LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012819\
Data File : BF112284.D
Acq On : 28 Jan 2019 19:39
Operator : JU/SJ
Sample : K1011-09 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-012519-A

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-BF012519.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	5.469	572	575	591	rBV	768116	815113	15.87%	2.718%
2	6.481	744	747	764	rBV	840837	896536	17.45%	2.989%
3	6.610	766	769	777	rBV	1031780	957340	18.63%	3.192%
4	6.839	804	808	826	rBV	1375081	1221562	23.78%	4.073%
5	6.992	830	834	841	rBV	781689	757182	14.74%	2.524%
6	7.398	899	903	915	rBV	542852	544910	10.61%	1.817%
7	8.122	1020	1026	1033	rBV	1784888	1635168	31.83%	5.452%
8	9.192	1204	1208	1218	rBV	1280041	1135462	22.10%	3.786%
9	9.586	1272	1275	1279	rBV2	72634	88006	1.71%	0.293%
10	9.804	1305	1312	1317	rBV	96870	83917	1.63%	0.280%
11	9.875	1317	1324	1329	rBV2	1993650	1850028	36.01%	6.168%
12	10.304	1395	1397	1400	rVB	106015	78521	1.53%	0.262%
13	10.522	1430	1434	1440	rVB2	38242	56567	1.10%	0.189%
14	10.663	1456	1458	1469	rVB	515928	555688	10.82%	1.853%
15	10.775	1474	1477	1485	rVB	116553	143107	2.79%	0.477%
16	11.222	1550	1553	1555	rBV	103748	84598	1.65%	0.282%
17	11.257	1555	1559	1564	rVB3	57100	73547	1.43%	0.245%
18	11.363	1573	1577	1579	rBV	1949108	1684426	32.79%	5.616%
19	11.386	1579	1581	1588	rVB	227973	220096	4.28%	0.734%
20	11.645	1622	1625	1628	rBV	77331	69160	1.35%	0.231%
21	11.745	1639	1642	1646	rBV	1918462	1503129	29.26%	5.012%
22	11.892	1664	1667	1673	rVB2	59905	76428	1.49%	0.255%
23	12.051	1691	1694	1700	rVB	72023	74722	1.45%	0.249%
24	12.433	1755	1759	1761	rBV	5460251	5137355	100.00%	17.128%
25	12.457	1761	1763	1769	rVB	4347272	3579212	69.67%	11.933%
26	12.539	1773	1777	1780	rVB	705062	608918	11.85%	2.030%
27	12.574	1780	1783	1788	rBV	326885	302109	5.88%	1.007%
28	12.804	1812	1822	1829	rBV	300161	381046	7.42%	1.270%
29	12.939	1840	1845	1849	rBV	1076372	908875	17.69%	3.030%
30	13.168	1881	1884	1892	rVB4	64214	123327	2.40%	0.411%
31	13.257	1897	1899	1902	rVB	57969	53518	1.04%	0.178%
32	13.839	1995	1998	2003	rVB4	61509	84628	1.65%	0.282%
33	13.927	2010	2013	2017	rBV2	58619	58921	1.15%	0.196%
34	13.998	2021	2025	2028	rVV	1346472	1390141	27.06%	4.635%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012819\
Data File : BF112284.D
Acq On : 28 Jan 2019 19:39
Operator : JU/SJ
Sample : K1011-09 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-012519-A

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-BF012519.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.027	2028	2030	2037	rVB	124349	127434	2.48%	0.425%
36	14.151	2048	2051	2057	rVB2	71052	70631	1.37%	0.235%
37	14.457	2099	2103	2106	rBV	115091	127748	2.49%	0.426%
38	14.757	2151	2154	2158	rBV	156822	156150	3.04%	0.521%
39	15.039	2199	2202	2205	rBV	96672	124560	2.42%	0.415%
40	15.092	2208	2211	2218	rVB	198070	233130	4.54%	0.777%
41	15.339	2251	2253	2258	rVB	61471	74263	1.45%	0.248%
42	15.404	2261	2264	2268	rVB	91122	109233	2.13%	0.364%
43	15.462	2269	2274	2283	rVV	1050393	1370984	26.69%	4.571%
44	15.898	2343	2348	2353	rBV	137254	209936	4.09%	0.700%
45	16.398	2428	2433	2439	rVB3	92402	156211	3.04%	0.521%

