

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121922\
 Data File : BF131695.D
 Acq On : 19 Dec 2022 18:33
 Operator : CG\JU
 Sample : N6087-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 12-15-2022-HOWE-AVE

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-BF120822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131695.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.487	575	578	585	rVB	1177552	1081597	2.02%	0.672%
2	6.510	747	752	758	rBV	583521	650051	1.22%	0.404%
3	7.445	906	911	914	rVB	1632774	1509825	2.82%	0.938%
4	7.975	917	1001	1002	rBV	4930542	53460200	100.00%	33.208%
5	8.569	1095	1102	1104	rBV3	3719625	4402762	8.24%	2.735%
6	8.657	1113	1117	1118	rBV	1599388	1518977	2.84%	0.944%
7	8.692	1118	1123	1124	rBV	1806806	2603484	4.87%	1.617%
8	8.834	1124	1147	1150	rBV3	6477655	37532263	70.21%	23.314%
9	9.028	1160	1180	1182	rBV4	5275893	25518799	47.73%	15.852%
10	9.128	1193	1197	1200	rVB3	7945608	14995657	28.05%	9.315%
11	9.151	1200	1201	1204	rVB2	3415671	2229240	4.17%	1.385%
12	9.181	1204	1206	1207	rBV	1264000	800039	1.50%	0.497%
13	9.198	1207	1209	1211	rBV2	847352	899517	1.68%	0.559%
14	9.257	1217	1219	1225	rVB3	1716846	2837306	5.31%	1.762%
15	9.328	1225	1231	1233	rVV4	713657	1332040	2.49%	0.827%
16	9.957	1332	1338	1350	rVB2	315830	602223	1.13%	0.374%
17	10.145	1361	1370	1377	rBV	1523557	2479959	4.64%	1.540%
18	10.369	1397	1408	1411	rBV	1846774	3804893	7.12%	2.363%
19	10.739	1466	1471	1474	rBV	1697695	1503048	2.81%	0.934%
20	13.010	1853	1857	1860	rBV	1523674	1224505	2.29%	0.761%

