

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030823\
 Data File : BF132699.D
 Acq On : 08 Mar 2023 20:00
 Operator : CG\JU
 Sample : 01829-06
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS-06-20230306

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_F\Methods\8270-BF022223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132699.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.222	443	448	458	rVB	1372927	1664865	44.39%	6.079%
2	5.616	511	515	518	rBV	3475830	3234586	86.24%	11.811%
3	6.616	680	685	688	rBV	3235984	3228154	86.07%	11.788%
4	6.987	744	748	752	rBV	1214619	938544	25.02%	3.427%
5	7.040	754	757	765	rVB	73556	62830	1.68%	0.229%
6	7.551	840	844	847	rBV	2535925	2127703	56.73%	7.769%
7	8.269	963	966	970	rBV	1392209	1185877	31.62%	4.330%
8	9.345	1145	1149	1152	rBV	4354356	3750703	100.00%	13.696%
9	10.033	1262	1266	1269	rBV	1560881	1324615	35.32%	4.837%
10	10.745	1383	1387	1390	rBV	468043	371448	9.90%	1.356%
11	10.822	1396	1400	1410	rBV	2093095	1976191	52.69%	7.216%
12	11.375	1491	1494	1497	rBV	66088	52620	1.40%	0.192%
13	11.528	1516	1520	1524	rBV	1516460	1280729	34.15%	4.677%
14	11.739	1552	1556	1564	rBV2	25945	46998	1.25%	0.172%
15	12.039	1604	1607	1612	rBV	247770	255330	6.81%	0.932%
16	12.563	1693	1696	1701	rBV	46464	75290	2.01%	0.275%
17	12.769	1723	1731	1738	rBV2	45018	91613	2.44%	0.335%
18	12.827	1738	1741	1746	rBV3	43900	56280	1.50%	0.206%
19	13.116	1786	1790	1793	rBV	3644385	3154390	84.10%	11.518%
20	13.586	1867	1870	1874	rVB	98174	76225	2.03%	0.278%
21	14.004	1938	1941	1954	rBV	235549	354046	9.44%	1.293%
22	14.145	1962	1965	1968	rBV	49977	44635	1.19%	0.163%
23	14.186	1968	1972	1978	rVV	979712	938437	25.02%	3.427%
24	14.633	2045	2048	2053	rBV4	26666	47554	1.27%	0.174%
25	15.727	2229	2234	2241	rVB2	773857	1045953	27.89%	3.819%

