LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111017\
Data File : BF100406.D
Acq On : 10 Nov 2017 22:04
Operator : SJ/JU
Sample : I6388-13
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-7

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-BF110817.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	5.134	513	518	528	rBV	411312	499902	17.52%	1.856%
2	5.522	579	584	587	rBV	2838291	2712841	95.09%	10.072%
3	6.528	749	755	765	rBV	2560199	2853020	100.00%	10.593%
4	6.669	775	779	783	rBV	2893035	2706253	94.86%	10.048%
5	6.904	815	819	822	rBV	1165867	1004389	35.20%	3.729%
6	7.057	841	845	848	rBV	2500119	2142040	75.08%	7.953%
7	7.463	909	914	917	rBV	1847372	1653998	57.97%	6.141%
8	8.187	1032	1037	1040	rBV	1386708	1246079	43.68%	4.627%
9	8.734	1127	1130	1133	rBV	161591	137347	4.81%	0.510%
10	9.257	1214	1219	1222	rBV	3196117	2812813	98.59%	10.444%
11	9.645	1282	1285	1293	rVB	272379	261852	9.18%	0.972%
12	9.939	1331	1335	1339	rBV	1374119	1210714	42.44%	4.495%
13	10.057	1347	1355	1360	rBV2	60329	67385	2.36%	0.250%
14	10.651	1452	1456	1459	rBV	498079	410550	14.39%	1.524%
15	10.728	1461	1469	1472	rVV	1355512	1330015	46.62%	4.938%
16	10.757	1472	1474	1479	rVB2	43247	44725	1.57%	0.166%
17	11.428	1584	1588	1591	rBV	1122816	1027570	36.02%	3.815%
18	11.939	1670	1675	1684	rBV2	118087	129181	4.53%	0.480%
19	12.633	1790	1793	1798	rBV	32031	30912	1.08%	0.115%
20	12.727	1805	1809	1813	rBV3	39199	47335	1.66%	0.176%
21	12.886	1829	1836	1847	rVB2	158661	262429	9.20%	0.974%
22	13.010	1852	1857	1860	rBV	2268101	1977311	69.31%	7.342%
23	13.898	2004	2008	2015	rVB	108800	125803	4.41%	0.467%
24	14.063	2032	2036	2039	rBV	1100641	943871	33.08%	3.504%
25	14.521	2111	2114	2120	rBV4	27123	40585	1.42%	0.151%
26	14.833	2164	2167	2173	rVB	45387	45368	1.59%	0.168%
27	15.180	2223	2226	2230	rVB	64525	70253	2.46%	0.261%
28	15.545	2283	2288	2297	rVB	555372	820275	28.75%	3.046%
29	16.010	2363	2367	2373	rBV	82585	126058	4.42%	0.468%
30	16.533	2451	2456	2461	rVB	72918	118308	4.15%	0.439%
31	17.139	2555	2559	2564	rVB2	44335	74108	2.60%	0.275%

