LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122917\
Data File : BF101826.D
Acq On : 29 Dec 2017 13:54
Operator : SJ/JU
Sample : I7040-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

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-BF121417.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	4.993	491	494	516	rBV	105363	202701	7.44%	0.774%
2	5.410	562	565	592	rBV	651029	1253756	46.03%	4.788%
3	6.440	737	740	757	rBV2	467340	1027174	37.71%	3.923%
4	6.557	757	760	776	rVB	1995878	2253642	82.73%	8.607%
5	6.781	795	798	806	rBV	1041246	994119	36.50%	3.797%
6	6.939	821	825	843	rBV	1833904	2021285	74.20%	7.720%
7	7.357	892	896	911	rBV	1397222	1726481	63.38%	6.594%
8	7.510	919	922	925	rVB	42549	36659	1.35%	0.140%
9	8.063	1013	1016	1031	rBV	1229076	1295814	47.57%	4.949%
10	8.510	1088	1092	1104	rVB	119879	219982	8.08%	0.840%
11	8.816	1138	1144	1148	rBV8	13690	28193	1.04%	0.108%
12	9.004	1173	1176	1181	rVB7	20320	33375	1.23%	0.127%
13	9.139	1195	1199	1207	rVB	2922005	2723946	100.00%	10.403%
14	9.245	1213	1217	1219	rBV4	28108	34588	1.27%	0.132%
15	9.539	1263	1267	1272	rVB	89866	100094	3.67%	0.382%
16	9.733	1296	1300	1303	rBV	43504	38702	1.42%	0.148%
17	9.822	1311	1315	1319	rBV	1317994	1229426	45.13%	4.695%
18	9.969	1336	1340	1342	rBV2	32932	42004	1.54%	0.160%
