

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
 Data File : BF136392.D
 Acq On : 04 Dec 2023 20:37
 Operator : CG\JU
 Sample : 05586-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VAULT-1

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-BF112723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136392.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.045	499	503	510	rVB	67961	86801	2.73%	0.432%
2	5.439	565	570	573	rBV	2729095	2464442	77.64%	12.256%
3	6.439	735	740	743	rBV	2351997	2493995	78.57%	12.403%
4	6.804	798	802	805	rBV	730926	589807	18.58%	2.933%
5	7.363	892	897	900	rBV	1793110	1595055	50.25%	7.933%
6	8.080	1015	1019	1022	rBV	887550	741736	23.37%	3.689%
7	9.157	1198	1202	1205	rBV	3863083	3174304	100.00%	15.787%
8	9.275	1218	1222	1231	rVB	613101	583043	18.37%	2.900%
9	9.745	1300	1302	1305	rVB2	55184	43632	1.37%	0.217%
10	9.833	1314	1317	1321	rVB	929976	754139	23.76%	3.751%
11	10.245	1383	1387	1389	rBV2	65810	61240	1.93%	0.305%
12	10.380	1407	1410	1413	rBV4	26613	39470	1.24%	0.196%
13	10.627	1448	1452	1455	rBV	1672299	1380243	43.48%	6.864%
14	10.757	1470	1474	1481	rBV2	77379	127910	4.03%	0.636%
15	11.227	1552	1554	1558	rVB	48877	50736	1.60%	0.252%