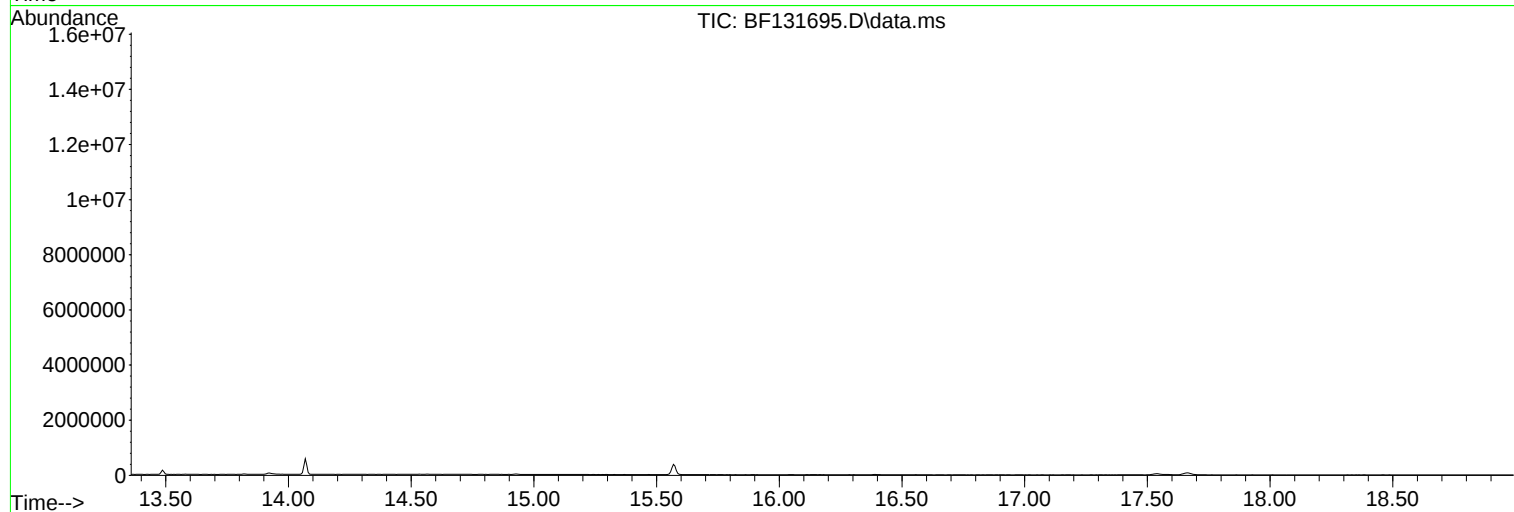
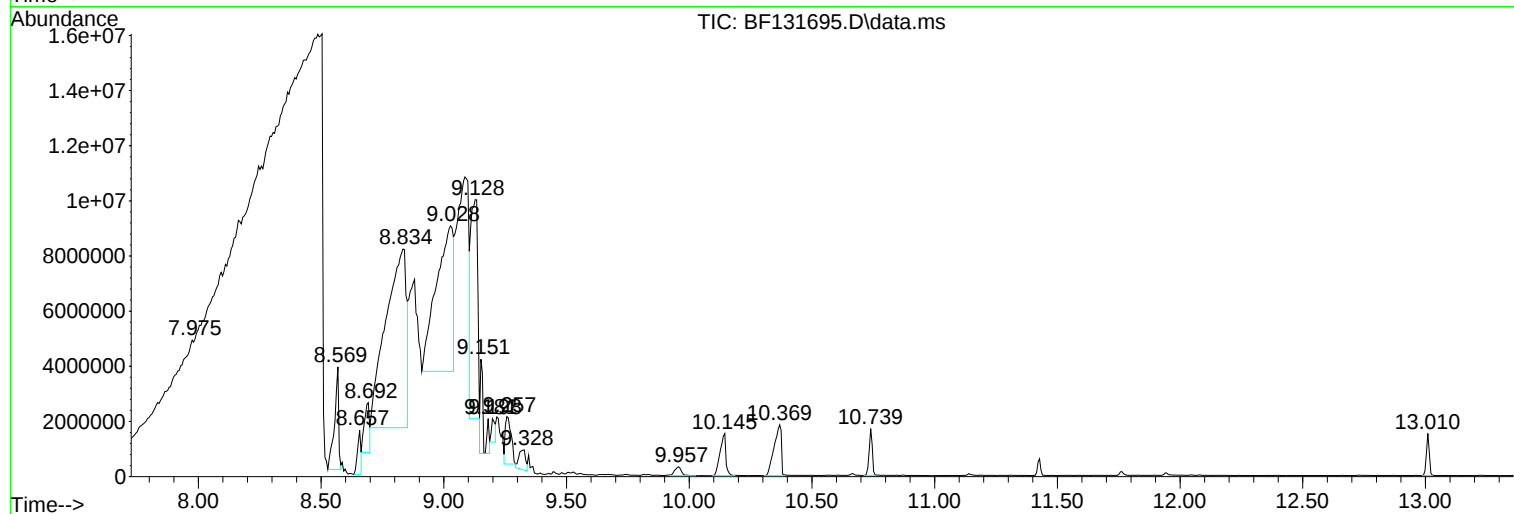
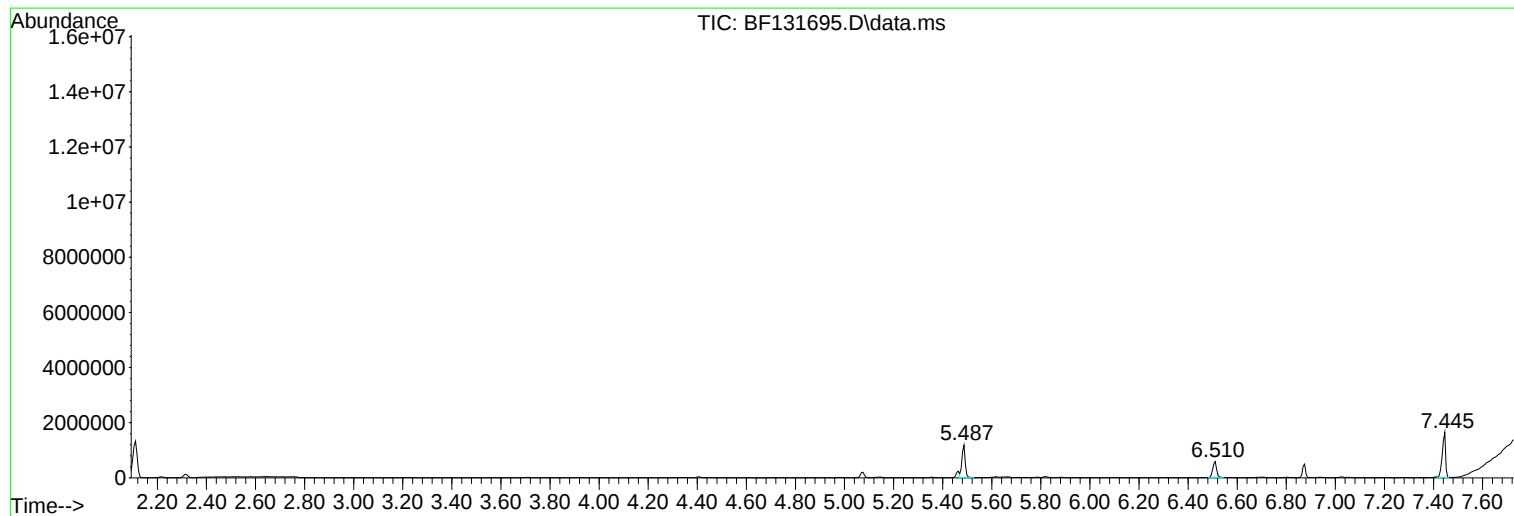
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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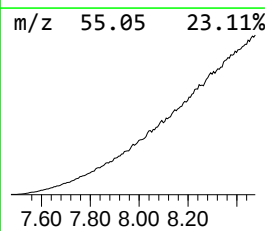
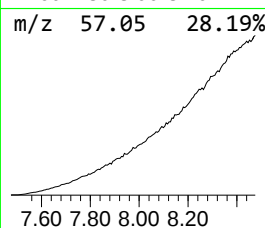
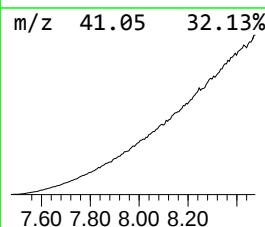
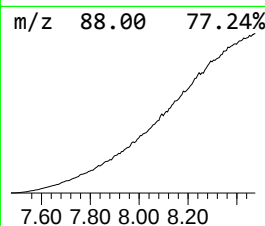
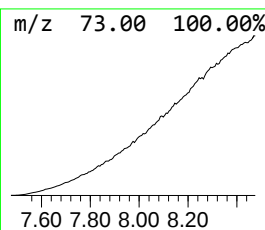
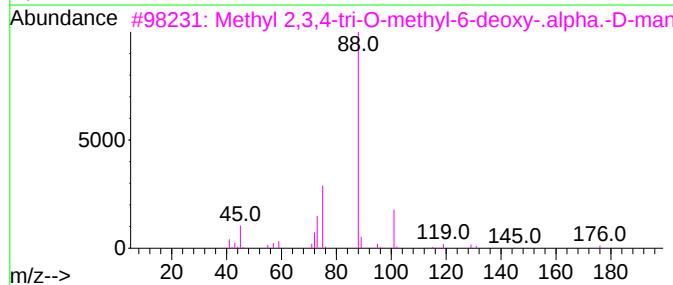
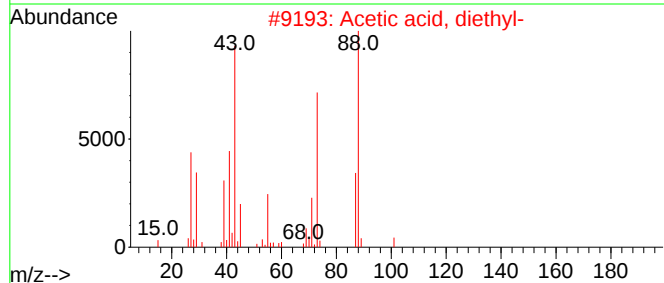
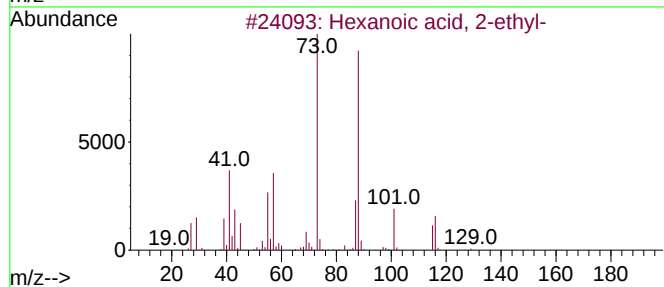
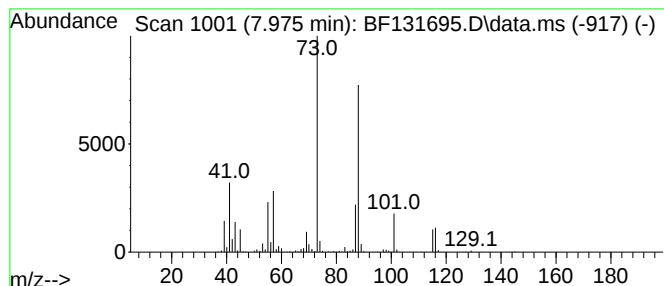
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hexanoic acid, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.975	20.00 ng	53460200	Naphthalene-d8	8.163

