LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072921\
Data File : BF124854.D
Acq On : 29 Jul 2021 16:41
Operator : JU/CG
Sample : M3176-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 18-B7-TP-(9.5-12)

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124854.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	22	24	25	rVB	306663	216099	66.68%	10.766%
2	2.263	25	30	38	rVB3	13112	29939	9.24%	1.492%
3	2.822	121	125	130	rBB	11745	16259	5.02%	0.810%
4	4.675	436	440	443	rBB	18158	18390	5.67%	0.916%
5	5.110	509	514	518	rBB2	16934	22751	7.02%	1.133%
6	5.498	575	580	583	rBV	154579	147515	45.52%	7.349%
7	6.498	745	750	753	rBV	135168	133140	41.08%	6.633%
8	6.869	811	813	816	rBB	37525	28565	8.81%	1.423%
9	7.433	905	909	912	rBV	116771	116102	35.83%	5.784%
10	8.051	1012	1014	1021	rBB	5475	6957	2.15%	0.347%
11	8.151	1028	1031	1034	rBV	48558	40792	12.59%	2.032%
12	9.233	1210	1215	1218	rBV	245255	229795	70.91%	11.449%
13	9.910	1327	1330	1333	rBV	66176	49917	15.40%	2.487%
14	10.704	1461	1465	1468	rBV	184995	161381	49.80%	8.040%
15	11.398	1579	1583	1586	rBV	73457	56580	17.46%	2.819%
16	12.745	1807	1812	1815	rBV	257963	261909	80.82%	13.049%
17	12.992	1848	1854	1857	rBV	343645	324061	100.00%	16.145%
18	13.145	1877	1880	1884	rBB	31175	26295	8.11%	1.310%
19	13.486	1935	1938	1941	rBB	43772	35818	11.05%	1.784%
20	14.039	2028	2032	2035	rBB	57645	48610	15.00%	2.422%
21	15.515	2278	2283	2288	rBB2	29715	36316	11.21%	1.809%

Sum of corrected areas: 2007191

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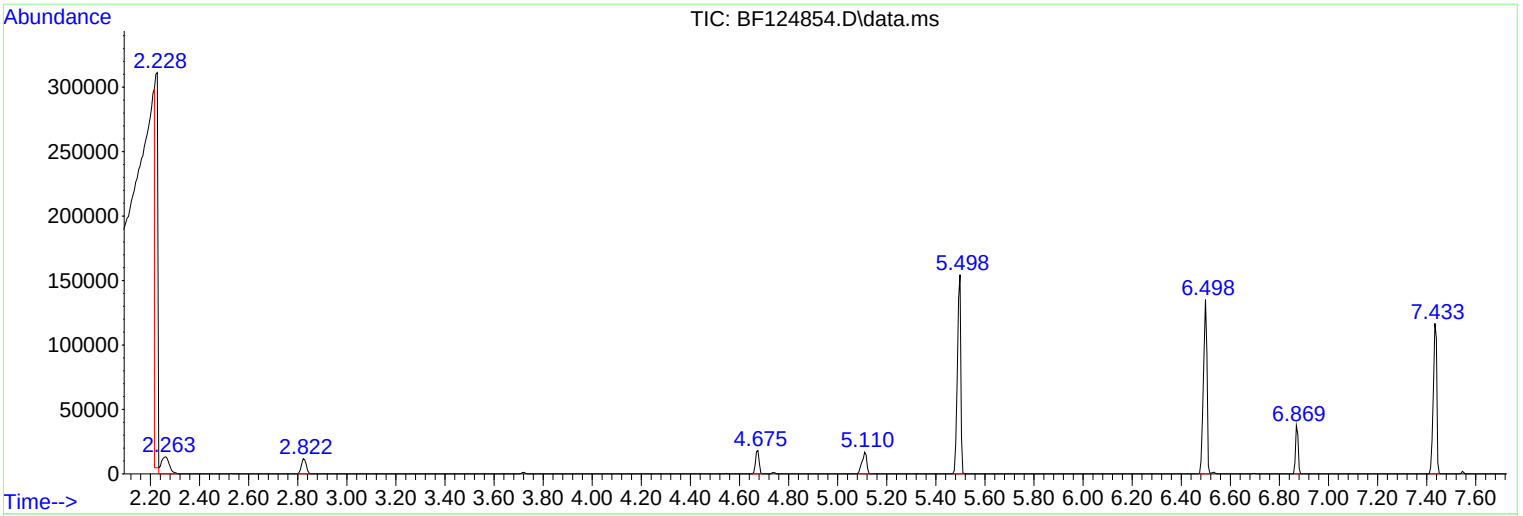
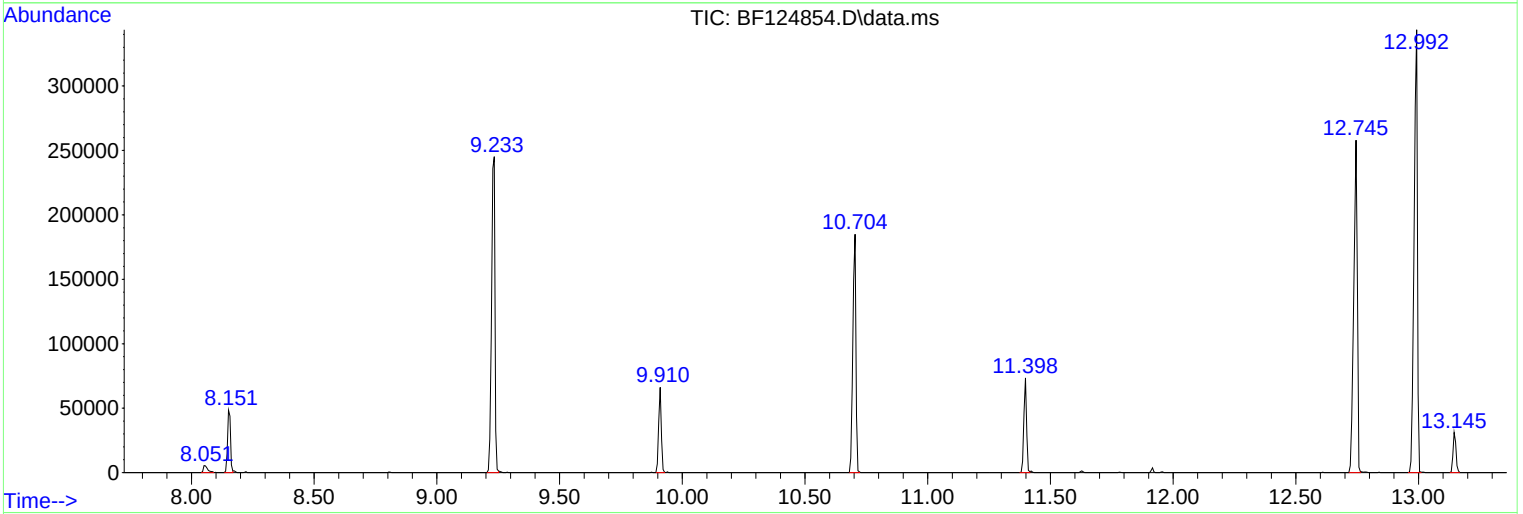
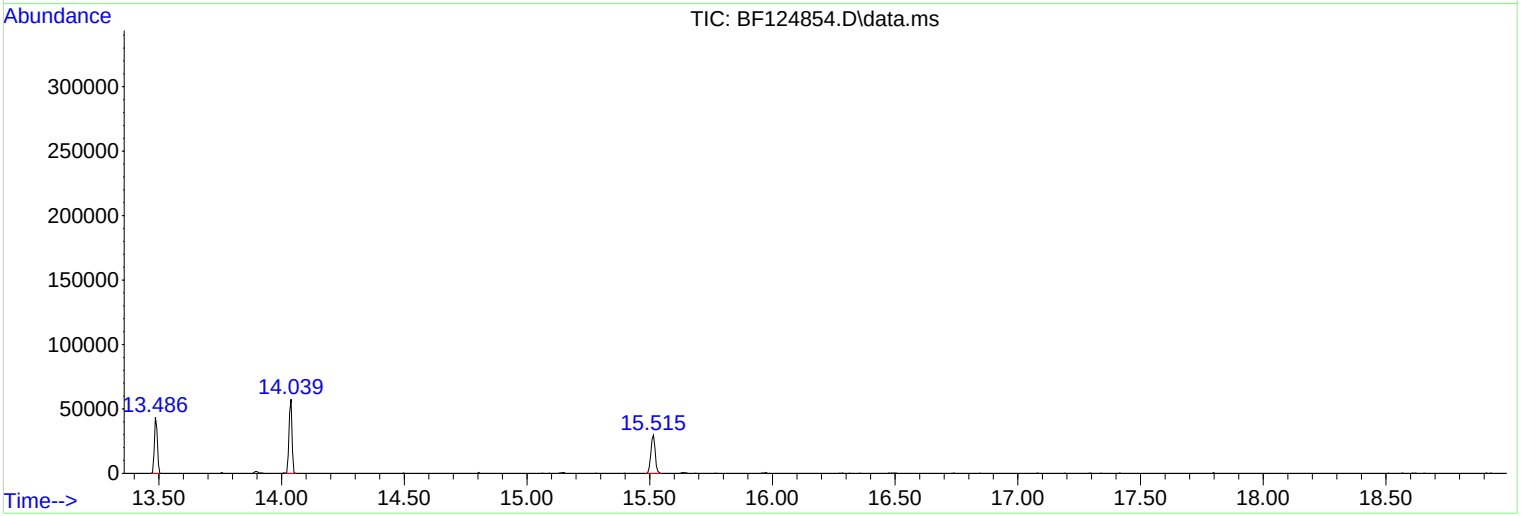
Instrument :
BNA_F
ClientSampleId :
18-B7-TP-(9.5-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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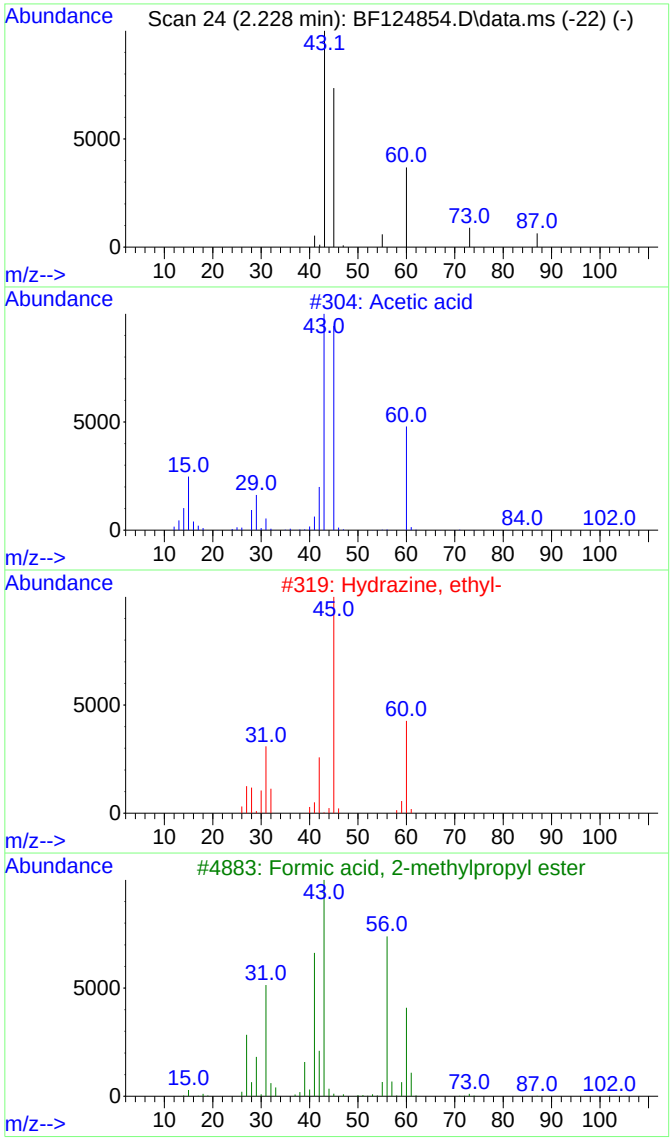
