

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
 Data File : BF136431.D
 Acq On : 06 Dec 2023 16:41
 Operator : CG\JU
 Sample : 05602-03
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SPRING-VALLEY-TP-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-BF120523.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136431.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	15	18	23	rVB	22740	30031	1.57%	0.227%
2	5.034	496	501	508	rVB	68790	80092	4.19%	0.605%
3	5.434	564	569	572	rBV	2082262	1912271	100.00%	14.438%
4	6.434	734	739	742	rBV	1933668	1828054	95.60%	13.802%
5	6.798	797	801	804	rBV	674717	562701	29.43%	4.249%
6	7.357	891	896	899	rBV	1365846	1171805	61.28%	8.847%
7	7.963	996	999	1003	rBV	89434	71569	3.74%	0.540%
8	8.075	1014	1018	1021	rBV	747393	661037	34.57%	4.991%
9	9.151	1197	1201	1204	rBV	2468027	1911124	99.94%	14.430%
10	9.828	1312	1316	1320	rBV	749660	582737	30.47%	4.400%
11	10.616	1446	1450	1454	rBV	973518	892388	46.67%	6.738%
12	11.316	1566	1569	1572	rBV	582159	528158	27.62%	3.988%
13	11.857	1657	1661	1670	rBV3	106684	136519	7.14%	1.031%
14	12.533	1773	1776	1779	rBV	65528	55290	2.89%	0.417%
15	12.645	1790	1795	1803	rBV5	36143	62012	3.24%	0.468%
16	12.763	1810	1815	1818	rBV	67565	64940	3.40%	0.490%
17	12.916	1837	1841	1844	rBV	2047025	1700730	88.94%	12.841%
18	13.968	2016	2020	2023	rBV	629365	599791	31.37%	4.529%
19	15.451	2268	2272	2279	rBV	338372	393229	20.56%	2.969%

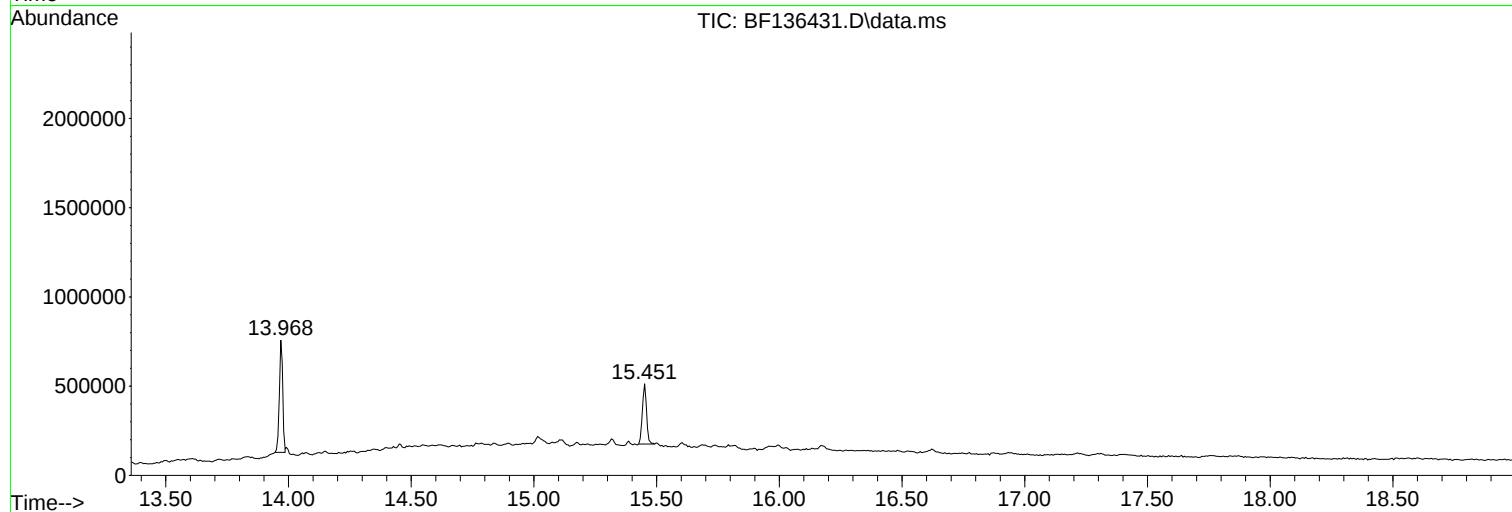
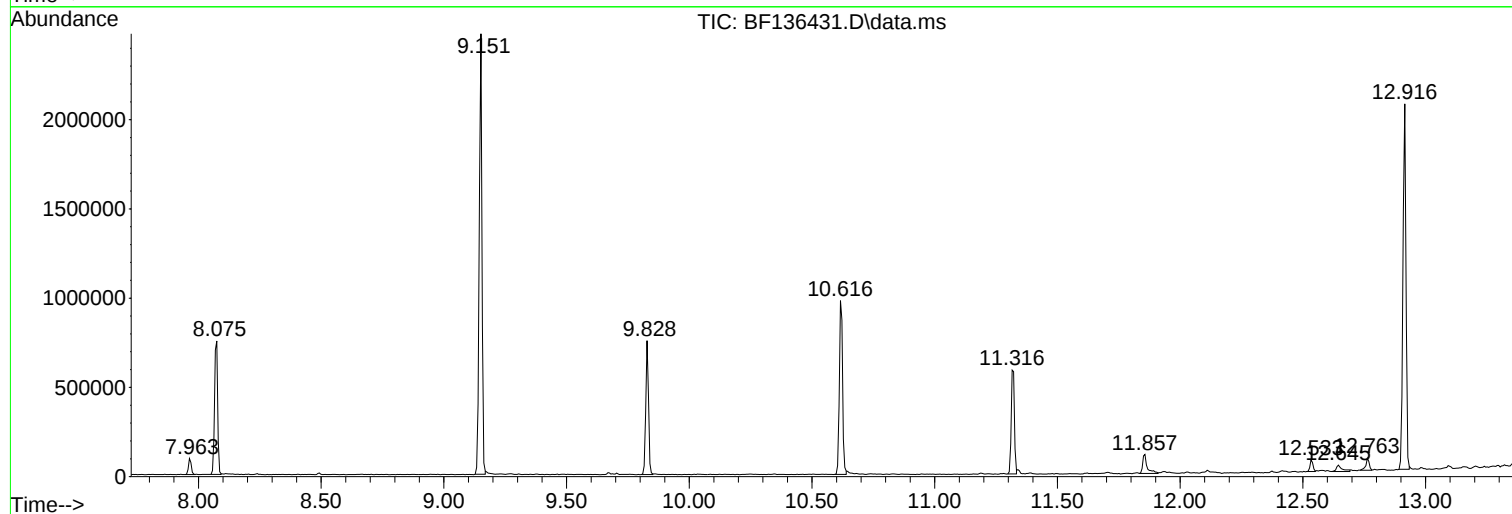
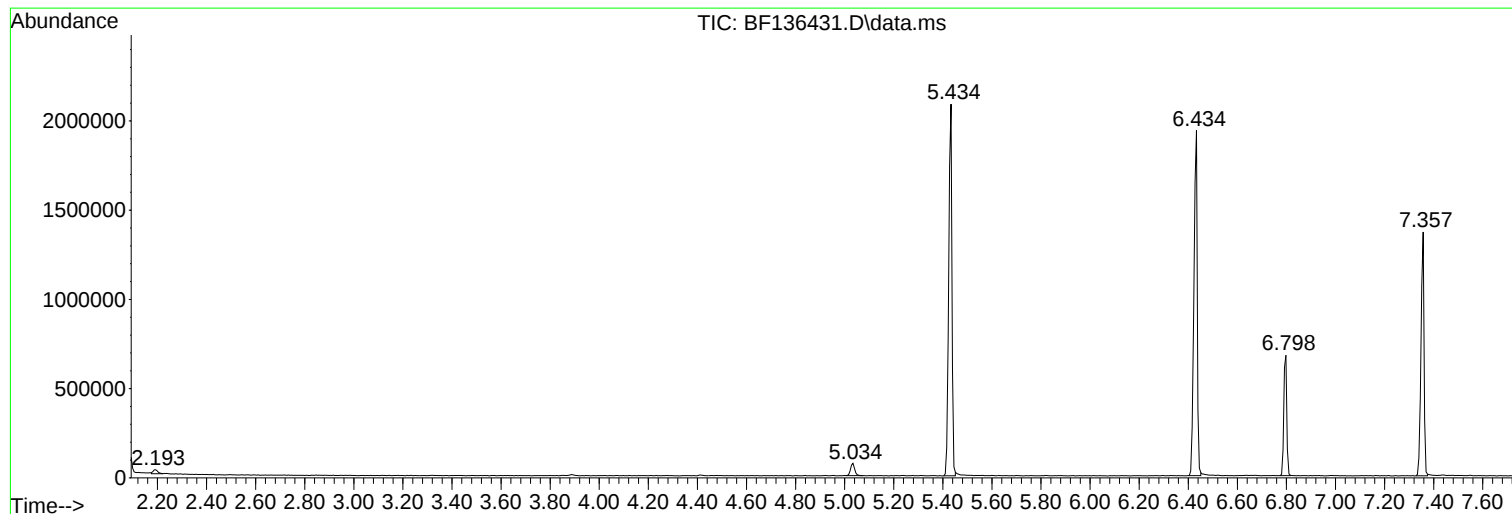
Sum of corrected areas: 13244478

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136431.D
