LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041015\
Data File : BF078408.D
Acq On : 10 Apr 2015 19:25
Operator : TP/IZ
Sample : G1791-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LS-SD08C

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-BF040115.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	1.013	9	11	14	rVV	303655	275589	26.50%	3.466%
2	1.127	18	21	24	rVB	85009	107849	10.37%	1.356%
3	1.264	31	33	36	rVB	59434	65613	6.31%	0.825%
4	1.527	54	56	63	rVV	30652	51618	4.96%	0.649%
5	1.618	63	64	87	rVB	613408	1040000	100.00%	13.079%
6	4.522	316	318	324	rBV	46596	65557	6.30%	0.824%
7	5.116	367	370	376	rBV	424399	541355	52.05%	6.808%
8	6.453	485	487	492	rVB	587046	560761	53.92%	7.052%
9	6.568	495	497	500	rVB	592849	593486	57.07%	7.463%
10	6.853	520	522	525	rBV	146433	163694	15.74%	2.059%
11	7.048	536	539	541	rBV	293528	403224	38.77%	5.071%
12	7.562	582	584	586	rBV	307562	337568	32.46%	4.245%
13	8.431	658	660	663	rBV	189552	228692	21.99%	2.876%
14	9.151	721	723	726	rVB	33557	31850	3.06%	0.401%
15	9.779	776	778	781	rBV	676764	605404	58.21%	7.613%
16	10.294	821	823	825	rBV	74359	64430	6.20%	0.810%
17	10.545	842	845	847	rBV2	6239	11002	1.06%	0.138%
18	10.591	847	849	852	rVB	308093	282823	27.19%	3.557%
19	11.151	896	898	899	rBV	11917	12642	1.22%	0.159%
20	11.494	926	928	932	rVB	132370	119035	11.45%	1.497%
21	11.562	932	934	937	rBV	433183	457532	43.99%	5.754%
22	12.420	1006	1009	1011	rBV	262532	307141	29.53%	3.862%
23	13.963	1142	1144	1146	rVB	44169	46304	4.45%	0.582%
24	14.408	1180	1183	1185	rBV	821647	804246	77.33%	10.114%
25	15.597	1284	1287	1291	rBV2	10375	21530	2.07%	0.271%
26	15.677	1291	1294	1296	rVV	327611	372113	35.78%	4.680%
27	17.357	1439	1441	1444	rBV	271733	369619	35.54%	4.648%
28	18.329	1524	1526	1529	rVB3	7145	11244	1.08%	0.141%

