LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111414\
Data File : BF075530.D
Acq On : 15 Nov 2014 9:43
Operator : TP / JJ
Sample : F4634-17
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-11052014

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	1.601	43	45	48	rVB	305491	377553	11.92%	2.653%
2	1.761	56	59	62	rVB	212280	279784	8.84%	1.966%
3	1.830	64	65	73	rVV	92035	168777	5.33%	1.186%
4	1.967	73	77	108	rVB	1562756	3166173	100.00%	22.247%
5	5.339	369	372	378	rVB	202185	226622	7.16%	1.592%
6	5.830	413	415	418	rBV	396281	472412	14.92%	3.319%
7	7.087	523	525	528	rBV	615962	535194	16.90%	3.760%
8	7.259	537	540	542	rBV	474418	508298	16.05%	3.571%
9	7.544	563	565	568	rBV	308029	341298	10.78%	2.398%
10	7.739	580	582	584	rBV	368409	373686	11.80%	2.626%
11	8.242	623	626	628	rBV	242009	313269	9.89%	2.201%
12	9.133	701	704	706	rBV	420003	482707	15.25%	3.392%
13	10.470	819	821	824	rBV	821725	780357	24.65%	5.483%
14	10.973	863	865	868	rBV	39628	33628	1.06%	0.236%
15	11.305	892	894	897	rBV	500663	528606	16.70%	3.714%
16	12.288	977	980	983	rBV	915790	865976	27.35%	6.085%
17	13.156	1053	1056	1059	rVB	599813	550755	17.39%	3.870%
18	13.854	1115	1117	1128	rBV	60504	74673	2.36%	0.525%
19	14.962	1212	1214	1216	rBV	37327	37083	1.17%	0.261%
20	15.157	1228	1231	1233	rBV	1566261	2022179	63.87%	14.208%
21	16.334	1330	1334	1342	rBV2	144245	486558	15.37%	3.419%
22	16.448	1342	1344	1347	rVB	623353	654327	20.67%	4.598%
23	16.585	1354	1356	1364	rVB2	16528	35055	1.11%	0.246%
24	18.174	1492	1495	1498	rBV	552563	675099	21.32%	4.743%
25	18.871	1553	1556	1563	rBV5	28488	107732	3.40%	0.757%
26	19.294	1591	1593	1600	rVB4	13150	34087	1.08%	0.240%
27	19.557	1613	1616	1620	rBV	50652	100337	3.17%	0.705%

Sum of corrected areas: 14232225

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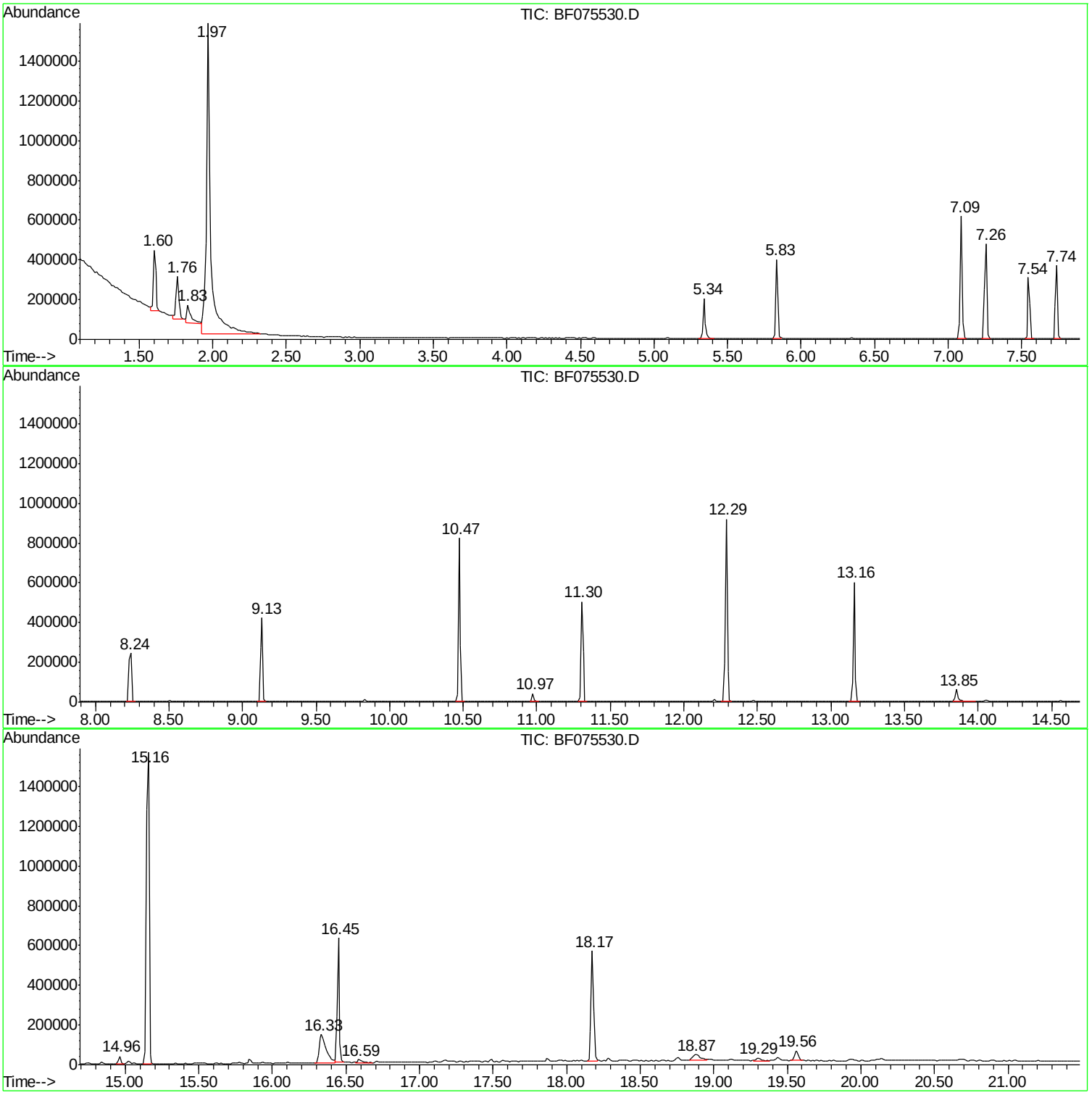
Instrument :
BNA_F
ClientSampleId :
DUP-11052014

