LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040418\
Data File : BF104234.D
Acq On : 4 Apr 2018 19:15
Operator : JU/SJ
Sample : J2151-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-040318-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:\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	5.592	592	596	628	rBV2	237391	1048075	9.40%	2.501%
2	6.592	763	766	785	rBV	374607	1185751	10.63%	2.829%
3	6.722	785	788	816	rVB	773575	1520999	13.64%	3.629%
4	6.951	824	827	849	rBV2	300790	656586	5.89%	1.567%
5	7.104	849	853	868	rBV	706286	1034182	9.27%	2.468%
6	7.522	920	924	945	rBV	275776	824582	7.39%	1.968%
7	8.233	1041	1045	1055	rBV	590126	942919	8.46%	2.250%
8	9.298	1223	1226	1235	rBV	1303277	1559085	13.98%	3.720%
9	9.575	1270	1273	1282	rBV8	42117	115809	1.04%	0.276%
10	9.986	1339	1343	1359	rBV	988117	1131150	10.14%	2.699%
11	10.786	1475	1479	1490	rBV	589170	933943	8.37%	2.229%
12	10.869	1490	1493	1497	rVB2	92670	130424	1.17%	0.311%
13	11.486	1594	1598	1609	rBV	677426	1113683	9.99%	2.657%
14	11.857	1656	1661	1680	rBV	4375000	5169237	46.35%	12.335%
15	12.557	1773	1780	1782	rBV	5223214	11151826	100.00%	26.610%
16	12.580	1782	1784	1792	rVV2	5312482	6221666	55.79%	14.846%
17	12.645	1792	1795	1803	rVV	2870623	2684128	24.07%	6.405%
18	12.710	1803	1806	1816	rVB	96841	211941	1.90%	0.506%
19	12.939	1842	1845	1851	rVB	105813	139168	1.25%	0.332%
20	13.068	1864	1867	1878	rBV	984059	1097580	9.84%	2.619%
21	13.292	1902	1905	1914	rVB2	261113	353215	3.17%	0.843%
22	13.368	1914	1918	1920	rBV	242422	240443	2.16%	0.574%
23	13.392	1920	1922	1927	rVV3	100253	115709	1.04%	0.276%
24	13.480	1934	1937	1942	rVB	223911	227315	2.04%	0.542%
25	13.804	1987	1992	2001	rVB2	145820	270110	2.42%	0.645%
26	13.939	2011	2015	2020	rVB	136527	154600	1.39%	0.369%
27	14.033	2028	2031	2037	rBV	218405	197677	1.77%	0.472%
28	14.139	2045	2049	2061	rBV	566159	828329	7.43%	1.977%
29	15.674	2306	2310	2325	rVB	376462	648256	5.81%	1.547%

Sum of corrected areas: 41908388

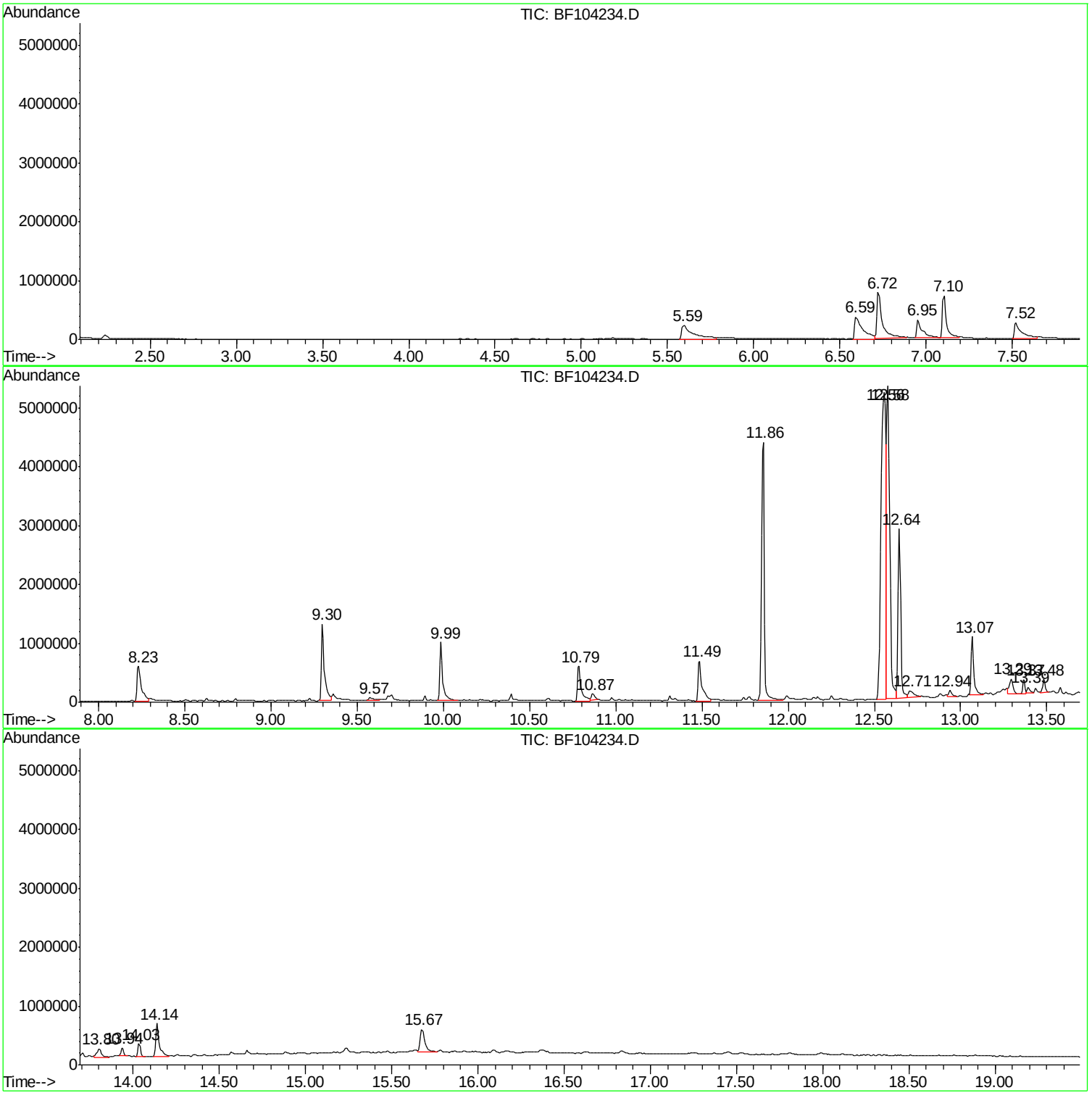
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040418\
Data File : BF104234.D
Acq On : 4 Apr 2018 19:15
Operator : JU/SJ
Sample : J2151-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

