LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090418\
Data File : BF108747.D
Acq On : 4 Sep 2018 18:07
Operator : JU/SJ
Sample : J4270-05 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-02-083018

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-BF083018.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	5.213	486	489	501	rBV	67624	81068	2.33%	0.542%
2	6.654	728	734	747	rBV3	38781	170062	4.90%	1.137%
3	6.772	750	754	786	rVB	98159	335390	9.65%	2.243%
4	6.995	788	792	807	rBV	224353	478731	13.78%	3.202%
5	7.142	814	817	832	rVB	138239	229925	6.62%	1.538%
6	7.583	886	892	894	rBV3	27043	57104	1.64%	0.382%
7	8.272	1006	1009	1033	rBV	386094	672206	19.35%	4.496%
8	9.342	1188	1191	1200	rBV	273069	372212	10.71%	2.489%
9	9.736	1252	1258	1264	rBV2	27666	43141	1.24%	0.289%
10	10.030	1304	1308	1320	rBV	630249	768671	22.13%	5.141%
11	11.019	1472	1476	1481	rBV	55872	51015	1.47%	0.341%
12	11.530	1559	1563	1575	rBV	552842	849616	24.46%	5.682%
13	11.818	1609	1612	1617	rVB	84459	77250	2.22%	0.517%
14	11.889	1621	1624	1640	rBV	1311092	1280789	36.87%	8.566%
15	12.583	1738	1742	1744	rBV	2557586	2699921	77.72%	18.058%
16	12.607	1744	1746	1753	rVV	3722586	3474079	100.00%	23.236%
17	12.683	1756	1759	1768	rVV	774526	748469	21.54%	5.006%
18	12.754	1768	1771	1781	rVV	93385	163139	4.70%	1.091%
19	12.924	1794	1800	1803	rBV4	57801	67405	1.94%	0.451%
20	12.983	1803	1810	1816	rVV	102061	156407	4.50%	1.046%
21	13.112	1828	1832	1839	rBV	438783	532668	15.33%	3.563%
22	13.289	1857	1862	1864	rBV4	46942	65373	1.88%	0.437%
23	13.336	1864	1870	1875	rVB2	55220	92436	2.66%	0.618%
24	13.412	1880	1883	1887	rBV2	56464	59981	1.73%	0.401%
25	14.189	2010	2015	2025	rBV	582382	865787	24.92%	5.791%
26	15.742	2275	2279	2291	rVB	276544	485435	13.97%	3.247%
27	16.165	2348	2351	2356	rVB	50013	73281	2.11%	0.490%

Sum of corrected areas: 14951561

LSC Report - Integrated Chromatogram

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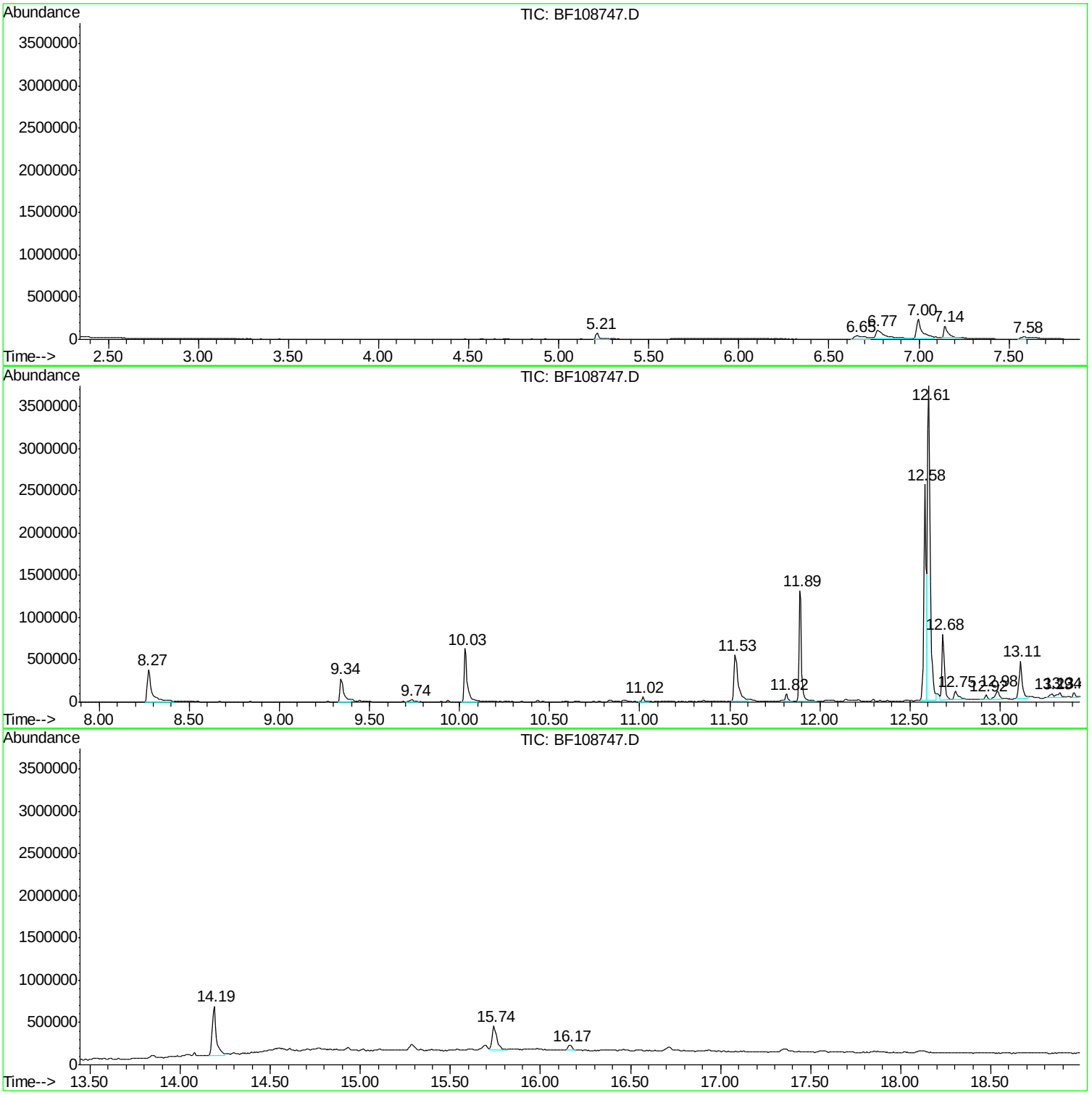
Sample : J4270-05 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-02-083018

