

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
 Data File : BF125521.D
 Acq On : 16 Sep 2021 00:21
 Operator : JU/CG
 Sample : M3687-30
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A003015

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-BF091521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125521.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.204	12	20	28	rVB	1532353	2046045	48.86%	6.186%
2	4.734	448	450	452	rVB	171632	121325	2.90%	0.367%
3	5.110	510	514	522	rVB	74425	95949	2.29%	0.290%
4	5.216	523	532	541	rBV	48122	116751	2.79%	0.353%
5	5.316	543	549	554	rVB2	27474	47845	1.14%	0.145%
6	5.498	575	580	583	rBV	3563620	3572291	85.31%	10.800%
7	5.716	599	617	621	rBV2	119443	449868	10.74%	1.360%
8	6.263	707	710	715	rBV4	25397	52173	1.25%	0.158%
9	6.504	746	751	754	rBV	3307860	3735607	89.21%	11.294%
10	6.587	758	765	769	rVB	271544	571366	13.65%	1.727%
11	6.863	809	812	816	rBV	1166855	1053031	25.15%	3.184%
12	7.275	876	882	899	rBV7	23004	73550	1.76%	0.222%
13	7.434	903	909	912	rBV	2473204	2518292	60.14%	7.613%
14	7.581	925	934	947	rBV	422235	855980	20.44%	2.588%
15	7.922	986	992	1002	rBV	374096	554574	13.24%	1.677%
16	8.057	1012	1015	1026	rBV	358798	646933	15.45%	1.956%
17	8.151	1026	1031	1034	rVB	1442307	1380599	32.97%	4.174%
18	8.528	1088	1095	1113	rBV	589487	939937	22.45%	2.842%
19	9.081	1185	1189	1198	rBV	435598	513927	12.27%	1.554%
20	9.157	1200	1202	1208	rVB	49968	66990	1.60%	0.203%
21	9.228	1208	1214	1217	rBV	4562920	4187250	100.00%	12.659%
22	9.610	1276	1279	1293	rBV	75422	174743	4.17%	0.528%
23	9.904	1323	1329	1333	rBV	1660395	1467653	35.05%	4.437%
24	10.698	1460	1464	1474	rBV	1551846	1482469	35.40%	4.482%
25	11.392	1579	1582	1586	rBV	1404313	1283345	30.65%	3.880%
