
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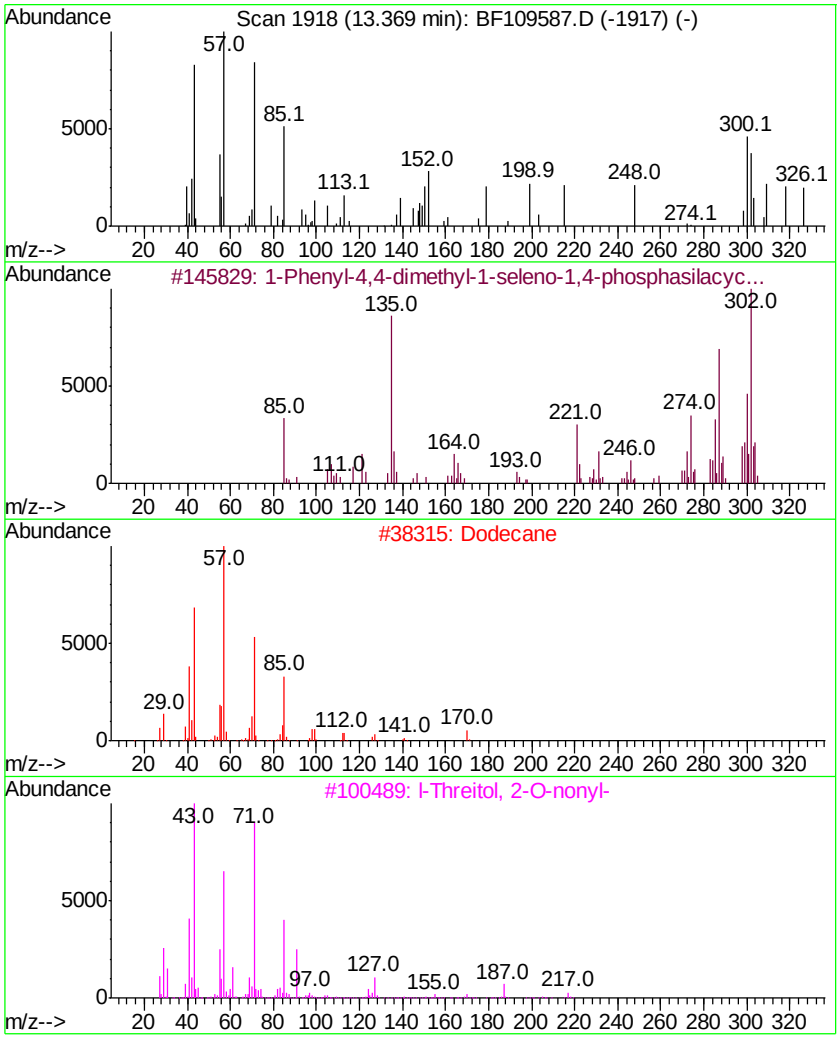
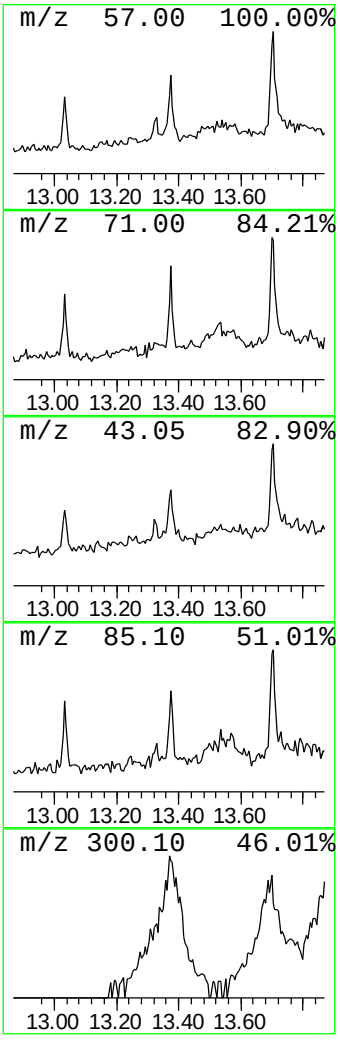
Peak Number 4 1-Phenyl-4,4-dimethyl-1-sel... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.37	2.53 ng	78424	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenyl-4,4-dimethyl-1-seleno-1...	302	C12H19PSeSi	111514-27-3	53
2	Dodecane	170	C12H26	000112-40-3	35
3	l-Threitol, 2-O-nonyl-	248	C13H28O4	163776-15-6	35
4	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	35
5	Dibenzo[fg,op]naphthacene	302	C24H14	000192-51-8	35