Sum of corrected areas: 29993543

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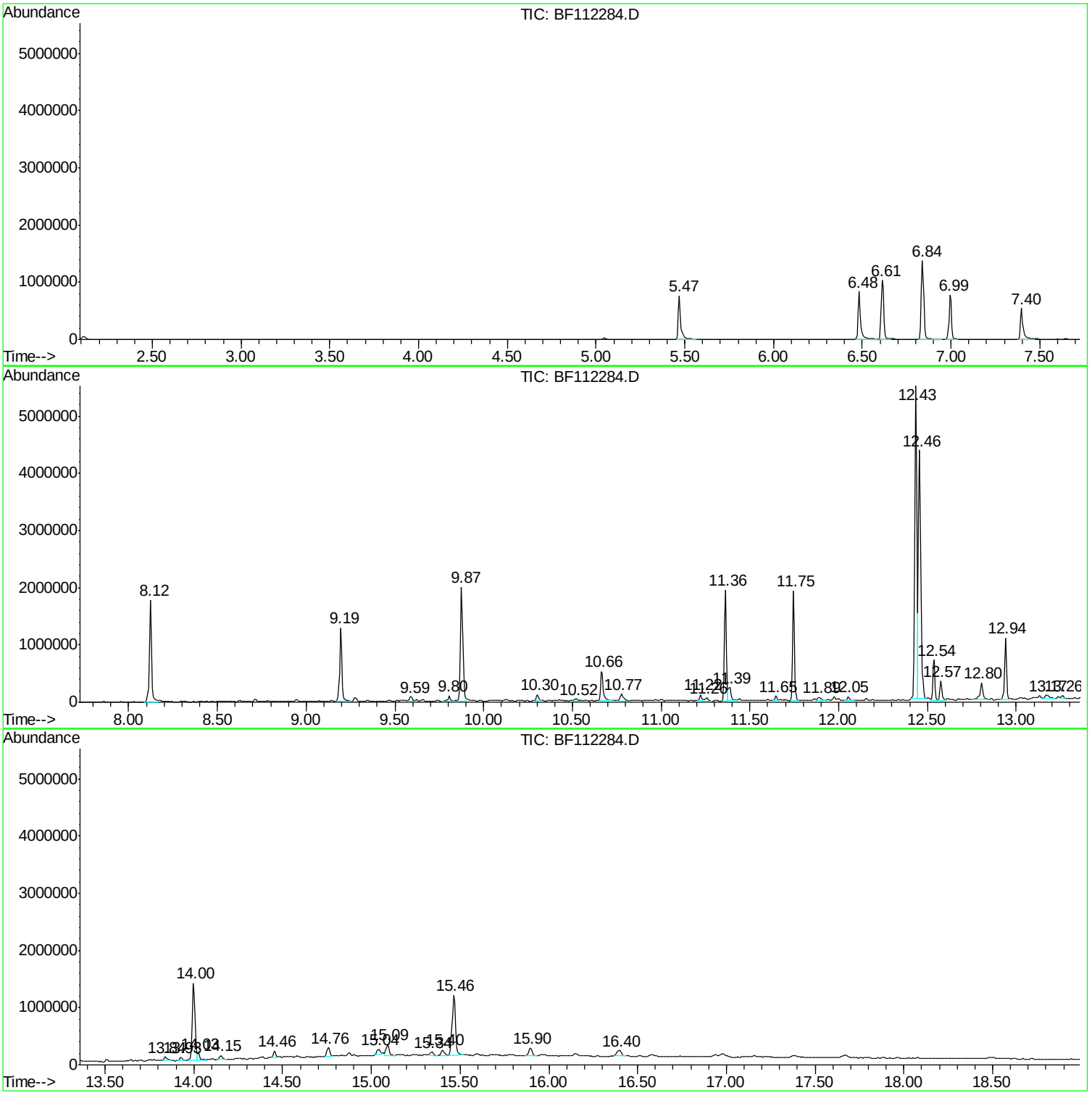
BNA_F
ClientSampleId :
OR-01-012519-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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 F\DATA\BF012819\
Data File : BF112284.D
Acq On : 28 Jan 2019 19:39
Operator : JU/SJ
Sample : K1011-09 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-01-012519-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

