LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112917\
Data File : BF100989.D
Acq On : 29 Nov 2017 20:18
Operator : SJ/JU
Sample : I6304-28 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-112817-D

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-BF110817.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	5.057	503	505	513	rBB	12365	12679	2.39%	0.235%
2	5.463	570	574	585	rBB	252758	226849	42.68%	4.209%
3	6.475	743	746	756	rVB	291397	238097	44.79%	4.417%
4	6.616	767	770	774	rBV	283588	246317	46.34%	4.570%
5	6.851	807	810	814	rBV	547070	428534	80.62%	7.951%
6	7.004	833	836	840	rBV	210030	188282	35.42%	3.493%
7	7.410	902	905	909	rBV	160748	129983	24.45%	2.412%
8	8.133	1025	1028	1032	rBV	651368	531553	100.00%	9.862%
9	9.204	1207	1210	1214	rBV	334143	266903	50.21%	4.952%
10	9.280	1221	1223	1227	rBB	7798	6574	1.24%	0.122%
11	9.598	1274	1277	1280	rBV	18149	15769	2.97%	0.293%
12	9.810	1307	1313	1316	rBB2	16008	15109	2.84%	0.280%
13	9.892	1323	1327	1330	rBV	590450	490970	92.37%	9.109%
14	10.310	1396	1398	1401	rVB	16870	12249	2.30%	0.227%
15	10.675	1458	1460	1465	rBV	121223	106772	20.09%	1.981%
16	10.786	1475	1479	1484	rBV	12944	14779	2.78%	0.274%
17	11.380	1576	1580	1583	rBV	471144	413670	77.82%	7.675%
18	11.763	1641	1645	1648	rVB	137839	119816	22.54%	2.223%
19	11.992	1675	1684	1687	rBV6	10608	25588	4.81%	0.475%
20	12.445	1758	1761	1763	rBV	549317	470082	88.44%	8.722%
21	12.469	1763	1765	1771	rVB2	351833	293291	55.18%	5.441%
22	12.551	1776	1779	1782	rBV	55468	42974	8.08%	0.797%
23	12.592	1783	1786	1789	rBV	32726	28272	5.32%	0.525%
24	12.692	1796	1803	1808	rBV6	5179	13895	2.61%	0.258%
25	12.821	1822	1825	1827	rBV	28860	24692	4.65%	0.458%
26	12.957	1845	1848	1853	rVB	242319	187849	35.34%	3.485%
27	13.151	1867	1881	1883	rBV9	19630	55912	10.52%	1.037%
28	13.627	1959	1962	1964	rBV4	8409	12230	2.30%	0.227%
29	13.851	1997	2000	2006	rBV6	12038	18591	3.50%	0.345%
30	13.945	2014	2016	2018	rBV3	8713	8975	1.69%	0.167%
31	14.021	2024	2029	2032	rBV	460100	423384	79.65%	7.855%
32	15.492	2274	2279	2286	rBV2	246301	319271	60.06%	5.923%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112917\
Data File : BF100989.D
Acq On : 29 Nov 2017 20:18
Operator : SJ/JU
Sample : I6304-28 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-112817-D

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-BF110817.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 5389911

