LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111117\
Data File : BF100448.D
Acq On : 11 Nov 2017 18:37
Operator : SJ/JU
Sample : I6388-17
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-9

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	2.216	19	22	34	rVB3	20963	39535	1.67%	0.165%
2	4.522	409	414	422	rBV	26664	30536	1.29%	0.127%
3	5.128	513	517	525	rBV	385722	451768	19.13%	1.884%
4	5.522	579	584	587	rBV	2410999	2306353	97.68%	9.619%
5	6.528	749	755	765	rBV	2230721	2361062	100.00%	9.847%
6	6.604	765	768	771	rVB	32971	25375	1.07%	0.106%
7	6.669	775	779	783	rBV	2372010	2284310	96.75%	9.527%
8	6.904	815	819	822	rBV	1140744	913496	38.69%	3.810%
9	7.057	841	845	849	rVB	1944912	1811266	76.71%	7.554%
10	7.463	909	914	917	rBV	1579180	1368257	57.95%	5.707%
11	7.492	917	919	923	rVB	37217	31292	1.33%	0.131%
12	8.157	1030	1032	1034	rBV	83807	80932	3.43%	0.338%
13	8.187	1034	1037	1040	rVV	1280712	1073429	45.46%	4.477%
14	8.239	1042	1046	1049	rVB	42867	37153	1.57%	0.155%
15	8.475	1082	1086	1091	rVB5	15626	24381	1.03%	0.102%
16	8.598	1104	1107	1110	rBV	62676	50927	2.16%	0.212%
17	8.739	1124	1131	1133	rBV	106367	111162	4.71%	0.464%
18	8.769	1133	1136	1140	rVB	162200	121676	5.15%	0.507%
19	9.198	1207	1209	1212	rVB	71076	52107	2.21%	0.217%
20	9.257	1215	1219	1226	rBV	2542130	2246800	95.16%	9.371%
21	9.334	1229	1232	1235	rVB	218046	185170	7.84%	0.772%
22	9.651	1283	1286	1289	rBV2	239911	235946	9.99%	0.984%
23	9.863	1315	1322	1325	rBV	228390	187196	7.93%	0.781%
24	9.916	1326	1331	1332	rVV4	33905	38172	1.62%	0.159%
25	9.939	1332	1335	1338	rVV2	1085656	958439	40.59%	3.997%
26	9.969	1338	1340	1342	rVB	48778	41445	1.76%	0.173%
27	10.092	1357	1361	1364	rBV	118264	108125	4.58%	0.451%
28	10.122	1364	1366	1370	rVV4	29324	43985	1.86%	0.183%
29	10.186	1373	1377	1381	rBV4	52884	77240	3.27%	0.322%
30	10.363	1400	1407	1410	rBV	233413	198258	8.40%	0.827%
31	10.581	1439	1444	1450	rBV	82821	102423	4.34%	0.427%
32	10.651	1450	1456	1462	rBV	272422	252440	10.69%	1.053%
33	10.728	1465	1469	1472	rVB	1112878	963812	40.82%	4.020%
34	10.833	1484	1487	1492	rBV2	204016	298848	12.66%	1.246%

LSC Area Percent Report

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Acq On : 11 Nov 2017 18:37
Operator : SJ/JU
Sample : I6388-17
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-9

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

35	11.063	1522	1526	1529	rVB4	20297	24367	1.03%	0.102%
36	11.280	1560	1563	1566	rBV	142098	122379	5.18%	0.510%
37	11.316	1566	1569	1575	rVB2	74375	82802	3.51%	0.345%
38	11.428	1584	1588	1591	rBV	977780	834451	35.34%	3.480%
39	11.710	1633	1636	1639	rVB	102298	77415	3.28%	0.323%
40	11.939	1670	1675	1680	rBV2	49255	49573	2.10%	0.207%
41	12.116	1703	1705	1709	rVB	46104	35854	1.52%	0.150%
42	13.010	1853	1857	1860	rBV	1999957	1735510	73.51%	7.238%
43	13.898	2004	2008	2016	rBV	134535	157648	6.68%	0.658%
44	14.063	2033	2036	2040	rBV	954782	878830	37.22%	3.665%
45	14.527	2111	2115	2121	rBV	63791	77485	3.28%	0.323%
46	15.180	2222	2226	2229	rBV	84837	89334	3.78%	0.373%
47	15.551	2284	2289	2299	rVB	492862	650708	27.56%	2.714%
48	16.015	2364	2368	2373	rBV3	33198	47047	1.99%	0.196%

Sum of corrected areas: 23976719

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111117\
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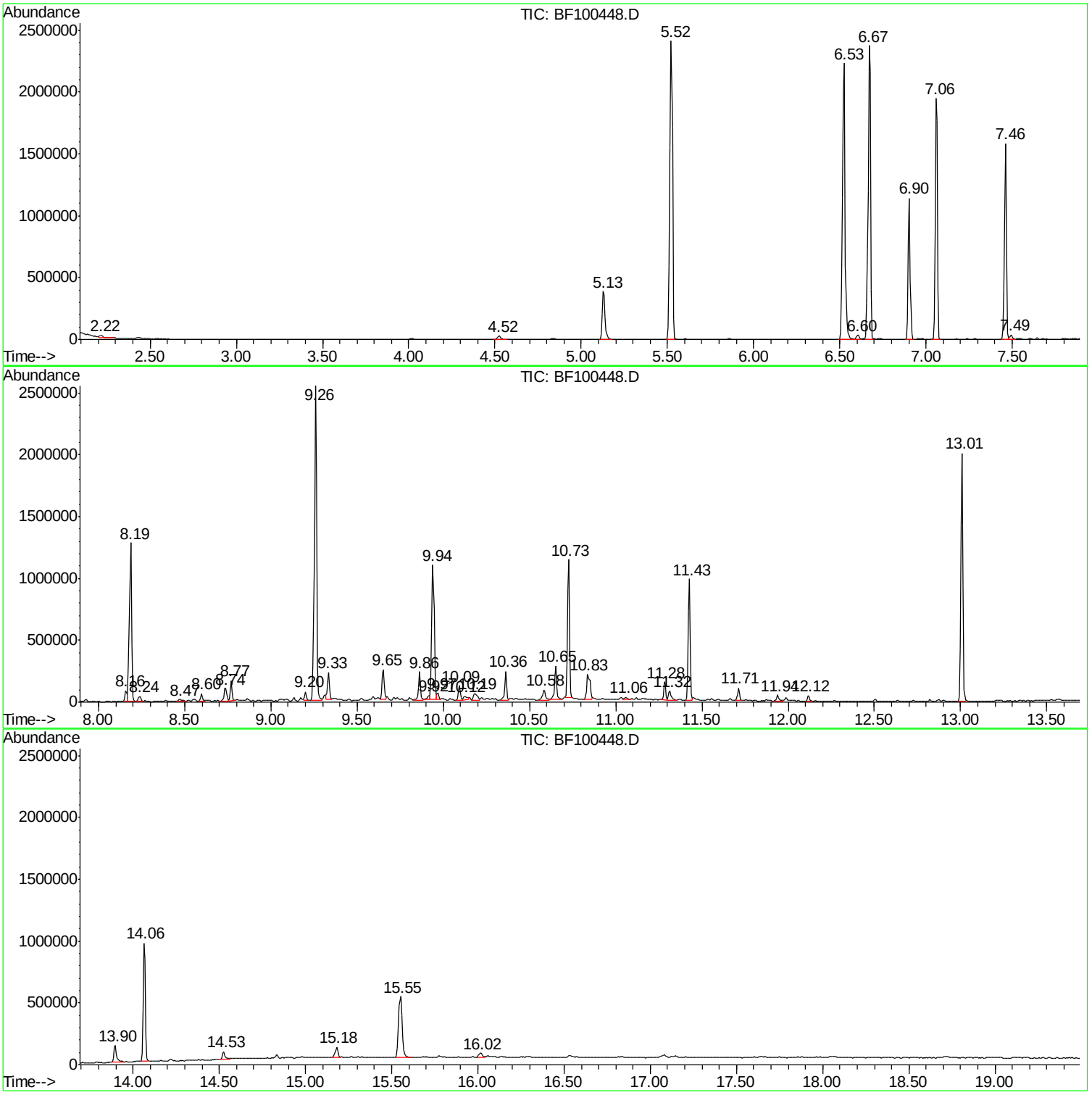
Instrument :
BNA_F
ClientSampleId :
3N-9

