

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
 Data File : BM039984.D
 Acq On : 24 May 2023 15:09
 Operator : CG/JU
 Sample : 02899-11
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TWP01

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-BM052323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039984.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.640	208	230	231	rBV4	44220	185326	1.12%	0.246%
2	5.093	300	307	313	rBV	241230	324929	1.96%	0.432%
3	5.563	380	387	394	rBV	2982769	4121004	24.88%	5.480%
4	7.169	652	660	669	rBV	1581043	2500489	15.10%	3.325%
5	8.016	796	804	811	rVB	1193553	1798783	10.86%	2.392%
6	9.181	993	1002	1011	rBV	3239675	5316098	32.10%	7.069%
7	10.833	1275	1283	1289	rBV	1419107	2368608	14.30%	3.150%
8	12.445	1548	1557	1572	rBV	595610	1086286	6.56%	1.445%
9	13.280	1691	1699	1707	rBV	8379409	11708756	70.70%	15.570%
10	14.651	1925	1932	1941	rVB	1865431	2647813	15.99%	3.521%
11	16.004	2156	2162	2169	rBV	939124	1239178	7.48%	1.648%
12	16.133	2178	2184	2195	rBV	6269649	8507608	51.37%	11.314%
13	16.333	2212	2218	2227	rBV	310738	430029	2.60%	0.572%
14	16.880	2305	2311	2330	rBV	1005301	1653908	9.99%	2.199%
15	17.392	2392	2398	2404	rBV	2078983	2921917	17.64%	3.886%
16	18.286	2545	2550	2559	rBV	468555	746479	4.51%	0.993%
17	18.362	2559	2563	2574	rVB	94570	176344	1.06%	0.235%
18	19.562	2762	2767	2778	rBV	310657	563037	3.40%	0.749%
19	19.780	2800	2804	2808	rBV	509661	756231	4.57%	1.006%