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.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

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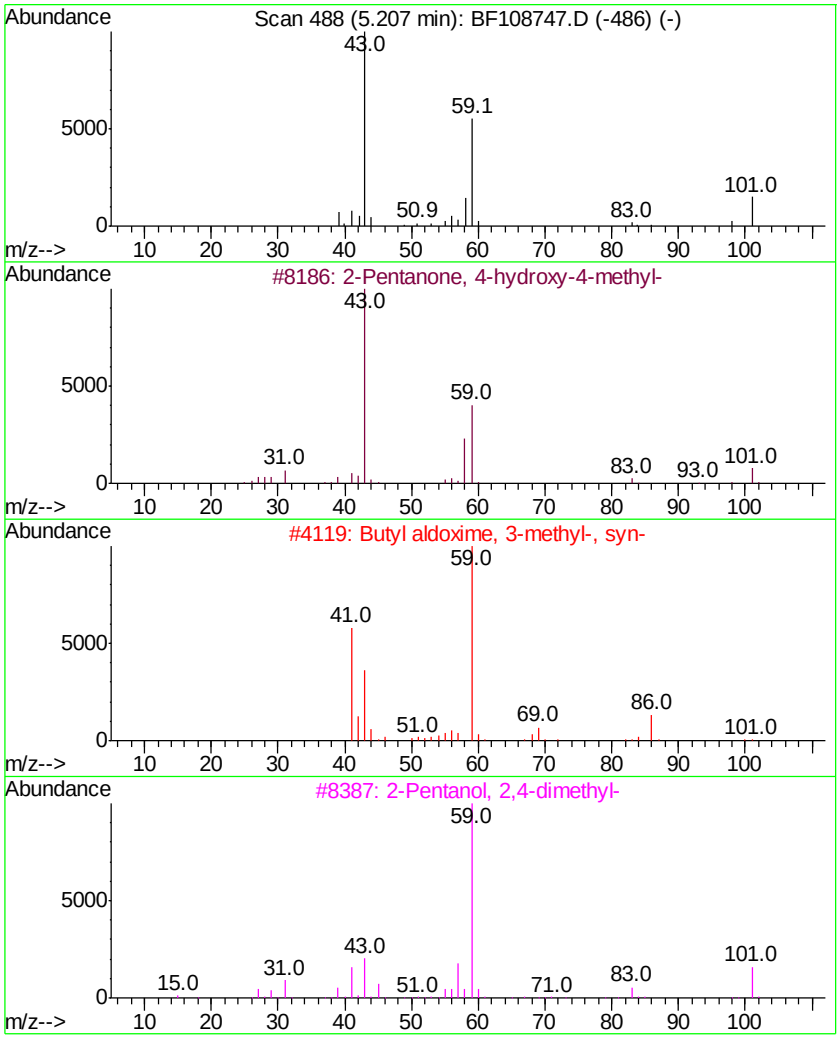
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

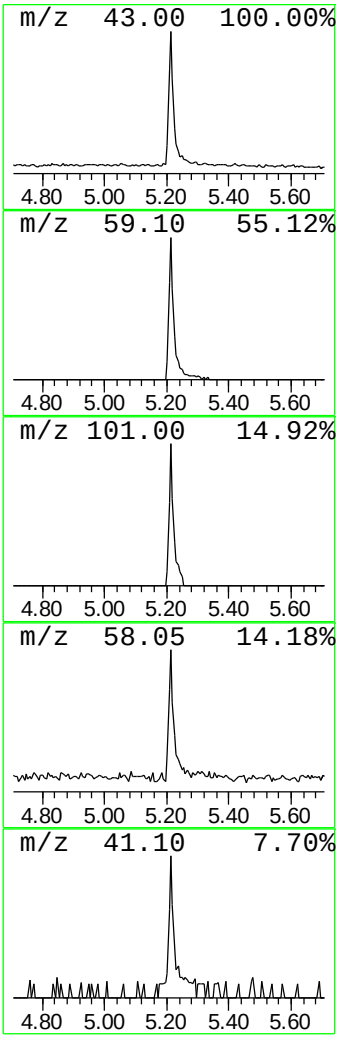
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	3.39 ng	81068	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	43
3	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	40
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





