LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111221\
Data File : BF126158.D
Acq On : 12 Nov 2021 18:00
Operator : JU/CG
Sample : M4644-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C-5

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-BF110321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126158.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	20	22	23	rVB	7875705	5500307	100.00%	14.593%
2	2.234	23	25	40	rVB	987343	2000128	36.36%	5.307%
3	2.787	114	119	125	rVB	248701	345618	6.28%	0.917%
4	4.640	429	434	442	rBV	408680	414351	7.53%	1.099%
5	5.057	501	505	507	rBV	213845	236918	4.31%	0.629%
6	5.081	507	509	518	rVB	289790	290524	5.28%	0.771%
7	5.463	569	574	577	rBV	3481572	3364399	61.17%	8.926%
8	6.469	740	745	748	rBV	3196690	3138506	57.06%	8.327%
9	6.840	805	808	812	rBV	983571	787466	14.32%	2.089%
10	7.404	899	904	907	rBV	2862745	2515668	45.74%	6.674%
11	8.034	1007	1011	1022	rBV	217992	380543	6.92%	1.010%
12	8.122	1022	1026	1030	rBV	1147796	1003938	18.25%	2.664%
13	9.204	1205	1210	1213	rBV	5189039	4793266	87.15%	12.717%
14	9.881	1321	1325	1328	rBV	1265303	1166818	21.21%	3.096%
15	10.669	1454	1459	1462	rBV	3568804	3195180	58.09%	8.477%
16	11.363	1573	1577	1580	rBV	1525109	1258799	22.89%	3.340%
17	12.951	1843	1847	1850	rBV	5748019	5339100	97.07%	14.165%
18	14.004	2022	2026	2033	rVB	1186805	998693	18.16%	2.650%
19	14.986	2187	2193	2207	rVB3	39156	141636	2.58%	0.376%
20	15.468	2270	2275	2279	rBV	653771	820111	14.91%	2.176%

