

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
 Data File : BM038731.D
 Acq On : 14 Feb 2023 15:40
 Operator : CG/JU
 Sample : 01328-06
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 COMP-2-BORING-1-7-14

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: BM038731.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.987	301	306	318	rVB	242031	335891	14.54%	2.716%
2	5.457	381	386	399	rBV	693403	977319	42.29%	7.902%
3	7.075	654	661	675	rBV	633402	966687	41.83%	7.816%
4	7.898	795	801	807	rBV	162635	244542	10.58%	1.977%
5	9.075	992	1001	1011	rBV	386978	602419	26.07%	4.871%
6	10.710	1272	1279	1287	rBV	171041	283479	12.27%	2.292%
7	13.169	1690	1697	1708	rBV	1108154	1553499	67.23%	12.560%
8	14.539	1924	1930	1938	rBV	269391	377768	16.35%	3.054%
9	15.898	2156	2161	2168	rVB	35598	46344	2.01%	0.375%
10	16.033	2178	2184	2192	rBV	834337	1136768	49.19%	9.191%
11	17.286	2391	2397	2402	rBV	304172	422034	18.26%	3.412%
12	18.168	2541	2547	2557	rBV	146388	219308	9.49%	1.773%
13	19.339	2741	2746	2751	rVB4	21374	35519	1.54%	0.287%
14	19.445	2759	2764	2773	rBV	66248	107687	4.66%	0.871%
15	19.580	2784	2787	2792	rBV2	22135	27008	1.17%	0.218%
16	19.721	2804	2811	2819	rBV2	19523	41304	1.79%	0.334%
17	19.904	2836	2842	2849	rVB	2077677	2310741	100.00%	18.682%
18	21.156	3051	3055	3062	rBV	141854	208226	9.01%	1.683%
19	21.462	3102	3107	3112	rBV	490196	589081	25.49%	4.763%
20	22.327	3249	3254	3261	rVB	837063	1072633	46.42%	8.672%
21	23.839	3505	3511	3522	rVB	413419	810426	35.07%	6.552%