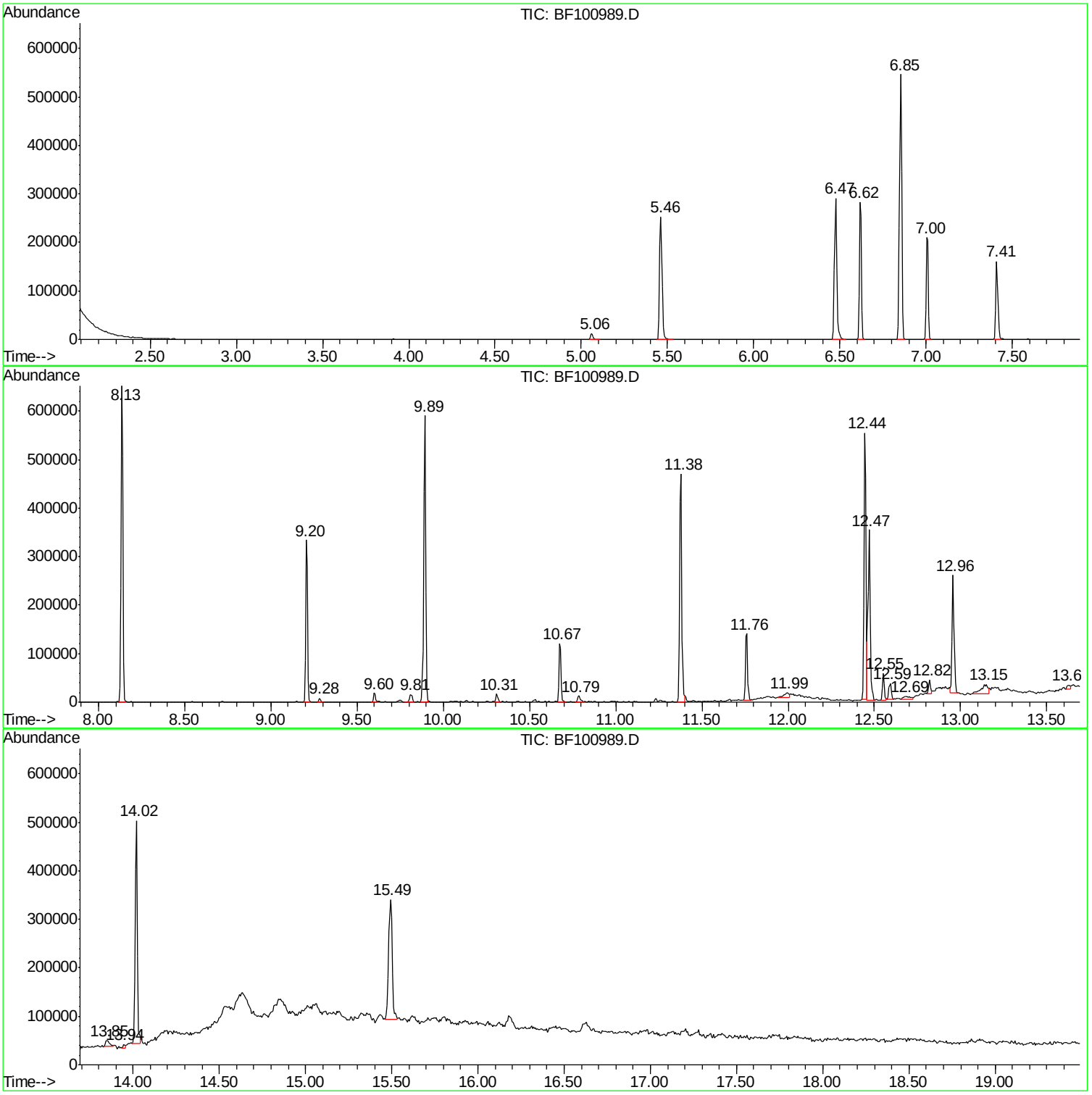
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112917\
Data File : BF100989.D
Acq On : 29 Nov 2017 20:18
Operator : SJ/JU
Sample : I6304-28 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-112817-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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\BF112917\
Data File : BF100989.D
Acq On : 29 Nov 2017 20:18
Operator : SJ/JU
Sample : I6304-28 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-112817-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

