

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
 Data File : BM038729.D
 Acq On : 14 Feb 2023 14:26
 Operator : CG/JU
 Sample : 01328-11
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 COMP-3-BORING-1-14-23

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: BM038729.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	315	rVB	228319	307103	16.48%	2.850%
2	5.457	380	386	397	rBV	640686	917316	49.23%	8.512%
3	7.075	654	661	675	rBV	602887	903300	48.48%	8.382%
4	7.898	795	801	808	rVB	168982	250771	13.46%	2.327%
5	9.075	994	1001	1011	rBV	355624	560958	30.10%	5.205%
6	10.710	1270	1279	1286	rBV	193335	313339	16.82%	2.907%
7	13.163	1690	1696	1704	rBV	951665	1356110	72.78%	12.583%
8	14.539	1924	1930	1941	rBV	311797	427077	22.92%	3.963%
9	15.898	2155	2161	2166	rBV	34268	44686	2.40%	0.415%
10	16.033	2177	2184	2195	rBV	816359	1133697	60.84%	10.520%
11	17.286	2391	2397	2403	rBV	348337	481542	25.84%	4.468%
12	18.168	2541	2547	2557	rBV	203701	313498	16.82%	2.909%
13	18.245	2557	2560	2565	rVB	11906	19966	1.07%	0.185%
14	19.327	2741	2744	2751	rVB7	13645	24230	1.30%	0.225%
15	19.445	2759	2764	2777	rBV2	106400	177662	9.53%	1.649%
16	19.721	2807	2811	2818	rVB	19677	31171	1.67%	0.289%
17	19.903	2836	2842	2848	rBV	1573867	1863366	100.00%	17.290%
18	21.156	3051	3055	3061	rBV	70581	110678	5.94%	1.027%
19	21.462	3102	3107	3112	rBV	490991	602122	32.31%	5.587%
20	22.327	3250	3254	3261	rVB	145686	187862	10.08%	1.743%
21	23.838	3505	3511	3520	rBV2	377252	750628	40.28%	6.965%