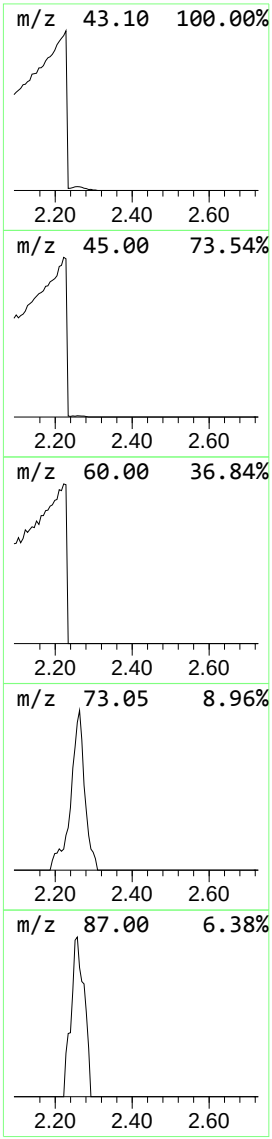
Peak Number 1 Acetic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.228	151.30 ng	216099	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	56
2	Hydrazine, ethyl-	60	C2H8N2	000624-80-6	7
3	Formic acid, 2-methylpropyl ester	102	C5H10O2	000542-55-2	4
4	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	4
5	Aziridine, 1-(methoxymethyl)-	87	C4H9NO	001497-83-2	4





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Operator : JU/CG
Sample : M3176-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
18-B7-TP-(9.5-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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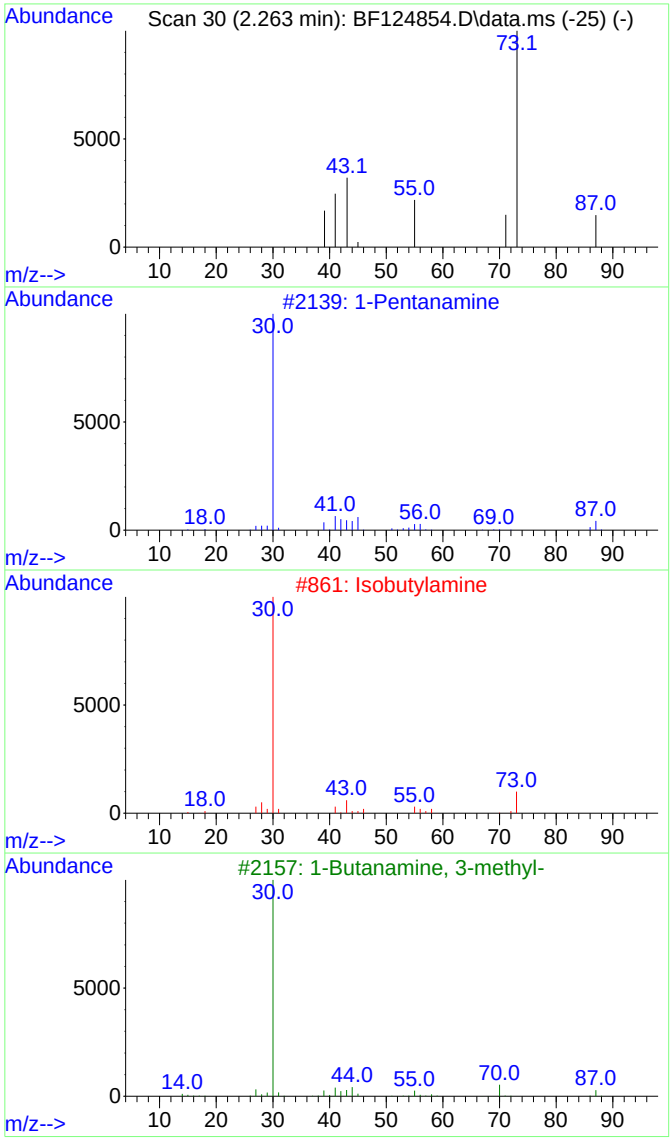
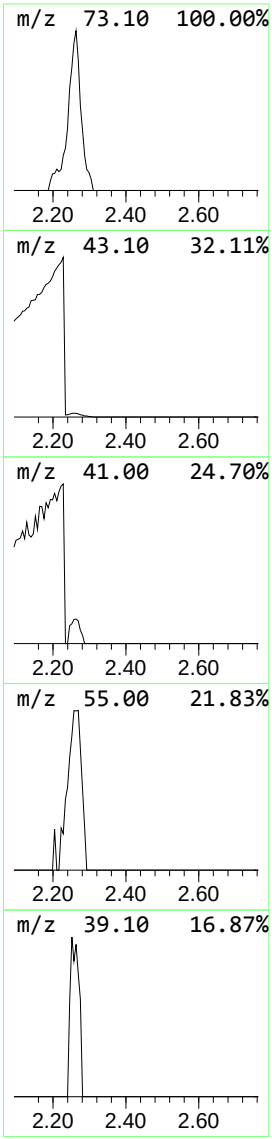
Peak Number 2 unknown2.263 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.263	20.96 ng	29939	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanamine	87	C5H13N	000110-58-7	4