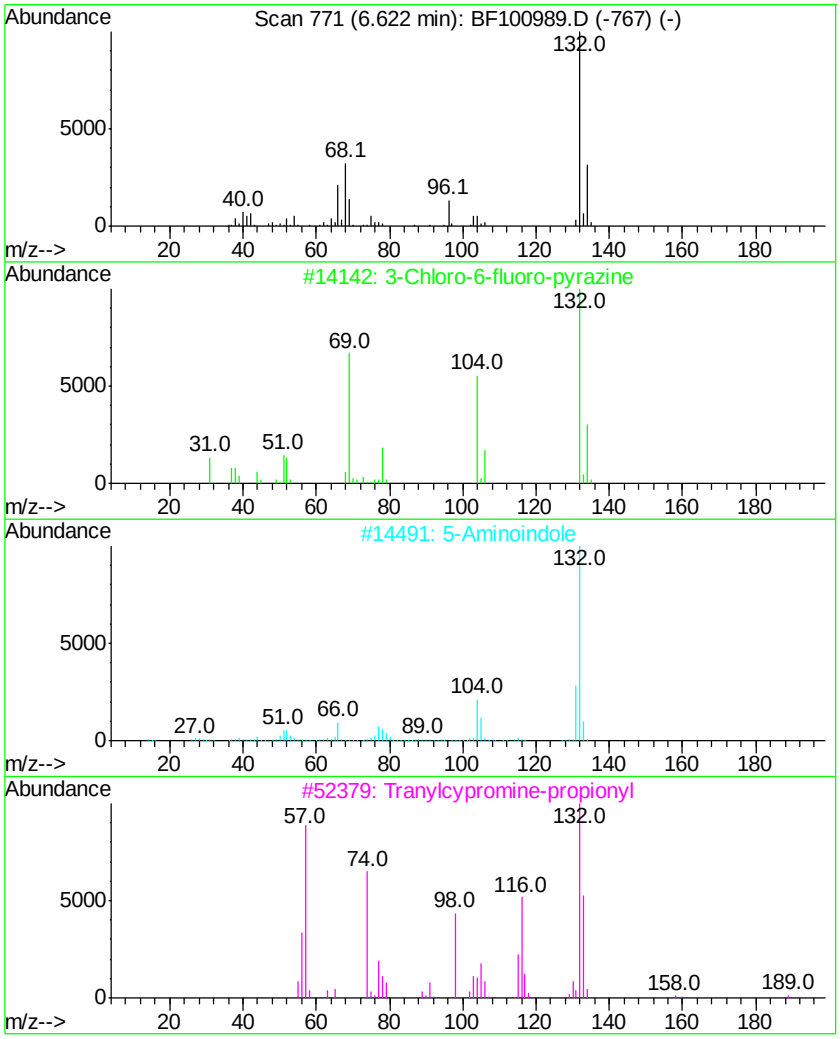
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

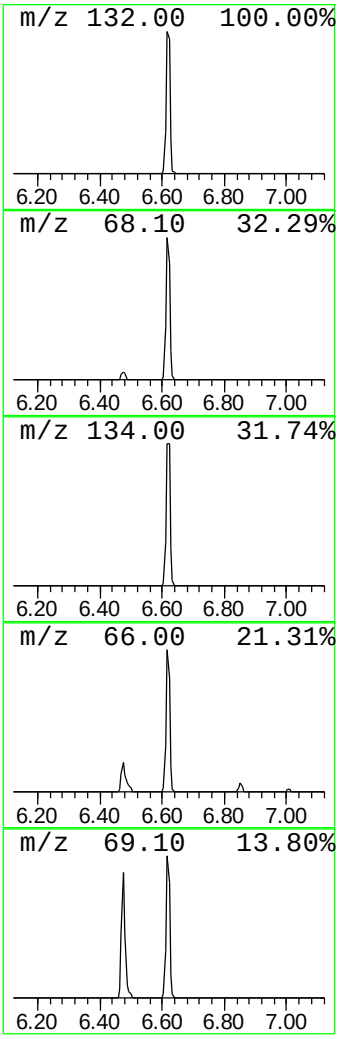
****

Peak Number 1 unknown6.62 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	11.50 ng	246317	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	35
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112917\
Data File : BF100989.D
Acq On : 29 Nov 2017 20:18
Operator : SJ/JU
Sample : I6304-28 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-112817-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