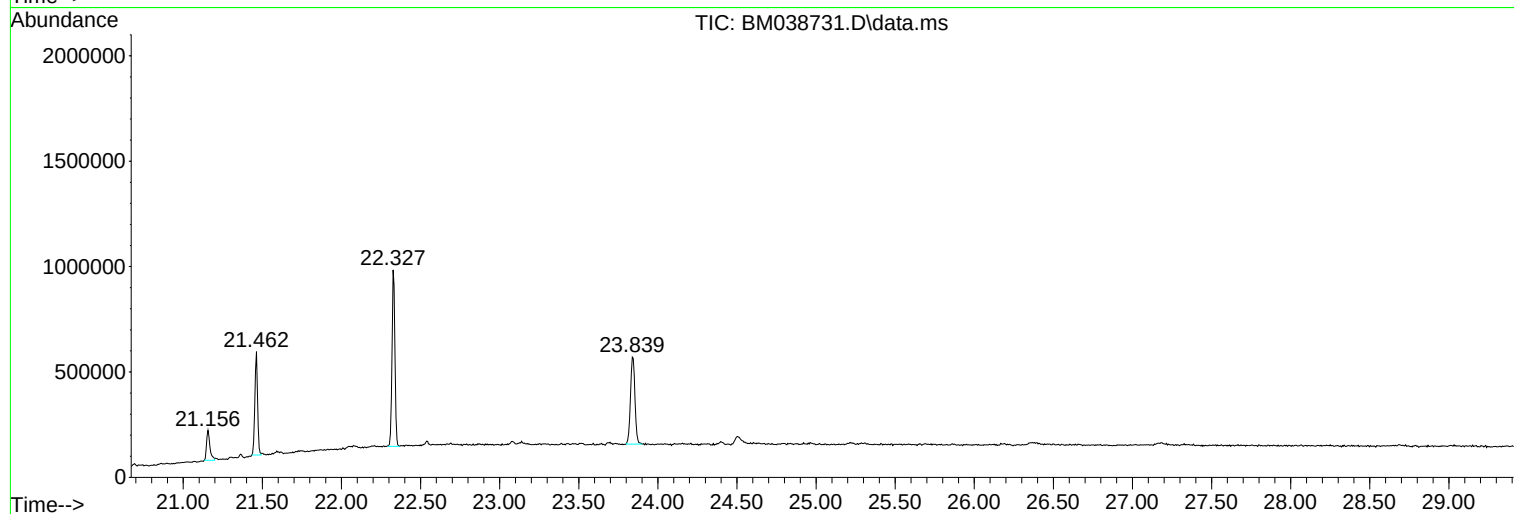
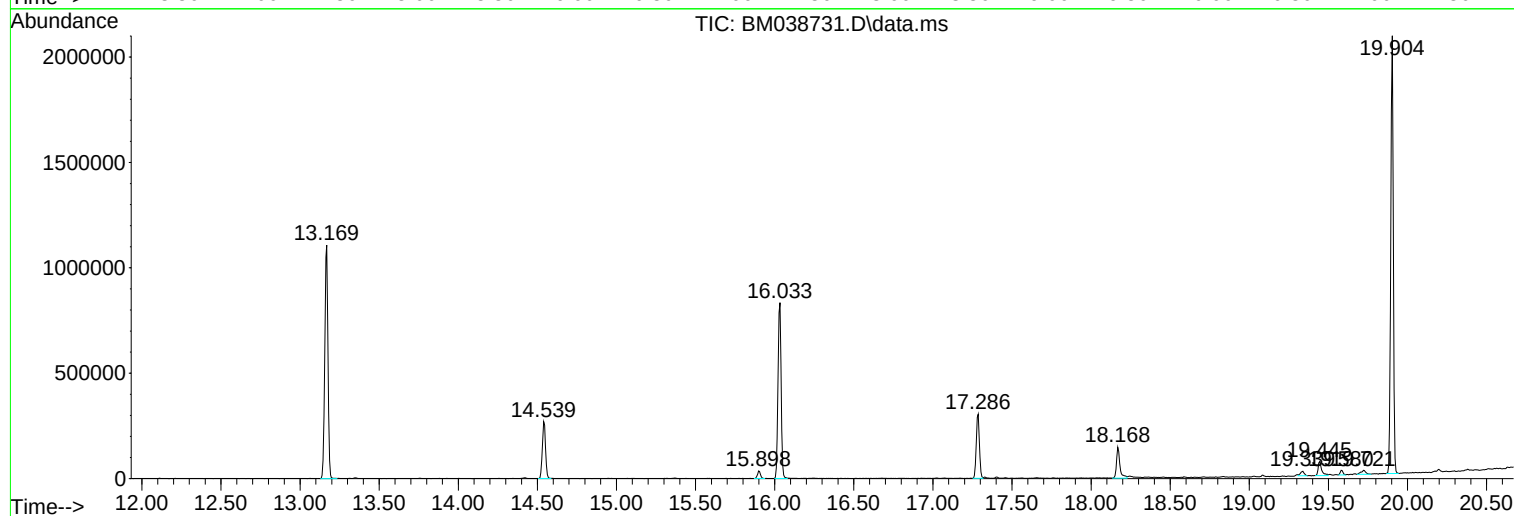
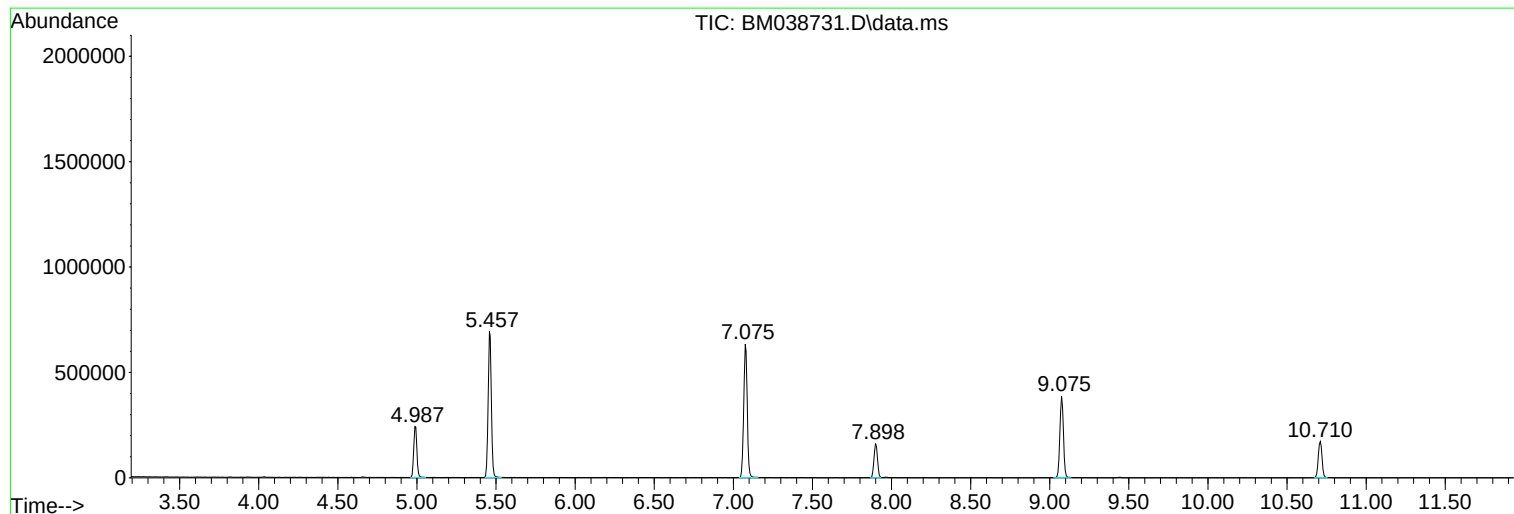
Sum of corrected areas: 12368683

