

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021623\
 Data File : BF132441.D
 Acq On : 16 Feb 2023 19:19
 Operator : CG\JU
 Sample : 01553-03
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TWP-01-DUP

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-BF021623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132441.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.260	409	412	422	rVB	886952	1017669	14.61%	2.576%
2	5.649	474	478	482	rBV	2956978	2900505	41.64%	7.343%
3	6.643	643	647	657	rBV	2117870	1936866	27.80%	4.903%
4	7.025	709	712	716	rVB	1353835	1142659	16.40%	2.893%
5	7.595	799	809	812	rBV	4206573	4313407	61.92%	10.920%
6	8.313	927	931	934	rBV	1868233	1485776	21.33%	3.761%
7	9.072	1057	1060	1066	rBV2	88048	72529	1.04%	0.184%
8	9.395	1109	1115	1118	rBV	7199761	6823099	97.94%	17.273%
9	9.642	1154	1157	1161	rBV	204406	178425	2.56%	0.452%
10	10.078	1227	1231	1234	rBV	2047441	1690315	24.26%	4.279%
11	10.484	1297	1300	1304	rVB	850606	727189	10.44%	1.841%
12	10.789	1347	1352	1357	rBV	140508	139996	2.01%	0.354%
13	10.872	1361	1366	1369	rBV	4503107	4457854	63.99%	11.285%
14	11.572	1481	1485	1488	rBV	2139952	1791085	25.71%	4.534%
15	12.107	1570	1576	1586	rBV5	64606	194975	2.80%	0.494%
16	13.172	1751	1757	1760	rBV	6727270	6966391	100.00%	17.636%
17	14.230	1933	1937	1941	rBV	1744956	1541667	22.13%	3.903%
18	14.319	1947	1952	1959	rBV	535274	560301	8.04%	1.418%
19	15.101	2081	2085	2090	rVB	203713	222528	3.19%	0.563%
20	15.789	2196	2202	2212	rBV	956546	1338545	19.21%	3.389%

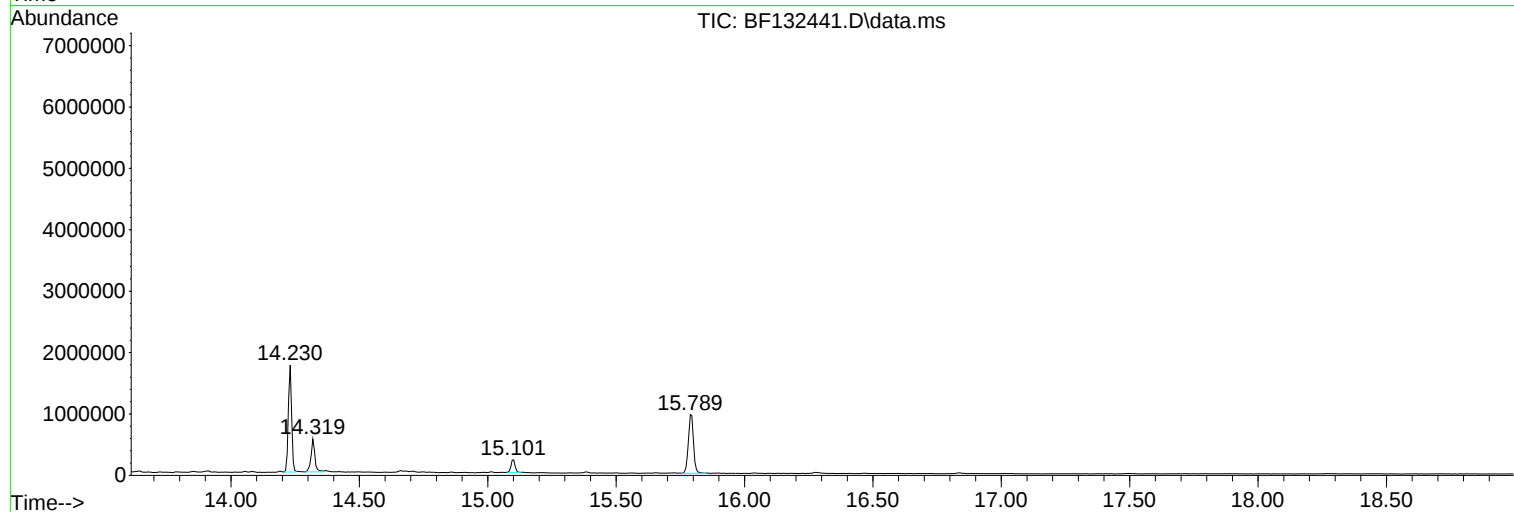
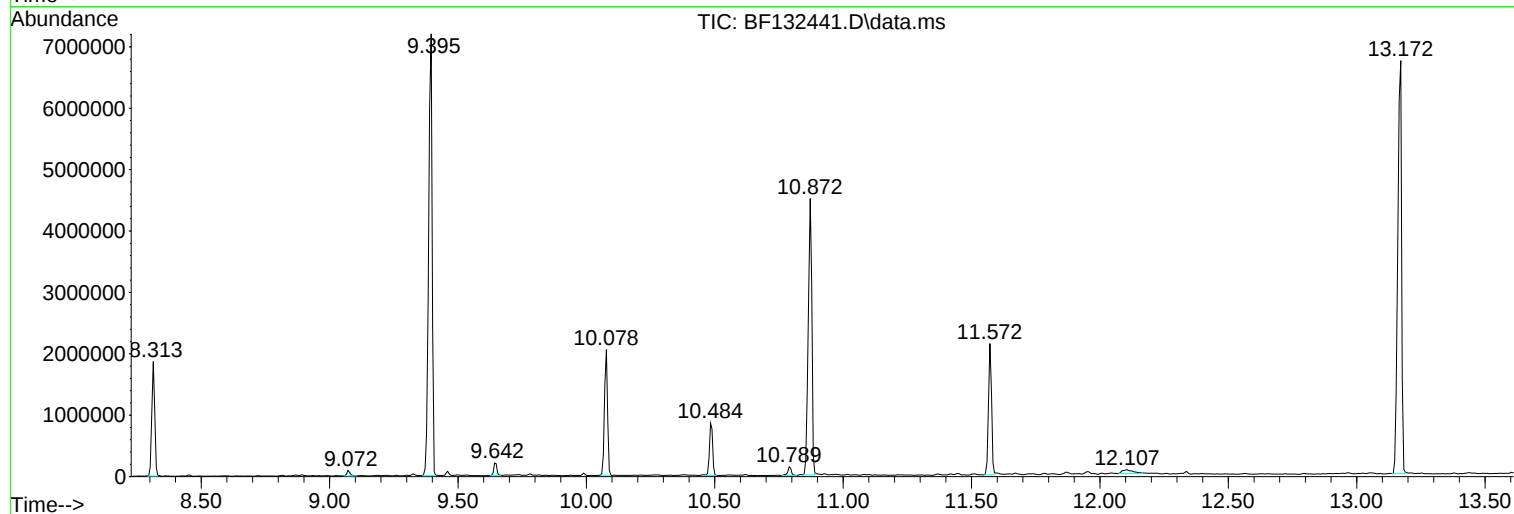
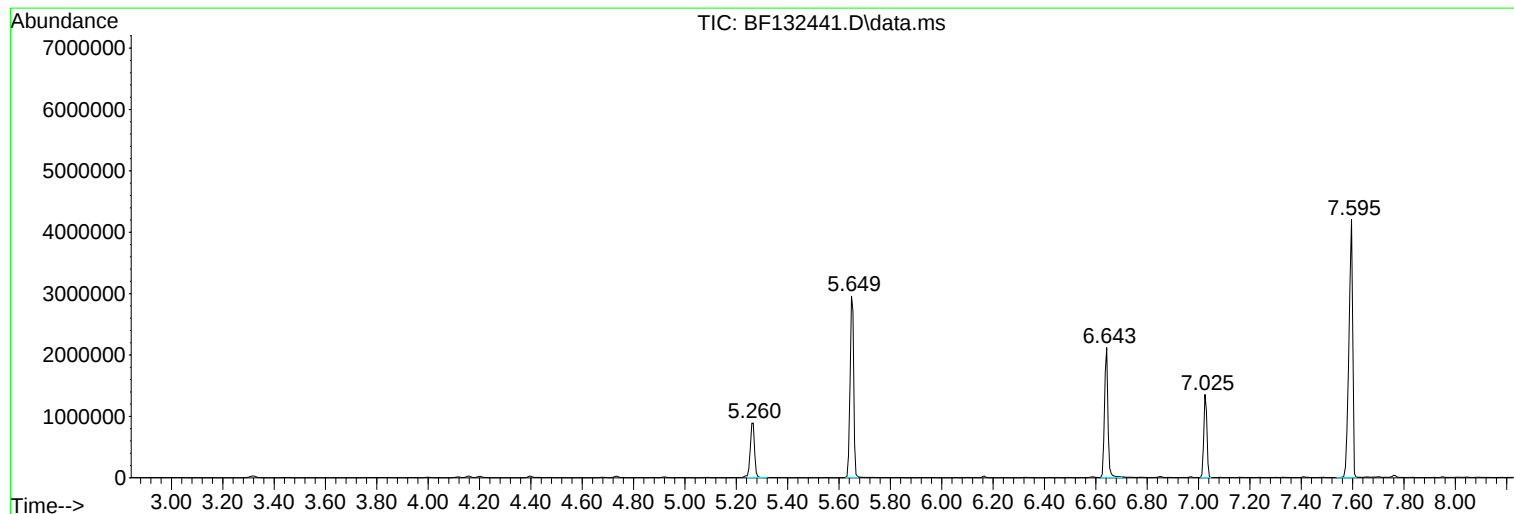
Sum of corrected areas: 39501781

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021623\
Data File : BF132441.D
Acq On : 16 Feb 2023 19:19
Operator : CG\JU
