

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022023\
 Data File : BM038797.D
 Acq On : 20 Feb 2023 21:27
 Operator : CG/JU
 Sample : 01597-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 NYE-WATER-0217

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_M\Methods\8270-BM020123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM038797.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.957	291	301	308	rBV	95711	133379	3.25%	0.934%
2	5.428	375	381	392	rVB	358015	483035	11.77%	3.383%
3	7.051	651	657	668	rVB	185947	285704	6.96%	2.001%
4	7.875	791	797	804	rBV	162755	237612	5.79%	1.664%
5	9.051	990	997	1007	rVB	483639	774417	18.88%	5.423%
6	10.687	1268	1275	1282	rVB	200844	318700	7.77%	2.232%
7	11.310	1372	1381	1388	rBV2	20056	42494	1.04%	0.298%
8	12.086	1506	1513	1521	rBV	37075	68099	1.66%	0.477%
9	13.151	1687	1694	1701	rVB	1602420	2182837	53.21%	15.286%
10	13.504	1746	1754	1758	rBV4	23334	44326	1.08%	0.310%
11	13.675	1775	1783	1786	rBV	31441	51517	1.26%	0.361%
12	14.533	1922	1929	1934	rBV	323172	496439	12.10%	3.476%
13	15.492	2088	2092	2100	rVB9	24651	56463	1.38%	0.395%
14	15.898	2157	2161	2165	rBV3	28112	50134	1.22%	0.351%
15	16.027	2177	2183	2195	rVB	1459735	1931970	47.09%	13.529%
16	17.280	2391	2396	2401	rVB	396217	542444	13.22%	3.799%
17	17.386	2409	2414	2419	rBV	106350	161878	3.95%	1.134%
18	17.486	2427	2431	2439	rVB3	38530	70680	1.72%	0.495%
19	17.657	2457	2460	2471	rVB4	40511	89850	2.19%	0.629%
20	18.168	2542	2547	2554	rBV3	184555	279667	6.82%	1.958%
21	18.474	2596	2599	2609	rVB5	33996	71358	1.74%	0.500%
22	19.445	2760	2764	2773	rVB	88737	124610	3.04%	0.873%
23	19.904	2837	2842	2847	rBV	3836824	4102645	100.00%	28.730%
24	21.156	3052	3055	3061	rVB2	101270	121272	2.96%	0.849%
25	21.462	3102	3107	3113	rBV	556576	675024	16.45%	4.727%
26	22.674	3310	3313	3318	rVB	74478	101425	2.47%	0.710%
27	23.839	3505	3511	3519	rVB2	401226	782202	19.07%	5.478%

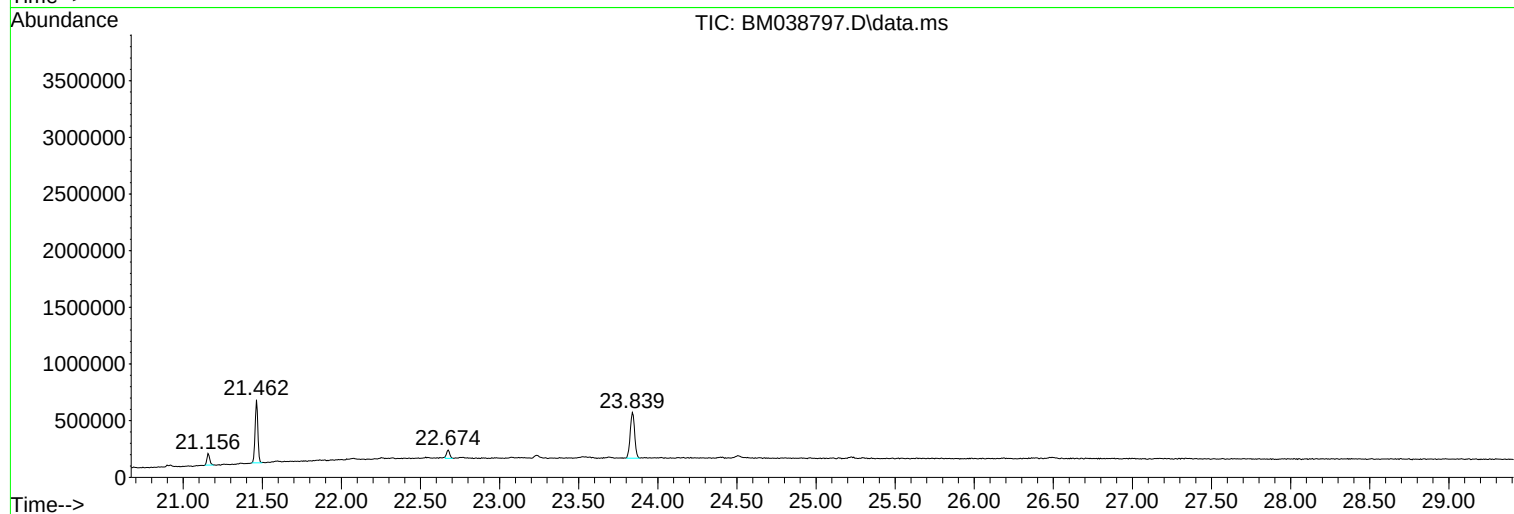
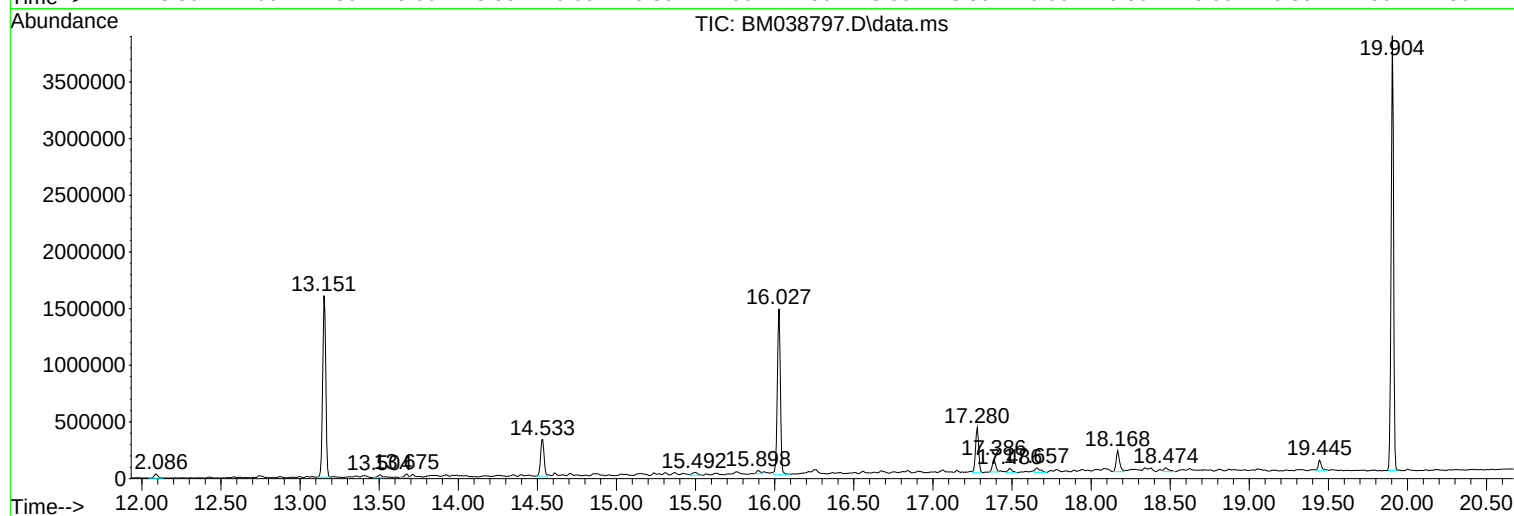
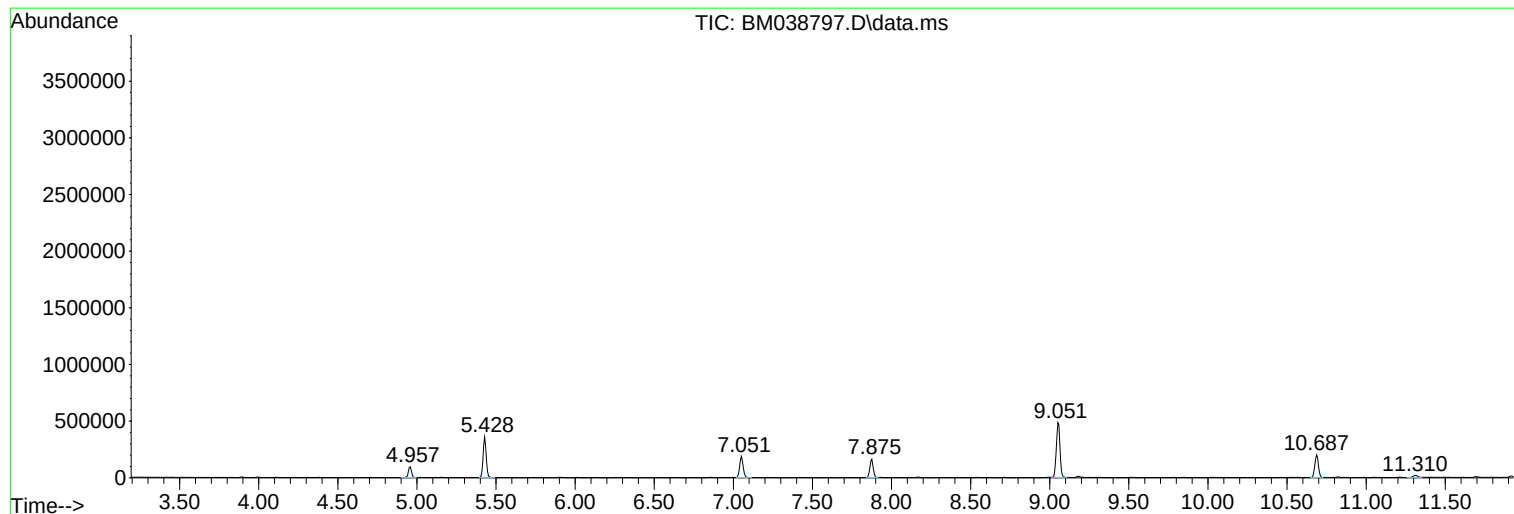
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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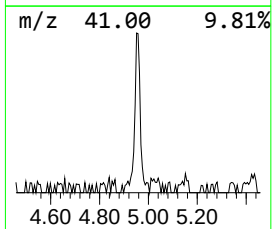
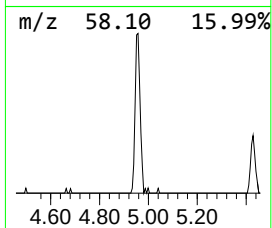
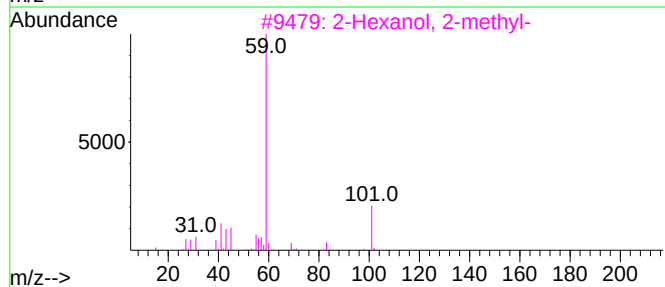
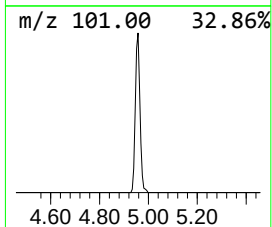
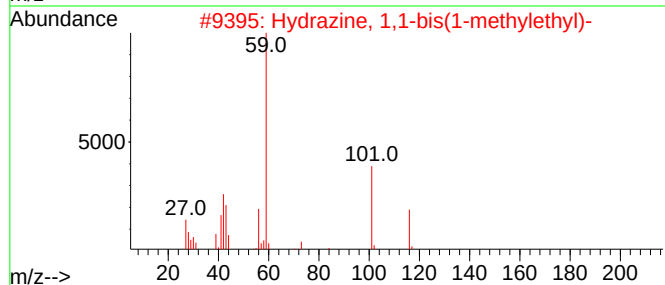
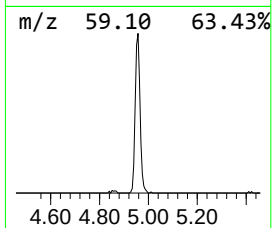
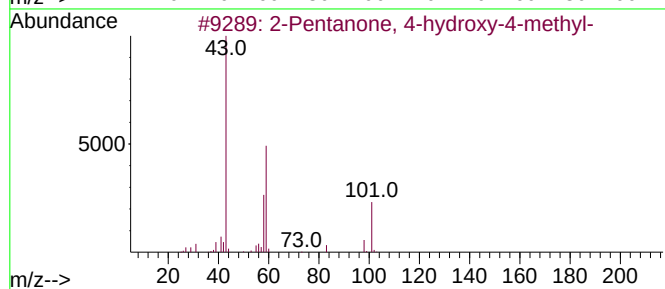
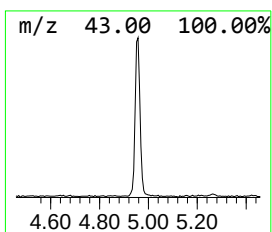
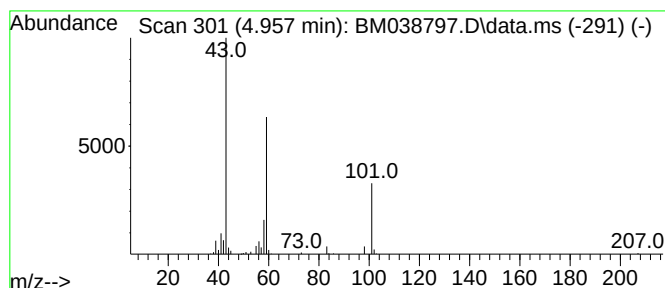
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.957	11.23 ng	133379	1,4-Dichlorobenzene-d4	7.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	43		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	42		
4	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	38		
5	Butanoic acid, 4-iodo-, methyl e...	228	C5H9IO2	014273-85-9	36		