19	10.033	1347	1351	1359	rBV	89612	124685	4.58%	0.476%
20	10.233	1382	1385	1388	rVB	69787	57163	2.10%	0.218%
21	10.445	1417	1421	1424	rBV3	23706	36921	1.36%	0.141%
22	10.616	1447	1450	1458	rBV	1296457	1394017	51.18%	5.324%
23	10.704	1462	1465	1470	rVB	67556	72239	2.65%	0.276%
24	10.969	1507	1510	1518	rBV2	116497	153038	5.62%	0.584%
25	11.151	1539	1541	1543	rBV	44127	29995	1.10%	0.115%
26	11.316	1565	1569	1576	rVB	1017625	1053105	38.66%	4.022%
27	11.522	1601	1604	1610	rVV2	119024	115340	4.23%	0.441%
28	11.575	1611	1613	1620	rVB4	25764	33239	1.22%	0.127%
29	11.680	1628	1631	1634	rBV2	61020	48078	1.77%	0.184%
30	11.839	1653	1658	1670	rBV	1253695	1558386	57.21%	5.952%
31	12.227	1721	1724	1728	rBV5	27640	33459	1.23%	0.128%
32	12.339	1740	1743	1748	rBV	177935	188723	6.93%	0.721%
33	12.386	1749	1751	1754	rVB	102292	81512	2.99%	0.311%
34	12.516	1770	1773	1775	rBV2	57111	67685	2.48%	0.259%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122917\
Data File : BF101826.D
Acq On : 29 Dec 2017 13:54
Operator : SJ/JU
Sample : I7040-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

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-BF121417.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.621	1786	1791	1801	rBV	1405366	1712520	62.87%	6.540%