2	Isobutylamine	73	C4H11N	000078-81-9	4
3	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	3
4	1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	3
5	1-Butanamine	73	C4H11N	000109-73-9	3





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Operator : JU/CG
Sample : M3176-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
18-B7-TP-(9.5-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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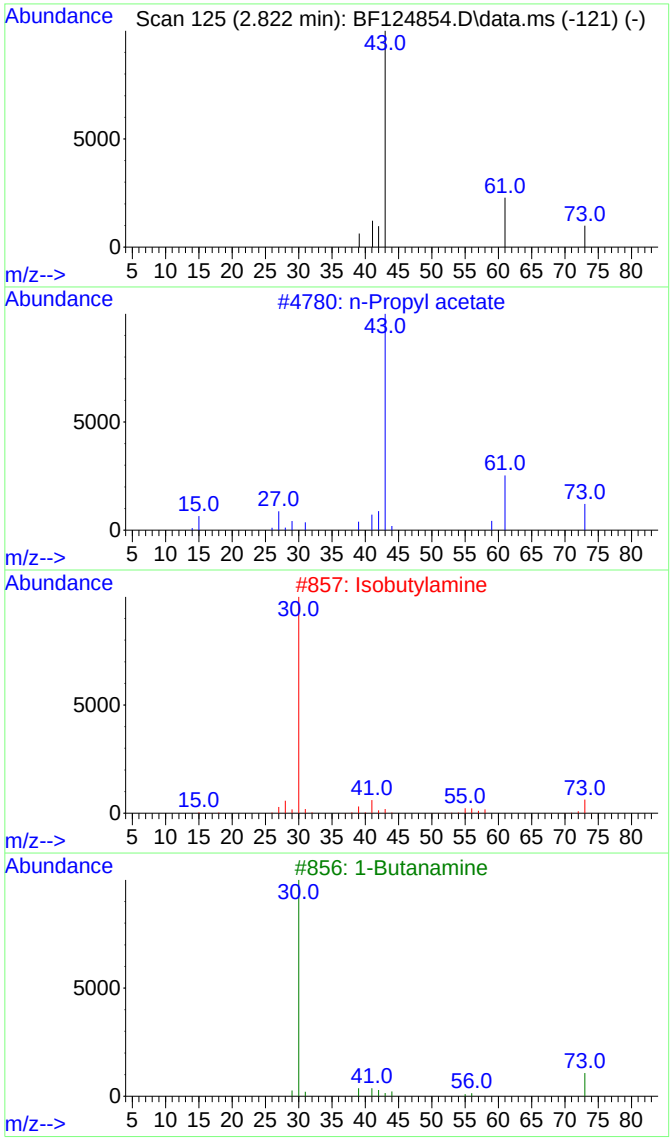
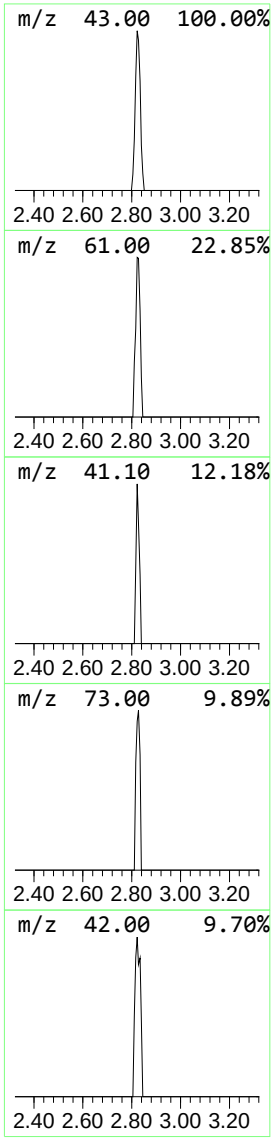
Peak Number 3 n-Propyl acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.822	11.38 ng	16259	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	64
2	Isobutylamine	73	C4H11N	000078-81-9	3
3	1-Butanamine	73	C4H11N	000109-73-9	3
4	Hydrogen azide	43	HN3	007782-79-8	3
5	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	2