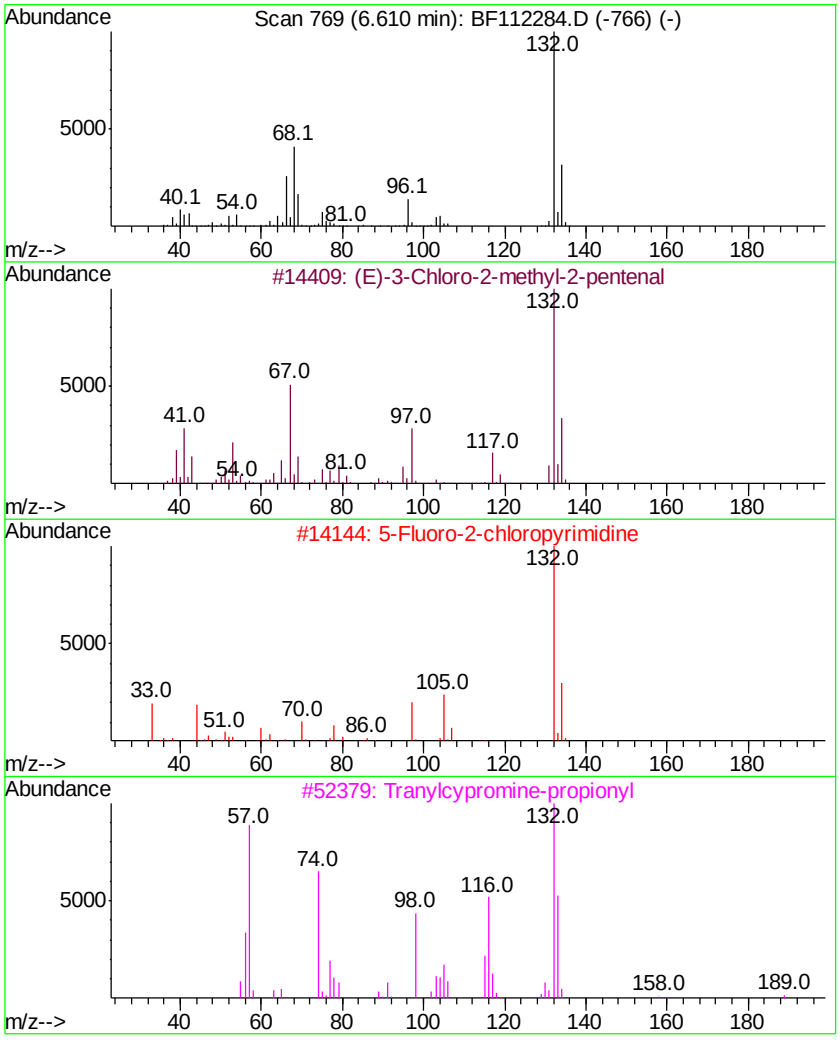
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

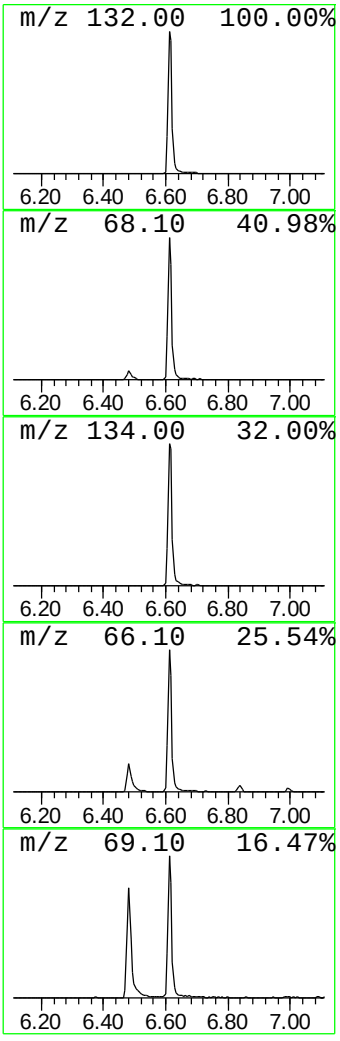
****

Peak Number 1 unknown6.61 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	15.67 ng	957340	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012819\
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Misc :
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Instrument : BNA_F
ClientSampleId : OR-01-012519-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

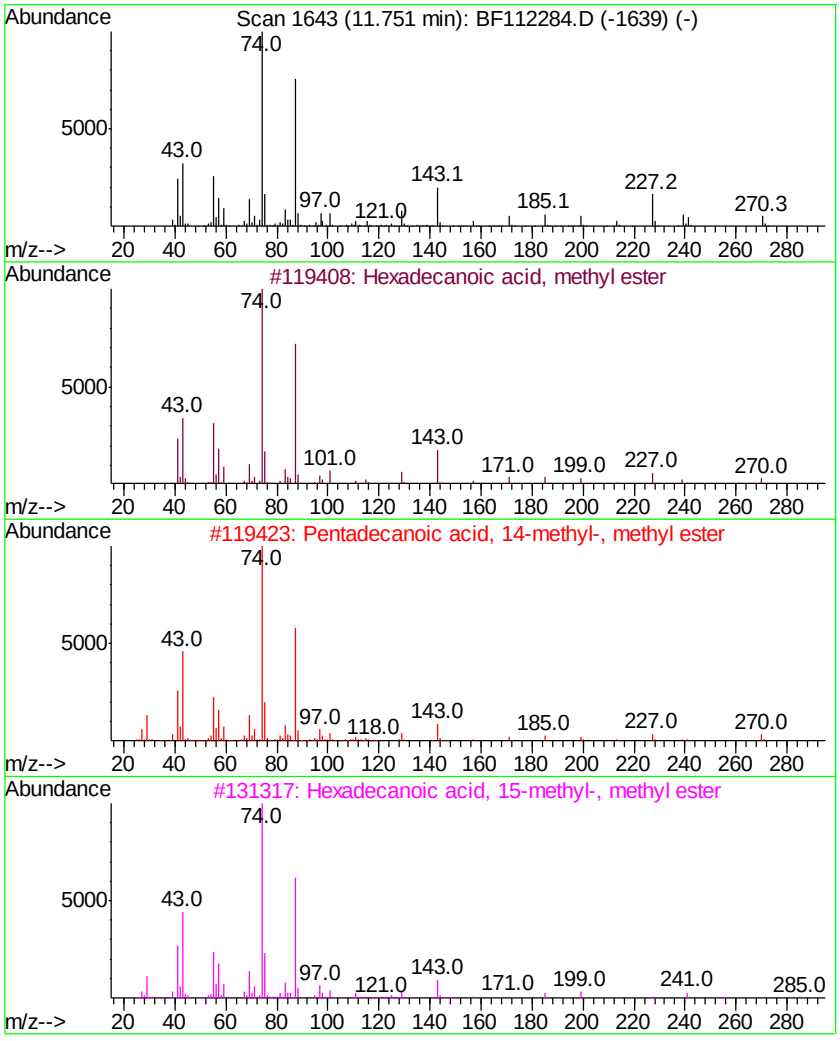
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