20	20.015	2838	2844	2849	rBV	13762171	16561036	100.00%	22.023%
21	21.274	3054	3058	3068	rBV	461845	633185	3.82%	0.842%
22	21.486	3090	3094	3099	rBV	245381	301022	1.82%	0.400%
23	21.568	3102	3108	3113	rVV	2792181	3952519	23.87%	5.256%
24	21.609	3113	3115	3122	rVB	328694	377252	2.28%	0.502%
25	22.856	3324	3327	3333	rVB	143067	200330	1.21%	0.266%
26	23.274	3394	3398	3402	rBV2	223179	355814	2.15%	0.473%
27	24.021	3519	3525	3539	rVB	1875974	3764687	22.73%	5.006%

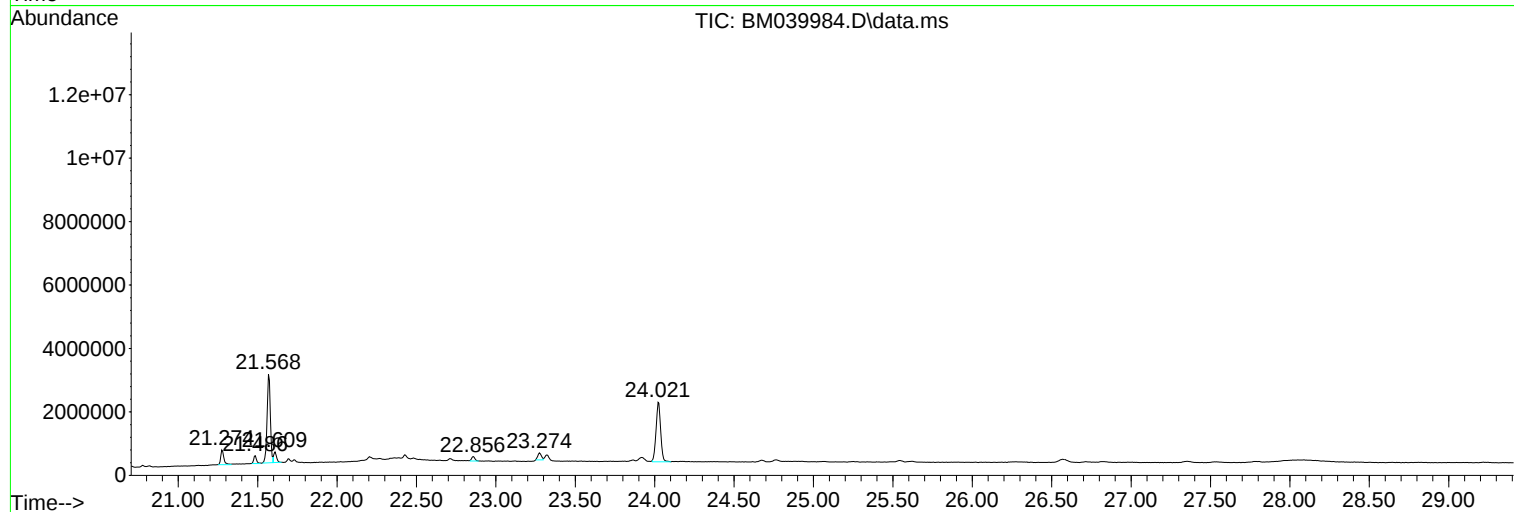
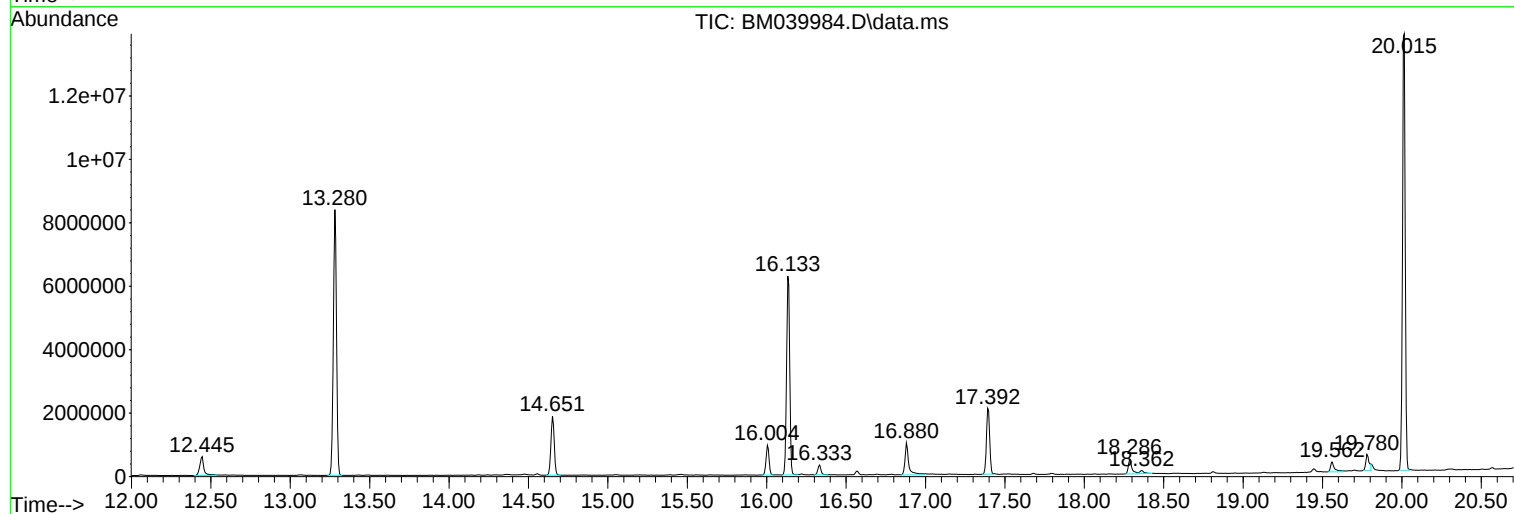
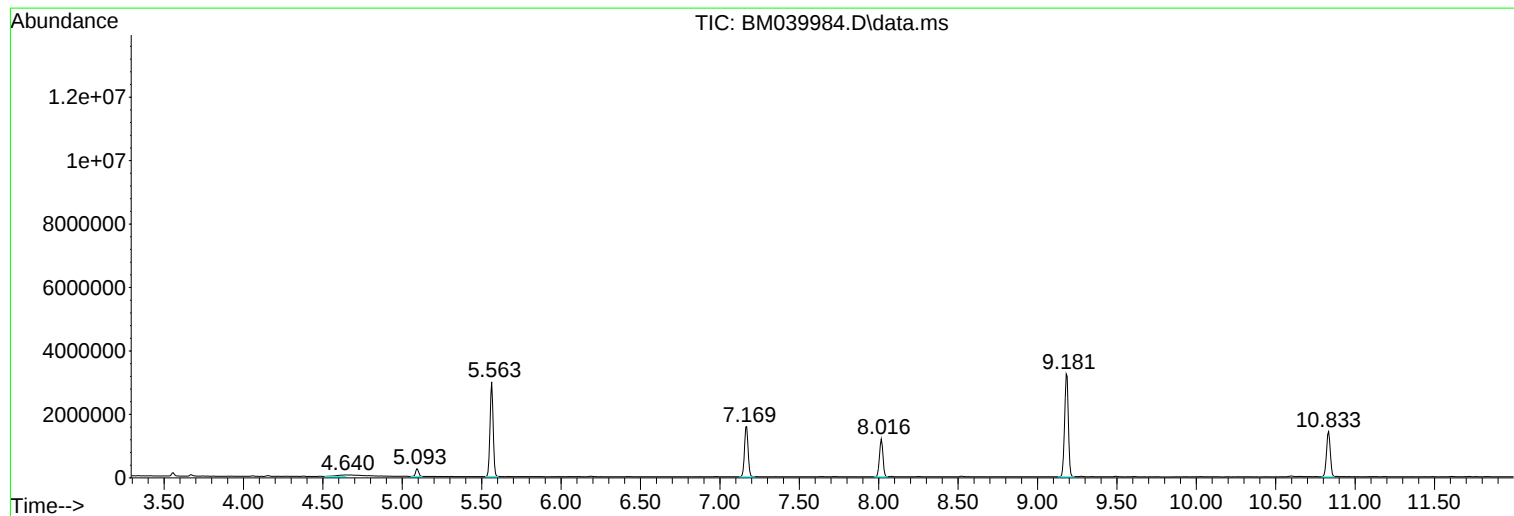
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Instrument :
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ClientSampleId :
TWP01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.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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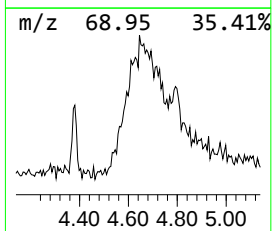
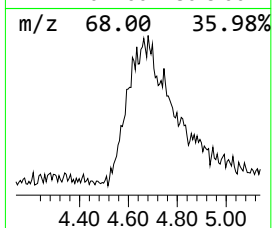
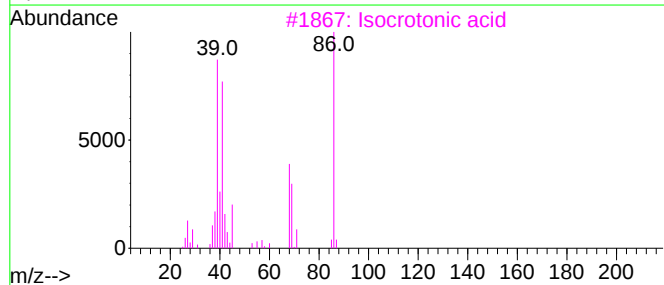
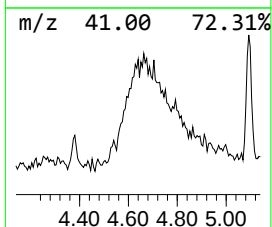
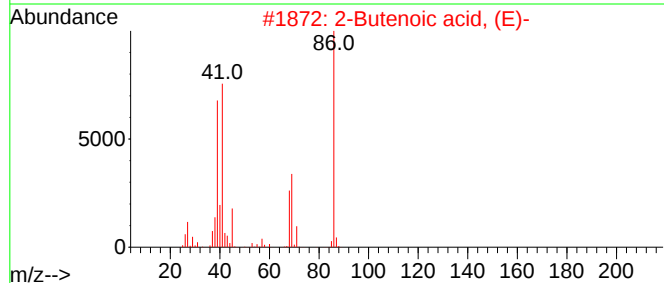
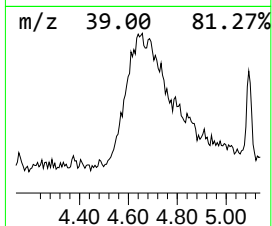
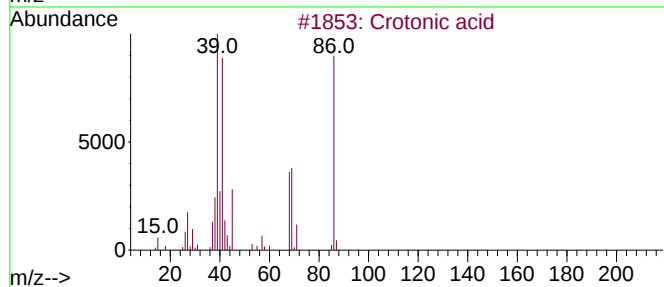
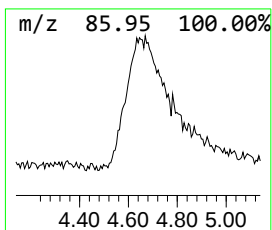
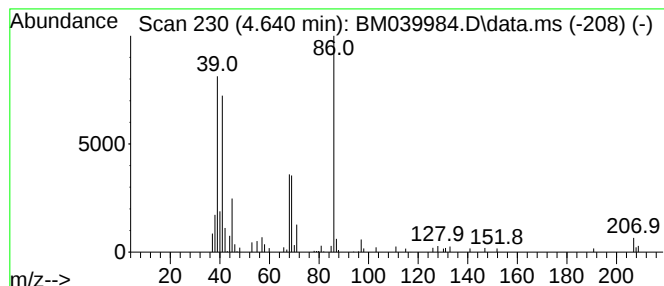
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Crotonic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.640	2.06 ng	185326	1,4-Dichlorobenzene-d4	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Crotonic acid	86	C4H6O2	003724-65-0	96
