

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022723\
 Data File : BF132555.D
 Acq On : 27 Feb 2023 16:32
 Operator : CG\JU
 Sample : 01703-05
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 T2-STONE

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: BF132555.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.237	403	408	416	rVB	1576670	1918085	53.43%	6.494%
2	5.631	471	475	478	rBV	3197612	2883944	80.33%	9.764%
3	6.019	537	541	545	rBV	78034	63501	1.77%	0.215%
4	6.631	640	645	648	rBV	3122619	3005447	83.71%	10.175%
5	7.001	705	708	712	rVB	1118673	880043	24.51%	2.979%
6	7.566	800	804	807	rBV	2326607	2060418	57.39%	6.975%
7	7.913	859	863	869	rBV	73003	78611	2.19%	0.266%
8	8.289	923	927	930	rBV	1395217	1097774	30.58%	3.716%
9	9.366	1106	1110	1113	rBV	4503112	3590104	100.00%	12.154%
10	9.430	1118	1121	1125	rVV	64865	57329	1.60%	0.194%
11	9.754	1173	1176	1179	rBV	118846	123947	3.45%	0.420%
12	9.789	1179	1182	1184	rBV3	64601	63551	1.77%	0.215%
13	9.913	1200	1203	1205	rBV2	78706	75513	2.10%	0.256%
14	9.960	1208	1211	1214	rVB3	103995	116534	3.25%	0.395%
15	10.054	1223	1227	1229	rVB	1210137	1107140	30.84%	3.748%
16	10.366	1277	1280	1281	rBV3	104025	104506	2.91%	0.354%
17	10.460	1294	1296	1300	rVB2	146229	123820	3.45%	0.419%
18	10.689	1333	1335	1340	rVB	244149	229949	6.41%	0.778%
19	10.766	1345	1348	1350	rVV	672235	506370	14.10%	1.714%
20	10.848	1358	1362	1366	rBV	1633451	1641903	45.73%	5.559%
21	10.960	1378	1381	1384	rBV	566698	458577	12.77%	1.553%
22	11.430	1458	1461	1463	rBV	447744	422304	11.76%	1.430%
23	11.548	1478	1481	1484	rBV	1013758	1026954	28.61%	3.477%
24	12.066	1566	1569	1572	rBV2	420991	421648	11.74%	1.427%
25	12.348	1615	1617	1621	rBV	630741	446671	12.44%	1.512%
26	13.142	1749	1752	1757	rVB	2672609	2589225	72.12%	8.766%
27	14.171	1924	1927	1930	rVB	489446	416689	11.61%	1.411%
28	14.207	1931	1933	1940	rVB	780873	838024	23.34%	2.837%
29	15.765	2195	2198	2207	rVB	507556	717770	19.99%	2.430%
30	16.530	2323	2328	2335	rVB	543793	1099480	30.63%	3.722%
31	17.001	2403	2408	2421	rVB	694224	1372121	38.22%	4.645%

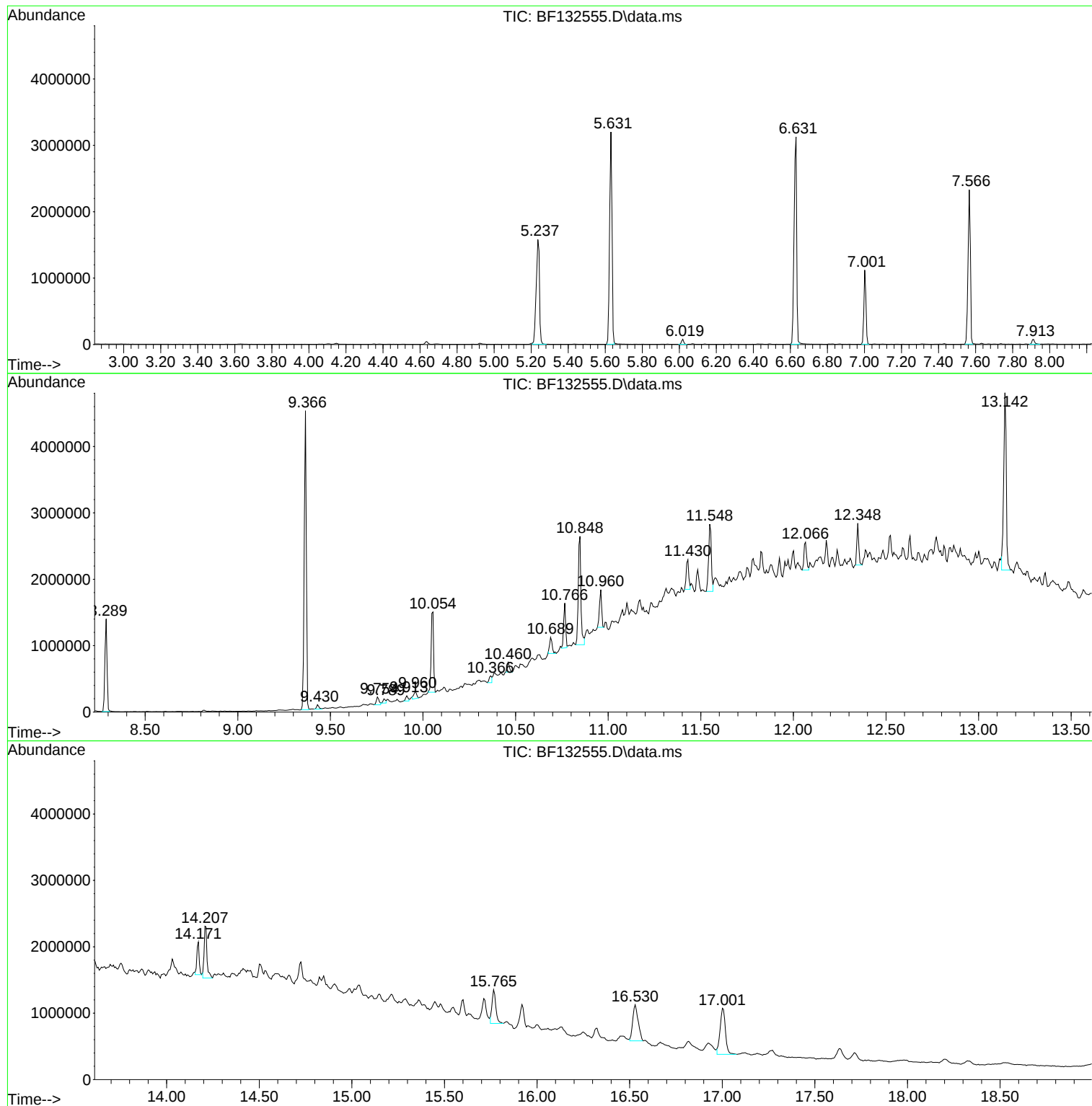
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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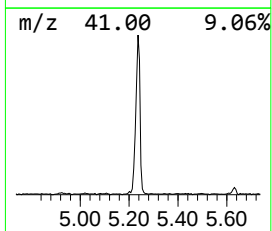
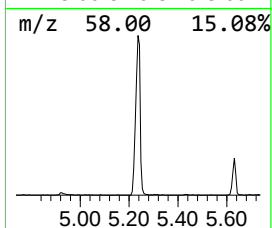
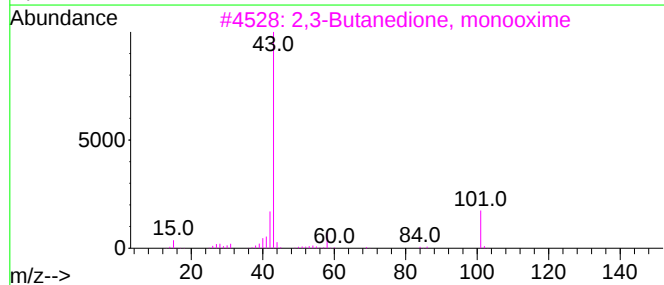
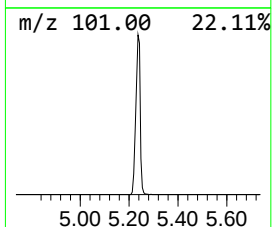
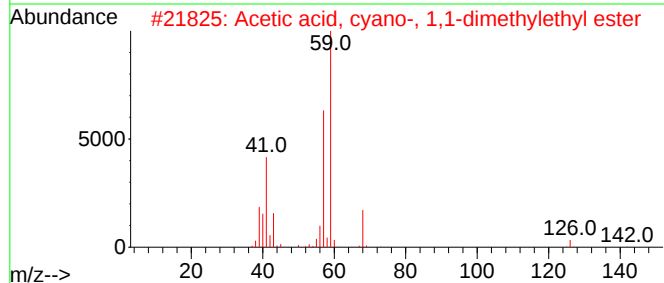
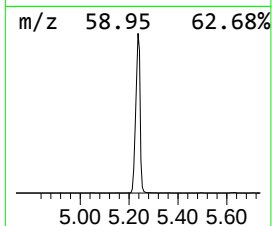
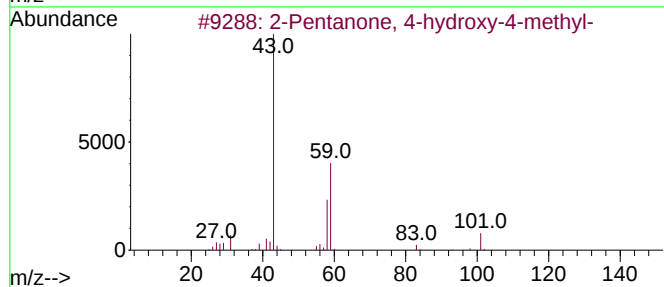
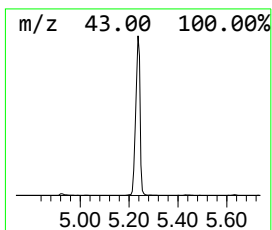
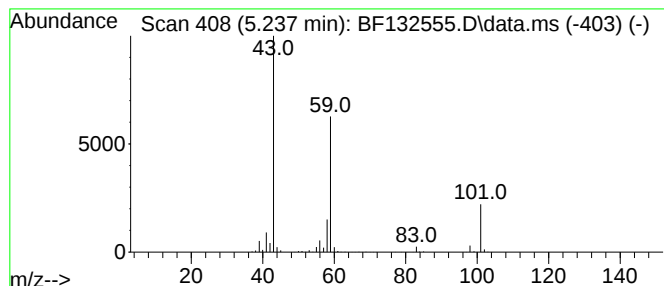
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.237	43.59 ng	1918090	1,4-Dichlorobenzene-d4	7.001