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

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

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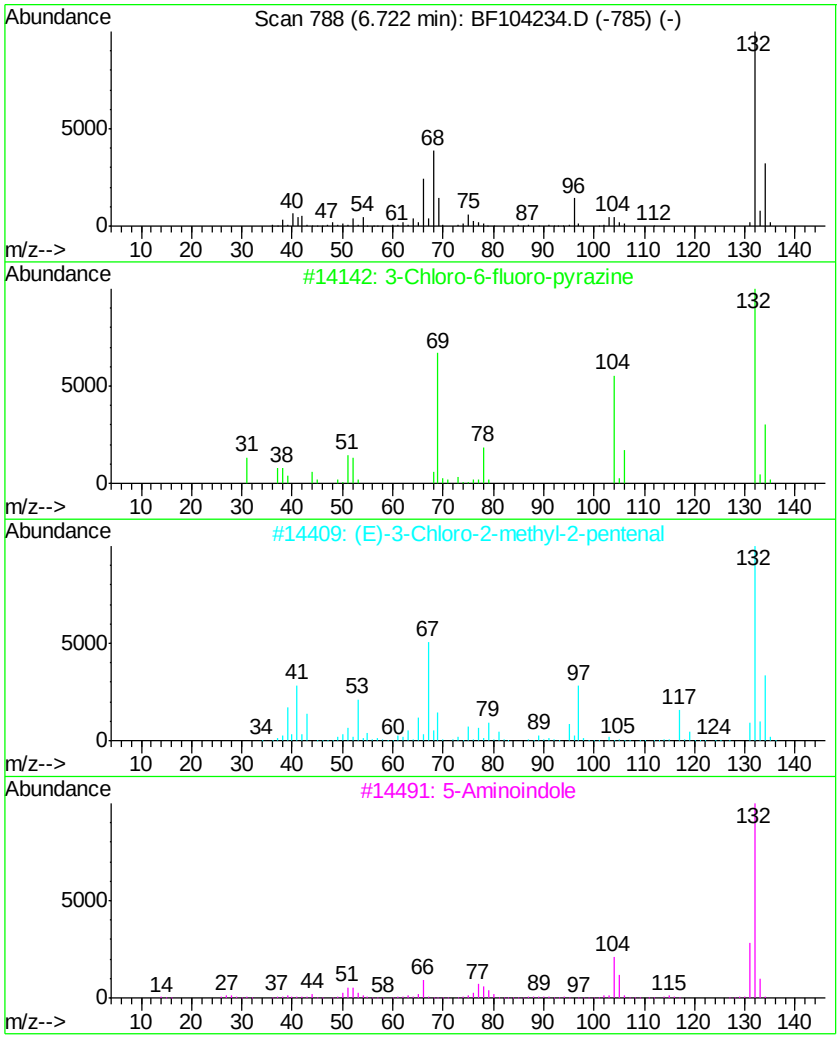
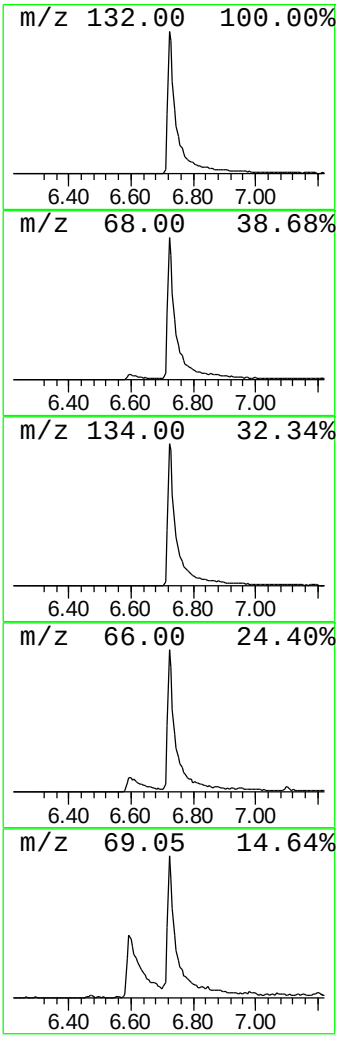
****

Peak Number 1 unknown6.72 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	46.33 ng	1521000	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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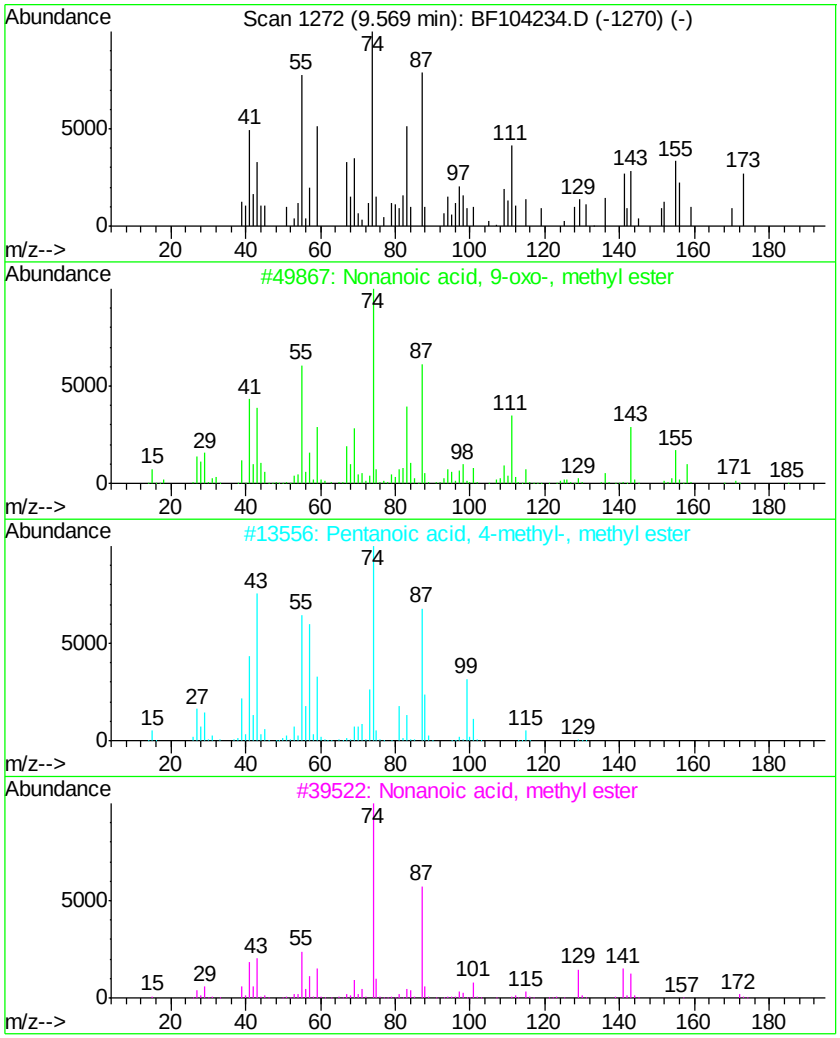
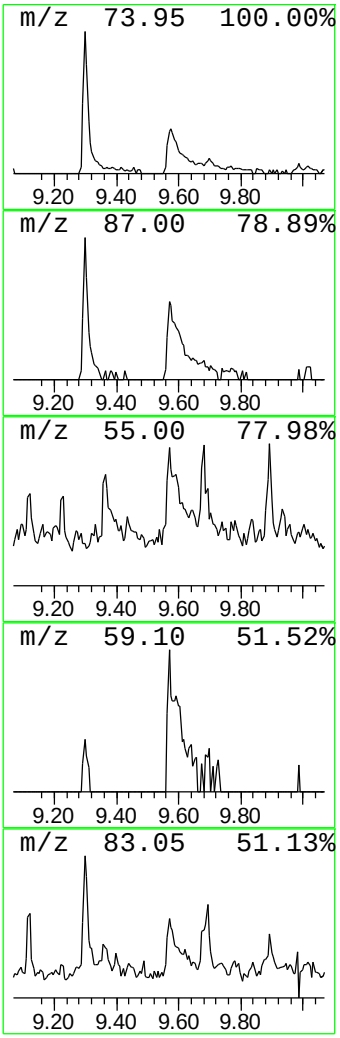
****

Peak Number 3 Nonanoic acid, 9-oxo-, meth... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.57	2.05 ng	115809	Acenaphthene-d10	9.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid, 9-oxo-, methyl ester	186	C10H18O3	001931-63-1	64
2	Pentanoic acid, 4-methyl-, methy...	130	C7H14O2	002412-80-8	35
3	Nonanoic acid, methyl ester	172	C10H20O2	001731-84-6	35
4	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	27
5	Undecanoic acid, methyl ester	200	C12H24O2	001731-86-8	27





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ClientSampleId : AU-06-040318-A