Sum of corrected areas: 37691969

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Instrument :
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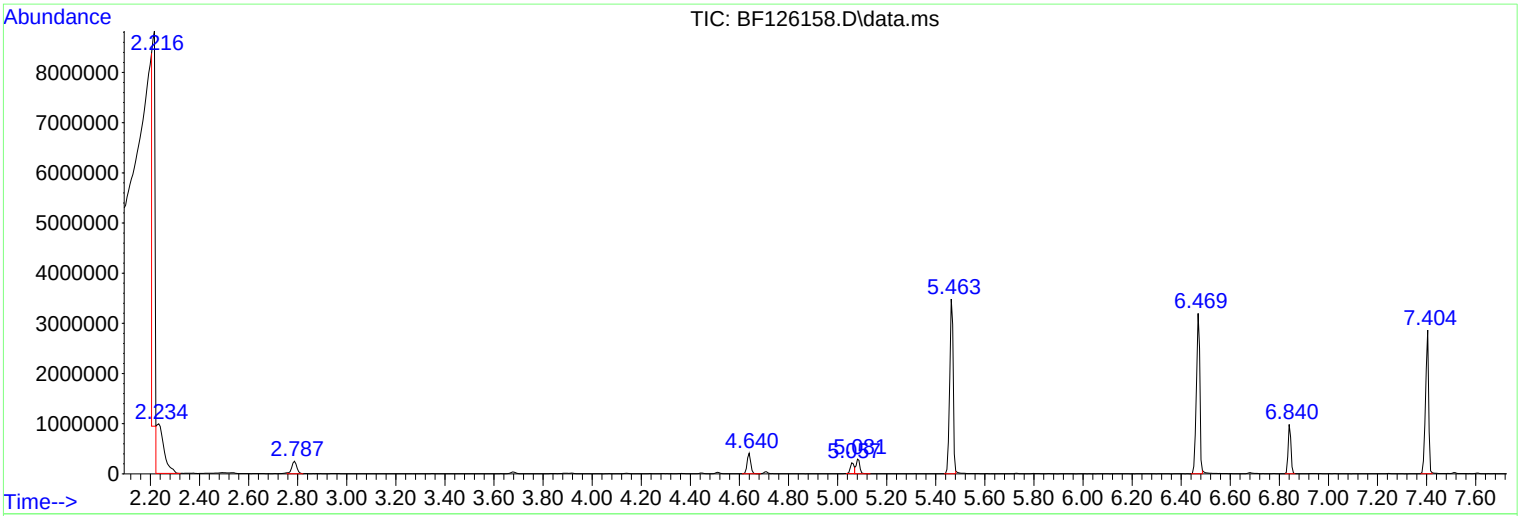
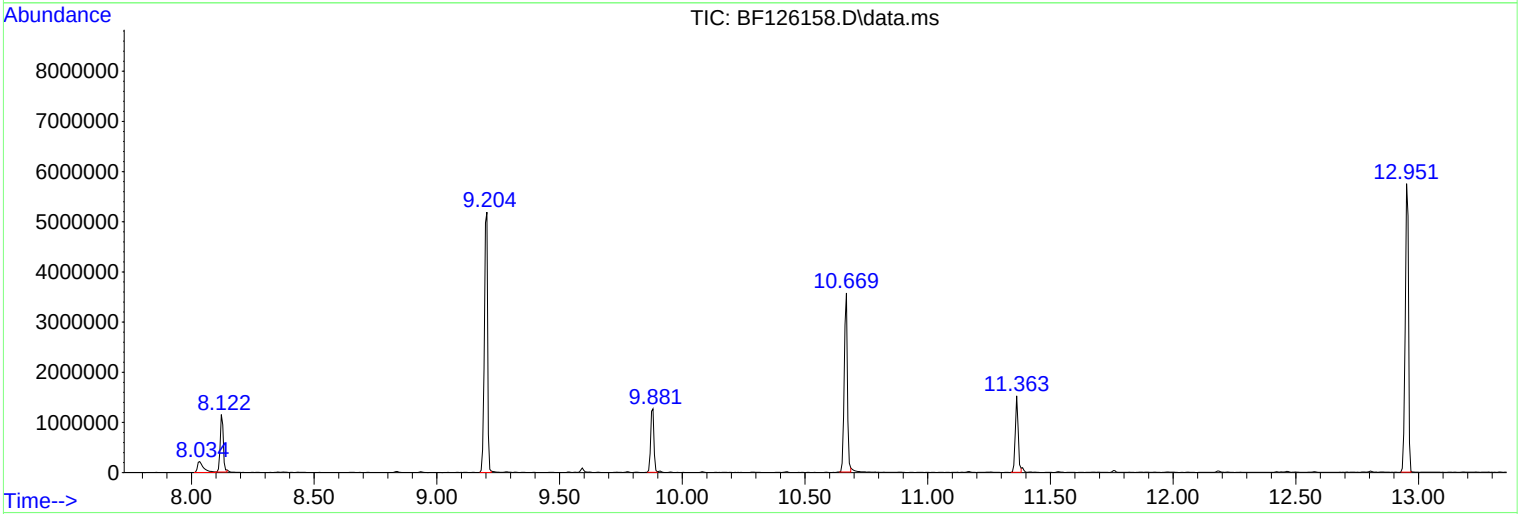
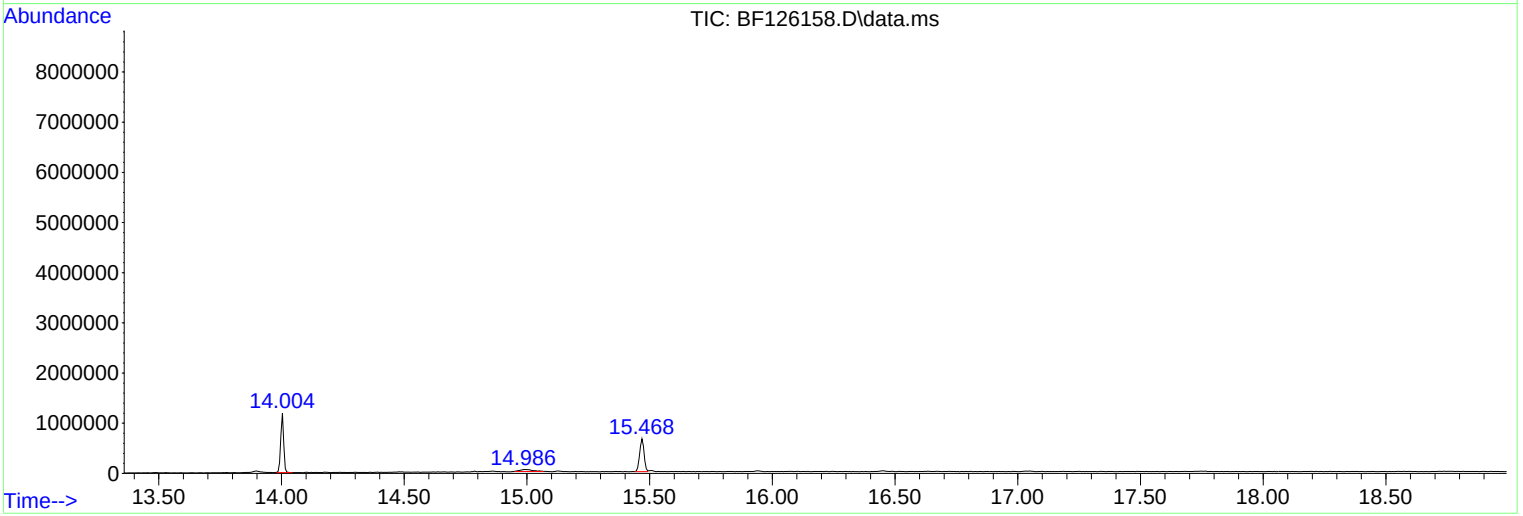