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038731.D
Acq On : 14 Feb 2023 15:40
Operator : CG/JU
Sample : 01328-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-2-BORING-1-7-14

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038731.D
Acq On : 14 Feb 2023 15:40
Operator : CG/JU
Sample : 01328-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-2-BORING-1-7-14

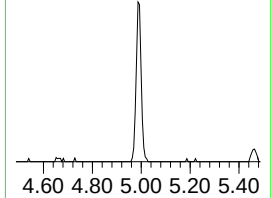
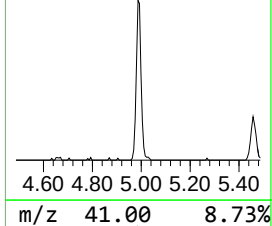
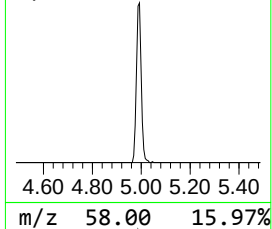
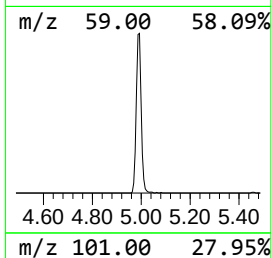
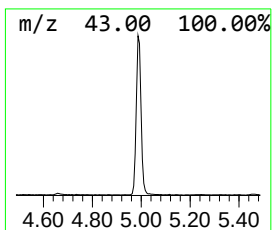
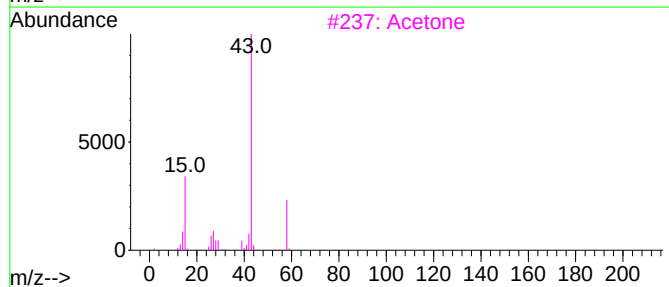
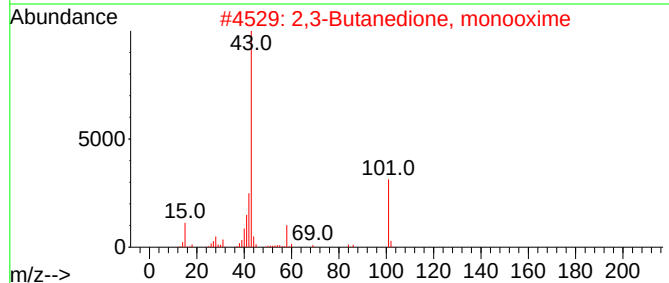
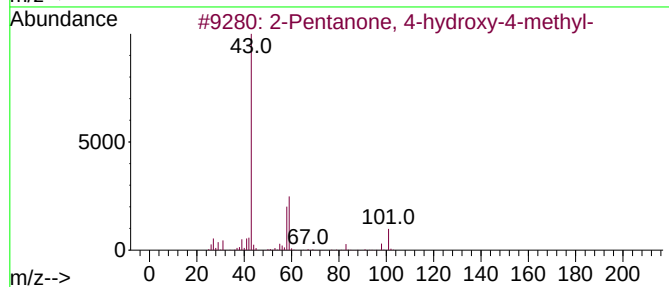
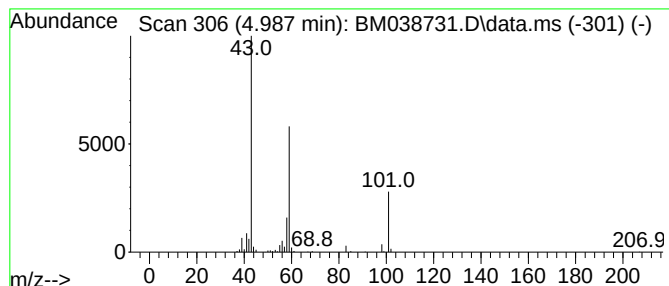
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	27.47 ng	335891	1,4-Dichlorobenzene-d4	7.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
3	Acetone	58	C3H6O	000067-64-1	10		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038731.D
Acq On : 14 Feb 2023 15:40
Operator : CG/JU
Sample : 01328-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-2-BORING-1-7-14

