LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100215\
Data File : BF082029.D
Acq On : 3 Oct 2015 18:56
Operator : UM/IZ
Sample : G3867-05
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-03-6.5-7.0-092915

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-BF092815.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	5.074	254	257	272	rVB	860725	1297769	46.45%	5.320%
2	5.486	290	293	295	rBV	2076785	2429230	86.95%	9.959%
3	6.514	380	383	386	rBV	2057072	2207607	79.02%	9.051%
4	6.652	392	395	397	rBV	2447999	2345057	83.94%	9.614%
5	6.880	414	415	418	rBV	324841	438957	15.71%	1.800%
6	7.040	427	429	432	rBV	1989913	1742151	62.36%	7.142%
7	7.452	463	465	479	rBV	1382990	1503876	53.83%	6.165%
8	8.172	525	528	530	rBV	702359	621353	22.24%	2.547%
9	9.258	620	623	625	rBV	1841370	2660274	95.22%	10.906%
10	9.646	655	657	660	rBV	557365	539563	19.31%	2.212%
11	9.932	679	682	684	rBV	870795	771937	27.63%	3.165%
12	10.355	715	719	721	rVB	30908	64145	2.30%	0.263%
13	10.721	749	751	754	rBV2	1509617	1910870	68.40%	7.834%
14	10.835	759	761	766	rVB	53488	69854	2.50%	0.286%
15	11.281	798	800	802	rBV	31081	38637	1.38%	0.158%
16	11.418	810	812	815	rBV	591392	746962	26.74%	3.062%
17	11.955	857	859	865	rBV2	126619	168115	6.02%	0.689%
18	12.835	934	936	938	rVB	128035	109549	3.92%	0.449%
19	12.904	938	942	949	rVB	52084	106902	3.83%	0.438%
20	13.018	949	952	954	rBV	2757209	2793800	100.00%	11.454%
21	13.544	995	998	1000	rBV	80889	74306	2.66%	0.305%
22	13.921	1028	1031	1041	rBV	90921	184246	6.59%	0.755%
23	14.069	1041	1044	1056	rVV	710303	833780	29.84%	3.418%
24	14.229	1056	1058	1062	rVB	22109	33156	1.19%	0.136%
25	14.538	1083	1085	1090	rBV2	25340	38899	1.39%	0.159%
26	14.847	1109	1112	1116	rBV	24863	29458	1.05%	0.121%
27	14.927	1116	1119	1121	rVB	28834	37983	1.36%	0.156%
28	15.532	1169	1172	1185	rBV	372723	593505	21.24%	2.433%

