LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030218\
Data File : BF103364.D
Acq On : 2 Mar 2018 14:10
Operator : SJ/JU
Sample : J1402-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-01-022818-D

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-BF022218.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	21	rVB	281269	391904	9.80%	1.100%
2	5.116	512	515	528	rBV	94953	140504	3.51%	0.394%
3	5.504	577	581	598	rBV	3736233	3977427	99.48%	11.161%
4	6.516	748	753	764	rBV	3234450	3998086	100.00%	11.219%
5	6.651	771	776	779	rBV	3535829	3701869	92.59%	10.388%
6	6.875	810	814	820	rBV	1275614	1072598	26.83%	3.010%
7	7.034	836	841	844	rBV	2744812	2756701	68.95%	7.736%
8	7.440	906	910	921	rBV	2140784	2369024	59.25%	6.648%
9	8.157	1028	1032	1053	rVB	1366578	1331961	33.31%	3.738%
10	9.234	1210	1215	1224	rBV	2801164	2849455	71.27%	7.996%
11	9.298	1224	1226	1229	rVB	85074	71270	1.78%	0.200%
12	9.563	1267	1271	1276	rVV4	37624	48922	1.22%	0.137%
13	9.622	1276	1281	1289	rBV	213415	276482	6.92%	0.776%
14	9.828	1312	1316	1320	rBV	199855	167585	4.19%	0.470%
15	9.916	1327	1331	1338	rVB	1397314	1292061	32.32%	3.626%
16	10.151	1368	1371	1375	rVB3	45251	43684	1.09%	0.123%
17	10.328	1398	1401	1404	rVB	239117	190643	4.77%	0.535%
18	10.551	1434	1439	1441	rBV	68256	78760	1.97%	0.221%
19	10.710	1462	1466	1474	rBV	1570299	1659282	41.50%	4.656%
20	10.804	1479	1482	1492	rVB	194452	234522	5.87%	0.658%
21	11.251	1555	1558	1561	rBV	105170	88119	2.20%	0.247%
22	11.410	1581	1585	1587	rBV	1125795	1046597	26.18%	2.937%
23	11.433	1587	1589	1593	rVB	208914	210423	5.26%	0.590%
24	11.922	1668	1672	1674	rBV2	210195	204885	5.12%	0.575%
25	12.022	1686	1689	1697	rVB3	46035	71267	1.78%	0.200%
26	12.092	1697	1701	1707	rVB2	55967	68818	1.72%	0.193%
27	12.469	1761	1765	1767	rBV3	133417	144570	3.62%	0.406%
28	12.492	1767	1769	1772	rVB3	72626	64130	1.60%	0.180%
29	12.574	1781	1783	1788	rVB4	39890	48292	1.21%	0.136%
30	12.627	1788	1792	1795	rBV	361426	344833	8.62%	0.968%
31	12.657	1795	1797	1800	rVV	78096	66148	1.65%	0.186%
32	12.710	1803	1806	1811	rVB4	39369	50216	1.26%	0.141%
33	12.857	1825	1831	1837	rVB	328824	368375	9.21%	1.034%
34	12.992	1850	1854	1857	rBV	1800987	1632655	40.84%	4.581%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030218\
Data File : BF103364.D
Acq On : 2 Mar 2018 14:10
Operator : SJ/JU
Sample : J1402-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-01-022818-D

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-BF022218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.186	1884	1887	1889	rBV3	42771	40712	1.02%	0.114%
36	13.421	1923	1927	1930	rBV2	58685	70360	1.76%	0.197%
37	13.545	1945	1948	1951	rBV2	44308	48909	1.22%	0.137%
38	13.874	2000	2004	2009	rBV2	539442	625220	15.64%	1.754%
39	14.063	2031	2036	2038	rBV2	789232	924404	23.12%	2.594%
40	14.086	2038	2040	2047	rVB	178449	169924	4.25%	0.477%
41	14.198	2056	2059	2061	rBV	70137	64700	1.62%	0.182%
42	14.510	2109	2112	2118	rBV2	128841	207869	5.20%	0.583%
43	14.816	2162	2164	2167	rVB	78069	70457	1.76%	0.198%
44	14.968	2187	2190	2194	rBV2	122015	125277	3.13%	0.352%
45	15.127	2213	2217	2219	rBV	153810	203179	5.08%	0.570%
46	15.157	2219	2222	2226	rVV2	325180	422904	10.58%	1.187%
47	15.192	2226	2228	2234	rVB3	128356	147429	3.69%	0.414%
48	15.439	2267	2270	2275	rVB	100392	117777	2.95%	0.330%
49	15.504	2278	2281	2285	rVB	105284	125772	3.15%	0.353%
50	15.568	2285	2292	2296	rBV	486802	732611	18.32%	2.056%
51	15.992	2359	2364	2369	rVB	307296	476803	11.93%	1.338%

Sum of corrected areas: 35636375

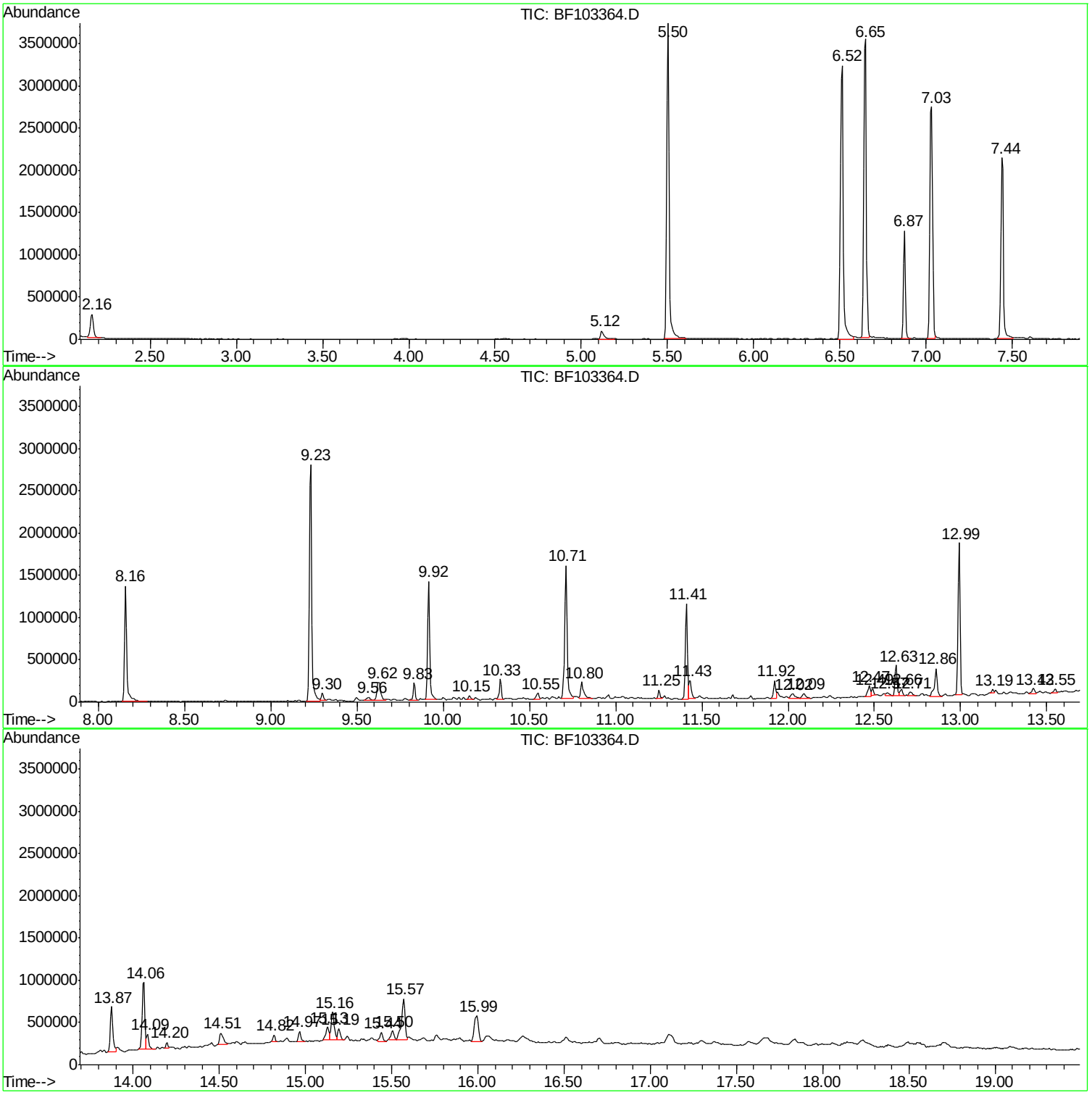
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030218\
Data File : BF103364.D
Acq On : 2 Mar 2018 14:10
Operator : SJ/JU
Sample : J1402-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-01-022818-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030218\
Data File : BF103364.D
Acq On : 2 Mar 2018 14:10
Operator : SJ/JU
Sample : J1402-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-01-022818-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