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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Data File : BF100448.D
Acq On : 11 Nov 2017 18:37
Operator : SJ/JU
Sample : I6388-17
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-9

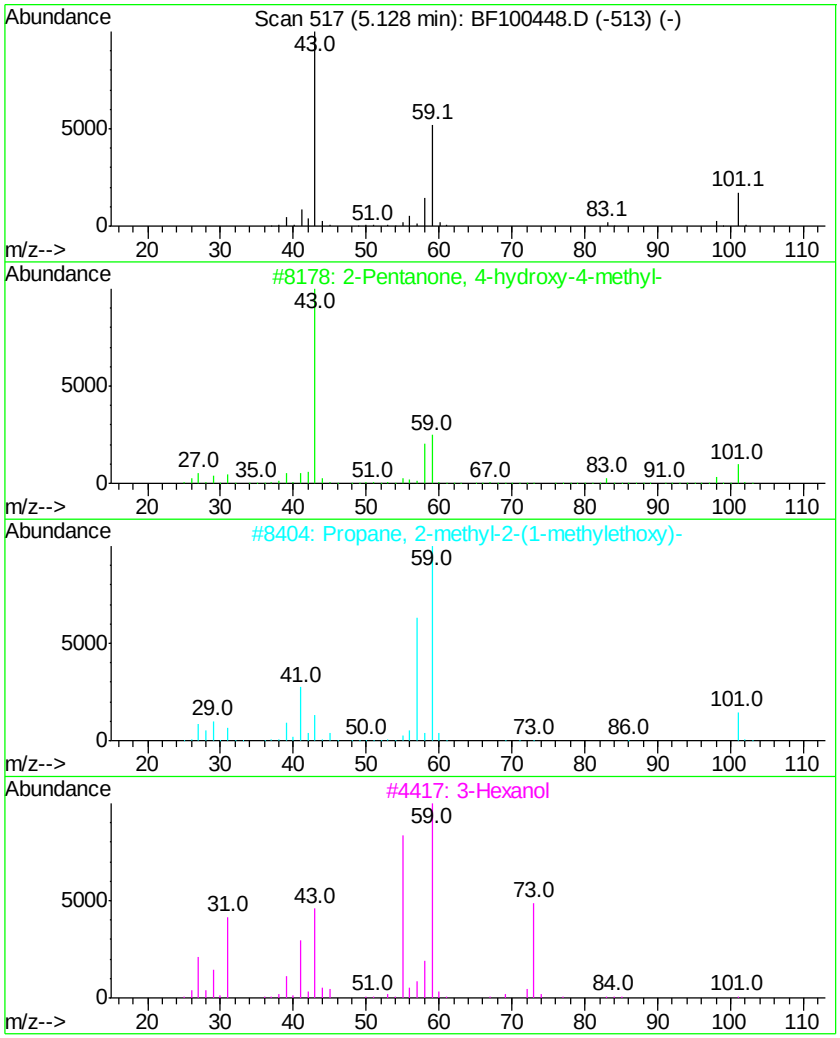
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

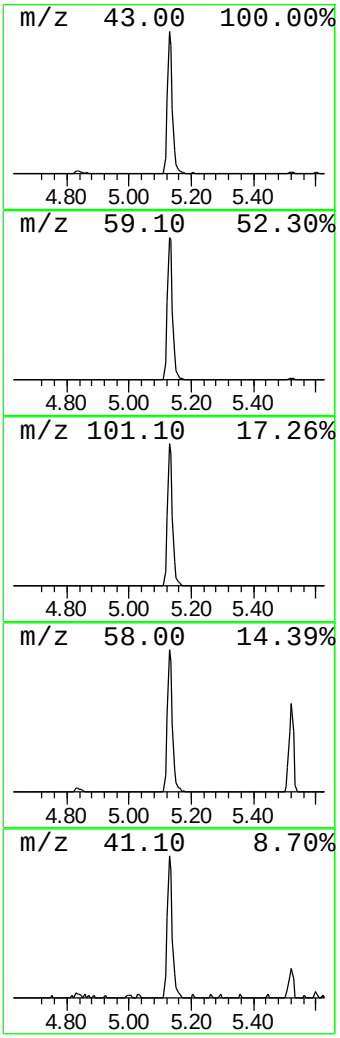
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	9.89 ng	451768	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	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	3-Hexanol	102	C6H14O	000623-37-0	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111117\
Data File : BF100448.D
Acq On : 11 Nov 2017 18:37
Operator : SJ/JU
Sample : I6388-17
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-9

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

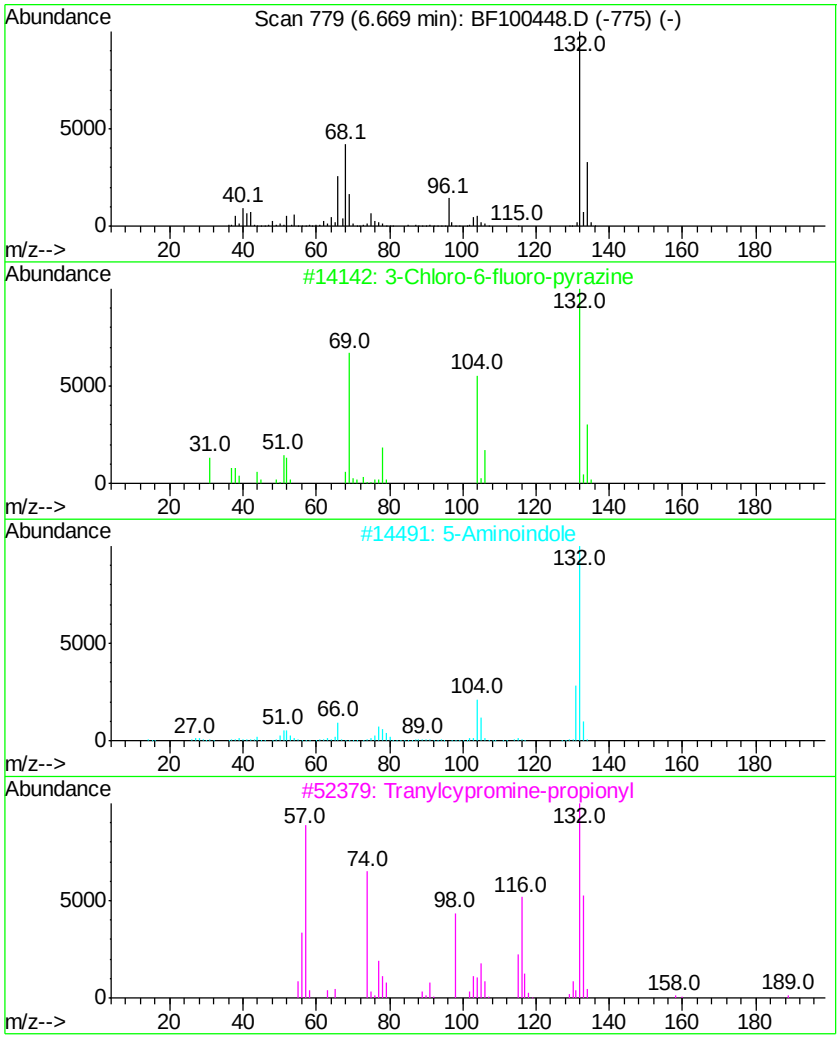
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