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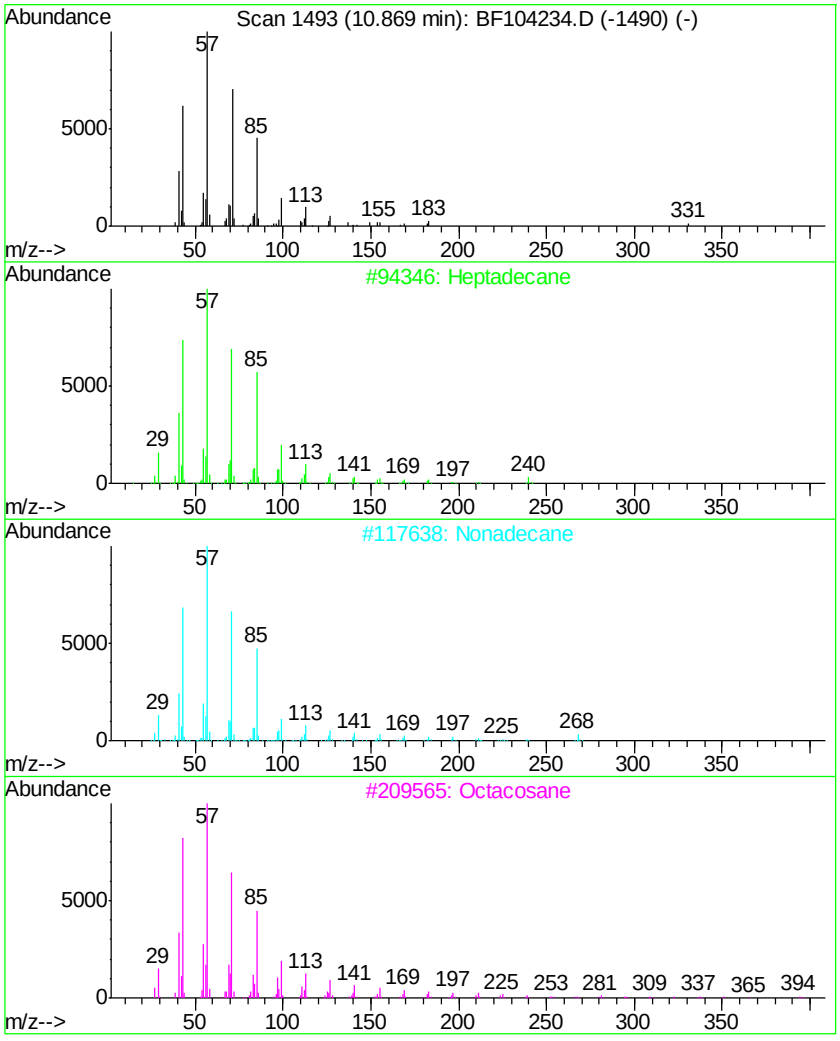
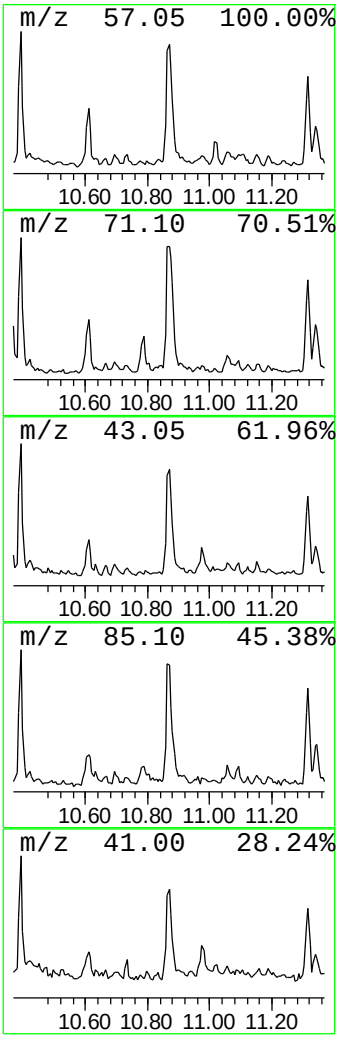
****

Peak Number 4 Heptadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.87	2.34 ng	130424	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Nonadecane	268	C19H40	000629-92-5	90
3	Octacosane	394	C28H58	000630-02-4	90
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	90
5	Pentadecane	212	C15H32	000629-62-9	90





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Misc :
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Instrument : BNA_F
ClientSampleId : AU-06-040318-A

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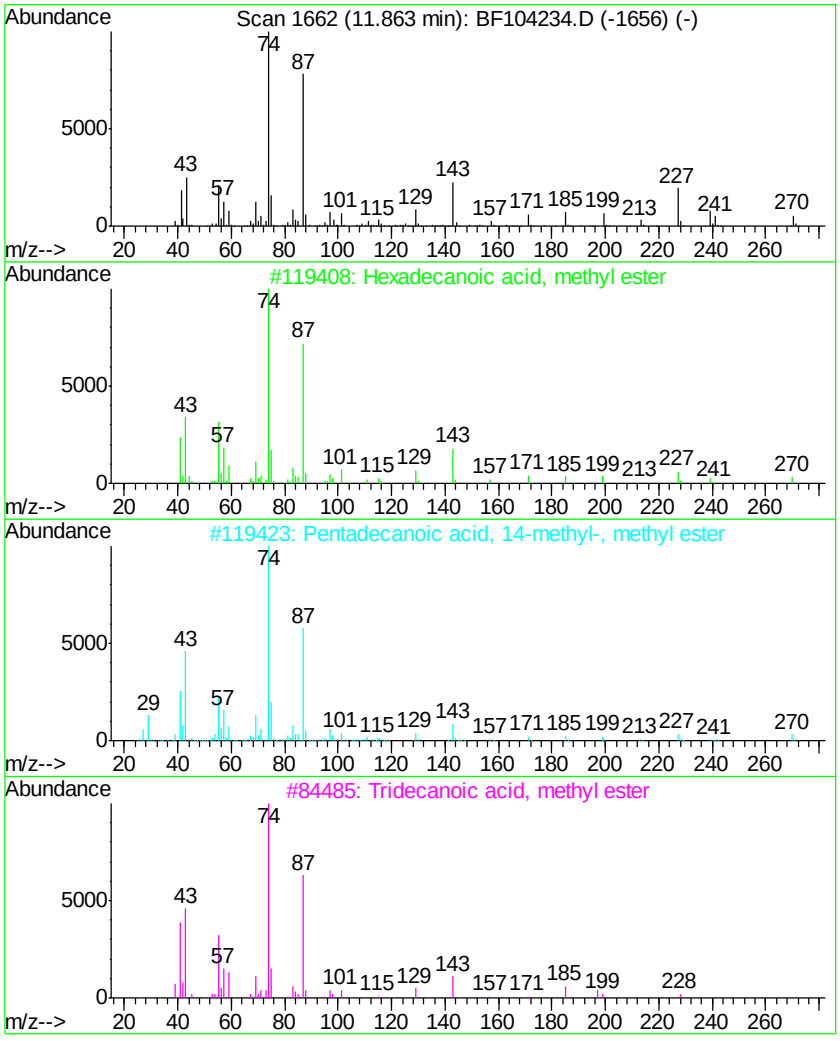
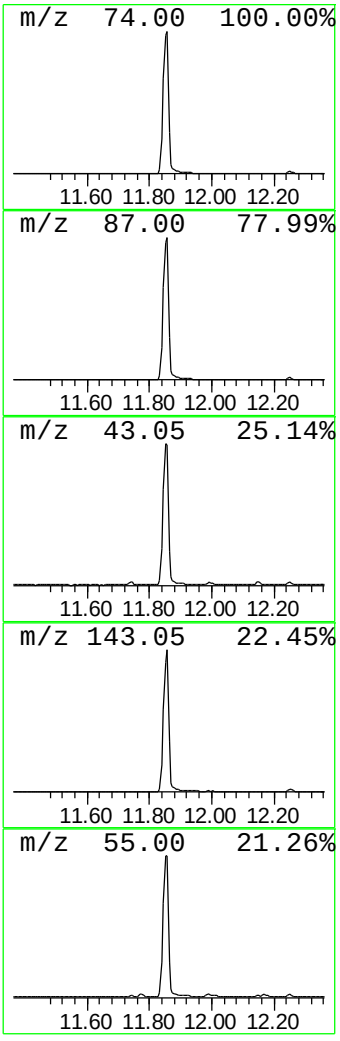
****
Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	92.83 ng	5169240	Phenanthrene-d10	11.49

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	92
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
4	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86





