LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106397.D
Acq On : 13 Jun 2018 17:59
Operator : JU/SJ
Sample : J3251-03 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-03-061118

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-BF061118.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	4.084	291	297	302	rBV	87232	109438	2.75%	0.367%
2	5.190	481	485	490	rVB	123501	132875	3.33%	0.446%
3	5.613	553	557	564	rBV	1331180	1449615	36.37%	4.861%
4	6.613	723	727	744	rVB	1280786	1574321	39.50%	5.279%
5	6.748	746	750	753	rBV	1833396	1496123	37.54%	5.017%
6	6.966	783	787	790	rVB	1209053	917812	23.03%	3.078%
7	7.119	810	813	817	rVB	1358927	1164181	29.21%	3.904%
8	7.525	878	882	885	rBV	1187852	949324	23.82%	3.183%
9	8.248	1001	1005	1008	rBV	1544433	1205127	30.24%	4.041%
10	9.319	1184	1187	1191	rVB	2041972	1739698	43.65%	5.834%
11	9.389	1196	1199	1203	rBV2	48250	42004	1.05%	0.141%
12	9.713	1251	1254	1257	rBV	364221	270037	6.78%	0.906%
13	9.919	1287	1289	1293	rVB	110821	84891	2.13%	0.285%
14	10.007	1300	1304	1307	rBV2	1569648	1297067	32.55%	4.349%
15	10.207	1335	1338	1342	rVB2	71470	67484	1.69%	0.226%
16	10.419	1372	1374	1378	rVB	157558	127547	3.20%	0.428%
17	10.554	1394	1397	1400	rVB	108079	85440	2.14%	0.287%
18	10.642	1406	1412	1414	rBV	69876	85823	2.15%	0.288%
19	10.795	1435	1438	1442	rBV	1116827	1005521	25.23%	3.372%
20	10.895	1452	1455	1461	rBV	185096	200517	5.03%	0.672%
21	11.342	1528	1531	1534	rBV	158564	132087	3.31%	0.443%
22	11.371	1534	1536	1538	rVV	64053	65171	1.64%	0.219%
23	11.395	1538	1540	1543	rVB	56368	49514	1.24%	0.166%
24	11.501	1554	1558	1560	rBV	1304371	1298893	32.59%	4.356%
25	11.524	1560	1562	1565	rVV	617136	494572	12.41%	1.658%
26	11.571	1567	1570	1574	rVB	114927	94643	2.37%	0.317%
27	11.771	1601	1604	1606	rBV	128485	91809	2.30%	0.308%
28	11.830	1611	1614	1618	rVB4	30749	41683	1.05%	0.140%
29	11.871	1618	1621	1625	rBV	1493013	1330675	33.39%	4.462%
30	12.013	1640	1645	1646	rBV2	109530	144396	3.62%	0.484%
31	12.113	1659	1662	1664	rBV2	85377	76048	1.91%	0.255%
32	12.177	1670	1673	1676	rBV	104418	91044	2.28%	0.305%
33	12.324	1695	1698	1704	rVB4	36813	49768	1.25%	0.167%
34	12.566	1735	1739	1741	rBV	3845346	3985327	100.00%	13.364%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
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Acq On : 13 Jun 2018 17:59
Operator : JU/SJ
Sample : J3251-03 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-03-061118

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-BF061118.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.589	1741	1743	1749	rVV2	2971323	2766012	69.40%	9.275%
36	12.666	1753	1756	1761	rVB	687600	600727	15.07%	2.014%
37	12.713	1761	1764	1768	rBV	514454	431978	10.84%	1.449%
38	12.907	1792	1797	1798	rBV3	71650	86767	2.18%	0.291%
39	12.942	1801	1803	1810	rVB	393225	364046	9.13%	1.221%
40	13.083	1823	1827	1830	rBV	1473180	1290206	32.37%	4.326%
41	13.230	1850	1852	1854	rBV	102178	84113	2.11%	0.282%
42	13.395	1878	1880	1884	rVB	63662	51173	1.28%	0.172%
43	13.971	1976	1978	1982	rVB3	96707	92030	2.31%	0.309%
44	14.148	2004	2008	2011	rBV	1123485	1146251	28.76%	3.844%
45	15.695	2266	2271	2277	rVB	714777	957830	24.03%	3.212%