26	11.780	1645	1648	1651	rBV	42460	44737	1.07%	0.135%
27	11.922	1668	1672	1680	rBV5	141799	253056	6.04%	0.765%
28	12.710	1803	1806	1811	rBV6	78151	110596	2.64%	0.334%
29	12.980	1848	1852	1855	rBV	3306211	2960478	70.70%	8.950%
30	13.904	2007	2009	2011	rVB	63475	44949	1.07%	0.136%
31	14.039	2029	2032	2036	rVB	947583	813508	19.43%	2.459%
32	15.527	2280	2285	2294	rVB2	661186	841603	20.10%	2.544%

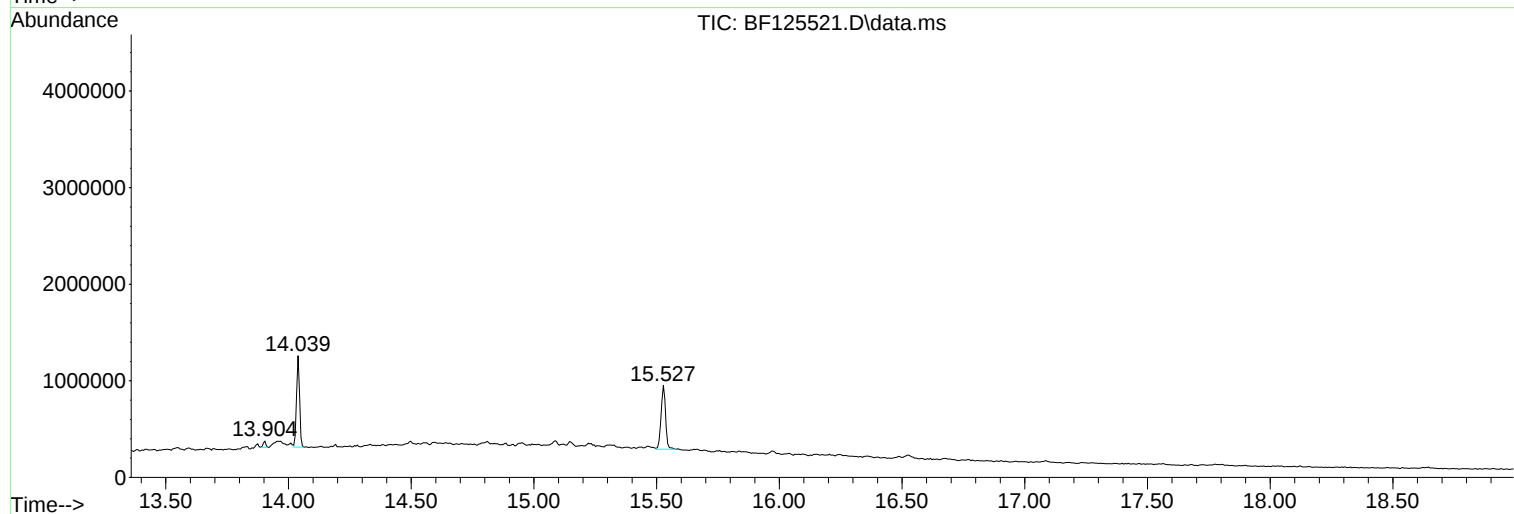
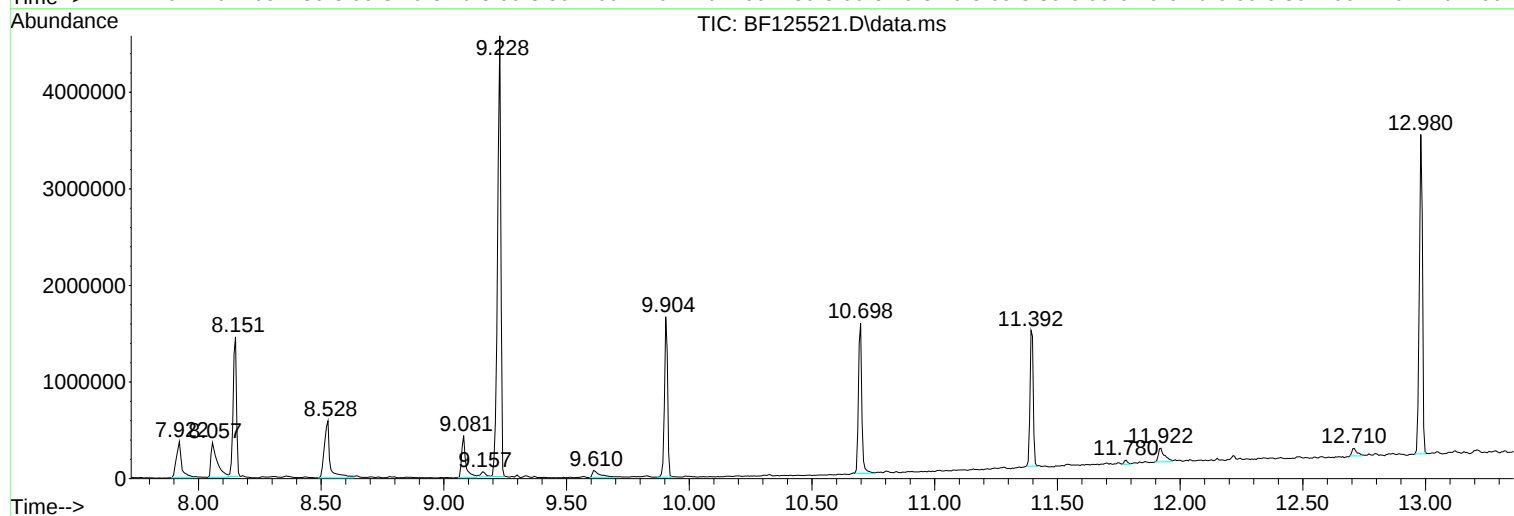
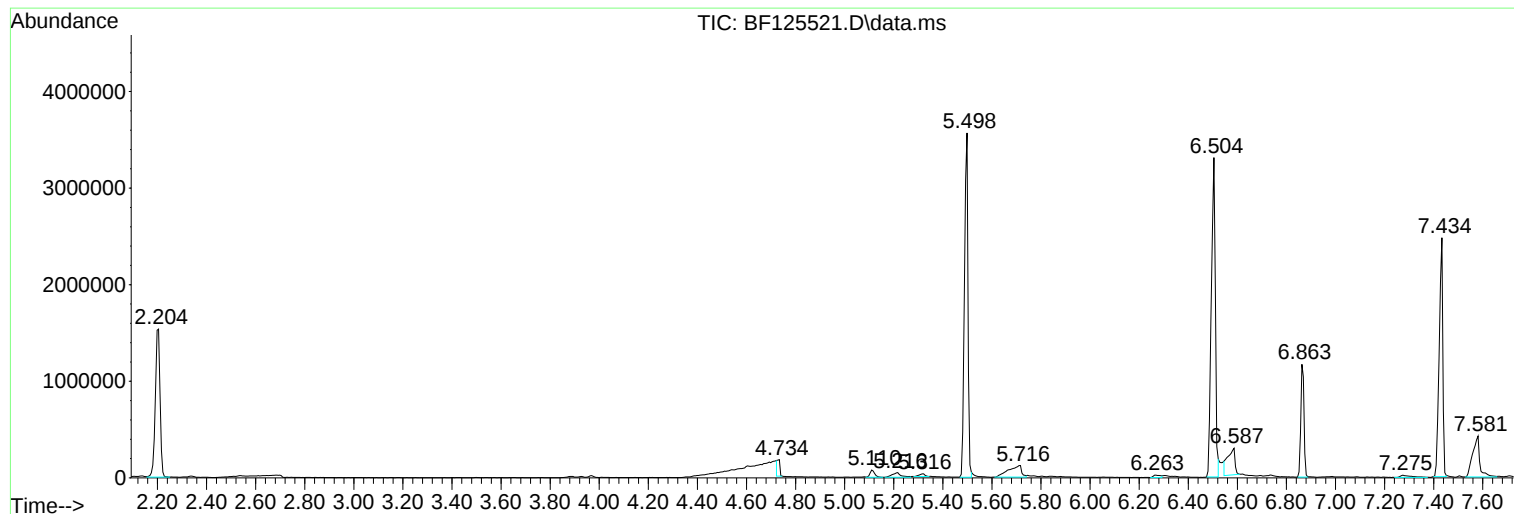
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ClientSampleId :
A003015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.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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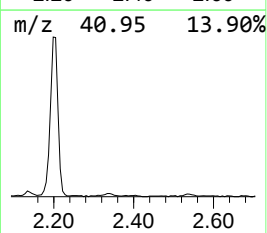
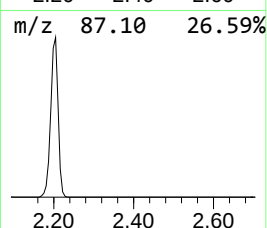
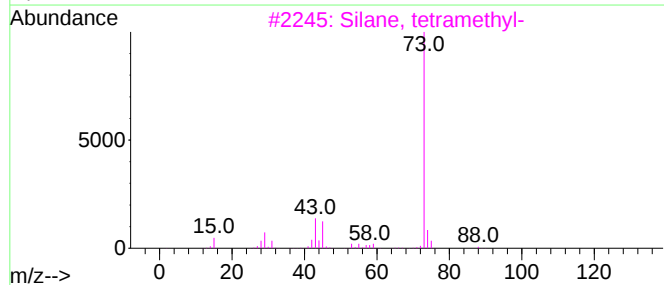
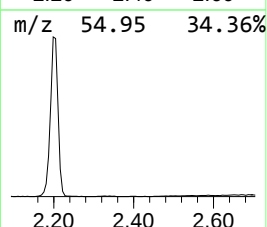
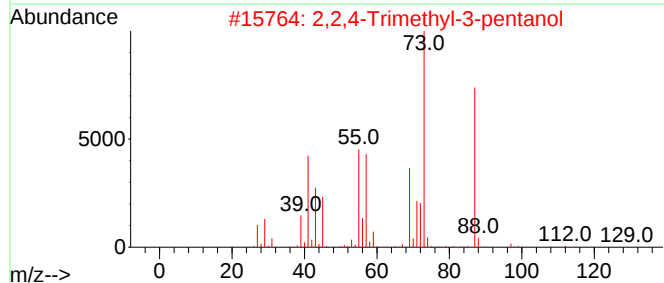
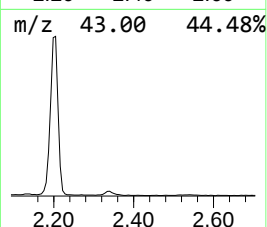
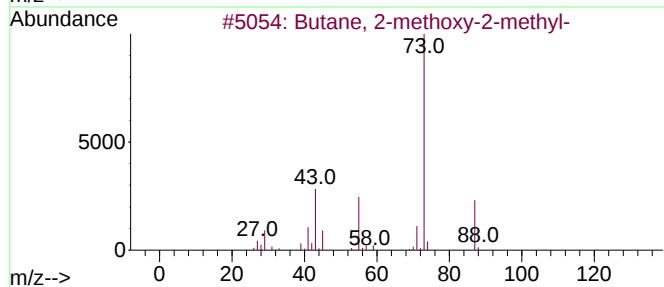
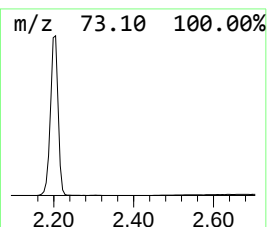
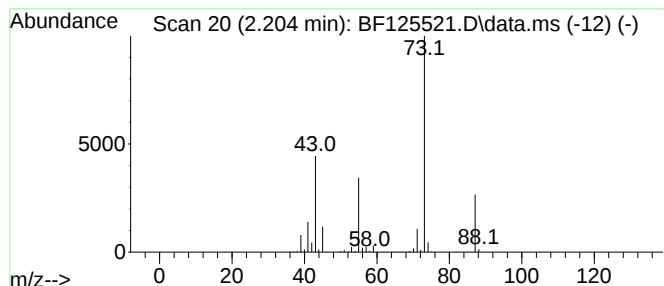
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.204	38.86 ng	2046050	1,4-Dichlorobenzene-d4	6.863

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	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	28
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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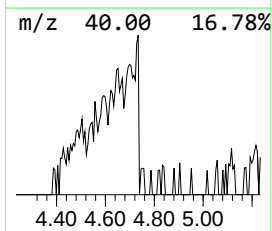
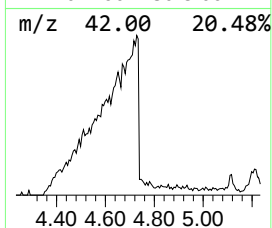
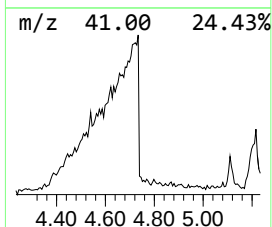
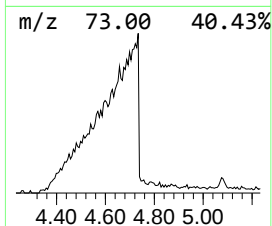
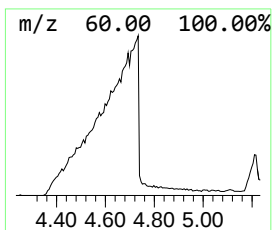
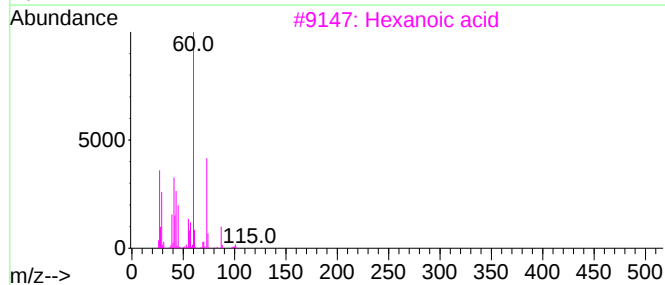
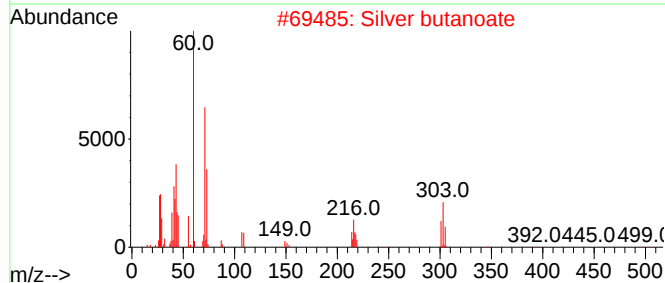