36	12.698	1801	1804	1806	rVB	58493	58081	2.13%	0.222%
37	12.786	1814	1819	1828	rVB2	94293	155550	5.71%	0.594%
38	12.892	1833	1837	1841	rBV	1898792	1756303	64.48%	6.708%
39	13.086	1868	1870	1875	rBV3	45491	52932	1.94%	0.202%
40	13.327	1909	1911	1914	rVB2	36159	28733	1.05%	0.110%
41	13.445	1928	1931	1934	rBV	43024	43703	1.60%	0.167%
42	13.774	1984	1987	1998	rBV	367007	389375	14.29%	1.487%
43	13.910	2008	2010	2016	rVB	48912	36792	1.35%	0.141%
44	13.968	2016	2020	2025	rBV	852214	828496	30.42%	3.164%
45	15.439	2266	2270	2277	rVB	636615	811445	29.79%	3.099%

Sum of corrected areas: 26183456

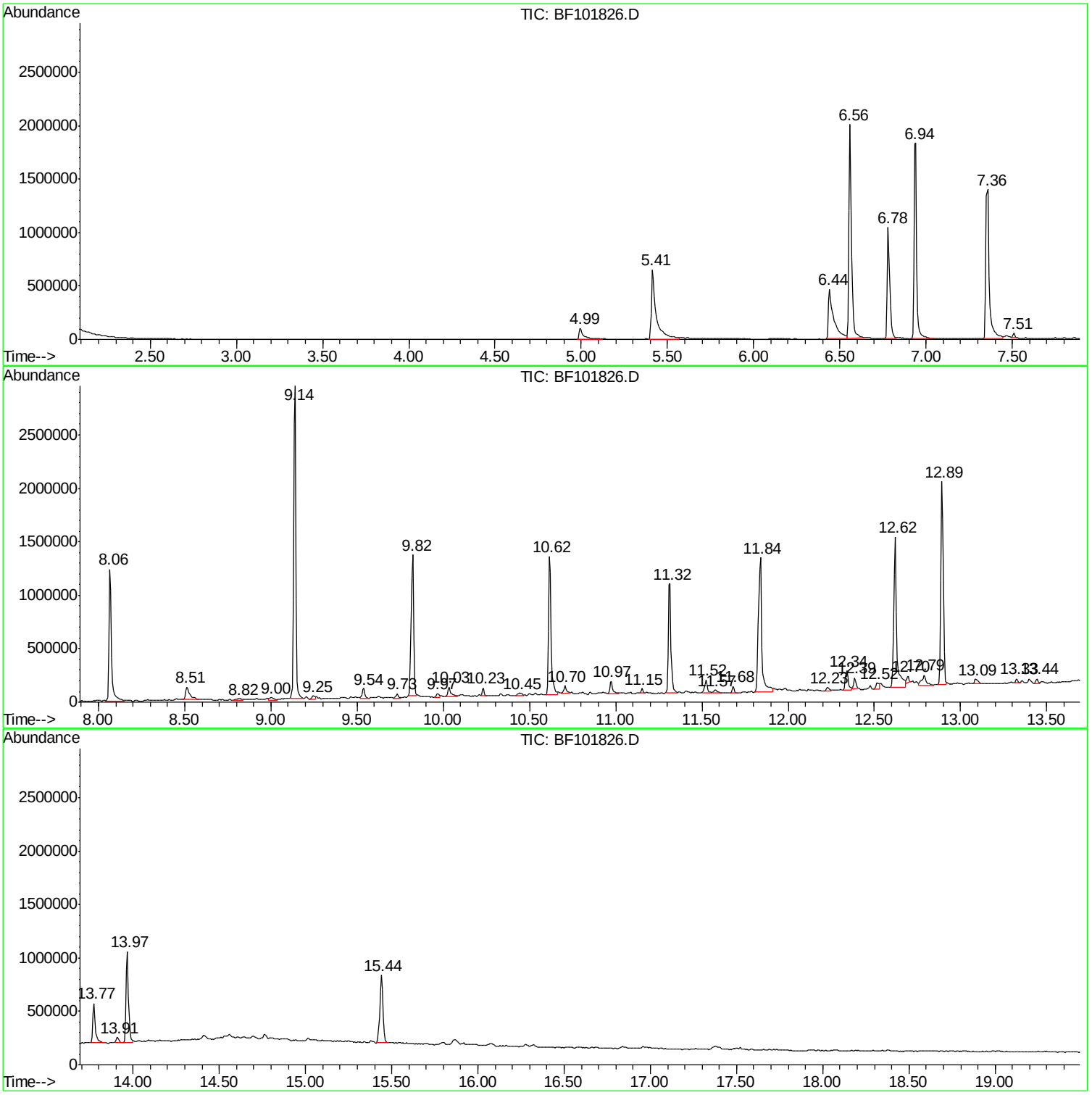
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122917\
Data File : BF101826.D
Acq On : 29 Dec 2017 13:54
Operator : SJ/JU
Sample : I7040-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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\BF122917\
Data File : BF101826.D
Acq On : 29 Dec 2017 13:54
Operator : SJ/JU
Sample : I7040-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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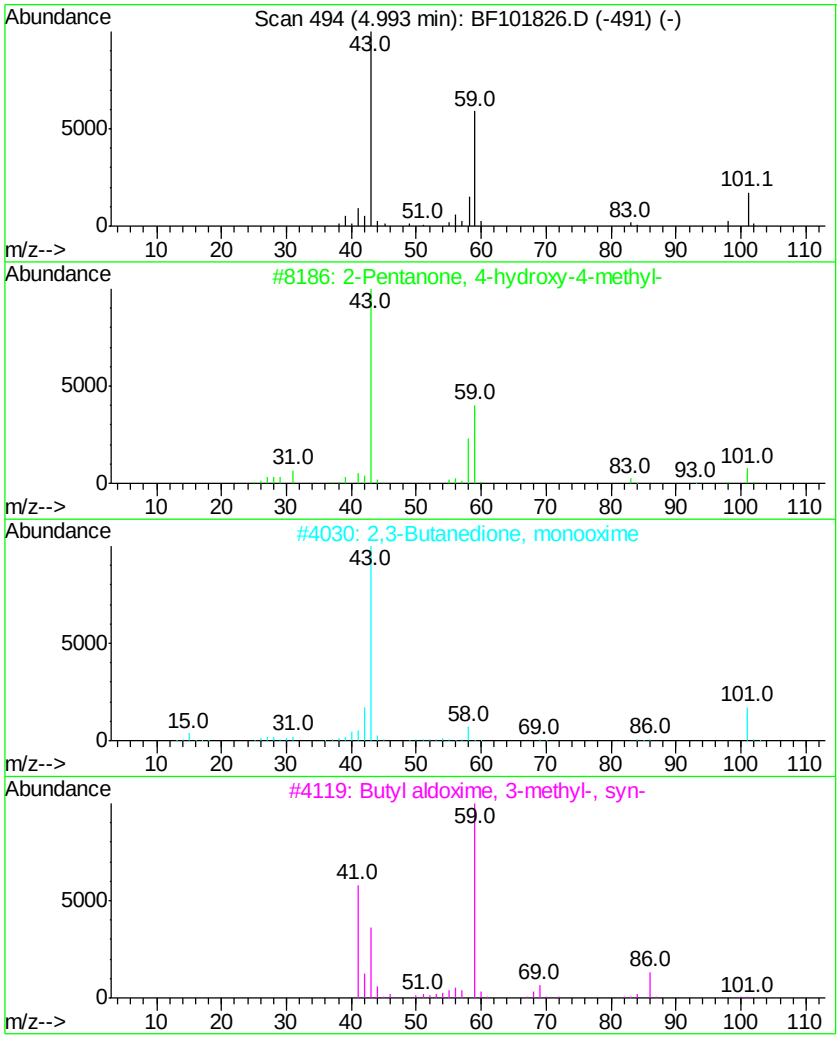
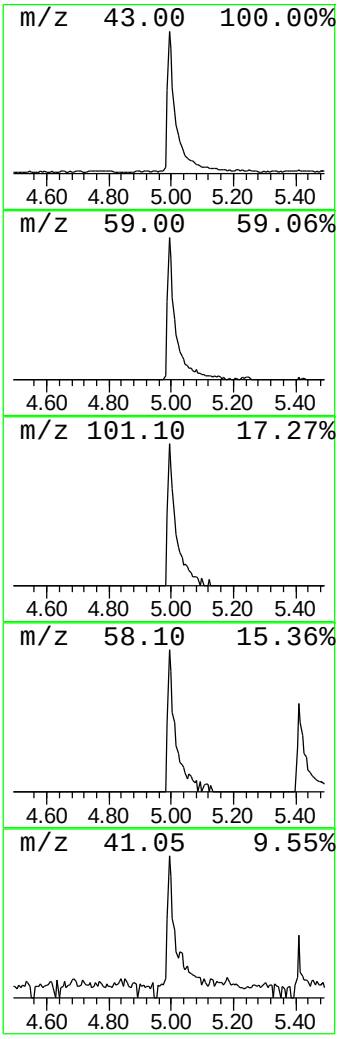
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	4.08 ng	202701	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122917\