Sum of corrected areas: 29821608

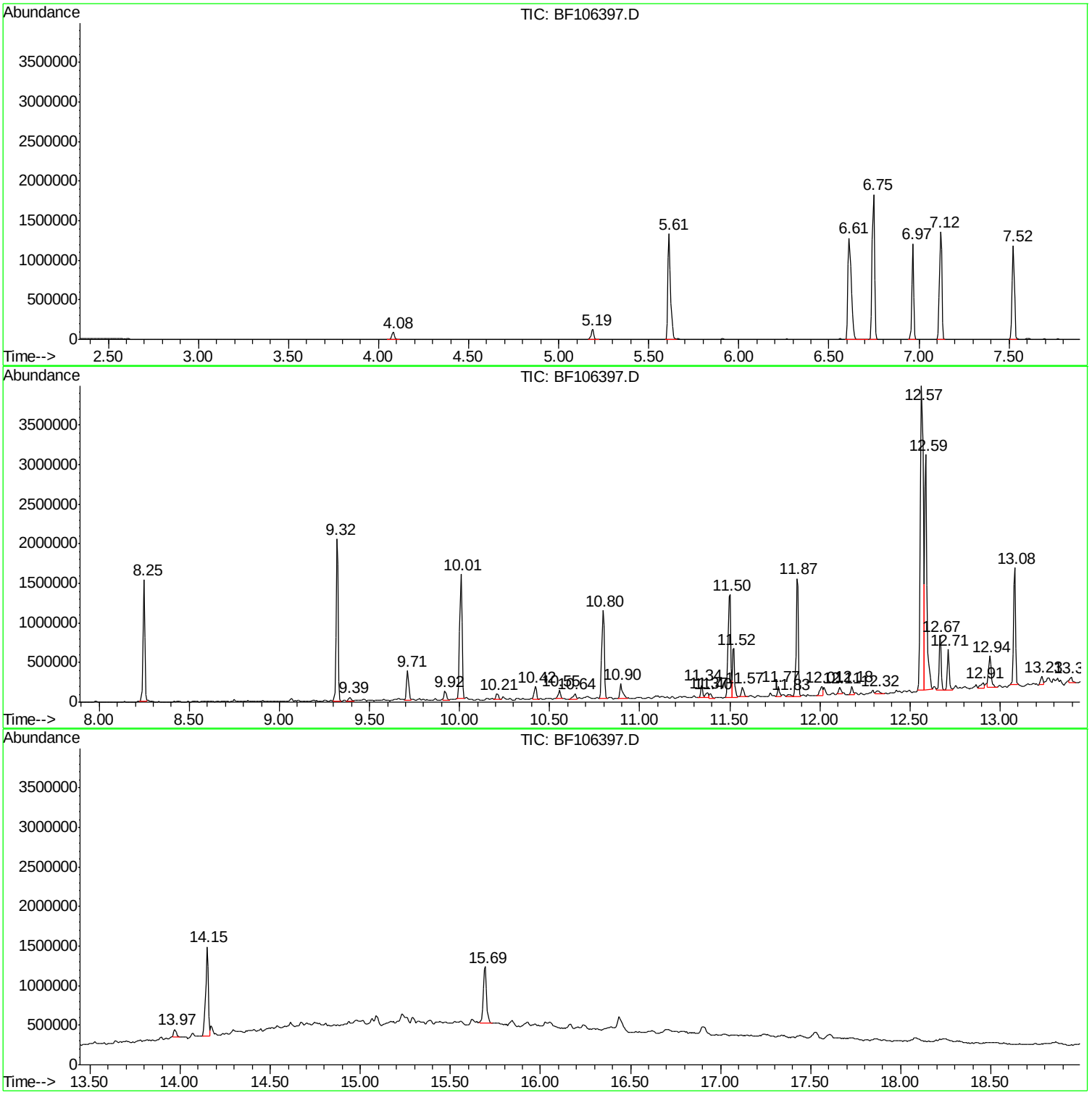
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106397.D
Acq On : 13 Jun 2018 17:59
Operator : JU/SJ
Sample : J3251-03 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-03-061118

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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\BF061318\
Data File : BF106397.D
Acq On : 13 Jun 2018 17:59
Operator : JU/SJ
Sample : J3251-03 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-03-061118

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

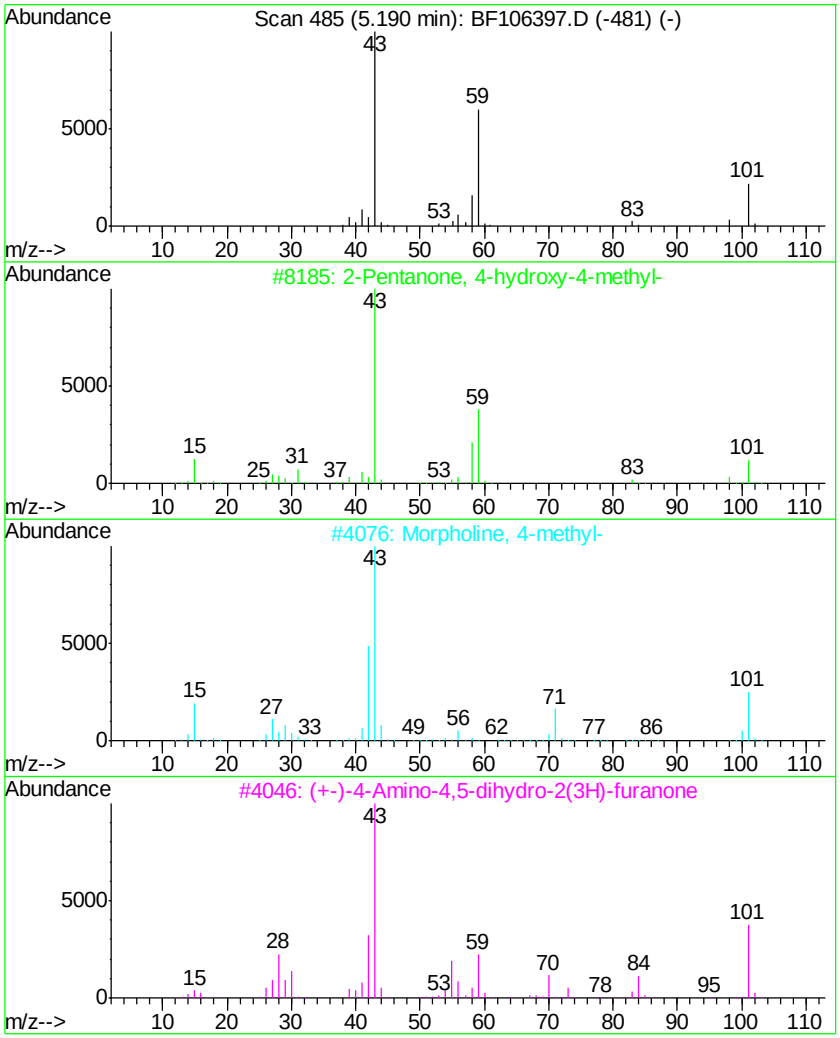
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

