LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041015\
Data File : BF078407.D
Acq On : 10 Apr 2015 18:55
Operator : TP/IZ
Sample : G1791-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LS-SD08B

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	1.127	19	21	23	rBV	1366749	1248965	44.91%	5.154%
2	1.230	23	30	32	rVB	147592	347793	12.51%	1.435%
3	1.367	40	42	45	rVB	214432	257558	9.26%	1.063%
4	1.618	62	64	73	rBV	36910	62824	2.26%	0.259%
5	4.567	320	322	329	rBV	164346	285633	10.27%	1.179%
6	5.139	369	372	375	rBV	1926859	2322400	83.52%	9.583%
7	6.464	485	488	491	rBV	1723754	2213378	79.59%	9.133%
8	6.579	495	498	500	rBV	2346489	2406299	86.53%	9.930%
9	6.865	520	523	525	rBV	405611	482981	17.37%	1.993%
10	7.047	536	539	541	rBV	1921319	1842431	66.26%	7.603%
11	7.562	581	584	587	rBV	1227317	1385916	49.84%	5.719%
12	8.442	658	661	663	rBV	474498	642985	23.12%	2.653%
13	9.150	721	723	726	rBV	120310	115591	4.16%	0.477%
14	9.779	776	778	781	rBV	1944885	2594118	93.29%	10.705%
15	10.293	821	823	826	rBV	224857	196425	7.06%	0.811%
16	10.545	843	845	847	rBV	29525	37734	1.36%	0.156%
17	10.591	847	849	852	rVB	747854	729260	26.22%	3.009%
18	10.911	874	877	888	rBV	15296	44732	1.61%	0.185%
19	11.151	895	898	900	rBV	30130	36070	1.30%	0.149%
20	11.494	926	928	931	rBV	307413	351729	12.65%	1.451%
21	11.574	932	935	937	rBV	1106317	1565280	56.29%	6.459%
22	12.419	1006	1009	1011	rBV	639164	719401	25.87%	2.969%
23	13.962	1142	1144	1147	rVB	69761	102856	3.70%	0.424%
24	14.408	1180	1183	1186	rBV	2063032	2780814	100.00%	11.475%
25	15.597	1284	1287	1291	rBV2	26187	45315	1.63%	0.187%
26	15.677	1291	1294	1297	rBV	683064	725916	26.10%	2.995%
27	17.368	1439	1442	1445	rBV	574839	689302	24.79%	2.844%