Sum of corrected areas: 7951921

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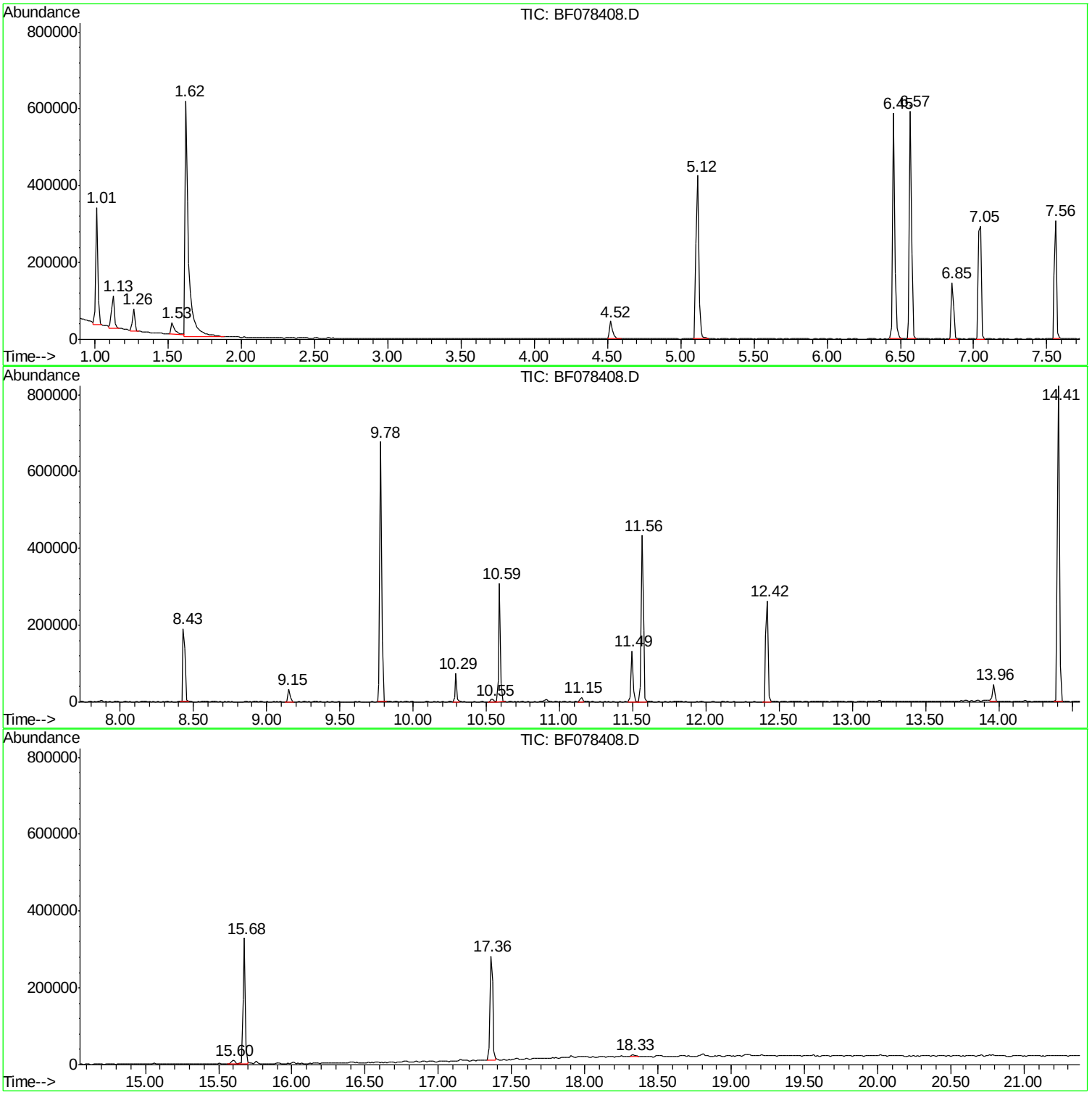
Instrument : BNA_F
ClientSampleId : LS-SD08C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.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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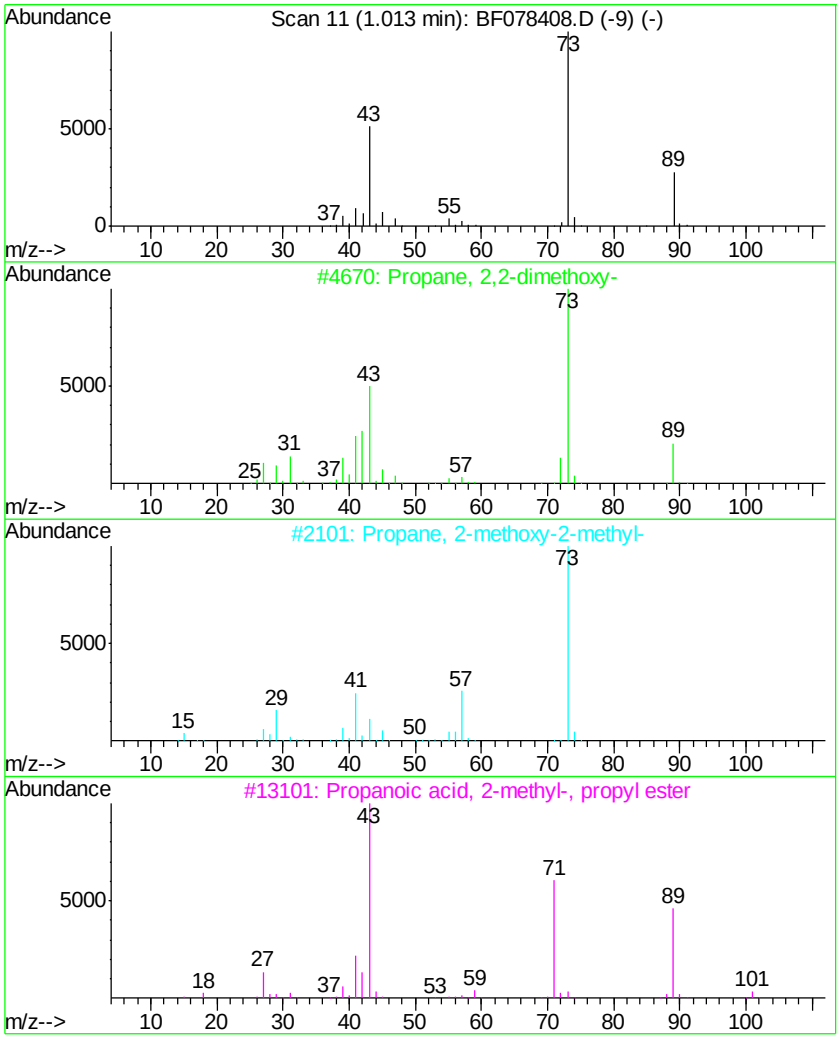
TIC Integration Parameters: LSCINT.P