Data File : BF101826.D
Acq On : 29 Dec 2017 13:54
Operator : SJ/JU
Sample : I7040-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

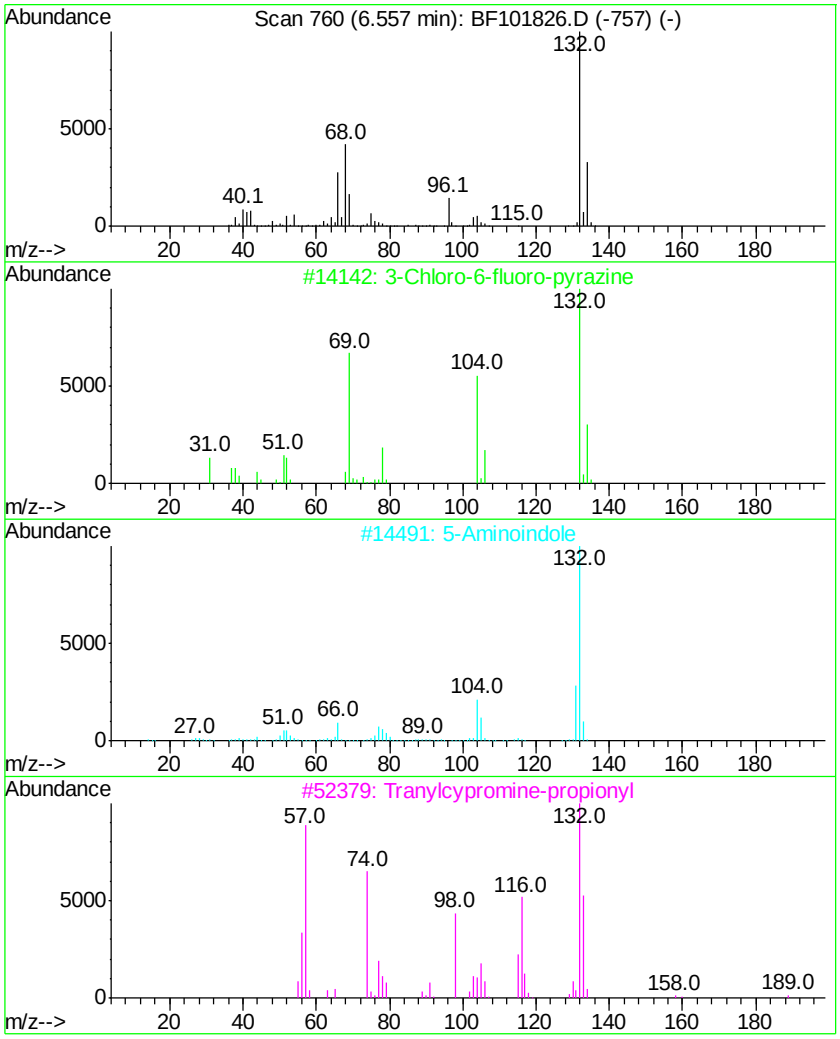
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

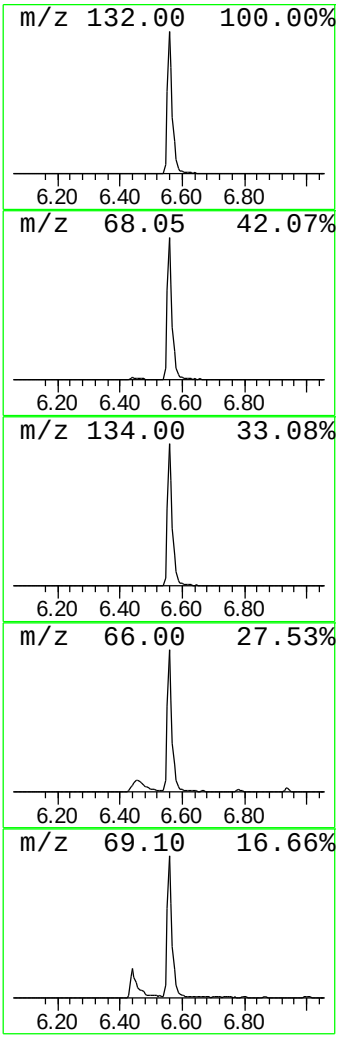
****

Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	45.34 ng	2253640	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122917\
Data File : BF101826.D
Acq On : 29 Dec 2017 13:54
Operator : SJ/JU
Sample : I7040-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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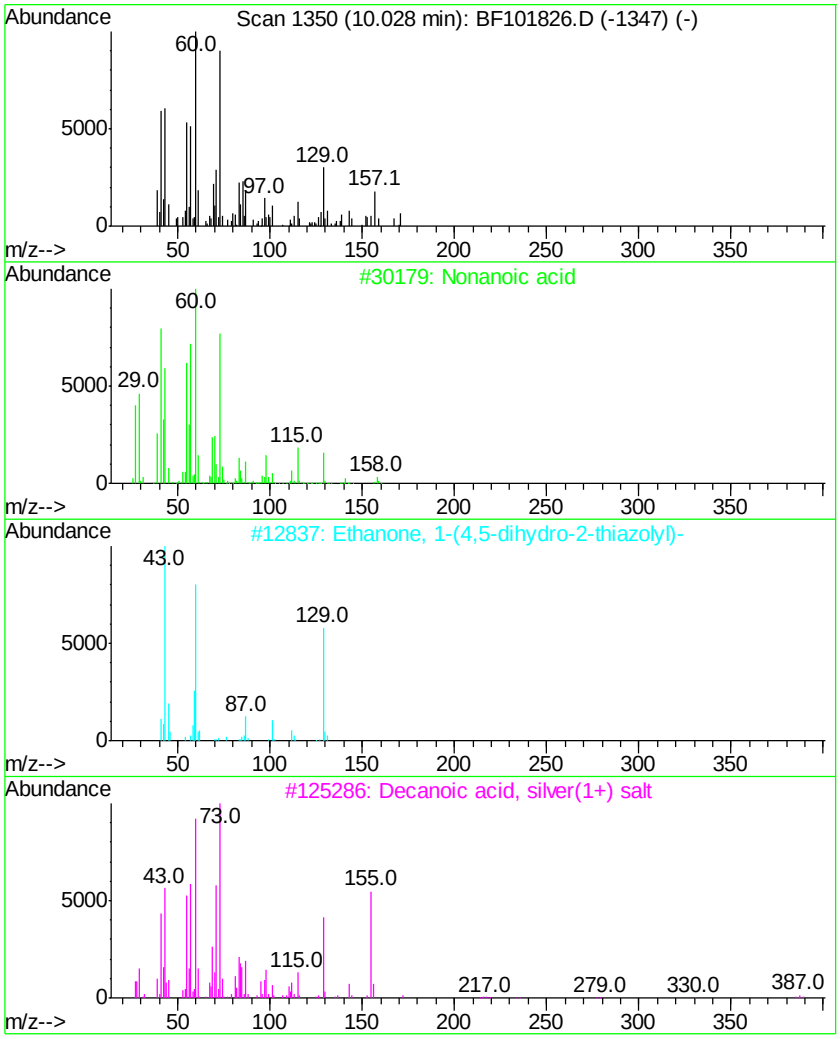
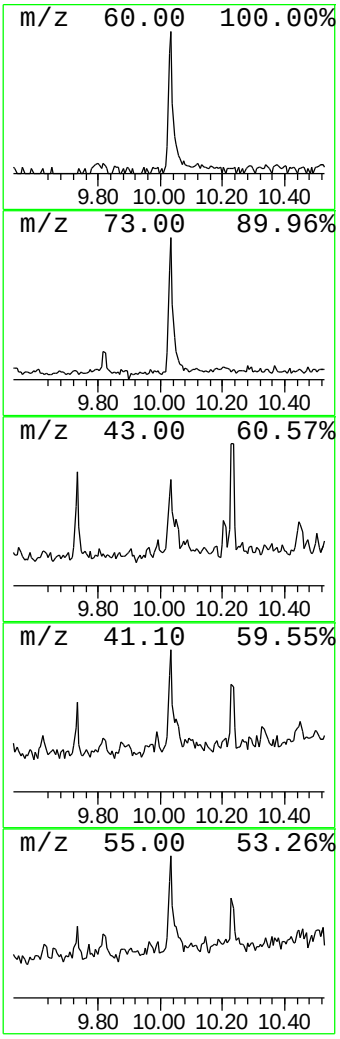
Peak Number 4 unknown10.03 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.03	2.03 ng	124685	Acenaphthene-d10	9.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid	158	C9H18O2	000112-05-0	47
2	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	46
3	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	45
4	1-(p-Toluidino)-1-deoxy-.beta.-d...	269	C13H19NO5	1000226-06-4	43
5	Heptanoic acid	130	C7H14O2	000111-14-8	43





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122917\
Data File : BF101826.D
Acq On : 29 Dec 2017 13:54