Sample : 01553-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TWP-01-DUP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.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\BF021623\
Data File : BF132441.D
Acq On : 16 Feb 2023 19:19
Operator : CG\JU
Sample : 01553-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TWP-01-DUP

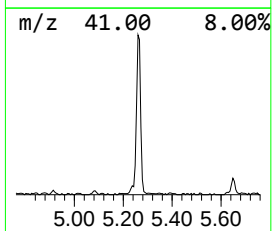
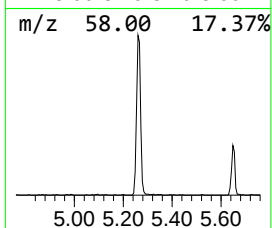
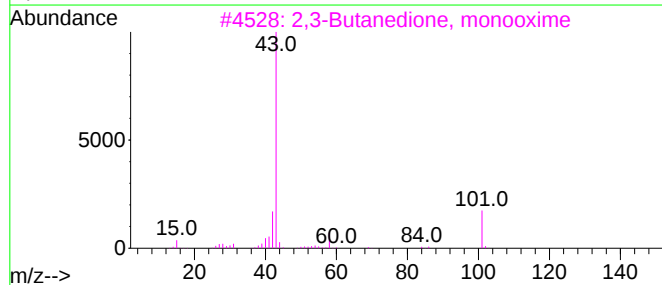
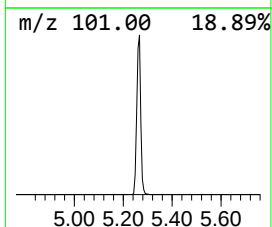
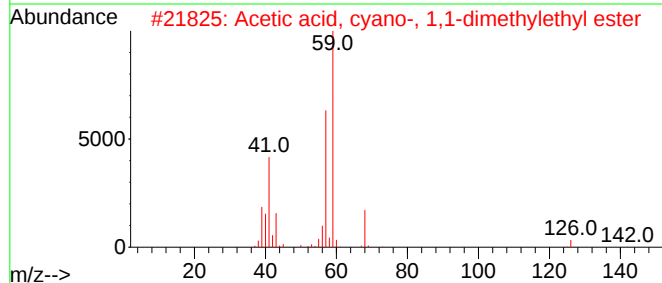
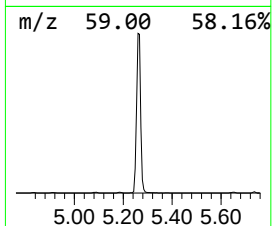
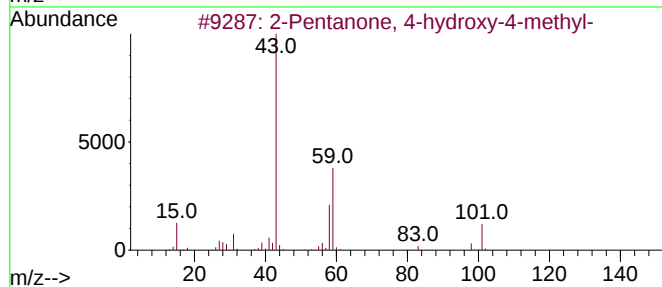
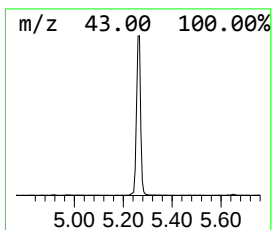
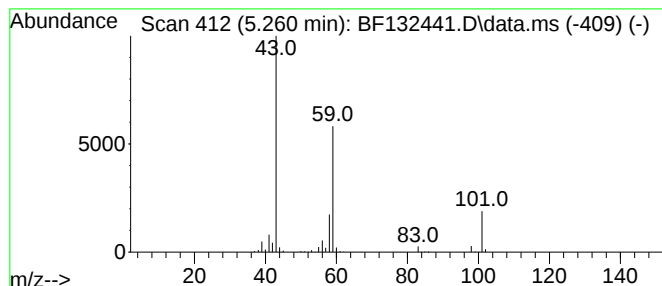
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.260	17.81 ng	1017670	1,4-Dichlorobenzene-d4	7.025

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	Acetone	58	C3H6O	000067-64-1	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021623\