Sum of corrected areas: 26933290

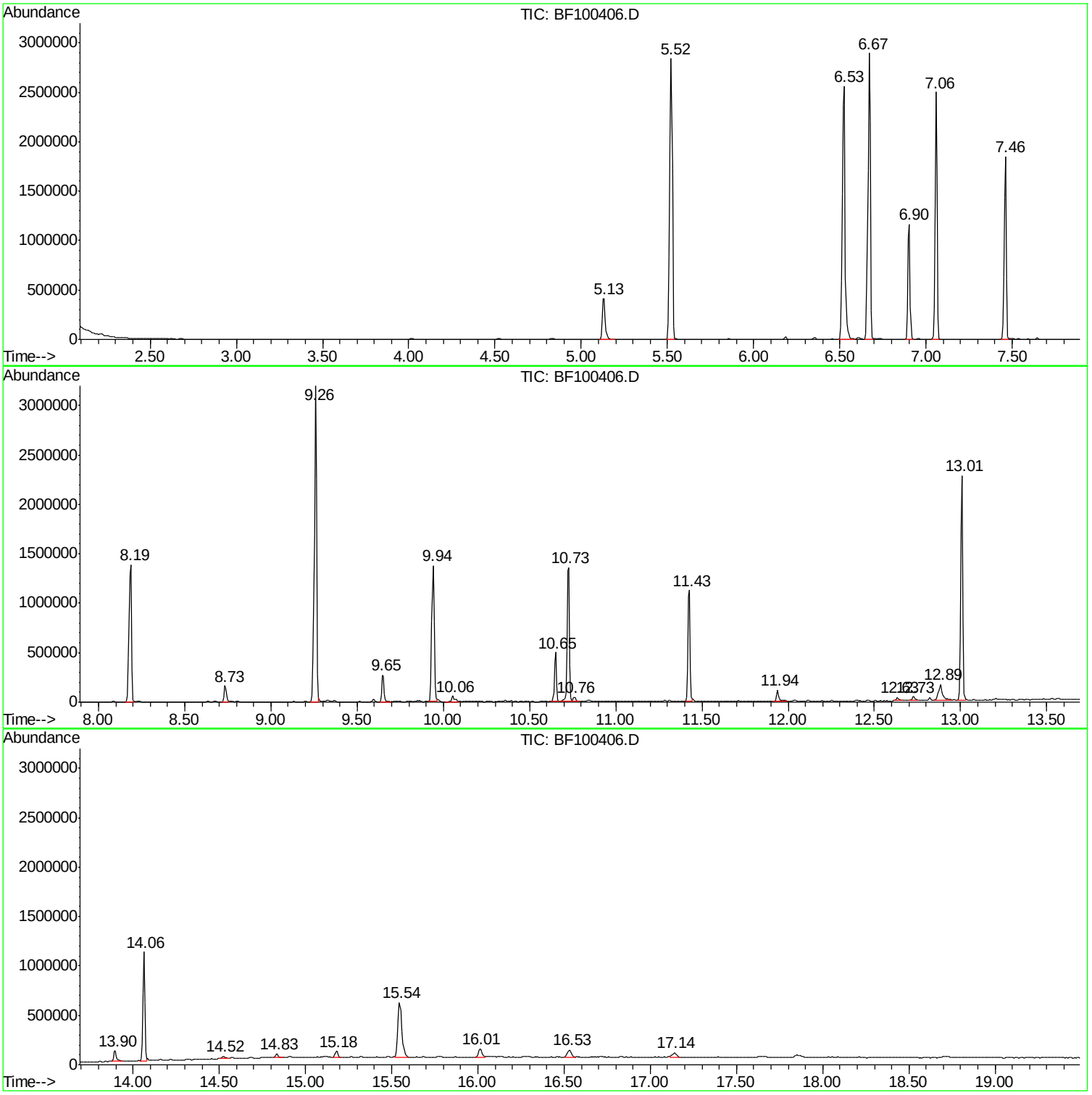
LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111017\
Data File : BF100406.D
Acq On : 10 Nov 2017 22:04
Operator : SJ/JU
Sample : I6388-13
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3N-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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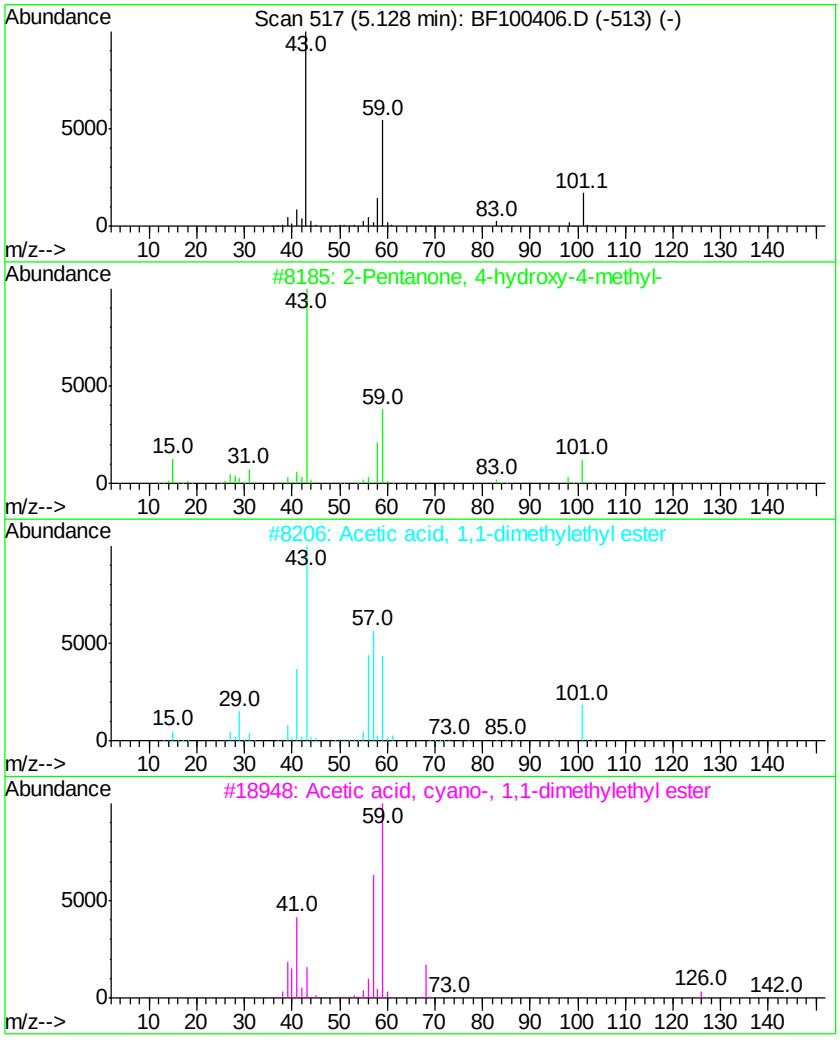
TIC Integration Parameters: LSCINT.P

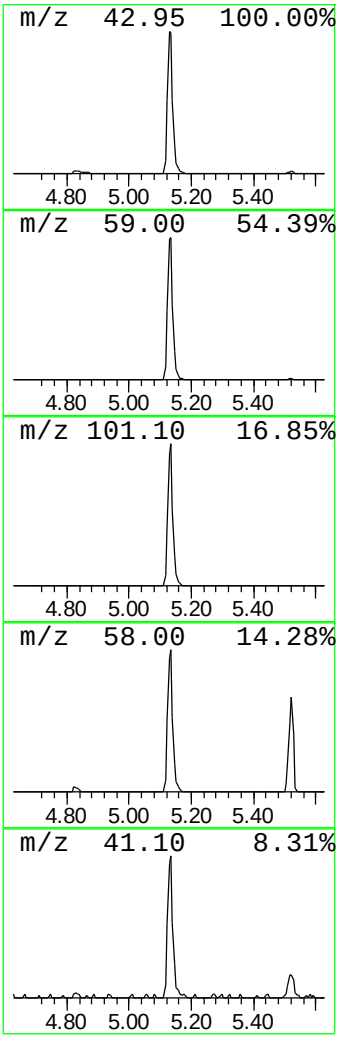
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	9.95 ng	499902	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