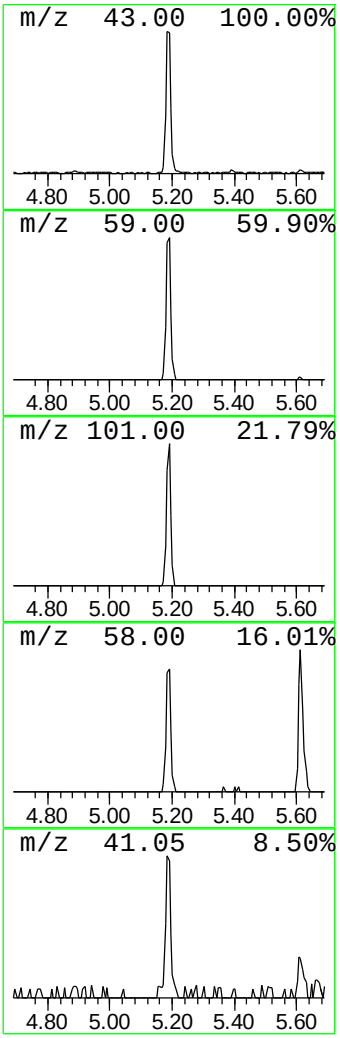
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	2.90 ng	132875	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106397.D
Acq On : 13 Jun 2018 17:59
Operator : JU/SJ
Sample : J3251-03 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-03-061118

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

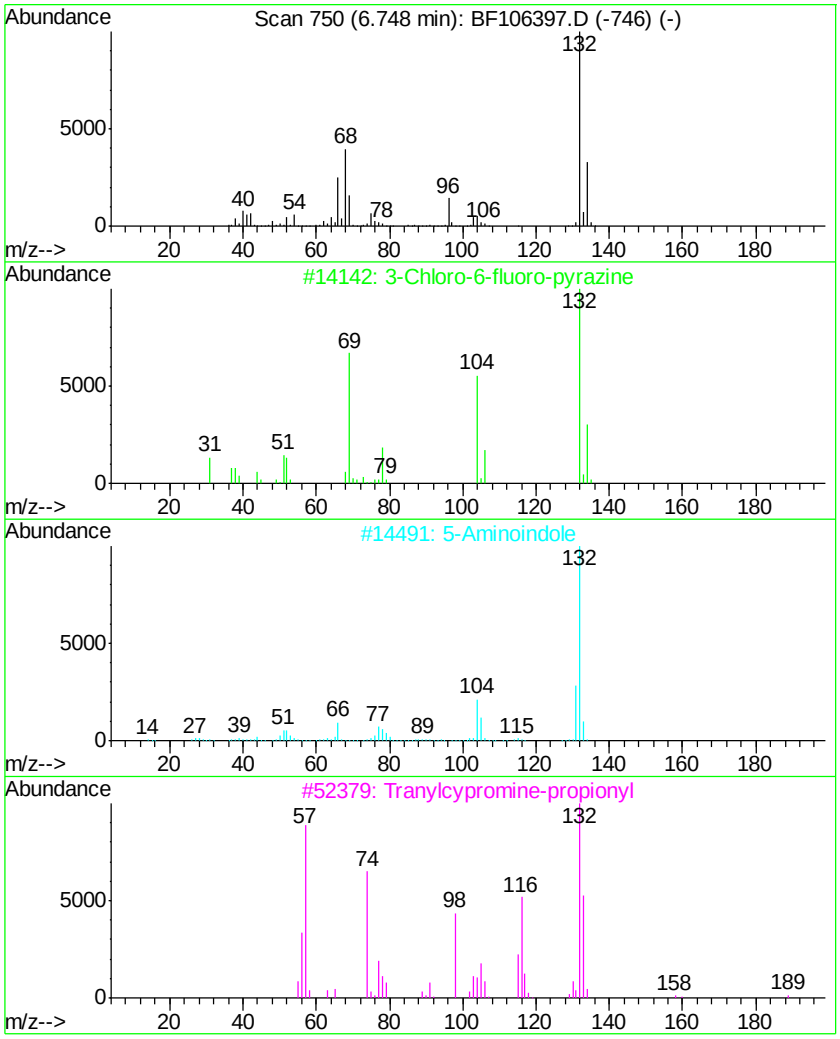
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

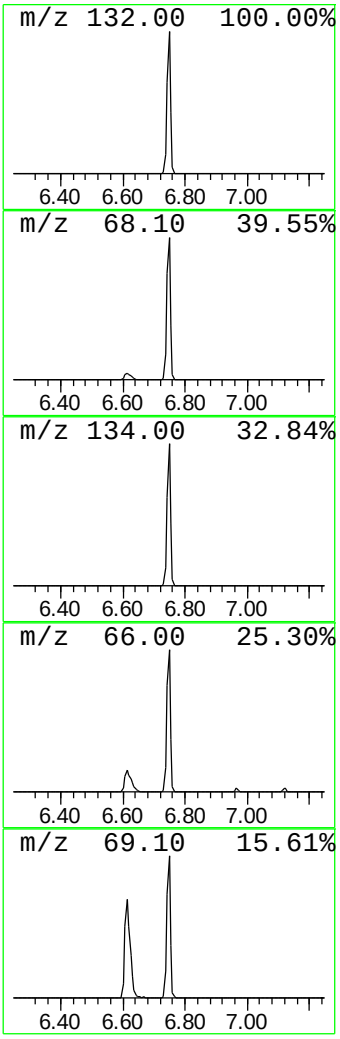
****

Peak Number 3 unknown6.75 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	32.60 ng	1496120	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106397.D
Acq On : 13 Jun 2018 17:59
Operator : JU/SJ
Sample : J3251-03 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-03-061118

