LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102247.D
Acq On : 20 Jan 2018 5:06
Operator : SJ/JU
Sample : J1113-11
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-16-2.5-3.0

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-BF010918.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	4.922	477	482	492	rVB	163226	232852	7.18%	0.838%
2	5.334	547	552	555	rBV	3216328	3206953	98.88%	11.536%
3	6.363	721	727	736	rBV	3020865	3243440	100.00%	11.667%
4	6.492	744	749	752	rBV	3402646	3241234	99.93%	11.659%
5	6.716	784	787	791	rBV	927742	788904	24.32%	2.838%
6	6.875	810	814	817	rBV	2923669	2511262	77.43%	9.033%
7	7.287	878	884	887	rBV	2139457	2035388	62.75%	7.321%
8	7.469	912	915	919	rVB	44292	35977	1.11%	0.129%
9	7.998	1001	1005	1009	rBV	1147123	1003608	30.94%	3.610%
10	9.081	1183	1189	1192	rBV	3263094	3119821	96.19%	11.222%
11	9.469	1252	1255	1258	rBV	294502	256764	7.92%	0.924%
12	9.686	1283	1292	1295	rBV	127194	104025	3.21%	0.374%
13	9.751	1299	1303	1307	rVB	1087714	966861	29.81%	3.478%
14	10.186	1373	1377	1380	rVB	128479	116436	3.59%	0.419%
15	10.404	1409	1414	1416	rBV	35428	41948	1.29%	0.151%
16	10.539	1431	1437	1441	rBV	1628022	1622134	50.01%	5.835%
17	10.657	1454	1457	1462	rBV	115097	109893	3.39%	0.395%
18	11.104	1530	1533	1536	rBV	41198	34487	1.06%	0.124%
19	11.233	1552	1555	1559	rBV	878683	797375	24.58%	2.868%
20	12.645	1791	1795	1798	rBV	143533	114863	3.54%	0.413%
21	12.821	1821	1825	1828	rBV	2228881	1964439	60.57%	7.066%
22	13.351	1911	1915	1917	rBV	84262	76727	2.37%	0.276%
23	13.716	1973	1977	1985	rBV	403836	393934	12.15%	1.417%
24	13.868	1999	2003	2007	rBV	789425	703852	21.70%	2.532%
25	14.345	2079	2084	2090	rBV3	62458	107309	3.31%	0.386%
26	14.639	2129	2134	2137	rBV4	30110	42902	1.32%	0.154%
27	15.292	2240	2245	2258	rVB	642172	803537	24.77%	2.890%
28	15.774	2323	2327	2334	rVB2	57250	87242	2.69%	0.314%
29	16.198	2396	2399	2403	rBV4	20717	36279	1.12%	0.130%

