LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF020318\
Data File : BF102724.D
Acq On : 3 Feb 2018 18:30
Operator : SJ/JU
Sample : J1436-13
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B18

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-BF020318.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	2.163	8	13	19	rVB	403623	526938	11.26%	1.316%
2	5.116	512	515	521	rVB	115395	144940	3.10%	0.362%
3	5.498	574	580	583	rBV	4302491	4629293	98.90%	11.557%
4	6.504	745	751	763	rVB	4121545	4680682	100.00%	11.685%
5	6.651	770	776	779	rBV	4261228	4526078	96.70%	11.299%
6	6.704	782	785	790	rVB	144229	134875	2.88%	0.337%
7	6.881	811	815	818	rBV	1288248	1109687	23.71%	2.770%
8	7.034	837	841	845	rVB	3640995	3485231	74.46%	8.701%
9	7.440	905	910	913	rBV	2907594	2757274	58.91%	6.884%
10	7.540	924	927	931	rVB	63316	51081	1.09%	0.128%
11	8.163	1029	1033	1036	rVB	1644538	1453751	31.06%	3.629%
12	8.710	1123	1126	1130	rBV	102250	87658	1.87%	0.219%
13	9.239	1211	1216	1219	rBV	4516982	4528075	96.74%	11.304%
14	9.628	1278	1282	1285	rBV	394377	344282	7.36%	0.859%
15	9.839	1316	1318	1322	rVB	81872	65832	1.41%	0.164%
16	9.916	1327	1331	1335	rVB	1718673	1461562	31.23%	3.649%
17	10.339	1401	1403	1406	rVB	95408	74957	1.60%	0.187%
18	10.628	1447	1452	1455	rBV	261106	207853	4.44%	0.519%
19	10.704	1459	1465	1468	rBV	2520098	2332738	49.84%	5.824%
20	10.816	1481	1484	1489	rVB	72390	76706	1.64%	0.191%
21	11.398	1580	1583	1587	rBV	1265727	1151711	24.61%	2.875%
22	11.922	1668	1672	1681	rBV	496570	513250	10.97%	1.281%
23	12.622	1786	1791	1796	rBV3	44855	92152	1.97%	0.230%
24	12.704	1802	1805	1819	rBV	280581	374418	8.00%	0.935%
25	12.986	1849	1853	1856	rBV	3306856	2927950	62.55%	7.310%
26	13.874	2000	2004	2007	rBV	232250	261308	5.58%	0.652%
27	13.904	2007	2009	2013	rVB	82846	75656	1.62%	0.189%
28	14.039	2028	2032	2035	rVB	974668	911093	19.46%	2.275%
29	15.510	2278	2282	2292	rVB	738064	1069061	22.84%	2.669%