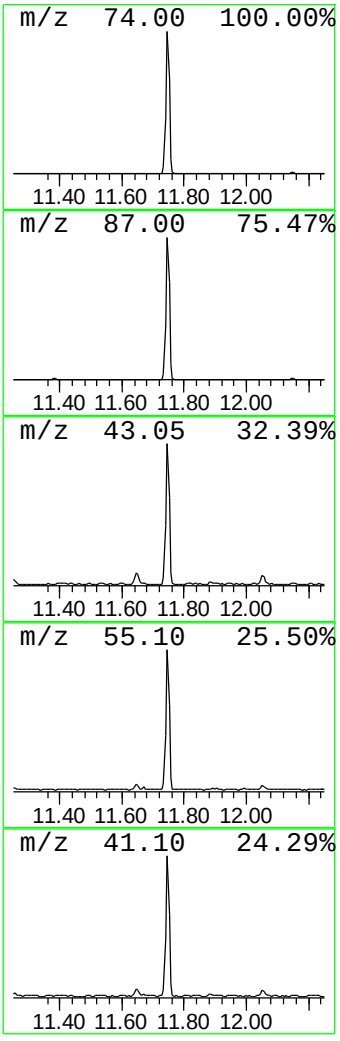
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	17.85 ng	1503130	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
3	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	87
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
5	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012819\
Data File : BF112284.D
Acq On : 28 Jan 2019 19:39
Operator : JU/SJ
Sample : K1011-09 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-012519-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

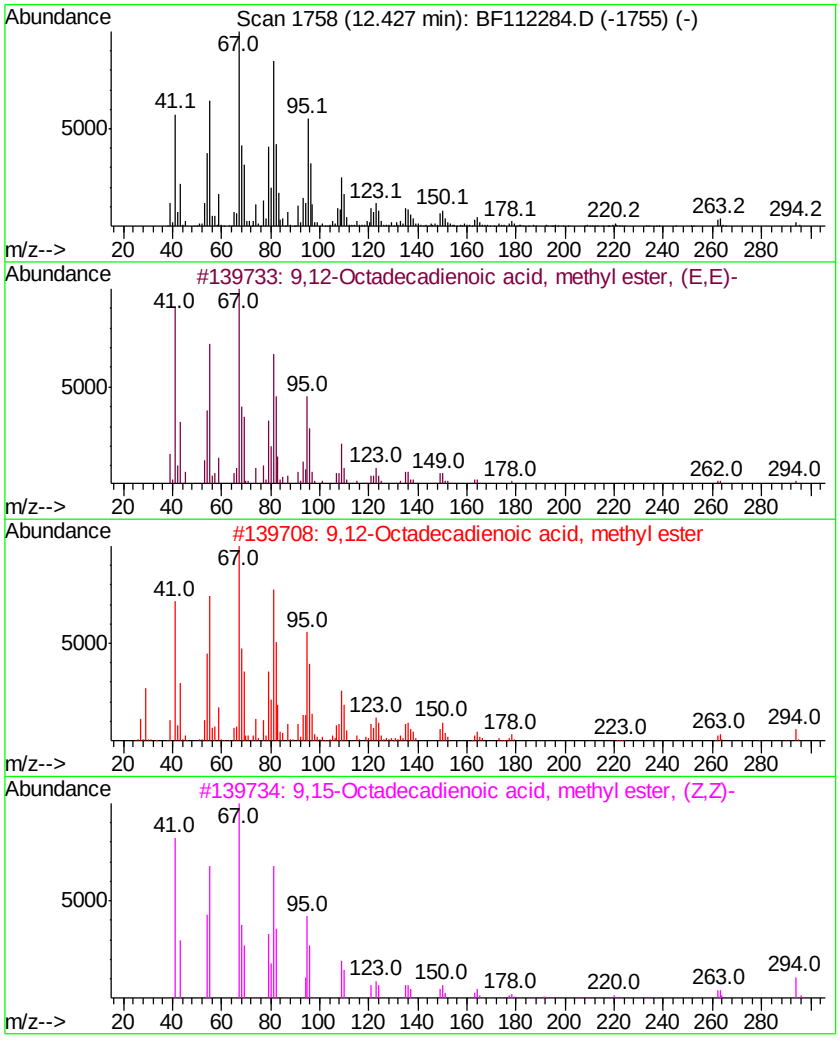
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