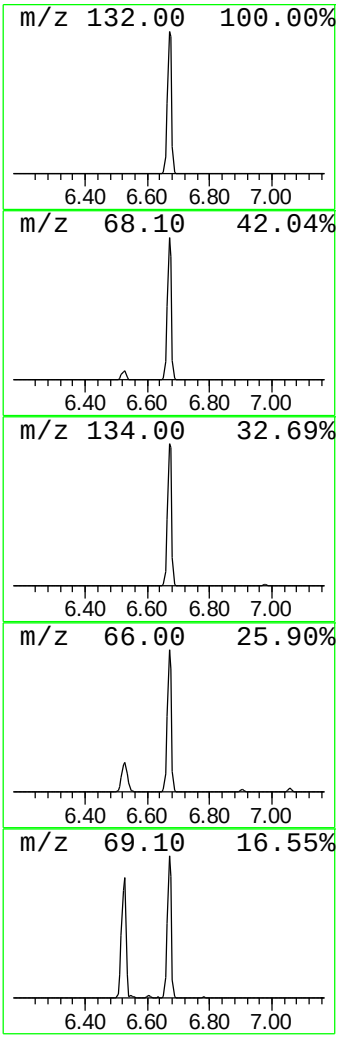
****

Peak Number 2 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	50.01 ng	2284310	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	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Data File : BF100448.D
Acq On : 11 Nov 2017 18:37
Operator : SJ/JU
Sample : I6388-17
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-9

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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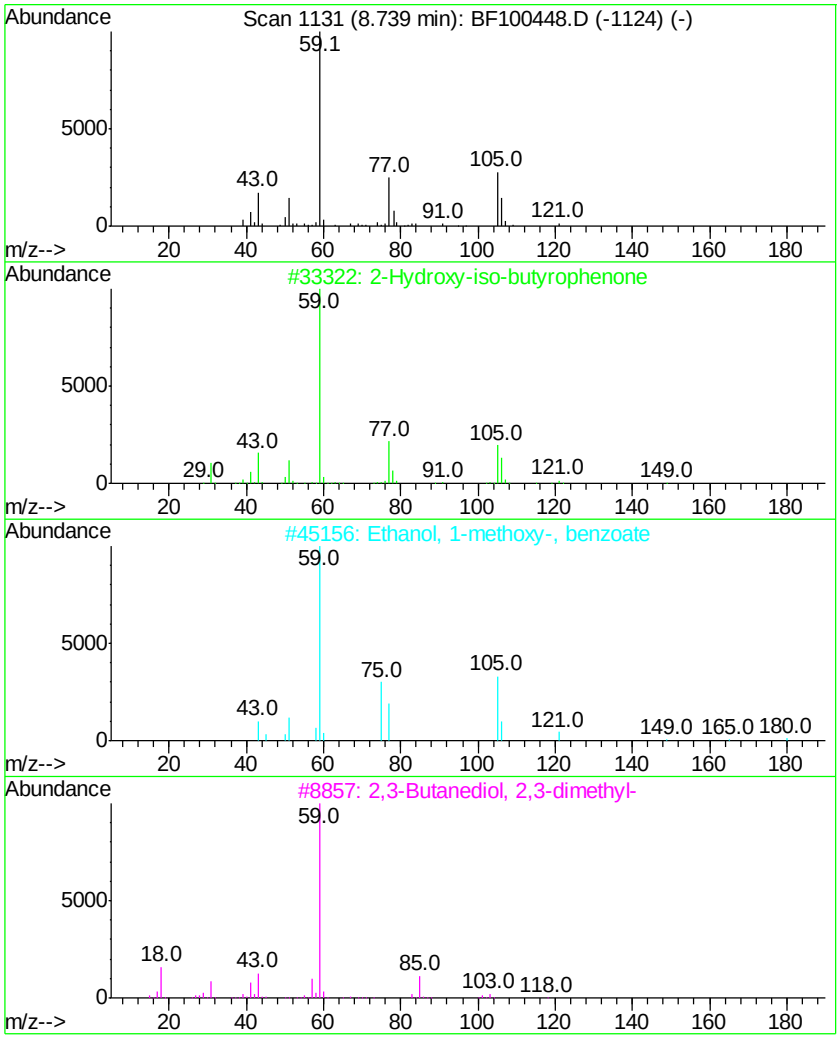
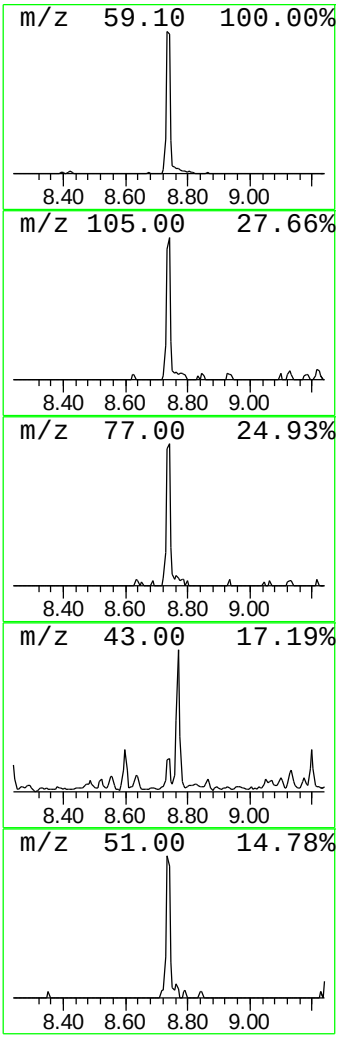
Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.74	2.07 ng	111162	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	50
3	2,3-Butanediol, 2,3-dimethyl-	118	C6H14O2	000076-09-5	23
4	Formamide, N-methyl-	59	C2H5NO	000123-39-7	9
5	Oxirane, tetramethyl-	100	C6H12O	005076-20-0	9





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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-9

