LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111414\
Data File : BF075550.D
Acq On : 15 Nov 2014 19:35
Operator : TP / JJ
Sample : F4649-02
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S32-FILL05

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-BF111214.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	1.624	44	47	49	rVB	2979456	4291400	100.00%	19.824%
2	1.761	56	59	63	rVB	136110	251867	5.87%	1.163%
3	1.830	63	65	74	rVV	163908	282482	6.58%	1.305%
4	1.967	74	77	84	rVV2	810566	1303197	30.37%	6.020%
5	2.070	84	86	91	rVB	34816	60485	1.41%	0.279%
6	5.339	370	372	376	rBV	548396	784263	18.28%	3.623%
7	5.842	413	416	419	rBV	1434277	1538378	35.85%	7.107%
8	7.099	523	526	528	rBV	1803697	1607916	37.47%	7.428%
9	7.259	538	540	543	rBV	1679865	1564039	36.45%	7.225%
10	7.545	563	565	568	rBV	219508	282528	6.58%	1.305%
11	7.739	579	582	584	rBV	1335410	1183685	27.58%	5.468%
12	8.242	623	626	628	rBV	1105559	1009548	23.52%	4.664%
13	9.133	702	704	706	rBV	399529	405877	9.46%	1.875%
14	10.471	819	821	824	rVB	1274241	1537658	35.83%	7.103%
15	10.973	863	865	868	rVB	467417	428423	9.98%	1.979%
16	11.305	892	894	897	rBV	382366	443510	10.33%	2.049%
17	12.288	978	980	983	rBV	1010112	1062915	24.77%	4.910%
18	13.157	1054	1056	1059	rBV	496635	457879	10.67%	2.115%
19	14.962	1211	1214	1216	rVB	78271	68332	1.59%	0.316%
20	15.157	1228	1231	1233	rBV	1312399	1634569	38.09%	7.551%
21	15.842	1289	1291	1294	rBV	38367	44166	1.03%	0.204%
22	16.334	1330	1334	1342	rBV	51960	121356	2.83%	0.561%
23	16.448	1342	1344	1347	rBV	504386	539131	12.56%	2.491%
24	16.917	1380	1385	1388	rBV4	58820	124256	2.90%	0.574%
25	18.197	1494	1497	1500	rBV	410400	563554	13.13%	2.603%
26	18.871	1550	1556	1563	rBV9	12104	55949	1.30%	0.258%

Sum of corrected areas: 21647363

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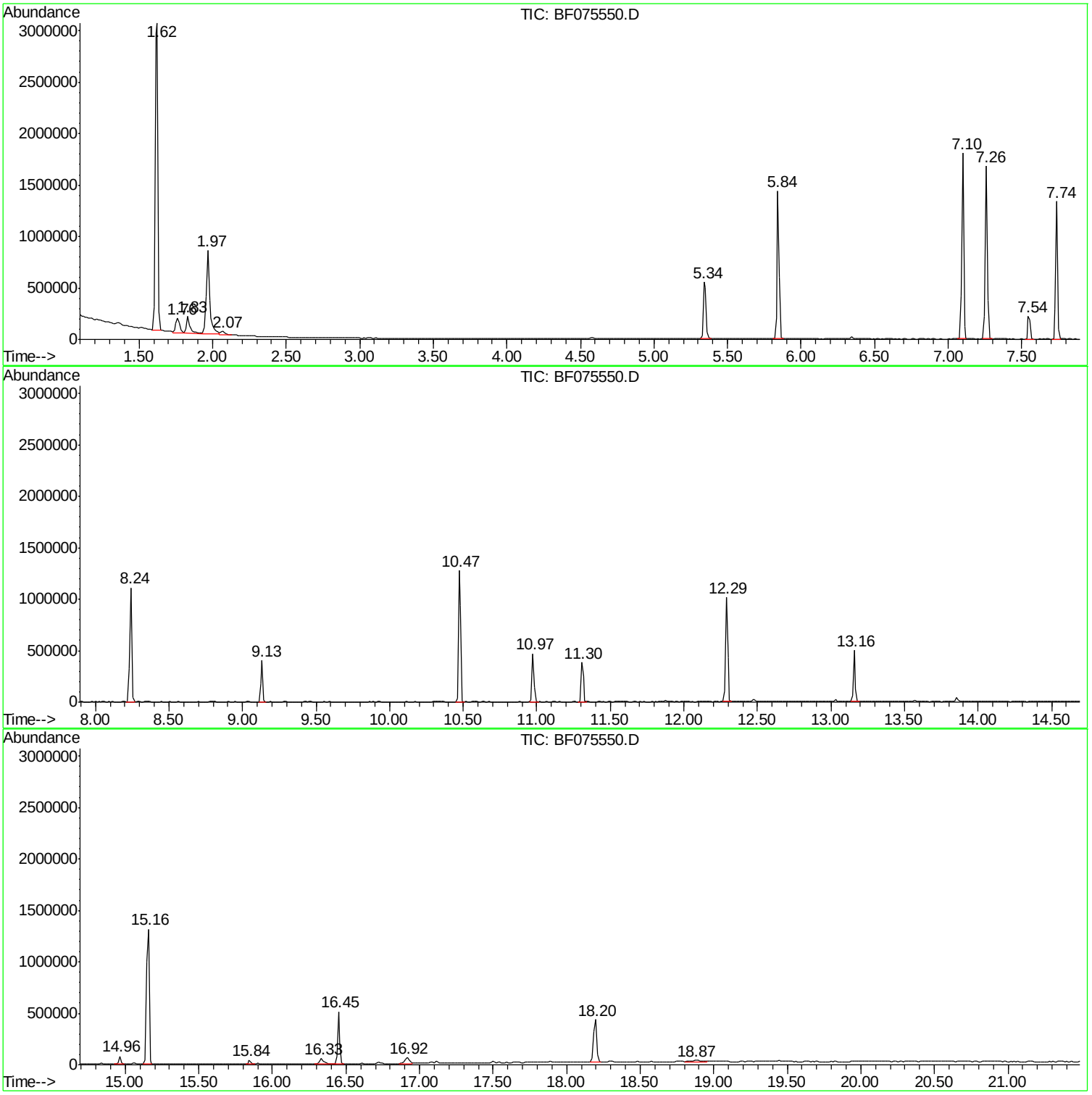
BNA_F
ClientSampleId :
S32-FILL05