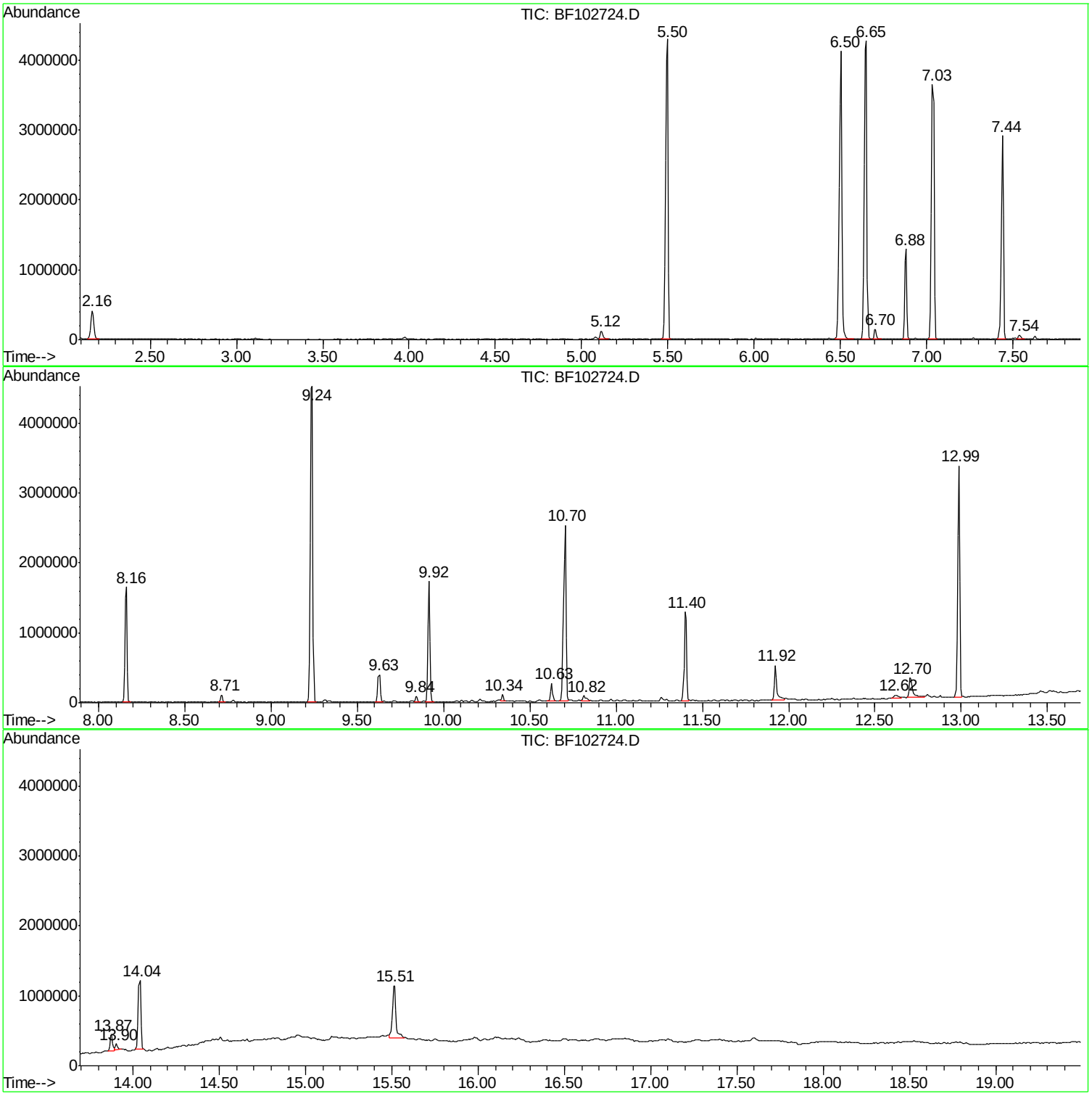
Sum of corrected areas: 40056092

Data Path : U:\HPCHEM1\BNA F\DATA\BF020318\
Data File : BF102724.D
Acq On : 3 Feb 2018 18:30
Operator : SJ/JU
Sample : J1436-13
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : U:\HPCHEM1\BNA F\DATA\BF020318\
Data File : BF102724.D
Acq On : 3 Feb 2018 18:30
Operator : SJ/JU
Sample : J1436-13
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

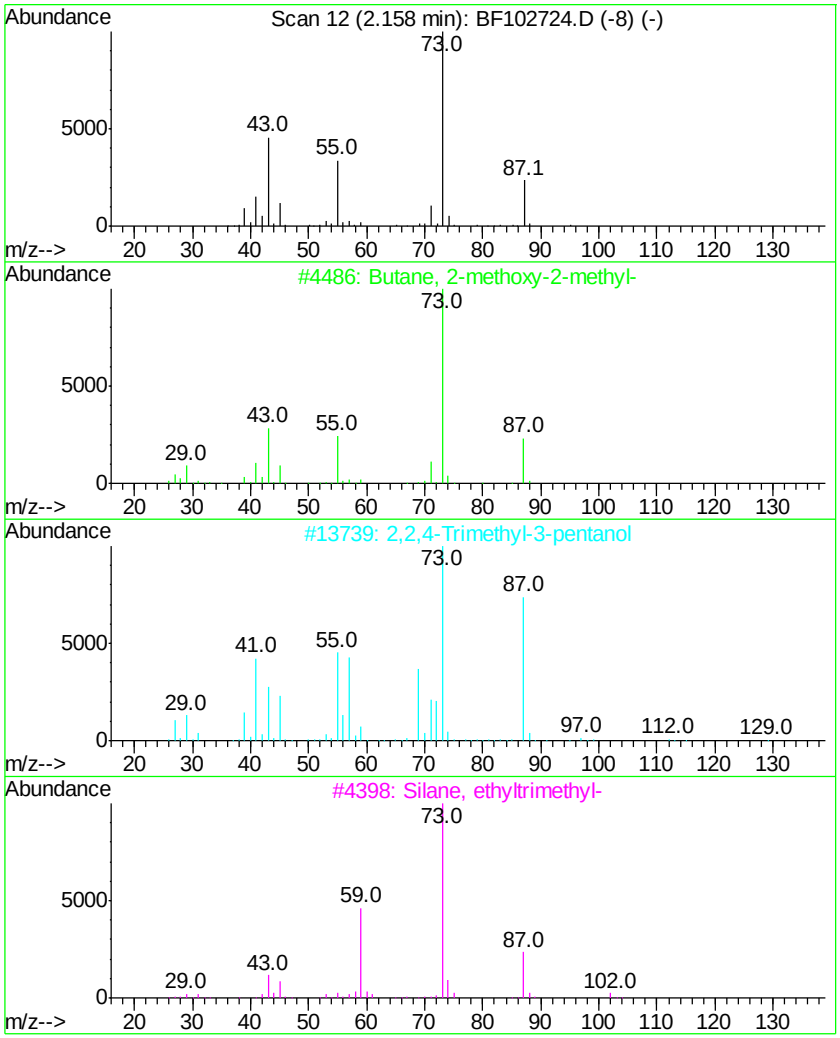
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

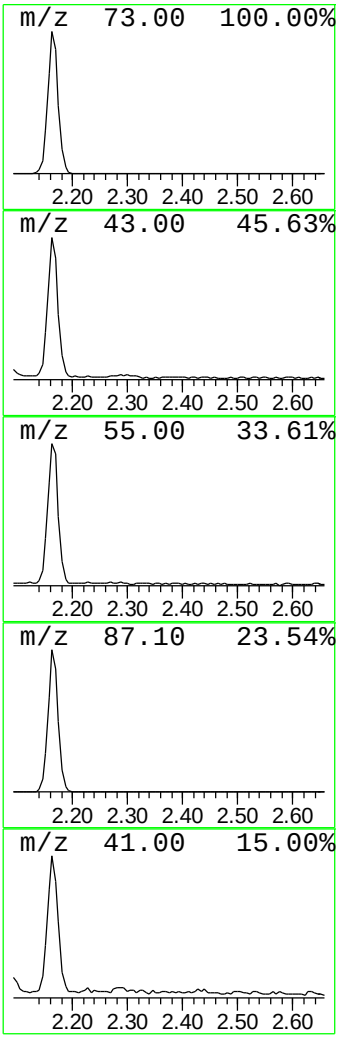
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	9.50 ng	526938	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	33
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25





