LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040418\
Data File : BF104236.D
Acq On : 4 Apr 2018 20:08
Operator : JU/SJ
Sample : J2151-05 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-040318-C

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-BF032818.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	2.234	22	25	32	rVB	48751	65012	4.75%	0.440%
2	5.175	522	525	531	rBV	15445	23741	1.74%	0.161%
3	5.598	592	597	630	rBV2	140289	709932	51.92%	4.801%
4	6.598	763	767	785	rBV	209626	768461	56.20%	5.197%
5	6.722	785	788	808	rVB	483154	940386	68.78%	6.360%
6	6.951	824	827	849	rBV	270632	560564	41.00%	3.791%
7	7.104	849	853	877	rVB	530017	815004	59.61%	5.512%
8	7.522	920	924	945	rBV	161685	529019	38.69%	3.578%
9	8.234	1041	1045	1066	rBV	499251	852126	62.32%	5.763%
10	9.298	1223	1226	1235	rBV	951888	1131867	82.78%	7.655%
11	9.363	1235	1237	1249	rVB2	55974	88338	6.46%	0.597%
12	9.698	1288	1294	1300	rBV2	54723	93912	6.87%	0.635%
13	9.892	1323	1327	1330	rVB	52508	42805	3.13%	0.290%
14	9.986	1339	1343	1355	rBV	846535	912868	66.77%	6.174%
15	10.392	1409	1412	1415	rVB	65043	46699	3.42%	0.316%
16	10.610	1445	1449	1452	rBV2	27083	28439	2.08%	0.192%
17	10.786	1475	1479	1490	rBV	377162	583800	42.70%	3.948%
18	10.869	1490	1493	1498	rVB	56985	81447	5.96%	0.551%
19	11.316	1566	1569	1571	rBV	38837	30660	2.24%	0.207%
20	11.345	1571	1574	1577	rVB	22256	20105	1.47%	0.136%
21	11.486	1594	1598	1610	rBV	547181	839532	61.40%	5.678%
22	11.739	1638	1641	1645	rBV	29534	26195	1.92%	0.177%
23	11.845	1656	1659	1668	rBV	562076	496107	36.28%	3.355%
24	11.986	1680	1683	1688	rBV5	34542	50616	3.70%	0.342%
25	12.151	1708	1711	1715	rVB3	23777	19999	1.46%	0.135%
26	12.304	1734	1737	1741	rBV5	10968	14511	1.06%	0.098%
27	12.533	1773	1776	1778	rBV	1412300	1367280	100.00%	9.247%
28	12.557	1778	1780	1791	rVV2	1169880	1176887	86.08%	7.960%
29	12.639	1791	1794	1800	rVB	251248	222150	16.25%	1.502%
30	12.704	1802	1805	1812	rBV	64363	92854	6.79%	0.628%
31	12.916	1838	1841	1842	rBV2	20943	18962	1.39%	0.128%
32	12.939	1842	1845	1850	rVB	47407	63543	4.65%	0.430%
33	13.063	1863	1866	1877	rBV	688207	812249	59.41%	5.493%
34	13.939	2012	2015	2022	rVB2	83814	93574	6.84%	0.633%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040418\
Data File : BF104236.D
Acq On : 4 Apr 2018 20:08
Operator : JU/SJ
Sample : J2151-05 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-040318-C

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-BF032818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.139	2045	2049	2061	rBV	462281	675874	49.43%	4.571%
36	15.674	2307	2310	2319	rVB2	280757	490271	35.86%	3.316%