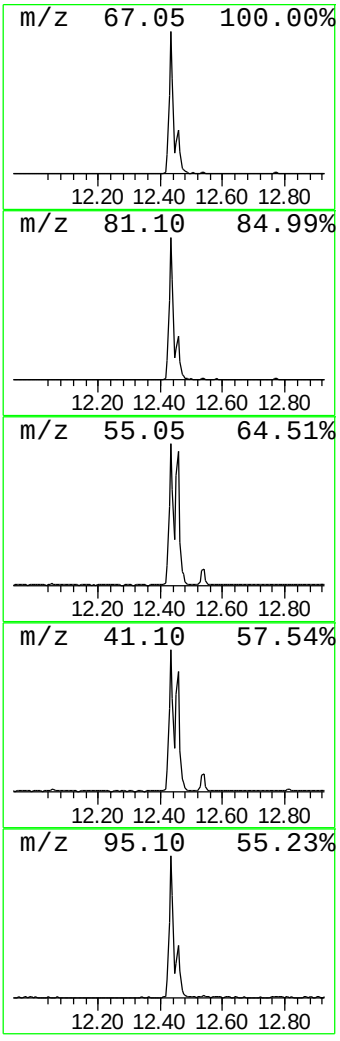
****

Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.43	61.00 ng	5137360	Phenanthrene-d10	11.36

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	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
4	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
5	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	99





Library Search Compound Report

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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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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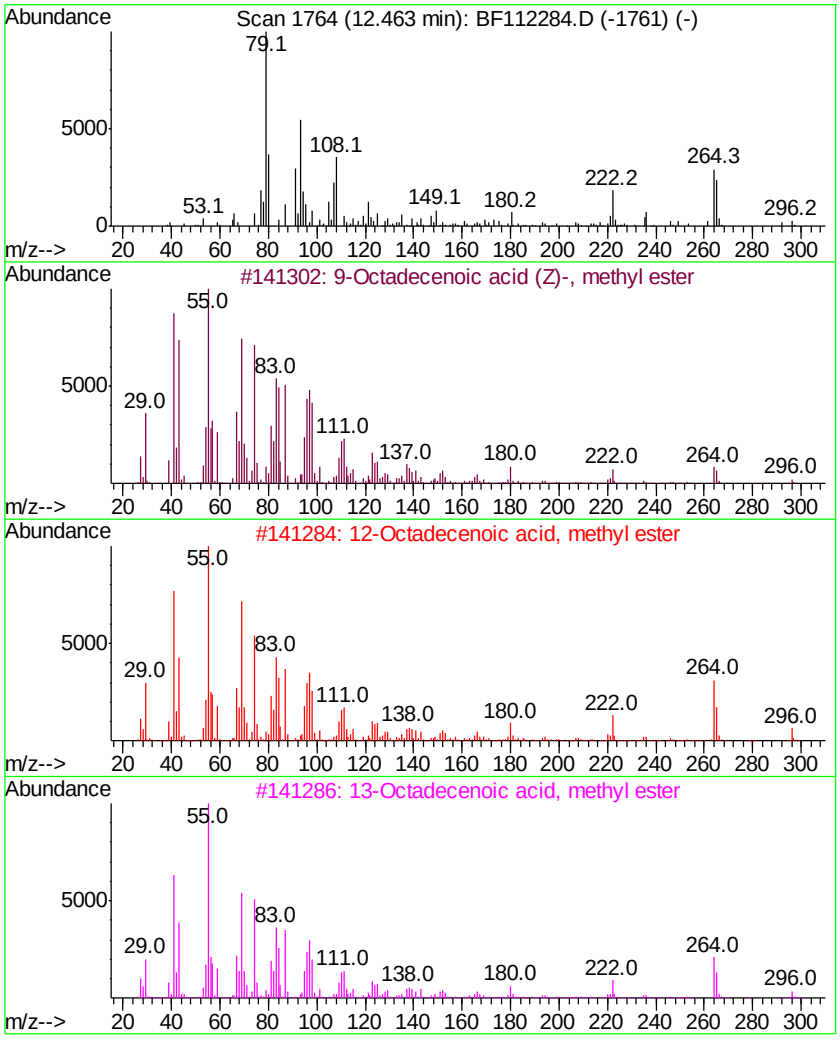
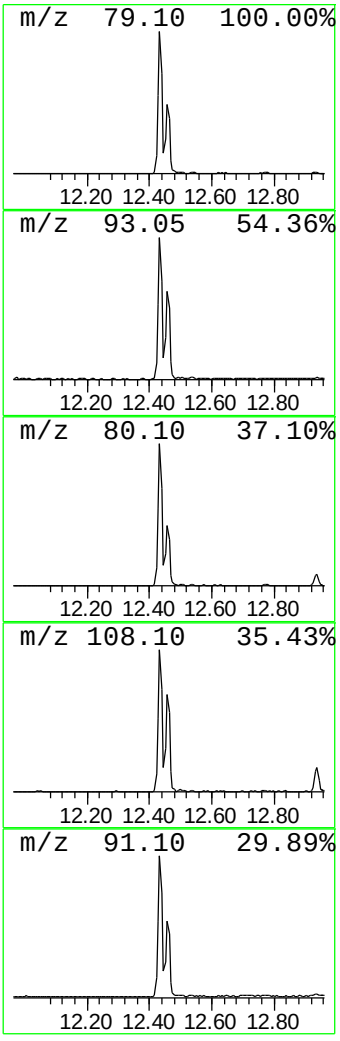
Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.46	42.50 ng	3579210	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
4	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
5	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012819\
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Misc :
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Instrument : BNA_F
ClientSampleId : OR-01-012519-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