Library Search Compound Report

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Instrument : BNA_F
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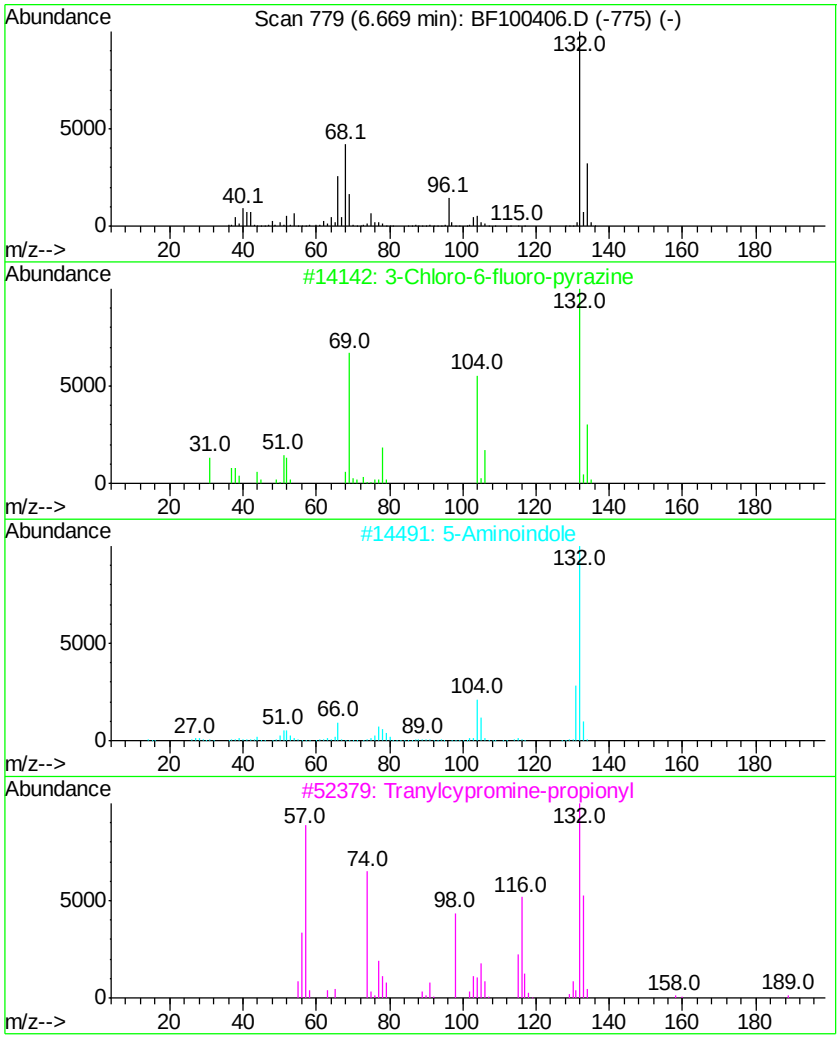
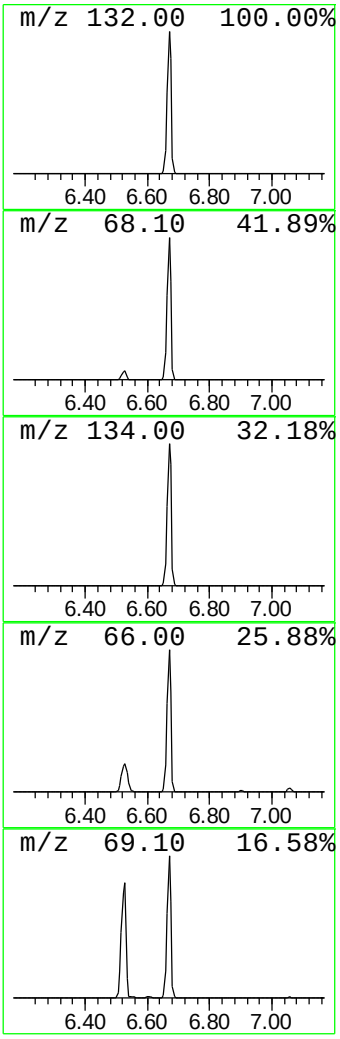
****

Peak Number 2 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	53.89 ng	2706250	1,4-Dichlorobenzene-d4	6.90