Operator : SJ/JU
Sample : I7040-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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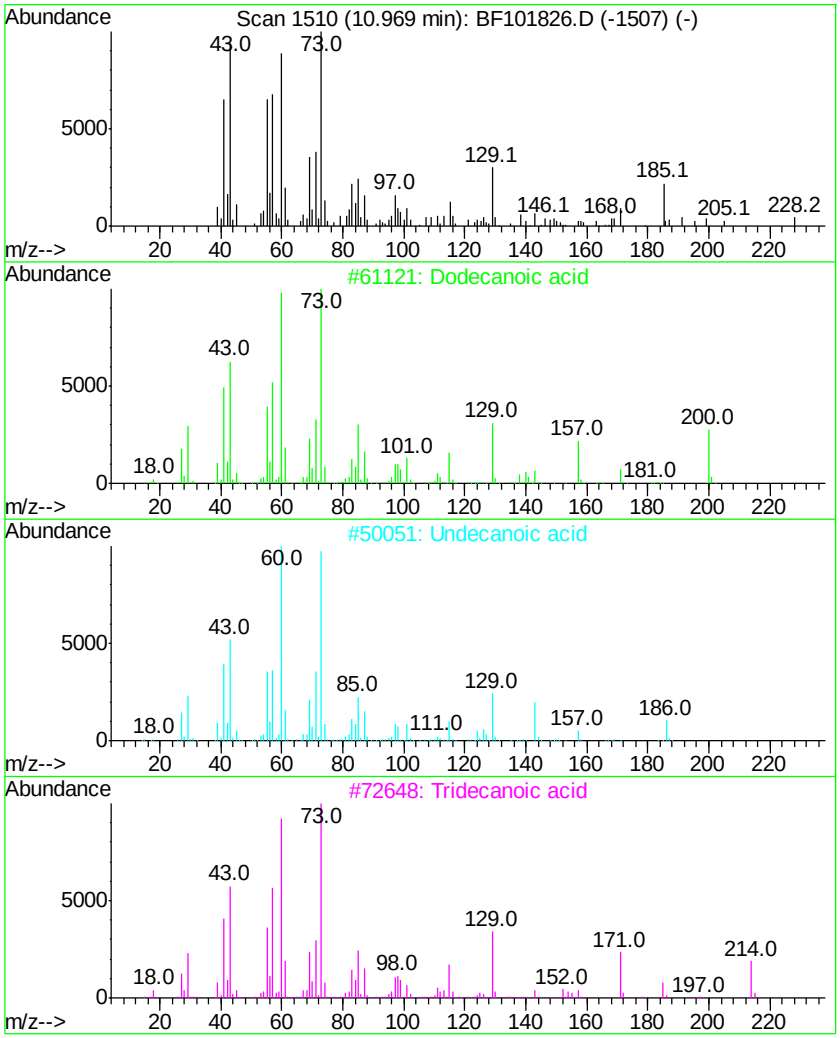
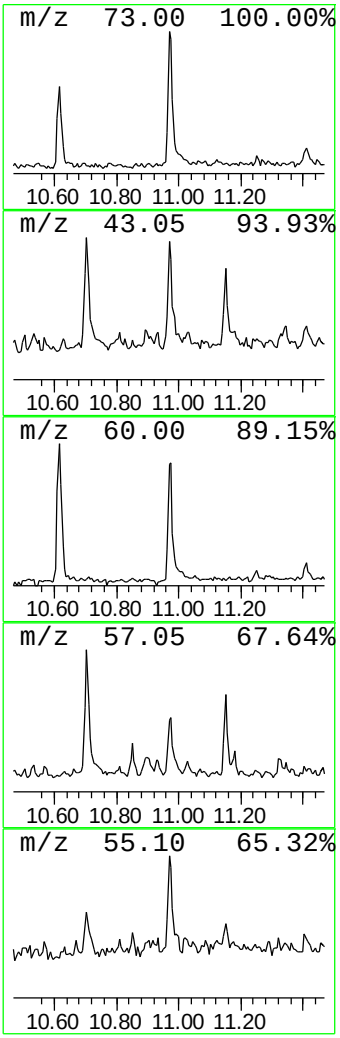
Peak Number 5 Dodecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.97	2.91 ng	153038	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	86
2	Undecanoic acid	186	C11H22O2	000112-37-8	72
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	n-Decanoic acid	172	C10H20O2	000334-48-5	59
5	Methyl-.alpha.-d-ribofuranoside	164	C6H12O5	1000129-83-1	46





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122917\
Data File : BF101826.D
Acq On : 29 Dec 2017 13:54
Operator : SJ/JU
Sample : I7040-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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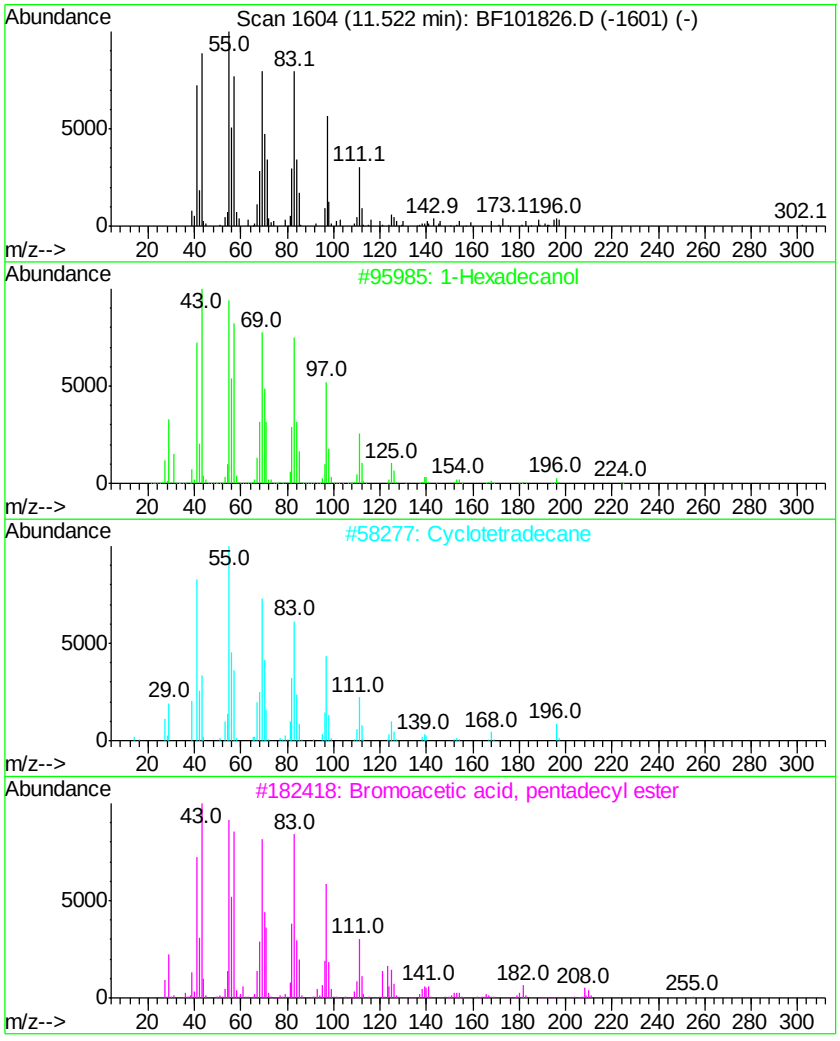
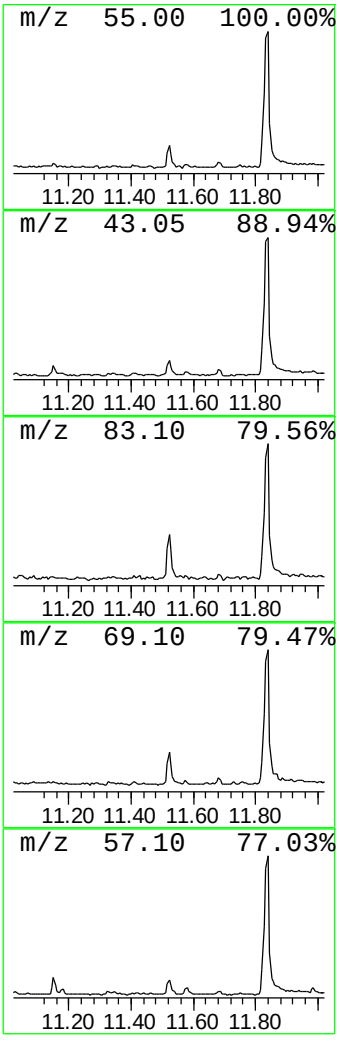
Peak Number 6 1-Hexadecanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.52	2.19 ng	115340	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	94
2	Cyclotetradecane	196	C14H28	000295-17-0	91
3	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	91
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	Cyclohexadecane	224	C16H32	000295-65-8	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122917\