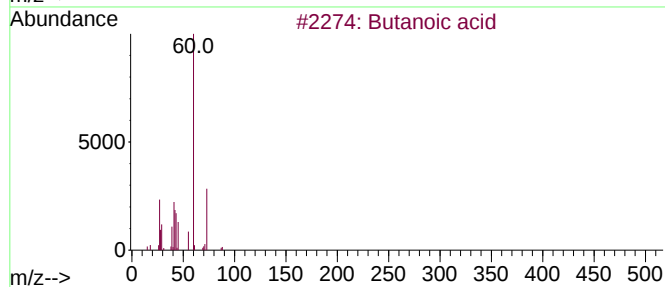
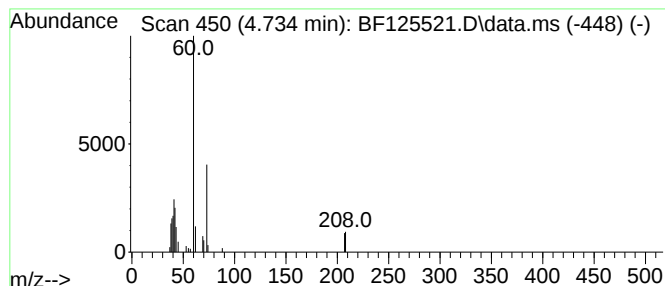
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown4.734 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.734	2.30 ng	121325	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid	88	C4H8O2	000107-92-6	47
2			Silver butanoate	194	C4H7AgO2	005076-24-4	28
3			Hexanoic acid	116	C6H12O2	000142-62-1	9
4			Pentanoic acid	102	C5H10O2	000109-52-4	9
5			1,6-Anhydro-.beta.-d-talopyranose	162	C6H10O5	1000133-05-8	9



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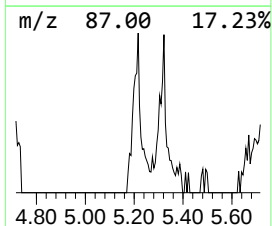
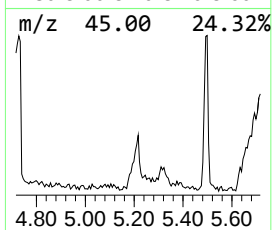
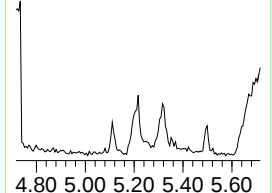
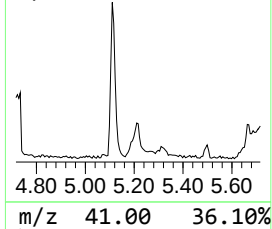
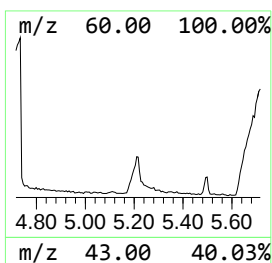
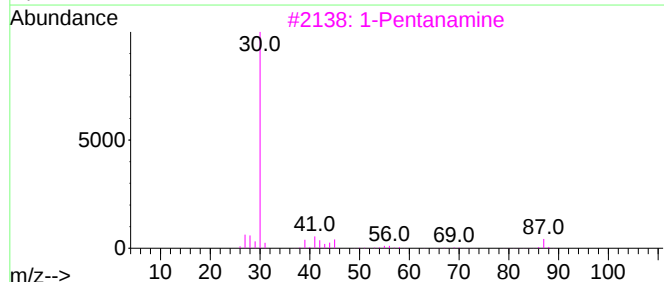
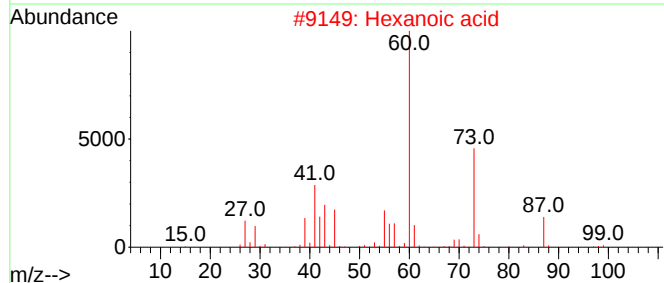
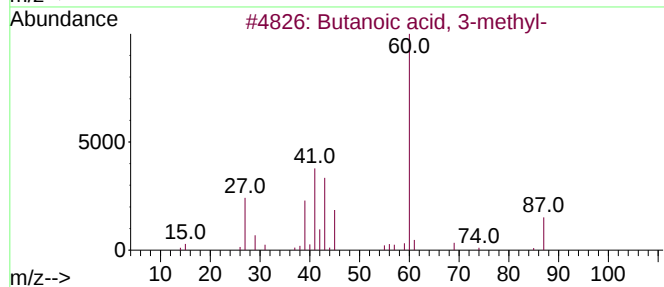
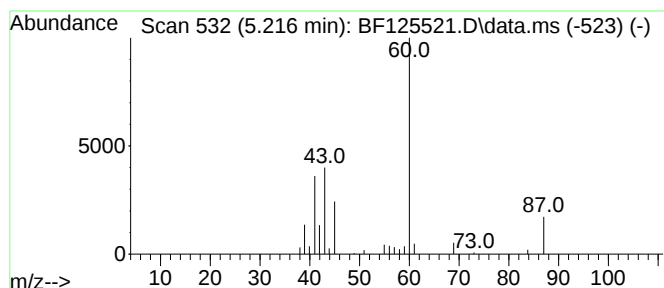
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Butanoic acid, 3-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.216	2.22 ng	116751	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	83
2			Hexanoic acid	116	C6H12O2	000142-62-1	40
3			1-Pentanamine	87	C5H13N	000110-58-7	9
4			Pentanoic acid	102	C5H10O2	000109-52-4	9
5			Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	9



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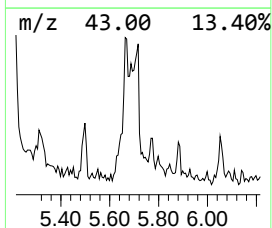
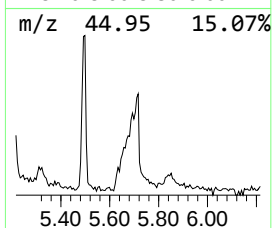
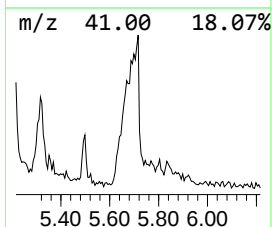
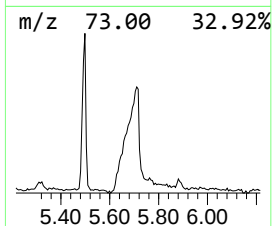
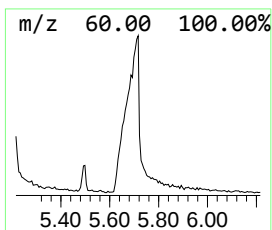
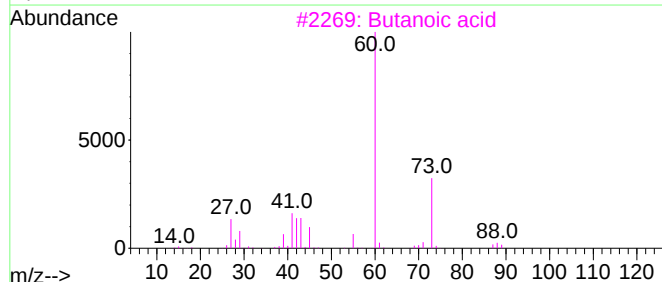
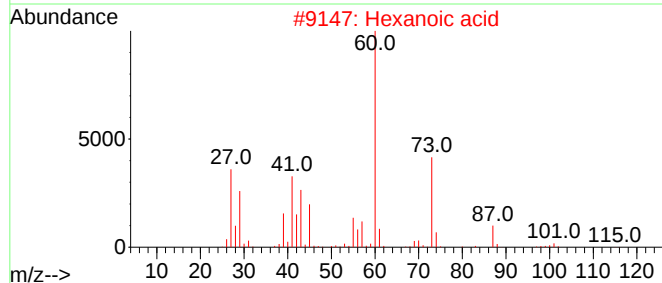
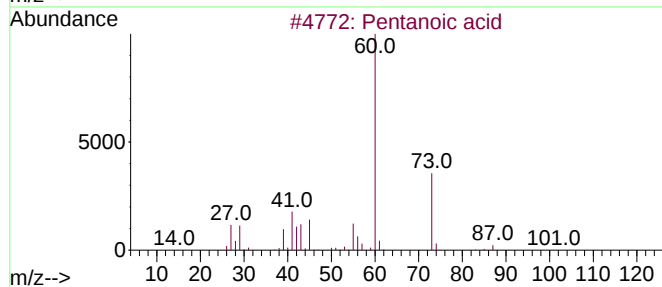
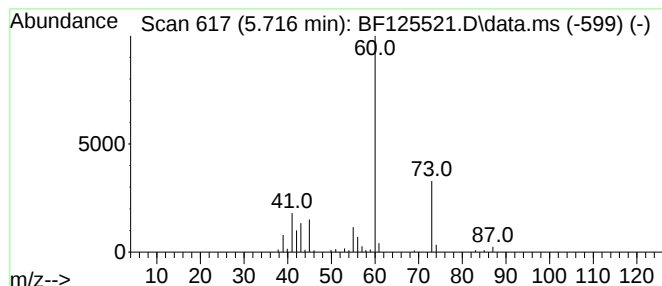