ClientSampleId :
C-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.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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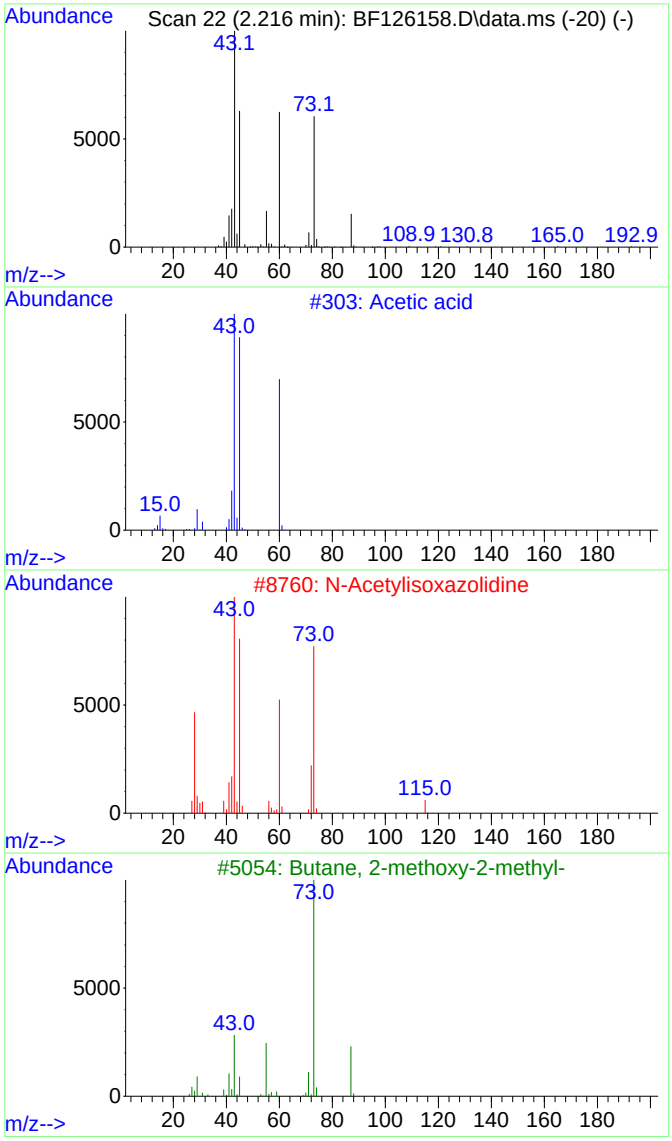
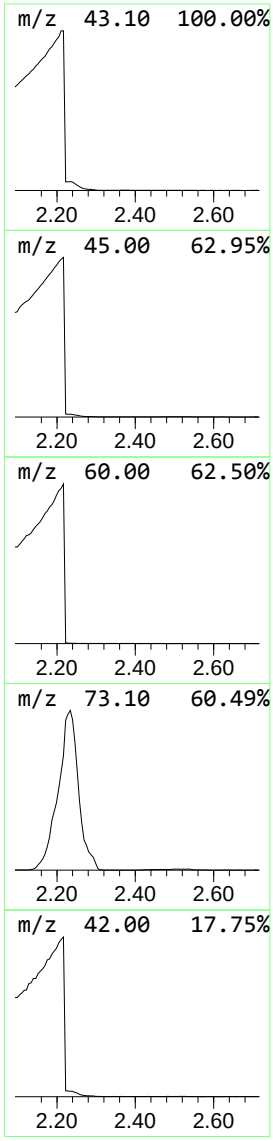
****