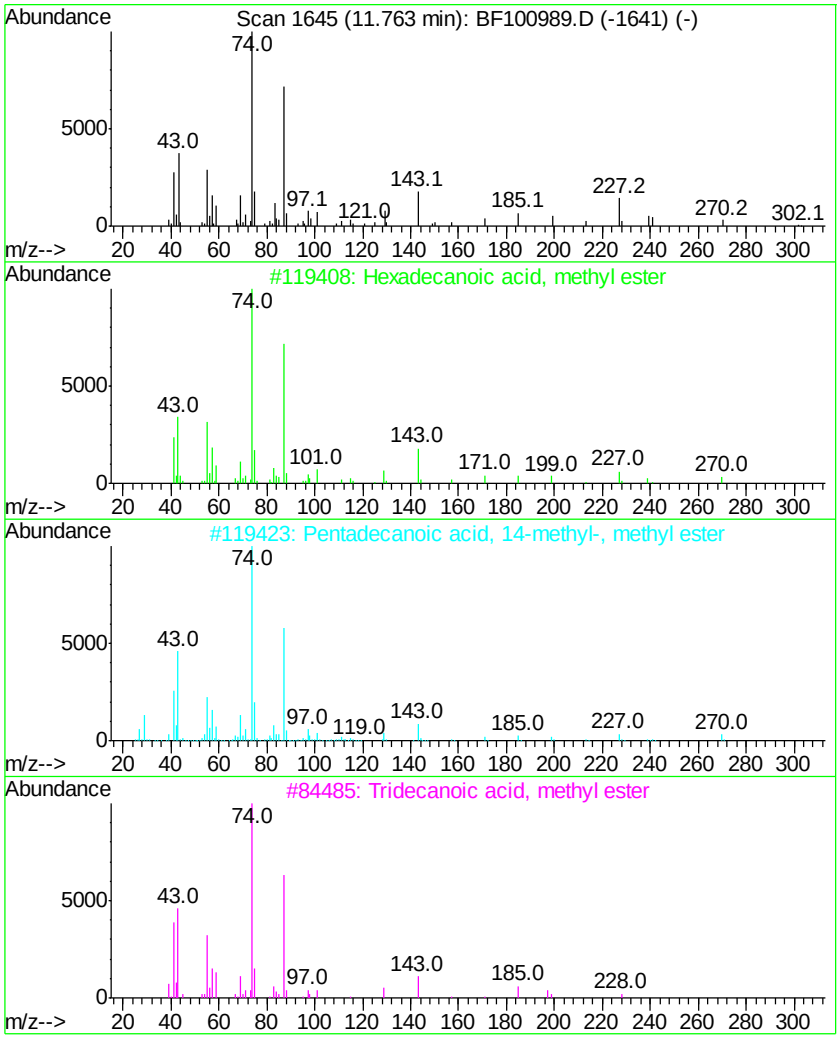
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

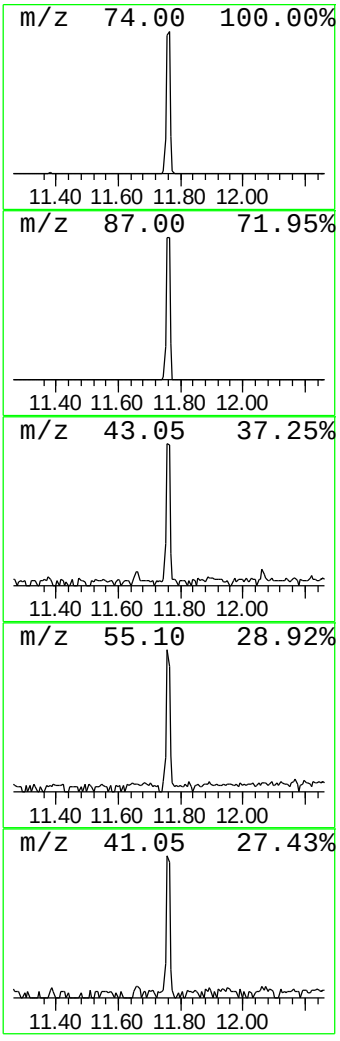
****

Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.76	5.79 ng	119816	Phenanthrene-d10	11.38

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	94
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
4	Methyl stearate	298	C19H38O2	000112-61-8	83
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112917\
Data File : BF100989.D
Acq On : 29 Nov 2017 20:18
Operator : SJ/JU
Sample : I6304-28 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-112817-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

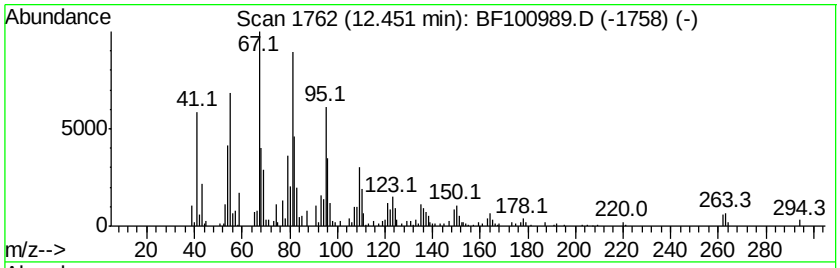
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