Sum of corrected areas: 24391941

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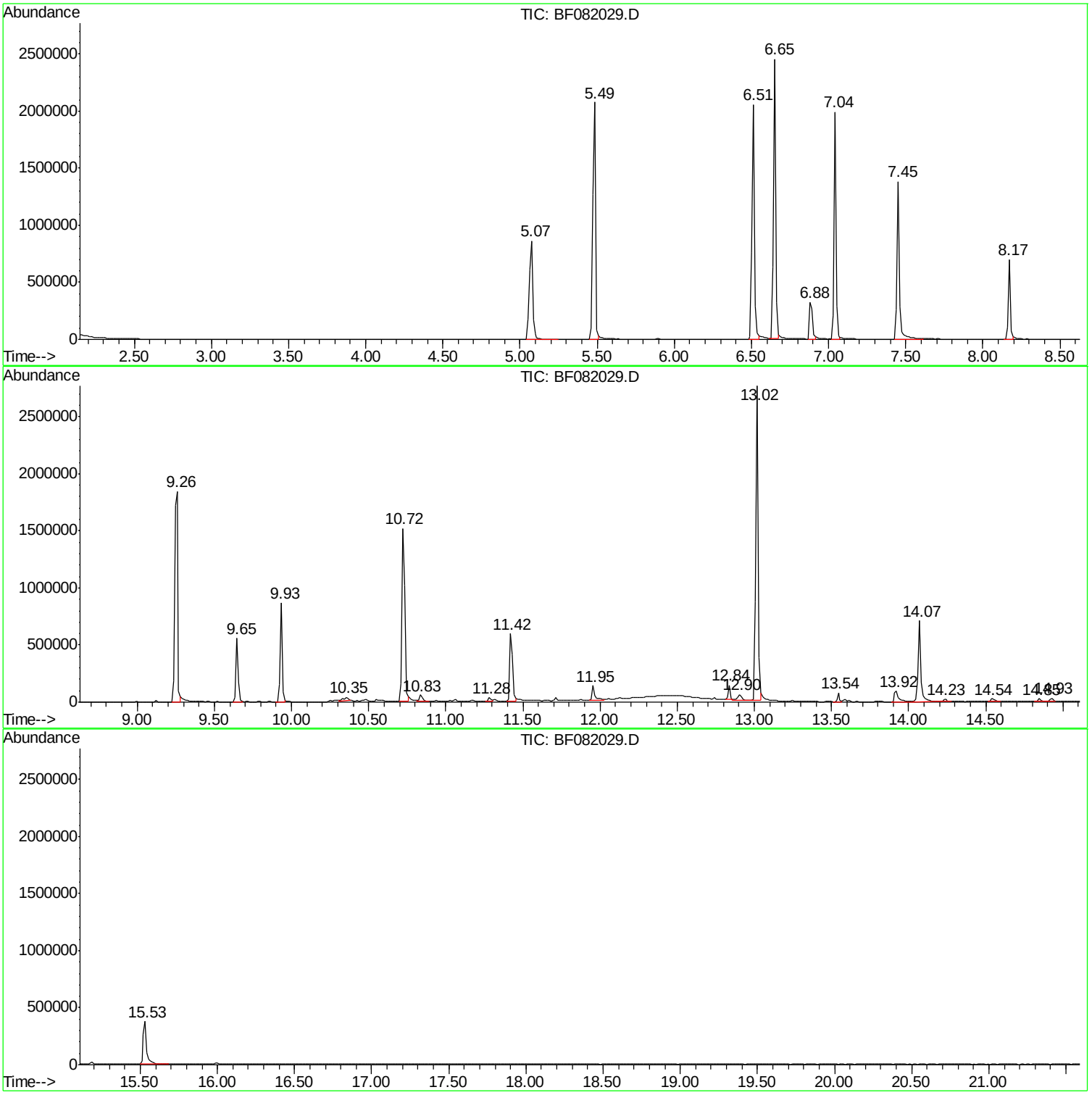
BNA_F
ClientSampleId :
SB-03-6.5-7.0-092915