Sum of corrected areas: 24233706

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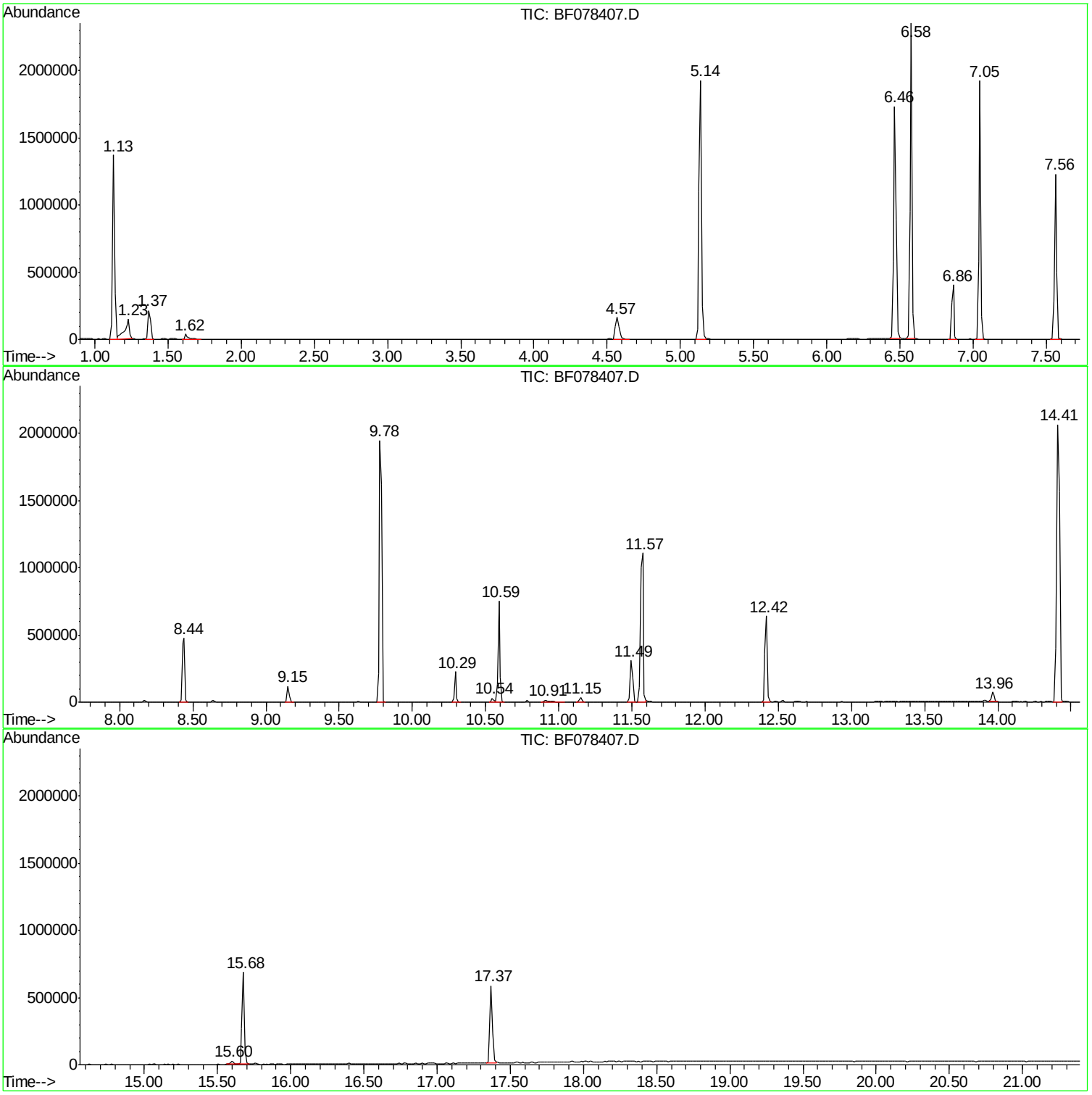
Instrument :
BNA_F
ClientSampleId :
LS-SD08B

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041015\
Data File : BF078407.D
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Operator : TP/IZ
Sample : G1791-01
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Instrument : BNA_F
ClientSampleId : LS-SD08B