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

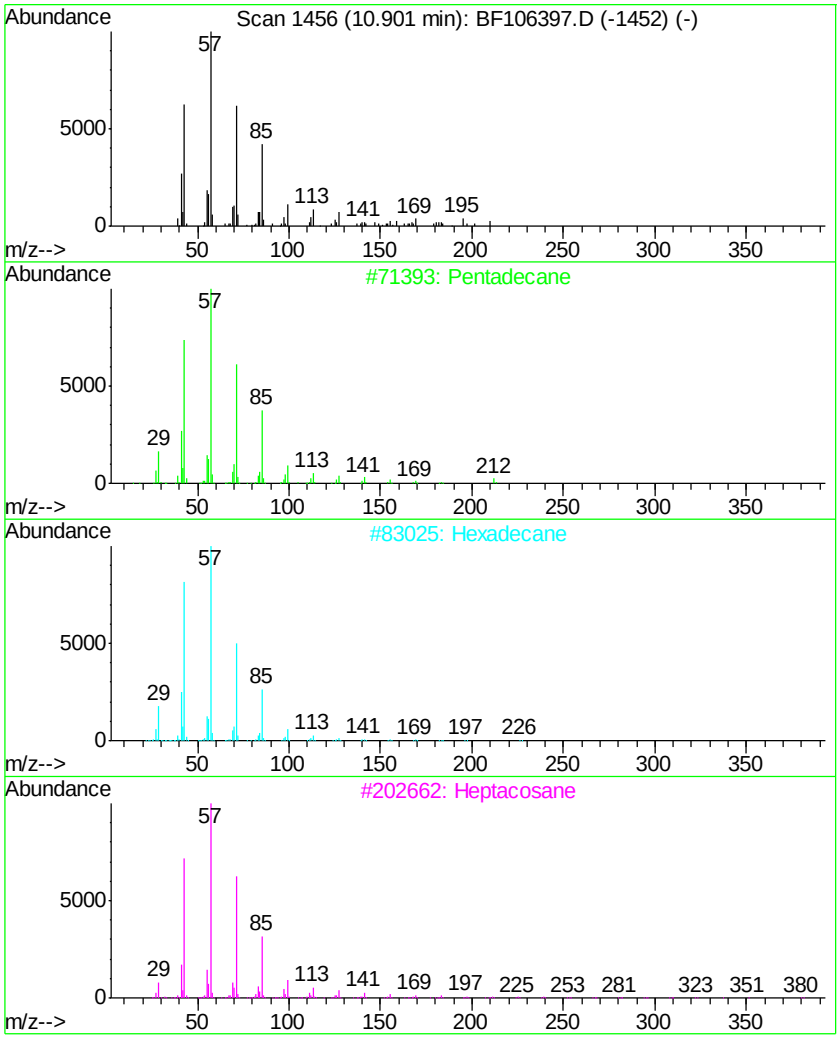
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

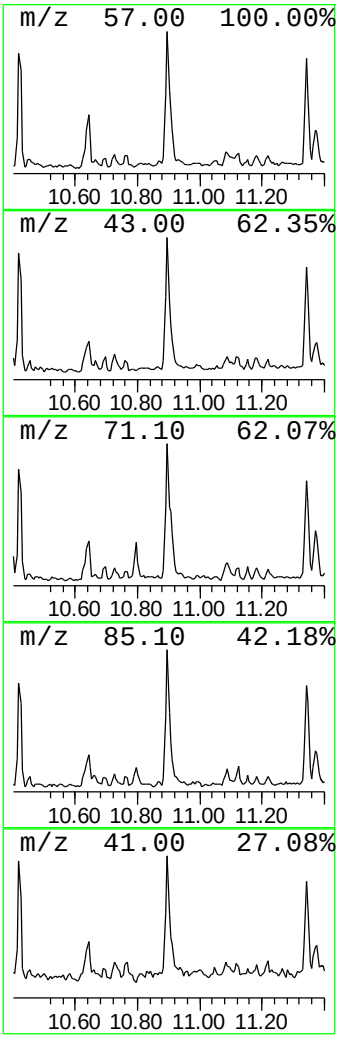
****

Peak Number 5 Pentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.90	3.09 ng	200517	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Heptacosane	380	C27H56	000593-49-7	86
4	Dodecane, 2-methyl-	184	C13H28	001560-97-0	72
5	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
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Operator : JU/SJ
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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-03-061118