Peak Number 1 Acetic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.216	139.70 ng	5500310	1,4-Dichlorobenzene-d4	6.840

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	64
2	N-Acetylisoxazolidine	115	C5H9NO2	115615-36-6	50
3	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	35
4	Heptanoic acid	130	C7H14O2	000111-14-8	28
5	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	25





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
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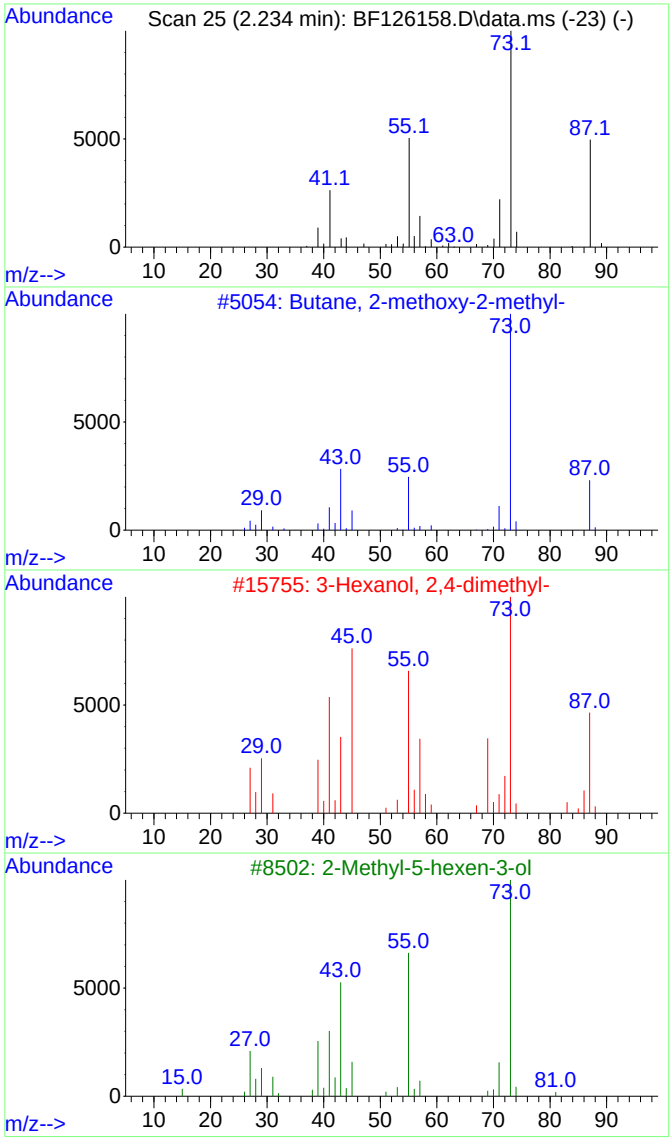
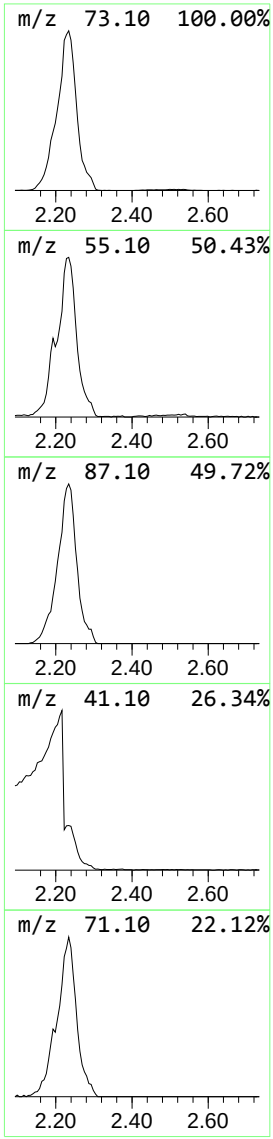
Peak Number 2 unknown2.234 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.234	50.80 ng	2000130	1,4-Dichlorobenzene-d4	6.840

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	36
2	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	36
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
4	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





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Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
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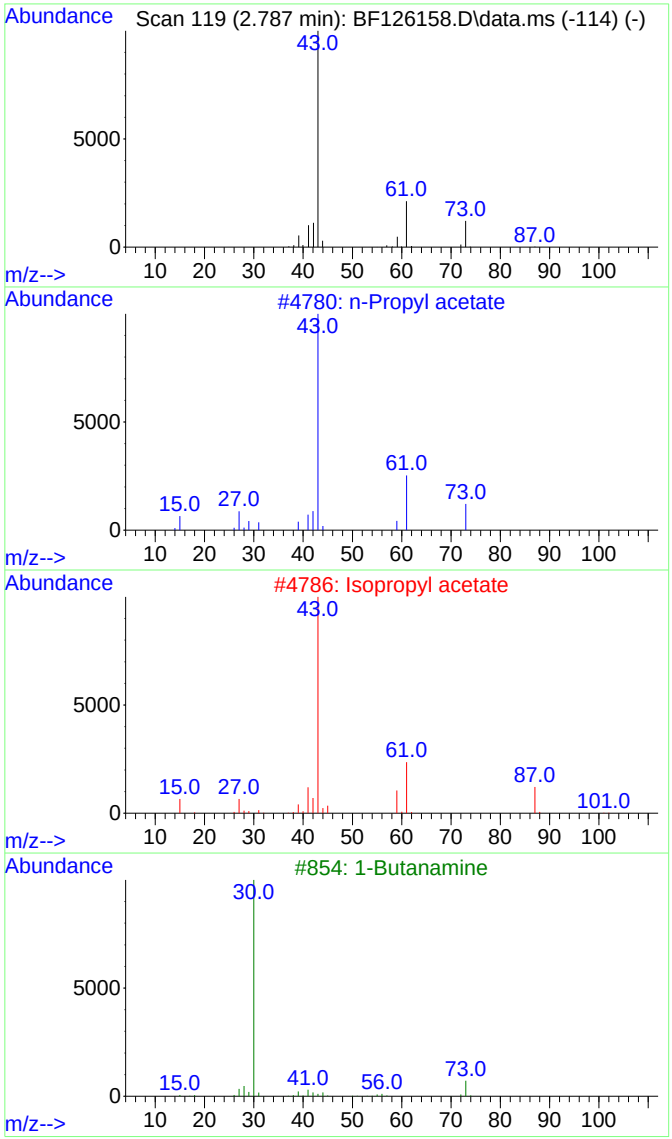
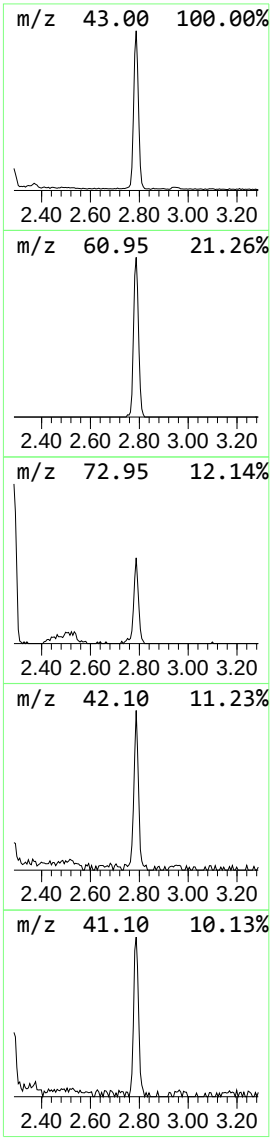
Peak Number 3 n-Propyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.787	8.78 ng	345618	1,4-Dichlorobenzene-d4	6.840