Sum of corrected areas: 14785789

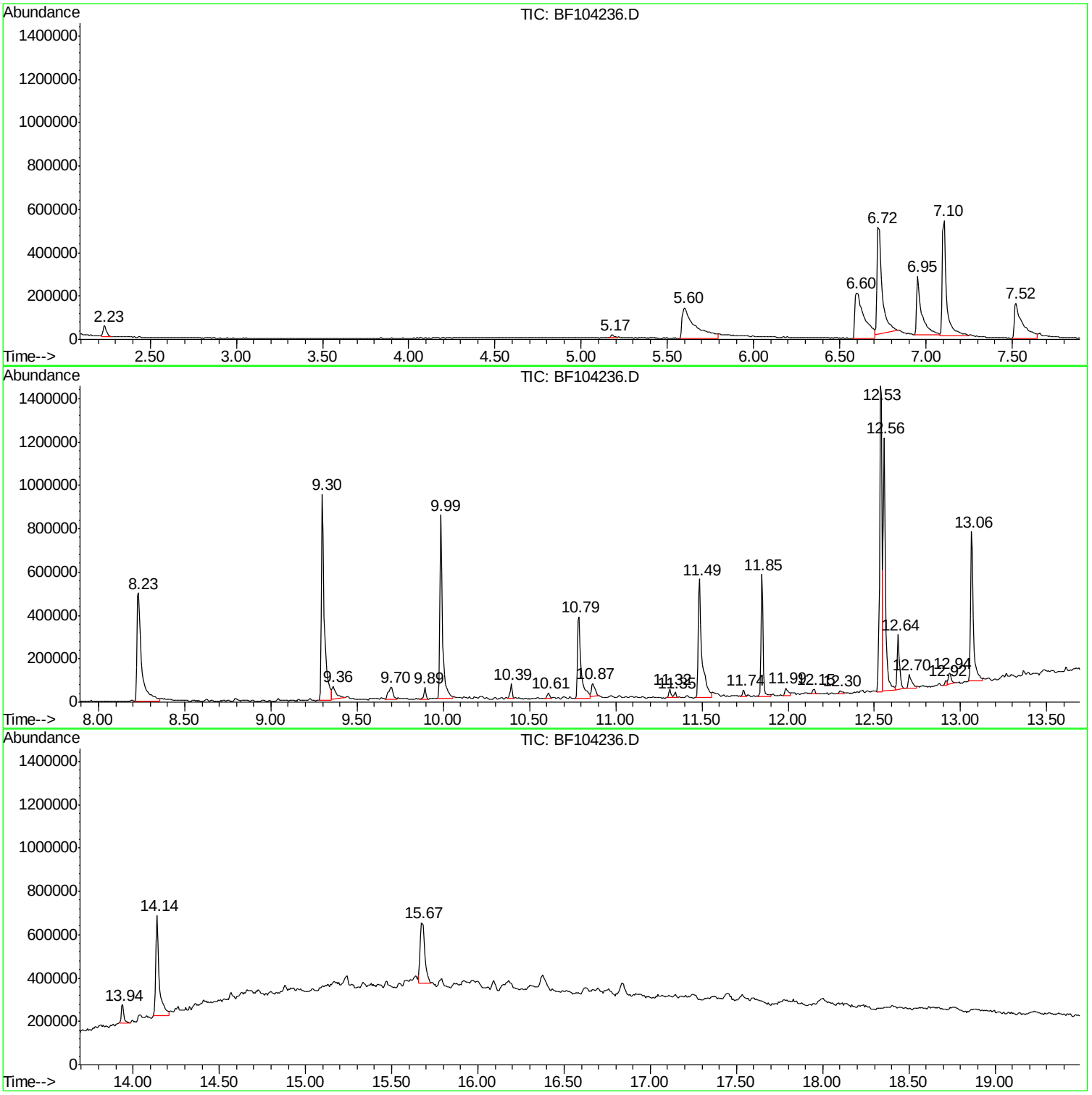
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040418\
Data File : BF104236.D
Acq On : 4 Apr 2018 20:08
Operator : JU/SJ
Sample : J2151-05 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-040318-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.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\BF040418\
Data File : BF104236.D
Acq On : 4 Apr 2018 20:08
Operator : JU/SJ
Sample : J2151-05 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-040318-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

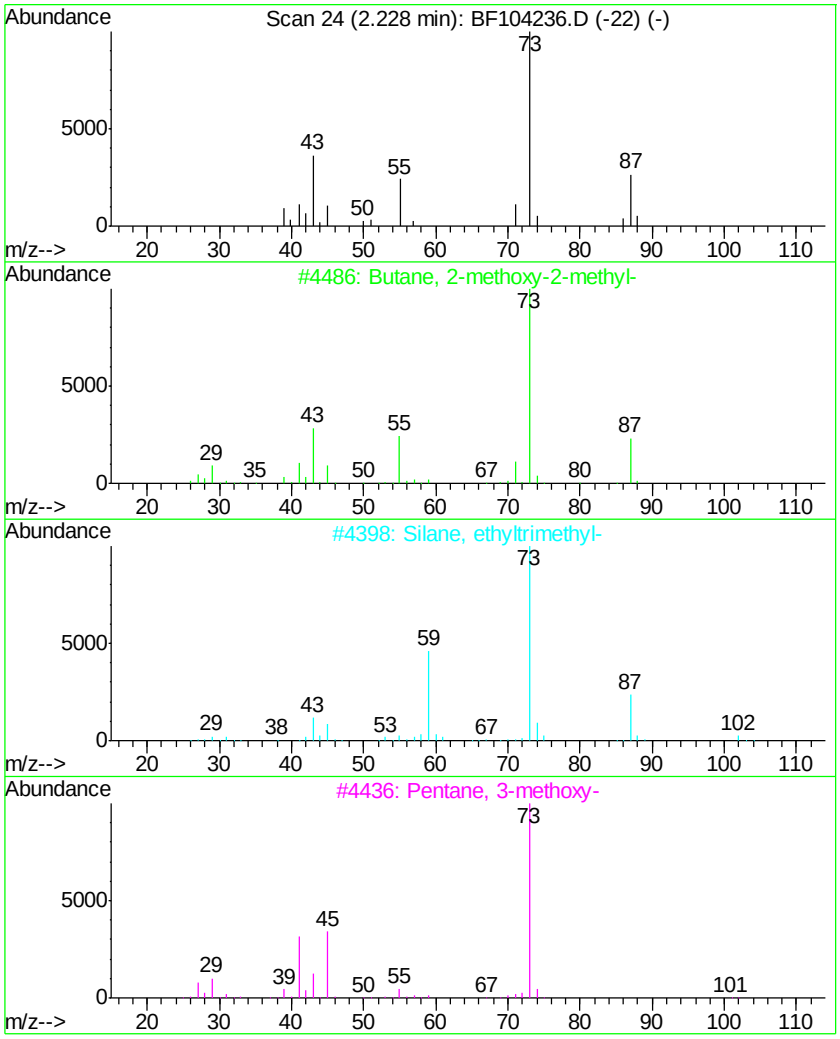
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