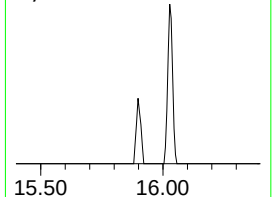
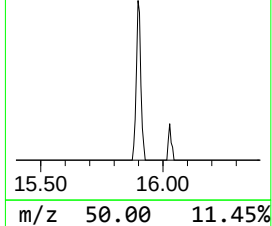
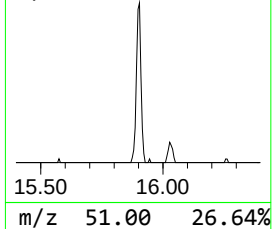
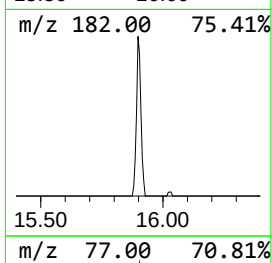
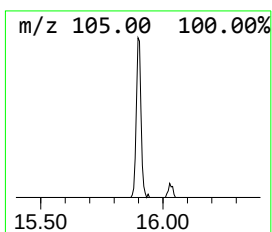
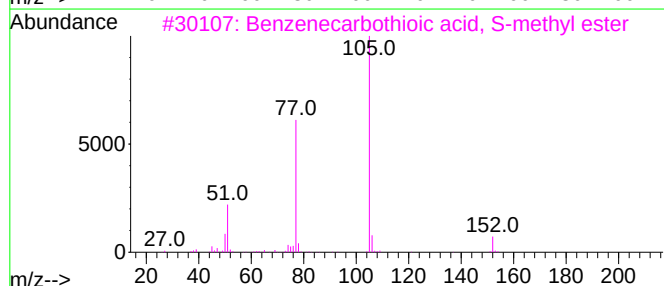
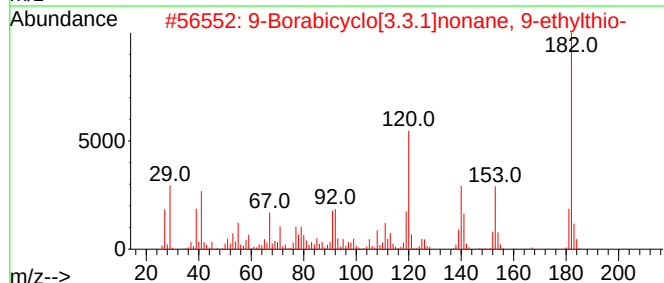
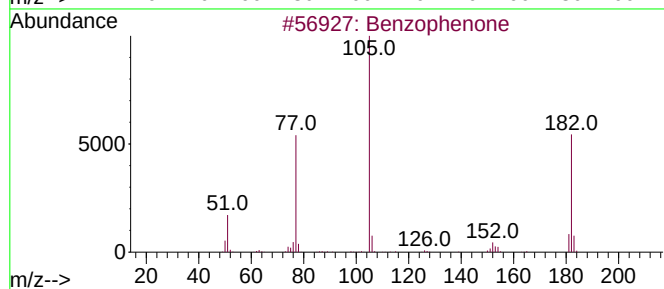
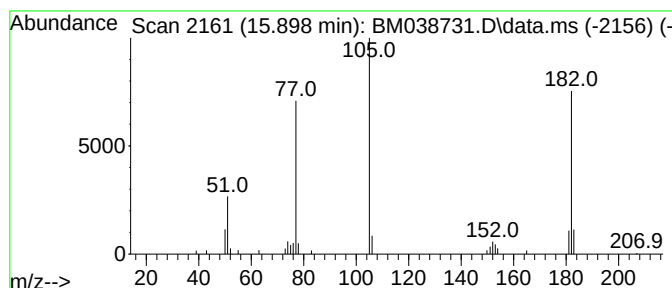
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.898	2.45 ng	46344	Acenaphthene-d10	14.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	95
2			9-Borabicyclo[3.3.1]nonane, 9-ethylthio-	182	C10H19BS	1000155-58-6	43
3			Benzenecarbothioic acid, S-methyl ester	152	C8H8OS	005925-68-8	41
4			Glyoxylohydroximoyl chloride, 2-oxo-	183	C8H6ClNO2	004937-87-5	38
5			1-Methyl-1,6-diazaplenalene	182	C12H10N2	079691-99-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038731.D
Acq On : 14 Feb 2023 15:40
Operator : CG/JU
Sample : 01328-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