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 18-B7-TP-(9.5-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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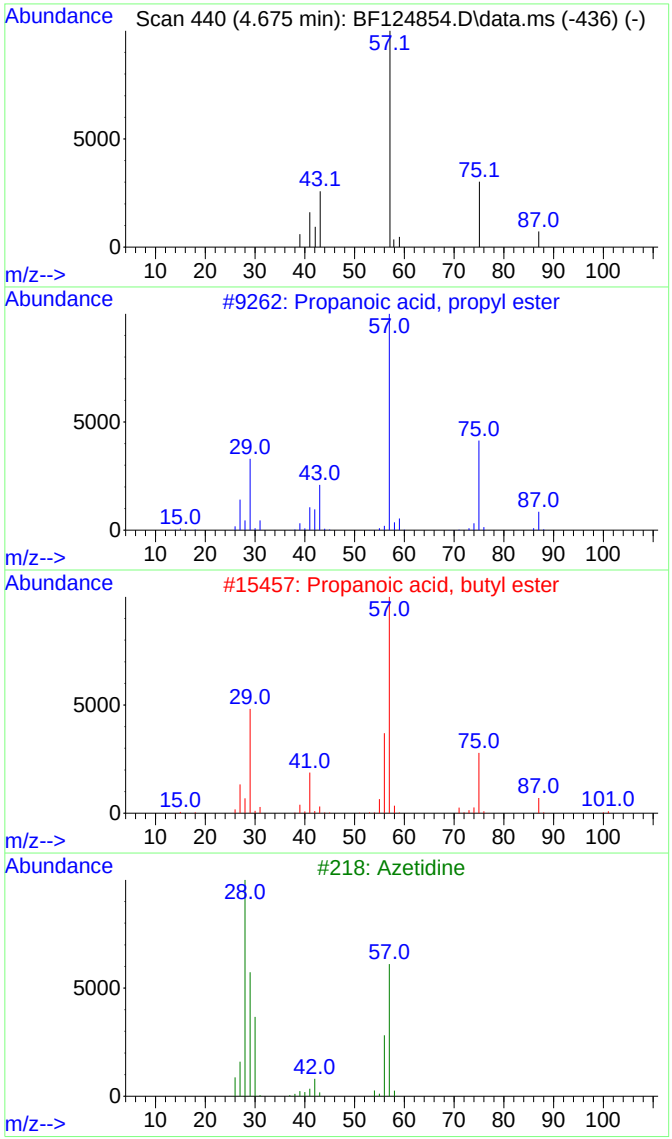
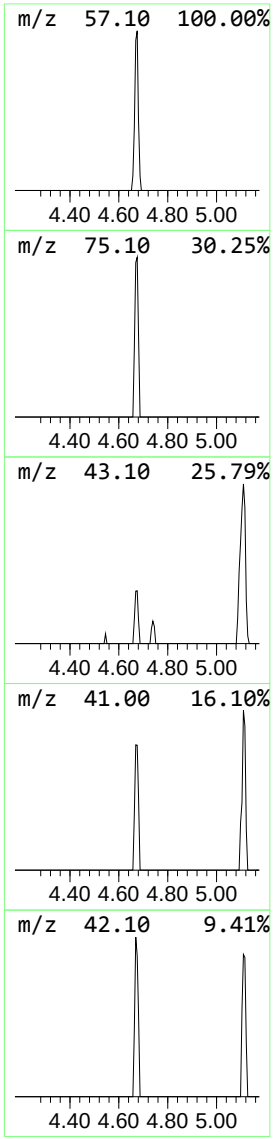
Peak Number 4 Propanoic acid, propyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.675	12.88 ng	18390	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	74
2	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	9
3	Azetidine	57	C3H7N	000503-29-7	7
4	1-Pentanamine	87	C5H13N	000110-58-7	5
5	1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	4





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Operator : JU/CG
Sample : M3176-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
18-B7-TP-(9.5-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
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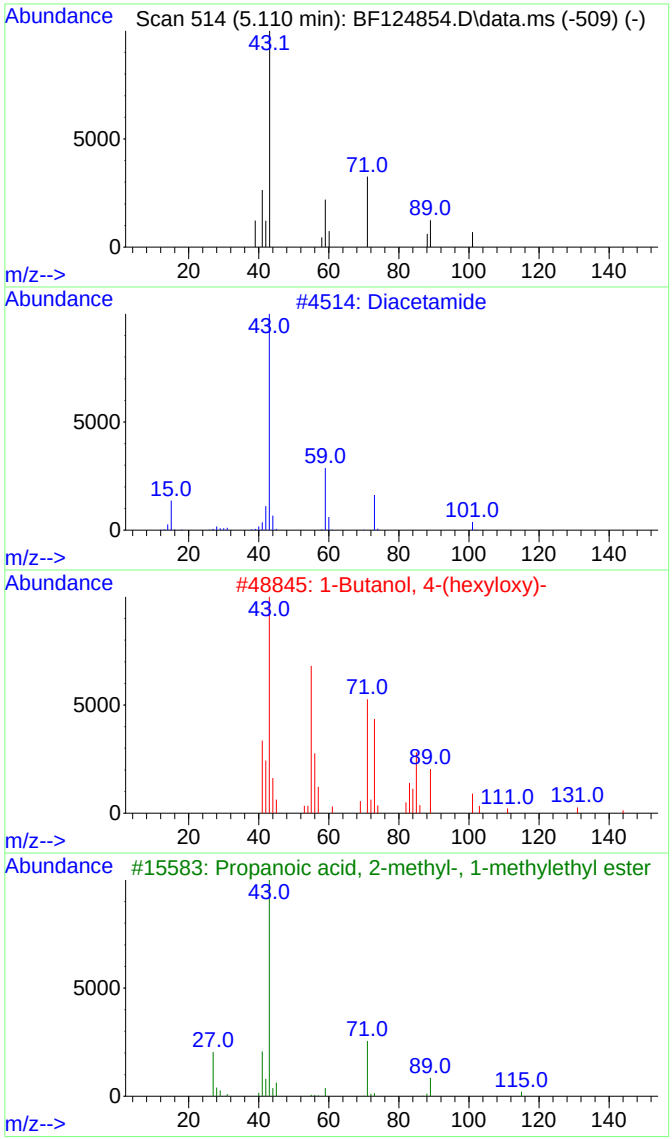
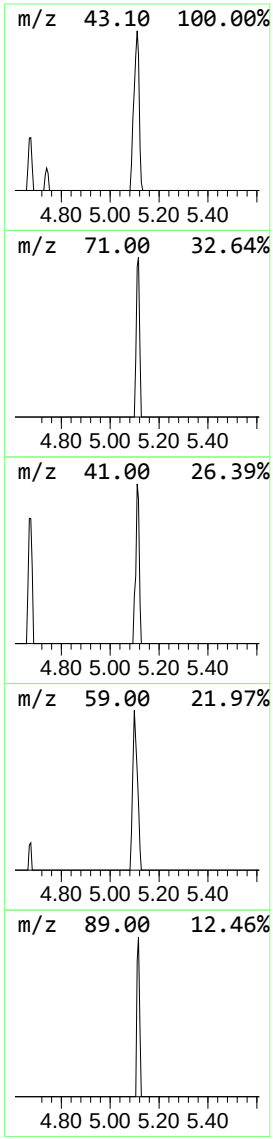
