

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020723\
 Data File : BF132346.D
 Acq On : 07 Feb 2023 16:01
 Operator : CG\JU
 Sample : 01466-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A-2

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-BF013123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132346.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.290	408	417	424	rBV	995339	1303304	26.66%	3.914%
2	5.678	477	483	486	rBV	3100997	3194311	65.33%	9.592%
3	6.337	591	595	598	rVB	61497	51100	1.05%	0.153%
4	6.666	645	651	654	rBV	2930283	3214947	65.76%	9.654%
5	7.048	713	716	720	rBV	1080755	888374	18.17%	2.668%
6	7.613	807	812	815	rBV	2382226	2158462	44.15%	6.482%
7	8.007	874	879	886	rBV	41413	49319	1.01%	0.148%
8	8.336	931	935	938	rBV	1560429	1213867	24.83%	3.645%
9	9.413	1114	1118	1121	rBV	5052188	4388017	89.75%	13.177%
10	10.101	1231	1235	1238	rBV	1794845	1439549	29.44%	4.323%
11	10.813	1353	1356	1360	rVB	245542	188473	3.85%	0.566%
12	10.895	1365	1370	1373	rBV	3696333	3244314	66.36%	9.742%
13	11.595	1485	1489	1493	rBV	1781211	1566260	32.04%	4.703%
14	12.107	1568	1576	1591	rBV	814984	839451	17.17%	2.521%
15	12.818	1691	1697	1702	rBV	57913	81359	1.66%	0.244%
16	12.895	1706	1710	1721	rBV	271712	278821	5.70%	0.837%
17	13.048	1729	1736	1747	rVB	143447	191053	3.91%	0.574%
18	13.189	1756	1760	1764	rBV	5007931	4889199	100.00%	14.682%
19	13.701	1844	1847	1851	rBV3	61383	60489	1.24%	0.182%
20	14.077	1908	1911	1930	rVB	357388	630192	12.89%	1.892%
21	14.254	1937	1941	1944	rBV	1280207	1143569	23.39%	3.434%
22	14.348	1951	1957	1963	rBV	809499	879782	17.99%	2.642%
23	14.736	2020	2023	2034	rVB5	38487	82810	1.69%	0.249%
24	15.830	2203	2209	2221	rBV2	755809	1030229	21.07%	3.094%
25	16.130	2255	2260	2269	rBV	40530	76000	1.55%	0.228%
26	16.395	2299	2305	2322	rBV6	47595	217917	4.46%	0.654%

