LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020217\
Data File : BF092757.D
Acq On : 3 Feb 2017 1:21
Operator : SJ/MA
Sample : I1650-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39-COMP

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-BF013017.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	5.127	263	266	277	rBV	1553873	2392807	46.38%	5.491%
2	5.550	300	303	306	rBV	4018415	4733577	91.76%	10.863%
3	6.579	390	393	396	rBV	4104840	5158652	100.00%	11.839%
4	6.704	401	404	407	rBV	4001819	4805732	93.16%	11.029%
5	6.933	422	424	427	rVB	1069971	885980	17.17%	2.033%
6	7.093	435	438	440	rBV	3640373	3358784	65.11%	7.708%
7	7.504	471	474	476	rBV	2747237	2905202	56.32%	6.667%
8	8.224	534	537	539	rBV	1265355	1145811	22.21%	2.630%
9	9.299	628	631	634	rBV	3987890	4275971	82.89%	9.813%
10	9.687	663	665	668	rVB	422717	524669	10.17%	1.204%
11	9.973	688	690	692	rBV	1039447	1144617	22.19%	2.627%
12	10.408	724	728	729	rVV2	66087	114082	2.21%	0.262%
13	10.522	736	738	741	rVB	70759	72668	1.41%	0.167%
14	10.625	741	747	750	rBV4	34243	93771	1.82%	0.215%
15	10.762	757	759	762	rBV2	1591773	2323971	45.05%	5.333%
16	10.876	766	769	774	rVB2	125198	183317	3.55%	0.421%
17	11.322	805	808	809	rBV	129416	113867	2.21%	0.261%
18	11.356	809	811	814	rVB	45961	55313	1.07%	0.127%
19	11.459	818	820	824	rBV2	1133161	1431362	27.75%	3.285%
20	11.539	824	827	828	rVB	76100	93462	1.81%	0.214%
21	11.745	843	845	847	rVB	90997	81905	1.59%	0.188%
22	11.962	861	864	865	rBV	80176	73856	1.43%	0.169%
23	11.985	865	866	868	rVV	77045	83766	1.62%	0.192%
24	12.076	872	874	878	rVB3	85114	159080	3.08%	0.365%
25	12.511	909	912	913	rBV	55091	54156	1.05%	0.124%
26	12.545	913	915	918	rVB2	37213	55725	1.08%	0.128%
27	12.671	924	926	928	rBV	312978	263692	5.11%	0.605%
28	12.899	941	946	949	rBV	283416	332352	6.44%	0.763%
29	13.048	956	959	961	rBV	3238568	3174990	61.55%	7.286%
30	13.231	971	975	976	rBV	50427	65976	1.28%	0.151%
31	13.299	976	981	982	rBV2	38925	61696	1.20%	0.142%
32	13.939	1035	1037	1042	rVB	74886	117298	2.27%	0.269%
33	14.099	1048	1051	1052	rBV	833026	936367	18.15%	2.149%
34	14.122	1052	1053	1056	rVB	125285	103616	2.01%	0.238%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020217\
Data File : BF092757.D
Acq On : 3 Feb 2017 1:21
Operator : SJ/MA
Sample : I1650-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39-COMP

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-BF013017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.476	1080	1084	1086	rBV	26519	55718	1.08%	0.128%
36	14.557	1089	1091	1094	rBV2	40950	66494	1.29%	0.153%
37	15.128	1139	1141	1145	rBV	76800	153132	2.97%	0.351%
38	15.197	1145	1147	1149	rVB	100730	116844	2.27%	0.268%
39	15.425	1165	1167	1170	rVB	41161	62706	1.22%	0.144%
40	15.494	1170	1173	1176	rBV	65659	93623	1.81%	0.215%
41	15.551	1176	1178	1185	rVV	555534	906515	17.57%	2.080%
42	16.008	1215	1218	1221	rBV	134285	202573	3.93%	0.465%
43	16.511	1259	1262	1270	rBV2	23025	66840	1.30%	0.153%
44	17.002	1302	1305	1309	rBV2	27663	56117	1.09%	0.129%
45	17.094	1309	1313	1317	rVV2	67046	146388	2.84%	0.336%
46	17.174	1317	1320	1323	rVB3	45172	80785	1.57%	0.185%
47	17.437	1340	1343	1348	rVB	23142	63132	1.22%	0.145%
48	17.528	1348	1351	1354	rBV3	28060	58439	1.13%	0.134%
49	18.603	1441	1445	1453	rVB6	19142	67559	1.31%	0.155%