Data Path : U:\HPCHEM1\BNA F\DATA\BF020318\
Data File : BF102724.D
Acq On : 3 Feb 2018 18:30
Operator : SJ/JU
Sample : J1436-13
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

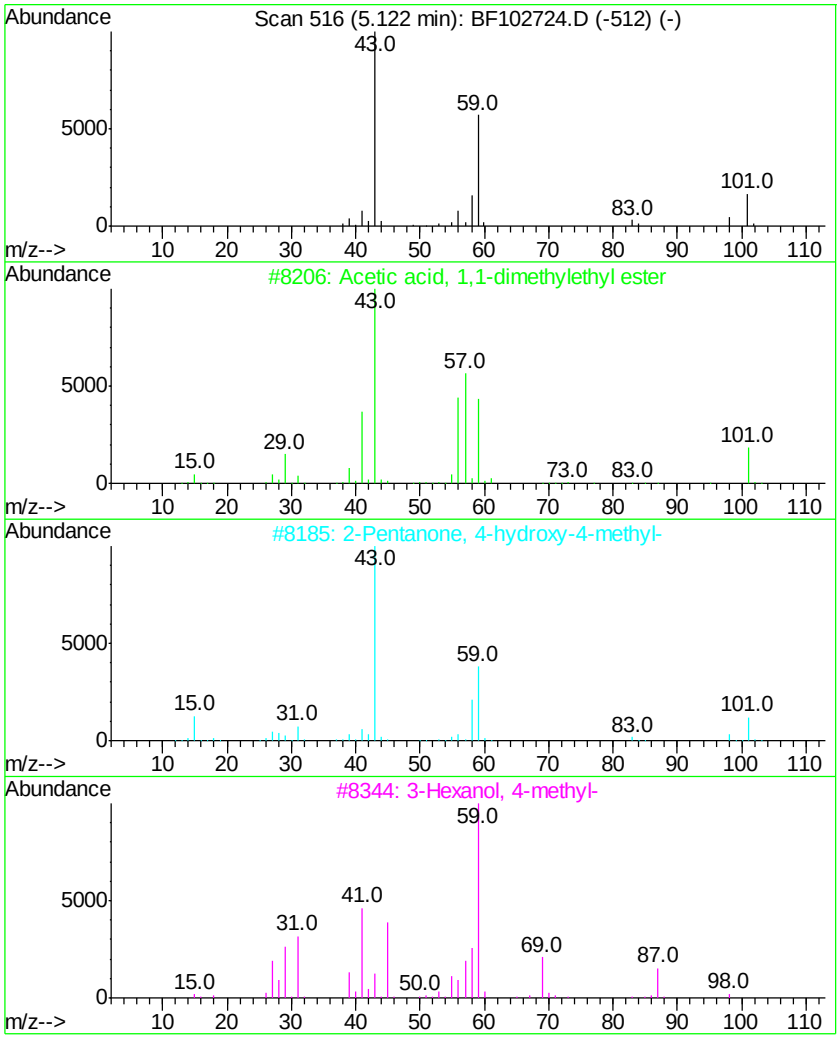
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

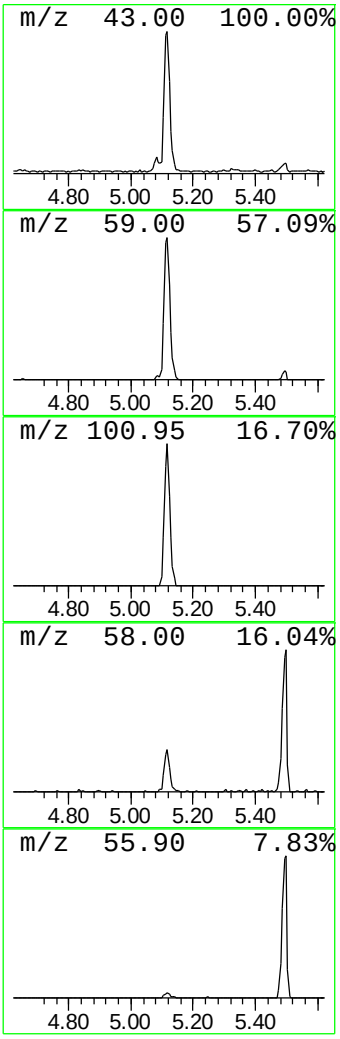
****

Peak Number 2 unknown5.12 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	2.61 ng	144940	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16





Data Path : U:\HPCHEM1\BNA F\DATA\BF020318\
Data File : BF102724.D
Acq On : 3 Feb 2018 18:30
Operator : SJ/JU
Sample : J1436-13
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

