LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042915\
Data File : BF078841.D
Acq On : 30 Apr 2015 6:36
Operator : TP/IZ
Sample : G2021-02
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-17-0-2

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-BF042815.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	1.290	5	9	12	rVB	9881482	14763833	100.00%	23.644%
2	1.427	20	21	28	rVB	98738	178490	1.21%	0.286%
3	1.541	28	31	33	rBV	6089581	8548956	57.90%	13.691%
4	1.678	40	43	46	rBV	7202389	11444530	77.52%	18.328%
5	1.781	51	52	57	rBV	200682	349078	2.36%	0.559%
6	1.861	57	59	62	rVB	771990	940384	6.37%	1.506%
7	1.918	62	64	70	rBV	1745886	2480653	16.80%	3.973%
8	2.010	70	72	86	rVB	236800	561808	3.81%	0.900%
9	2.215	88	90	109	rVB	120619	278785	1.89%	0.446%
10	5.187	349	350	357	rVB	260441	304793	2.06%	0.488%
11	5.679	390	393	396	rBV	2183518	2138543	14.49%	3.425%
12	6.924	500	502	505	rBV	2136365	2127935	14.41%	3.408%
13	7.096	514	517	519	rBV	1844511	2327448	15.76%	3.727%
14	7.382	540	542	544	rBV	539607	478173	3.24%	0.766%
15	7.564	556	558	561	rVB	1257607	1747239	11.83%	2.798%
16	8.067	600	602	605	rBV	1174237	1332933	9.03%	2.135%
17	8.959	678	680	683	rBV	780477	677698	4.59%	1.085%
18	10.308	795	798	800	rBV	3373530	2889129	19.57%	4.627%
19	11.142	868	871	873	rVB	690454	728194	4.93%	1.166%
20	12.114	954	956	959	rBV2	1494840	1787242	12.11%	2.862%
21	12.982	1030	1032	1034	rBV	720287	801832	5.43%	1.284%
22	14.491	1162	1164	1166	rBV	128419	158641	1.07%	0.254%
23	14.777	1184	1189	1192	rBV	144488	169644	1.15%	0.272%
24	14.982	1204	1207	1210	rBV	2803372	3102829	21.02%	4.969%
25	16.285	1318	1321	1323	rBV	847632	1019136	6.90%	1.632%
26	17.577	1432	1434	1440	rBV	66937	159998	1.08%	0.256%
27	18.034	1472	1474	1477	rBV	586747	944229	6.40%	1.512%

Sum of corrected areas: 62442153

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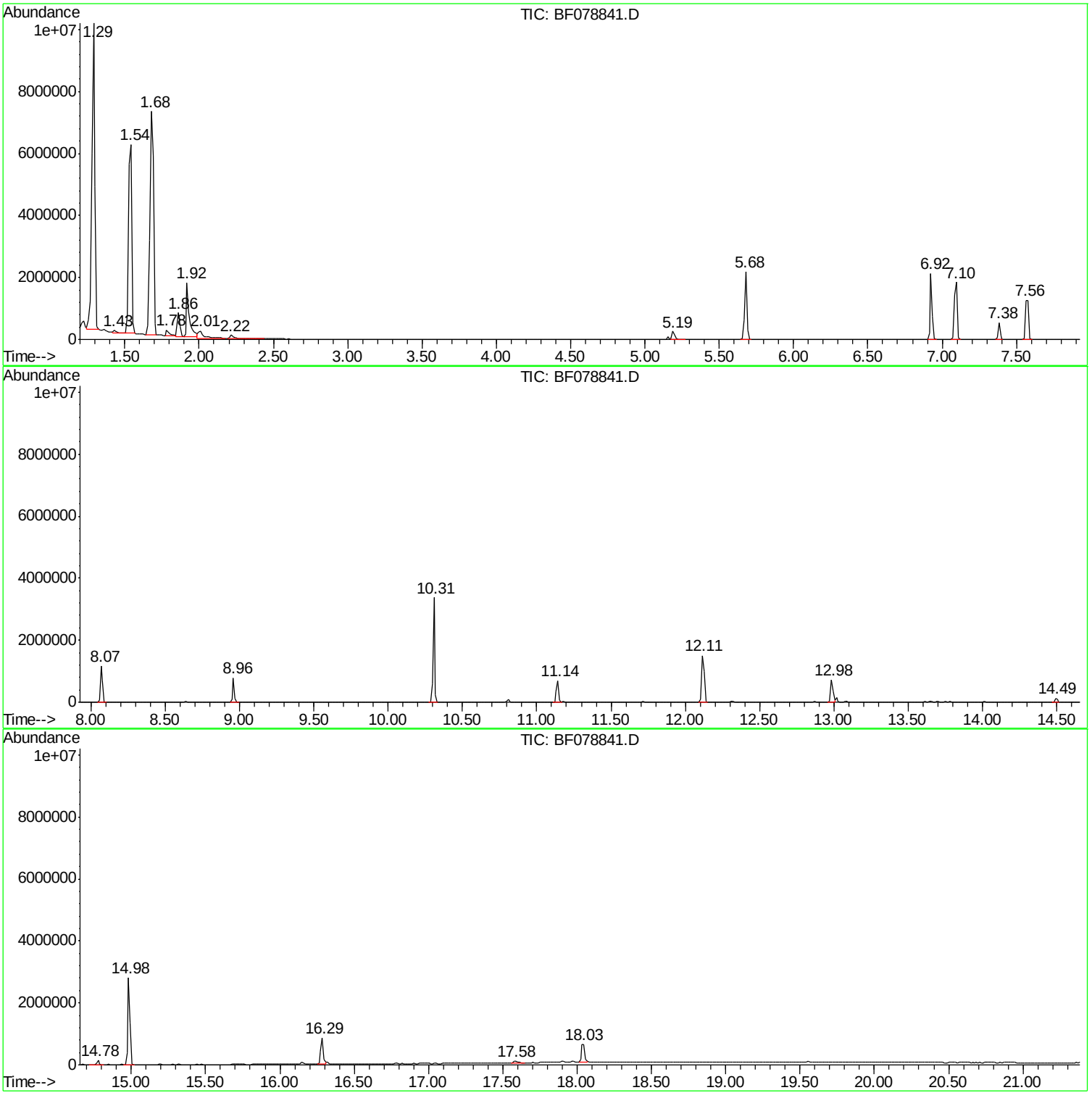
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PS-17-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.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\BF042915\
Data File : BF078841.D
Acq On : 30 Apr 2015 6:36
Operator : TP/IZ
Sample : G2021-02
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-17-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