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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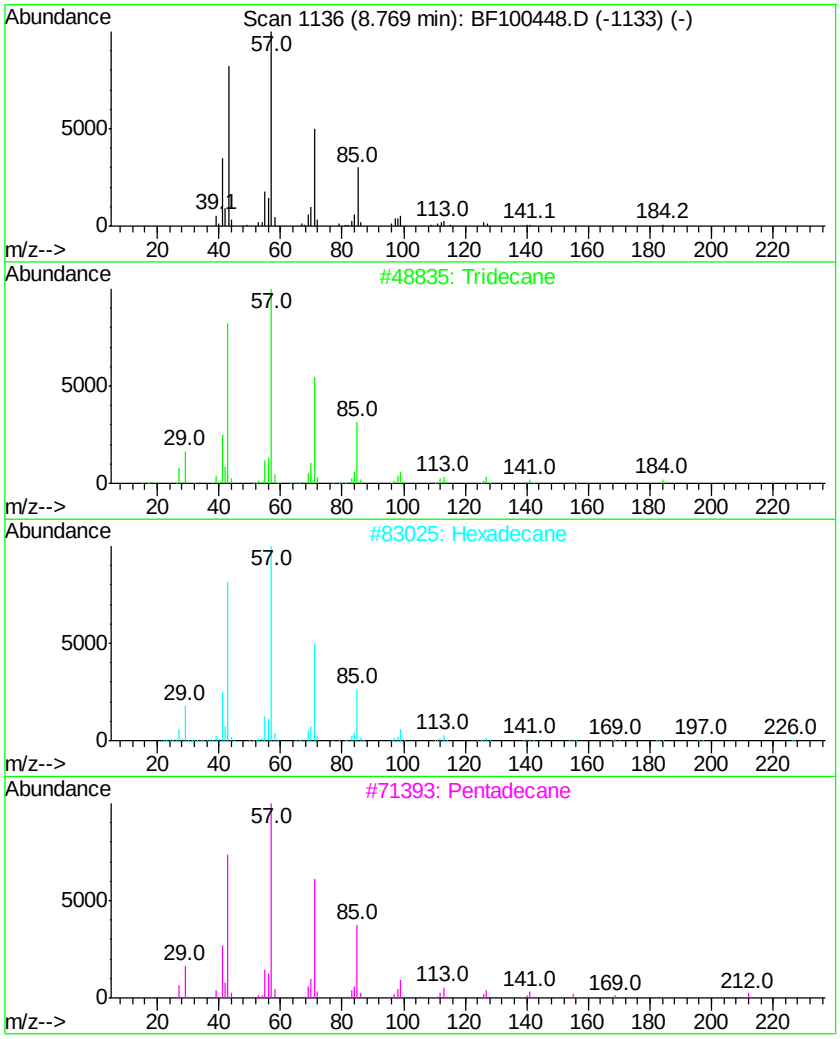
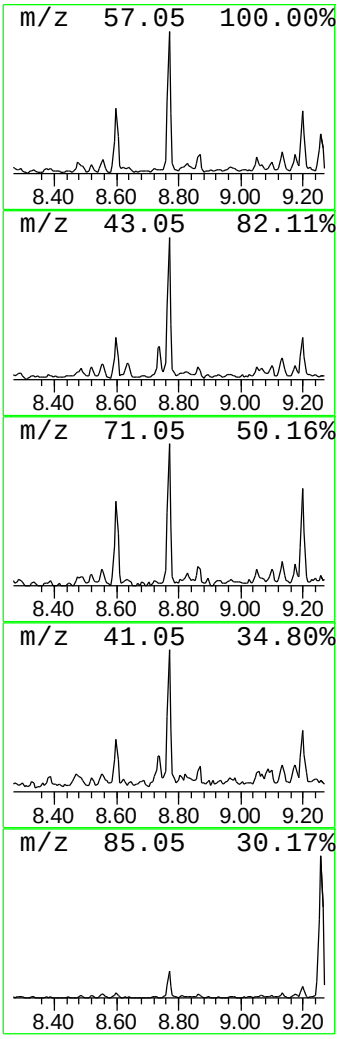
Peak Number 5 Tridecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.77	2.27 ng	121676	Naphthalene-d8	8.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	94
2	Hexadecane	226	C16H34	000544-76-3	90
3	Pentadecane	212	C15H32	000629-62-9	83
4	Undecane	156	C11H24	001120-21-4	83
5	Nonane, 5-butyl-	184	C13H28	017312-63-9	81





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Sample : I6388-17
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-9

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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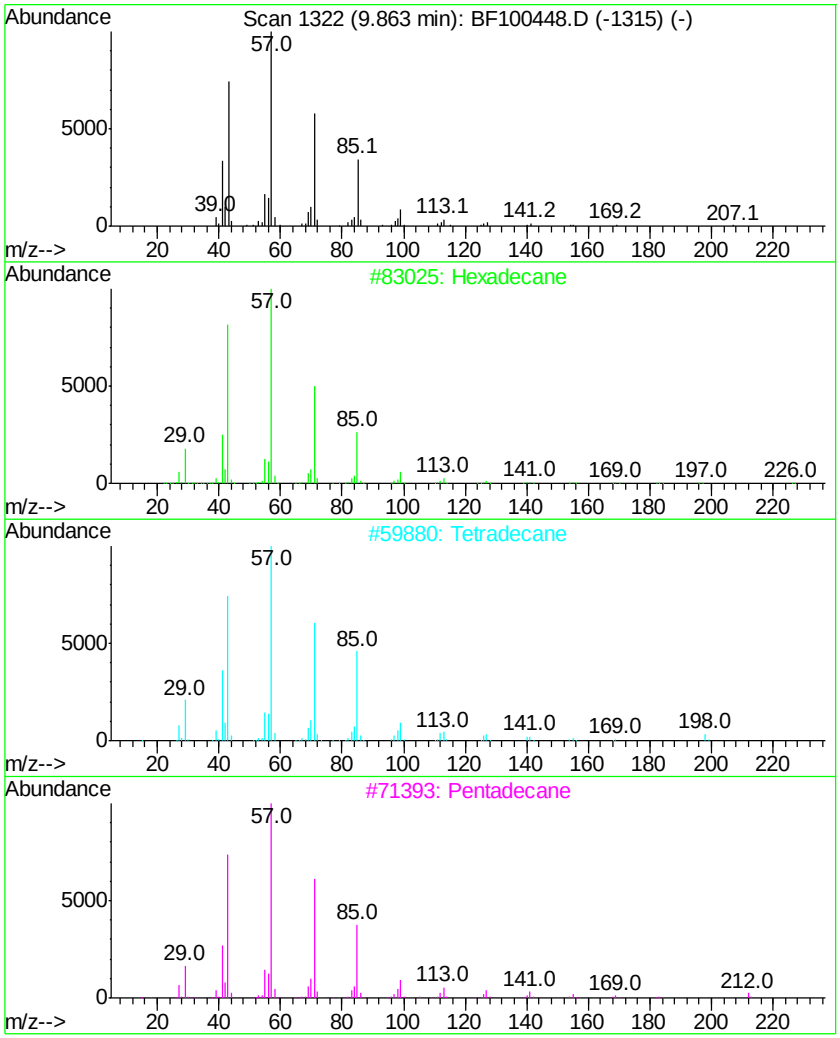
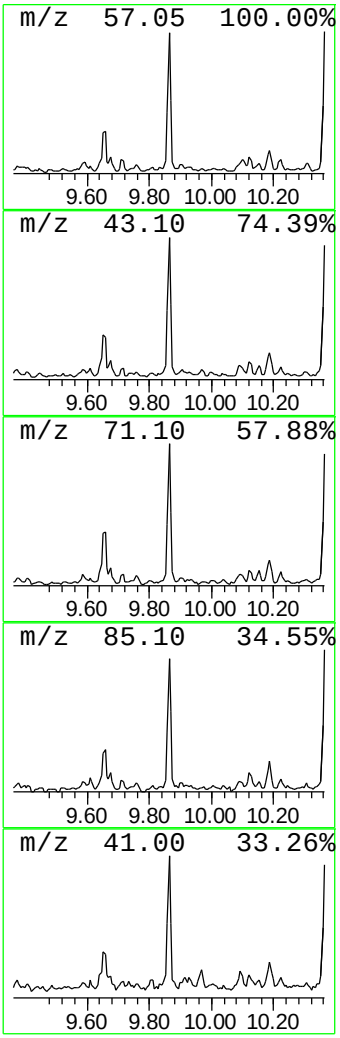
****

Peak Number 7 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.86	3.91 ng	187196	Acenaphthene-d10	9.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Tetradecane	198	C14H30	000629-59-4	90
3	Pentadecane	212	C15H32	000629-62-9	90
4	Tridecane	184	C13H28	000629-50-5	83
5	1-Decene, 4-methyl-	154	C11H22	013151-29-6	68





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Data File : BF100448.D
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Operator : SJ/JU
Sample : I6388-17
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-9