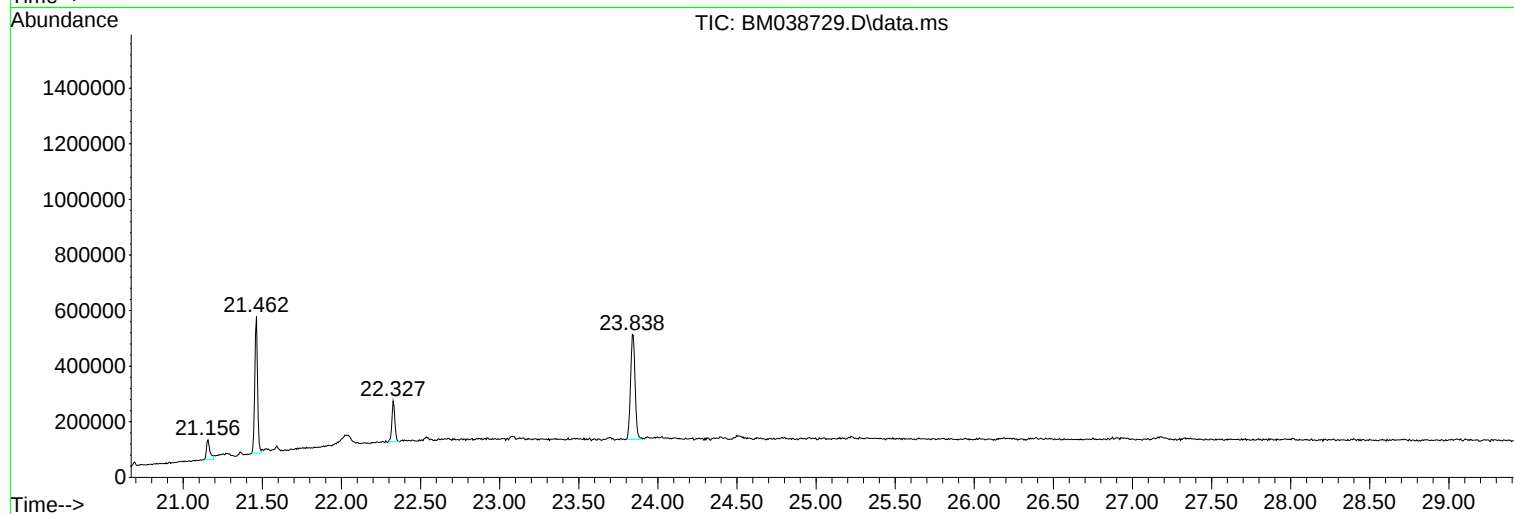
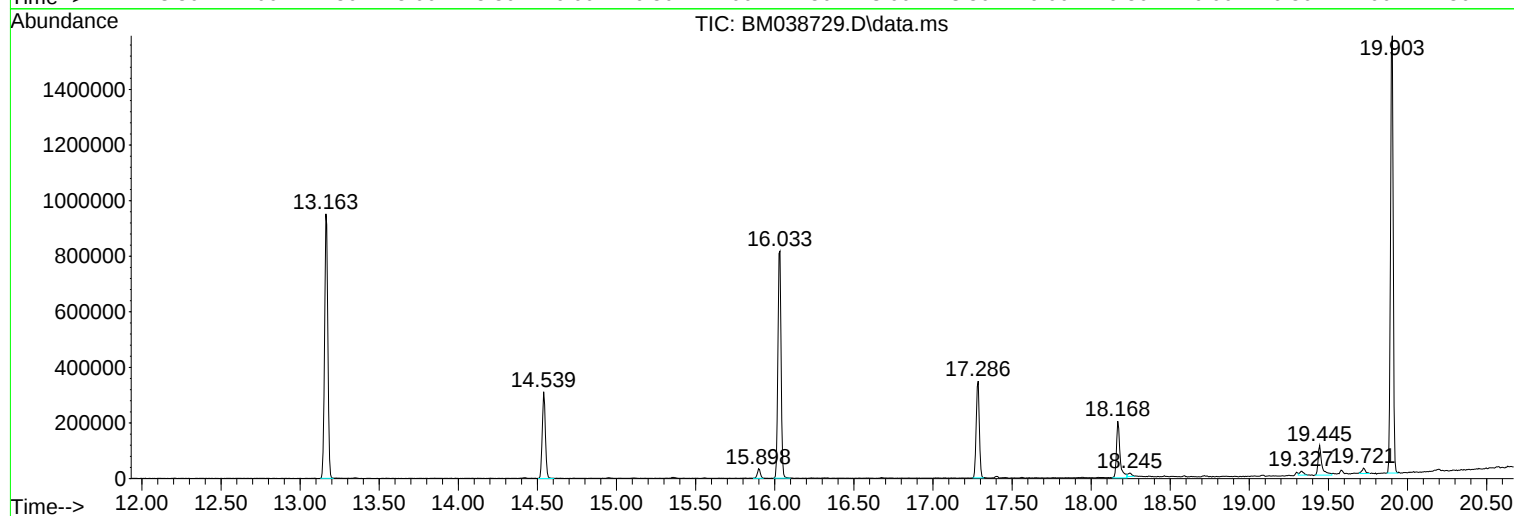
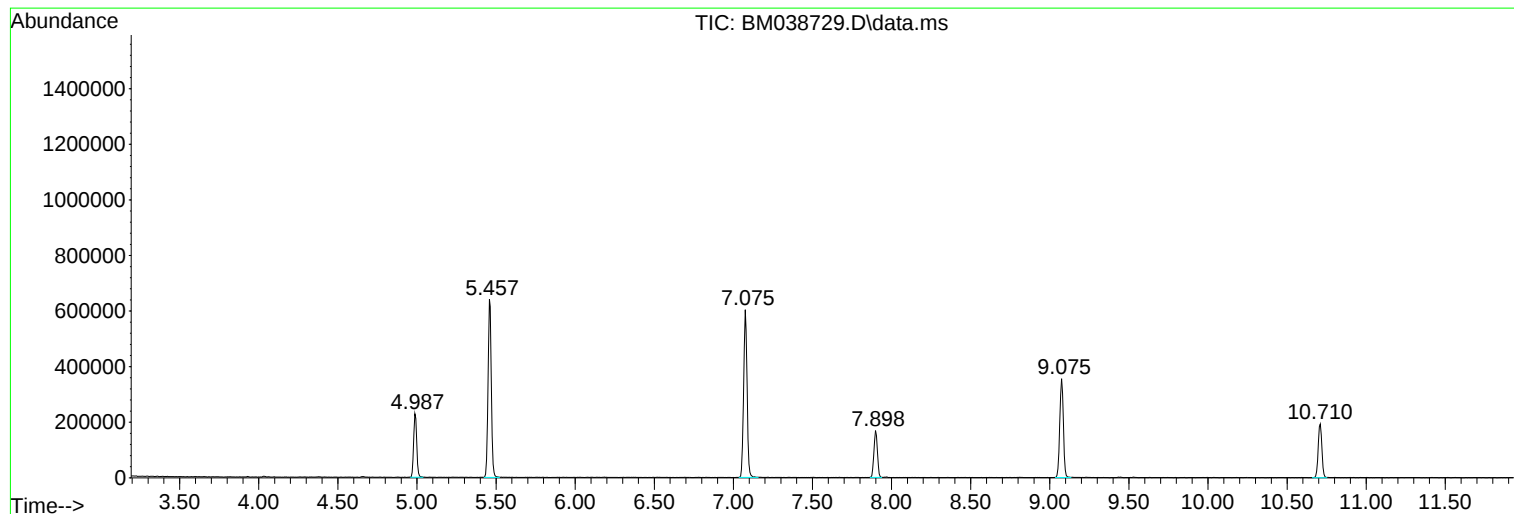
Sum of corrected areas: 10777082