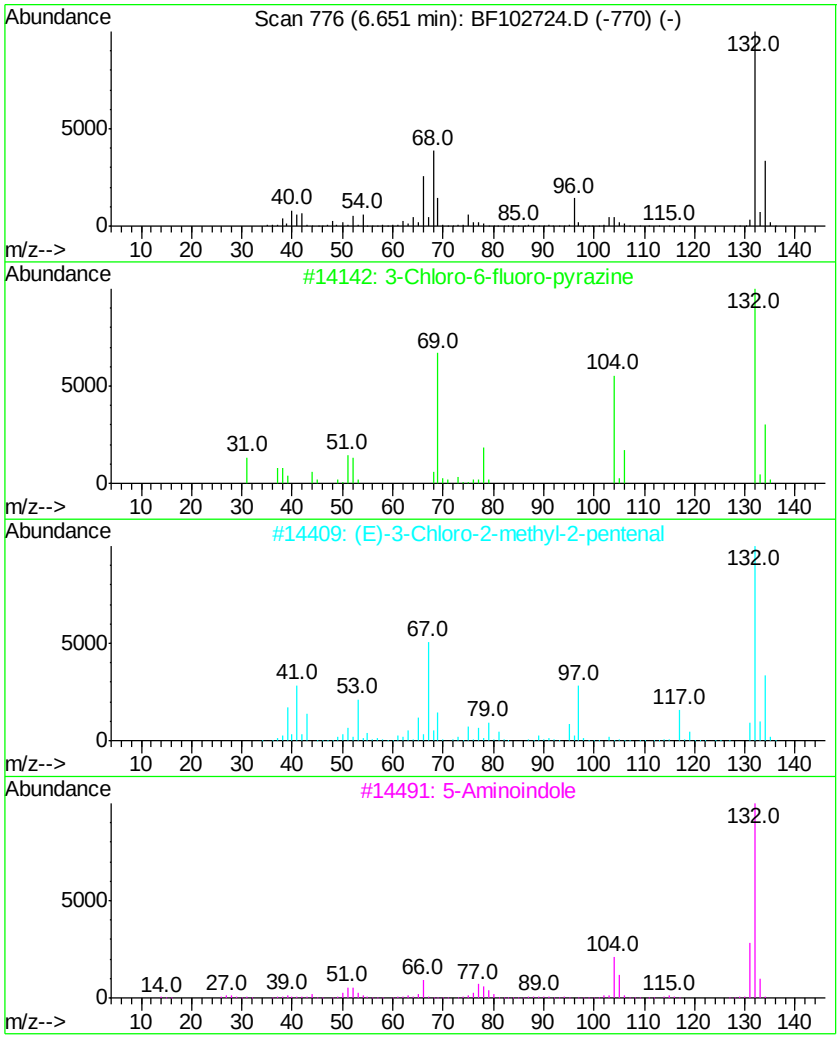
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

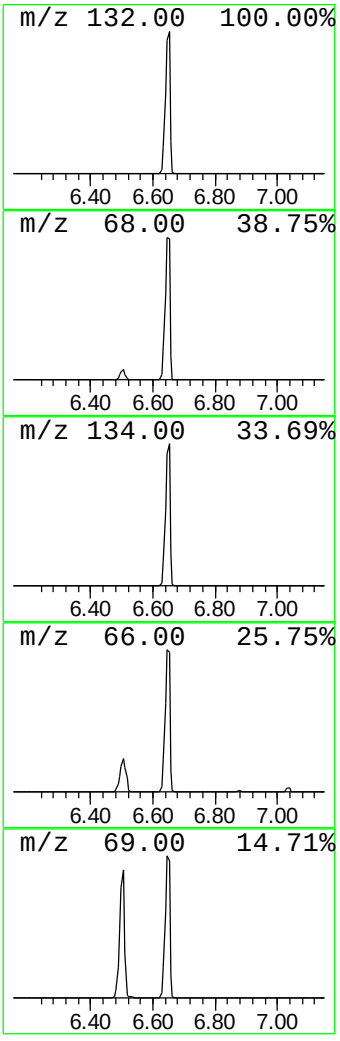
****

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	81.57 ng	4526080	1,4-Dichlorobenzene-d4	6.88

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	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Data Path : U:\HPCHEM1\BNA F\DATA\BF020318\
Data File : BF102724.D
Acq On : 3 Feb 2018 18:30
Operator : SJ/JU
Sample : J1436-13
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

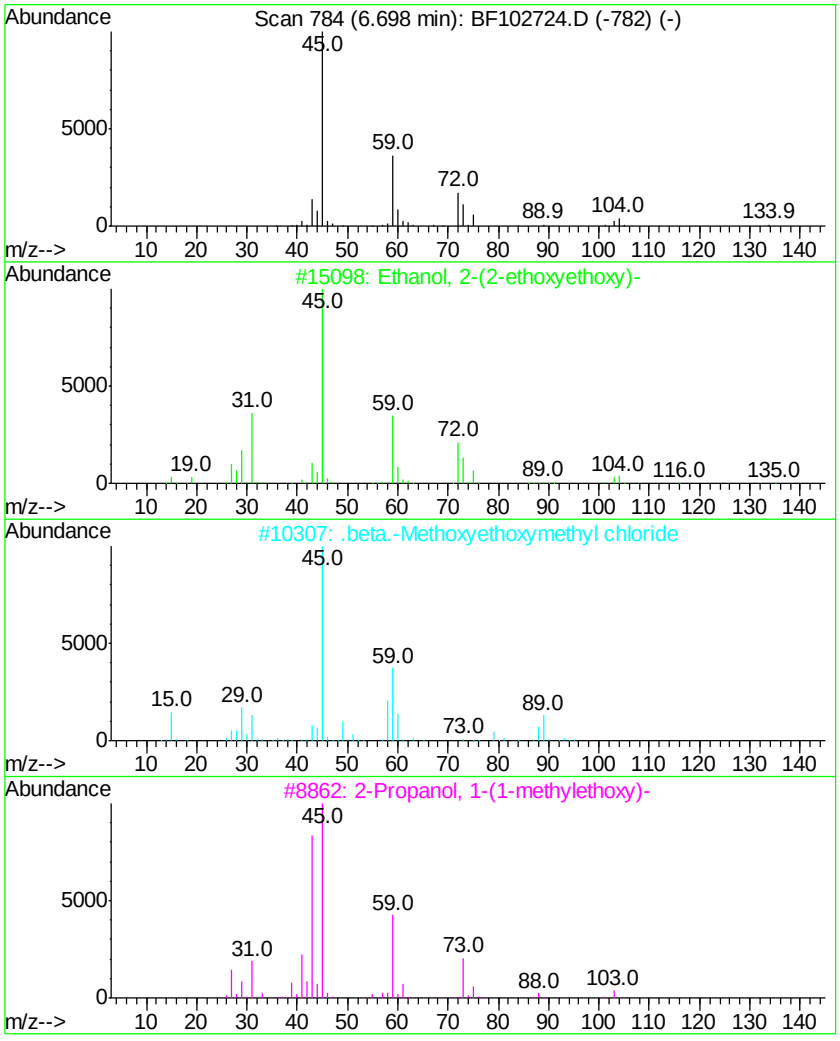
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