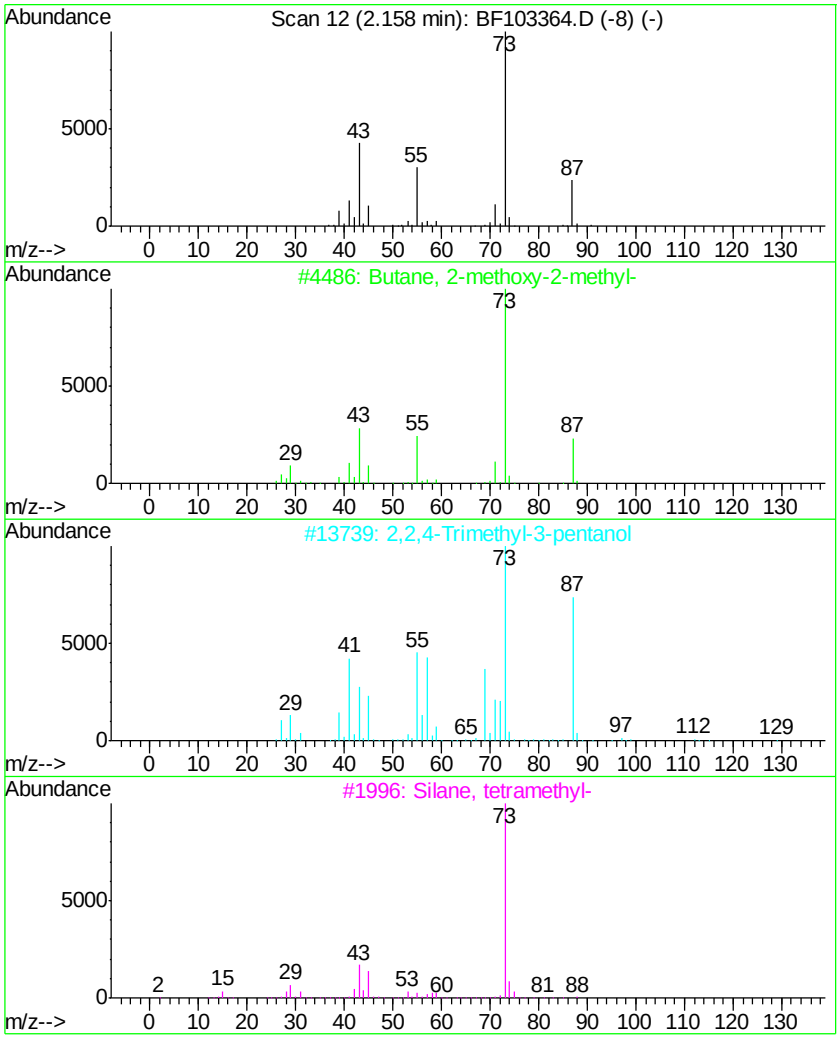
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

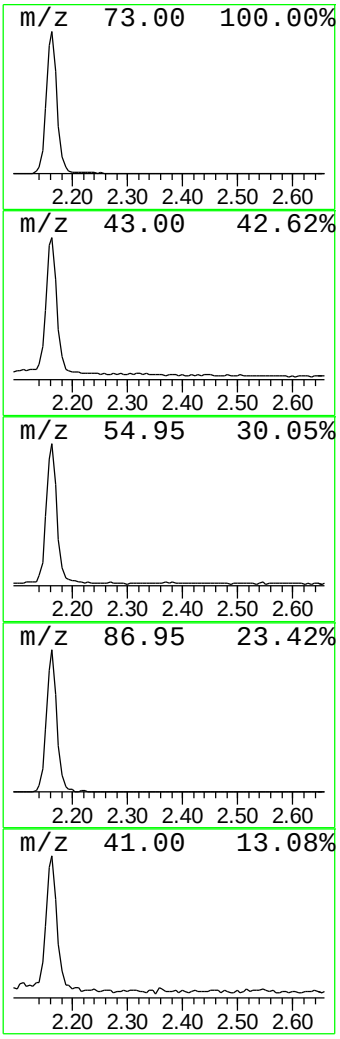
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	7.31 ng	391904	1,4-Dichlorobenzene-d4	6.87

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, tetramethyl-	88	C4H12Si	000075-76-3	35
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030218\
Data File : BF103364.D
Acq On : 2 Mar 2018 14:10
Operator : SJ/JU
Sample : J1402-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-01-022818-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