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.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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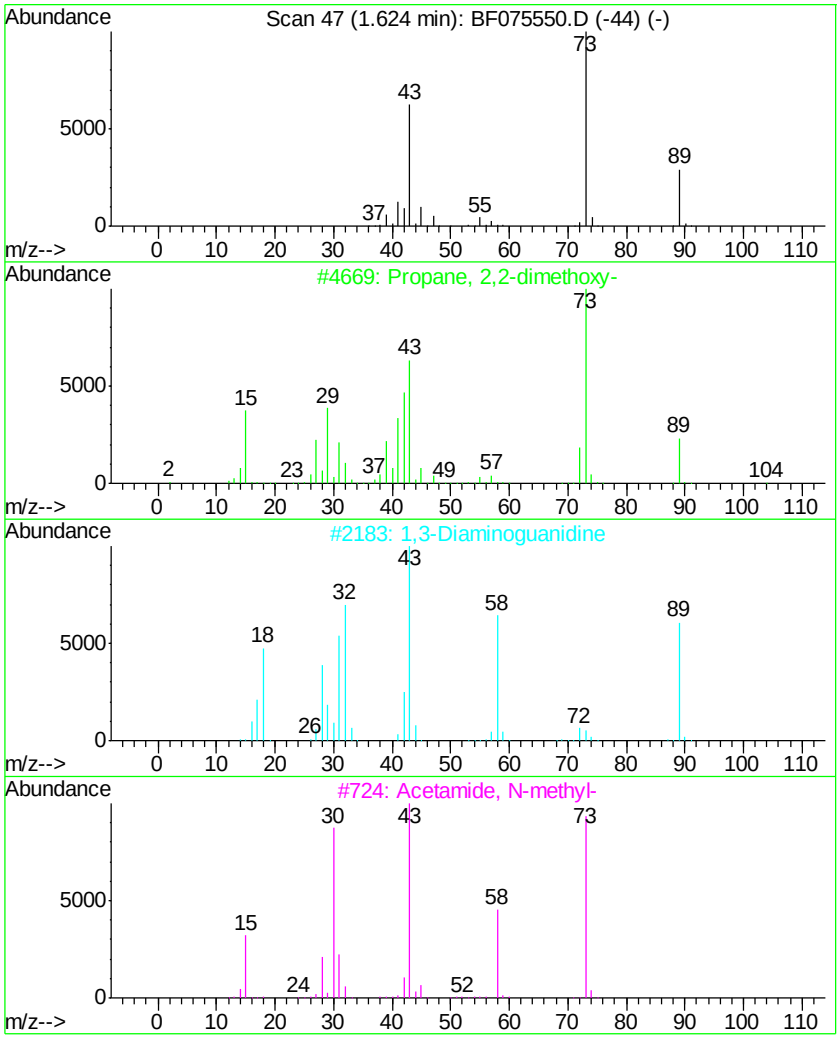
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

