LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032415\
Data File : BF077936.D
Acq On : 25 Mar 2015 5:03
Operator : TP/IZ
Sample : G1613-08
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4-2

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-BF031115.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	1.047	11	14	17	rVB	824635	1418856	51.38%	8.903%
2	1.264	31	33	36	rVV	2136668	2761614	100.00%	17.329%
3	1.390	40	44	47	rVB	747331	1200260	43.46%	7.532%
4	1.550	57	58	65	rVB	50828	81617	2.96%	0.512%
5	1.652	65	67	75	rVV	130639	272675	9.87%	1.711%
6	1.767	75	77	97	rVB	853015	1617472	58.57%	10.150%
7	2.018	97	99	107	rVB3	13112	28570	1.03%	0.179%
8	4.864	346	348	356	rVB	68163	89179	3.23%	0.560%
9	5.401	393	395	398	rBV	617866	690452	25.00%	4.333%
10	6.693	506	508	511	rBV	710438	702096	25.42%	4.406%
11	6.830	518	520	523	rBV	845305	779149	28.21%	4.889%
12	7.116	543	545	548	rBV	270735	238528	8.64%	1.497%
13	7.299	559	561	564	rBV	596911	599327	21.70%	3.761%
14	7.813	604	606	608	rBV	489132	450613	16.32%	2.828%
15	8.693	681	683	686	rBV	381785	333874	12.09%	2.095%
16	10.042	799	801	803	rBV	1127826	1002607	36.31%	6.291%
17	10.865	871	873	875	rBV	395006	385873	13.97%	2.421%
18	11.836	956	958	961	rBV2	467285	536202	19.42%	3.365%
19	12.694	1031	1033	1036	rBV	333599	398385	14.43%	2.500%
20	14.522	1190	1193	1196	rVB	28456	30885	1.12%	0.194%
21	14.694	1205	1208	1210	rBV	1136730	1171021	42.40%	7.348%
22	15.882	1309	1312	1317	rBV	41290	99944	3.62%	0.627%
23	15.974	1317	1320	1323	rBV	479623	482424	17.47%	3.027%
24	16.145	1332	1335	1337	rBV	26885	29459	1.07%	0.185%
25	16.625	1374	1377	1379	rBV2	24512	32138	1.16%	0.202%
26	17.700	1468	1471	1474	rBV	371516	502811	18.21%	3.155%

