

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022823\
 Data File : BF132579.D
 Acq On : 28 Feb 2023 18:57
 Operator : CG\JU
 Sample : 01701-04
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-13-GW02

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-BF022223.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132579.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.616	3	5	14	rVB	839097	1017763	1.64%	0.734%
2	5.240	446	451	460	rVB	1360789	1460704	2.35%	1.053%
3	5.628	510	517	521	rBV	3167485	3148754	5.07%	2.271%
4	6.622	682	686	689	rBV	2754795	2294665	3.70%	1.655%
5	6.998	747	750	754	rBV	1667710	1435153	2.31%	1.035%
6	7.569	841	847	850	rBV	4131485	4275435	6.89%	3.083%
7	7.987	853	918	921	rBV	5948003	62048249	100.00%	44.745%
8	8.287	965	969	972	rVB	2302204	1857790	2.99%	1.340%
9	8.475	995	1001	1002	rVV	817647	1324905	2.14%	0.955%
10	8.534	1003	1011	1013	rVV	2241277	5221591	8.42%	3.765%
11	8.569	1013	1017	1021	rVV2	2527486	3895273	6.28%	2.809%
12	8.651	1021	1031	1034	rVV3	2013268	5067254	8.17%	3.654%
13	8.757	1037	1049	1051	rVV	3031580	8643154	13.93%	6.233%
14	8.798	1053	1056	1057	rVV	1882904	2343314	3.78%	1.690%
15	8.822	1057	1060	1061	rVV	2839362	2866277	4.62%	2.067%
16	9.369	1147	1153	1156	rBV	7964730	7807178	12.58%	5.630%
17	10.051	1265	1269	1272	rVB	2598918	2183366	3.52%	1.574%
18	10.763	1387	1390	1394	rVB	767508	673016	1.08%	0.485%
19	10.845	1399	1404	1408	rBV	5301268	5854661	9.44%	4.222%
20	11.545	1519	1523	1526	rBV	2686093	2318565	3.74%	1.672%
21	12.057	1606	1610	1626	rBV	893143	1001351	1.61%	0.722%
22	13.139	1789	1794	1797	rBV	8444246	9021287	14.54%	6.506%
23	14.198	1970	1974	1978	rBV	1828978	1681316	2.71%	1.212%
24	15.751	2233	2238	2246	rBV2	951320	1229736	1.98%	0.887%