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Misc :
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Instrument : BNA_F
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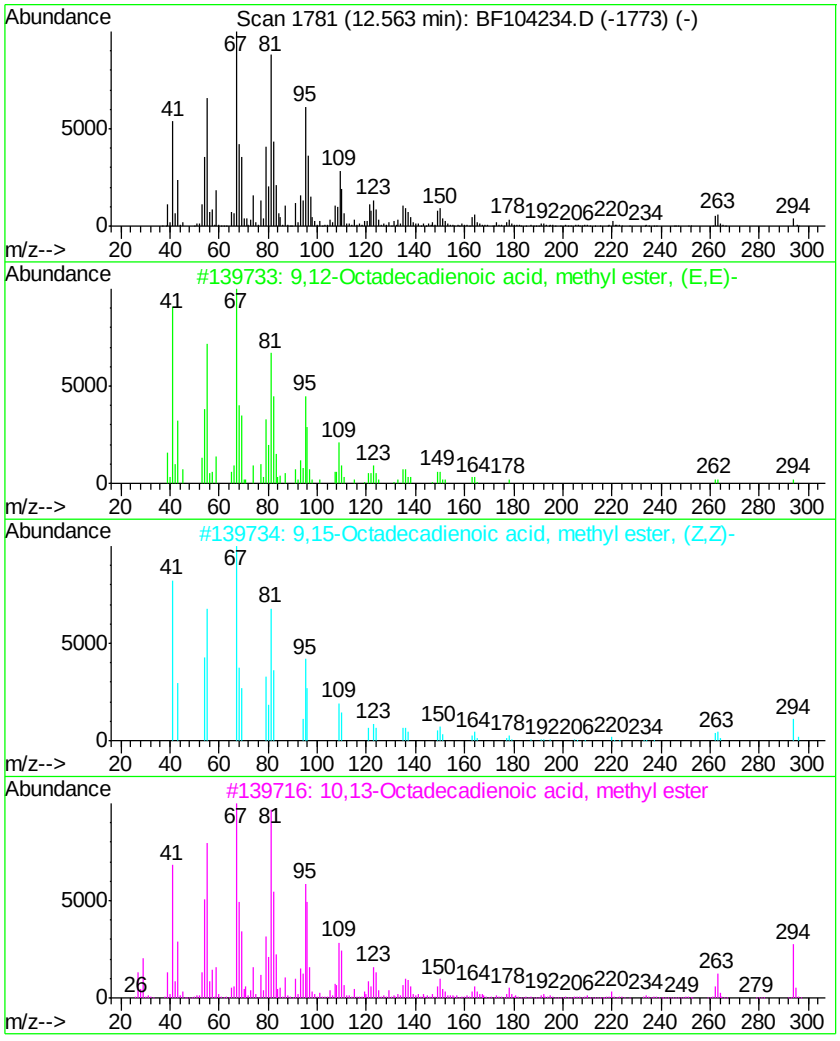
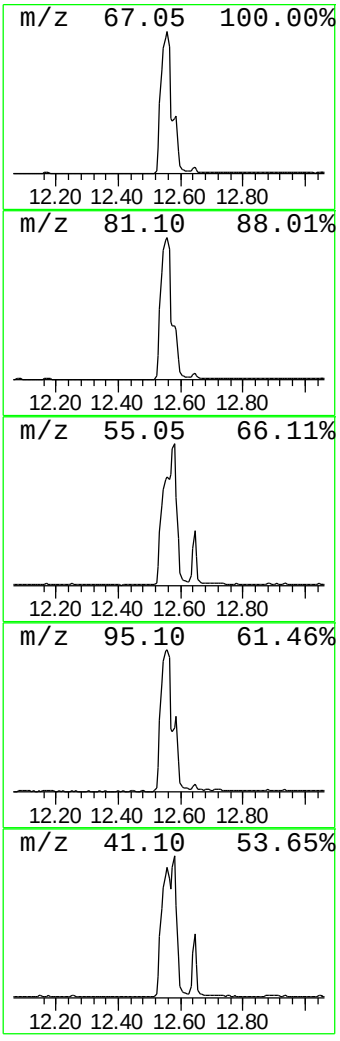
****
Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	200.27 ng	11151800	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	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	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	98





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Instrument : BNA_F
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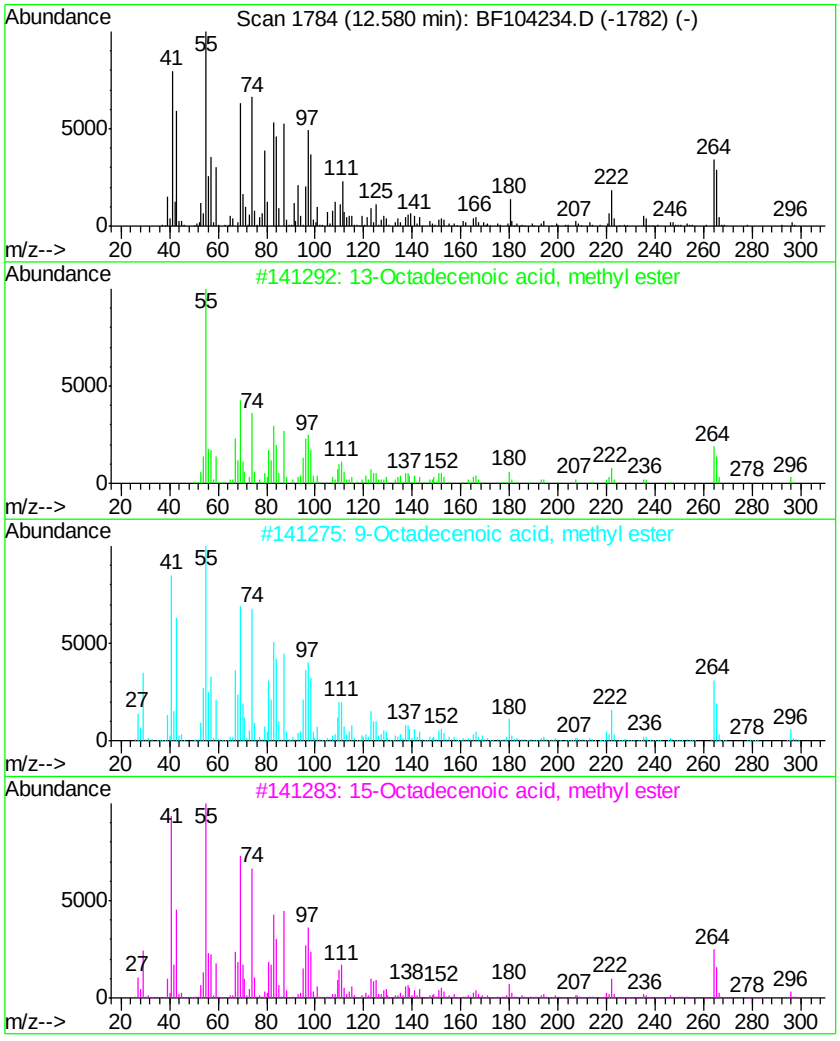
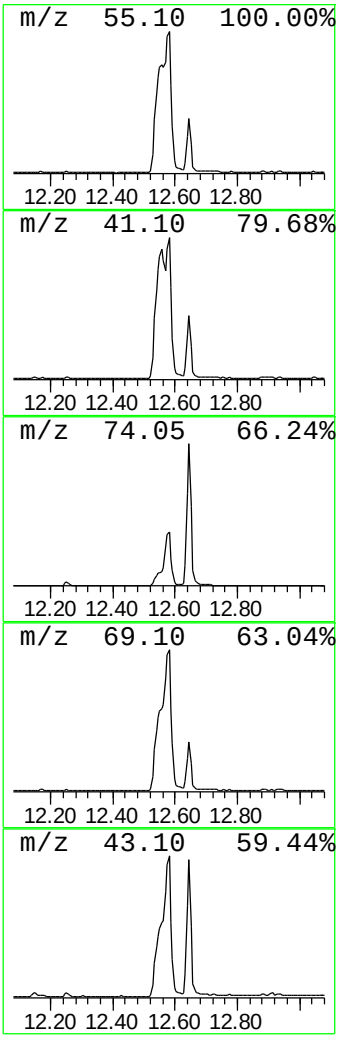
****

Peak Number 7 13-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.58	111.73 ng	6221670	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	90
2	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	87
3	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	86
4	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	86
5	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	83





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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
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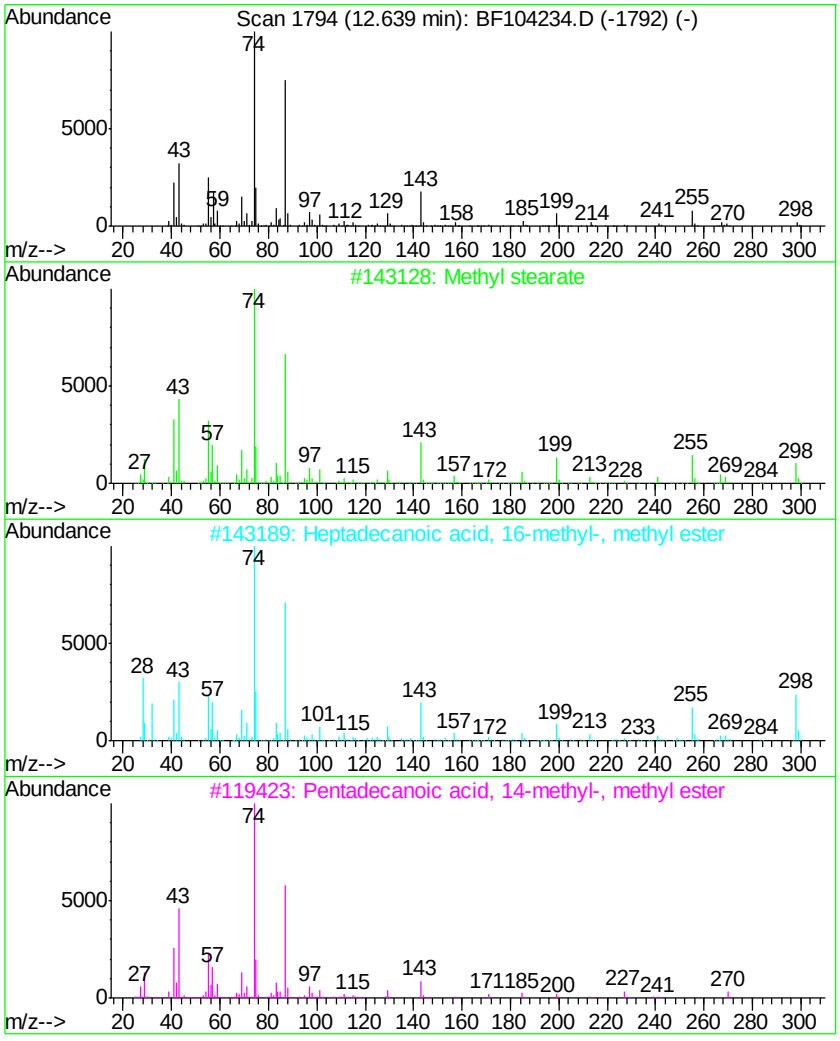
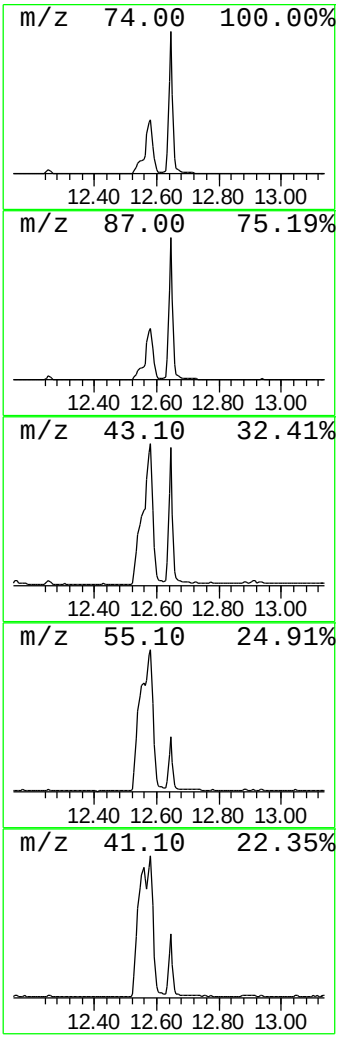
****