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





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Misc :
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Instrument : BNA_F
ClientSampleId : 3N-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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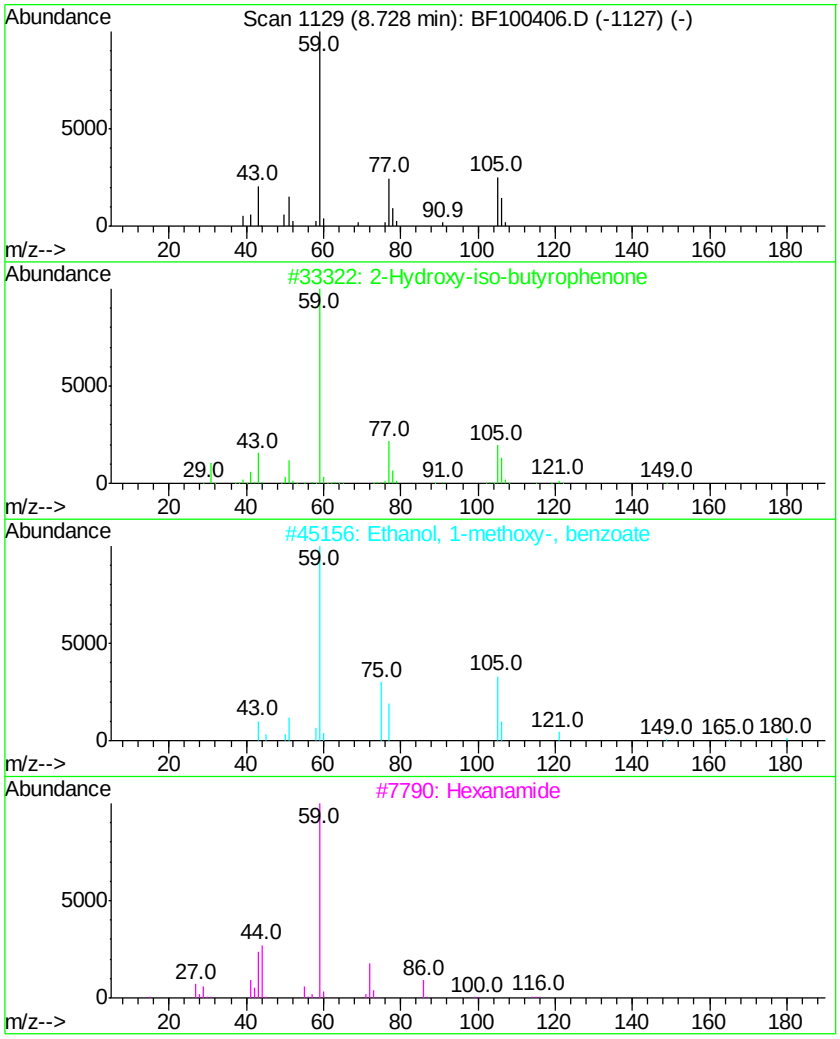
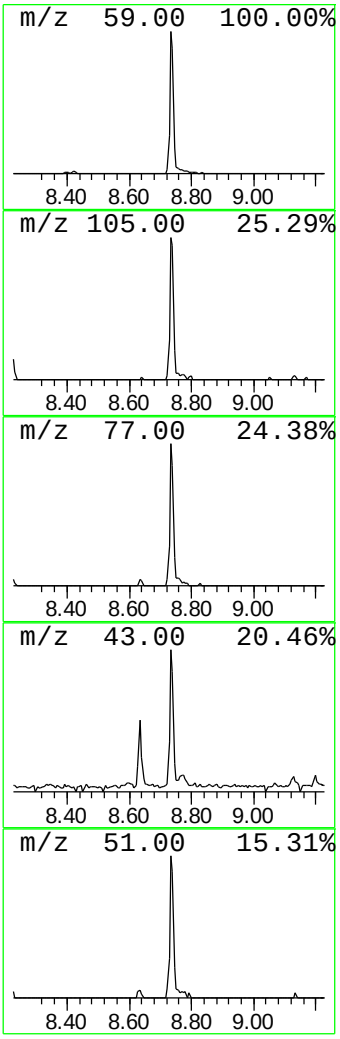
Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.73	2.20 ng	137347	Naphthalene-d8	8.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	64
3	Hexanamide	115	C6H13NO	000628-02-4	9
4	Formamide, N-methyl-	59	C2H5NO	000123-39-7	7
5	2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	7





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Data File : BF100406.D
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Operator : SJ/JU
Sample : I6388-13
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

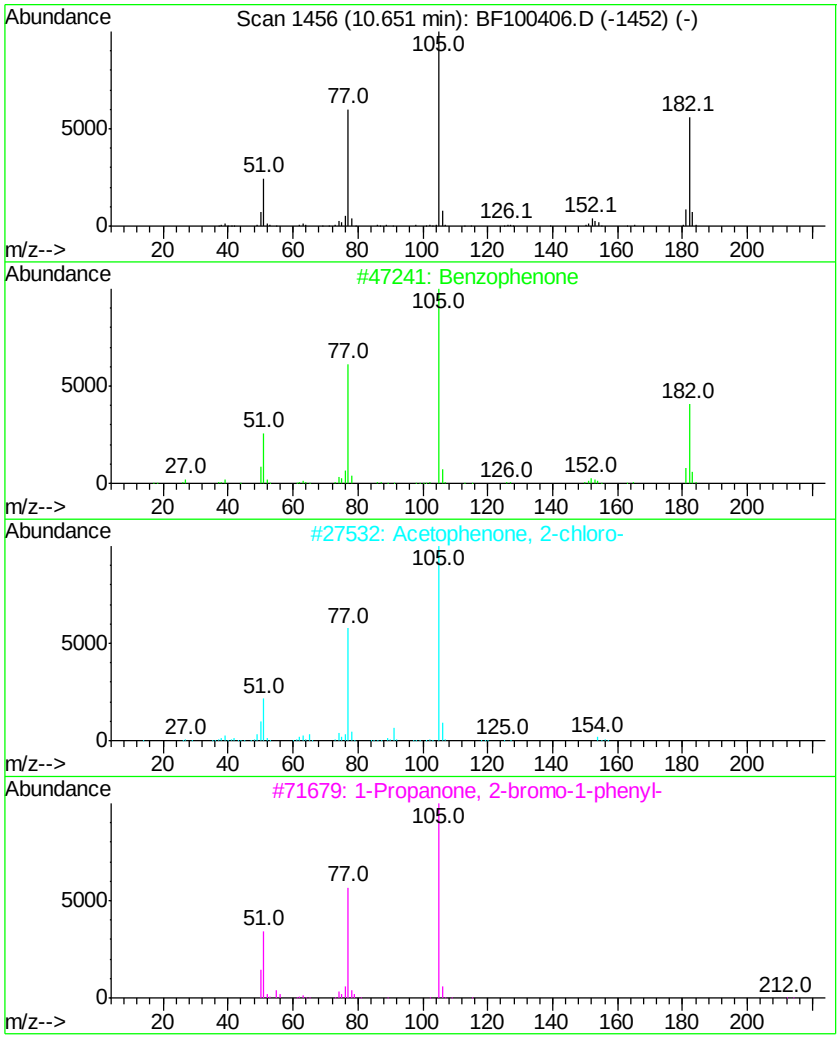
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