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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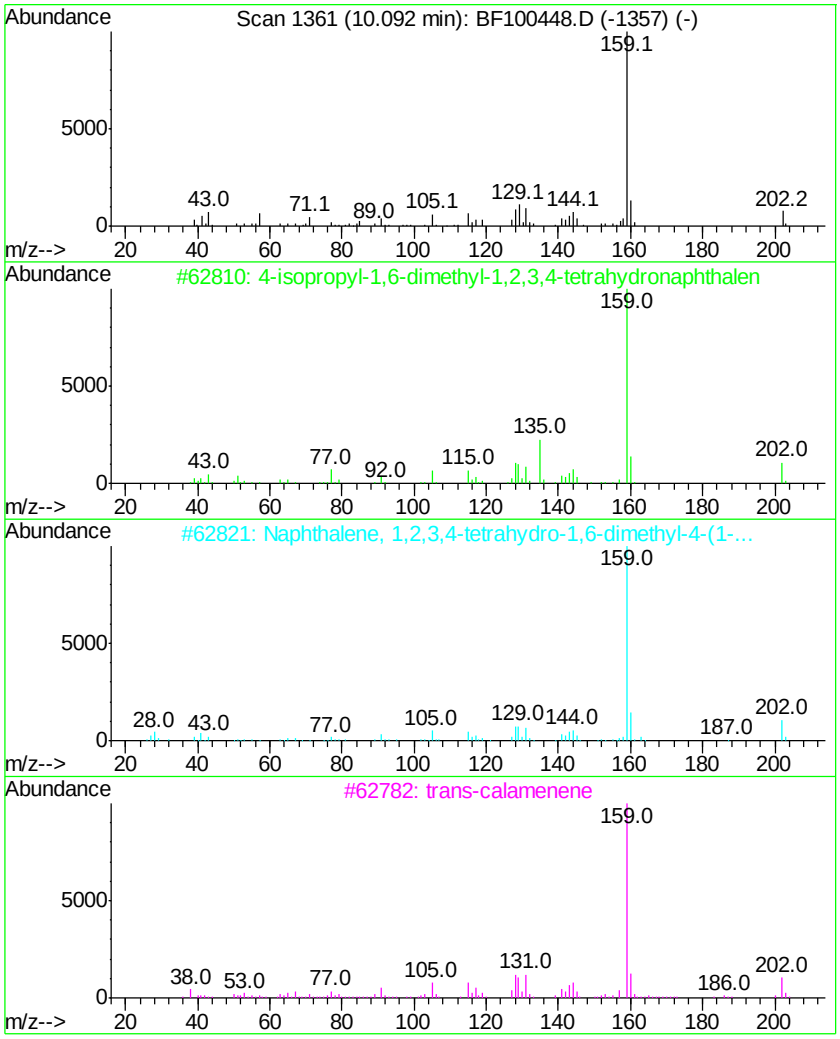
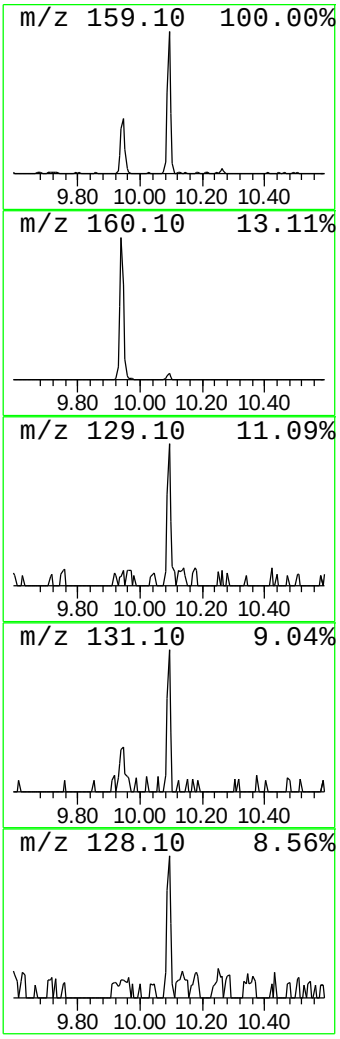
Peak Number 8 4-isopropyl-1,6-dimethyl-1,... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.09	2.26 ng	108125	Acenaphthene-d10	9.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-isopropyl-1,6-dimethyl-1,2,3,4...	202	C15H22	1000378-99-6	97
2	Naphthalene, 1,2,3,4-tetrahydro-...	202	C15H22	000483-77-2	95
3	trans-calamenene	202	C15H22	1000374-17-3	91
4	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	000475-03-6	86
5	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	030316-36-0	78





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Instrument : BNA_F
ClientSampleId : 3N-9

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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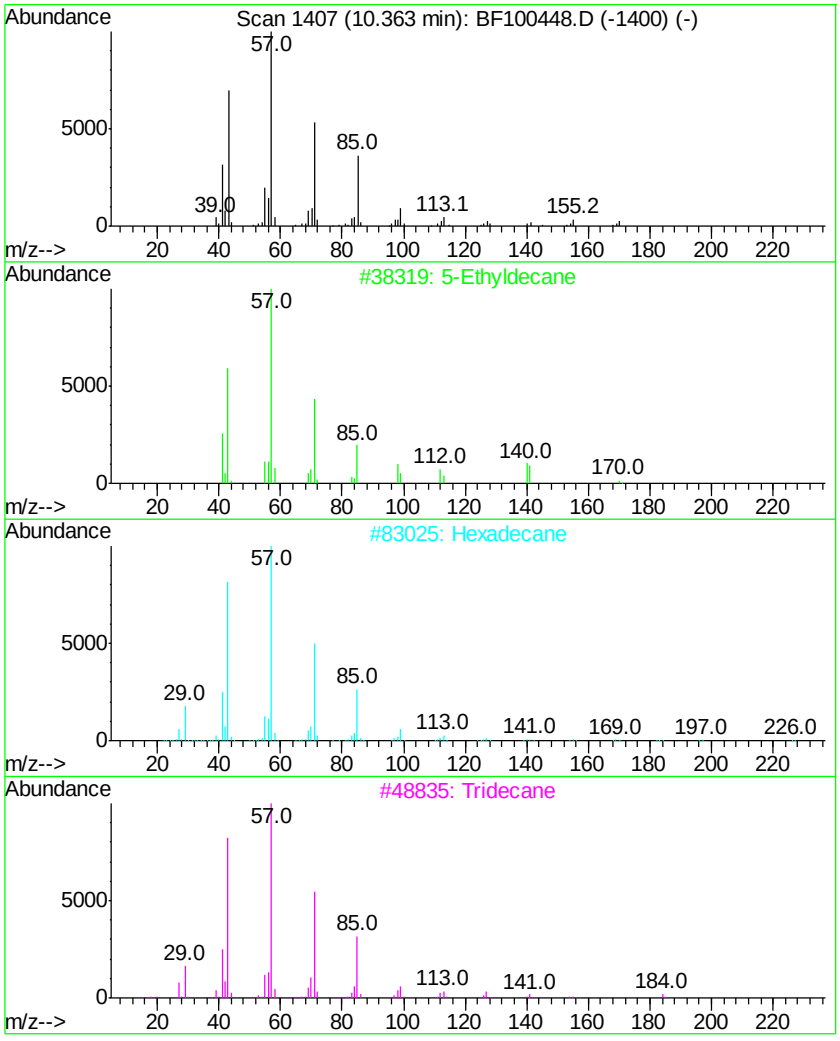
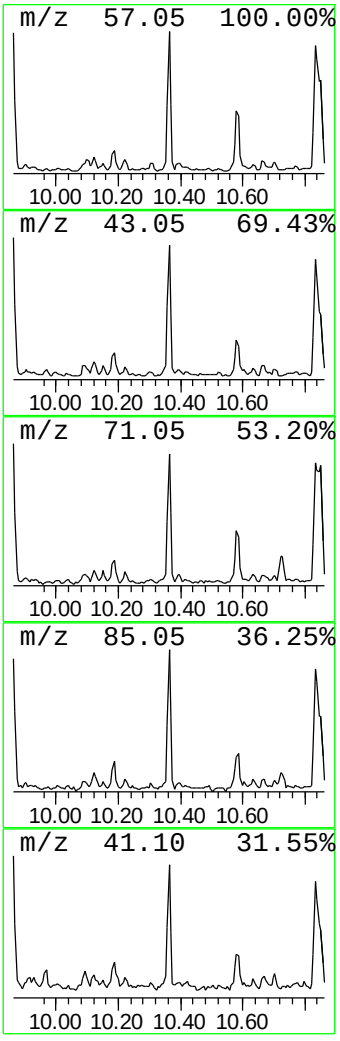
Peak Number 9 5-Ethyldecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.36	4.14 ng	198258	Acenaphthene-d10	9.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Ethyldecane	170	C12H26	017302-36-2	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Tridecane	184	C13H28	000629-50-5	90
4	Heptadecane	240	C17H36	000629-78-7	90
5	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	80