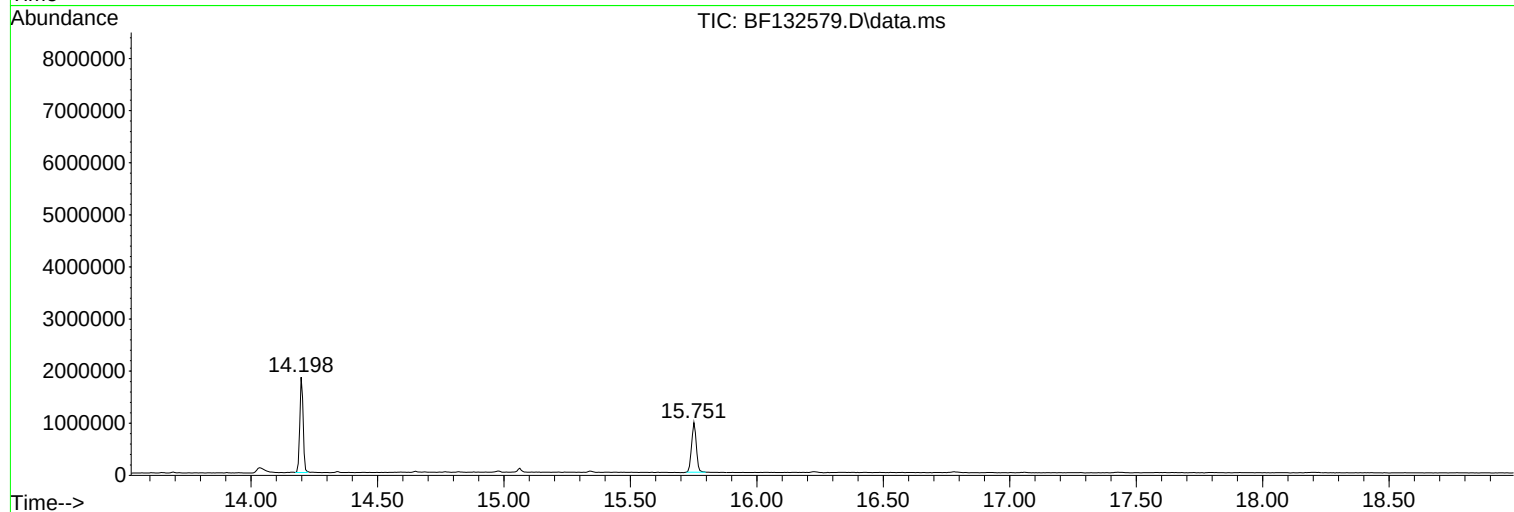
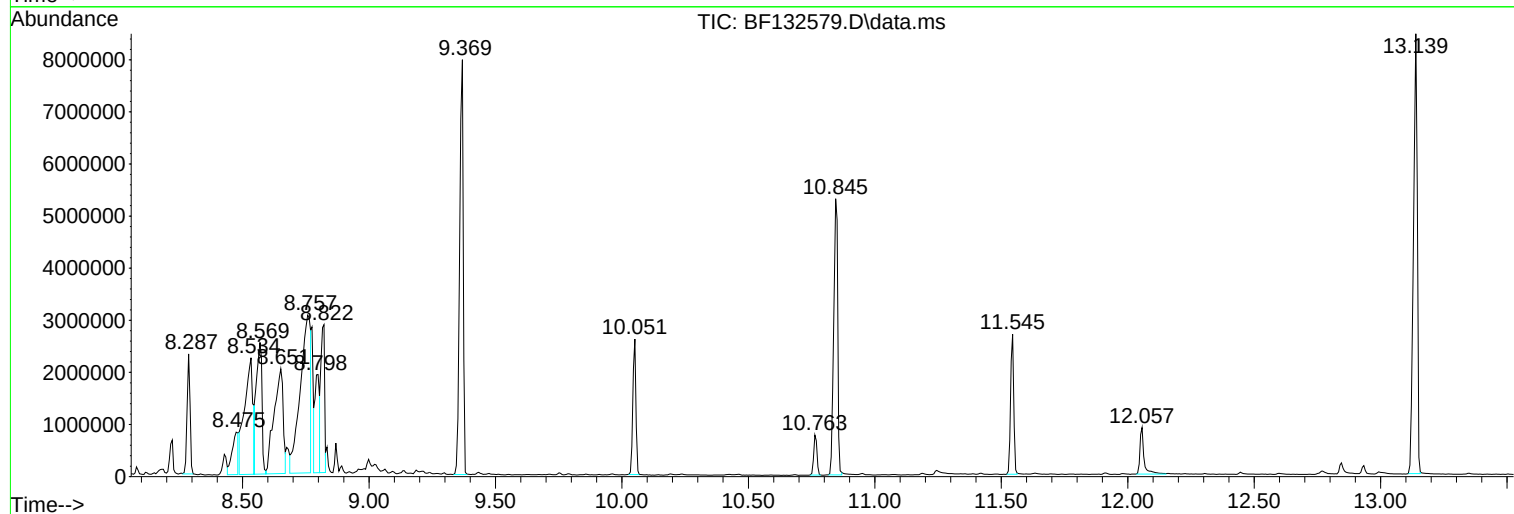
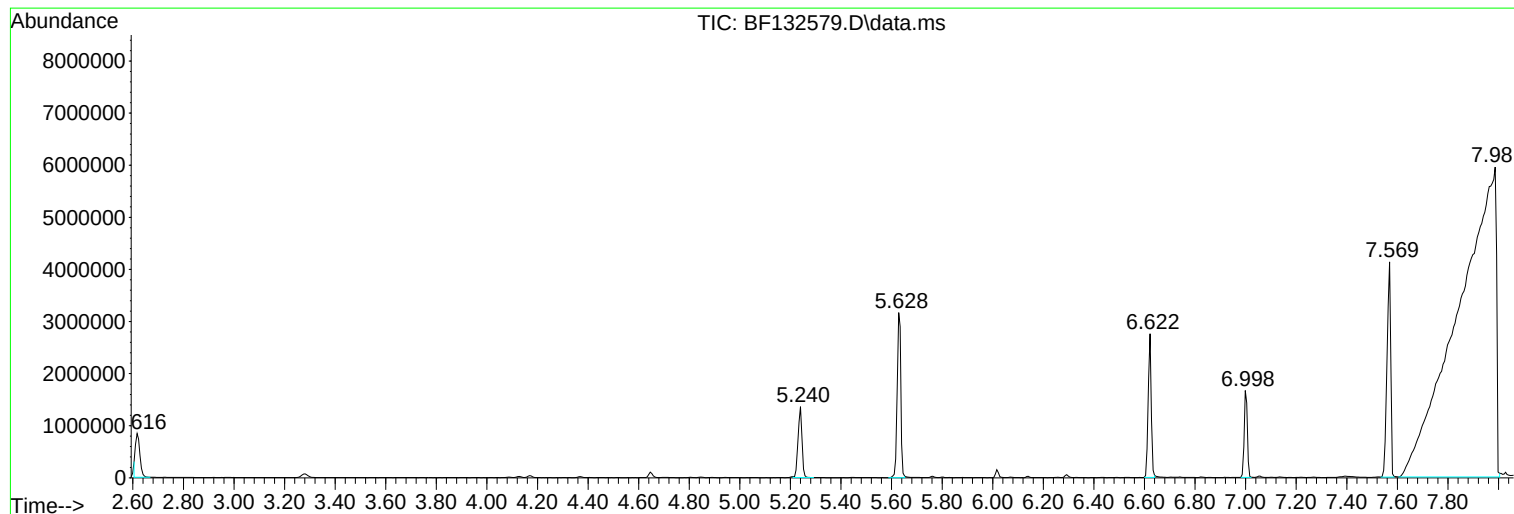
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B-13-GW02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.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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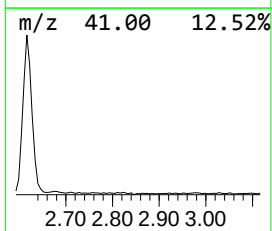
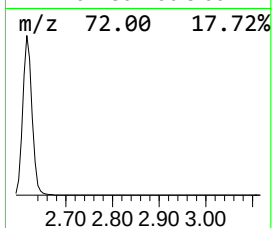
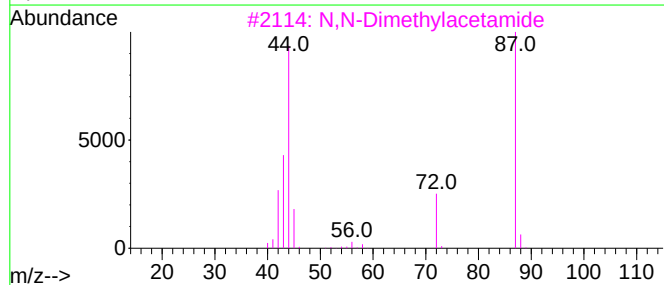
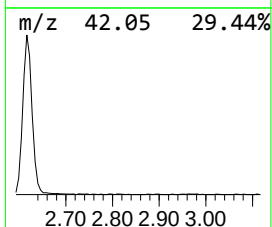
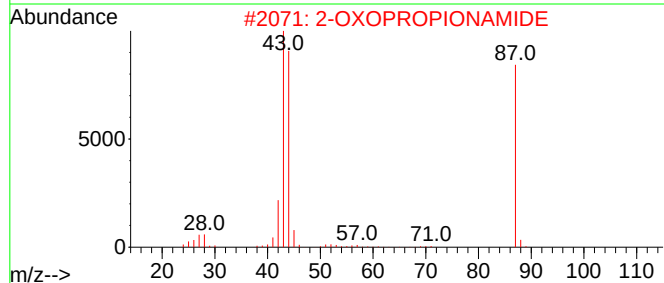
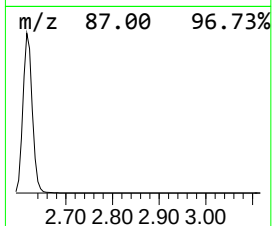
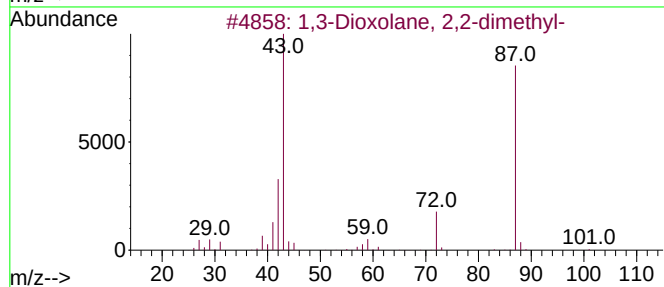
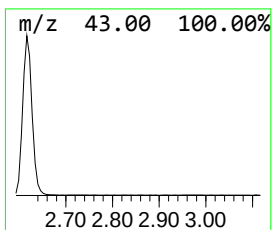
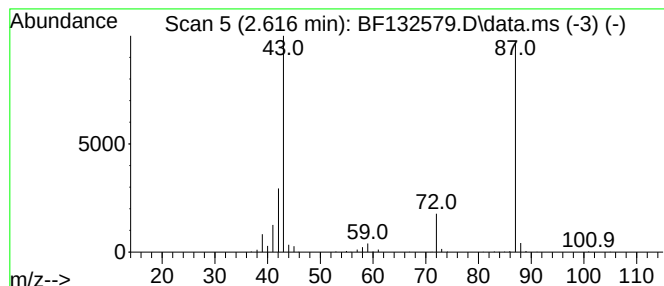
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1,3-Dioxolane, 2,2-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.616	14.18 ng	1017760	1,4-Dichlorobenzene-d4	6.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2,2-dimethyl-	102	C5H10O2	002916-31-6	83
2			2-OXOPROPIONAMIDE	87	C3H5NO2	000631-66-3	56
3			N,N-Dimethylacetamide	87	C4H9NO	000127-19-5	53
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	50
5			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	42



