LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022615\
Data File : BF077471.D
Acq On : 26 Feb 2015 18:06
Operator : TP/IZ
Sample : G1384-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
36A-B-022515

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: CENTROID

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.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	1.424	44	47	50	rVB	4560542	4723640	100.00%	22.287%
2	1.561	55	59	72	rVB2	141473	331230	7.01%	1.563%
3	1.733	72	74	81	rVB	121864	196052	4.15%	0.925%
4	1.847	82	84	109	rVB	526066	1202214	25.45%	5.672%
5	5.047	362	364	370	rBV	213939	247868	5.25%	1.169%
6	5.550	406	408	411	rBV	880832	1210288	25.62%	5.710%
7	6.819	517	519	522	rBV	1295075	1210089	25.62%	5.709%
8	6.979	530	533	535	rBV	1242843	1338339	28.33%	6.315%
9	7.265	556	558	560	rVB	367626	326088	6.90%	1.539%
10	7.448	572	574	577	rBV	817961	1044899	22.12%	4.930%
11	7.950	616	618	621	rBV	612912	773560	16.38%	3.650%
12	8.842	694	696	698	rBV	518019	447023	9.46%	2.109%
13	10.191	811	814	816	rBV	1922823	1786027	37.81%	8.427%
14	10.694	855	858	860	rBV	62324	54003	1.14%	0.255%
15	11.014	884	886	889	rBV	550443	530564	11.23%	2.503%
16	11.917	963	965	968	rBV	127949	113544	2.40%	0.536%
17	11.997	969	972	974	rBV	1068505	1069618	22.64%	5.047%
18	12.854	1045	1047	1050	rBV2	475391	551832	11.68%	2.604%
19	14.854	1220	1222	1225	rBV	1980769	2175400	46.05%	10.264%
20	16.020	1322	1324	1330	rBV	328745	390696	8.27%	1.843%
21	16.146	1332	1335	1338	rVV	659386	674434	14.28%	3.182%
22	17.300	1433	1436	1440	rBV	39116	51227	1.08%	0.242%
23	17.860	1482	1485	1488	rBV	521212	667439	14.13%	3.149%
24	18.489	1538	1540	1543	rBV	50061	78611	1.66%	0.371%