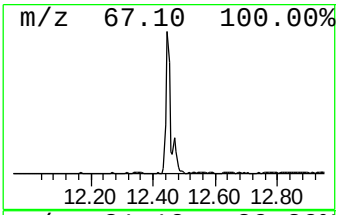
****

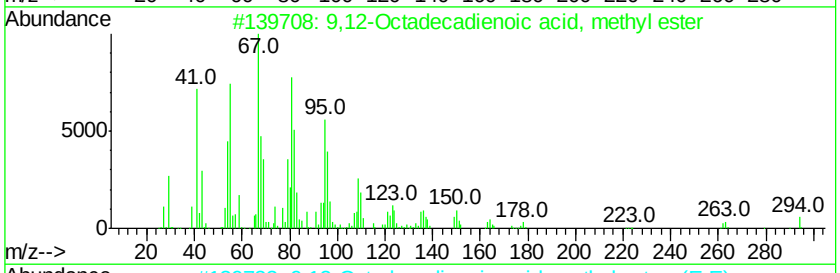
Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 1

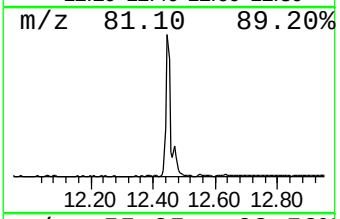
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.45	22.73 ng	470082	Phenanthrene-d10	11.38

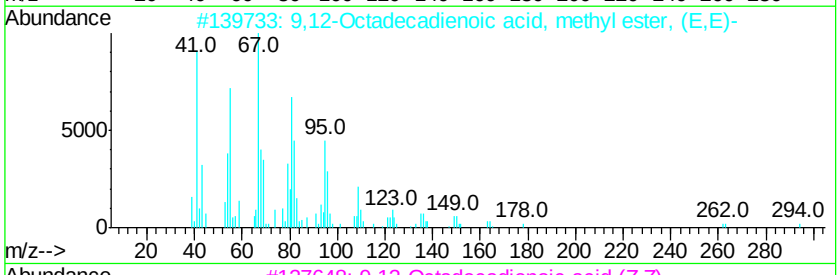
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	98
3	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	95
4	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	94
5	9,17-Octadecadienal, (Z)-	264	C18H32O	056554-35-9	93

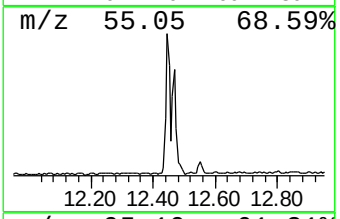


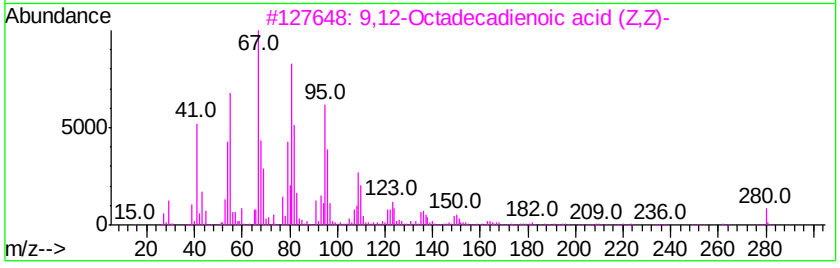


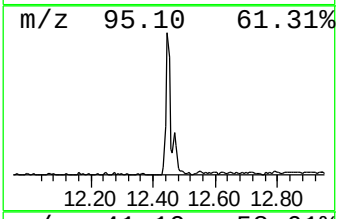


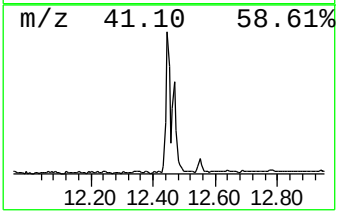












Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112917\
Data File : BF100989.D
Acq On : 29 Nov 2017 20:18
Operator : SJ/JU
Sample : I6304-28 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-112817-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