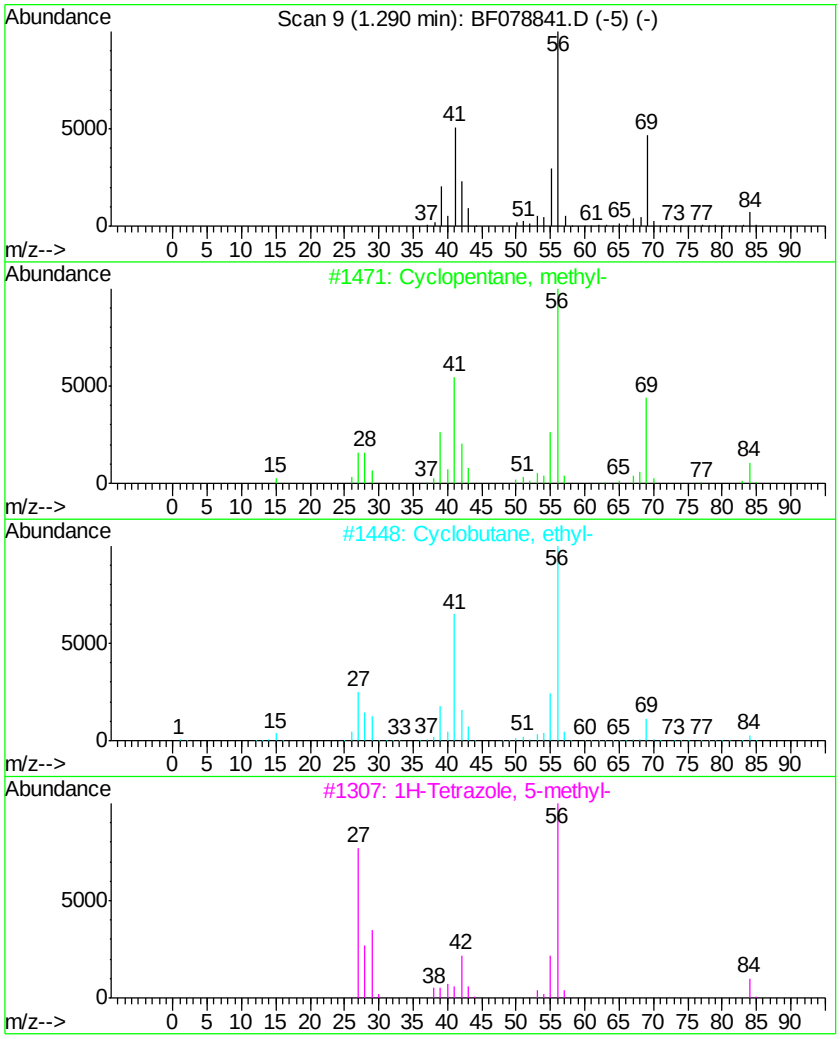
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

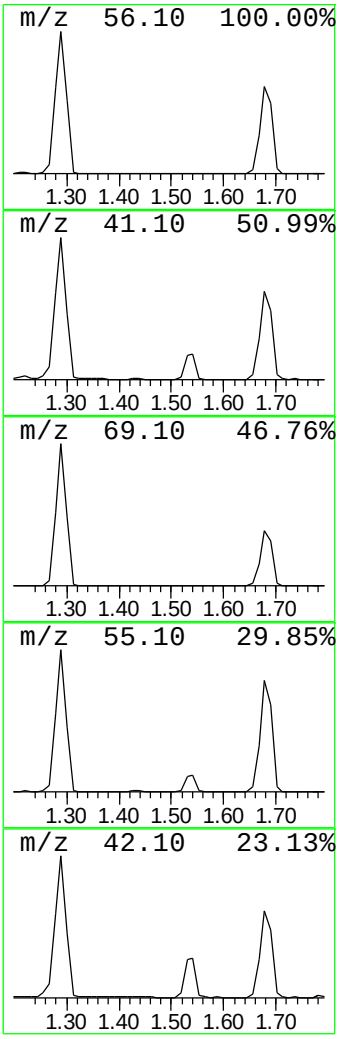
****

Peak Number 1 Cyclopentane, methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.29	617.51 ng	14763800	1,4-Dichlorobenzene-d4	7.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	87
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	80
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
4	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	64
5	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	56