16	11.327	1568	1571	1574	rBV	840232	675510	21.28%	3.360%
17	11.863	1659	1662	1666	rBV2	153871	157100	4.95%	0.781%
18	12.927	1839	1843	1846	rBV	3284056	2869258	90.39%	14.270%
19	13.980	2019	2022	2028	rVB	714767	649682	20.47%	3.231%
20	15.468	2271	2275	2288	rVB	407476	585713	18.45%	2.913%
21	15.615	2298	2300	2306	rVB3	127459	169523	5.34%	0.843%
22	16.198	2395	2399	2407	rVB2	186065	353246	11.13%	1.757%
23	16.645	2470	2475	2484	rVB	259158	460860	14.52%	2.292%

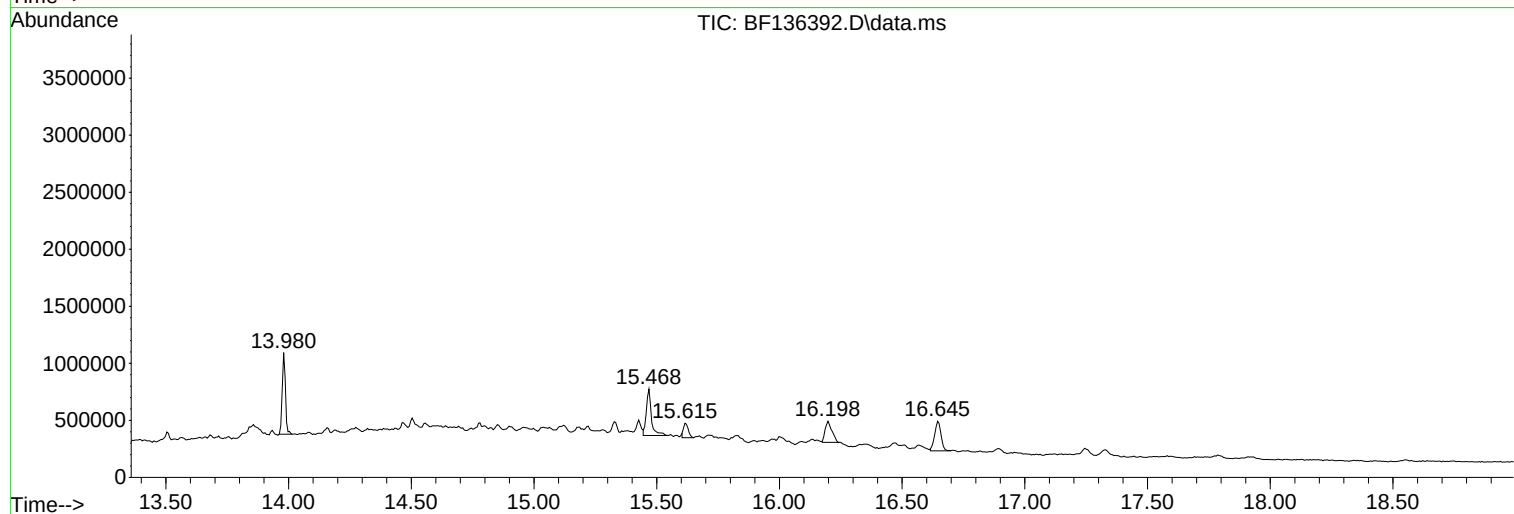
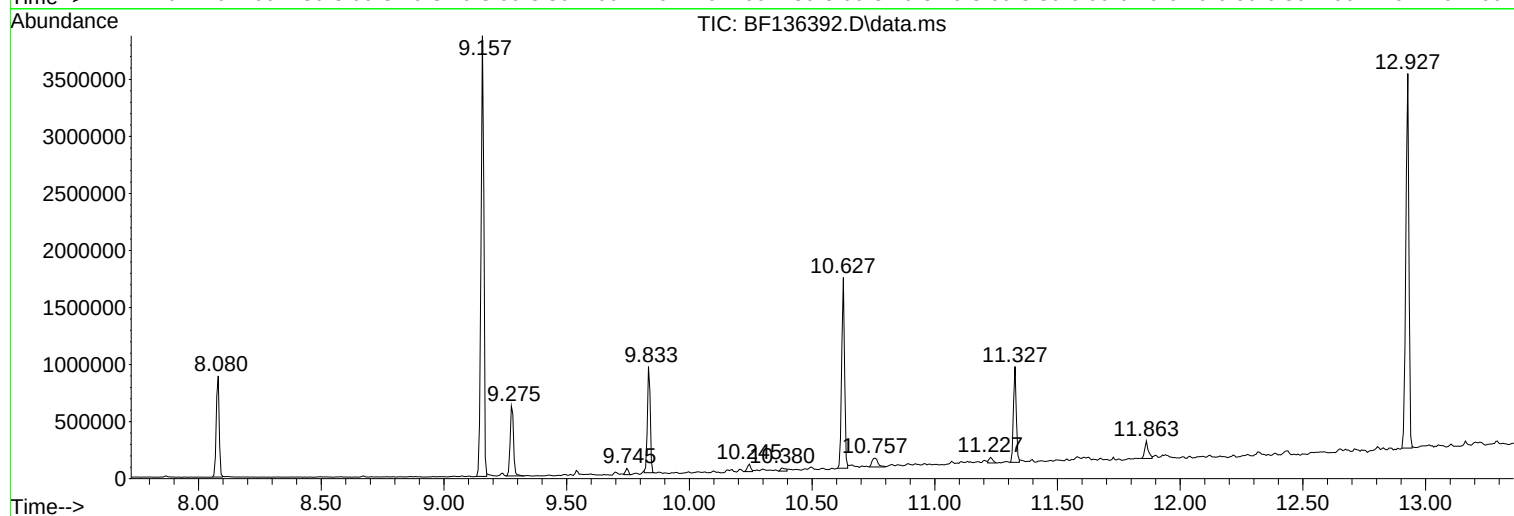
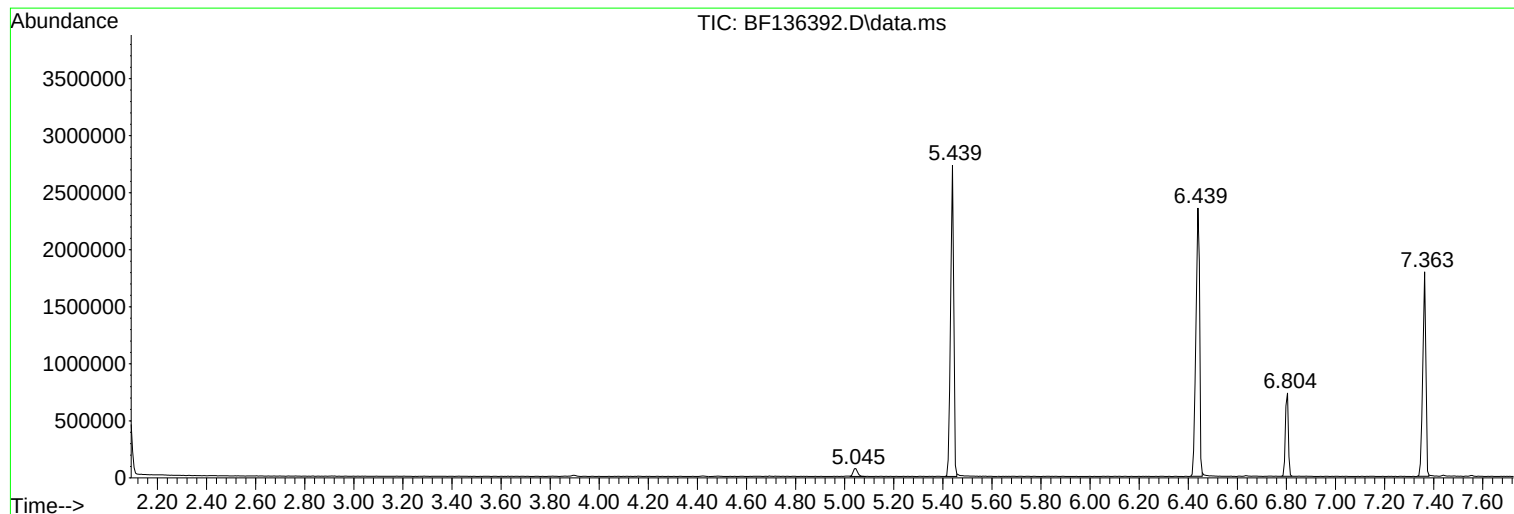
Sum of corrected areas: 20107445

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136392.D
Acq On : 04 Dec 2023 20:37
Operator : CG\JU
Sample : 05586-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VAULT-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.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\BF120423\
Data File : BF136392.D
Acq On : 04 Dec 2023 20:37
Operator : CG\JU
Sample : 05586-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VAULT-1

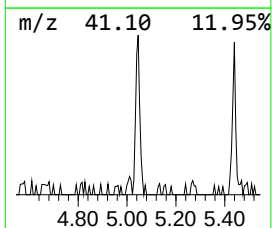
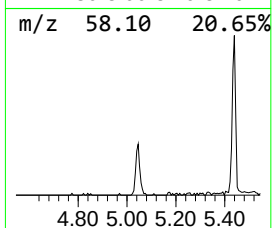
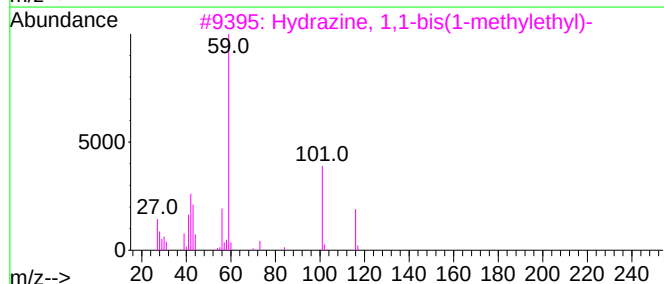
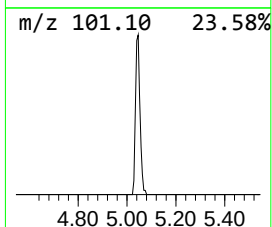