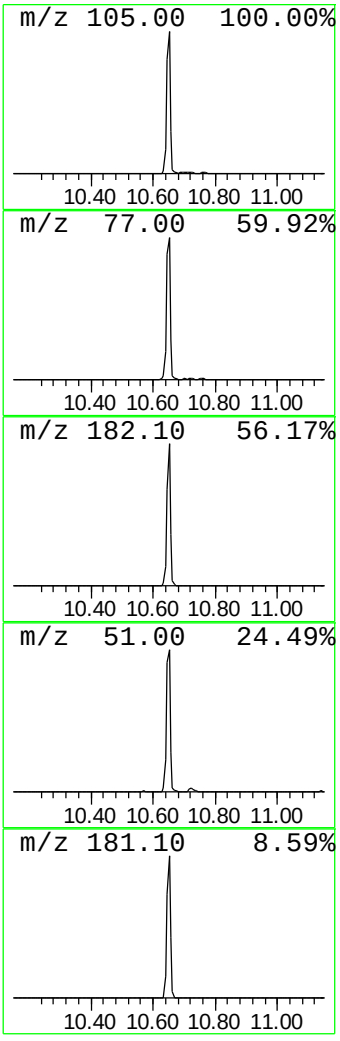
****

Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	6.78 ng	410550	Acenaphthene-d10	9.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47
3	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47
5	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47





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Misc :
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Instrument : BNA_F
ClientSampleId : 3N-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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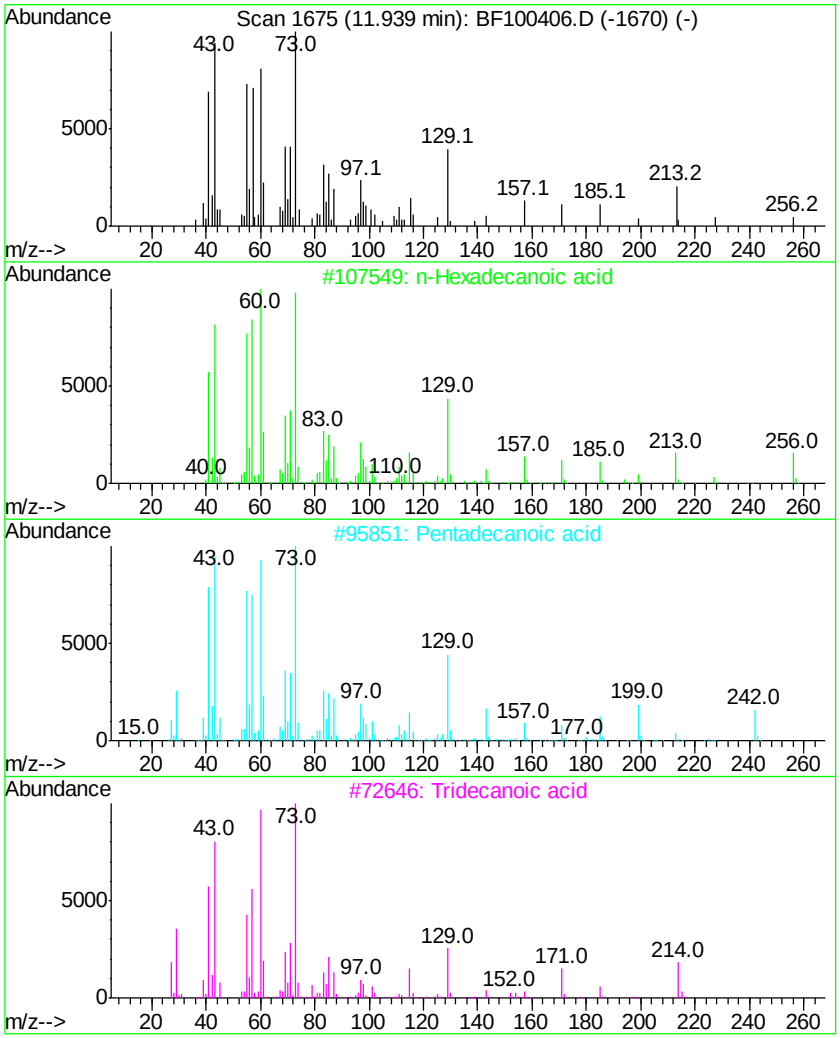
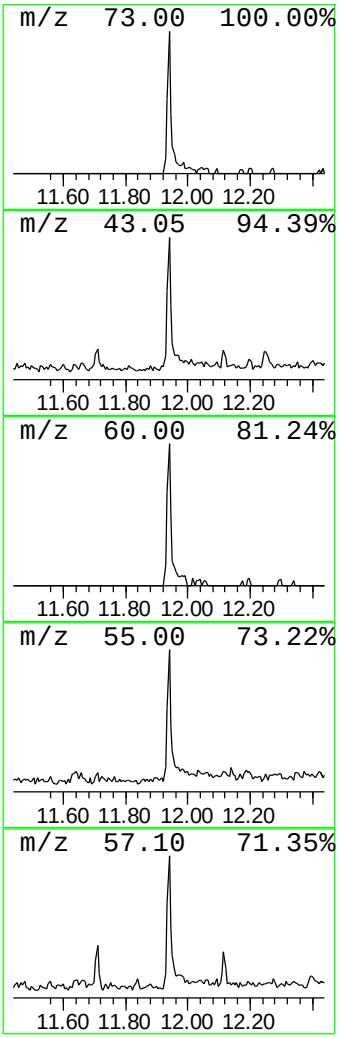
Peak Number 6 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	2.51 ng	129181	Phenanthrene-d10	11.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	30





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TIC Integration Parameters: LSCINT.P