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.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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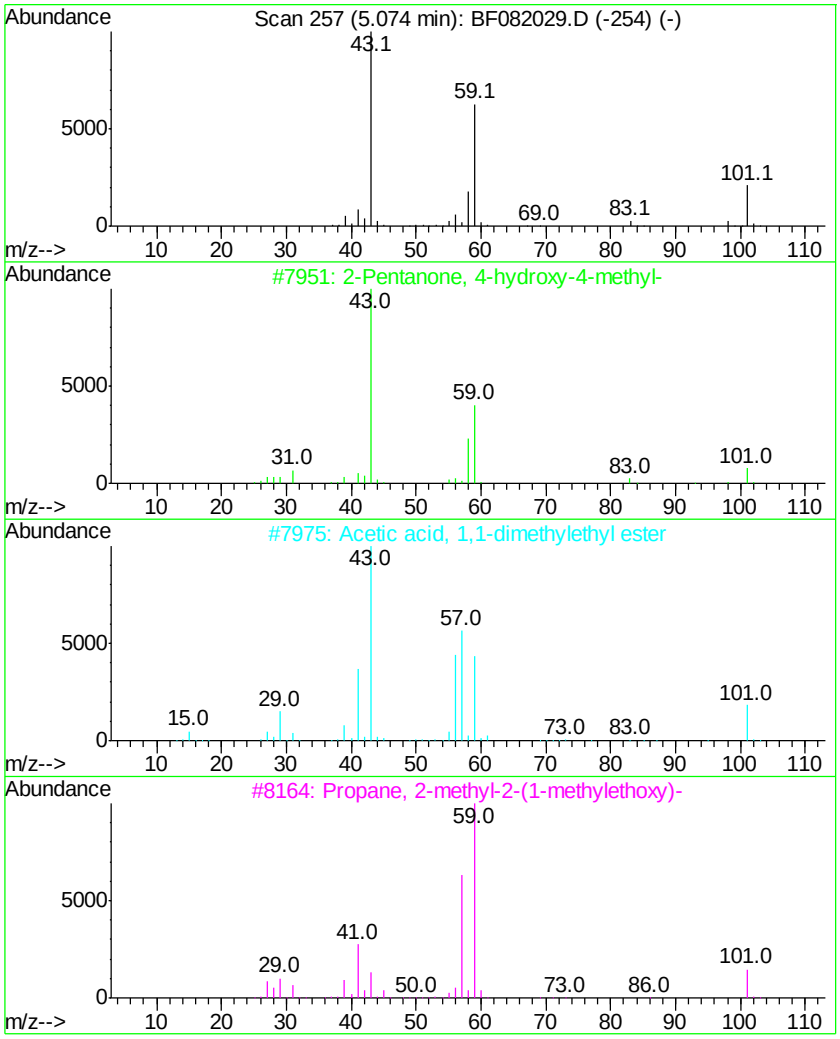
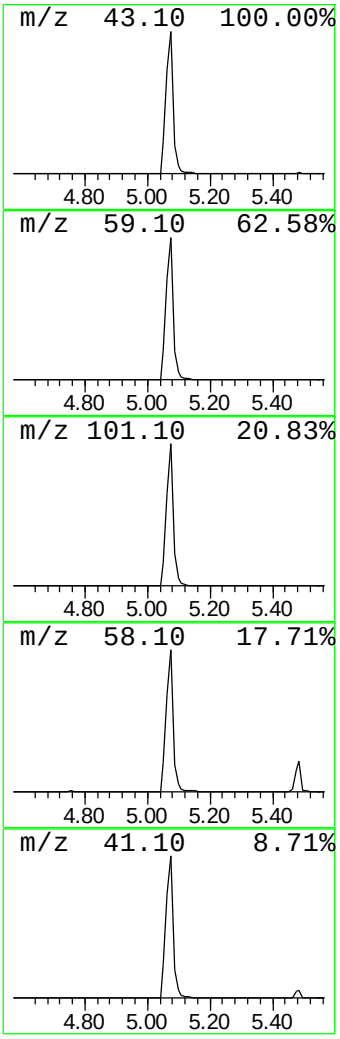
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	59.13 ng	1297770	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Acetone	58	C3H6O	000067-64-1	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100215\
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Acq On : 3 Oct 2015 18:56
Operator : UM/IZ
Sample : G3867-05
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-03-6.5-7.0-092915

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

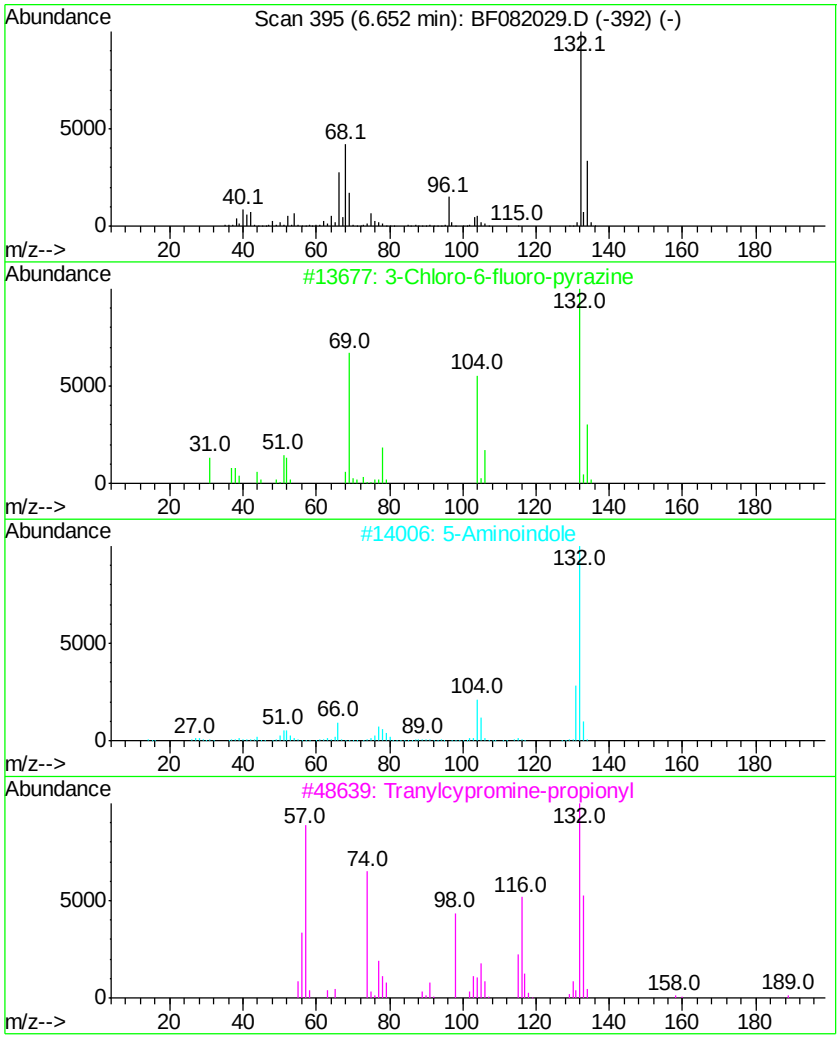
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