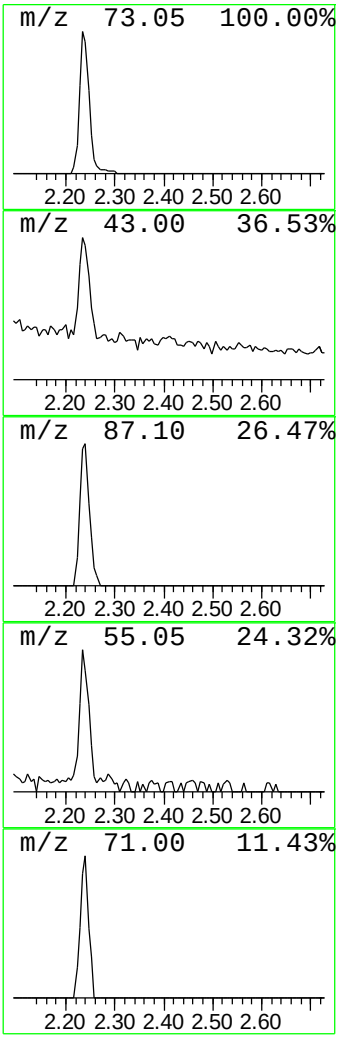
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	2.32 ng	65012	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	33
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040418\
Data File : BF104236.D
Acq On : 4 Apr 2018 20:08
Operator : JU/SJ
Sample : J2151-05 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-040318-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.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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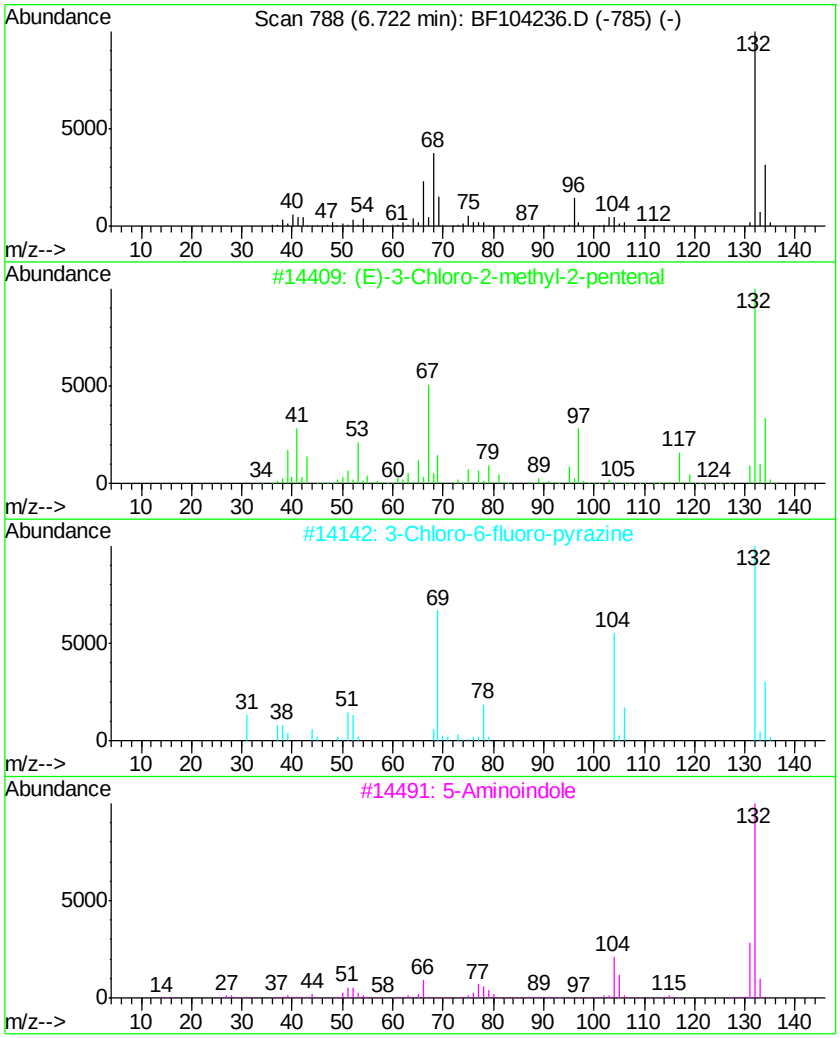
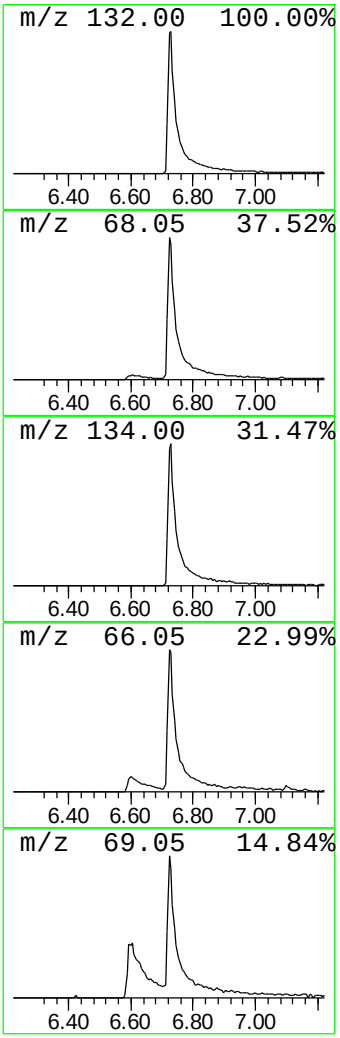
Peak Number 2 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	33.55 ng	940386	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040418\
Data File : BF104236.D
Acq On : 4 Apr 2018 20:08
Operator : JU/SJ
Sample : J2151-05 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-040318-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

