

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031623\
 Data File : BM039026.D
 Acq On : 16 Mar 2023 21:22
 Operator : CG/JU
 Sample : 01923-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SAMPLE-1

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-BM030823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039026.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.057	296	301	313	rVB	1309760	1772343	11.44%	2.167%
2	5.528	374	381	389	rBV	2245038	3166153	20.44%	3.871%
3	6.004	453	462	476	rBV	1140605	1784831	11.52%	2.182%
4	7.128	646	653	669	rVB	1341672	2060797	13.31%	2.519%
5	7.975	787	797	804	rBV	1259244	1963894	12.68%	2.401%
6	9.145	989	996	1005	rVB	4488005	7176958	46.34%	8.774%
7	9.304	1009	1023	1036	rBV	776089	1857688	12.00%	2.271%
8	10.787	1268	1275	1281	rBV	1684038	2803020	18.10%	3.427%
9	10.845	1281	1285	1290	rVB	283643	423376	2.73%	0.518%
10	12.398	1544	1549	1554	rBV	170849	289037	1.87%	0.353%
11	13.245	1683	1693	1704	rBV	10837960	15486742	100.00%	18.933%
12	14.616	1916	1926	1933	rBV	2451906	3518677	22.72%	4.302%
13	15.969	2151	2156	2162	rVB	528669	699062	4.51%	0.855%
14	16.098	2172	2178	2189	rBV	4970150	6798273	43.90%	8.311%
15	16.845	2300	2305	2311	rBV	169627	265633	1.72%	0.325%
16	17.116	2345	2351	2355	rBV2	390552	512594	3.31%	0.627%
17	17.357	2387	2392	2402	rVB	2769213	3768522	24.33%	4.607%
18	18.257	2539	2545	2554	rBV	1024923	1642224	10.60%	2.008%
19	19.527	2757	2761	2770	rBV3	342108	555922	3.59%	0.680%
20	19.792	2802	2806	2813	rVB	258859	330204	2.13%	0.404%
21	19.980	2832	2838	2843	rBV	12556399	15183061	98.04%	18.562%
22	21.221	3045	3049	3050	rBV	489610	518466	3.35%	0.634%
23	21.245	3050	3053	3062	rVB	1132710	1488263	9.61%	1.819%