Data File : BF101826.D
Acq On : 29 Dec 2017 13:54
Operator : SJ/JU
Sample : I7040-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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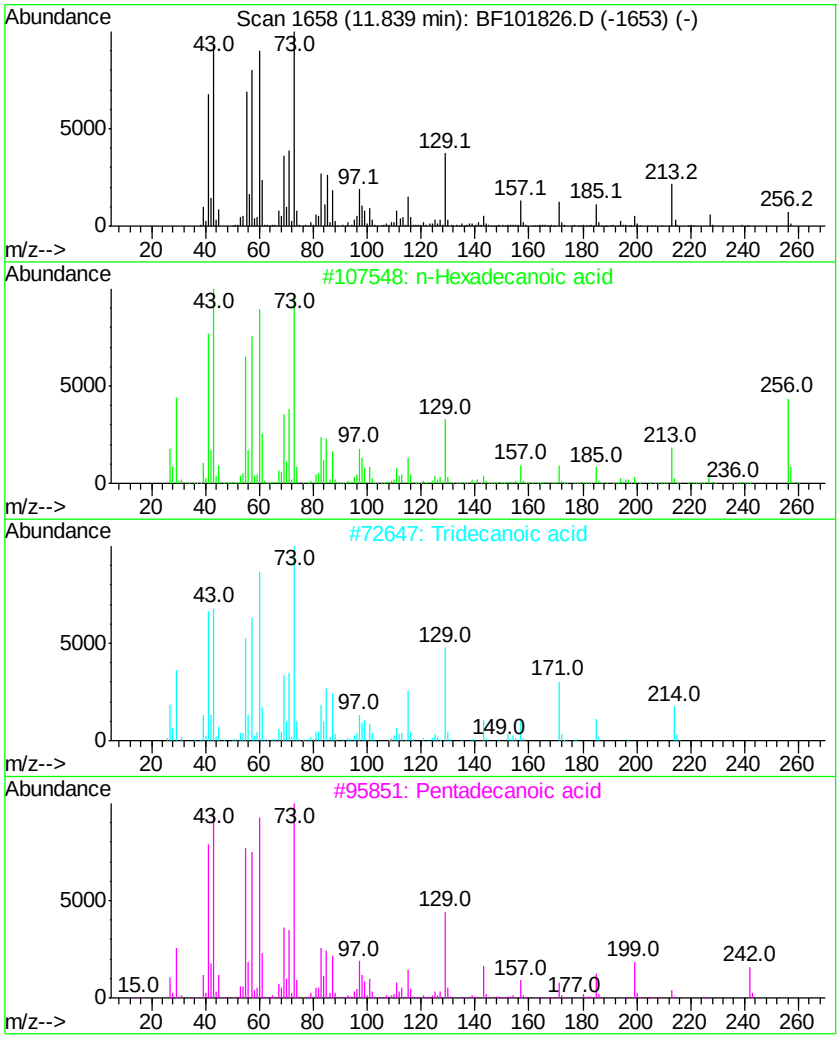
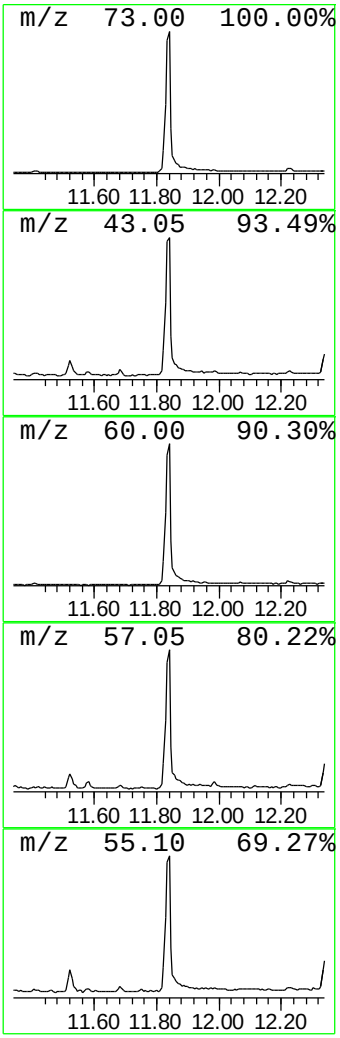
Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	29.60 ng	1558390	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	96
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Hydroxylamine, O-decyl-	173	C10H23NO	029812-79-1	15





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122917\
Data File : BF101826.D
Acq On : 29 Dec 2017 13:54
Operator : SJ/JU
Sample : I7040-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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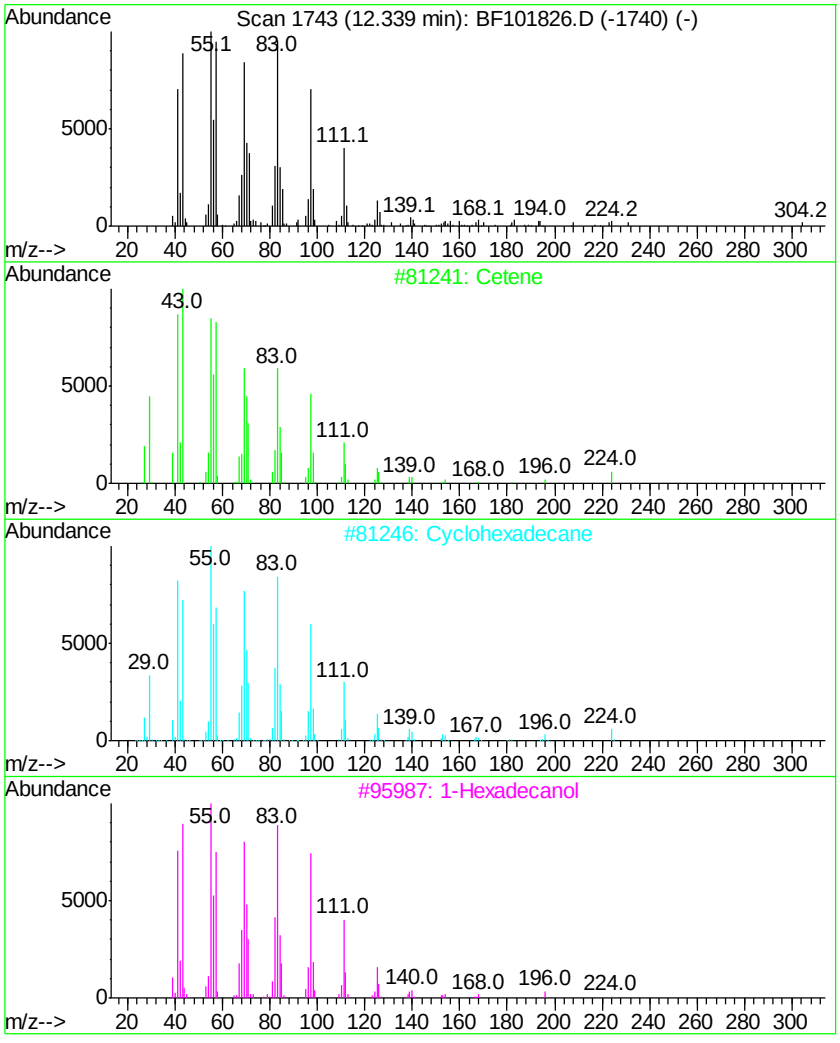
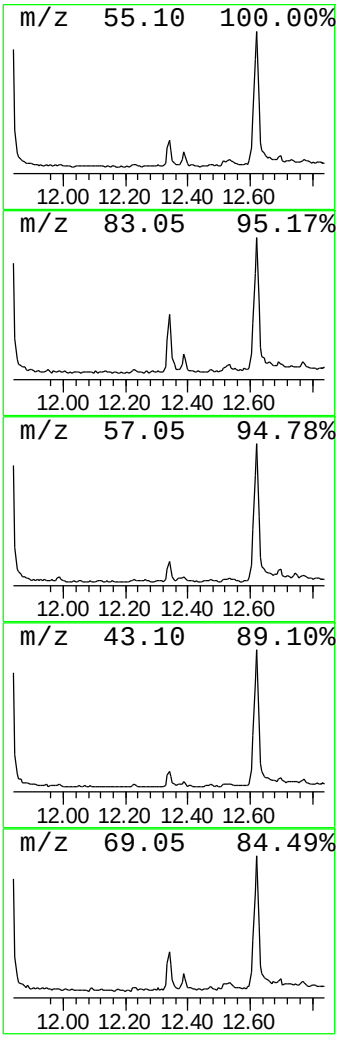
Peak Number 8 Cetene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	3.58 ng	188723	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cetene	224	C16H32	000629-73-2	97
2	Cyclohexadecane	224	C16H32	000295-65-8	96
3	1-Hexadecanol	242	C16H34O	036653-82-4	94
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	91





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122917\