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	78
2	Isopropyl acetate	102	C5H10O2	000108-21-4	38
3	1-Butanamine	73	C4H11N	000109-73-9	5
4	Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	5
5	Isobutylamine	73	C4H11N	000078-81-9	5





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

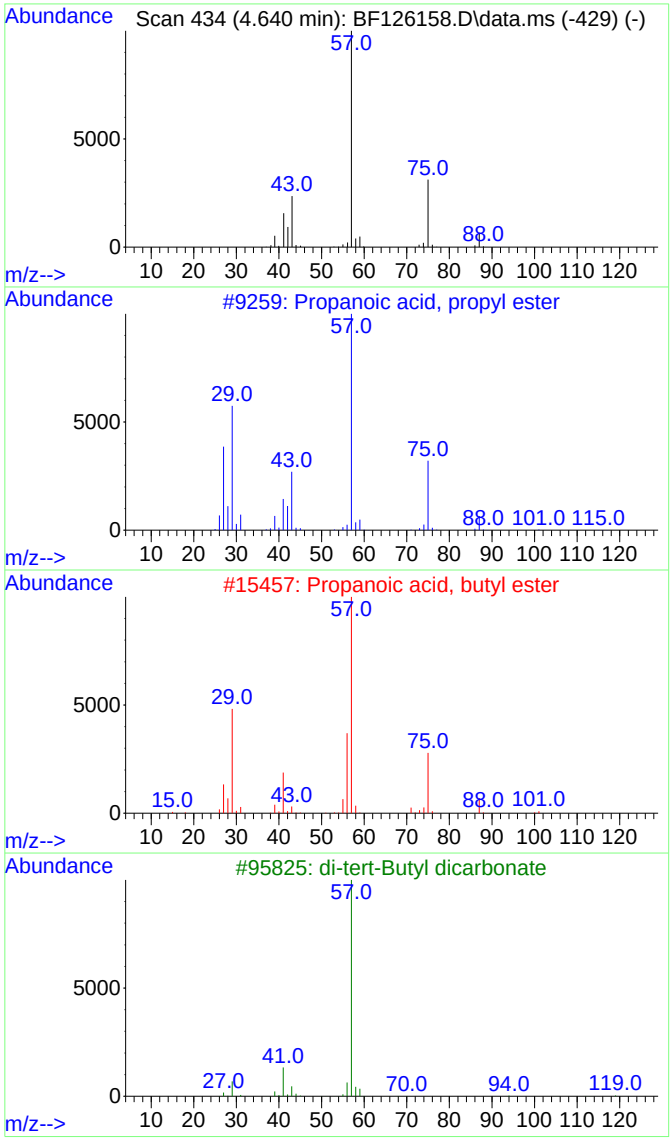
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

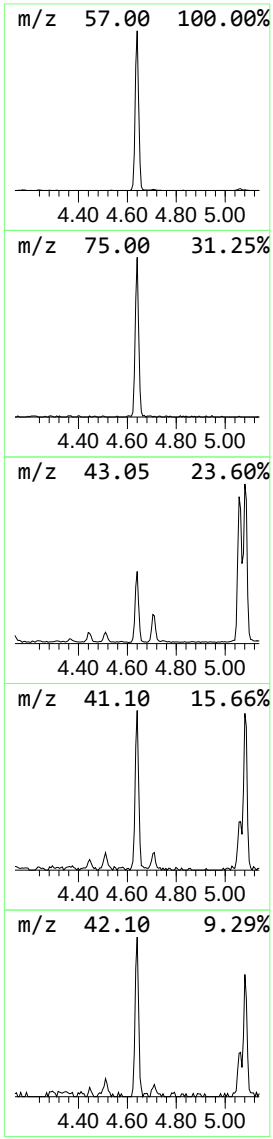
****

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.640	10.52 ng	414351	1,4-Dichlorobenzene-d4	6.840

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	42
3	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
4	1-Penten-3-ol	86	C5H10O	000616-25-1	7
5	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	5