Sum of corrected areas: 43574955

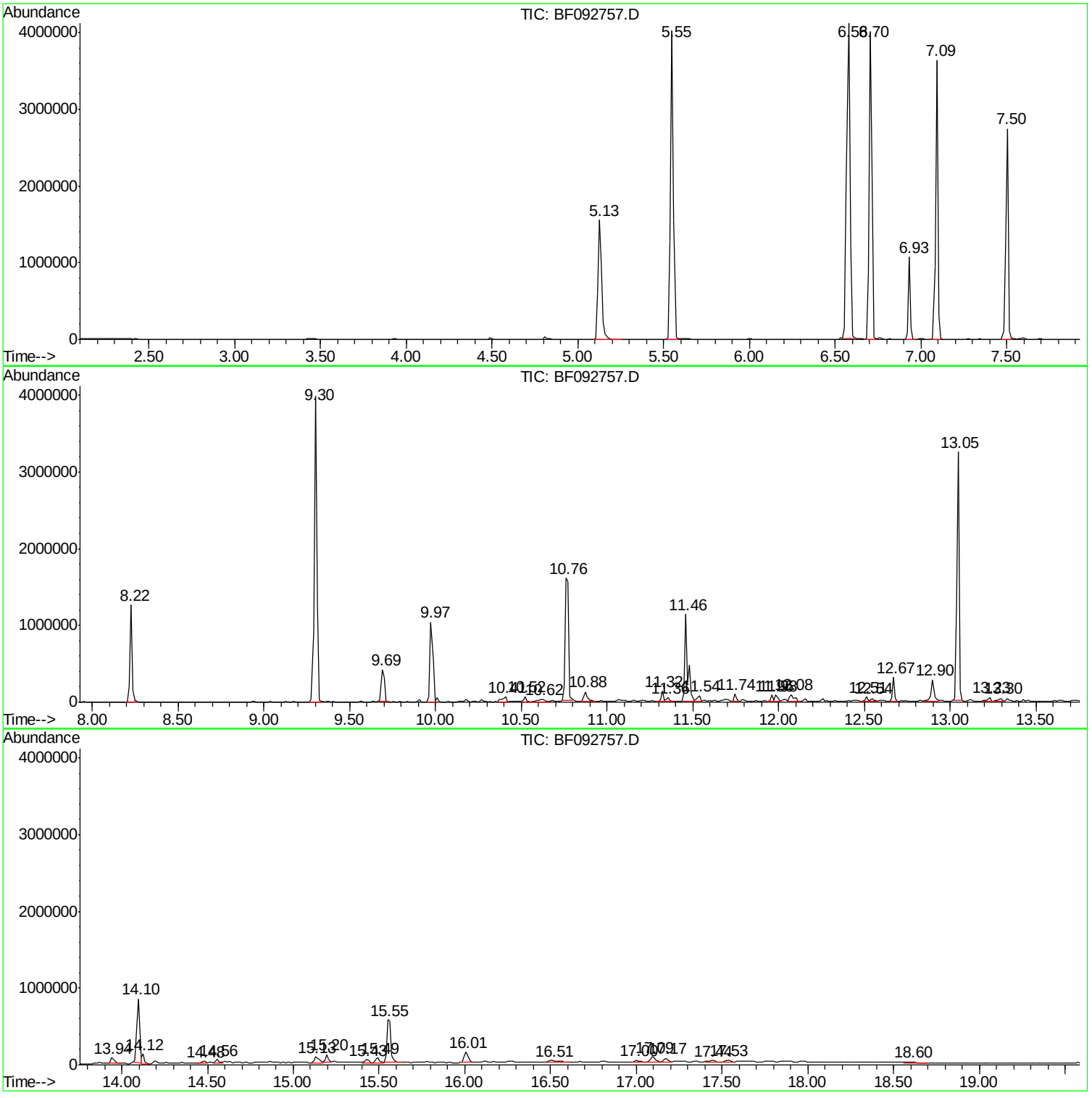
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020217\
Data File : BF092757.D
Acq On : 3 Feb 2017 1:21
Operator : SJ/MA
Sample : I1650-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020217\
Data File : BF092757.D
Acq On : 3 Feb 2017 1:21
Operator : SJ/MA
Sample : I1650-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

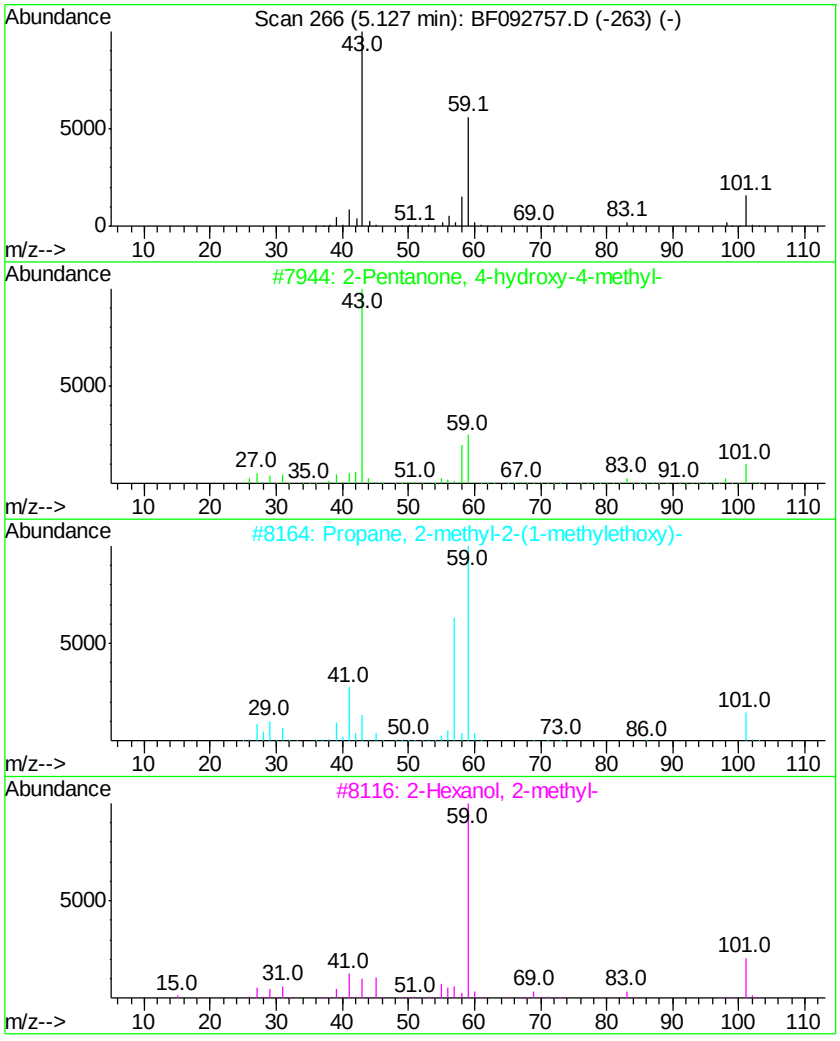
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