Peak Number 5 unknown5.110 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	15.93 ng	22751	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diacetamide	101	C4H7NO2	000625-77-4	9
2	1-Butanol, 4-(hexyloxy)-	174	C10H22O2	004541-13-3	9
3	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	9
4	1,4-Butanediamine	88	C4H12N2	000110-60-1	7
5	Propyl nitrite	89	C3H7NO2	000543-67-9	5





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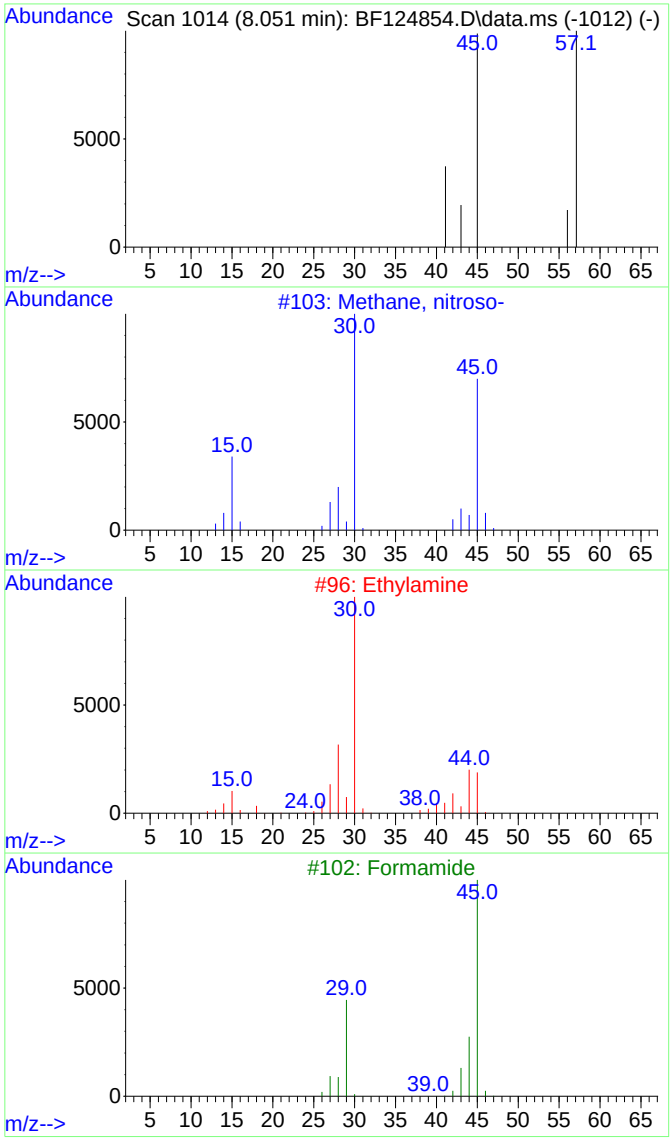
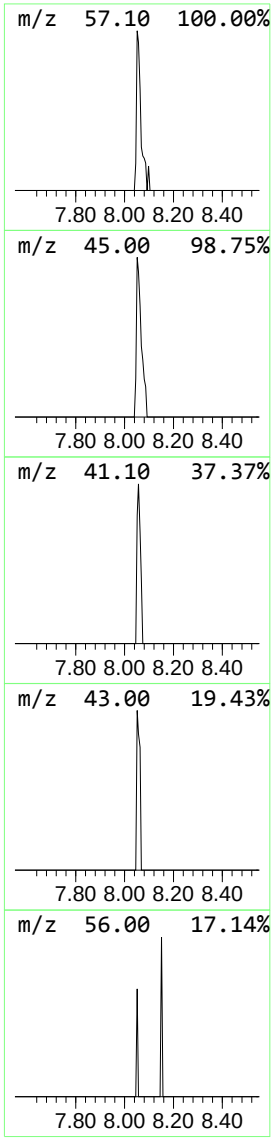
Peak Number 6 unknown8.051 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	3.41 ng	6957	Naphthalene-d8	8.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methane, nitroso-	45	CH3NO	000865-40-7	3
2	Ethylamine	45	C2H7N	000075-04-7	3
3	Formamide	45	CH3NO	000075-12-7	2
4	3-Hydroxy-2-methylbutanenitrile	99	C5H9NO	038046-46-7	1
5	Butane, 1-methoxy-	88	C5H12O	000628-28-4	1