Sum of corrected areas: 21194685

LSC Report - Integrated Chromatogram

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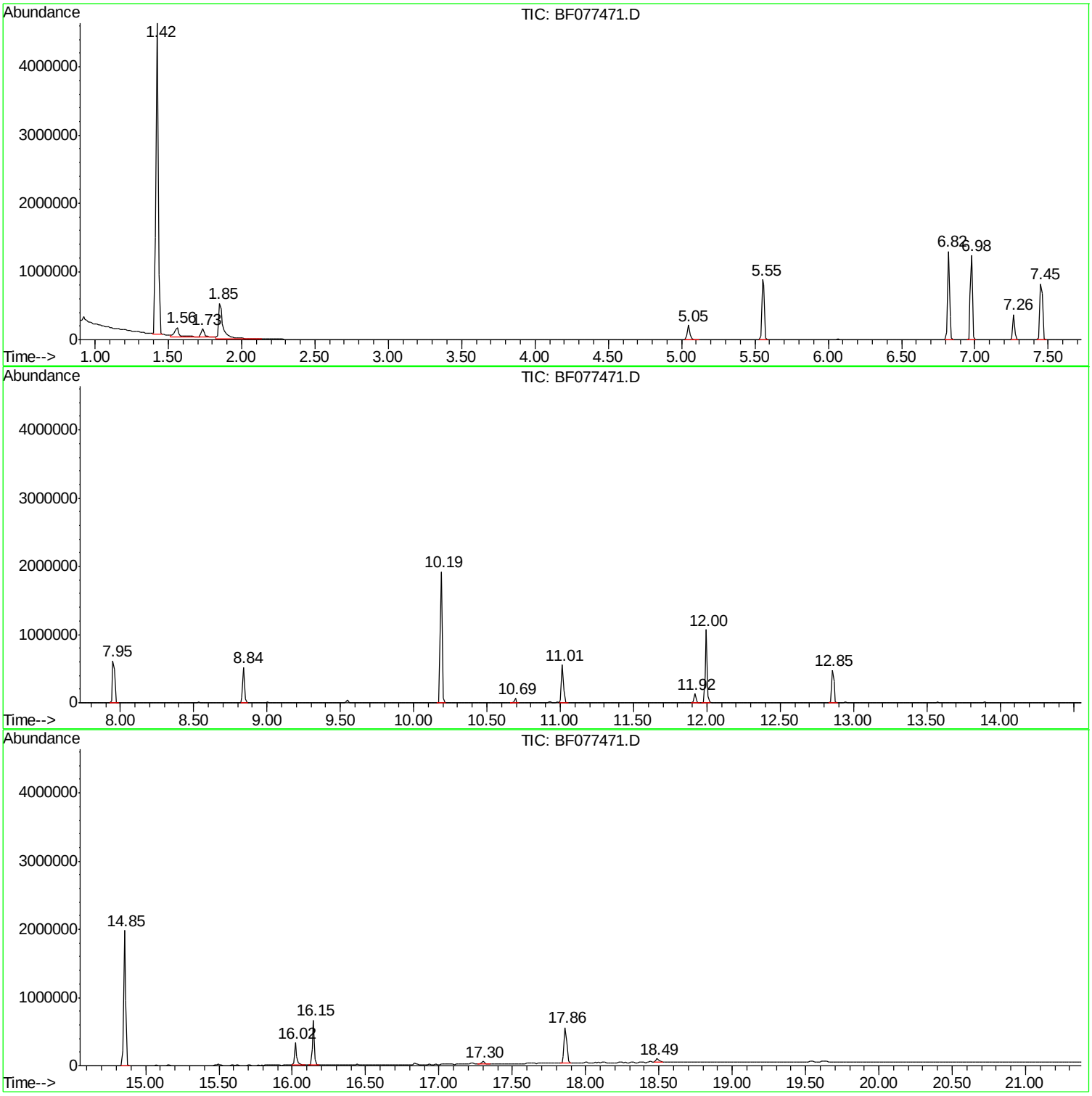
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
36A-B-022515