Acq On : 06 Dec 2023 16:41
Operator : CG\JU
Sample : 05602-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPRING-VALLEY-TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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\BF120623\
Data File : BF136431.D
Acq On : 06 Dec 2023 16:41
Operator : CG\JU
Sample : 05602-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPRING-VALLEY-TP-2

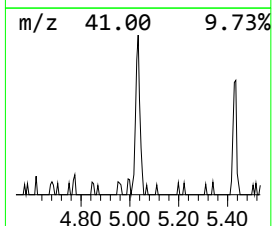
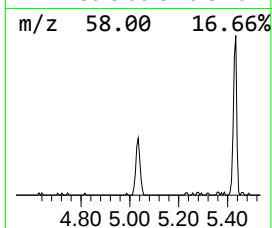
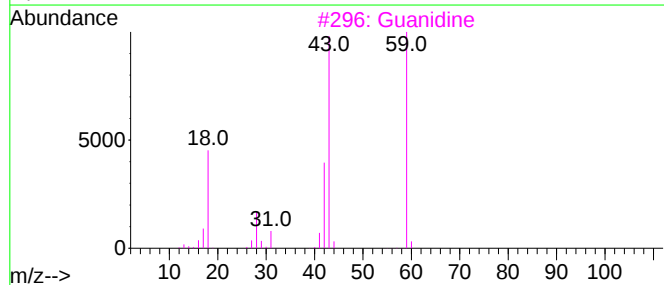
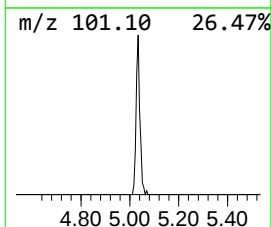
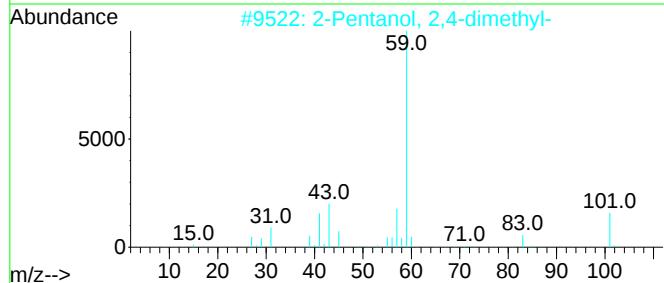
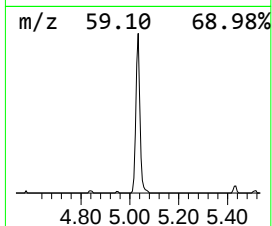
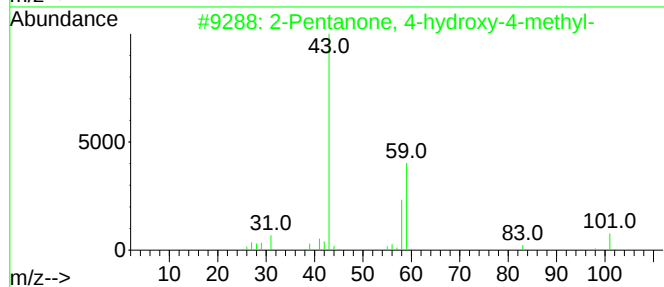
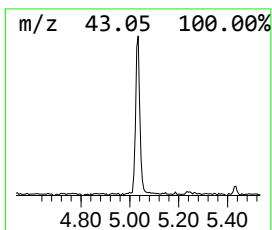
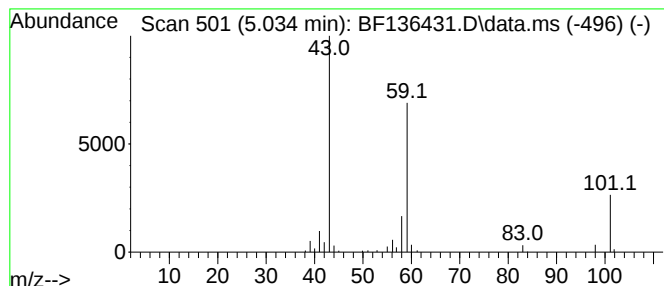