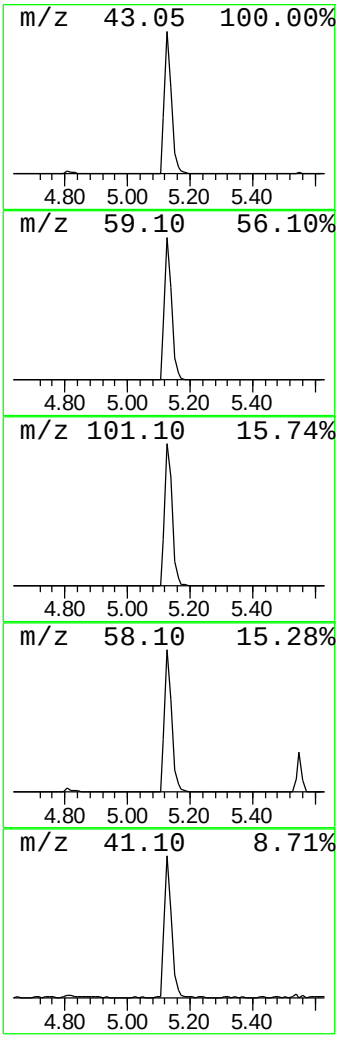
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	54.01 ng	2392810	1,4-Dichlorobenzene-d4	6.93

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	42
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020217\
Data File : BF092757.D
Acq On : 3 Feb 2017 1:21
Operator : SJ/MA
Sample : I1650-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

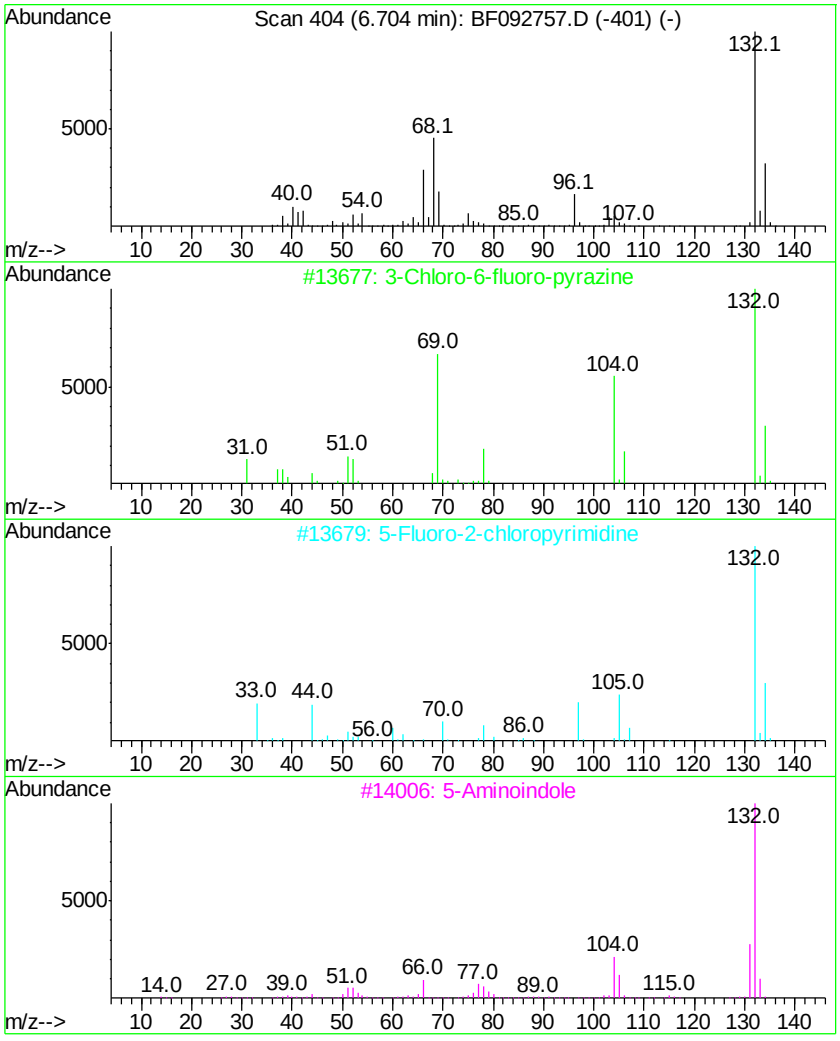
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

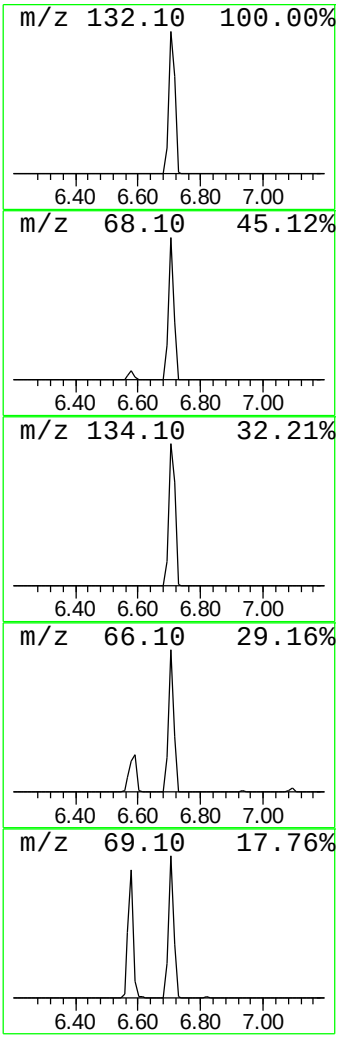
****

Peak Number 2 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	108.48 ng	4805730	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Xenon	132	Xe	007440-63-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020217\
Data File : BF092757.D
Acq On : 3 Feb 2017 1:21
Operator : SJ/MA
Sample : I1650-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