Peak Number 8 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	48.20 ng	2684130	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	98
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	90
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	86
5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	86





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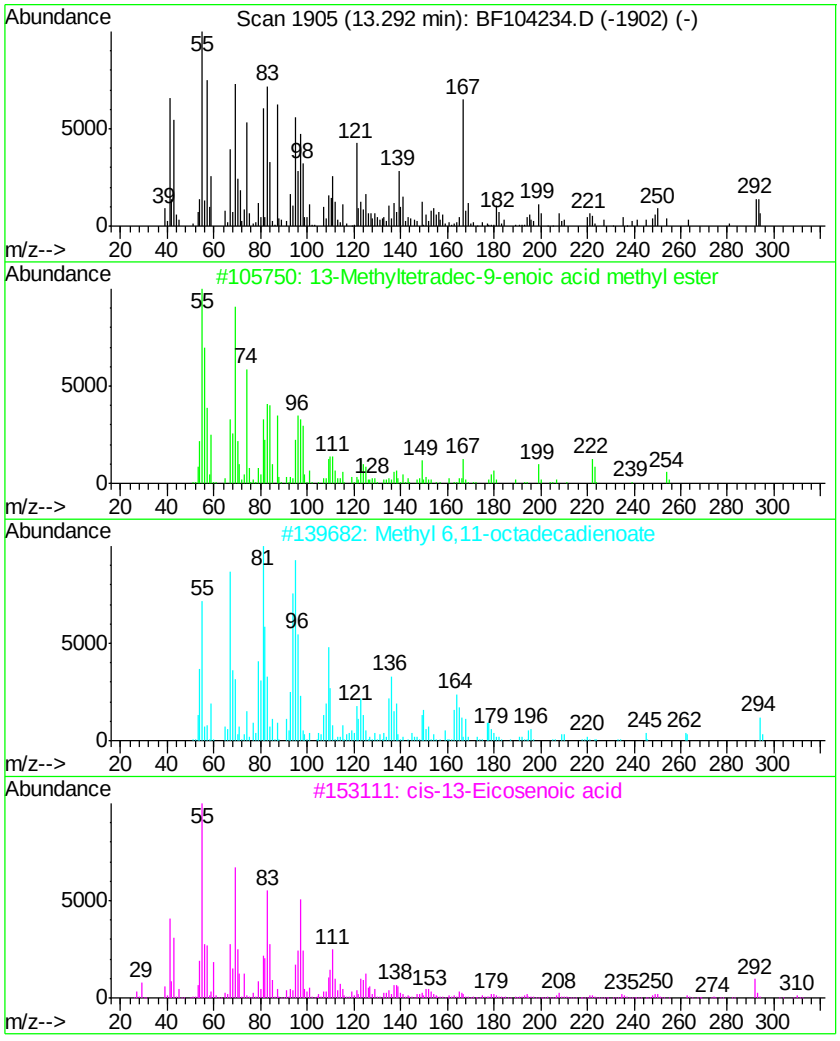
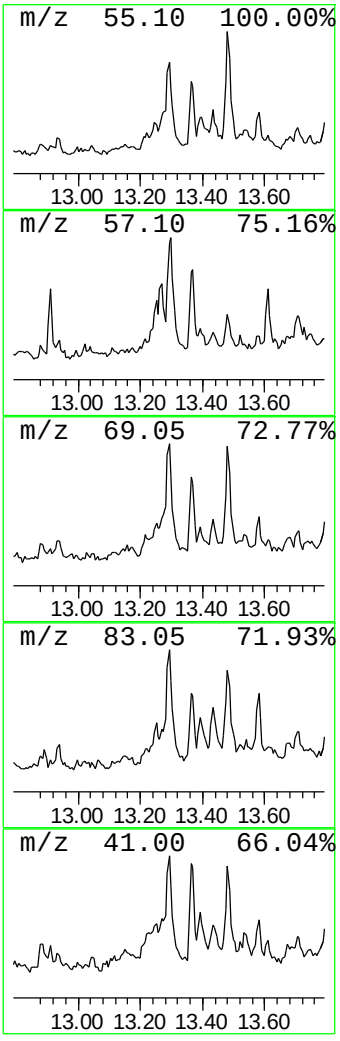
Peak Number 9 13-Methyltetradec-9-enoic a... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.29	8.53 ng	353215	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Methyltetradec-9-enoic acid m...	254	C16H30O2	1000365-89-8	52
2	Methyl 6,11-octadecadienoate	294	C19H34O2	1000336-43-2	42
3	cis-13-Eicosenoic acid	310	C20H38O2	017735-94-3	38
4	cis-11-Eicosenoic acid	310	C20H38O2	005561-99-9	38
5	cis-9-Hexadecenoic acid	254	C16H30O2	1000333-19-5	38





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
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TIC Library : C:\DATABASE\NIST11.L
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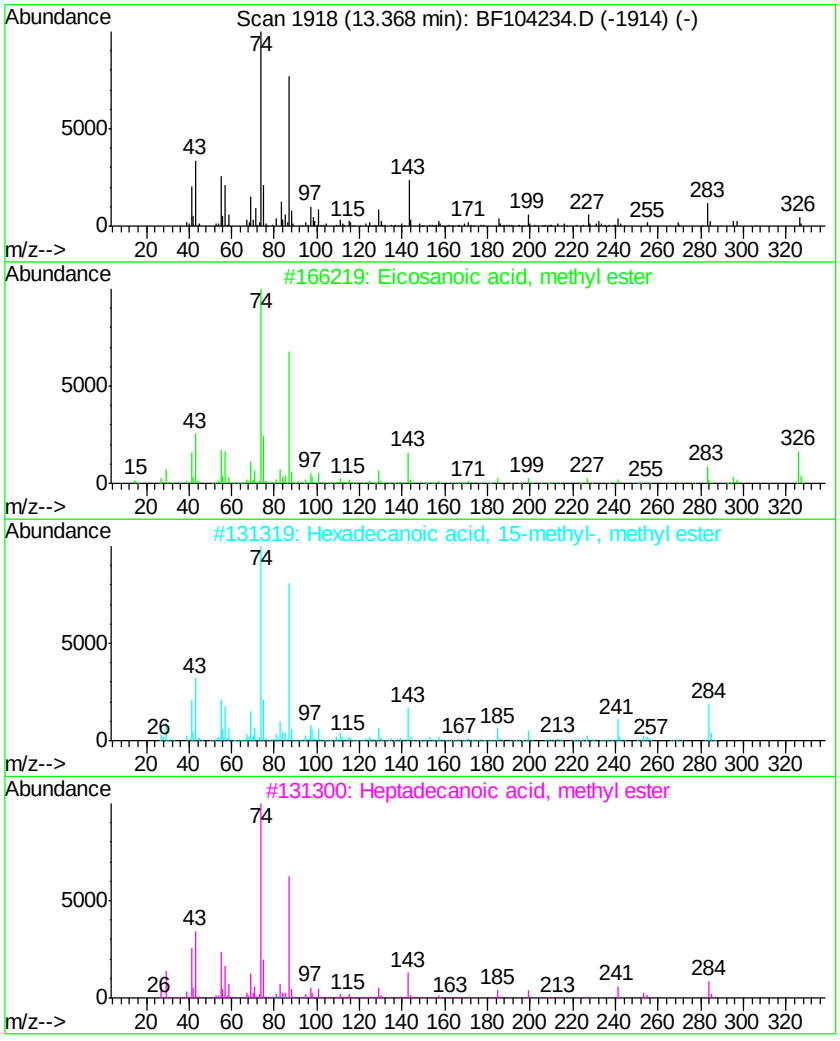
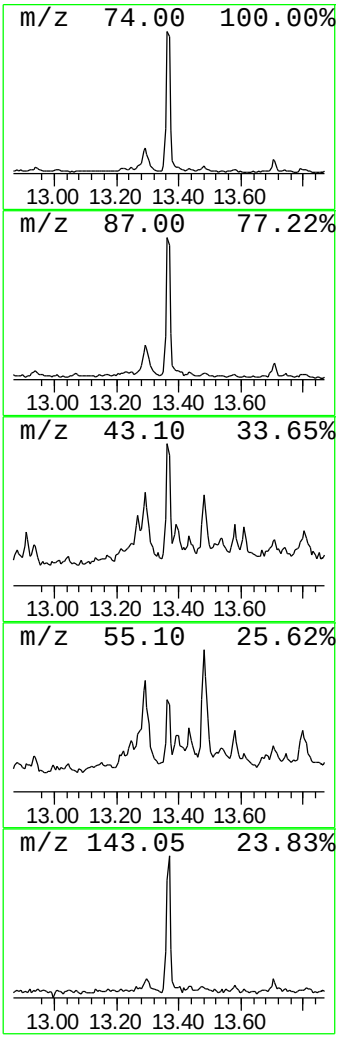
Peak Number 10 Eicosanoic acid, methyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.37	5.81 ng	240443	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	97
2	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	95
3	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	93
4	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	93
5	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	87