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Data File : BF077471.D
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Sample : G1384-10
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.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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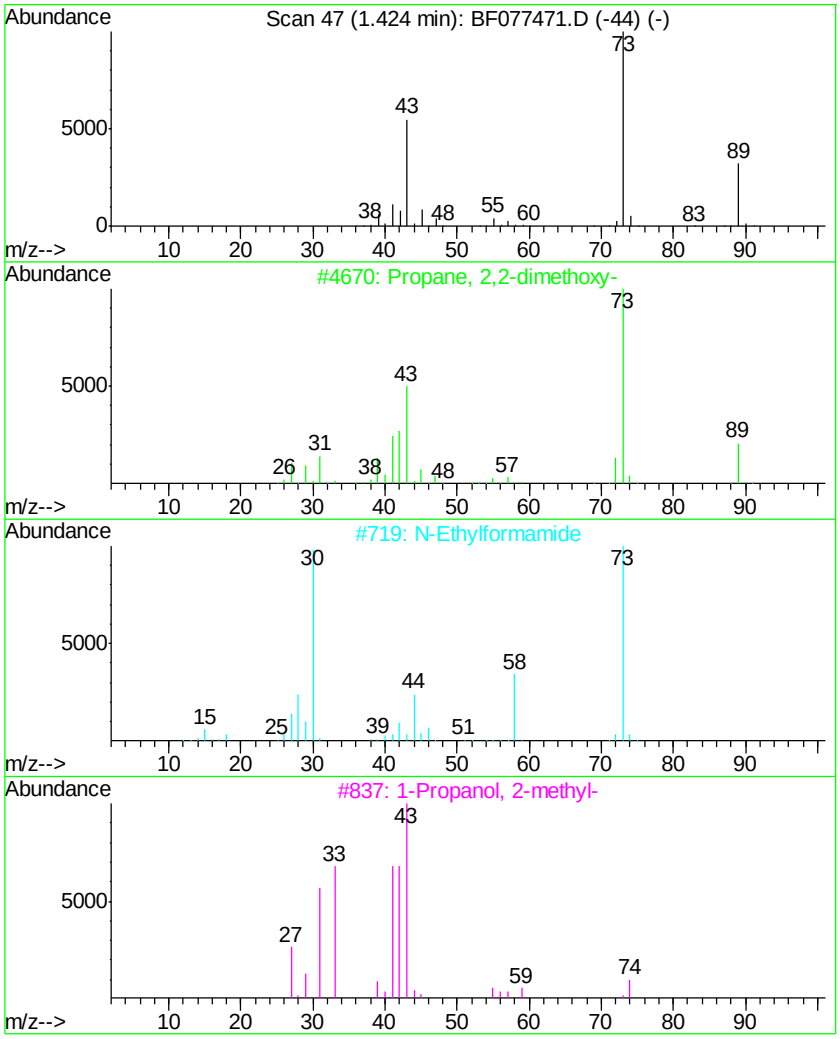
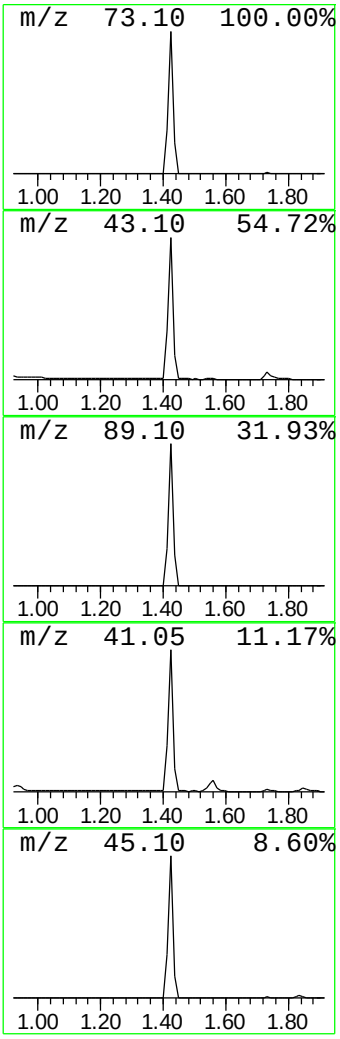
Peak Number 1 unknown1.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.42	289.72 ng	4723640	1,4-Dichlorobenzene-d4	7.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
4	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
5	2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	9





Library Search Compound Report

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Sample : G1384-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
36A-B-022515