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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

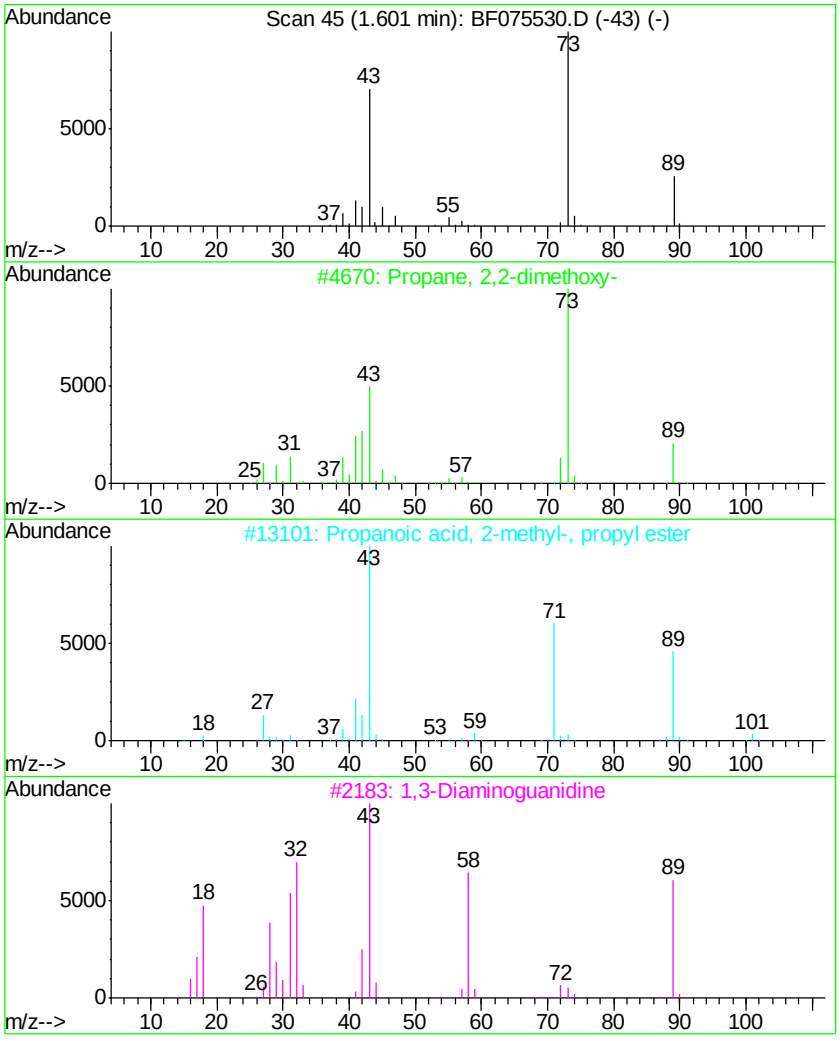
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