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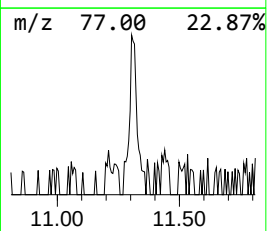
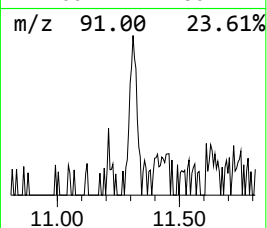
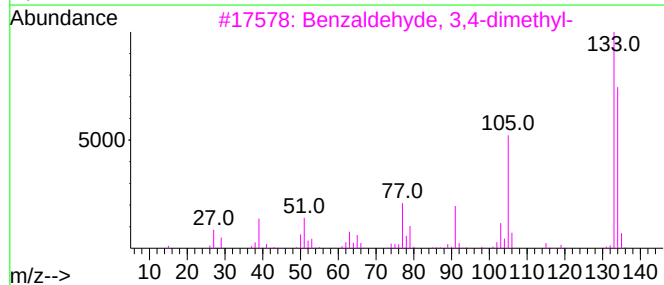
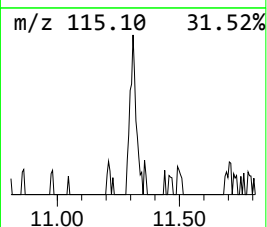
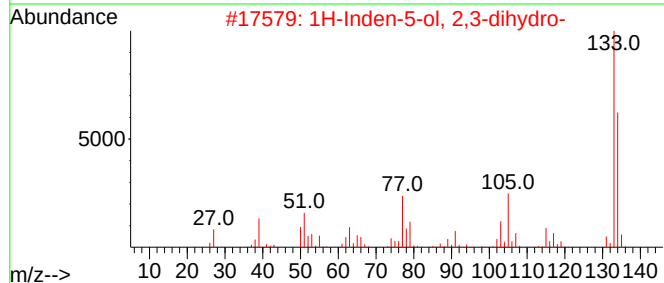
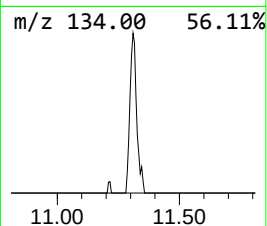
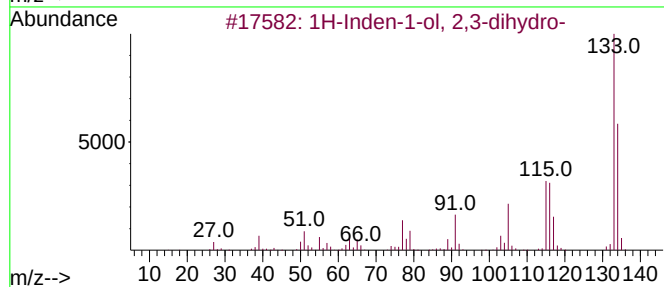
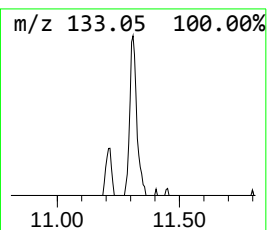
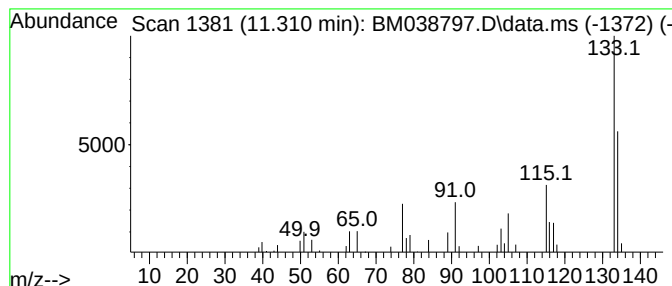
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1H-Inden-1-ol, 2,3-dihydro- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.310	2.67 ng	42494	Naphthalene-d8	10.687