Data File : BF132441.D
Acq On : 16 Feb 2023 19:19
Operator : CG\JU
Sample : 01553-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TWP-01-DUP

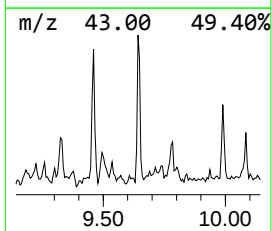
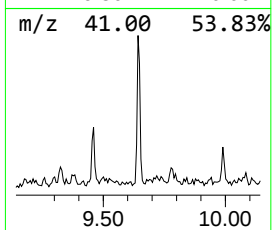
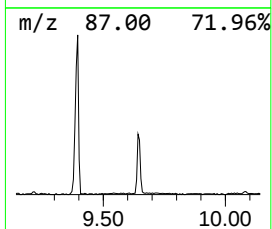
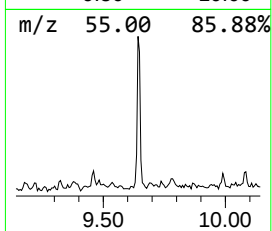
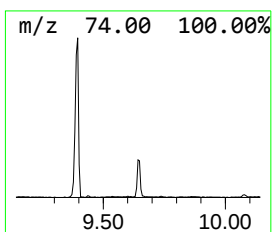
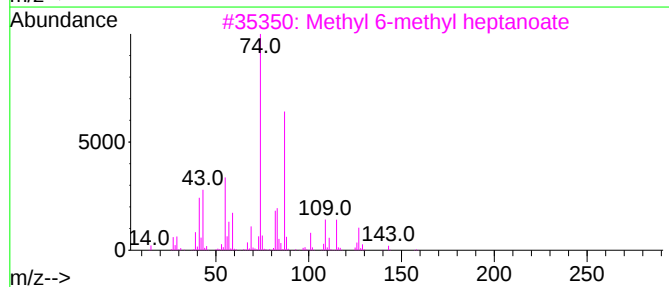
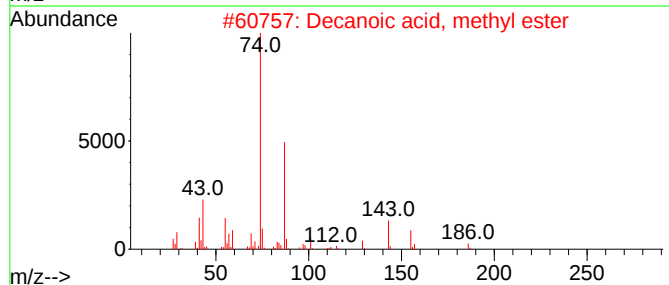
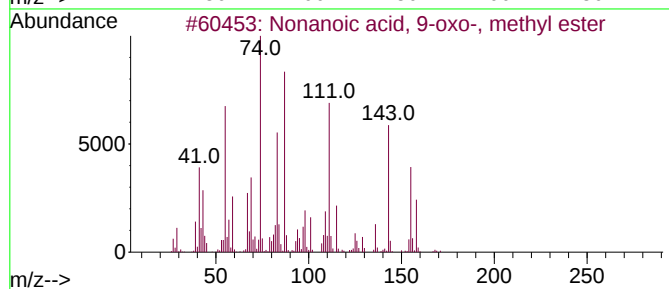
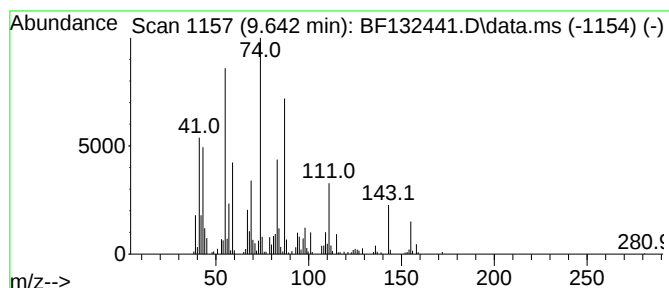
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Nonanoic acid, 9-oxo-, meth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.642	2.11 ng	178425	Acenaphthene-d10	10.078

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanoic acid, 9-oxo-, methyl ester	186	C10H18O3	001931-63-1	90