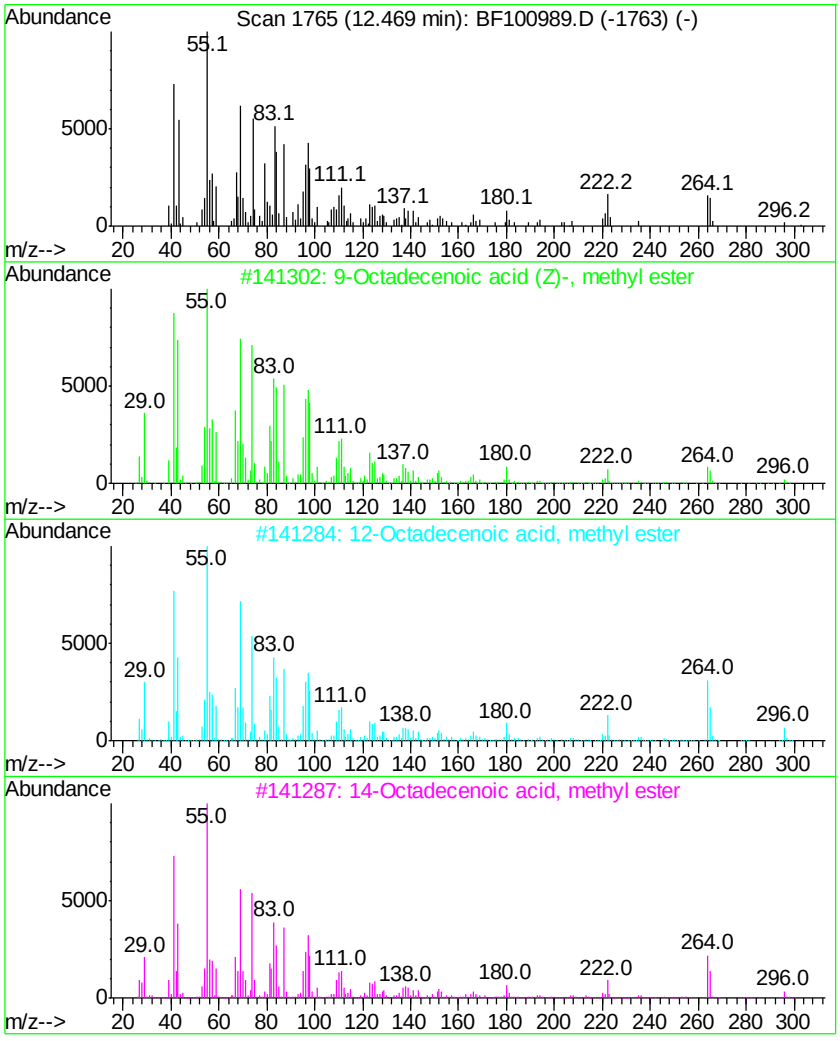
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

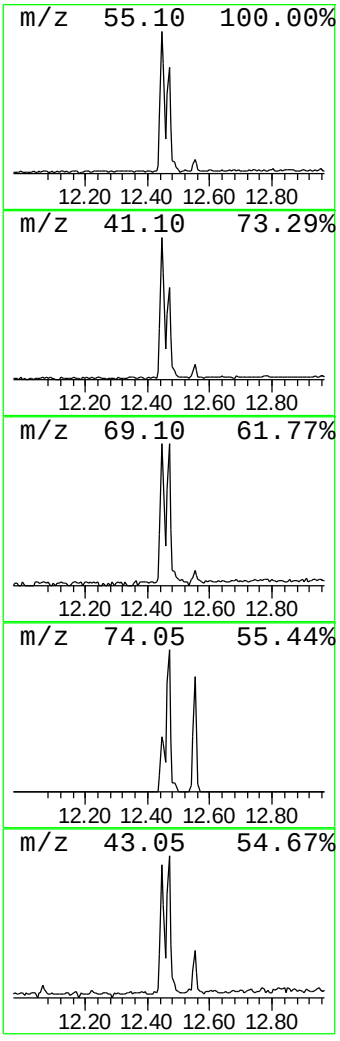
****

Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.47	14.18 ng	293291	Phenanthrene-d10	11.38

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	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
4	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
5	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99





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Acq On : 29 Nov 2017 20:18
Operator : SJ/JU
Sample : I6304-28 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-112817-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

