

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022823\
 Data File : BF132578.D
 Acq On : 28 Feb 2023 18:25
 Operator : CG\JU
 Sample : 01701-03
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-13-GW01

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: BF132578.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.240	447	451	459	rVB	1520837	1848517	3.34%	1.432%
2	5.634	511	518	521	rBV	3881783	3716653	6.71%	2.879%
3	6.622	682	686	691	rBV	3013927	2806673	5.07%	2.174%
4	6.998	747	750	757	rBV	1504677	1453801	2.63%	1.126%
5	7.569	841	847	850	rBV	4261205	4732273	8.55%	3.666%
6	7.969	854	915	918	rBV	5568372	55361394	100.00%	42.889%
7	8.210	952	956	961	rVB2	589867	572164	1.03%	0.443%
8	8.287	966	969	972	rBV	2135352	1755707	3.17%	1.360%
9	8.469	994	1000	1001	rVV	695794	1070459	1.93%	0.829%
10	8.522	1001	1009	1011	rVV	1843894	4235254	7.65%	3.281%
11	8.563	1011	1016	1019	rVV2	2109996	3698000	6.68%	2.865%
12	8.645	1020	1030	1033	rVV3	1785097	4143271	7.48%	3.210%
13	8.751	1036	1048	1052	rVV3	2574460	8433755	15.23%	6.534%
14	8.787	1052	1054	1055	rVV	1708388	1551062	2.80%	1.202%
15	8.810	1055	1058	1060	rVV	2460303	2653669	4.79%	2.056%
16	8.998	1087	1090	1093	rBV2	675446	568074	1.03%	0.440%
17	9.369	1148	1153	1156	rVB	8330155	7803349	14.10%	6.045%
18	10.051	1265	1269	1272	rBV	2411982	2008919	3.63%	1.556%
19	10.851	1399	1405	1408	rBV	5109288	5595633	10.11%	4.335%
20	11.545	1519	1523	1525	rBV	2578907	2201326	3.98%	1.705%
21	12.057	1606	1610	1614	rBV	574174	589677	1.07%	0.457%
22	13.139	1789	1794	1797	rBV	8350372	9203995	16.63%	7.130%
23	14.198	1970	1974	1977	rVV	1902027	1825083	3.30%	1.414%
24	15.751	2232	2238	2245	rBV2	918305	1252898	2.26%	0.971%