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Data File : BF078841.D
Acq On : 30 Apr 2015 6:36
Operator : TP/IZ
Sample : G2021-02
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-17-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.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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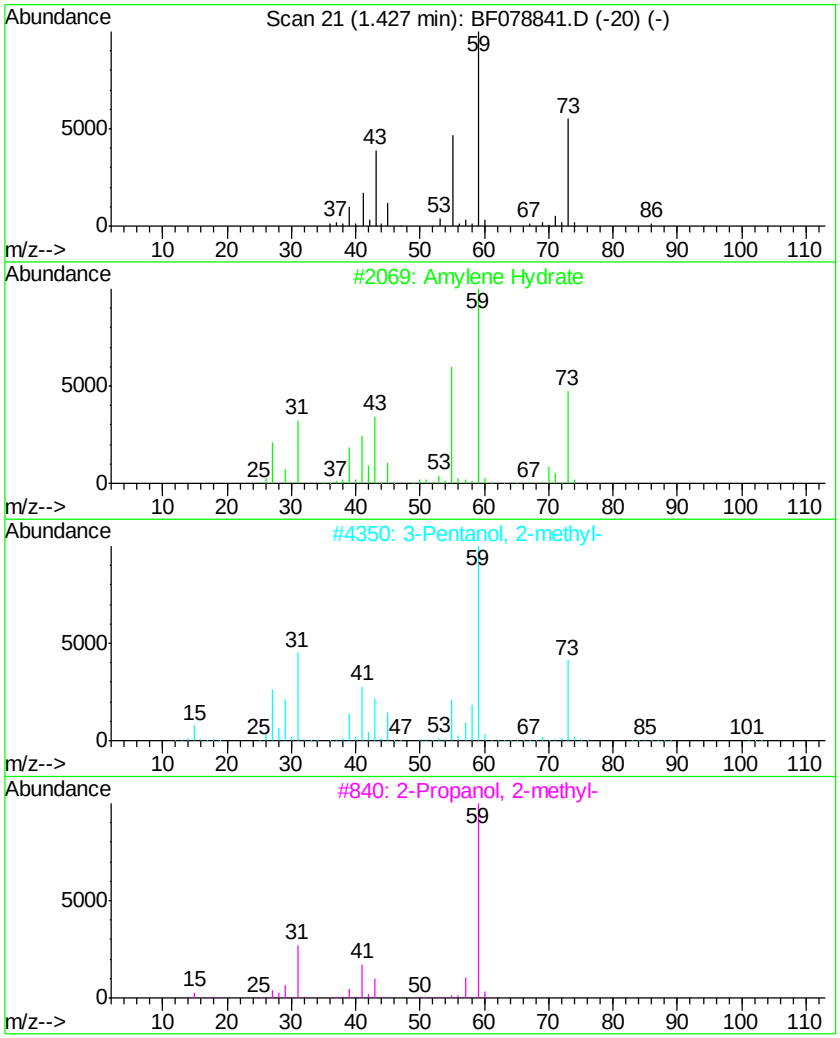
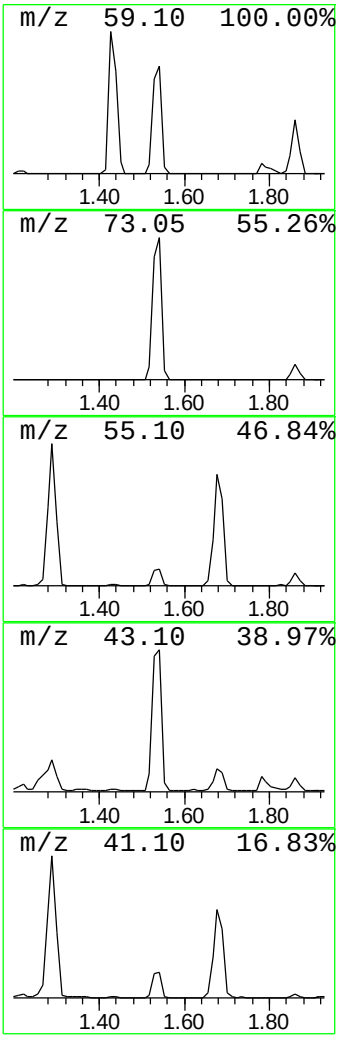
Peak Number 2 Amylene Hydrate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.43	7.47 ng	178490	1,4-Dichlorobenzene-d4	7.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Amylene Hydrate	88	C5H12O	000075-85-4	83
2	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	64
3	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	40
4	Silane, trimethyl-	74	C3H10Si	000993-07-7	39
5	6-Nitrohexan-2-ol	147	C6H13NO3	062224-53-7	38