24	21.539	3098	3103	3108	rBV	2803372	3580574	23.12%	4.377%
25	22.809	3316	3319	3327	rVB	489965	692575	4.47%	0.847%
26	23.974	3511	3517	3526	rVB2	1697536	3456960	22.32%	4.226%

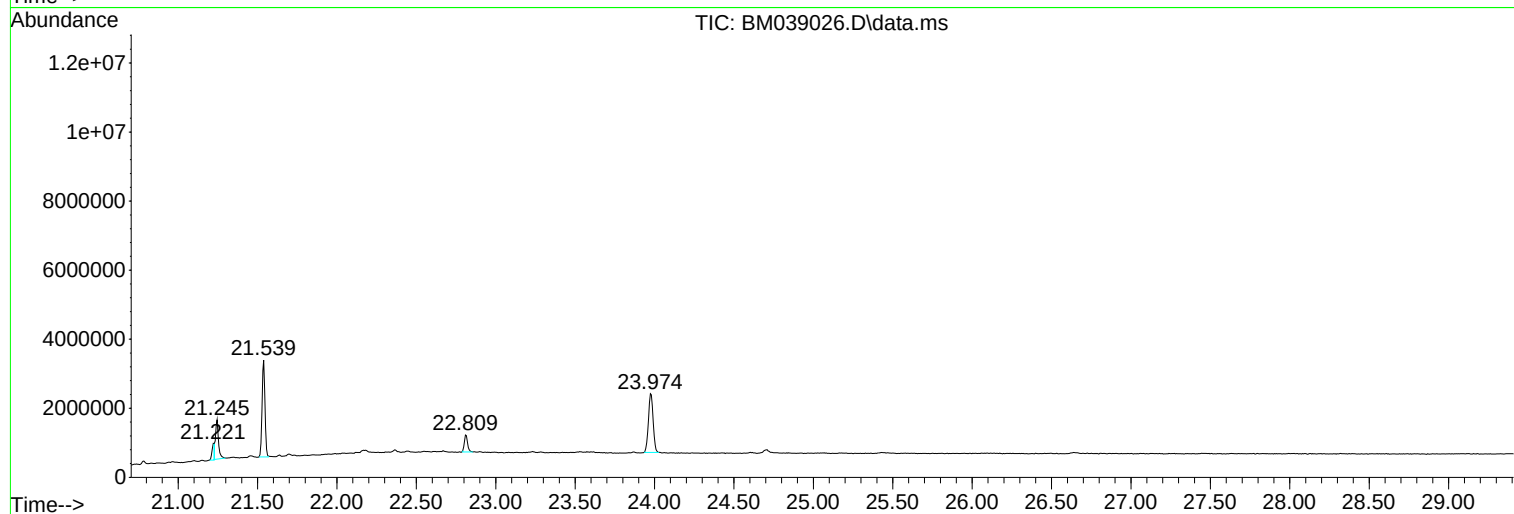
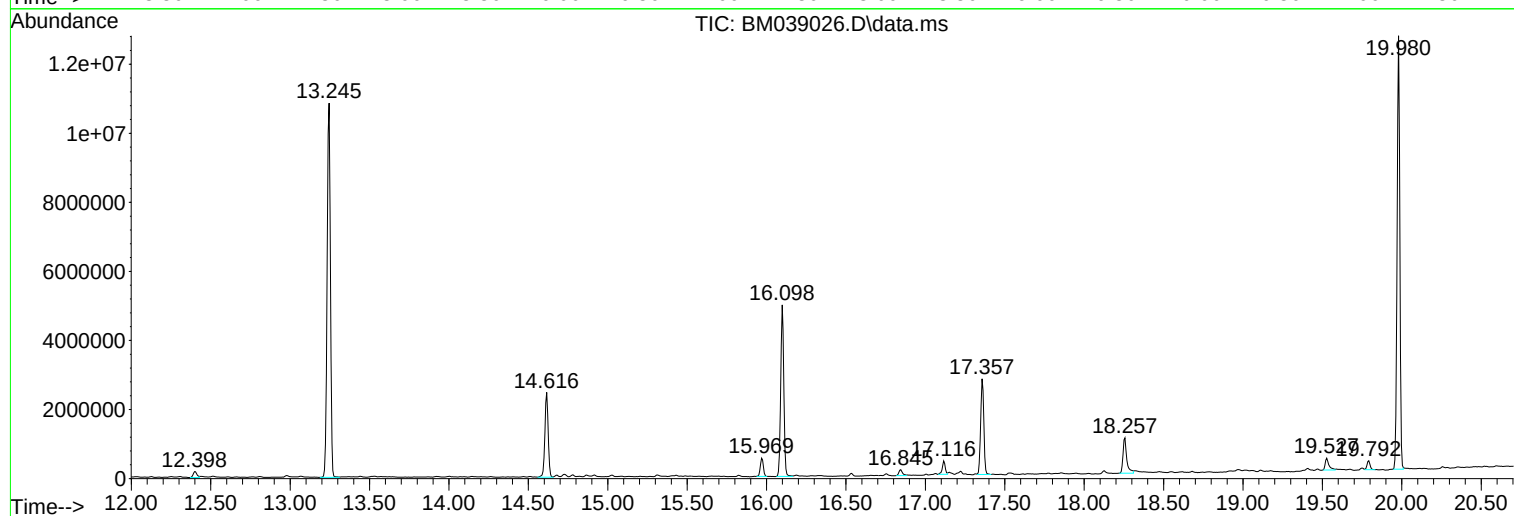
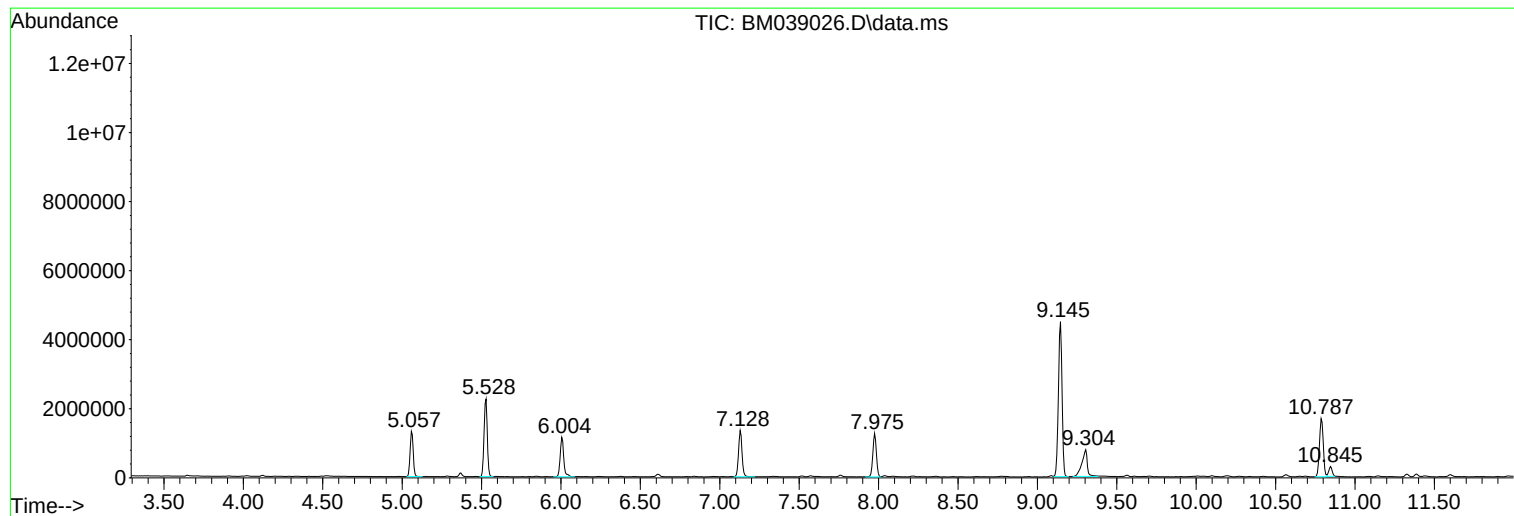
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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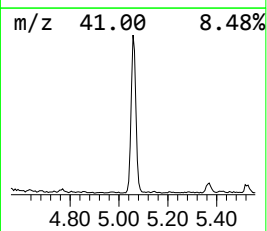
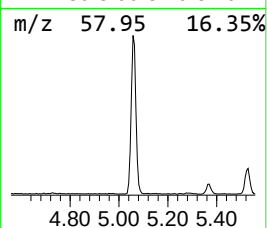
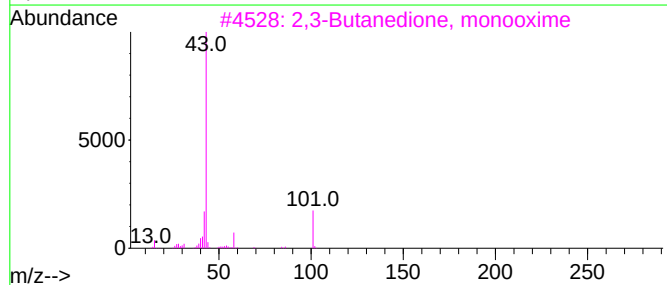
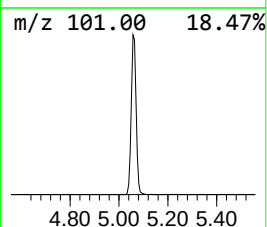
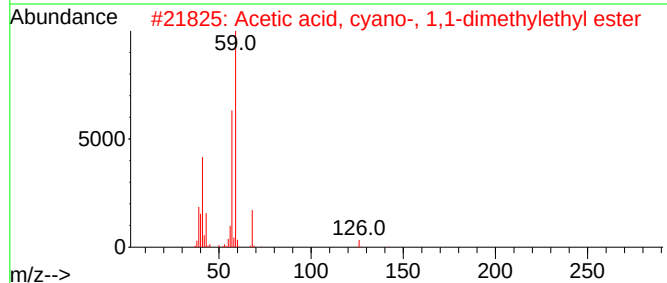
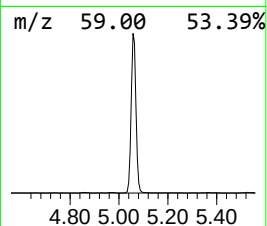
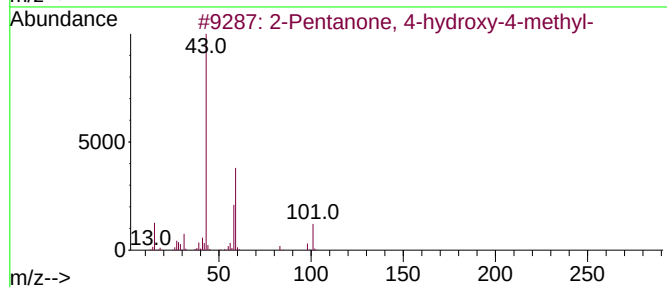
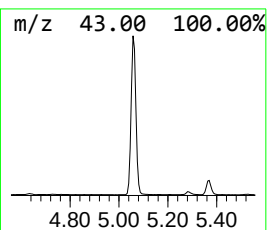
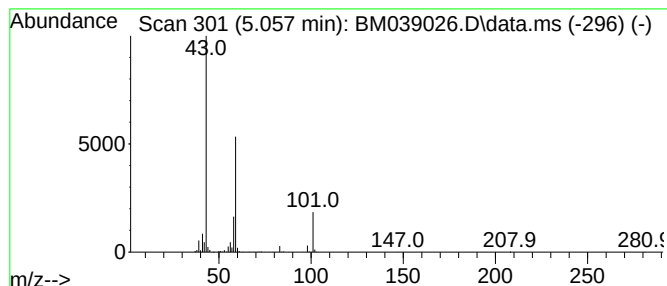
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	18.05 ng	1772340	1,4-Dichlorobenzene-d4	7.975

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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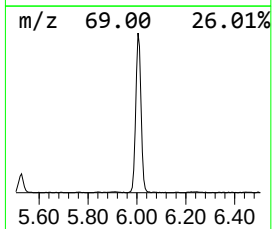
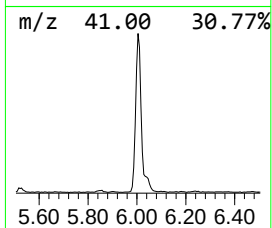
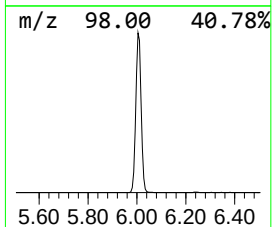
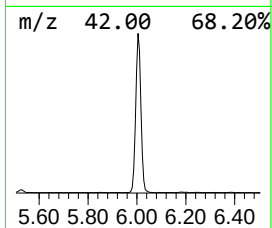
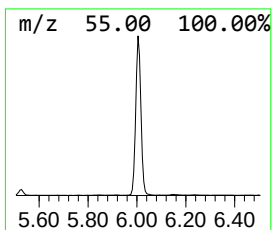
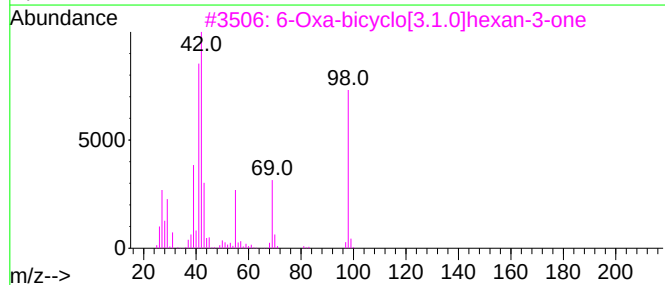
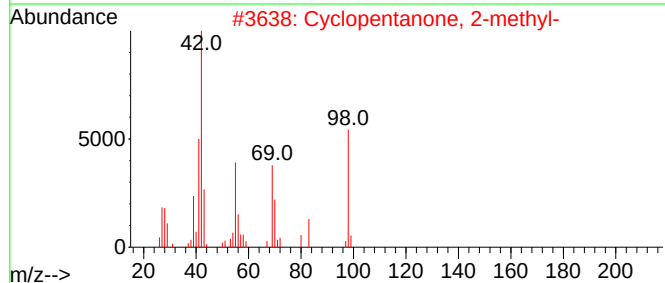
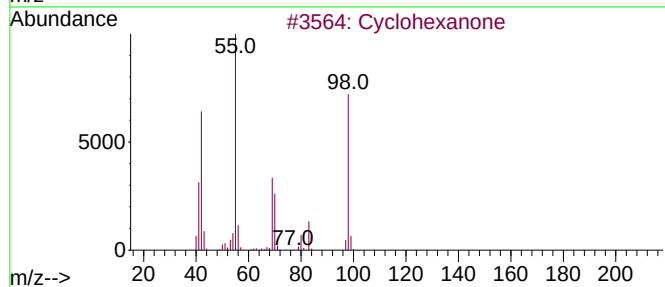
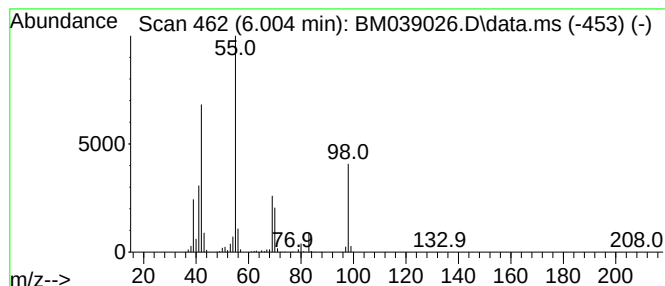
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclohexanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.004	18.18 ng	1784830	1,4-Dichlorobenzene-d4	7.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone	98	C6H10O	000108-94-1	95
2			Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	72