Sum of corrected areas: 15936031

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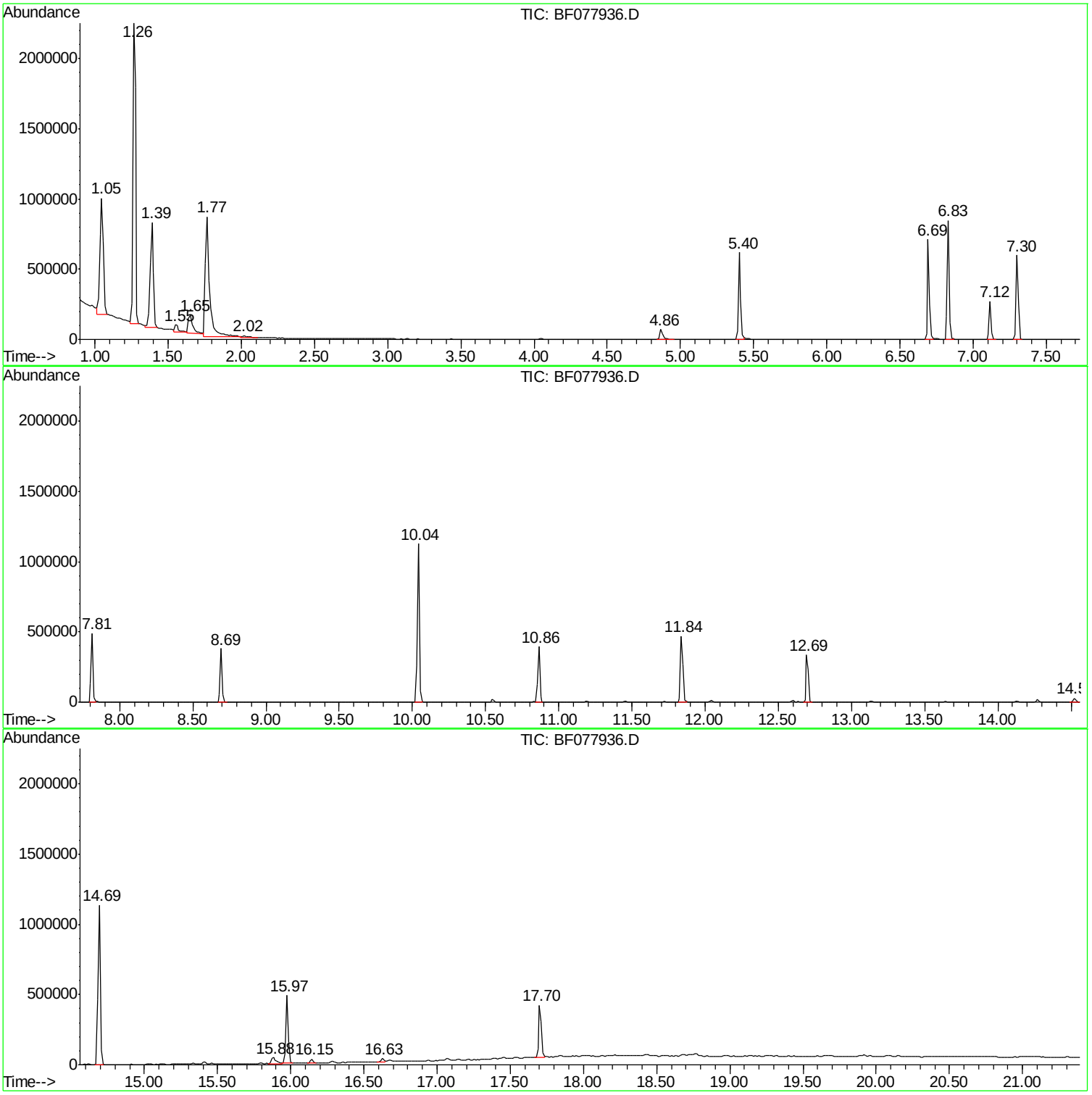
Instrument : BNA_F
ClientSampleId : SB-4-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.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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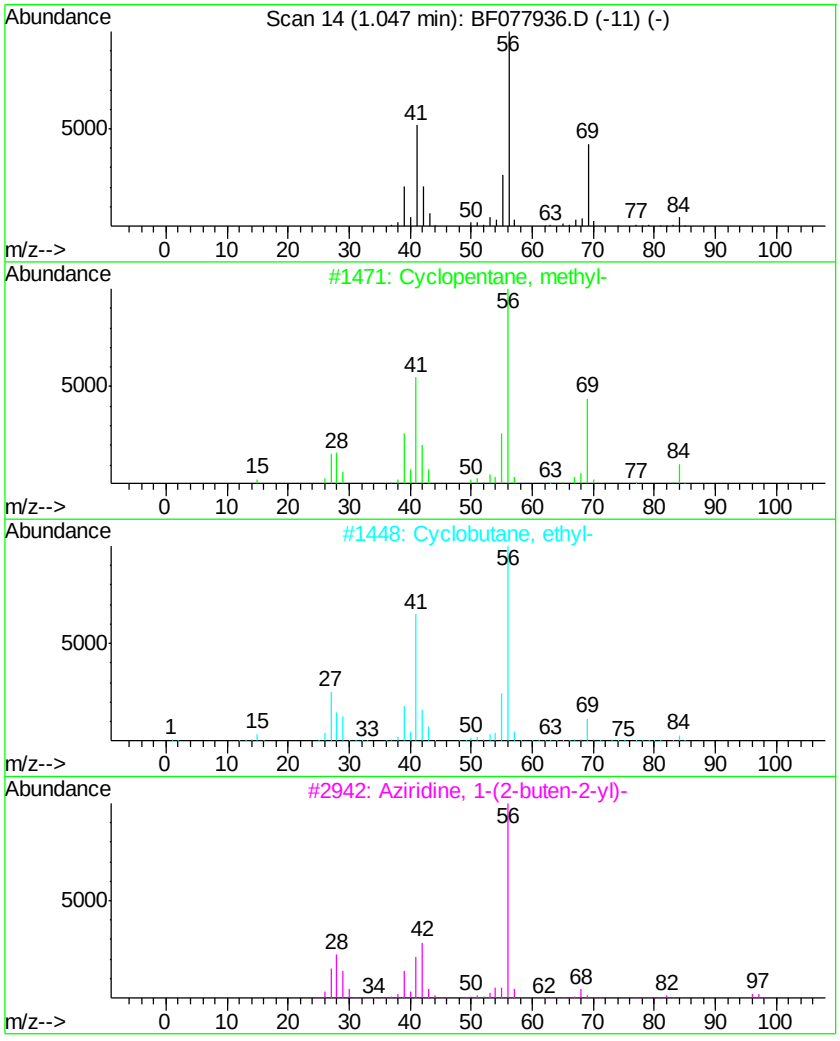
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