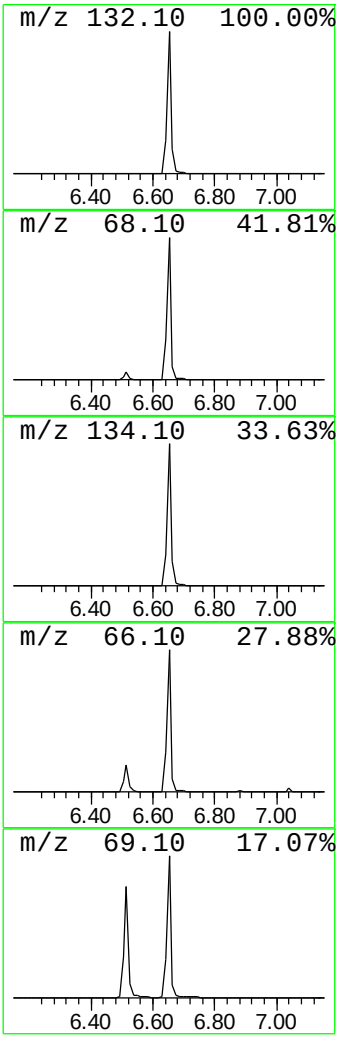
****

Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	106.85 ng	2345060	1,4-Dichlorobenzene-d4	6.89

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	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Operator : UM/IZ
Sample : G3867-05
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-03-6.5-7.0-092915