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Inden-1-ol, 2,3-dihydro-	134	C9H10O	006351-10-6	87
2			1H-Inden-5-ol, 2,3-dihydro-	134	C9H10O	001470-94-6	76
3			Benzaldehyde, 3,4-dimethyl-	134	C9H10O	005973-71-7	62
4			Tetrahydroquinoxaline	134	C8H10N2	003476-89-9	50
5			Pyrazine, 2-methyl-6-(1-propenyl...	134	C8H10N2	055138-67-5	49



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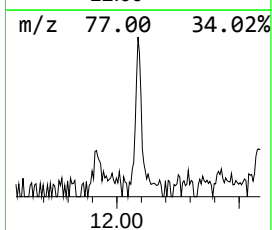
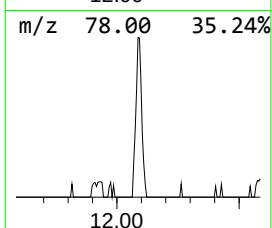
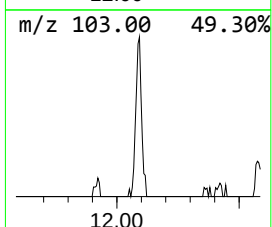
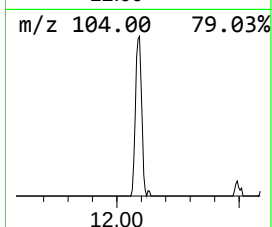
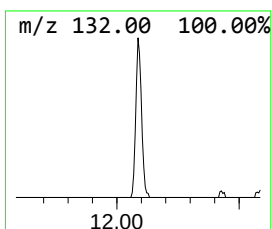
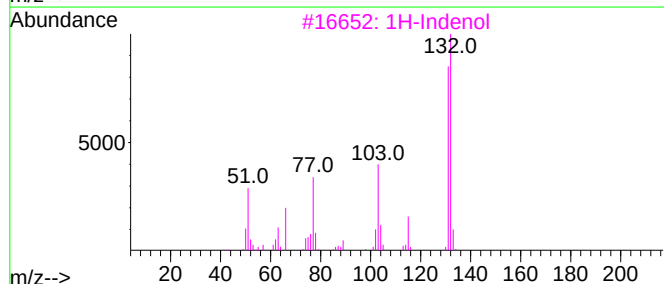
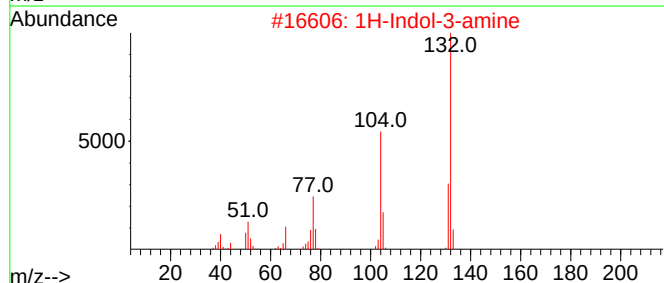
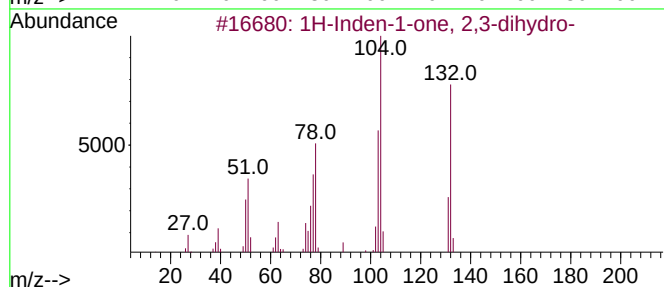
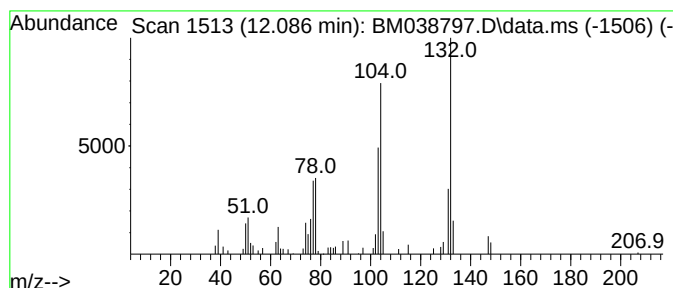
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1H-Inden-1-one, 2,3-dihydro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.086	4.27 ng	68099	Naphthalene-d8	10.687	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Inden-1-one, 2,3-dihydro-	132	C9H8O	000083-33-0	96
2	1H-Indol-3-amine	132	C8H8N2	007250-19-3	81
3	1H-Indenol	132	C9H8O	056631-57-3	49
4	2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	49
5	Benzonitrile, 4-(hydroxymethyl)-	133	C8H7NO	000874-89-5	43



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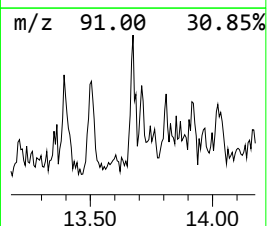
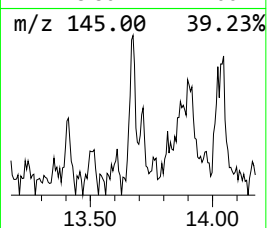
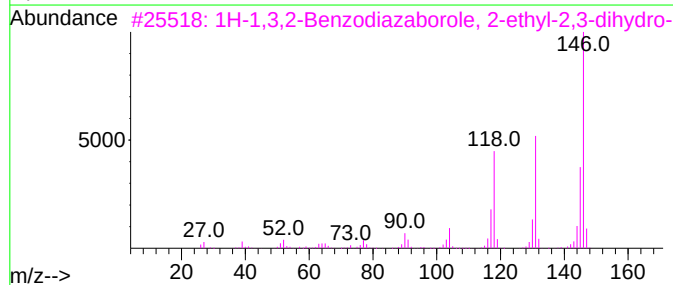
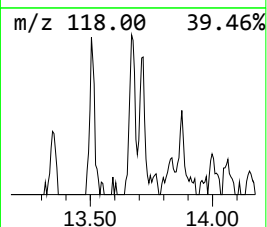
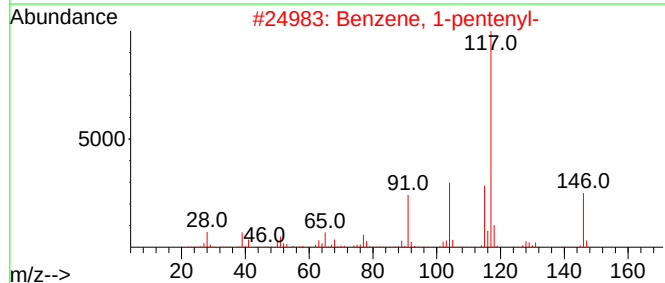
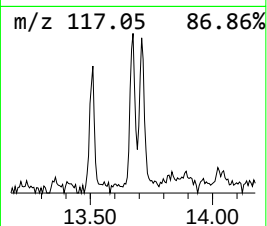
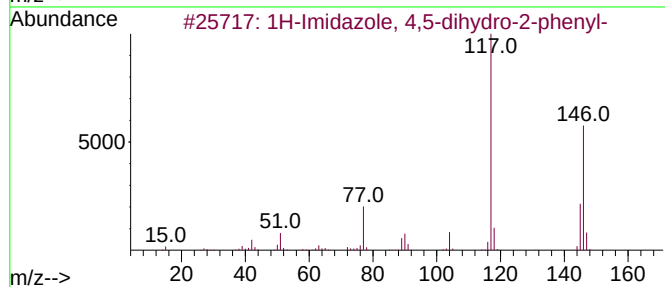
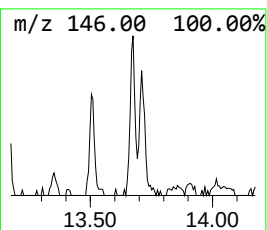
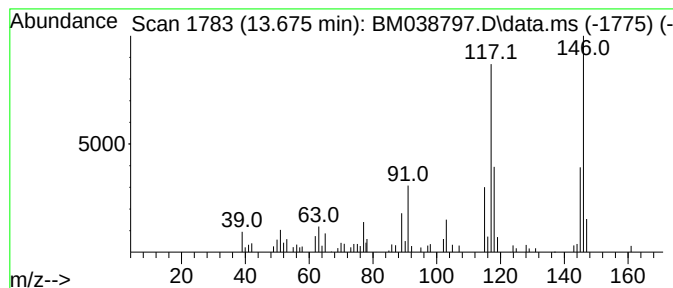
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Peak Number 4 1H-Imidazole, 4,5-dihydro-2... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.675	2.08 ng	51517	Acenaphthene-d10	14.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Imidazole, 4,5-dihydro-2-phenyl-	146	C9H10N2	000936-49-2	68
2			Benzene, 1-pentenyl-	146	C11H14	000826-18-6	52
3			1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	49
4			Indane	118	C9H10	000496-11-7	46
5			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	42