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Data File : BF108747.D
Acq On : 4 Sep 2018 18:07
Operator : JU/SJ
Sample : J4270-05 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-02-083018

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

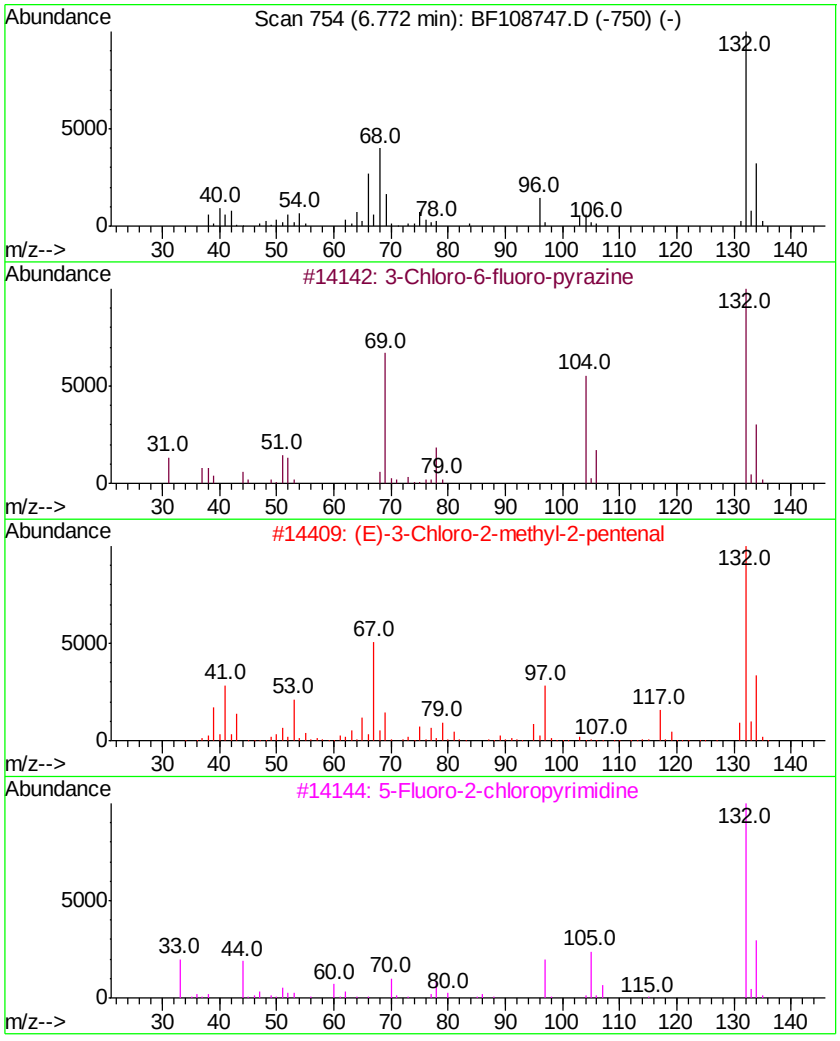
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

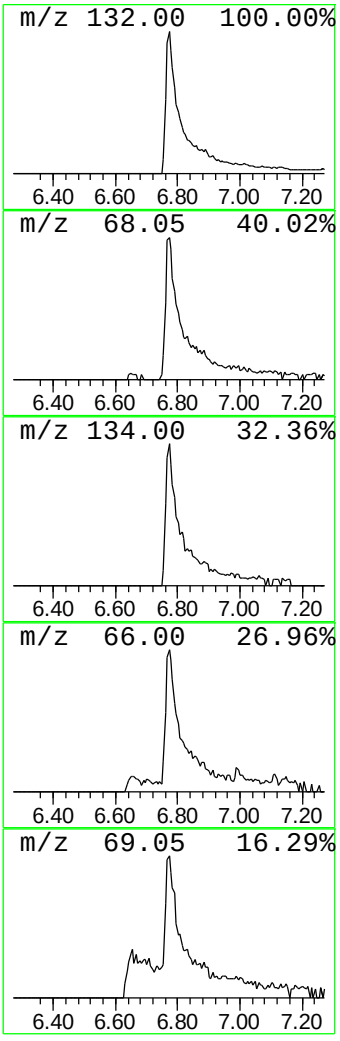
****

Peak Number 2 unknown6.77 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	14.01 ng	335390	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10





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Sample : J4270-05 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-02-083018