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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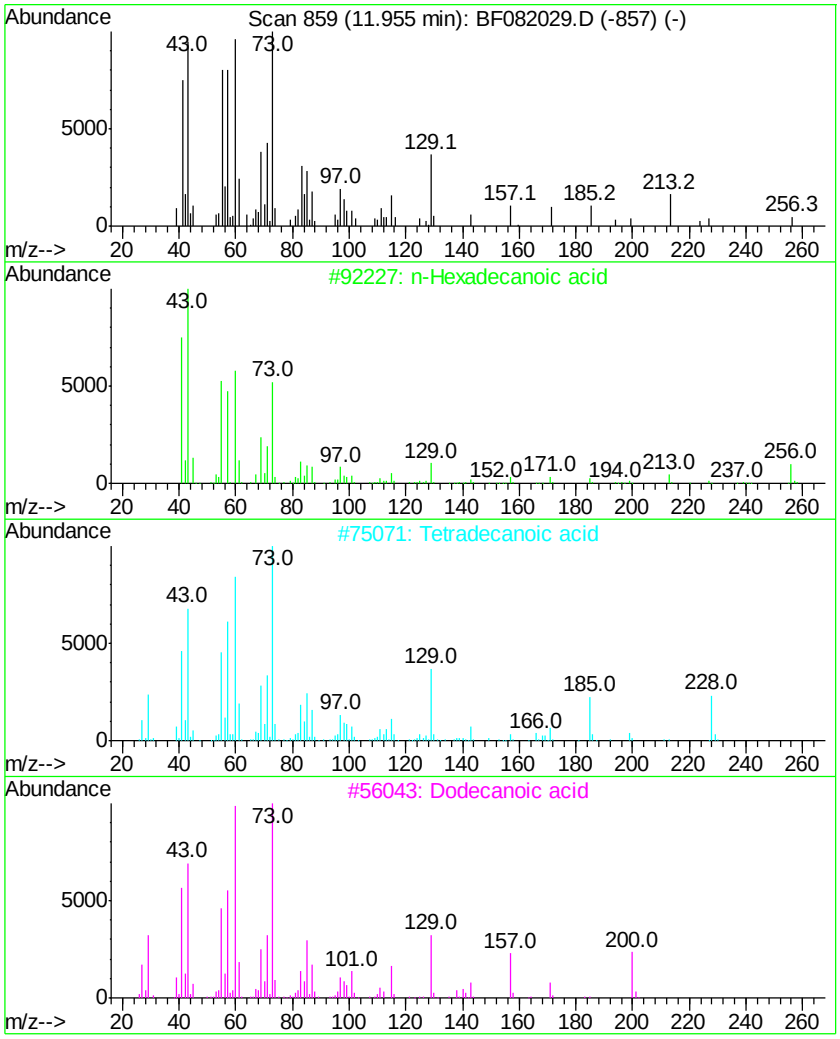
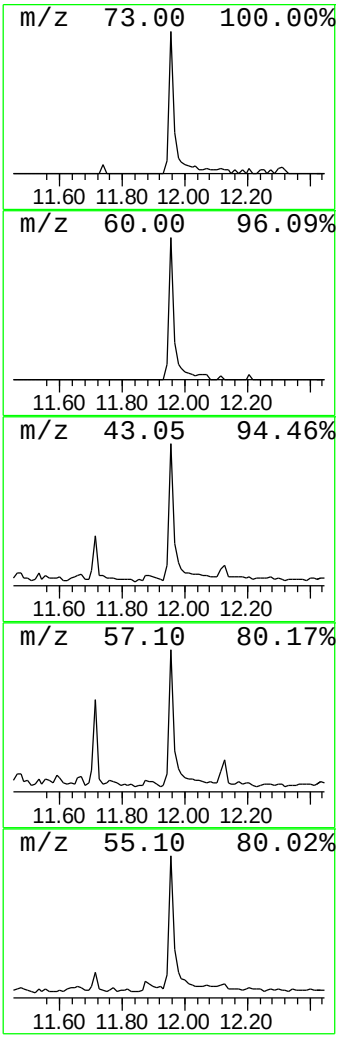
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	4.50 ng	168115	Phenanthrene-d10	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3	Dodecanoic acid	200	C12H24O2	000143-07-7	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Heptanoic acid	130	C7H14O2	000111-14-8	11





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Sample : G3867-05
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-03-6.5-7.0-092915