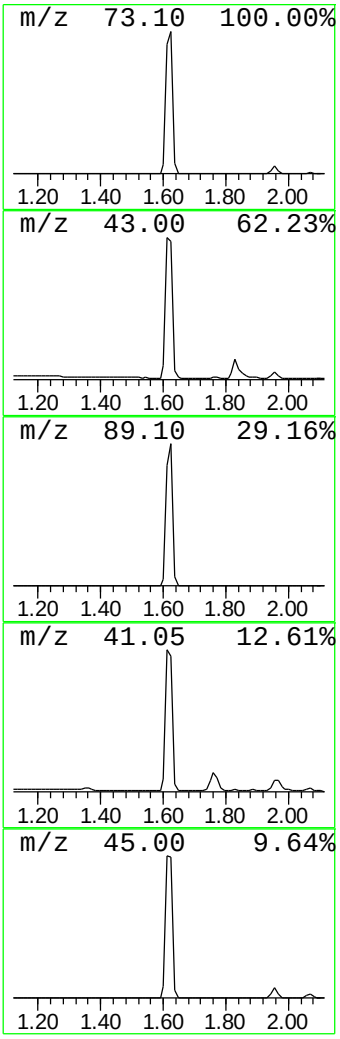
****

Peak Number 1 unknown1.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.62	303.79 ng	4291400	1,4-Dichlorobenzene-d4	7.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	45
2	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
3	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	9
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9





Library Search Compound Report

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Acq On : 15 Nov 2014 19:35
Operator : TP / JJ
Sample : F4649-02
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S32-FILL05

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

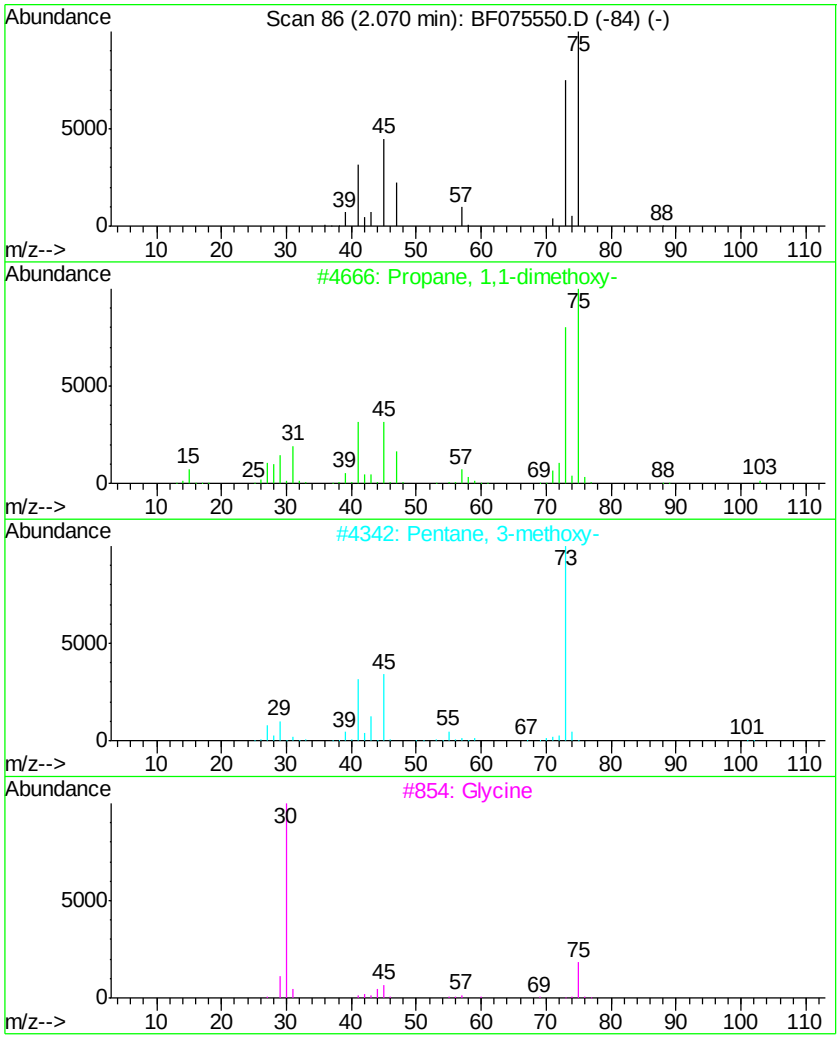
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