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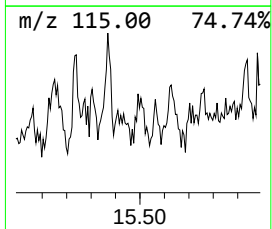
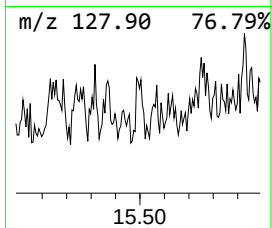
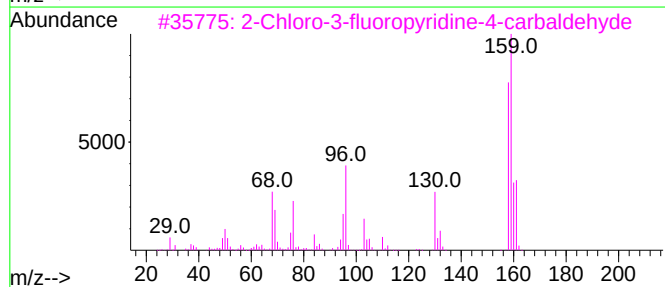
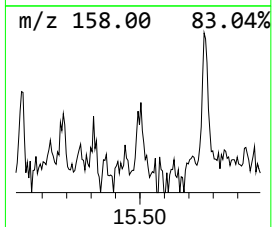
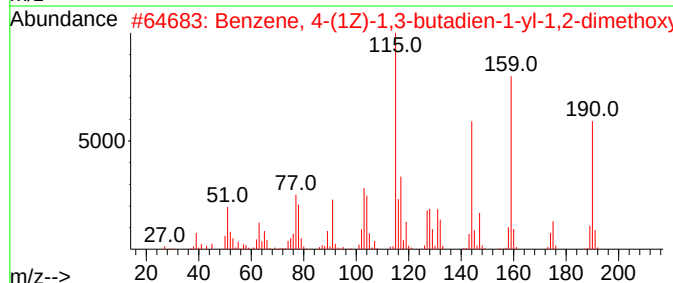
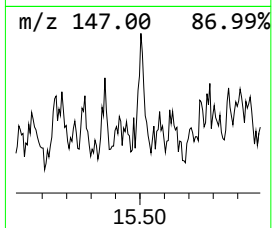
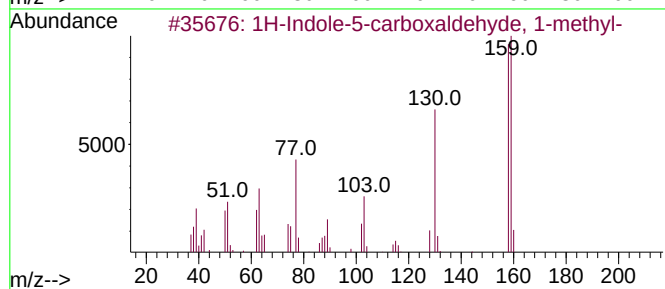
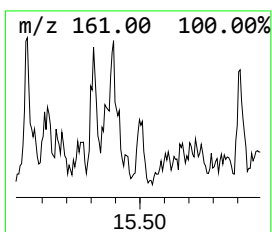
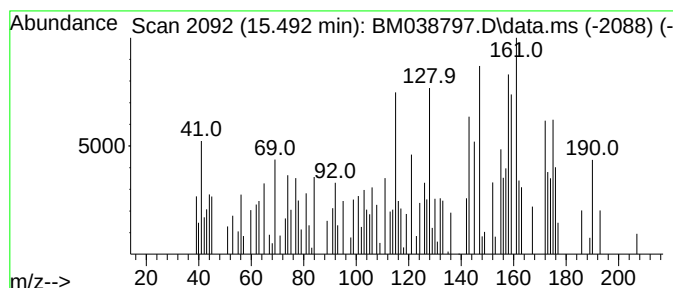
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Peak Number 5 unknown15.492 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.492	2.27 ng	56463	Acenaphthene-d10	14.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indole-5-carboxaldehyde, 1-me...	159	C10H9NO	090923-75-4	18
2			Benzene, 4-(1Z)-1,3-butadien-1-y...	190	C12H14O2	088909-06-2	15
3			2-Chloro-3-fluoropyridine-4-carb...	159	C6H3ClFNO	329794-28-7	14
4			6-Phenyl-3,5-hexadien-2-one	172	C12H12O	004173-44-8	11
5			Benzene, [(2-methylenecyclopropy...	162	C10H10S	078656-80-1	11



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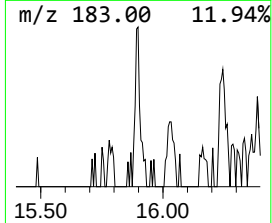
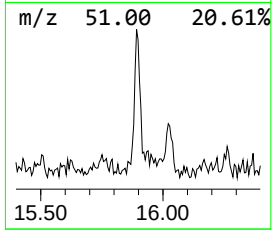
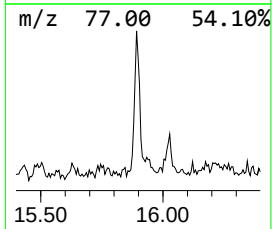
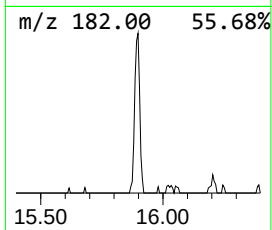
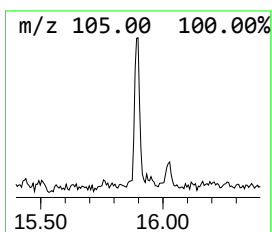
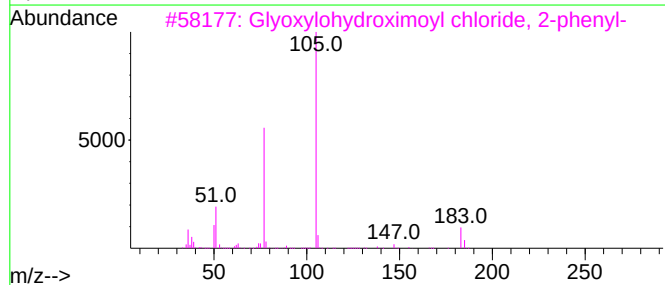
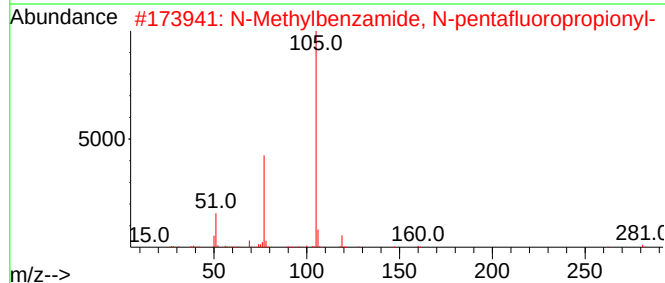
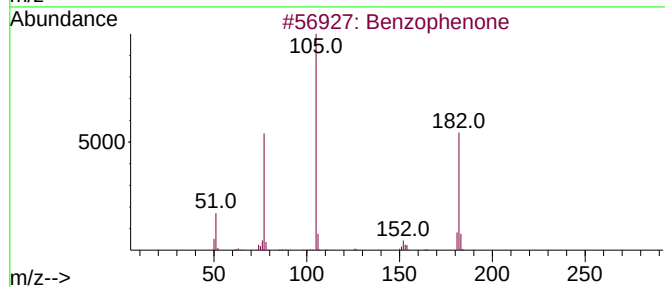
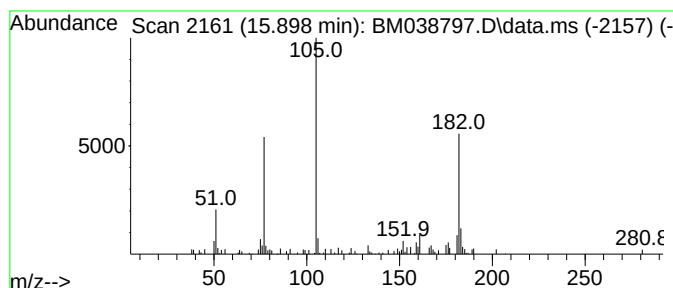
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzophenone Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.898	2.02 ng	50134	Acenaphthene-d10	14.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	94
2			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	49
3			Glyoxylohydroximoyl chloride, 2-...	183	C8H6ClNO2	004937-87-5	49
4			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	43
5			1,3-Butanedione, 2-allyl-1-phenyl-	202	C13H14O2	010225-38-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022023\
Data File : BM038797.D
Acq On : 20 Feb 2023 21:27
Operator : CG/JU
Sample : 01597-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
NYE-WATER-0217