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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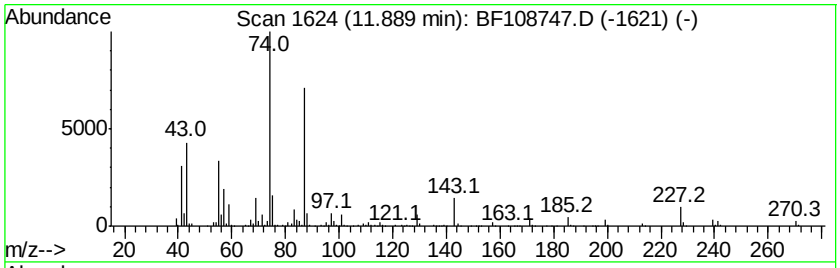
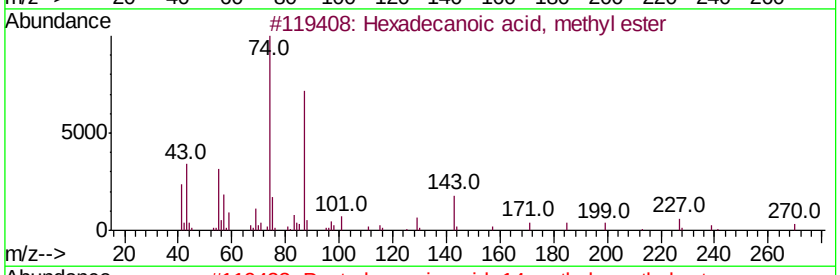
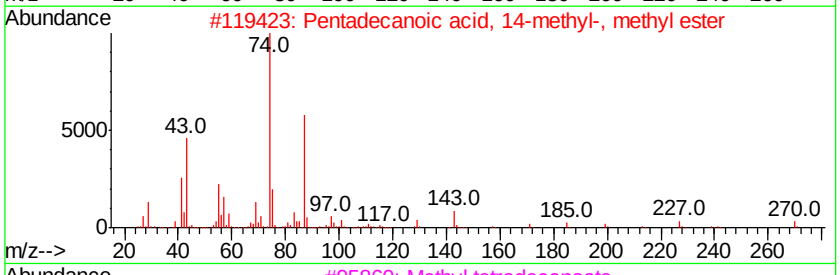
Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 3

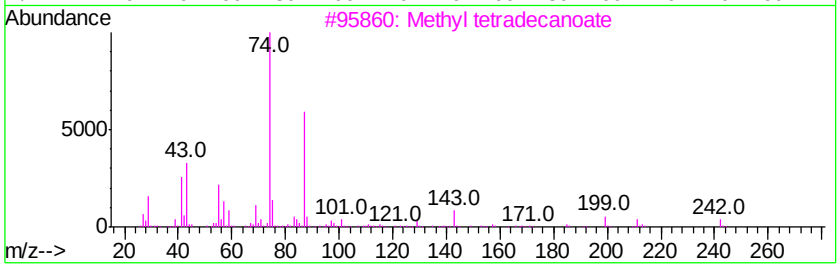
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	30.15 ng	1280790	Phenanthrene-d10	11.53

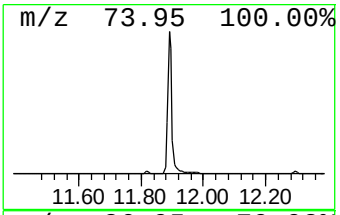
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	99
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	94
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	93
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86

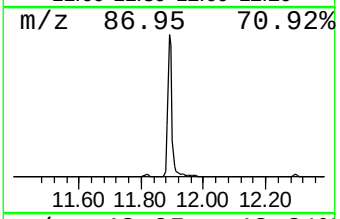


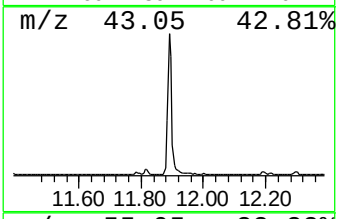


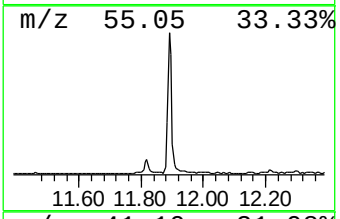


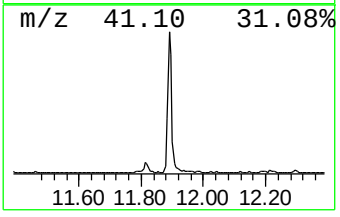












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Acq On : 4 Sep 2018 18:07
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Sample : J4270-05 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-02-083018

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

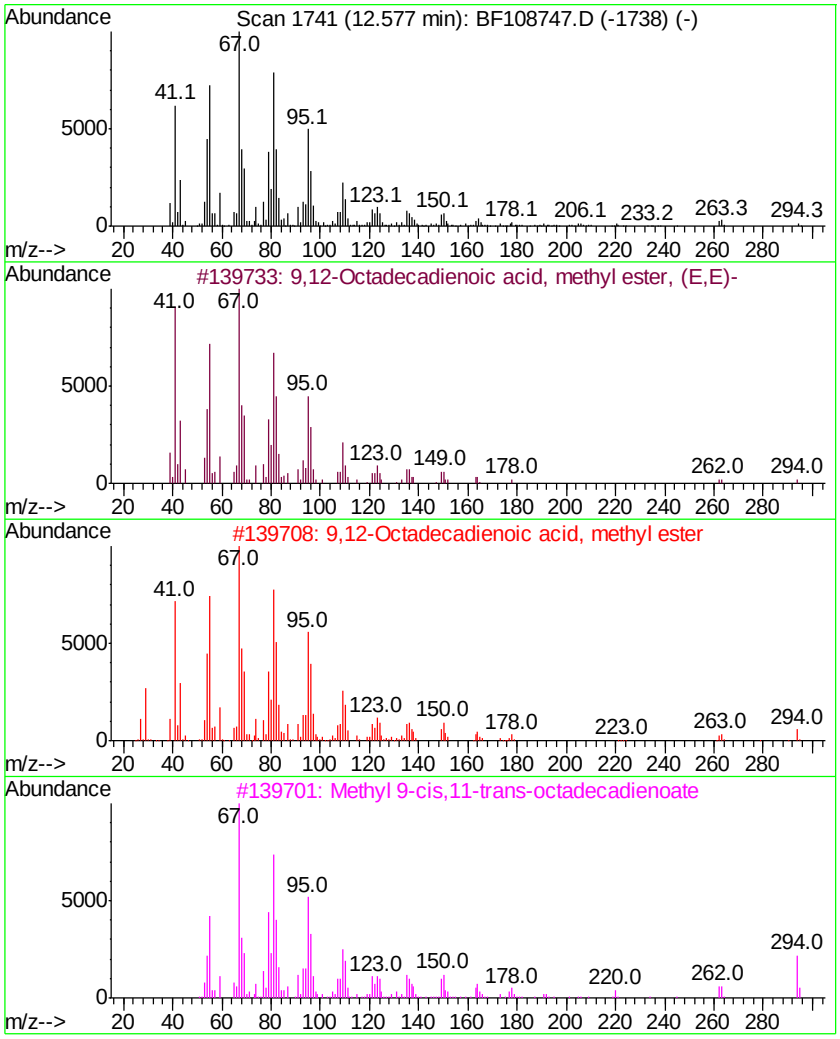
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

