

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030223\
 Data File : BF132616.D
 Acq On : 02 Mar 2023 19:46
 Operator : CG\JU
 Sample : 01749-11
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CF-13

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: BF132616.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.228	444	449	462	rVB	1554168	1929591	51.54%	6.962%
2	5.622	512	516	520	rBV	3267552	3257421	87.00%	11.754%
3	6.622	682	686	689	rBV	3387953	3334852	89.07%	12.033%
4	6.998	747	750	754	rBV	1499861	1220243	32.59%	4.403%
5	7.563	842	846	849	rBV	2676599	2281017	60.93%	8.230%
6	8.287	965	969	972	rBV	1949953	1539437	41.12%	5.555%
7	9.363	1148	1152	1155	rBV	4233833	3743947	100.00%	13.509%
8	10.045	1265	1268	1272	rVB	1815260	1512696	40.40%	5.458%
9	10.757	1386	1389	1392	rBV	120434	96669	2.58%	0.349%
10	10.839	1399	1403	1411	rBV	2101712	1767730	47.22%	6.378%
11	11.545	1519	1523	1526	rBV	1394015	1265252	33.79%	4.565%
12	12.057	1606	1610	1624	rBV3	162492	283068	7.56%	1.021%
13	12.763	1727	1730	1733	rBV	66601	64251	1.72%	0.232%
14	12.851	1742	1745	1753	rBV7	28108	61319	1.64%	0.221%
15	12.998	1764	1770	1776	rBV	69246	90947	2.43%	0.328%
16	13.133	1789	1793	1797	rBV	3042065	2709576	72.37%	9.777%
17	14.045	1942	1948	1959	rBV6	100848	364924	9.75%	1.317%
18	14.204	1971	1975	1978	rBV	1308483	1154127	30.83%	4.164%
19	15.063	2119	2121	2125	rVB	106734	105914	2.83%	0.382%
20	15.757	2234	2239	2248	rVB2	708730	931242	24.87%	3.360%