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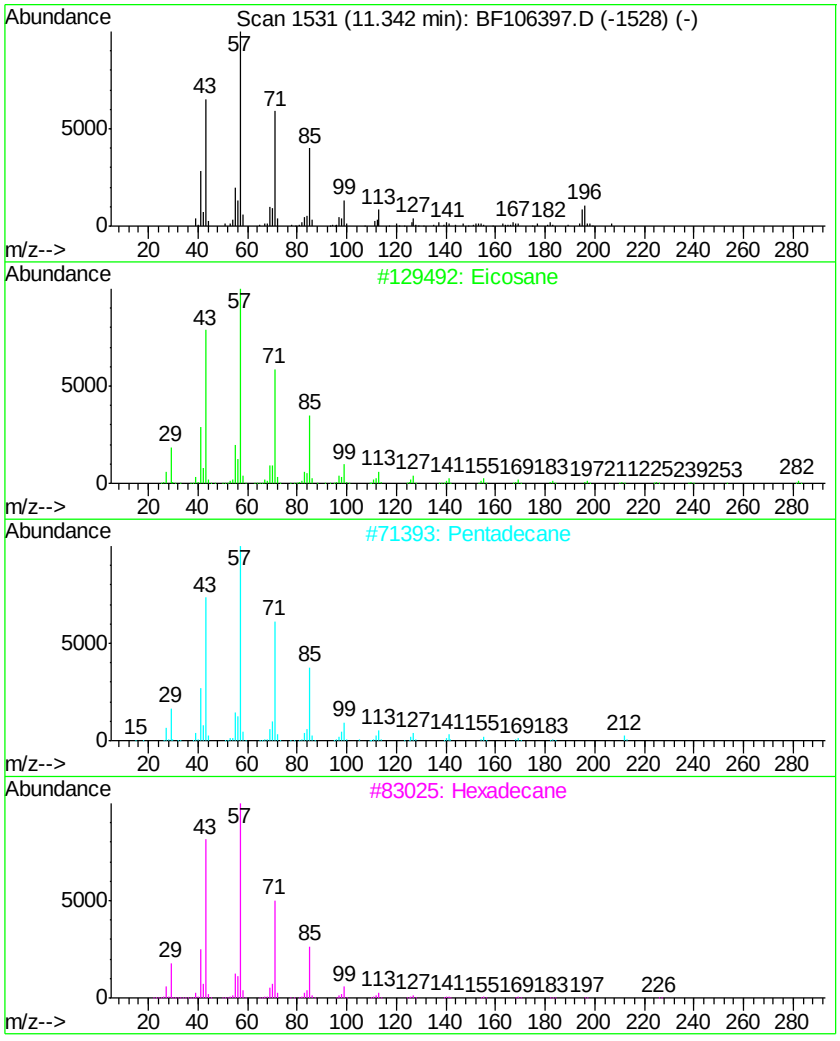
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

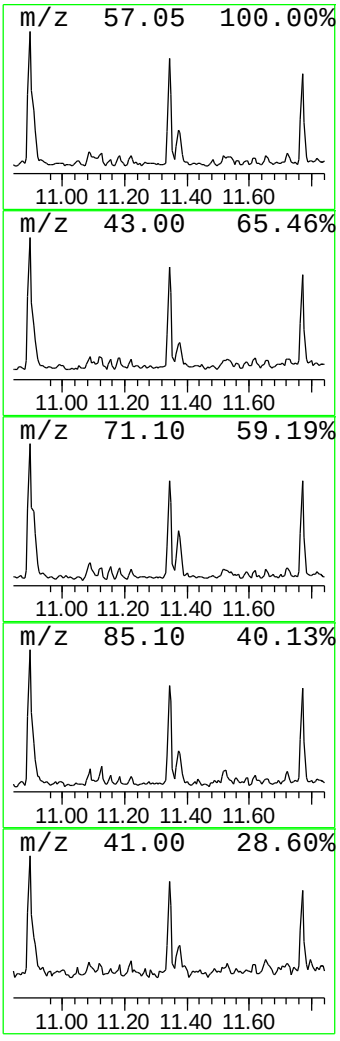
****

Peak Number 6 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.34	2.03 ng	132087	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	83
2	Pentadecane	212	C15H32	000629-62-9	80
3	Hexadecane	226	C16H34	000544-76-3	80
4	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	80
5	Tetratetracontane	619	C44H90	007098-22-8	80





Library Search Compound Report

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Sample : J3251-03 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-03-061118

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

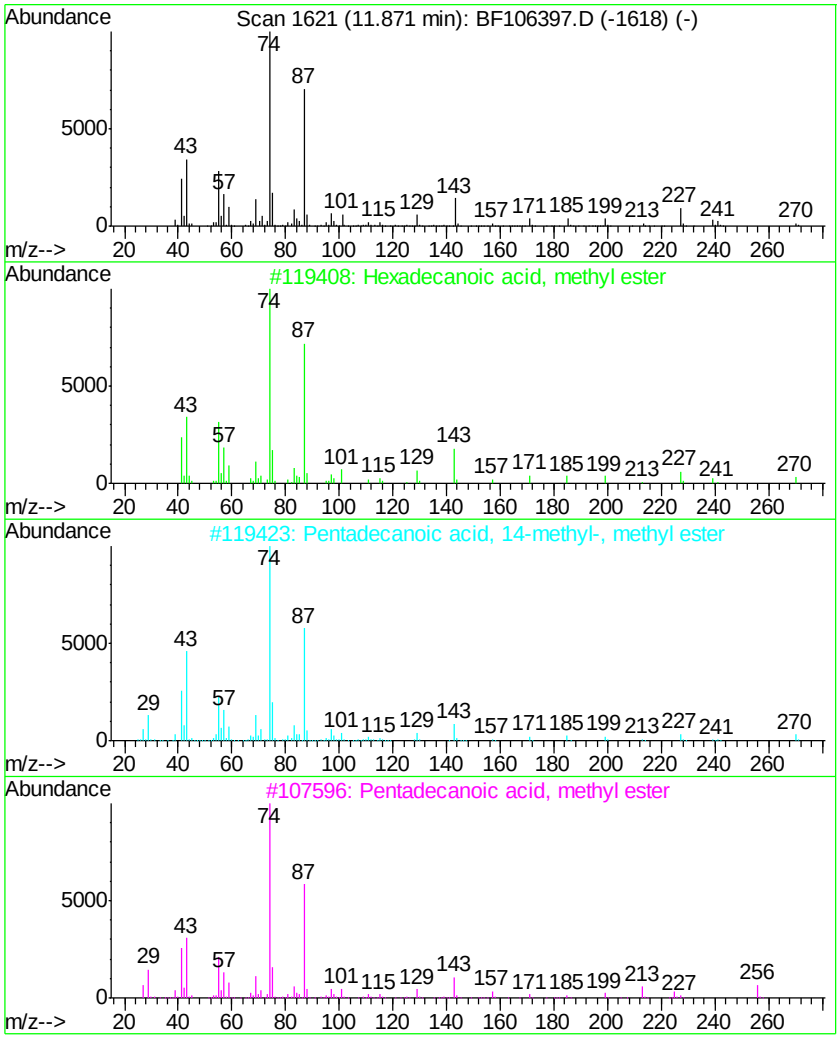
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