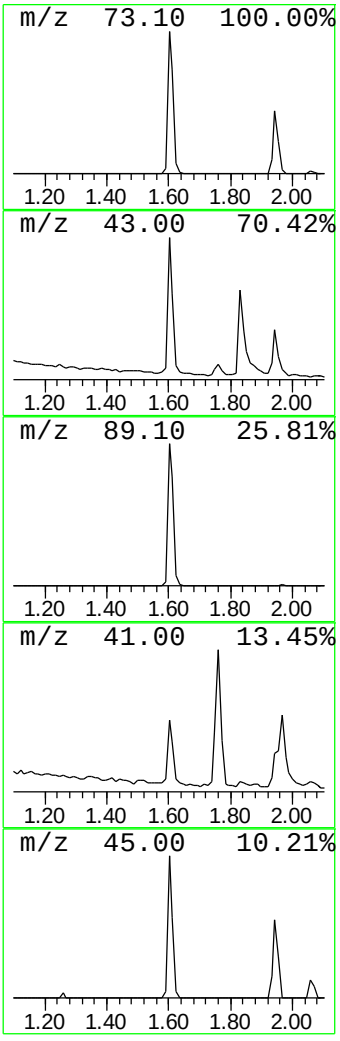
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.60	22.12 ng	377553	1,4-Dichlorobenzene-d4	7.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	59
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	17
3	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5	1-Propanol, 2-methyl-2-nitro-	119	C4H9NO3	000076-39-1	9





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Sample : F4634-17
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Instrument : BNA_F
ClientSampleId : DUP-11052014

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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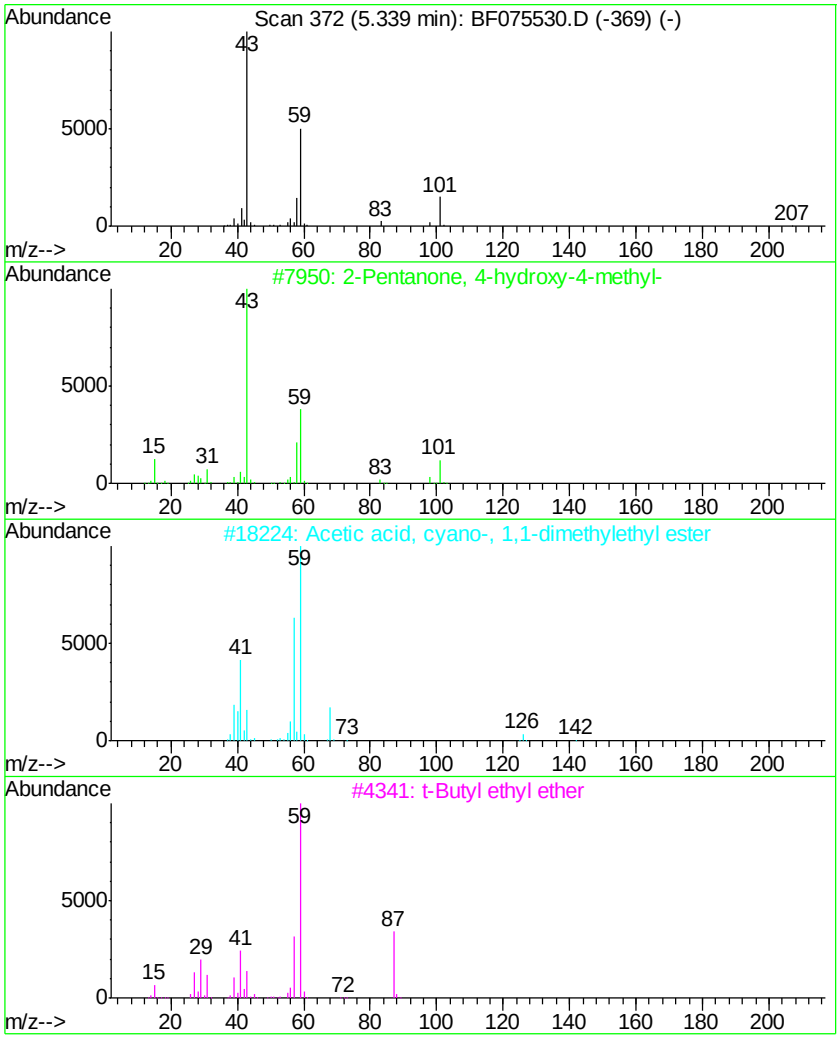
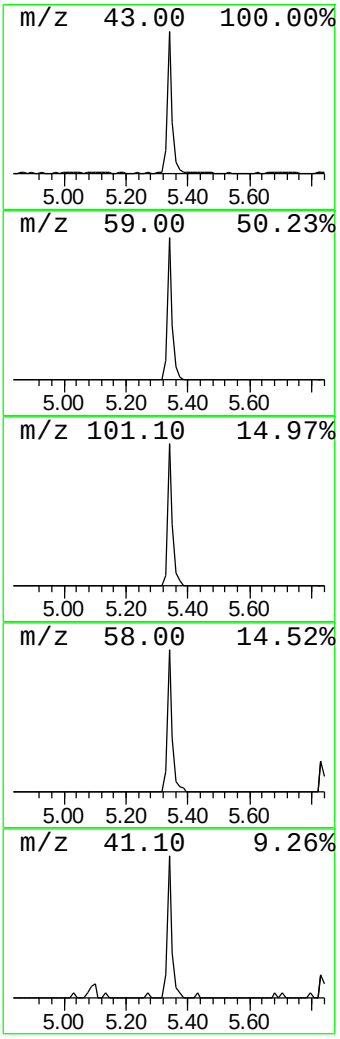
Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.34	13.28 ng	226622	1,4-Dichlorobenzene-d4	7.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	t-Butyl ethyl ether	102	C6H14O	1000118-18-4	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111414\
Data File : BF075530.D
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Sample : F4634-17
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-11052014