Sum of corrected areas: 27800446

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102247.D
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Operator : SJ/JU
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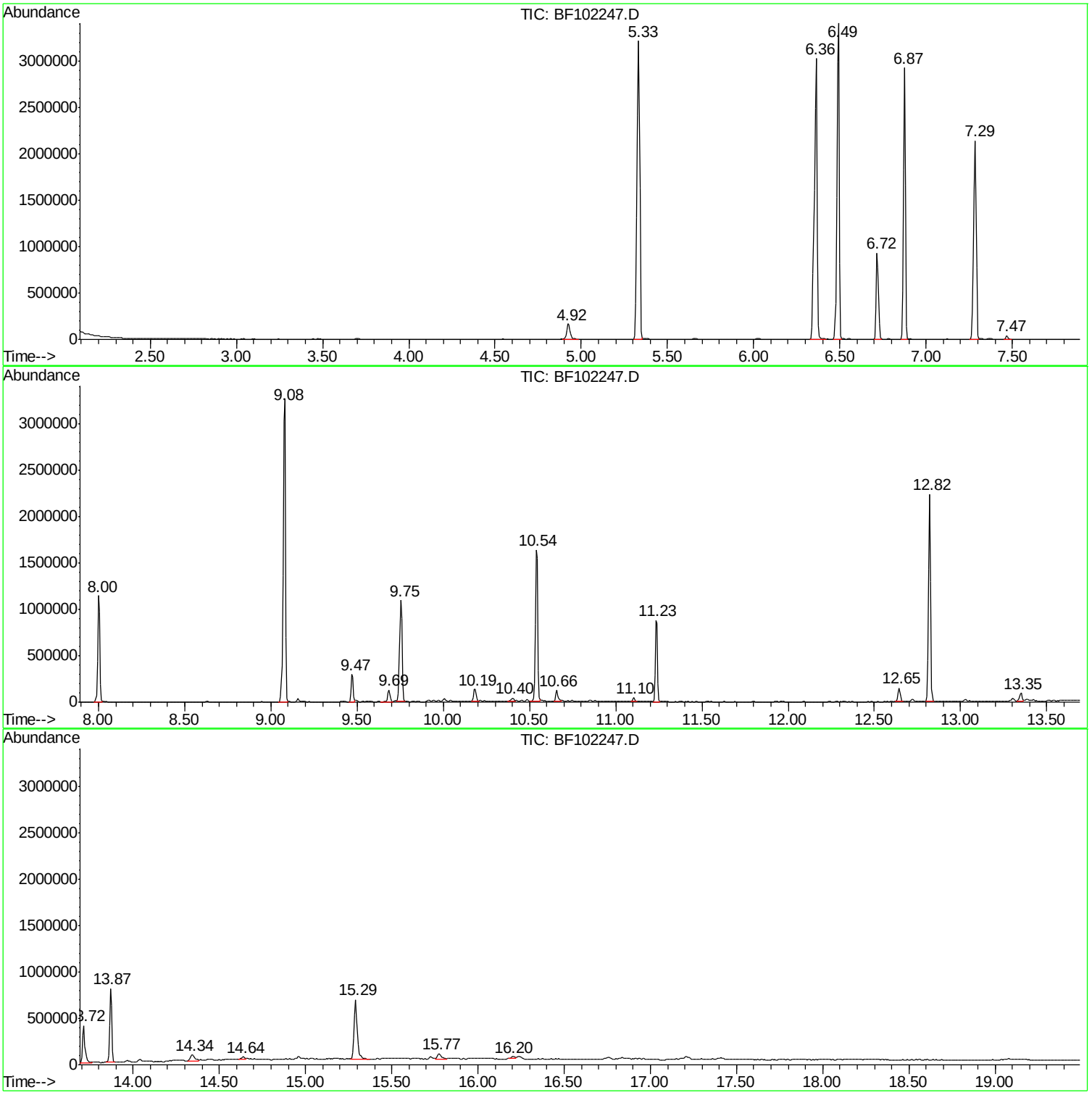
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-16-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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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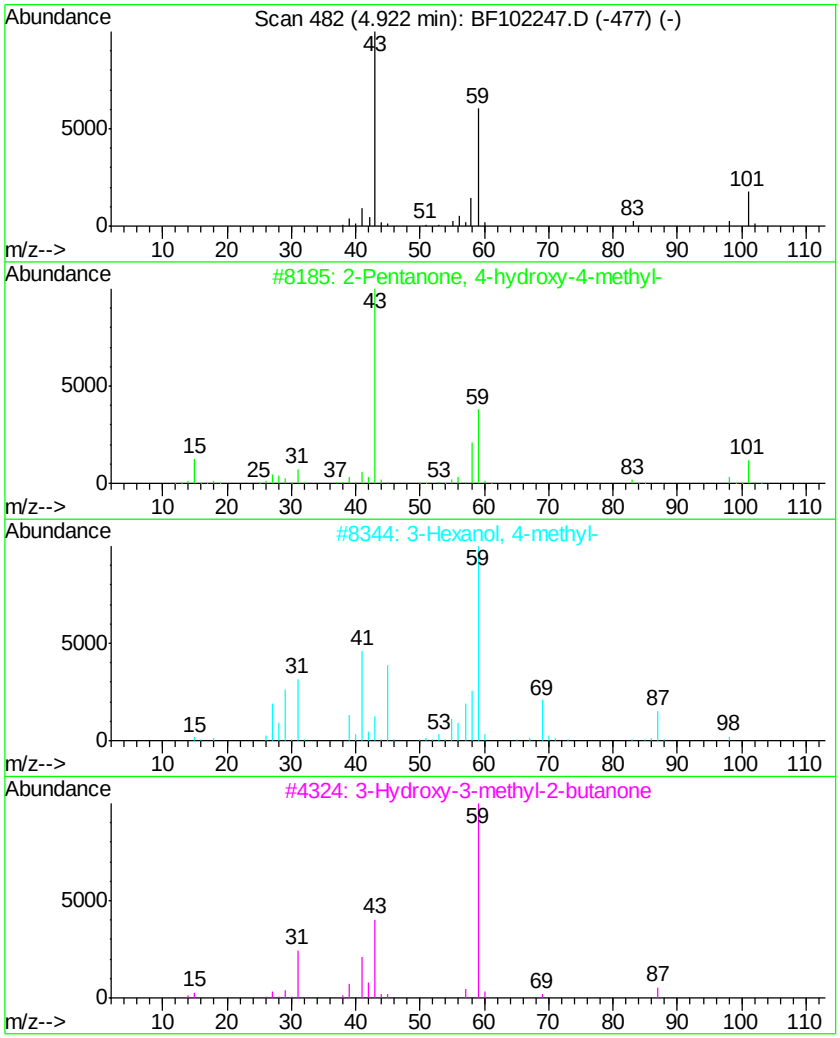
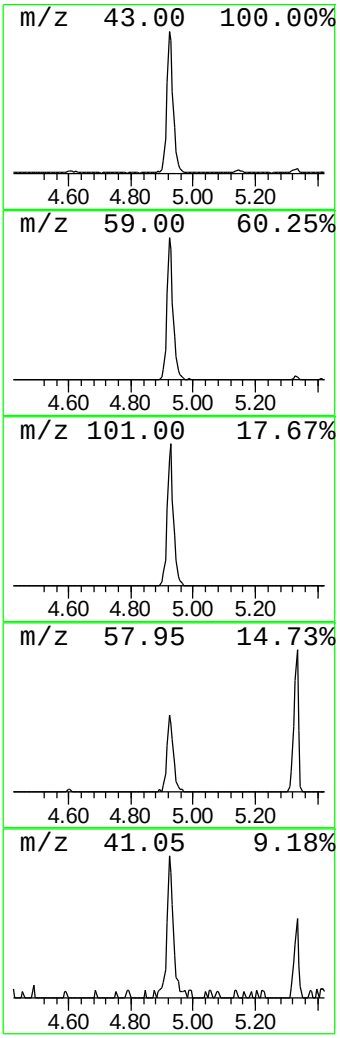
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	5.90 ng	232852	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
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TIC Library : C:\DATABASE\NIST11.L
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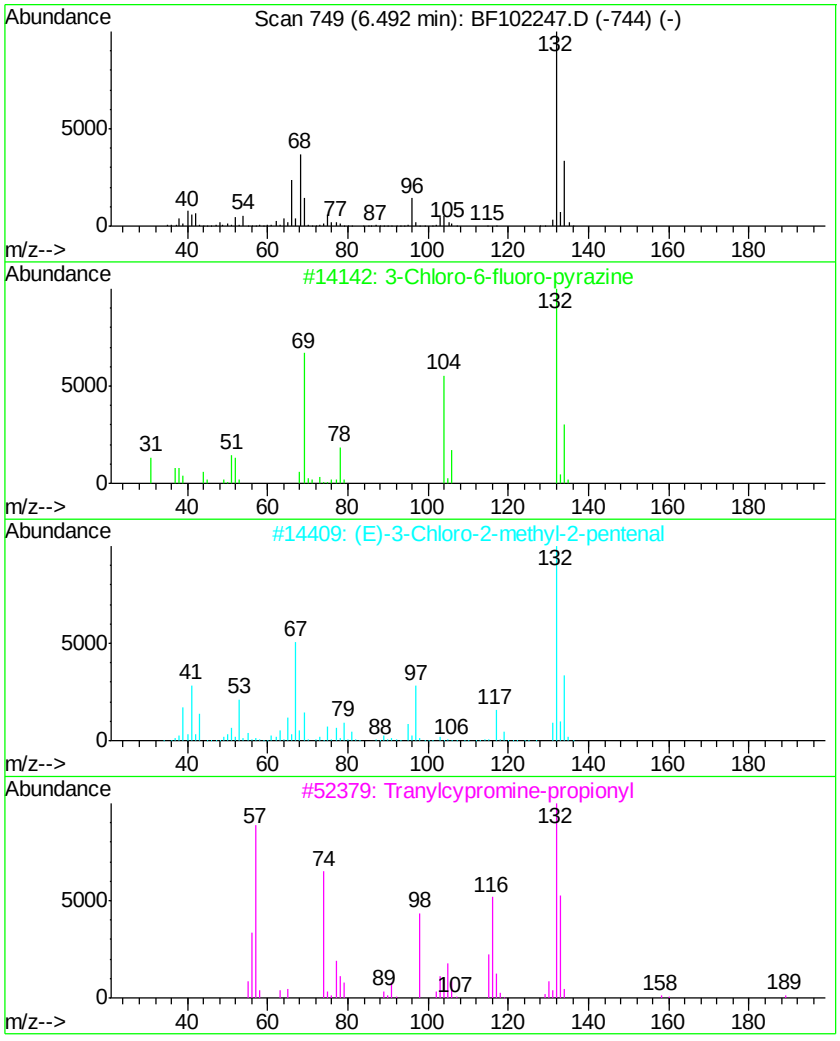
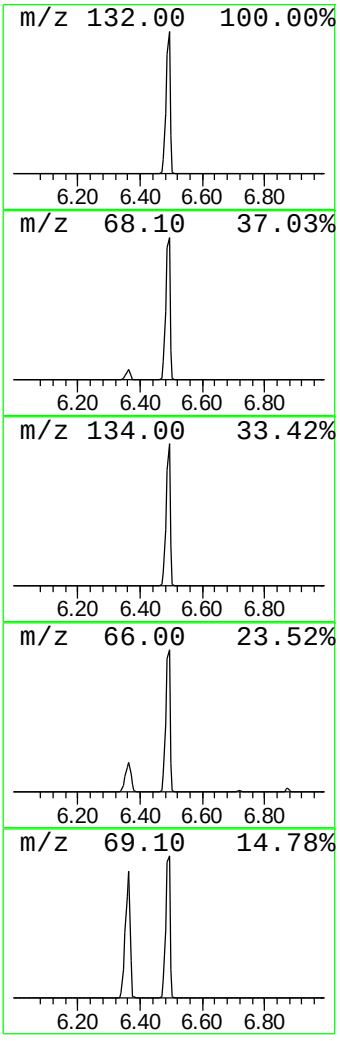
****