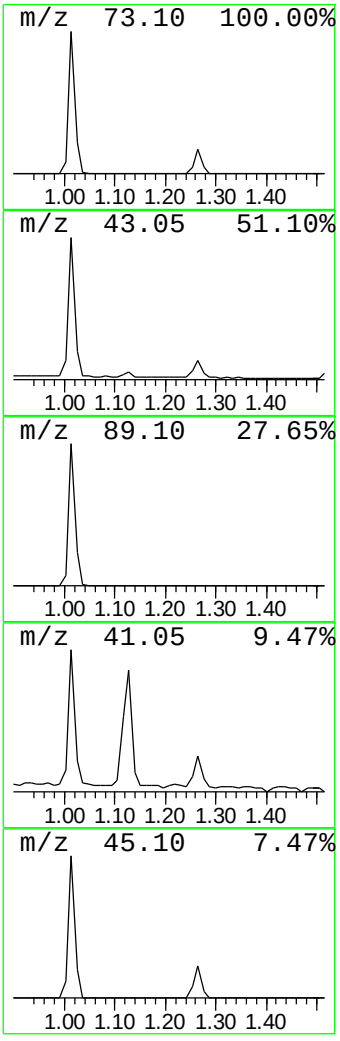
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.01	33.67 ng	275589	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	9
4	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





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Data File : BF078408.D
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Operator : TP/IZ
Sample : G1791-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LS-SD08C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.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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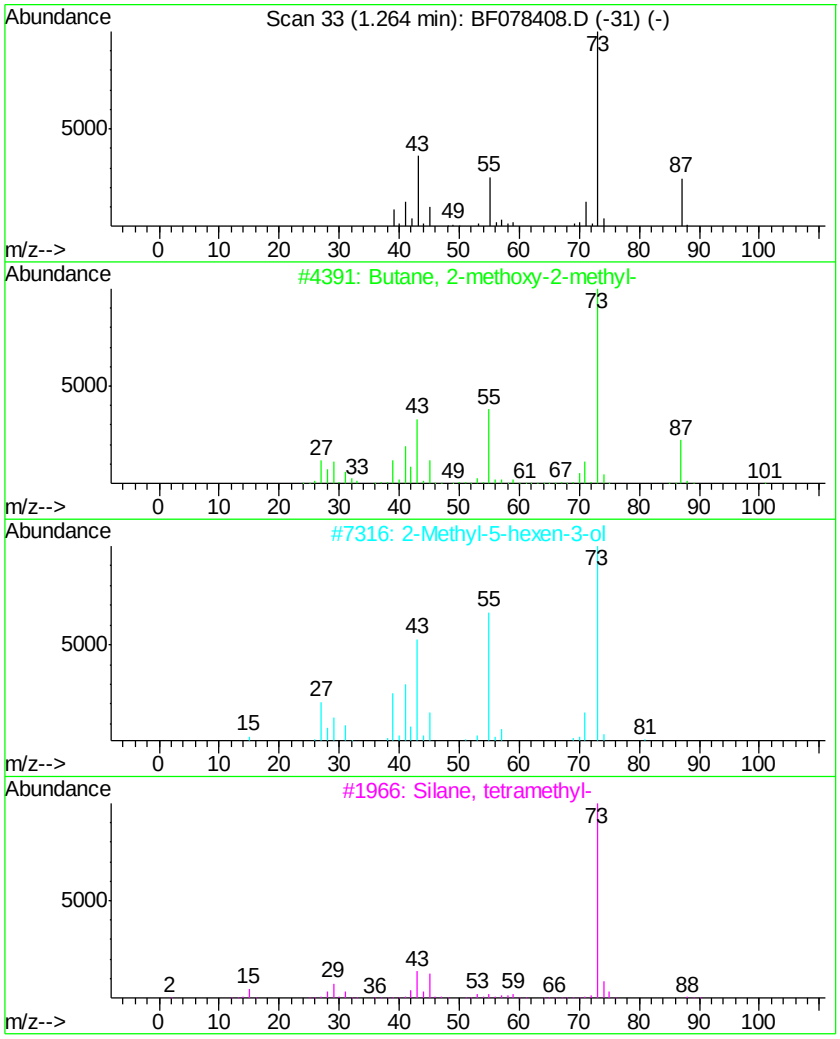
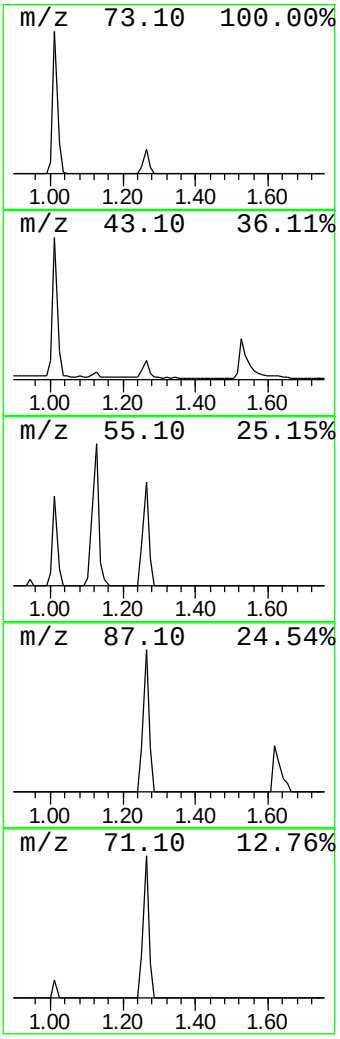
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.26	8.02 ng	65613	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	50
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	17