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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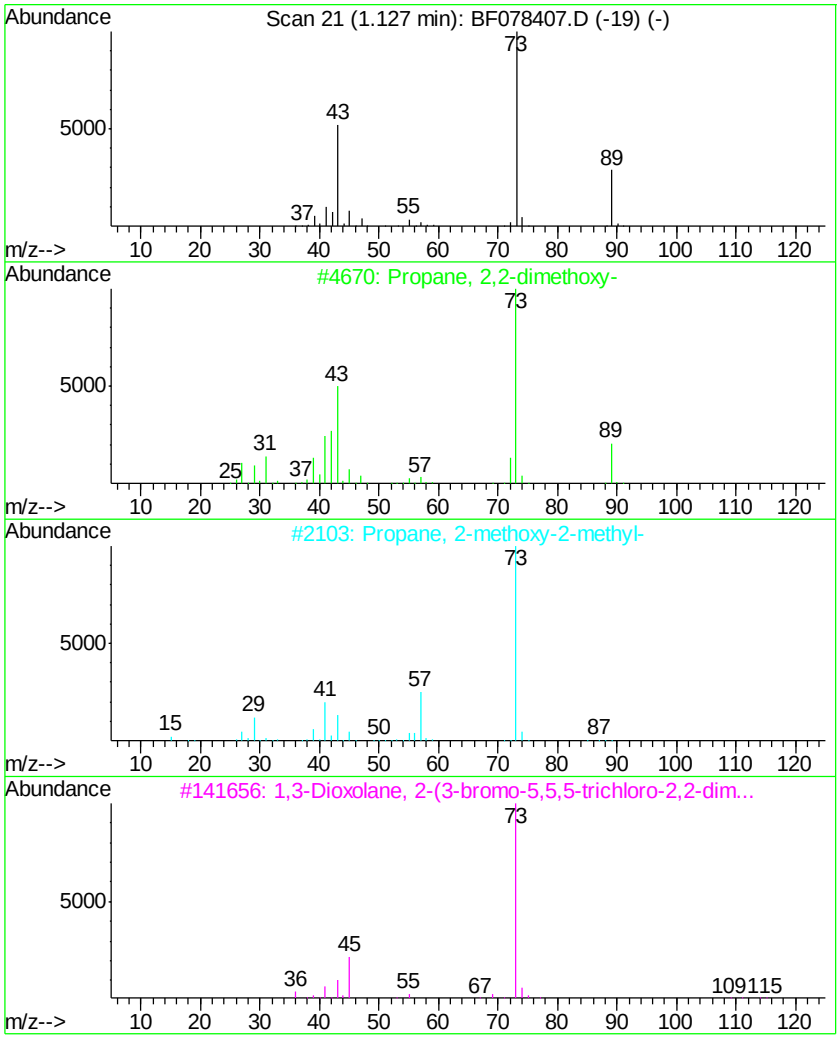
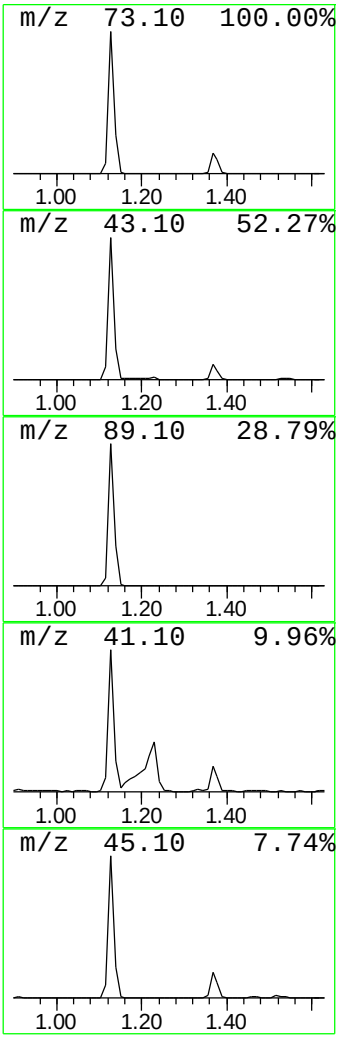
Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.13	51.72 ng	1248970	1,4-Dichlorobenzene-d4	6.86

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	1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9
4	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	9





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Data File : BF078407.D
Acq On : 10 Apr 2015 18:55
Operator : TP/IZ
Sample : G1791-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LS-SD08B