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.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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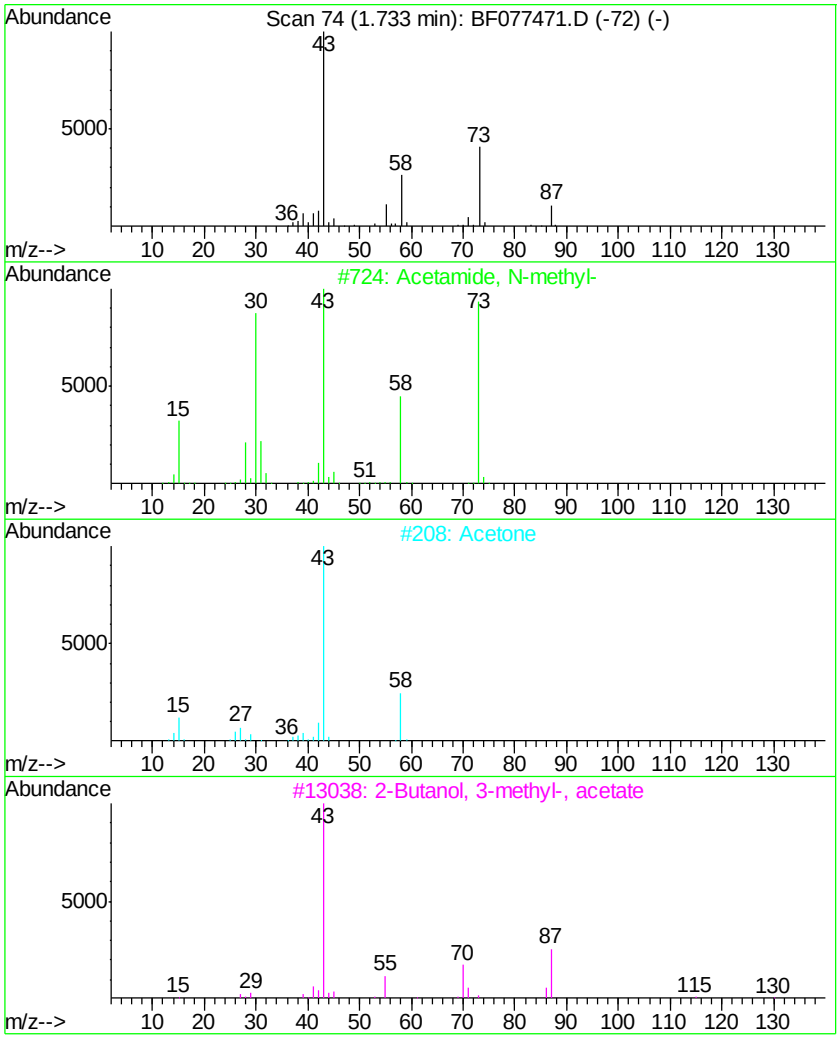
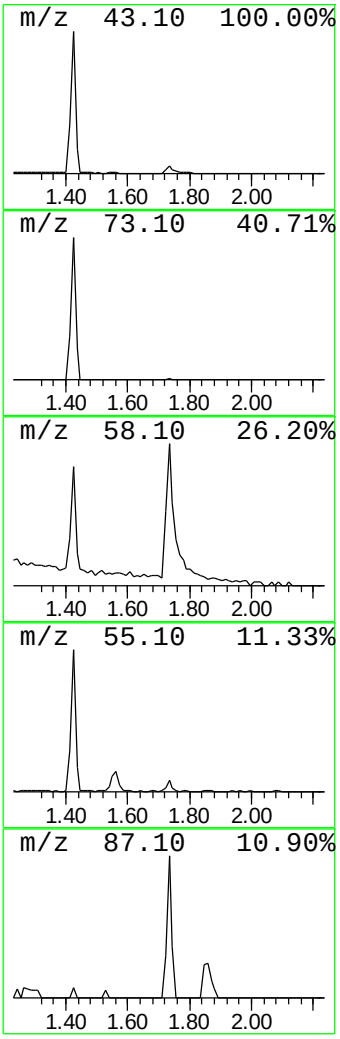
Peak Number 3 unknown1.73 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.73	12.02 ng	196052	1,4-Dichlorobenzene-d4	7.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	47
2	Acetone	58	C3H6O	000067-64-1	37
3	2-Butanol, 3-methyl-, acetate	130	C7H14O2	005343-96-4	37
4	1-Pentanamine	87	C5H13N	000110-58-7	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

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Data File : BF077471.D
Acq On : 26 Feb 2015 18:06
Operator : TP/IZ
Sample : G1384-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
36A-B-022515

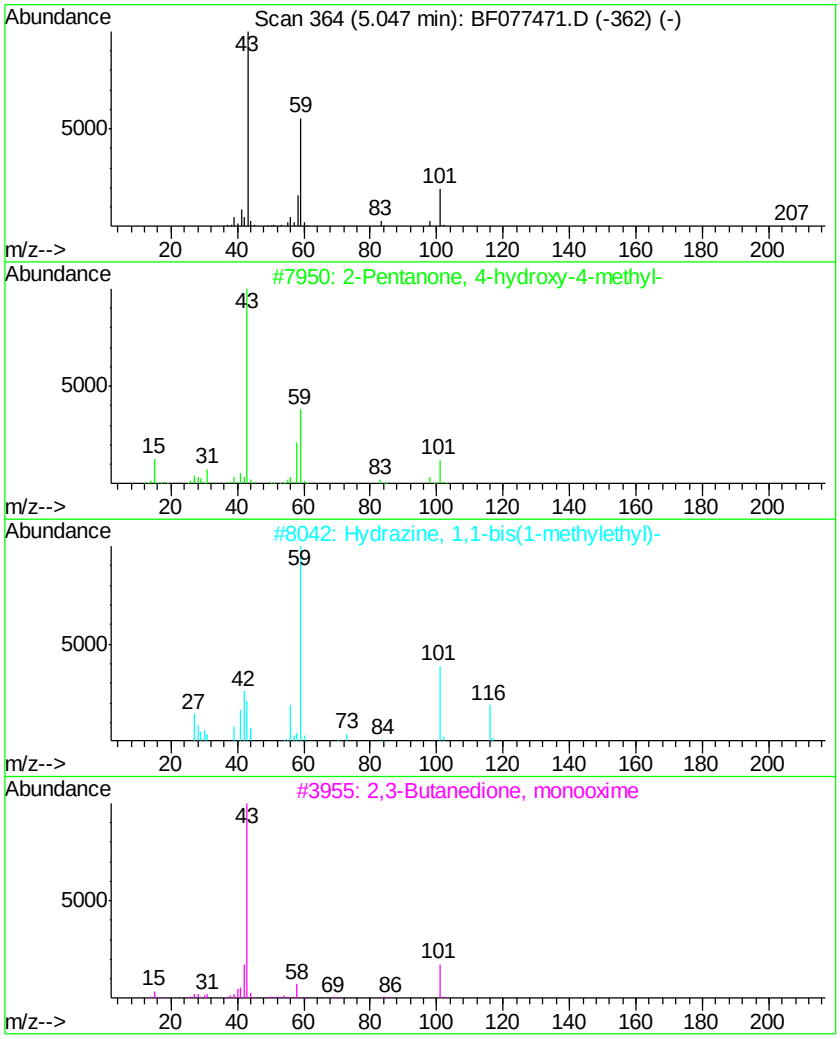
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