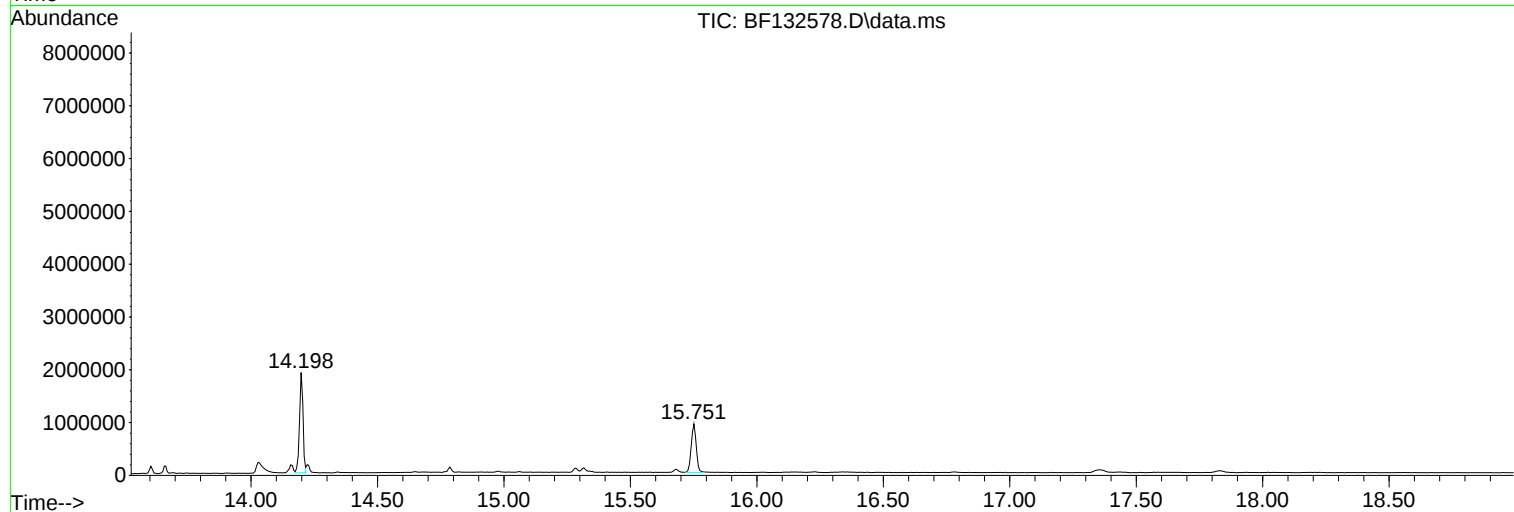
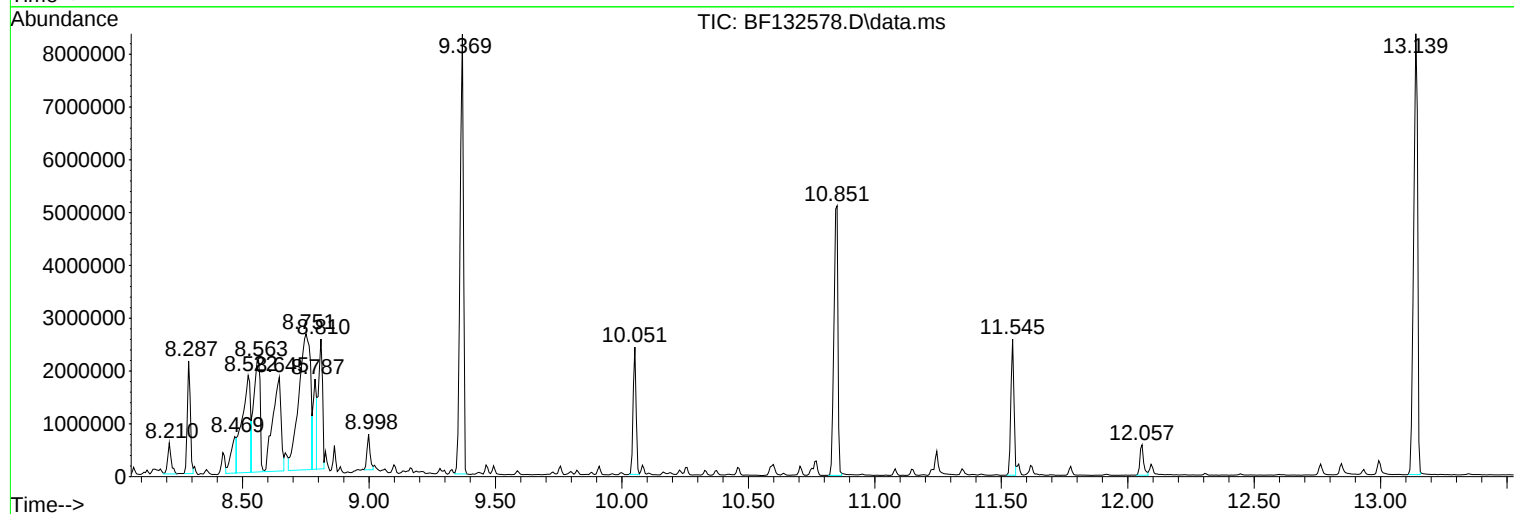
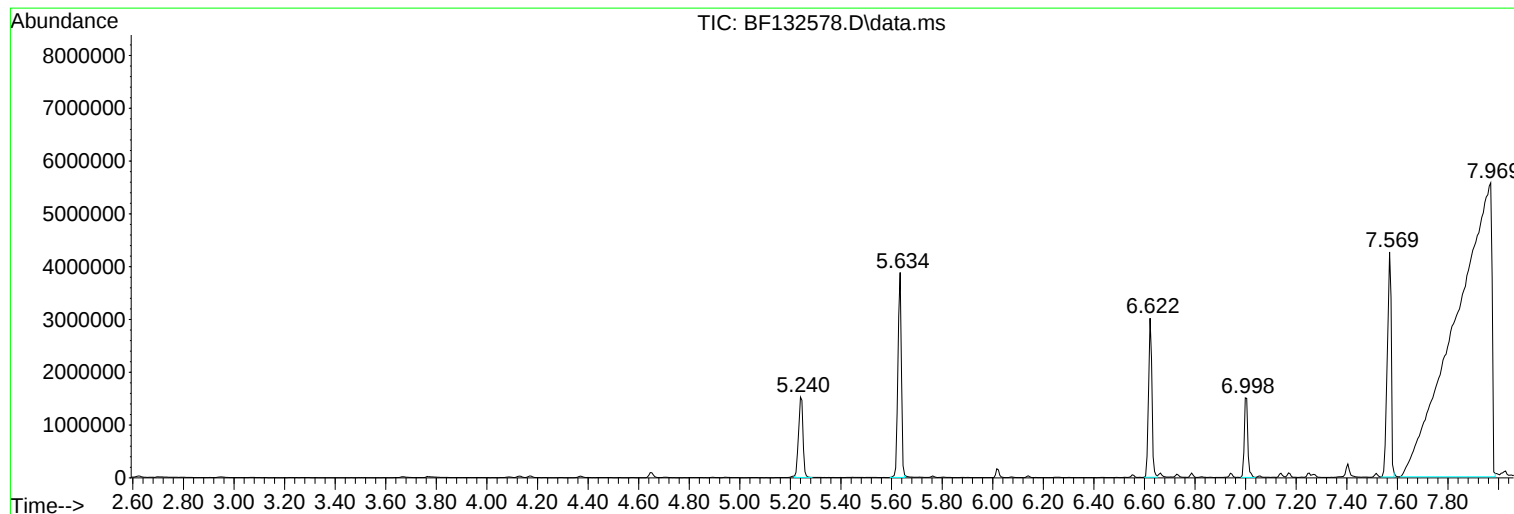
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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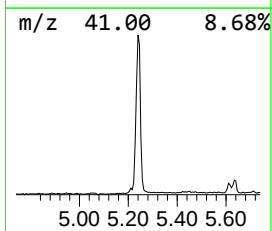
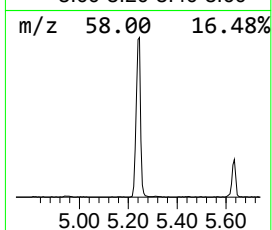
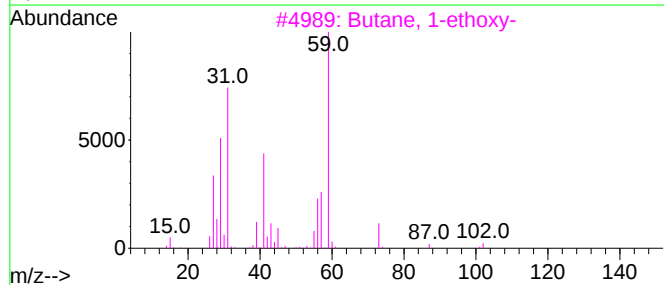
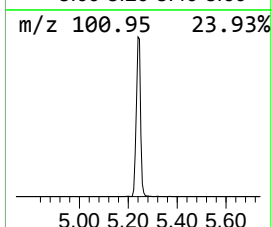
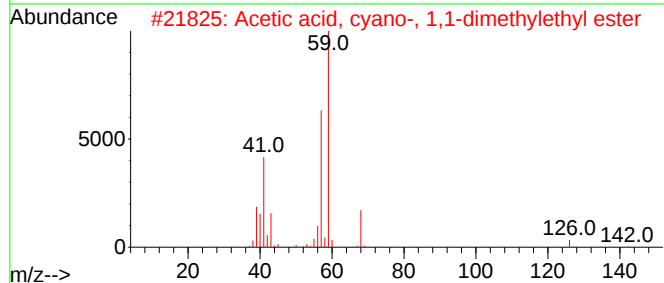
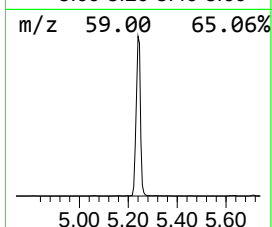
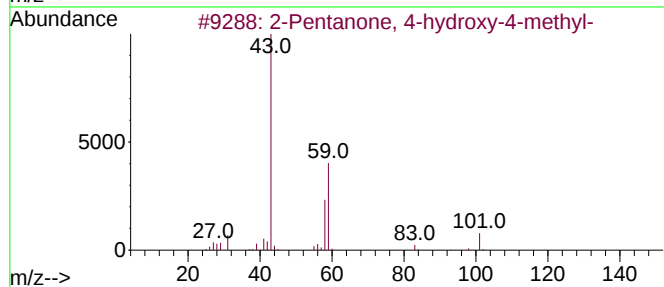
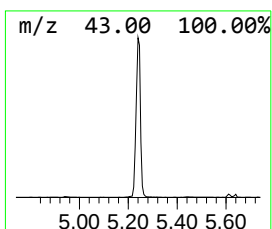
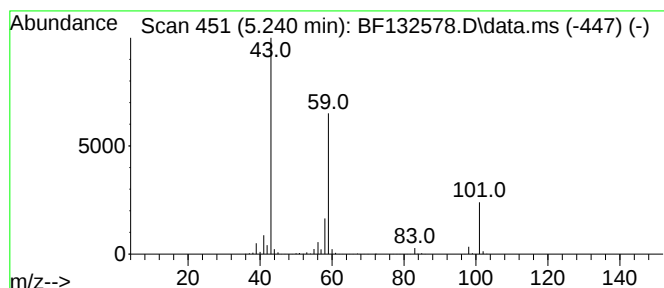
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.240	25.43 ng	1848520	1,4-Dichlorobenzene-d4	7.004

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Guanidine	59	CH5N3	000113-00-8	9