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	82.17 ng	3241230	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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ClientSampleId : SB-16-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
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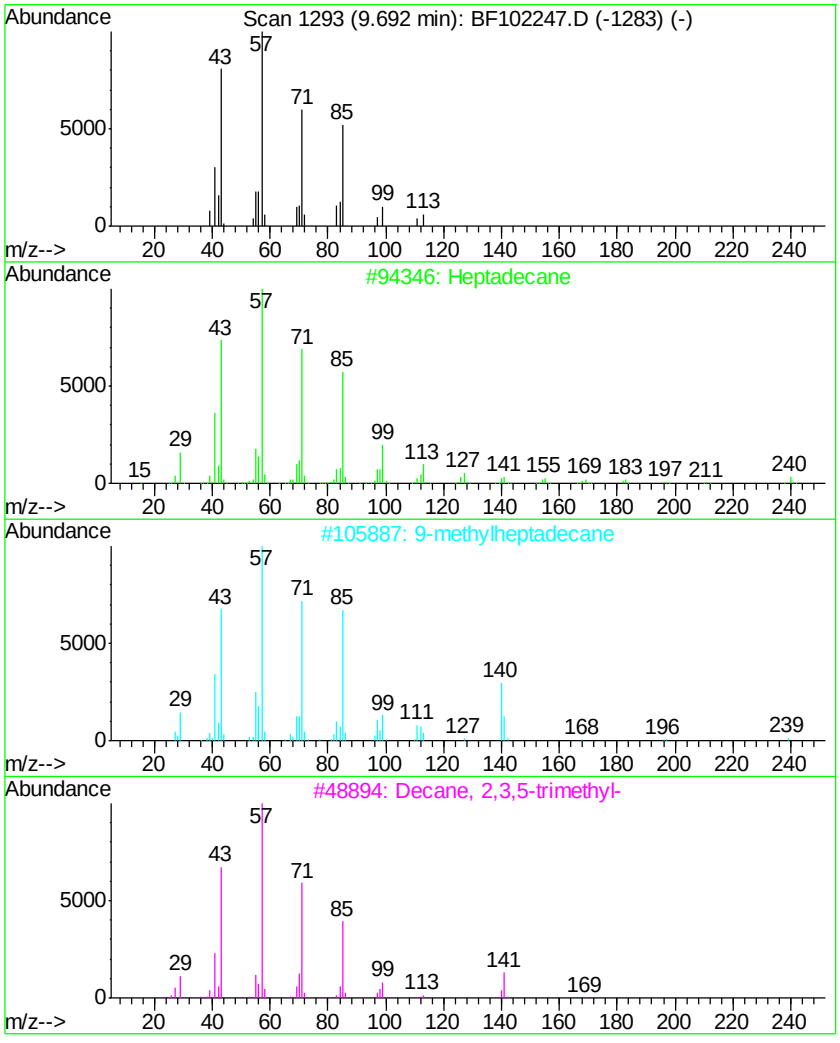
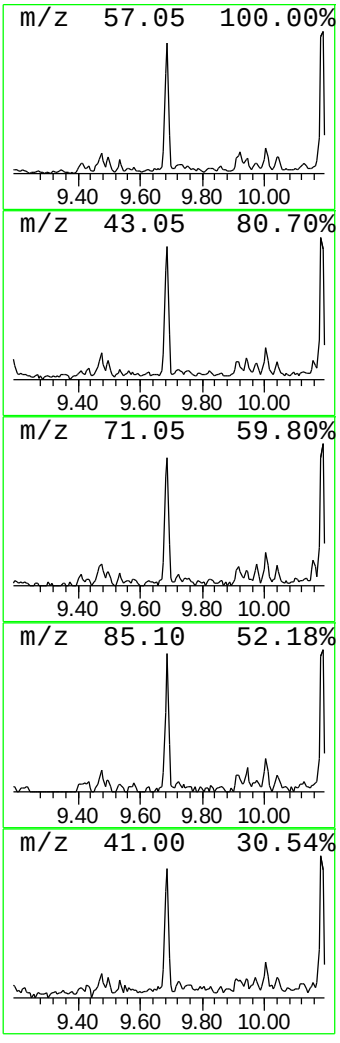
****