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TIC Library : C:\Database\NIST20.L
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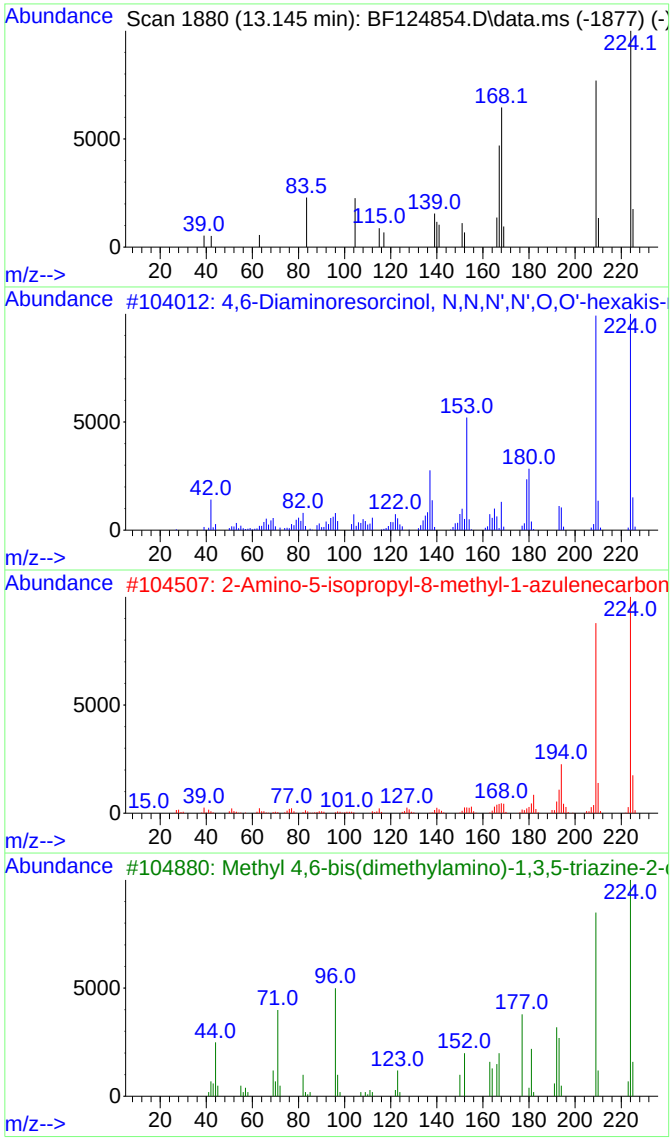
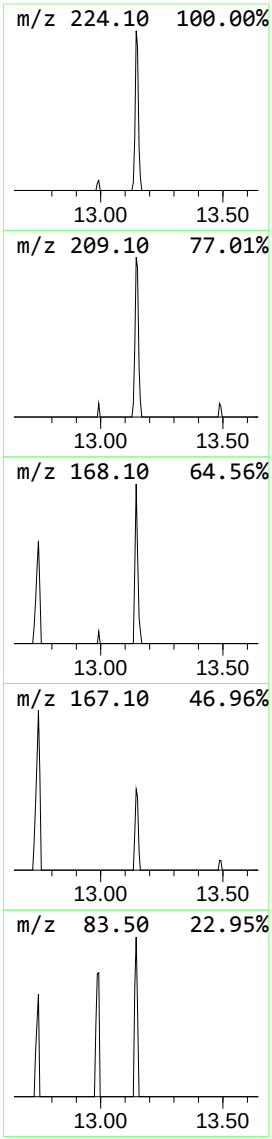
****
Peak Number 8 4,6-Diaminoresorcinol, N,N,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.145	10.82 ng	26295	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,6-Diaminoresorcinol, N,N,N',N'...	224	C12H20N2O2	1000494-57-0	52
2	2-Amino-5-isopropyl-8-methyl-1-a...	224	C15H16N2	093946-48-6	50
3	Methyl 4,6-bis(dimethylamino)-1,...	224	C9H16N6O	1000101-98-0	49
4	1H-1,3-Benzimidazole, 5-methoxy-...	224	C14H12N2O	1000350-62-4	47
5	2-(4-Methoxyphenyl)-1-benzofuran	224	C15H12O2	019234-04-9	47





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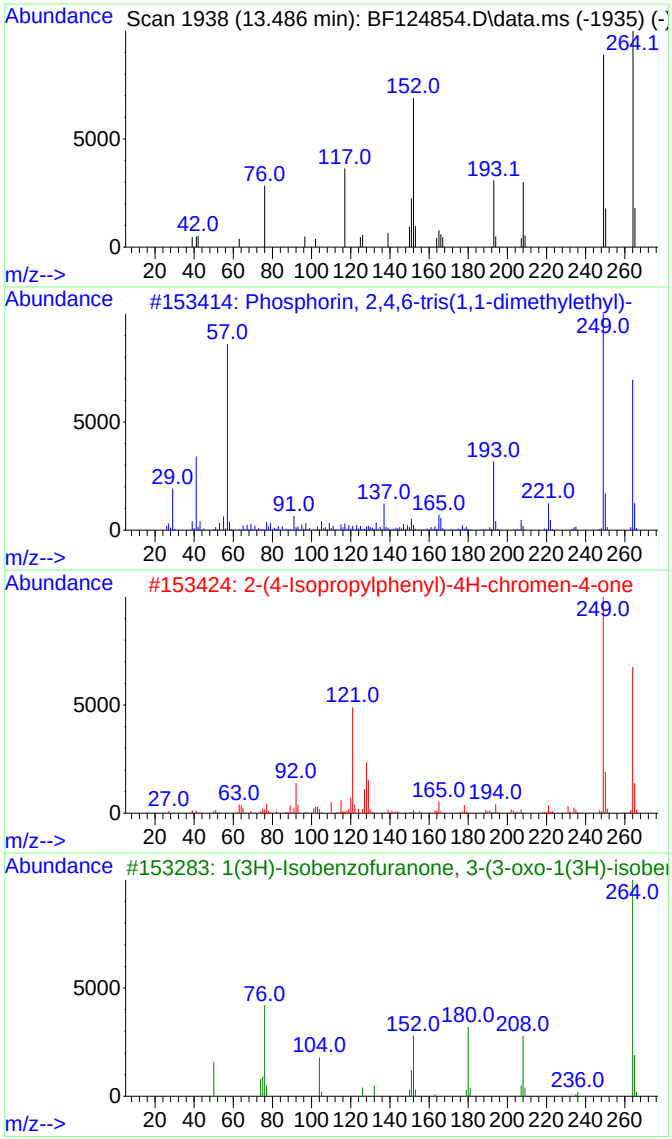
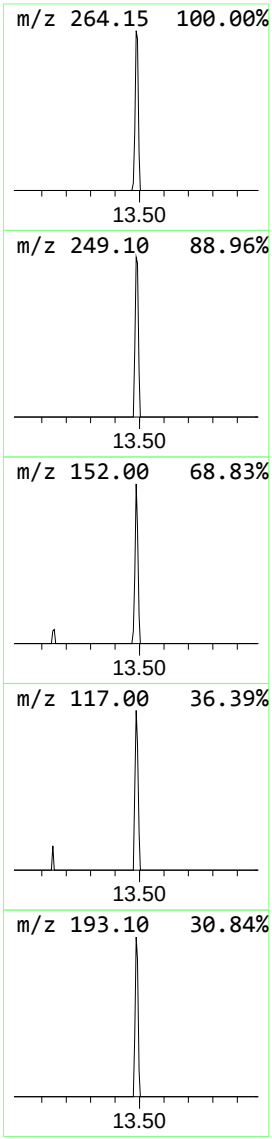