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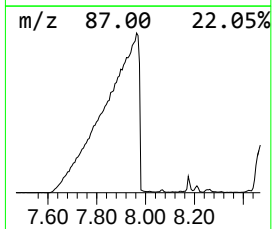
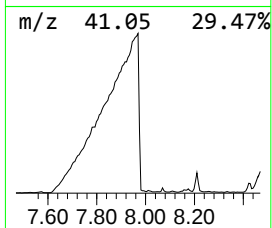
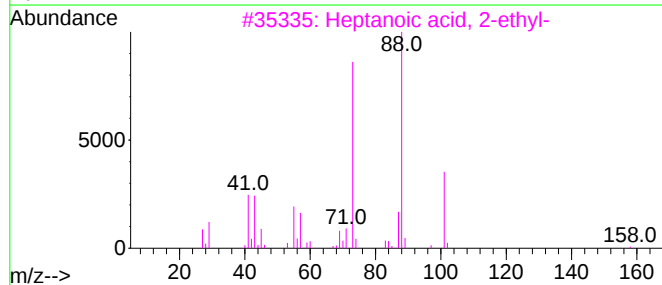
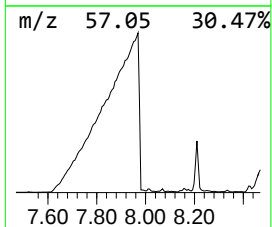
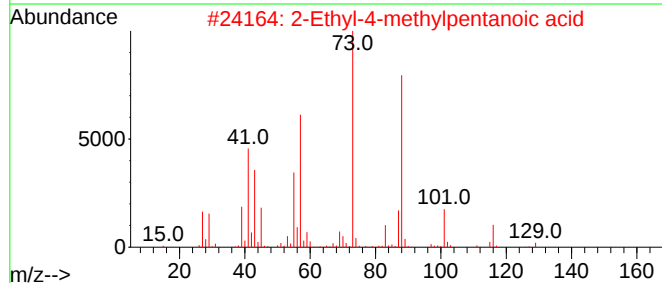
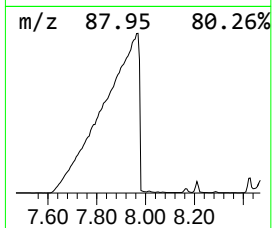
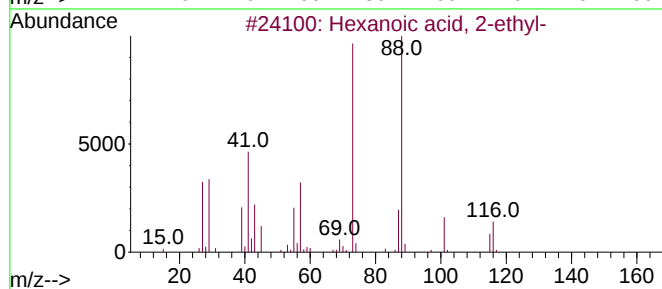
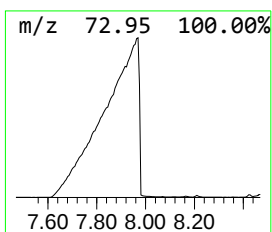
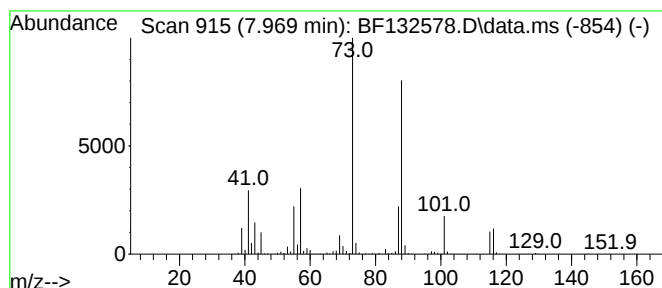
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Hexanoic acid, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.969	630.64 ng	55361400	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			2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	64
3			Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	59
4			Acetic acid, diethyl-	116	C6H12O2	000088-09-5	59
5			Methyl-4-deoxy-2,3-di-O-methyl.b...	218	C9H14O6	1000312-09-9	47



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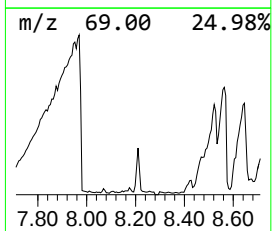
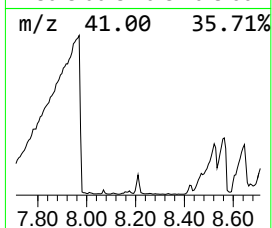
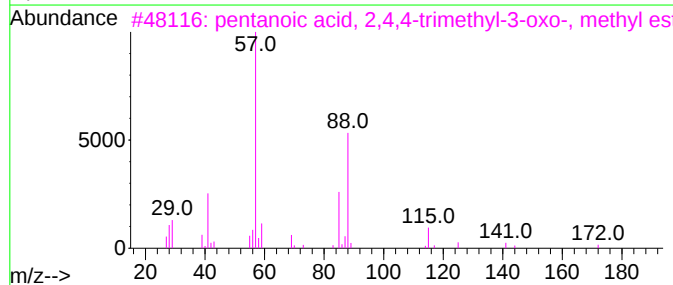
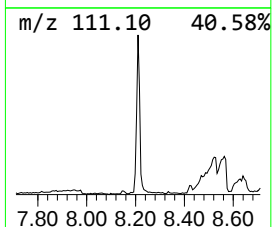
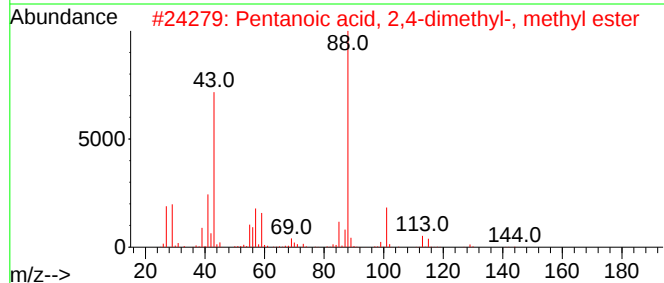
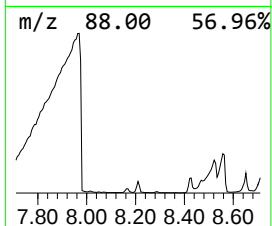
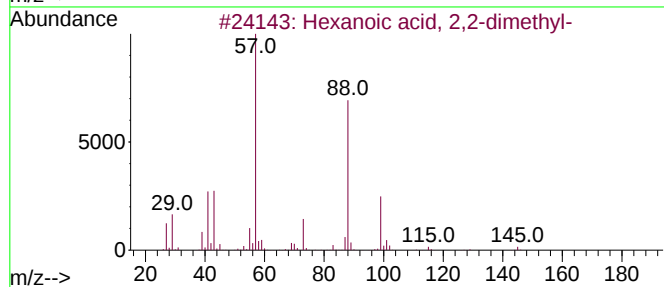
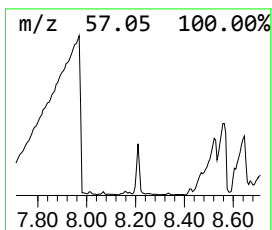
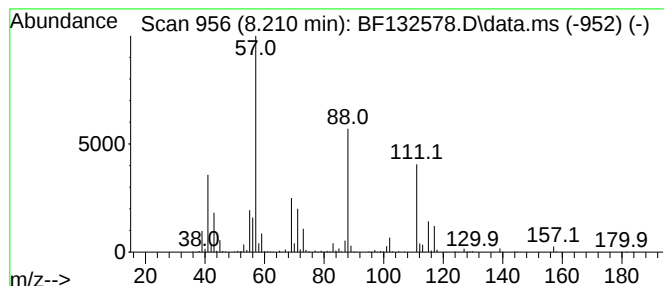
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown8.210 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.210	6.52 ng	572164	Naphthalene-d8	8.287

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2,2-dimethyl-	144	C8H16O2	000813-72-9	25
2			Pentanoic acid, 2,4-dimethyl-, m...	144	C8H16O2	071672-33-8	22
3			pentanoic acid, 2,4,4-trimethyl-...	172	C9H16O3	1000404-62-8	17
4			Pentanoic acid, 2-methyl-, methy...	130	C7H14O2	002177-77-7	17
5			Methyl propionate	88	C4H8O2	000554-12-1	16