Peak Number 4 Heptadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.69	2.15 ng	104025	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	9-methylheptadecane	254	C18H38	026741-18-4	86
3	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83
4	Pentadecane	212	C15H32	000629-62-9	78
5	Tetradecane	198	C14H30	000629-59-4	78





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Instrument : BNA_F
ClientSampleId : SB-16-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
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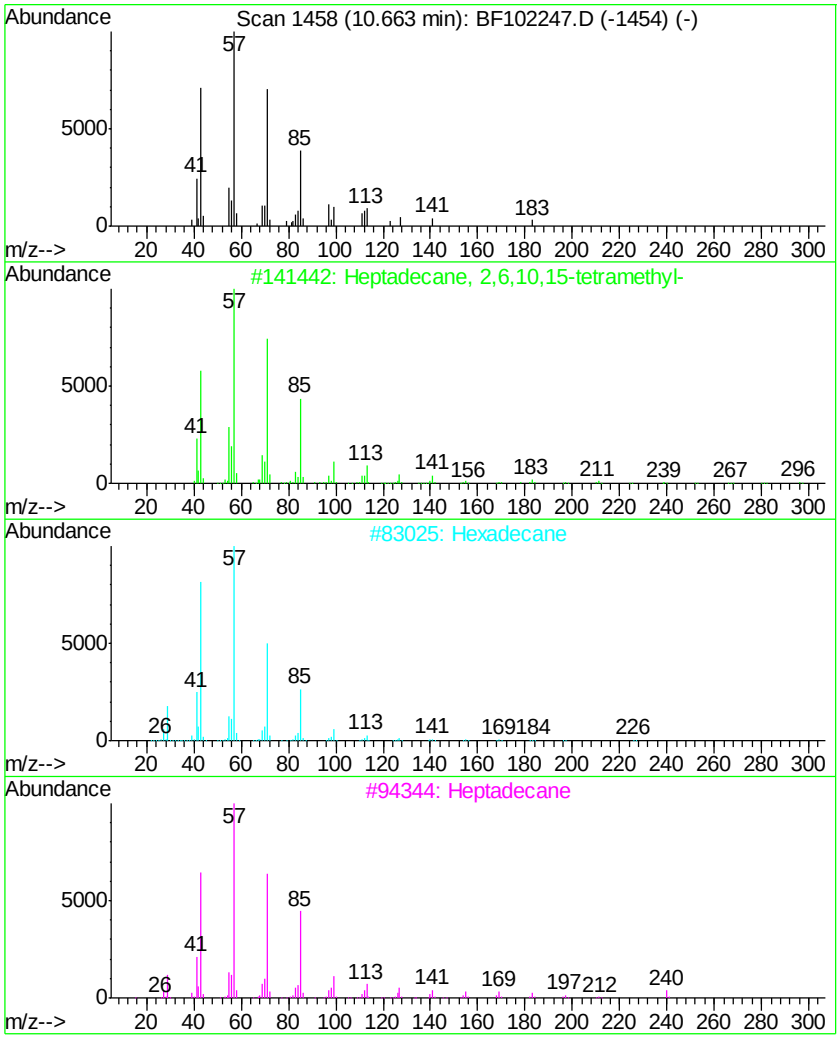
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