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	64
3			Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	50
4			Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	50
5			2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	42



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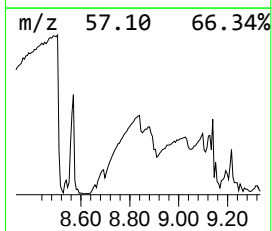
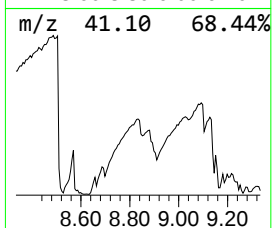
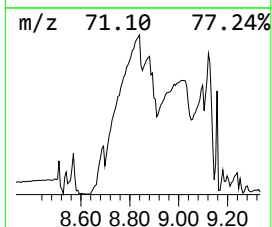
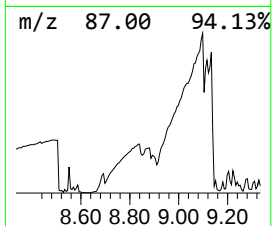
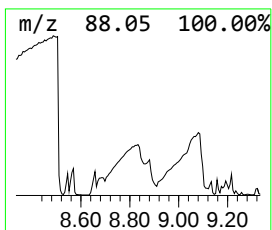
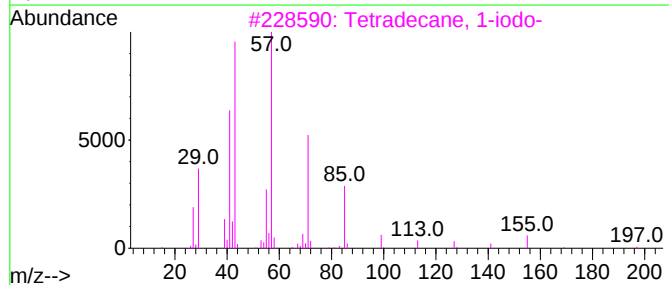
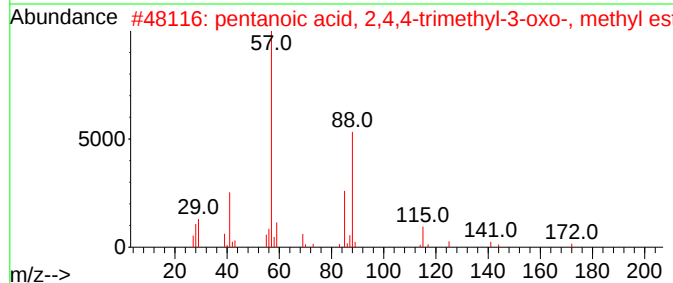
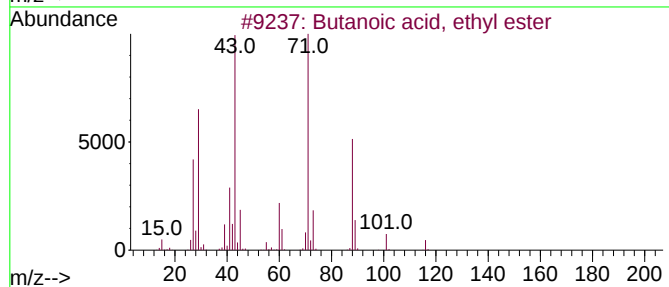
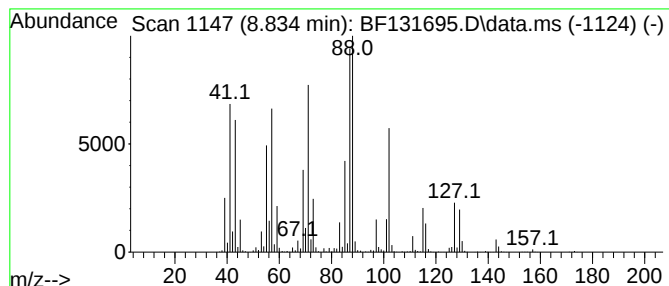
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown8.834 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.834	14.04 ng	37532300	Naphthalene-d8	8.163

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	27
2		pentanoic acid, 2,4,4-trimethyl-...	172	C9H16O3	1000404-62-8	22
3		Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	14
4		Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	14
5		Oxalic acid, isohexyl neopentyl ...	244	C13H24O4	1000309-73-0	14



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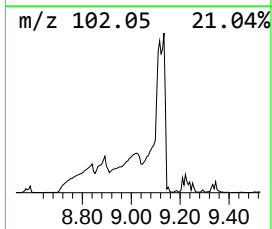
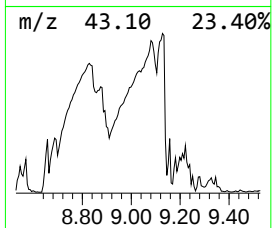
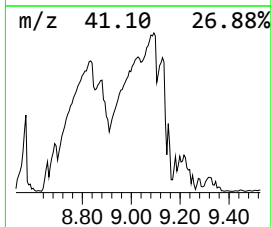
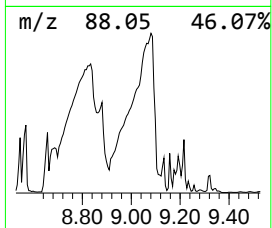
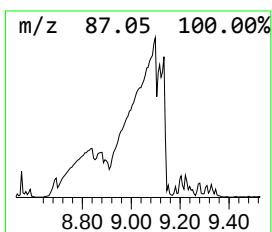
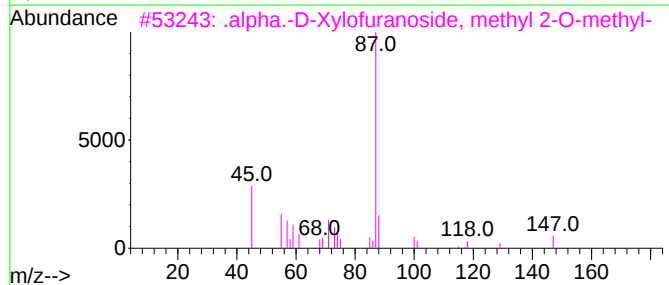
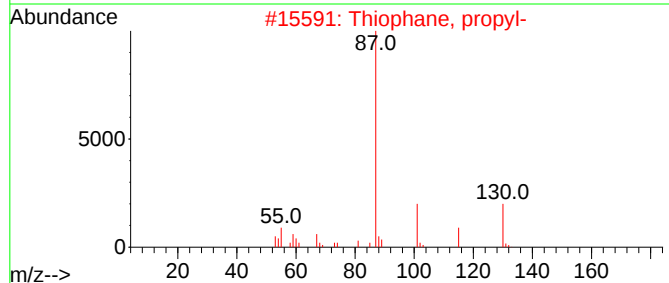
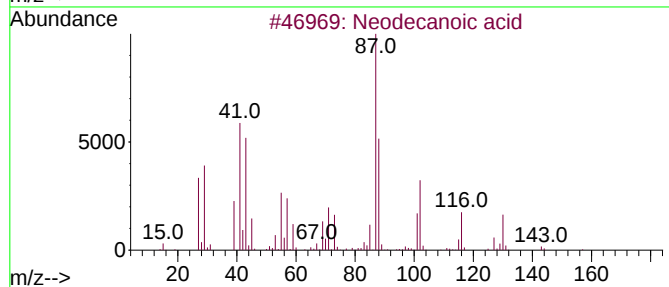
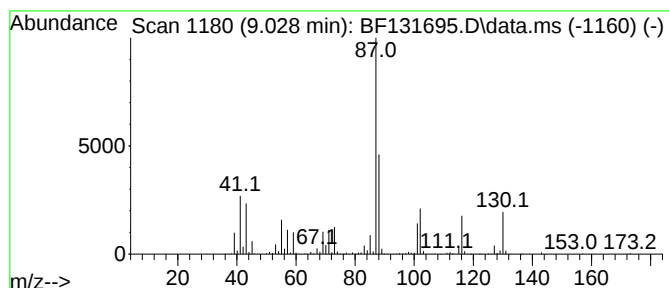
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Neodecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.028	9.55 ng	25518800	Naphthalene-d8	8.163