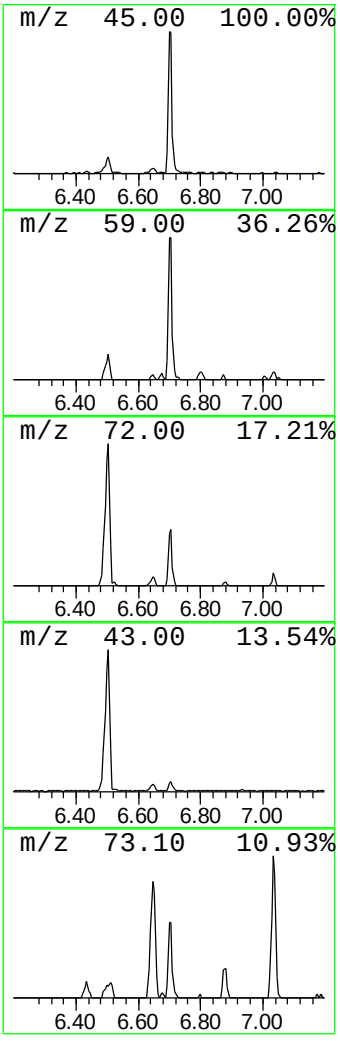
****

Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	2.43 ng	134875	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	.beta.-Methoxyethoxymethyl chloride	124	C4H9ClO2	003970-21-6	38
3	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38
4	Methoxyacetic acid, butyl ester	146	C7H14O3	017640-22-1	33
5	Methoxyacetic acid, 2-methylprop...	146	C7H14O3	1000282-40-9	33





Data Path : U:\HPCHEM1\BNA F\DATA\BF020318\
Data File : BF102724.D
Acq On : 3 Feb 2018 18:30
Operator : SJ/JU
Sample : J1436-13
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

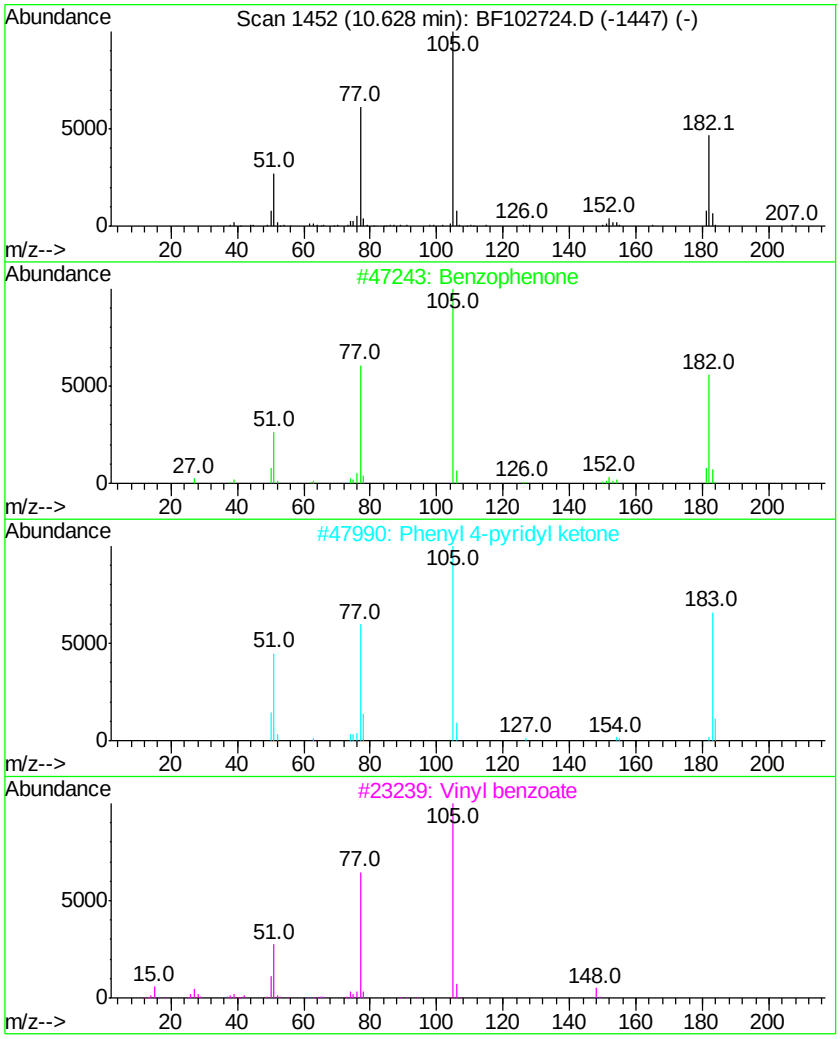
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