2			2-Butenoic acid, (E)-	86	C4H6O2	000107-93-7	96
3			Isocrotonic acid	86	C4H6O2	000503-64-0	95
4			2-Propenoic acid, 2-methyl-	86	C4H6O2	000079-41-4	87
5			2-Butenedioic acid, 2-methyl-, (Z)-	130	C5H6O4	000498-23-7	83



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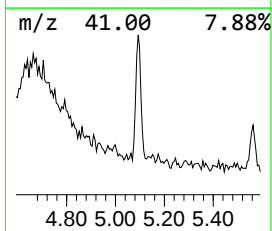
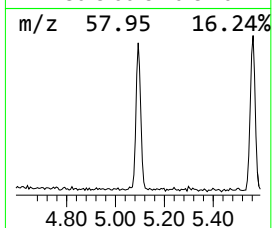
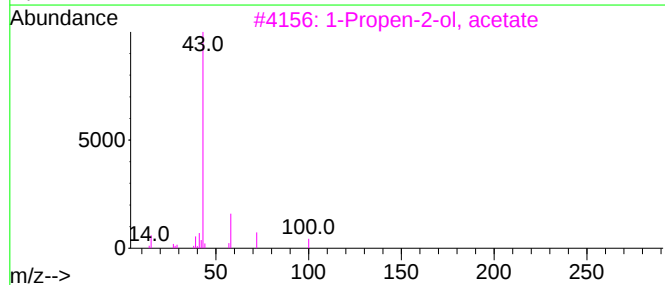
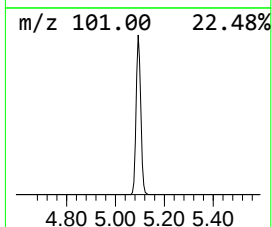
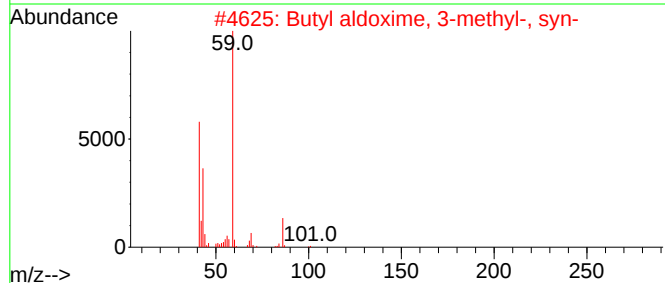
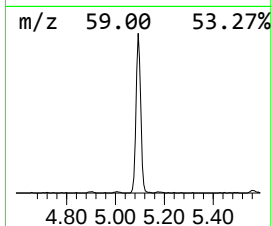
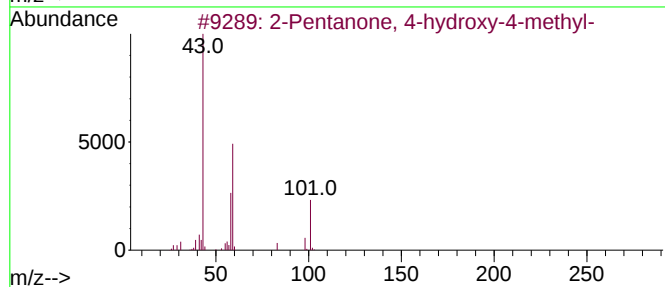
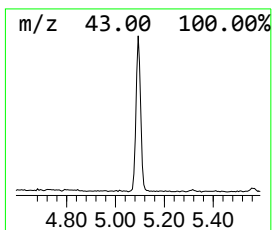
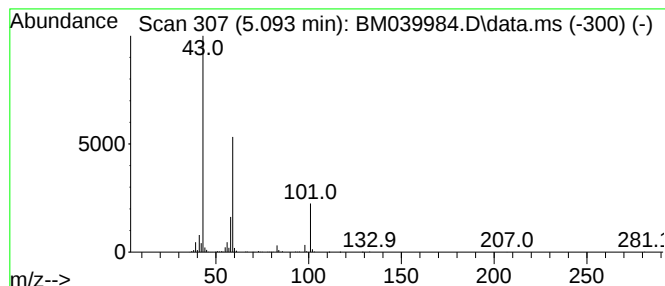
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	3.61 ng	324929	1,4-Dichlorobenzene-d4	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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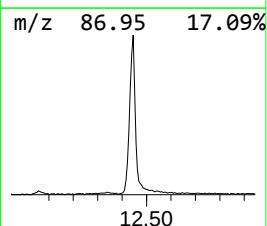
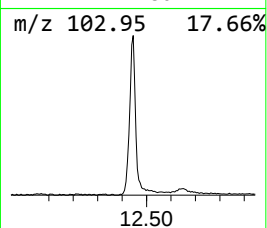
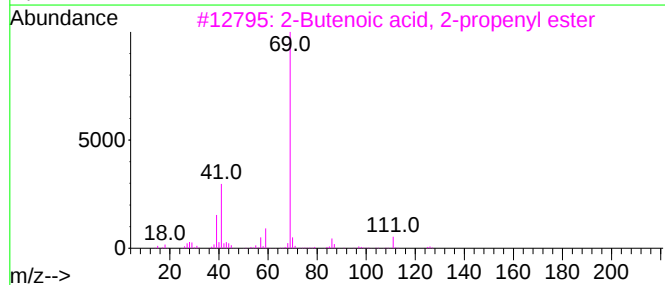
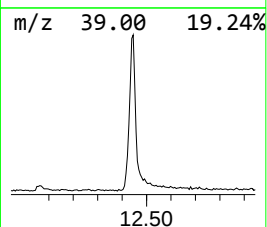
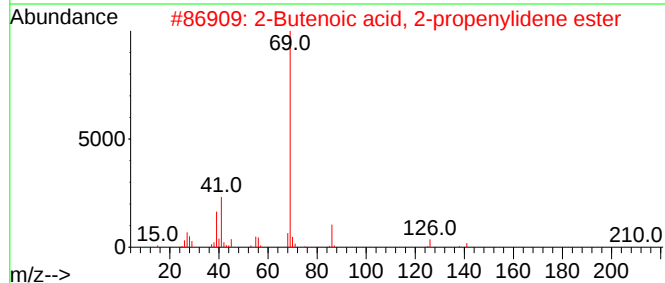
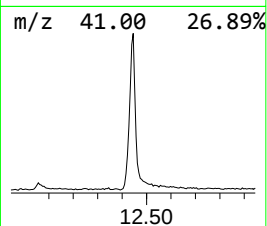
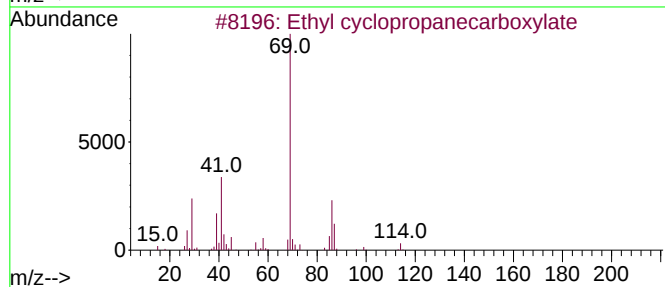
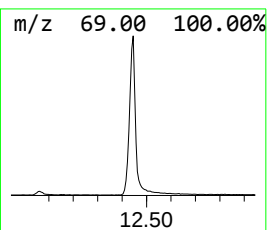
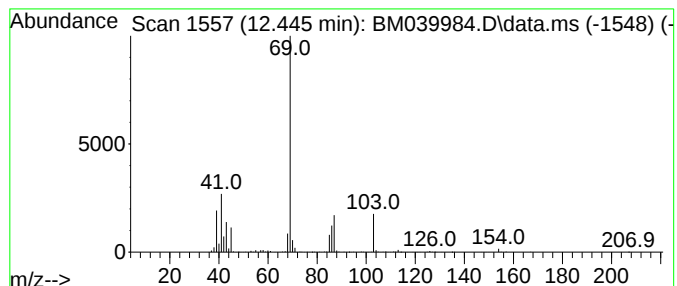
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown12.445 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.445	9.17 ng	1086290	Naphthalene-d8	10.833

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	45