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111117\
Data File : BF100448.D
Acq On : 11 Nov 2017 18:37
Operator : SJ/JU
Sample : I6388-17
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-9

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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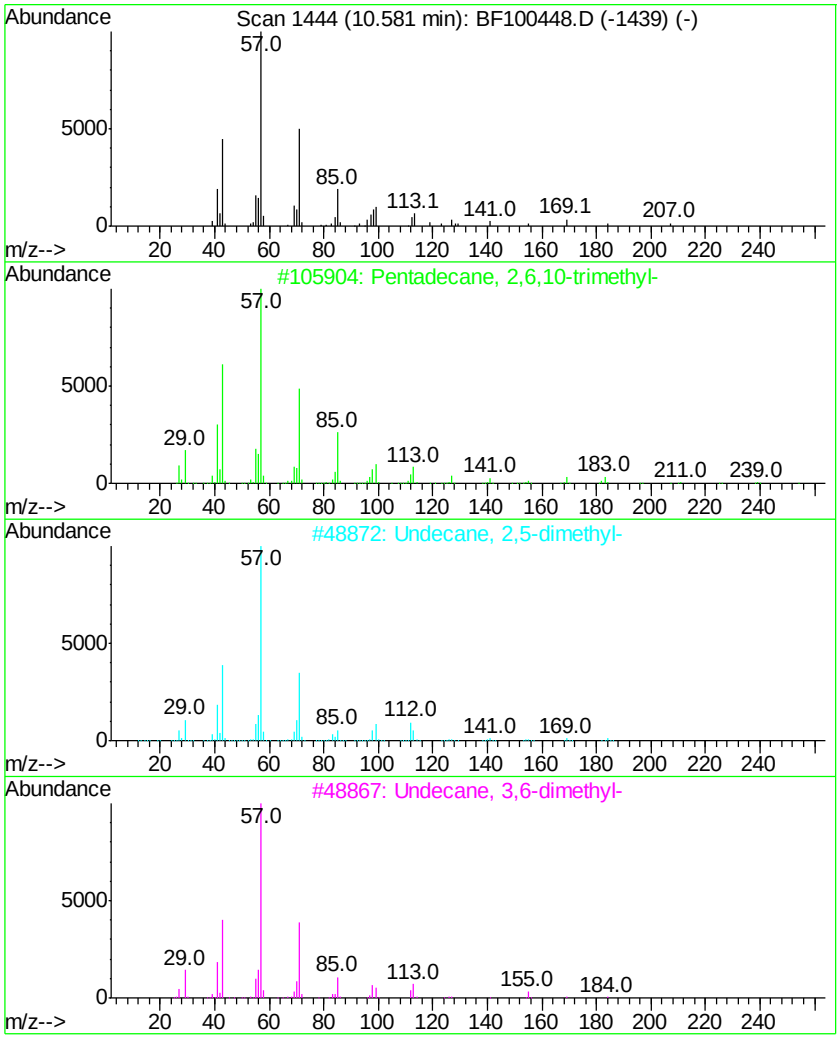
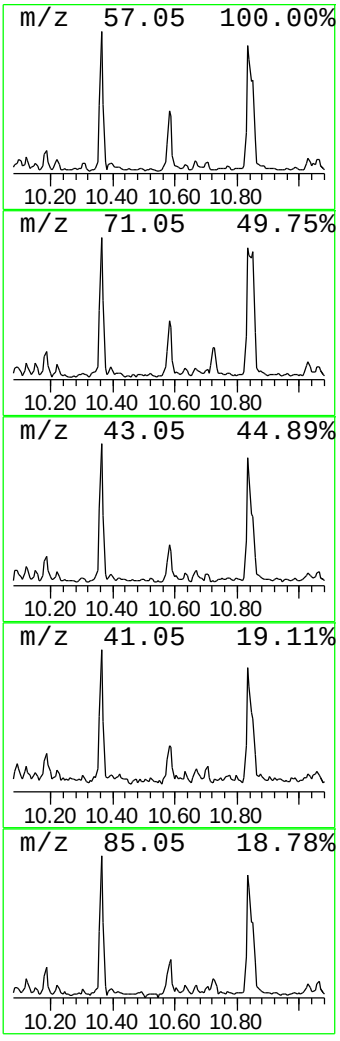
Peak Number 10 Pentadecane, 2,6,10-trimethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.58	2.14 ng	102423	Acenaphthene-d10	9.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	90
2	Undecane, 2,5-dimethyl-	184	C13H28	017301-22-3	81
3	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	78
4	Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	74
5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	72





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Acq On : 11 Nov 2017 18:37
Operator : SJ/JU
Sample : I6388-17
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-9

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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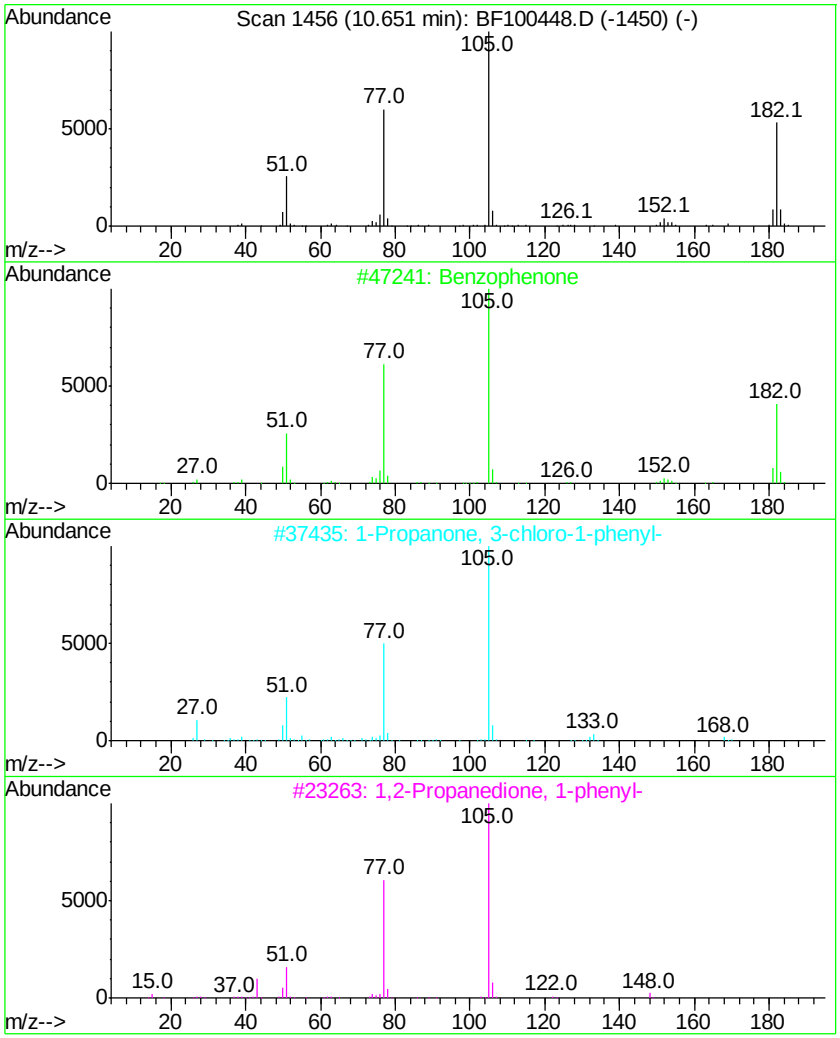
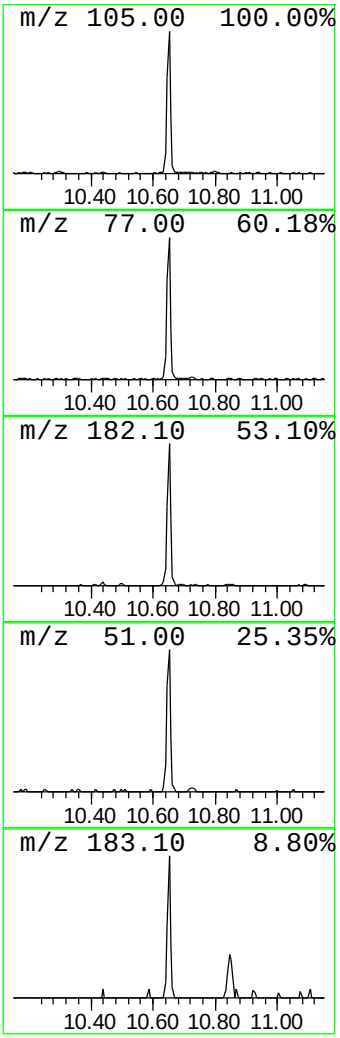
Peak Number 11 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	5.27 ng	252440	Acenaphthene-d10	9.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
3	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
4	Benzoyl bromide	184	C7H5BrO	000618-32-6	47
5	Benzenecarbothioic acid	138	C7H6OS	000098-91-9	47