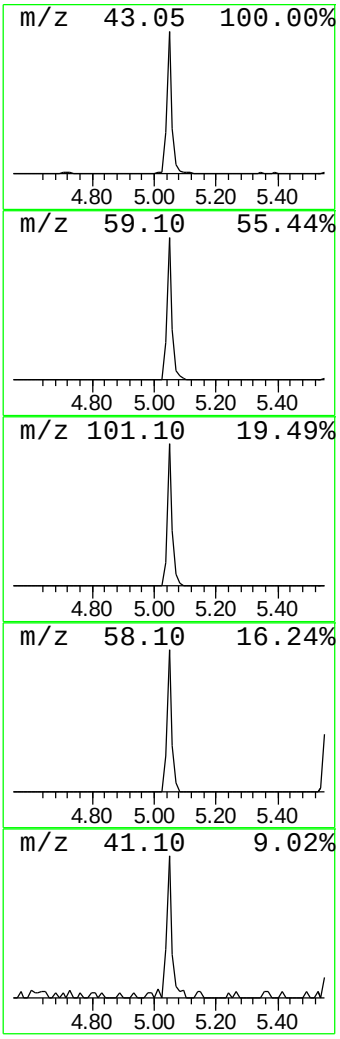
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	15.20 ng	247868	1,4-Dichlorobenzene-d4	7.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Butane	58	C4H10	000106-97-8	9





Library Search Compound Report

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Sample : G1384-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
36A-B-022515