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Data File : BF078841.D
Acq On : 30 Apr 2015 6:36
Operator : TP/IZ
Sample : G2021-02
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-17-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.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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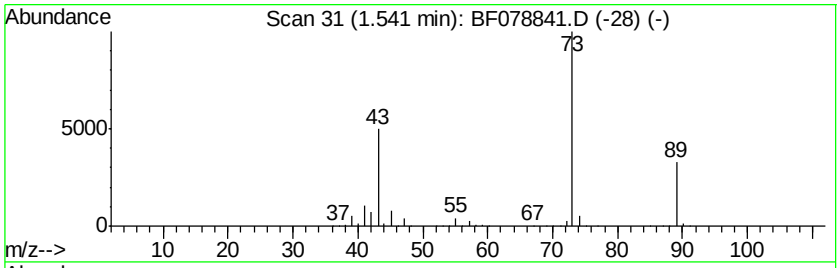
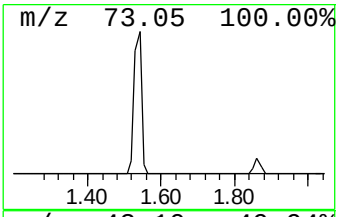
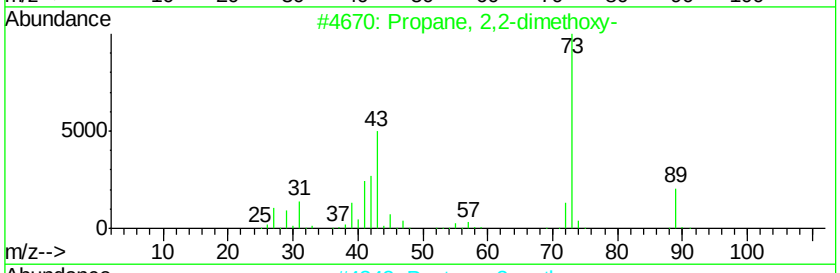
Peak Number 3 unknown1.54 Concentration Rank 3

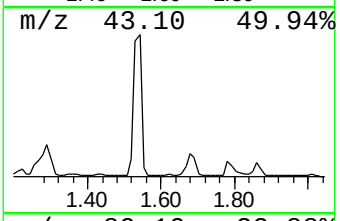
R.T.	EstConc	Area	Relative to ISTD	R.T.
1.54	357.57 ng	8548960	1,4-Dichlorobenzene-d4	7.38

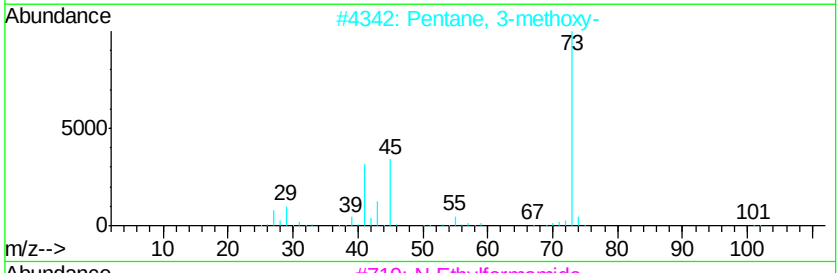
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9

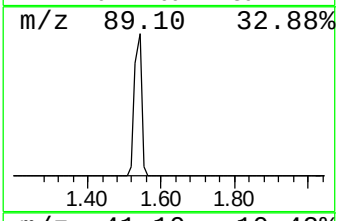


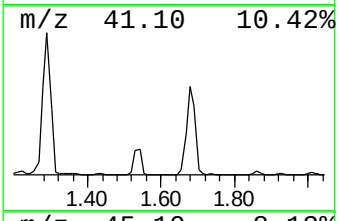


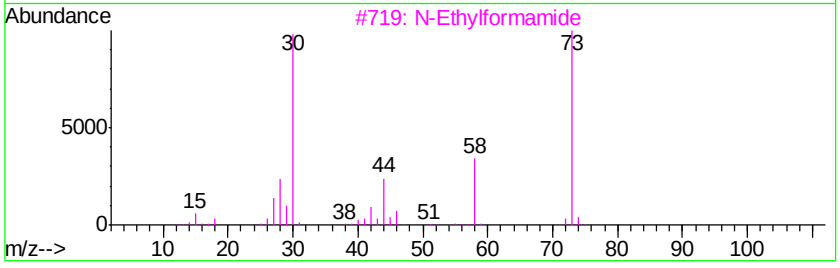


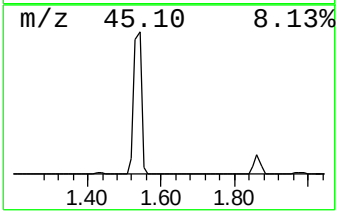












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Operator : TP/IZ
Sample : G2021-02
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-17-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