Library Search Compound Report

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TIC Integration Parameters: LSCINT.P

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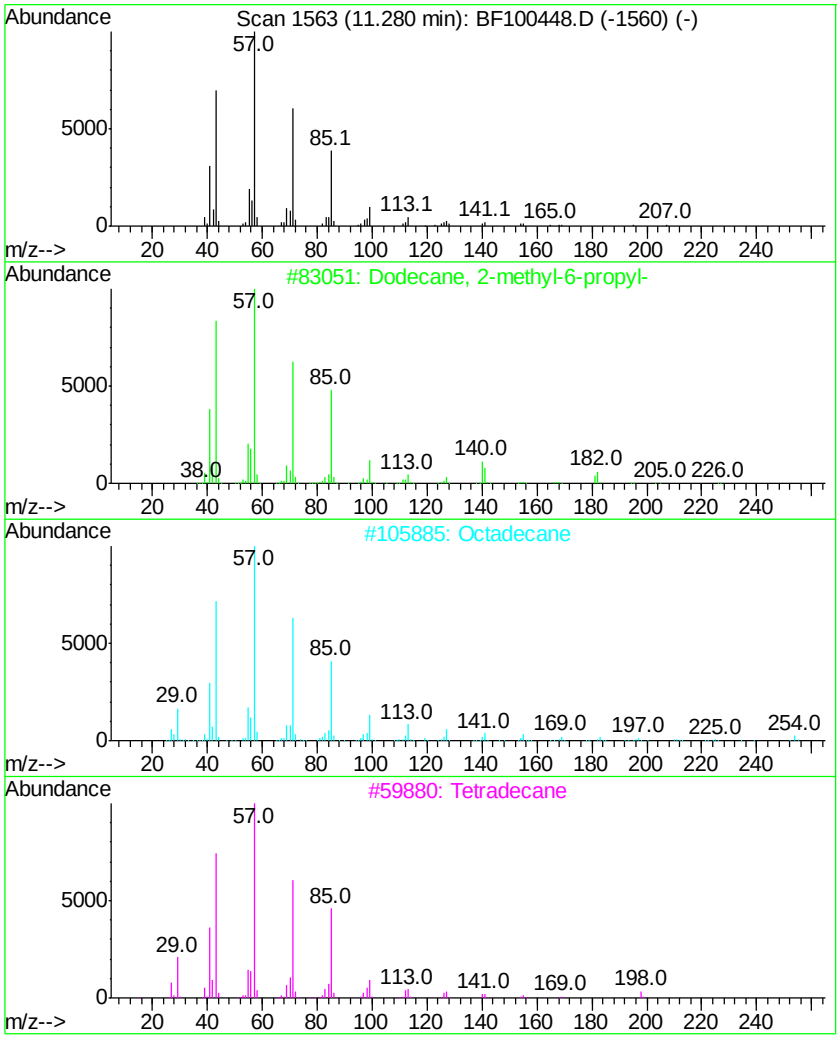
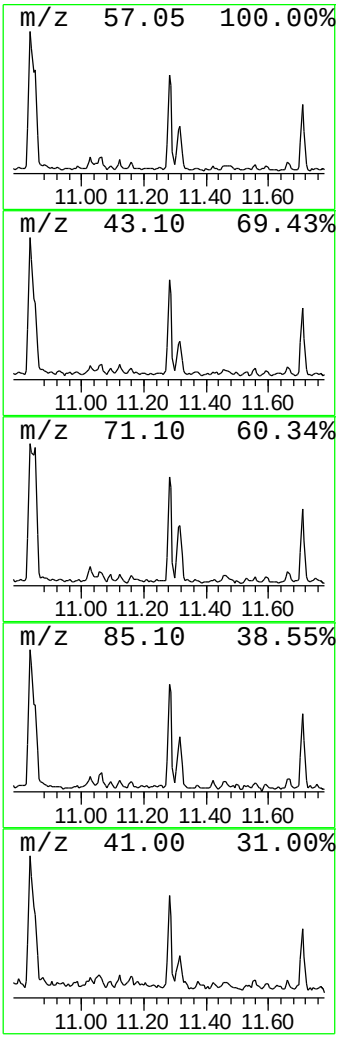
Peak Number 13 Dodecane, 2-methyl-6-propyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.28	2.93 ng	122379	Phenanthrene-d10	11.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	90
2	Octadecane	254	C18H38	000593-45-3	86
3	Tetradecane	198	C14H30	000629-59-4	86
4	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	80
5	Hexadecane	226	C16H34	000544-76-3	80