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038729.D
Acq On : 14 Feb 2023 14:26
Operator : CG/JU
Sample : 01328-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-3-BORING-1-14-23

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 : BM038729.D
Acq On : 14 Feb 2023 14:26
Operator : CG/JU
Sample : 01328-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-3-BORING-1-14-23

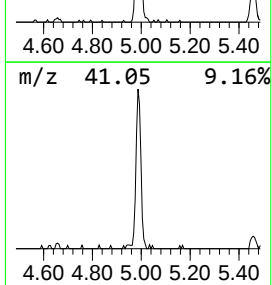
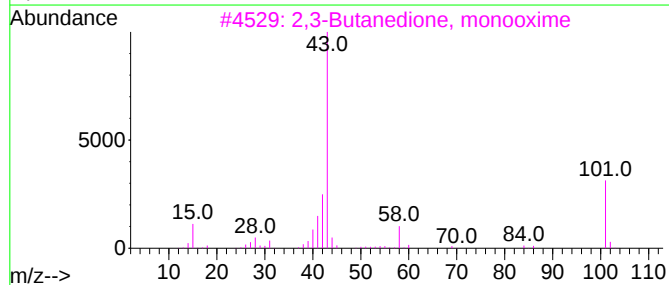
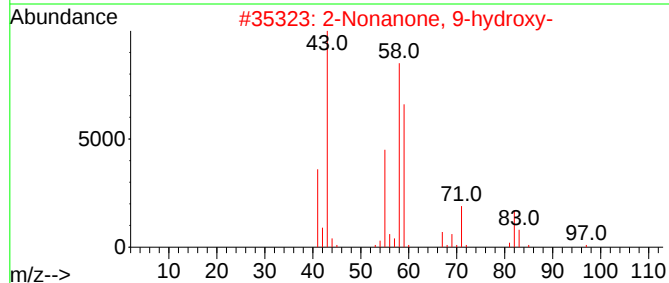
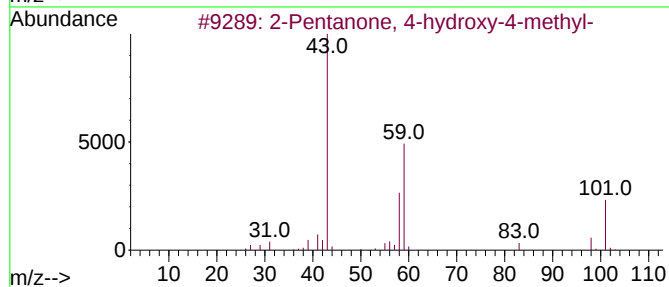
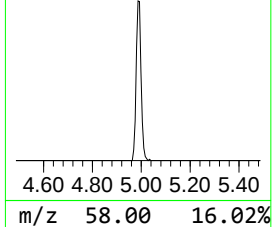
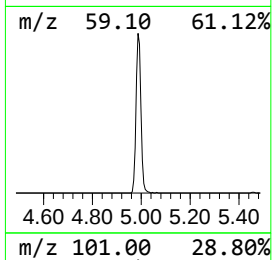
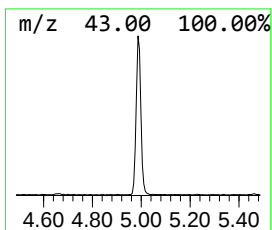
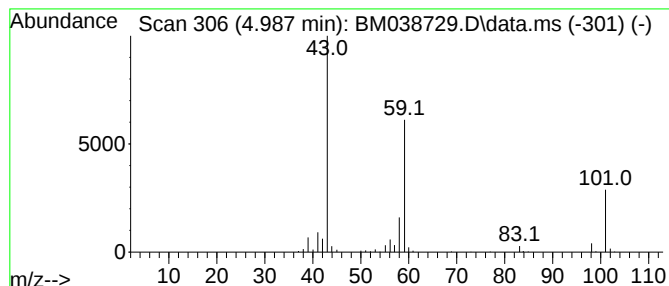
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	24.49 ng	307103	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	56
2		2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	28
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
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 : BM038729.D
Acq On : 14 Feb 2023 14:26
Operator : CG/JU
Sample : 01328-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-3-BORING-1-14-23