3			6-Oxa-bicyclo[3.1.0]hexan-3-one	98	C5H6O2	074017-10-0	47
4			Cyclohexane, methyl-	98	C7H14	000108-87-2	45
5			2-Pentene, (Z)-	70	C5H10	000627-20-3	43



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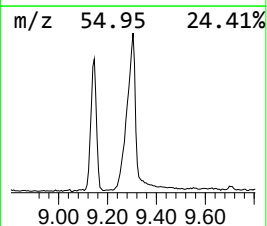
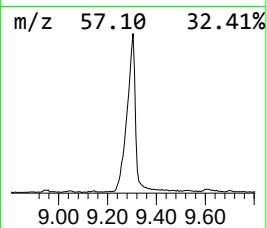
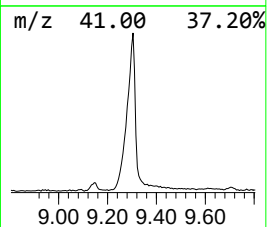
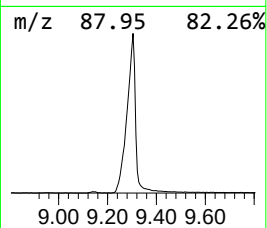
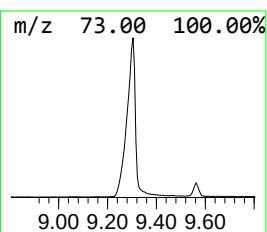
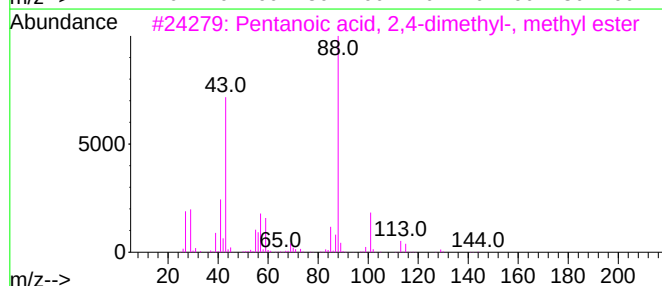
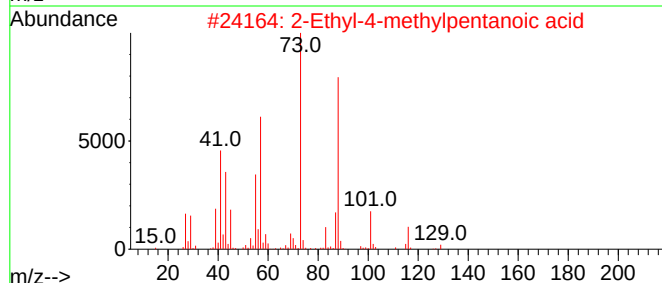
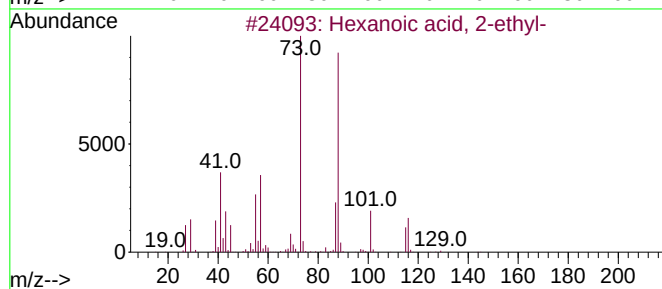
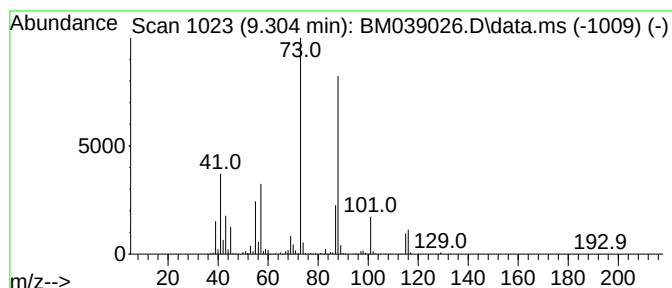
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Hexanoic acid, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.304	18.92 ng	1857690	1,4-Dichlorobenzene-d4	7.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2			2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	50
3			Pentanoic acid, 2,4-dimethyl-, m...	144	C8H16O2	071672-33-8	47
4			Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	45
5			Acetic acid, diethyl-	116	C6H12O2	000088-09-5	45



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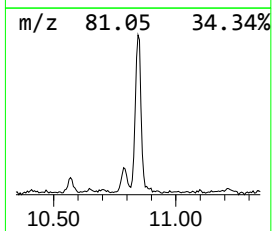
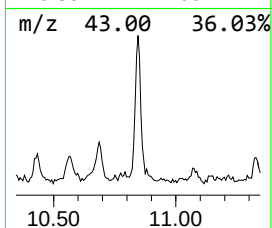
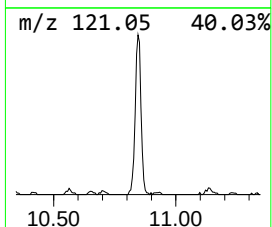
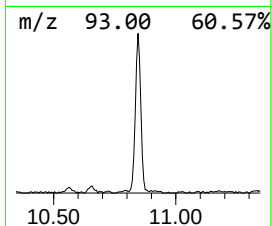
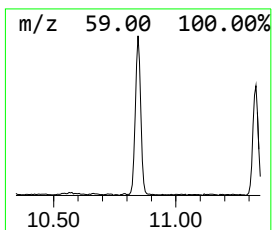
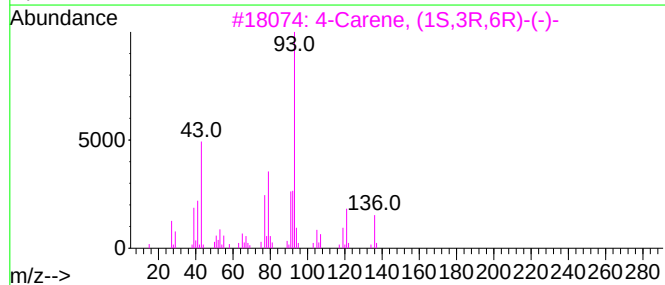
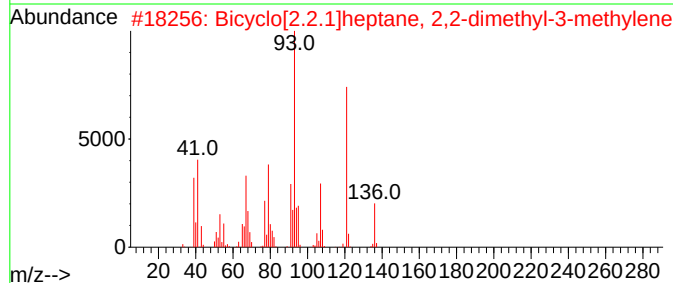
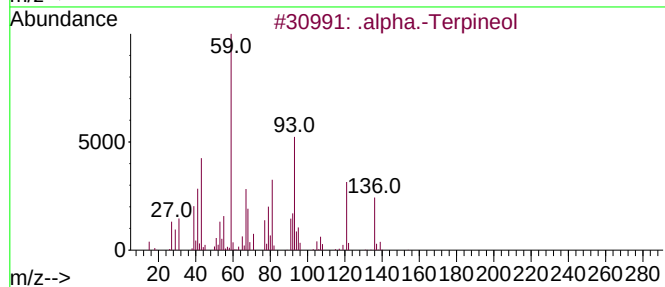
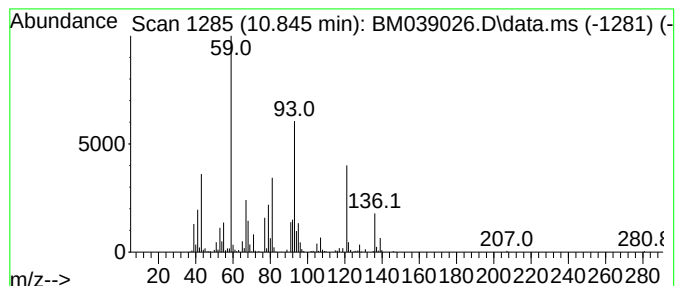
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Peak Number 4 .alpha.-Terpineol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.845	3.02 ng	423376	Naphthalene-d8	10.787