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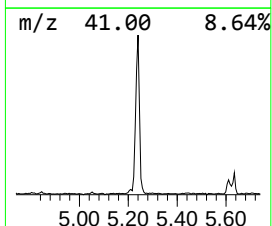
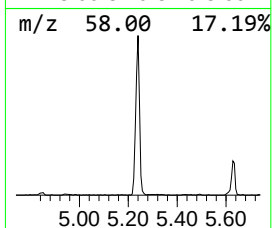
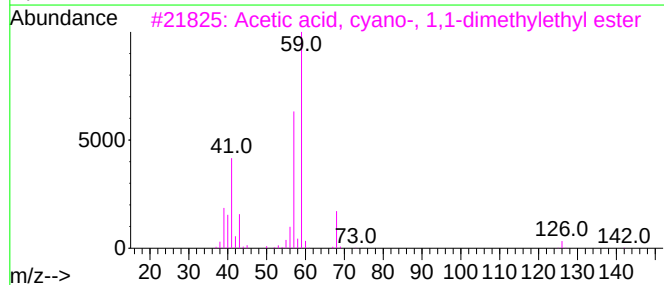
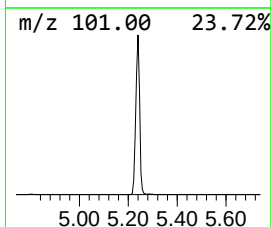
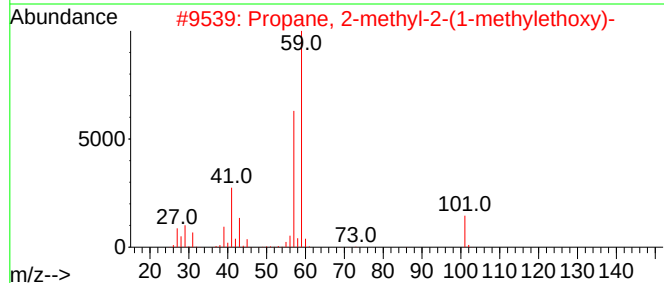
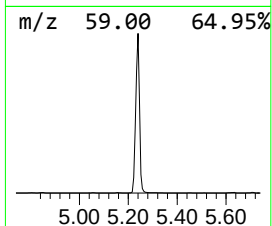
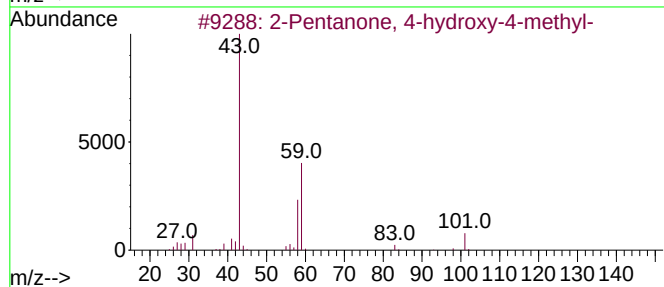
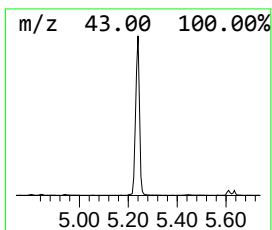
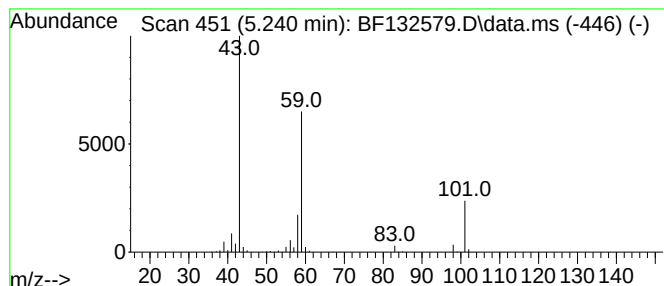
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.240	20.36 ng	1460700	1,4-Dichlorobenzene-d4	6.998

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	53
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Guanidine	59	CH5N3	000113-00-8	9



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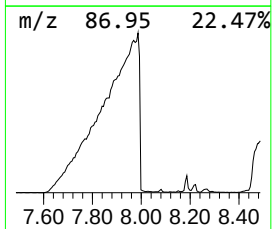
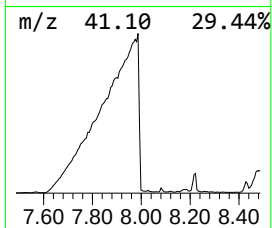
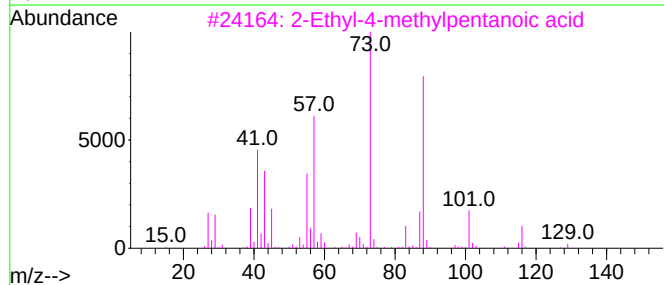
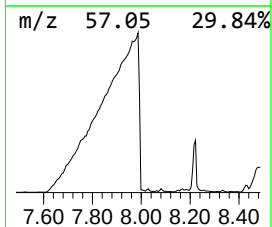
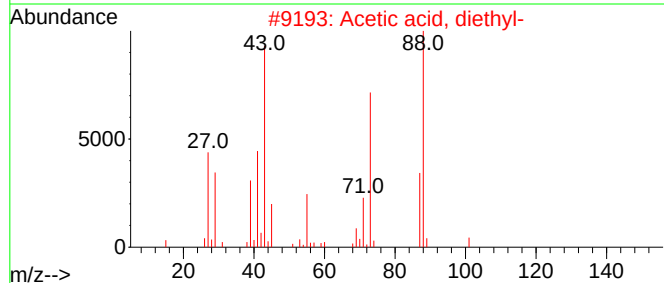
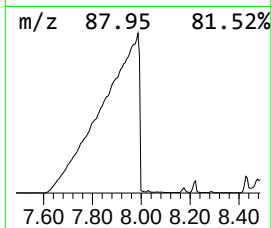
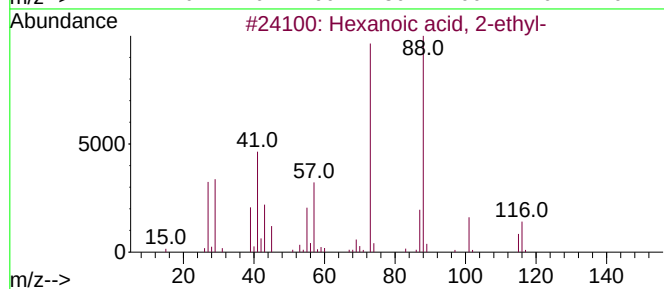
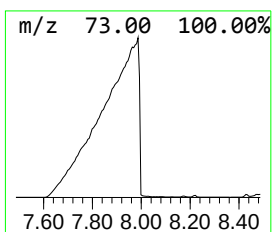
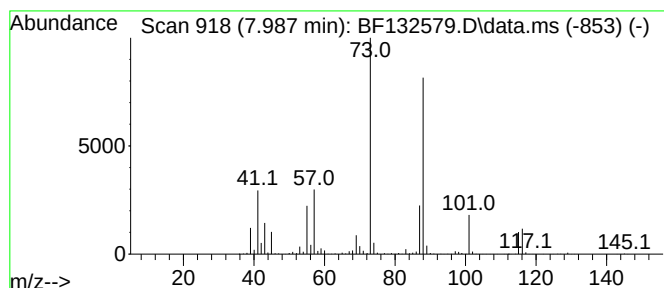
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Hexanoic acid, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.987	667.98 ng	62048200	Naphthalene-d8	8.287

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2			Acetic acid, diethyl-	116	C6H12O2	000088-09-5	59
3			2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	56
4			Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	50
5			Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	45