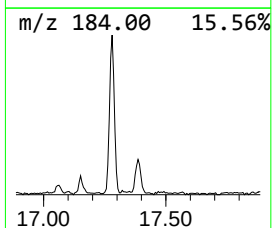
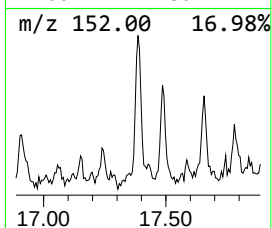
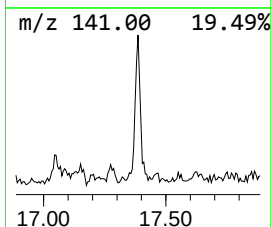
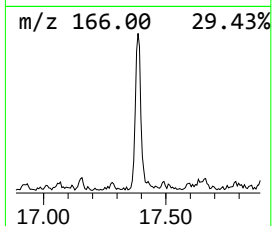
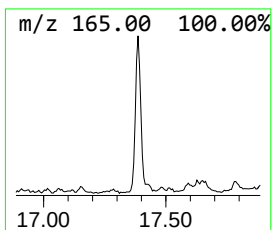
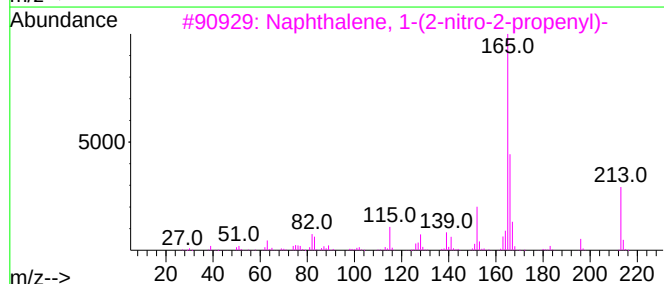
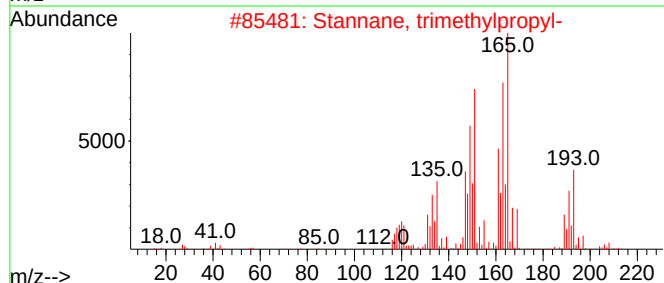
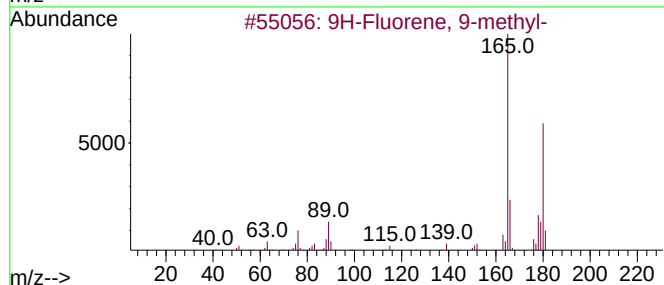
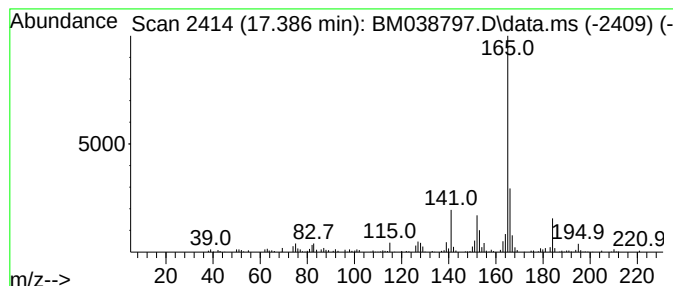
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown17.386 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.386	5.97 ng	161878	Phenanthrene-d10	17.280