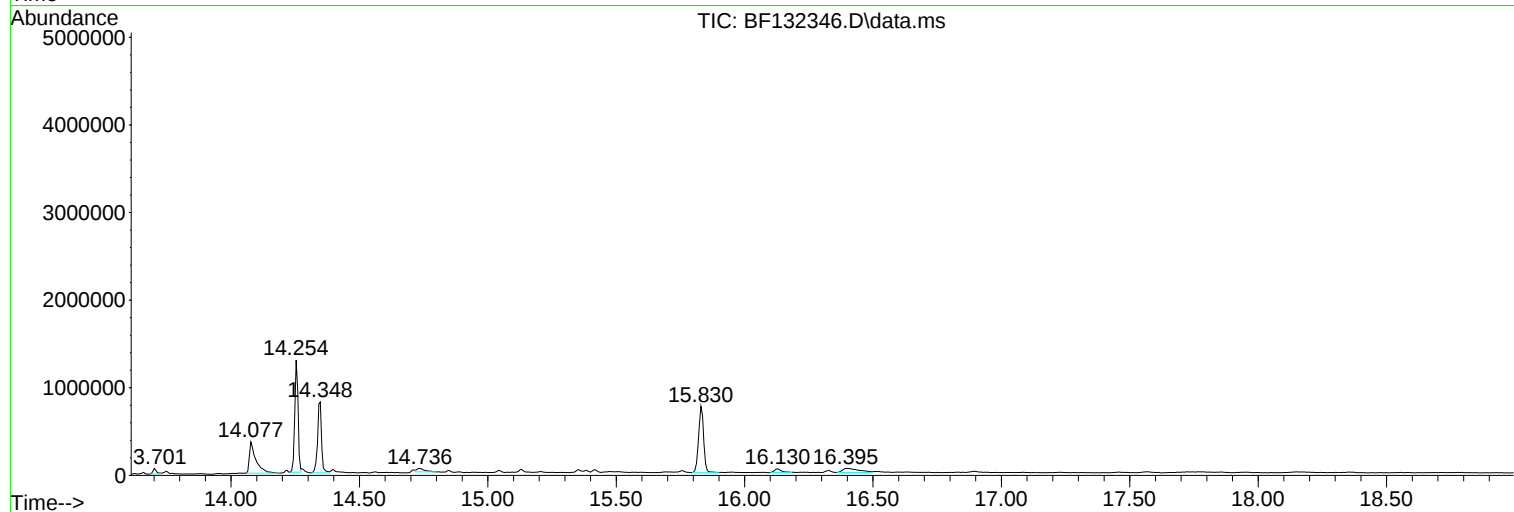
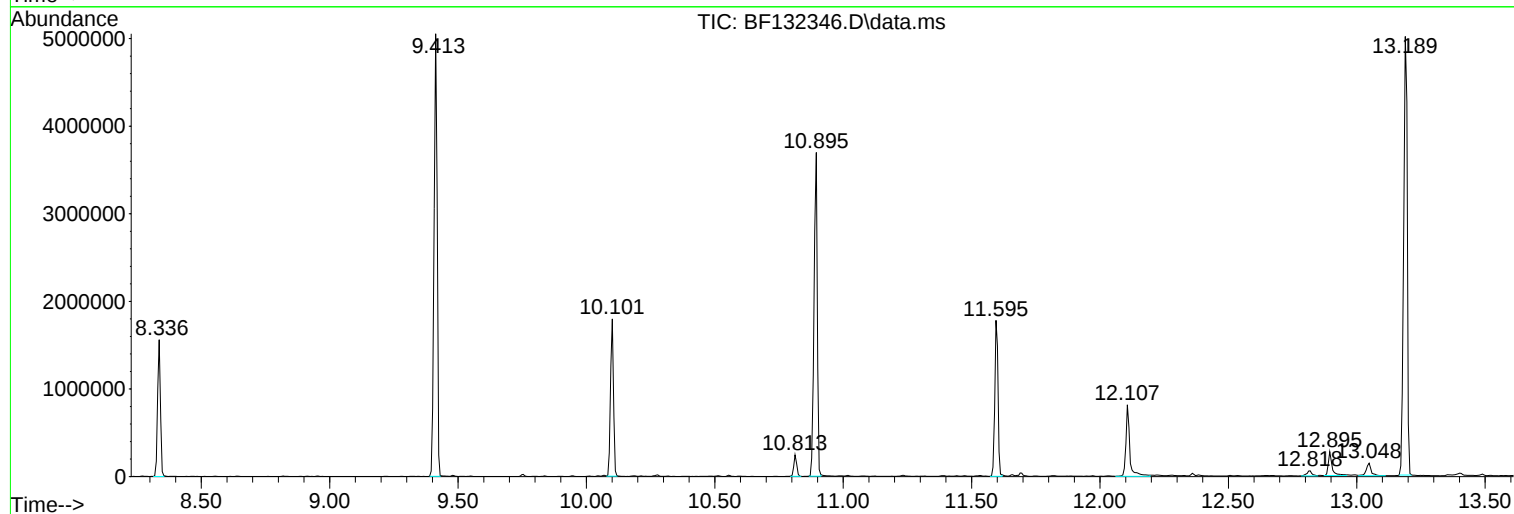
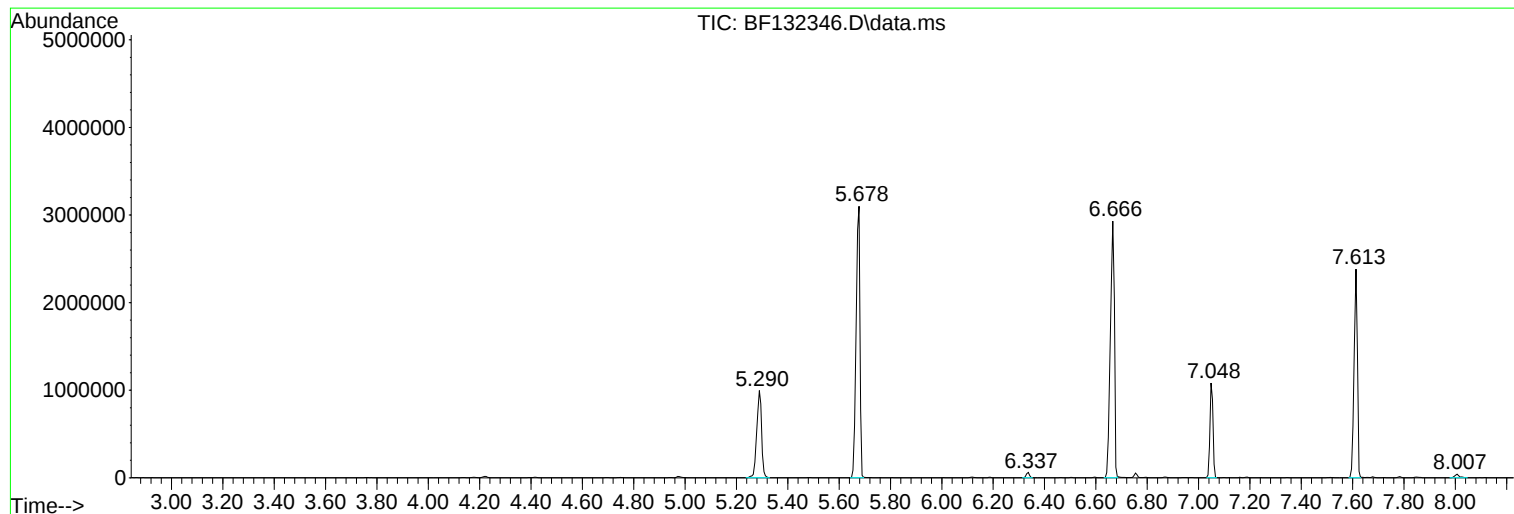
Sum of corrected areas: 33301168