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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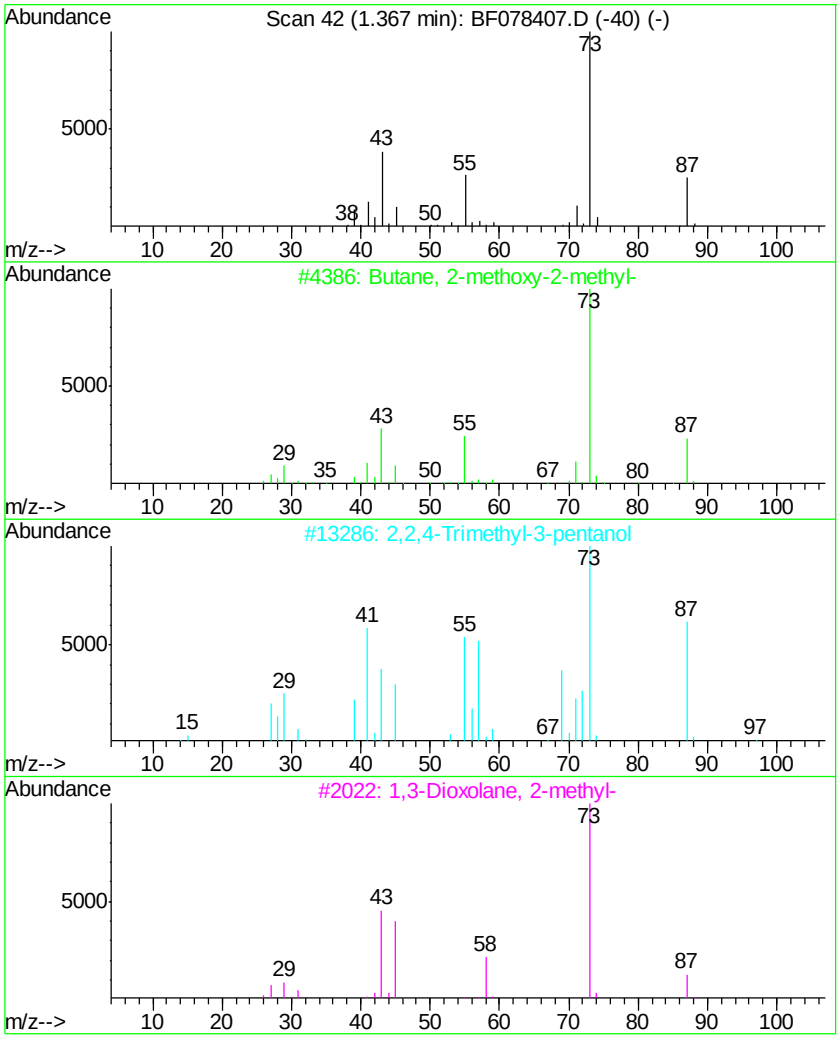
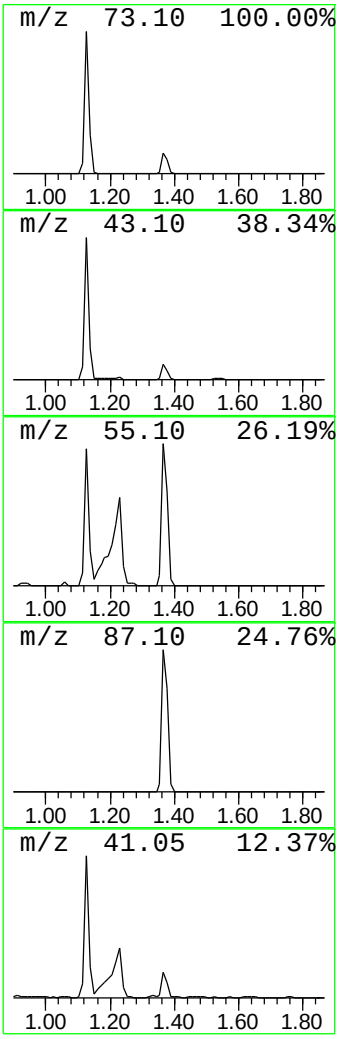
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.37	10.67 ng	257558	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041015\
Data File : BF078407.D
Acq On : 10 Apr 2015 18:55
Operator : TP/IZ
Sample : G1791-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LS-SD08B