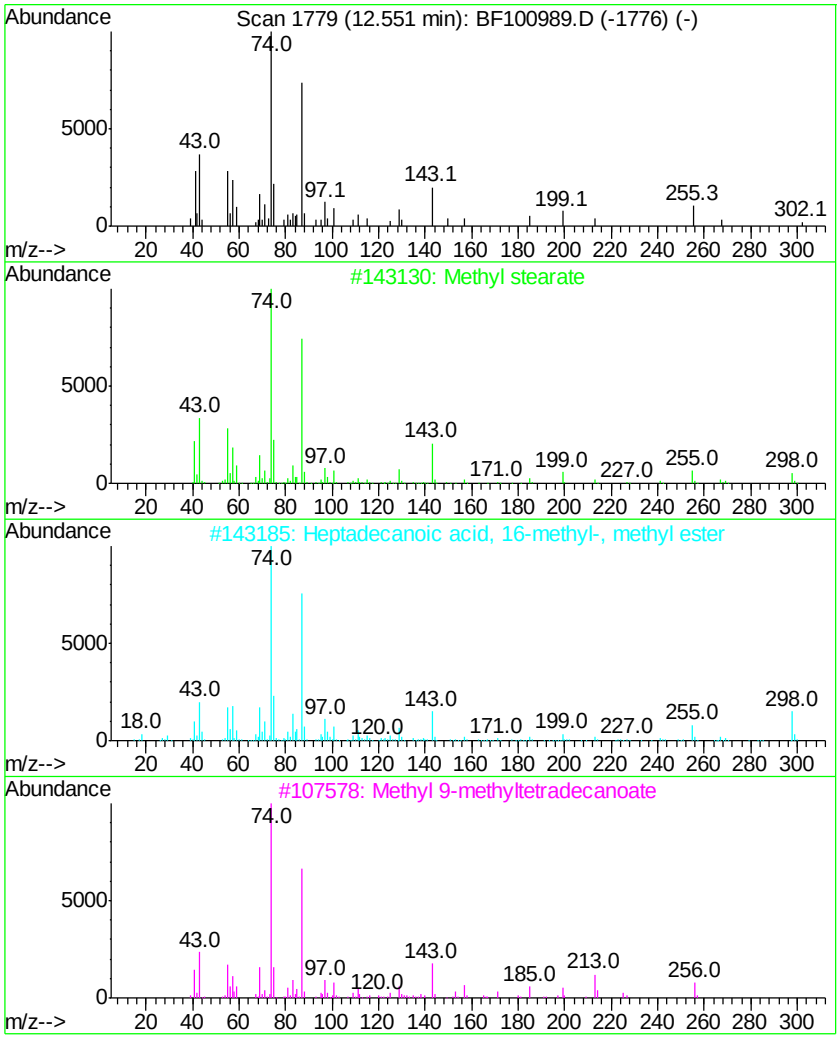
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

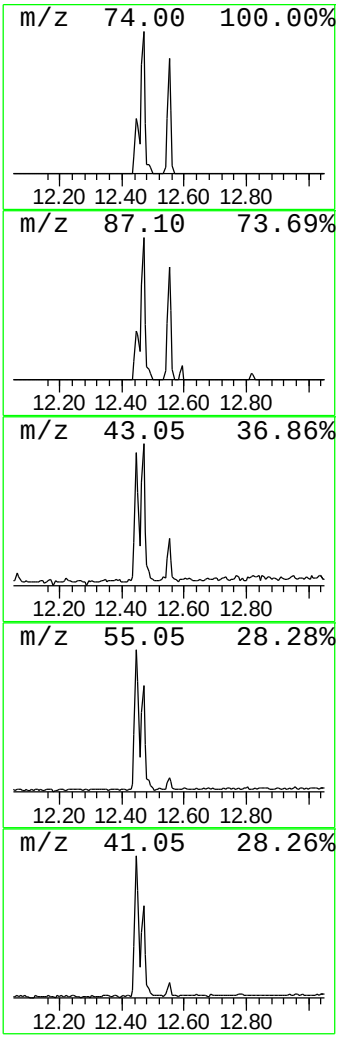
****

Peak Number 6 Methyl stearate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.55	2.08 ng	42974	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	91
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	87
3	Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	86
4	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	86
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