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020723\
Data File : BF132346.D
Acq On : 07 Feb 2023 16:01
Operator : CG\JU
Sample : 01466-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.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\BF020723\
Data File : BF132346.D
Acq On : 07 Feb 2023 16:01
Operator : CG\JU
Sample : 01466-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A-2

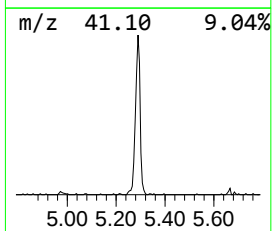
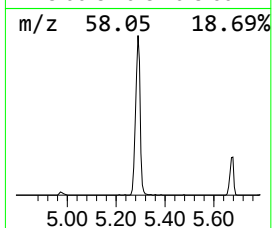
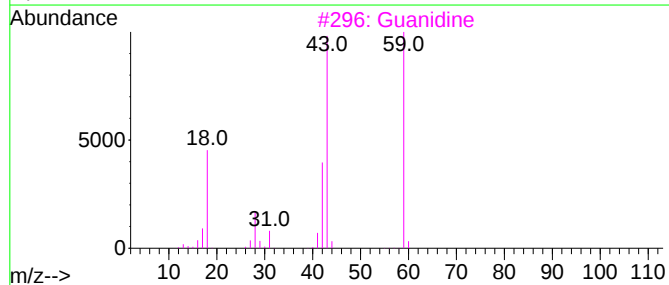
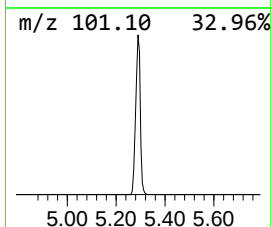
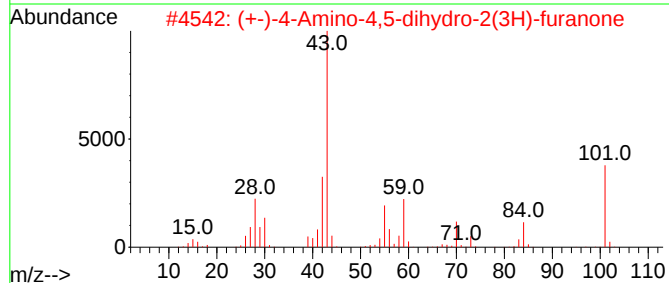
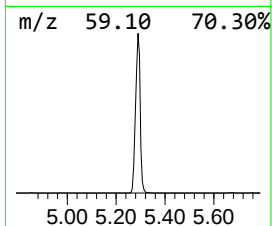
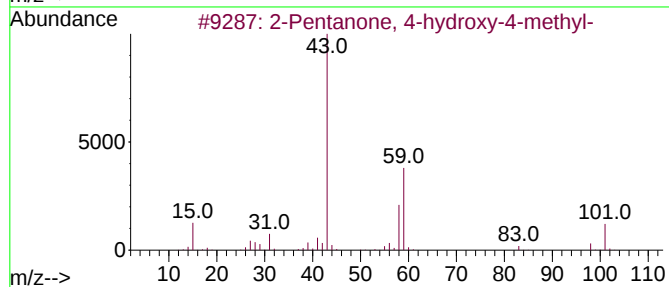
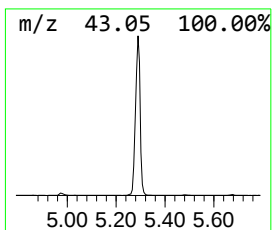
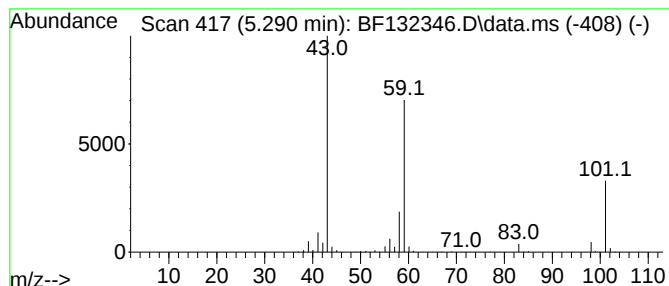
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.290	29.34 ng	1303300	1,4-Dichlorobenzene-d4	7.048

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3			Guanidine	59	CH5N3	000113-00-8	43
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020723\
Data File : BF132346.D
Acq On : 07 Feb 2023 16:01
Operator : CG\JU
Sample : 01466-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