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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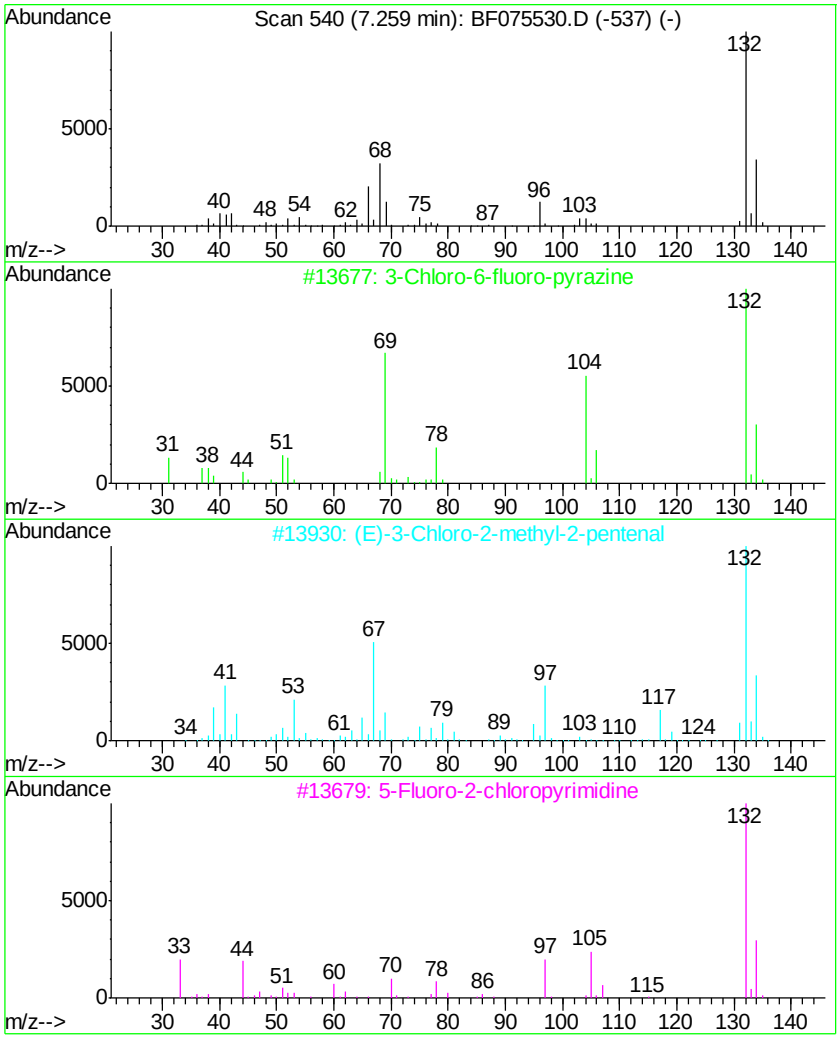
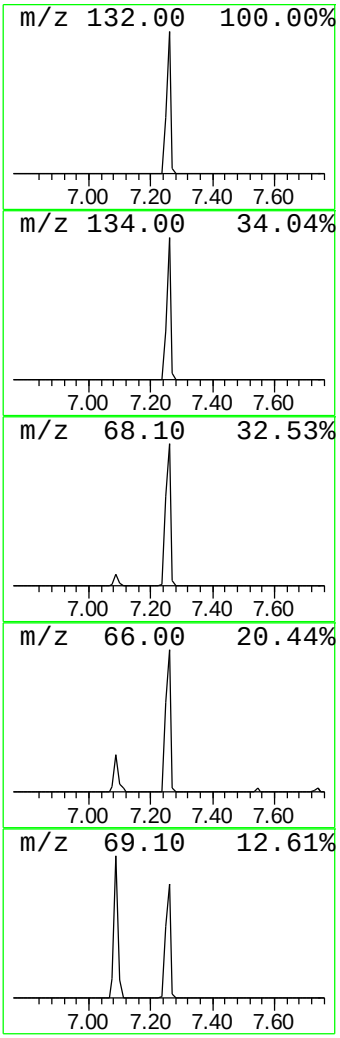
Peak Number 6 unknown7.26 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.26	29.79 ng	508298	1,4-Dichlorobenzene-d4	7.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Data File : BF075530.D
Acq On : 15 Nov 2014 9:43
Operator : TP / JJ
Sample : F4634-17
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-11052014