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	17
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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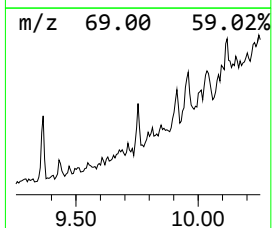
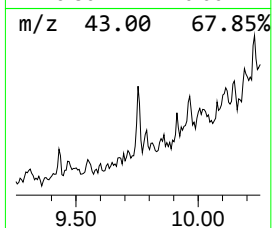
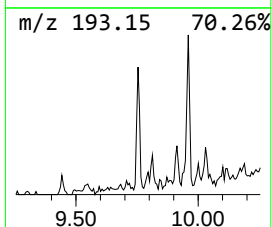
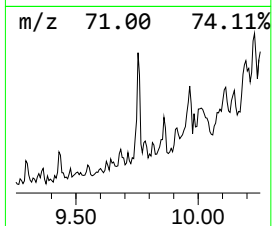
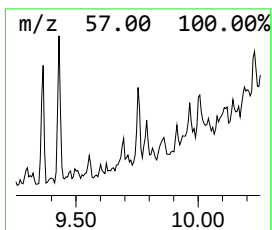
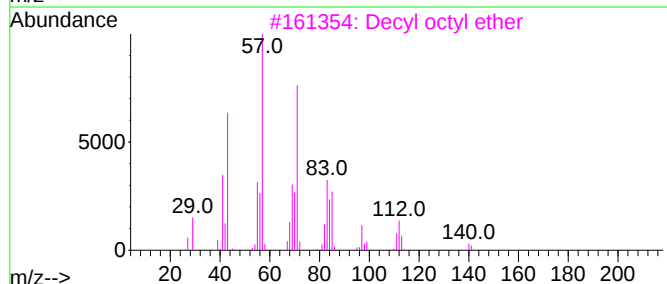
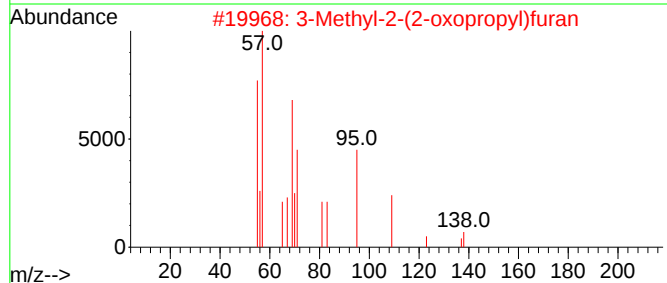
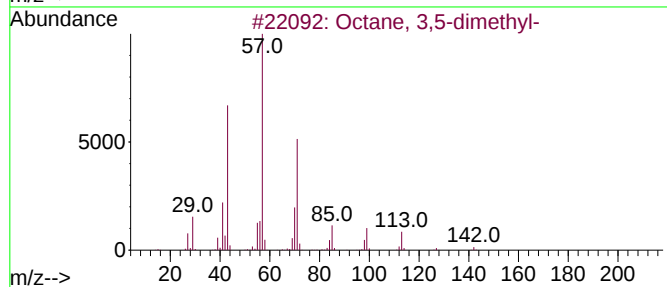
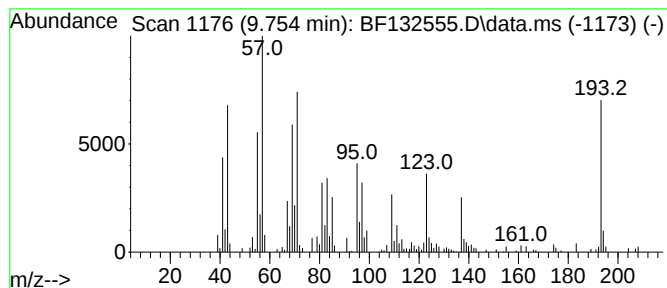
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown9.754 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.754	2.24 ng	123947	Acenaphthene-d10	10.054

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3,5-dimethyl-		142	C10H22		015869-93-9	35
2	3-Methyl-2-(2-oxopropyl)furan		138	C8H10O2		087773-62-4	30
3	Decyl octyl ether		270	C18H38O		1000406-38-3	30
4	2,6,10-Trimethylundeca-1,3-diene		194	C14H26		1000222-09-1	25
5	Decane, 2,3,5,8-tetramethyl-		198	C14H30		192823-15-7	25