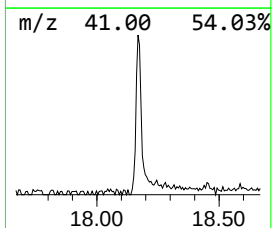
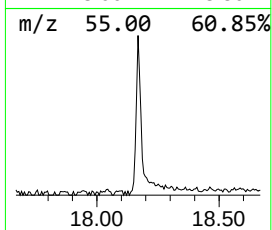
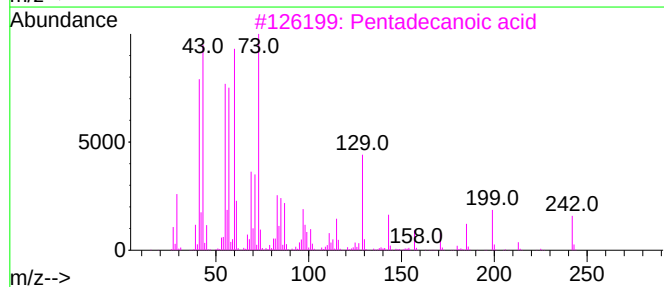
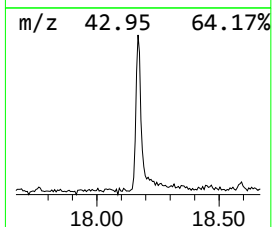
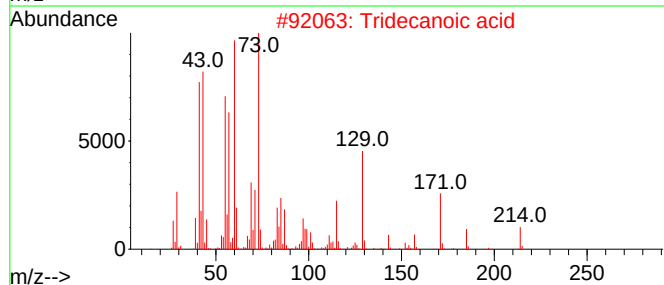
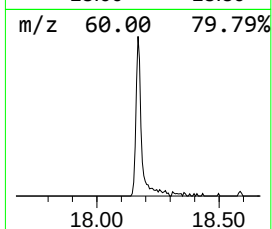
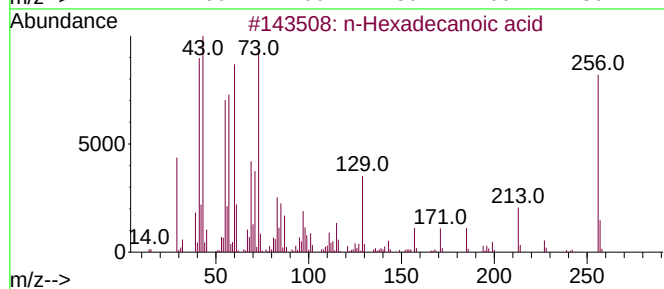
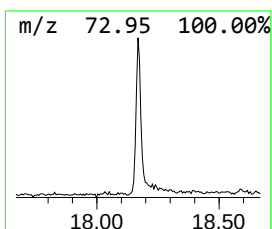
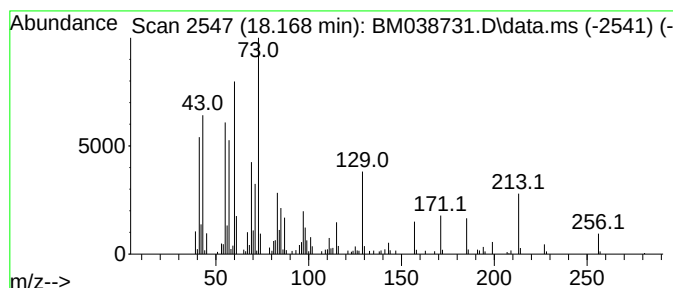
Instrument :
BNA_M
ClientSampleId :
COMP-2-BORING-1-7-14

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.168	10.39 ng	219308	Phenanthrene-d10	17.286	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038731.D
Acq On : 14 Feb 2023 15:40
Operator : CG/JU
Sample : 01328-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-2-BORING-1-7-14