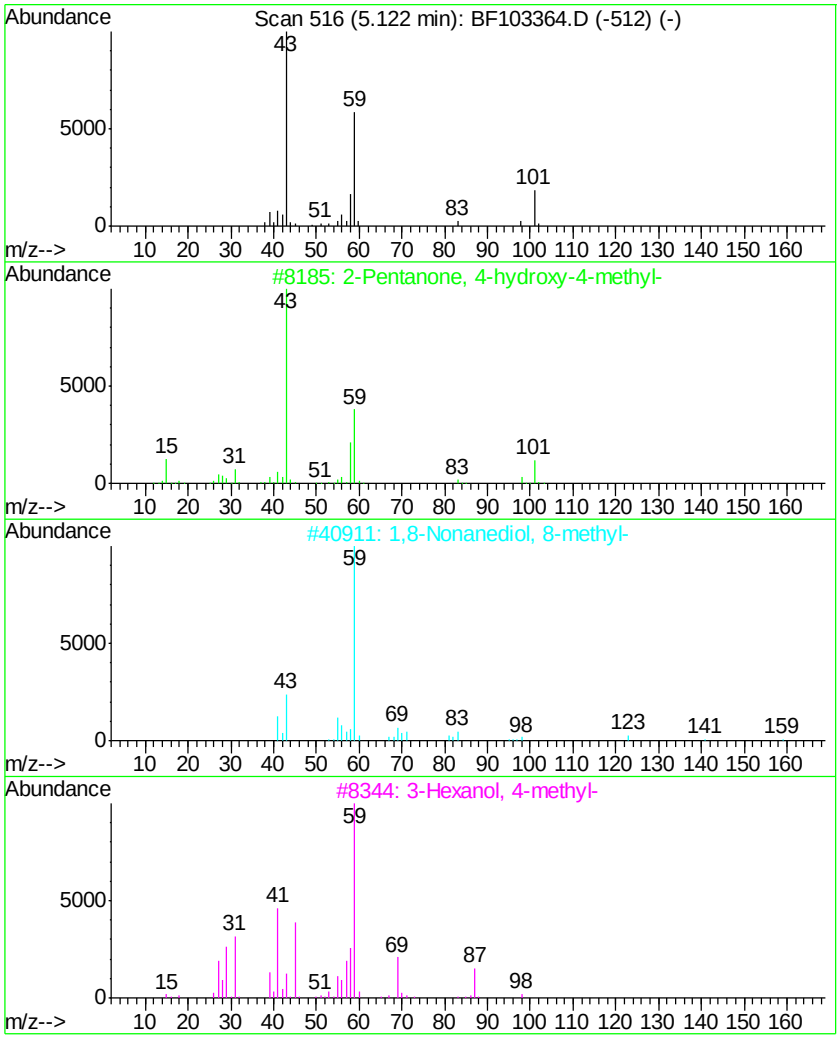
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

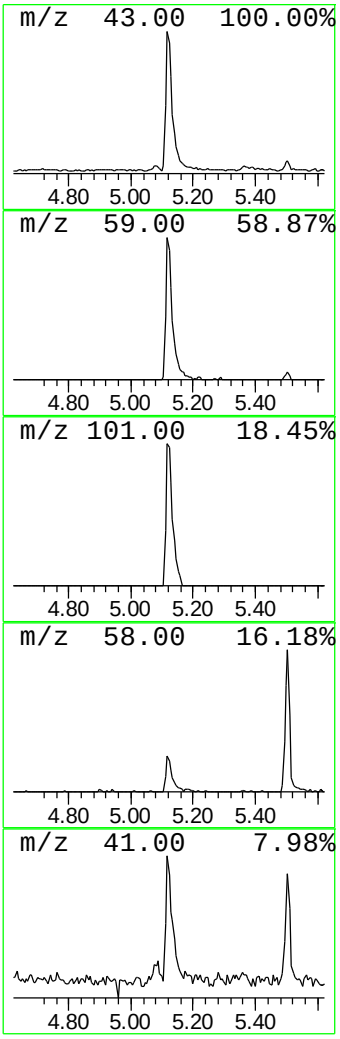
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	2.62 ng	140504	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	38
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030218\
Data File : BF103364.D
Acq On : 2 Mar 2018 14:10
Operator : SJ/JU
Sample : J1402-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-01-022818-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

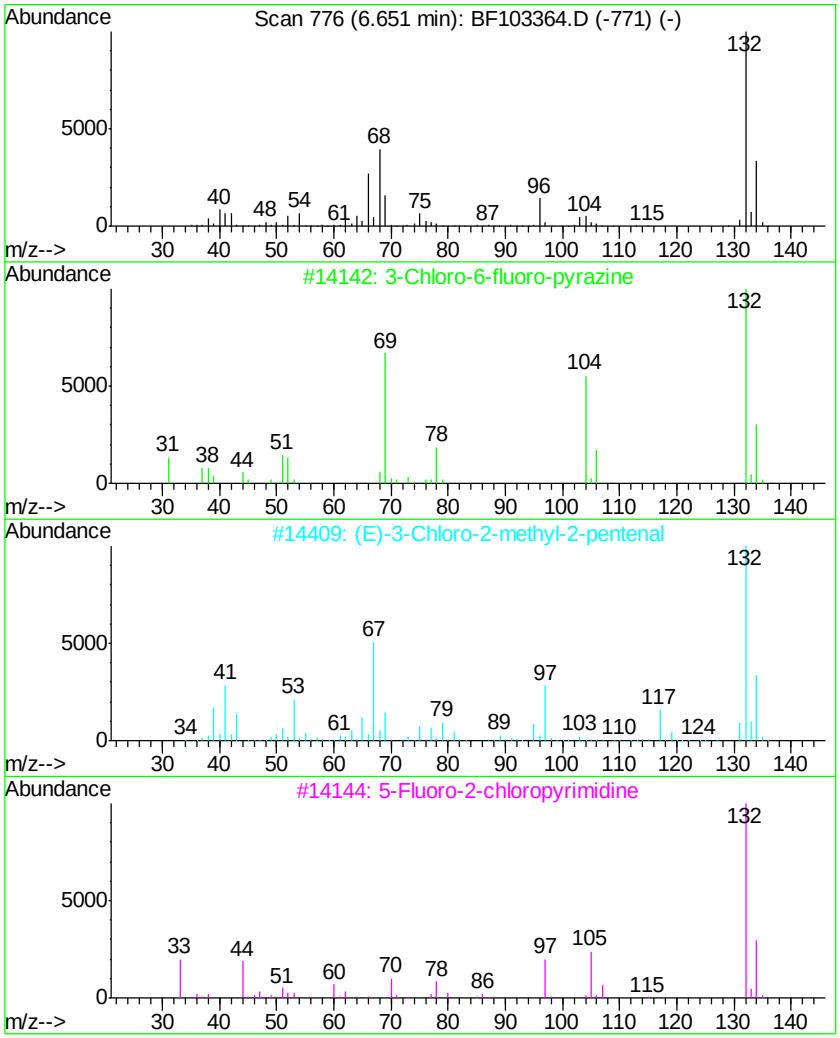
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

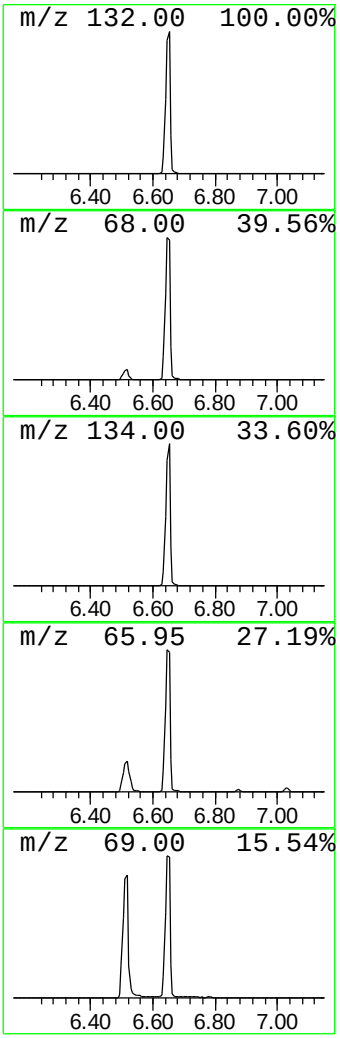
****

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	69.03 ng	3701870	1,4-Dichlorobenzene-d4	6.87