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.034	2.85 ng	80092	1,4-Dichlorobenzene-d4	6.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	45		
3	Guanidine	59	CH5N3	000113-00-8	43		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136431.D
Acq On : 06 Dec 2023 16:41
Operator : CG\JU
Sample : 05602-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPRING-VALLEY-TP-2

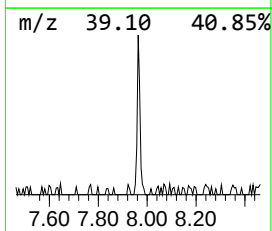
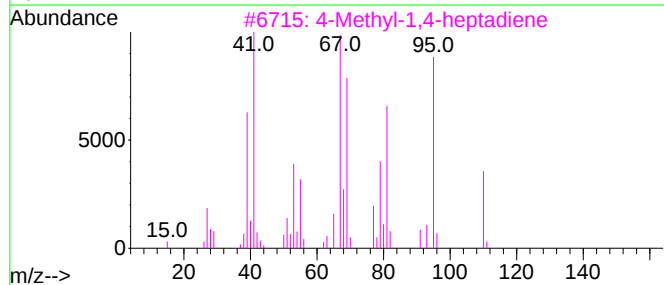
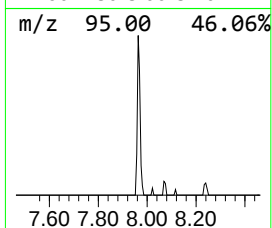
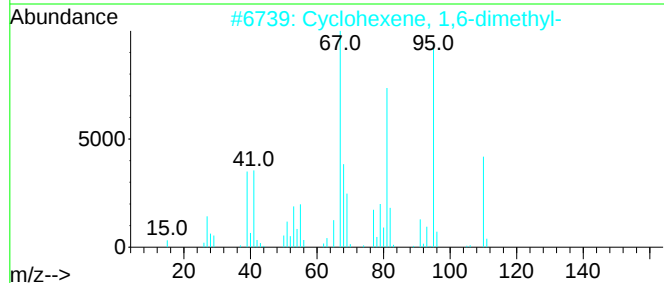
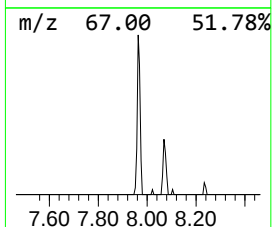
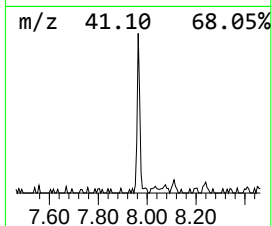
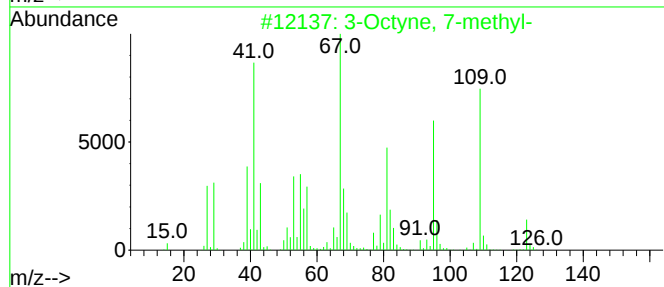
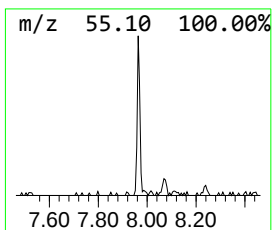
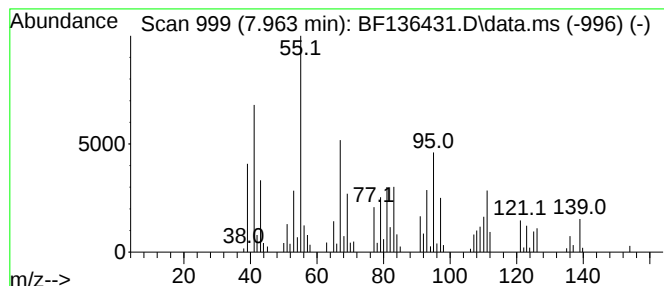