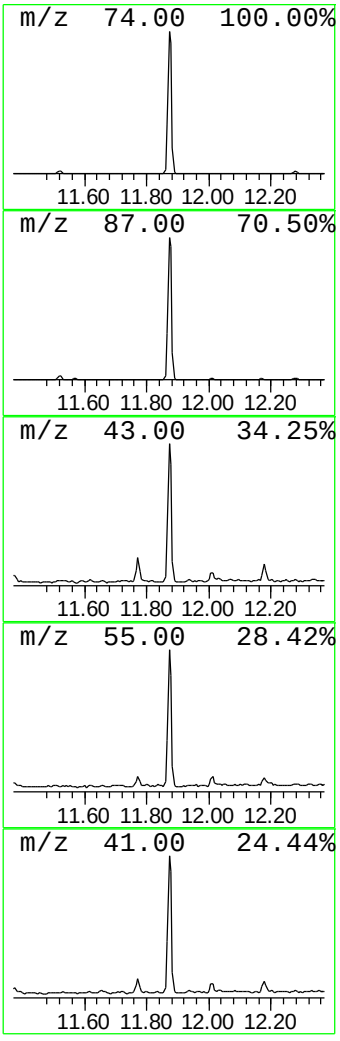
****

Peak Number 7 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	20.49 ng	1330680	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	91
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	83
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	80





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106397.D
Acq On : 13 Jun 2018 17:59
Operator : JU/SJ
Sample : J3251-03 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-03-061118

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

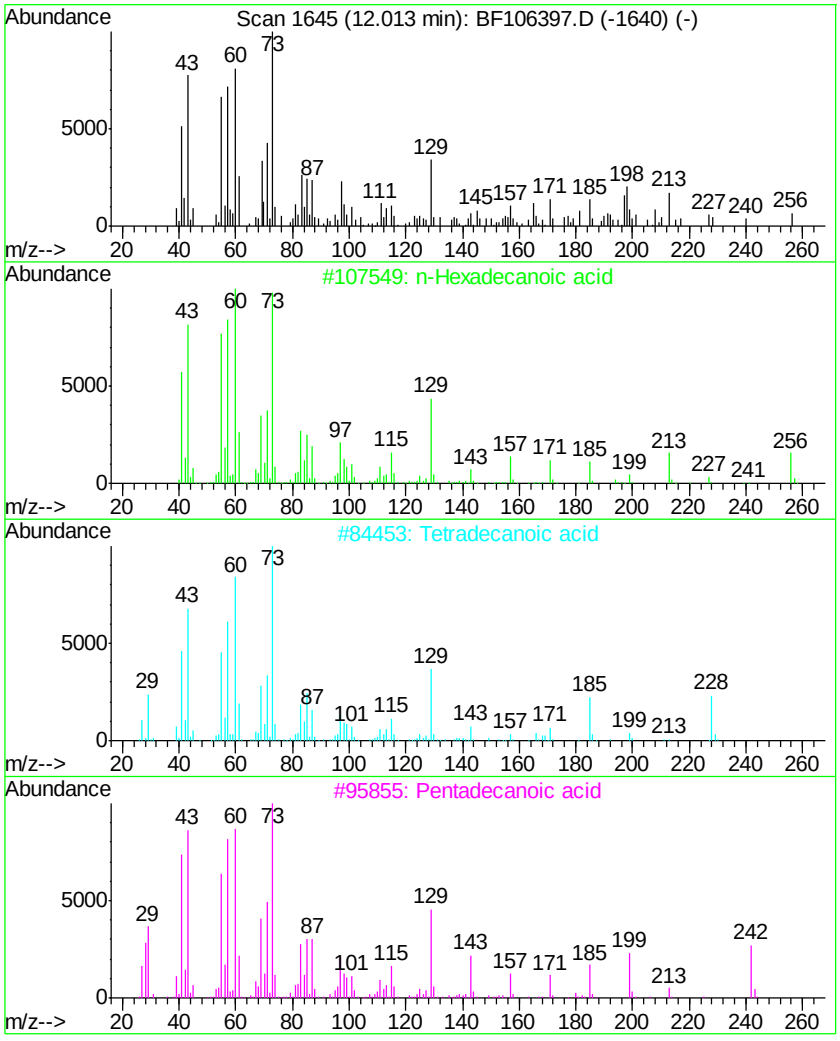
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