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9H-Fluorene, 9-methyl-	180	C14H12	002523-37-7	40
2		Stannane, trimethylpropyl-	208	C6H16Sn	003531-45-1	38
3		Naphthalene, 1-(2-nitro-2-propen...	213	C13H11NO2	080255-13-6	38
4		Diphenylacetyl chloride	230	C14H11ClO	001871-76-7	30
5		1H-Phenylene	166	C13H10	000203-80-5	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022023\
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Sample : 01597-01
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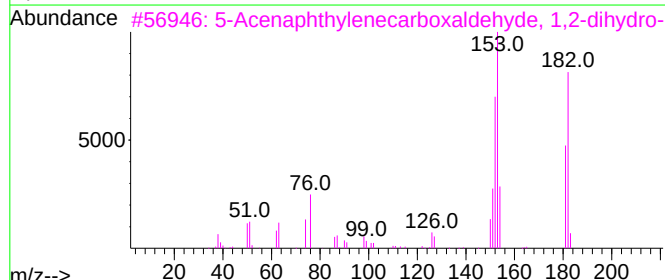
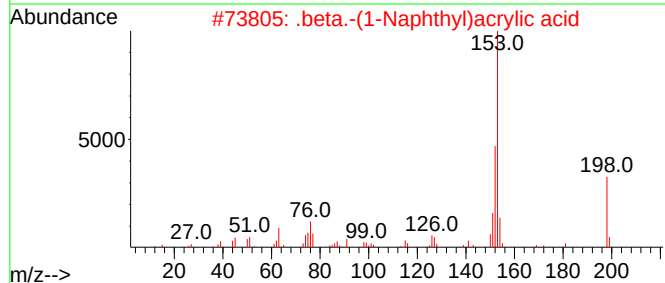
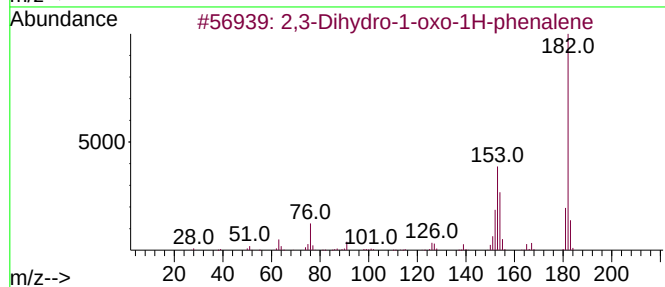
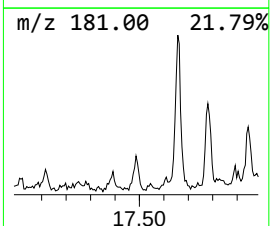
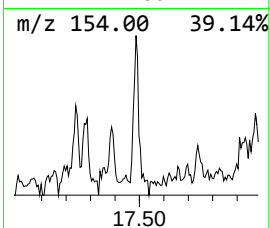
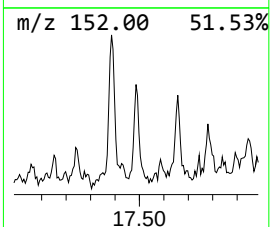
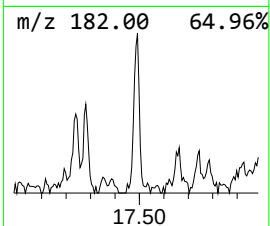
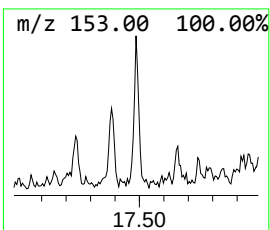
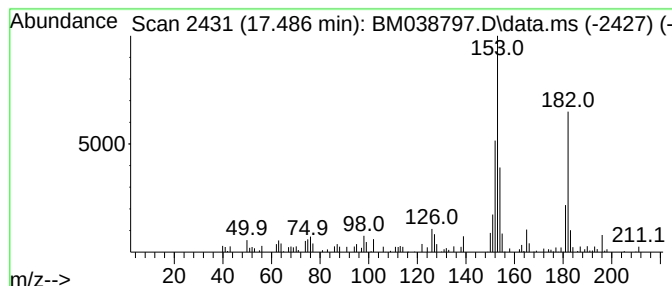
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2,3-Dihydro-1-oxo-1H-phenalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.486	2.61 ng	70680	Phenanthrene-d10	17.280	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Dihydro-1-oxo-1H-phenalene	182	C13H10O	000518-85-4	74
2	.beta.-(1-Naphthyl)acrylic acid	198	C13H10O2	013026-12-5	43
3	5-Acenaphthylenecarboxaldehyde, ...	182	C13H10O	1000362-64-3	43
4	3-Ethoxy-1,4,4a,5,6,7,8,8a-octah...	181	C11H19NO	076097-57-9	35
5	7-Chloro-1H-indole-2,3-dione	181	C8H4ClNO2	007477-63-6	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022023\
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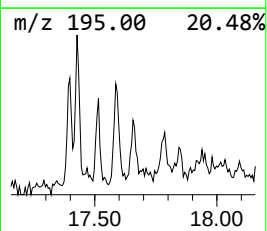
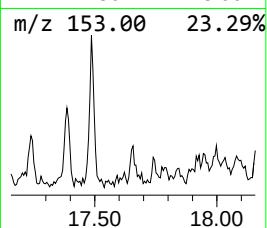
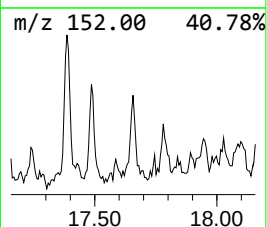
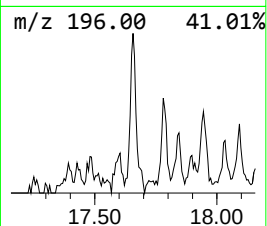
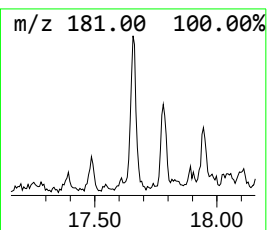
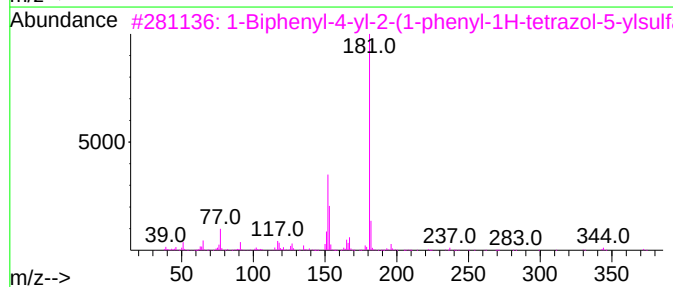
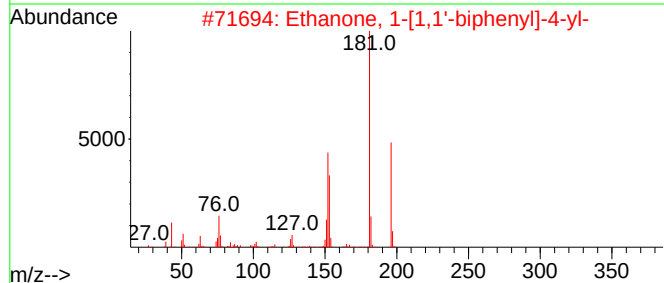
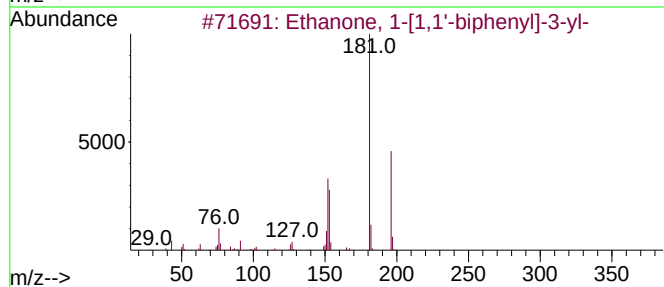
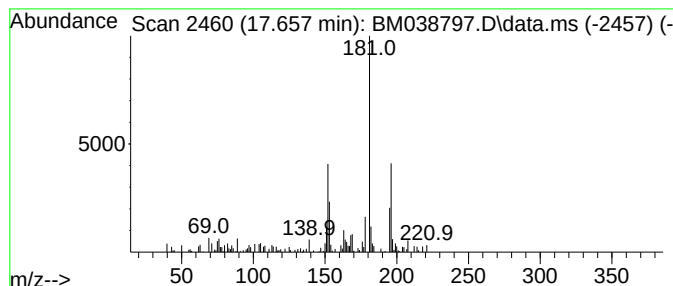
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Ethanone, 1-[1,1'-biphenyl]... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.657	3.31 ng	89850	Phenanthrene-d10	17.280	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-[1,1'-biphenyl]-3-yl-	196	C14H12O	003112-01-4	81
2	Ethanone, 1-[1,1'-biphenyl]-4-yl-	196	C14H12O	000092-91-1	81
3	1-Biphenyl-4-yl-2-(1-phenyl-1H-t...	372	C21H16N4OS	1000300-31-5	50
4	3'-Hydroxy-2',4'-dimethoxyacetop...	196	C10H12O4	1000433-07-3	49
5	9H-Carbazole, 2-methyl-	181	C13H11N	003652-91-3	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022023\
Data File : BM038797.D