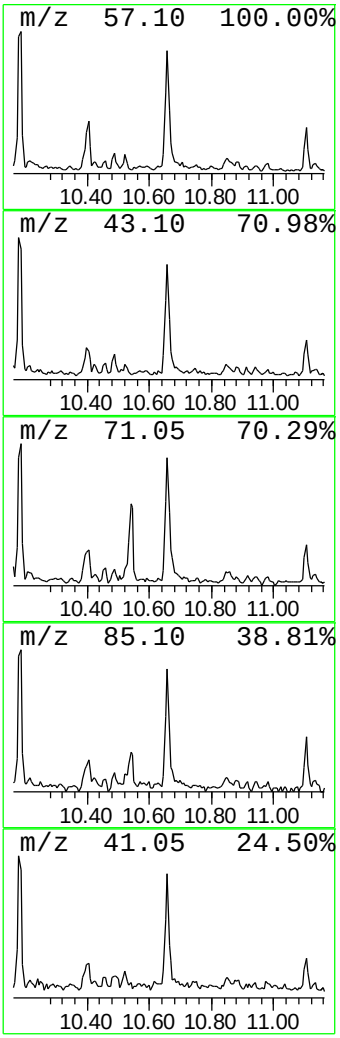
****

Peak Number 6 Heptadecane, 2,6,10,15-tetr... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	2.76 ng	109893	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Heptadecane	240	C17H36	000629-78-7	90
4	Heptacosane	380	C27H56	000593-49-7	90
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
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Sample : J1113-11
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-16-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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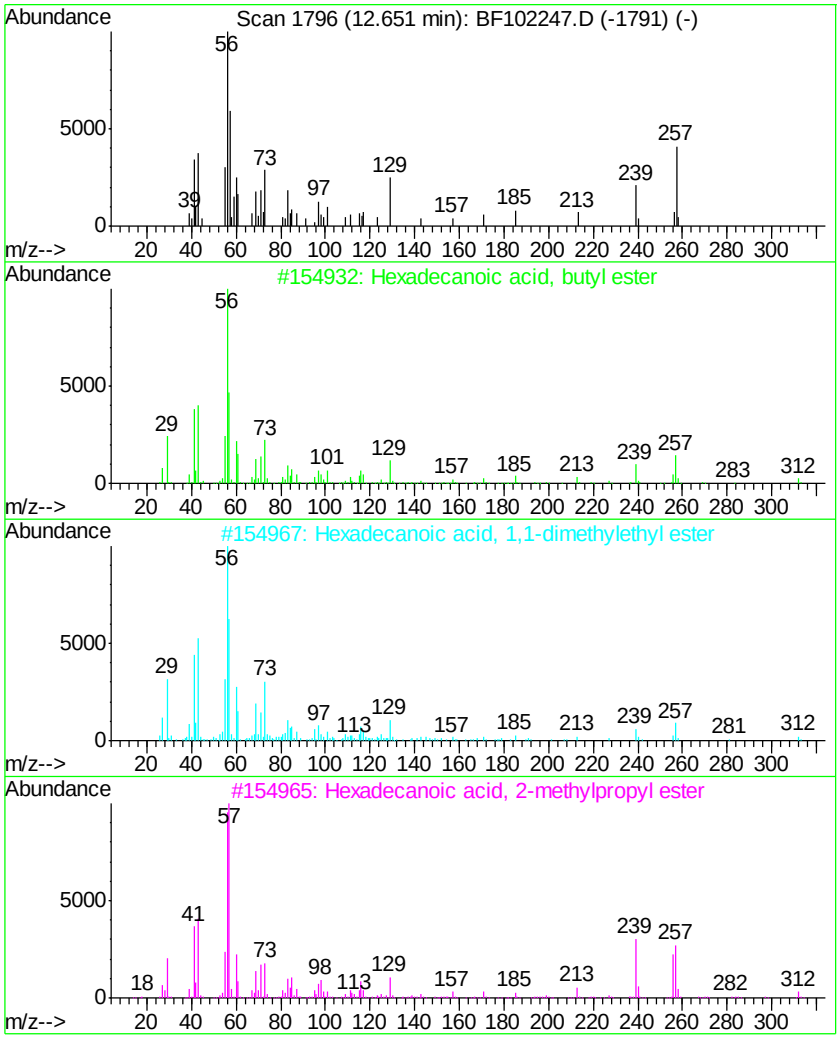
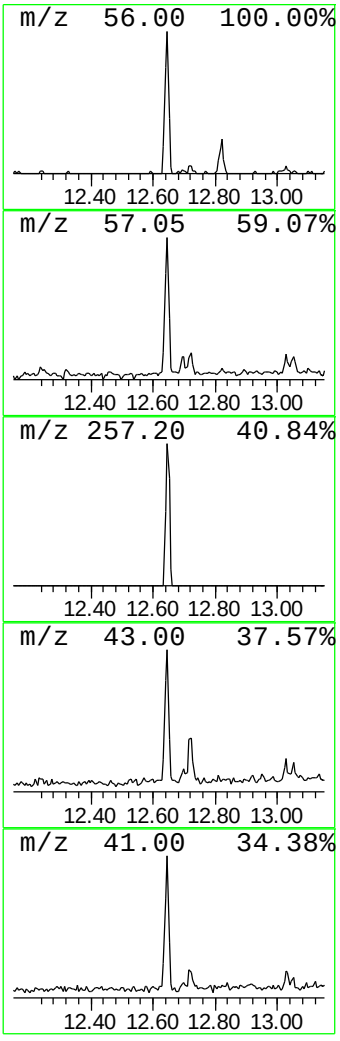
Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	3.26 ng	114863	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	64
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	53
4	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	43
5	5-Methyl-5-hexen-3-ol	114	C7H14O	067760-89-8	35





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Instrument : BNA_F
ClientSampleId : SB-16-2.5-3.0