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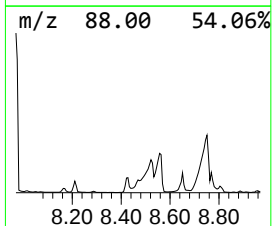
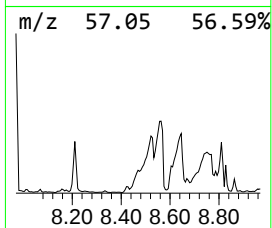
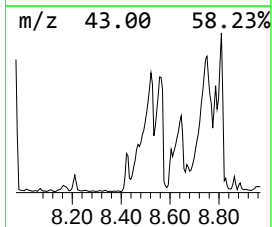
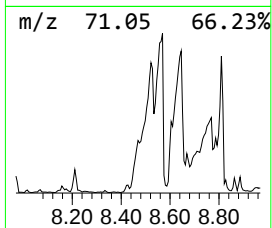
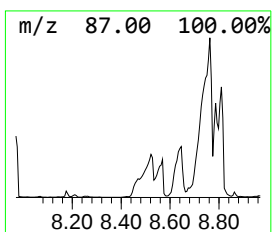
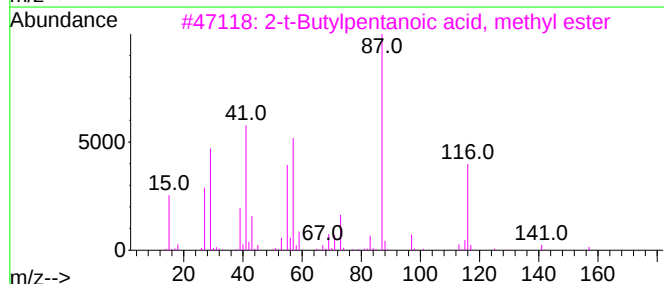
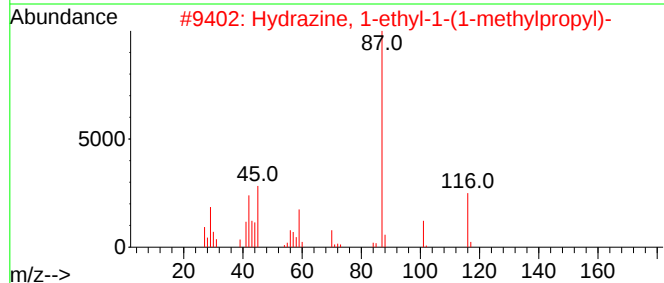
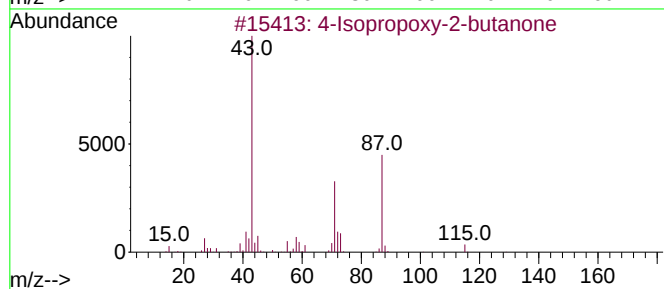
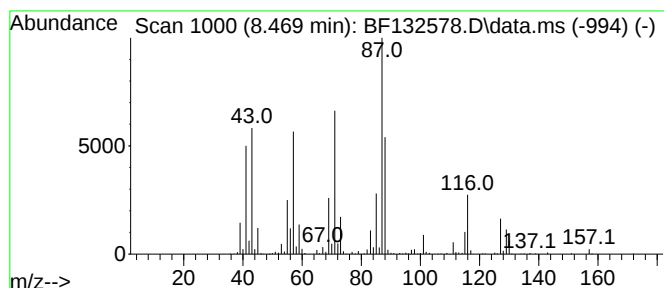
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown8.469 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.469	12.19 ng	1070460	Naphthalene-d8	8.287

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Isopropoxy-2-butanone	130	C7H14O2	032541-58-5	47	
2	Hydrazine, 1-ethyl-1-(1-methylpr...	116	C6H16N2	020325-97-7	38	
3	2-t-Butylpentanoic acid, methyl ...	172	C10H20O2	1000202-22-5	38	
4	Tetraethylene glycol, diacetate	278	C12H22O7	022790-12-1	22	
5	1,2-Butanediol, 3,3-dimethyl-	118	C6H14O2	059562-82-2	22	



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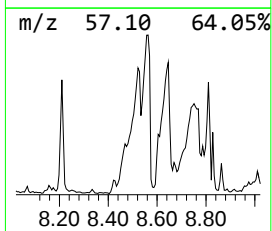
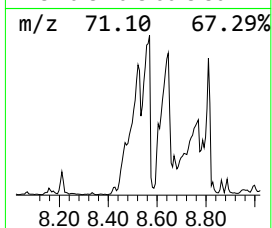
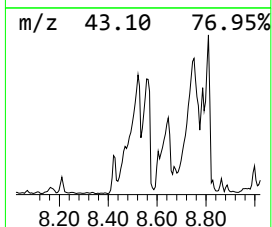
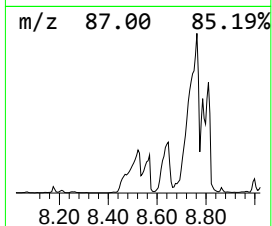
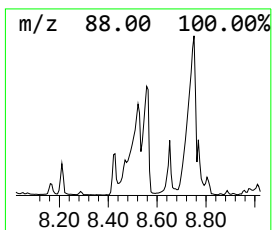
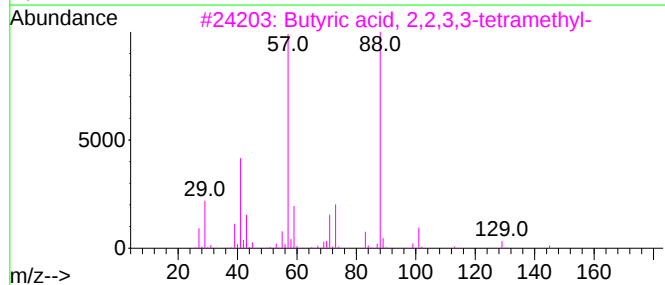
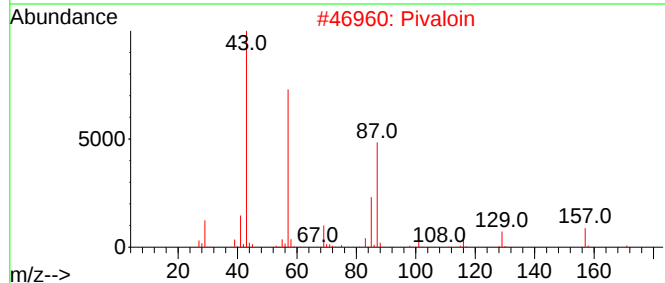
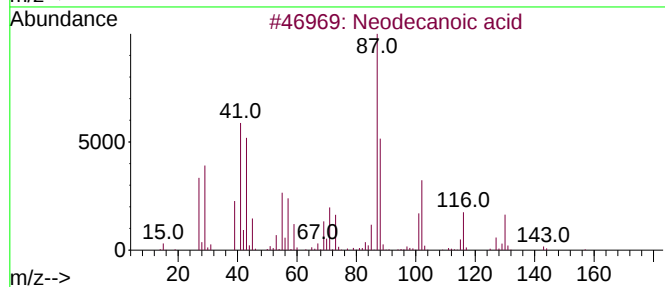
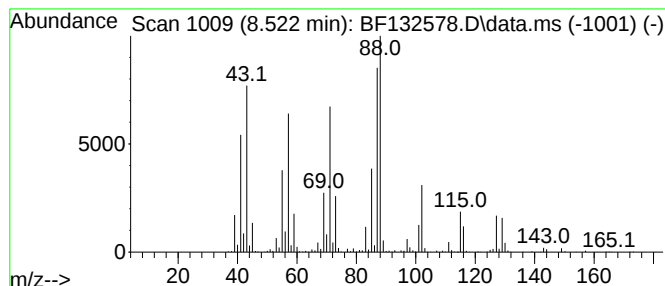
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown8.522 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.522	48.25 ng	4235250	Naphthalene-d8	8.287

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Neodecanoic acid	172	C10H20O2	026896-20-8	38
2		Pivaloin	172	C10H20O2	000815-66-7	35
3		Butyric acid, 2,2,3,3-tetramethyl-	144	C8H16O2	030407-41-1	22
4		t-C4H9CH2C(O)OCH2CH3	144	C8H16O2	005340-78-3	22
5		Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	22