2			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	47
3			Methyl 6-methyl heptanoate	158	C9H18O2	002519-37-1	43
4			Dodecanoic acid, 2-methyl-	214	C13H26O2	002874-74-0	38
5			Methyl 8-methyl-nonanoate	186	C11H22O2	1000452-00-9	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021623\
Data File : BF132441.D
Acq On : 16 Feb 2023 19:19
Operator : CG\JU
Sample : 01553-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TWP-01-DUP

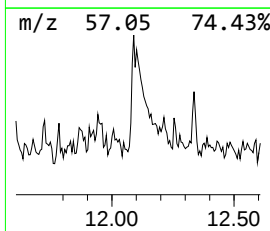
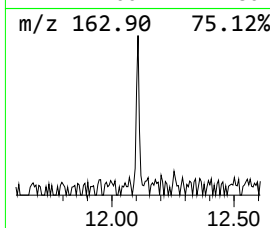
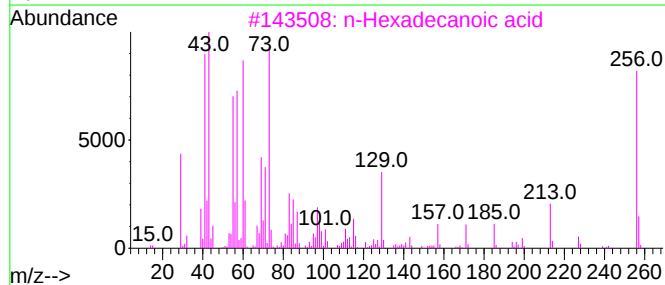
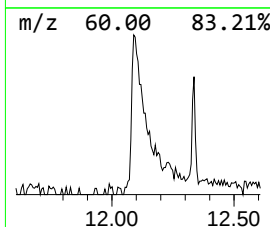
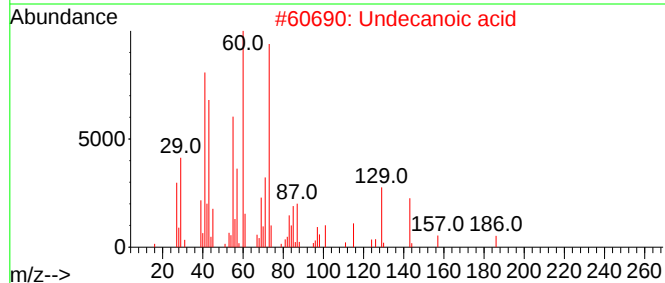
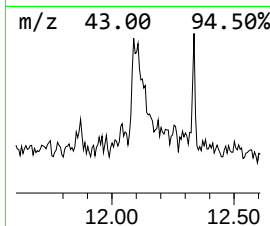
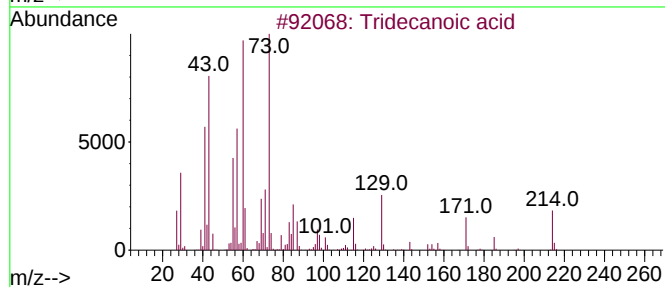
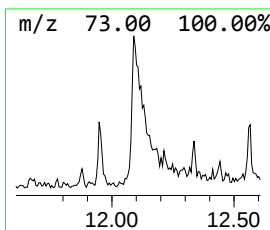
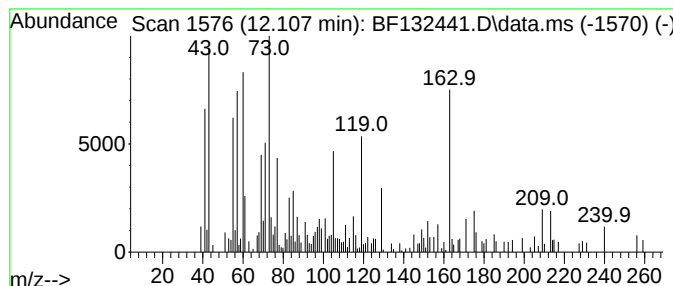
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown12.107 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.107	2.18 ng	194975	Phenanthrene-d10	11.572