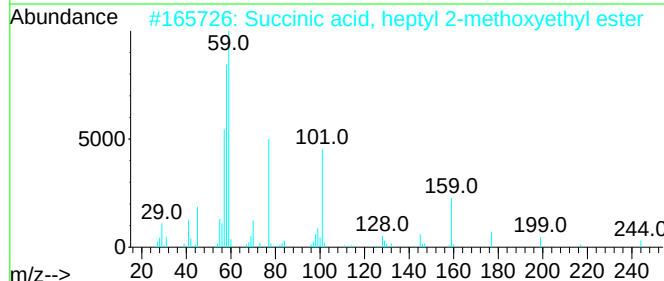
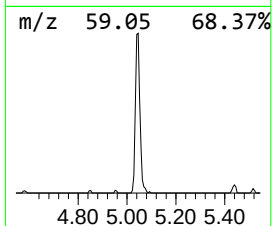
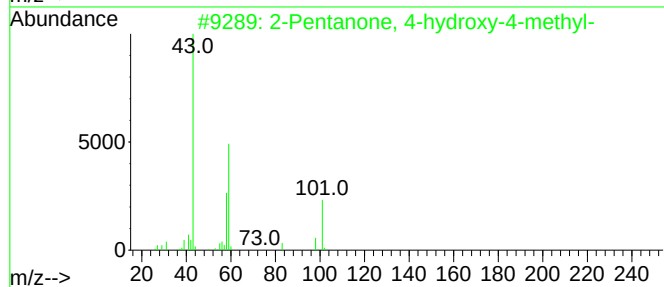
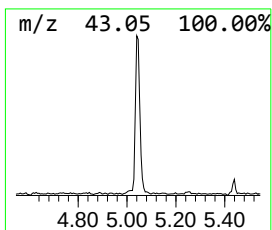
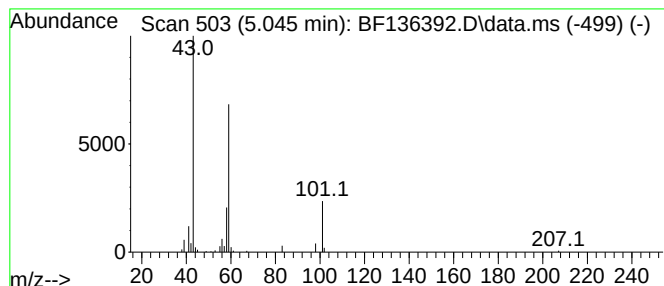
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.045	2.94 ng	86801	1,4-Dichlorobenzene-d4	6.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	28		
3	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	25		
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	17		
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	16		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136392.D
Acq On : 04 Dec 2023 20:37
Operator : CG\JU
Sample : 05586-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VAULT-1

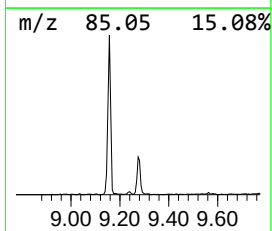
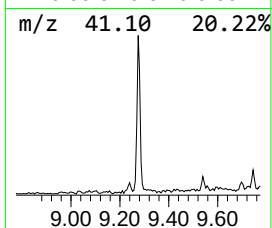
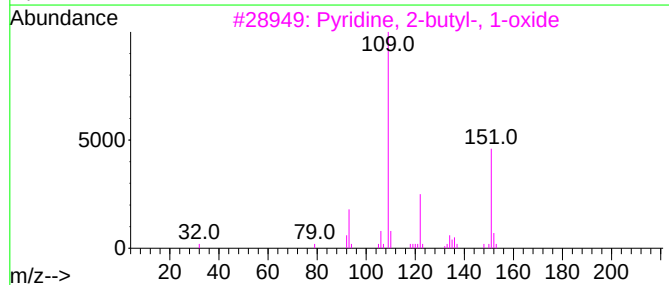
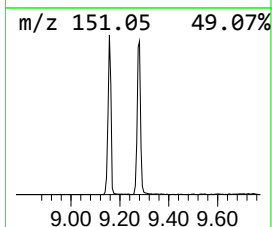
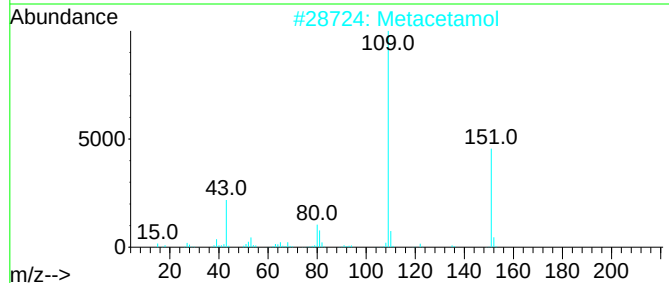
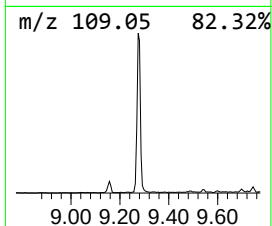
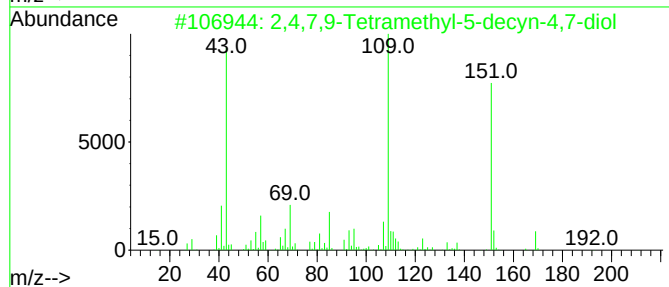
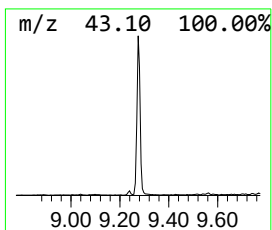
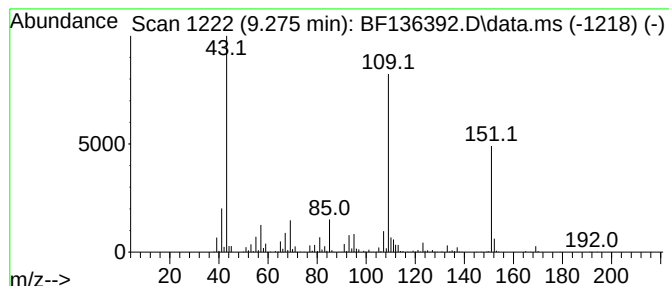
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD			R.T.
9.275	15.46 ng	583043	Acenaphthene-d10			9.833