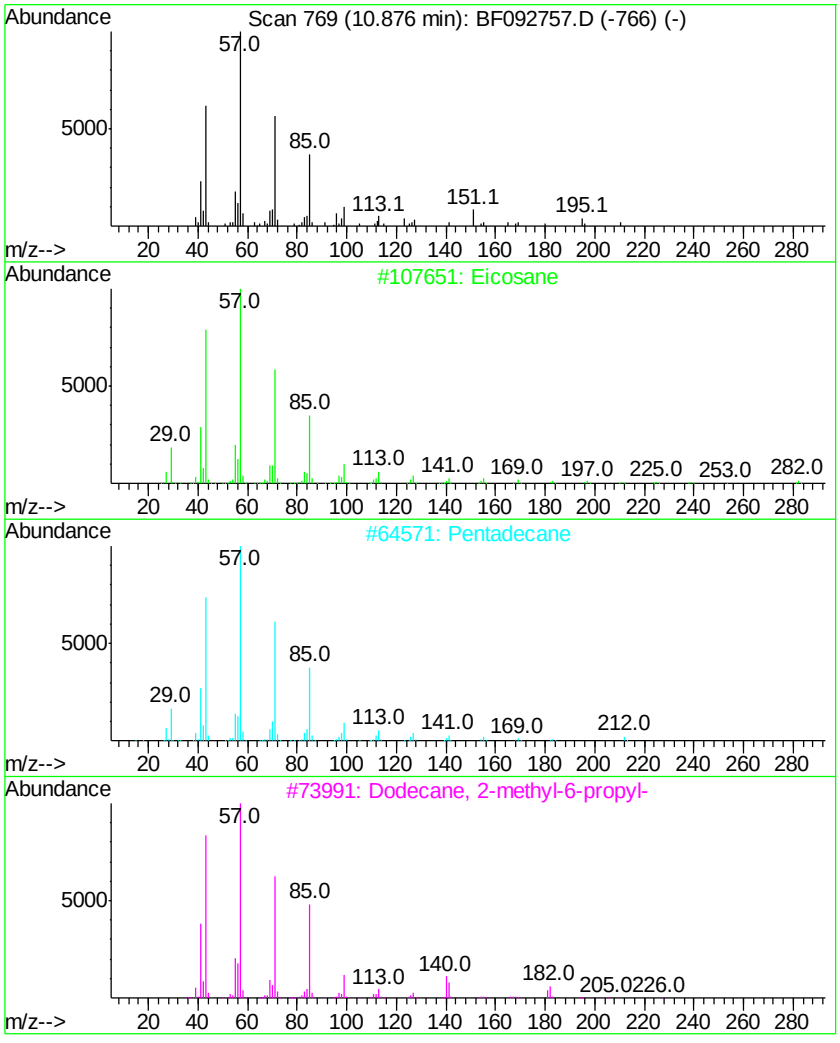
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

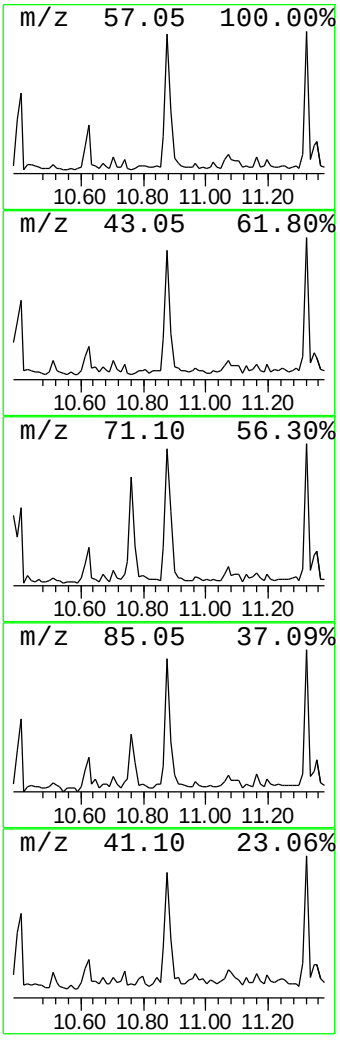
****

Peak Number 4 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.88	2.56 ng	183317	Phenanthrene-d10	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	74
2	Pentadecane	212	C15H32	000629-62-9	74
3	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	72
4	Tetradecane	198	C14H30	000629-59-4	72
5	Hexadecane	226	C16H34	000544-76-3	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020217\
Data File : BF092757.D
Acq On : 3 Feb 2017 1:21
Operator : SJ/MA
Sample : I1650-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