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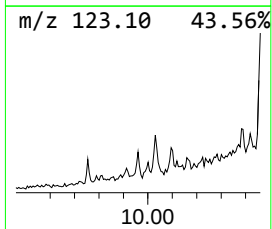
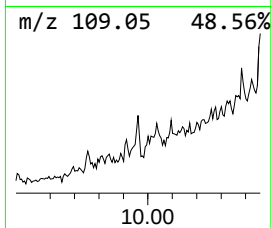
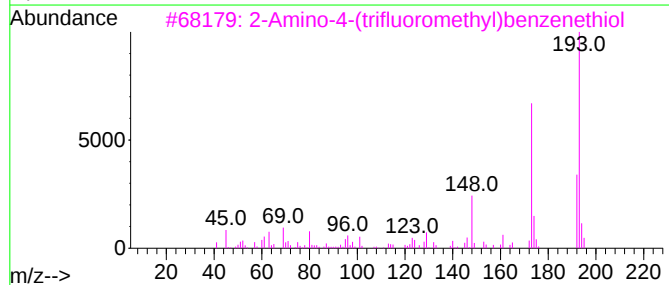
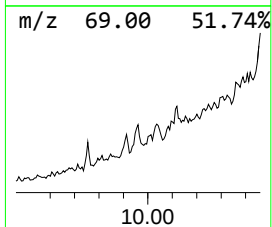
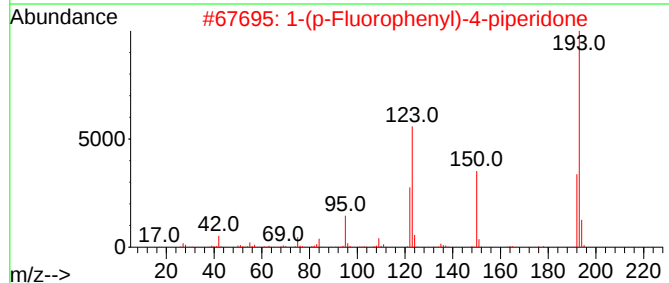
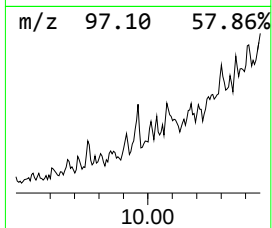
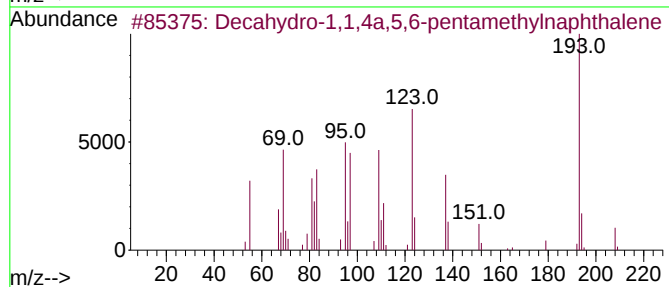
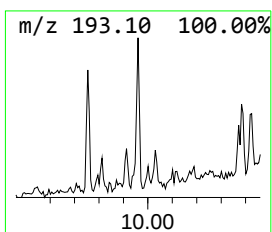
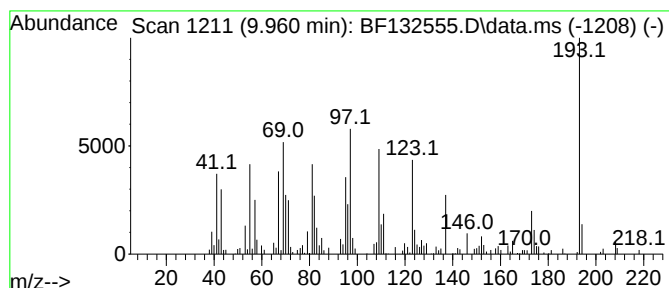
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown9.960 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.960	2.11 ng	116534	Acenaphthene-d10	10.054

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	38
2			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	30
3			2-Amino-4-(trifluoromethyl)benze...	193	C7H6F3NS	004274-38-8	27
4			2-Anthracenamine	193	C14H11N	000613-13-8	27
5			Neopentylidenecyclohexane	152	C11H20	039546-80-0	14



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Misc :
ALS Vial : 12 Sample Multiplier: 1

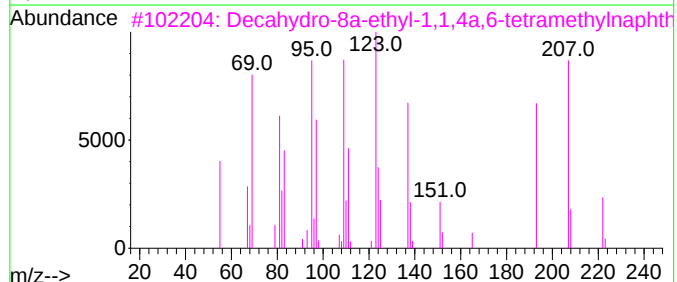
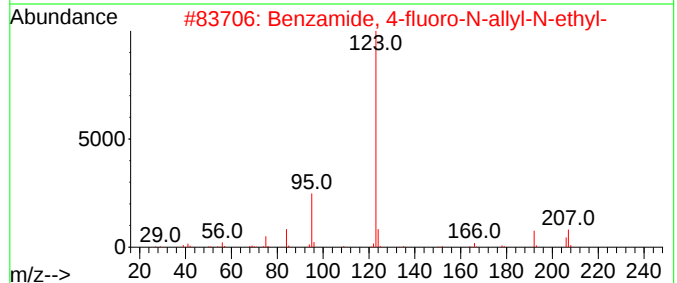
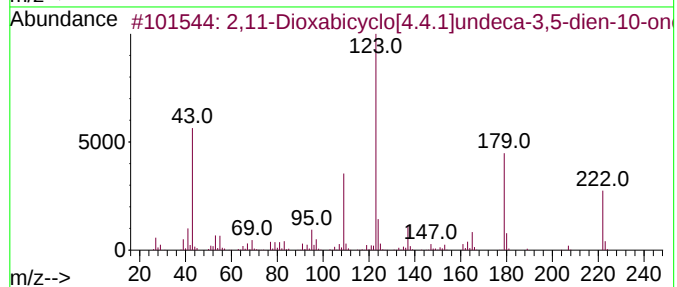
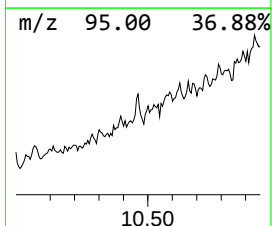
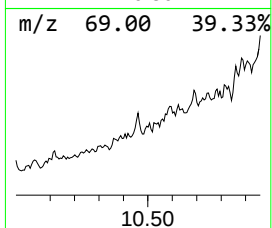
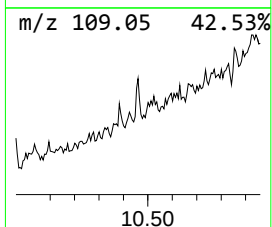
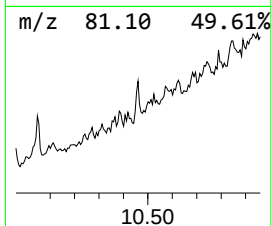
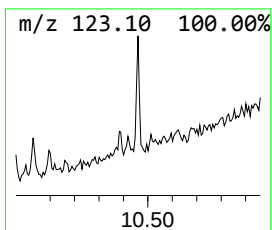
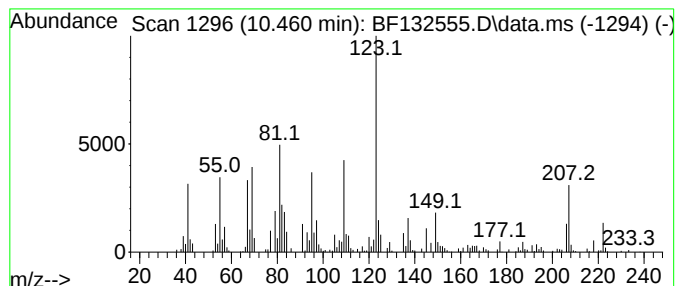
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Peak Number 4 2,11-Dioxabicyclo[4.4.1]und... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.460	2.24 ng	123820	Acenaphthene-d10	10.054	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,11-Dioxabicyclo[4.4.1]undeca-3...	222	C13H18O3	070412-52-1	53
2	Benzamide, 4-fluoro-N-allyl-N-et...	207	C12H14FNO	1000446-42-7	49
3	Decahydro-8a-ethyl-1,1,4a,6-tetr...	222	C16H30	1000100-23-6	49
4	6-Methyl-6-(5-methyl-furan-2-yl)...	206	C13H18O2	077822-40-3	43
5	Bicyclo[4.1.0]heptane-7-carboxam...	222	C11H14N2O5	329912-72-3	43