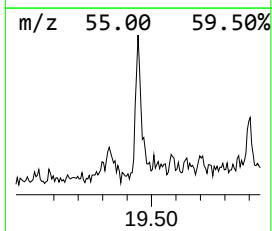
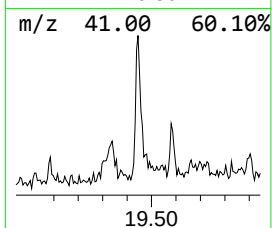
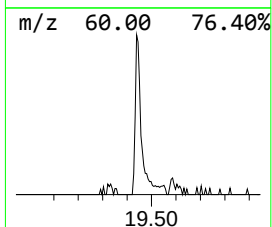
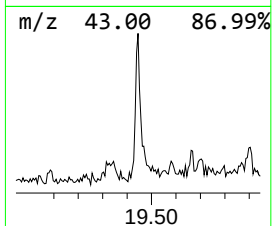
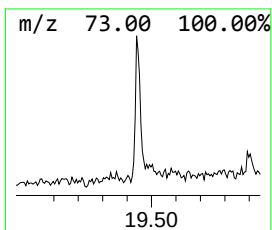
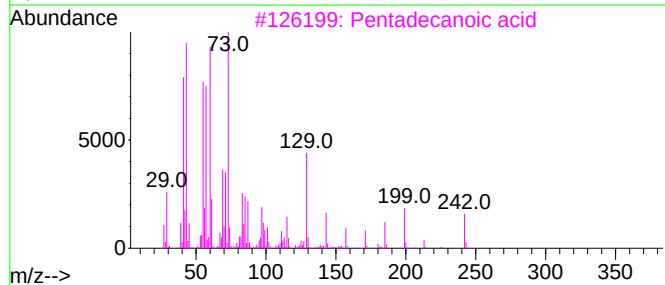
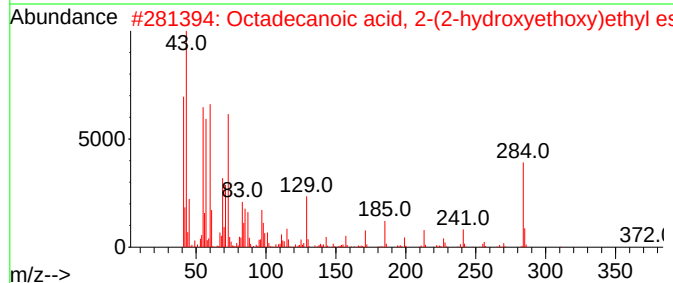
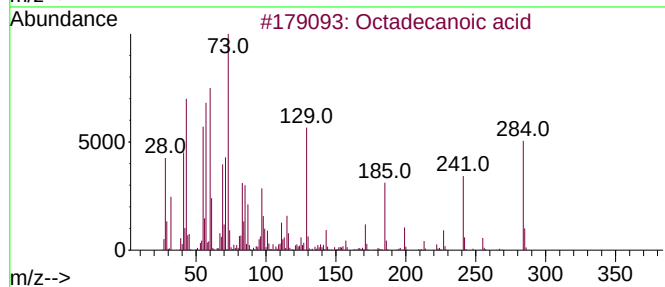
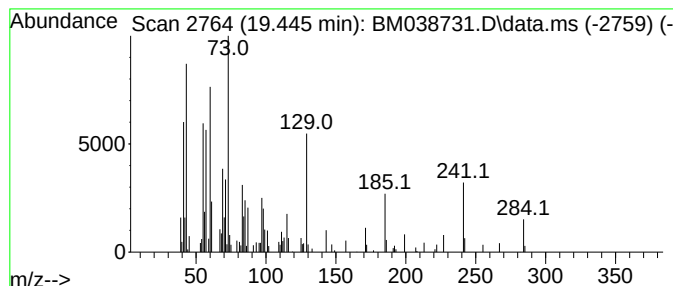
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.445	3.66 ng	107687	Chrysene-d12	21.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Tridecanoic acid	214	C13H26O2	000638-53-9	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038731.D
Acq On : 14 Feb 2023 15:40
Operator : CG/JU
Sample : 01328-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-2-BORING-1-7-14