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-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030218\
Data File : BF103364.D
Acq On : 2 Mar 2018 14:10
Operator : SJ/JU
Sample : J1402-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-01-022818-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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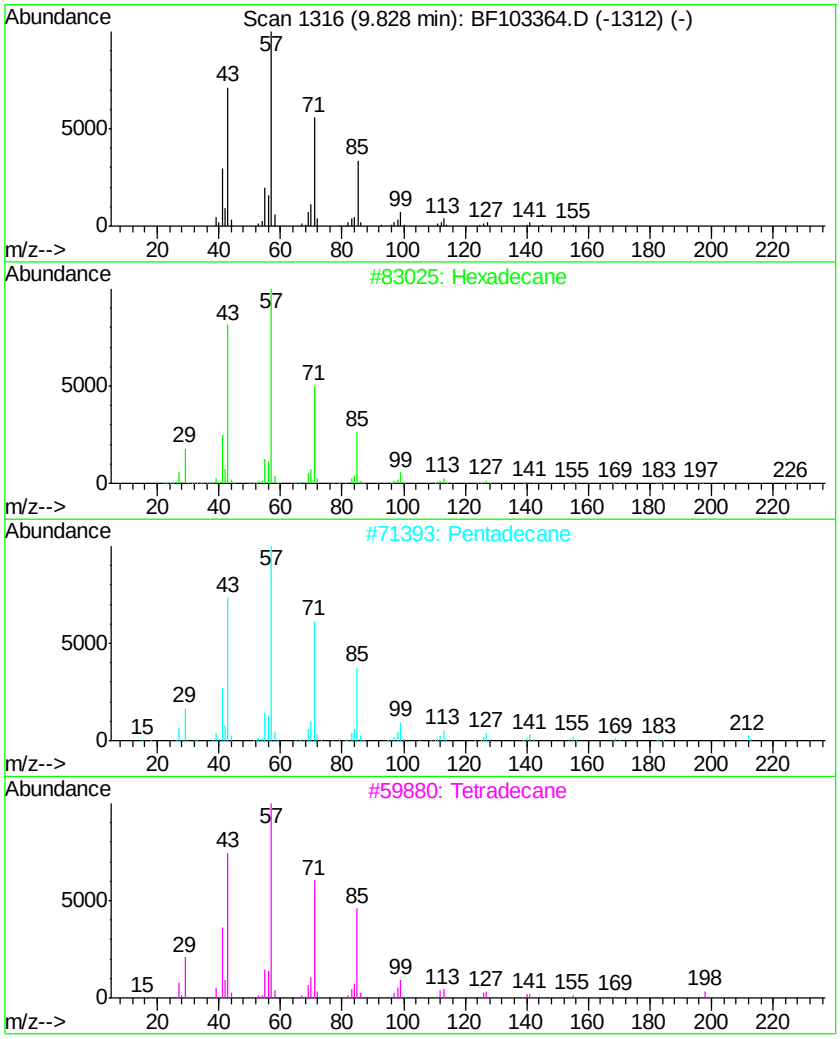
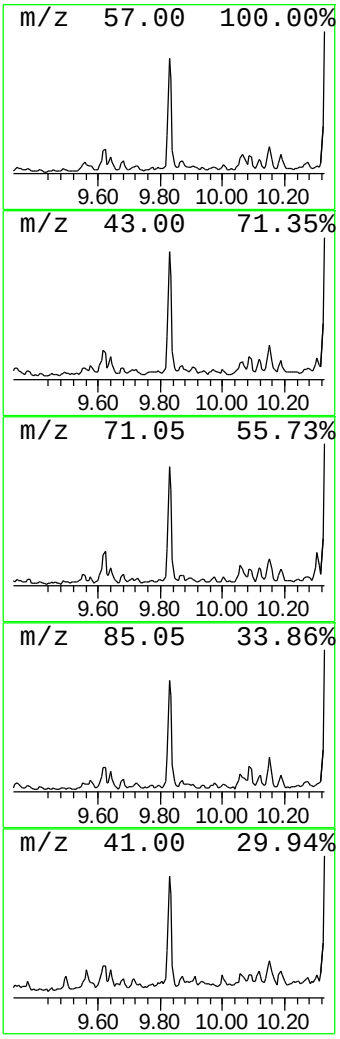
Peak Number 5 Hexadecane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.83	2.59 ng	167585	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Pentadecane	212	C15H32	000629-62-9	90
3	Tetradecane	198	C14H30	000629-59-4	90
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	86
5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	64





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030218\
Data File : BF103364.D
Acq On : 2 Mar 2018 14:10
Operator : SJ/JU
Sample : J1402-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-01-022818-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

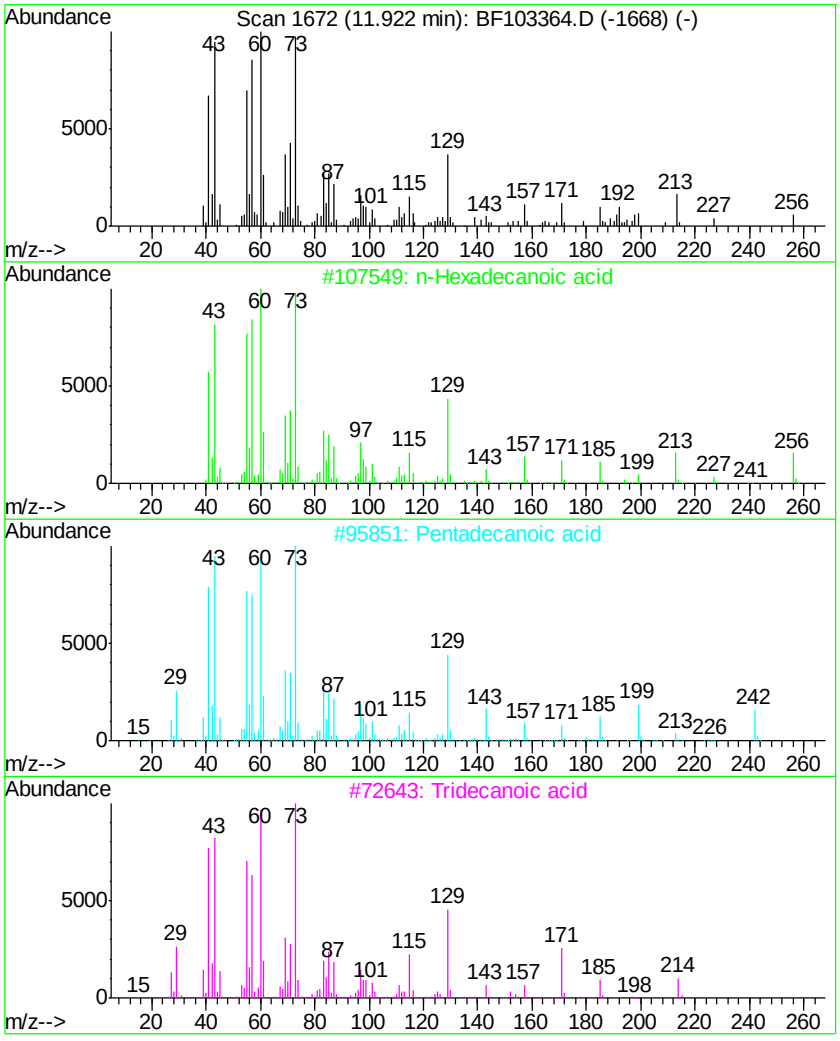
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