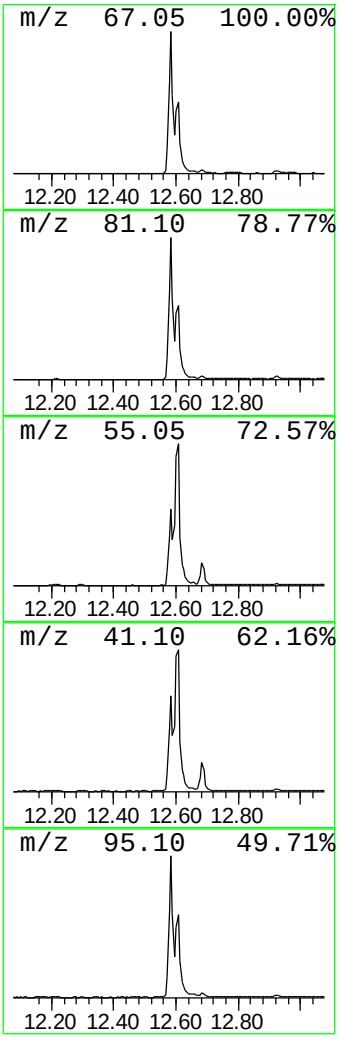
****

Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.58	63.56 ng	2699920	Phenanthrene-d10	11.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
3	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	99
4	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
5	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	98





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Instrument : BNA_F
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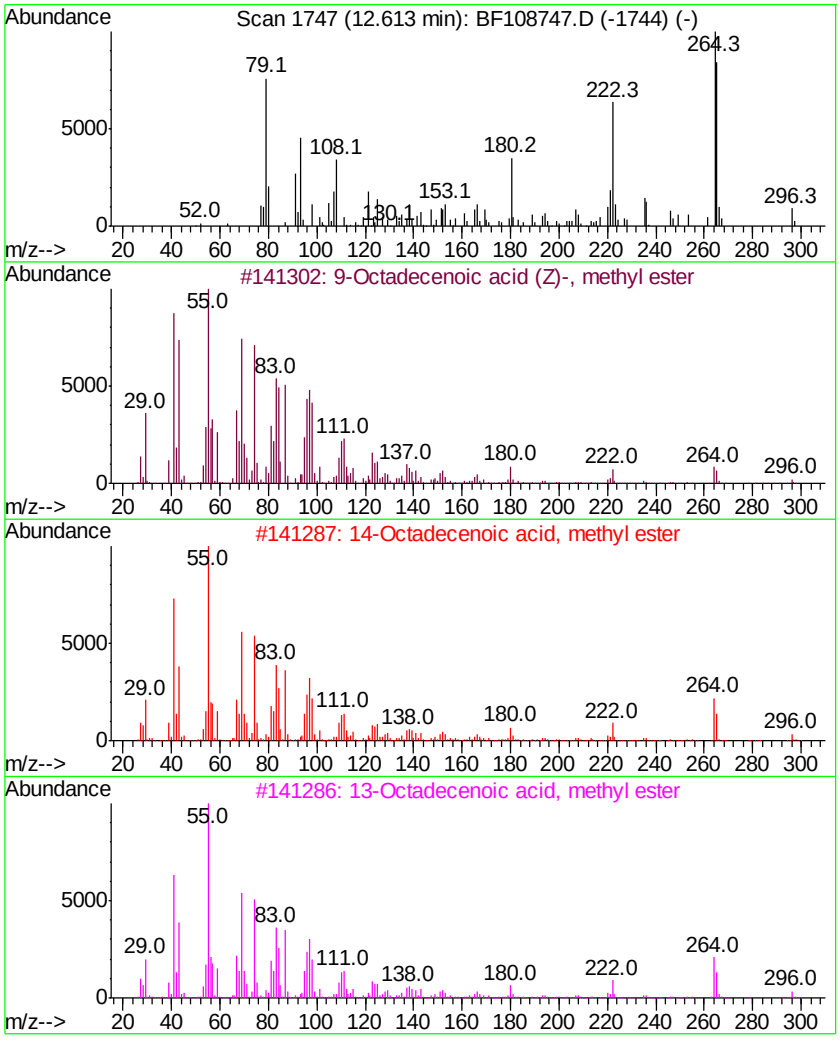
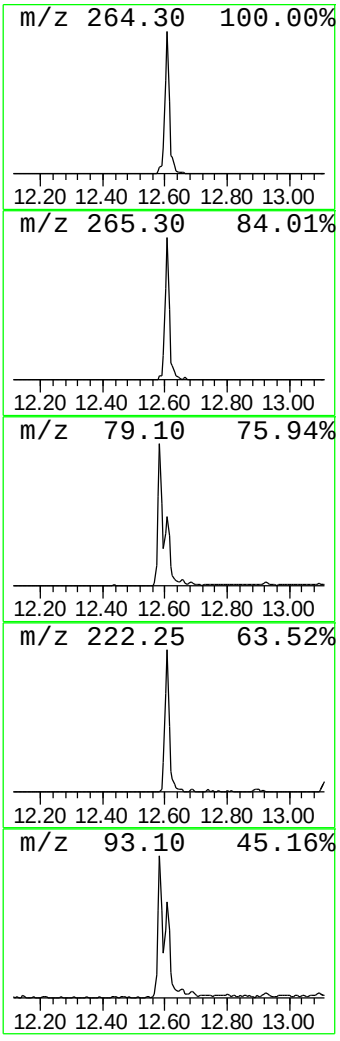
****