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.alpha.-Terpineol	154	C10H18O	000098-55-5	90
2			Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	005794-04-7	47
3			4-Carene, (1S,3R,6R)-(-)-	136	C10H16	005208-49-1	46
4			Bicyclo[2.2.1]hept-2-ene, 1,7,7-...	136	C10H16	000464-17-5	46
5			Bicyclo[2.2.1]hept-2-ene, 2,7,7-...	136	C10H16	000514-14-7	46



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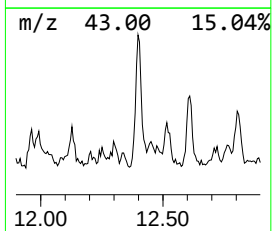
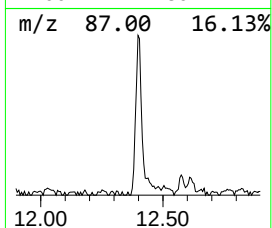
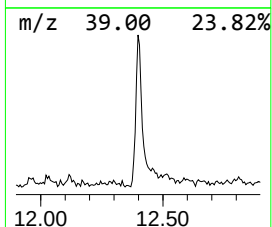
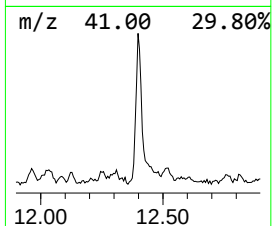
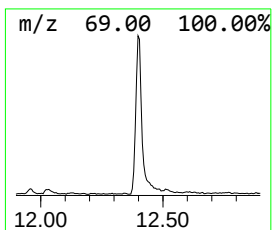
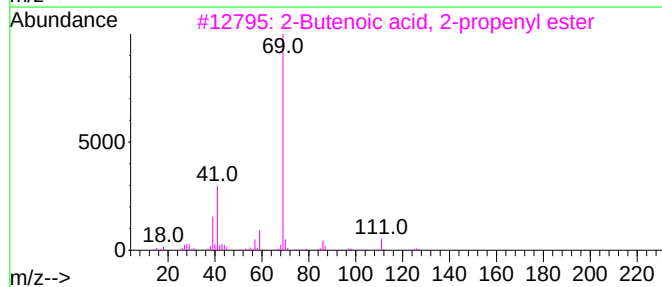
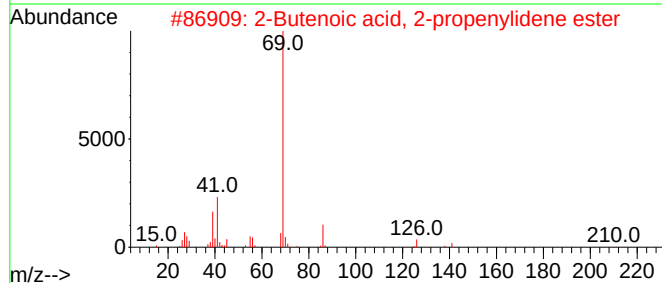
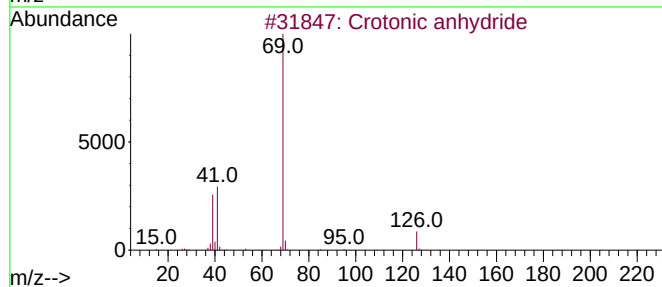
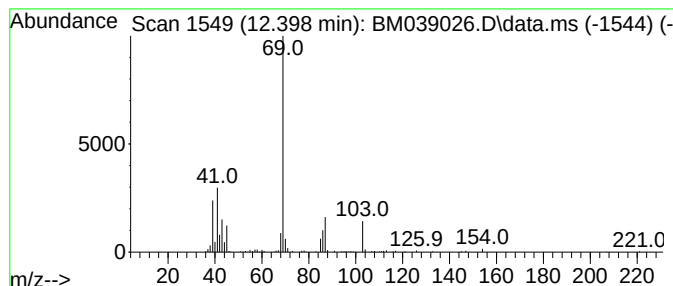
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Peak Number 5 unknown12.398 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.398	2.06 ng	289037	Naphthalene-d8	10.787

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Crotonic anhydride	154	C8H10O3	000623-68-7	47
2			2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	45
3			2-Butenoic acid, 2-propenyl ester	126	C7H10O2	020474-93-5	42
4			Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	39
5			2-propenoic acid, 2-methyl-, 2-(...	167	C7H9N3O2	1000404-53-2	33



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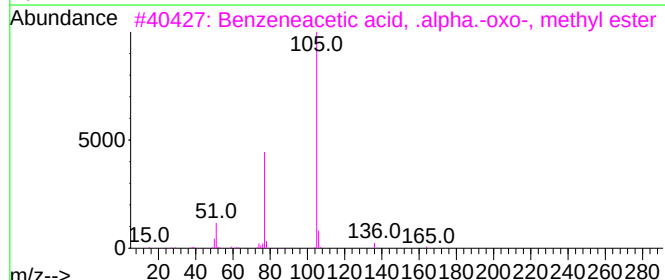
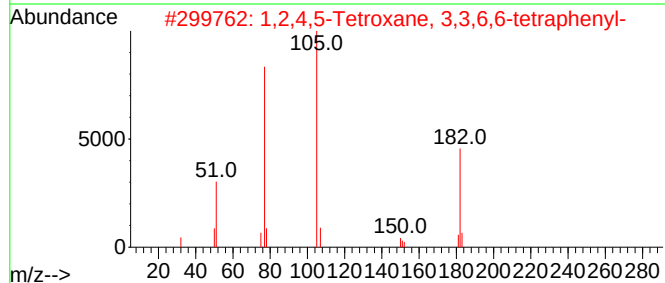
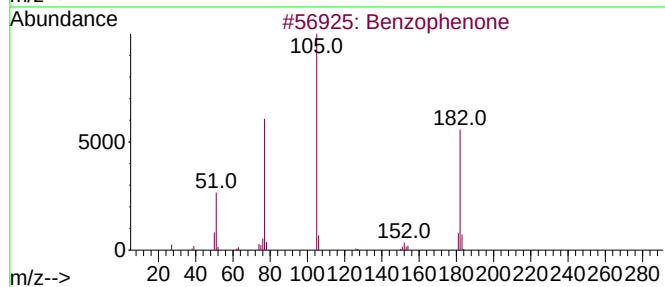
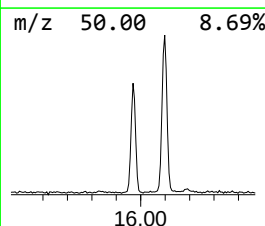
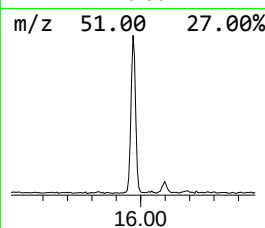
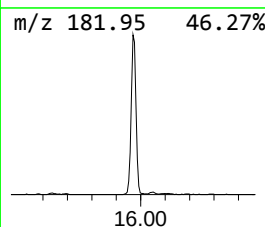
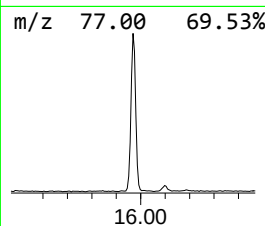