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Sample : J5221-01
Misc :
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Instrument : BNA_F
ClientSampleId : 100118-JETT-E-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

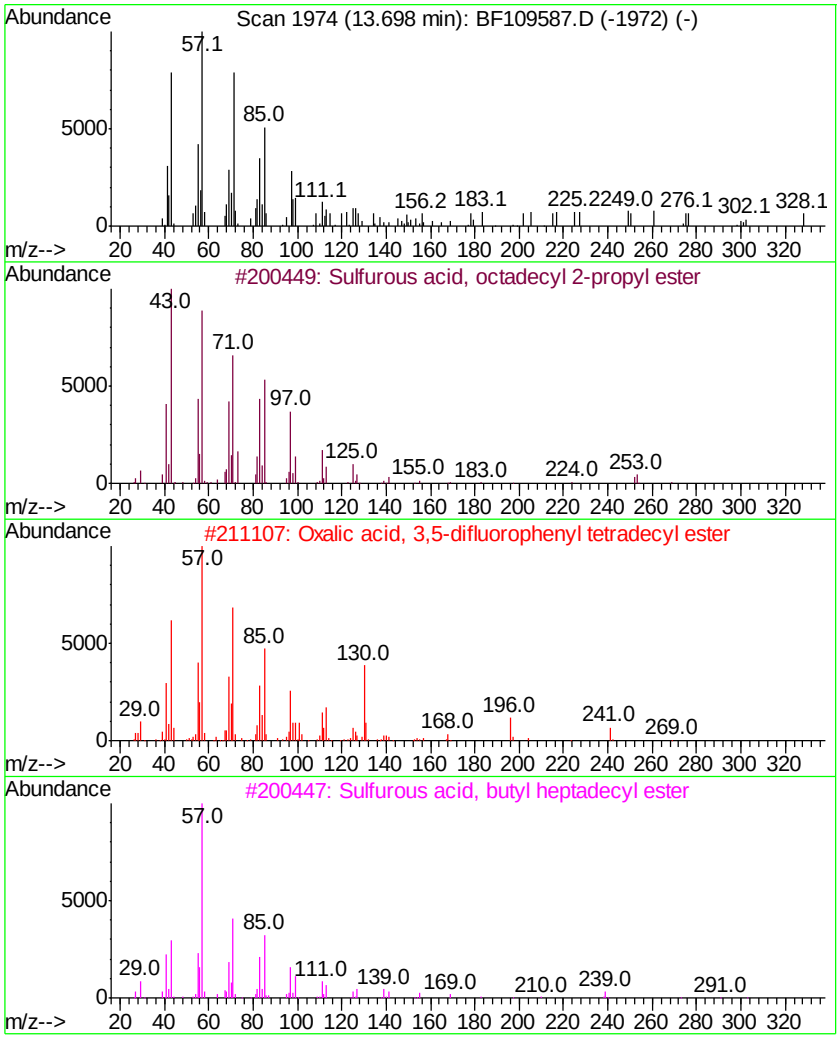
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

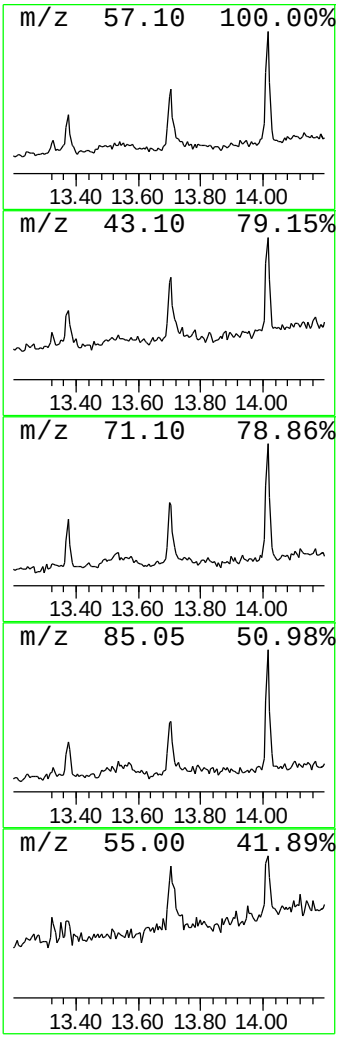
****

Peak Number 5 Sulfurous acid, octadecyl 2... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	2.77 ng	85729	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	68
2	Oxalic acid, 3,5-difluorophenyl ...	398	C22H32F2O4	1000309-67-8	64
3	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	64
4	Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	64
5	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	52