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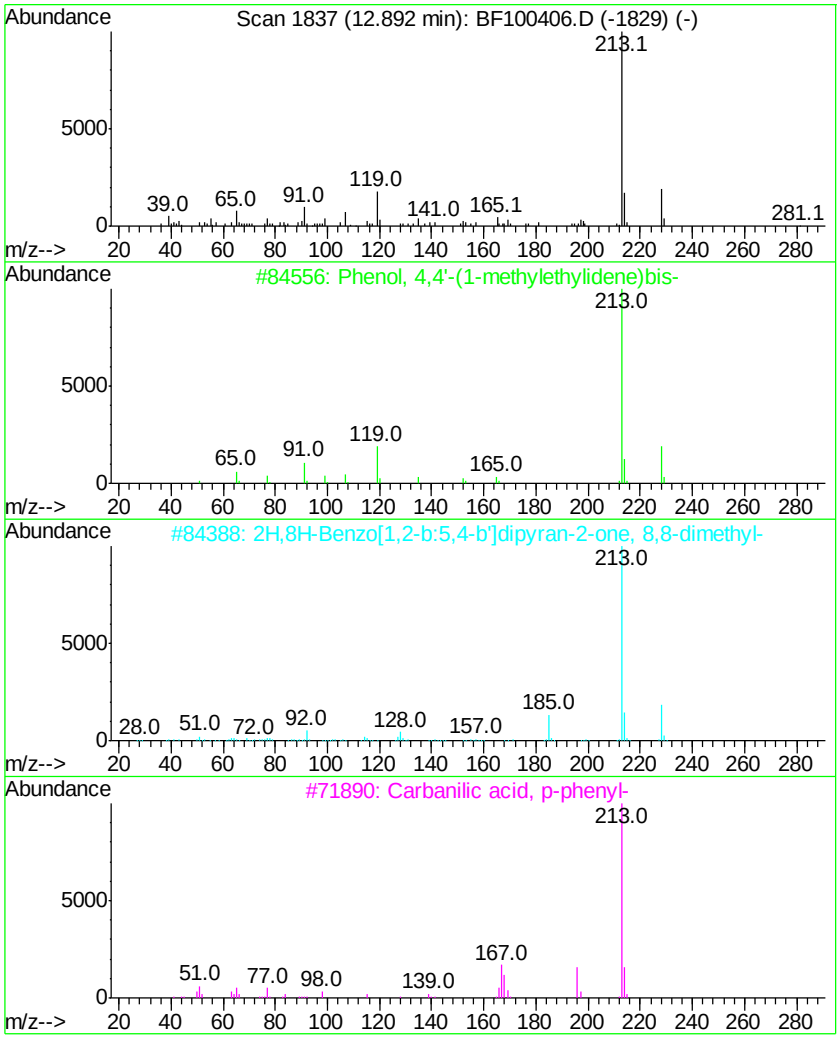
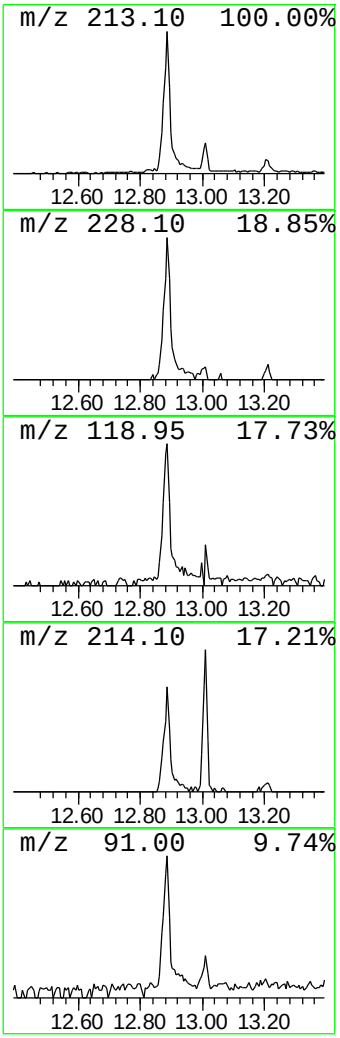
Peak Number 7 Phenol, 4,4'-(1-methylethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.89	5.56 ng	262429	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	97
2	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	59
3	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	58
4	Indole,6-methyl-2-(2-thienyl)-	213	C13H11NS	296245-70-0	53
5	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	45





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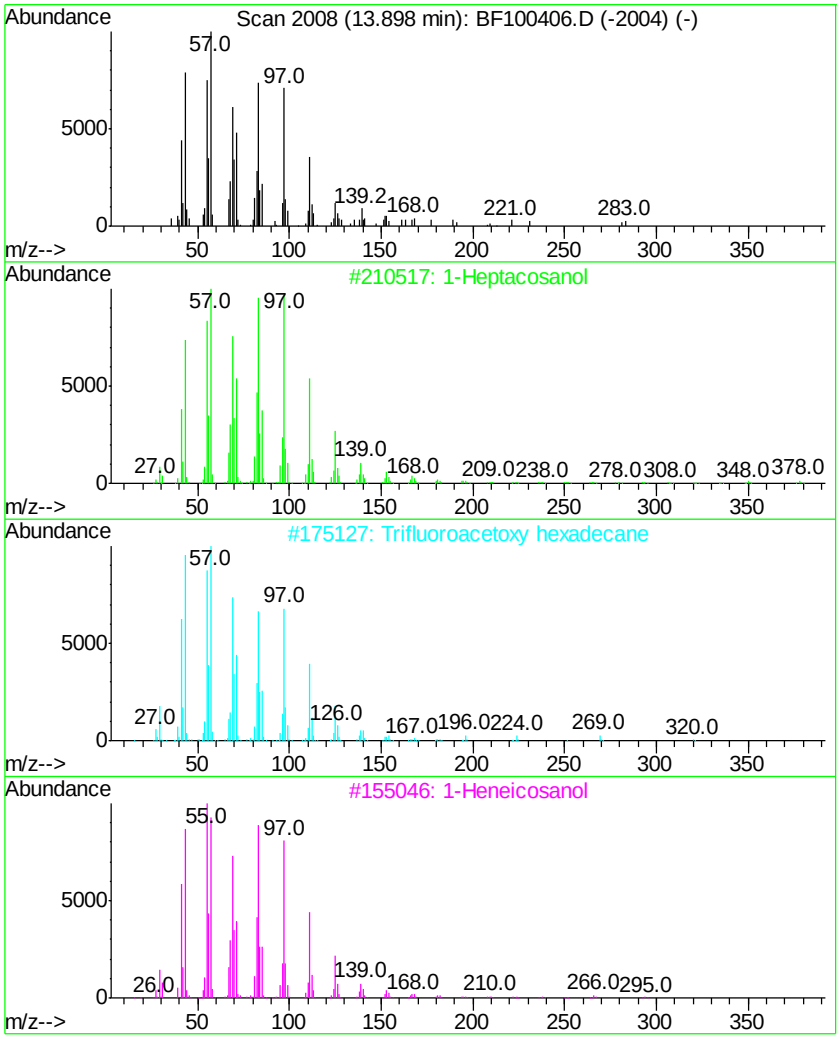
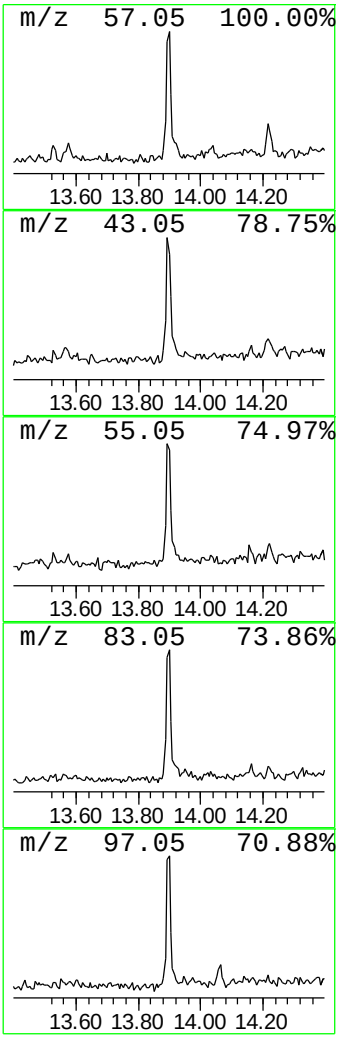
Peak Number 8 1-Heptacosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	2.67 ng	125803	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	91
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3	1-Heneicosanol	312	C21H44O	015594-90-8	90
4	Behenic alcohol	326	C22H46O	000661-19-8	90
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	87