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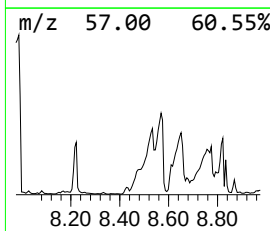
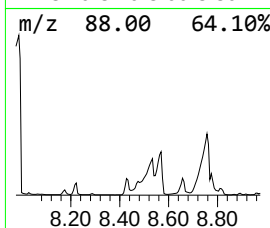
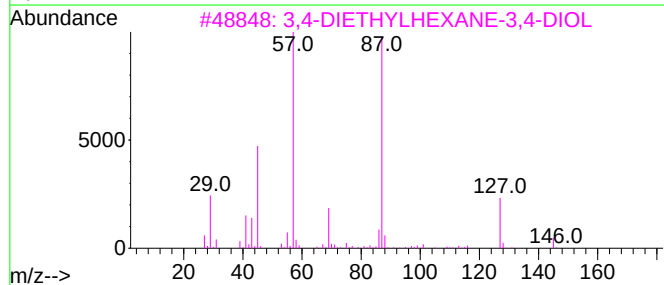
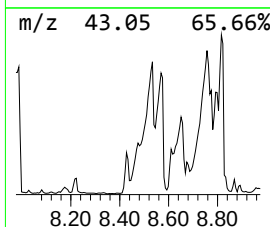
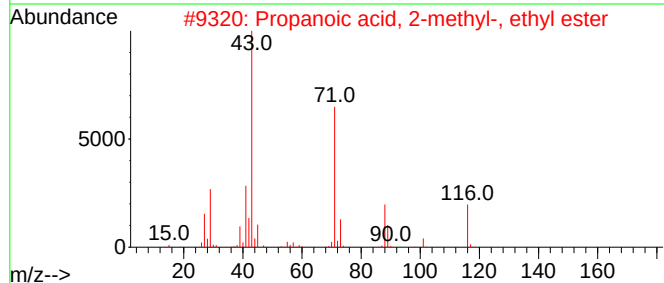
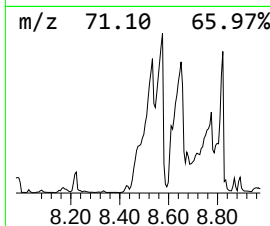
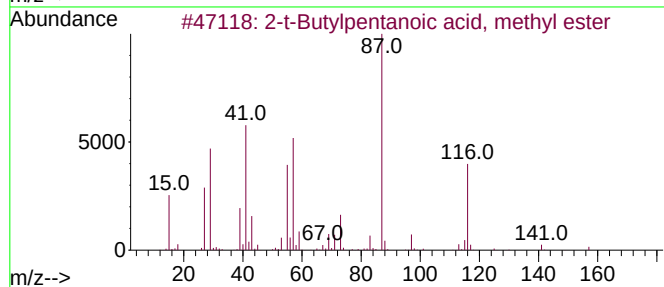
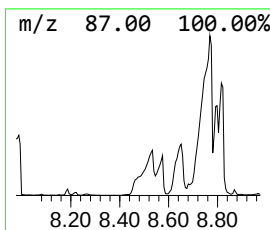
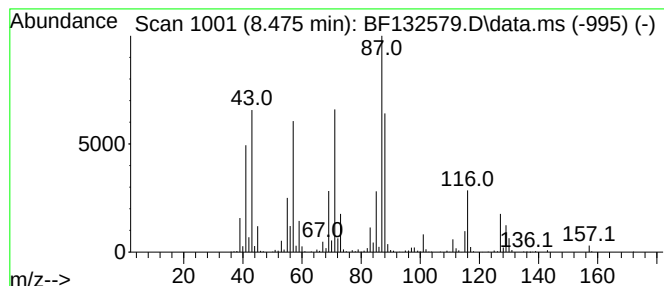
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown8.475 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.475	14.26 ng	1324910	Naphthalene-d8	8.287

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-t-Butylpentanoic acid, methyl ...	172	C10H20O2	1000202-22-5	38		
2	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	22		
3	3,4-DIETHYLHEXANE-3,4-DIOL	174	C10H22O2	006931-71-1	22		
4	Acetic acid, 3-ethylpent-3-yl ester	158	C9H18O2	1000368-76-0	22		
5	2-(Oxolan-2-yl)-1,2-oxazinane	157	C8H15N02	1000445-08-1	22		



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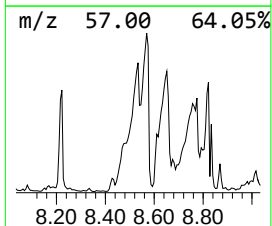
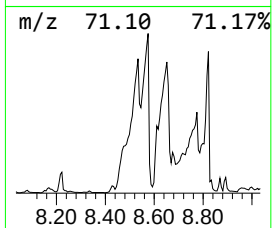
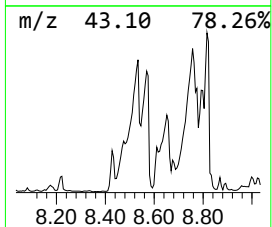
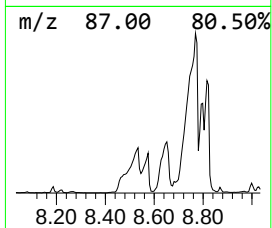
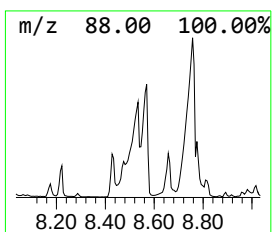
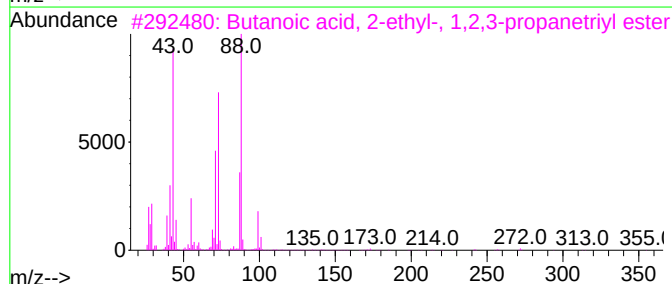
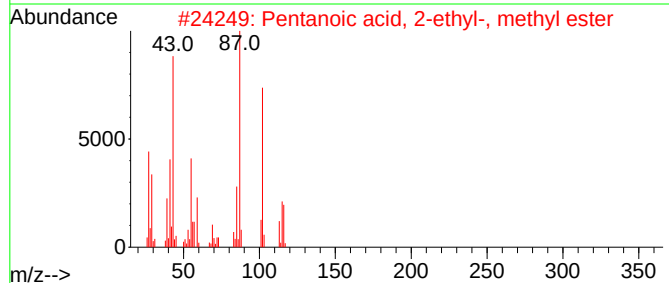
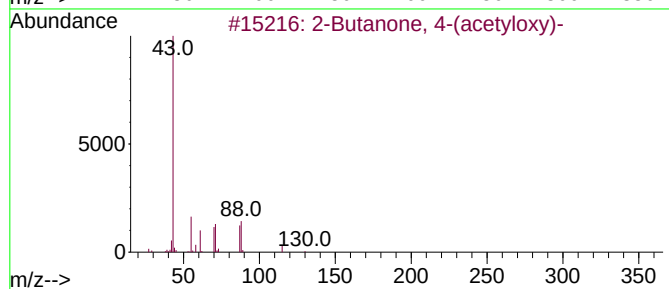
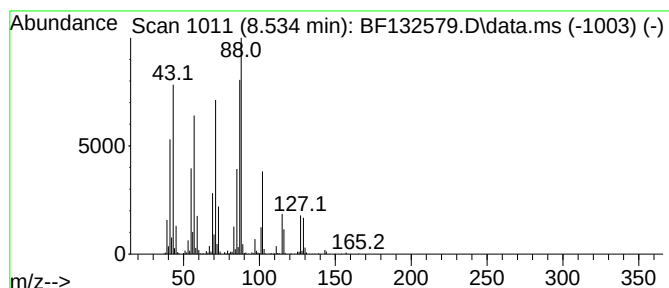
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown8.534 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.534	56.21 ng	5221590	Naphthalene-d8	8.287

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 4-(acetyloxy)-	130	C6H10O3	010150-87-5	47		
2	Pentanoic acid, 2-ethyl-, methyl...	144	C8H16O2	000816-16-0	27		
3	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	27		
4	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	27		
5	Butyric acid, 2,2,3,3-tetramethyl-	144	C8H16O2	030407-41-1	22		