Library Search Compound Report

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Sample : J5221-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100118-JETT-E-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

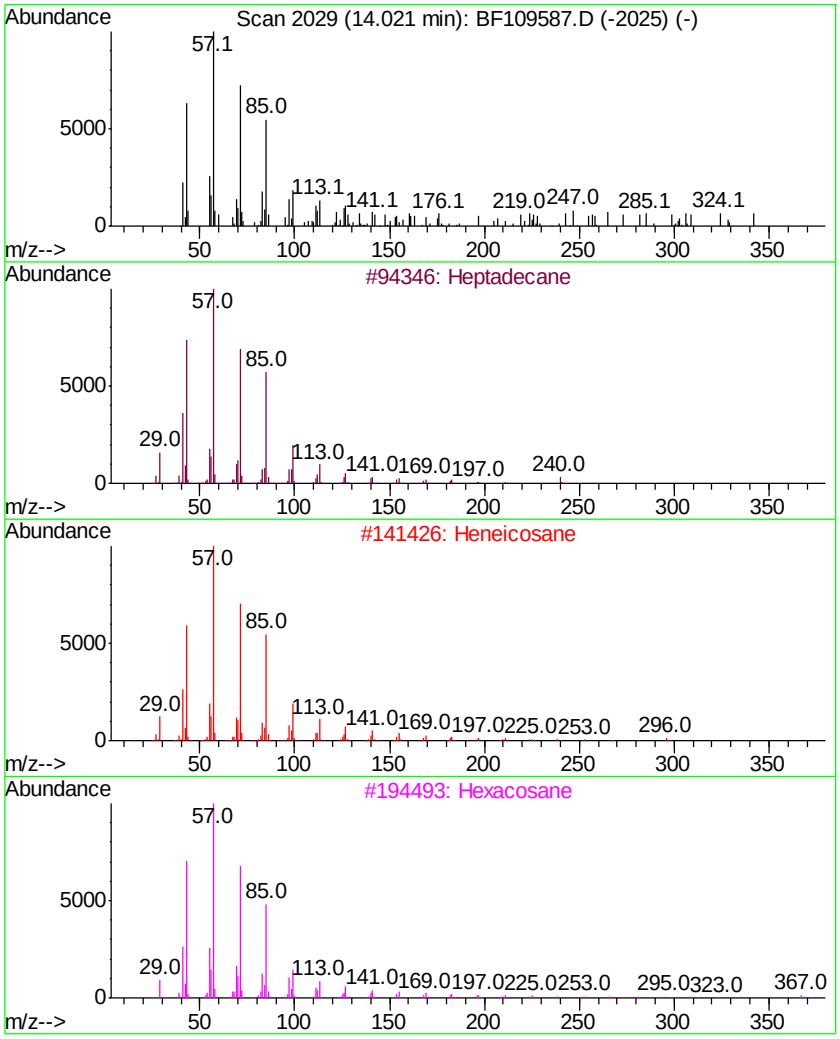
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

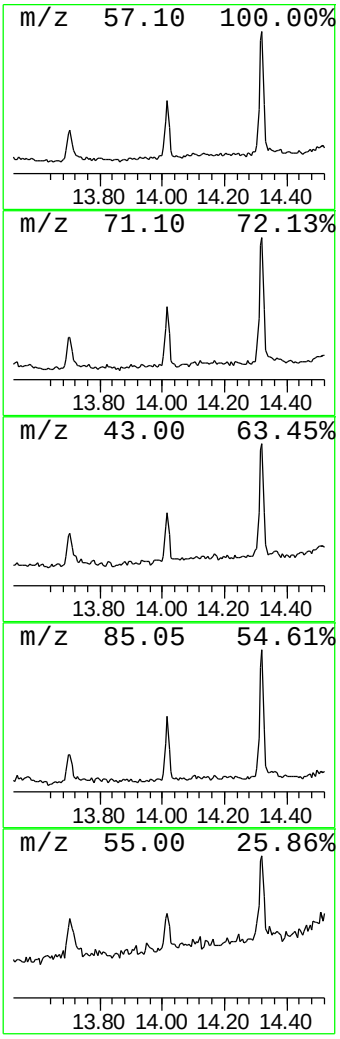
****

Peak Number 6 Heptadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.02	2.07 ng	64174	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Heneicosane	296	C21H44	000629-94-7	90
3	Hexacosane	366	C26H54	000630-01-3	87
4	Octadecane	254	C18H38	000593-45-3	86
5	Hexadecane	226	C16H34	000544-76-3	86





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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100118-JETT-E-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