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Neodecanoic acid	172	C10H20O2	026896-20-8	50
2		Thiophane, propyl-	130	C7H14S	001551-34-4	47
3		.alpha.-D-Xylofuranoside, methyl...	178	C7H14O5	032469-86-6	43
4		Heptanoic acid, 2-propyl-, methy...	186	C11H22O2	056247-53-1	43
5		Uridine, 2'-O-methyl-	258	C10H14N2O6	002140-76-3	38



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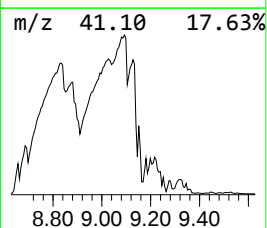
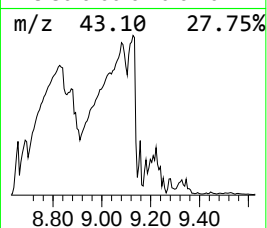
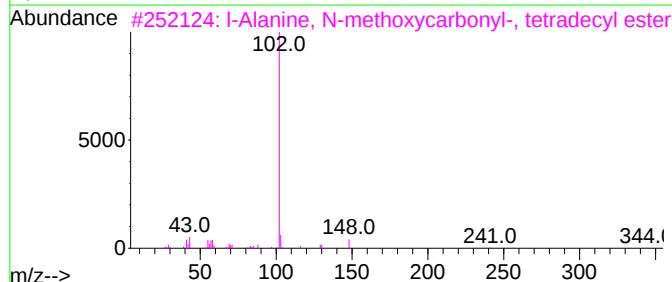
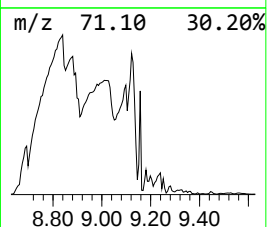
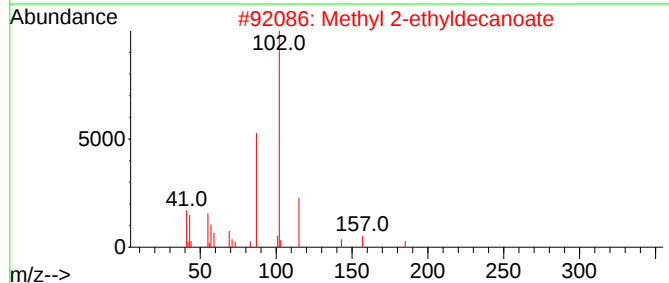
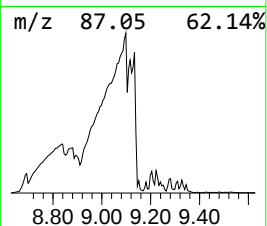
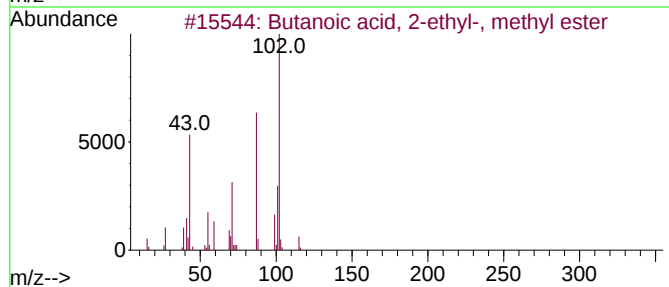
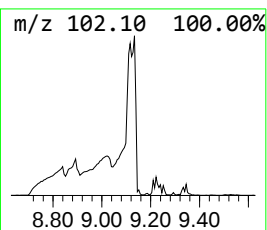
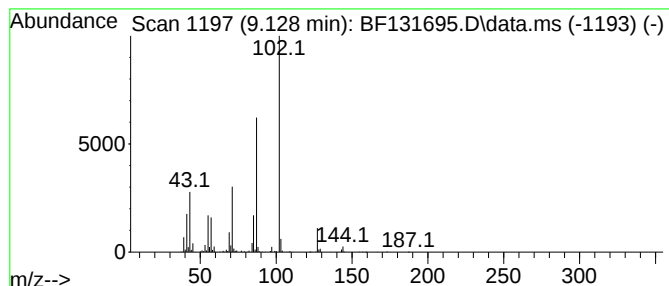
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Peak Number 4 unknown9.128 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.128	498.01 ng	14995700	Acenaphthene-d10	9.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 2-ethyl-, methyl ...	130	C7H14O2	000816-11-5	39
2			Methyl 2-ethyldecanoate	214	C13H26O2	020483-47-0	38
3			l-Alanine, N-methoxycarbonyl-, t...	343	C19H37NO4	1000313-38-2	37
4			l-Alanine, N-methoxycarbonyl-, o...	399	C23H45NO4	1000313-38-6	37
5			l-Alanine, N-methoxycarbonyl-, p...	357	C20H39NO4	1000313-38-3	37