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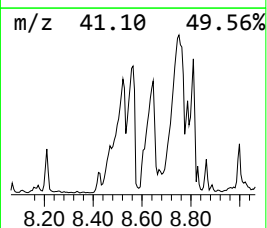
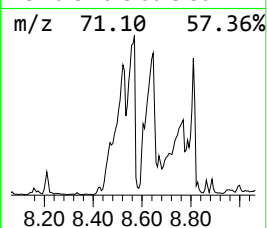
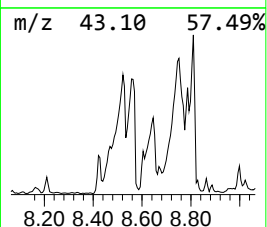
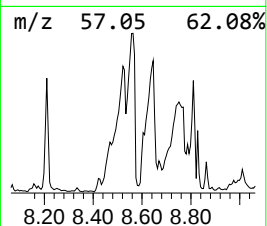
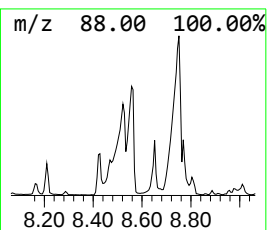
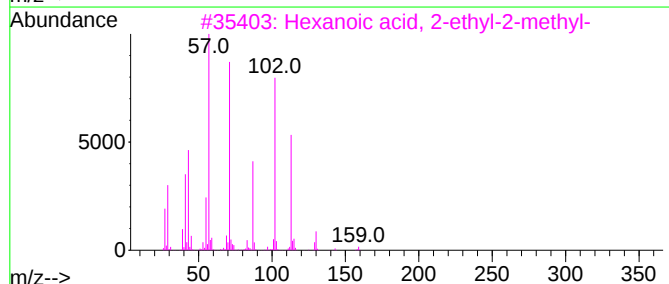
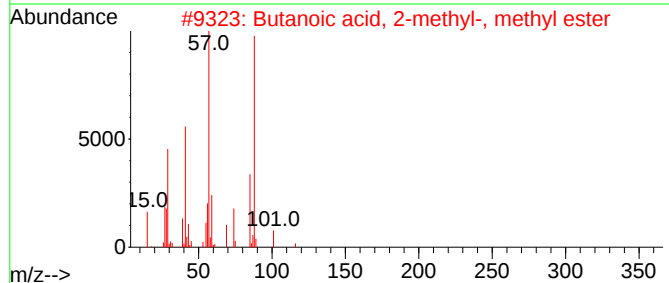
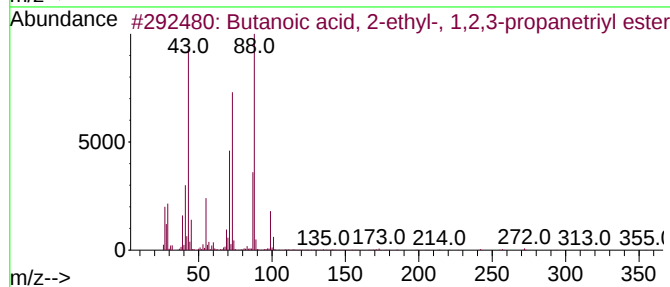
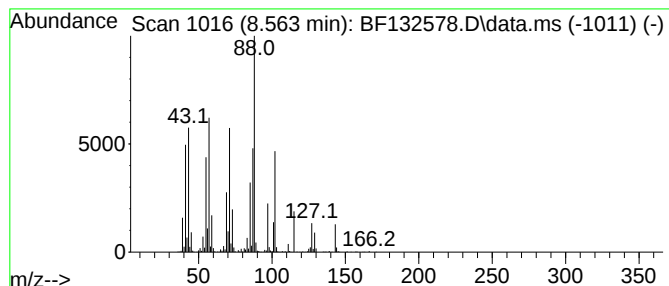
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown8.563 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.563	42.13 ng	3698000	Naphthalene-d8	8.287

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	32
2			Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	27
3			Hexanoic acid, 2-ethyl-2-methyl-	158	C9H18O2	001185-29-1	22
4			Methyl-4-deoxy-2,3-di-O-methyl.b...	218	C9H14O6	1000312-09-9	22
5			Butanoic acid, 2,3-dimethyl-, me...	130	C7H14O2	030540-29-5	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022823\
Data File : BF132578.D
Acq On : 28 Feb 2023 18:25
Operator : CG\JU
Sample : 01701-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-13-GW01

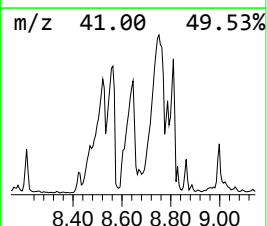
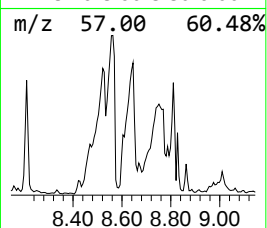
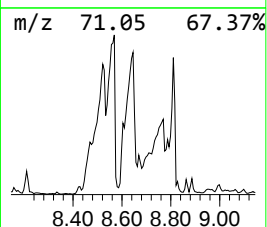
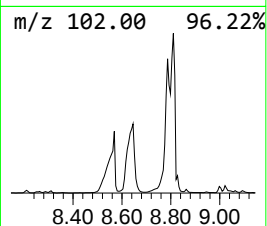
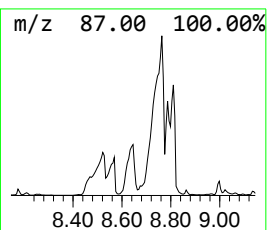
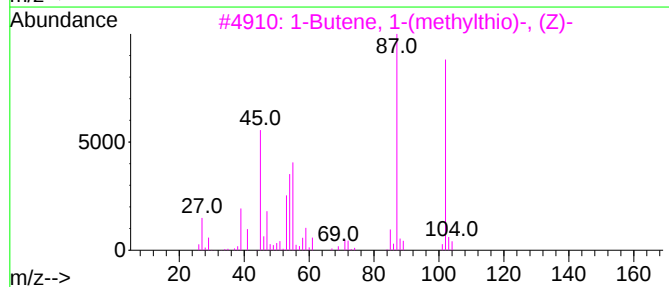
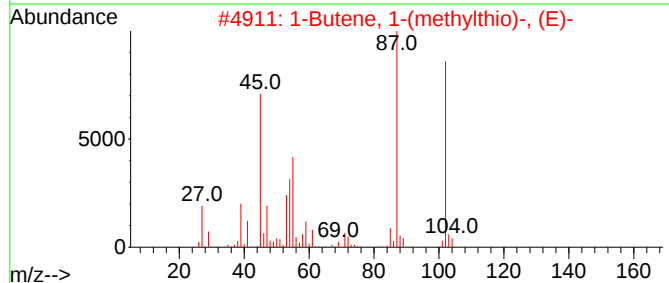
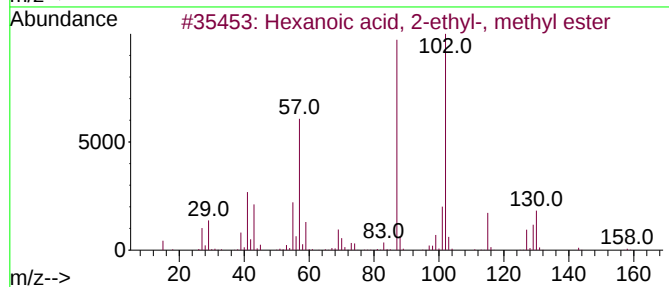
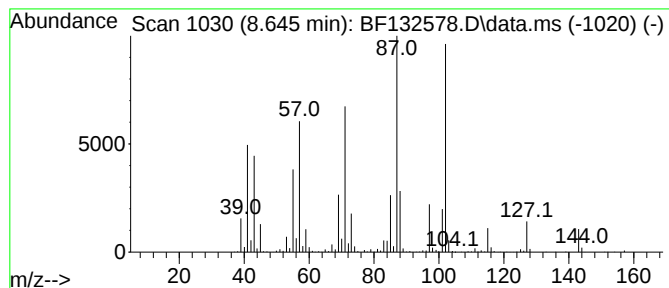
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown8.645 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.645	47.20 ng	4143270	Naphthalene-d8	8.287