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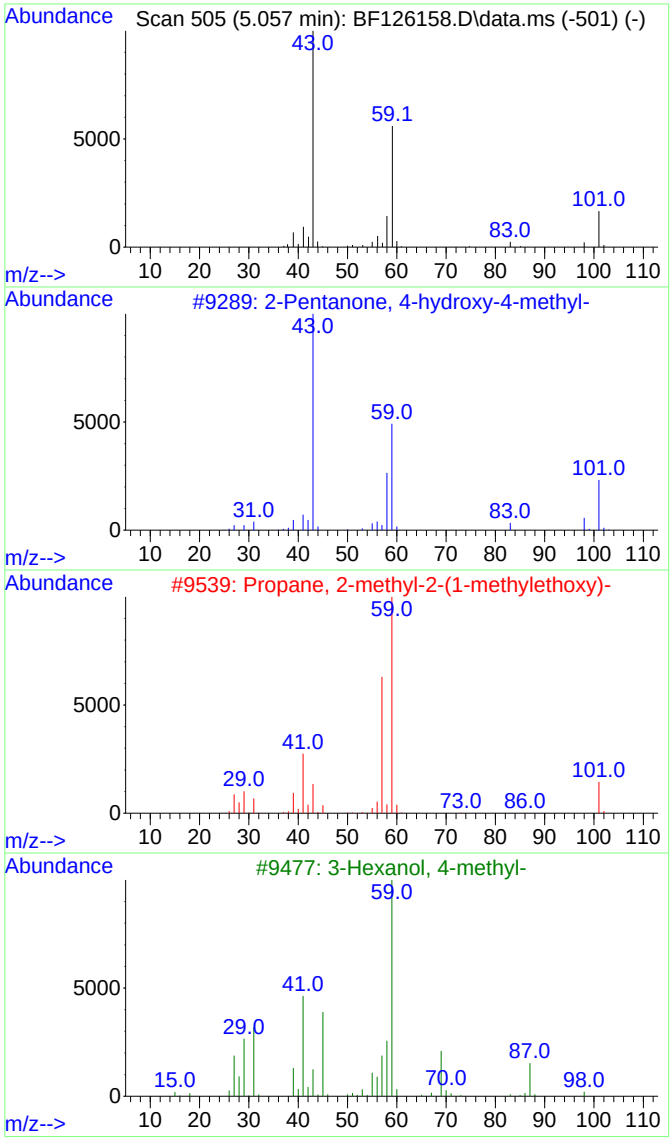
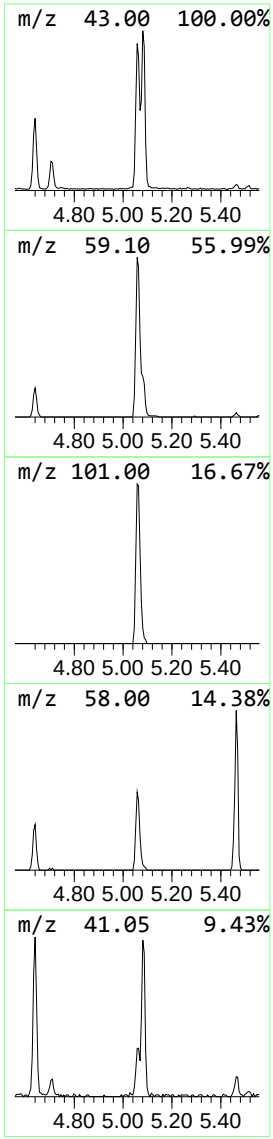
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	6.02 ng	236918	1,4-Dichlorobenzene-d4	6.840

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	1,2-Butanediol	90	C4H10O2	000584-03-2	28





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TIC Library : C:\Database\NIST20.L
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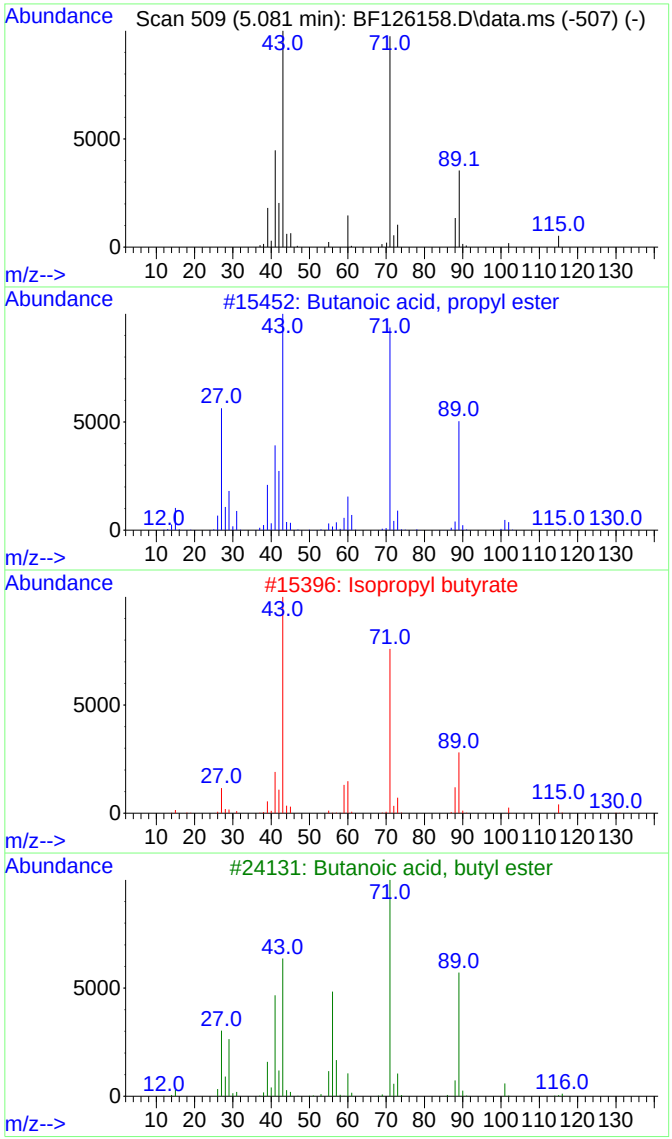
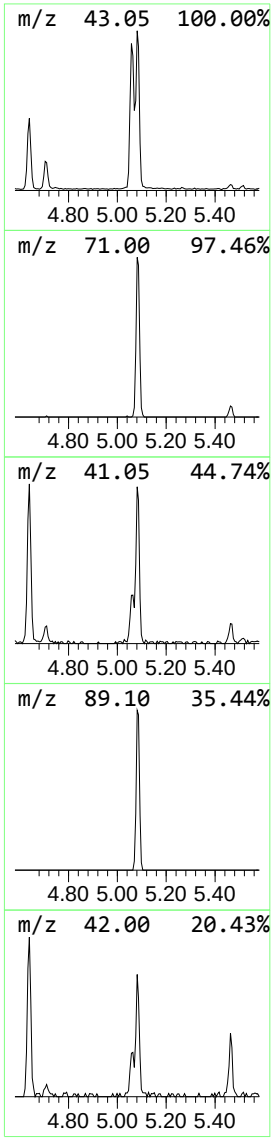
****