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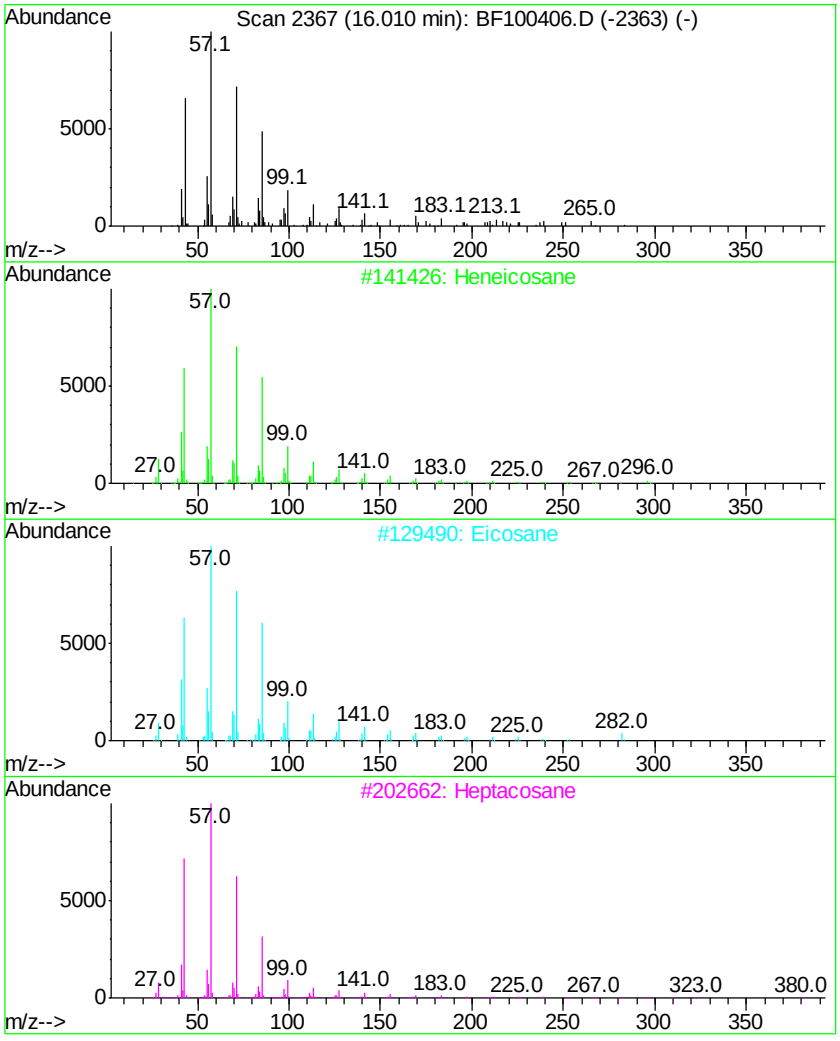
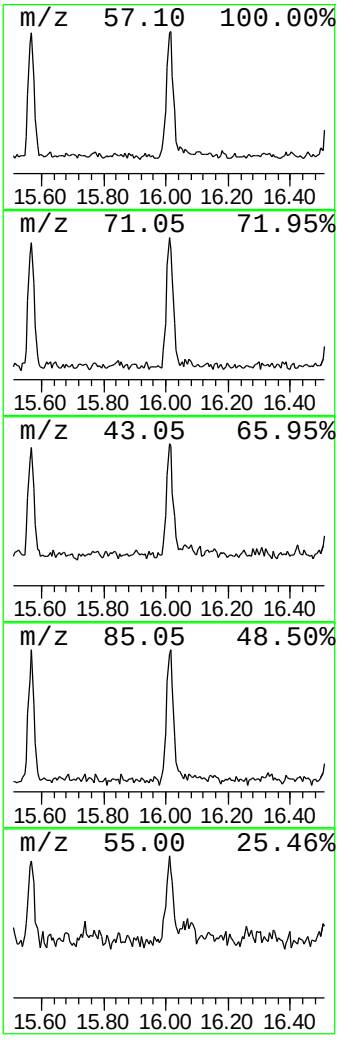
Peak Number 9 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.01	3.07 ng	126058	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Docosane	310	C22H46	000629-97-0	91