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-, methyl ...	158	C9H18O2	000816-19-3	47
2			1-Butene, 1-(methylthio)-, (E)-	102	C5H10S	017414-27-6	43
3			1-Butene, 1-(methylthio)-, (Z)-	102	C5H10S	017414-15-2	37
4			Butanoic acid, 2,3-dimethyl-, et...	144	C8H16O2	054004-42-1	30
5			2,3-Di-O-methyl-D-xylopyranose	178	C7H14O5	018186-26-0	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022823\
Data File : BF132578.D
Acq On : 28 Feb 2023 18:25
Operator : CG\JU
Sample : 01701-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
B-13-GW01

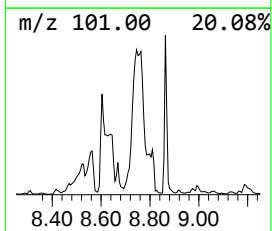
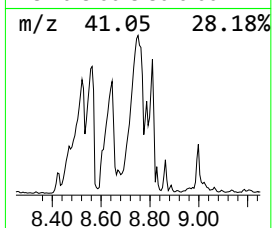
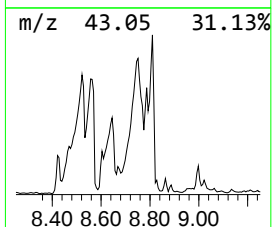
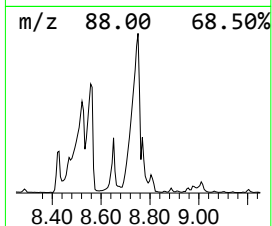
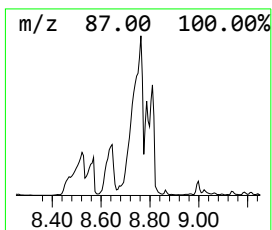
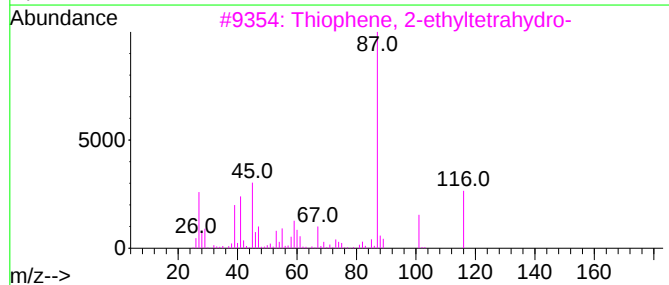
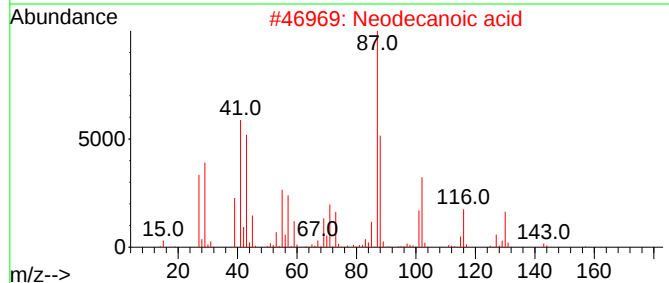
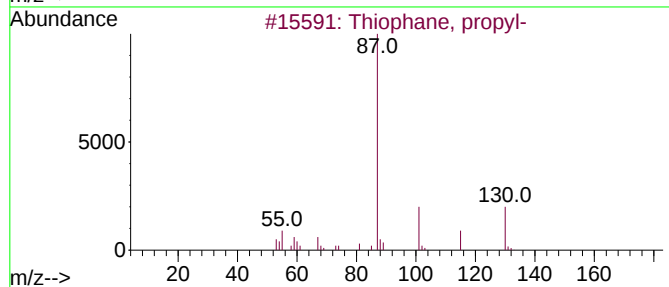
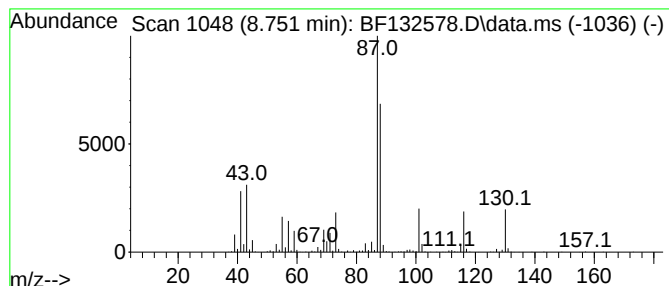
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
8.751	96.07 ng	8433760	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	43
4		Nonanoic acid, 2,4-dimethyl-, me...	200	C12H24O2	054889-61-1	25
5		Hexanoic acid, 2,4-dimethyl-, me...	158	C9H18O2	014251-45-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022823\
Data File : BF132578.D
Acq On : 28 Feb 2023 18:25
Operator : CG\JU
Sample : 01701-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-13-GW01

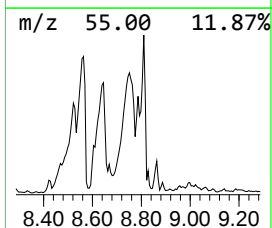
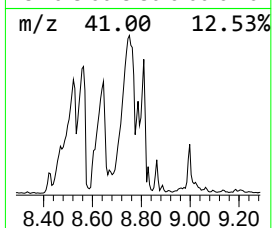
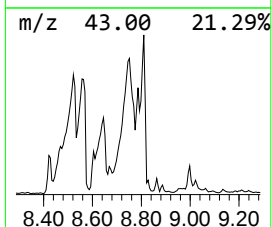
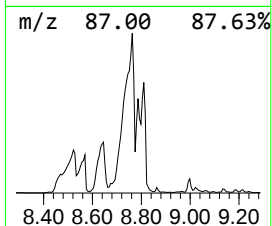
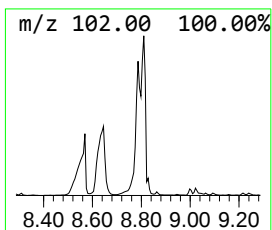
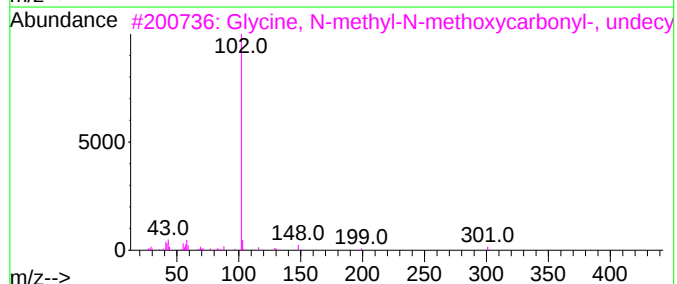
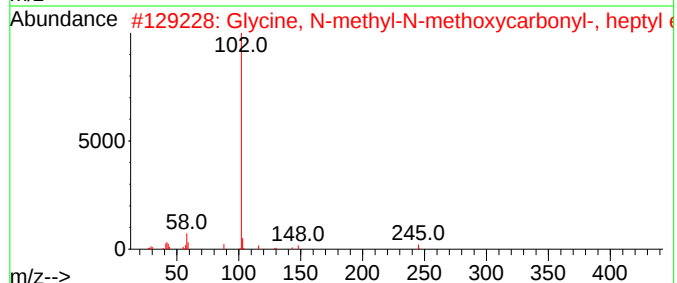
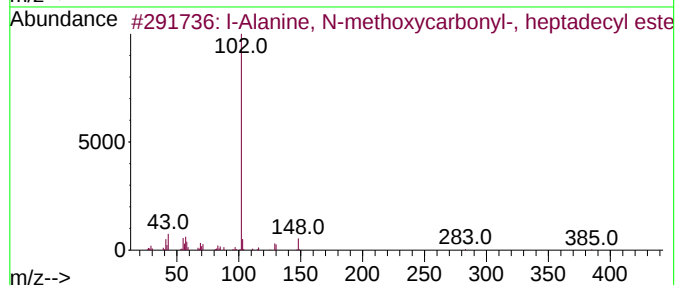
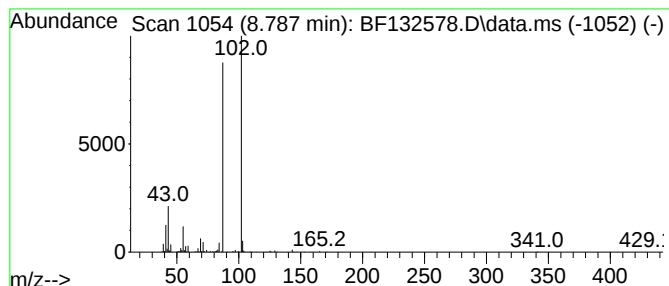
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown8.787 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.787	17.67 ng	1551060	Naphthalene-d8	8.287