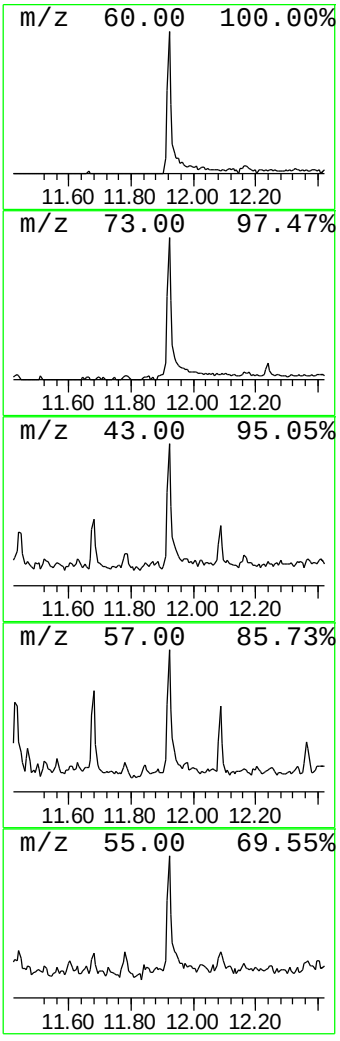
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	3.92 ng	204885	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030218\
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-01-022818-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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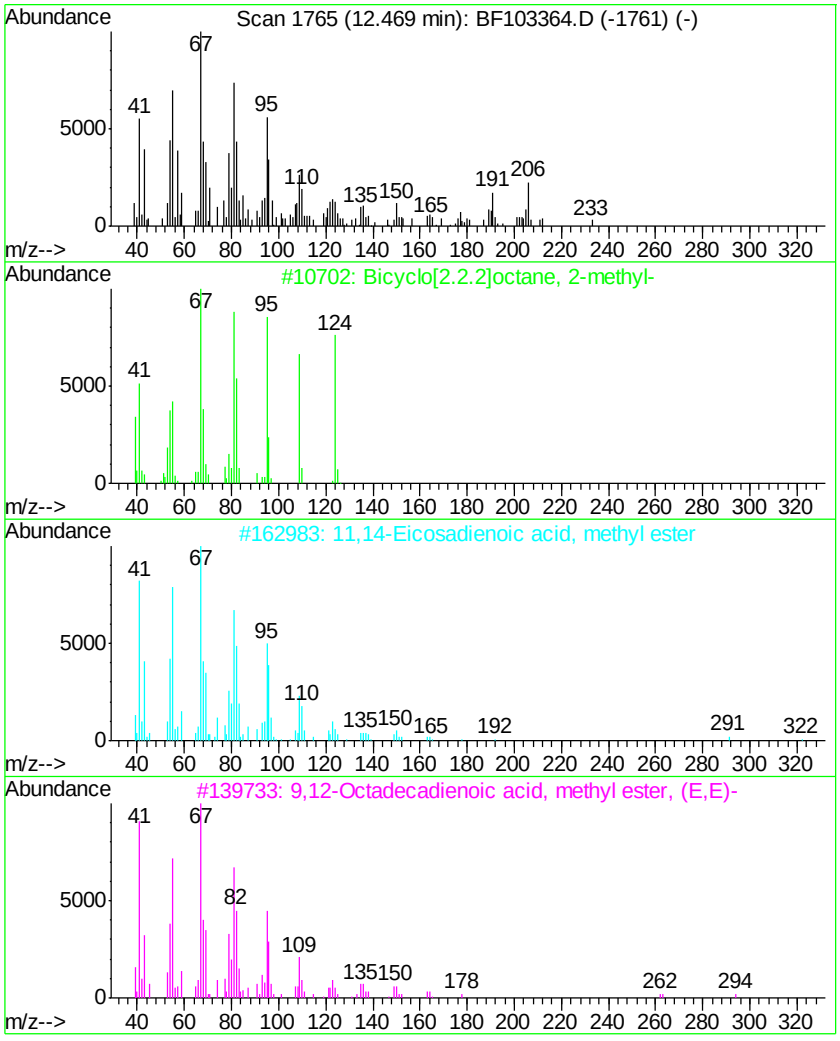
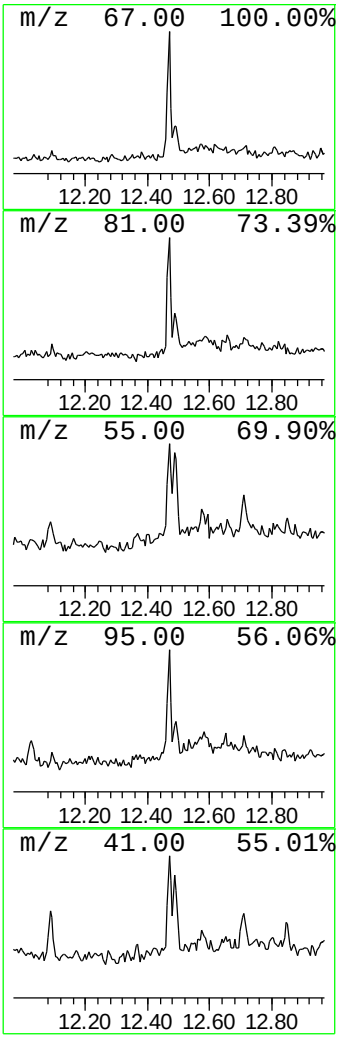
Peak Number 9 Bicyclo[2.2.2]octane, 2-met... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.47	2.76 ng	144570	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.2]octane, 2-methyl-	124	C9H16	000766-53-0	87
2	11,14-Eicosadienoic acid, methyl...	322	C21H38O2	002463-02-7	76
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	76
4	9-Octadecyne	250	C18H34	035365-59-4	72
5	7-Tetradecyne	194	C14H26	035216-11-6	72