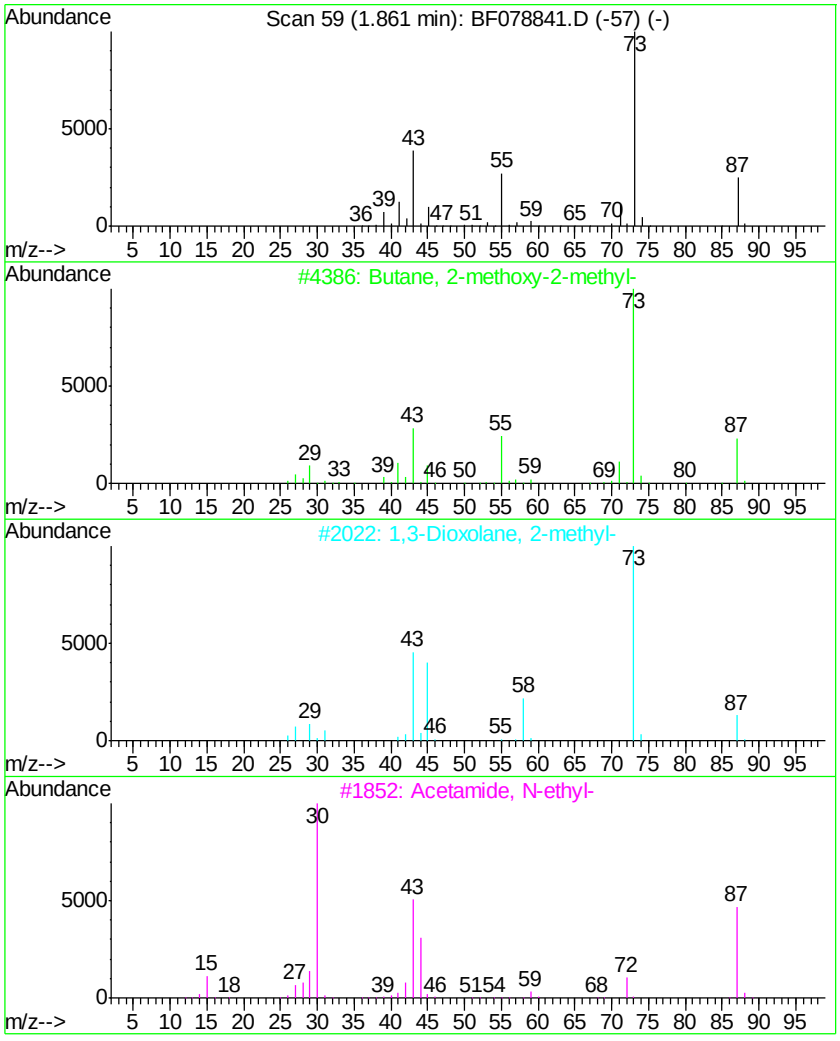
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

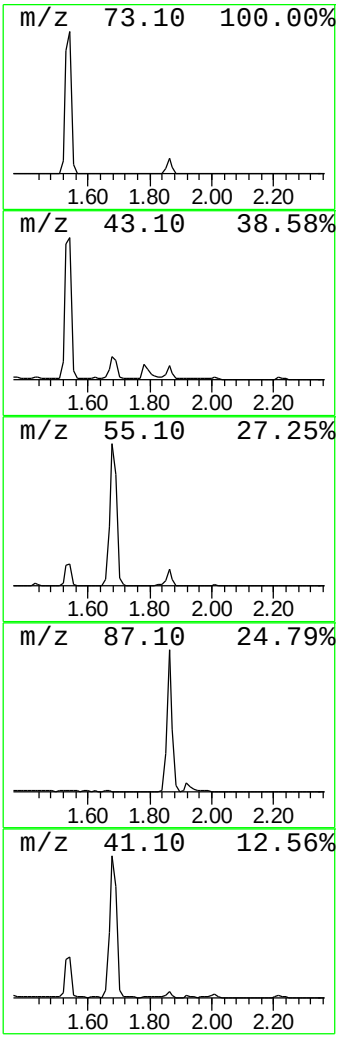
****

Peak Number 6 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.86	39.33 ng	940384	1,4-Dichlorobenzene-d4	7.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10





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Sample : G2021-02
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-17-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

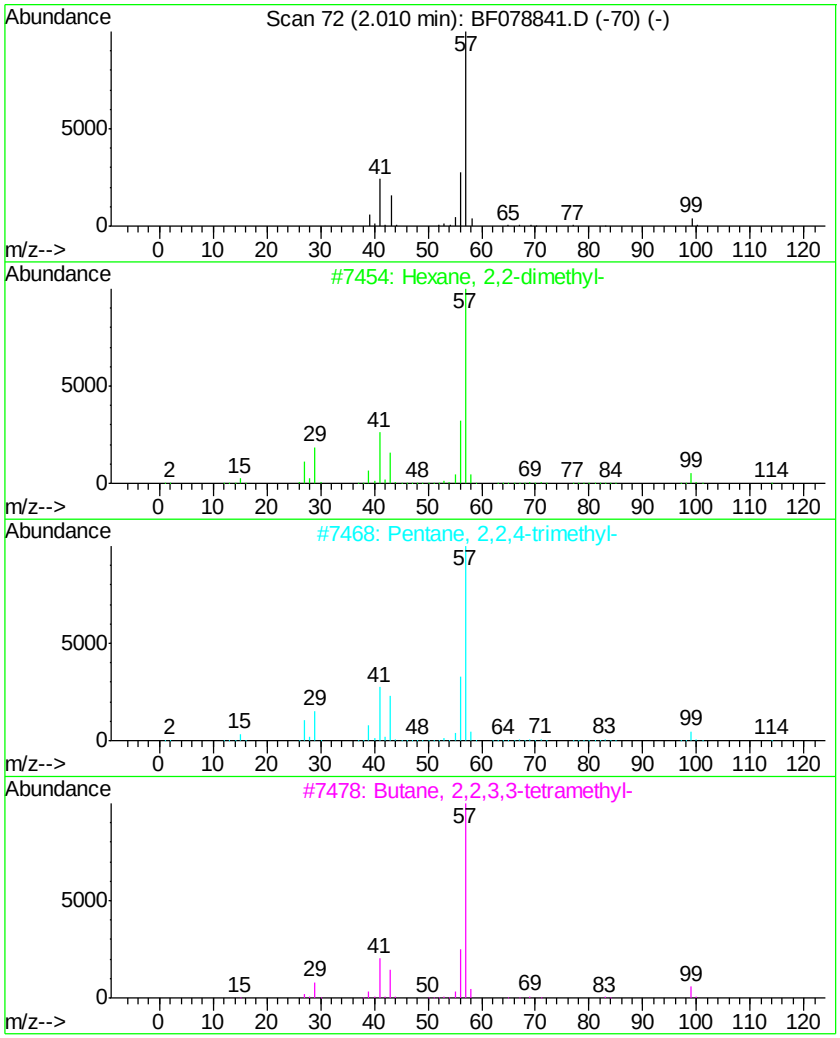
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