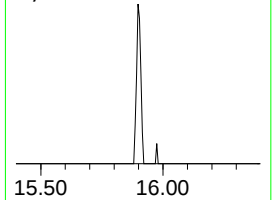
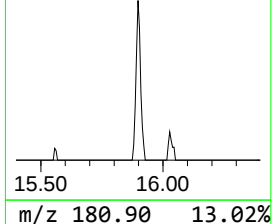
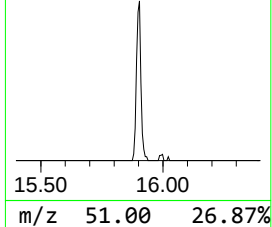
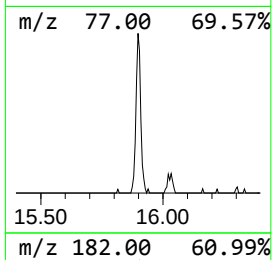
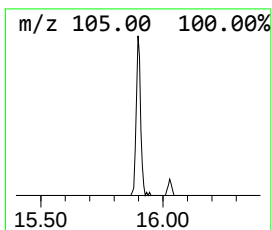
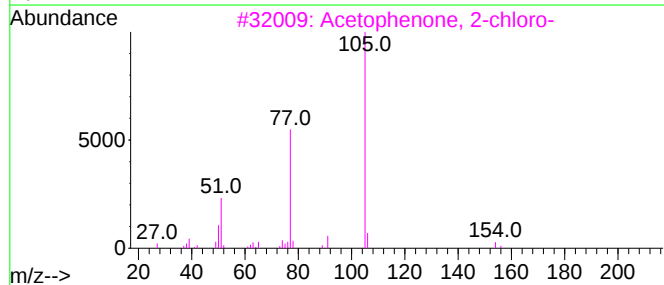
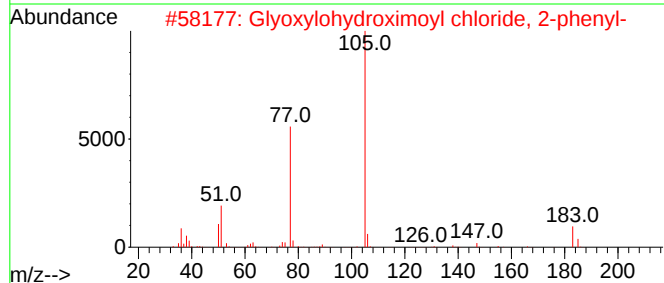
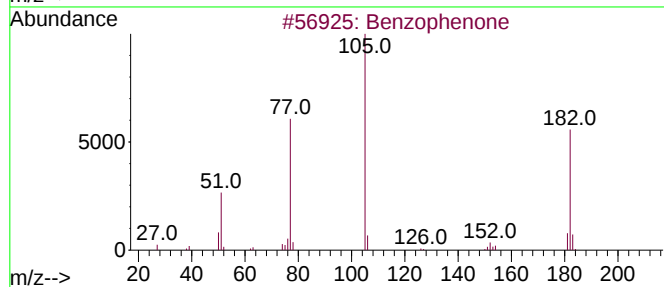
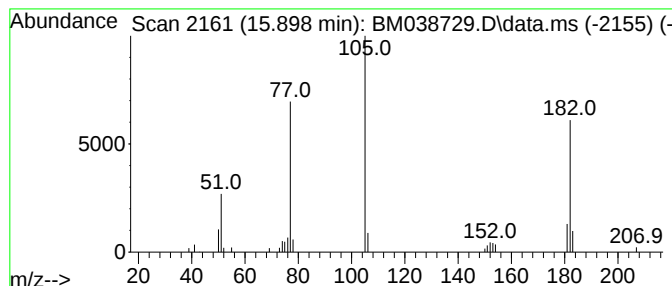
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	2.09 ng	44686	Acenaphthene-d10	14.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Glyoxylohydroximoyl chloride, 2-...	183	C8H6ClNO2	004937-87-5	49
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
4			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	46
5			Benzoylformic acid	150	C8H6O3	000611-73-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038729.D
Acq On : 14 Feb 2023 14:26
Operator : CG/JU
Sample : 01328-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