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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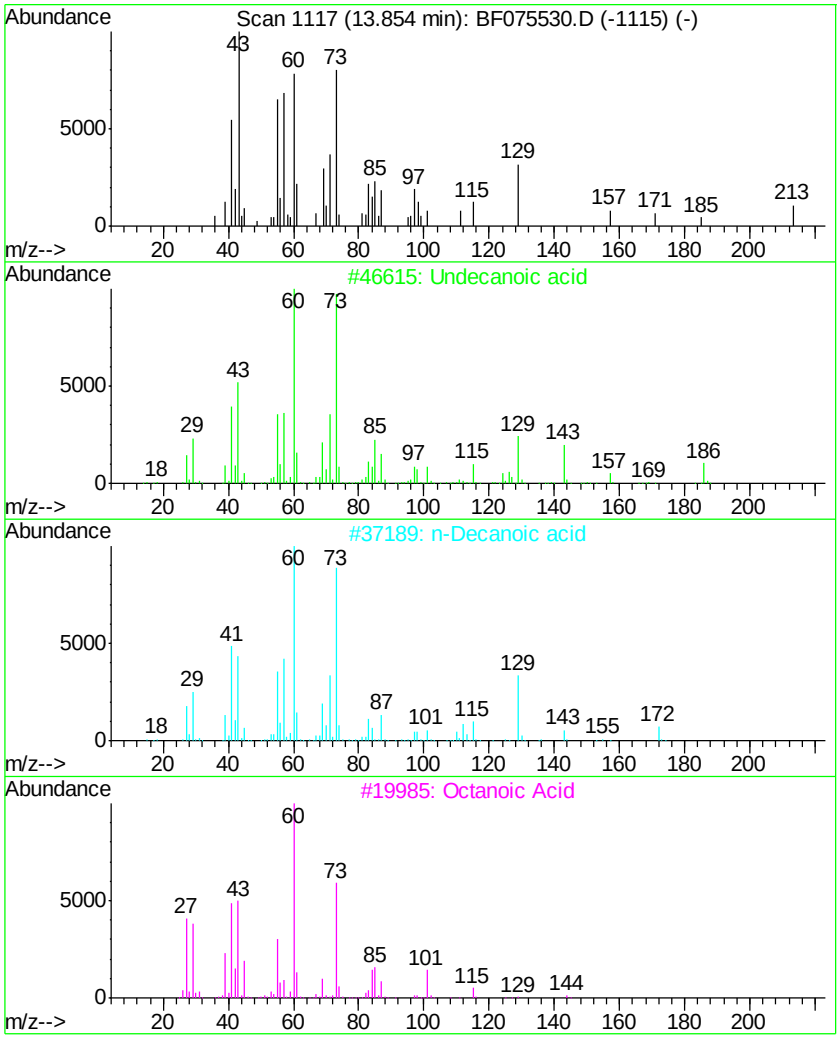
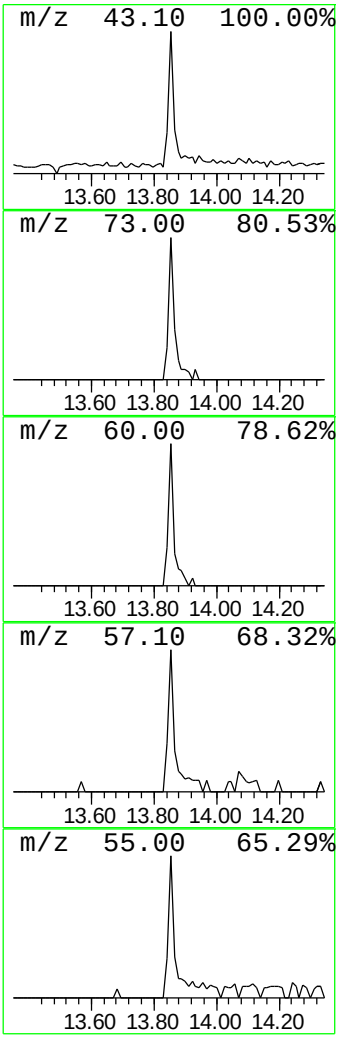
Peak Number 8 Undecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	2.71 ng	74673	Phenanthrene-d10	13.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	64
2	n-Decanoic acid	172	C10H20O2	000334-48-5	53
3	Octanoic Acid	144	C8H16O2	000124-07-2	50
4	Nonanoic acid	158	C9H18O2	000112-05-0	47
5	.alpha.-D-Glucopyranoside, .alph...	342	C12H22O11	000099-20-7	47