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Sample : I6388-17
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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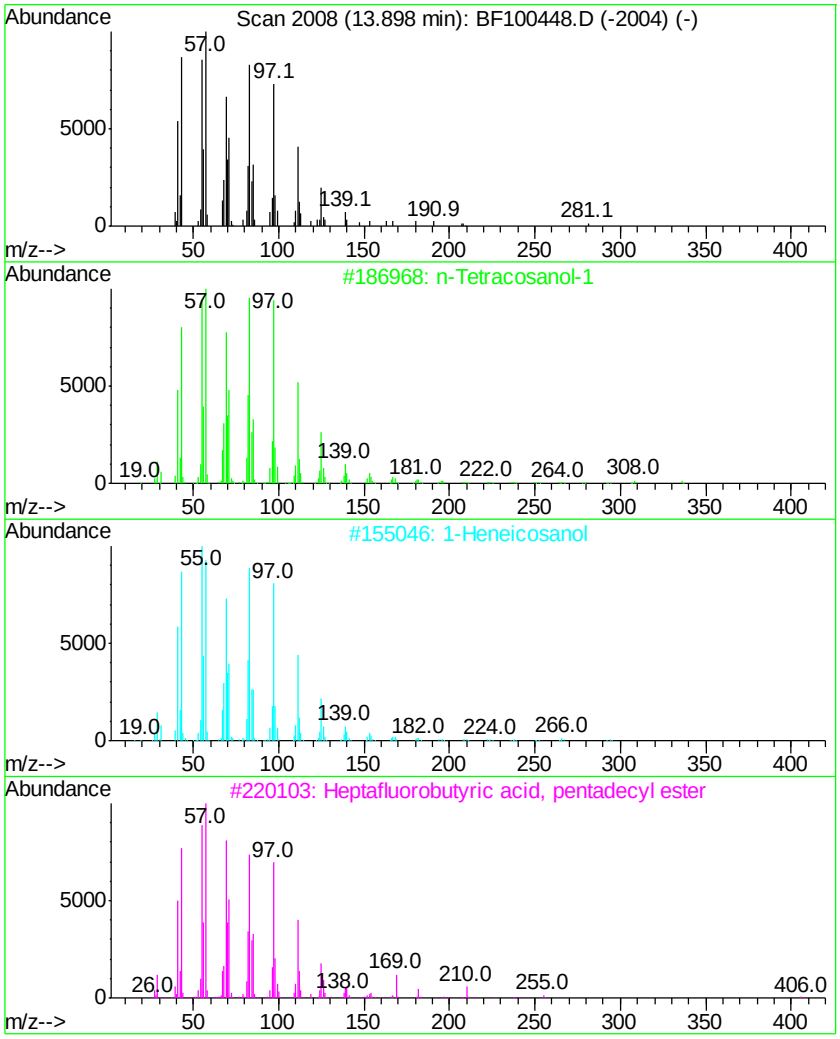
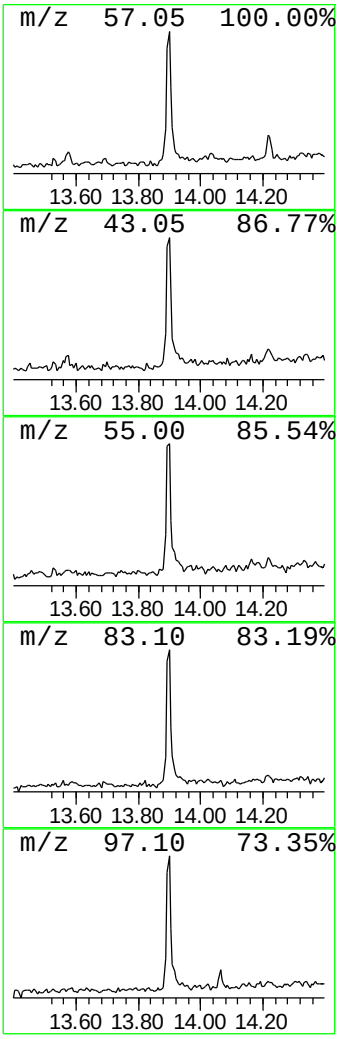
Peak Number 14 n-Tetracosanol-1 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	3.59 ng	157648	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94





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TIC Integration Parameters: LSCINT.P

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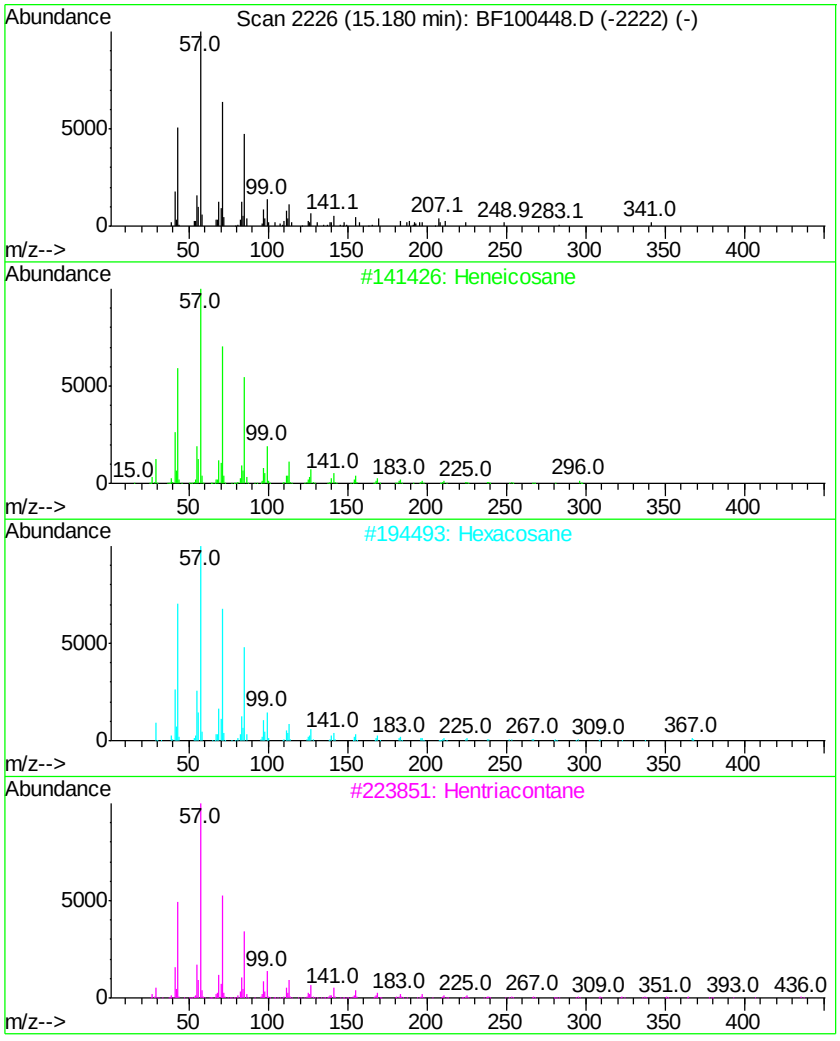
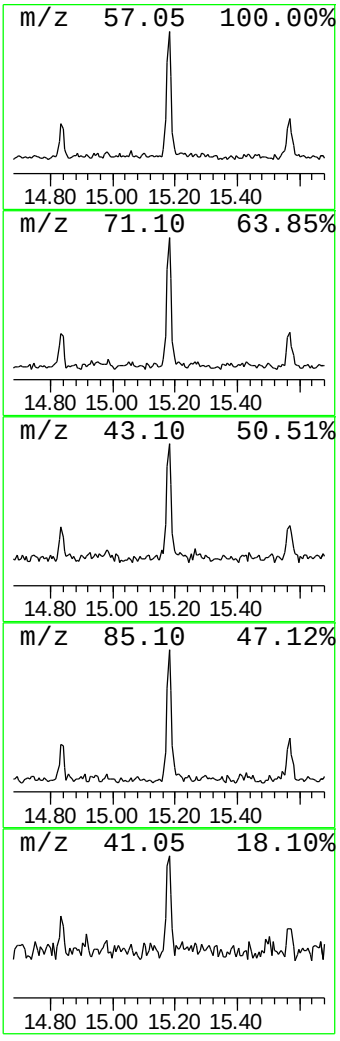
Peak Number 15 Heneicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.18	2.75 ng	89334	Perylene-d12	15.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	87
2	Hexacosane	366	C26H54	000630-01-3	87
3	Hentriacontane	437	C31H64	000630-04-6	87
4	Octadecane	254	C18H38	000593-45-3	83
5	Docosane	310	C22H46	000629-97-0	83





Tentatively Identified Compound (LSC) summary

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Sample : I6388-17
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-9

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	451768	1	6.90	913496	20.0
unknown6.67	6.67	50.0	ng	2284310	1	6.90	913496	20.0
2-Hydroxy-iso-but...	8.74	2.1	ng	111162	2	8.19	1073430	20.0
Tridecane	8.77	2.3	ng	121676	2	8.19	1073430	20.0
Hexadecane	9.86	3.9	ng	187196	3	9.94	958439	20.0
4-isopropyl-1,6-d...	10.09	2.3	ng	108125	3	9.94	958439	20.0
5-Ethyldecane	10.36	4.1	ng	198258	3	9.94	958439	20.0
Pentadecane, 2,6,...	10.58	2.1	ng	102423	3	9.94	958439	20.0
Benzophenone	10.65	5.3	ng	252440	3	9.94	958439	20.0
Dodecane, 2-methy...	11.28	2.9	ng	122379	4	11.43	834451	20.0
n-Tetracosanol-1	13.90	3.6	ng	157648	5	14.06	878830	20.0
Heneicosane	15.18	2.8	ng	89334	6	15.55	650708	20.0