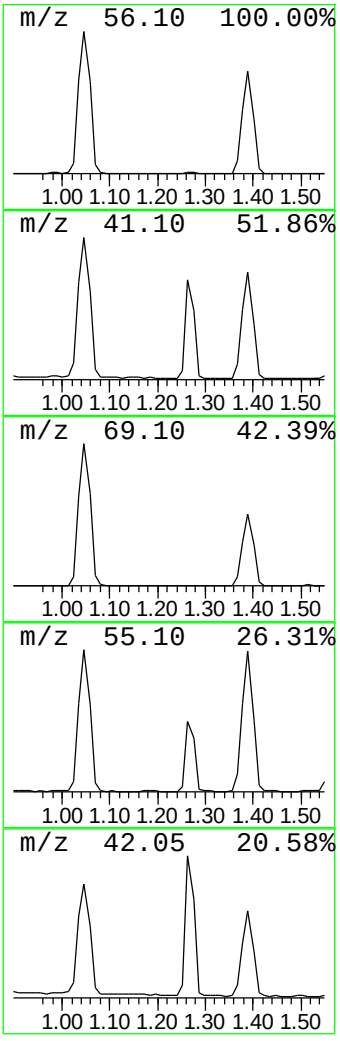
****

Peak Number 1 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.05	118.97 ng	1418860	1,4-Dichlorobenzene-d4	7.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	80
3	Aziridine, 1-(2-buten-2-yl)-	97	C6H11N	1000158-95-2	40
4	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	39
5	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	39





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Acq On : 25 Mar 2015 5:03
Operator : TP/IZ
Sample : G1613-08
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.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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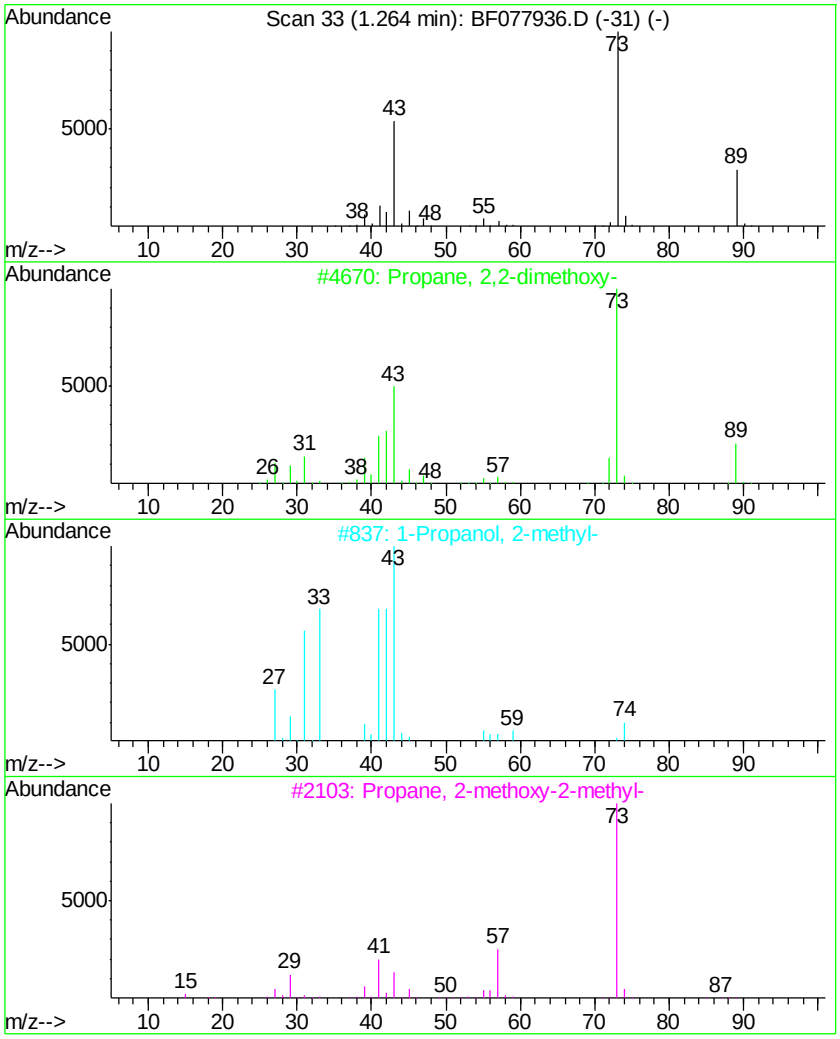
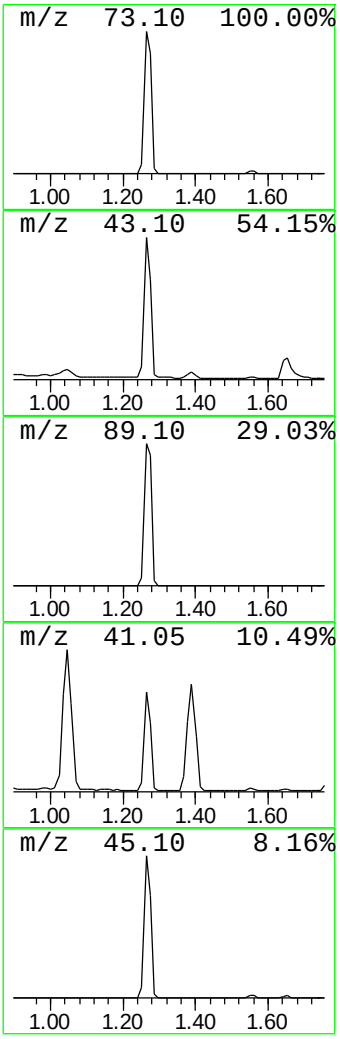
Peak Number 2 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.26	231.56 ng	2761610	1,4-Dichlorobenzene-d4	7.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	78
2	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
3	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	9
5	1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9