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111414\
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Acq On : 15 Nov 2014 9:43
Operator : TP / JJ
Sample : F4634-17
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-11052014

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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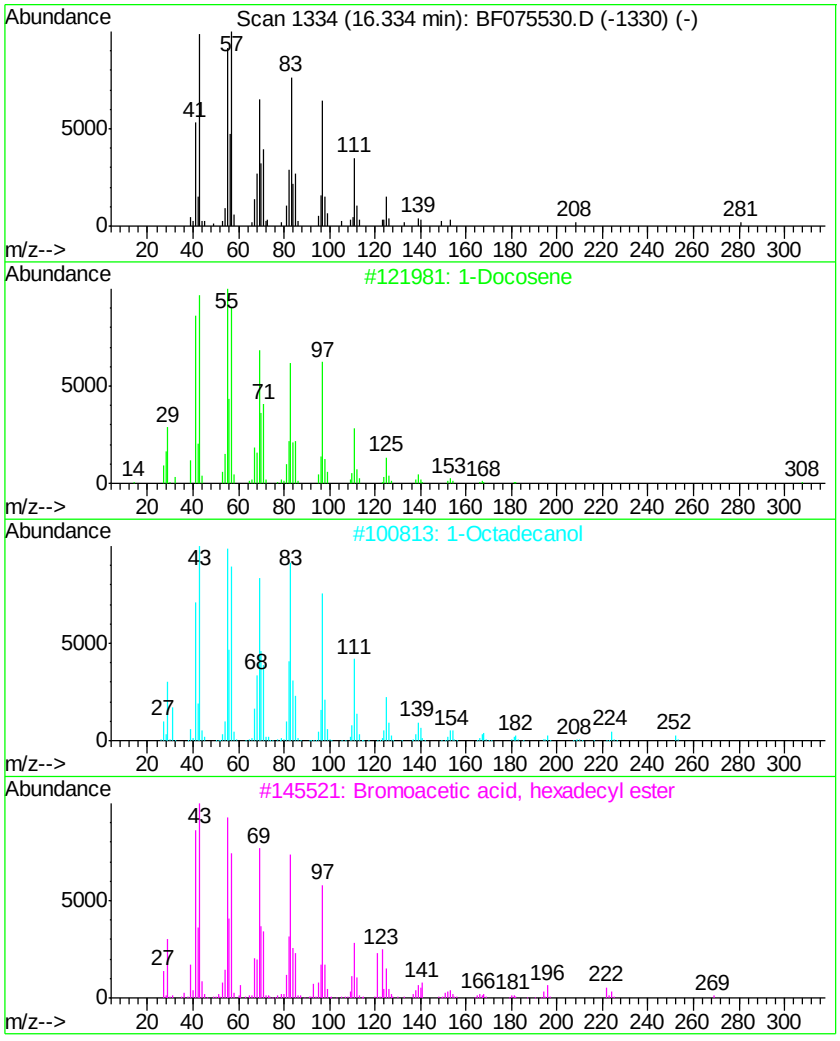
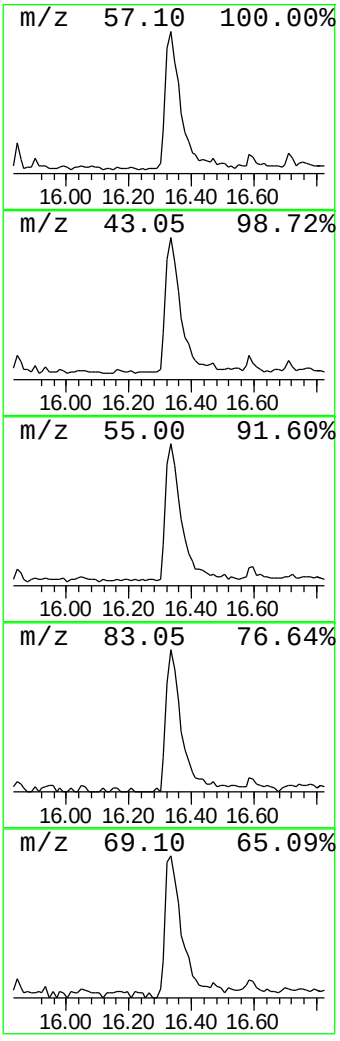
Peak Number 9 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.33	14.87 ng	486558	Chrysene-d12	16.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	94
2	1-Octadecanol	270	C18H38O	000112-92-5	91
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
4	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	91
5	1-Nonadecene	266	C19H38	018435-45-5	91





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ClientSampleId : DUP-11052014