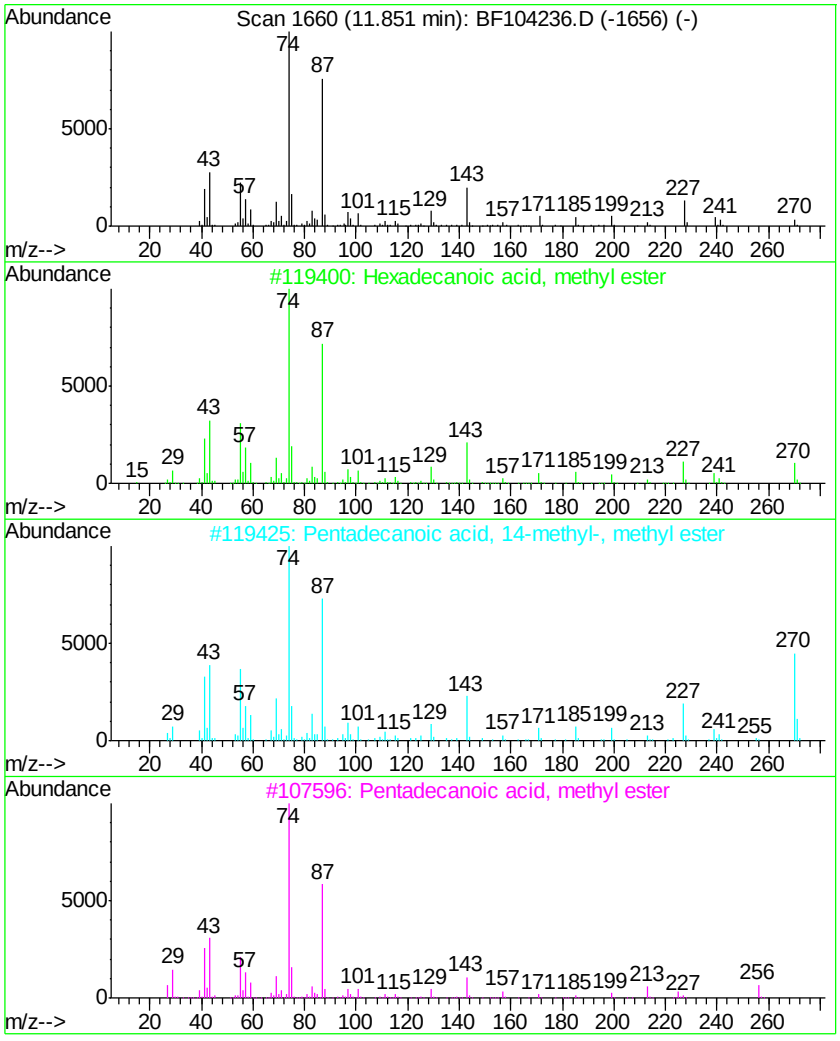
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