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Misc :
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Instrument : BNA_F
ClientSampleId : PL-01-022818-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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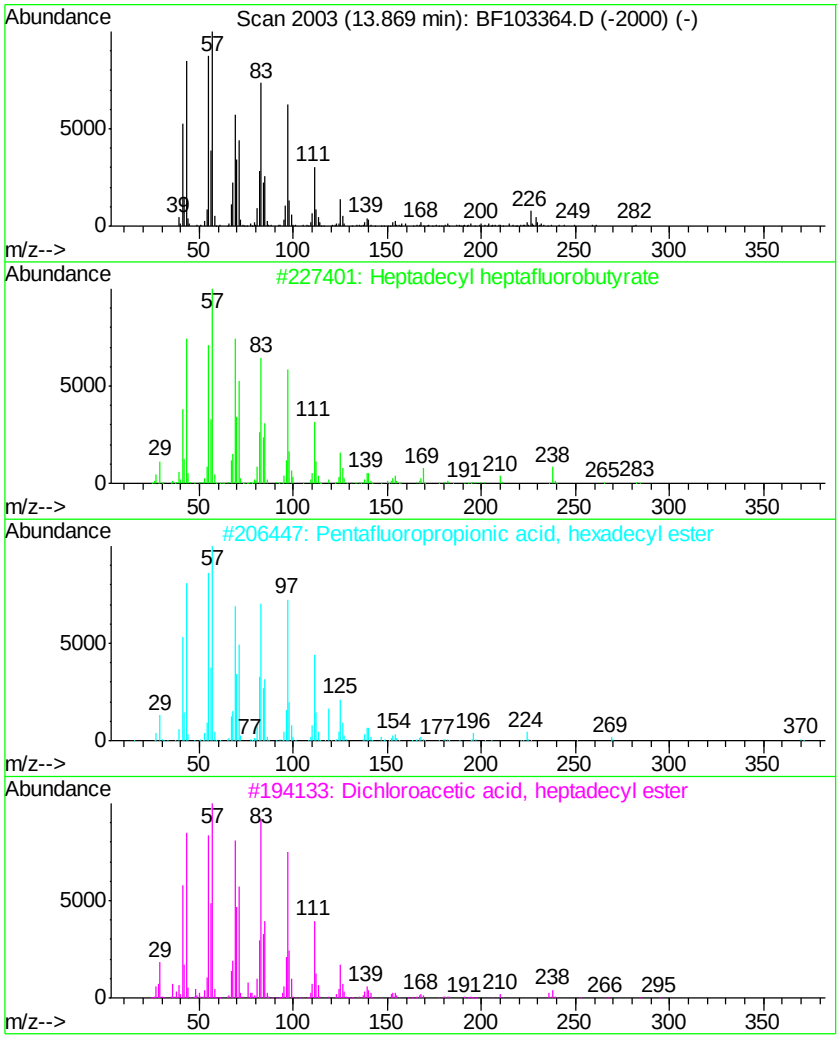
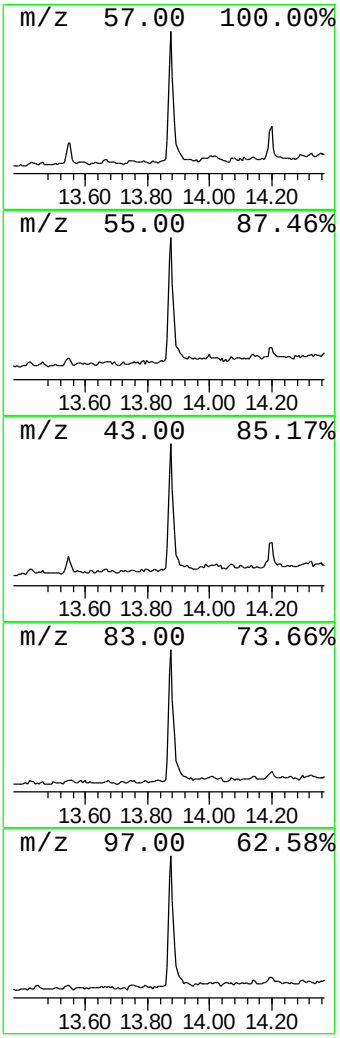
Peak Number 10 Heptadecyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	13.53 ng	625220	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030218\
Data File : BF103364.D
Acq On : 2 Mar 2018 14:10
Operator : SJ/JU
Sample : J1402-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-01-022818-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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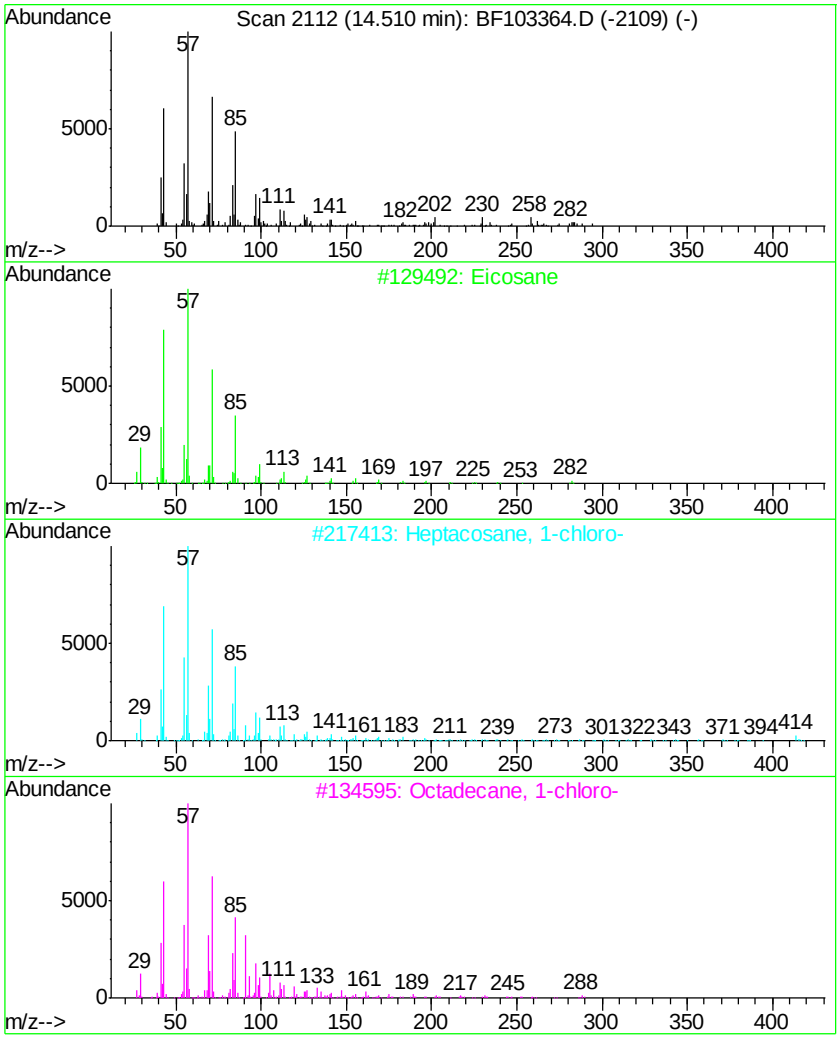
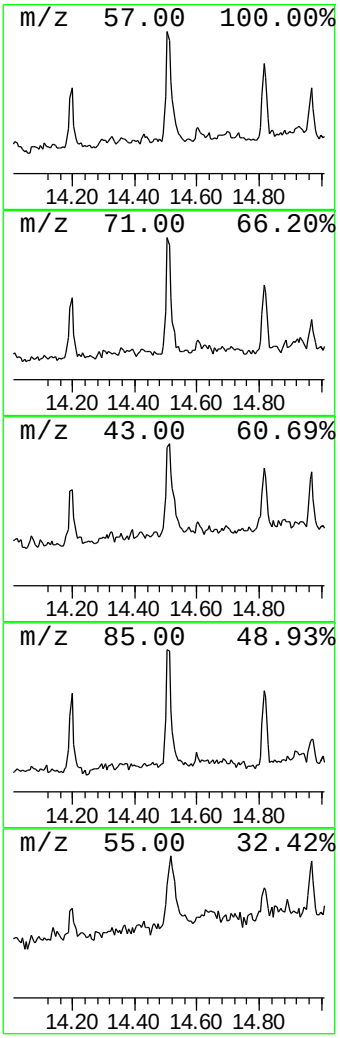
Peak Number 11 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.51	4.50 ng	207869	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	89
2	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	87
3	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	87
4	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	87
5	Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	86