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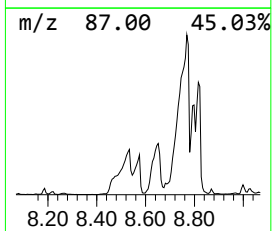
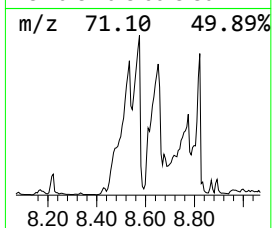
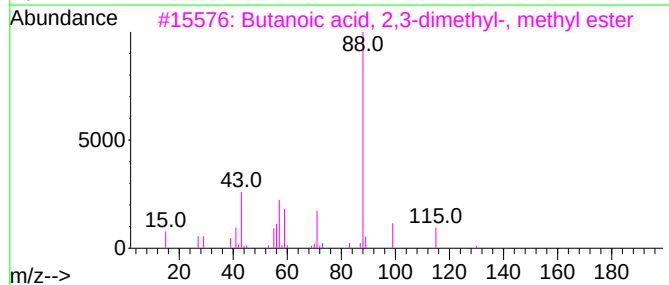
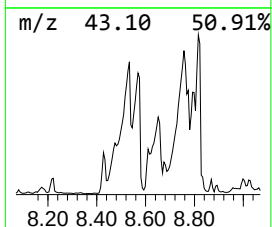
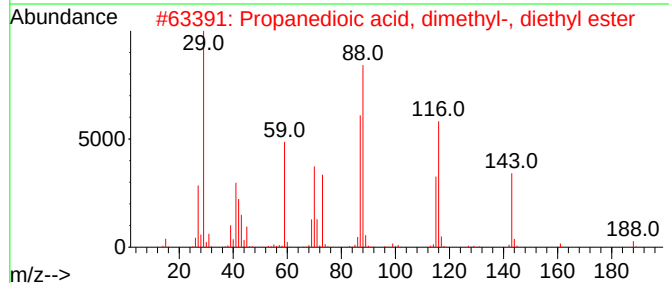
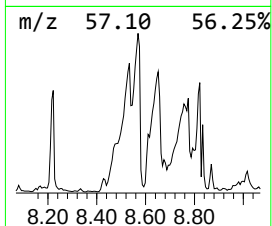
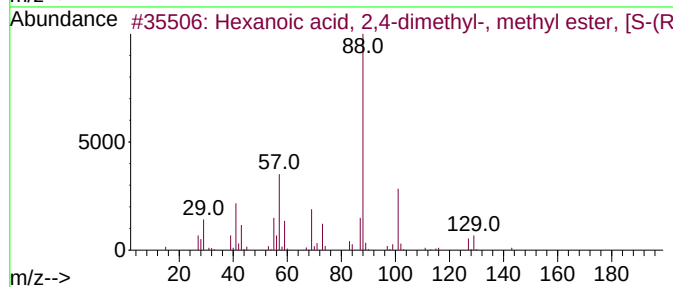
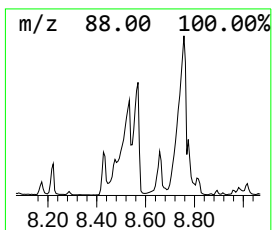
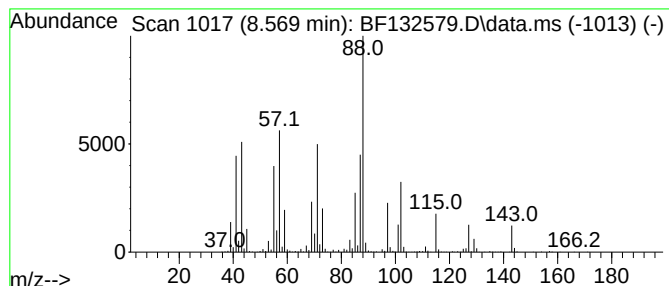
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown8.569 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.569	41.93 ng	3895270	Naphthalene-d8	8.287

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2,4-dimethyl-, me...	158	C9H18O2	014251-45-7	38
2			Propanedioic acid, dimethyl-, di...	188	C9H16O4	001619-62-1	27
3			Butanoic acid, 2,3-dimethyl-, me...	130	C7H14O2	030540-29-5	27
4			Butyric acid, 2,2,3,3-tetramethyl-	144	C8H16O2	030407-41-1	27
5			Glycine, N-(methoxycarbonyl)-, m...	147	C5H9NO4	070288-73-2	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022823\
Data File : BF132579.D
Acq On : 28 Feb 2023 18:57
Operator : CG\JU
Sample : 01701-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
B-13-GW02

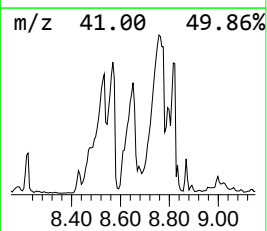
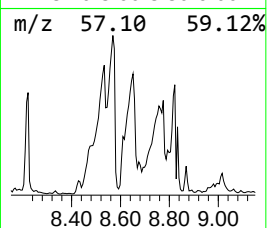
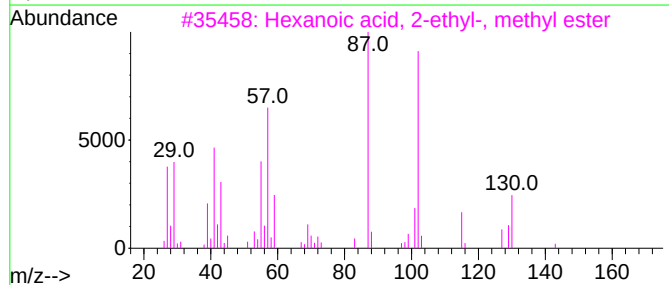
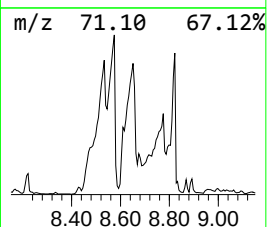
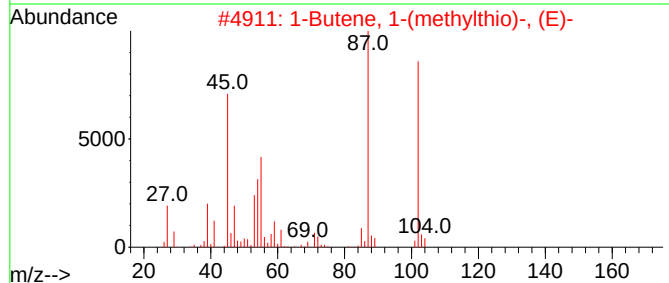
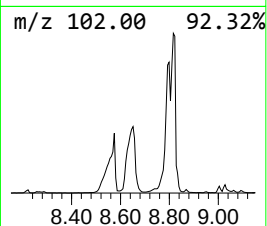
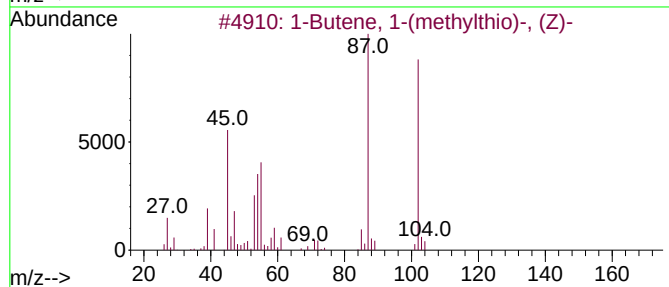
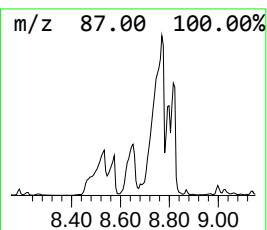
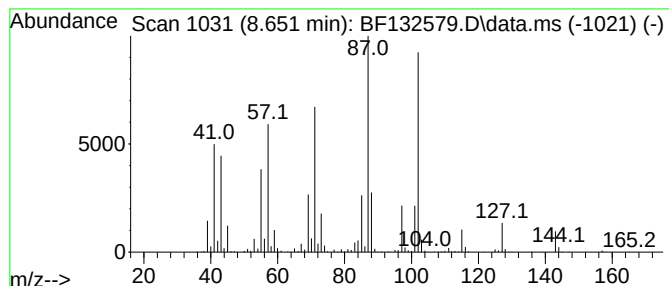
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown8.651 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.651	54.55 ng	5067250	Naphthalene-d8	8.287