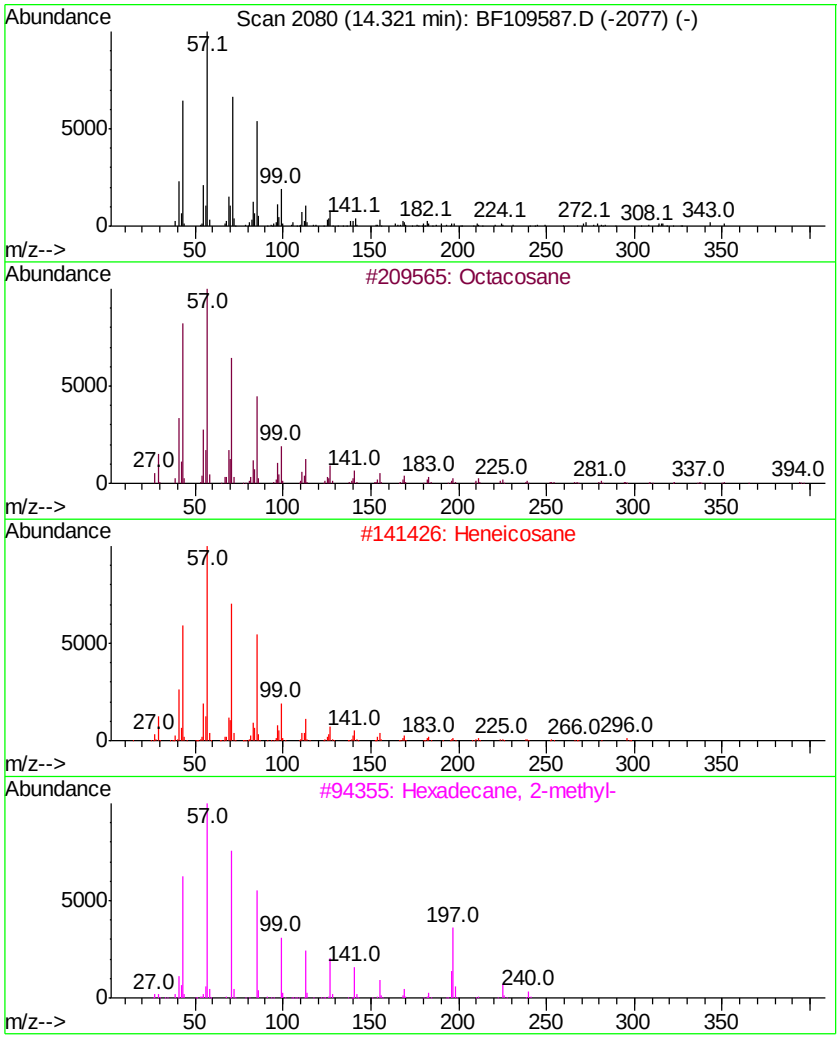
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

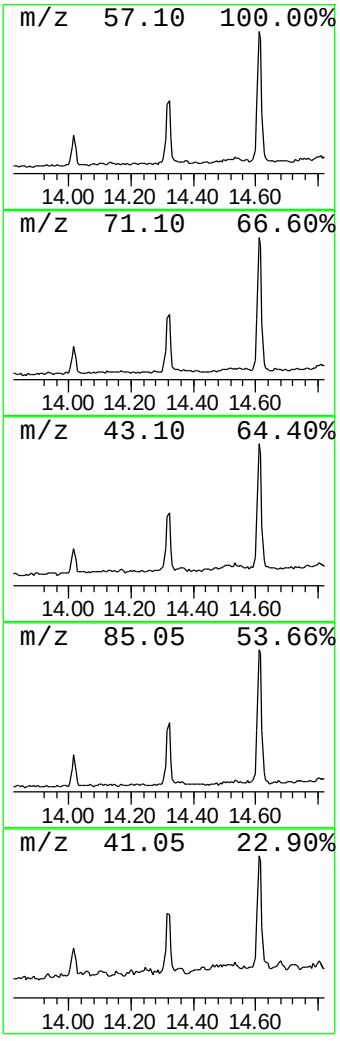
****

Peak Number 7 Hexadecane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.32	4.03 ng	124758	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	87
2	Heneicosane	296	C21H44	000629-94-7	87
3	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	87
4	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	87
5	Heptadecane	240	C17H36	000629-78-7	86