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Data File : BF077936.D
Acq On : 25 Mar 2015 5:03
Operator : TP/IZ
Sample : G1613-08
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.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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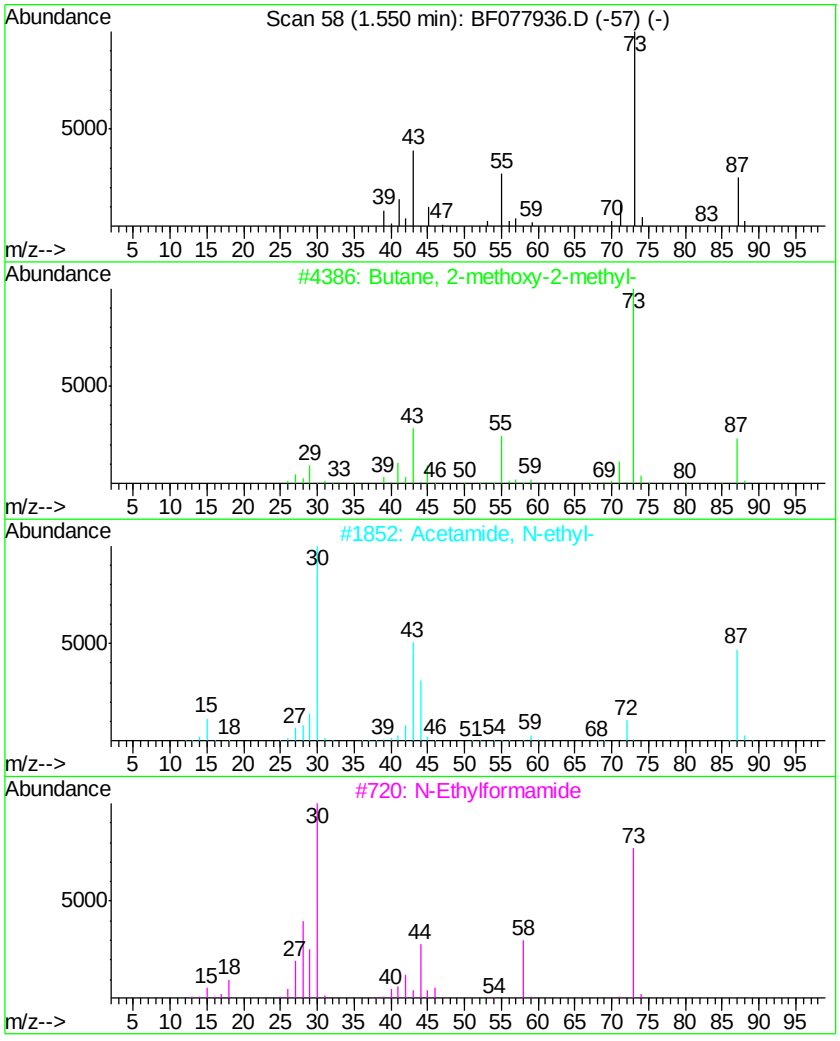
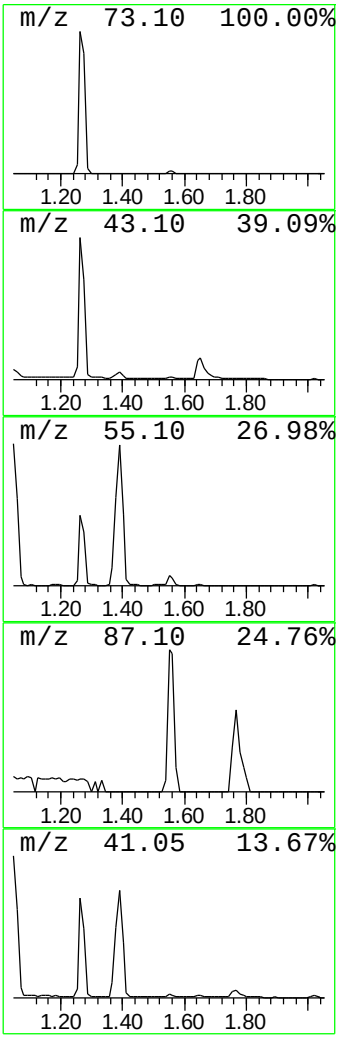
Peak Number 4 Butane, 2-methoxy-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.55	6.84 ng	81617	1,4-Dichlorobenzene-d4	7.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5	1,4-Butanediamine	88	C4H12N2	000110-60-1	9