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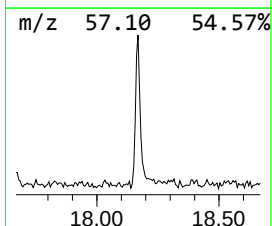
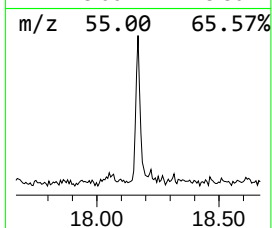
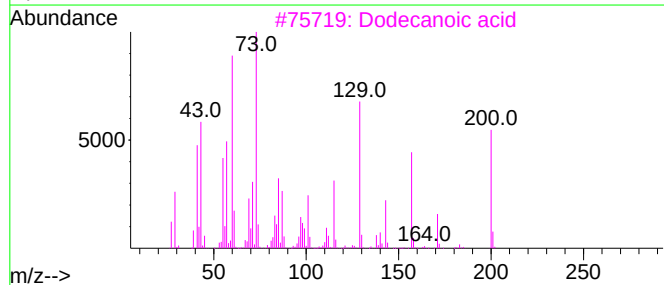
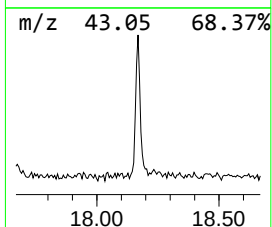
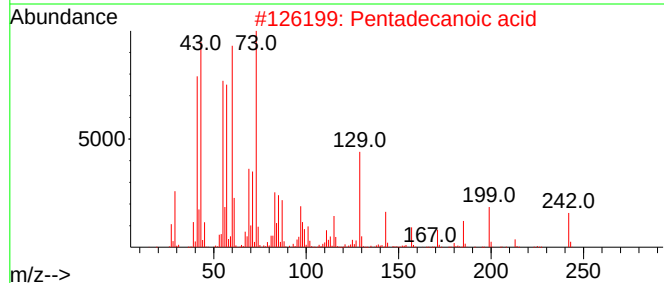
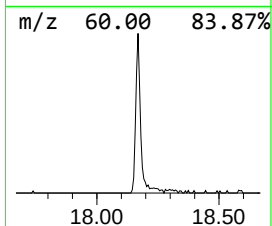
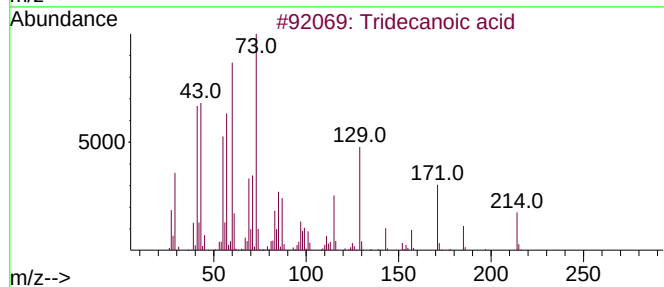
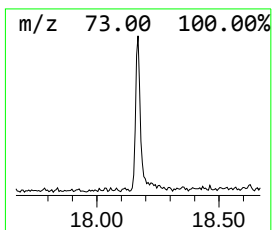
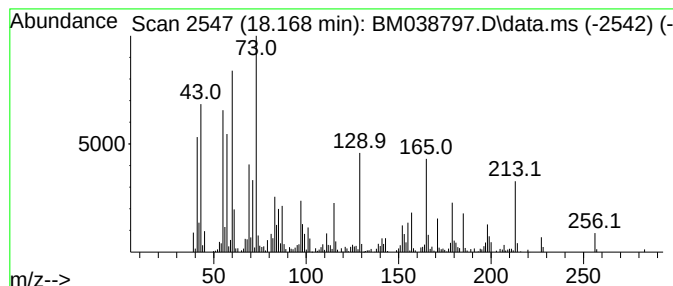
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tridecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.168	10.31 ng	279667	Phenanthrene-d10		17.280	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Tridecanoic acid		214	C13H26O2	000638-53-9	93
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	64
3	Dodecanoic acid		200	C12H24O2	000143-07-7	55
4	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	53
5	Tetradecanoic acid		228	C14H28O2	000544-63-8	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022023\
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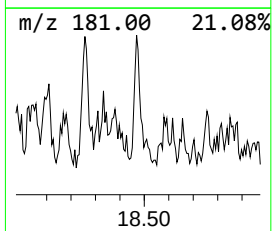
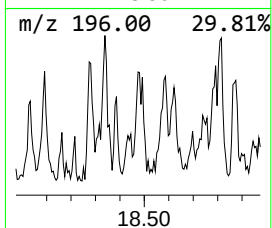
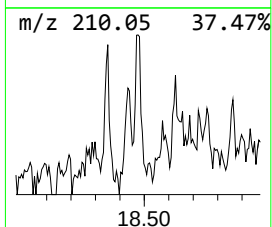
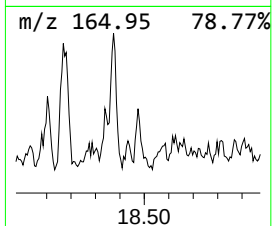
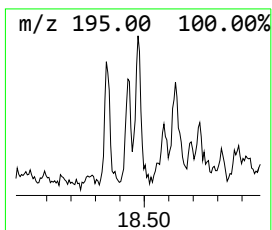
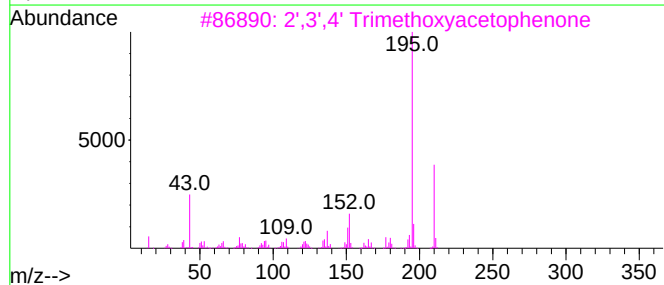
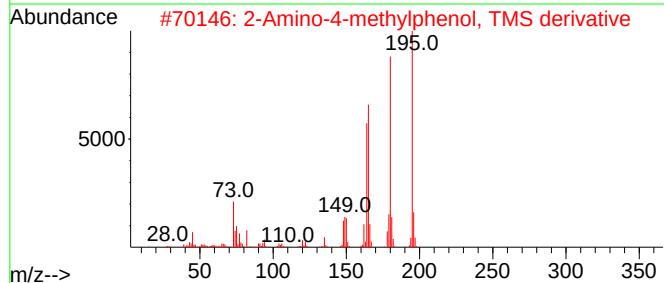
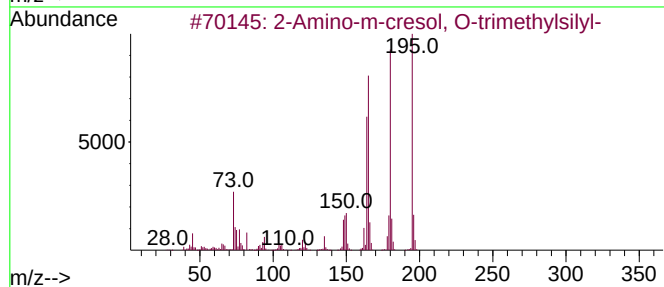
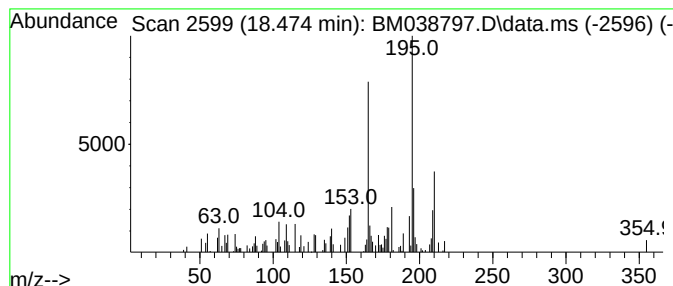
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2-Amino-m-cresol, O-trimeth... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD			R.T.
18.474	2.63 ng	71358	Phenanthrene-d10			17.280
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Amino-m-cresol, O-trimethylsilyl-		195	C10H17NOSi	1000473-45-2	50
2	2-Amino-4-methylphenol, TMS deri...		195	C10H17NOSi	1000373-18-0	43
3	2',3',4' Trimethoxyacetophenone		210	C11H14O4	013909-73-4	30
4	Fluorene-9-methanol		196	C14H12O	024324-17-2	30
5	3-Dimethylaminomethyl-4-(1-pyrro...		210	C11H18N2O2	1010427-46-2	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022023\
Data File : BM038797.D
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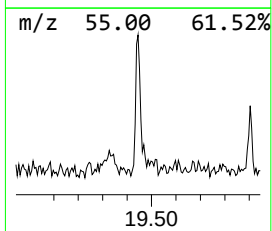
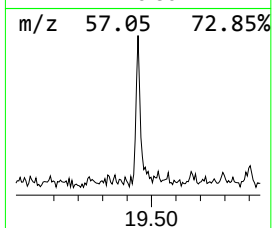
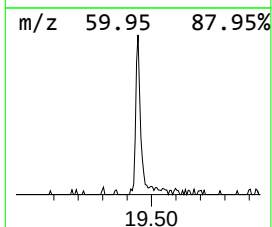
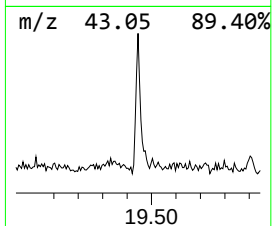
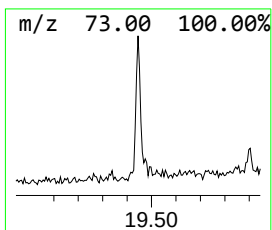
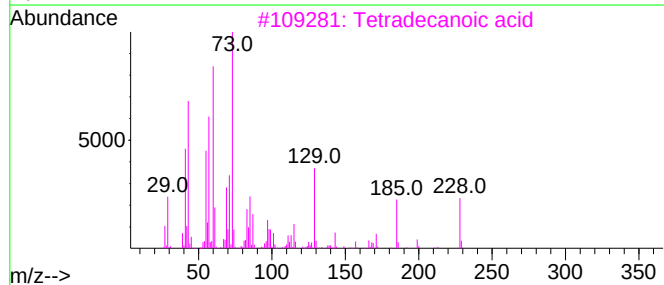
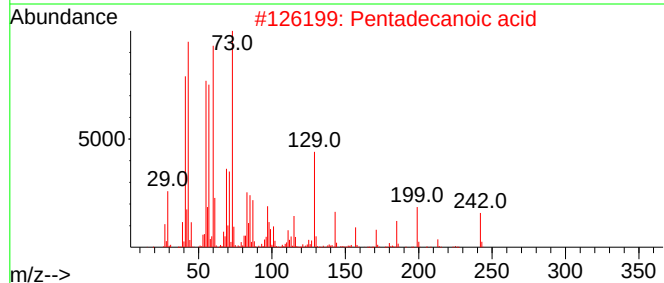
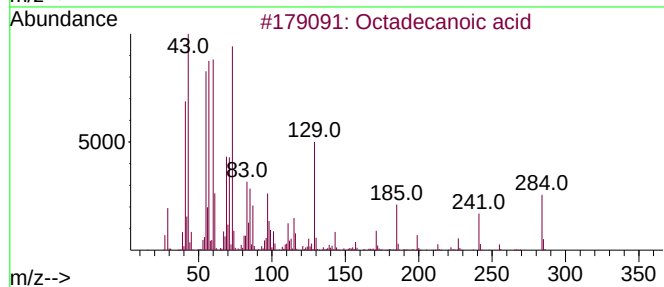
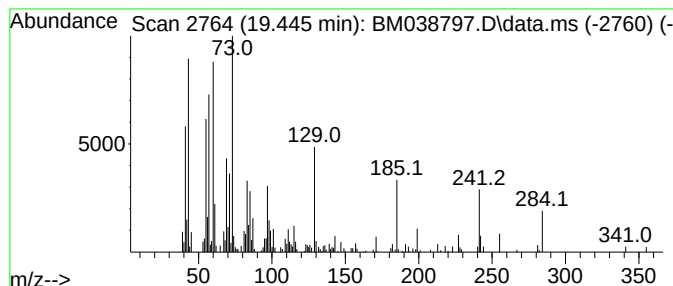
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.445	3.69 ng	124610	Chrysene-d12	21.462