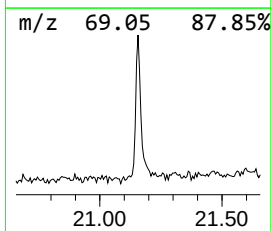
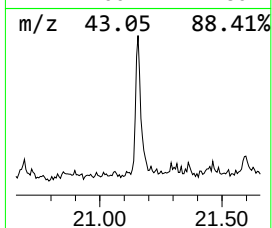
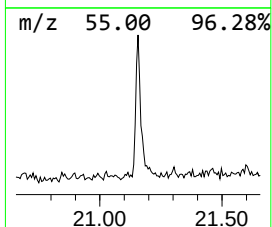
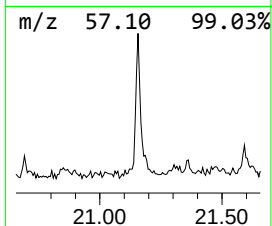
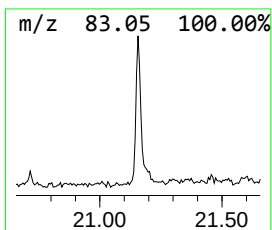
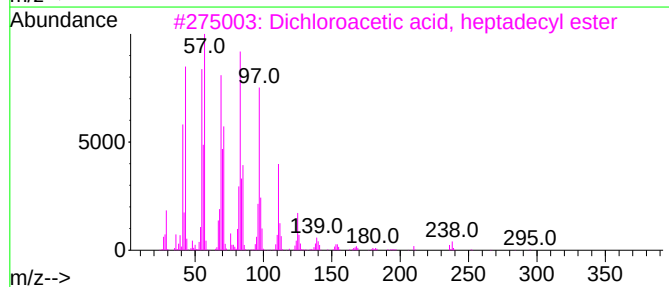
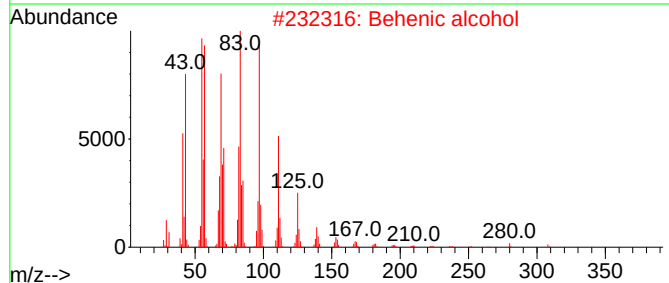
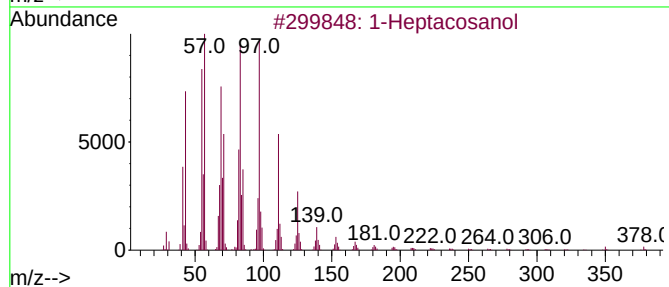
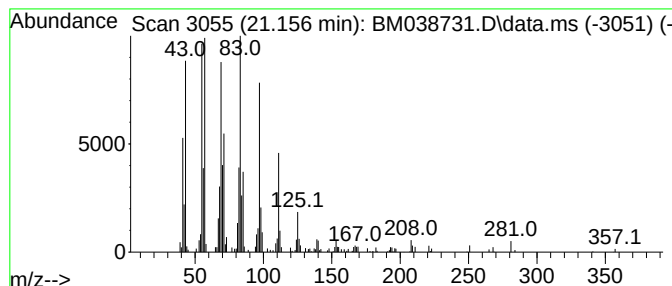
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Heptacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.156	7.07 ng	208226	Chrysene-d12	21.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptacosanol	396	C27H56O	002004-39-9	94
2			Behenic alcohol	326	C22H46O	000661-19-8	94
3			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5			n-Nonadecanol-1	284	C19H40O	001454-84-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038731.D
Acq On : 14 Feb 2023 15:40
Operator : CG/JU
Sample : 01328-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