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Butene, 1-(methylthio)-, (Z)-	102	C5H10S	017414-15-2	46
2		1-Butene, 1-(methylthio)-, (E)-	102	C5H10S	017414-27-6	43
3		Hexanoic acid, 2-ethyl-, methyl ...	158	C9H18O2	000816-19-3	38
4		Heptanoic acid, 2-ethyl-, methyl...	172	C10H20O2	000816-63-7	37
5		2,3-Di-O-methyl-D-xylopyranose	178	C7H14O5	018186-26-0	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022823\
Data File : BF132579.D
Acq On : 28 Feb 2023 18:57
Operator : CG\JU
Sample : 01701-04
Misc :
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ClientSampleId :
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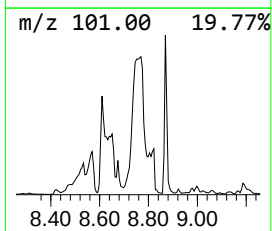
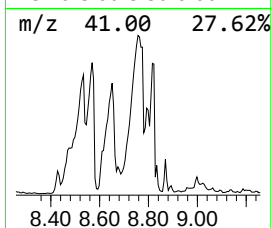
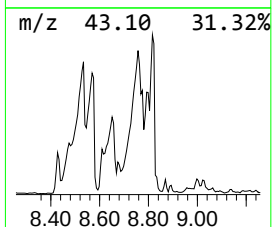
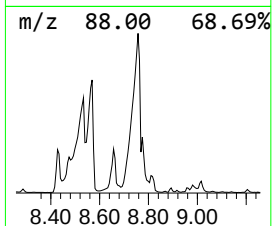
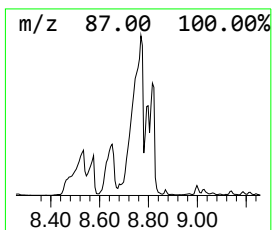
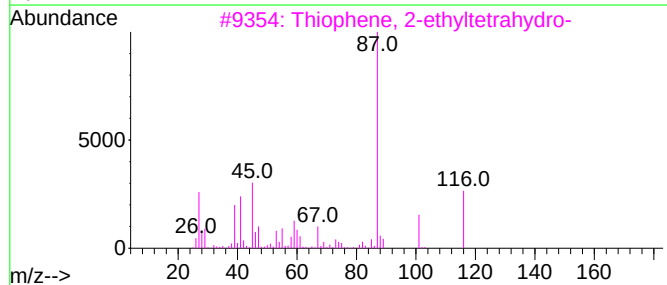
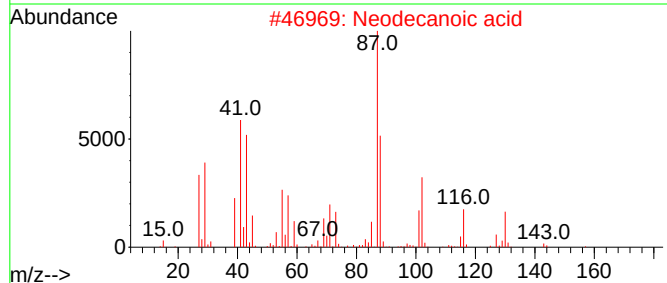
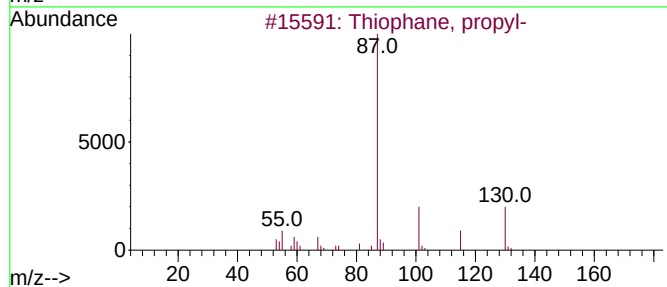
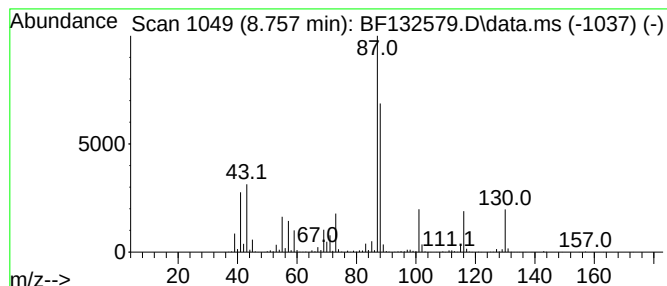
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Thiophane, propyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.757	93.05 ng	8643150	Naphthalene-d8	8.287

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophane, propyl-	130	C7H14S	001551-34-4	58
2			Neodecanoic acid	172	C10H20O2	026896-20-8	56
3			Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	47
4			Heptanoic acid, 2,4-dimethyl-, m...	172	C10H20O2	018450-78-7	35
5			Hydrazine, 1-ethyl-1-(1-methylpr...	116	C6H16N2	020325-97-7	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022823\
Data File : BF132579.D
Acq On : 28 Feb 2023 18:57
Operator : CG\JU
Sample : 01701-04
Misc :
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ClientSampleId :
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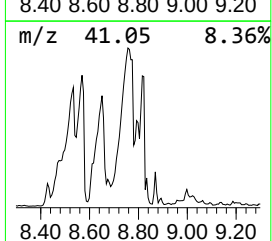
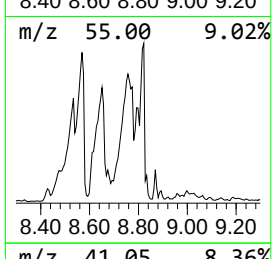
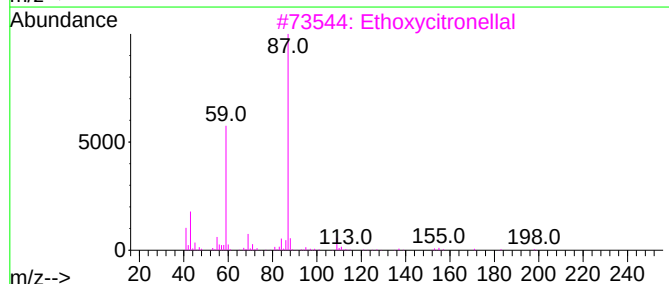
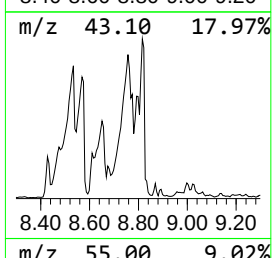
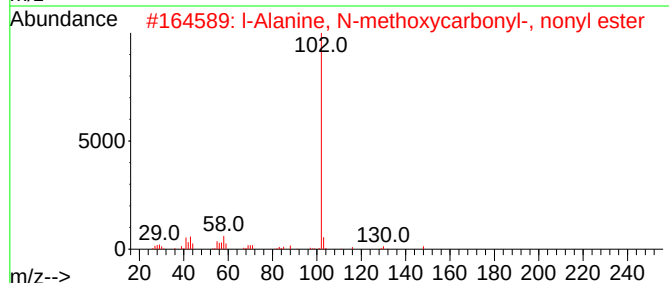
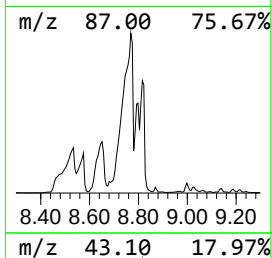
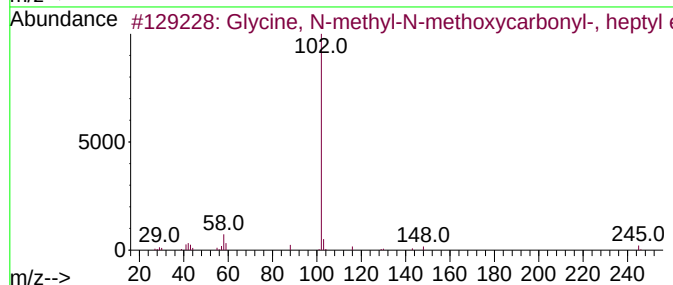
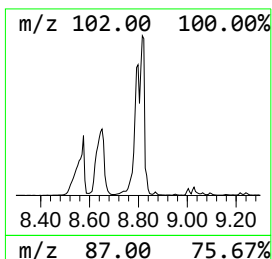
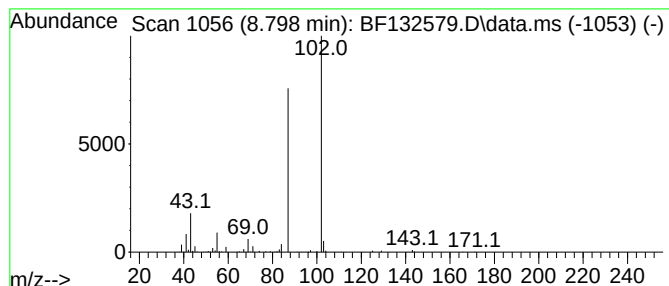
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown8.798 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.798	25.23 ng	2343310	Naphthalene-d8	8.287