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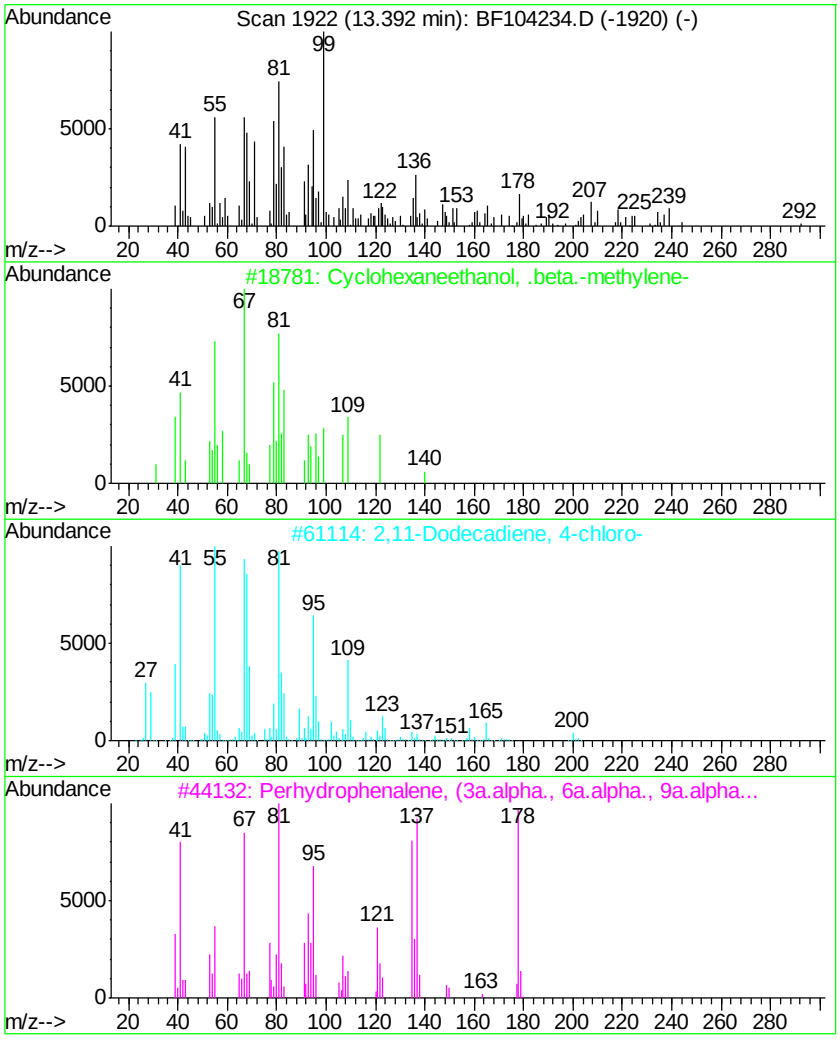
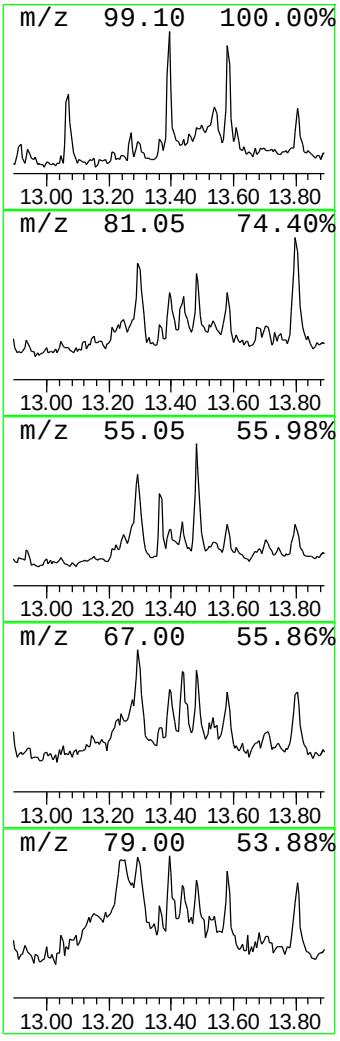
Peak Number 11 unknown13.39 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.39	2.79 ng	115709	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexaneethanol, .beta.-methy...	140	C9H16O	007697-55-4	38
2	2,11-Dodecadiene, 4-chloro-	200	C12H21Cl	1000155-54-5	30
3	Perhydrophenalene, (3a.alpha., 6...	178	C13H22	040250-64-4	30
4	Bicyclo[10.1.0]tridec-1-ene	178	C13H22	054766-91-5	30
5	1,2-Dioctylcyclopropene	264	C19H36	001089-40-3	25





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Data File : BF104234.D
Acq On : 4 Apr 2018 19:15
Operator : JU/SJ
Sample : J2151-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