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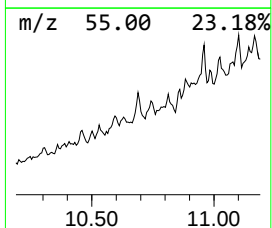
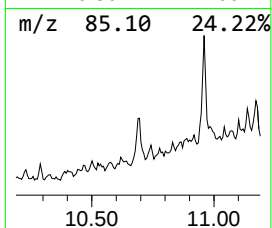
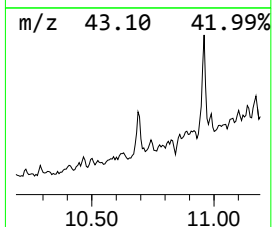
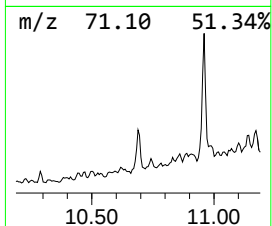
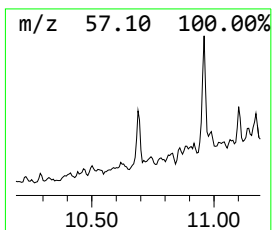
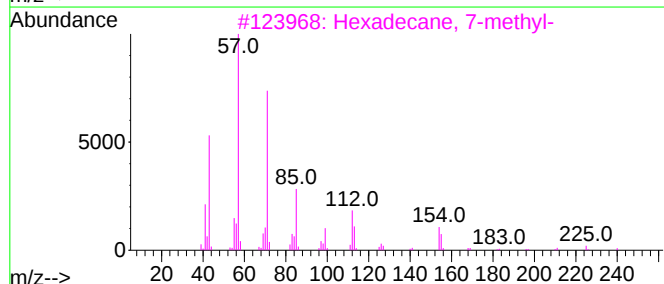
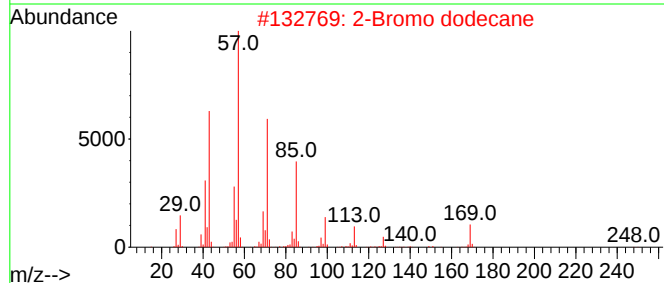
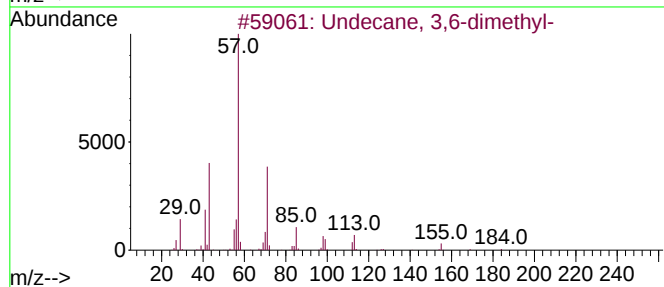
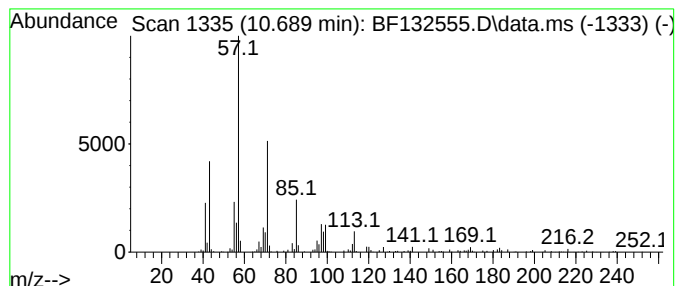
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Peak Number 5 Undecane, 3,6-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.689	4.15 ng	229949	Acenaphthene-d10	10.054

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	76
2			2-Bromo dodecane	248	C12H25Br	013187-99-0	70
3			Hexadecane, 7-methyl-	240	C17H36	026730-20-1	59
4			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	53
5			3,5-Dimethyldodecane	198	C14H30	107770-99-0	52