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Data File : BF078408.D
Acq On : 10 Apr 2015 19:25
Operator : TP/IZ
Sample : G1791-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LS-SD08C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.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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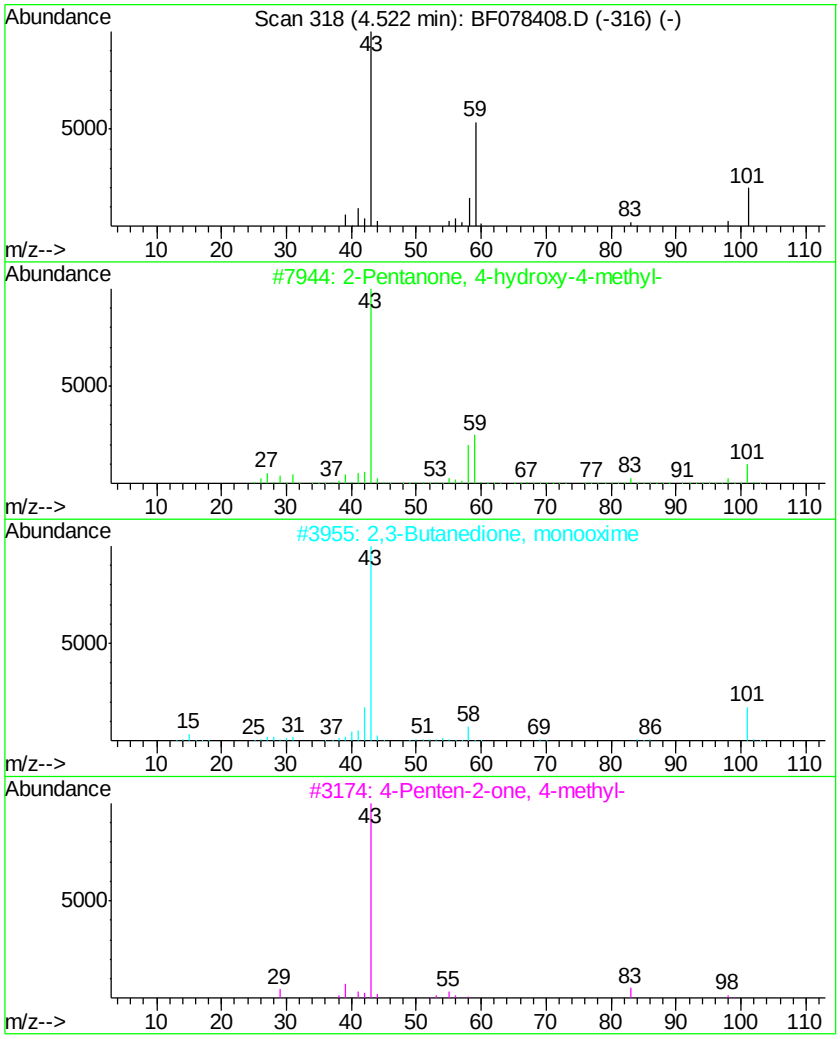
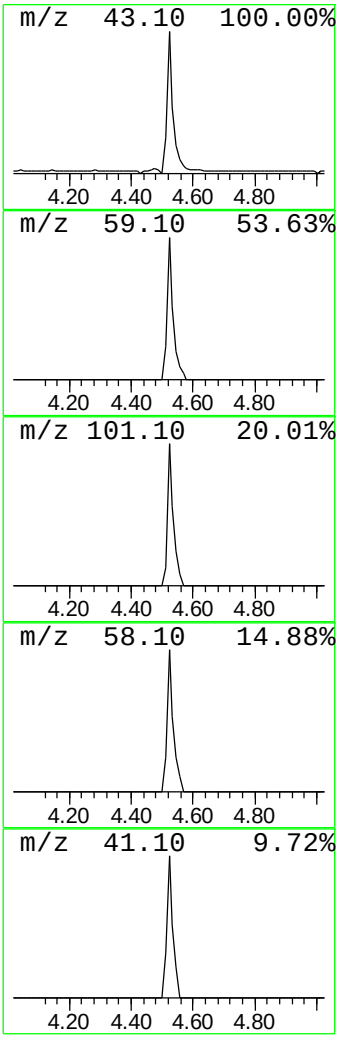
Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.52	8.01 ng	65557	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	9
5	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9