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	49
2		Undecanoic acid	186	C11H22O2	000112-37-8	38
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	30
4		Dodecanoic acid	200	C12H24O2	000143-07-7	30
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021623\
Data File : BF132441.D
Acq On : 16 Feb 2023 19:19
Operator : CG\JU
Sample : 01553-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TWP-01-DUP

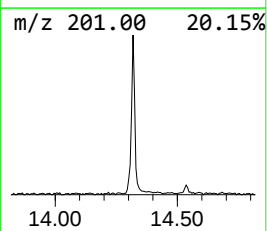
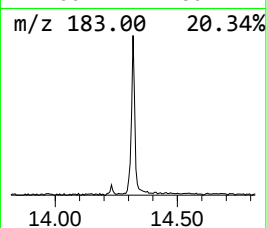
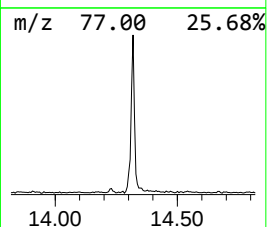
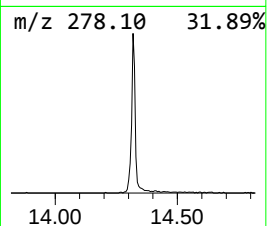
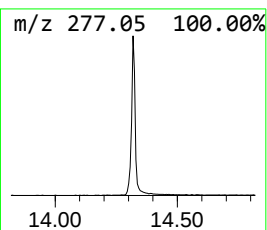
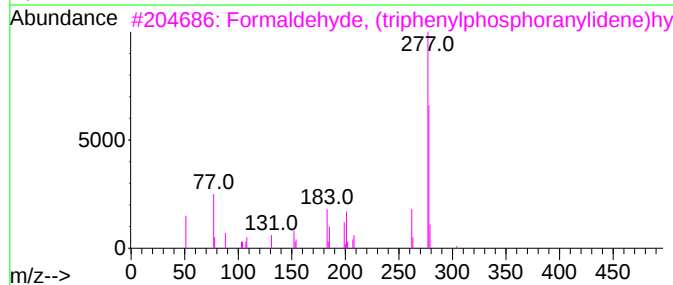
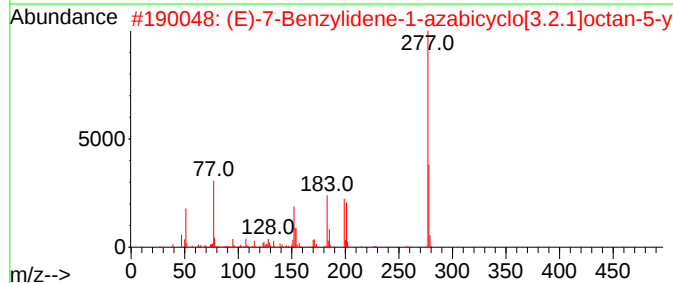
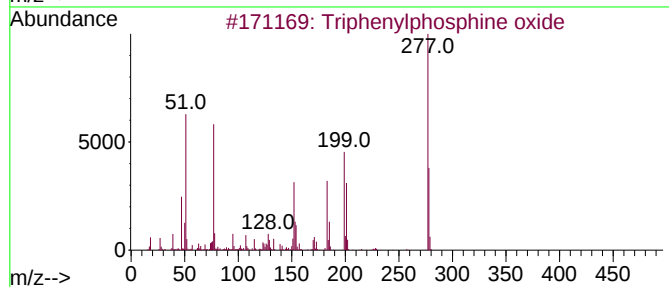
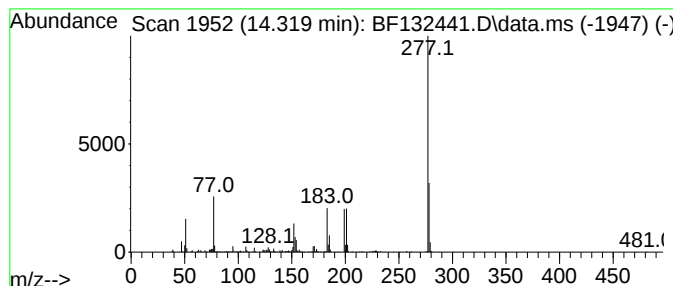