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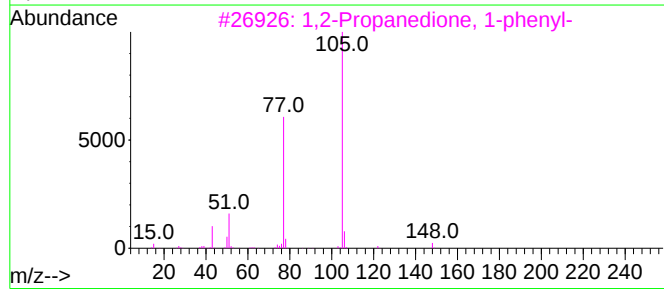
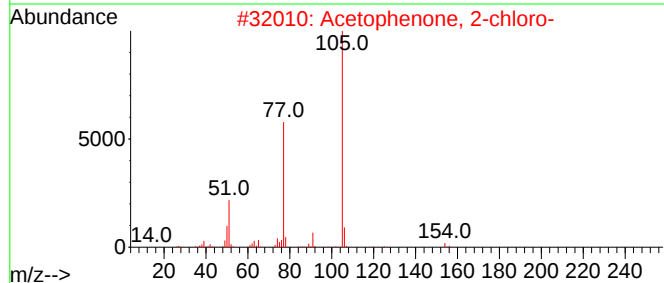
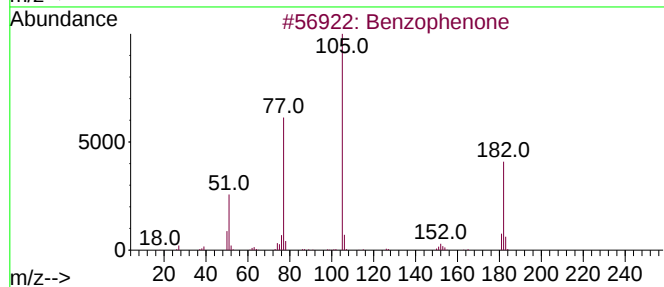
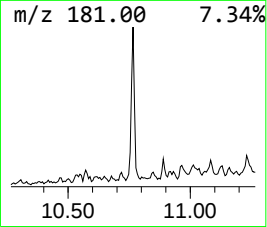
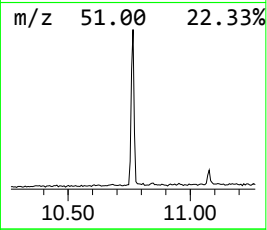
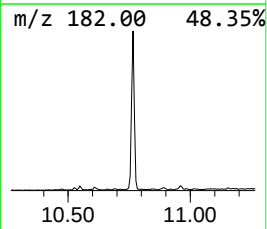
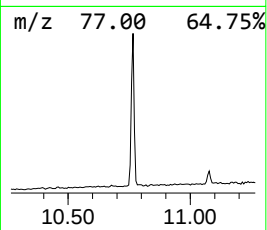
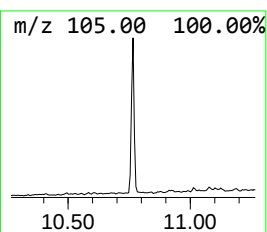
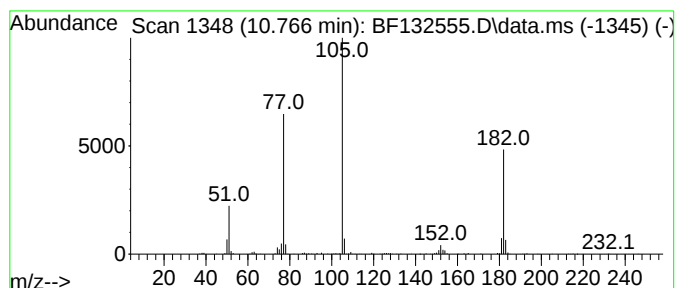
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.766	9.15 ng	506370	Acenaphthene-d10	10.054

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
4			Vinyl benzoate	148	C9H8O2	000769-78-8	47
5			Methyl 2-benzoyl-4-cyanobutanoate	231	C13H13NO3	1010486-83-8	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022723\
Data File : BF132555.D
Acq On : 27 Feb 2023 16:32
Operator : CG\JU
Sample : 01703-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