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Sample : G1791-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LS-SD08C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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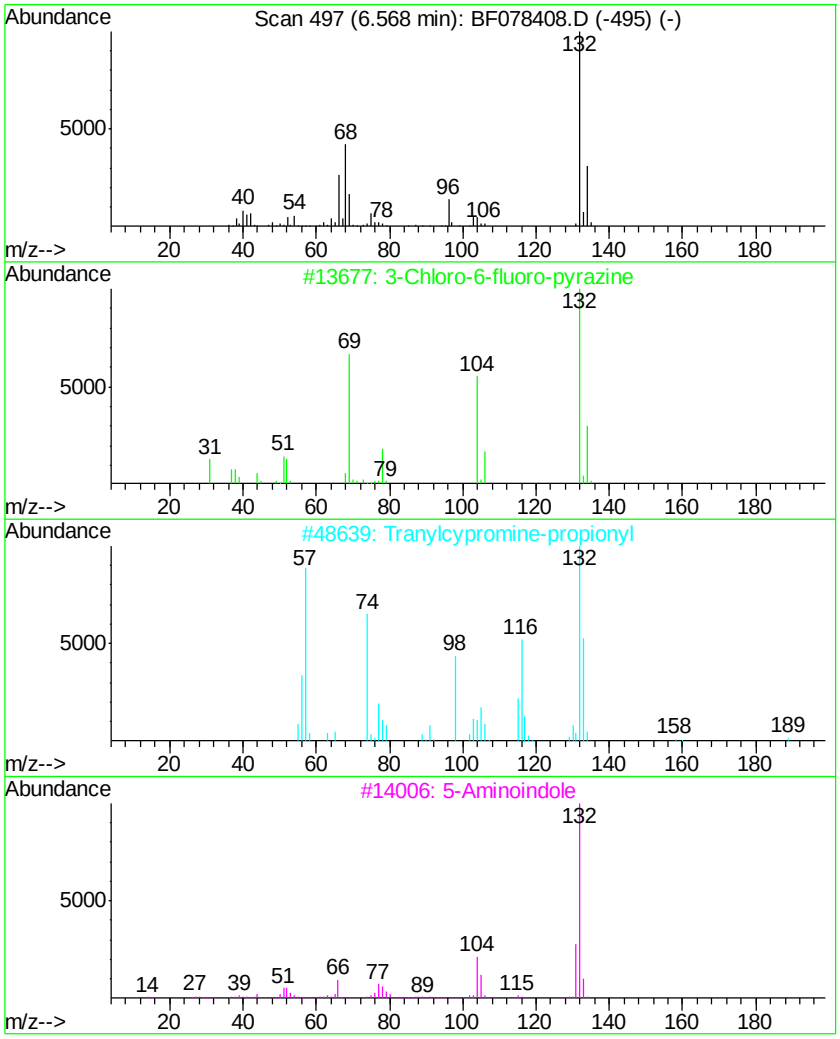
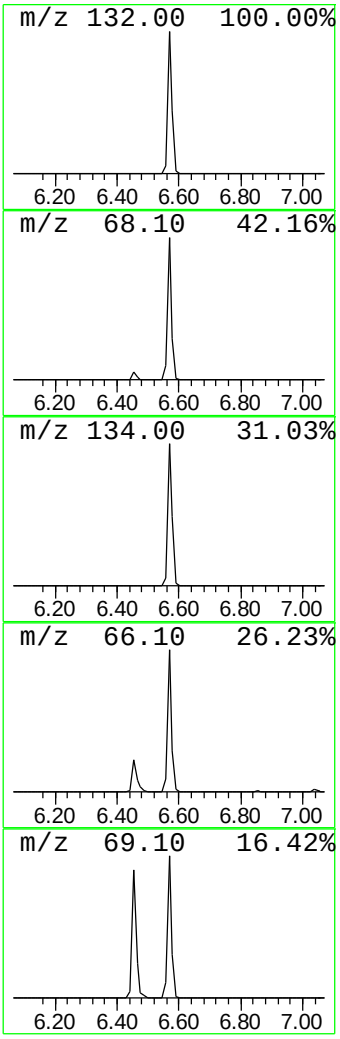
Peak Number 7 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	72.51 ng	593486	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	5-Aminoindole	132	C8H8N2	005192-03-0	10
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Sample : G1791-02
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ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LS-SD08C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