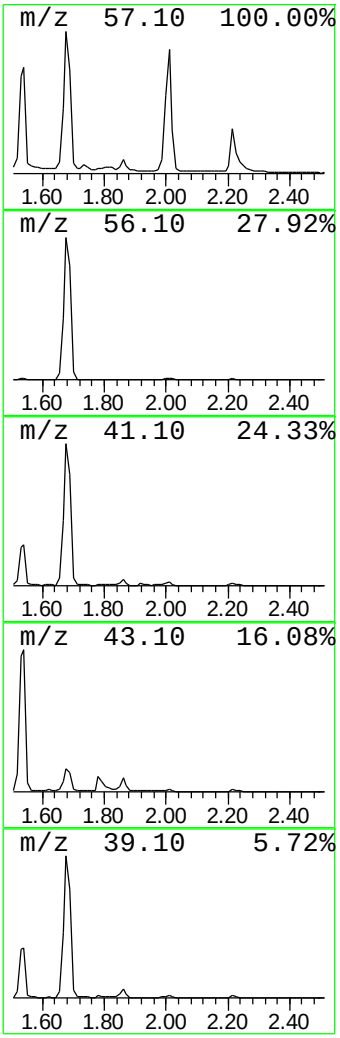
****

Peak Number 8 Hexane, 2,2-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.01	23.50 ng	561808	1,4-Dichlorobenzene-d4	7.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	83
2	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	78
3	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
4	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	56
5	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	40





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Sample : G2021-02
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-17-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

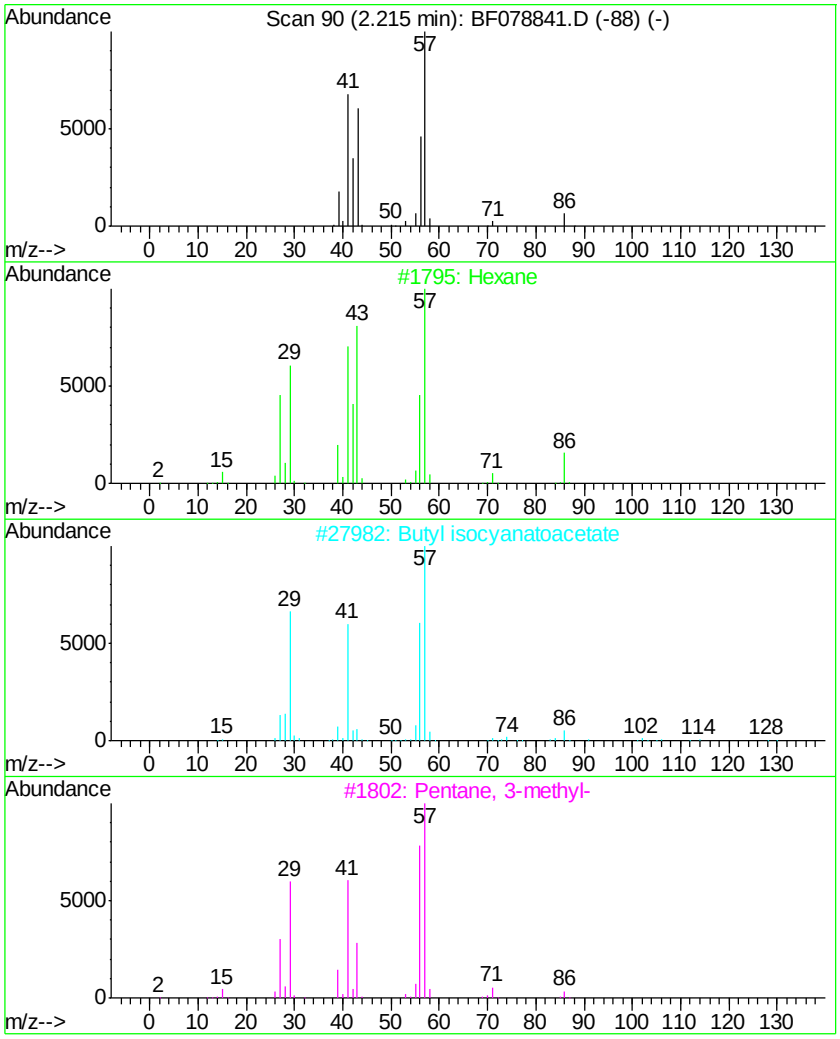
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