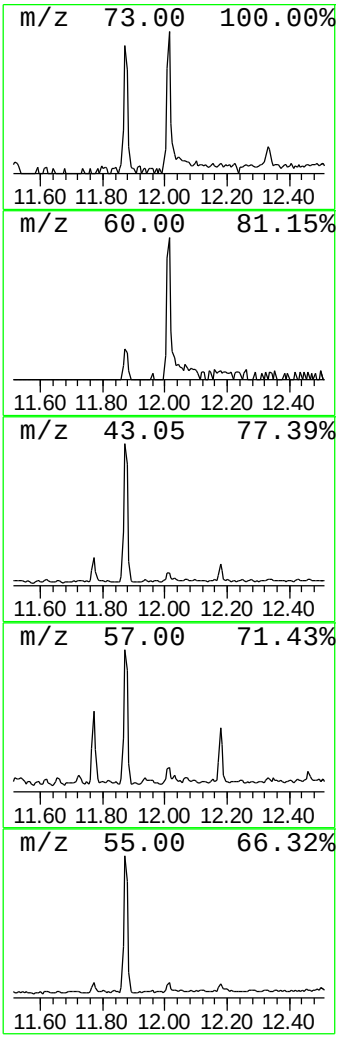
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	2.22 ng	144396	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Undecanoic acid	186	C11H22O2	000112-37-8	58
5	n-Decanoic acid	172	C10H20O2	000334-48-5	52





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106397.D
Acq On : 13 Jun 2018 17:59
Operator : JU/SJ
Sample : J3251-03 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-03-061118

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

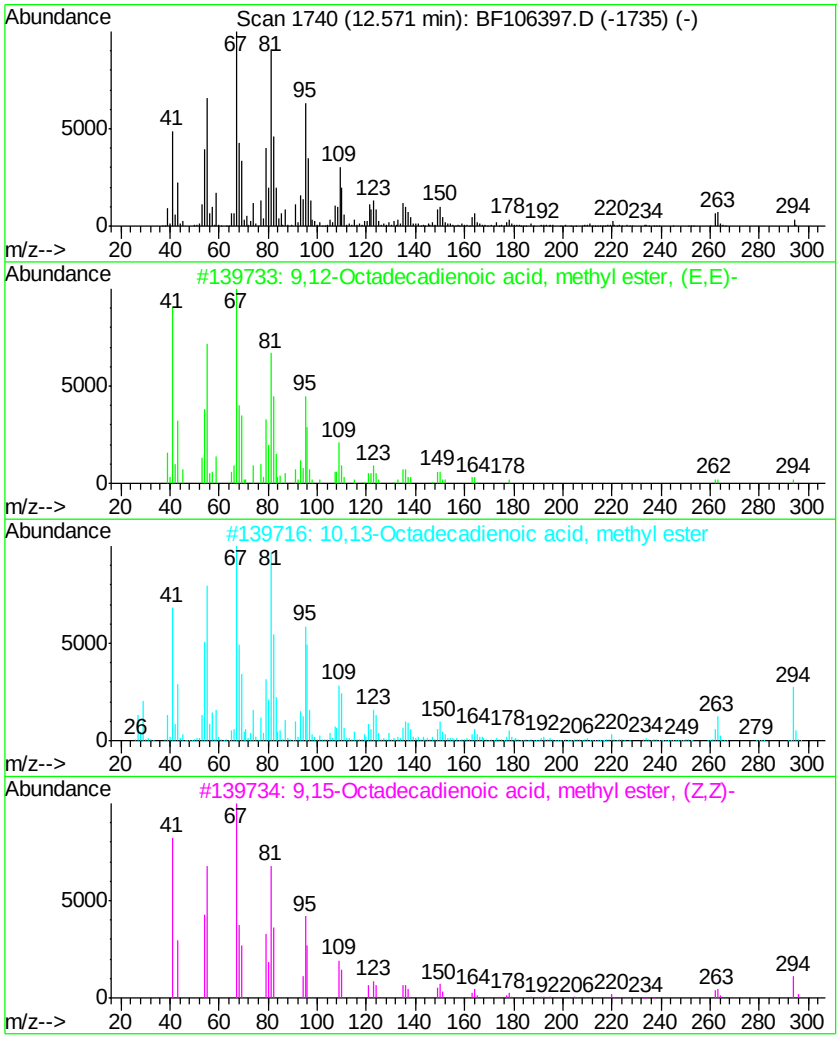
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

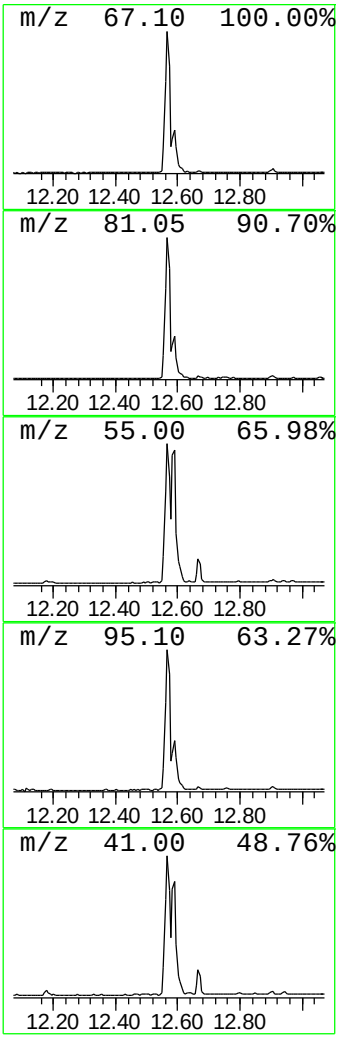
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	61.37 ng	3985330	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
5	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106397.D
Acq On : 13 Jun 2018 17:59
Operator : JU/SJ
Sample : J3251-03 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-03-061118