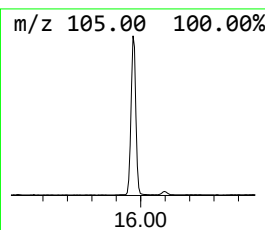
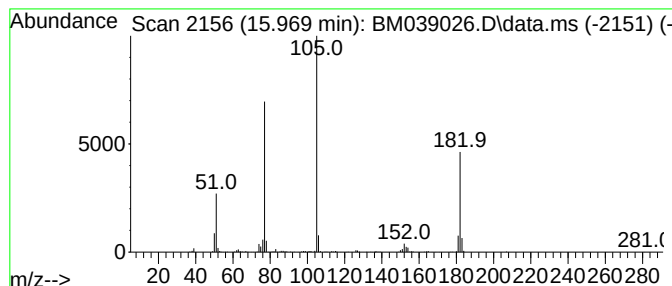
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.969	3.97 ng	699062	Acenaphthene-d10	14.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	53
4			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
5			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031623\
Data File : BM039026.D
Acq On : 16 Mar 2023 21:22
Operator : CG/JU
Sample : 01923-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

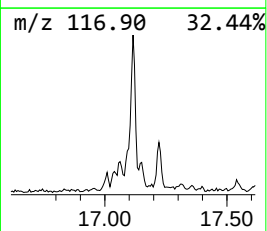
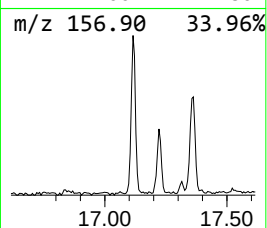
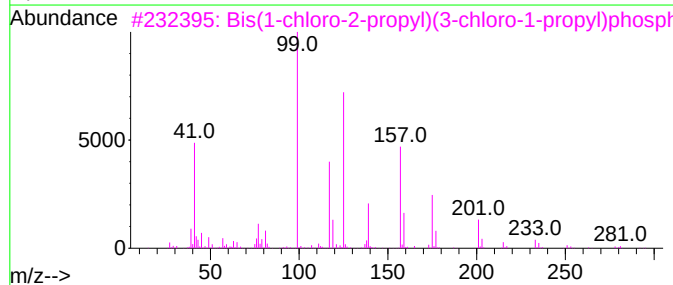
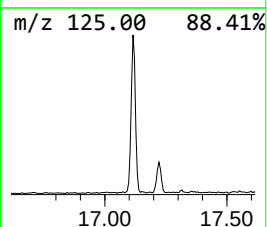
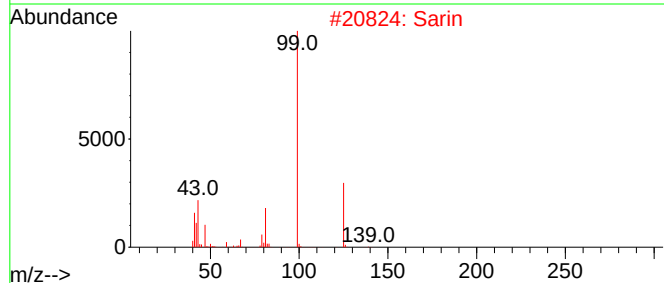
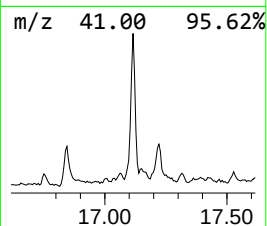
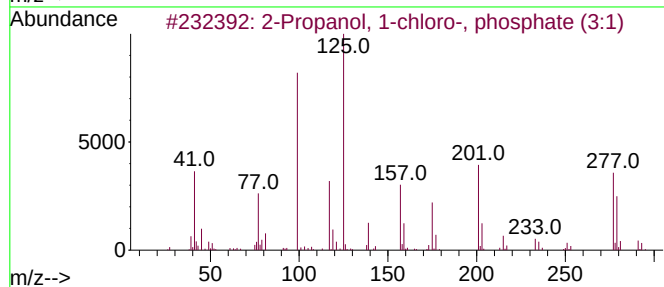
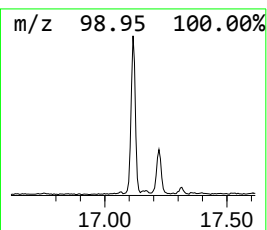
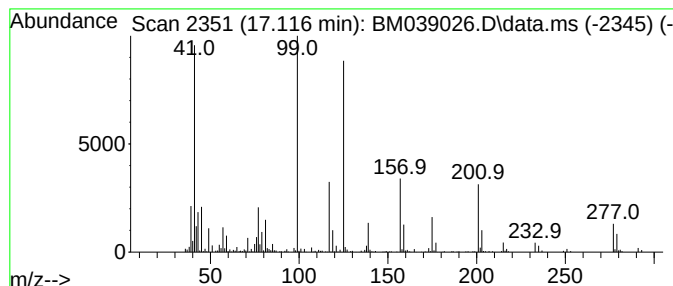
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-Propanol, 1-chloro-, phos... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
17.116	2.72 ng	512594	Phenanthrene-d10		17.357	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Propanol, 1-chloro-, phosphate...		326	C9H18Cl13O4P	013674-84-5	91
2	Sarin		140	C4H10FO2P	000107-44-8	47
3	Bis(1-chloro-2-propyl)(3-chloro-...		326	C9H18Cl13O4P	137909-40-1	43
4	Triisopropylphosphate		224	C9H21O4P	000513-02-0	38
5	Tris(2-chloropropyl) phosphate		326	C9H18Cl13O4P	006145-73-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031623\
Data File : BM039026.D
Acq On : 16 Mar 2023 21:22
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Sample : 01923-01
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Instrument :
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ClientSampleId :