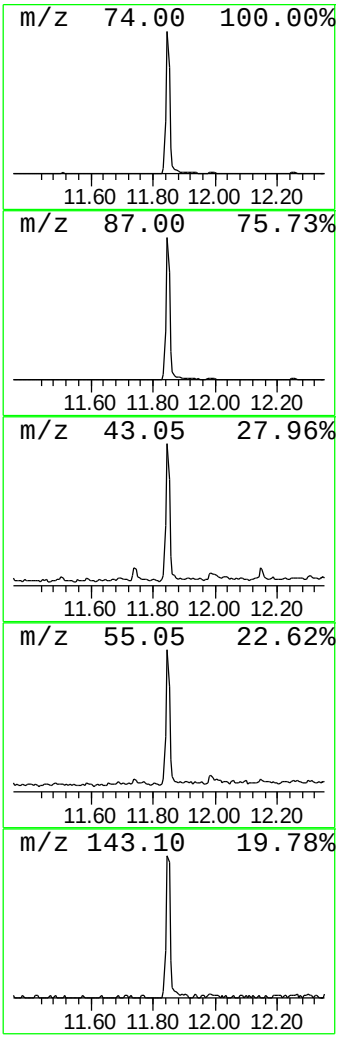
****

Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	11.82 ng	496107	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	96
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	94
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	86
5	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	86





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Acq On : 4 Apr 2018 20:08
Operator : JU/SJ
Sample : J2151-05 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-040318-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.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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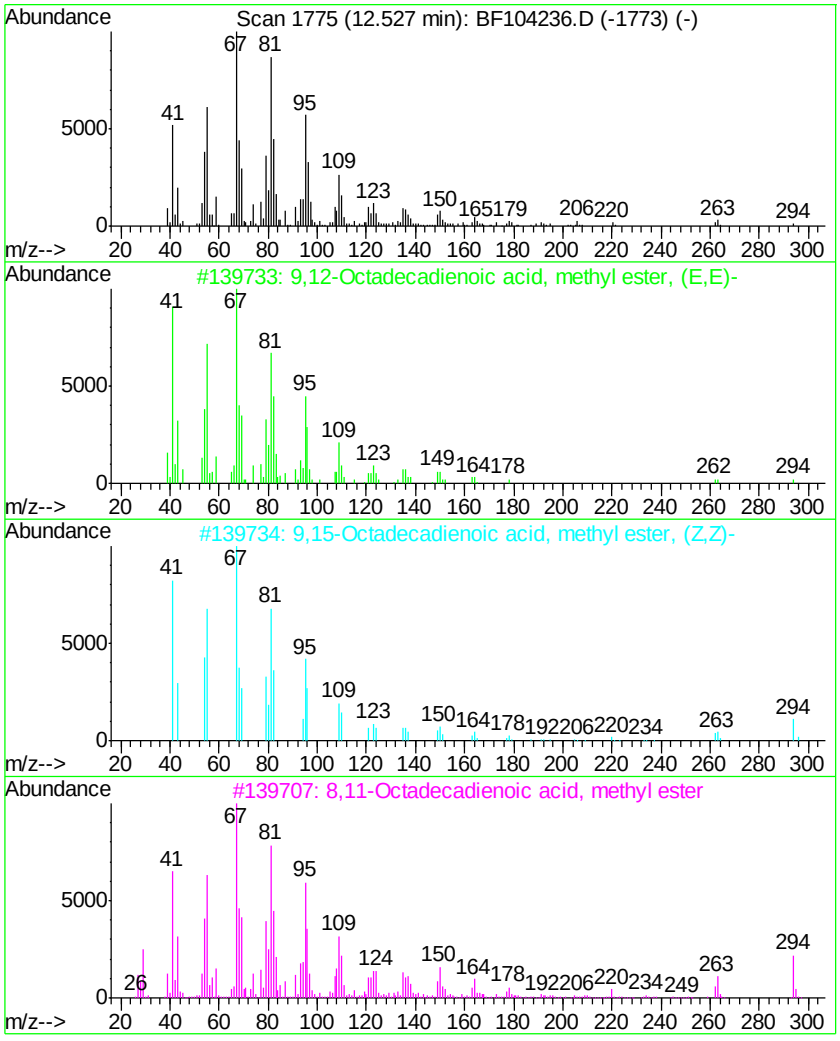
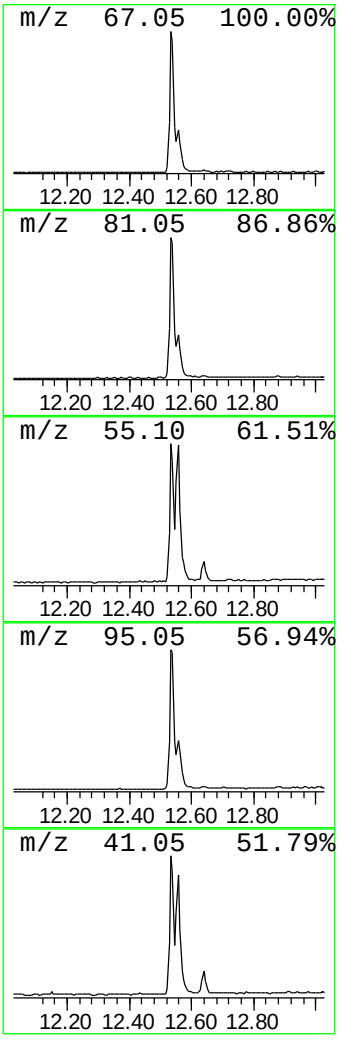
Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.53	32.57 ng	1367280	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
3	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	99
4	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
5	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	99