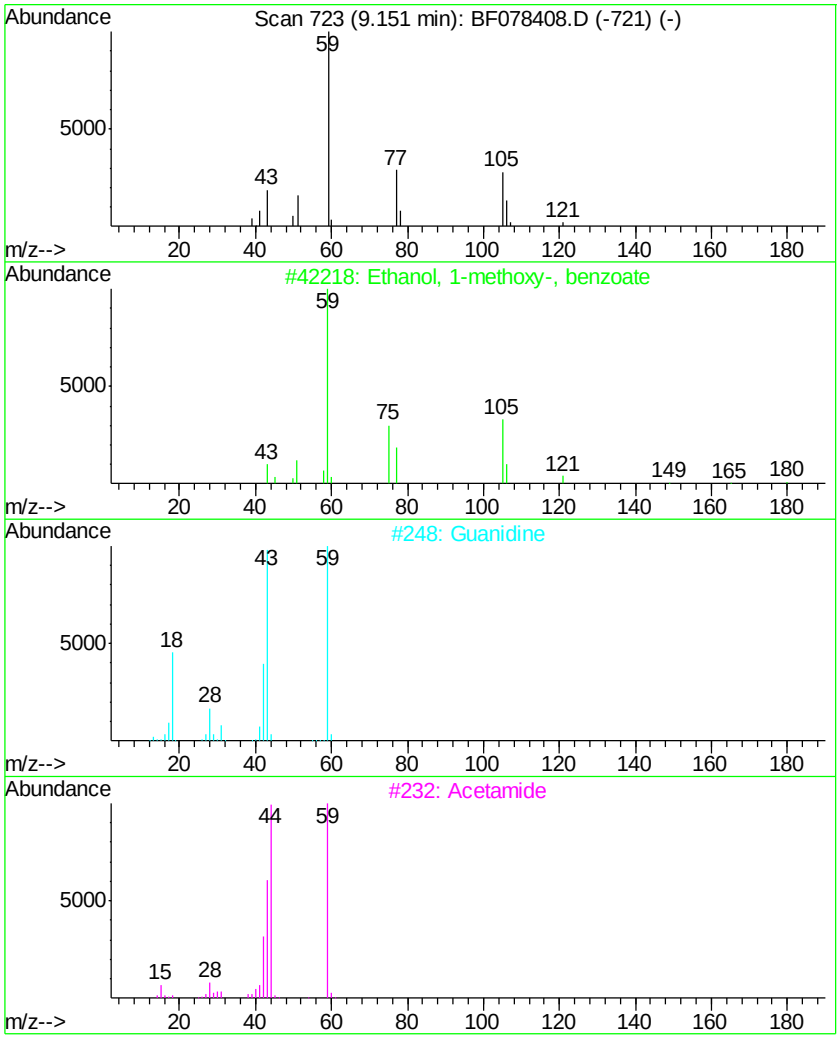
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

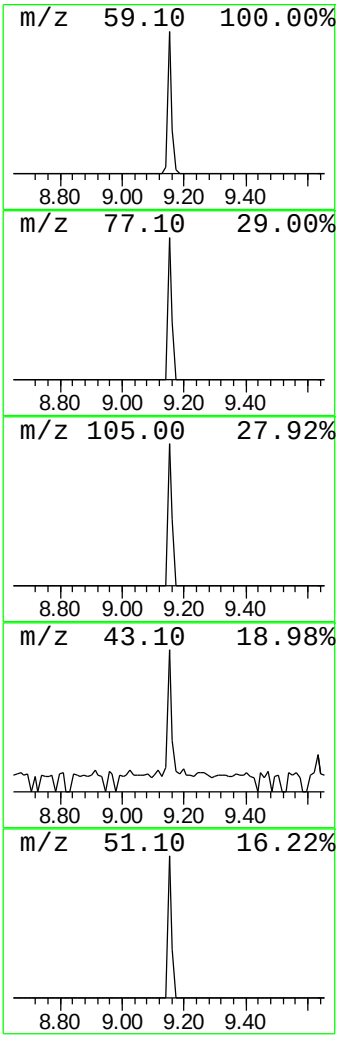
****

Peak Number 9 Ethanol, 1-methoxy-, benzoate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.15	2.79 ng	31850	Naphthalene-d8	8.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	72
2	Guanidine	59	CH5N3	000113-00-8	7
3	Acetamide	59	C2H5NO	000060-35-5	5
4	Acetaldoxime	59	C2H5NO	000107-29-9	4
5	Methyl difluoro(fluorosulfonyl)a...	192	C3H3F3O4S	000680-15-9	4





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Instrument : BNA_F
ClientSampleId : LS-SD08C