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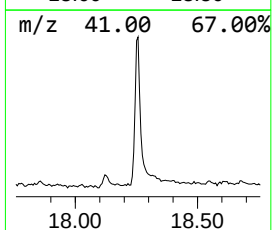
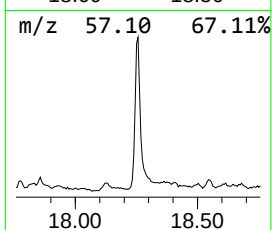
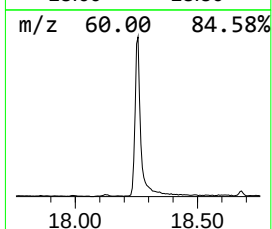
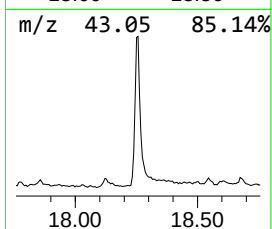
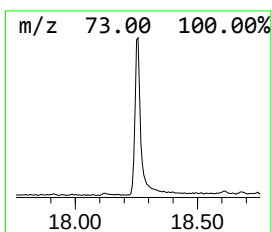
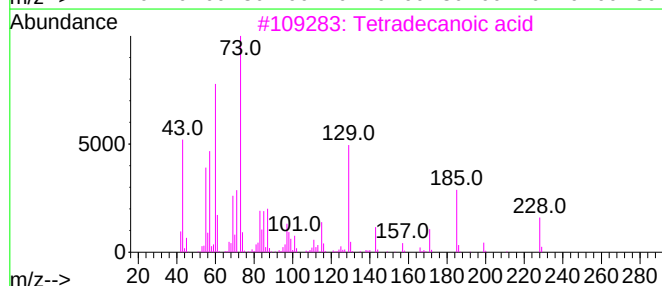
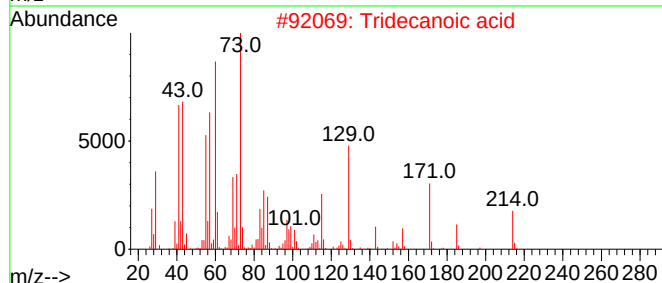
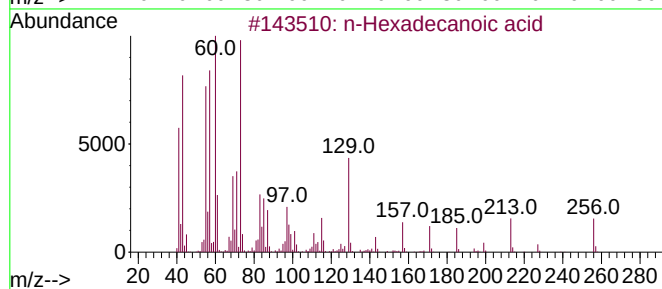
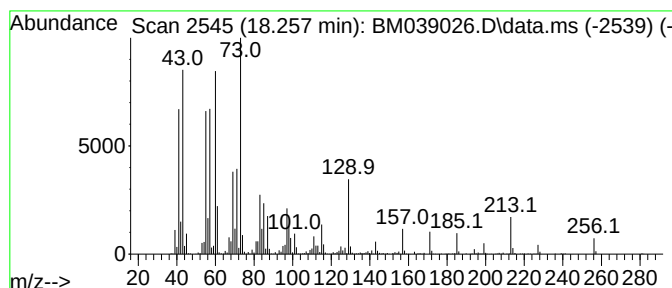
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.257	8.72 ng	1642220	Phenanthrene-d10	17.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	92
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	20



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031623\
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Sample : 01923-01
Misc :
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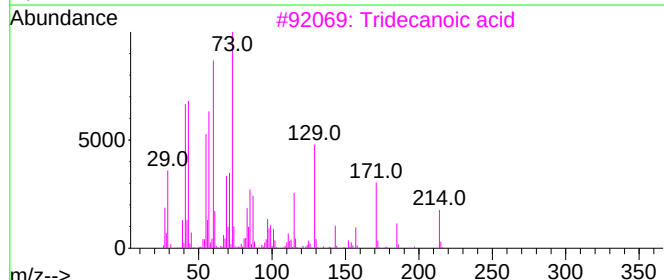
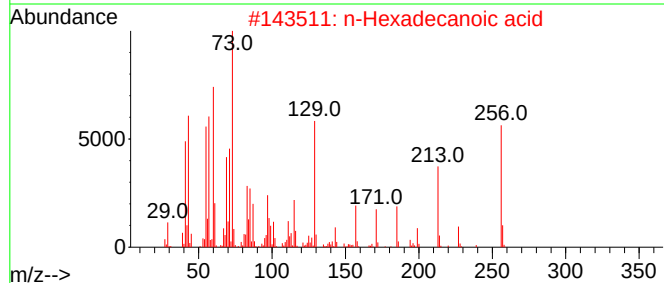
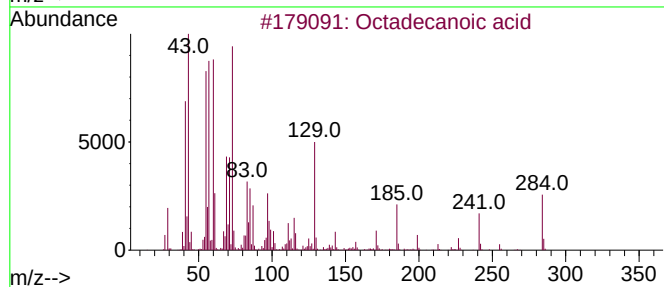
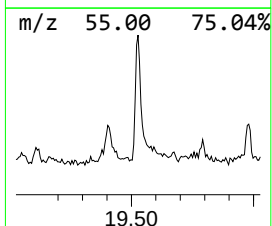
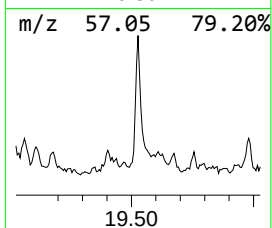
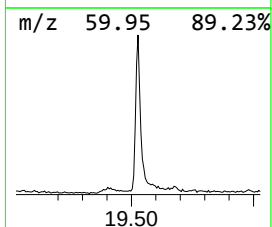
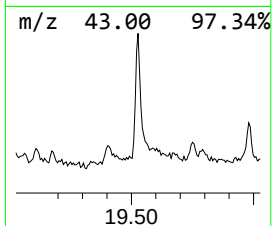
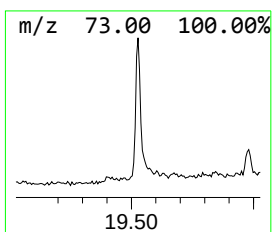
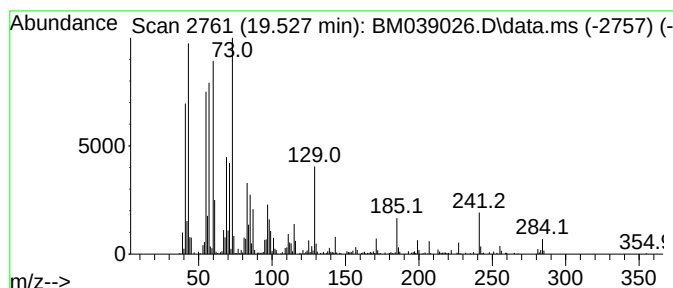
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.527	3.11 ng	555922	Chrysene-d12	21.539	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031623\
Data File : BM039026.D
Acq On : 16 Mar 2023 21:22
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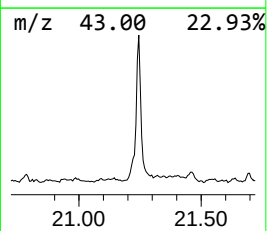
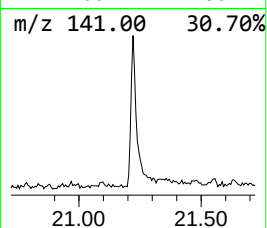
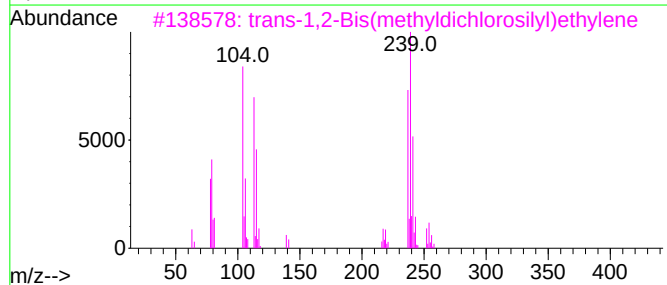
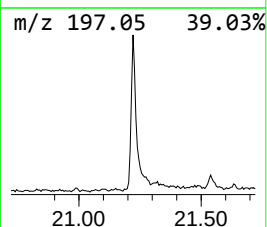
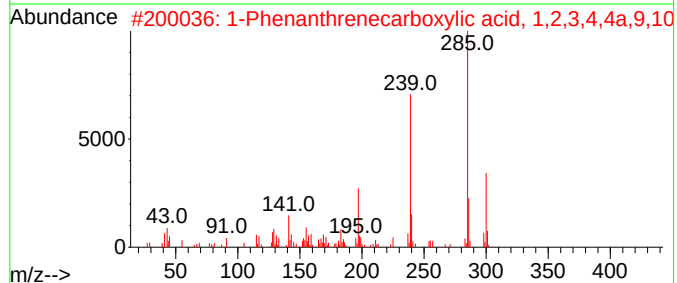