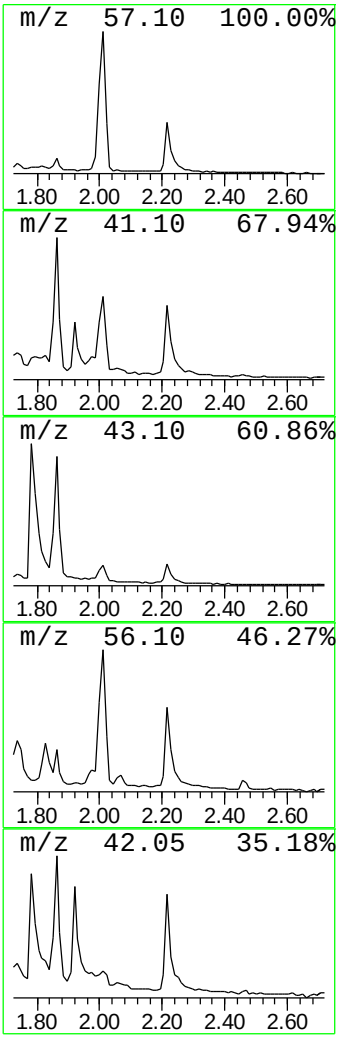
****

Peak Number 9 Hexane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	11.66 ng	278785	1,4-Dichlorobenzene-d4	7.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane	86	C6H14	000110-54-3	64
2	Butyl isocyanatoacetate	157	C7H11NO3	017046-22-9	38
3	Pentane, 3-methyl-	86	C6H14	000096-14-0	17
4	Butane, 2-methyl-	72	C5H12	000078-78-4	17
5	Borinic acid, diethyl-	86	C4H11BO	004426-31-7	9





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Instrument : BNA_F
ClientSampleId : PS-17-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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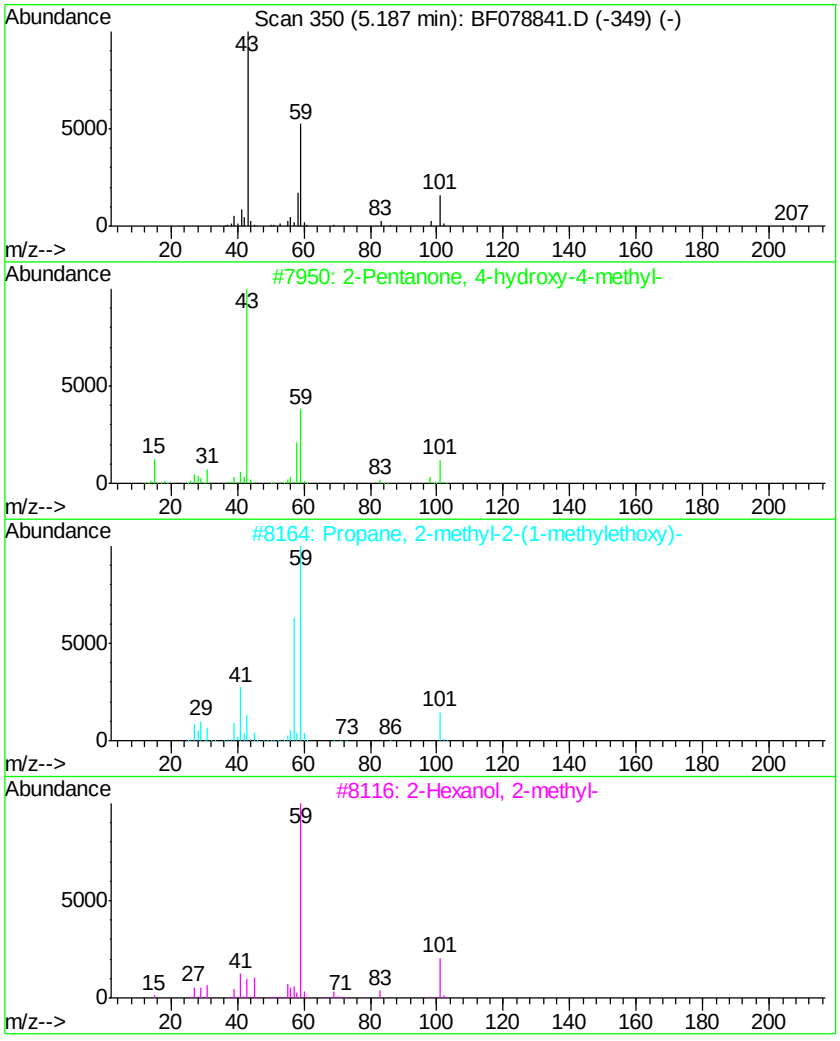
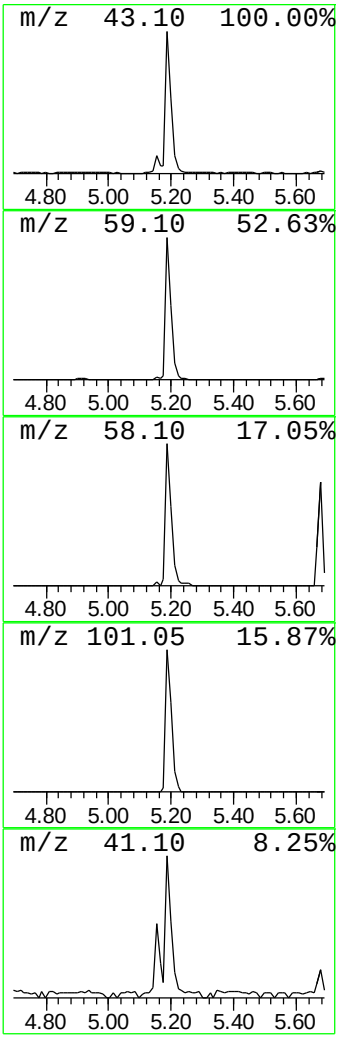
Peak Number 10 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	12.75 ng	304793	1,4-Dichlorobenzene-d4	7.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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