Peak Number 6 Butanoic acid, propyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	7.38 ng	290524	1,4-Dichlorobenzene-d4	6.840

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	78
2	Isopropyl butyrate	130	C7H14O2	000638-11-9	78
3	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	64
4	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	56
5	Butanoic acid, 2,2-dimethyl-	116	C6H12O2	000595-37-9	53





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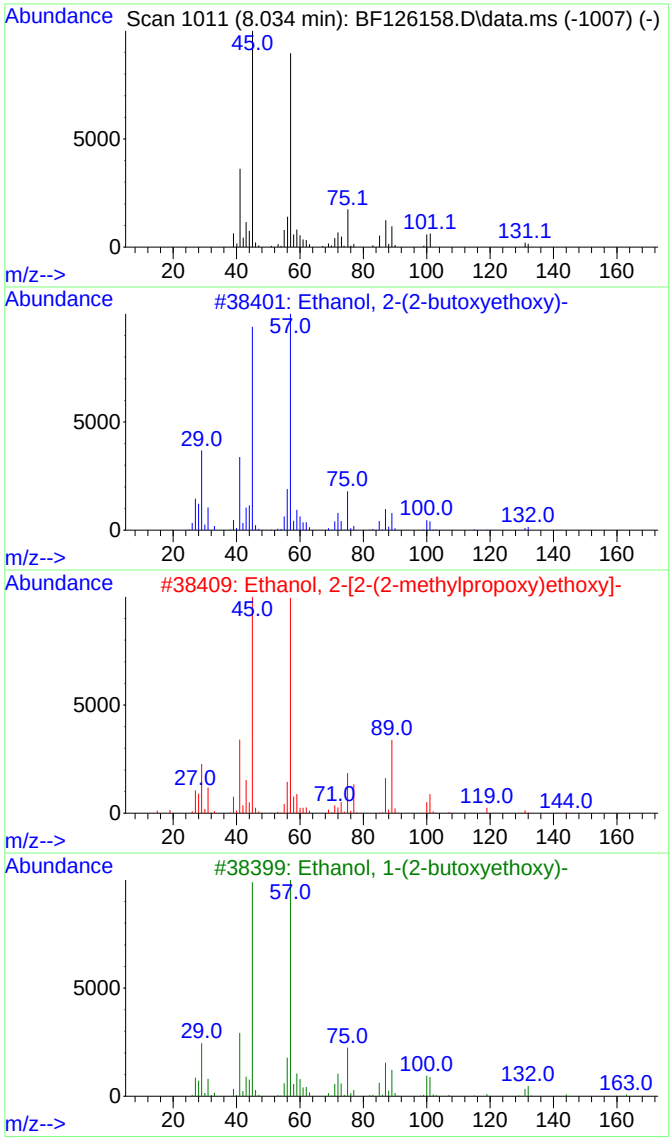
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

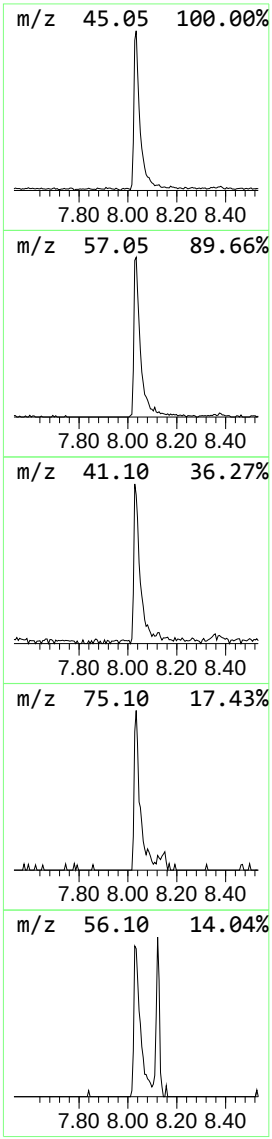
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.034	7.58 ng	380543	Naphthalene-d8	8.122