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.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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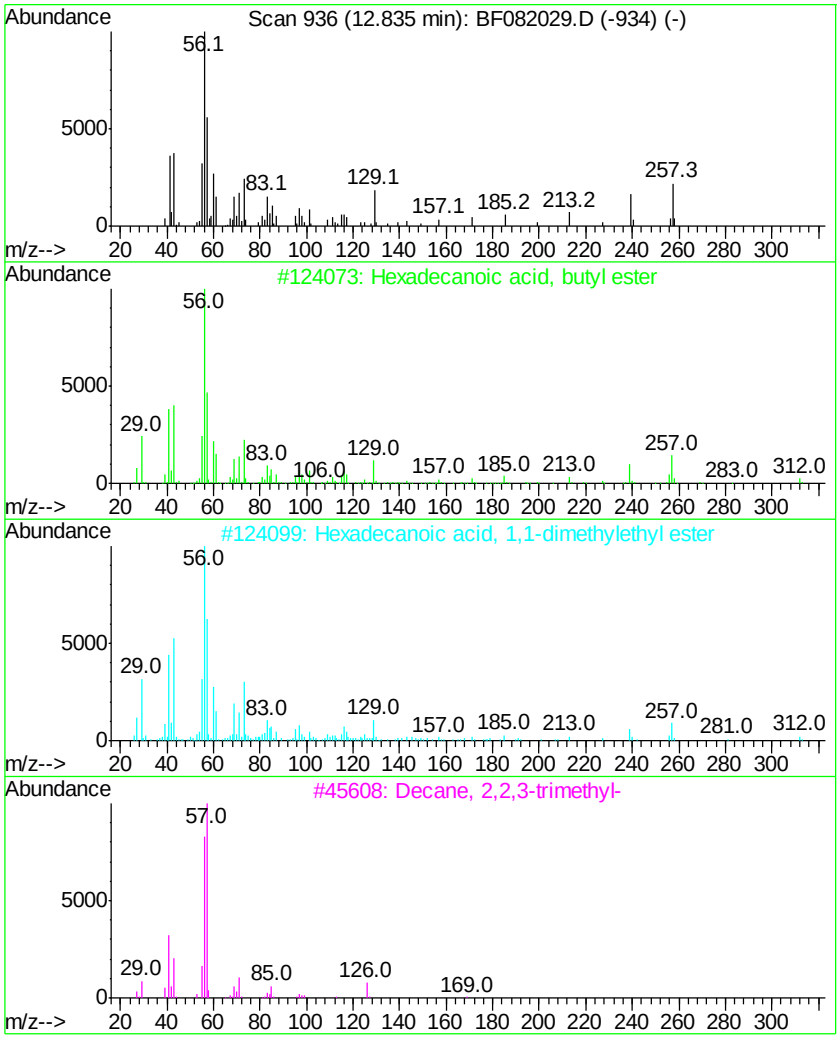
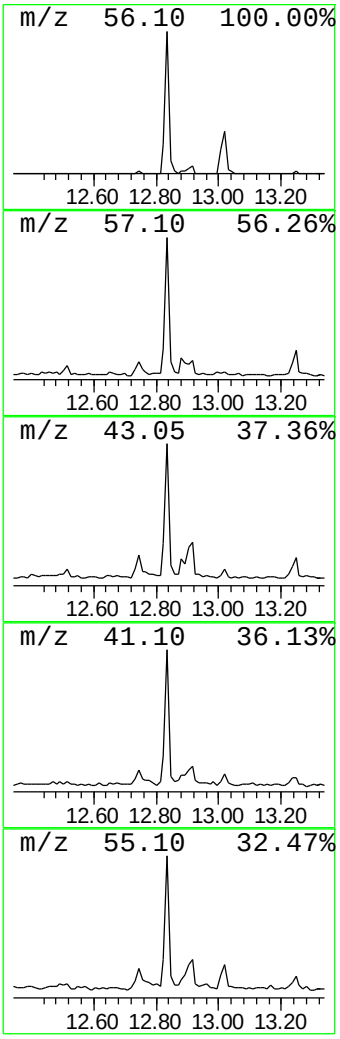
Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	2.63 ng	109549	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	83
3	Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	35
4	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35
5	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	32





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TIC Integration Parameters: LSCINT.P