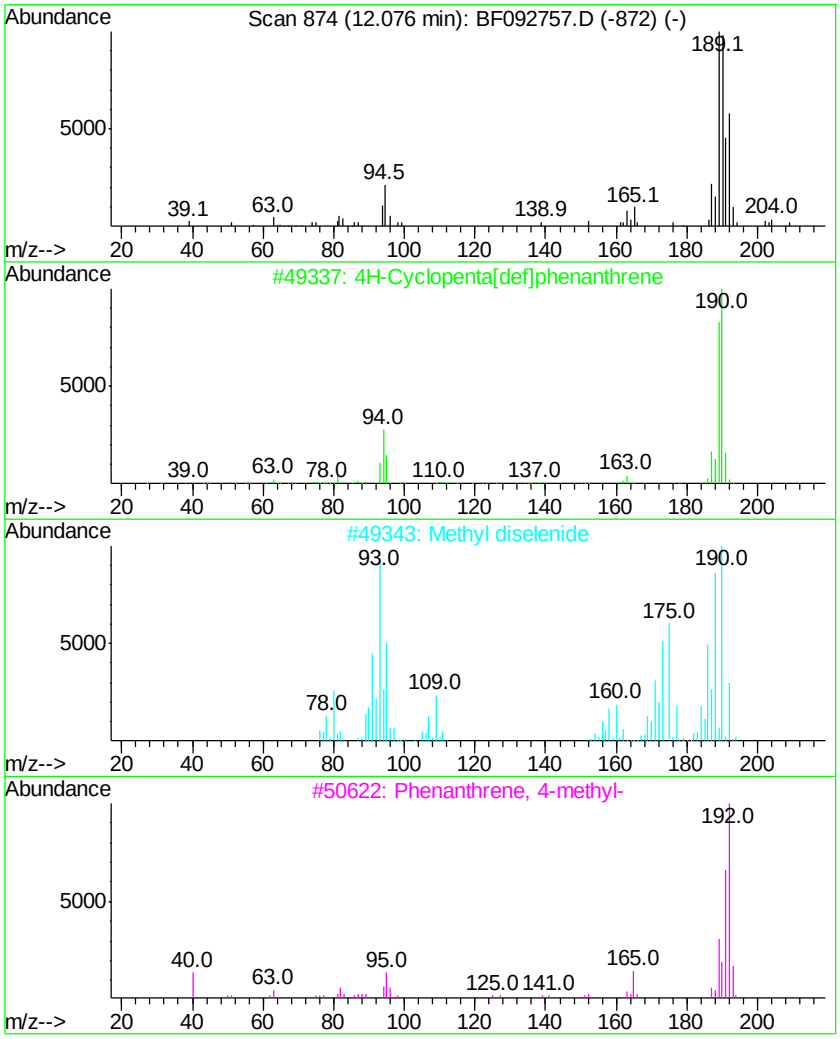
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

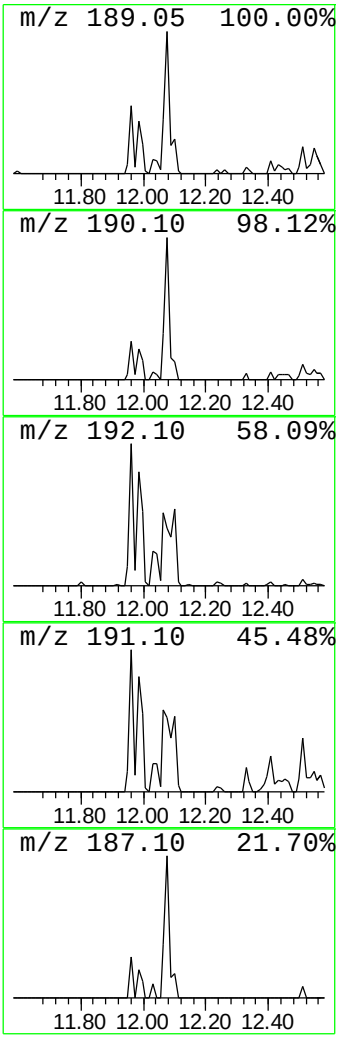
****

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.08	2.22 ng	159080	Phenanthrene-d10	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	92
2	Methyl diselenide	190	C2H6Se2	007101-31-7	41
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	38
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	30
5	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	30