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
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TIC Library : C:\DATABASE\NIST02.L
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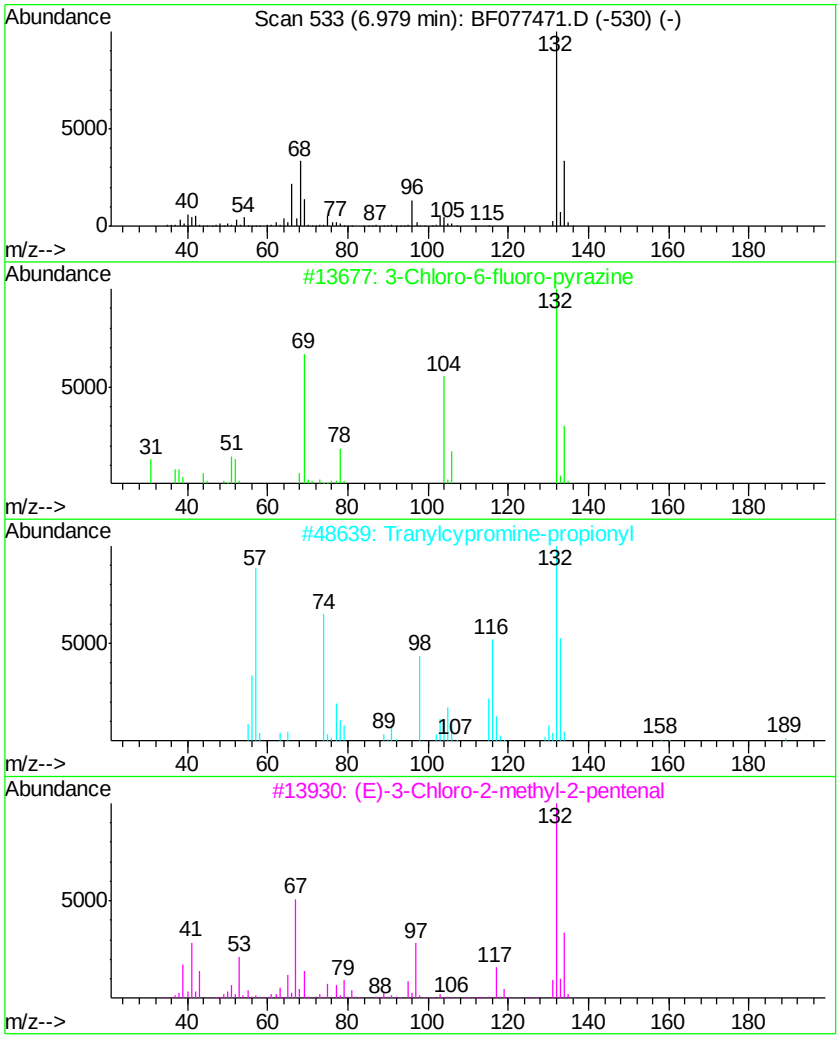
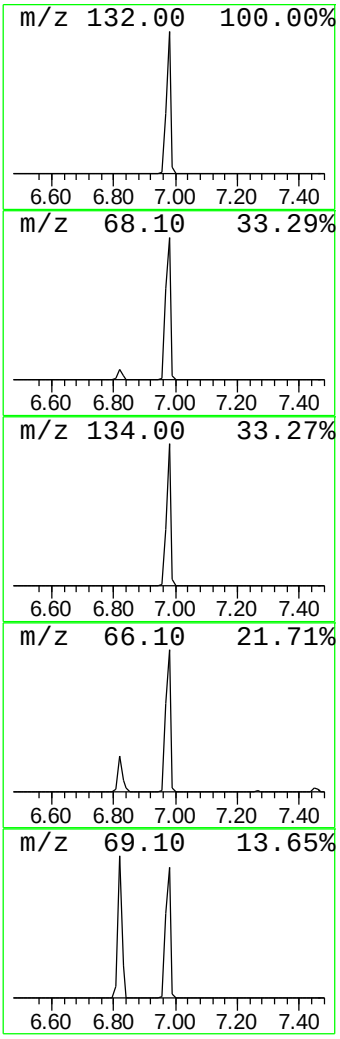
****

Peak Number 6 unknown6.98 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.98	82.08 ng	1338340	1,4-Dichlorobenzene-d4	7.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4	Amphetaminil	250	C17H18N2	017590-01-1	12
5	5-Aminoindole	132	C8H8N2	005192-03-0	12





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022615\
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Instrument :
BNA_F
ClientSampleId :
36A-B-022515