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Instrument : BNA_F
ClientSampleId : 100118-JETT-E-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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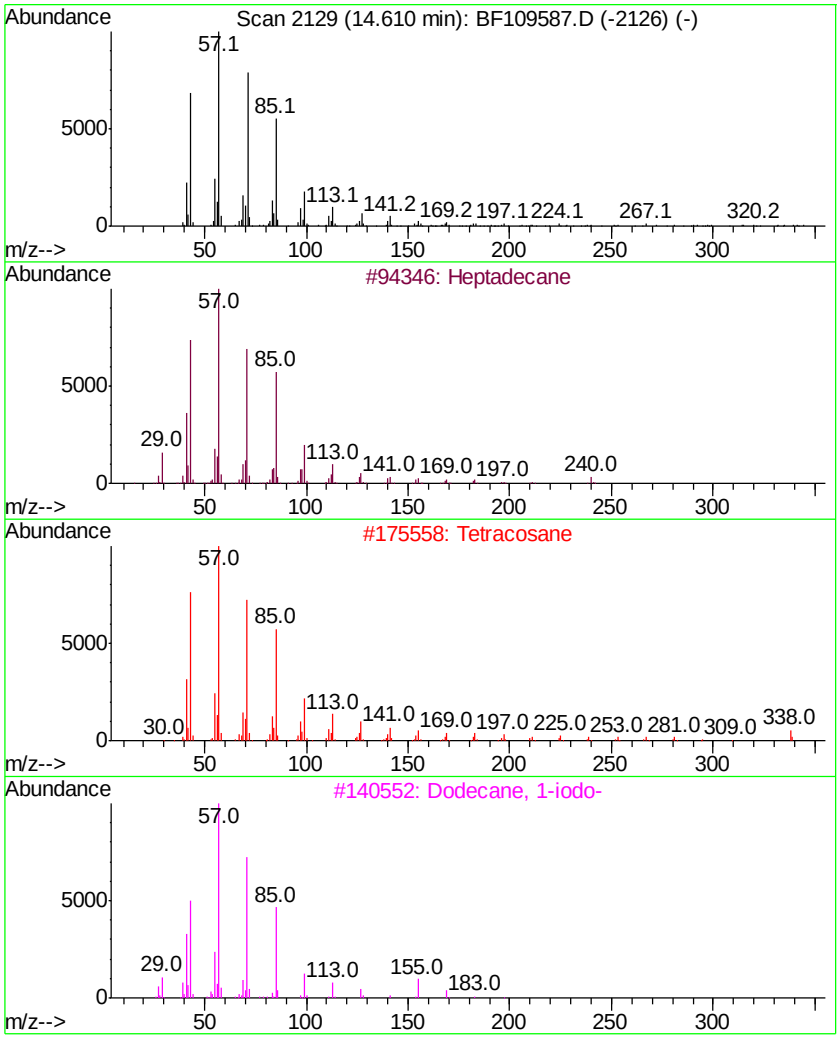
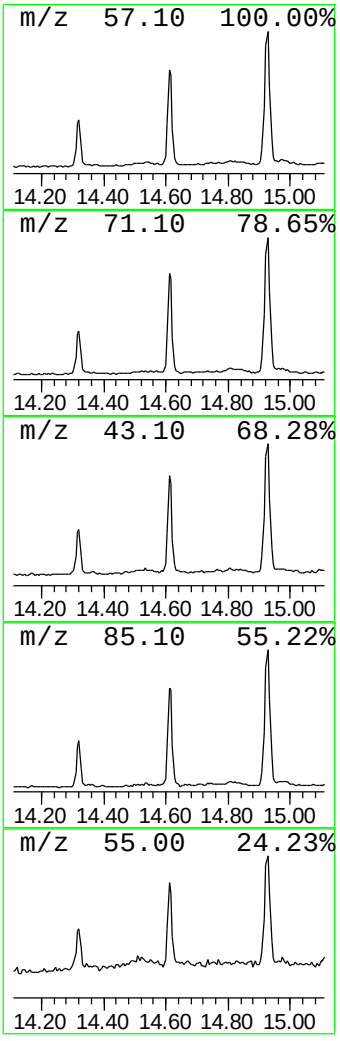
Peak Number 8 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.61	9.52 ng	252614	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Tetracosane	338	C24H50	000646-31-1	90
3	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
4	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	83
5	Heptacosane	380	C27H56	000593-49-7	83