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

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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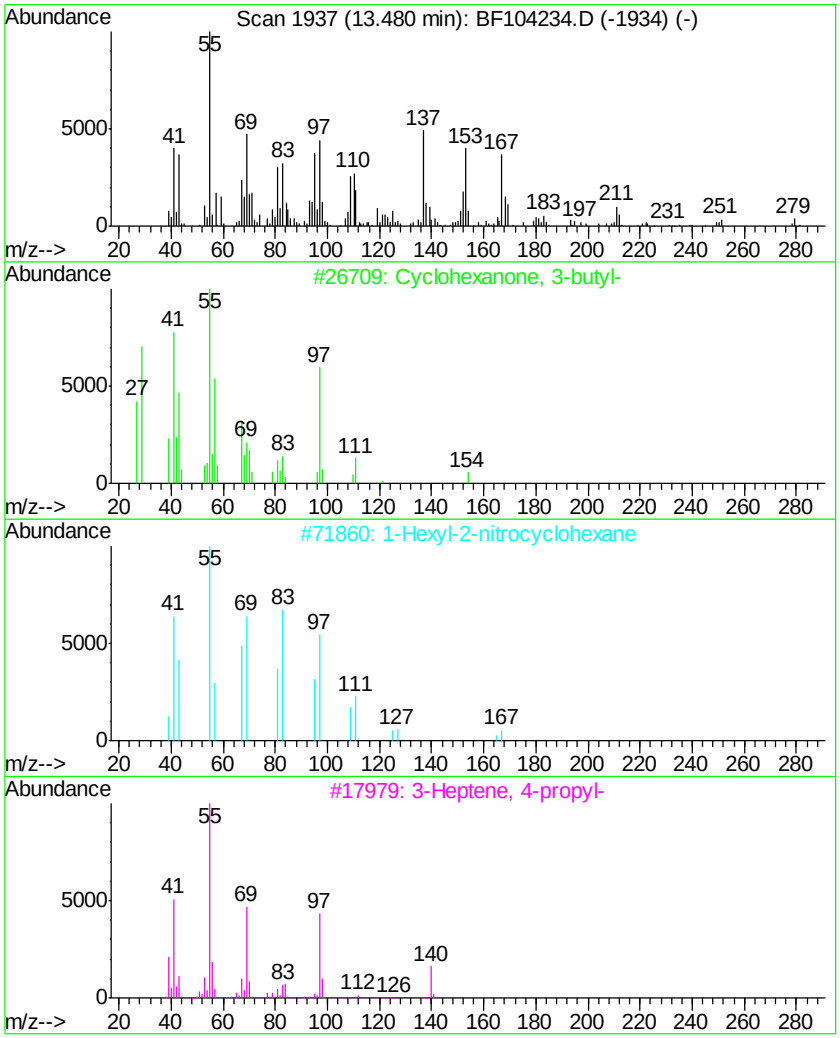
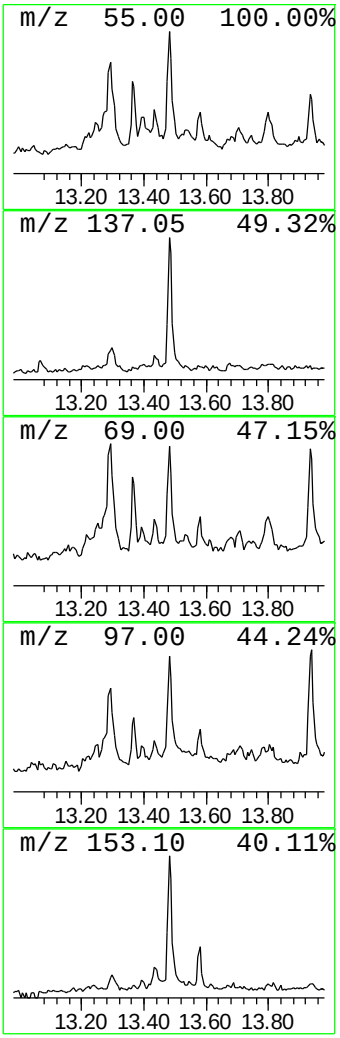
Peak Number 12 unknown13.48 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	5.49 ng	227315	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 3-butyl-	154	C10H18O	039178-69-3	11
2	1-Hexyl-2-nitrocyclohexane	213	C12H23NO2	118252-04-3	10
3	3-Heptene, 4-propyl-	140	C10H20	004485-13-6	10
4	1,7-Dimethyl-4-(1-methylethyl)cy...	210	C15H30	000645-10-3	10
5	Cyclohexanemethanol, 4-methyl-, ...	128	C8H16O	003937-48-2	10





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Operator : JU/SJ
Sample : J2151-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

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

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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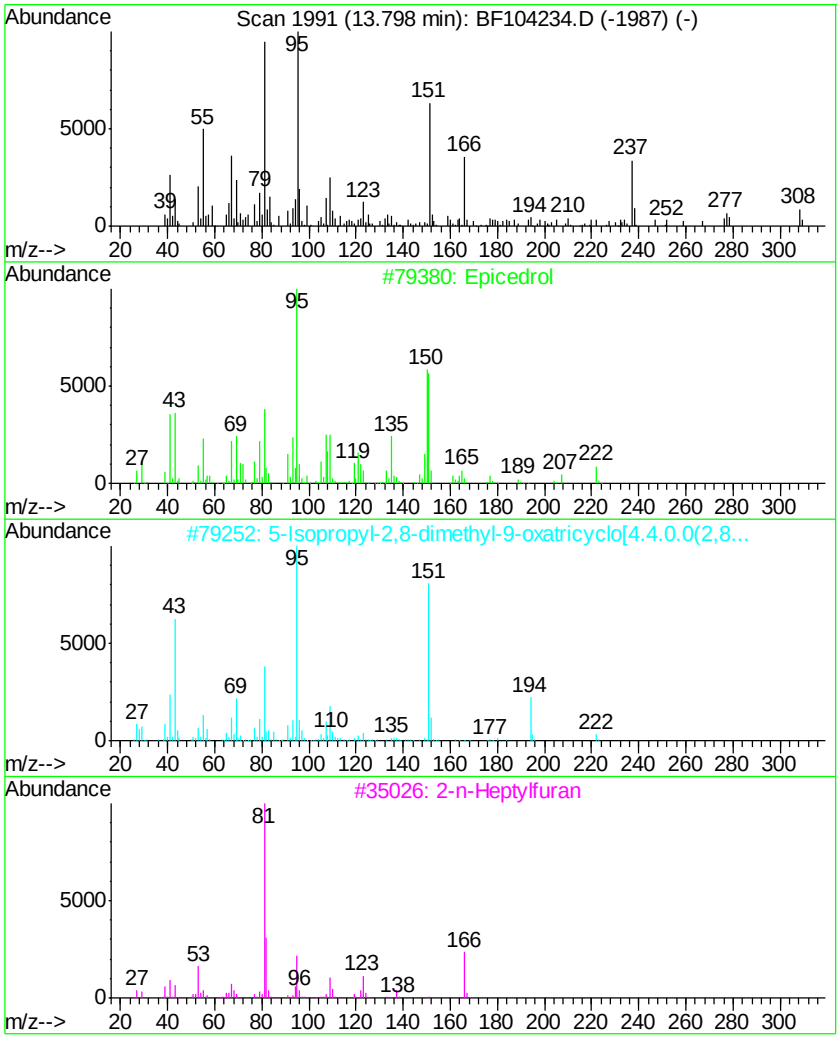
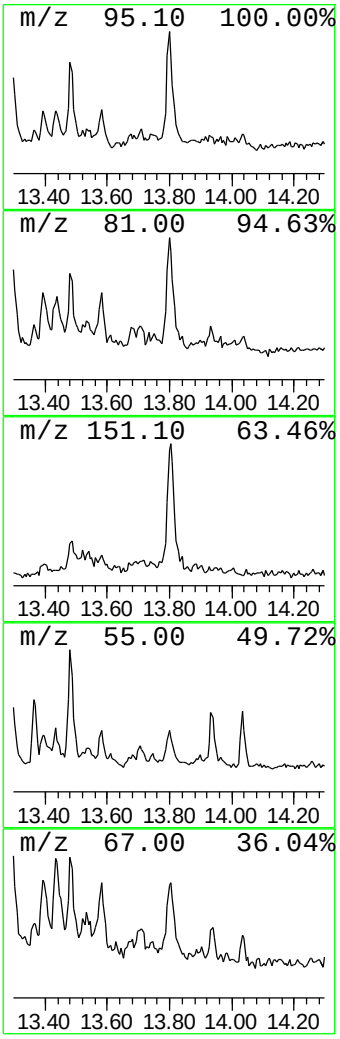
Peak Number 13 unknown13.80 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	6.52 ng	270110	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Epicedrol	222	C15H26O	1000156-22-8	41
2	5-Isopropyl-2,8-dimethyl-9-oxatr...	222	C14H22O2	1000185-23-8	38
3	2-n-Heptylfuran	166	C11H18O	003777-71-7	25
4	Butyric acid, 2-(3-oxo-3H-benzo[...	237	C11H11NO3S	1000316-00-8	18
5	cis-3-Methyl-endo-tricyclo[5.2.1...	150	C11H18	1000215-29-0	18





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Data File : BF104234.D
Acq On : 4 Apr 2018 19:15
Operator : JU/SJ
Sample : J2151-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