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Peak Number 4 Pentanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.716	8.54 ng	449868	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanoic acid	102	C5H10O2	000109-52-4	90
2			Hexanoic acid	116	C6H12O2	000142-62-1	78
3			Butanoic acid	88	C4H8O2	000107-92-6	78
4			Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	53
5			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	38



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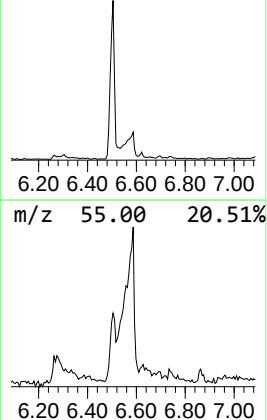
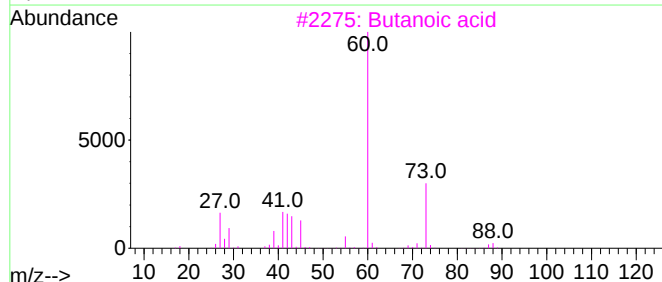
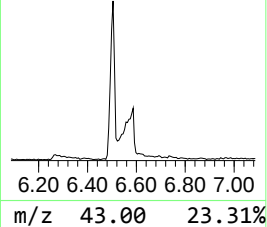
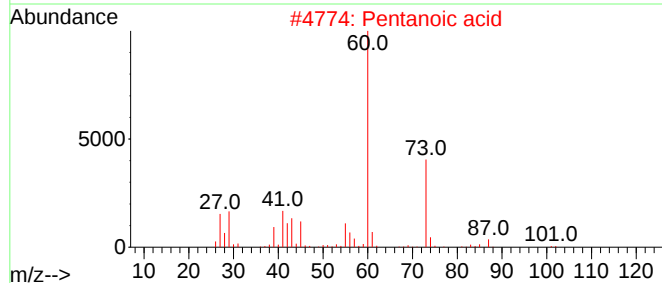
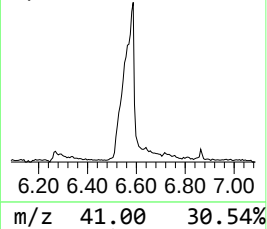
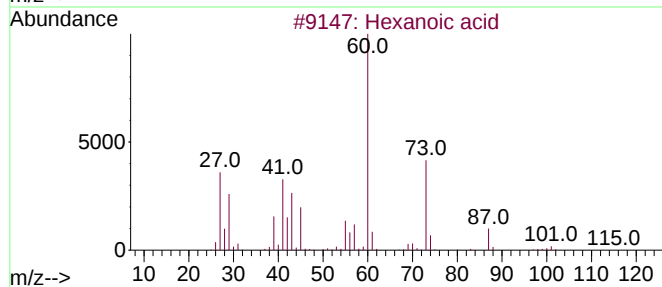
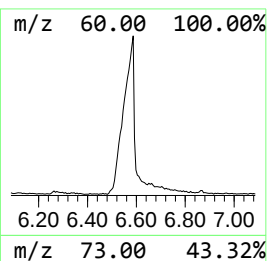
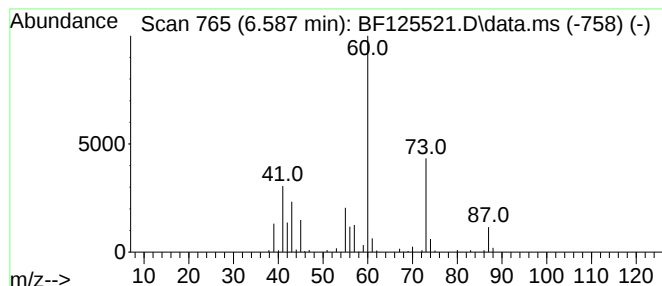
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Hexanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.587	10.85 ng	571366	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid	116	C6H12O2	000142-62-1	83
2			Pentanoic acid	102	C5H10O2	000109-52-4	78
3			Butanoic acid	88	C4H8O2	000107-92-6	72
4			Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	64
5			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	59



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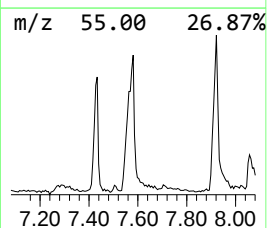
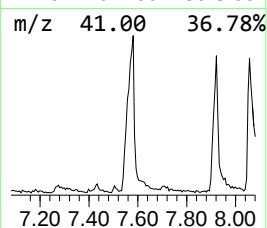
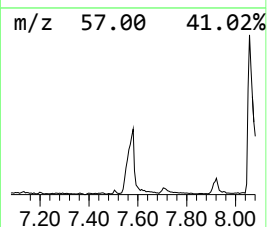
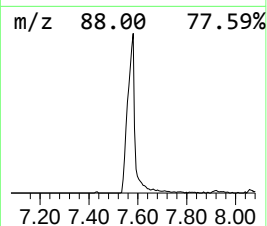
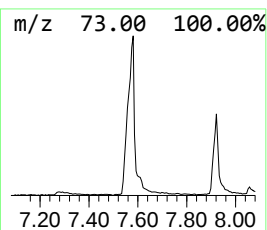
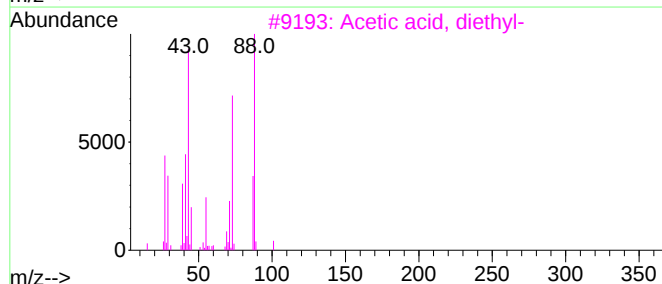
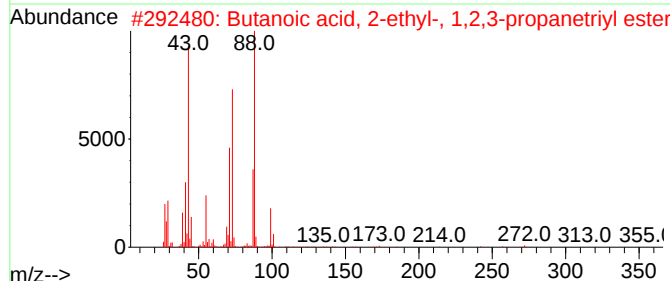
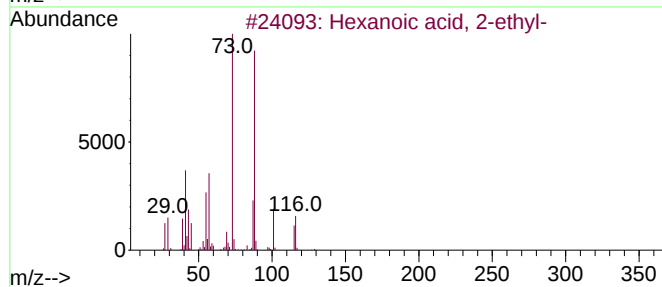
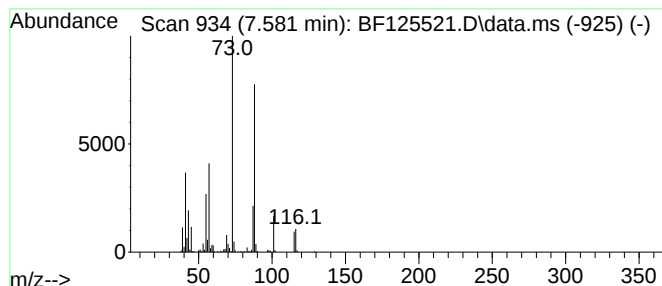