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2		000126-86-3	91
2	Metacetamol	151	C8H9NO2		000621-42-1	64
3	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO		031396-32-4	59
4	m-Isopropoxyaniline	151	C9H13NO		041406-00-2	59
5	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3		1000107-08-7	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136392.D
Acq On : 04 Dec 2023 20:37
Operator : CG\JU
Sample : 05586-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VAULT-1

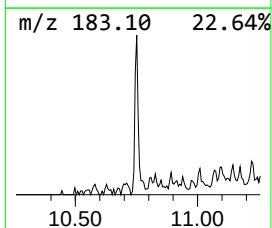
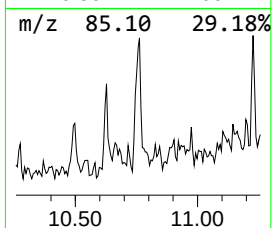
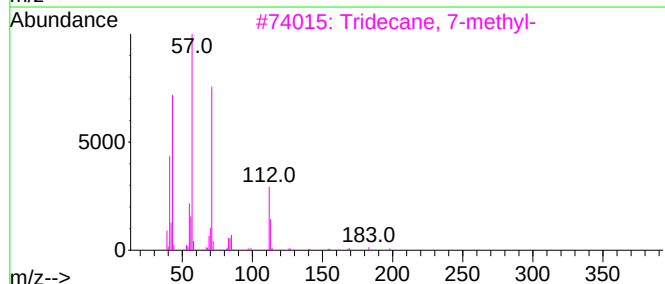
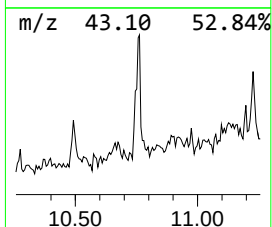
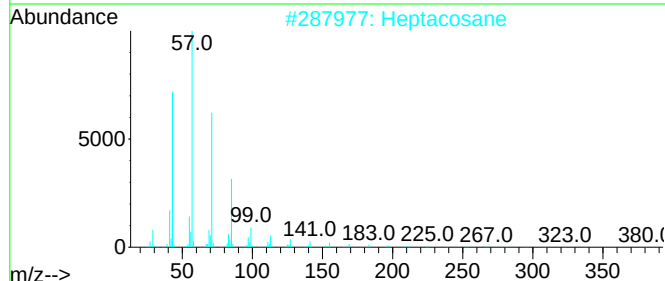
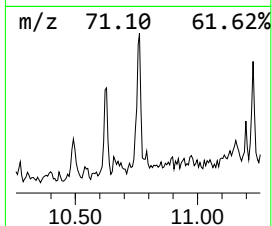
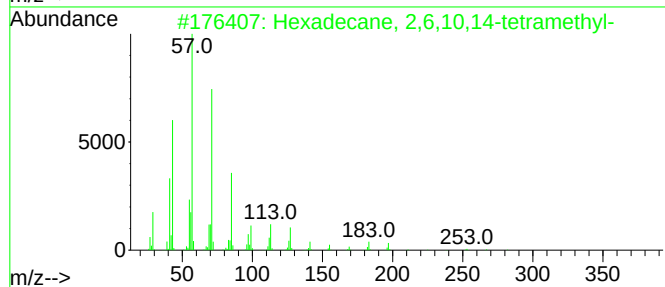
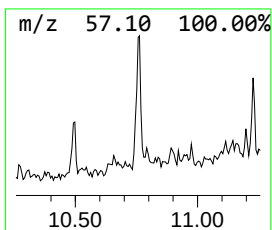
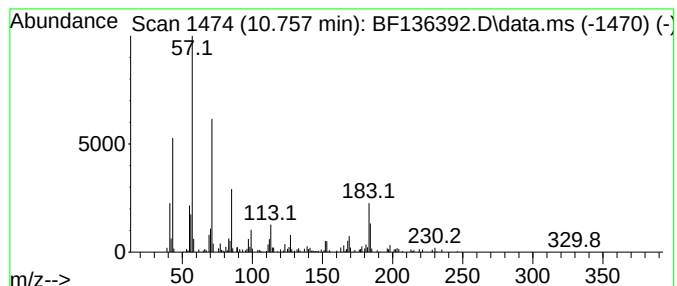
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Hexadecane, 2,6,10,14-tetra... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.757	3.79 ng	127910	Phenanthrene-d10	11.327

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	68
2			Heptacosane	380	C27H56	000593-49-7	58
3			Tridecane, 7-methyl-	198	C14H30	026730-14-3	55