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040418\
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Sample : J2151-05 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-040318-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

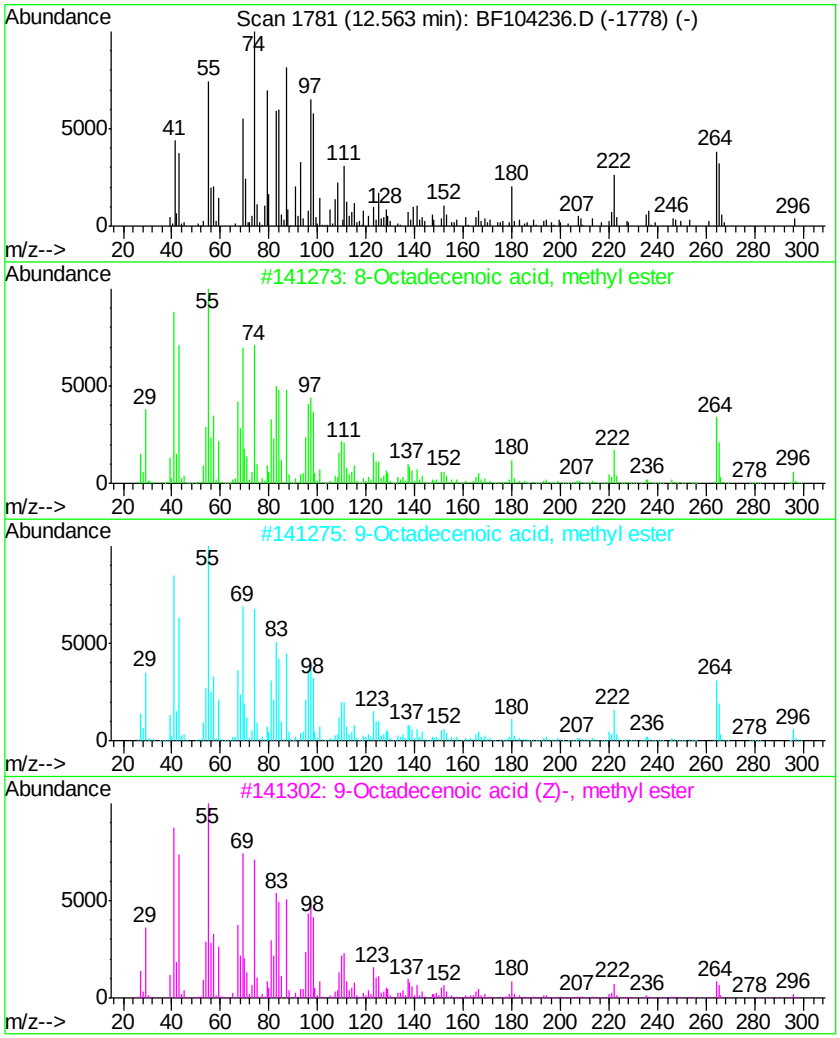
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

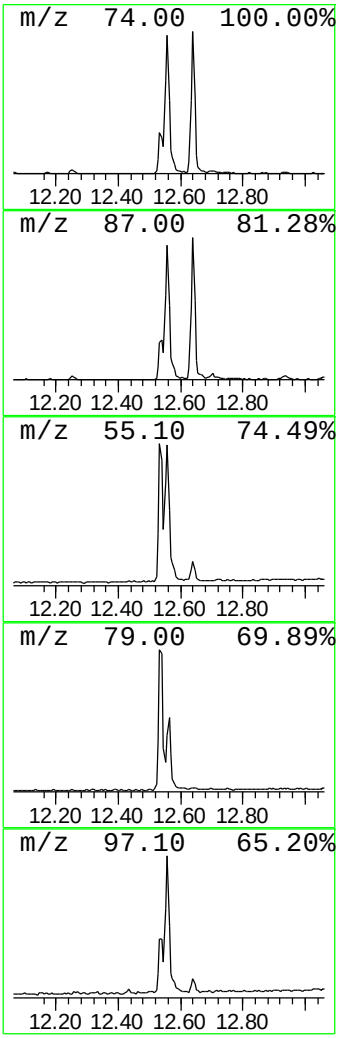
****

Peak Number 6 8-Octadecenoic acid, methyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	28.04 ng	1176890	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	98
2	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	98
3	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	97
4	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	97
5	7-Octadecenoic acid, methyl ester	296	C19H36O2	057396-98-2	96