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Glycine, N-methyl-N-methoxycarbo...	245	C12H23NO4	1000320-60-8	9
2			l-Alanine, N-methoxycarbonyl-, n...	273	C14H27NO4	1000313-37-8	9
3			Ethoxycitronellal	198	C12H22O2	1000132-02-6	9
4			l-Alanine, N-methoxycarbonyl-, t...	329	C18H35NO4	1010313-38-1	9
5			Aziridine-2-carbothioamide	102	C3H6N2S	1000189-98-7	7



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022823\
Data File : BF132579.D
Acq On : 28 Feb 2023 18:57
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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
B-13-GW02

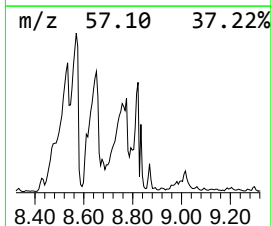
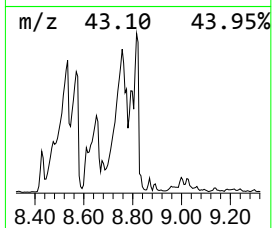
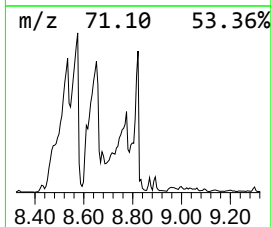
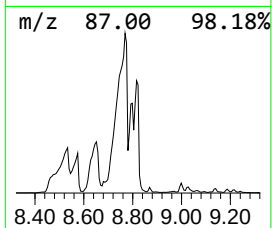
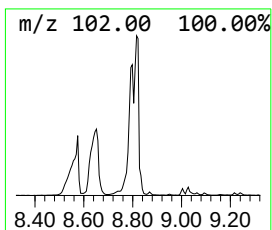
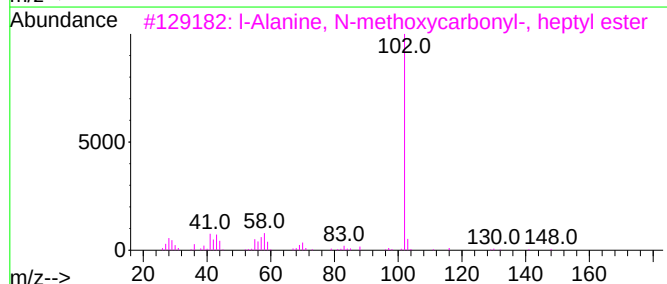
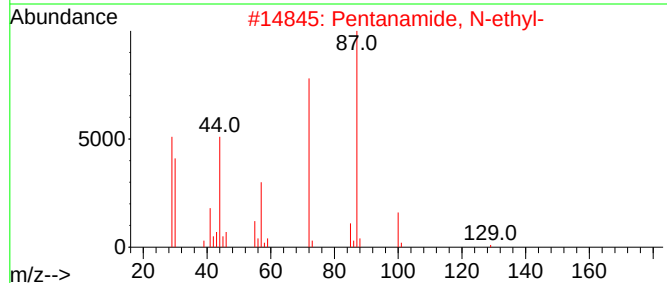
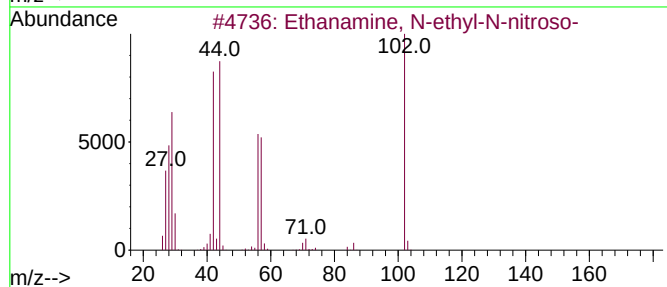
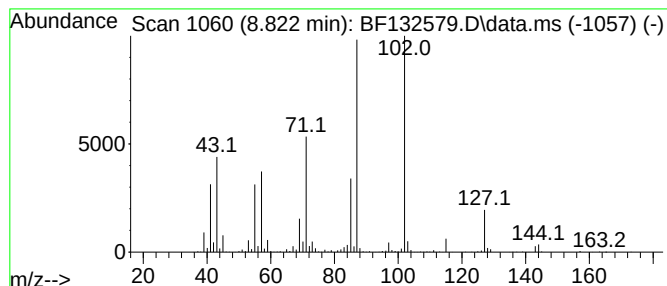
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown8.822 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.822	30.86 ng	2866280	Naphthalene-d8	8.287

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanamine, N-ethyl-N-nitroso-	102	C4H10N2O	000055-18-5	14
2		Pentanamide, N-ethyl-	129	C7H15NO	054007-33-9	14
3		L-Alanine, N-methoxycarbonyl-, h...	245	C12H23NO4	1000313-37-7	14
4		3-Pentanol, 2,3,4-trimethyl-	130	C8H18O	003054-92-0	10
5		3-Hexanol, 2,3-dimethyl-	130	C8H18O	004166-46-5	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022823\
Data File : BF132579.D
Acq On : 28 Feb 2023 18:57
Operator : CG\JU
Sample : 01701-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
B-13-GW02