Peak Number 9 unknown13.486 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.486	14.74 ng	35818	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phosphorin, 2,4,6-tris(1,1-dimet...	264	C17H29P	017420-29-0	47
2	2-(4-Isopropylphenyl)-4H-chromen...	264	C18H16O2	092831-11-3	43
3	1(3H)-Isobenzofuranone, 3-(3-oxo...	264	C16H8O4	000482-23-5	30
4	hydrazine, 1-formyl-2-[4-(octylo...	264	C15H24N2O2	1000396-88-6	27
5	1H-Indole, 3-(2-nitroethenyl)-1-...	264	C16H12N2O2	063050-02-2	22





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Acetic acid	2.228	151.3	ng	216099	1	6.869	28565	20.0
unknown2.263	2.263	21.0	ng	29939	1	6.869	28565	20.0
n-Propyl acetate	2.822	11.4	ng	16259	1	6.869	28565	20.0
Propanoic acid,...	4.675	12.9	ng	18390	1	6.869	28565	20.0
unknown5.110	5.110	15.9	ng	22751	1	6.869	28565	20.0
unknown8.051	8.051	3.4	ng	6957	2	8.151	40792	20.0
4,6-Diaminoreso...	13.145	10.8	ng	26295	5	14.039	48610	20.0
unknown13.486	13.486	14.7	ng	35818	5	14.039	48610	20.0