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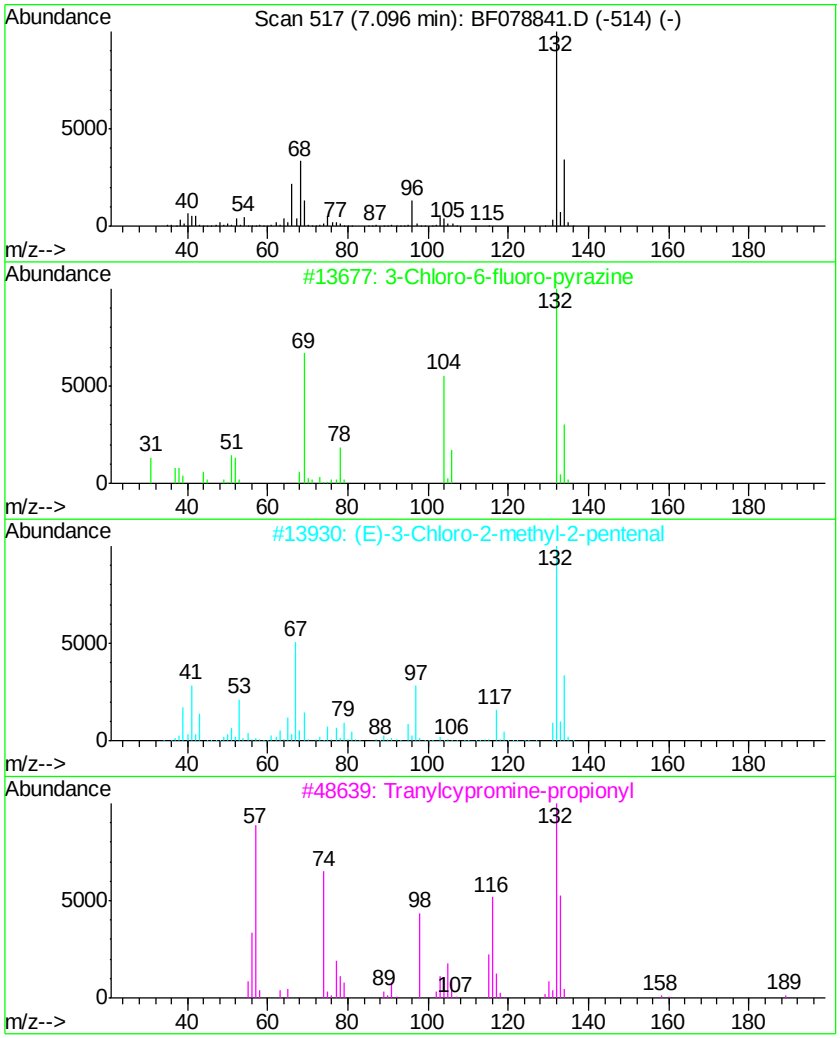
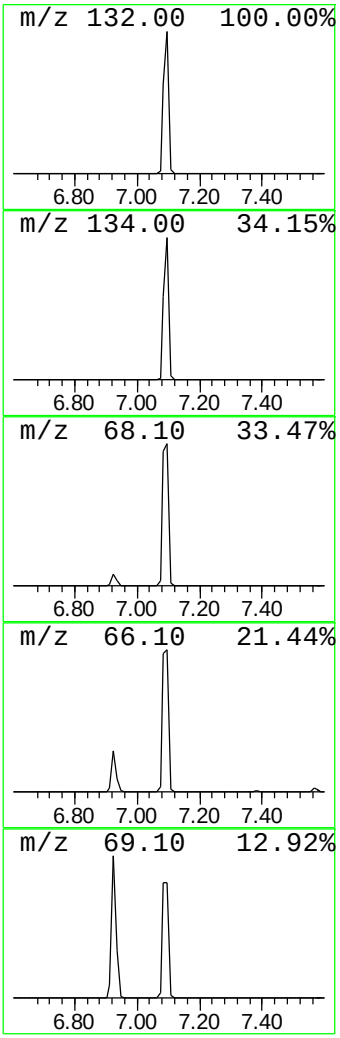
Peak Number 11 unknown7.10 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.10	97.35 ng	2327450	1,4-Dichlorobenzene-d4	7.38

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	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Amphetaminil	250	C17H18N2	017590-01-1	12
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042915\
Data File : BF078841.D
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Instrument : BNA_F
ClientSampleId : PS-17-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.M
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
Cyclopentane, met...	1.29	617.5	ng	14763800	1	7.38	478173	20.0
Amylene Hydrate	1.43	7.5	ng	178490	1	7.38	478173	20.0
unknown1.54	1.54	357.6	ng	8548960	1	7.38	478173	20.0
Butane, 2-methoxy...	1.86	39.3	ng	940384	1	7.38	478173	20.0
Hexane, 2,2-dimet...	2.01	23.5	ng	561808	1	7.38	478173	20.0
Hexane	2.22	11.7	ng	278785	1	7.38	478173	20.0
2-Pentanone, 4-hy...	5.19	12.8	ng	304793	1	7.38	478173	20.0
unknown7.10	7.10	97.3	ng	2327450	1	7.38	478173	20.0