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
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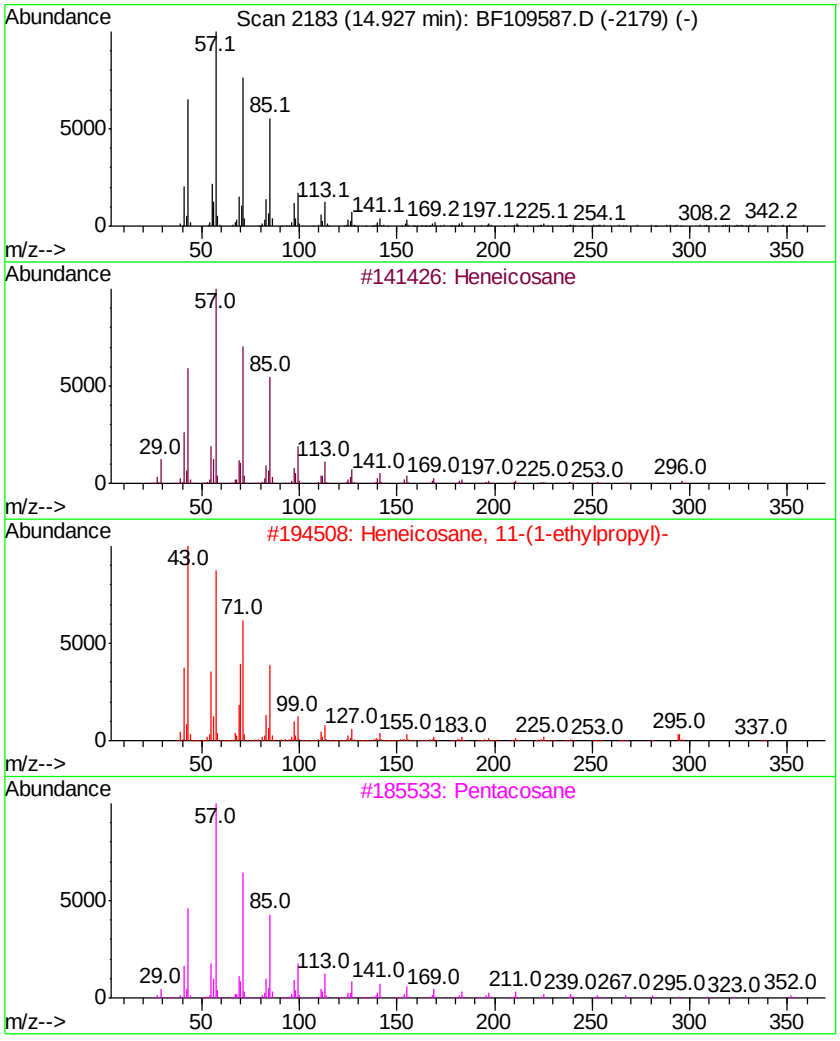
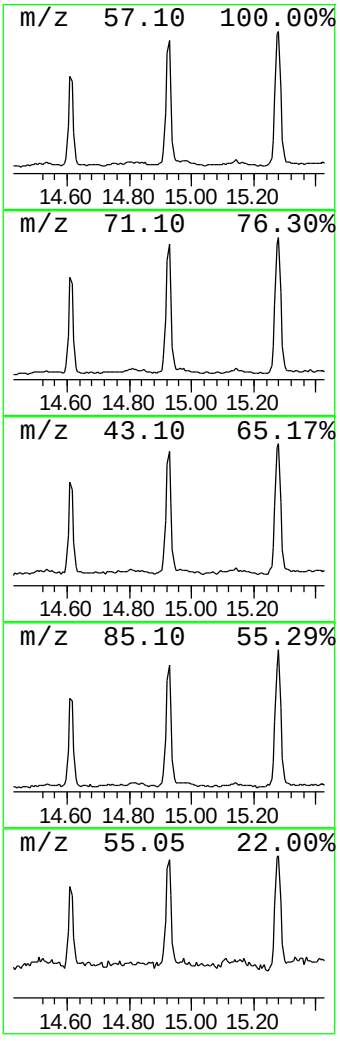
Peak Number 9 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	16.52 ng	438433	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
3	Pentacosane	352	C25H52	000629-99-2	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91