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Operator : TP/IZ
Sample : G1613-08
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.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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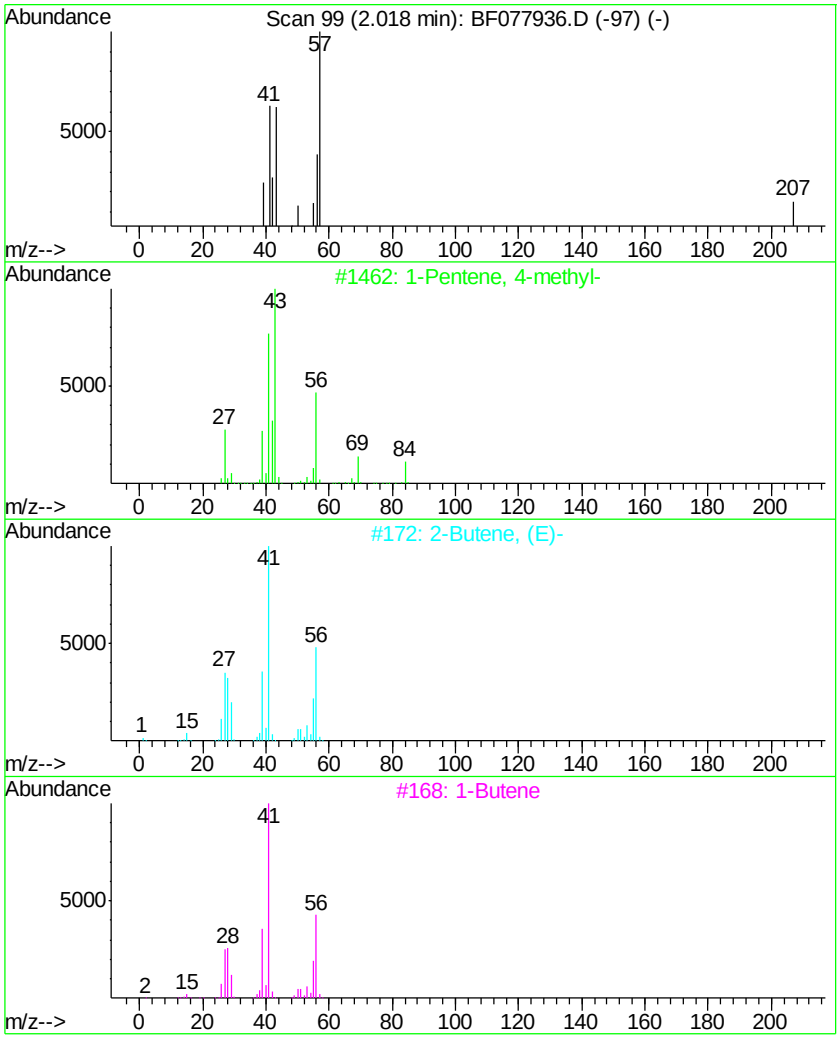
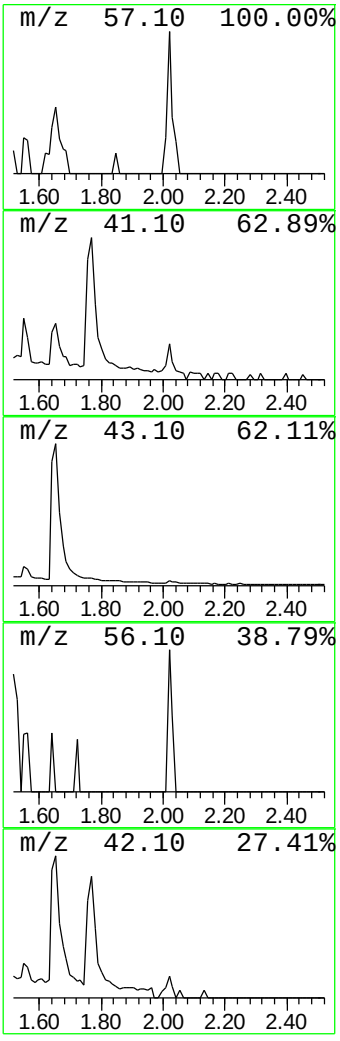
Peak Number 7 unknown2.02 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.02	2.40 ng	28570	1,4-Dichlorobenzene-d4	7.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene, 4-methyl-	84	C6H12	000691-37-2	28
2	2-Butene, (E)-	56	C4H8	000624-64-6	9
3	1-Butene	56	C4H8	000106-98-9	9