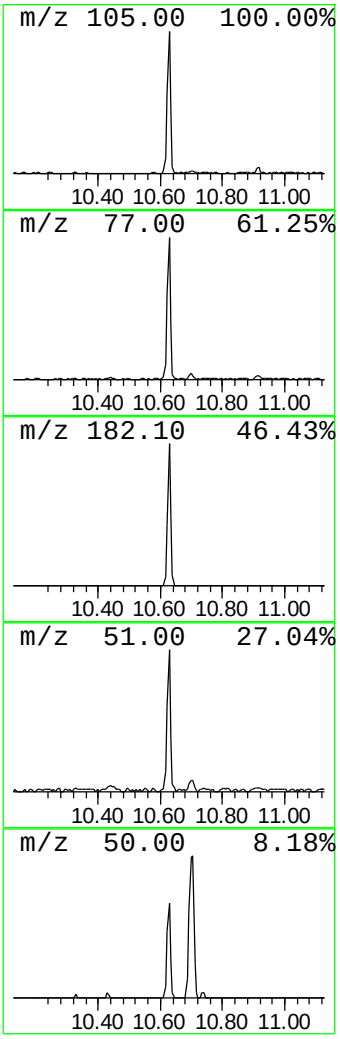
****

Peak Number 6 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	2.84 ng	207853	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	58
3	Vinyl benzoate	148	C9H8O2	000769-78-8	47
4	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
5	1-Butanone, 1-phenyl-	148	C10H12O	000495-40-9	47





Data Path : U:\HPCHEM1\BNA F\DATA\BF020318\
Data File : BF102724.D
Acq On : 3 Feb 2018 18:30
Operator : SJ/JU
Sample : J1436-13
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

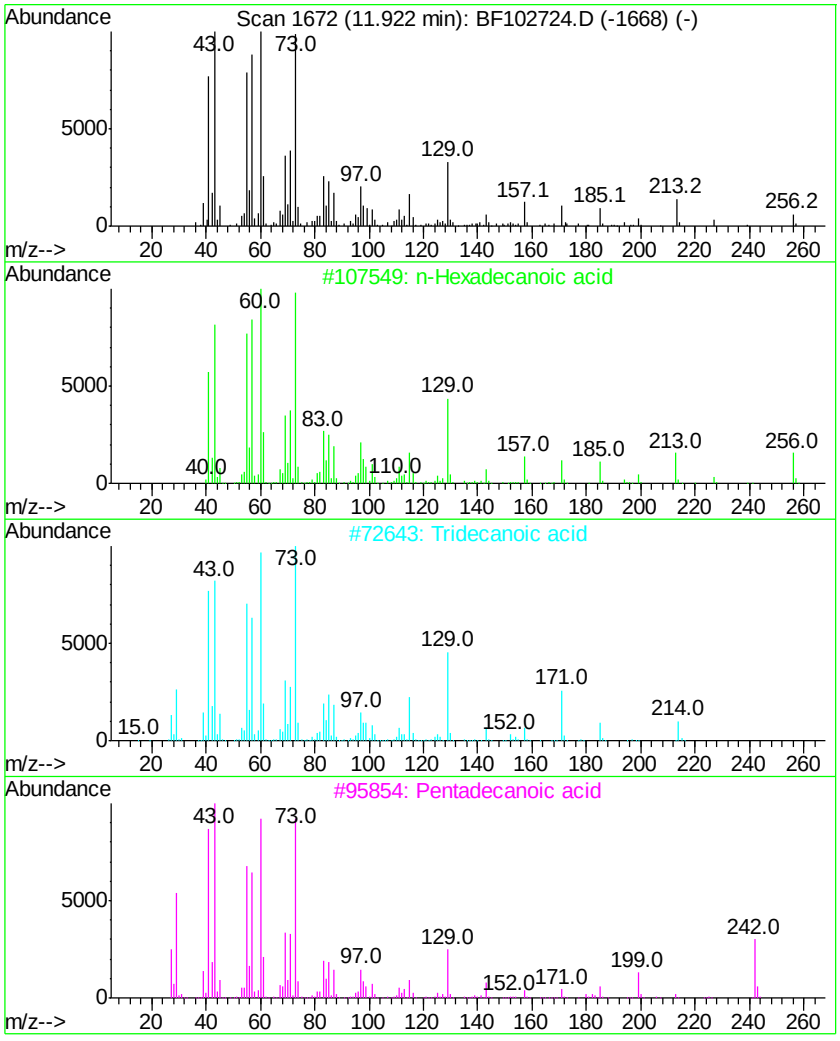
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