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexanoic acid, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.581	12.40 ng	855980	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2			Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	59
3			Acetic acid, diethyl-	116	C6H12O2	000088-09-5	53
4			2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	50
5			1,4-Dioxane	88	C4H8O2	000123-91-1	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125521.D
Acq On : 16 Sep 2021 00:21
Operator : JU/CG
Sample : M3687-30
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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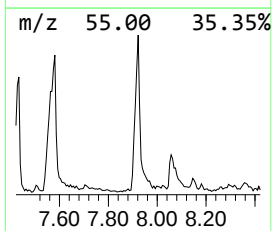
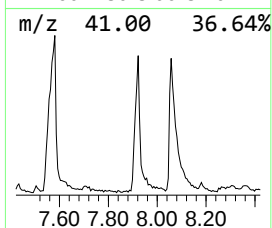
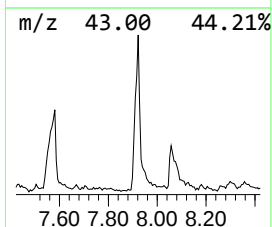
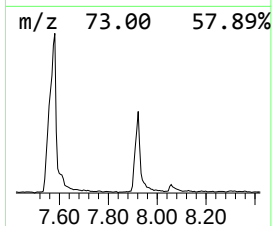
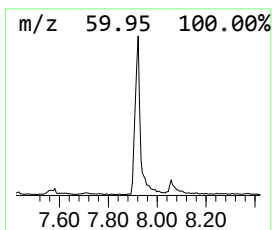
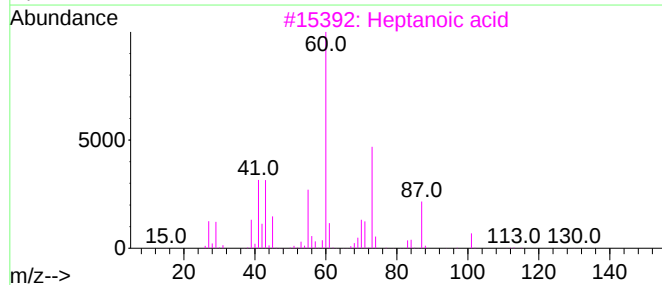
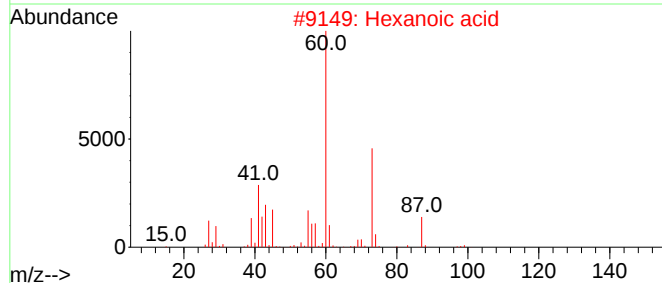
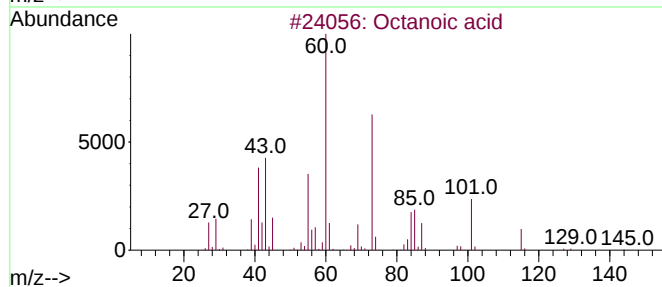
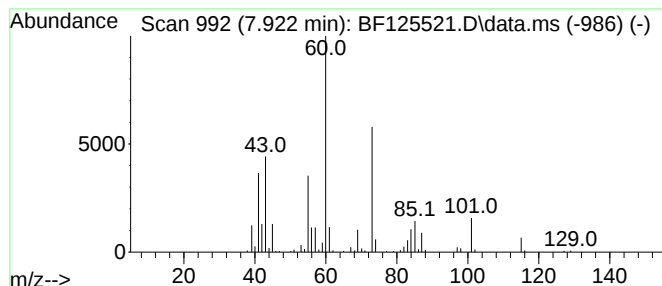
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.922	8.03 ng	554574	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octanoic acid	144	C8H16O2	000124-07-2	90
2			Hexanoic acid	116	C6H12O2	000142-62-1	64
3			Heptanoic acid	130	C7H14O2	000111-14-8	53
4			Pentanoic acid	102	C5H10O2	000109-52-4	53
5			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125521.D
Acq On : 16 Sep 2021 00:21
Operator : JU/CG
Sample : M3687-30
Misc :
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Instrument :
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ClientSampleId :
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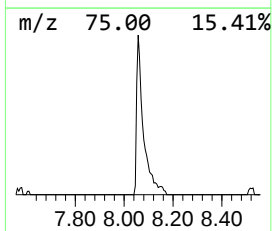
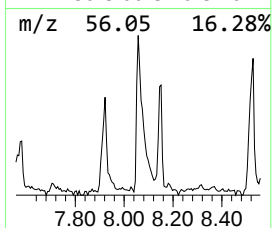
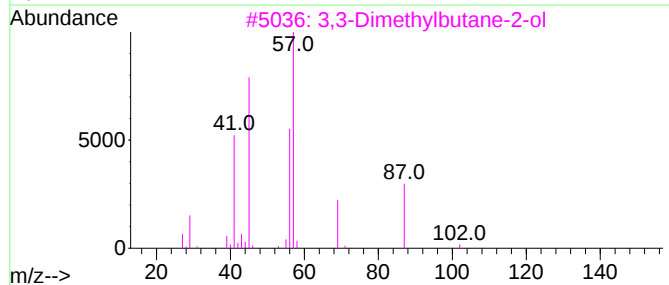
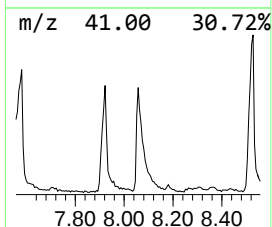
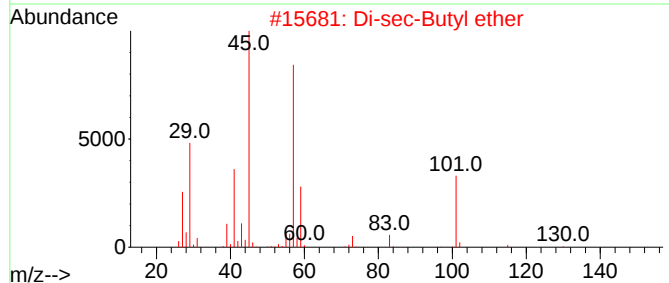