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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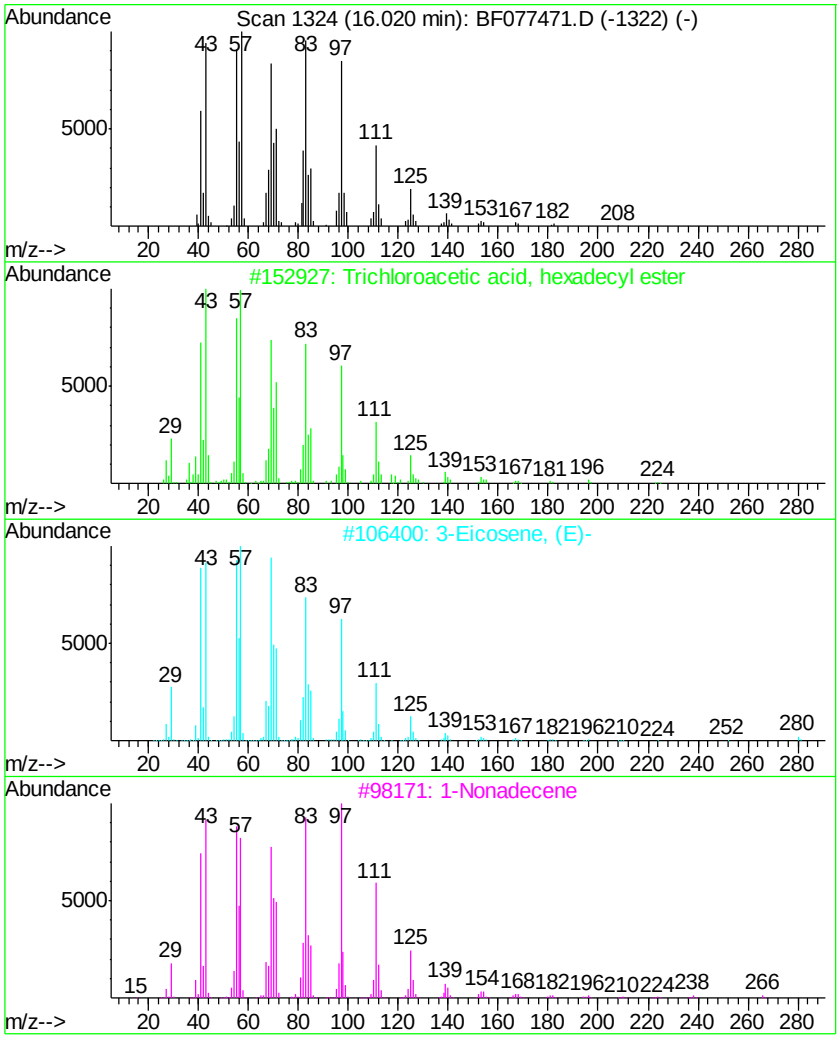
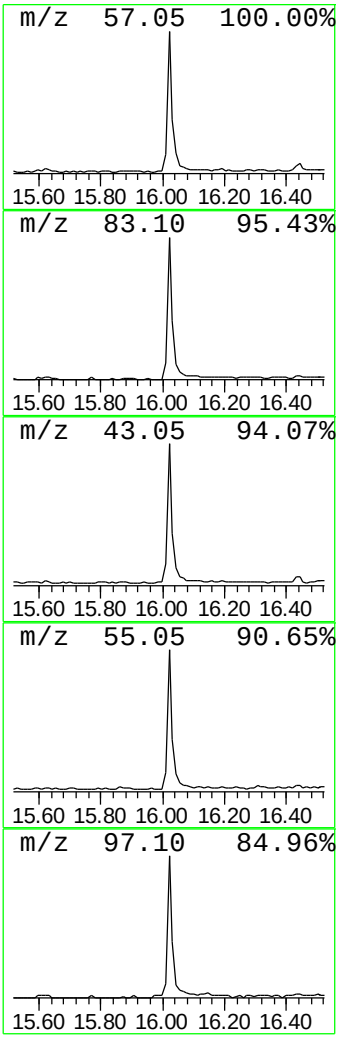
****

Peak Number 8 Trichloroacetic acid, hexad... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	11.59 ng	390696	Chrysene-d12	16.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	1-Heptadecanol	256	C17H36O	001454-85-9	87
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	87