2			2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	45
3			2-Butenoic acid, 2-propenyl ester	126	C7H10O2	020474-93-5	40
4			Crotonic anhydride	154	C8H10O3	000623-68-7	38
5			Cyclopropanecarboxylic acid, 3-m...	154	C9H14O2	1000299-37-4	9



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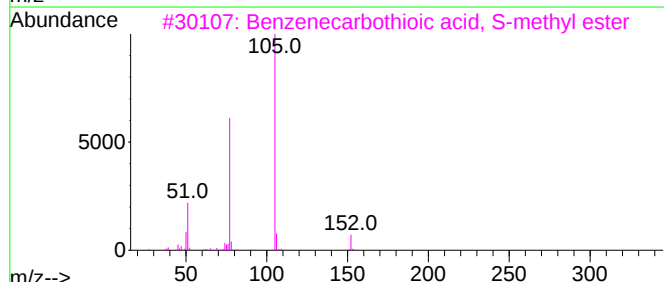
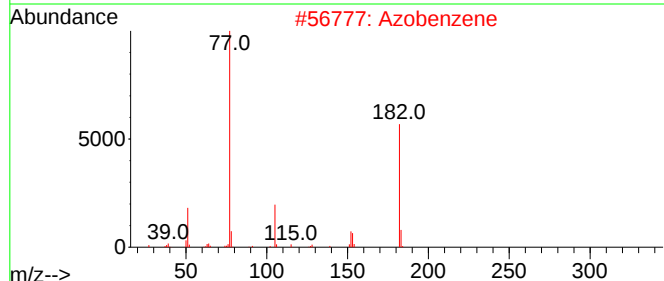
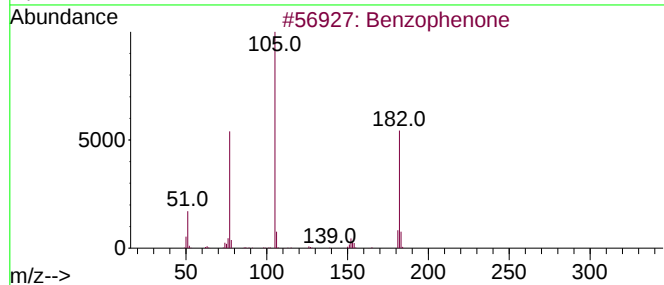
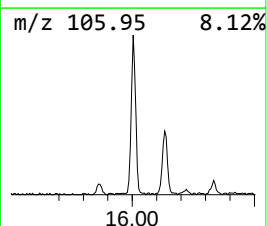
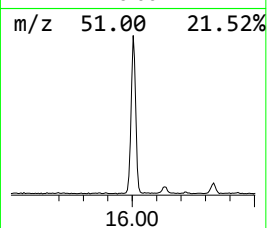
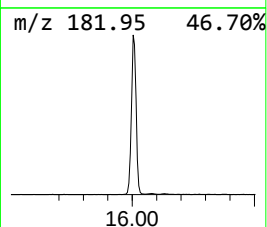
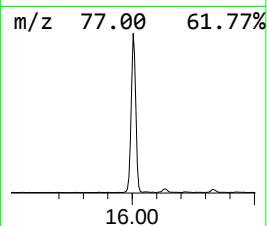
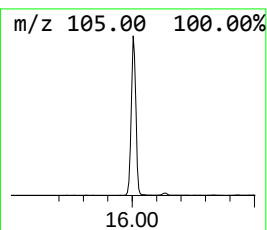
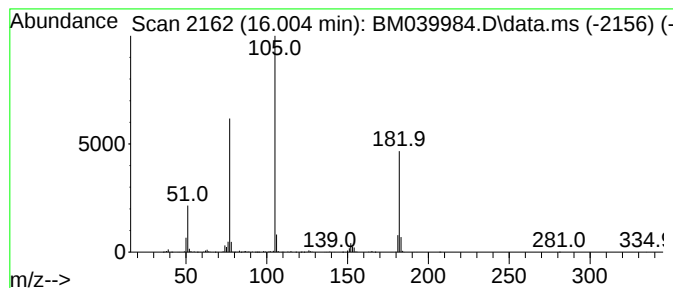
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.004	9.36 ng	1239180	Acenaphthene-d10	14.651

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	59
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
4			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	49
5			Methyl 2-benzoyl-4-cyanobutanoate	231	C13H13NO3	1010486-83-8	47



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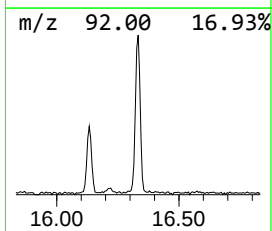
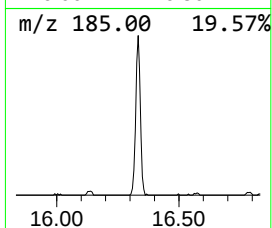
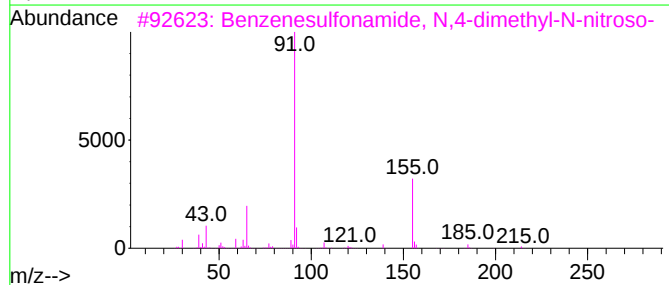
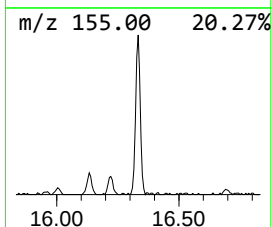
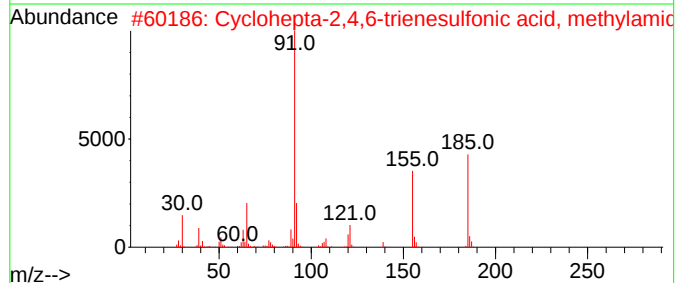
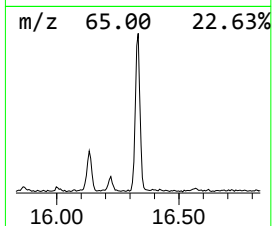
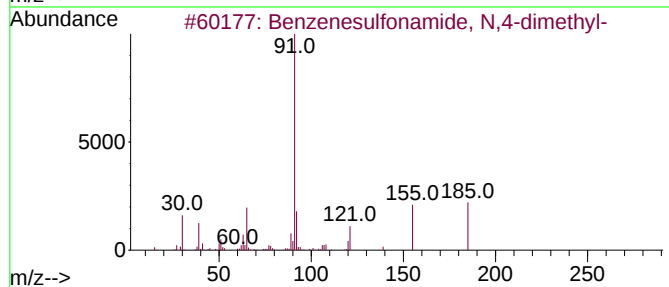
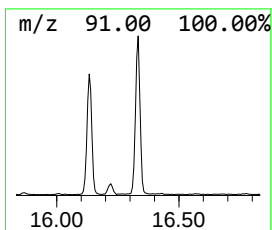
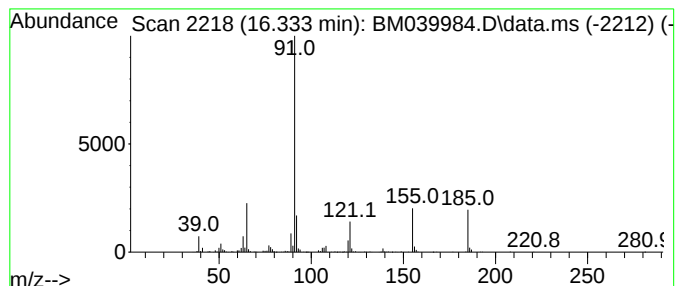