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020217\
Data File : BF092757.D
Acq On : 3 Feb 2017 1:21
Operator : SJ/MA
Sample : I1650-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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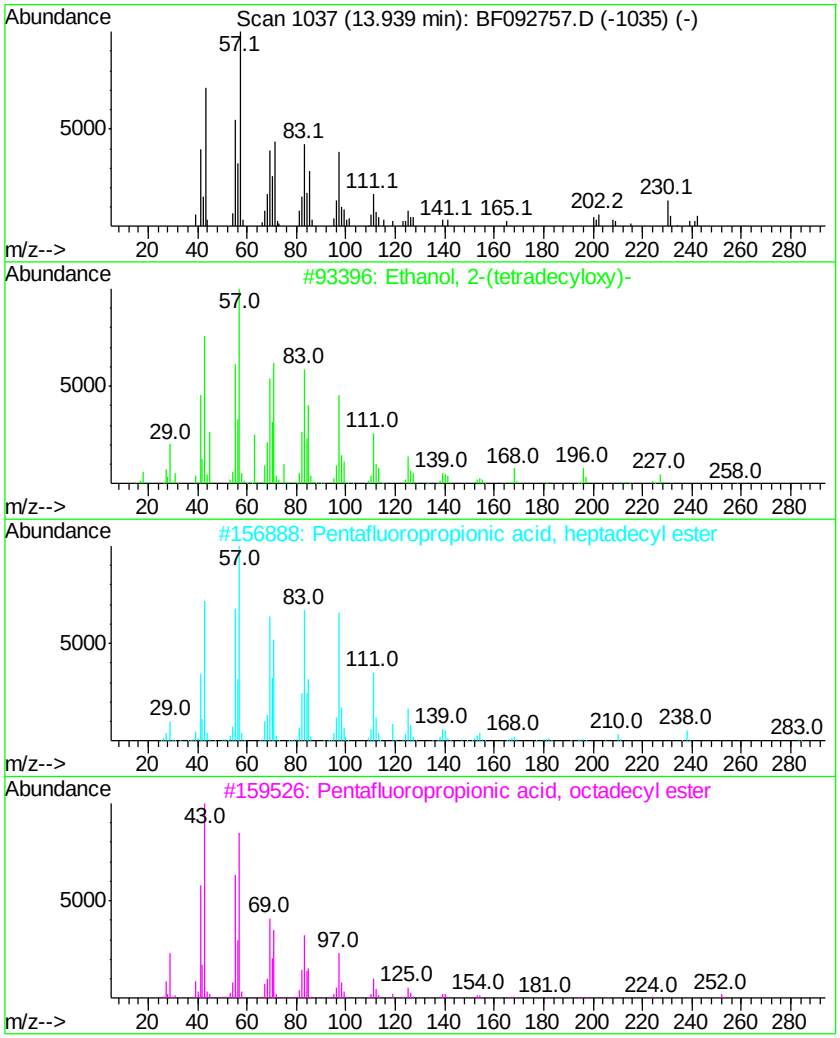
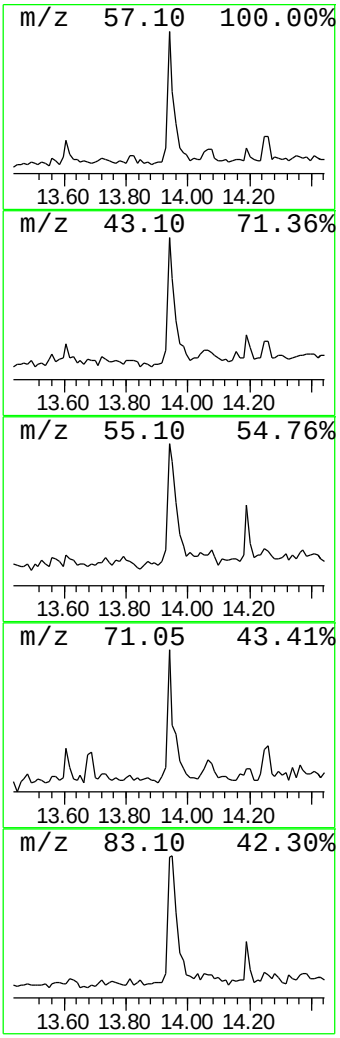
Peak Number 6 Ethanol, 2-(tetradecyloxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	2.51 ng	117298	Chrysene-d12	14.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
2	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	87
3	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	83
4	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	76
5	Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	76





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020217\
Data File : BF092757.D
Acq On : 3 Feb 2017 1:21
Operator : SJ/MA
Sample : I1650-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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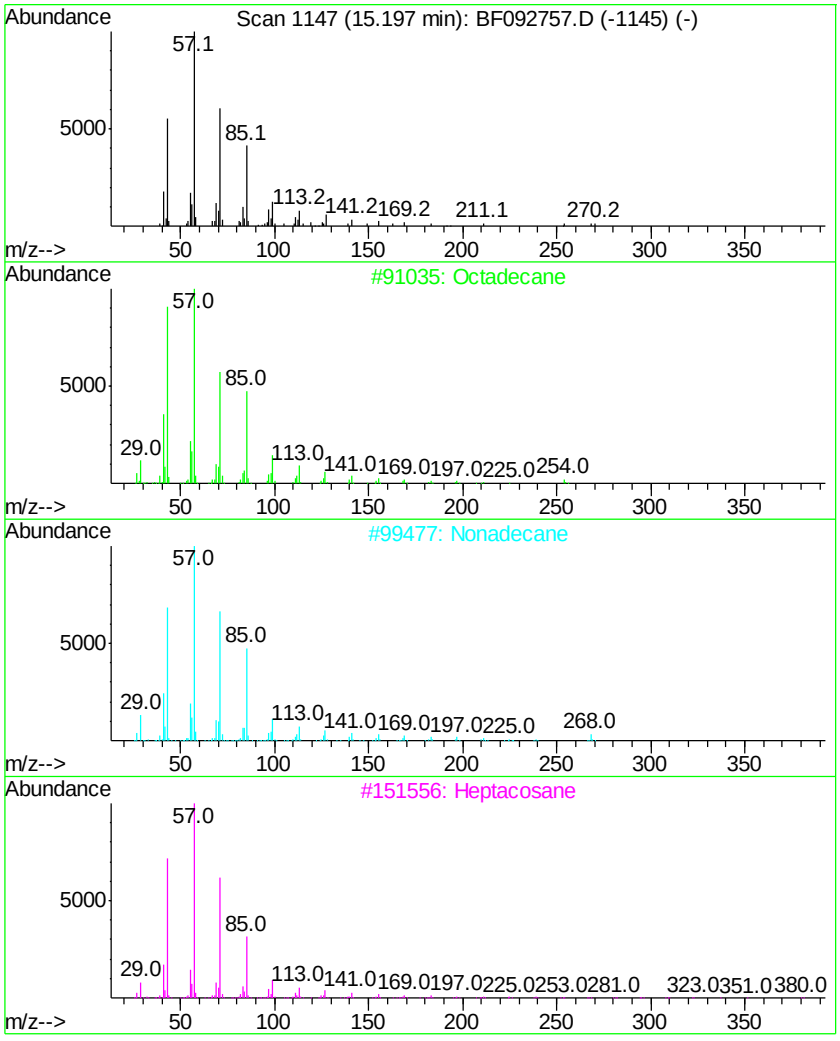
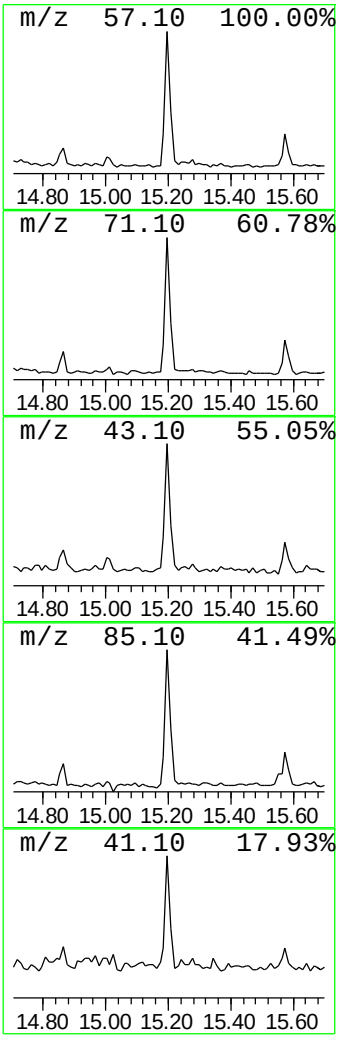
Peak Number 7 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.20	2.58 ng	116844	Perylene-d12	15.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	96
2	Nonadecane	268	C19H40	000629-92-5	93
3	Heptacosane	380	C27H56	000593-49-7	91
4	Pentacosane	352	C25H52	000629-99-2	91
5	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020217\
Data File : BF092757.D
Acq On : 3 Feb 2017 1:21
Operator : SJ/MA
Sample : I1650-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