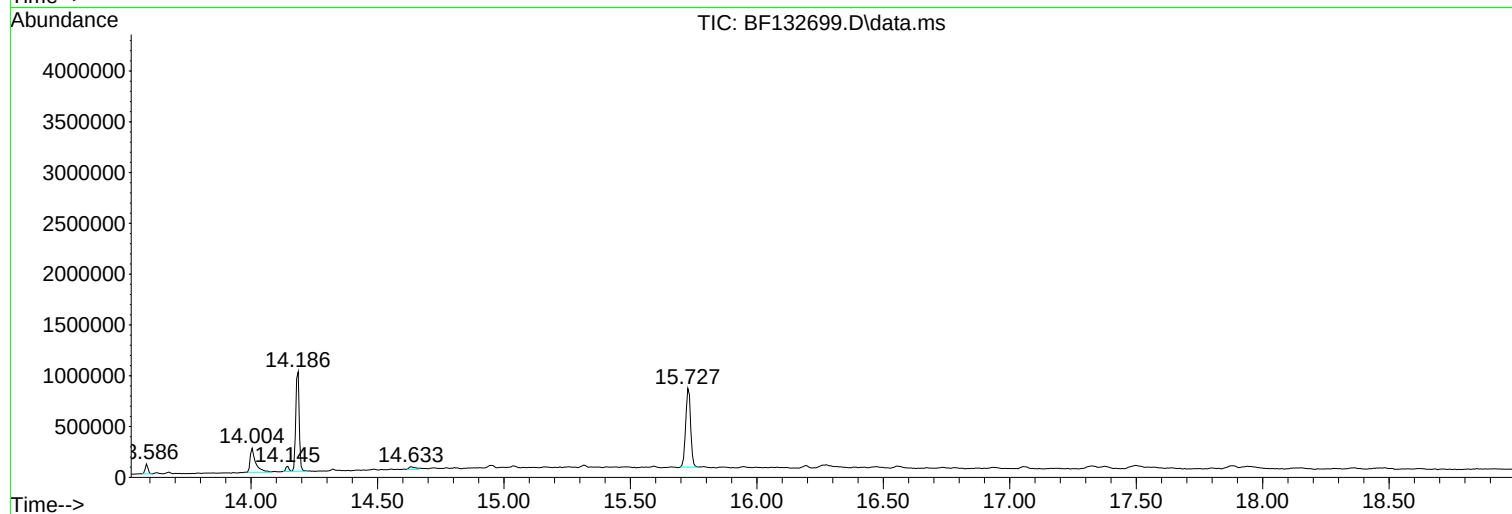
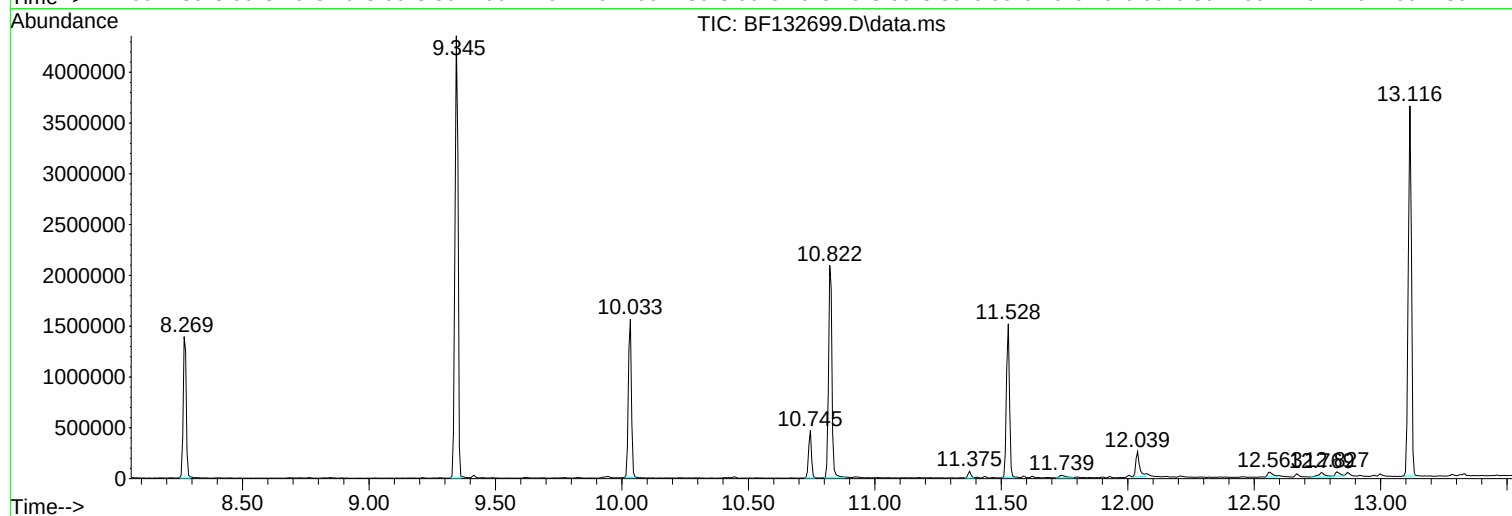