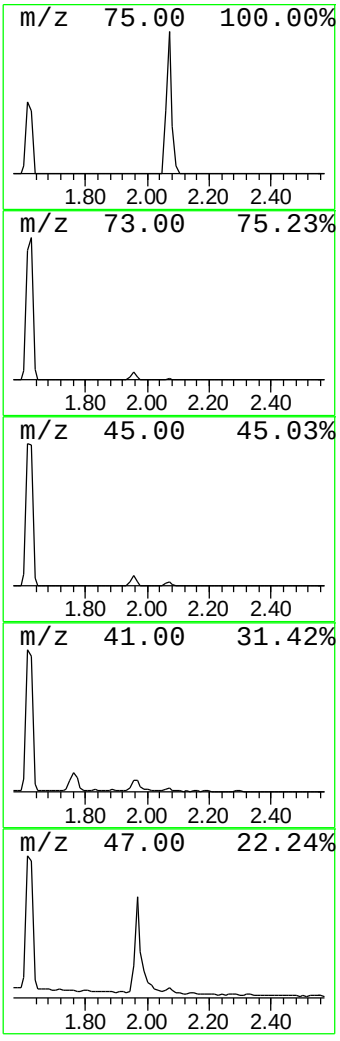
****

Peak Number 5 Propane, 1,1-dimethoxy- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.07	4.28 ng	60485	1,4-Dichlorobenzene-d4	7.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
3	Glycine	75	C2H5NO2	000056-40-6	7
4	1-Butanamine	73	C4H11N	000109-73-9	4
5	Methane, nitroso-	45	CH3NO	000865-40-7	4





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Acq On : 15 Nov 2014 19:35
Operator : TP / JJ
Sample : F4649-02
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S32-FILL05

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
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TIC Library : C:\DATABASE\NIST02.L
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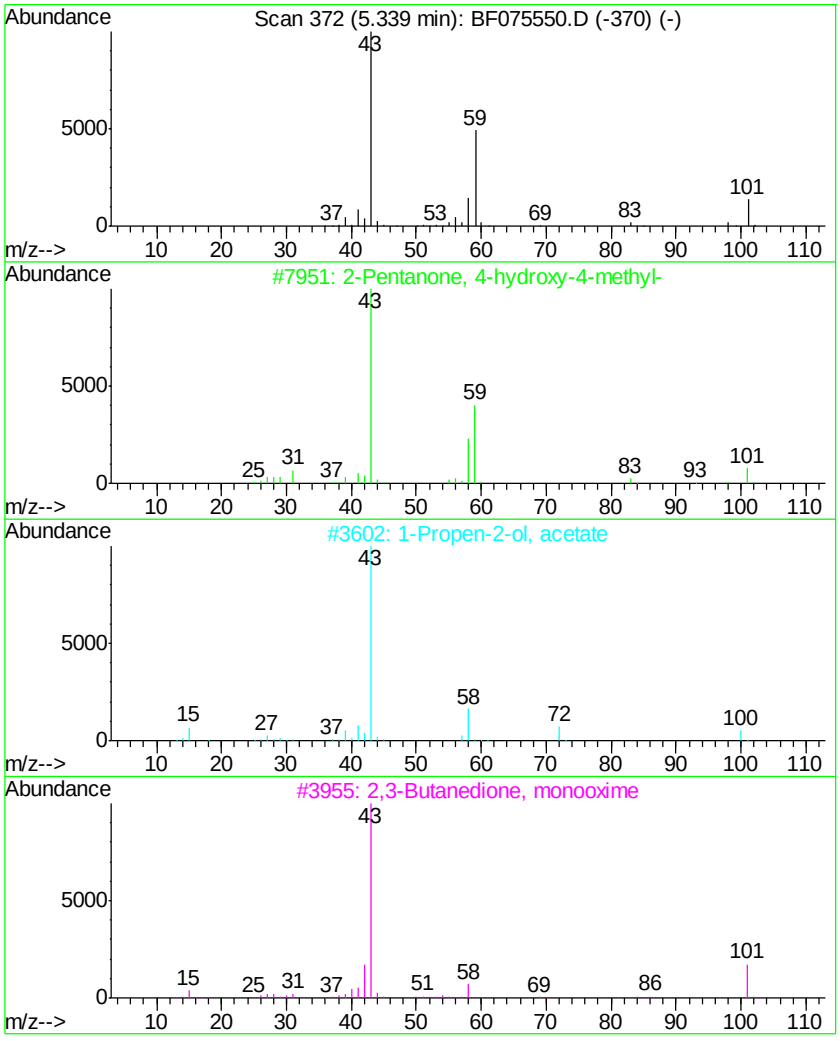
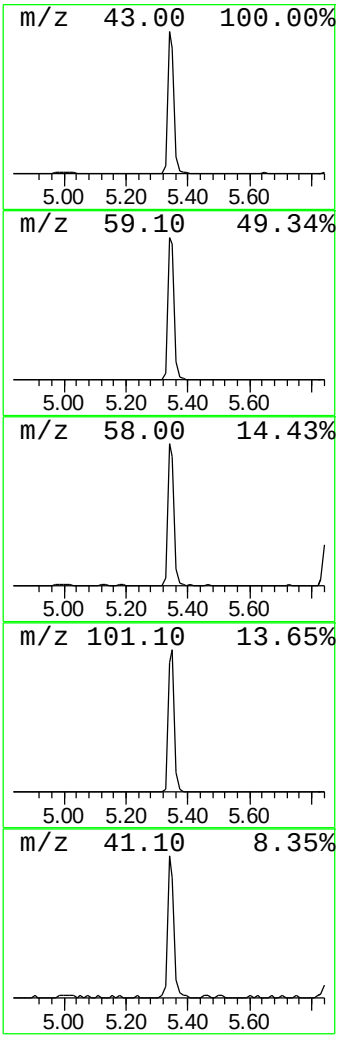
Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.34	55.52 ng	784263	1,4-Dichlorobenzene-d4	7.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	7
5	Acetone	58	C3H6O	000067-64-1	7