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TIC Library : C:\DATABASE\NIST11.L
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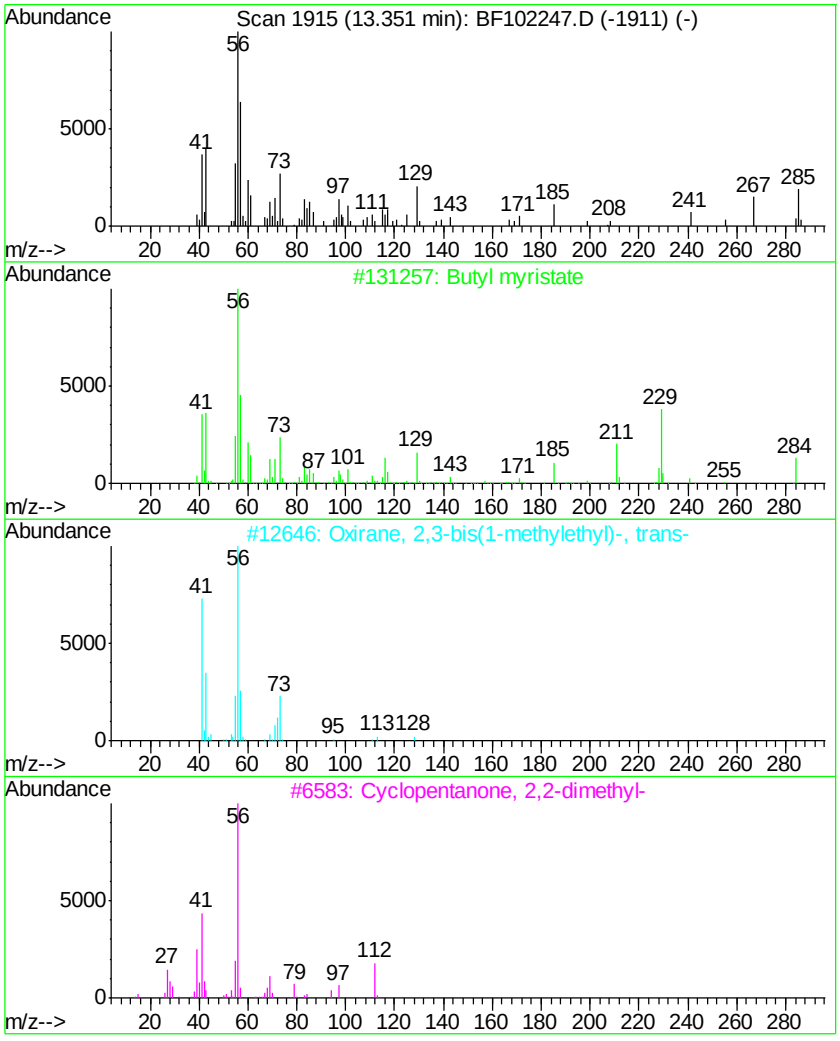
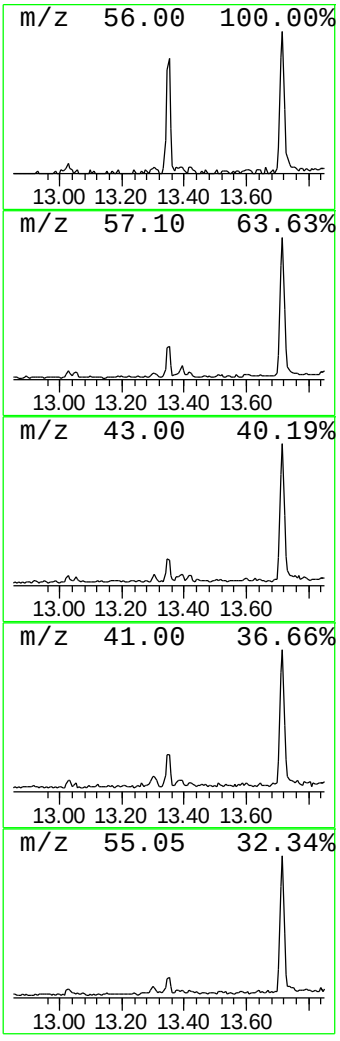
Peak Number 8 Butyl myristate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	2.18 ng	76727	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	72
2	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	32
3	Cyclopentanone, 2,2-dimethyl-	112	C7H12O	004541-32-6	30
4	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	27
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27





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TIC Library : C:\DATABASE\NIST11.L
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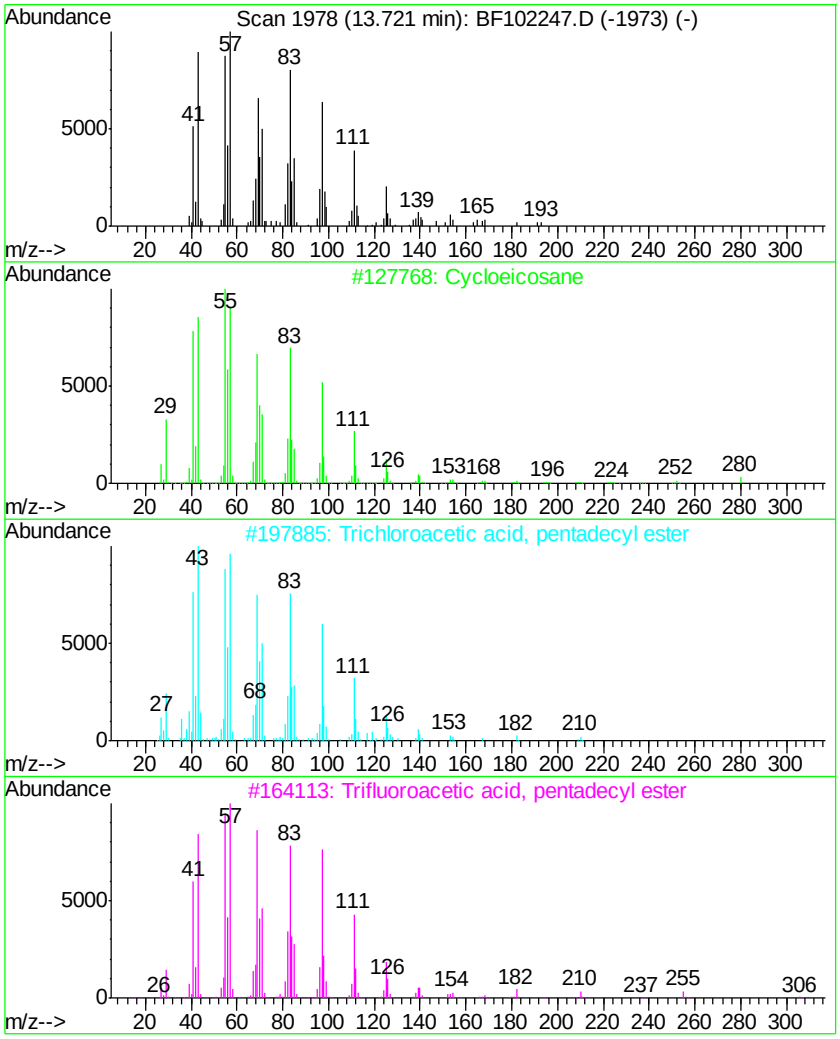
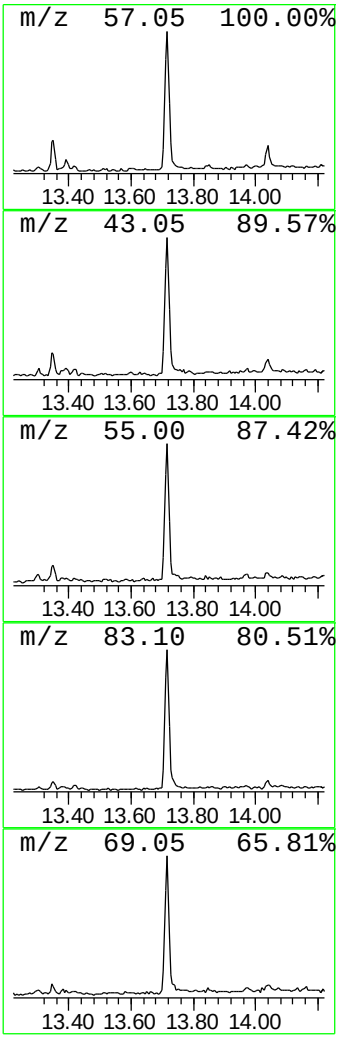
Peak Number 9 Cycloeicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	11.19 ng	393934	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloeicosane	280	C20H40	000296-56-0	99
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94