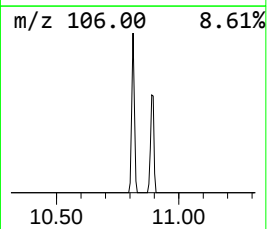
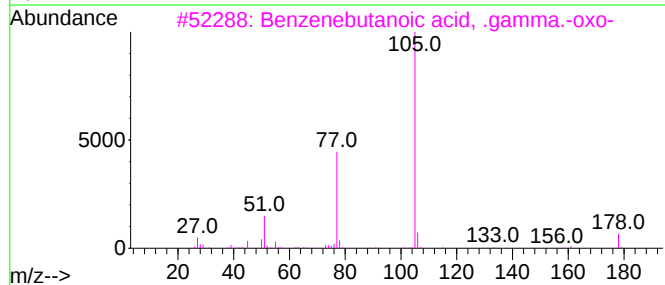
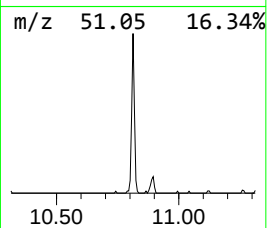
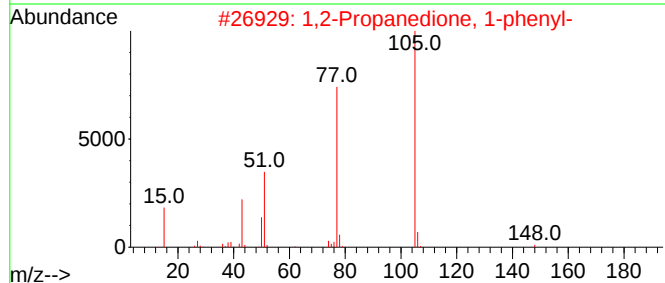
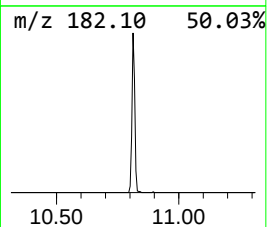
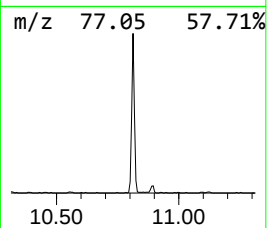
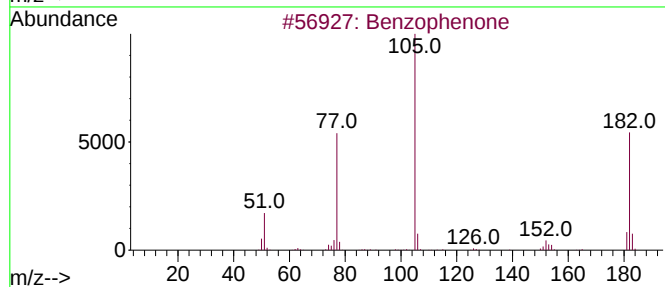
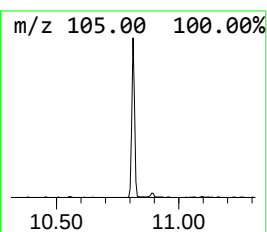
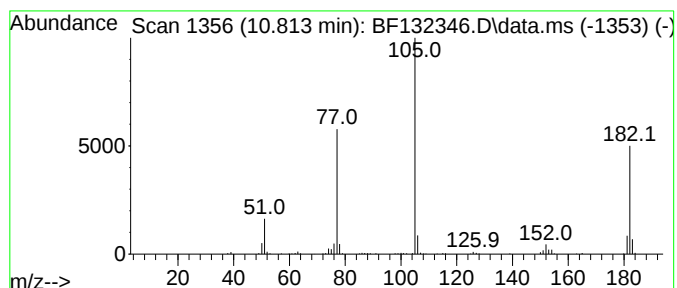
Instrument :
BNA_F
ClientSampleId :
A-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.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 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.813	2.62 ng	188473	Acenaphthene-d10	10.101	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	43
3	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	43
4	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	43
5	Ethanone, 1,2-diphenyl-	196	C14H12O	000451-40-1	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020723\
Data File : BF132346.D
Acq On : 07 Feb 2023 16:01
Operator : CG\JU
Sample : 01466-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