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Misc :
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Instrument : BNA_F
ClientSampleId : 100118-JETT-E-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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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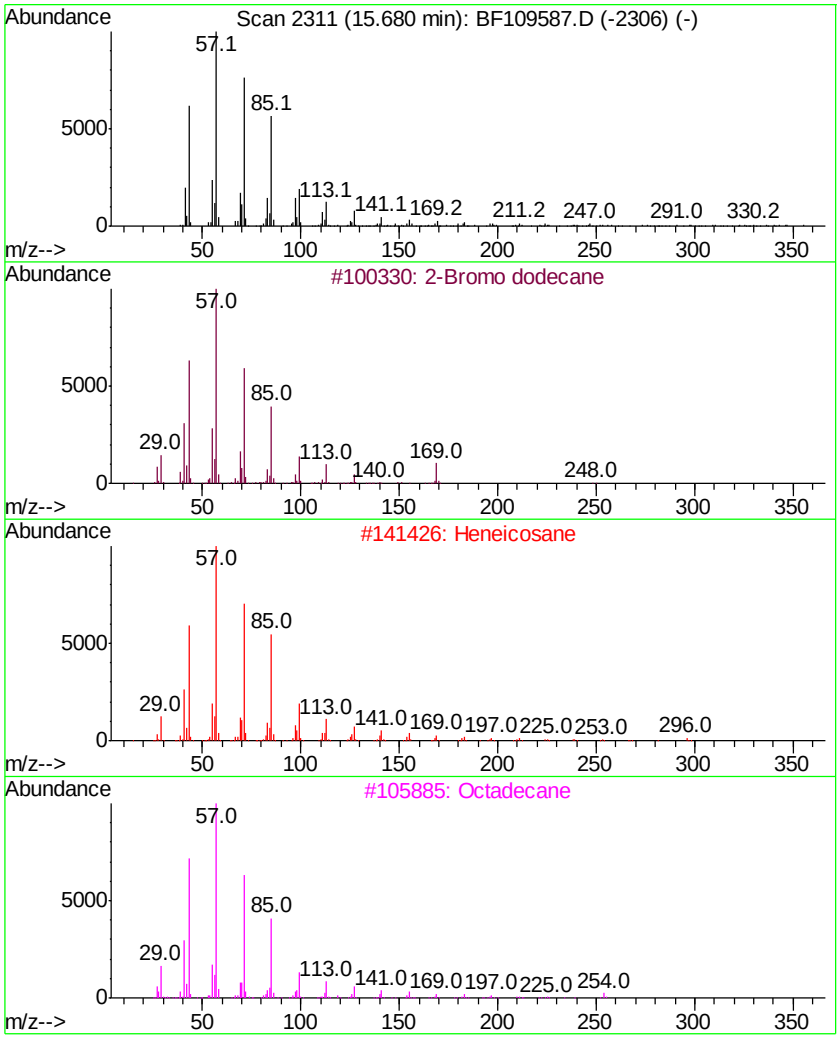
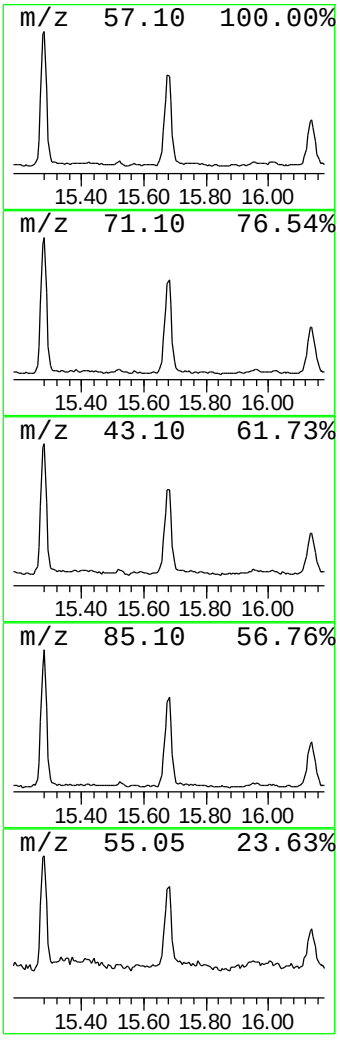
Peak Number 10 2-Bromo dodecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.68	15.07 ng	400019	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octadecane	254	C18H38	000593-45-3	86
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	83