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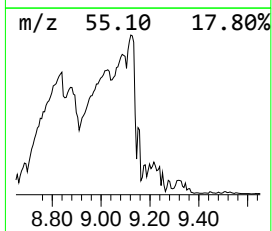
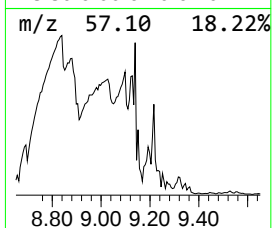
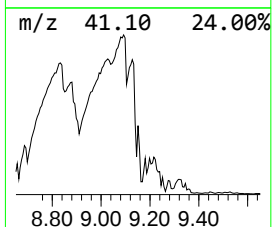
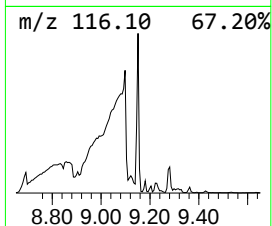
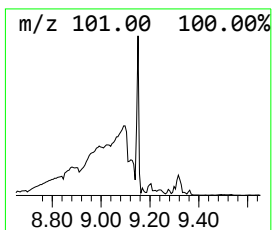
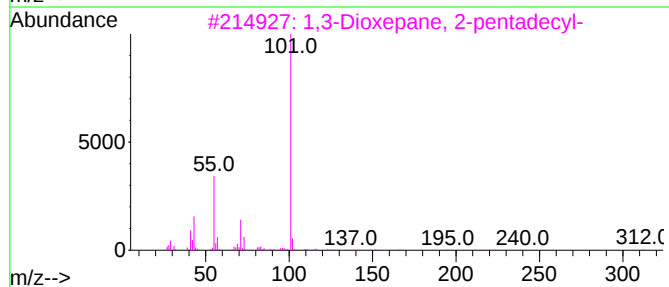
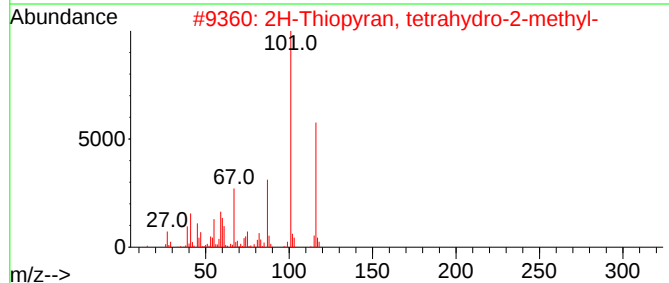
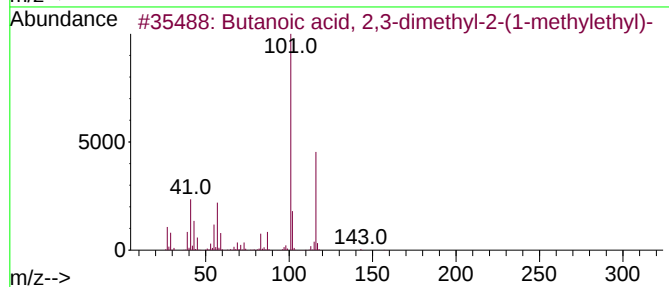
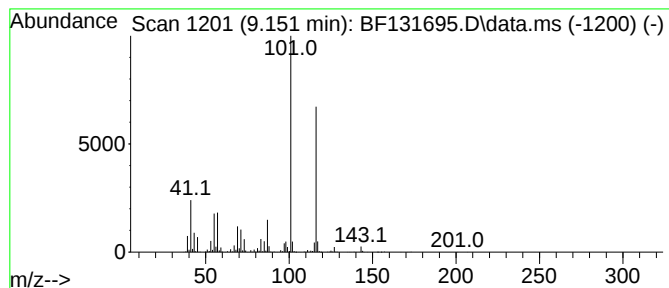
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Peak Number 5 Butanoic acid, 2,3-dimethyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.151	74.03 ng	2229240	Acenaphthene-d10	9.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 2,3-dimethyl-2-(1...	158	C9H18O2	023119-04-2	56
2			2H-Thiopyran, tetrahydro-2-methyl-	116	C6H12S	005161-16-0	47
3			1,3-Dioxepane, 2-pentadecyl-	312	C20H40O2	041563-29-5	43
4			Sulfurous acid, 2-methyl-4-metho...	336	C17H36O4S	1000309-21-1	40
5			1,3-Dioxolane, 2,2-diethyl-	130	C7H14O2	004362-57-6	38



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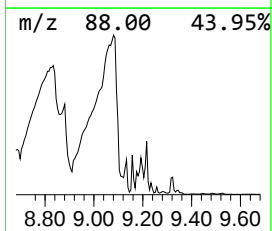
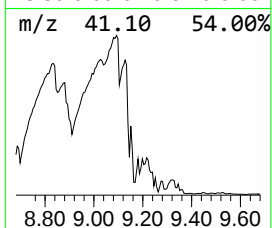
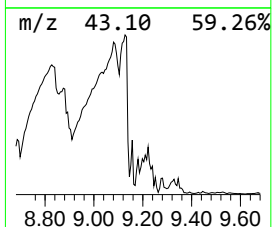
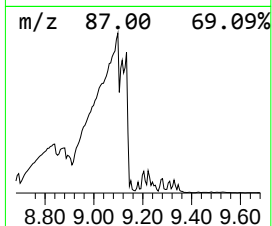
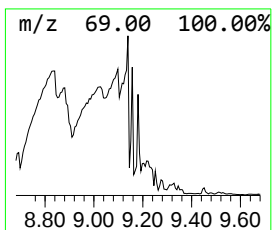
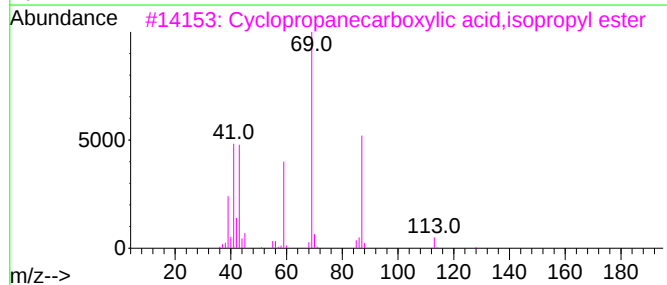
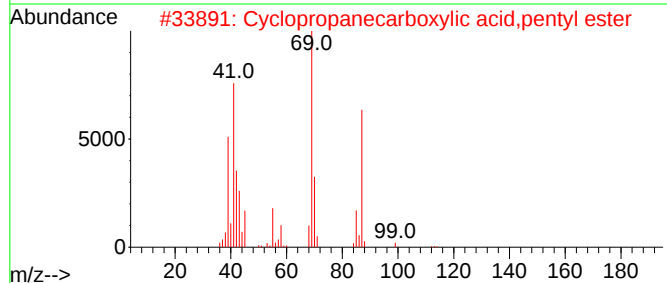
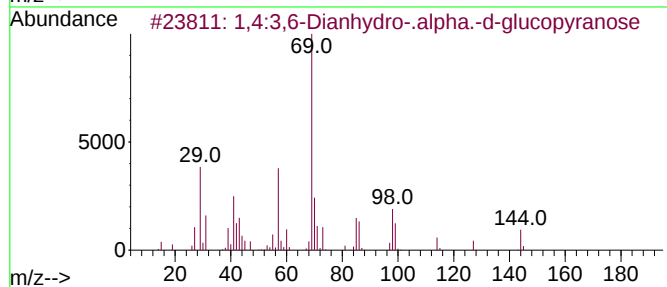
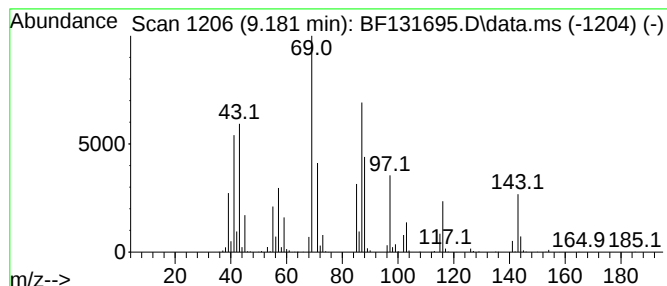
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown9.181 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.181	26.57 ng	800039	Acenaphthene-d10	9.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4:3,6-Dianhydro-.alpha.-d-gluc...	144	C6H8O4	1000098-14-8	22
2			Cyclopropanecarboxylic acid,pent...	156	C9H16O2	060128-02-1	17
3			Cyclopropanecarboxylic acid,isop...	128	C7H12O2	006887-83-8	17
4			Octyl crotonate	198	C12H22O2	1000429-17-5	16
5			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121922\
Data File : BF131695.D
Acq On : 19 Dec 2022 18:33
Operator : CG\JU
Sample : N6087-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
12-15-2022-HOWE-AVE