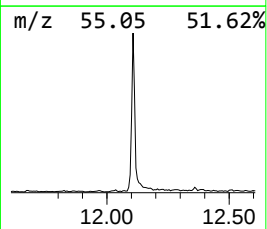
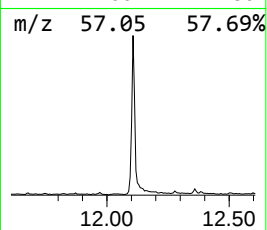
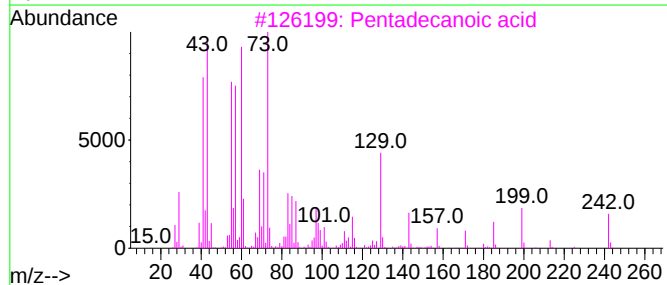
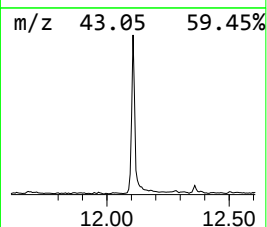
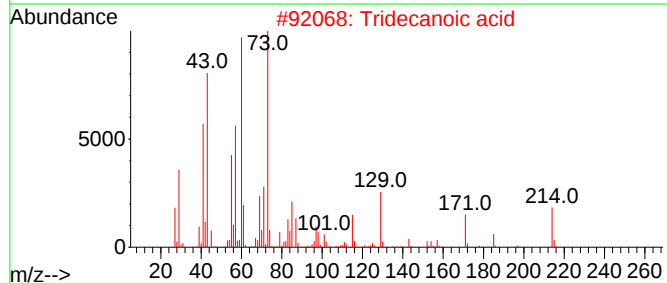
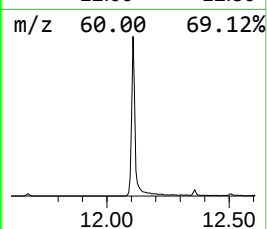
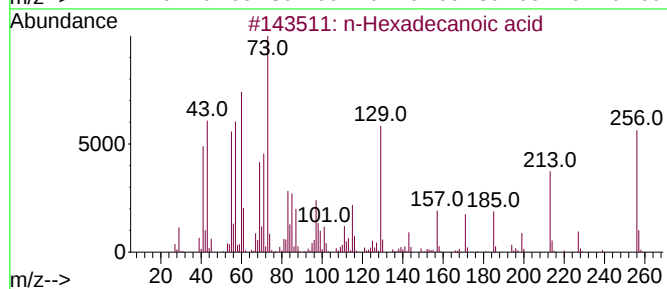
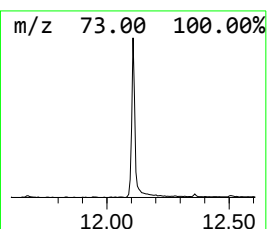
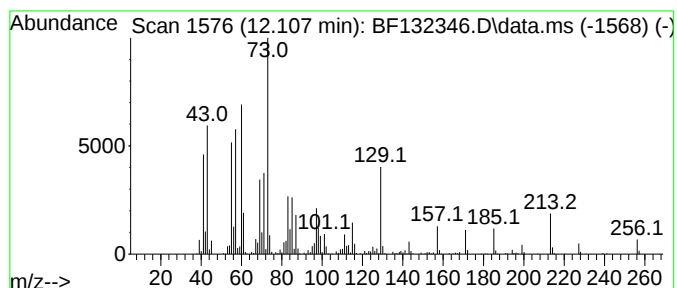
Instrument :
BNA_F
ClientSampleId :
A-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.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.	
12.107	10.72 ng	839451	Phenanthrene-d10		11.595	
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	89
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	64
5	n-Decanoic acid		172	C10H20O2	000334-48-5	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020723\
Data File : BF132346.D
Acq On : 07 Feb 2023 16:01
Operator : CG\JU
Sample : 01466-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A-2

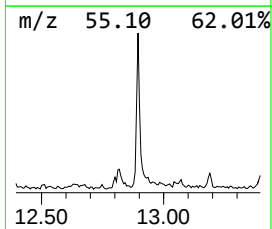
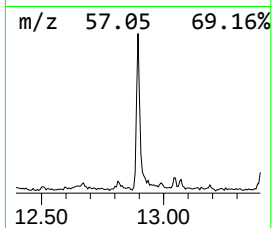
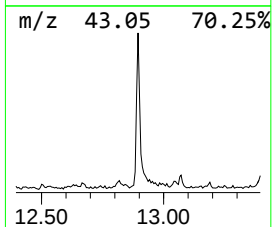
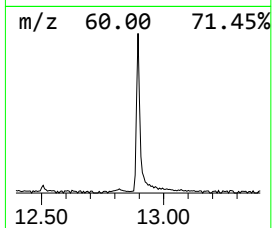
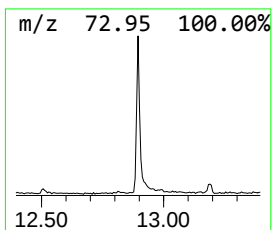
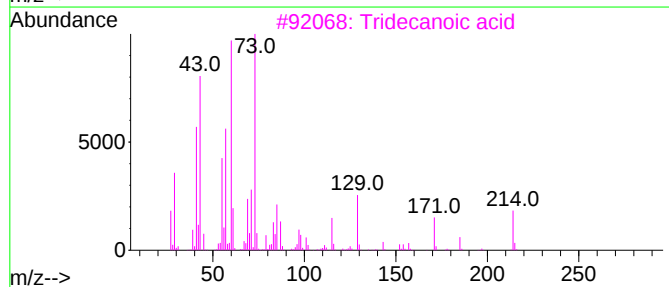
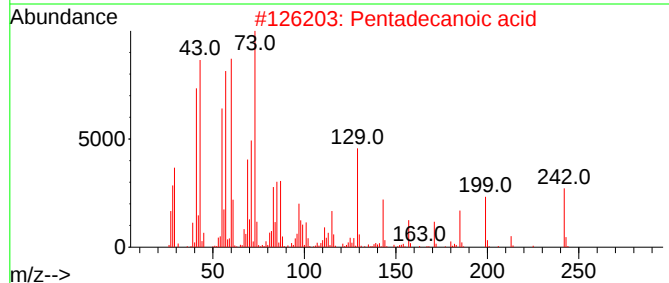
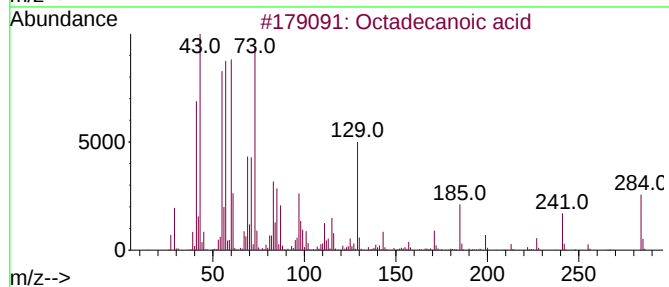
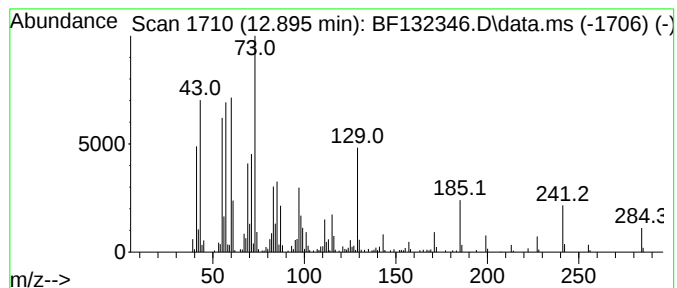
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.895	3.56 ng	278821	Phenanthrene-d10	11.595