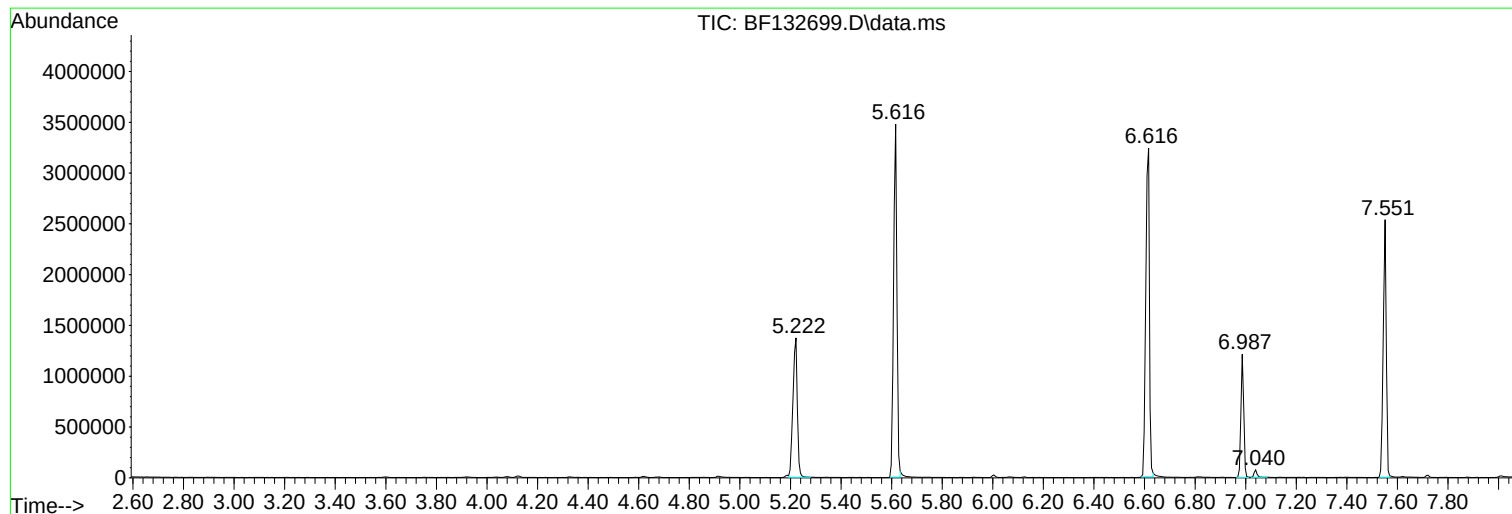
Sum of corrected areas: 27385616