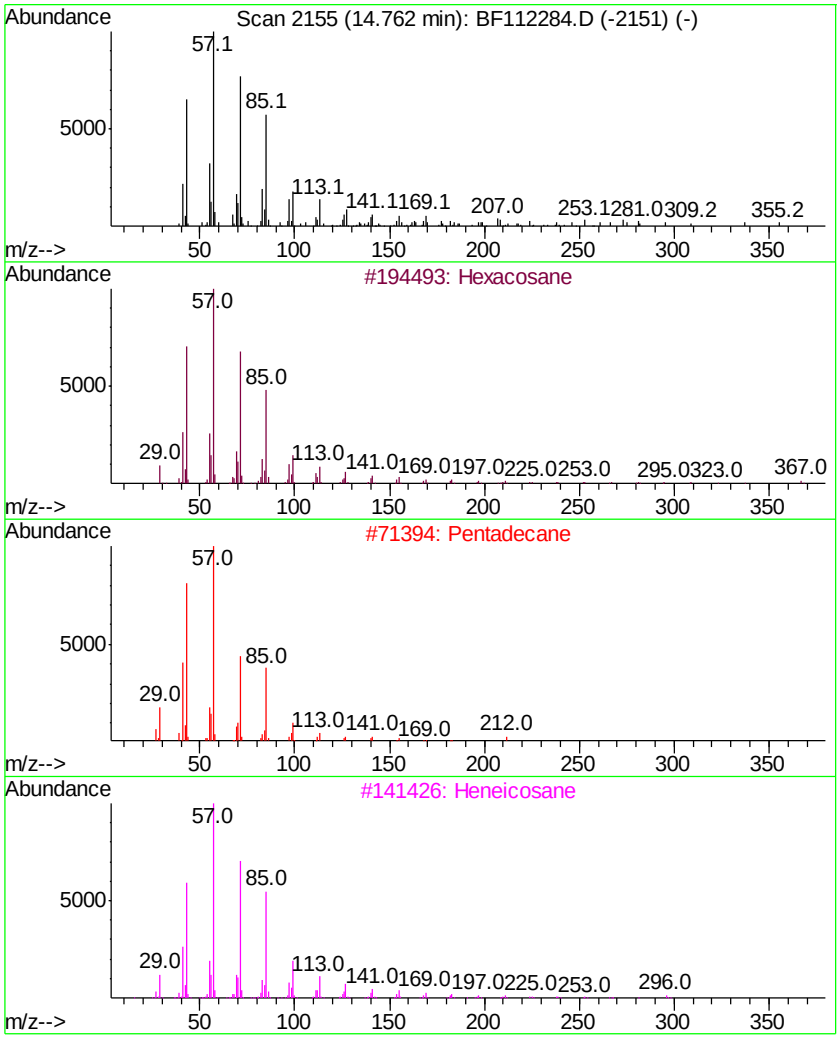
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

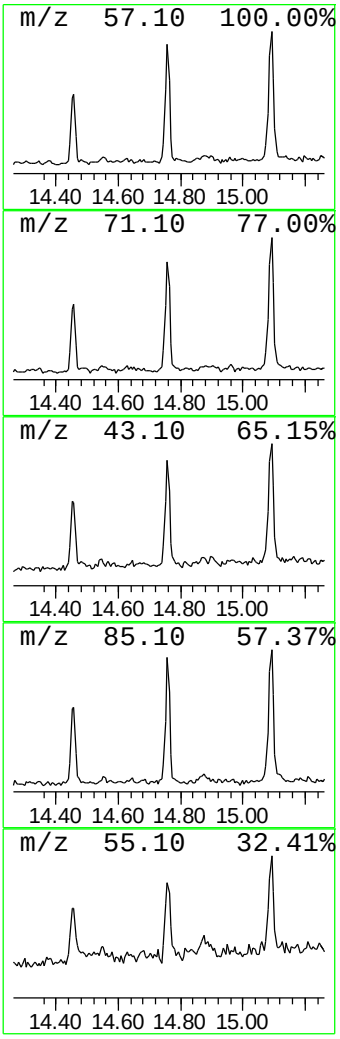
****

Peak Number 6 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.76	2.28 ng	156150	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	87
2	Pentadecane	212	C15H32	000629-62-9	87
3	Heneicosane	296	C21H44	000629-94-7	87
4	Octadecane, 2-methyl-	268	C19H40	001560-88-9	86
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : OR-01-012519-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