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	86
3			Tridecanoic acid	214	C13H26O2	000638-53-9	62
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	52
5			Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	20



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020723\
Data File : BF132346.D
Acq On : 07 Feb 2023 16:01
Operator : CG\JU
Sample : 01466-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

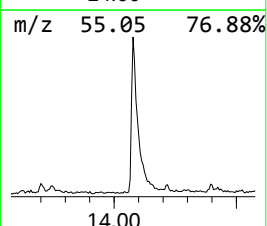
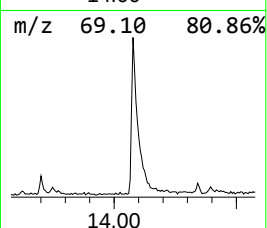
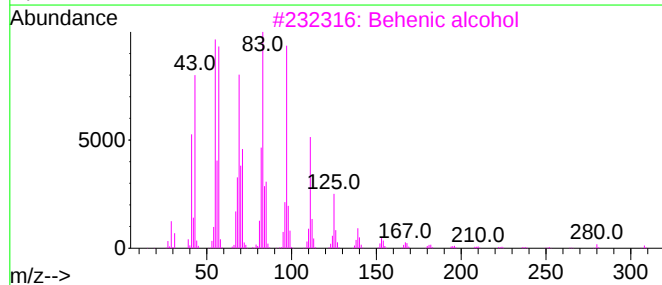
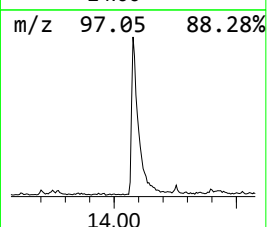
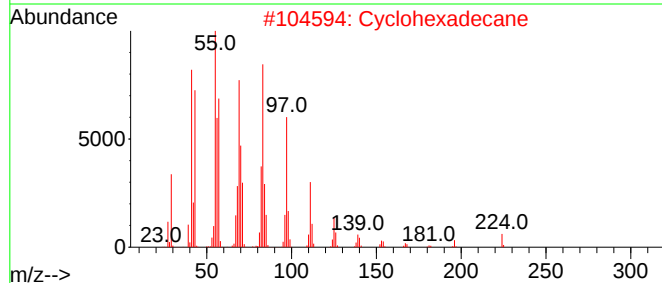
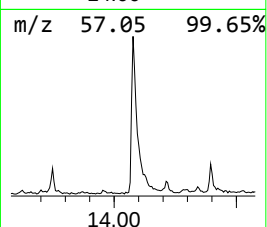
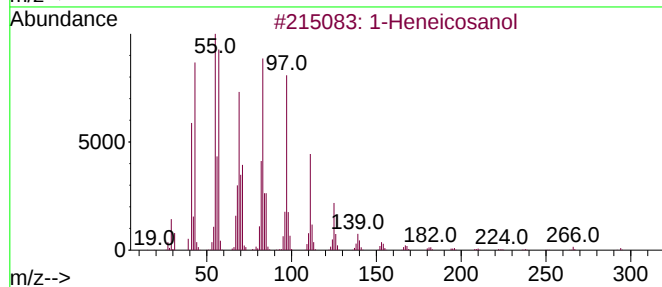
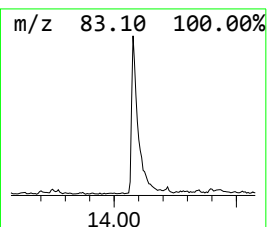
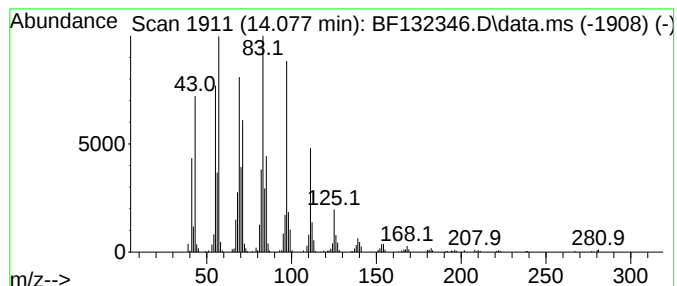
Instrument :
BNA_F
ClientSampleId :
A-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.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-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.077	11.02 ng	630192	Chrysene-d12	14.254	
Hit# of	5	Tentative ID	MW MolForm	CAS#	Qual
1		1-Heneicosanol	312 C21H44O	015594-90-8	93
2		Cyclohexadecane	224 C16H32	000295-65-8	93
3		Behenic alcohol	326 C22H46O	000661-19-8	93
4		Heptafluorobutyric acid, pentade...	424 C19H31F7O2	959261-23-5	91
5		Trichloroacetic acid, pentadecyl...	372 C17H31Cl3O2	074339-53-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020723\
Data File : BF132346.D
Acq On : 07 Feb 2023 16:01
Operator : CG\JU
Sample : 01466-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A-2