Data File : BF101826.D
Acq On : 29 Dec 2017 13:54
Operator : SJ/JU
Sample : I7040-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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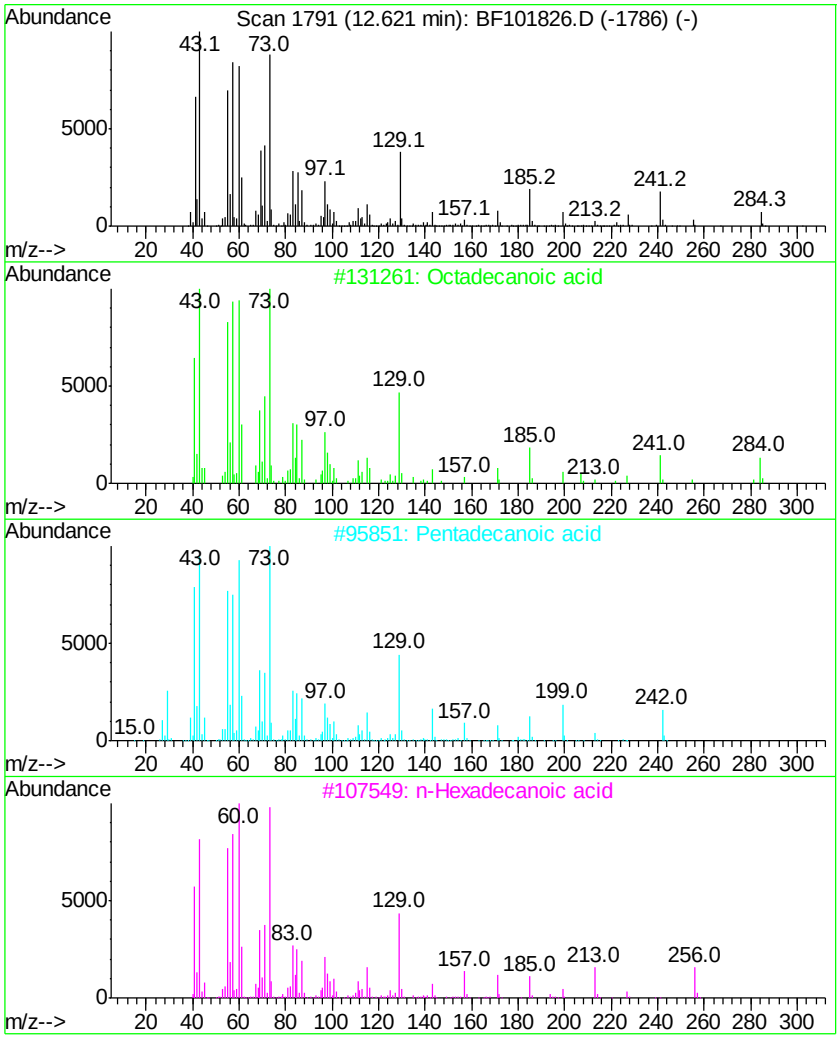
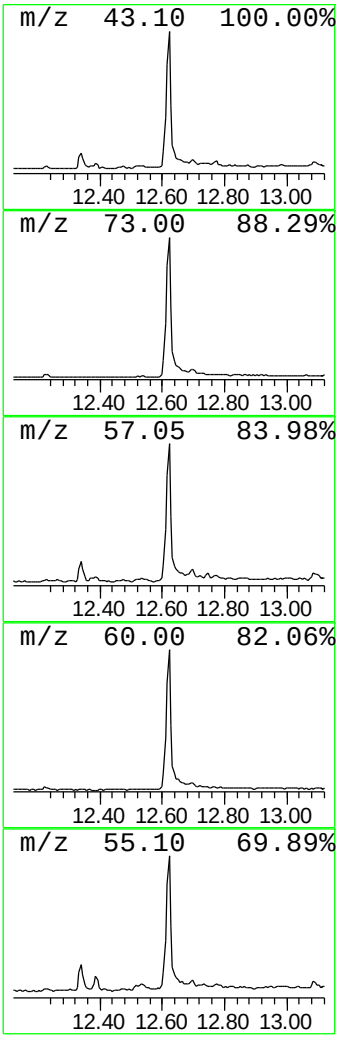
Peak Number 9 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.62	32.52 ng	1712520	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Tridecanoic acid	214	C13H26O2	000638-53-9	76





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122917\
Data File : BF101826.D
Acq On : 29 Dec 2017 13:54
Operator : SJ/JU
Sample : I7040-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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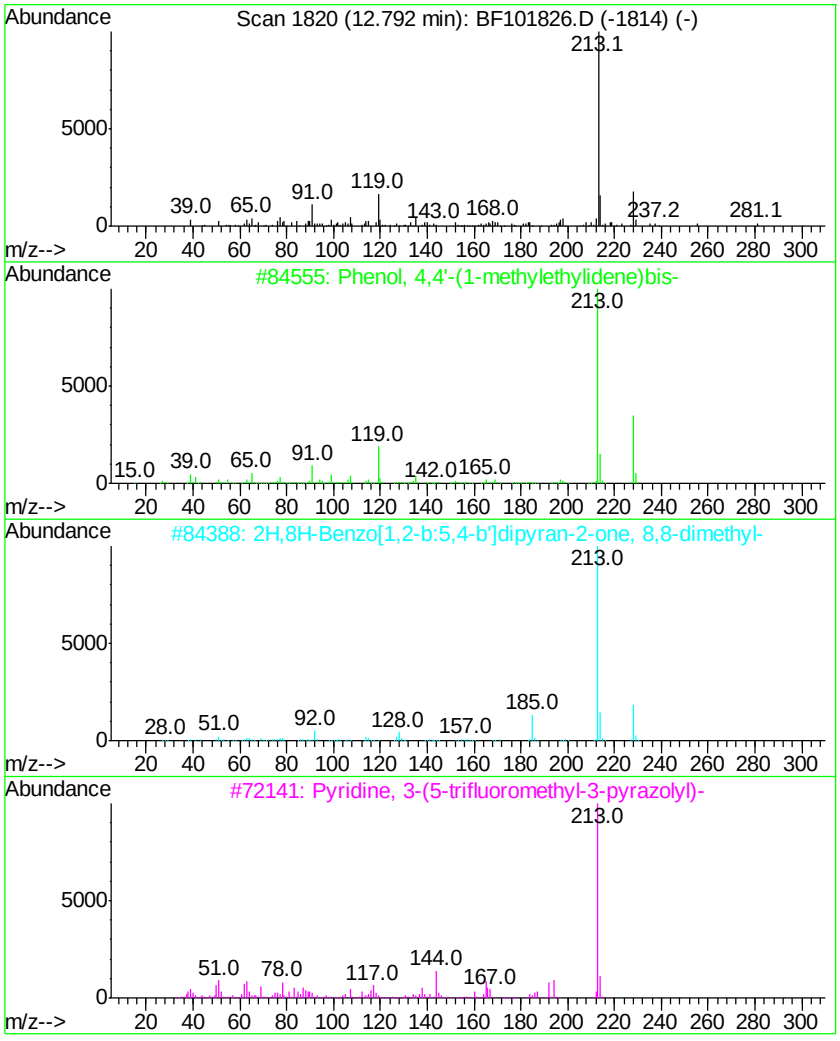
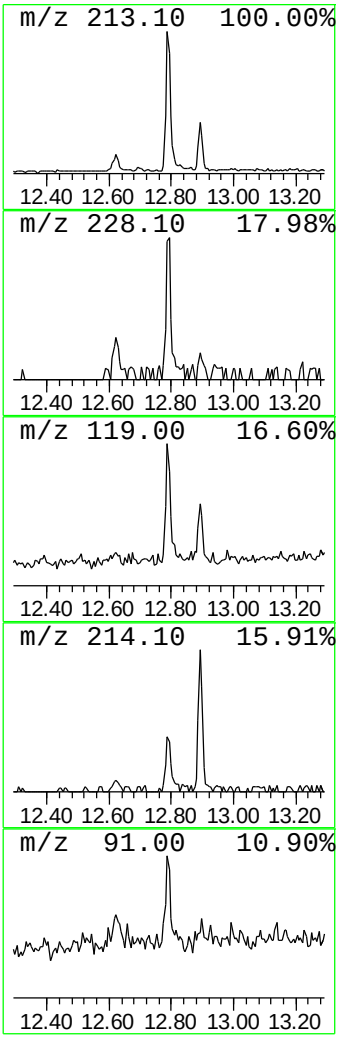
Peak Number 10 Phenol, 4,4'-(1-methylethyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	3.76 ng	155550	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	91
2	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	72
3	Pyridine, 3-(5-trifluoromethyl-3...	213	C9H6F3N3	003974-70-7	53
4	Indole,6-methyl-2-(2-thienyl)-	213	C13H11NS	296245-70-0	53
5	2-Trimethylsilyl-3-trimethylsily...	228	C8H20N4Si2	1000373-05-5	46