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030823\
Data File : BF132699.D
Acq On : 08 Mar 2023 20:00
Operator : CG\JU
Sample : 01829-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-06-20230306

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.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_F\Data\BF030823\
Data File : BF132699.D
Acq On : 08 Mar 2023 20:00
Operator : CG\JU
Sample : 01829-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-06-20230306

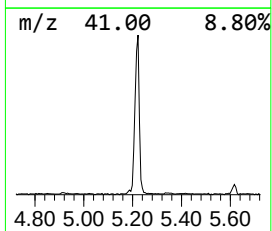
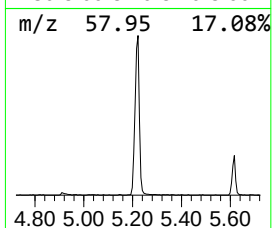
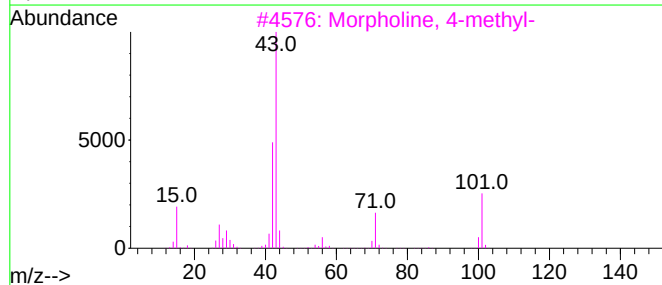
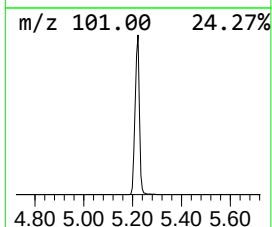
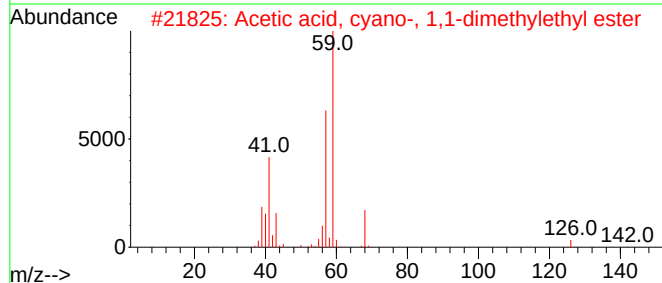
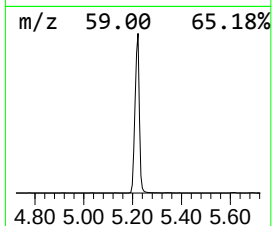
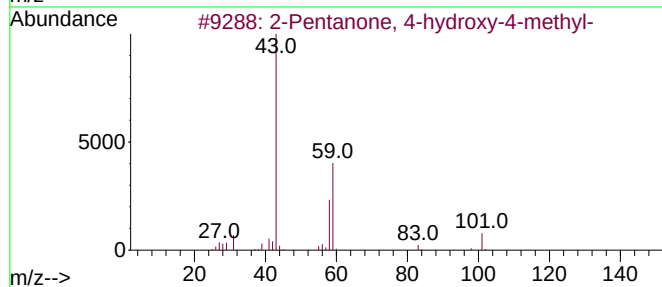
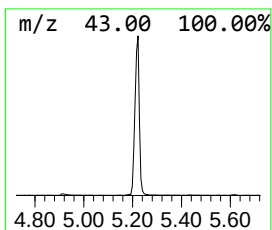
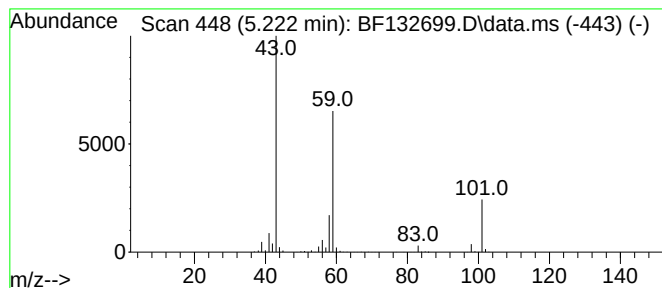
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.222	35.48 ng	1664870	1,4-Dichlorobenzene-d4	6.987

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030823\
Data File : BF132699.D
Acq On : 08 Mar 2023 20:00
Operator : CG\JU
Sample : 01829-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-06-20230306