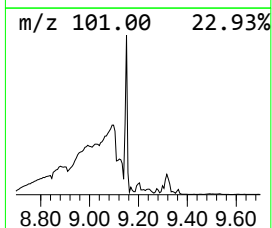
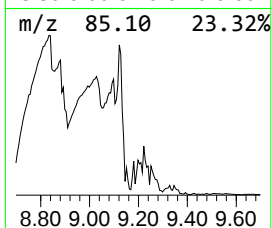
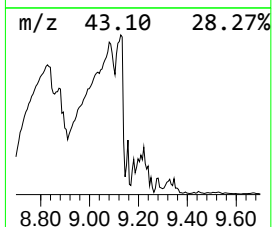
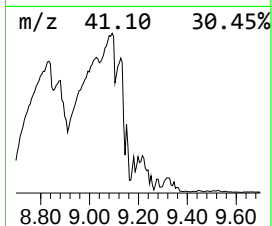
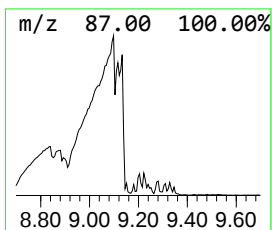
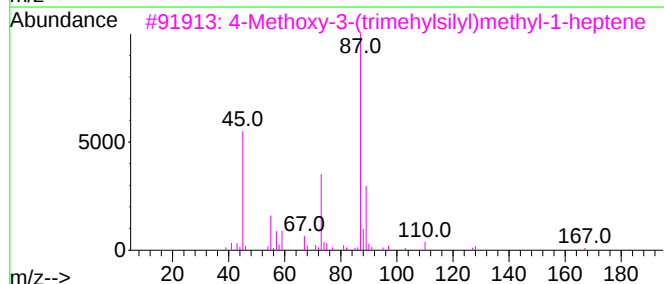
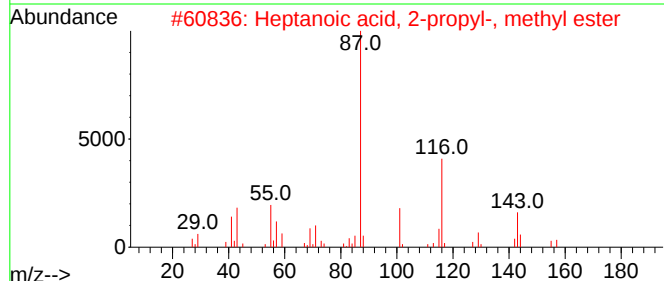
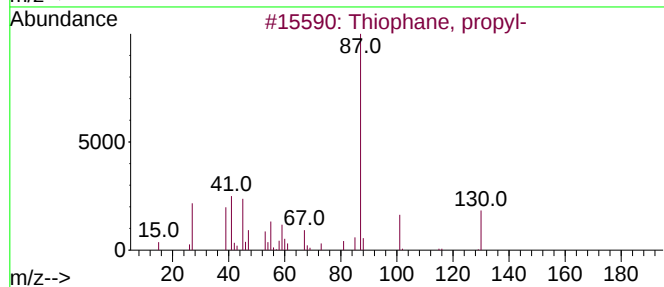
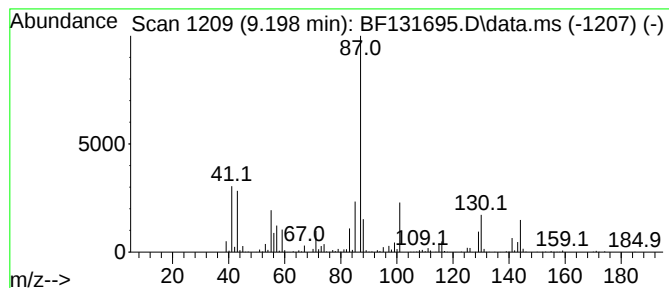
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Thiophane, propyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.198	29.87 ng	899517	Acenaphthene-d10	9.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophane, propyl-	130	C7H14S	001551-34-4	58
2			Heptanoic acid, 2-propyl-, methy...	186	C11H22O2	056247-53-1	38
3			4-Methoxy-3-(trimethylsilyl)methy...	214	C12H26OSi	1000433-72-9	32
4			3-Methyldodecanoic acid	214	C13H26O2	013490-36-3	28
5			Thiophene, 2-butyltetrahydro-	144	C8H16S	001613-49-6	28



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121922\
Data File : BF131695.D
Acq On : 19 Dec 2022 18:33
Operator : CG\JU
Sample : N6087-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
12-15-2022-HOWE-AVE