Peak Number 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.61	81.78 ng	3474080	Phenanthrene-d10	11.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
4	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
5	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	98





Library Search Compound Report

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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-02-083018

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
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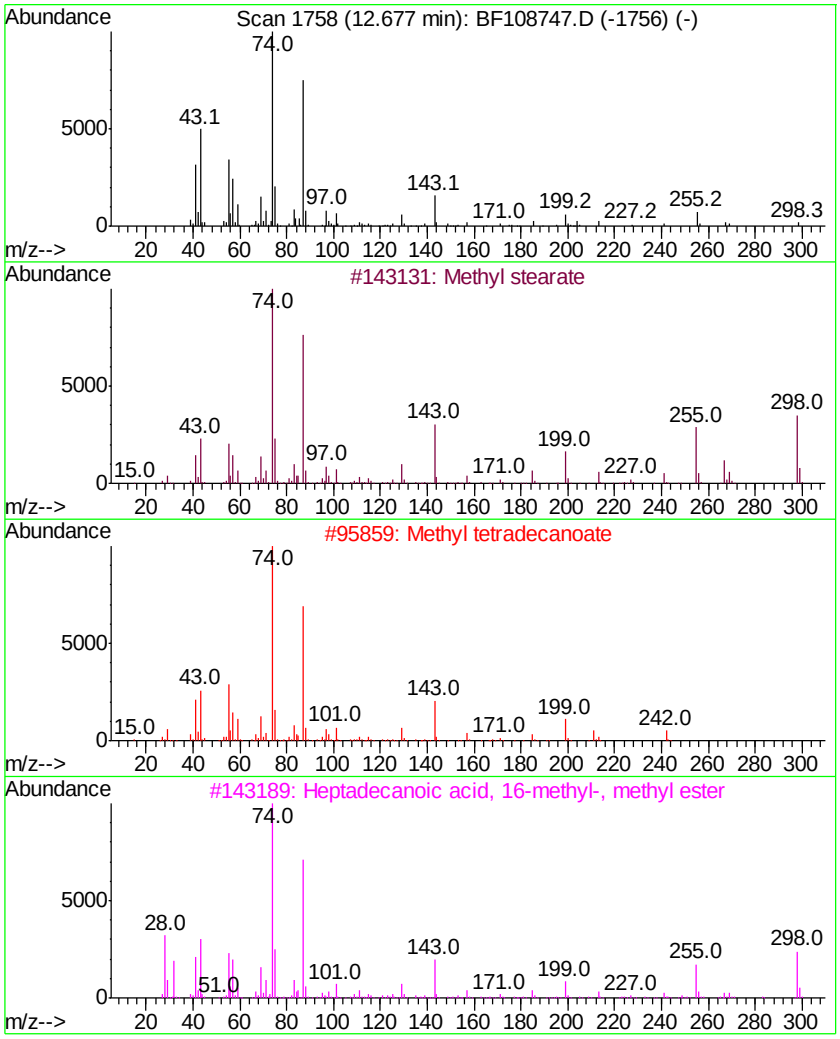
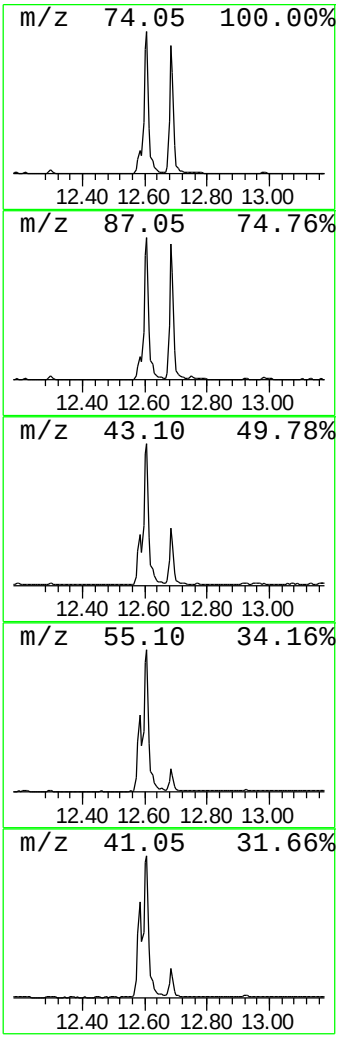
****