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ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-040318-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.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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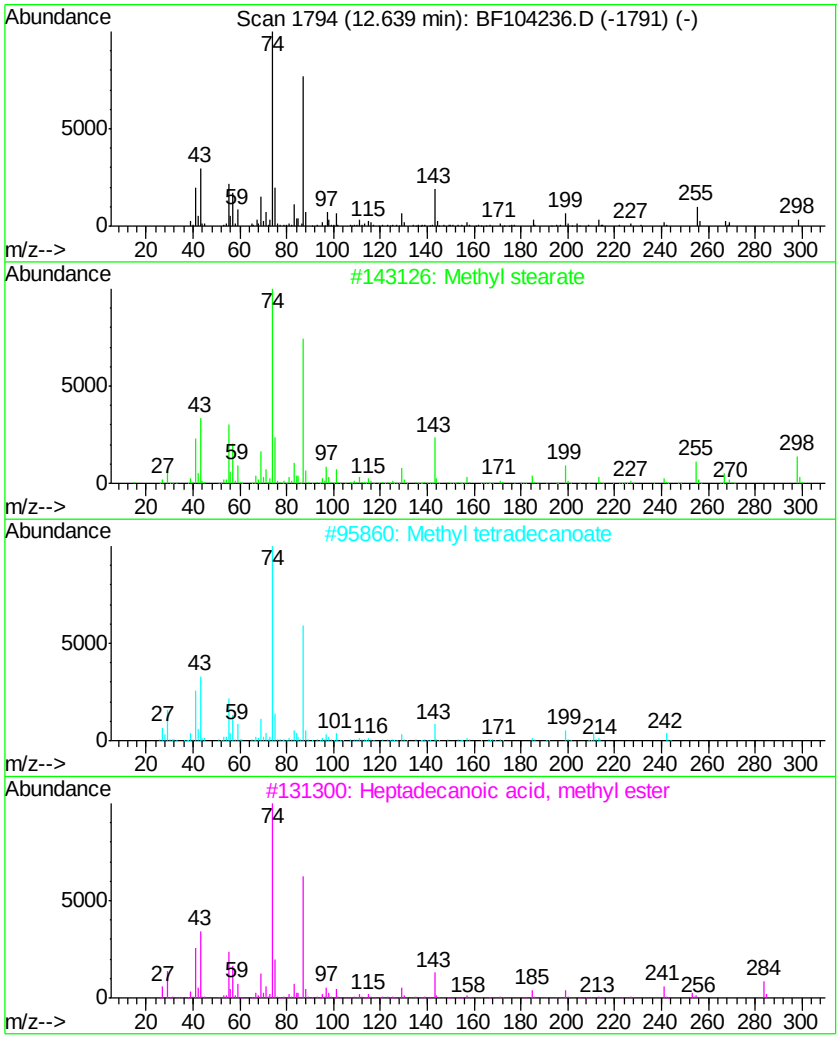
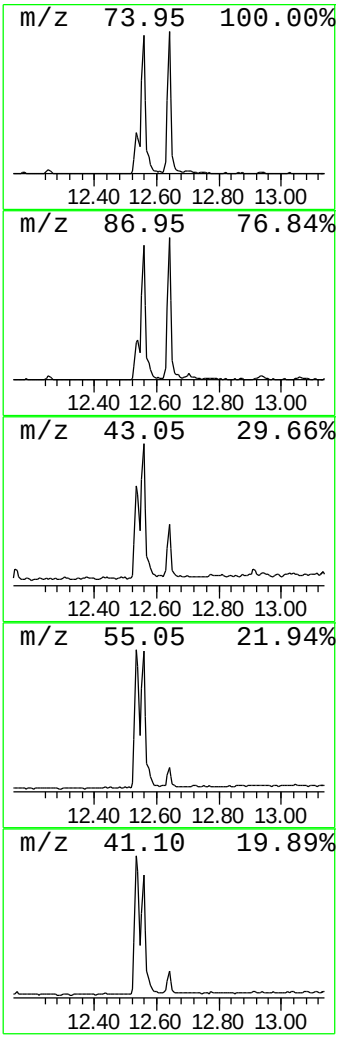
Peak Number 7 Methyl stearate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	5.29 ng	222150	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	97
2	Methyl tetradecanoate	242	C15H30O2	000124-10-7	93
3	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	87