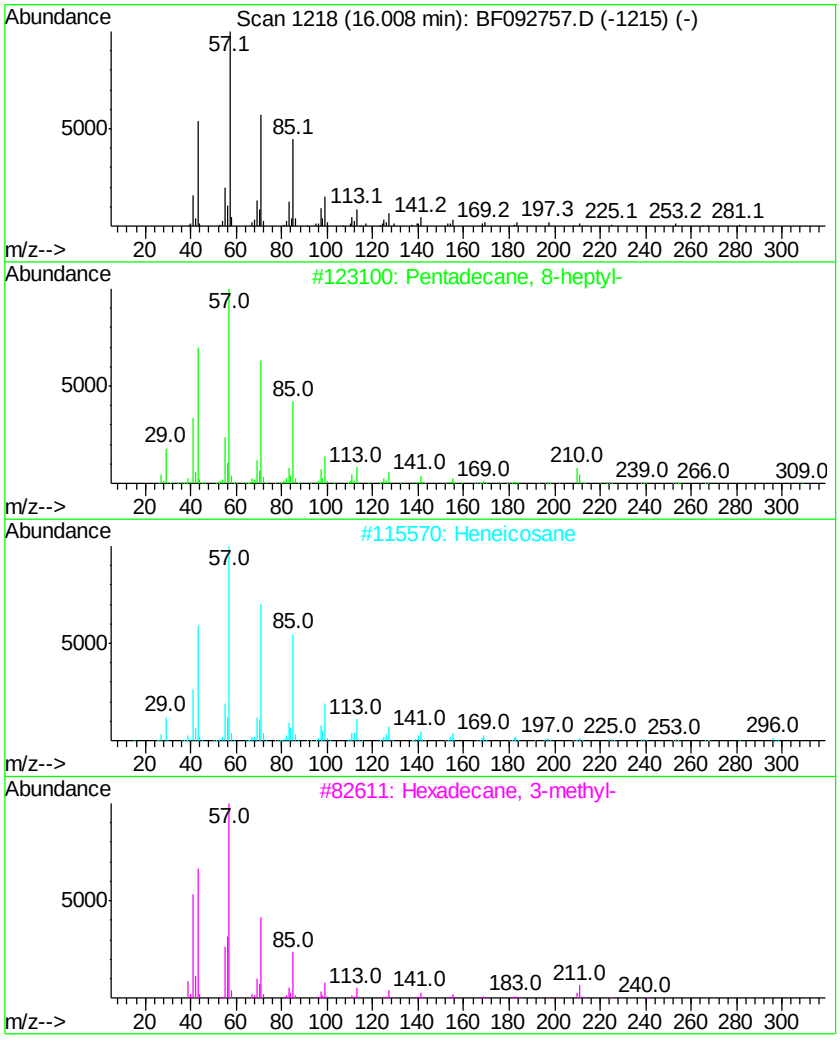
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