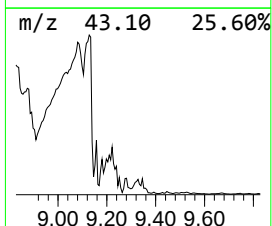
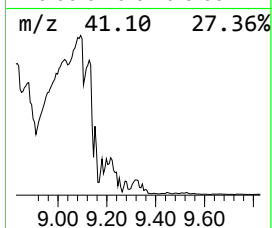
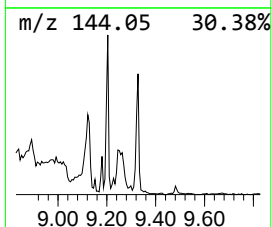
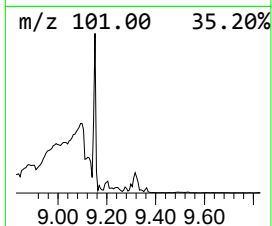
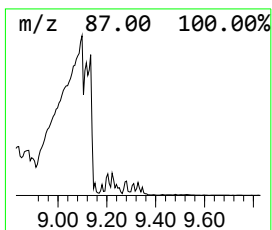
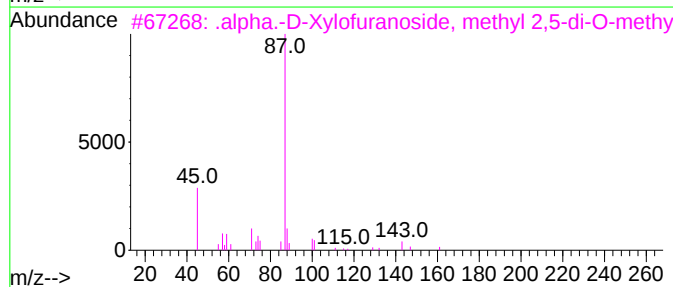
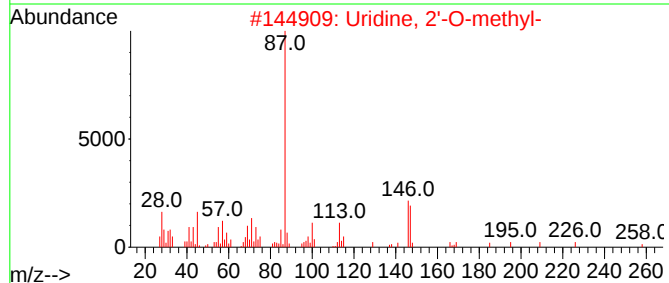
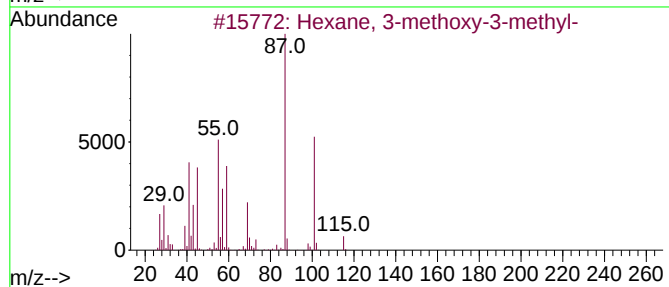
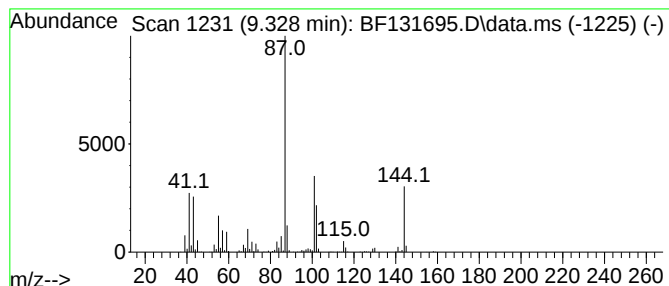
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown9.328 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.328	44.24 ng	1332040	Acenaphthene-d10	9.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methoxy-3-methyl-	130	C8H18O	074630-91-4	38
2			Uridine, 2'-O-methyl-	258	C10H14N2O6	002140-76-3	30
3			.alpha.-D-Xylofuranoside, methyl...	192	C8H16O5	035007-52-4	28
4			1,3-Dioxolane, 2-ethyl-2-methyl-	116	C6H12O2	000126-39-6	28
5			2-[2-[2-[2-(2-Butoxyethoxy)ethox...	336	C16H32O7	1000351-94-0	28



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121922\
Data File : BF131695.D
Acq On : 19 Dec 2022 18:33
Operator : CG\JU
Sample : N6087-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
12-15-2022-HOWE-AVE

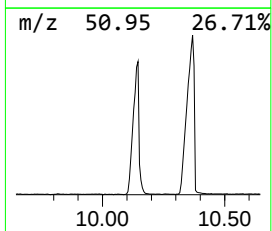
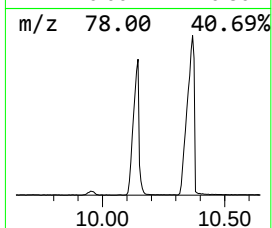
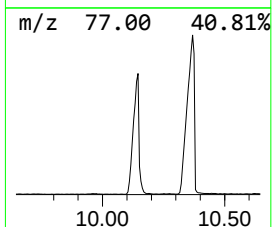
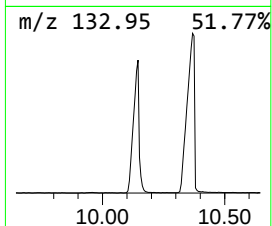
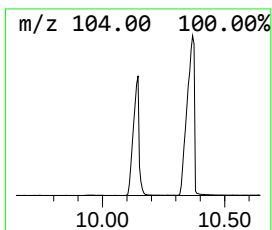
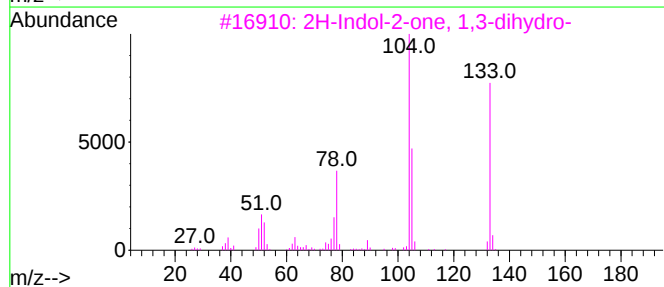
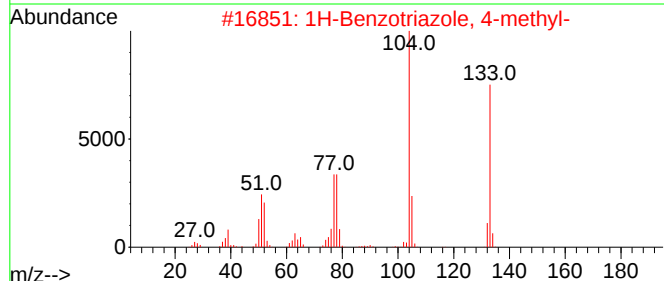
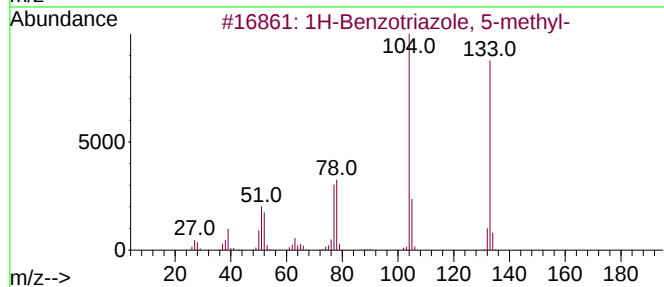
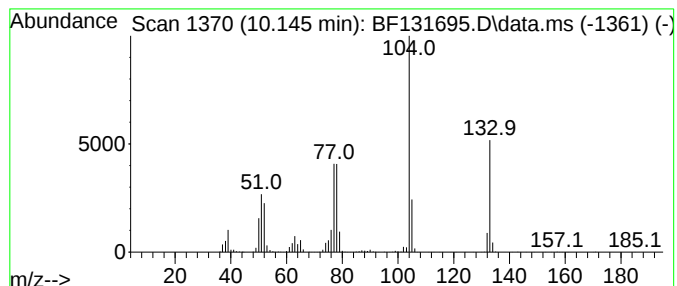
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1H-Benzotriazole, 5-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.145	82.36 ng	2479960	Acenaphthene-d10	9.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Benzotriazole, 5-methyl-	133	C7H7N3	000136-85-6	97
2			1H-Benzotriazole, 4-methyl-	133	C7H7N3	029878-31-7	97
3			2H-Indol-2-one, 1,3-dihydro-	133	C8H7NO	000059-48-3	83
4			Benzene, 1-azido-2-methyl-	133	C7H7N3	031656-92-5	72
5			1H-Indol-4-ol	133	C8H7NO	002380-94-1	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121922\
Data File : BF131695.D
Acq On : 19 Dec 2022 18:33
Operator : CG\JU
Sample : N6087-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
12-15-2022-HOWE-AVE