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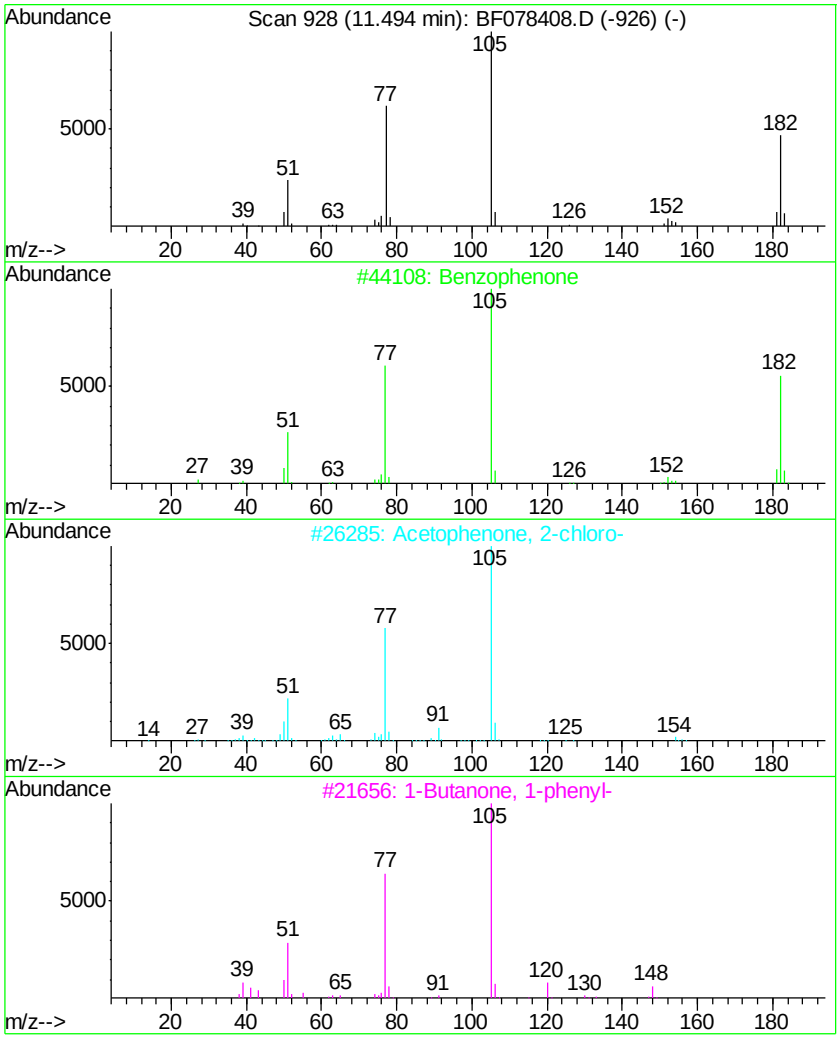
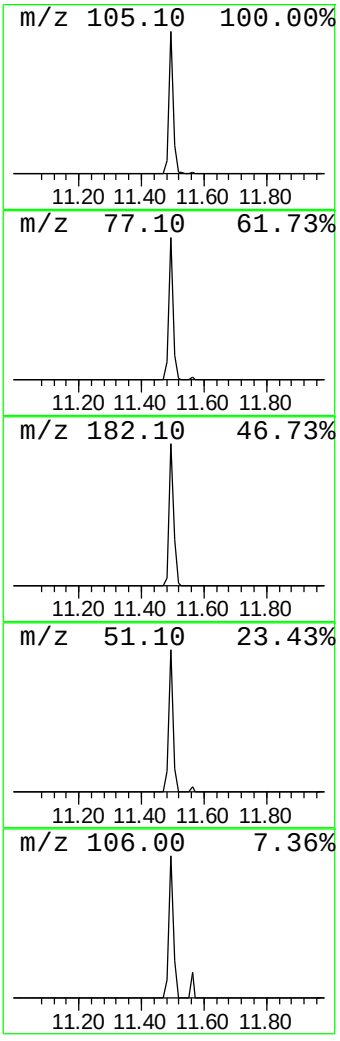
Peak Number 10 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.49	8.42 ng	119035	Acenaphthene-d10	10.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3	1-Butanone, 1-phenyl-	148	C10H12O	000495-40-9	47
4	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47
5	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.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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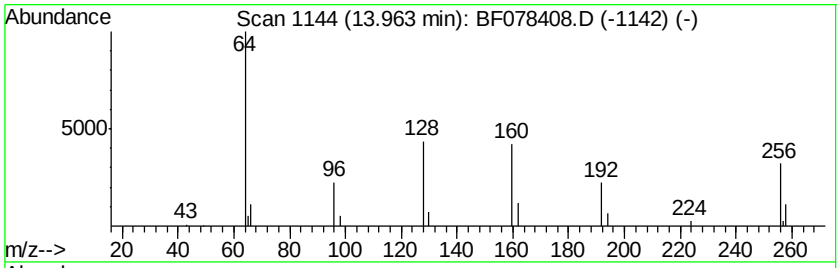
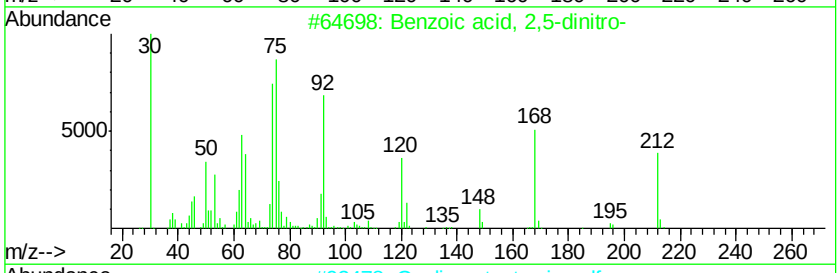
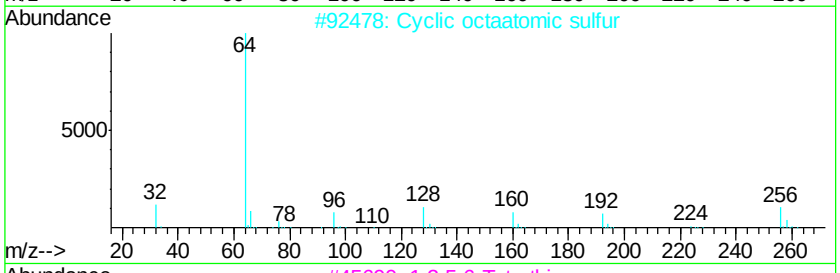
Peak Number 11 Benzoic acid, 2,5-dinitro- Concentration Rank 10