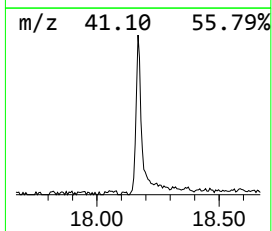
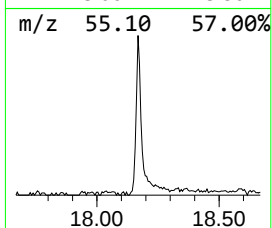
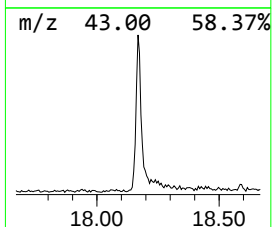
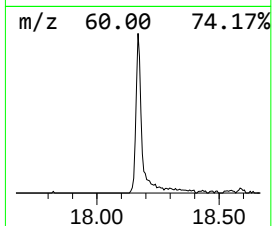
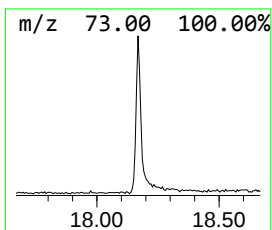
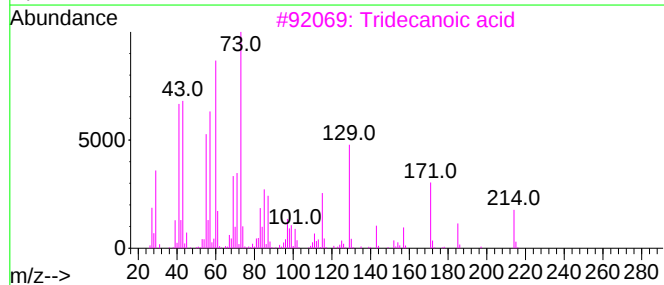
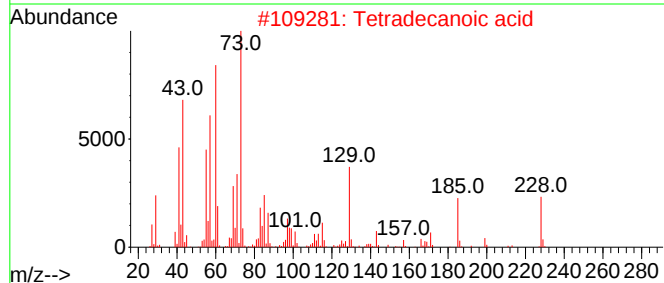
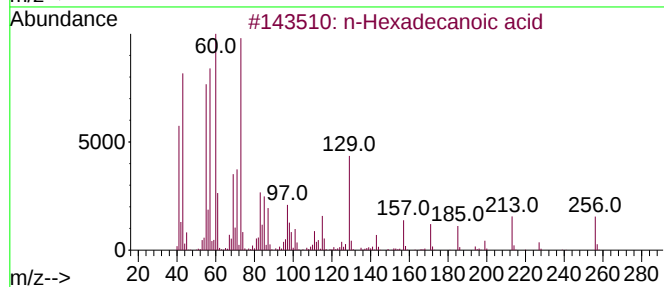
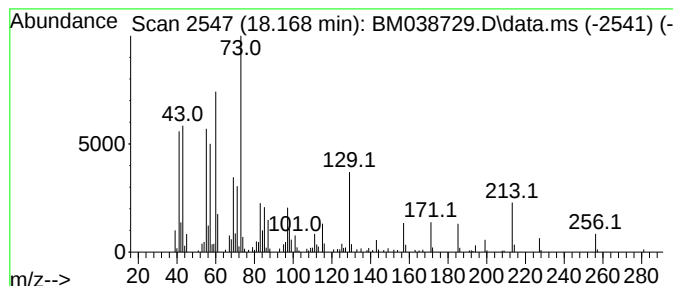
Instrument :
BNA_M
ClientSampleId :
COMP-3-BORING-1-14-23

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 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.168	13.02 ng	313498	Phenanthrene-d10		17.286	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid		228	C14H28O2	000544-63-8	94
3	Tridecanoic acid		214	C13H26O2	000638-53-9	70
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	62
5	Undecanoic acid		186	C11H22O2	000112-37-8	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038729.D
Acq On : 14 Feb 2023 14:26
Operator : CG/JU
Sample : 01328-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-3-BORING-1-14-23