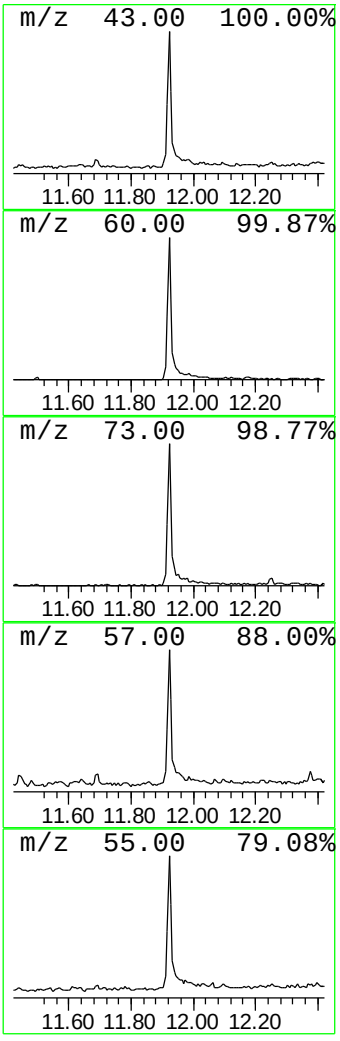
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	8.91 ng	513250	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





Library Search Compound Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF020318\
Data File : BF102724.D
Acq On : 3 Feb 2018 18:30
Operator : SJ/JU
Sample : J1436-13
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

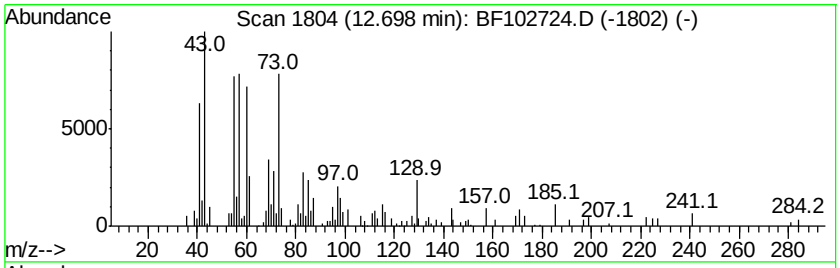
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

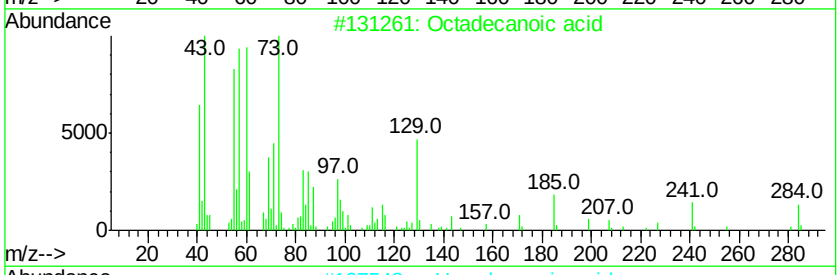
****

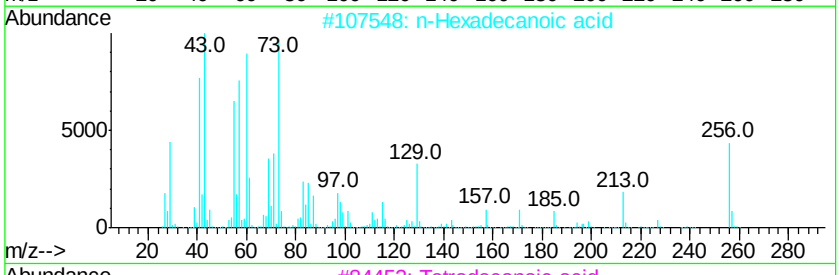
Peak Number 8 Octadecanoic acid Concentration Rank 5

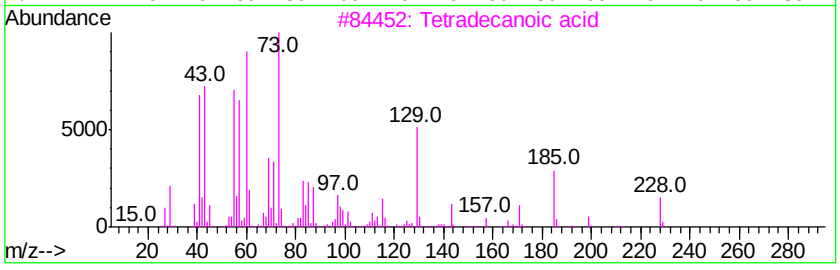
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	6.50 ng	374418	Phenanthrene-d10	11.40

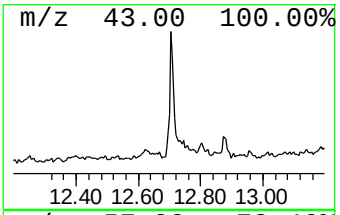
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	90
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Dodecanoic acid	200	C12H24O2	000143-07-7	62
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60

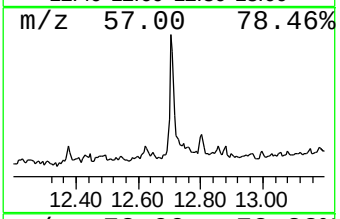


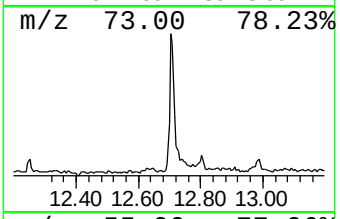


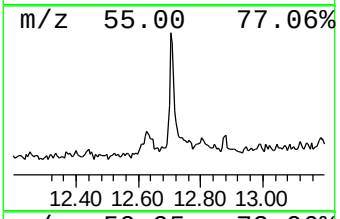


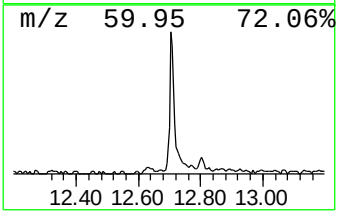












Data Path : U:\HPCHEM1\BNA F\DATA\BF020318\
Data File : BF102724.D
Acq On : 3 Feb 2018 18:30
Operator : SJ/JU
Sample : J1436-13
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