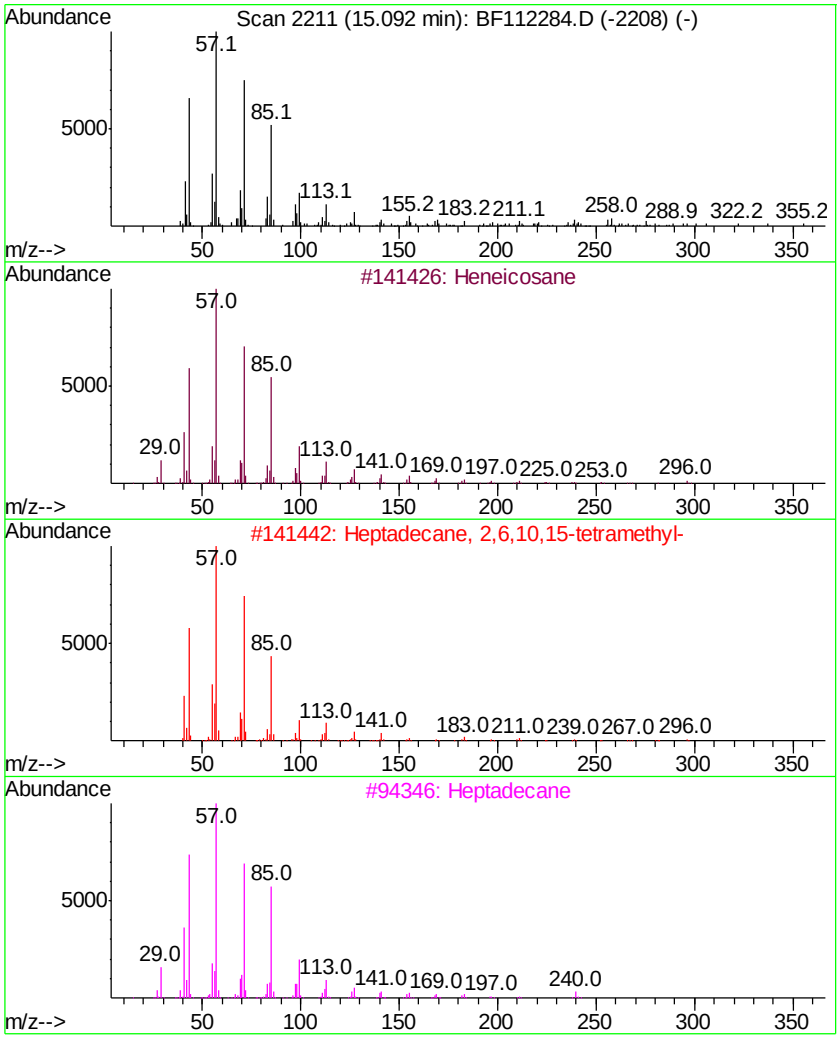
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

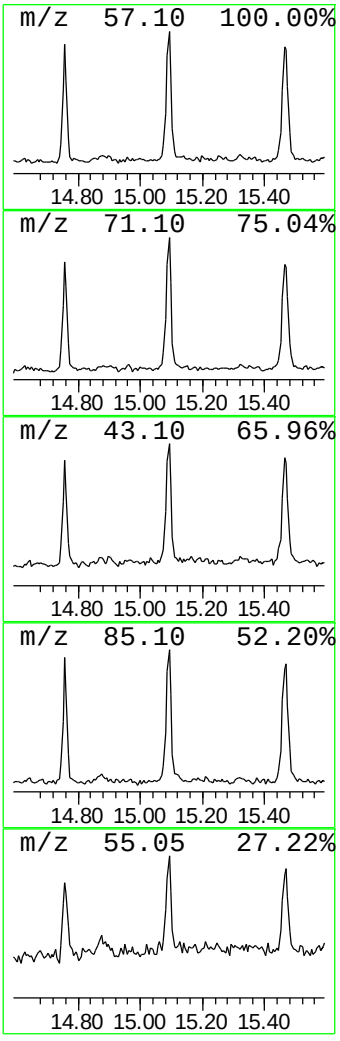
****

Peak Number 7 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	3.40 ng	233130	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	93
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
3	Heptadecane	240	C17H36	000629-78-7	93
4	Eicosane	282	C20H42	000112-95-8	93
5	Tetracosane	338	C24H50	000646-31-1	90





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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-012519-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