4			Tetradecane	198	C14H30	000629-59-4	53
5			Hexadecane	226	C16H34	000544-76-3	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136392.D
Acq On : 04 Dec 2023 20:37
Operator : CG\JU
Sample : 05586-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

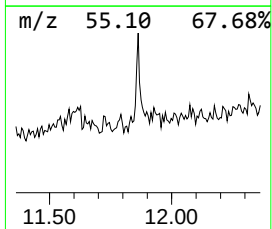
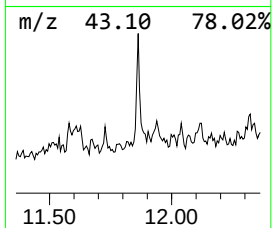
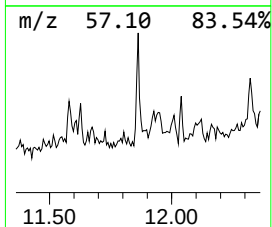
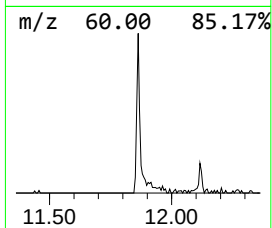
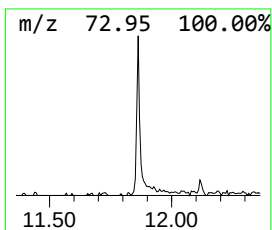
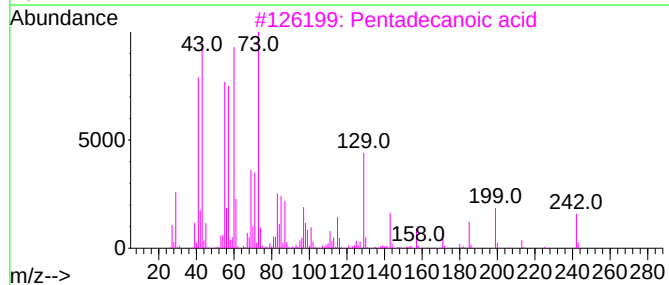
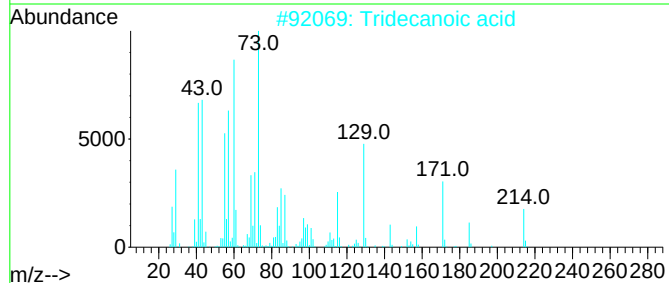
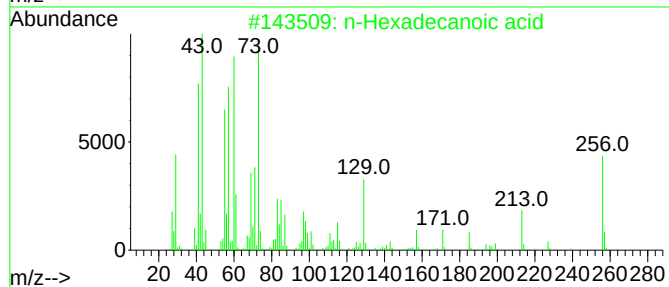
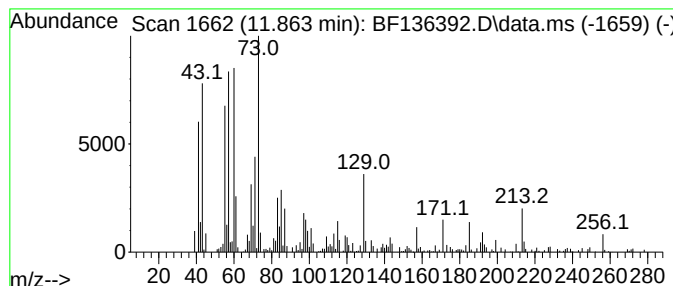
Instrument :
BNA_F
ClientSampleId :
VAULT-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.863	4.65 ng	157100	Phenanthrene-d10		11.327	
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	91
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	76
5	Tridecane, 2-methyl-		198	C14H30	001560-96-9	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136392.D
Acq On : 04 Dec 2023 20:37
Operator : CG\JU
Sample : 05586-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VAULT-1

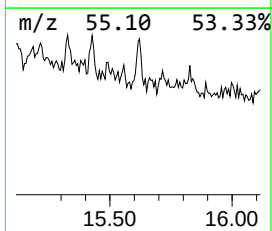
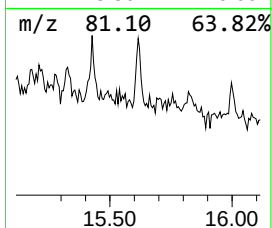
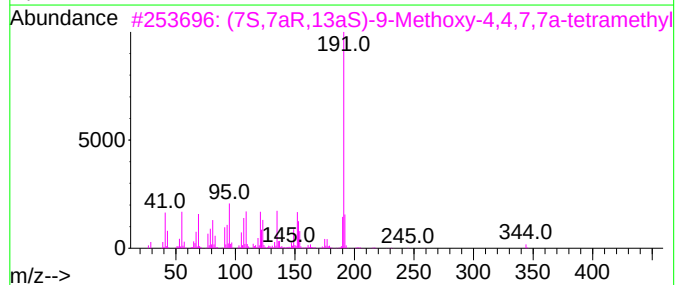