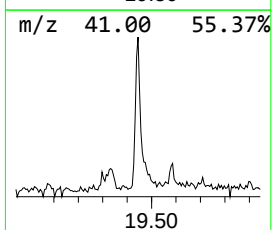
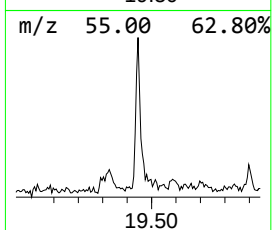
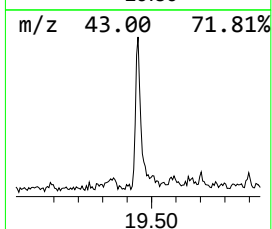
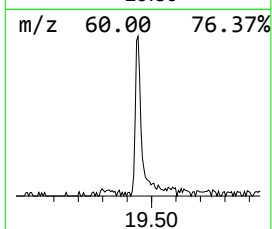
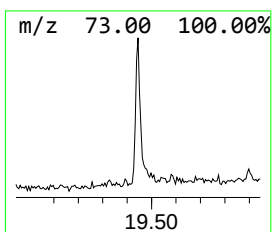
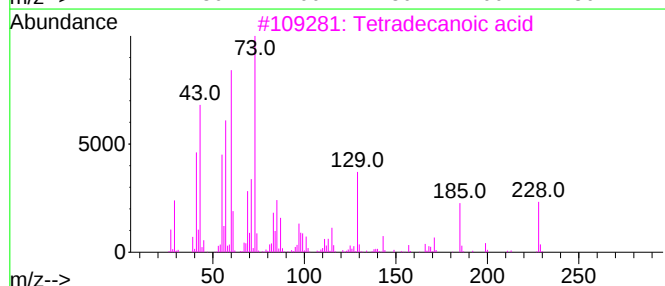
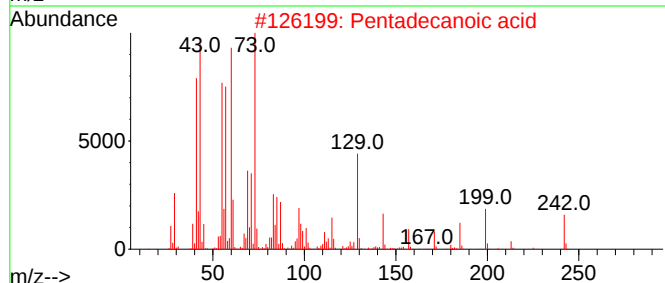
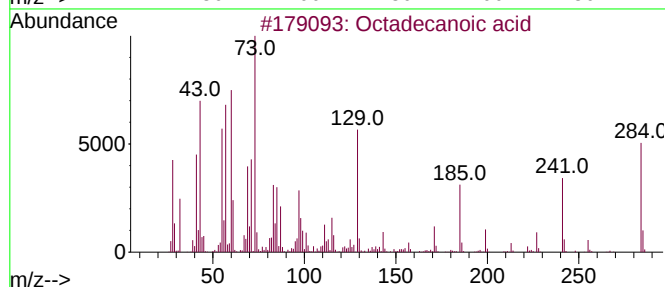
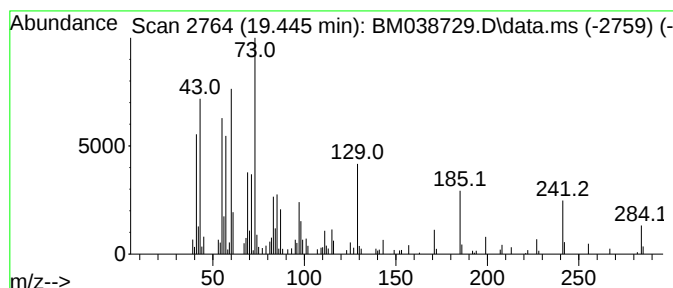
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.445	5.90 ng	177662	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	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			n-Decanoic acid	172	C10H20O2	000334-48-5	64
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038729.D
Acq On : 14 Feb 2023 14:26
Operator : CG/JU
Sample : 01328-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