Library Search Compound Report

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Operator : TP / JJ
Sample : F4649-02
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S32-FILL05

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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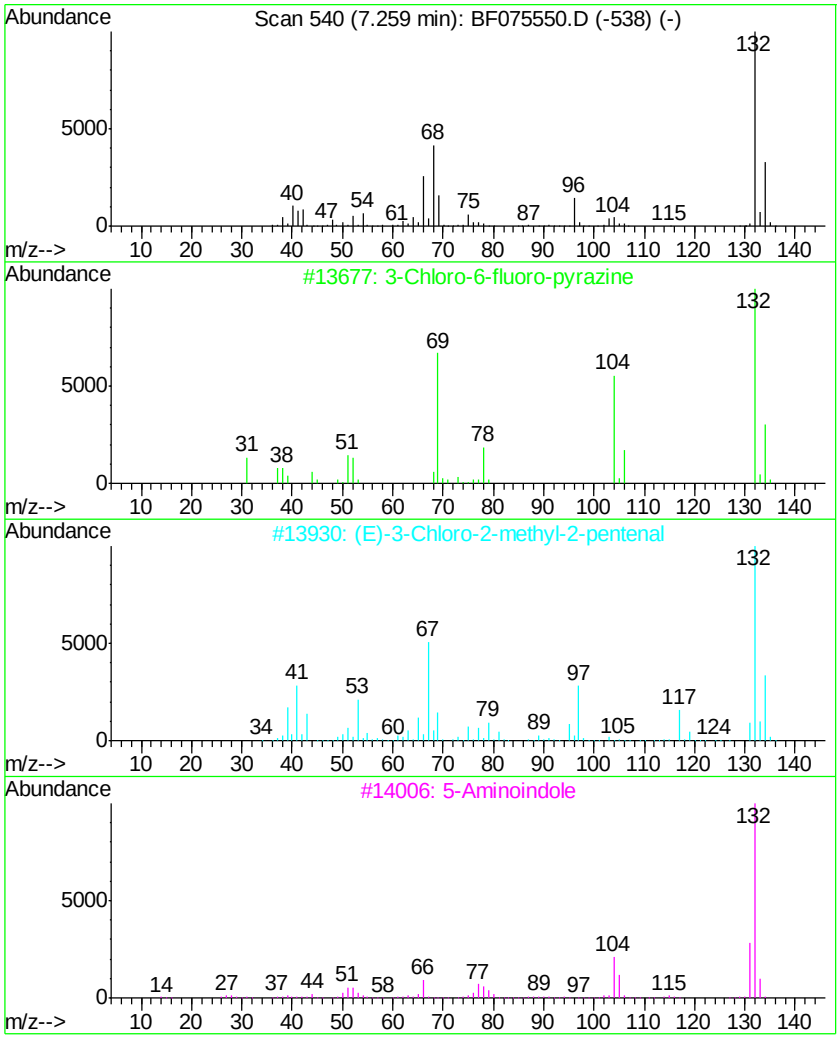
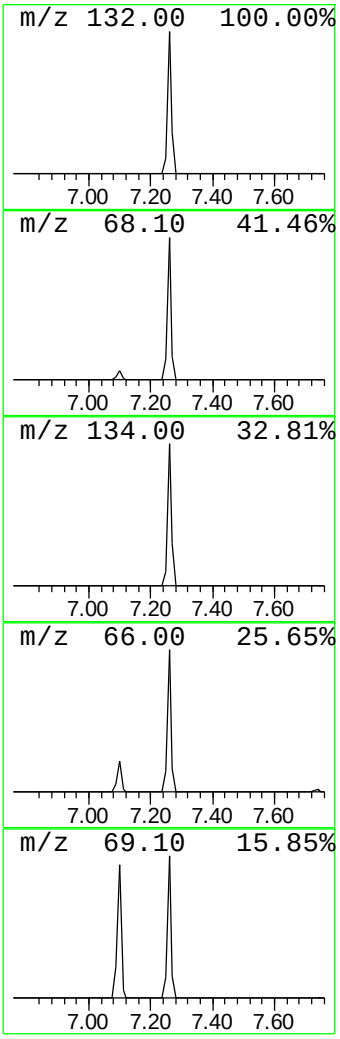
Peak Number 7 unknown7.26 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.26	110.72 ng	1564040	1,4-Dichlorobenzene-d4	7.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Sample : F4649-02
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S32-FILL05