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

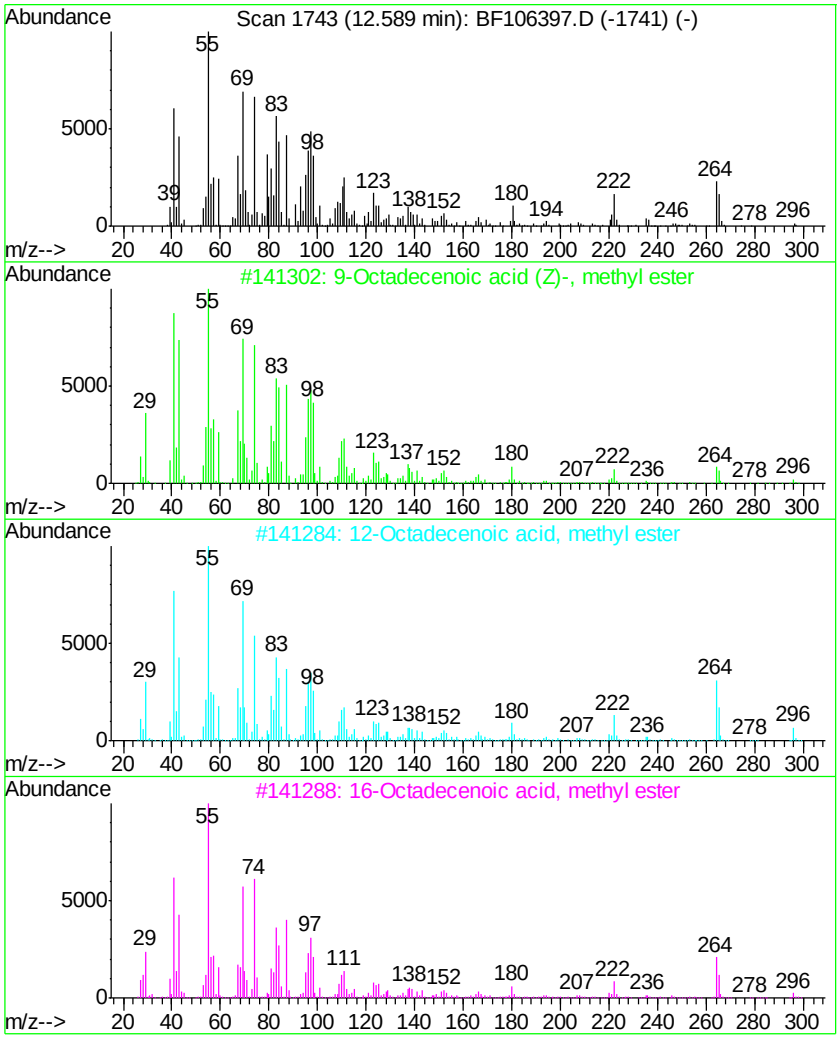
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

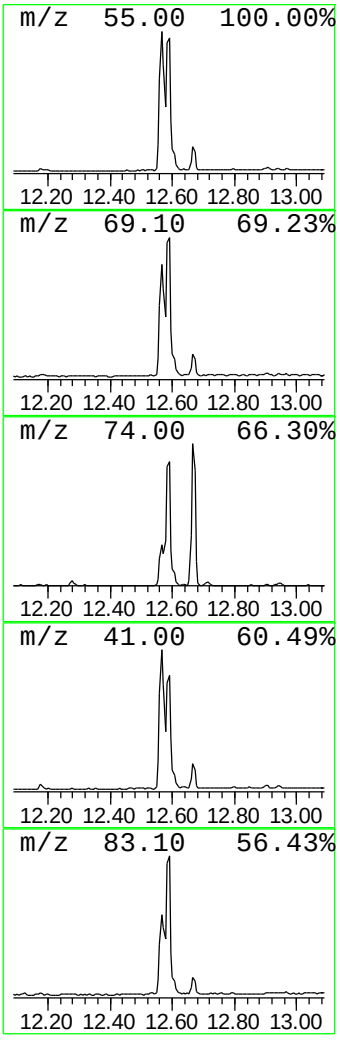
****

Peak Number 10 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.59	42.59 ng	2766010	Phenanthrene-d10	11.50

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	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	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





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061318\
Data File : BF106397.D
Acq On : 13 Jun 2018 17:59
Operator : JU/SJ
Sample : J3251-03 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-03-061118

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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...	5.19	2.9	ng	132875	1	6.97	917812	20.0
unknown6.75	6.75	32.6	ng	1496120	1	6.97	917812	20.0
Pentadecane	10.90	3.1	ng	200517	4	11.50	1298890	20.0
Eicosane	11.34	2.0	ng	132087	4	11.50	1298890	20.0
Hexadecanoic acid...	11.87	20.5	ng	1330680	4	11.50	1298890	20.0
n-Hexadecanoic acid	12.01	2.2	ng	144396	4	11.50	1298890	20.0
9,12-Octadecadien...	12.57	61.4	ng	3985330	4	11.50	1298890	20.0
9-Octadecenoic ac...	12.59	42.6	ng	2766010	4	11.50	1298890	20.0