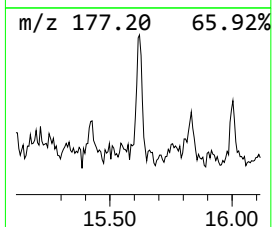
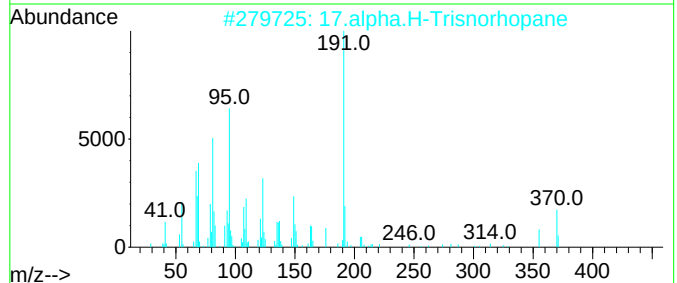
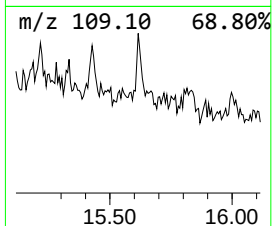
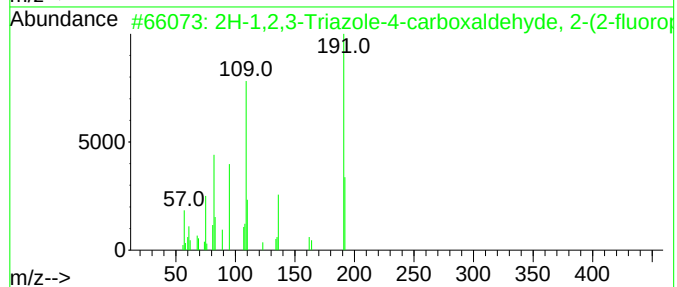
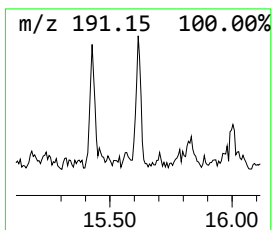
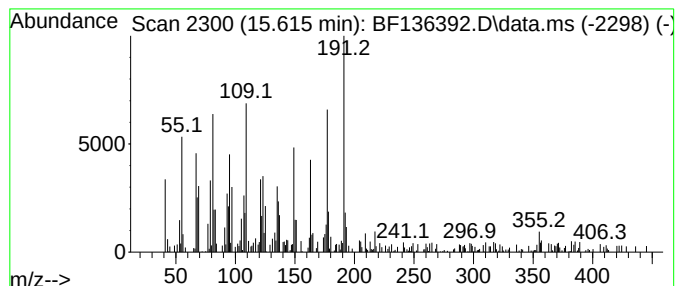
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown15.615 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	5.79 ng	169523	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2H-1,2,3-Triazole-4-carboxaldehy...	191	C9H6FN3O	051306-43-5	46
2			17.alpha.H-Trisnorhopane	370	C27H46	053584-59-1	41
3			(7S,7aR,13aS)-9-Methoxy-4,4,7,7a...	344	C22H32O3	1000482-45-3	38
4			23,28-Bisnor-17.alpha.(H)-hopane	384	C28H48	1000101-35-1	38
5			Benzamide, 3-fluoro-5-trifluorom...	305	C15H19F4NO	1000437-16-4	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136392.D
Acq On : 04 Dec 2023 20:37
Operator : CG\JU
Sample : 05586-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VAULT-1

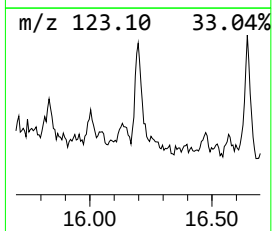
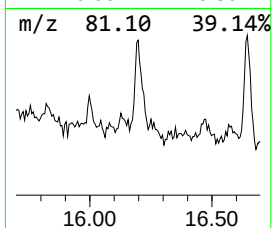
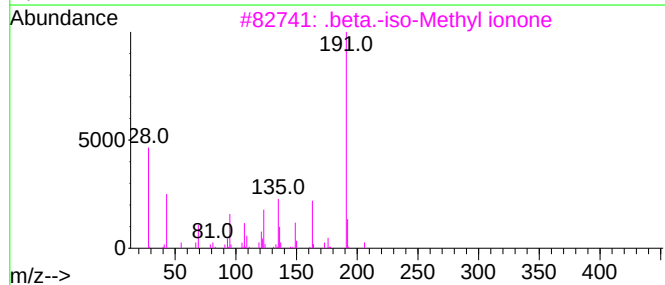
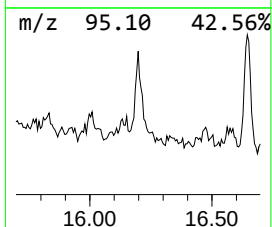
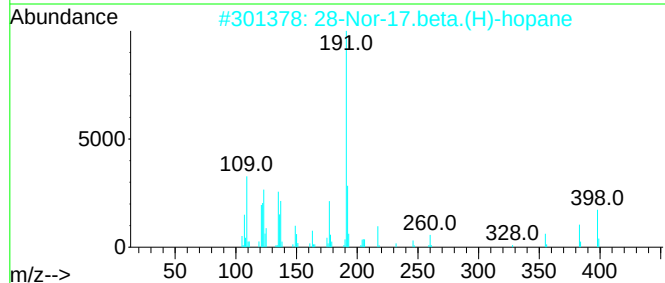
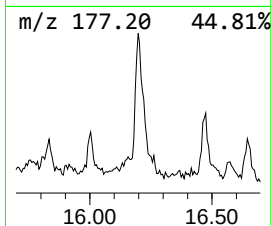