Peak Number 7 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.68	17.62 ng	748469	Phenanthrene-d10	11.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	98
2	Methyl tetradecanoate	242	C15H30O2	000124-10-7	94
3	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	92
4	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90





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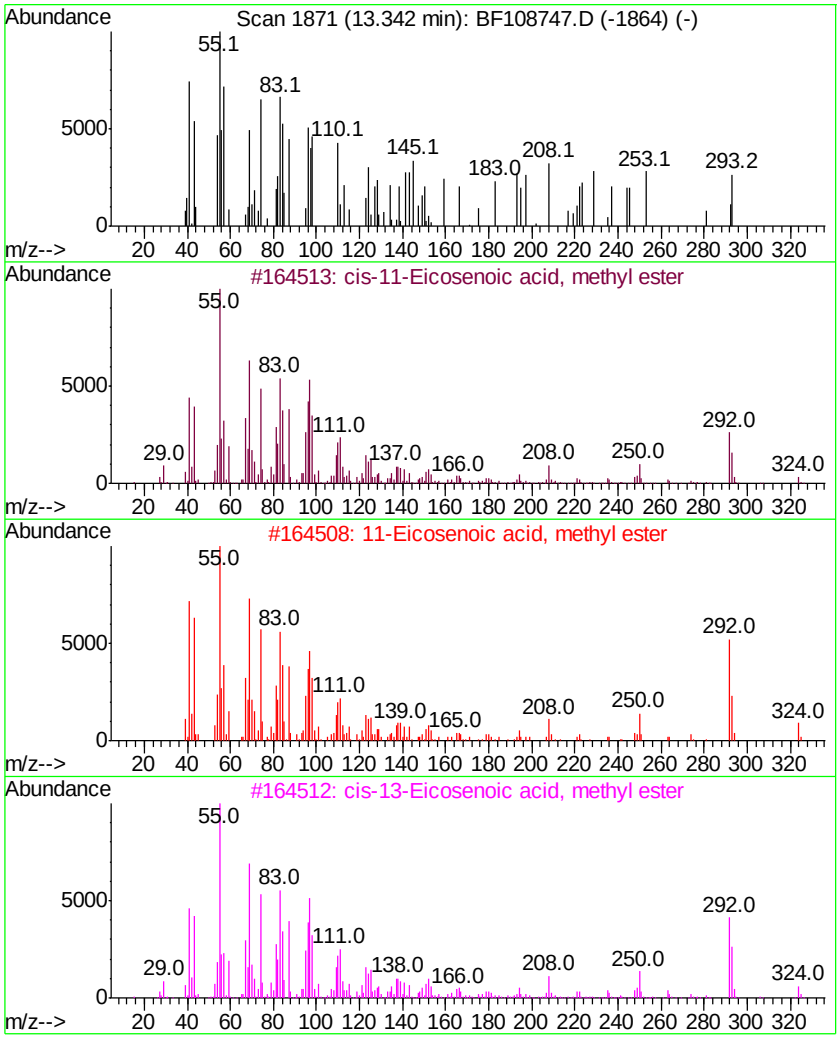
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

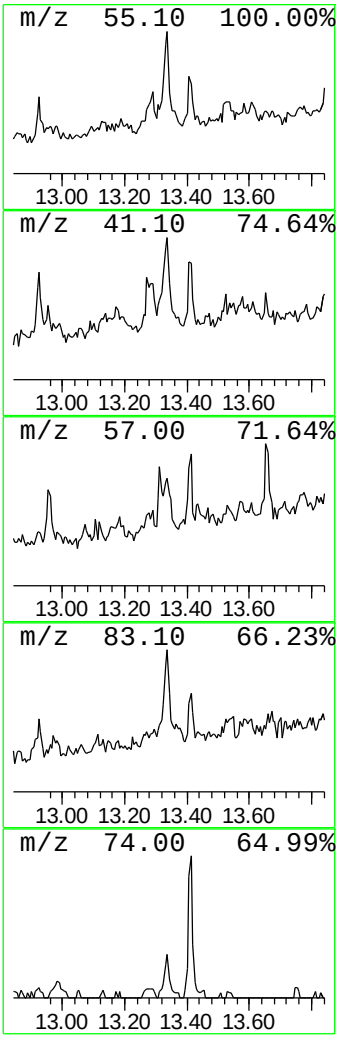
****

Peak Number 8 cis-11-Eicosenoic acid, met... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.34	2.14 ng	92436	Chrysene-d12	14.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-11-Eicosenoic acid, methyl e...	324	C21H40O2	1000333-63-8	91
2	11-Eicosenoic acid, methyl ester	324	C21H40O2	003946-08-5	91
3	cis-13-Eicosenoic acid, methyl e...	324	C21H40O2	1000333-52-1	91
4	cis-10-Heptadecenoic acid, methy...	282	C18H34O2	1000333-62-1	91
5	Methyl 9-eicosenoate	324	C21H40O2	1000336-50-5	83