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

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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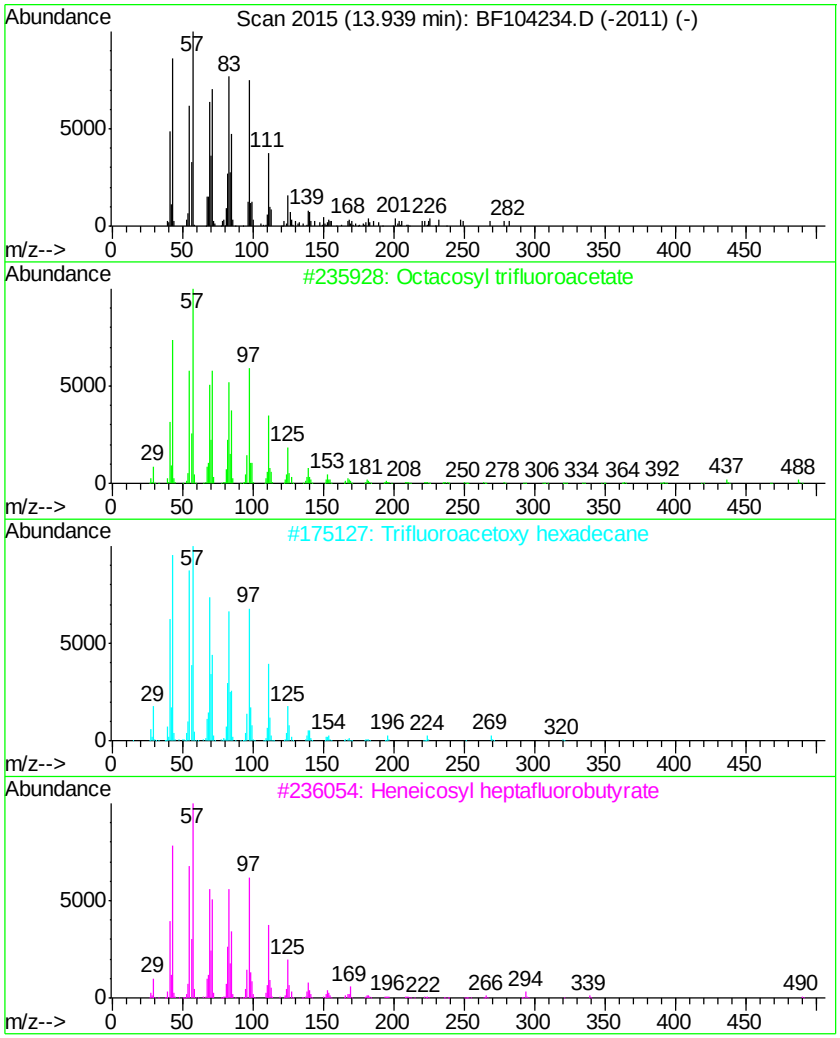
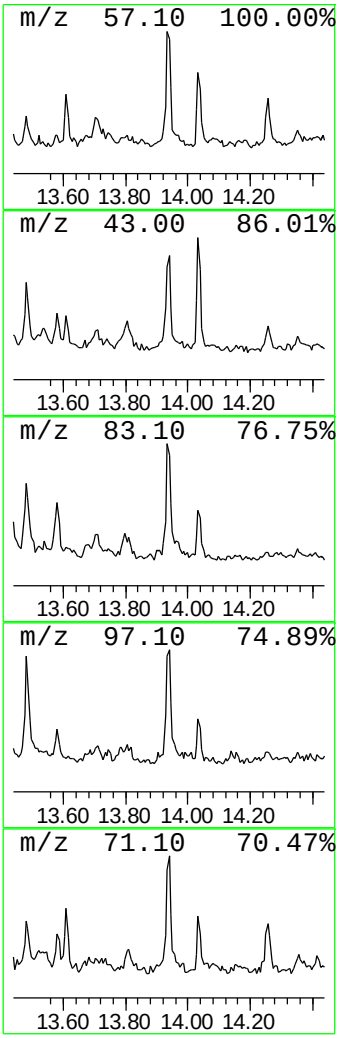
Peak Number 14 Octacosyl trifluoroacetate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	3.73 ng	154600	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	83
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	81
3	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	68
4	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	68
5	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	64





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Operator : JU/SJ
Sample : J2151-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

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

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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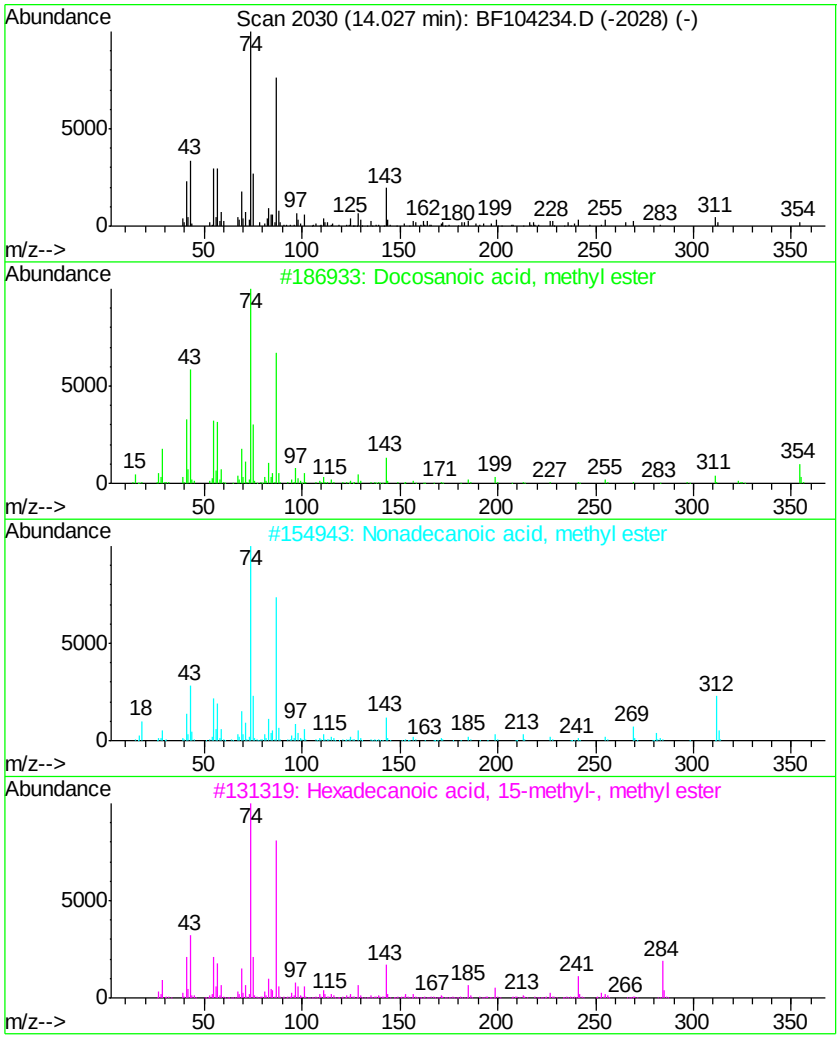
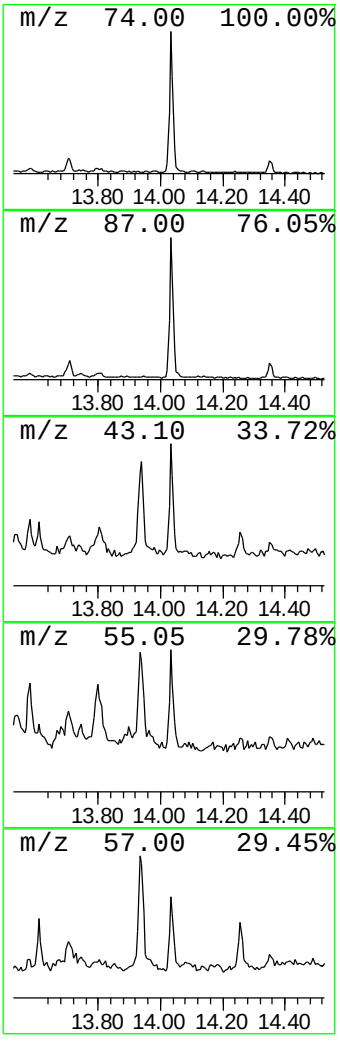
Peak Number 15 Docosanoic acid, methyl ester Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.03	4.77 ng	197677	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	99
2	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	94
3	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	87
4	Methyl stearate	298	C19H38O2	000112-61-8	86
5	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040418\
Data File : BF104234.D
Acq On : 4 Apr 2018 19:15
Operator : JU/SJ
Sample : J2151-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

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

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
unknown6.72	6.72	46.3	ng	1521000	1	6.95	656586	20.0
Nonanoic acid, 9-...	9.57	2.0	ng	115809	3	9.99	1131150	20.0
Heptadecane	10.87	2.3	ng	130424	4	11.49	1113680	20.0
Hexadecanoic acid...	11.86	92.8	ng	5169240	4	11.49	1113680	20.0
9,12-Octadecadien...	12.56	200.3	ng	11151800	4	11.49	1113680	20.0
13-Octadecenoic a...	12.58	111.7	ng	6221670	4	11.49	1113680	20.0
Methyl stearate	12.64	48.2	ng	2684130	4	11.49	1113680	20.0
13-Methyltetradec...	13.29	8.5	ng	353215	5	14.14	828329	20.0
Eicosanoic acid, ...	13.37	5.8	ng	240443	5	14.14	828329	20.0
unknown13.39	13.39	2.8	ng	115709	5	14.14	828329	20.0
unknown13.48	13.48	5.5	ng	227315	5	14.14	828329	20.0
unknown13.80	13.80	6.5	ng	270110	5	14.14	828329	20.0
Octacosyl trifluo...	13.94	3.7	ng	154600	5	14.14	828329	20.0
Docosanoic acid, ...	14.03	4.8	ng	197677	5	14.14	828329	20.0