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzenesulfonamide, N,4-dim... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.333	2.94 ng	430029	Phenanthrene-d10	17.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	94
2			Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	58
3			Benzenesulfonamide, N,4-dimethyl...	214	C8H10N2O3S	000080-11-5	50
4			4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	47
5			(O-p-Tosylisonitroso)malononitrile	249	C10H7N3O3S	020893-01-0	47



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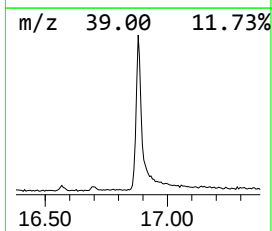
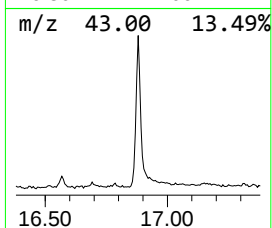
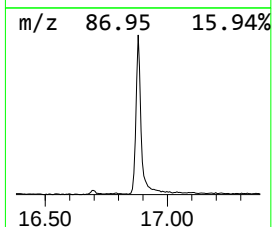
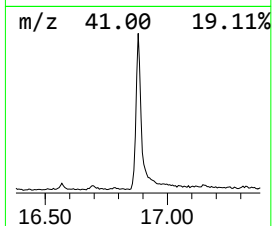
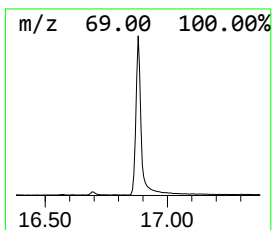
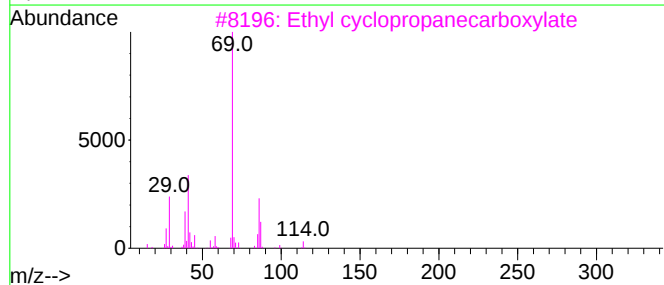
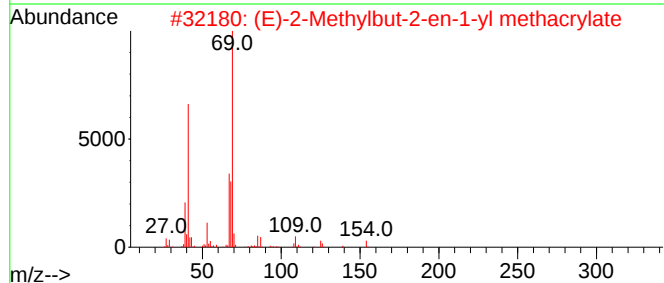
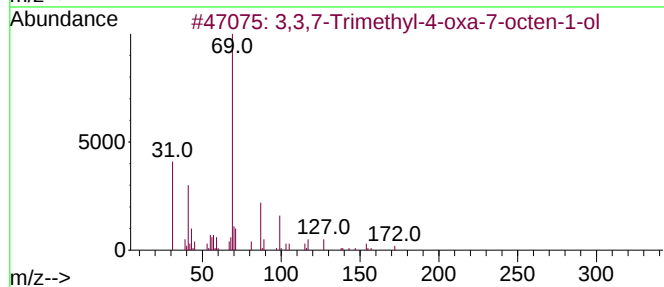
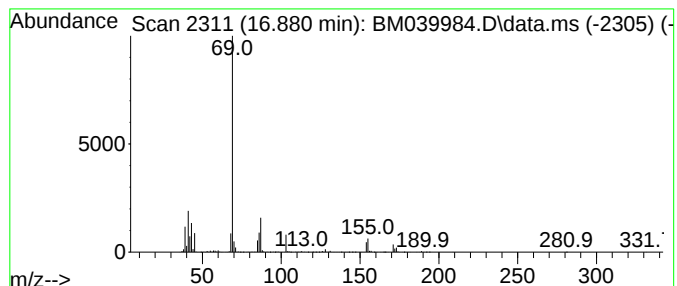
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown16.880 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.880	11.32 ng	1653910	Phenanthrene-d10	17.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,3,7-Trimethyl-4-oxa-7-octen-1-ol	172	C10H20O2	069161-47-3	39		
2	(E)-2-Methylbut-2-en-1-yl methac...	154	C9H14O2	088142-95-4	38		
3	Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	38		
4	Oxazolidin-2-one, N-[(E)-butenoyl]-	155	C7H9NO3	1010156-45-5	9		