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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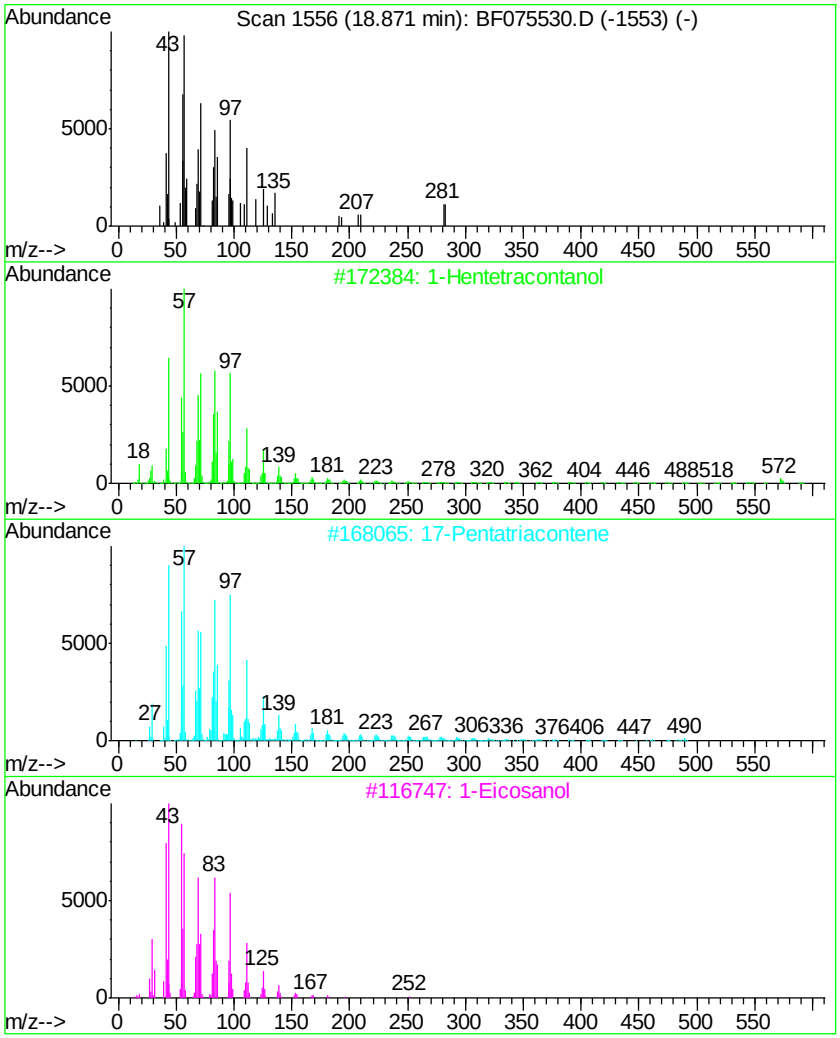
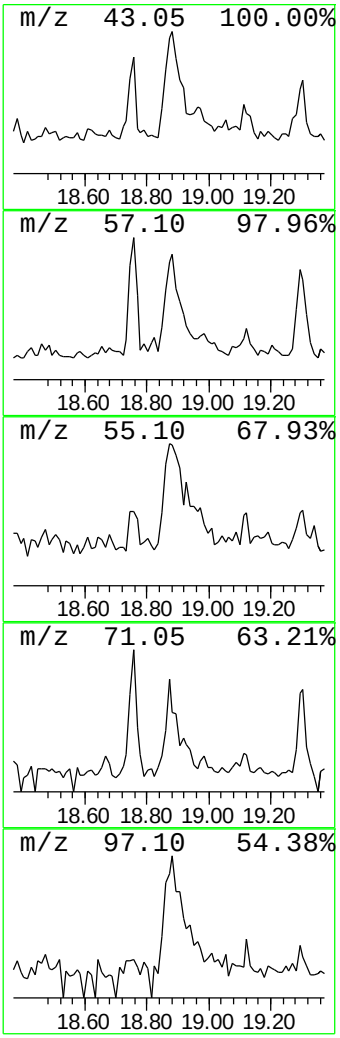
Peak Number 10 1-Hentetracontanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.87	3.19 ng	107732	Perylene-d12	18.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hentetracontanol	593	C41H84O	040710-42-7	70
2	17-Pentatriacontene	491	C35H70	006971-40-0	70
3	1-Eicosanol	298	C20H42O	000629-96-9	43
4	Cyclopentane, 2-isopropyl-1,3-di...	140	C10H20	032281-85-9	27
5	Eicosane	282	C20H42	000112-95-8	14