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
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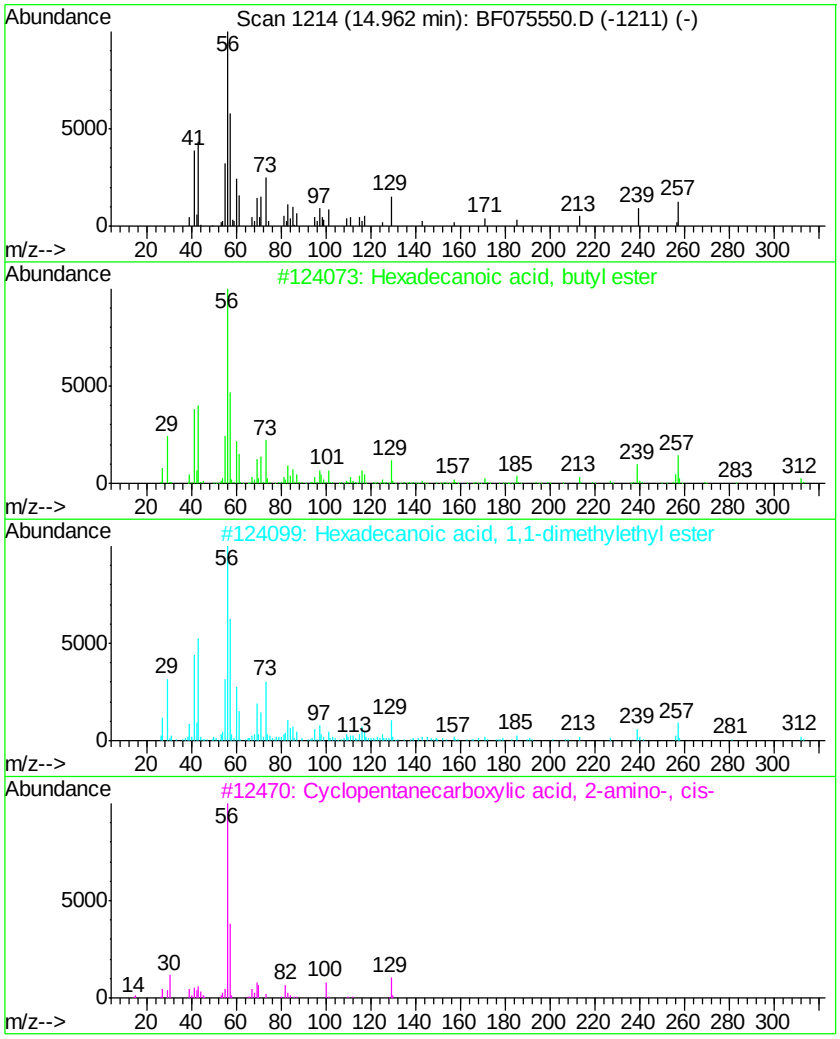
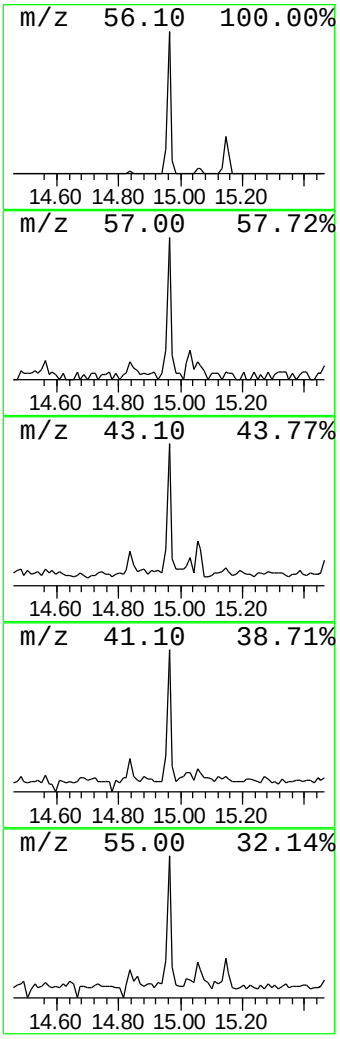
****

Peak Number 9 Hexadecanoic acid, butyl ester Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	2.53 ng	68332	Chrysene-d12	16.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	59
3	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	38
4	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	38
5	1-Pentadecene, 2-methyl-	224	C16H32	029833-69-0	37