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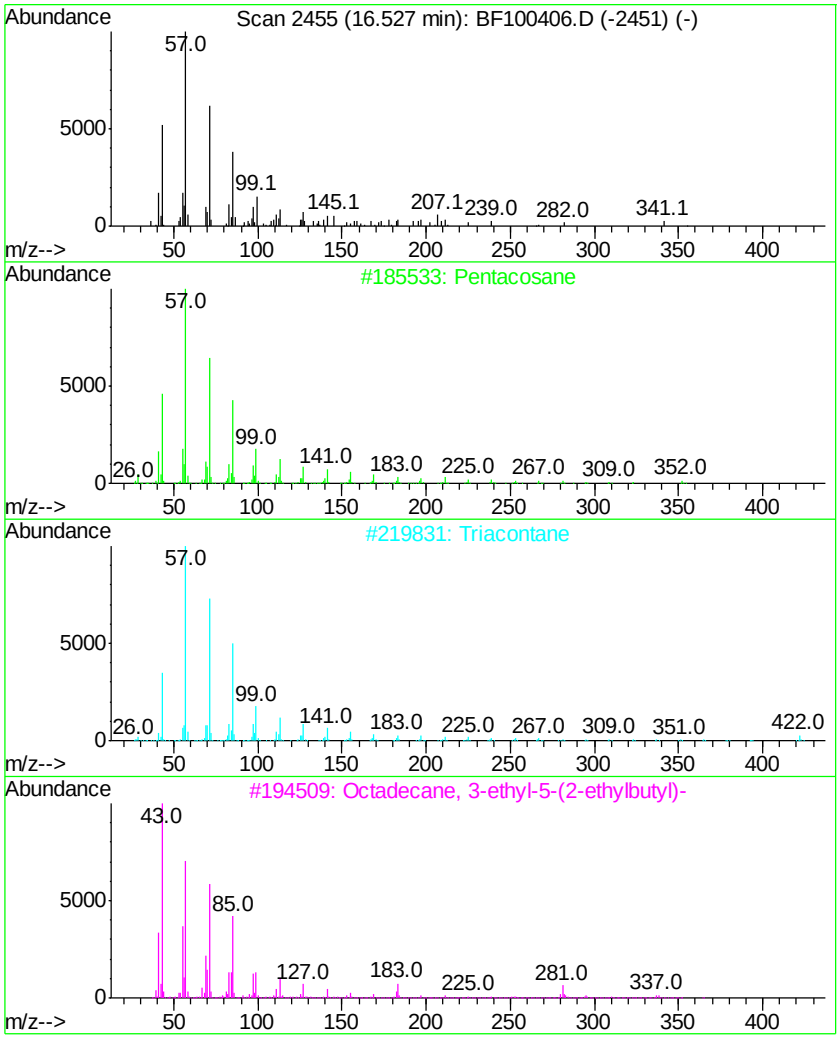
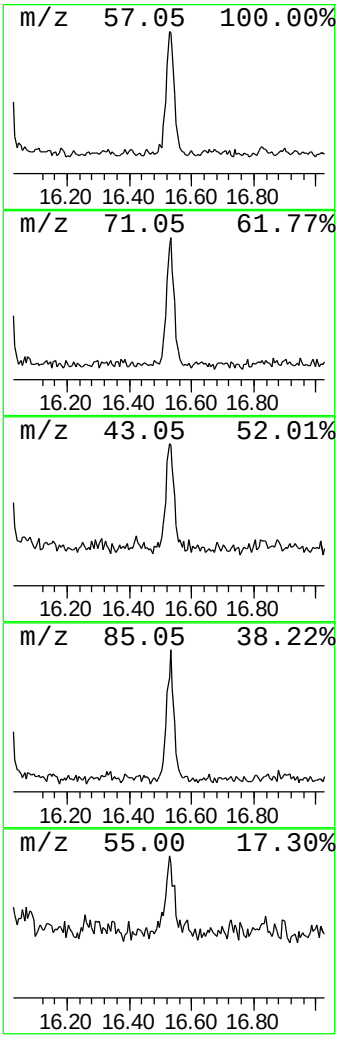
Peak Number 10 Pentacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	2.88 ng	118308	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	87
2	Triacontane	422	C30H62	000638-68-6	87
3	Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	86
4	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	80
5	Hexadecane, 5-butyl-	282	C20H42	006912-07-8	76





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF111017\
Data File : BF100406.D
Acq On : 10 Nov 2017 22:04
Operator : SJ/JU
Sample : I6388-13
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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...	5.13	9.9	ng	499902	1	6.90	1004390	20.0
unknown6.67	6.67	53.9	ng	2706250	1	6.90	1004390	20.0
2-Hydroxy-iso-but...	8.73	2.2	ng	137347	2	8.19	1246080	20.0
Benzophenone	10.65	6.8	ng	410550	3	9.94	1210710	20.0
n-Hexadecanoic acid	11.94	2.5	ng	129181	4	11.43	1027570	20.0
Phenol, 4,4'-(1-m...	12.89	5.6	ng	262429	5	14.06	943871	20.0
1-Heptacosanol	13.90	2.7	ng	125803	5	14.06	943871	20.0
Heneicosane	16.01	3.1	ng	126058	6	15.54	820275	20.0
Pentacosane	16.53	2.9	ng	118308	6	15.54	820275	20.0