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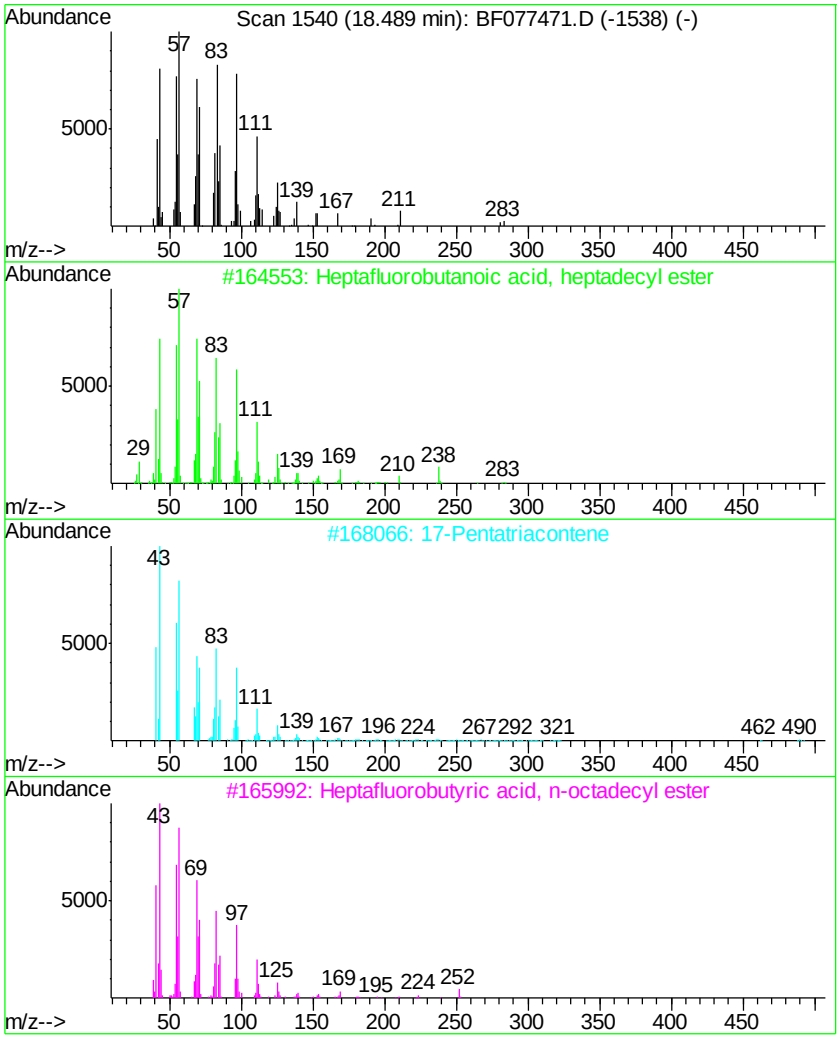
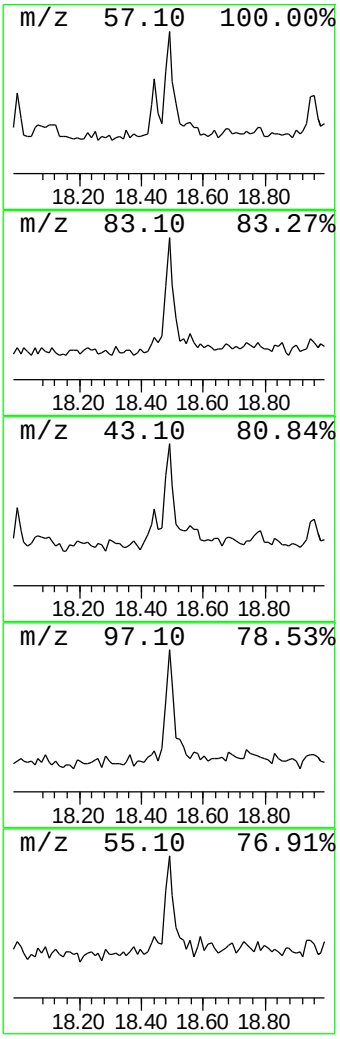
****

Peak Number 9 Heptafluorobutanoic acid, h... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.49	2.36 ng	78611	Perylene-d12	17.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	91
2	17-Pentatriacontene	491	C35H70	006971-40-0	91
3	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	87
4	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	87
5	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	80





Tentatively Identified Compound (LSC) summary

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
unknown1.42	1.42	289.7	ng	4723640	1	7.26	326088	20.0
unknown1.73	1.73	12.0	ng	196052	1	7.26	326088	20.0
2-Pentanone, 4-hy...	5.05	15.2	ng	247868	1	7.26	326088	20.0
unknown6.98	6.98	82.1	ng	1338340	1	7.26	326088	20.0
Trichloroacetic a...	16.02	11.6	ng	390696	5	16.15	674434	20.0
Heptafluorobutano...	18.49	2.4	ng	78611	6	17.86	667439	20.0