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TIC Library : C:\DATABASE\NIST11.L
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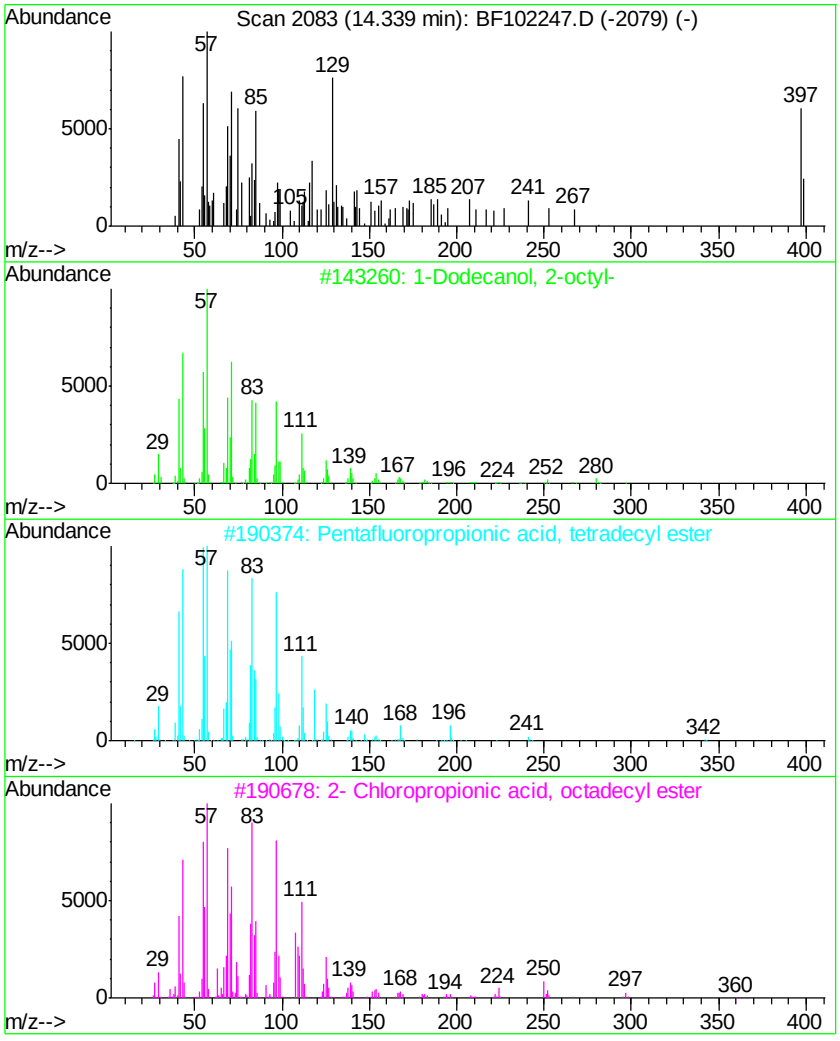
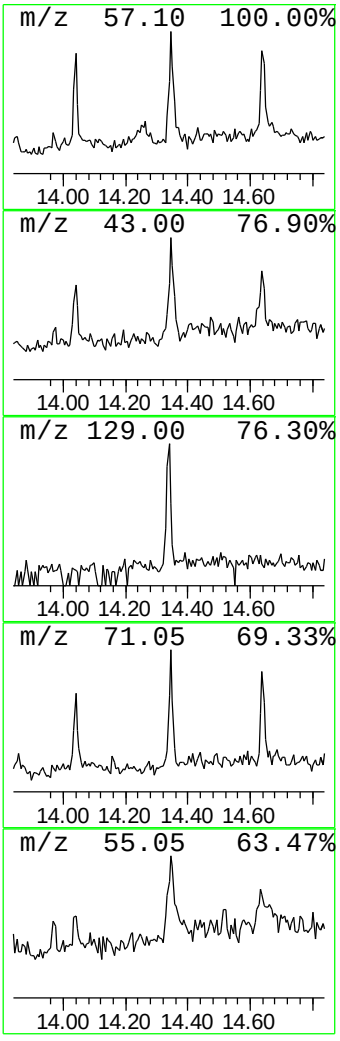
Peak Number 10 1-Dodecanol, 2-octyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	3.05 ng	107309	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	52
2	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	43
3	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	43
4	1-Tricosene	322	C23H46	018835-32-0	43
5	1-Docosene	308	C22H44	001599-67-3	43