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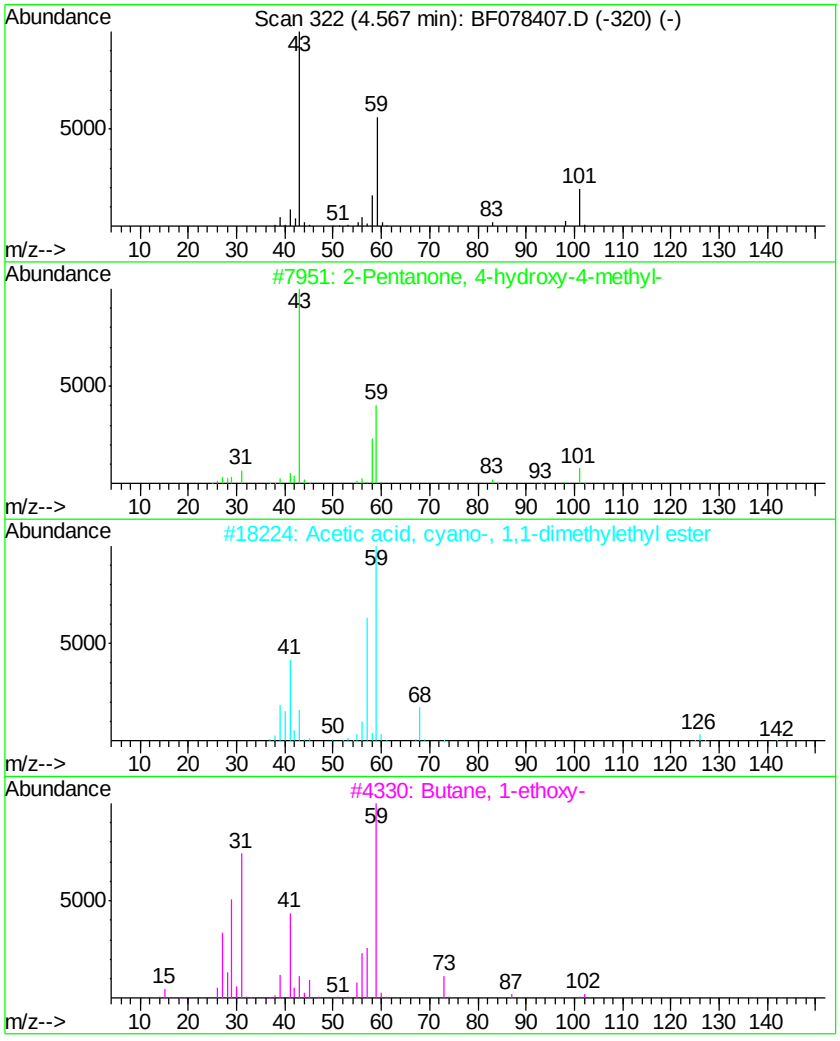
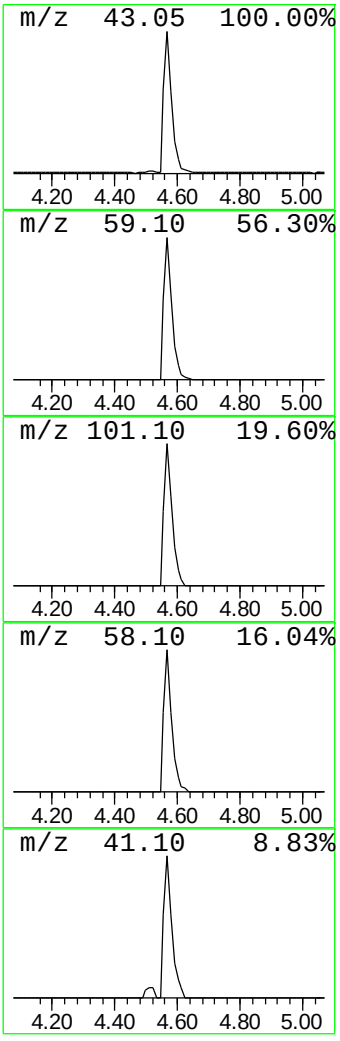
Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.57	11.83 ng	285633	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041015\
Data File : BF078407.D
Acq On : 10 Apr 2015 18:55
Operator : TP/IZ
Sample : G1791-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LS-SD08B