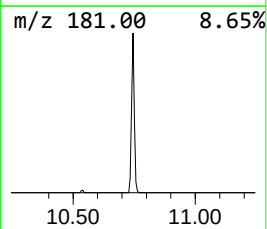
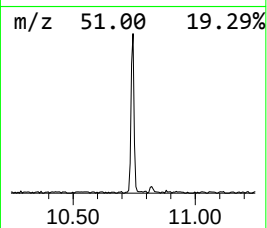
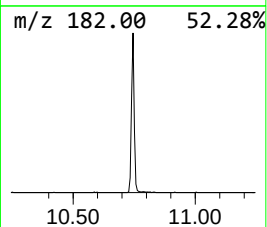
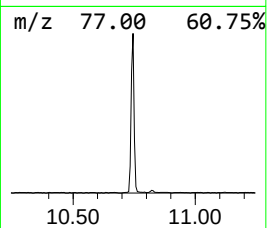
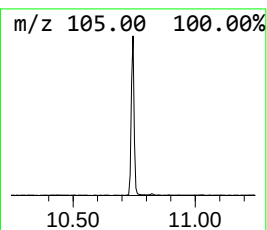
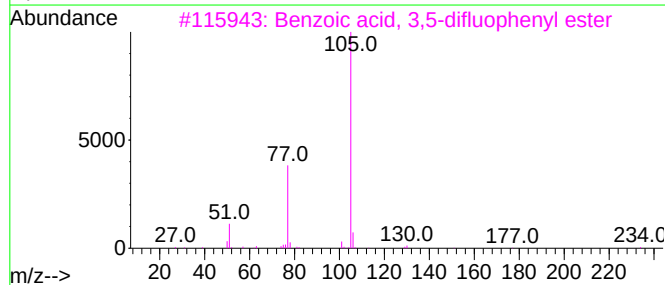
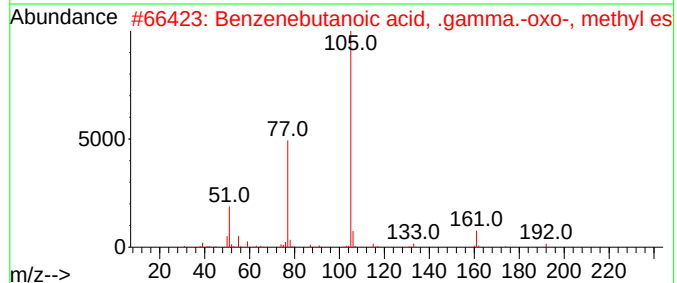
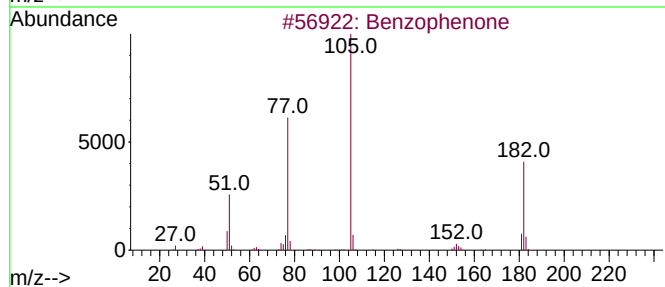
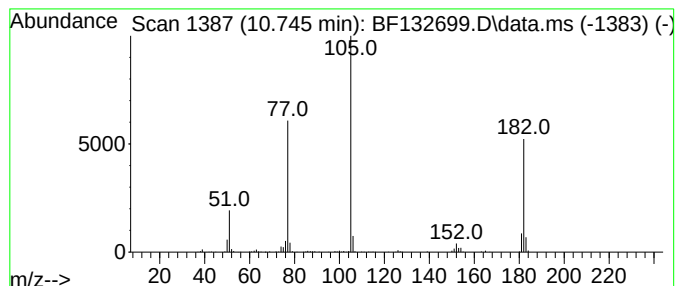
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.745	5.61 ng	371448	Acenaphthene-d10	10.034

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenebutanoic acid, .gamma.-ox...	192	C11H12O3	025333-24-8	47
3			Benzoic acid, 3,5-difluophenyl e...	234	C13H8F2O2	1000357-79-5	47
4			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47
5			2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030823\
Data File : BF132699.D
Acq On : 08 Mar 2023 20:00
Operator : CG\JU
Sample : 01829-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-06-20230306