4	1-Propene, 2-methyl-	56	C4H8	000115-11-7	9
5	2-Butene, (Z)-	56	C4H8	000590-18-1	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032415\
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Acq On : 25 Mar 2015 5:03
Operator : TP/IZ
Sample : G1613-08
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.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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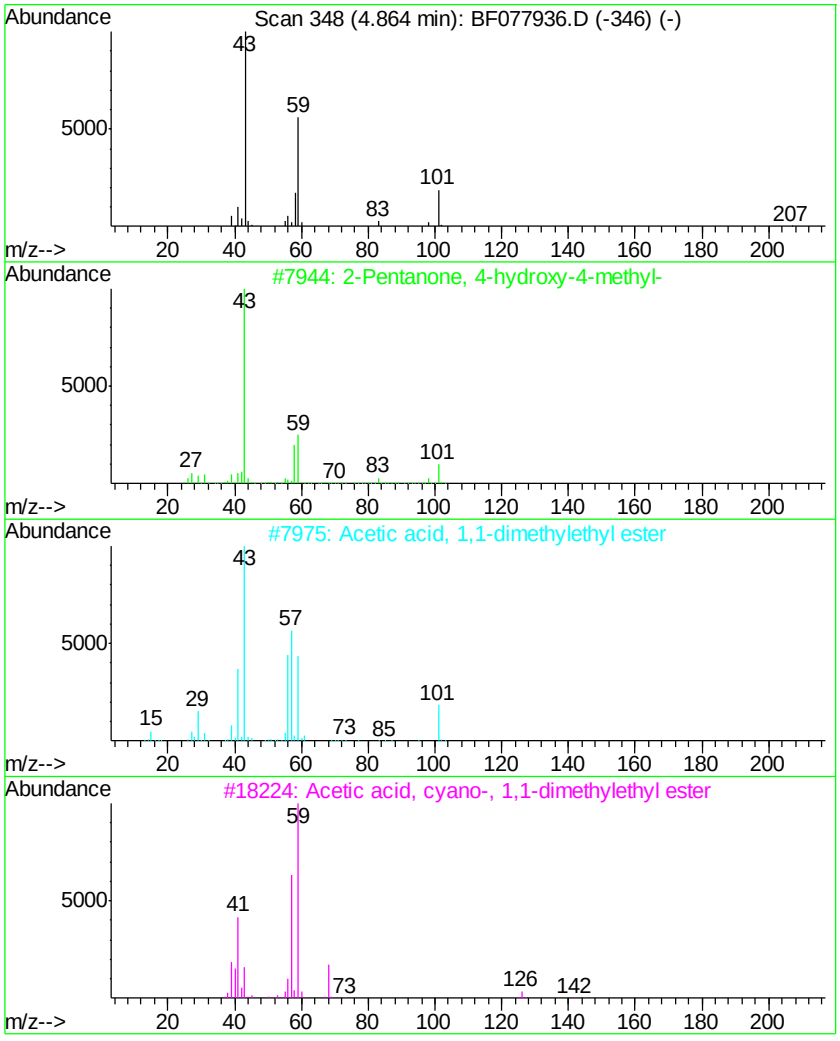
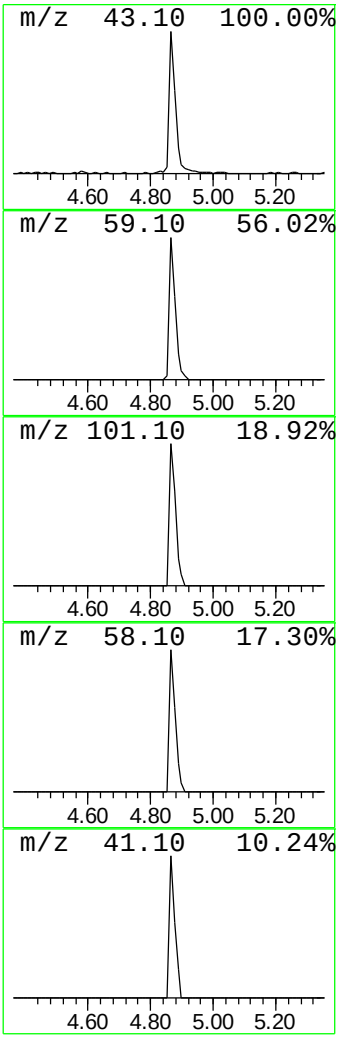
Peak Number 8 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	7.48 ng	89179	1,4-Dichlorobenzene-d4	7.12