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Data File : BF103364.D
Acq On : 2 Mar 2018 14:10
Operator : SJ/JU
Sample : J1402-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-01-022818-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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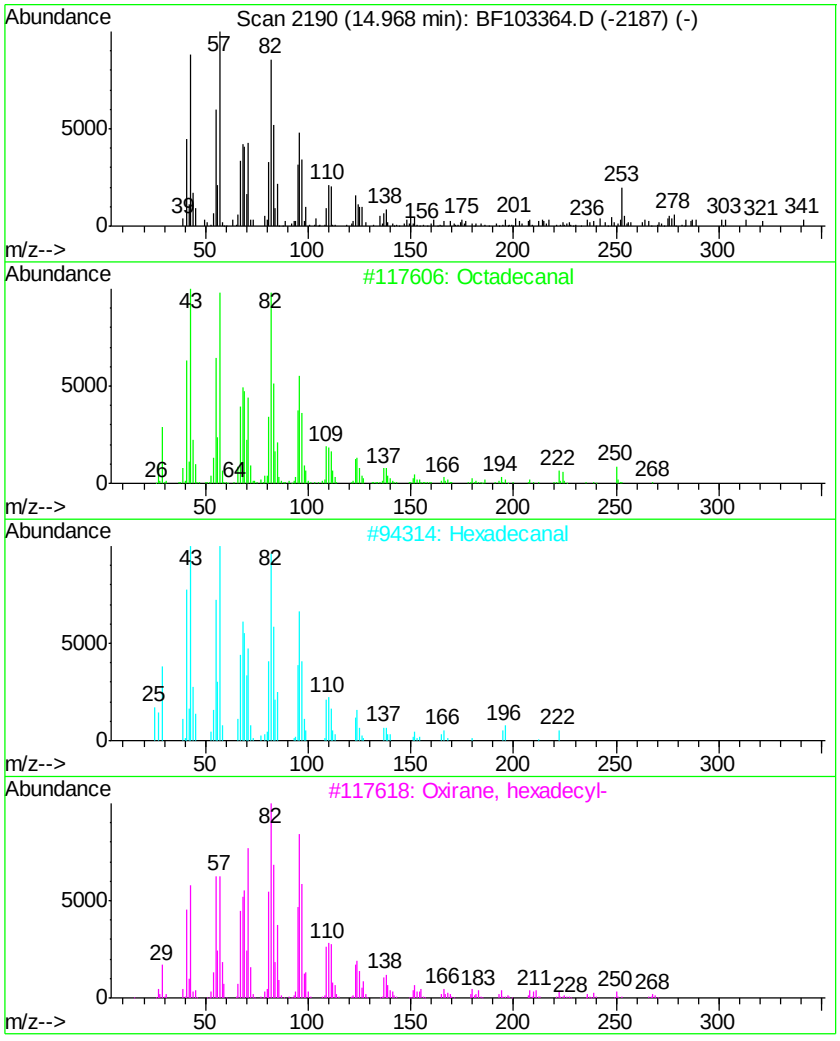
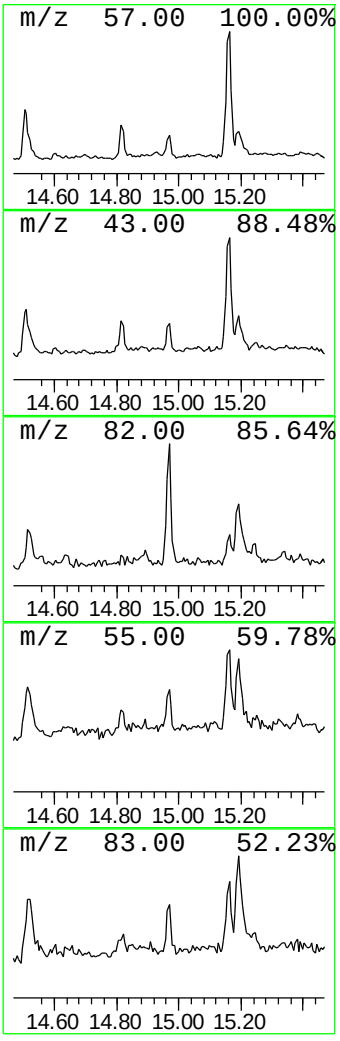
Peak Number 12 Octadecanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	3.42 ng	125277	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	87
2	Hexadecanal	240	C16H32O	000629-80-1	86
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	81
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	78
5	1,19-Eicosadiene	278	C20H38	014811-95-1	70