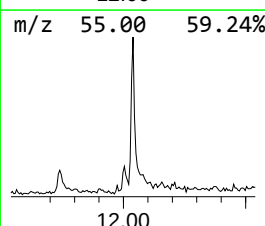
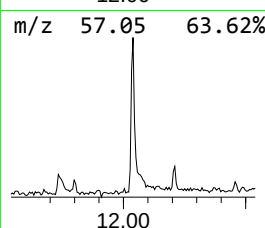
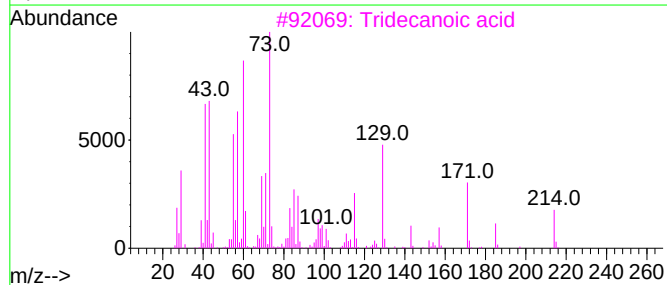
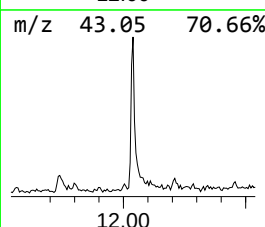
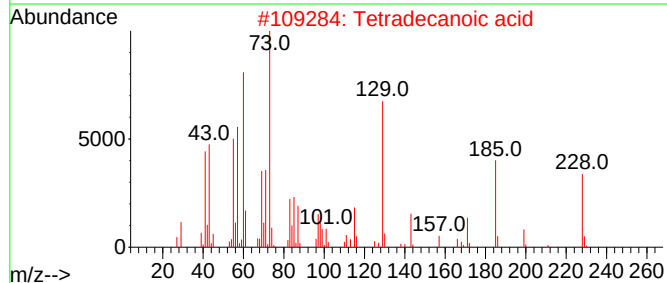
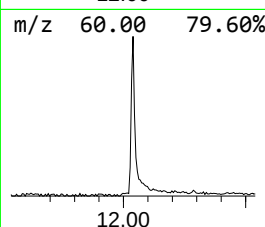
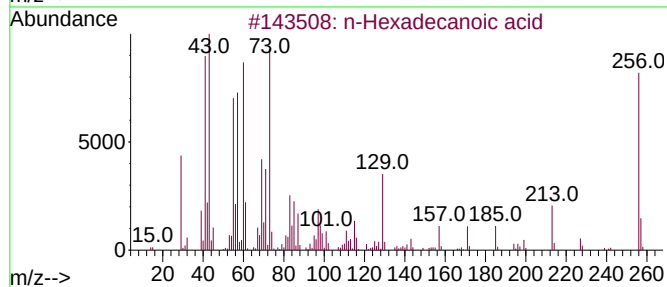
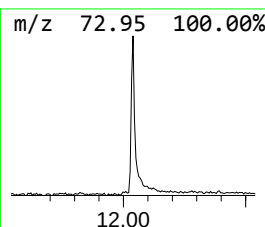
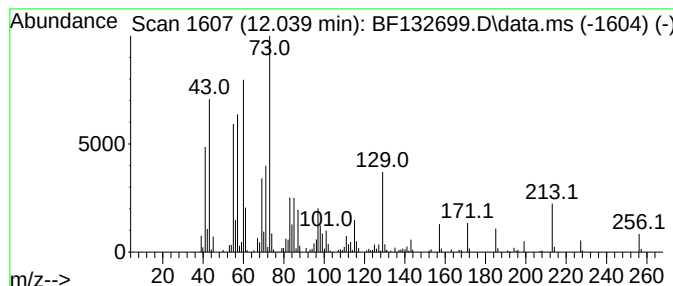
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.039	3.99 ng	255330	Phenanthrene-d10	11.528

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	91
3		Tridecanoic acid	214	C13H26O2	000638-53-9	91
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5		8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030823\
Data File : BF132699.D
Acq On : 08 Mar 2023 20:00
Operator : CG\JU
Sample : 01829-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-06-20230306