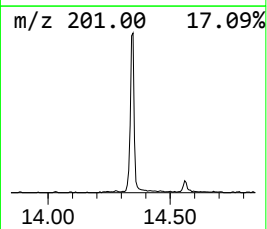
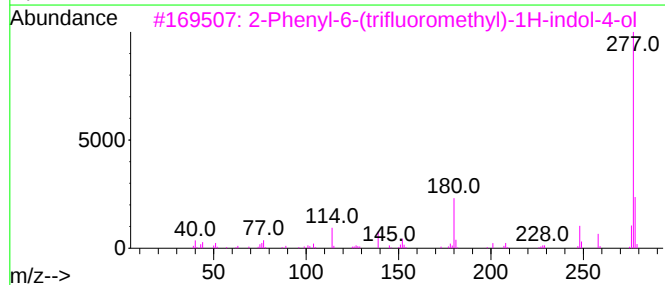
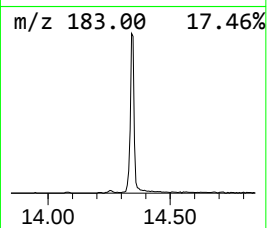
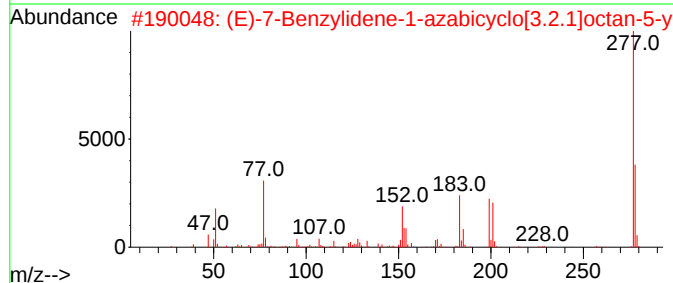
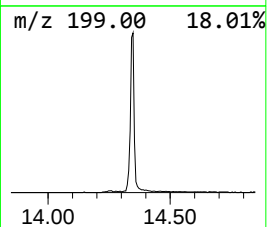
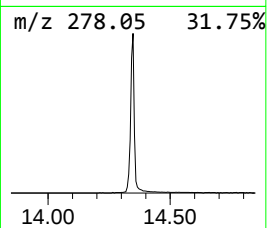
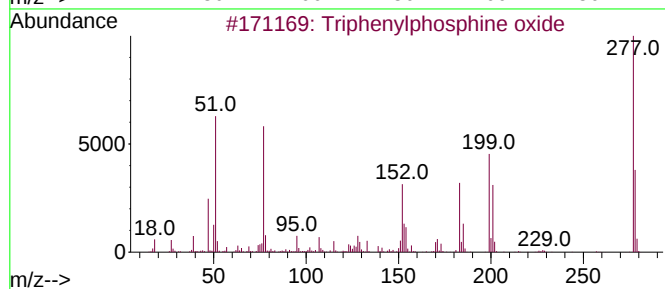
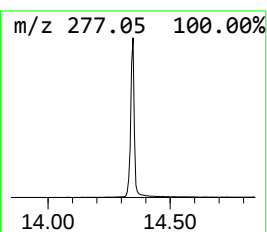
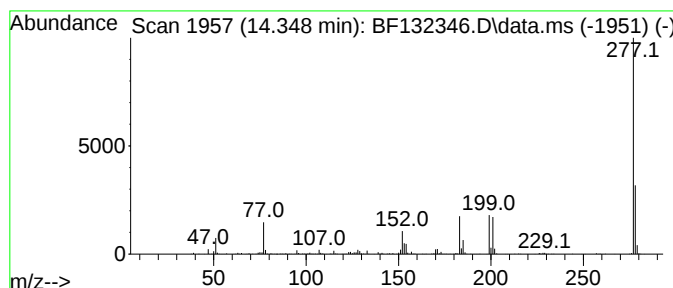
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.348	15.39 ng	879782	Chrysene-d12	14.254