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown7.963 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.963	2.17 ng	71569	Naphthalene-d8	8.075

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Octyne, 7-methyl-	124	C9H16	037050-06-9	43
2			Cyclohexene, 1,6-dimethyl-	110	C8H14	001759-64-4	38
3			4-Methyl-1,4-heptadiene	110	C8H14	013857-55-1	38
4			Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	38
5			3-Nonyne	124	C9H16	020184-89-8	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136431.D
Acq On : 06 Dec 2023 16:41
Operator : CG\JU
Sample : 05602-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPRING-VALLEY-TP-2

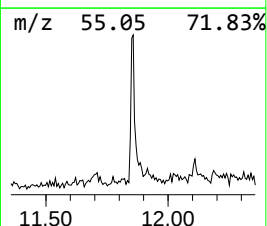
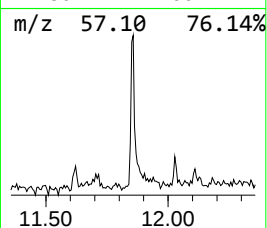
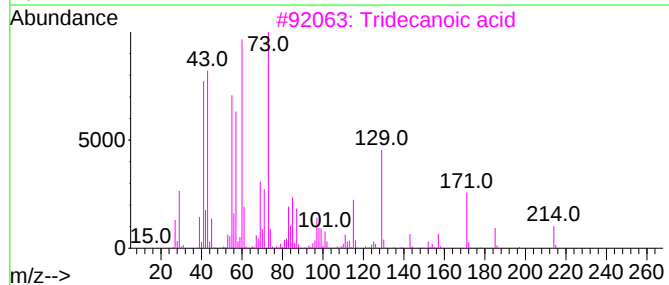
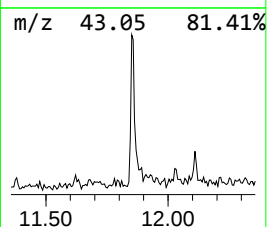
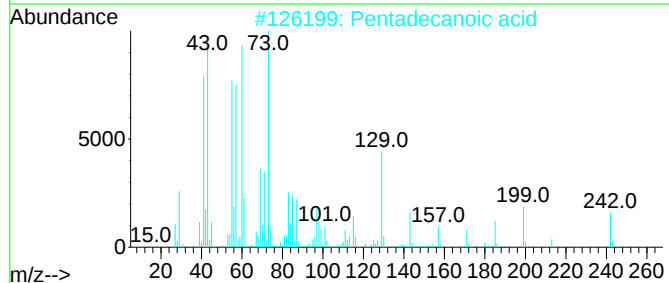