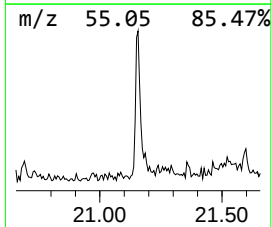
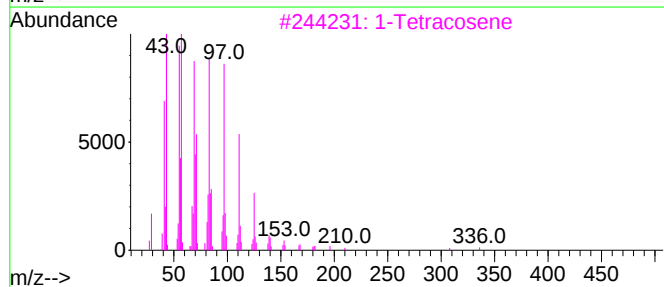
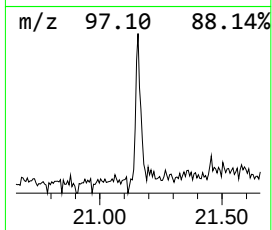
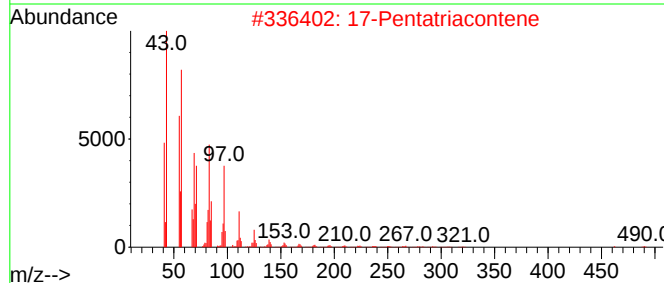
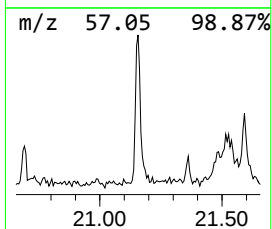
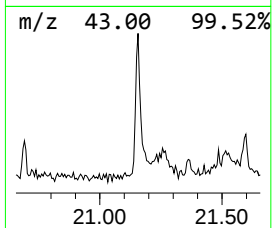
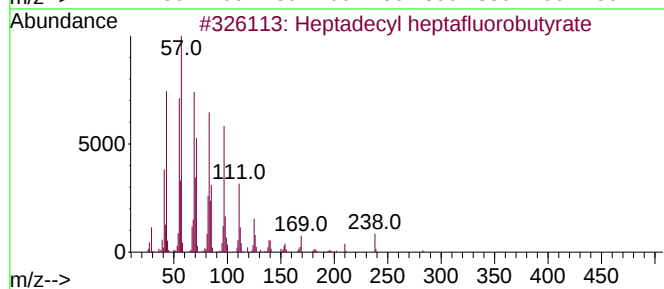
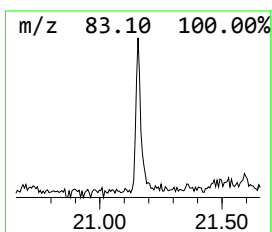
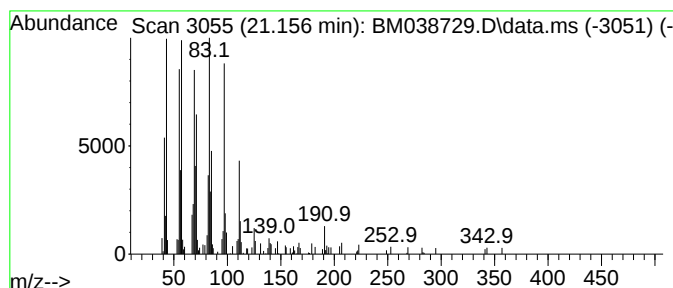
Instrument :
BNA_M
ClientSampleId :
COMP-3-BORING-1-14-23

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 Heptadecyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.156	3.68 ng	110678	Chrysene-d12	21.462	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2	17-Pentatriacontene	491	C35H70	006971-40-0	91
3	1-Tetracosene	336	C24H48	010192-32-2	87
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	83
5	1-Octadecanol	270	C18H38O	000112-92-5	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038729.D
Acq On : 14 Feb 2023 14:26
Operator : CG/JU
Sample : 01328-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