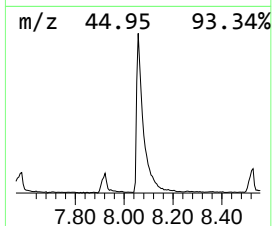
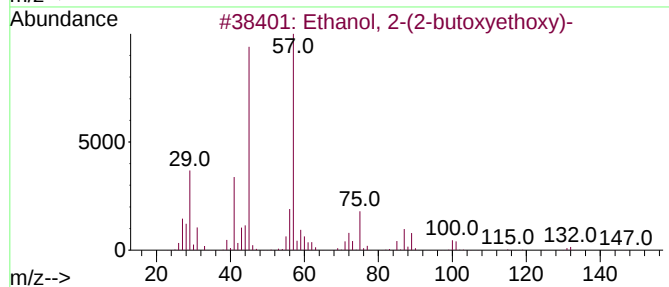
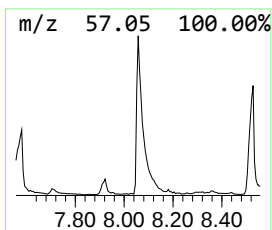
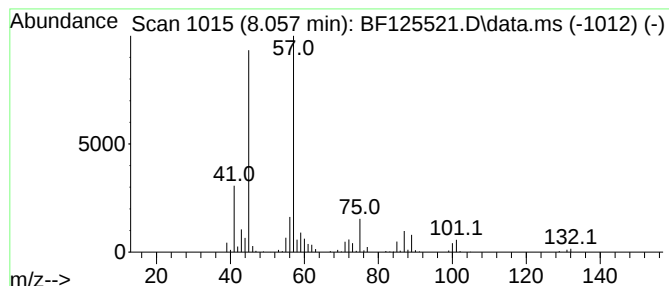
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.057	9.37 ng	646933	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
3			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
5			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125521.D
Acq On : 16 Sep 2021 00:21
Operator : JU/CG
Sample : M3687-30
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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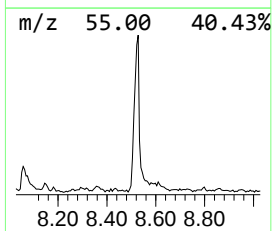
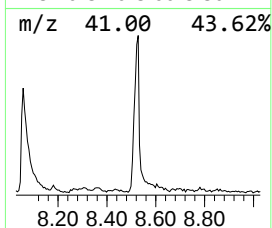
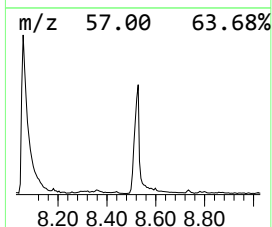
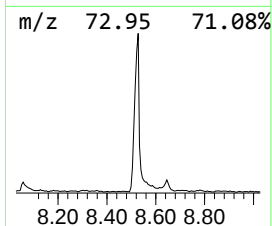
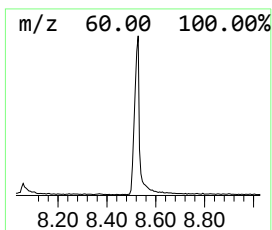
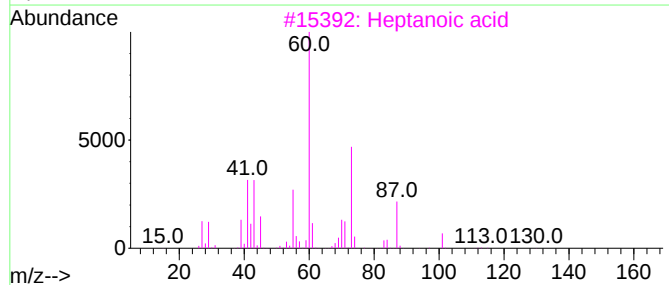
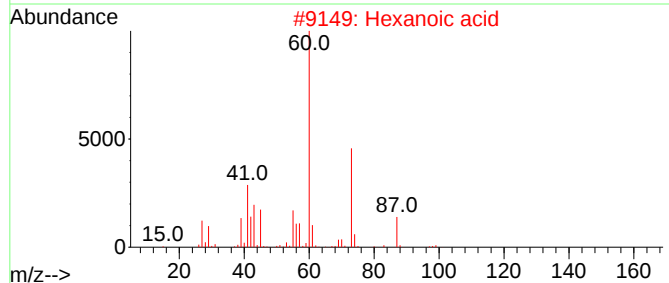
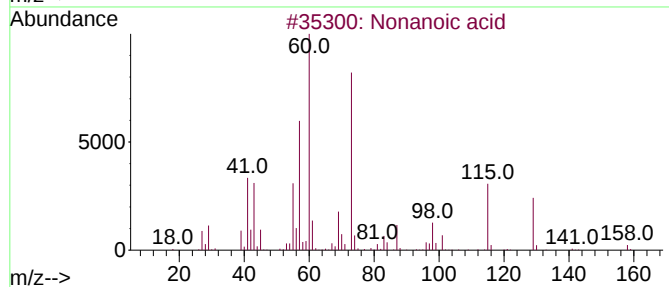
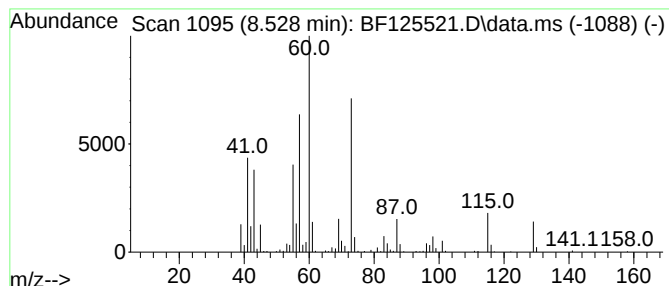
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.528	13.62 ng	939937	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanoic acid	158	C9H18O2	000112-05-0	83
2			Hexanoic acid	116	C6H12O2	000142-62-1	64
3			Heptanoic acid	130	C7H14O2	000111-14-8	64
4			Butanoic acid	88	C4H8O2	000107-92-6	58
5			Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125521.D
Acq On : 16 Sep 2021 00:21
Operator : JU/CG
Sample : M3687-30
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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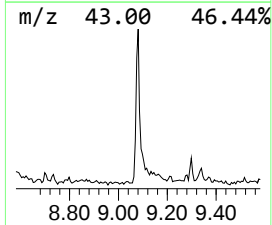
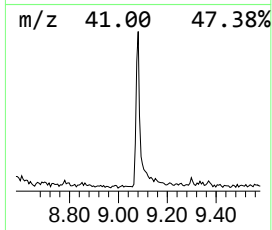
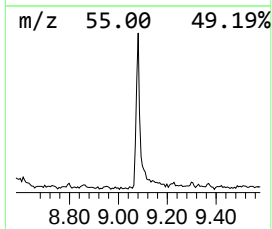
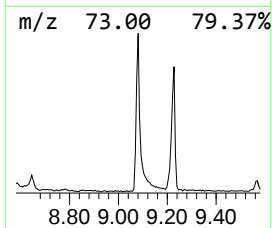
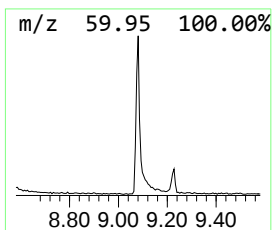
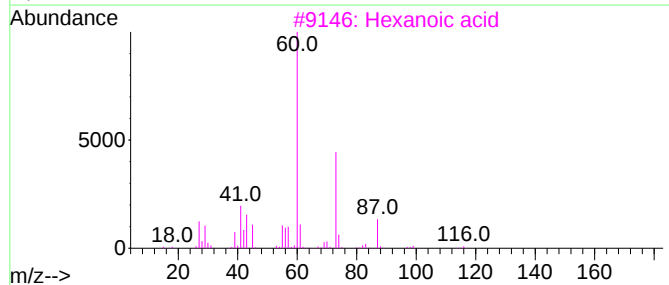