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030218\
Data File : BF103364.D
Acq On : 2 Mar 2018 14:10
Operator : SJ/JU
Sample : J1402-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-01-022818-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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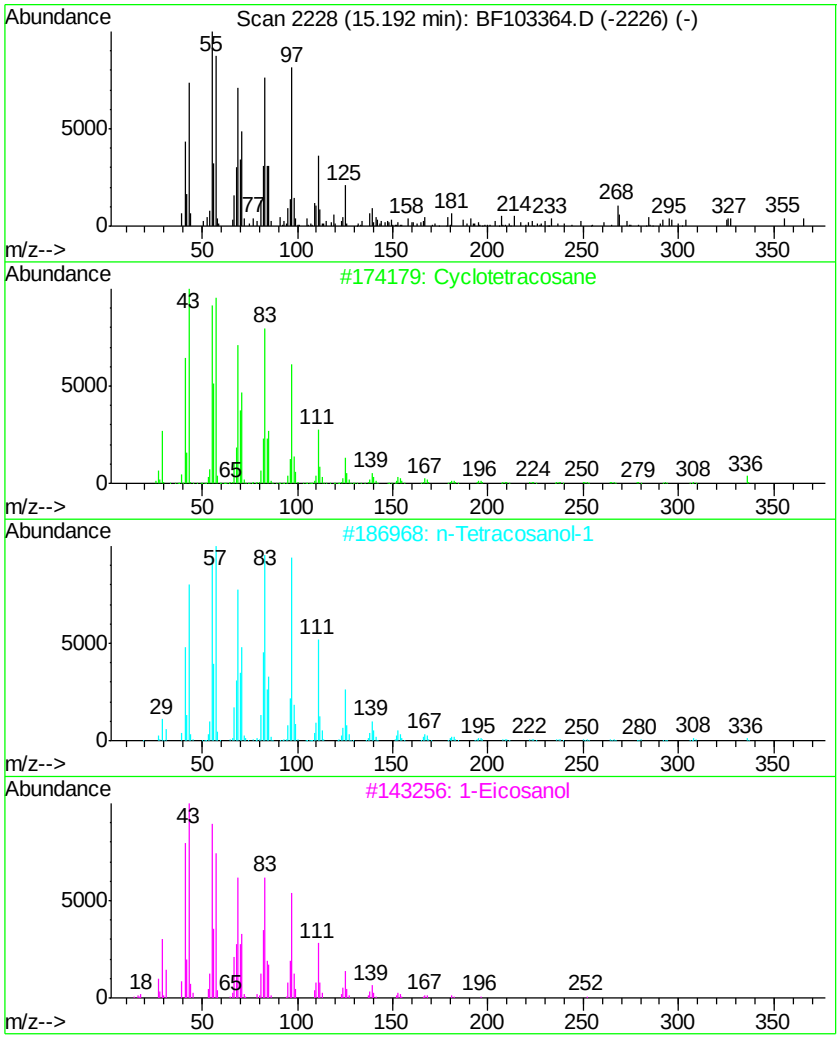
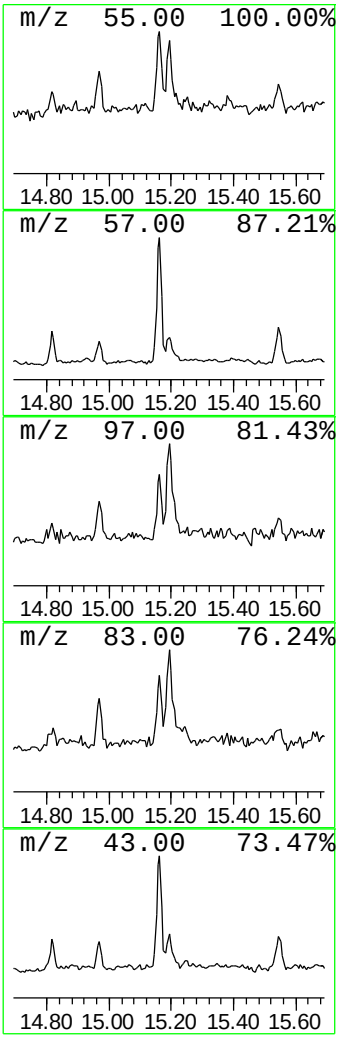
Peak Number 13 Cyclotetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.19	4.02 ng	147429	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	90
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
3	1-Eicosanol	298	C20H42O	000629-96-9	87
4	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	87
5	Octacosyl acetate	452	C30H60O2	018206-97-8	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030218\
Data File : BF103364.D
Acq On : 2 Mar 2018 14:10
Operator : SJ/JU
Sample : J1402-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-01-022818-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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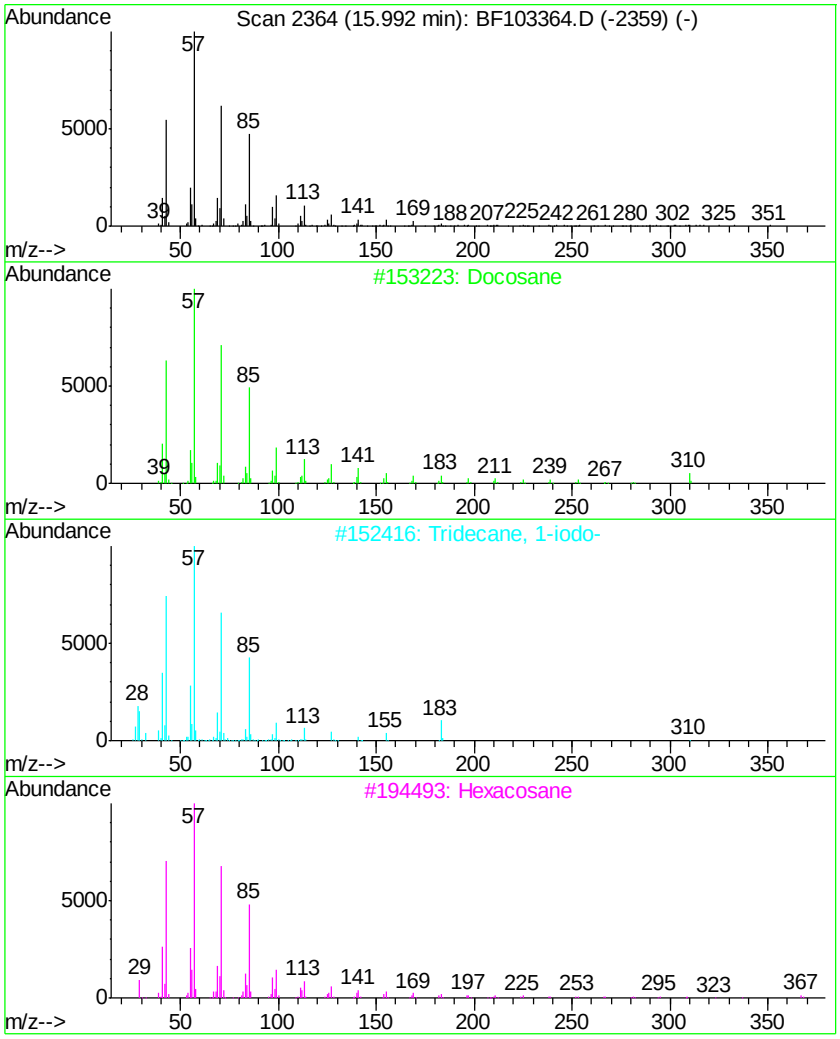
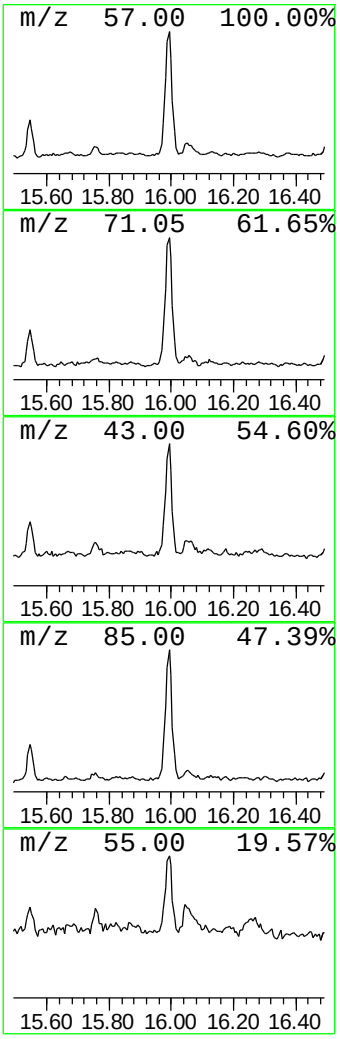
Peak Number 15 Docosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.99	13.02 ng	476803	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	93
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	93
3	Hexacosane	366	C26H54	000630-01-3	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030218\
Data File : BF103364.D
Acq On : 2 Mar 2018 14:10
Operator : SJ/JU
Sample : J1402-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-01-022818-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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	7.3	ng	391904	1	6.87	1072600	20.0
2-Pentanone, 4-hy...	5.12	2.6	ng	140504	1	6.87	1072600	20.0
unknown6.65	6.65	69.0	ng	3701870	1	6.87	1072600	20.0
Hexadecane	9.83	2.6	ng	167585	3	9.92	1292060	20.0
n-Hexadecanoic acid	11.92	3.9	ng	204885	4	11.41	1046600	20.0
Bicyclo[2.2.2]oct...	12.47	2.8	ng	144570	4	11.41	1046600	20.0
Heptadecyl heptaf...	13.87	13.5	ng	625220	5	14.06	924404	20.0
Eicosane	14.51	4.5	ng	207869	5	14.06	924404	20.0
Octadecanal	14.97	3.4	ng	125277	6	15.57	732611	20.0
Cyclotetracosane	15.19	4.0	ng	147429	6	15.57	732611	20.0
Docosane	15.99	13.0	ng	476803	6	15.57	732611	20.0