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4		Tridecanoic acid	214	C13H26O2	000638-53-9	62
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022023\
Data File : BM038797.D
Acq On : 20 Feb 2023 21:27
Operator : CG/JU
Sample : 01597-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NYE-WATER-0217

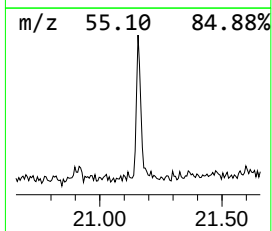
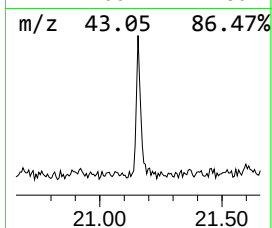
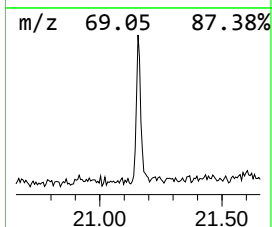
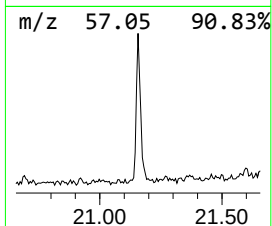
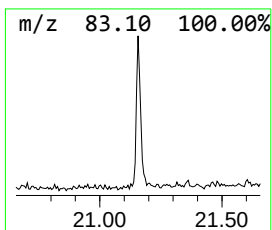
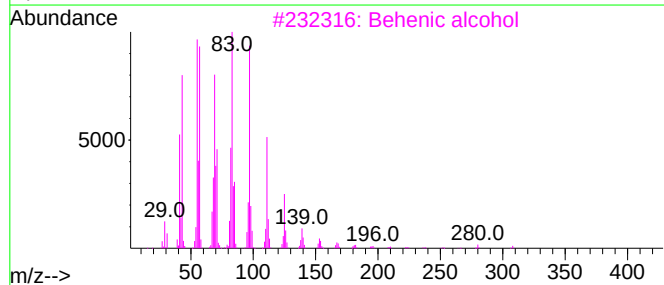
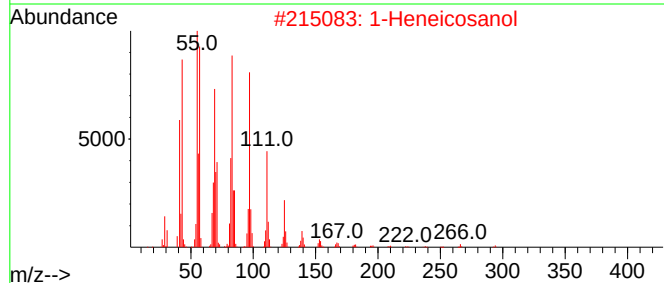
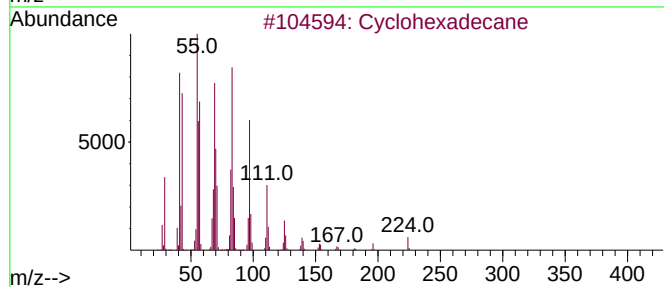
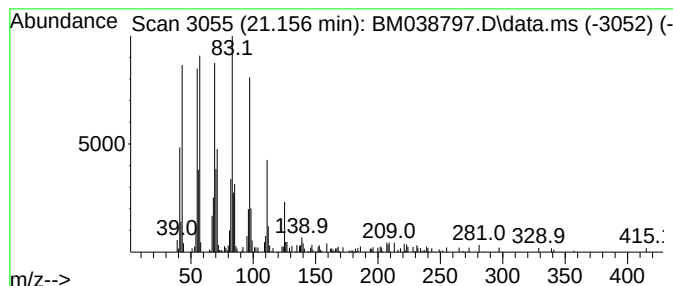
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Cyclohexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.156	3.59 ng	121272	Chrysene-d12	21.462

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexadecane	224	C16H32	000295-65-8	98
2		1-Heneicosanol	312	C21H44O	015594-90-8	95
3		Behenic alcohol	326	C22H46O	000661-19-8	94
4		1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022023\
Data File : BM038797.D
Acq On : 20 Feb 2023 21:27
Operator : CG/JU
Sample : 01597-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NYE-WATER-0217

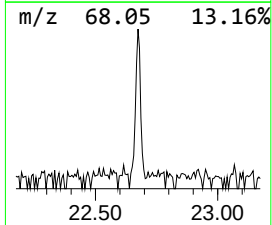
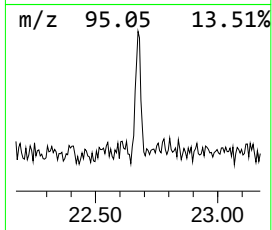
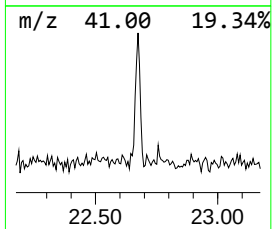
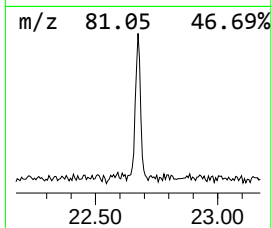
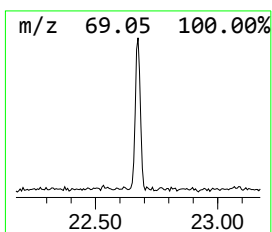
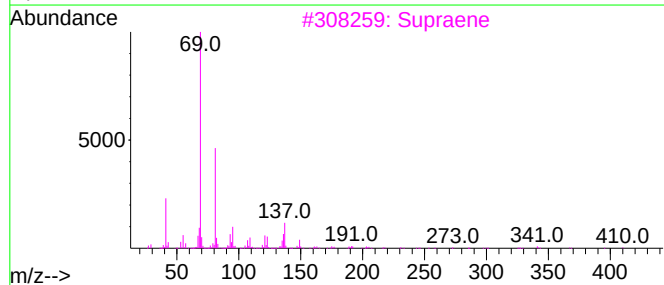
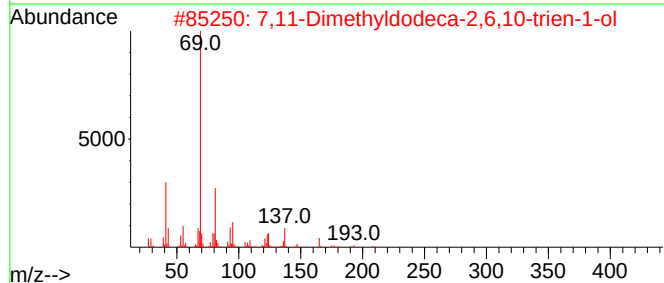
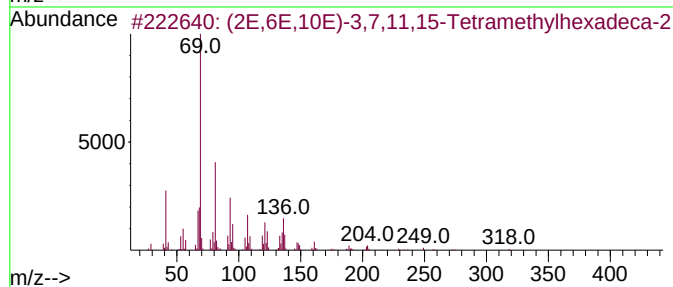
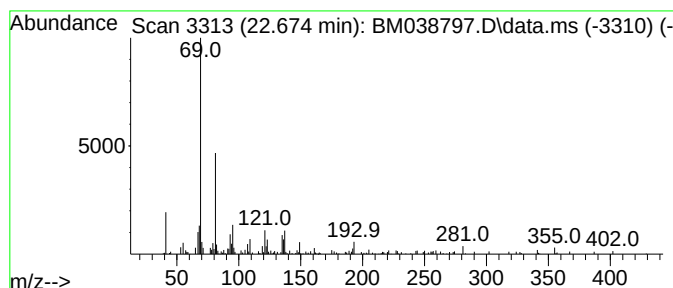
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 (2E,6E,10E)-3,7,11,15-Tetra... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.674	2.59 ng	101425	Perylene-d12	23.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(2E,6E,10E)-3,7,11,15-Tetramethy...	318	C21H34O2	125456-63-5	80		
2	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	74		
3	Supraene	410	C30H50	007683-64-9	74		
4	2,6,10,14-Hexadecatetraenoic aci...	318	C21H34O2	042207-88-5	64		
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022023\
Data File : BM038797.D
Acq On : 20 Feb 2023 21:27
Operator : CG/JU
Sample : 01597-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NYE-WATER-0217

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.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-...	4.957	11.2	ng	133379	1	7.875	237612	20.0
1H-Inden-1-ol, ...	11.310	2.7	ng	42494	2	10.687	318700	20.0
1H-Inden-1-one,...	12.086	4.3	ng	68099	2	10.687	318700	20.0
1H-Imidazole, 4...	13.675	2.1	ng	51517	3	14.533	496439	20.0
unknown15.492	15.492	2.3	ng	56463	3	14.533	496439	20.0
Benzophenone	15.898	2.0	ng	50134	3	14.533	496439	20.0
unknown17.386	17.386	6.0	ng	161878	4	17.280	542444	20.0
2,3-Dihydro-1-o...	17.486	2.6	ng	70680	4	17.280	542444	20.0
Ethanone, 1-[1,...	17.657	3.3	ng	89850	4	17.280	542444	20.0
Tridecanoic acid	18.168	10.3	ng	279667	4	17.280	542444	20.0
2-Amino-m-creso...	18.474	2.6	ng	71358	4	17.280	542444	20.0
Octadecanoic acid	19.445	3.7	ng	124610	5	21.462	675024	20.0
Cyclohexadecane	21.156	3.6	ng	121272	5	21.462	675024	20.0
(2E,6E,10E)-3,7...	22.674	2.6	ng	101425	6	23.839	782202	20.0