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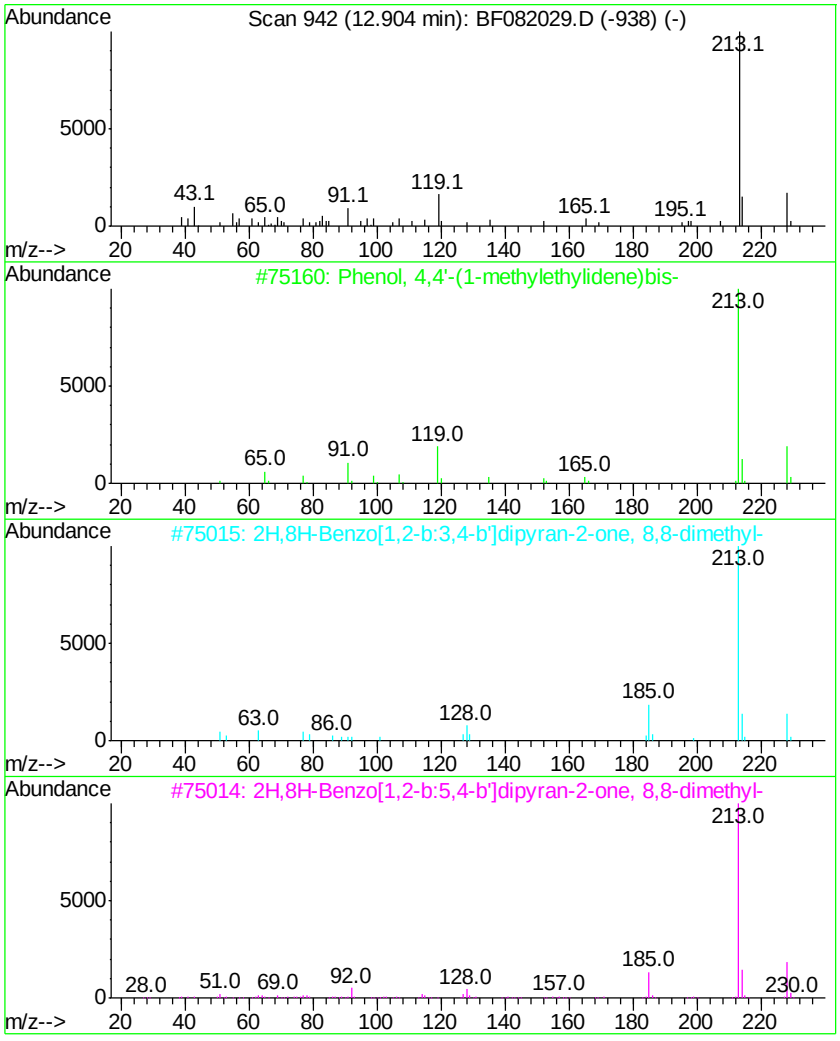
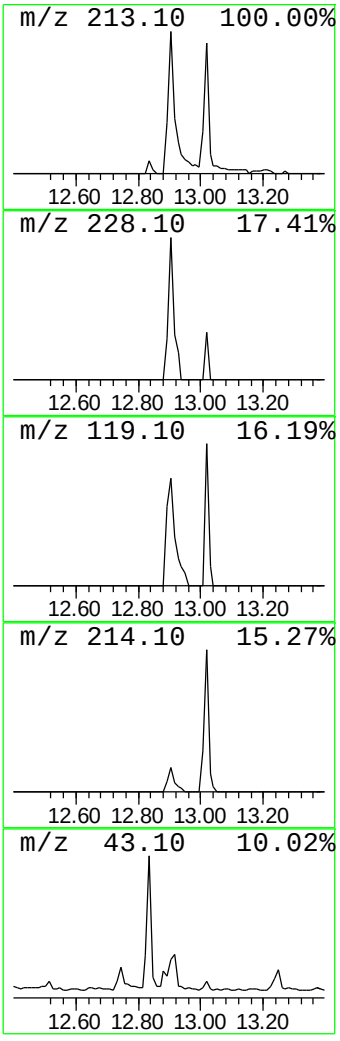
Peak Number 6 Phenol, 4,4'-(1-methylethyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.90	2.56 ng	106902	Chrysene-d12	14.07

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:3,4-b']dipyran...	228	C14H12O3	000523-59-1	53
3	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	36
4	Phenol, 2,4'-isopropylidenedi-	228	C15H16O2	000837-08-1	36
5	As-Indacen-1(2H)-one, 3,6,7,8-te...	228	C16H20O	055591-18-9	35