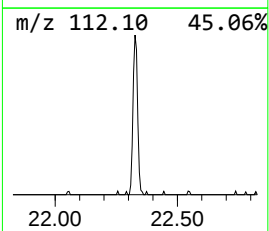
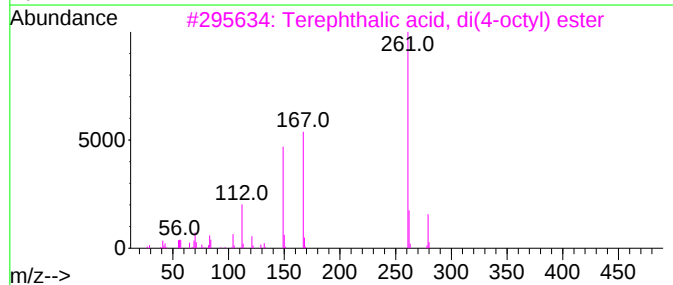
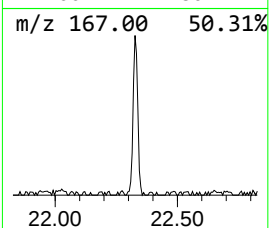
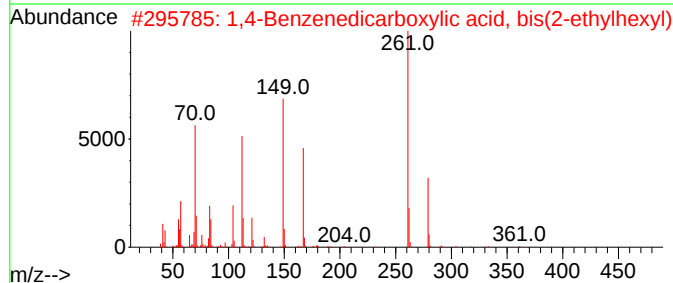
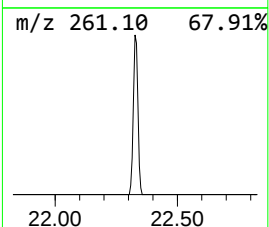
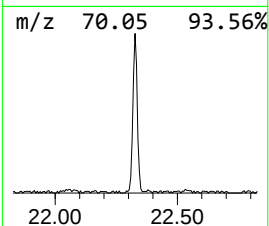
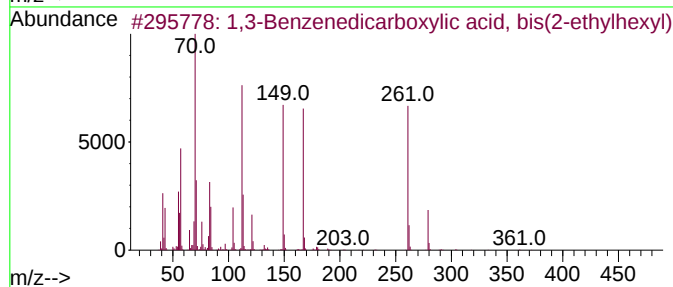
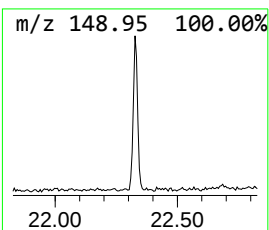
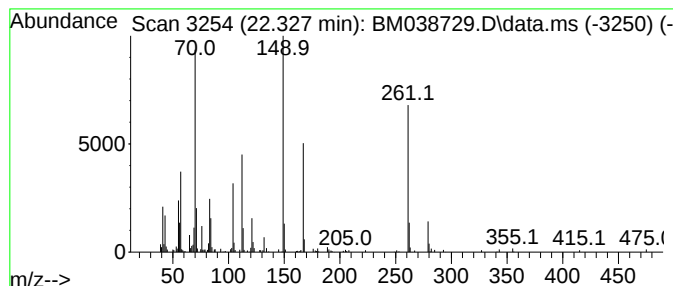
Instrument :
BNA_M
ClientSampleId :
COMP-3-BORING-1-14-23

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 1,3-Benzenedicarboxylic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.327	6.24 ng	187862	Chrysene-d12	21.462	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	53
2	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	52
3	Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	43
4	Phthalic acid, 6-ethyloct-3-yl 2...	418	C26H42O4	1000315-53-8	35
5	Terephthalic acid, 4,4-dimethylp...	376	C23H36O4	1000415-97-1	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038729.D
Acq On : 14 Feb 2023 14:26
Operator : CG/JU
Sample : 01328-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-3-BORING-1-14-23

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	24.5	ng	307103	1	7.898	250771	20.0
Benzophenone	15.898	2.1	ng	44686	3	14.539	427077	20.0
n-Hexadecanoic ...	18.168	13.0	ng	313498	4	17.286	481542	20.0
Octadecanoic acid	19.445	5.9	ng	177662	5	21.462	602122	20.0
Heptadecyl hept...	21.156	3.7	ng	110678	5	21.462	602122	20.0
1,3-Benzenedica...	22.327	6.2	ng	187862	5	21.462	602122	20.0