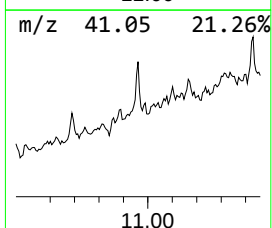
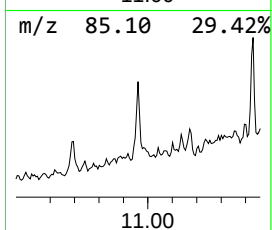
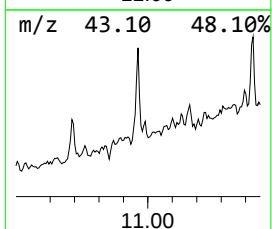
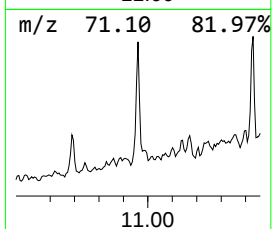
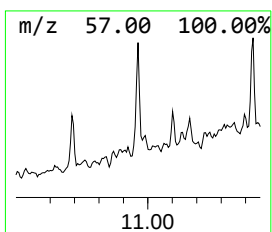
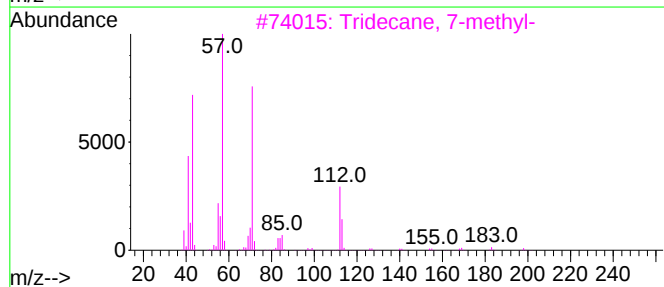
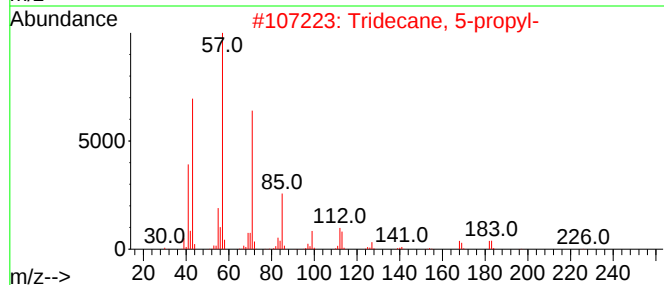
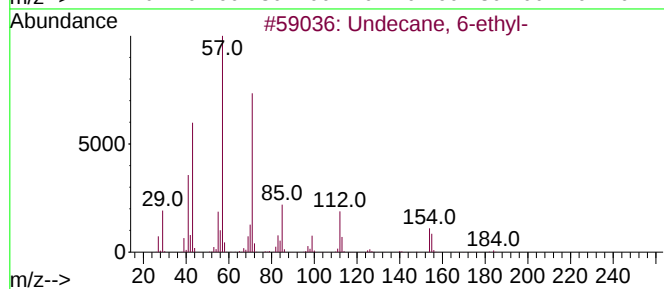
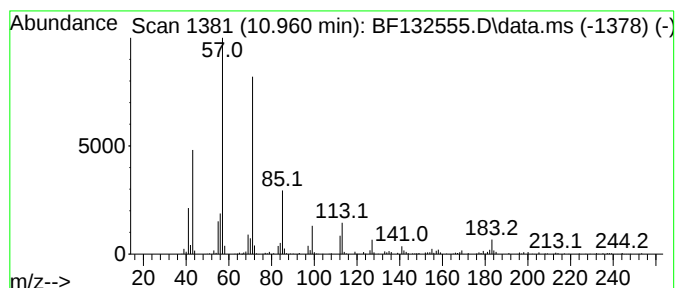
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Undecane, 6-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.960	8.93 ng	458577	Phenanthrene-d10		11.548	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Undecane, 6-ethyl-		184	C13H28	017312-60-6	87
2	Tridecane, 5-propyl-		226	C16H34	055045-11-9	86
3	Tridecane, 7-methyl-		198	C14H30	026730-14-3	70
4	2-Bromo dodecane		248	C12H25Br	013187-99-0	64
5	Octane, 2,6-dimethyl-		142	C10H22	002051-30-1	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022723\
Data File : BF132555.D
Acq On : 27 Feb 2023 16:32
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Sample : 01703-05
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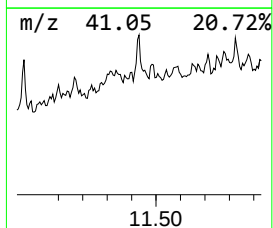
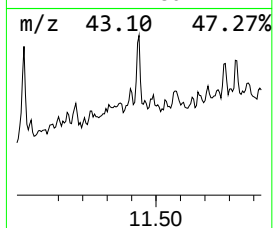
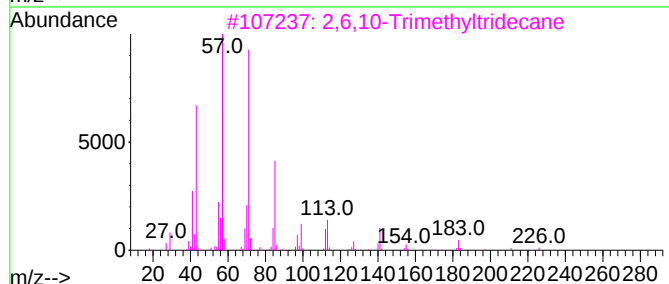
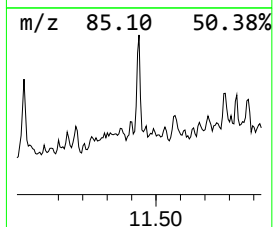
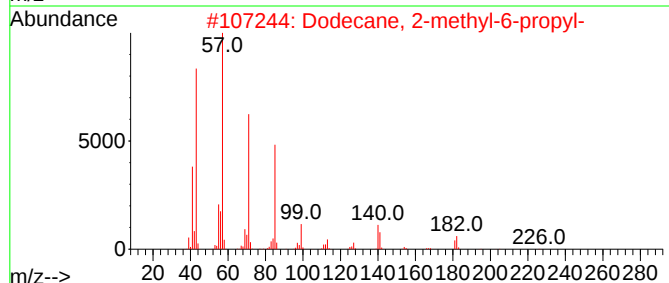
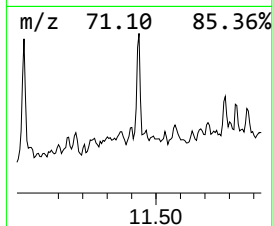
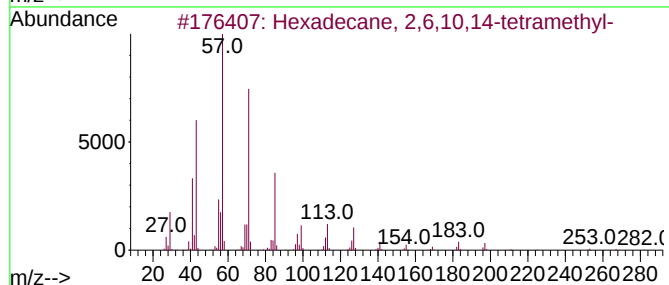
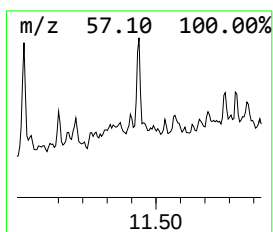
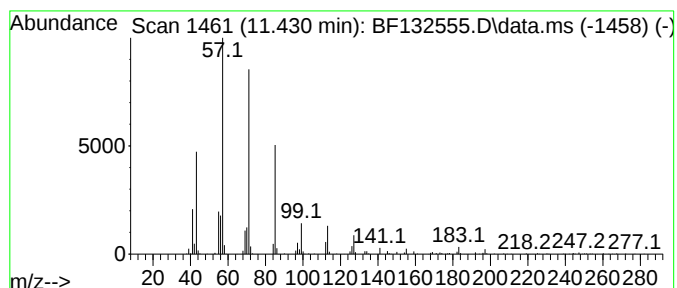
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecane, 2,6,10,14-tetra... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.430	8.22 ng	422304	Phenanthrene-d10		11.548	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-		282	C20H42	000638-36-8	91
2	Dodecane, 2-methyl-6-propyl-		226	C16H34	055045-08-4	87
3	2,6,10-Trimethyltridecane		226	C16H34	003891-99-4	86
4	2-Bromo dodecane		248	C12H25Br	013187-99-0	86
5	Dodecane, 2,6,10-trimethyl-		212	C15H32	003891-98-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022723\
Data File : BF132555.D
Acq On : 27 Feb 2023 16:32
Operator : CG\JU
Sample : 01703-05
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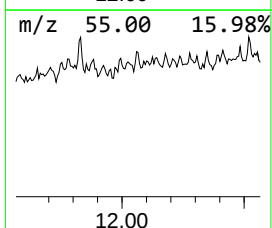
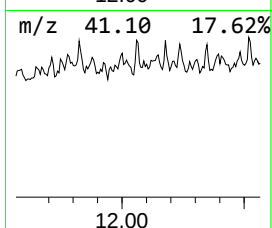
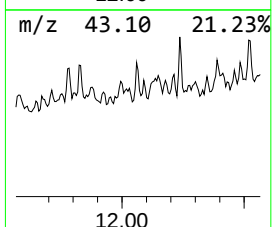
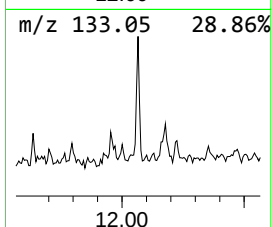
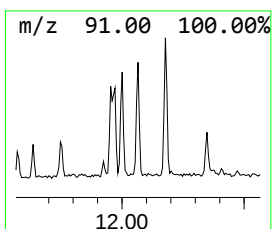
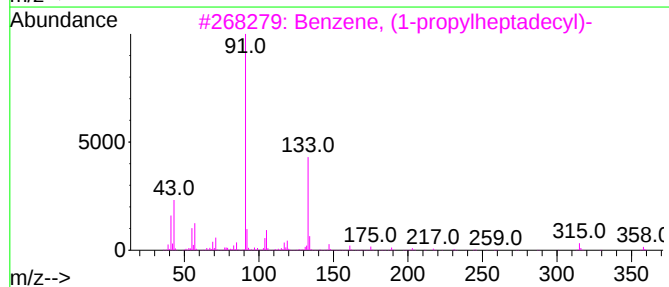
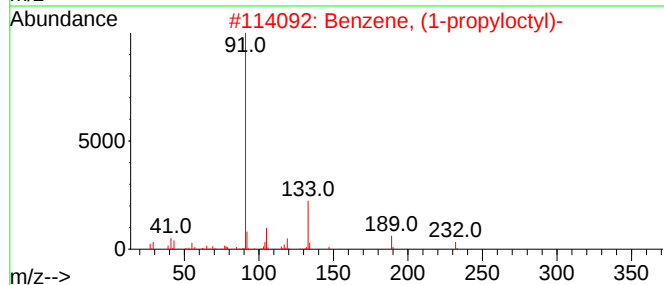
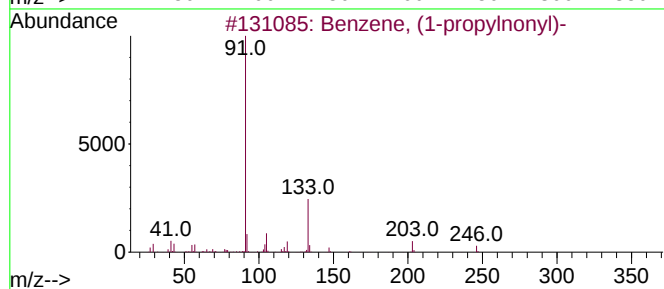
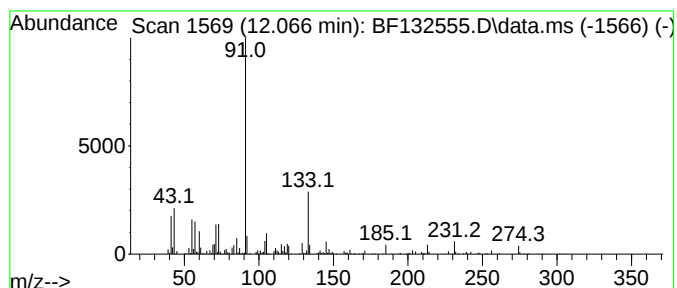
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown12.066 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.066	8.21 ng	421648	Phenanthrene-d10		11.548	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, (1-propylnonyl)-		246	C18H30	002719-64-4	35
2	Benzene, (1-propyloctyl)-		232	C17H28	004536-86-1	25
3	Benzene, (1-propylheptadecyl)-		358	C26H46	002400-03-5	25
4	Benzene, (1-propyldecyl)-		260	C19H32	004534-51-4	22
5	Benzene, (1-propylheptyl)-		218	C16H26	004537-12-6	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022723\
Data File : BF132555.D
Acq On : 27 Feb 2023 16:32
Operator : CG\JU
Sample : 01703-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