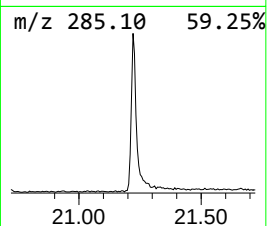
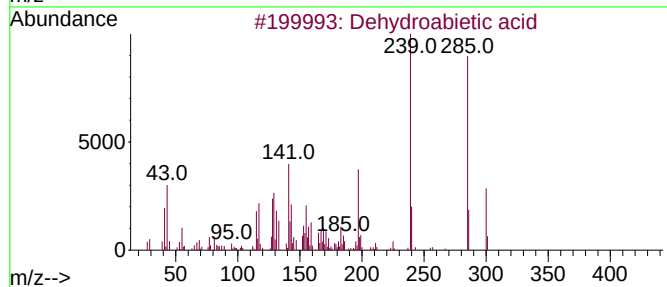
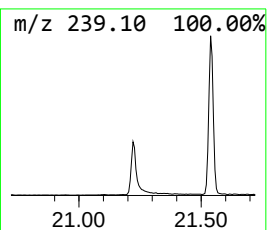
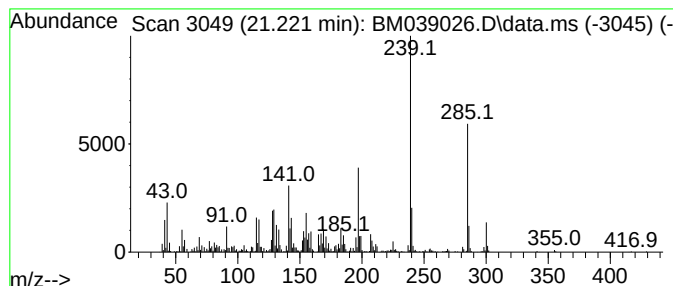
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Dehydroabietic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.221	2.90 ng	518466	Chrysene-d12	21.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dehydroabietic acid	300	C20H28O2	001740-19-8	99
2			1-Phenanthrenecarboxylic acid, 1...	300	C20H28O2	005155-70-4	90
3			trans-1,2-Bis(methyldichlorosilyl...)	252	C4H8Cl4Si2	065899-10-7	74
4			Butanoic acid, 2-(cyano)(2,4,6-t...	300	C17H20N2O3	1000267-71-7	58
5			Ethyl 4-hydroxy-7-trifluoromethy...	285	C13H10F3NO3	000391-02-6	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031623\
Data File : BM039026.D
Acq On : 16 Mar 2023 21:22
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Sample : 01923-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SAMPLE-1

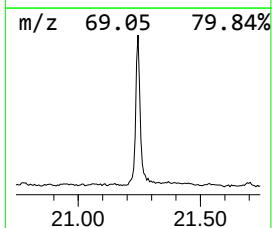
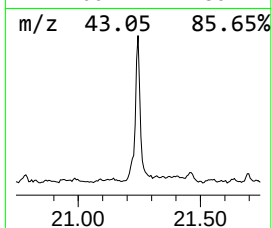
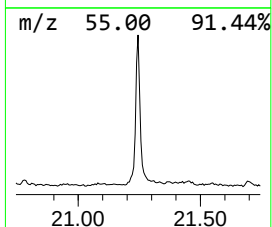
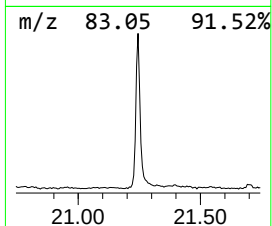
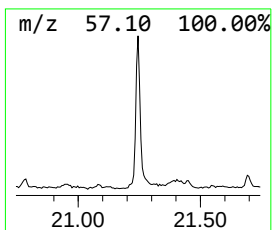
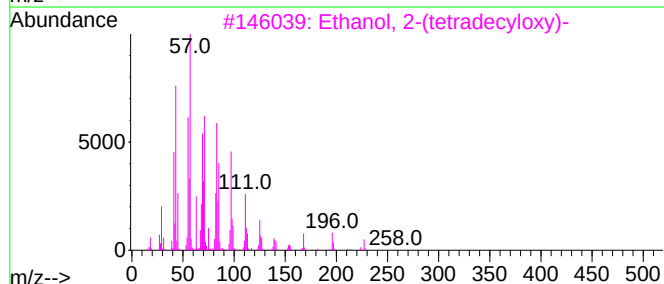
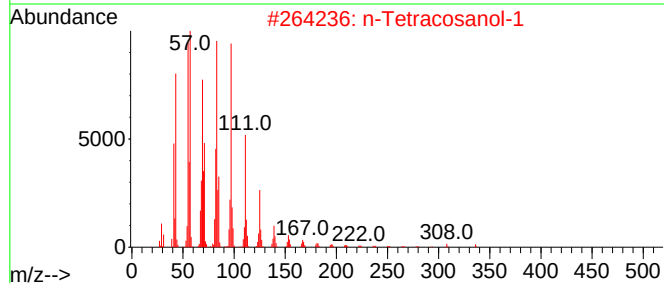
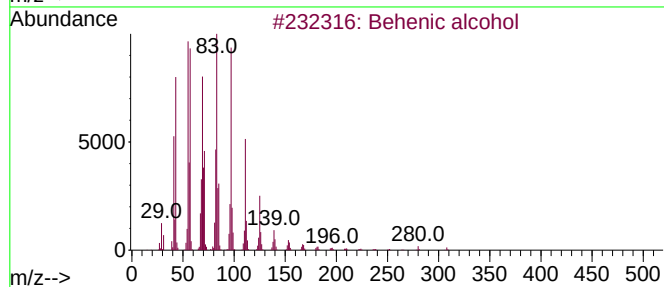
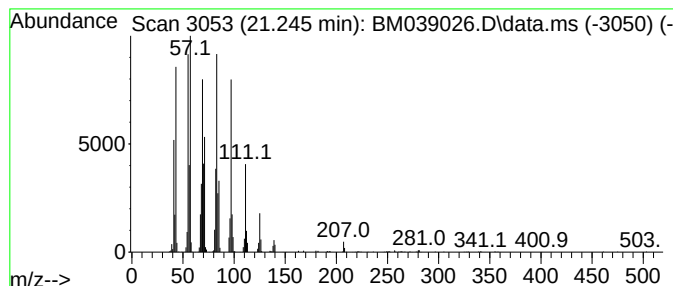
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.245	8.31 ng	1488260	Chrysene-d12	21.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	92
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5	Pentacos-1-ene	350	C25H50	016980-85-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031623\
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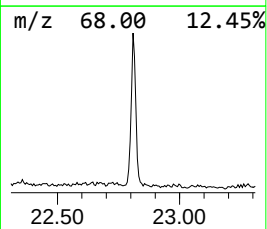