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

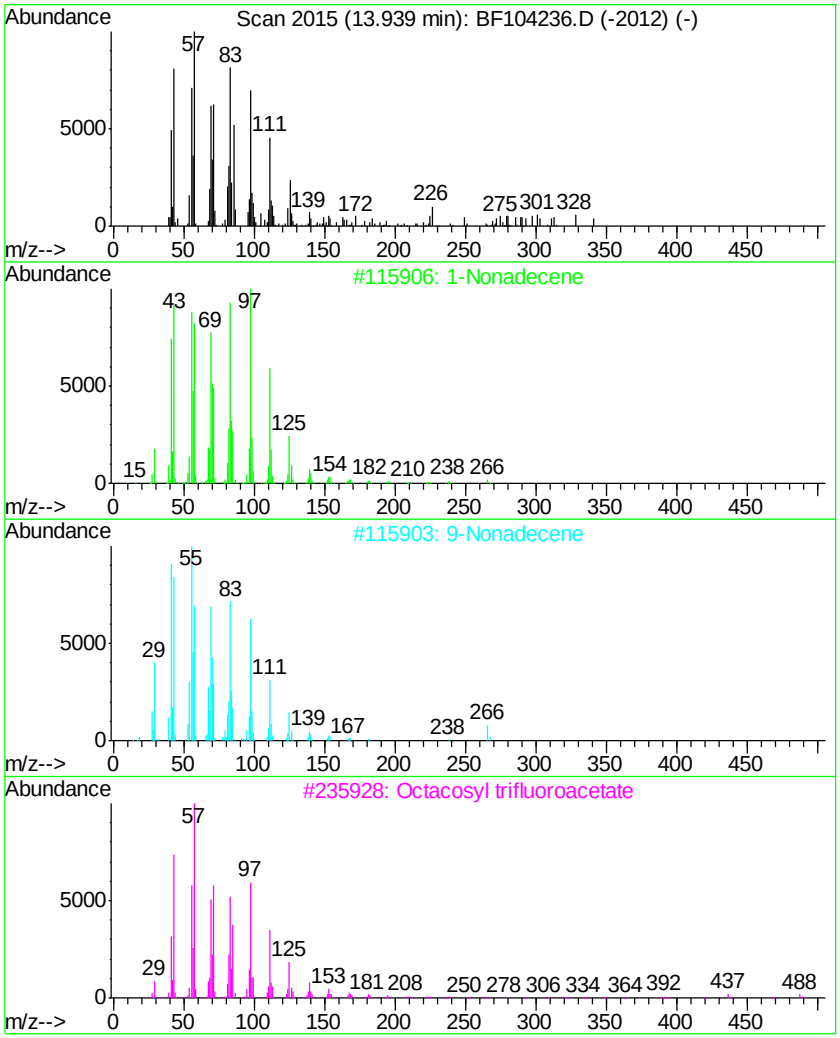
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

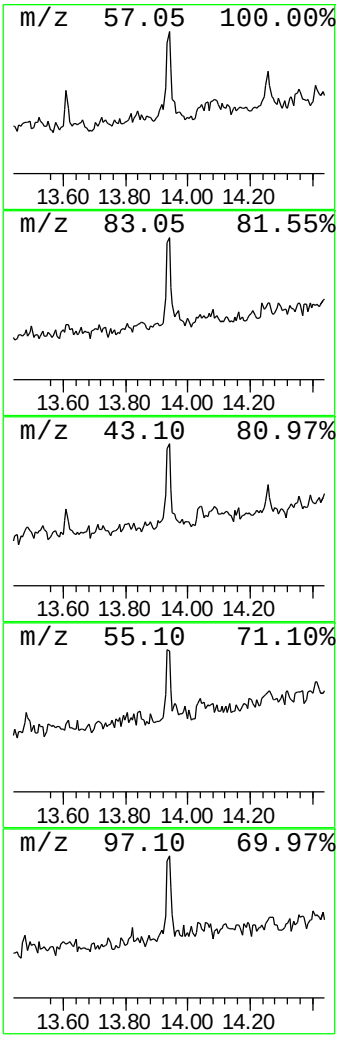
****

Peak Number 9 1-Nonadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	2.77 ng	93574	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	96
2	9-Nonadecene	266	C19H38	031035-07-1	95
3	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	94
4	Cyclooctadecane, ethyl-	280	C20H40	1000151-22-5	93
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040418\
Data File : BF104236.D
Acq On : 4 Apr 2018 20:08
Operator : JU/SJ
Sample : J2151-05 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-040318-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.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
Butane, 2-methoxy...	2.23	2.3	ng	65012	1	6.95	560564	20.0
unknown6.72	6.72	33.5	ng	940386	1	6.95	560564	20.0
Hexadecanoic acid...	11.85	11.8	ng	496107	4	11.49	839532	20.0
9,12-Octadecadien...	12.53	32.6	ng	1367280	4	11.49	839532	20.0
8-Octadecenoic ac...	12.56	28.0	ng	1176890	4	11.49	839532	20.0
Methyl stearate	12.64	5.3	ng	222150	4	11.49	839532	20.0
1-Nonadecene	13.94	2.8	ng	93574	5	14.14	675874	20.0