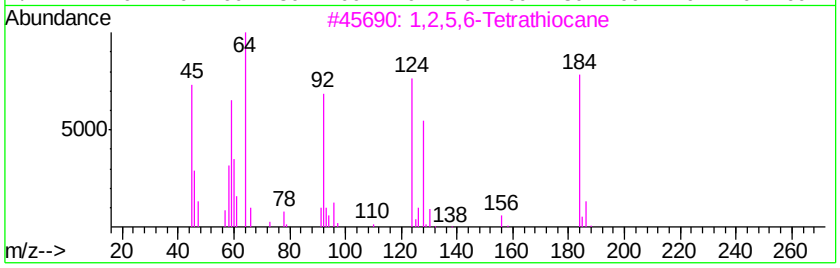
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	3.02 ng	46304	Phenanthrene-d10	12.42

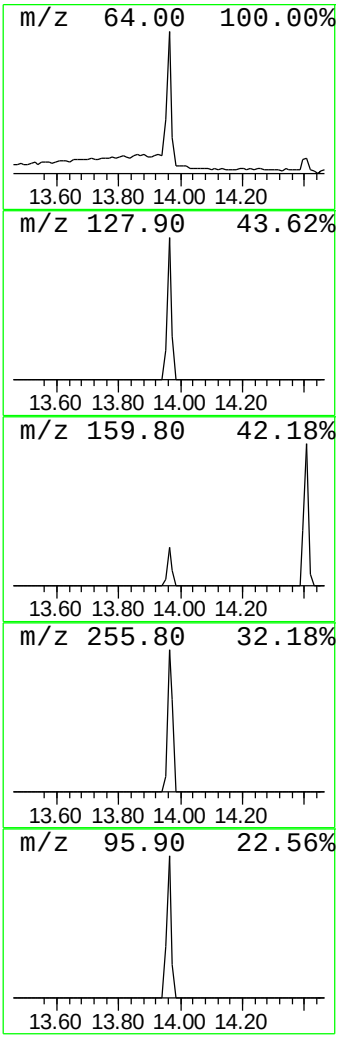
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2,5-dinitro-	212	C7H4N2O6	000610-28-6	50
2	Cyclic octaatomic sulfur	256	S8	010544-50-0	15
3	1,2,5,6-Tetrathiocane	184	C4H8S4	001940-01-8	9
4	Dihydropyrimidine-2-methyl thios...	208	C5H8N2O3S2	1000256-28-8	9
5	7-Amino-7H-S-triazolo[5,1-c]-S-t...	156	C3H4N6S	013728-28-4	9











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...	1.01	33.7	ng	275589	1	6.85	163694	20.0
Butane, 2-methoxy...	1.26	8.0	ng	65613	1	6.85	163694	20.0
2-Pentanone, 4-hy...	4.52	8.0	ng	65557	1	6.85	163694	20.0
unknown6.57	6.57	72.5	ng	593486	1	6.85	163694	20.0
Ethanol, 1-methox...	9.15	2.8	ng	31850	2	8.43	228692	20.0
Benzophenone	11.49	8.4	ng	119035	3	10.59	282823	20.0
Benzoic acid, 2,5...	13.96	3.0	ng	46304	4	12.42	307141	20.0