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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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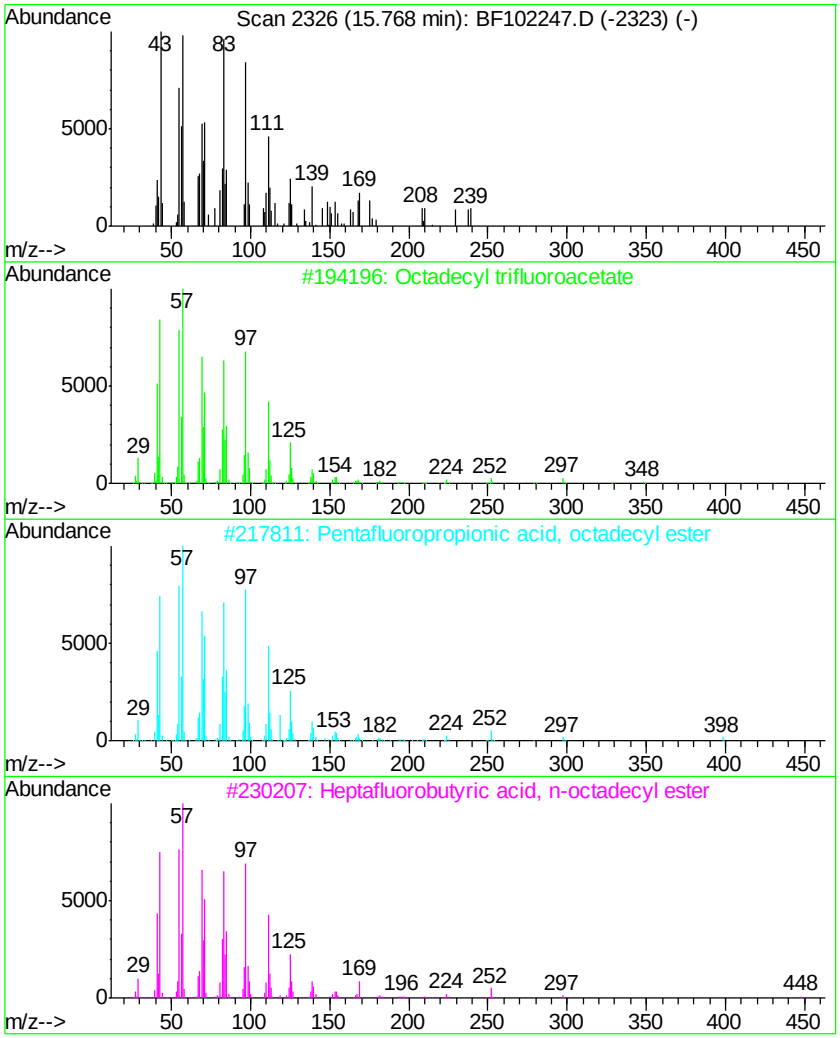
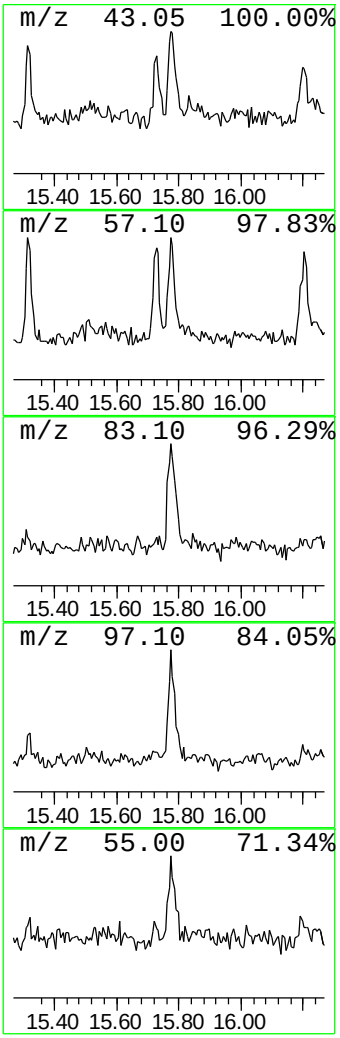
Peak Number 11 Octadecyl trifluoroacetate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	2.17 ng	87242	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
2	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	93
3	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
4	Heptacosyl acetate	438	C29H58O2	1000351-78-2	90
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90





Tentatively Identified Compound (LSC) summary

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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...	4.92	5.9	ng	232852	1	6.72	788904	20.0
unknown6.49	6.49	82.2	ng	3241230	1	6.72	788904	20.0
Heptadecane	9.69	2.1	ng	104025	3	9.75	966861	20.0
Heptadecane, 2,6,...	10.66	2.8	ng	109893	4	11.23	797375	20.0
Hexadecanoic acid...	12.65	3.3	ng	114863	5	13.87	703852	20.0
Butyl myristate	13.35	2.2	ng	76727	5	13.87	703852	20.0
Cycloeicosane	13.72	11.2	ng	393934	5	13.87	703852	20.0
1-Dodecanol, 2-oc...	14.34	3.0	ng	107309	5	13.87	703852	20.0
Octadecyl trifluo...	15.77	2.2	ng	87242	6	15.29	803537	20.0