5	Oxazolidin-2-one, N-[(Z)-butenoyl]-	155	C7H9NO3	1000156-45-4	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039984.D
Acq On : 24 May 2023 15:09
Operator : CG/JU
Sample : 02899-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

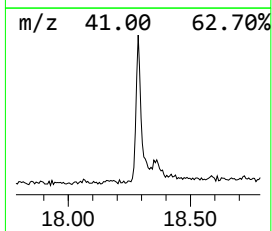
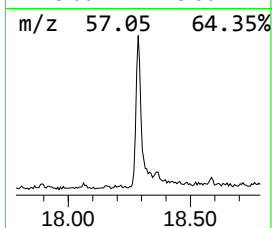
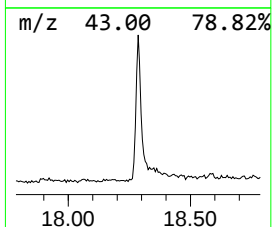
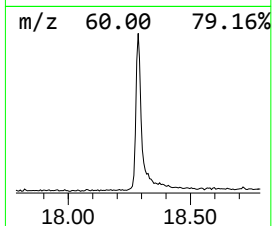
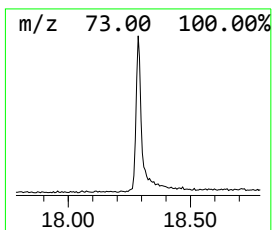
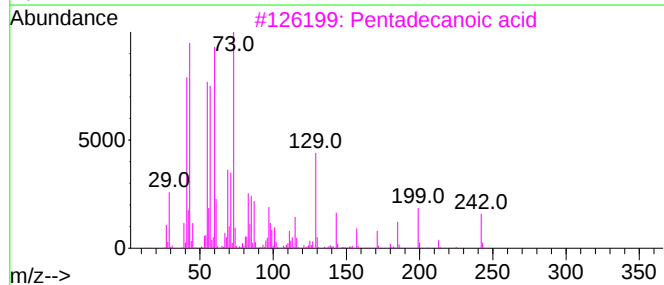
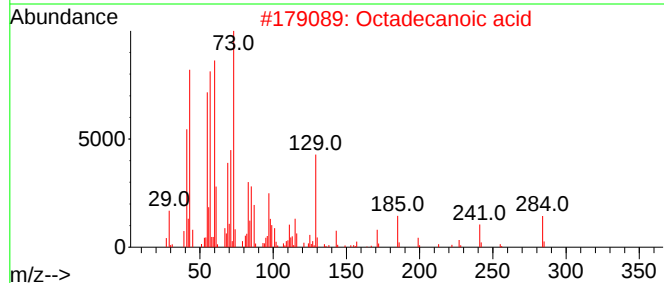
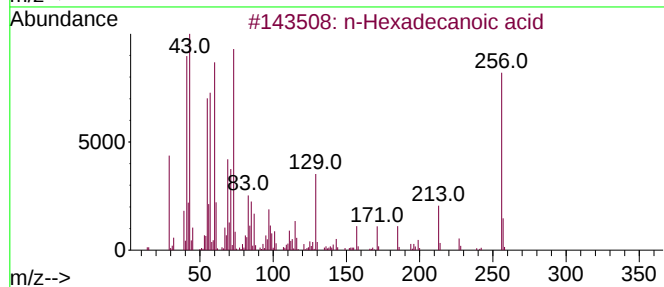
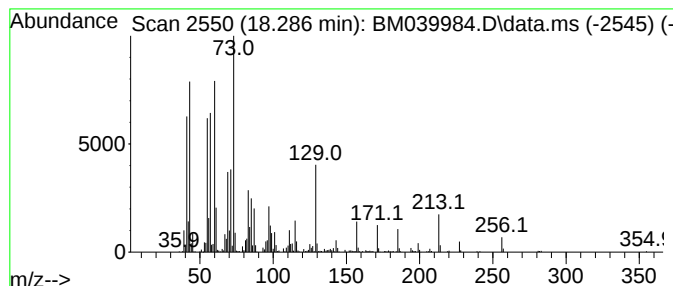
Instrument :
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ClientSampleId :
TWP01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.286	5.11 ng	746479	Phenanthrene-d10		17.392	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Octadecanoic acid		284	C18H36O2	000057-11-4	94
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	94
4	Tridecanoic acid		214	C13H26O2	000638-53-9	93
5	Tetradecanoic acid		228	C14H28O2	000544-63-8	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039984.D
Acq On : 24 May 2023 15:09
Operator : CG/JU
Sample : 02899-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

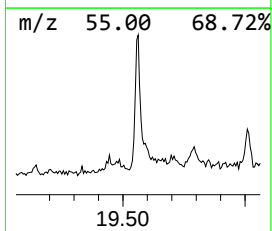
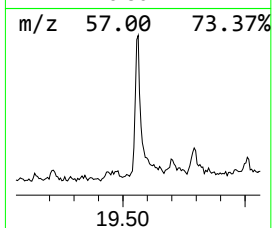
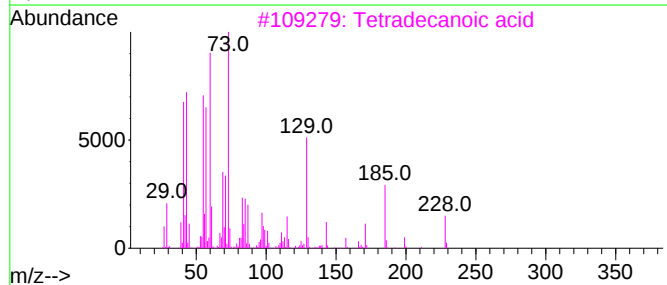
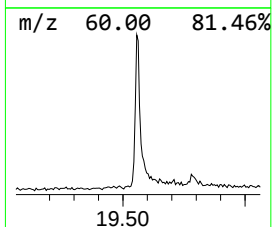
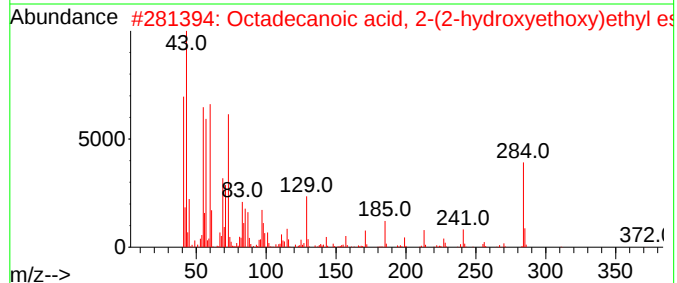
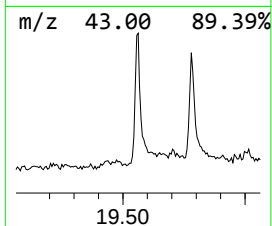
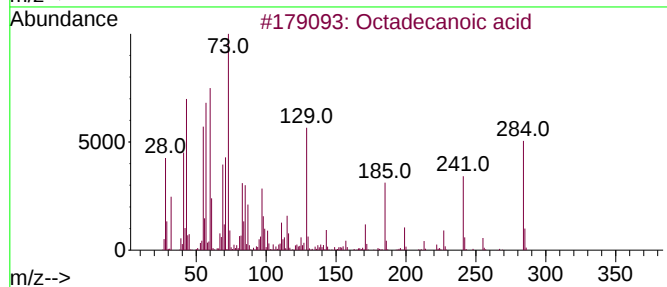