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	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Instrument : BNA_F
ClientSampleId : SB-4-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

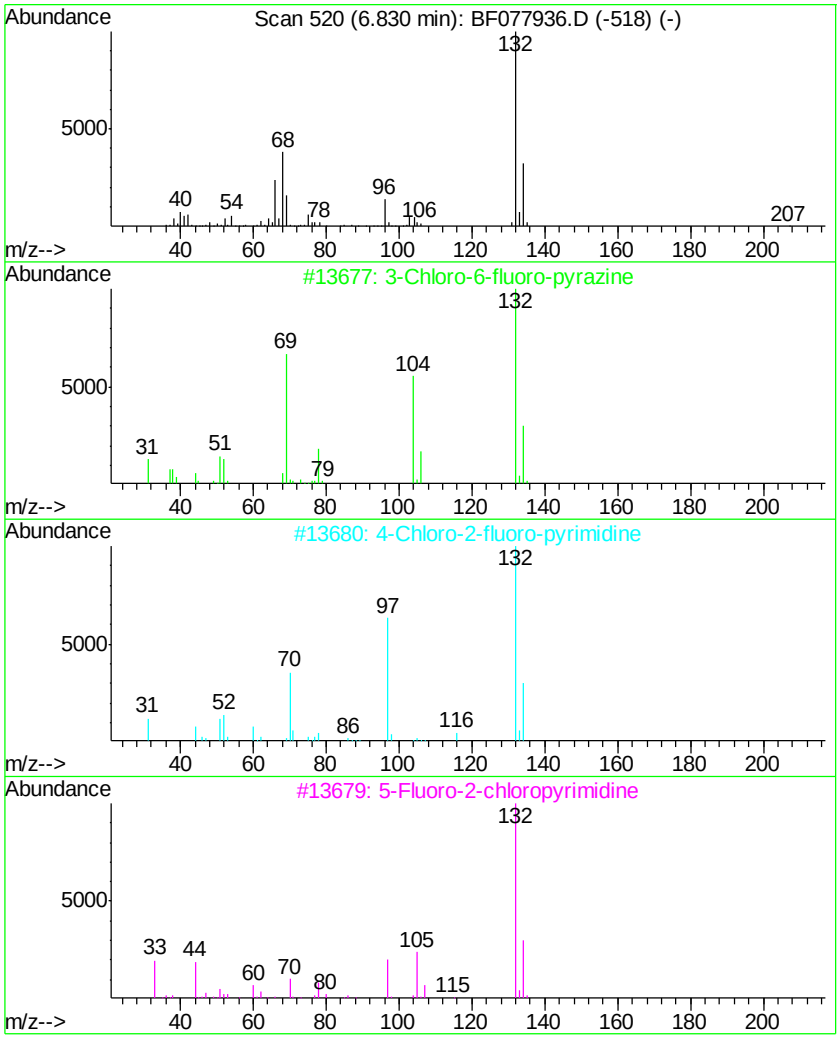
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

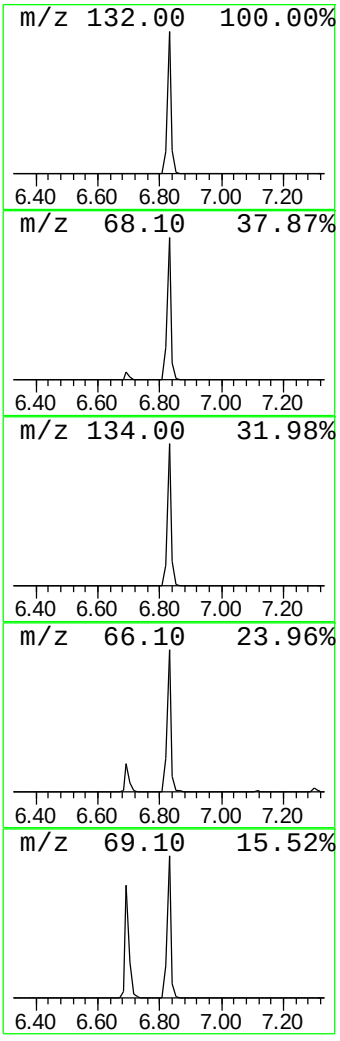
****

Peak Number 9 unknown6.83 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.83	65.33 ng	779149	1,4-Dichlorobenzene-d4	7.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