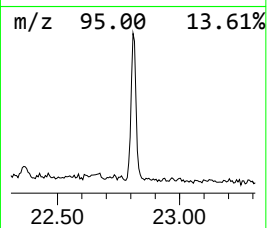
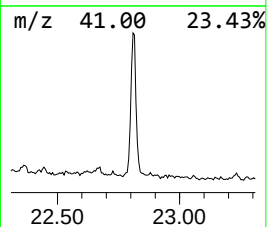
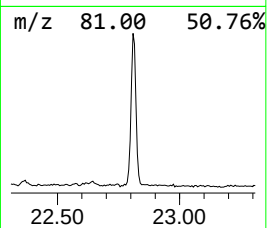
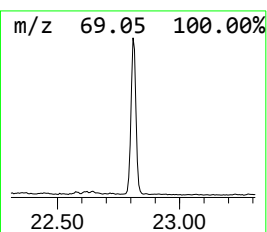
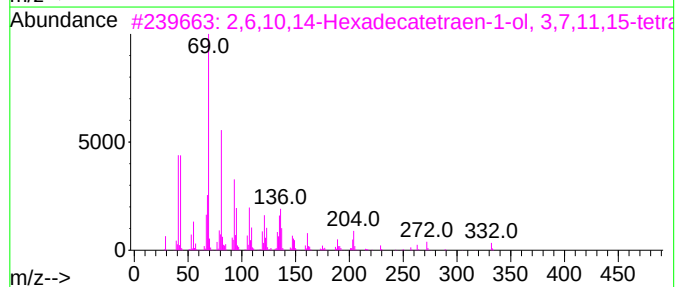
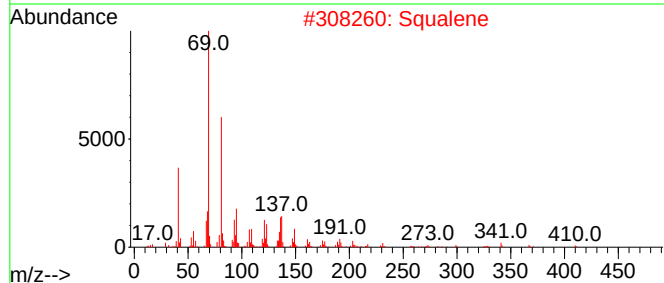
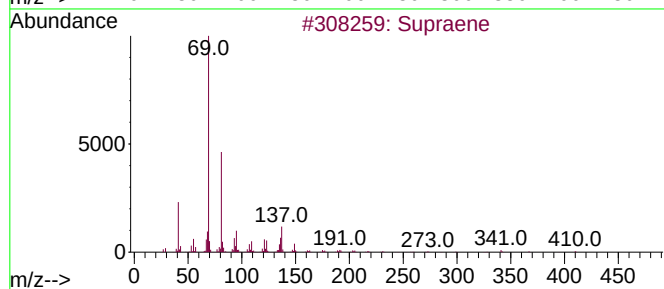
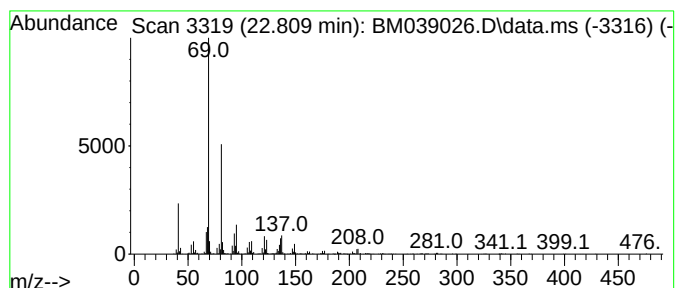
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.809	4.01 ng	692575	Perylene-d12	23.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	90
3			2,6,10,14-Hexadecatetraen-1-ol, ...	332	C22H36O2	061691-98-3	78
4			1-(Phenylthio)-3,7,11-trimethyl-...	314	C21H30S	028413-57-2	78
5			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031623\
Data File : BM039026.D
Acq On : 16 Mar 2023 21:22
Operator : CG/JU
Sample : 01923-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SAMPLE-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.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-...	5.057	18.1	ng	1772340	1	7.975	1963890	20.0
Cyclohexanone	6.004	18.2	ng	1784830	1	7.975	1963890	20.0
Hexanoic acid, ...	9.304	18.9	ng	1857690	1	7.975	1963890	20.0
.alpha.-Terpineol	10.845	3.0	ng	423376	2	10.787	2803020	20.0
unknown12.398	12.398	2.1	ng	289037	2	10.787	2803020	20.0
Benzophenone	15.969	4.0	ng	699062	3	14.616	3518680	20.0
2-Propanol, 1-c...	17.116	2.7	ng	512594	4	17.357	3768520	20.0
n-Hexadecanoic ...	18.257	8.7	ng	1642220	4	17.357	3768520	20.0
Octadecanoic acid	19.527	3.1	ng	555922	5	21.539	3580570	20.0
Dehydroabietic ...	21.221	2.9	ng	518466	5	21.539	3580570	20.0
Behenic alcohol	21.245	8.3	ng	1488260	5	21.539	3580570	20.0
Supraene	22.809	4.0	ng	692575	6	23.974	3456960	20.0