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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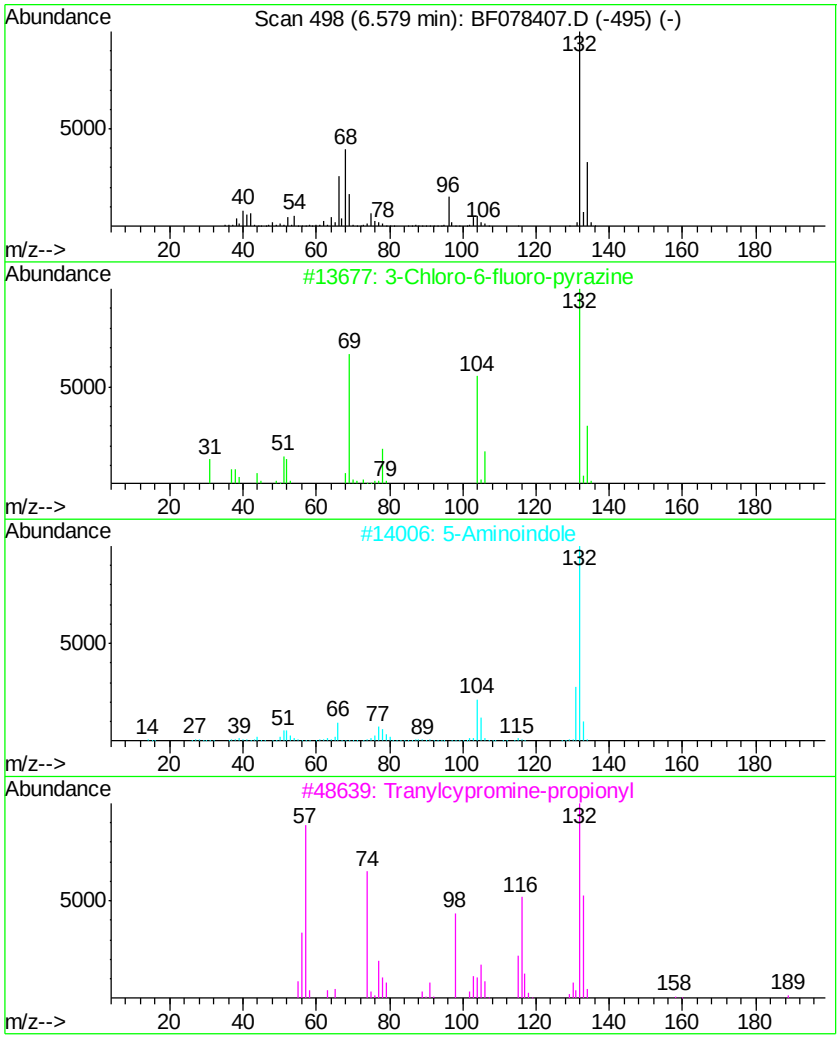
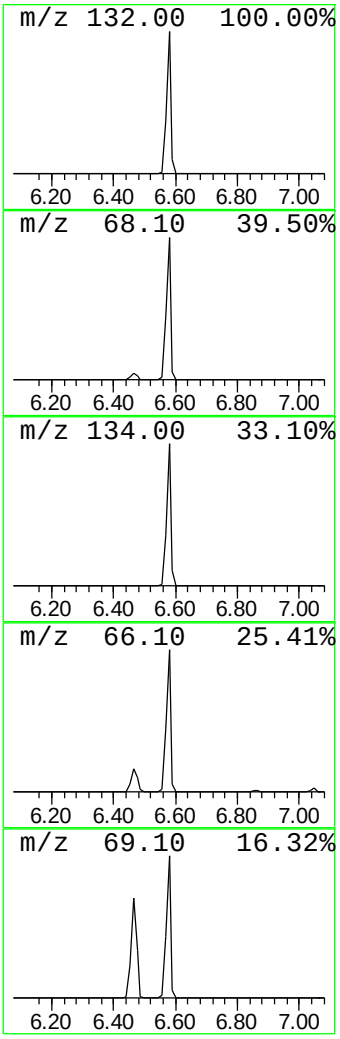
Peak Number 6 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	99.64 ng	2406300	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





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Operator : TP/IZ
Sample : G1791-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LS-SD08B