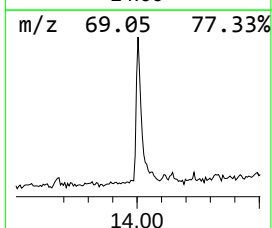
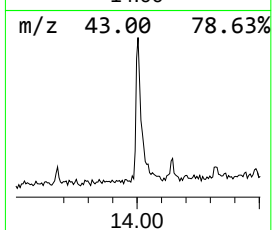
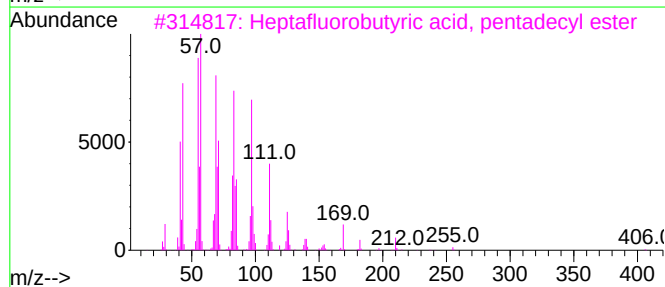
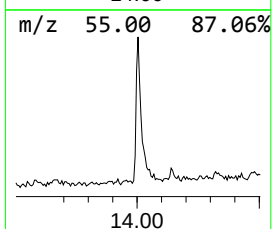
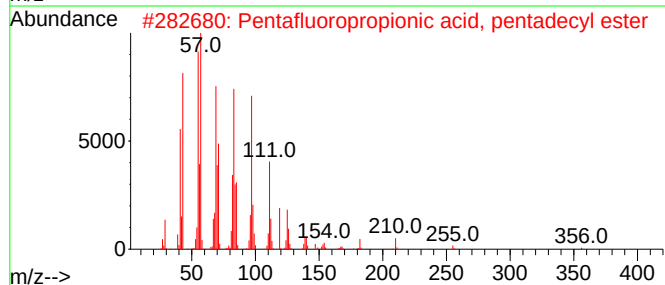
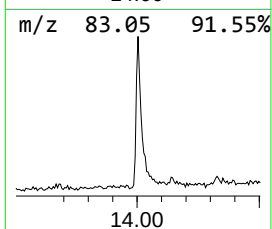
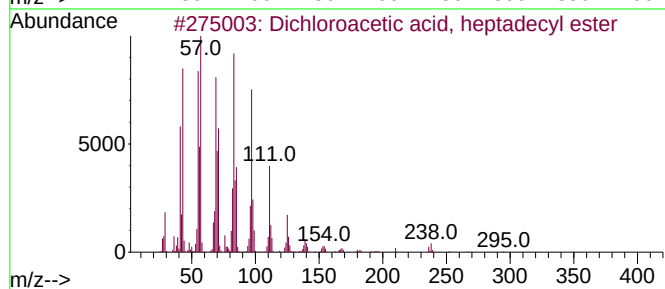
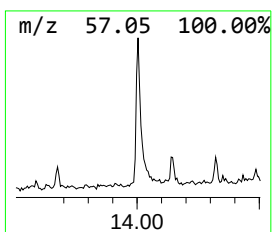
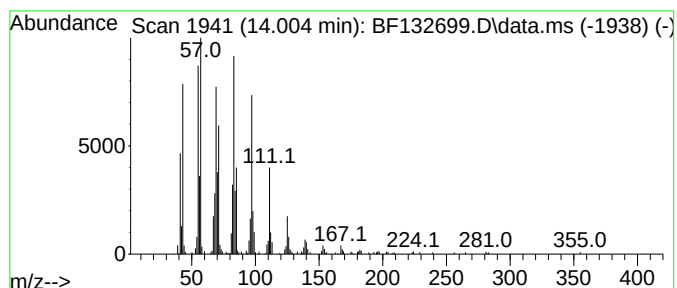
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Dichloroacetic acid, heptad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.004	7.55 ng	354046	Chrysene-d12	14.186

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5			1-Heneicosanol	312	C21H44O	015594-90-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030823\
Data File : BF132699.D
Acq On : 08 Mar 2023 20:00
Operator : CG\JU
Sample : 01829-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-06-20230306

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.222	35.5	ng	1664870	1	6.987	938544	20.0
Benzophenone	10.745	5.6	ng	371448	3	10.034	1324620	20.0
n-Hexadecanoic ...	12.039	4.0	ng	255330	4	11.528	1280730	20.0
Dichloroacetic ...	14.004	7.5	ng	354046	5	14.186	938437	20.0