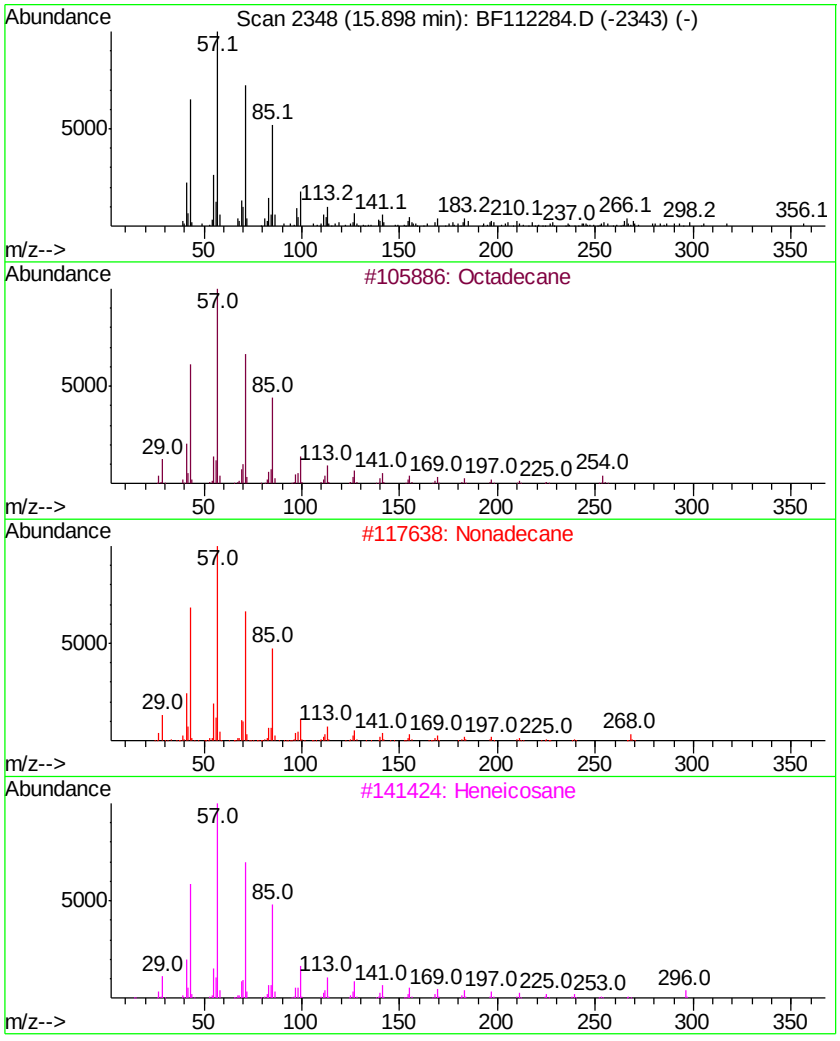
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

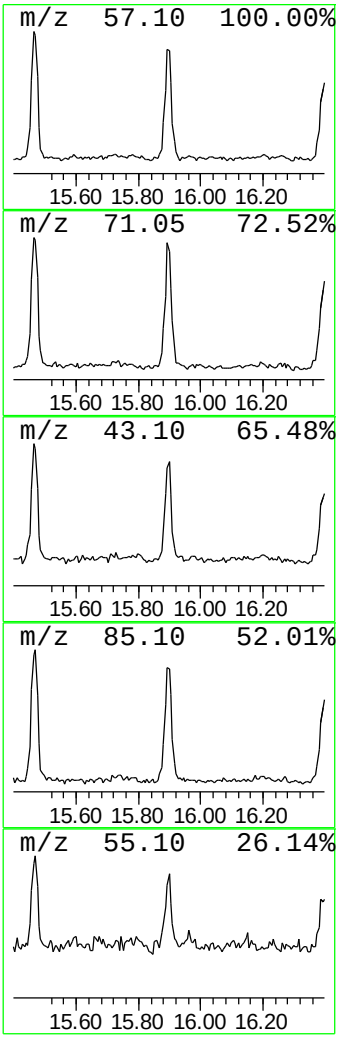
****

Peak Number 8 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.90	3.06 ng	209936	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	96
2	Nonadecane	268	C19H40	000629-92-5	95
3	Heneicosane	296	C21H44	000629-94-7	90
4	Docosane	310	C22H46	000629-97-0	90
5	Hexacosane	366	C26H54	000630-01-3	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF012819\
Data File : BF112284.D
Acq On : 28 Jan 2019 19:39
Operator : JU/SJ
Sample : K1011-09 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-01-012519-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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
unknown6.61	6.61	15.7	ng	957340	1	6.84	1221560	20.0
Hexadecanoic acid...	11.75	17.9	ng	1503130	4	11.36	1684430	20.0
9,12-Octadecadien...	12.43	61.0	ng	5137360	4	11.36	1684430	20.0
9-Octadecenoic ac...	12.46	42.5	ng	3579210	4	11.36	1684430	20.0
Hexacosane	14.76	2.3	ng	156150	6	15.46	1370980	20.0
Heneicosane	15.09	3.4	ng	233130	6	15.46	1370980	20.0
Octadecane	15.90	3.1	ng	209936	6	15.46	1370980	20.0