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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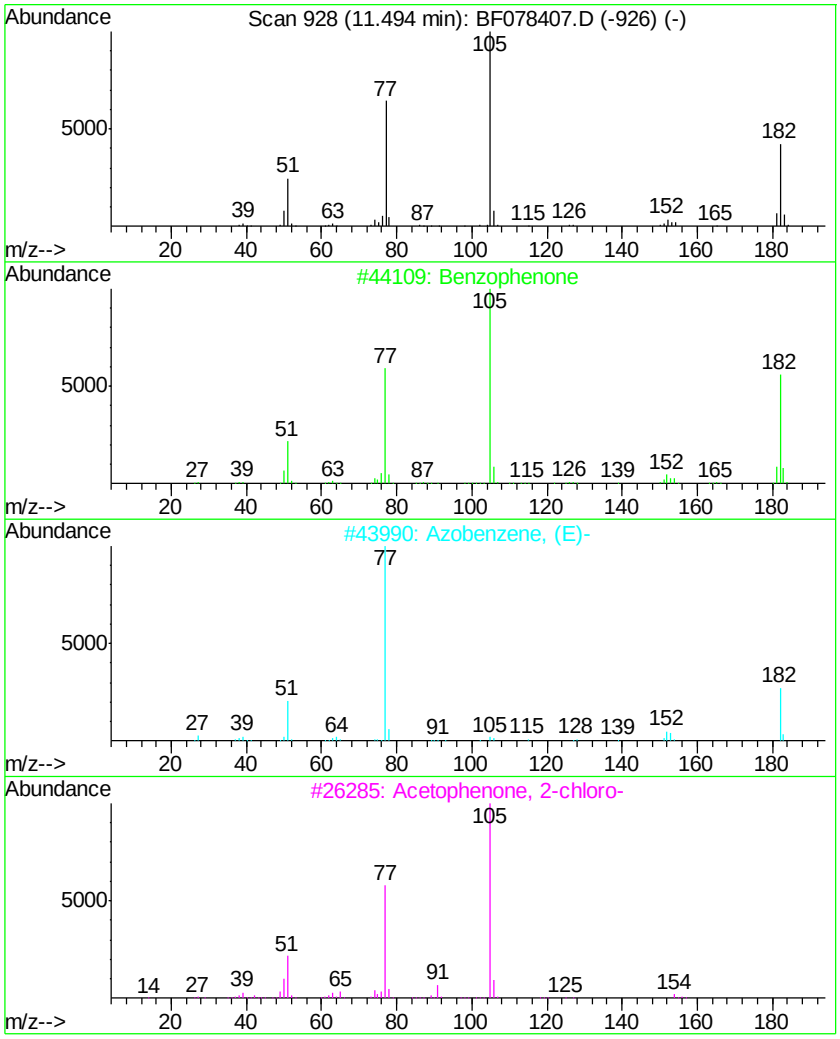
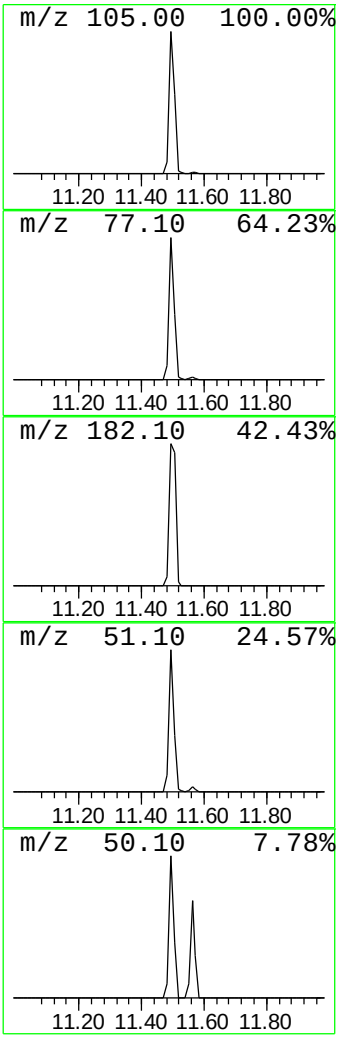
Peak Number 9 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.49	9.65 ng	351729	Acenaphthene-d10	10.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Azobenzene, (E)-	182	C12H10N2	017082-12-1	50
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47
5	Benzoyl bromide	184	C7H5BrO	000618-32-6	47





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Misc :
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Instrument : BNA_F
ClientSampleId : LS-SD08B