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
3	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	59
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53





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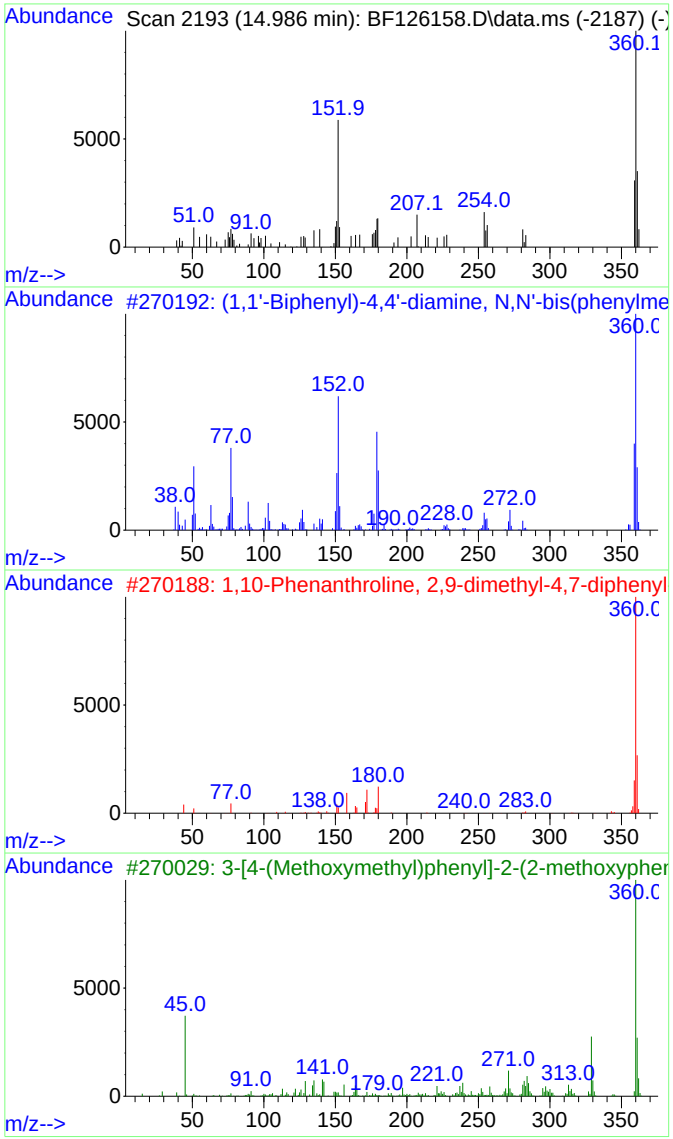
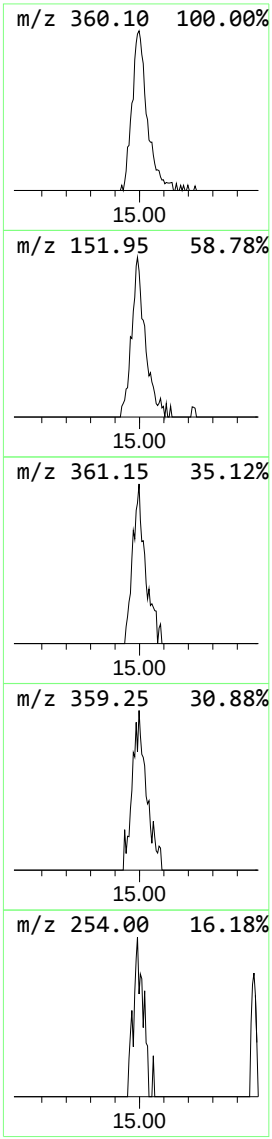
****
Peak Number 8 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.986	3.45 ng	141636	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1,1'-Biphenyl)-4,4'-diamine, N,...	360	C26H20N2	006311-48-4	64
2	1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	46
3	3-[4-(Methoxymethyl)phenyl]-2-(2...	360	C23H20O2S	1000458-33-8	43
4	Benzoic acid, 4-(3,4-dihydro-2,4...	361	C20H15N3O4	317326-96-8	43
5	Ethene, 1-(anthracen-9-yl)-2-(4-...	360	C27H20O	1000163-55-1	38





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	2.216	139.7	ng	5500310	1	6.840	787466	20.0
unknown2.234	2.234	50.8	ng	2000130	1	6.840	787466	20.0
n-Propyl acetate	2.787	8.8	ng	345618	1	6.840	787466	20.0
Propanoic acid,...	4.640	10.5	ng	414351	1	6.840	787466	20.0
2-Pentanone, 4-...	5.057	6.0	ng	236918	1	6.840	787466	20.0
Butanoic acid, ...	5.081	7.4	ng	290524	1	6.840	787466	20.0
Ethanol, 2-(2-b...	8.034	7.6	ng	380543	2	8.122	1003940	20.0
(1,1'-Biphenyl)...	14.986	3.5	ng	141636	6	15.468	820111	20.0