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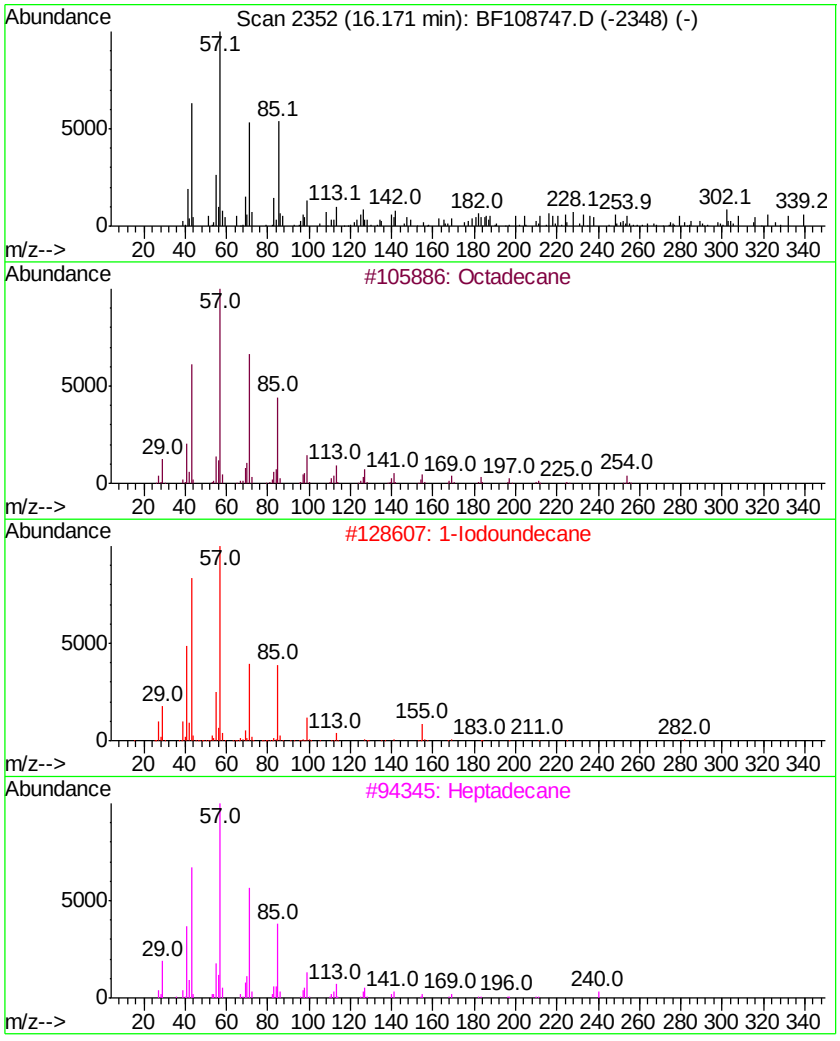
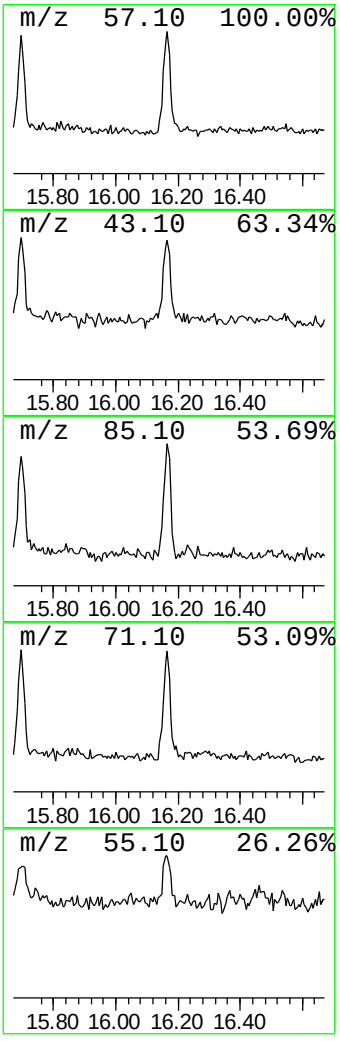
****

Peak Number 9 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.17	3.02 ng	73281	Perylene-d12	15.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	70
2	1-Iodoundecane	282	C11H23I	004282-44-4	64
3	Heptadecane	240	C17H36	000629-78-7	64
4	2-Thiopheneacetic acid, 4-tetrad...	338	C20H34O2S	1000280-67-0	52
5	2-methylhexacosane	380	C27H56	1000376-72-7	52





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090418\
Data File : BF108747.D
Acq On : 4 Sep 2018 18:07
Operator : JU/SJ
Sample : J4270-05 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-02-083018

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.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...	5.21	3.4	ng	81068	1	7.00	478731	20.0
unknown6.77	6.77	14.0	ng	335390	1	7.00	478731	20.0
Hexadecanoic acid...	11.89	30.1	ng	1280790	4	11.53	849616	20.0
9,12-Octadecadien...	12.58	63.6	ng	2699920	4	11.53	849616	20.0
9-Octadecenoic ac...	12.61	81.8	ng	3474080	4	11.53	849616	20.0
Methyl stearate	12.68	17.6	ng	748469	4	11.53	849616	20.0
cis-11-Eicosenoic...	13.34	2.1	ng	92436	5	14.19	865787	20.0
Octadecane	16.17	3.0	ng	73281	6	15.74	485435	20.0