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			l-Alanine, N-methoxycarbonyl-, h...	385	C22H43NO4	1000313-38-5	23
2			Glycine, N-methyl-N-methoxycarbo...	245	C12H23NO4	1000320-60-8	17
3			Glycine, N-methyl-N-methoxycarbo...	301	C16H31NO4	1000320-61-2	9
4			l-Alanine, N-methoxycarbonyl-, t...	343	C19H37NO4	1000313-38-2	9
5			l-Alanine, N-methoxycarbonyl-, o...	399	C23H45NO4	1000313-38-6	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022823\
Data File : BF132578.D
Acq On : 28 Feb 2023 18:25
Operator : CG\JU
Sample : 01701-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

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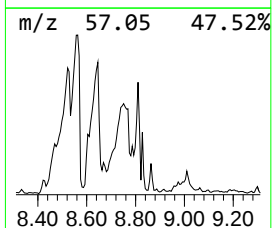
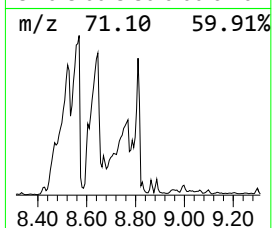
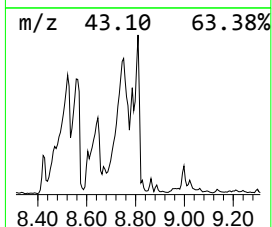
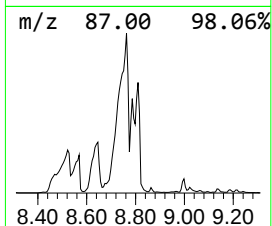
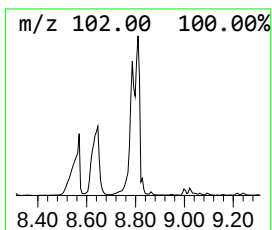
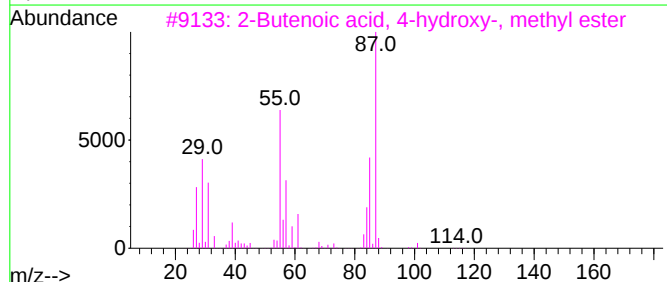
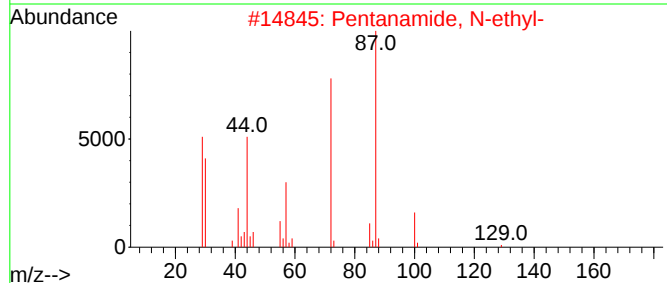
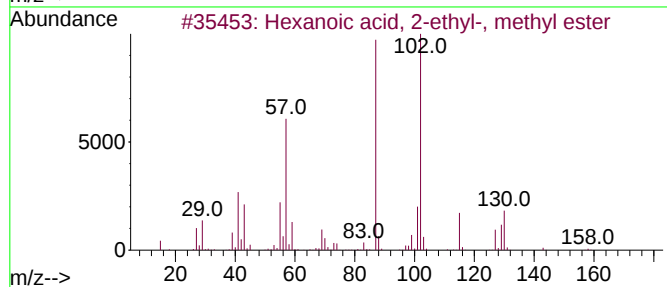
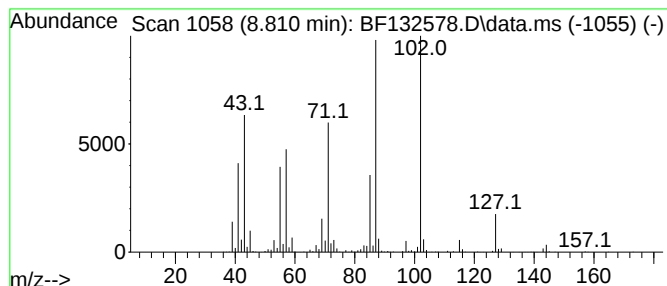
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown8.810 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.810	30.23 ng	2653670	Naphthalene-d8	8.287

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexanoic acid, 2-ethyl-, methyl ...	158	C9H18O2	000816-19-3	40
2		Pentanamide, N-ethyl-	129	C7H15NO	054007-33-9	30
3		2-Butenoic acid, 4-hydroxy-, met...	116	C5H8O3	004508-99-0	27
4		Ethanol, 2,2'-[1,2-ethanediylbis...	234	C10H18O6	000111-21-7	22
5		Tetraethylene glycol, diacetate	278	C12H22O7	022790-12-1	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022823\
Data File : BF132578.D
Acq On : 28 Feb 2023 18:25
Operator : CG\JU
Sample : 01701-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-13-GW01