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ClientSampleId : S32-FILL05

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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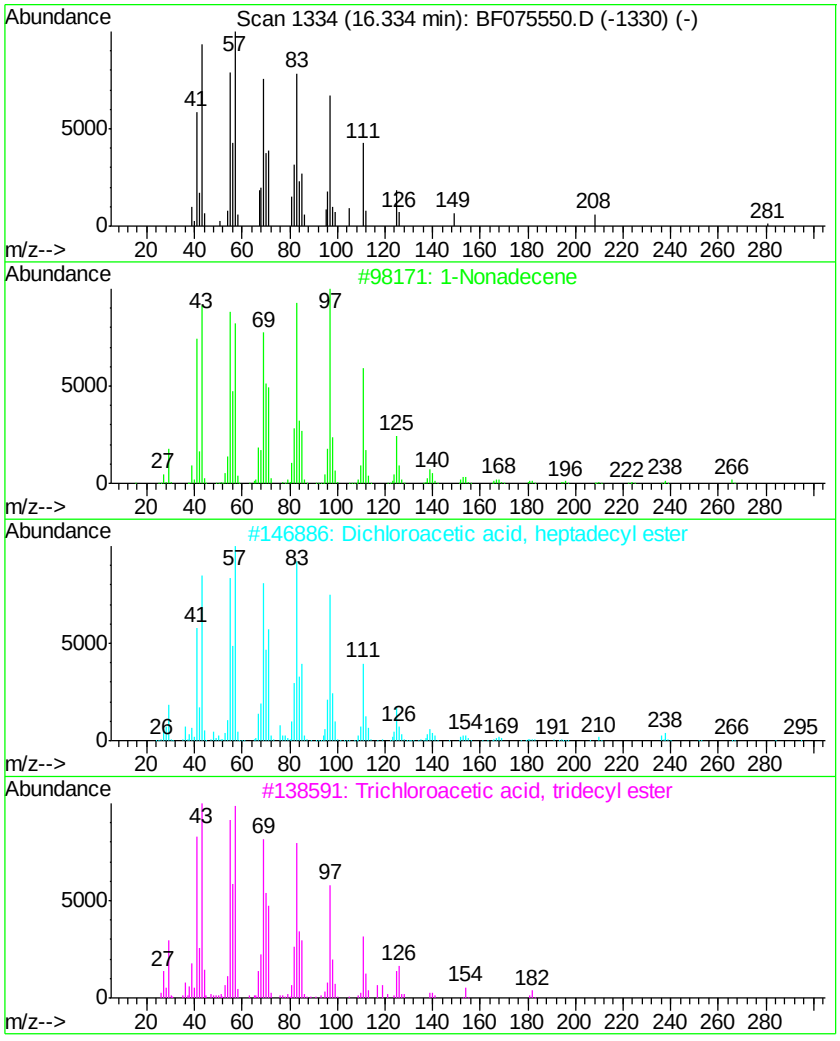
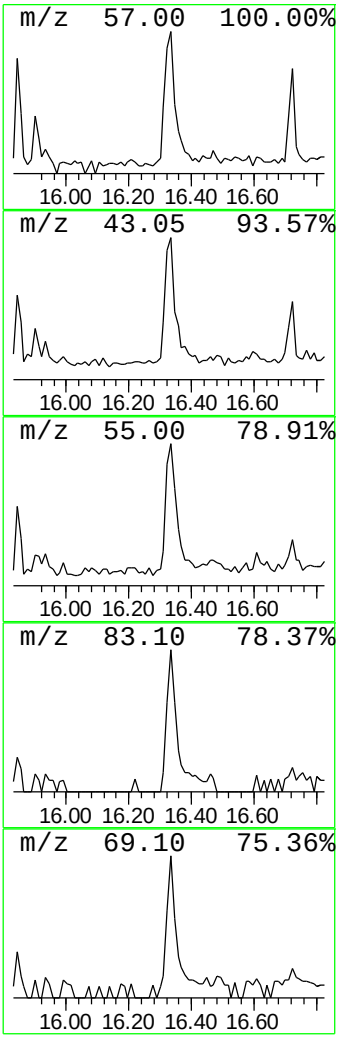
****

Peak Number 10 1-Nonadecene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.33	4.50 ng	121356	Chrysene-d12	16.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	90
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87
3	Trichloroacetic acid, tridecyl e...	344	C15H27Cl3O2	074339-51-8	86
4	1-Nonadecanol	284	C19H40O	001454-84-8	86
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	86