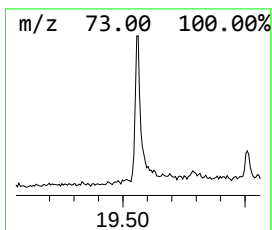
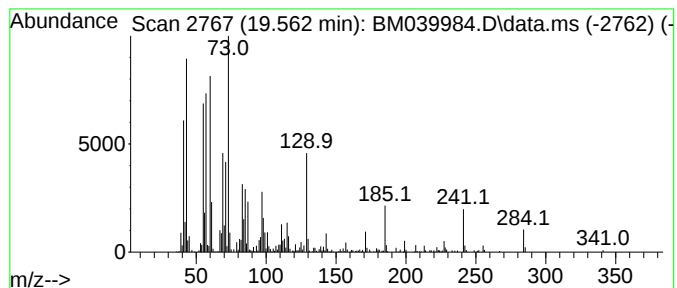
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.562	2.85 ng	563037	Chrysene-d12	21.568	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039984.D
Acq On : 24 May 2023 15:09
Operator : CG/JU
Sample : 02899-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TWP01

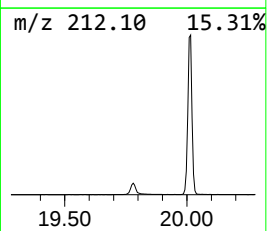
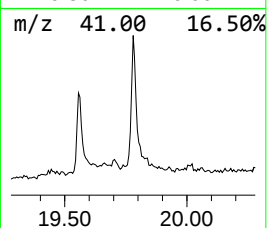
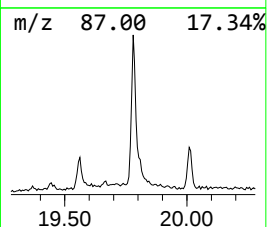
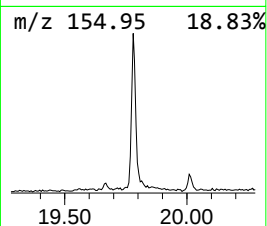
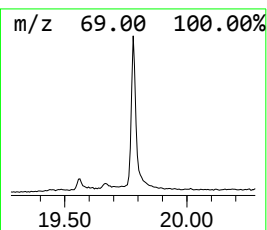
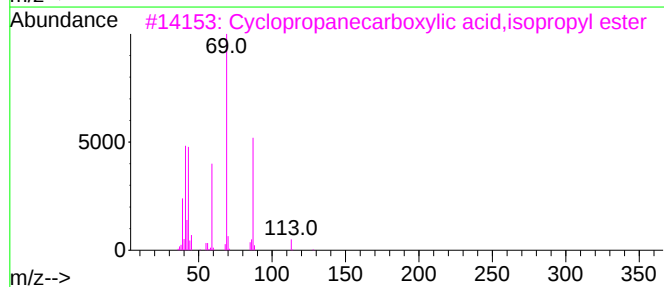
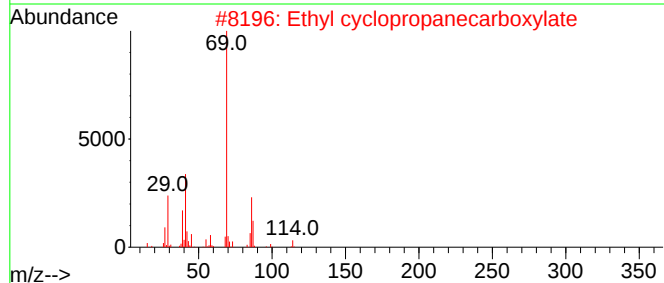
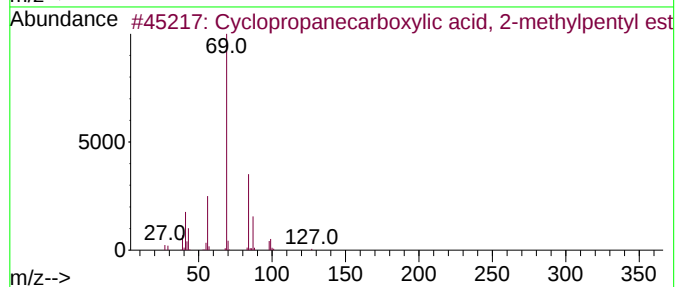
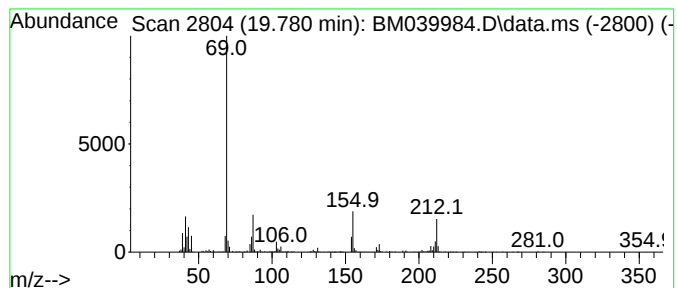
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown19.780 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.780	3.83 ng	756231	Chrysene-d12	21.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropanecarboxylic acid, 2-m...	170	C10H18O2	1000354-65-8	36
2			Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	33
3			Cyclopropanecarboxylic acid, isop...	128	C7H12O2	006887-83-8	28
4			2,3'-Bifuran, 2,2',3',5-tetrahydro-	138	C8H10O2	098869-93-3	28
5			Cyclopropanecarboxylic acid, buty...	142	C8H14O2	054947-39-6	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039984.D
Acq On : 24 May 2023 15:09
Operator : CG/JU
Sample : 02899-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

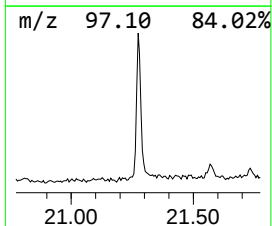