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

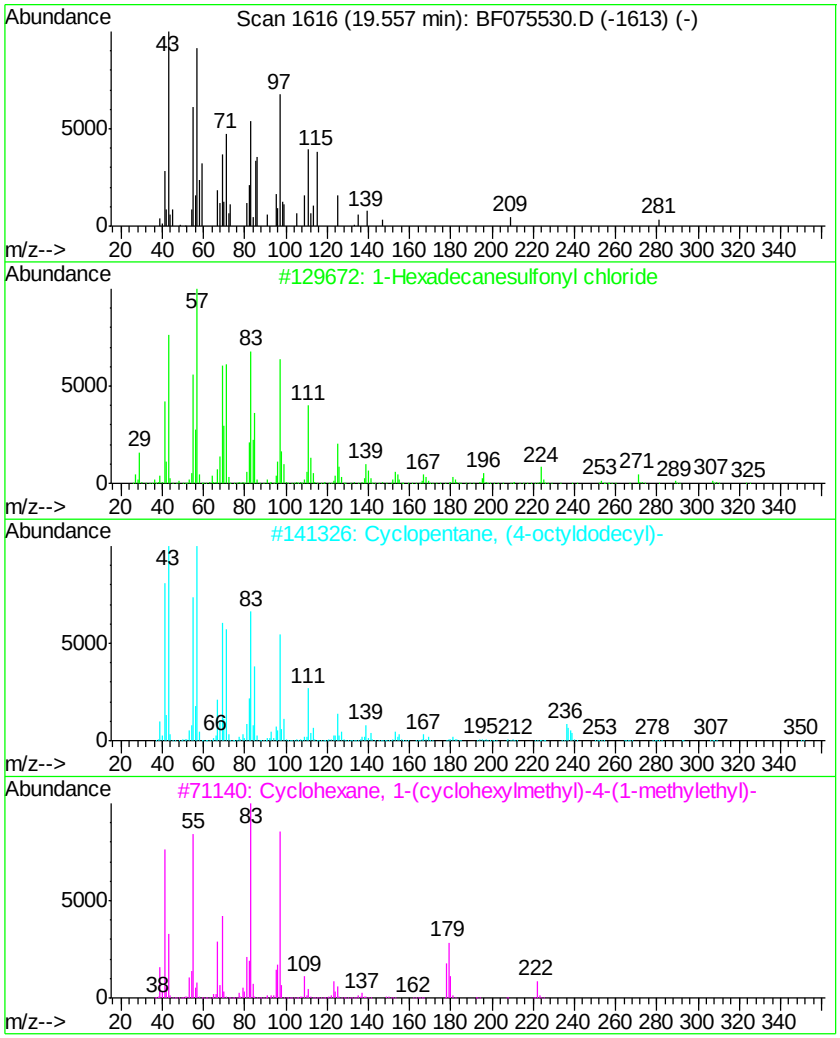
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

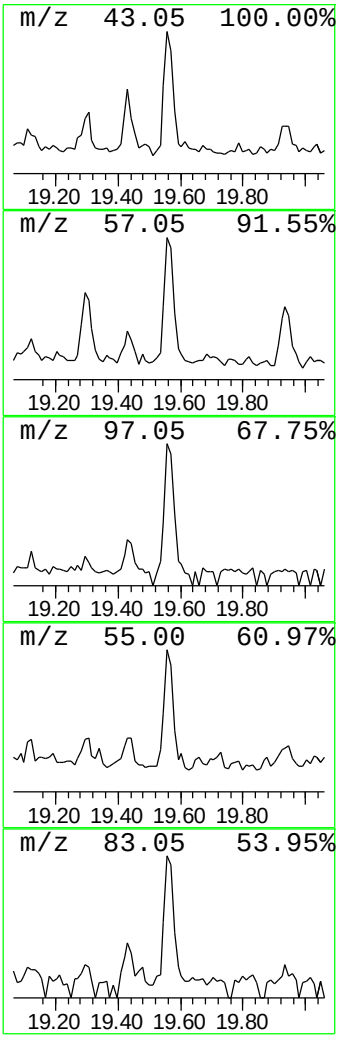
****

Peak Number 11 1-Hexadecanesulfonyl chloride Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.56	2.97 ng	100337	Perylene-d12	18.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	53
2	Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	49
3	Cyclohexane, 1-(cyclohexylmethyl...	222	C16H30	054965-61-6	14
4	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	14
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	10





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
Propane, 2,2-dime...	1.60	22.1	ng	377553	1	7.54	341298	20.0
2-Pentanone, 4-hy...	5.34	13.3	ng	226622	1	7.54	341298	20.0
unknown7.26	7.26	29.8	ng	508298	1	7.54	341298	20.0
Undecanoic acid	13.85	2.7	ng	74673	4	13.16	550755	20.0
1-Docosene	16.33	14.9	ng	486558	5	16.45	654327	20.0
1-Hentetracontanol	18.87	3.2	ng	107732	6	18.17	675099	20.0
1-Hexadecanesulfo...	19.56	3.0	ng	100337	6	18.17	675099	20.0