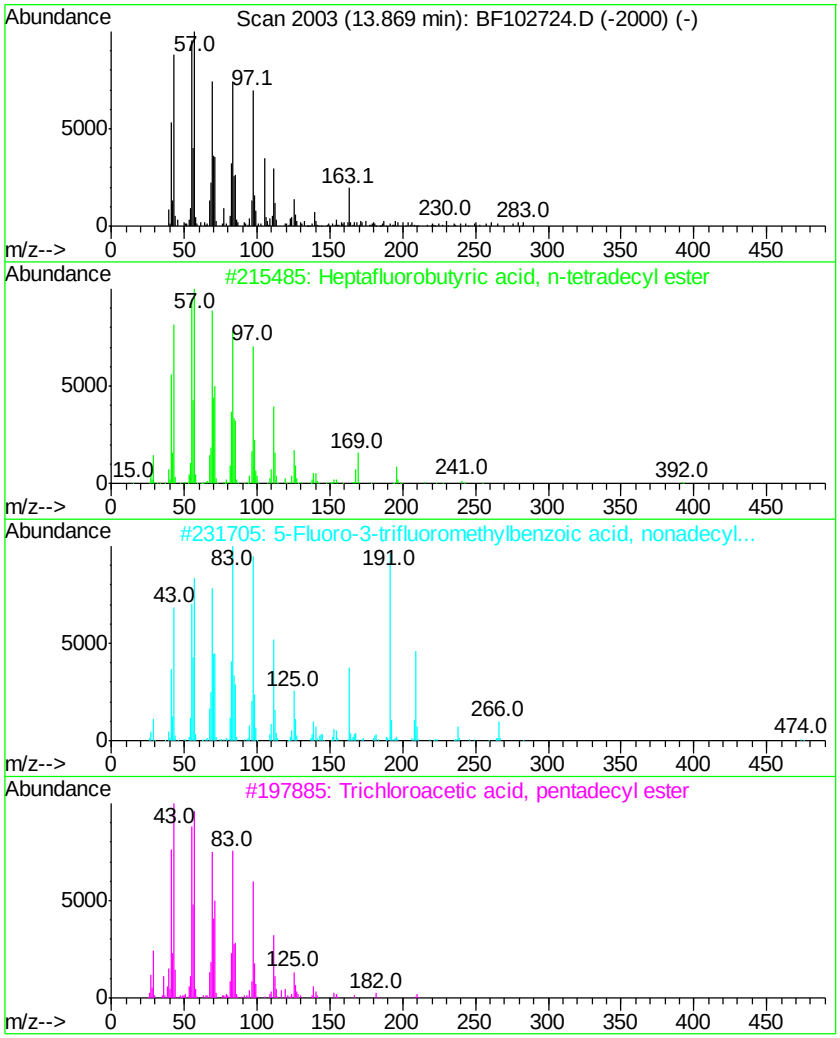
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

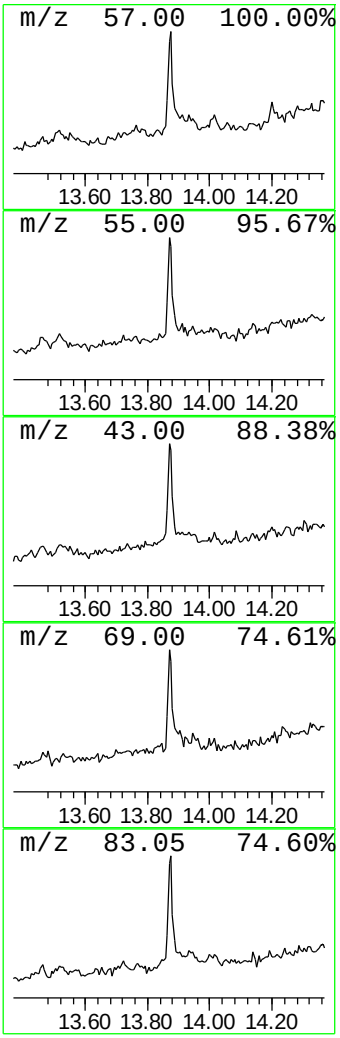
****

Peak Number 9 Heptafluorobutyric acid, n-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	5.74 ng	261308	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	93
2	5-Fluoro-3-trifluoromethylbenzoi...	474	C27H42F4O2	1000338-91-1	91
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
4	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	90
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90





Tentatively Identified Compound (LSC) summary

Data Path : U:\HPCHEM1\BNA_F\DATA\BF020318\
Data File : BF102724.D
Acq On : 3 Feb 2018 18:30
Operator : SJ/JU
Sample : J1436-13
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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...	2.16	9.5	ng	526938	1	6.88	1109690	20.0
unknown5.12	5.12	2.6	ng	144940	1	6.88	1109690	20.0
unknown6.65	6.65	81.6	ng	4526080	1	6.88	1109690	20.0
Ethanol, 2-(2-eth...	6.70	2.4	ng	134875	1	6.88	1109690	20.0
Benzophenone	10.63	2.8	ng	207853	3	9.92	1461560	20.0
n-Hexadecanoic acid	11.92	8.9	ng	513250	4	11.40	1151710	20.0
Octadecanoic acid	12.70	6.5	ng	374418	4	11.40	1151710	20.0
Heptafluorobutyri...	13.87	5.7	ng	261308	5	14.04	911093	20.0