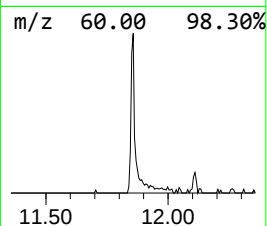
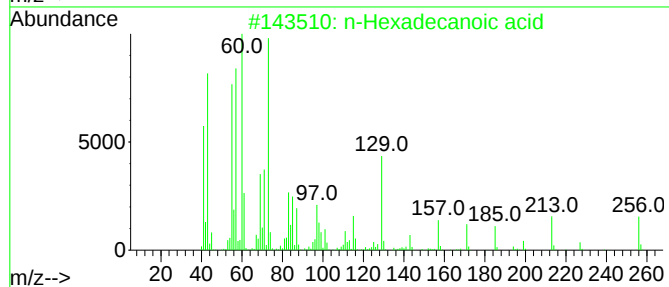
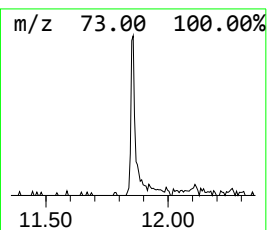
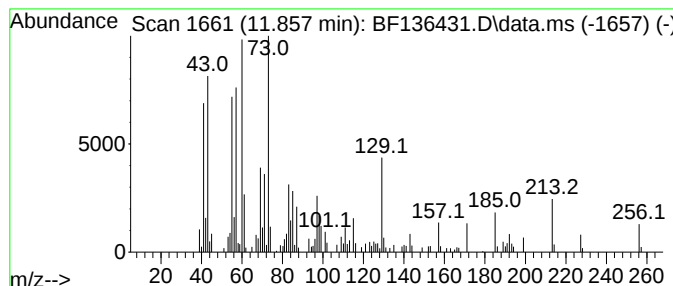
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	5.17 ng	136519	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136431.D
Acq On : 06 Dec 2023 16:41
Operator : CG\JU
Sample : 05602-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPRING-VALLEY-TP-2

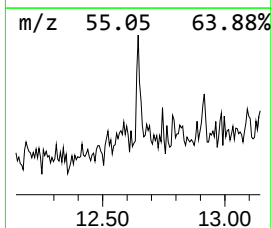
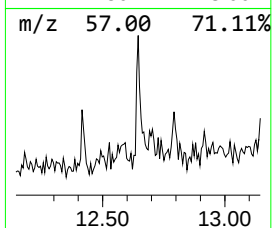
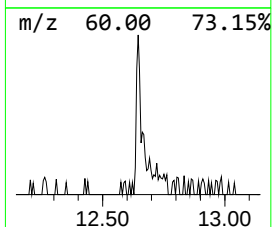
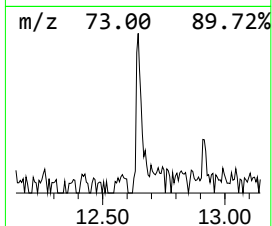
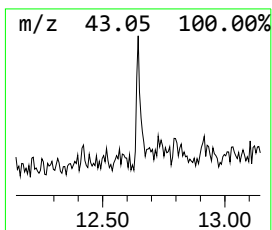
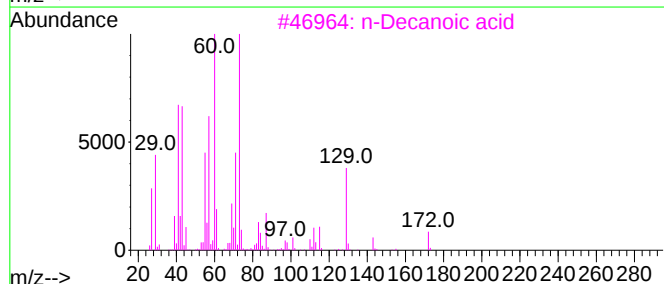
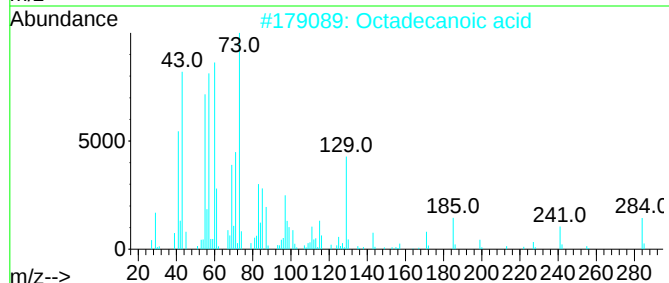
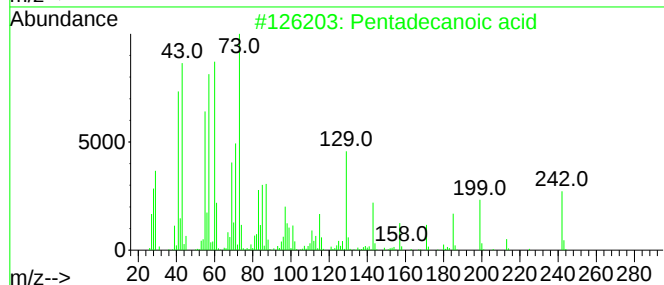
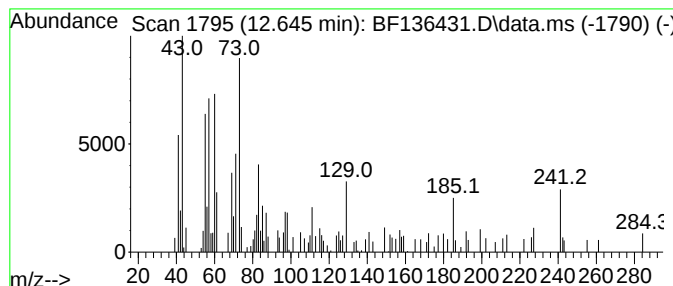
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	2.35 ng	62012	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
2			Octadecanoic acid	284	C18H36O2	000057-11-4	60
3			n-Decanoic acid	172	C10H20O2	000334-48-5	55
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	53
5			Undecanoic acid	186	C11H22O2	000112-37-8	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136431.D
Acq On : 06 Dec 2023 16:41
Operator : CG\JU
Sample : 05602-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPRING-VALLEY-TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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-...	5.034	2.9	ng	80092	1	6.798	562701	20.0
unknown7.963	7.963	2.2	ng	71569	2	8.075	661037	20.0
n-Hexadecanoic ...	11.857	5.2	ng	136519	4	11.322	528158	20.0
Pentadecanoic acid	12.645	2.4	ng	62012	4	11.322	528158	20.0