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122917\
Data File : BF101826.D
Acq On : 29 Dec 2017 13:54
Operator : SJ/JU
Sample : I7040-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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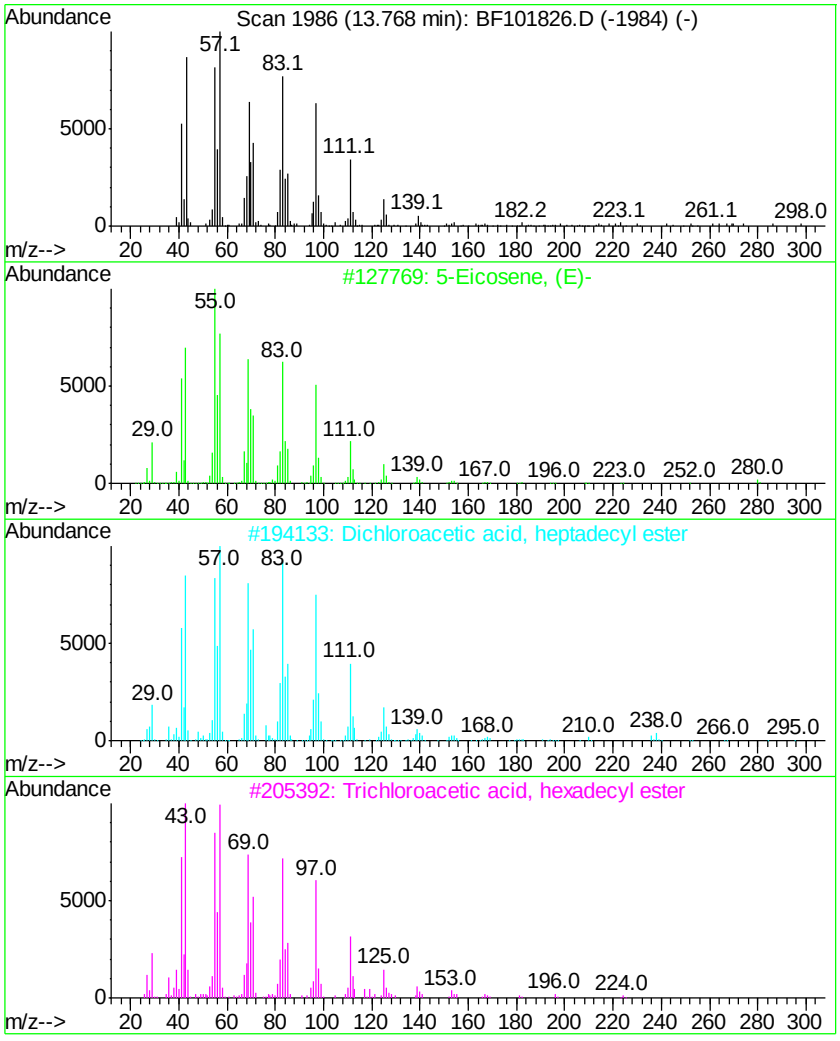
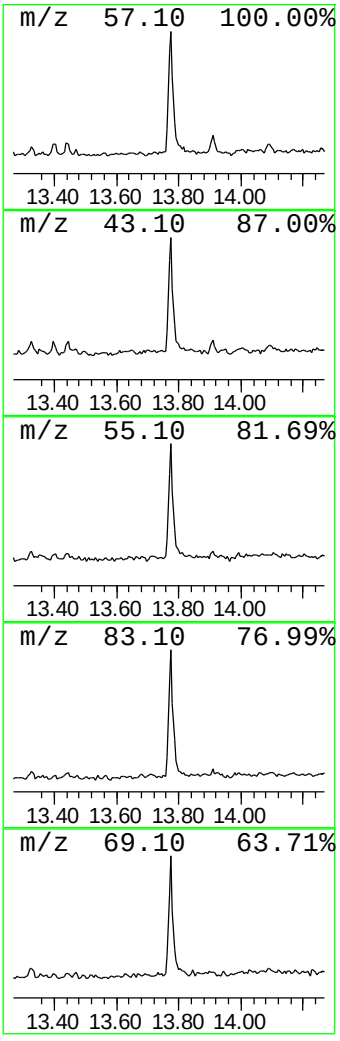
Peak Number 11 5-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	9.40 ng	389375	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	96
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122917\
Data File : BF101826.D
Acq On : 29 Dec 2017 13:54
Operator : SJ/JU
Sample : I7040-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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
2-Pentanone, 4-hy...	4.99	4.1	ng	202701	1	6.78	994119	20.0
unknown6.56	6.56	45.3	ng	2253640	1	6.78	994119	20.0
unknown10.03	10.03	2.0	ng	124685	3	9.82	1229430	20.0
Dodecanoic acid	10.97	2.9	ng	153038	4	11.32	1053110	20.0
1-Hexadecanol	11.52	2.2	ng	115340	4	11.32	1053110	20.0
n-Hexadecanoic acid	11.84	29.6	ng	1558390	4	11.32	1053110	20.0
Cetene	12.34	3.6	ng	188723	4	11.32	1053110	20.0
Octadecanoic acid	12.62	32.5	ng	1712520	4	11.32	1053110	20.0
Phenol, 4,4'-(1-m...	12.79	3.8	ng	155550	5	13.97	828496	20.0
5-Eicosene, (E)-	13.77	9.4	ng	389375	5	13.97	828496	20.0