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.319	7.27 ng	560301	Chrysene-d12	14.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2			(E)-7-Benzylidene-1-azabicyclo[3.2.1]octan-5-ylidene	293	C15H19N03S	1000483-83-4	70
3			Formaldehyde, (triphenylphosphoranylidene)hy	304	C19H17N2P	015990-54-2	64
4			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15N02	299962-12-2	38
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021623\
Data File : BF132441.D
Acq On : 16 Feb 2023 19:19
Operator : CG\JU
Sample : 01553-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TWP-01-DUP

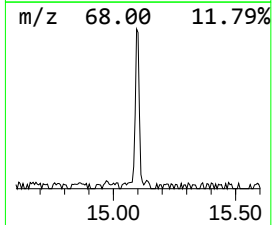
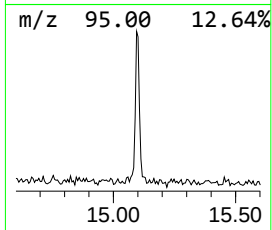
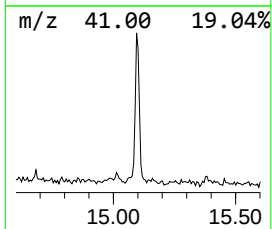
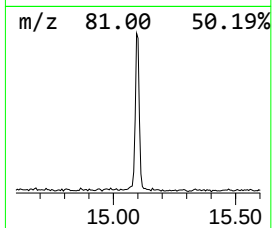
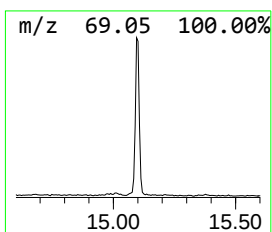
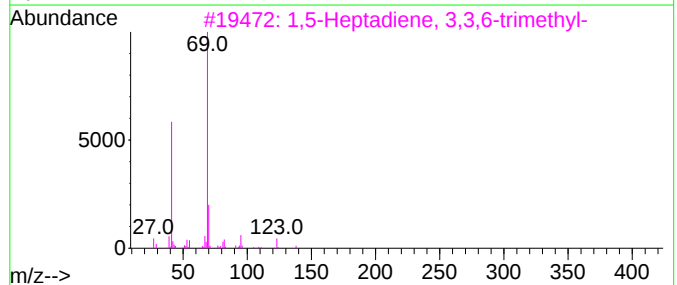
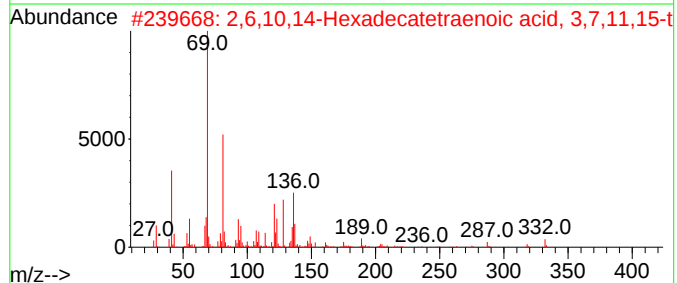
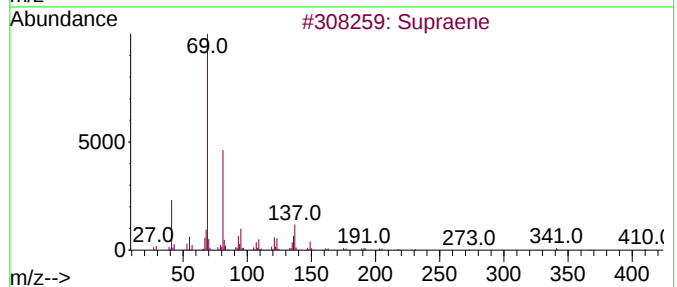
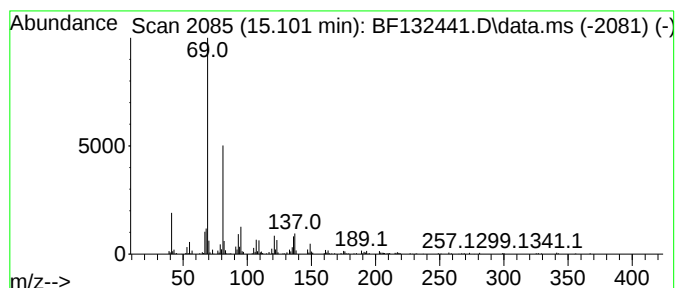
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.101	3.32 ng	222528	Perylene-d12	15.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
3			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52
4			1,5-Heptadiene, 2,6-dimethyl-	124	C9H16	006709-39-3	47
5			Squalene	410	C30H50	000111-02-4	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021623\
Data File : BF132441.D
Acq On : 16 Feb 2023 19:19
Operator : CG\JU
Sample : 01553-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TWP-01-DUP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.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-...	5.260	17.8	ng	1017670	1	7.025	1142660	20.0
Nonanoic acid, ...	9.642	2.1	ng	178425	3	10.078	1690320	20.0
unknown12.107	12.107	2.2	ng	194975	4	11.572	1791090	20.0
Triphenylphosph...	14.319	7.3	ng	560301	5	14.230	1541670	20.0
Supraene	15.101	3.3	ng	222528	6	15.795	1338550	20.0