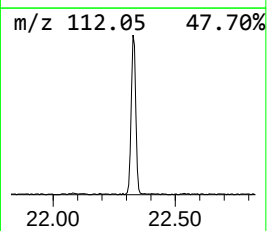
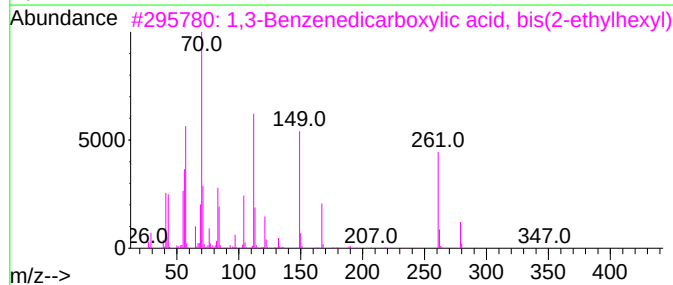
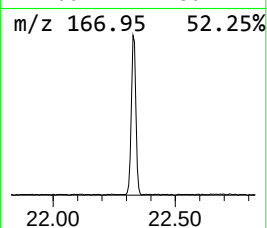
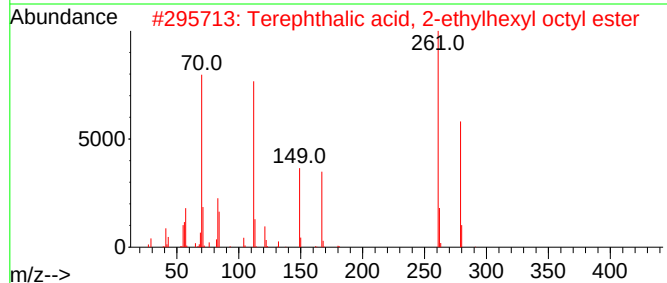
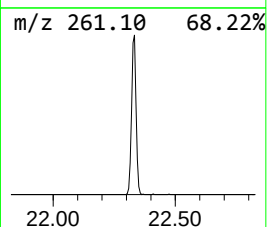
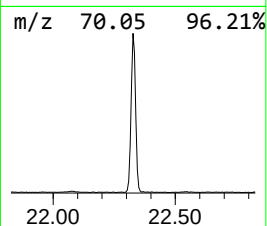
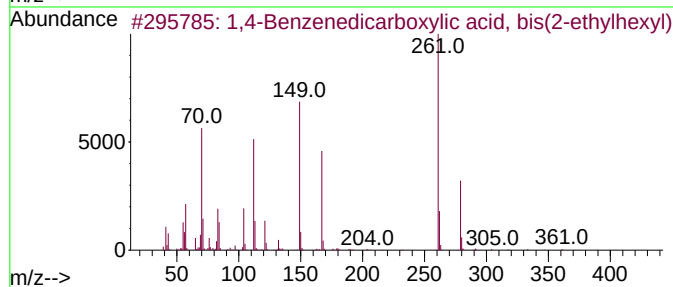
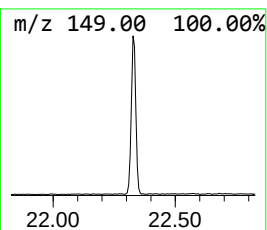
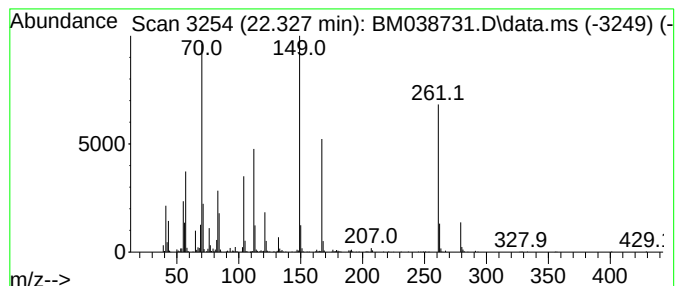
Instrument :
BNA_M
ClientSampleId :
COMP-2-BORING-1-7-14

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

Peak Number 6 1,4-Benzenedicarboxylic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.327	36.42 ng	1072630	Chrysene-d12	21.462
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		1,4-Benzenedicarboxylic acid, bi...	390 C24H38O4	006422-86-2 62
2		Terephthalic acid, 2-ethylhexyl ...	390 C24H38O4	1000324-00-5 50
3		1,3-Benzenedicarboxylic acid, bi...	390 C24H38O4	000137-89-3 49
4		Terephthalic acid, 3,5-difluorop...	390 C22H24F2O4	1000324-05-2 38
5		Terephthalic acid, di(4-octyl) e...	390 C24H38O4	1000323-74-2 38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038731.D
Acq On : 14 Feb 2023 15:40
Operator : CG/JU
Sample : 01328-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-2-BORING-1-7-14

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-...	4.987	27.5	ng	335891	1	7.898	244542	20.0
Benzophenone	15.898	2.5	ng	46344	3	14.539	377768	20.0
n-Hexadecanoic ...	18.168	10.4	ng	219308	4	17.286	422034	20.0
Octadecanoic acid	19.445	3.7	ng	107687	5	21.462	589081	20.0
1-Heptacosanol	21.156	7.1	ng	208226	5	21.462	589081	20.0
1,4-Benzenedica...	22.327	36.4	ng	1072630	5	21.462	589081	20.0