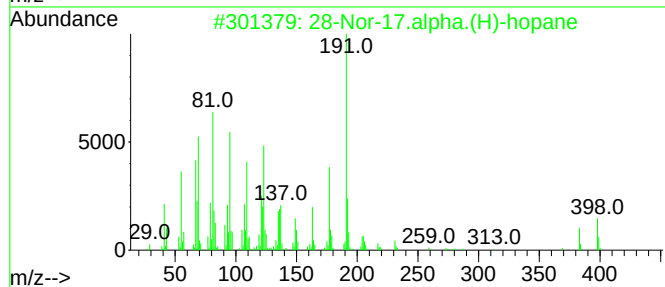
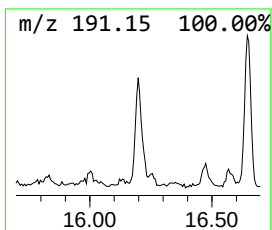
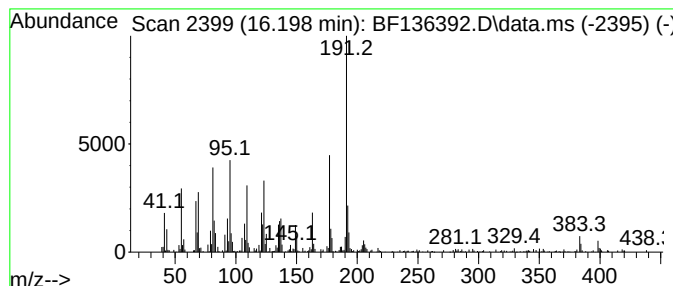
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 28-Nor-17.alpha.(H)-hopane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.198	12.06 ng	353246	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	95		
2	28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	59		
3	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	38		
4	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	38		
5	6-Fluoro-2-trifluoromethylbenzoi...	402	C18H8Cl2F4O2	1010343-74-7	38		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136392.D
Acq On : 04 Dec 2023 20:37
Operator : CG\JU
Sample : 05586-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

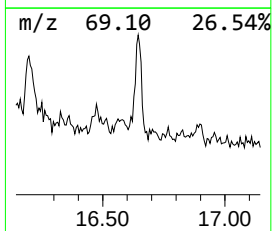
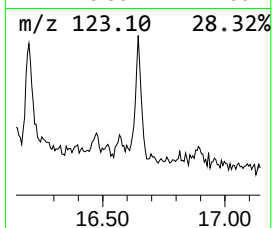
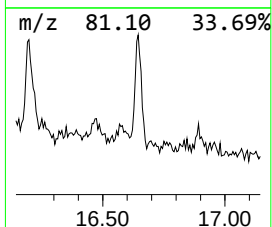
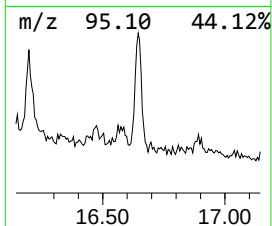
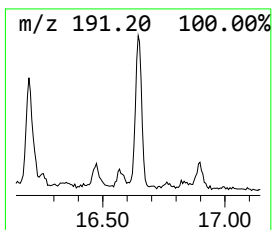
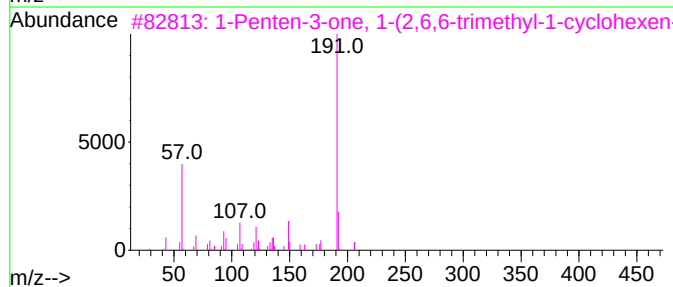
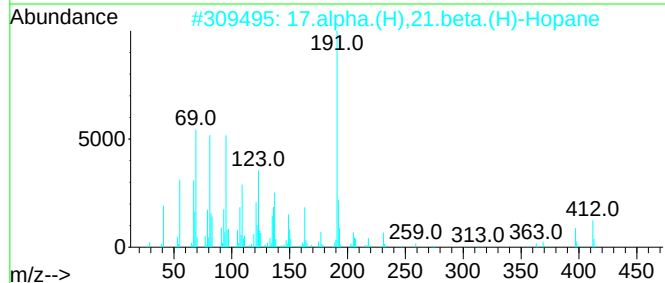
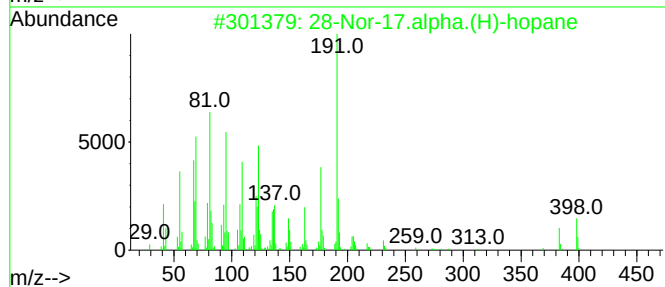
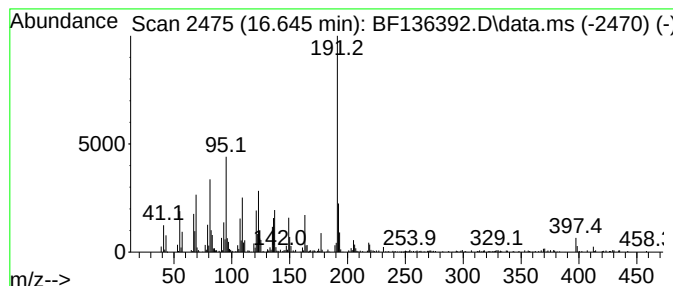
Instrument :
BNA_F
ClientSampleId :