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	91
3			2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	50
4			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	38
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020723\
Data File : BF132346.D
Acq On : 07 Feb 2023 16:01
Operator : CG\JU
Sample : 01466-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A-2

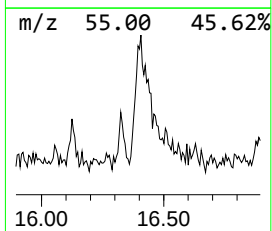
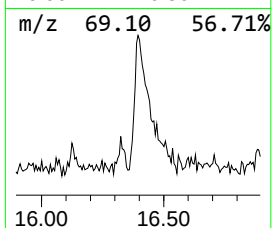
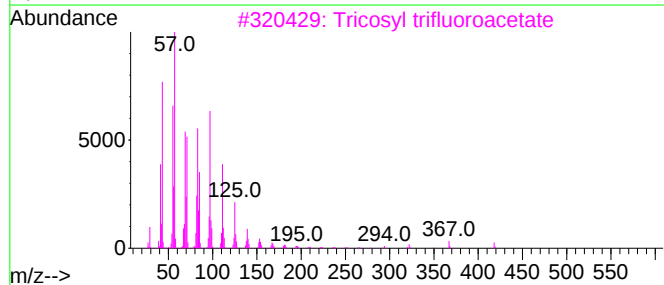
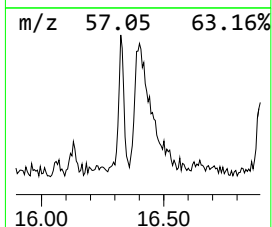
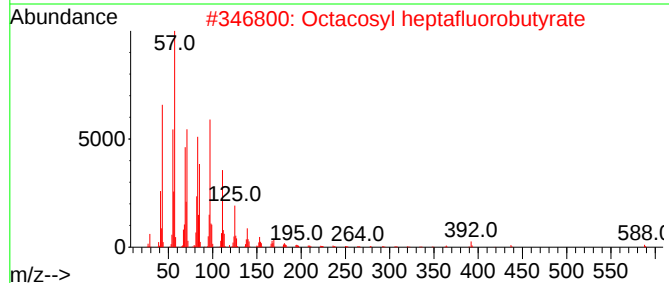
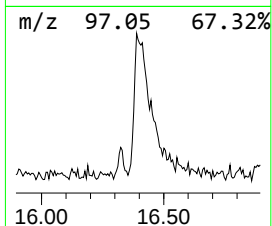
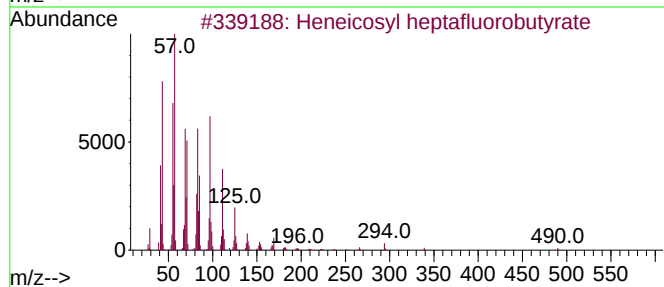
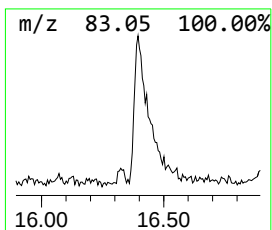
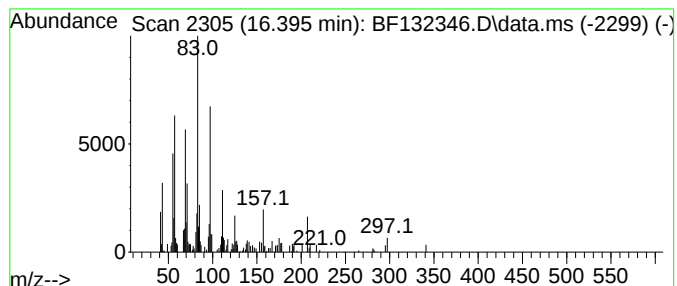
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown16.395 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.395	4.23 ng	217917	Perylene-d12	15.830

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	46
2			Octacosyl heptafluorobutyrate	606	C32H57F7O2	1010351-83-6	46
3			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	46
4			Triacontyl heptafluorobutyrate	634	C34H61F7O2	1000351-83-2	46
5			Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020723\
Data File : BF132346.D
Acq On : 07 Feb 2023 16:01
Operator : CG\JU
Sample : 01466-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.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-...	5.290	29.3	ng	1303300	1	7.048	888374	20.0
Benzophenone	10.813	2.6	ng	188473	3	10.101	1439550	20.0
n-Hexadecanoic ...	12.107	10.7	ng	839451	4	11.595	1566260	20.0
Octadecanoic acid	12.895	3.6	ng	278821	4	11.595	1566260	20.0
1-Heneicosanol	14.077	11.0	ng	630192	5	14.254	1143570	20.0
Triphenylphosph...	14.348	15.4	ng	879782	5	14.254	1143570	20.0
unknown16.395	16.395	4.2	ng	217917	6	15.830	1030230	20.0