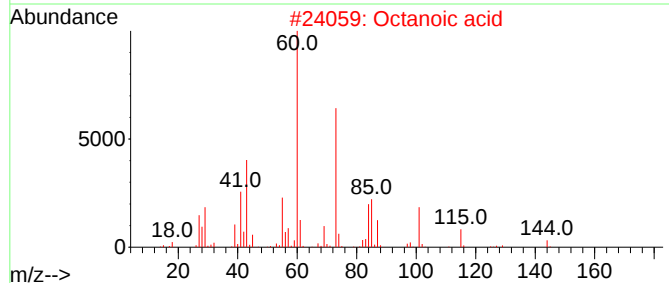
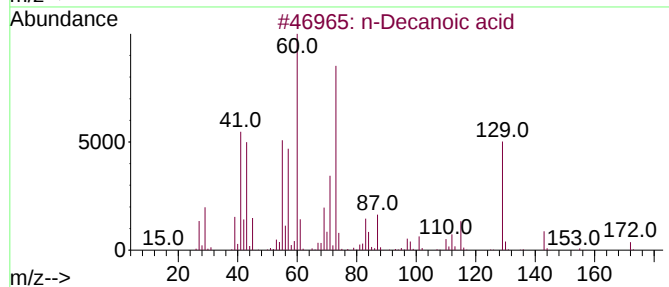
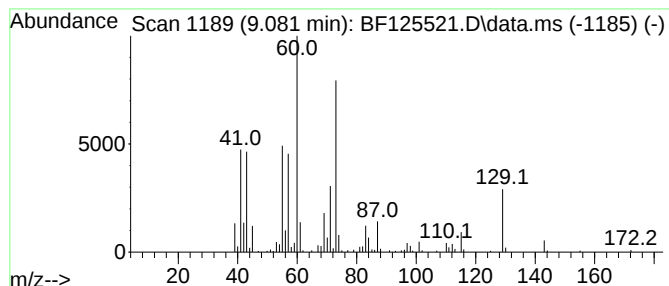
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 n-Decanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.081	7.00 ng	513927	Acenaphthene-d10	9.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Decanoic acid	172	C10H20O2	000334-48-5	97
2			Octanoic acid	144	C8H16O2	000124-07-2	53
3			Hexanoic acid	116	C6H12O2	000142-62-1	49
4			Pentanoic acid	102	C5H10O2	000109-52-4	46
5			Nonanoic acid	158	C9H18O2	000112-05-0	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125521.D
Acq On : 16 Sep 2021 00:21
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Sample : M3687-30
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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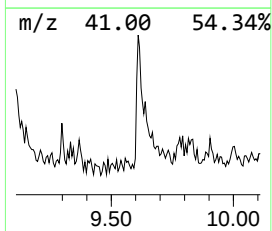
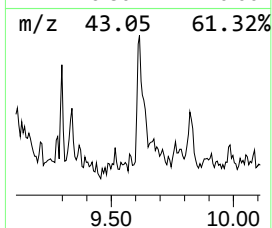
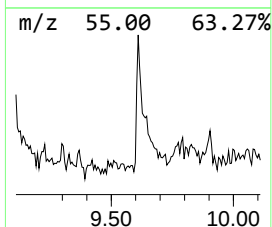
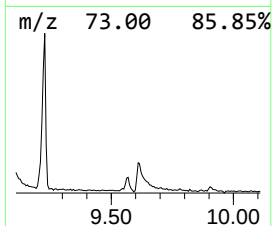
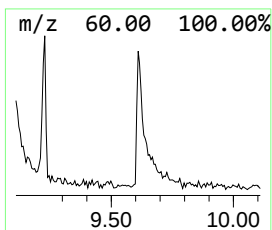
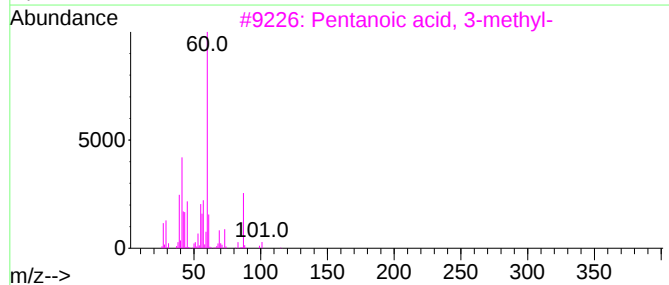
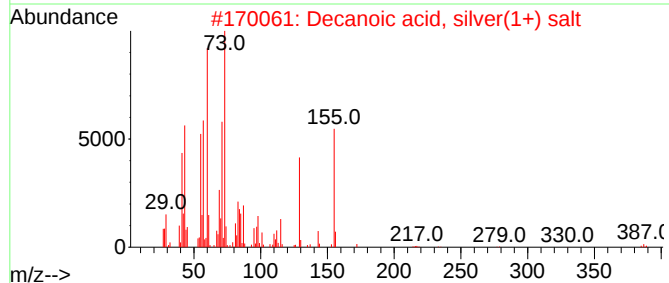
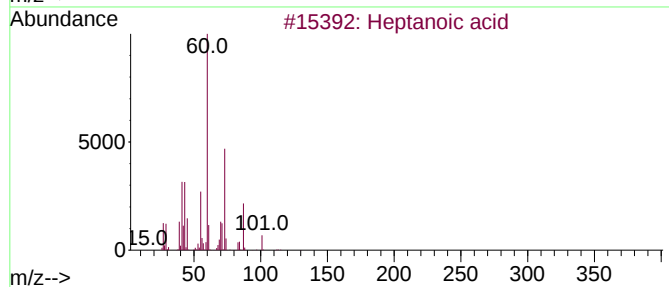
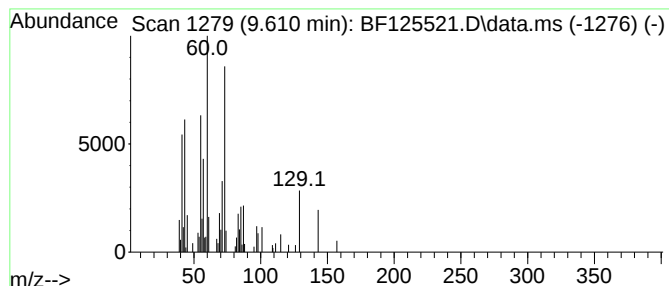
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown9.610 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.610	2.38 ng	174743	Acenaphthene-d10	9.904

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptanoic acid	130	C7H14O2	000111-14-8	47
2		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	43
3		Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	35
4		4-Bromobutyric acid	166	C4H7BrO2	002623-87-2	35
5		D-Allose	180	C6H12O6	002595-97-3	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
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Sample : M3687-30