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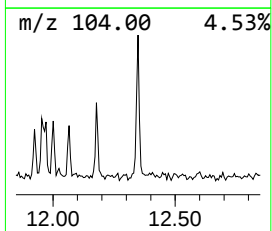
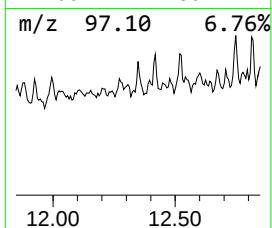
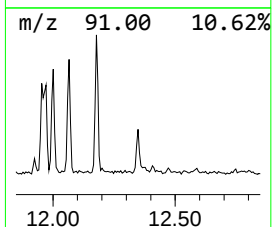
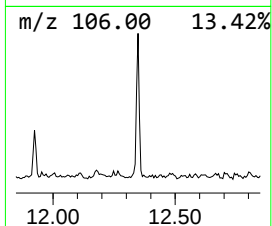
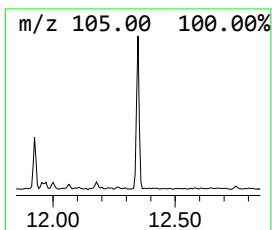
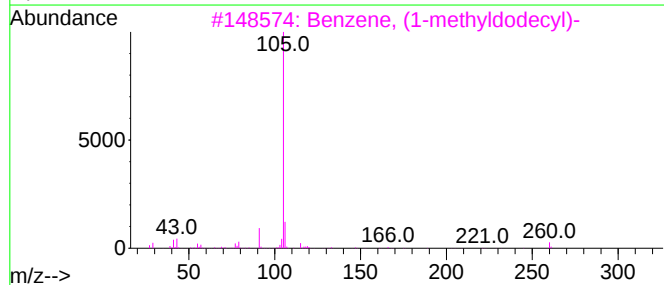
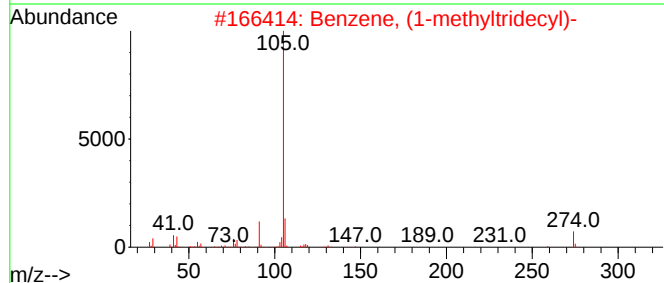
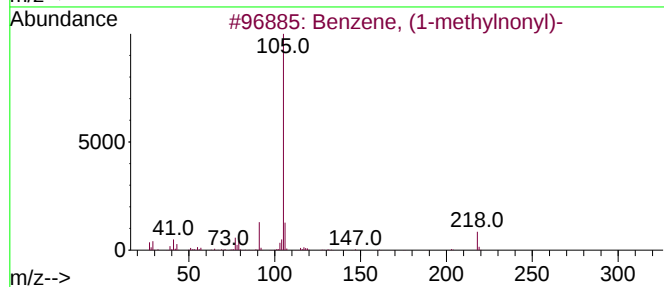
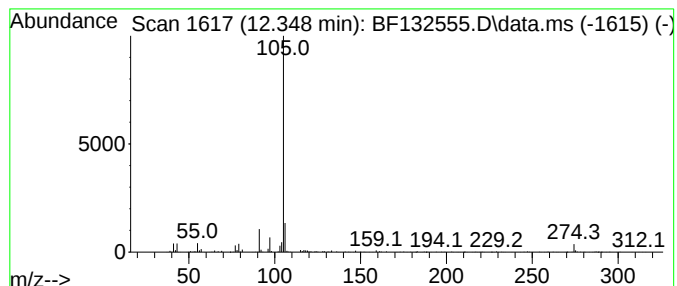
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzene, (1-methylnonyl)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.348	8.70 ng	446671	Phenanthrene-d10	11.548

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, (1-methylnonyl)-	218	C16H26	004537-13-7	59
2		Benzene, (1-methyltridecyl)-	274	C20H34	004534-59-2	58
3		Benzene, (1-methyldodecyl)-	260	C19H32	004534-53-6	53
4		Benzene, (1-methylundecyl)-	246	C18H30	002719-61-1	53
5		Benzene, (1-methyldecyl)-	232	C17H28	004536-88-3	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022723\
Data File : BF132555.D
Acq On : 27 Feb 2023 16:32
Operator : CG\JU
Sample : 01703-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

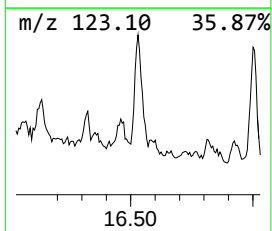
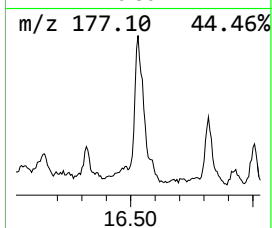
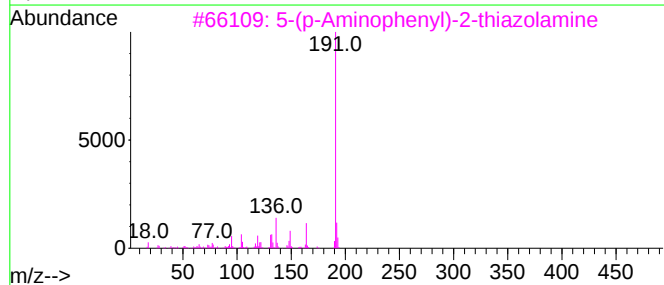
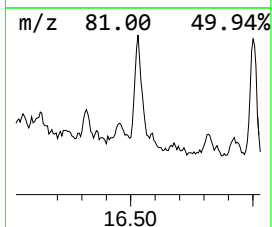
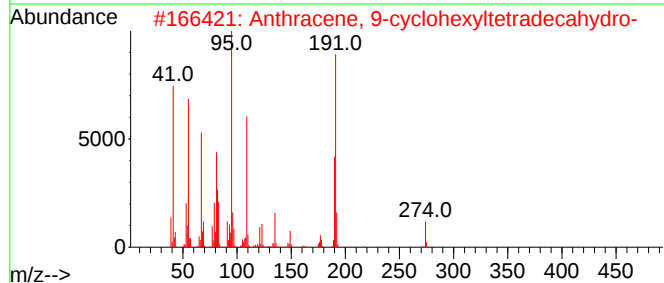
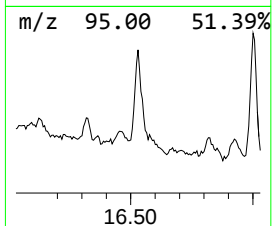
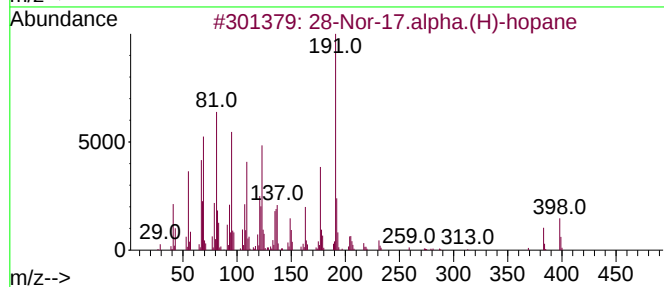
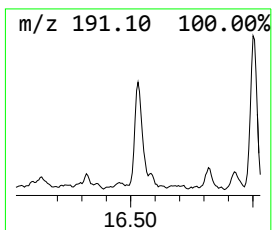
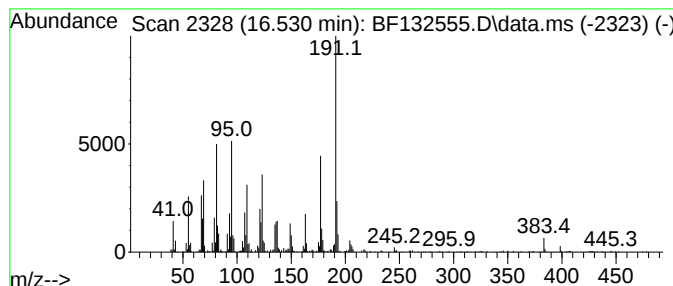
Instrument :
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ClientSampleId :
T2-STONE