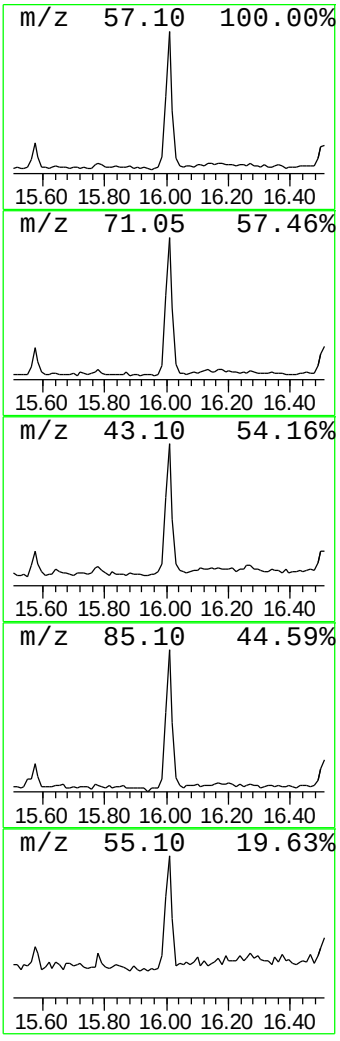
****

Peak Number 8 Pentadecane, 8-heptyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.01	4.47 ng	202573	Perylene-d12	15.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
2	Heneicosane	296	C21H44	000629-94-7	90
3	Hexadecane, 3-methyl-	240	C17H36	006418-43-5	90
4	Tetratetracontane	619	C44H90	007098-22-8	87
5	Octadecane	254	C18H38	000593-45-3	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020217\
Data File : BF092757.D
Acq On : 3 Feb 2017 1:21
Operator : SJ/MA
Sample : I1650-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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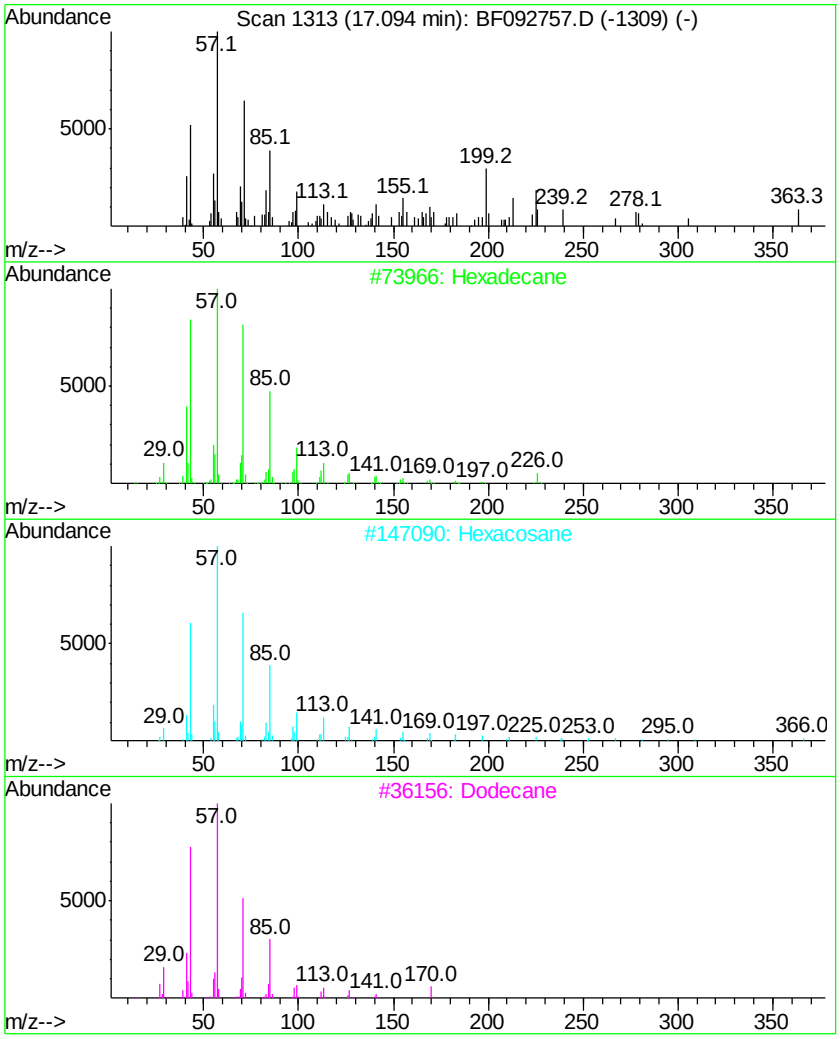
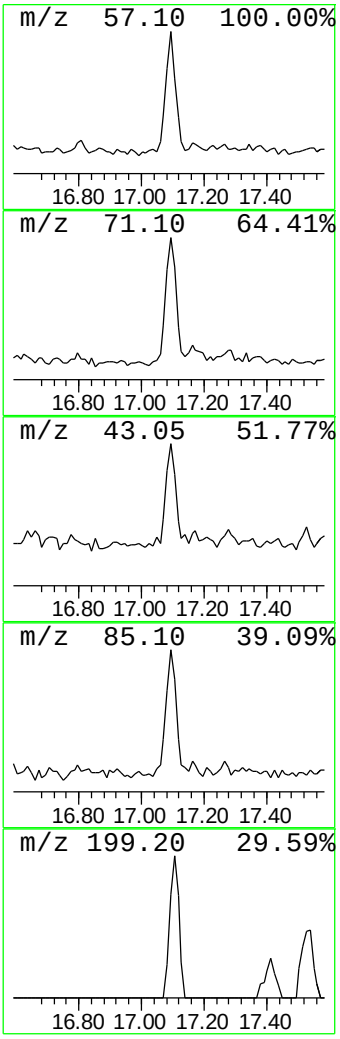
Peak Number 9 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.09	3.23 ng	146388	Perylene-d12	15.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Hexacosane	366	C26H54	000630-01-3	55
3	Dodecane	170	C12H26	000112-40-3	55
4	Heneicosane	296	C21H44	000629-94-7	49
5	Tetracosane	338	C24H50	000646-31-1	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020217\
Data File : BF092757.D
Acq On : 3 Feb 2017 1:21
Operator : SJ/MA
Sample : I1650-20
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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	54.0	ng	2392810	1	6.93	885980	20.0
unknown6.70	6.70	108.5	ng	4805730	1	6.93	885980	20.0
Eicosane	10.88	2.6	ng	183317	4	11.46	1431360	20.0
4H-Cyclopenta[def...	12.08	2.2	ng	159080	4	11.46	1431360	20.0
Ethanol, 2-(tetra...	13.94	2.5	ng	117298	5	14.10	936367	20.0
Octadecane	15.20	2.6	ng	116844	6	15.56	906515	20.0
Pentadecane, 8-he...	16.01	4.5	ng	202573	6	15.56	906515	20.0
Hexadecane	17.09	3.2	ng	146388	6	15.56	906515	20.0