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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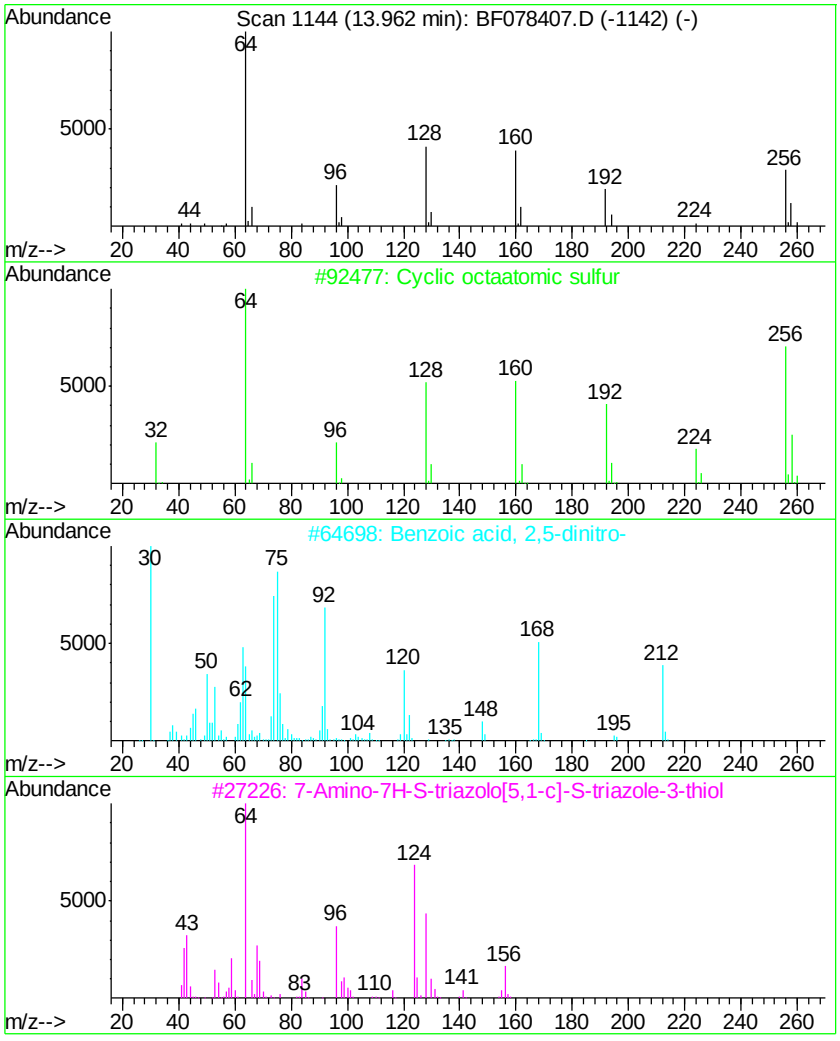
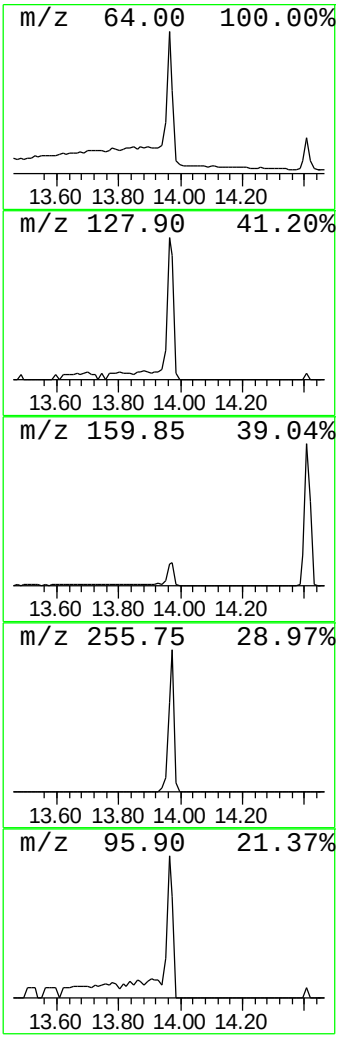
Peak Number 10 Cyclic octaatomic sulfur Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	2.86 ng	102856	Phenanthrene-d10	12.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclic octaatomic sulfur	256	S8	010544-50-0	94
2	Benzoic acid, 2,5-dinitro-	212	C7H4N2O6	000610-28-6	50
3	7-Amino-7H-S-triazolo[5,1-c]-S-t...	156	C3H4N6S	013728-28-4	38
4	Methanethiol, N-(p-methoxyphenet...	304	C11H16N2O4S2	040283-94-1	36
5	.alpha.-[9H-Purine-6-thiol-9-yl]...	321	C12H11N5O2S2	019271-00-2	9





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
Propane, 2,2-dime...	1.13	51.7	ng	1248970	1	6.86	482981	20.0
Butane, 2-methoxy...	1.37	10.7	ng	257558	1	6.86	482981	20.0
2-Pentanone, 4-hy...	4.57	11.8	ng	285633	1	6.86	482981	20.0
unknown6.58	6.58	99.6	ng	2406300	1	6.86	482981	20.0
Benzophenone	11.49	9.7	ng	351729	3	10.59	729260	20.0
Cyclic octaatomic...	13.96	2.9	ng	102856	4	12.42	719401	20.0