VAULT-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 17.alpha.(H),21.beta.(H)-Ho... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.645	15.74 ng	460860	Perylene-d12		15.468	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	28-Nor-17.alpha.(H)-hopane		398	C29H50	053584-60-4	76
2	17.alpha.(H),21.beta.(H)-Hopane		412	C30H52	013849-96-2	58
3	1-Penten-3-one, 1-(2,6,6-trimeth...		206	C14H22O	000127-43-5	45
4	Anthracene, 9-dodecyltetradecahy...		360	C26H48	055401-75-7	42
5	1-(2-Fluorobenzyl)-3-piperidinam...		278	C16H23FN2O	1546741-98-3	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136392.D
Acq On : 04 Dec 2023 20:37
Operator : CG\JU
Sample : 05586-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VAULT-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.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-...	5.045	2.9	ng	86801	1	6.804	589807	20.0
2,4,7,9-Tetrame...	9.275	15.5	ng	583043	3	9.833	754139	20.0
Hexadecane, 2,6...	10.757	3.8	ng	127910	4	11.327	675510	20.0
n-Hexadecanoic ...	11.863	4.7	ng	157100	4	11.327	675510	20.0
unknown15.615	15.615	5.8	ng	169523	6	15.468	585713	20.0
28-Nor-17.alpha...	16.198	12.1	ng	353246	6	15.468	585713	20.0
17.alpha.(H),21...	16.645	15.7	ng	460860	6	15.468	585713	20.0