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100418\
Data File : BF109587.D
Acq On : 4 Oct 2018 15:30
Operator : JU/SJ
Sample : J5221-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100118-JETT-E-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
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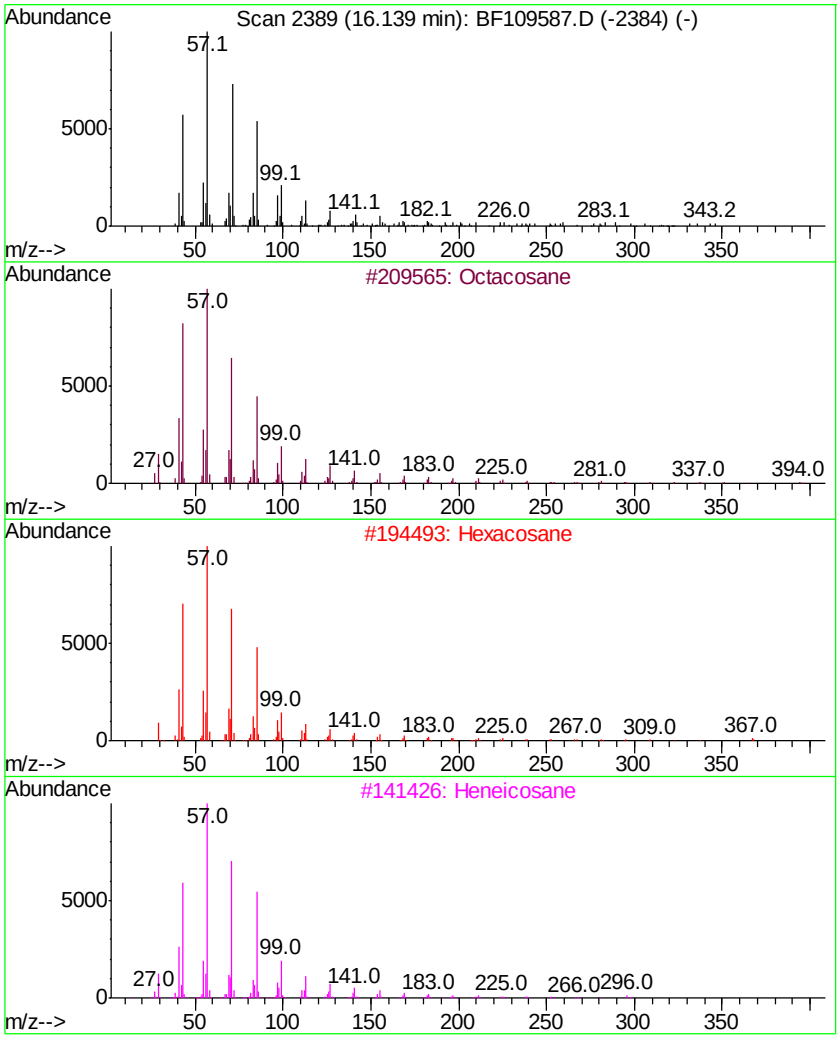
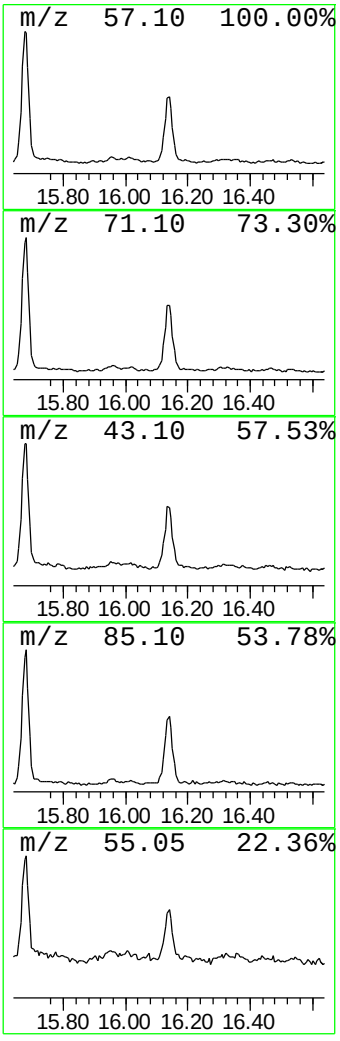
Peak Number 11 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.14	8.63 ng	229012	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
5	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100418\
Data File : BF109587.D
Acq On : 4 Oct 2018 15:30
Operator : JU/SJ
Sample : J5221-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100118-JETT-E-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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
2-Pentanone, 4-hy...	4.89	3.4	ng	87547	1	6.70	512764	20.0
unknown6.47	6.47	60.7	ng	1555680	1	6.70	512764	20.0
1-Phenyl-4,4-dime...	13.37	2.5	ng	78424	5	13.84	619491	20.0
Sulfurous acid, o...	13.70	2.8	ng	85729	5	13.84	619491	20.0
Heptadecane	14.02	2.1	ng	64174	5	13.84	619491	20.0
Hexadecane, 2-met...	14.32	4.0	ng	124758	5	13.84	619491	20.0
Tetracosane	14.61	9.5	ng	252614	6	15.24	530933	20.0
Heneicosane	14.93	16.5	ng	438433	6	15.24	530933	20.0
2-Bromo dodecane	15.68	15.1	ng	400019	6	15.24	530933	20.0
Octacosane	16.14	8.6	ng	229012	6	15.24	530933	20.0