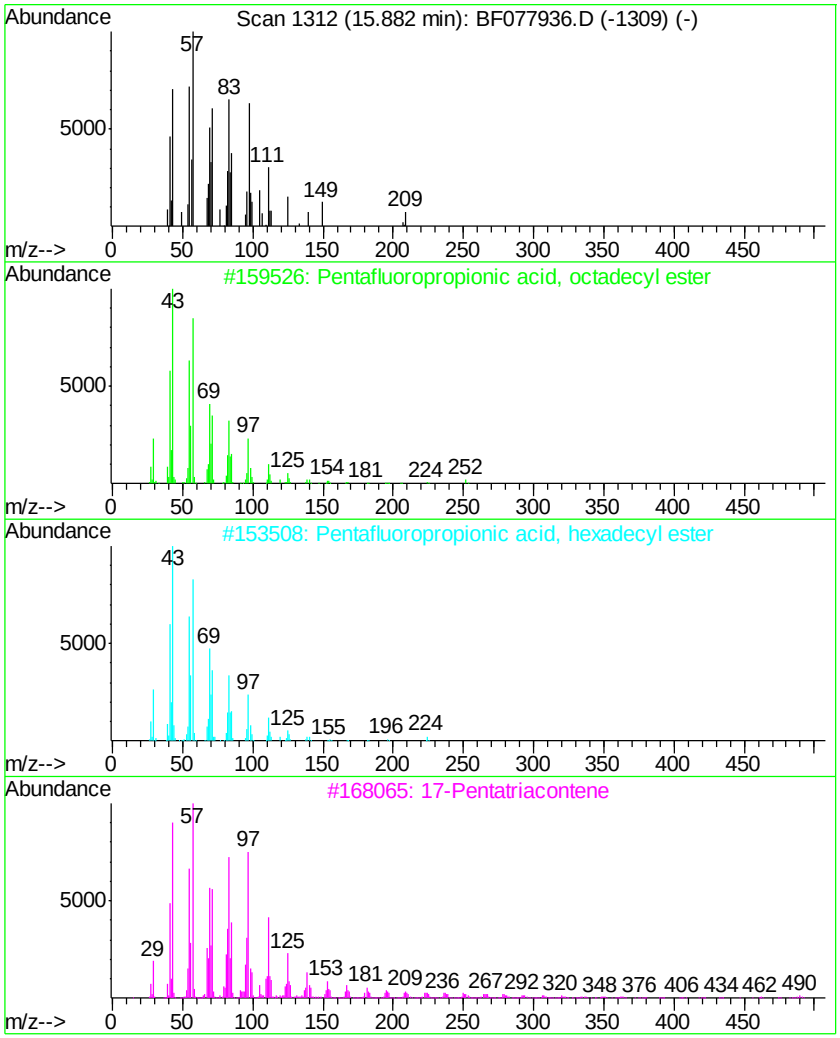
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

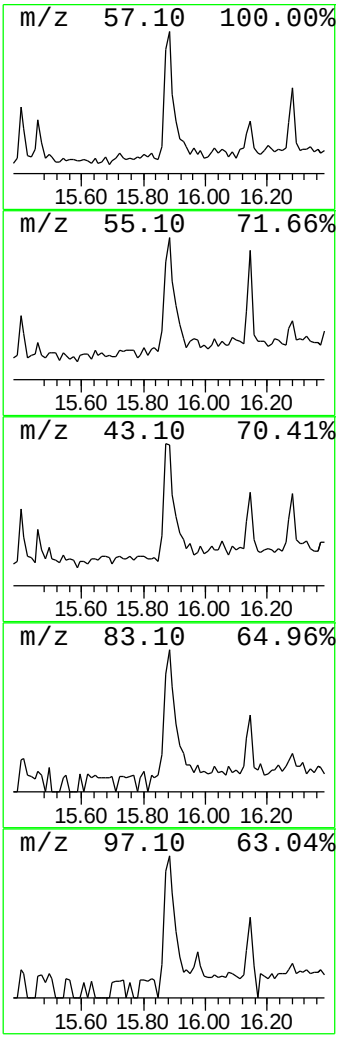
****

Peak Number 11 Pentafluoropropionic acid, ... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.88	4.14 ng	99944	Chrysene-d12	15.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	91
2	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	86
3	17-Pentatriacontene	491	C35H70	006971-40-0	86
4	1-Hentetracontanol	593	C41H84O	040710-42-7	86
5	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	76





Tentatively Identified Compound (LSC) summary

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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
Cyclopentane, met...	1.05	119.0	ng	1418860	1	7.12	238528	20.0
Propane, 2,2-dime...	1.26	231.6	ng	2761610	1	7.12	238528	20.0
Butane, 2-methoxy...	1.55	6.8	ng	81617	1	7.12	238528	20.0
unknown2.02	2.02	2.4	ng	28570	1	7.12	238528	20.0
2-Pentanone, 4-hy...	4.86	7.5	ng	89179	1	7.12	238528	20.0
unknown6.83	6.83	65.3	ng	779149	1	7.12	238528	20.0
Pentafluoropropio...	15.88	4.1	ng	99944	5	15.97	482424	20.0