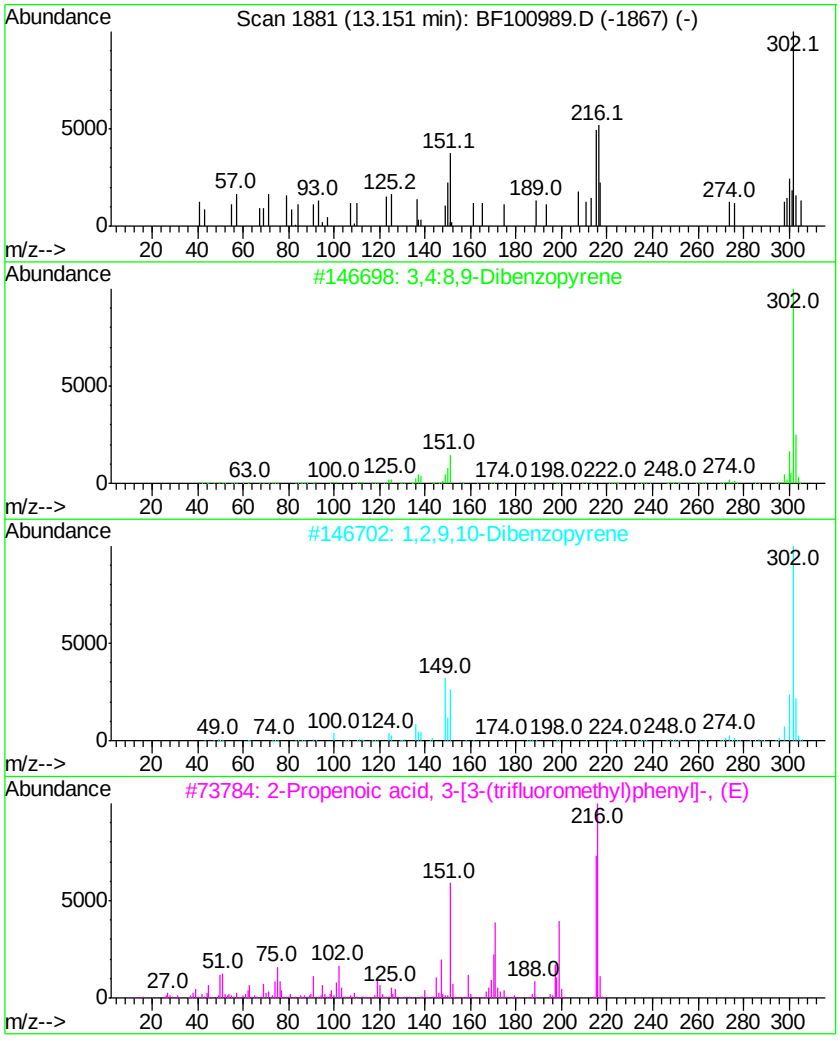
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

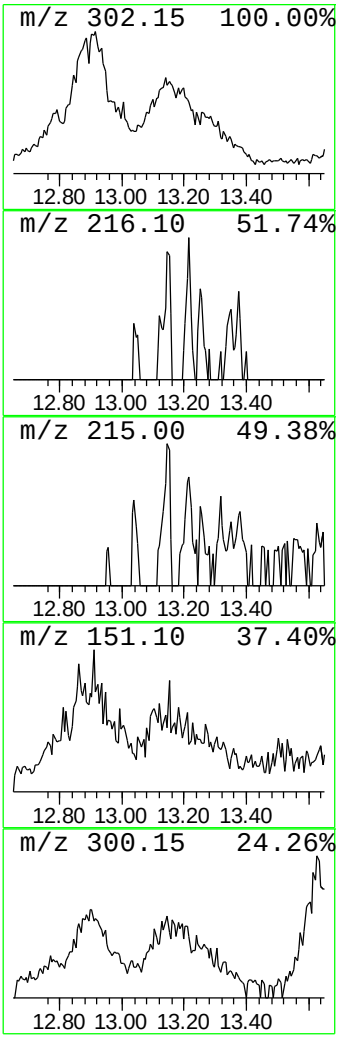
****

Peak Number 7 unknown13.15 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.15	2.64 ng	55912	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4:8,9-Dibenzopyrene	302	C24H14	000189-64-0	43
2	1,2,9,10-Dibenzopyrene	302	C24H14	000191-30-0	27
3	2-Propenoic acid, 3-[3-(trifluor...	216	C10H7F3O2	067801-07-4	25
4	Bicyclo[4.3.0]nonan-2-one, 8-(di...	302	C22H22O	082432-11-9	22
5	2H-Furo[3',2':4,5]furo[2,3-h]-1-...	302	C16H14O6	023315-33-5	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112917\
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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
unknown6.62	6.62	11.5	ng	246317	1	6.85	428534	20.0
Hexadecanoic acid...	11.76	5.8	ng	119816	4	11.38	413670	20.0
9,12-Octadecadien...	12.45	22.7	ng	470082	4	11.38	413670	20.0
9-Octadecenoic ac...	12.47	14.2	ng	293291	4	11.38	413670	20.0
Methyl stearate	12.55	2.1	ng	42974	4	11.38	413670	20.0
unknown13.15	13.15	2.6	ng	55912	5	14.02	423384	20.0