Misc :
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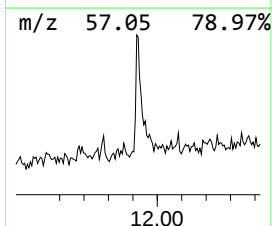
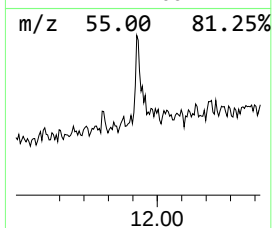
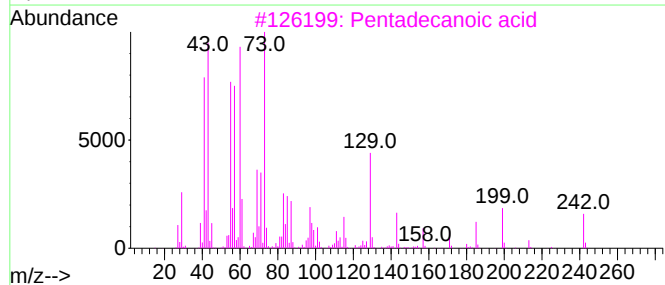
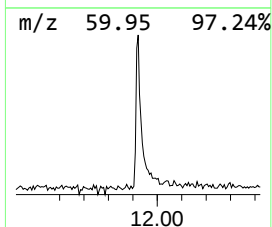
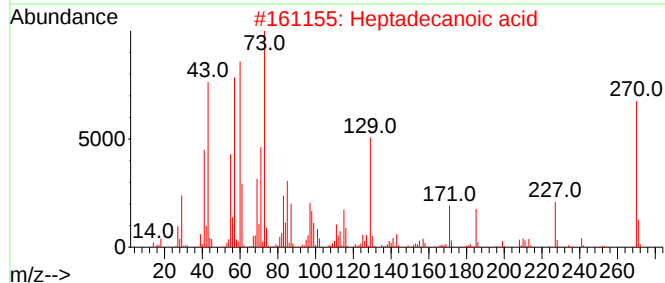
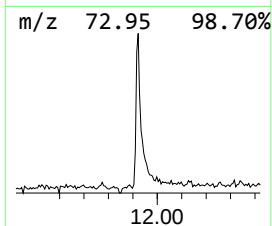
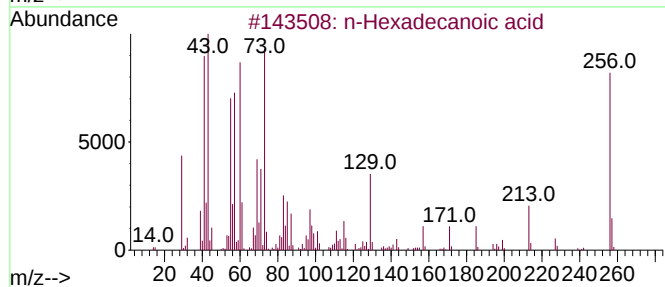
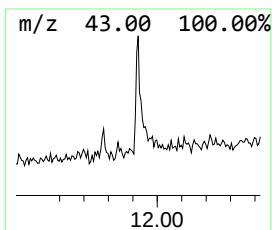
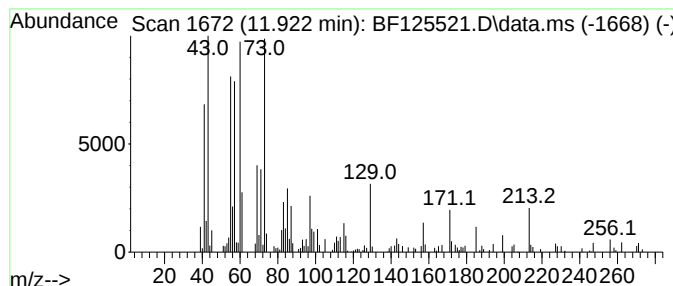
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.922	3.94 ng	253056	Phenanthrene-d10		11.392	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	97
2	Heptadecanoic acid		270	C17H34O2	000506-12-7	95
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	70
5	n-Decanoic acid		172	C10H20O2	000334-48-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125521.D
Acq On : 16 Sep 2021 00:21
Operator : JU/CG
Sample : M3687-30
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A003015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.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
Butane, 2-metho...	2.204	38.9	ng	2046050	1	6.863	1053030	20.0
unknown4.734	4.734	2.3	ng	121325	1	6.863	1053030	20.0
Butanoic acid, ...	5.216	2.2	ng	116751	1	6.863	1053030	20.0
Pentanoic acid	5.716	8.5	ng	449868	1	6.863	1053030	20.0
Hexanoic acid	6.587	10.9	ng	571366	1	6.863	1053030	20.0
Hexanoic acid, ...	7.581	12.4	ng	855980	2	8.151	1380600	20.0
Octanoic acid	7.922	8.0	ng	554574	2	8.151	1380600	20.0
Ethanol, 2-(2-b...	8.057	9.4	ng	646933	2	8.151	1380600	20.0
Nonanoic acid	8.528	13.6	ng	939937	2	8.151	1380600	20.0
n-Decanoic acid	9.081	7.0	ng	513927	3	9.904	1467650	20.0
unknown9.610	9.610	2.4	ng	174743	3	9.904	1467650	20.0
n-Hexadecanoic ...	11.922	3.9	ng	253056	4	11.392	1283350	20.0