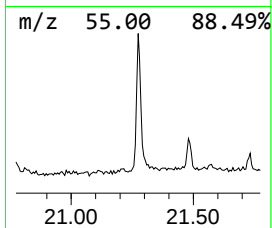
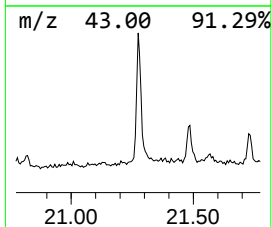
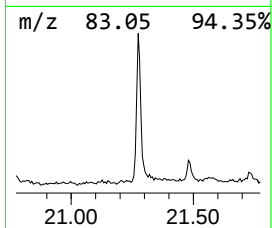
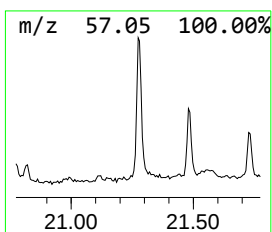
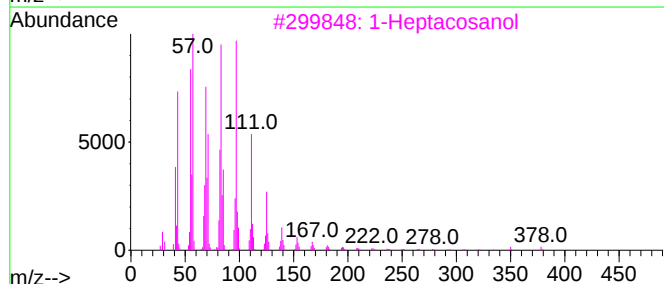
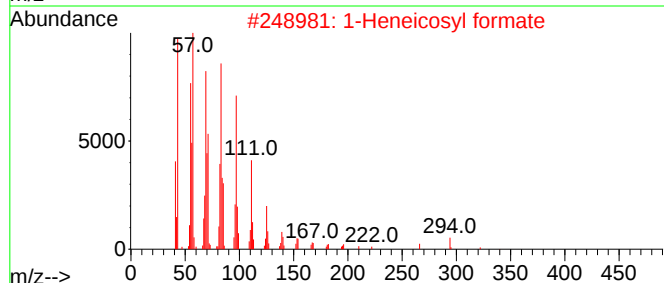
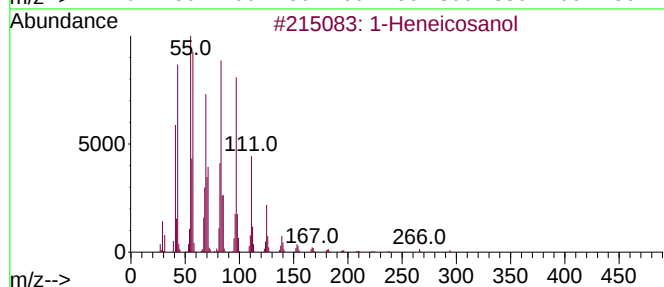
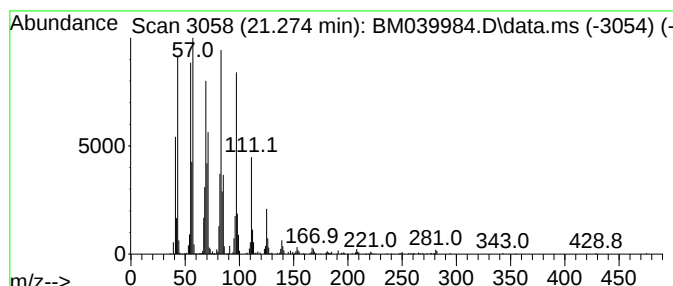
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.274	3.20 ng	633185	Chrysene-d12	21.568	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3	1-Heptacosanol	396	C27H56O	002004-39-9	94
4	Pentacos-1-ene	350	C25H50	016980-85-1	94
5	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039984.D
Acq On : 24 May 2023 15:09
Operator : CG/JU
Sample : 02899-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TWP01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.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
Crotonic acid	4.640	2.1	ng	185326	1	8.016	1798780	20.0
2-Pentanone, 4-...	5.093	3.6	ng	324929	1	8.016	1798780	20.0
unknown12.445	12.445	9.2	ng	1086290	2	10.833	2368610	20.0
Benzophenone	16.004	9.4	ng	1239180	3	14.651	2647810	20.0
Benzenesulfonam...	16.333	2.9	ng	430029	4	17.392	2921920	20.0
unknown16.880	16.880	11.3	ng	1653910	4	17.392	2921920	20.0
n-Hexadecanoic ...	18.286	5.1	ng	746479	4	17.392	2921920	20.0
Octadecanoic acid	19.562	2.9	ng	563037	5	21.568	3952520	20.0
unknown19.780	19.780	3.8	ng	756231	5	21.568	3952520	20.0
1-Heneicosanol	21.274	3.2	ng	633185	5	21.568	3952520	20.0