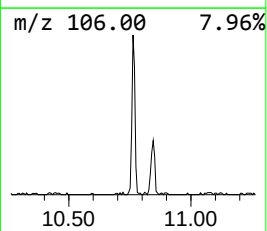
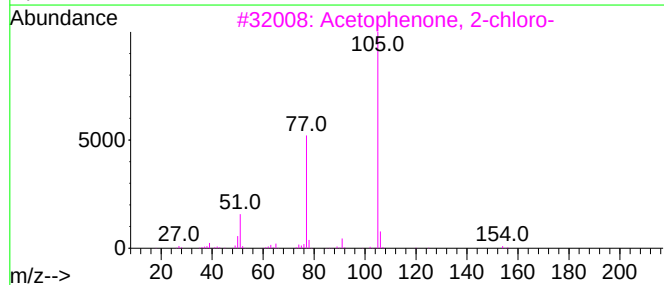
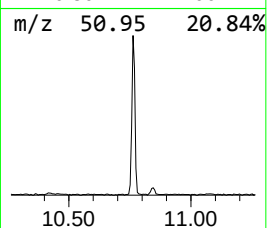
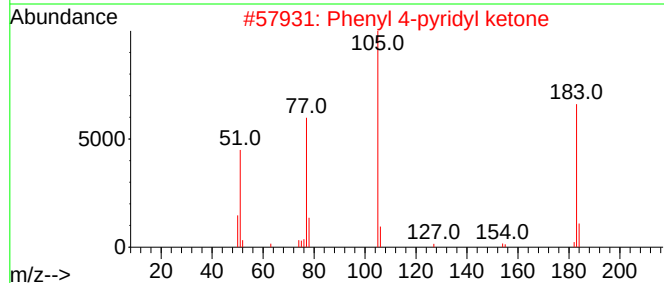
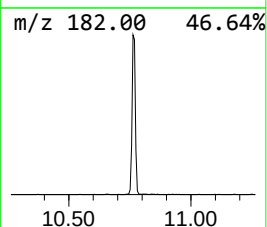
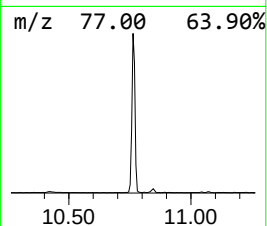
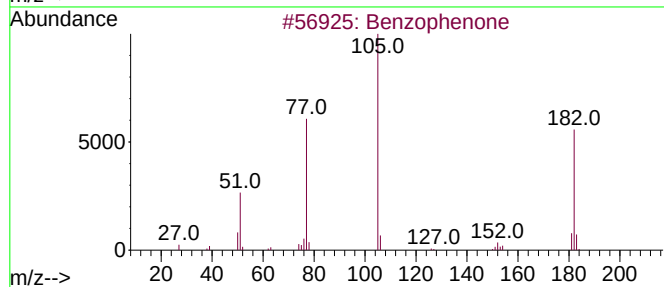
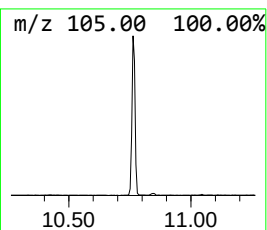
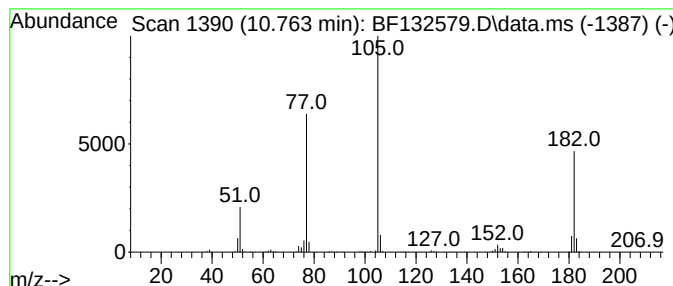
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzophenone Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.763	6.16 ng	673016	Acenaphthene-d10	10.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
5			S-Benzoyl(thiohydroxylamine)	153	C7H7NO S	025740-80-1	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022823\
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Sample : 01701-04
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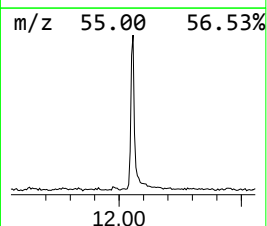
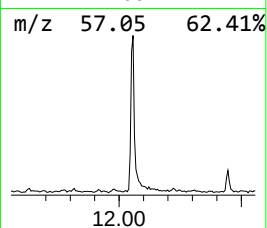
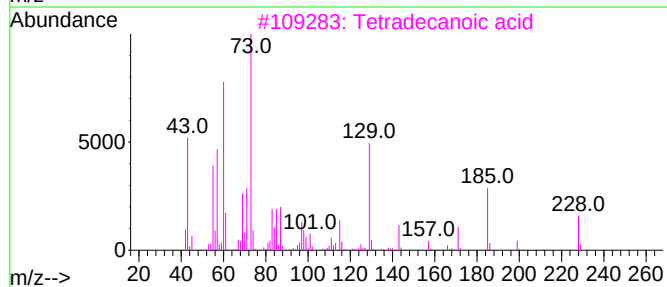
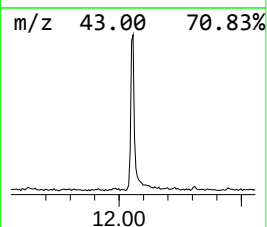
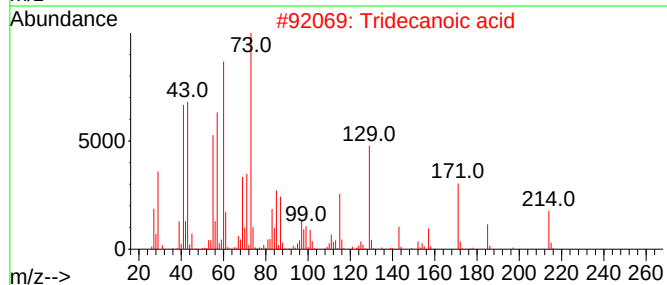
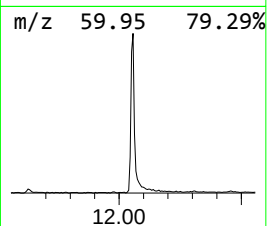
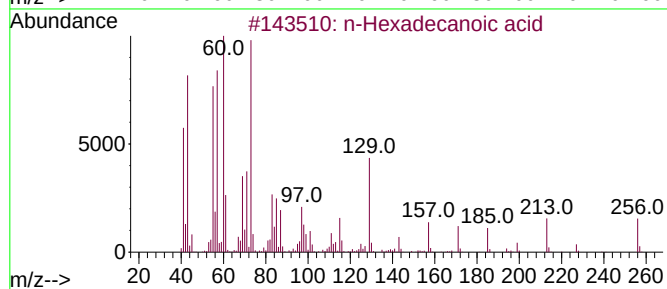
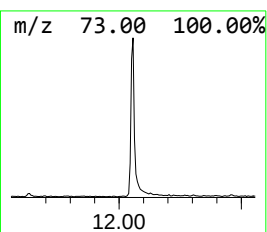
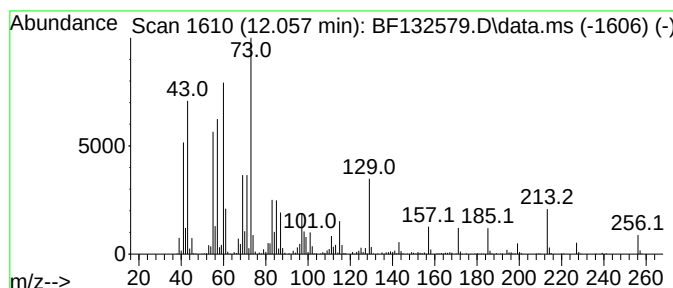
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.057	8.64 ng	1001350	Phenanthrene-d10	11.545	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022823\
Data File : BF132579.D
Acq On : 28 Feb 2023 18:57
Operator : CG\JU
Sample : 01701-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-13-GW02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,3-Dioxolane, ...	2.616	14.2	ng	1017760	1	6.998	1435150	20.0
2-Pentanone, 4-...	5.240	20.4	ng	1460700	1	6.998	1435150	20.0
Hexanoic acid, ...	7.987	668.0	ng	62048200	2	8.287	1857790	20.0
unknown8.475	8.475	14.3	ng	1324910	2	8.287	1857790	20.0
unknown8.534	8.534	56.2	ng	5221590	2	8.287	1857790	20.0
unknown8.569	8.569	41.9	ng	3895270	2	8.287	1857790	20.0
unknown8.651	8.651	54.5	ng	5067250	2	8.287	1857790	20.0
Thiophane, propyl-	8.757	93.0	ng	8643150	2	8.287	1857790	20.0
unknown8.798	8.798	25.2	ng	2343310	2	8.287	1857790	20.0
unknown8.822	8.822	30.9	ng	2866280	2	8.287	1857790	20.0
Benzophenone	10.763	6.2	ng	673016	3	10.051	2183370	20.0
n-Hexadecanoic ...	12.057	8.6	ng	1001350	4	11.545	2318570	20.0