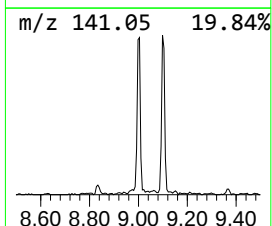
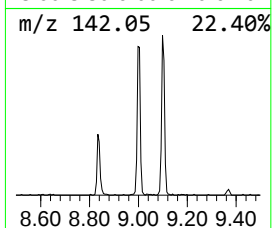
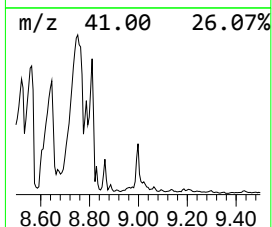
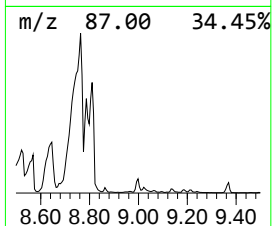
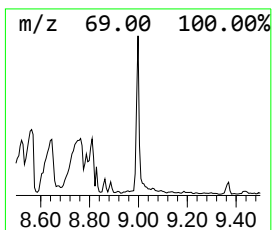
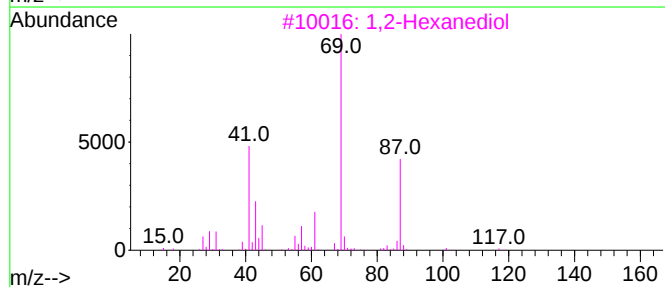
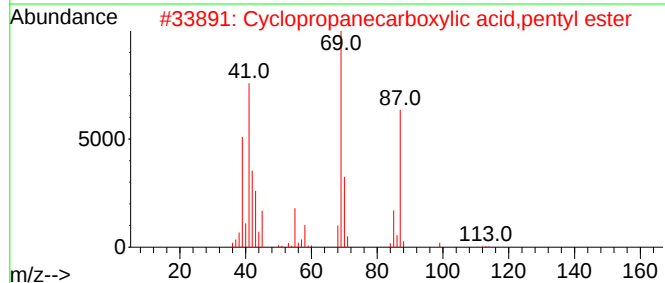
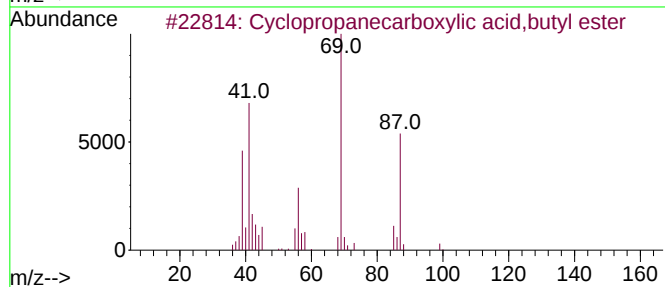
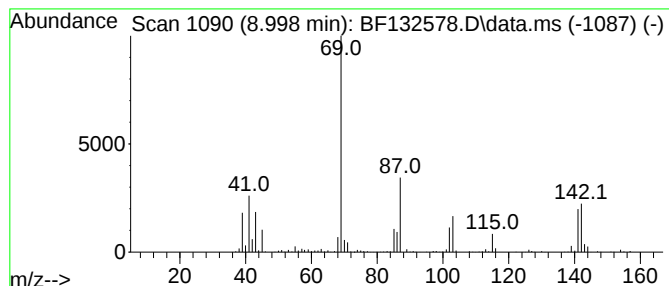
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Cyclopropanecarboxylic acid... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.998	6.47 ng	568074	Naphthalene-d8	8.287

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropanecarboxylic acid, buty...	142	C8H14O2	054947-39-6	50
2			Cyclopropanecarboxylic acid, pent...	156	C9H16O2	060128-02-1	38
3			1,2-Hexanediol	118	C6H14O2	006920-22-5	37
4			2-Hydroxyethyl methacrylate	130	C6H10O3	000868-77-9	37
5			4-Octanol, 2-methyl-	144	C9H20O	040575-41-5	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022823\
Data File : BF132578.D
Acq On : 28 Feb 2023 18:25
Operator : CG\JU
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Misc :
ALS Vial : 15 Sample Multiplier: 1

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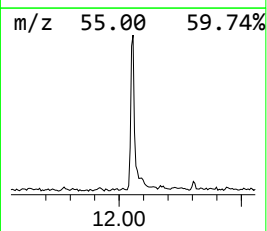
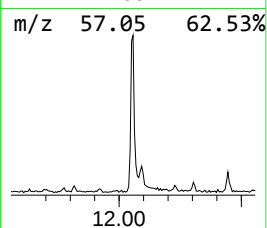
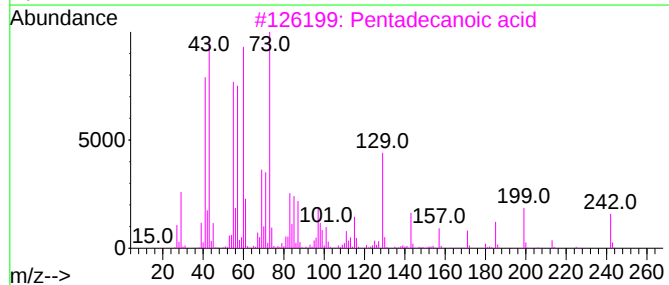
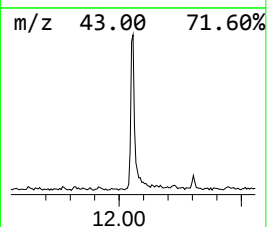
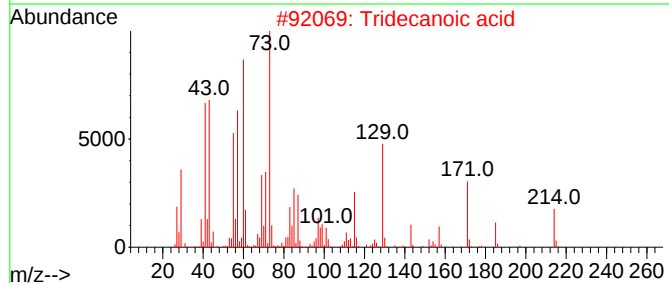
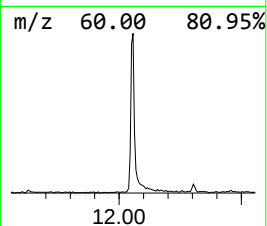
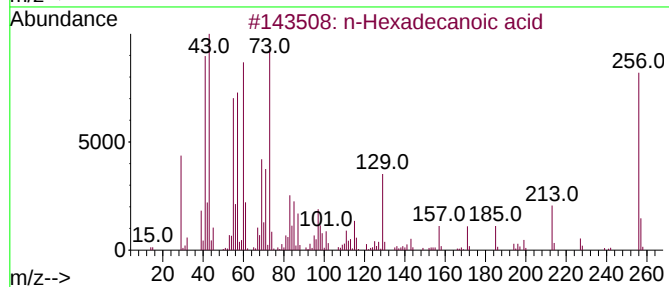
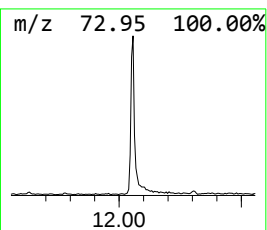
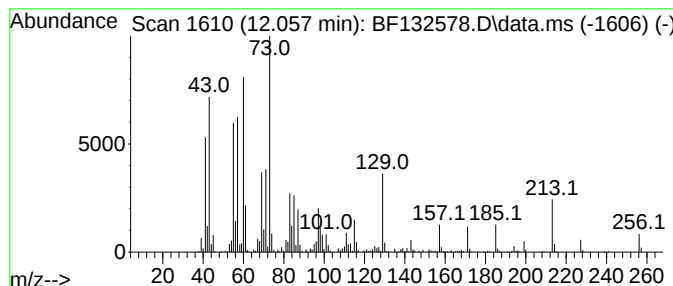
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.057	5.36 ng	589677	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	95
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5		8-Methylnonanoic acid	172	C10H20O2	005963-14-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022823\
Data File : BF132578.D
Acq On : 28 Feb 2023 18:25
Operator : CG\JU
Sample : 01701-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-13-GW01

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
2-Pentanone, 4-...	5.240	25.4	ng	1848520	1	7.004	1453800	20.0
Hexanoic acid, ...	7.969	630.6	ng	55361400	2	8.287	1755710	20.0
unknown8.210	8.210	6.5	ng	572164	2	8.287	1755710	20.0
unknown8.469	8.469	12.2	ng	1070460	2	8.287	1755710	20.0
unknown8.522	8.522	48.3	ng	4235250	2	8.287	1755710	20.0
unknown8.563	8.563	42.1	ng	3698000	2	8.287	1755710	20.0
unknown8.645	8.645	47.2	ng	4143270	2	8.287	1755710	20.0
Thiophane, propyl-	8.751	96.1	ng	8433760	2	8.287	1755710	20.0
unknown8.787	8.787	17.7	ng	1551060	2	8.287	1755710	20.0
unknown8.810	8.810	30.2	ng	2653670	2	8.287	1755710	20.0
Cyclopropanecar...	8.998	6.5	ng	568074	2	8.287	1755710	20.0
n-Hexadecanoic ...	12.057	5.4	ng	589677	4	11.545	2201330	20.0