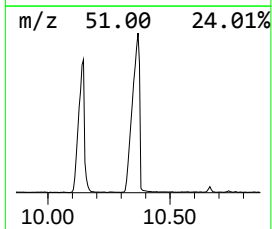
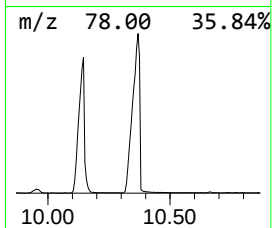
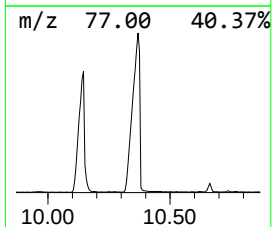
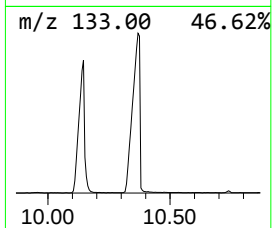
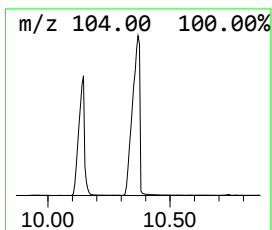
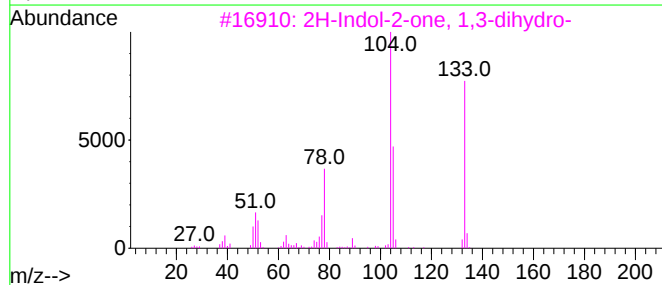
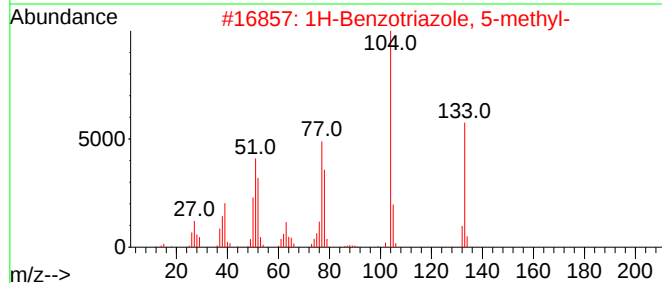
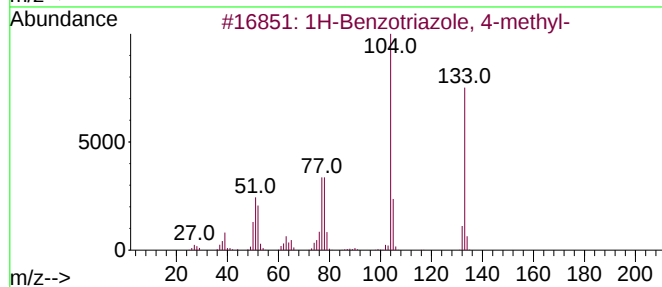
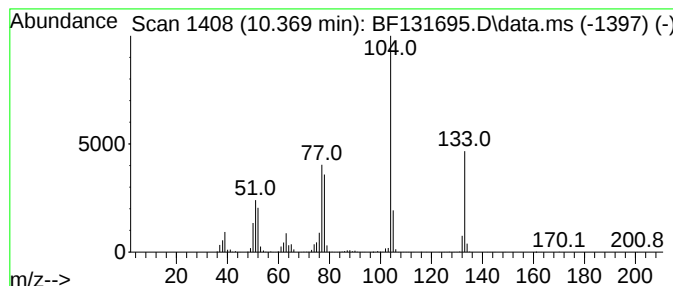
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1H-Benzotriazole, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.369	126.36 ng	3804890	Acenaphthene-d10	9.957

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Benzotriazole, 4-methyl-	133	C7H7N3	029878-31-7	97
2		1H-Benzotriazole, 5-methyl-	133	C7H7N3	000136-85-6	97
3		2H-Indol-2-one, 1,3-dihydro-	133	C8H7NO	000059-48-3	74
4		Benzene, 1-azido-2-methyl-	133	C7H7N3	031656-92-5	64
5		Styrene	104	C8H8	000100-42-5	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121922\
Data File : BF131695.D
Acq On : 19 Dec 2022 18:33
Operator : CG\JU
Sample : N6087-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
12-15-2022-HOWE-AVE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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
Hexanoic acid, ...	7.975	20.0	ng	53460200	2	8.163	53460200	20.0
unknown8.834	8.834	14.0	ng	37532300	2	8.163	53460200	20.0
Neodecanoic acid	9.028	9.6	ng	25518800	2	8.163	53460200	20.0
unknown9.128	9.128	498.0	ng	14995700	3	9.957	602223	20.0
Butanoic acid, ...	9.151	74.0	ng	2229240	3	9.957	602223	20.0
unknown9.181	9.181	26.6	ng	800039	3	9.957	602223	20.0
Thiophane, propyl-	9.198	29.9	ng	899517	3	9.957	602223	20.0
unknown9.328	9.328	44.2	ng	1332040	3	9.957	602223	20.0
1H-Benzotriazol...	10.145	82.4	ng	2479960	3	9.957	602223	20.0
1H-Benzotriazol...	10.369	126.4	ng	3804890	3	9.957	602223	20.0