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

Peak Number 11 28-Nor-17.alpha.(H)-hopane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.530	30.64 ng	1099480	Perylene-d12	15.765	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	60
2	Anthracene, 9-cyclohexyltetradec...	274	C20H34	055255-70-4	38
3	5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	27
4	Benzamide, 3-fluoro-4-trifluorom...	445	C25H39F4NO	1000437-19-1	22
5	2-Fluoro-3-trifluoromethylbenzoi...	404	C22H32F4O2	1000338-52-3	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022723\
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Acq On : 27 Feb 2023 16:32
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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
T2-STONE

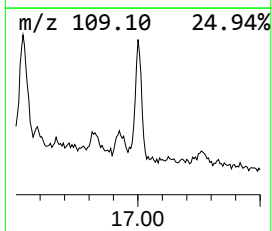
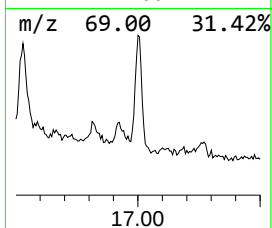
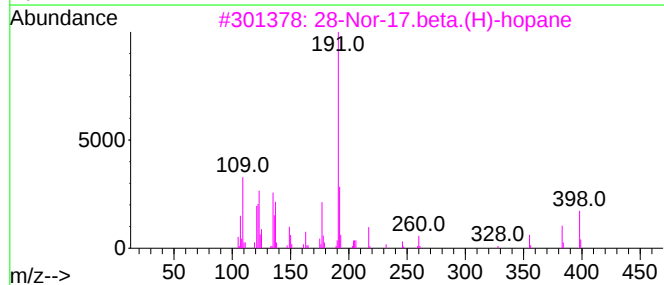
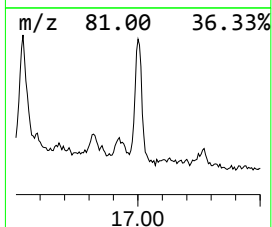
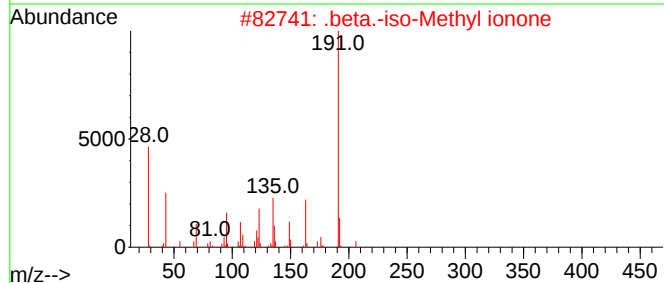
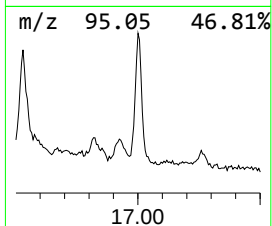
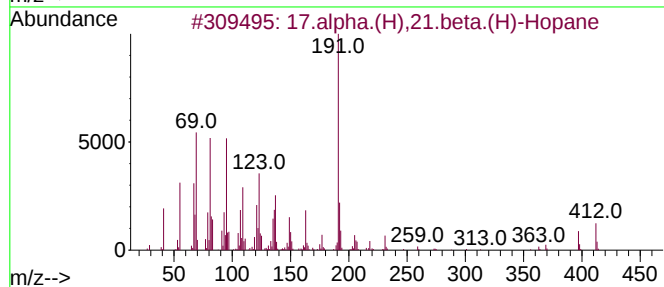
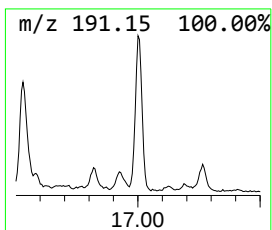
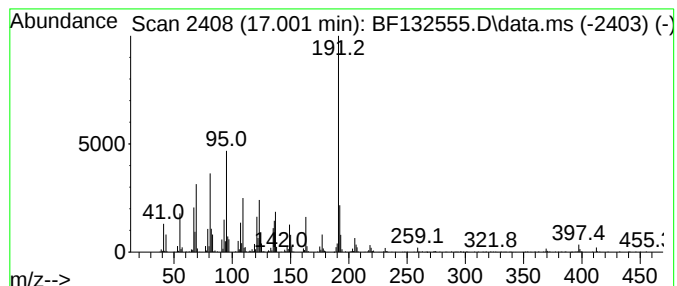
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 17.alpha.(H),21.beta.(H)-Ho... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.001	38.23 ng	1372120	Perylene-d12	15.765

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		17.alpha.(H),21.beta.(H)-Hopane	412	C30H52	013849-96-2	78
2		.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	64
3		28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	64
4		1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	53
5		Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022723\
Data File : BF132555.D
Acq On : 27 Feb 2023 16:32
Operator : CG\JU
Sample : 01703-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T2-STONE

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-...	5.237	43.6	ng	1918090	1	7.001	880043	20.0
unknown9.754	9.754	2.2	ng	123947	3	10.054	1107140	20.0
unknown9.960	9.960	2.1	ng	116534	3	10.054	1107140	20.0
2,11-Dioxabicyc...	10.460	2.2	ng	123820	3	10.054	1107140	20.0
Undecane, 3,6-d...	10.689	4.2	ng	229949	3	10.054	1107140	20.0
Benzophenone	10.766	9.2	ng	506370	3	10.054	1107140	20.0
Undecane, 6-ethyl-	10.960	8.9	ng	458577	4	11.548	1026950	20.0
Hexadecane, 2,6...	11.430	8.2	ng	422304	4	11.548	1026950	20.0
unknown12.066	12.066	8.2	ng	421648	4	11.548	1026950	20.0
Benzene, (1-met...	12.348	8.7	ng	446671	4	11.548	1026950	20.0
28-Nor-17.alpha...	16.530	30.6	ng	1099480	6	15.765	717770	20.0
17.alpha.(H),21...	17.001	38.2	ng	1372120	6	15.765	717770	20.0