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

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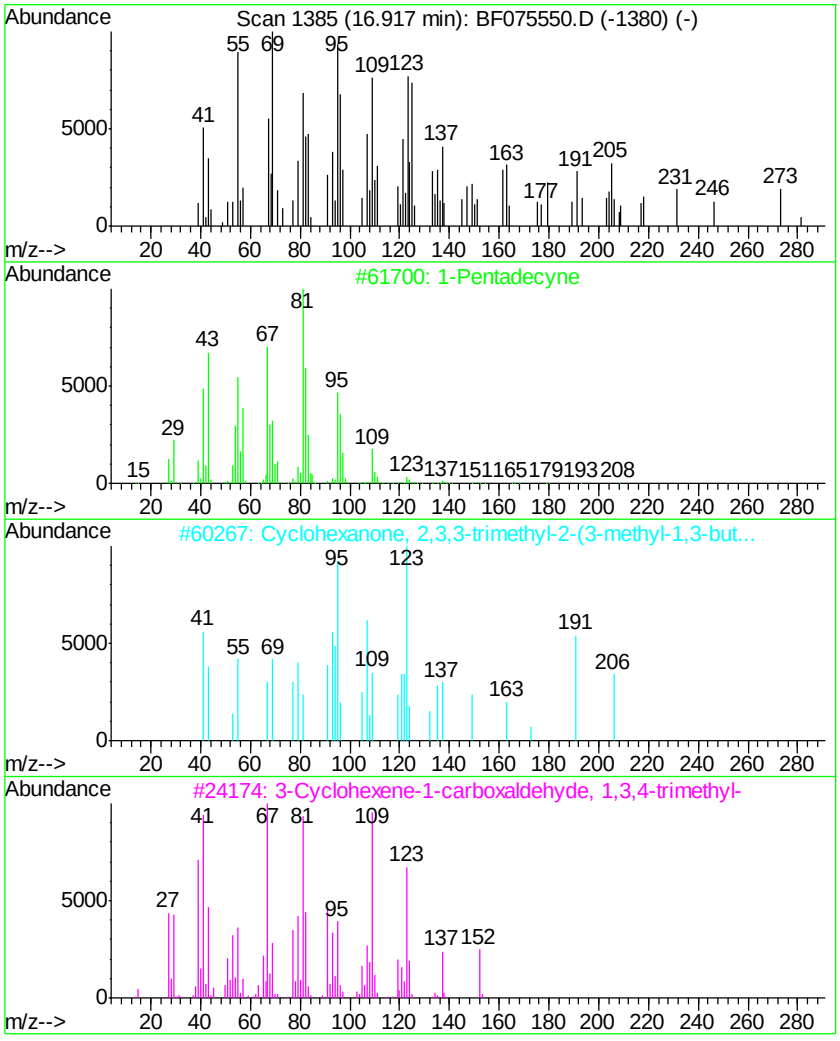
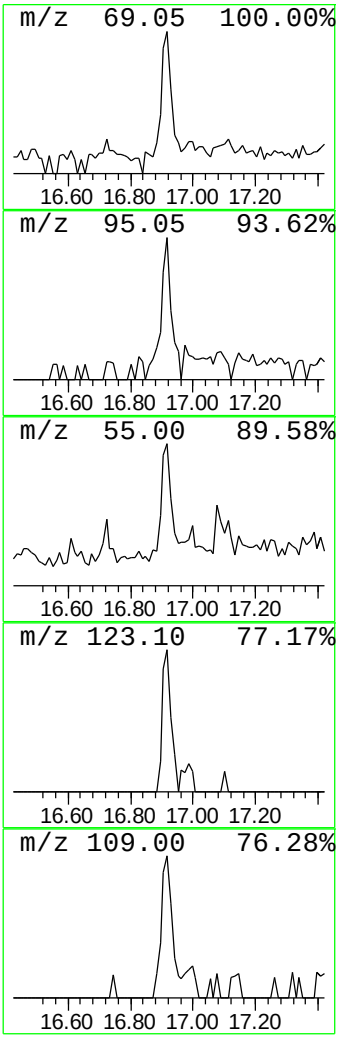
Peak Number 11 unknown16.92 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.92	4.61 ng	124256	Chrysene-d12	16.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentadecyne	208	C15H28	000765-13-9	42
2	Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-90-8	41
3	3-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	040702-26-9	27
4	Sesquirosefuran	218	C15H22O	039007-93-7	27
5	7-Tetradecyne	194	C14H26	035216-11-6	27





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
unknown1.62	1.62	303.8	ng	4291400	1	7.56	282528	20.0
Propane, 1,1-dime...	2.07	4.3	ng	60485	1	7.56	282528	20.0
2-Pentanone, 4-hy...	5.34	55.5	ng	784263	1	7.56	282528	20.0
unknown7.26	7.26	110.7	ng	1564040	1	7.56	282528	20.0
Hexadecanoic acid...	14.96	2.5	ng	68332	5	16.45	539131	20.0
1-Nonadecene	16.33	4.5	ng	121356	5	16.45	539131	20.0
unknown16.92	16.92	4.6	ng	124256	5	16.45	539131	20.0