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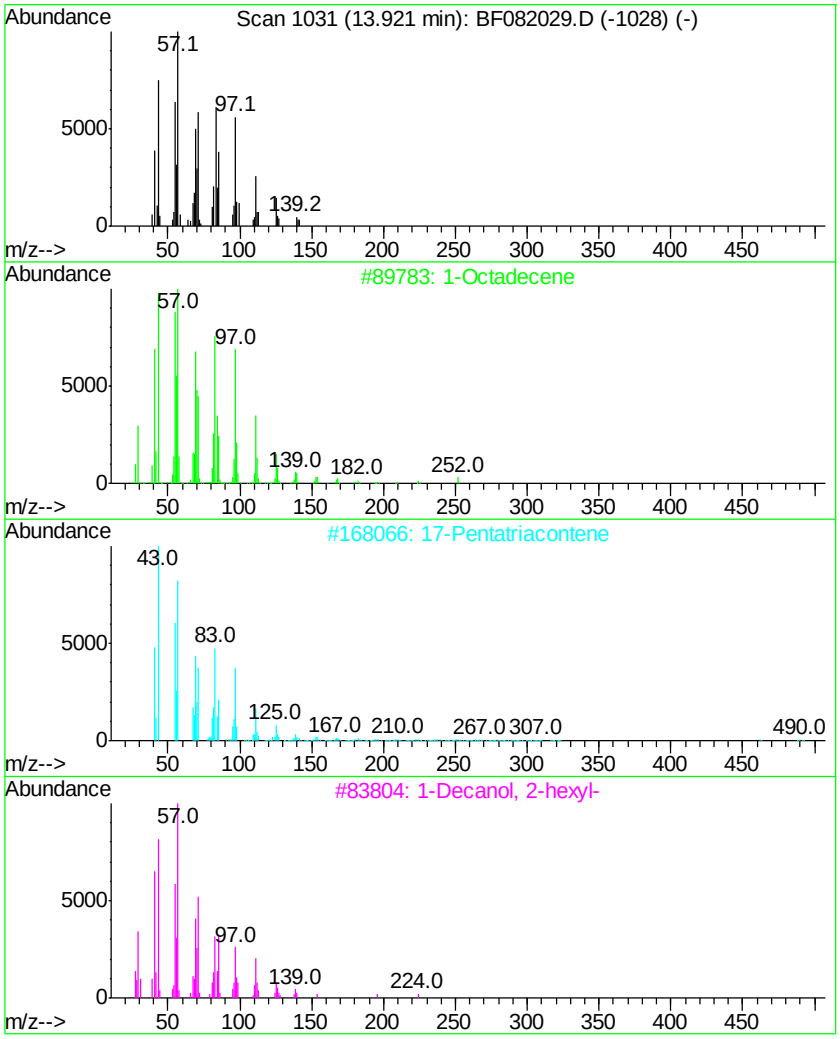
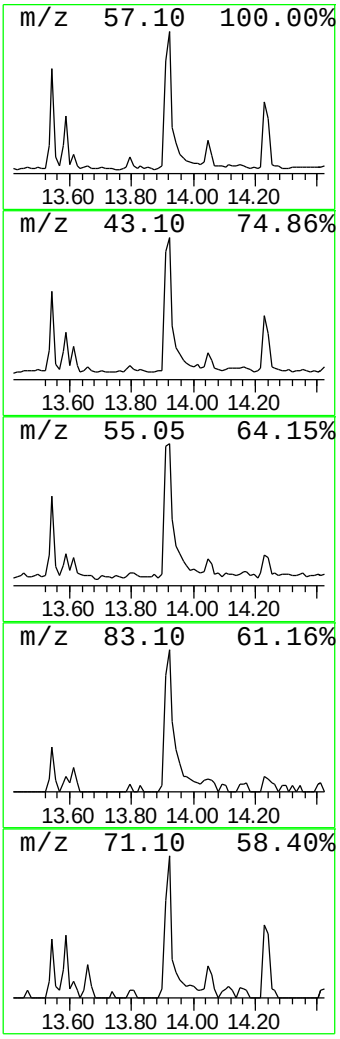
Peak Number 7 1-Octadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	4.42 ng	184246	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	76
2	17-Pentatriacontene	491	C35H70	006971-40-0	74
3	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	74
4	2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	72
5	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	68





Tentatively Identified Compound (LSC) summary

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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...	5.07	59.1	ng	1297770	1	6.89	438957	20.0
unknown6.65	6.65	106.8	ng	2345060	1	6.89	438957	20.0
n-Hexadecanoic acid	11.95	4.5	ng	168115	4	11.42	746962	20.0
Hexadecanoic acid...	12.84	2.6	ng	109549	5	14.07	833780	20.0
Phenol, 4,4'-(1-m...	12.90	2.6	ng	106902	5	14.07	833780	20.0
1-Octadecene	13.92	4.4	ng	184246	5	14.07	833780	20.0