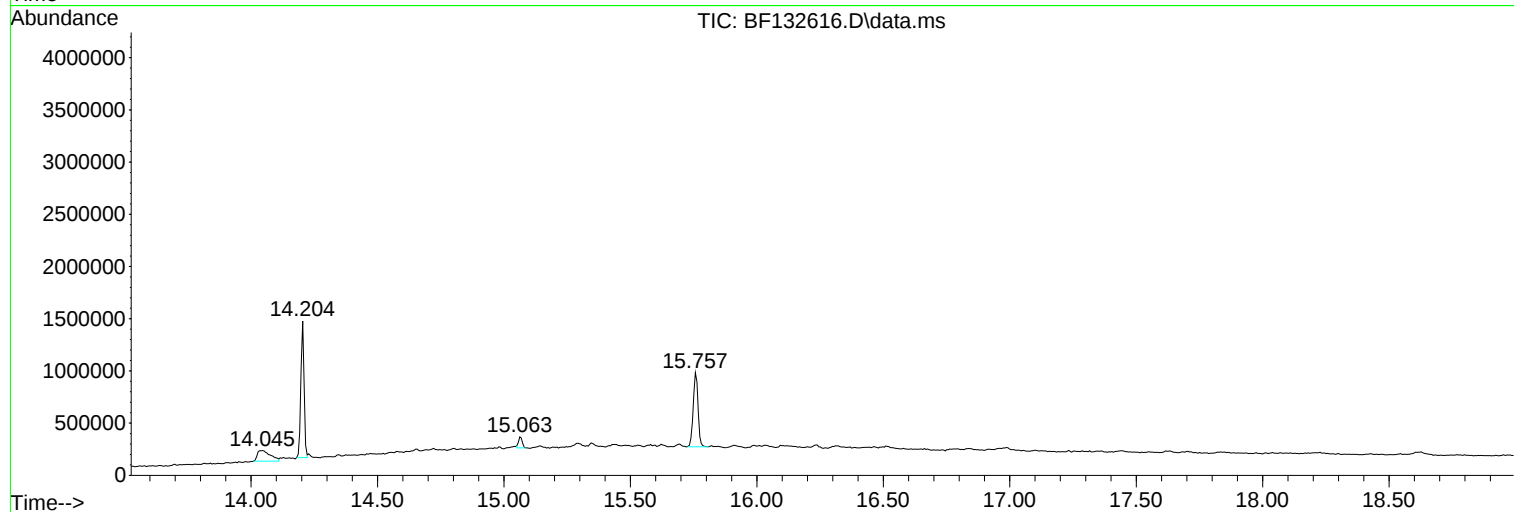
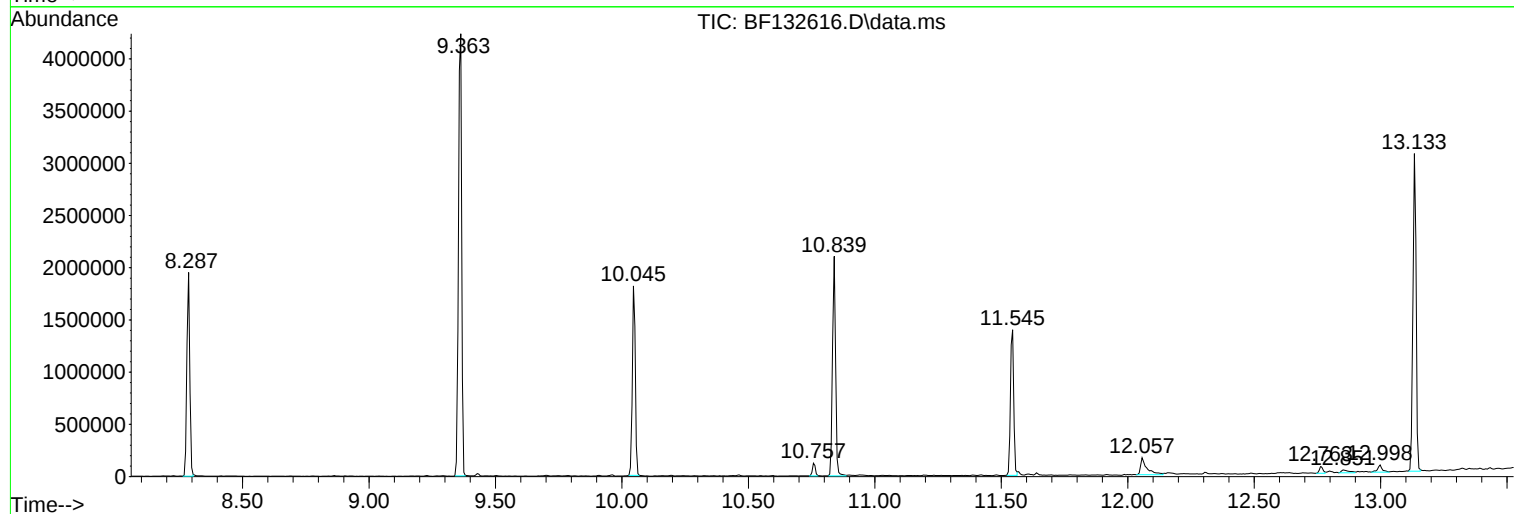
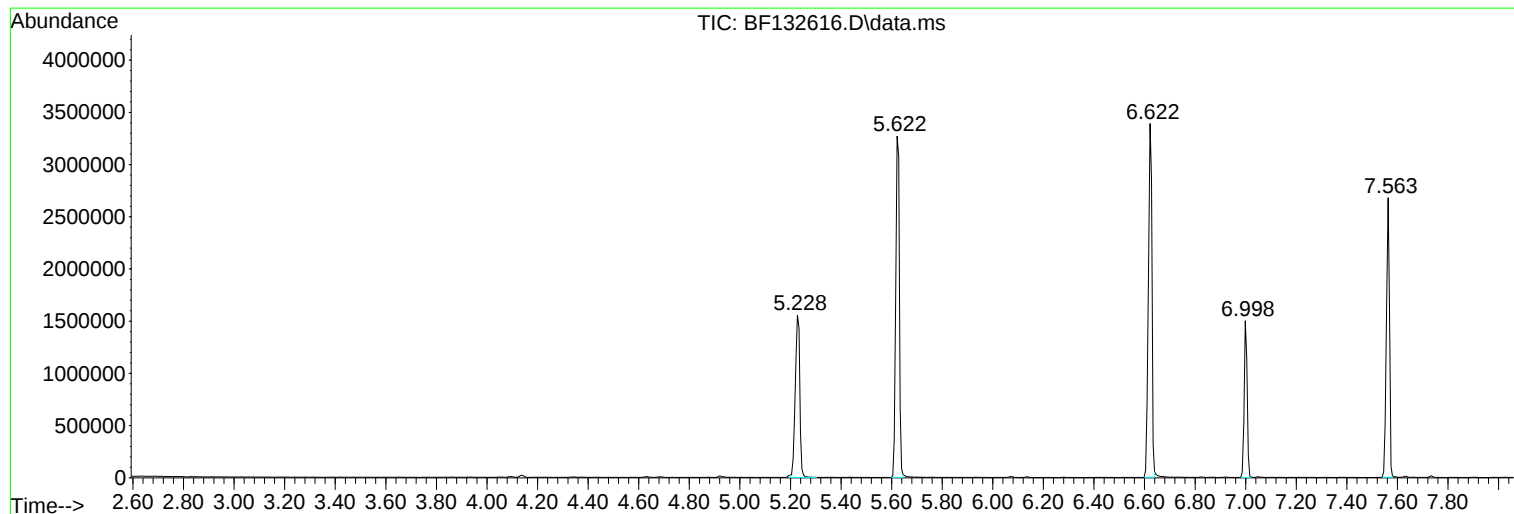
Sum of corrected areas: 27714223

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030223\
Data File : BF132616.D
Acq On : 02 Mar 2023 19:46
Operator : CG\JU
Sample : 01749-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CF-13

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\BF030223\
Data File : BF132616.D
Acq On : 02 Mar 2023 19:46
Operator : CG\JU
Sample : 01749-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CF-13

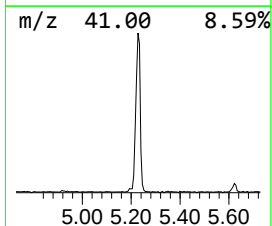
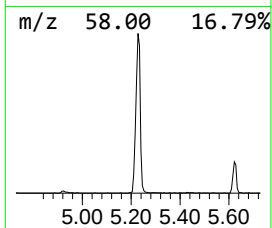
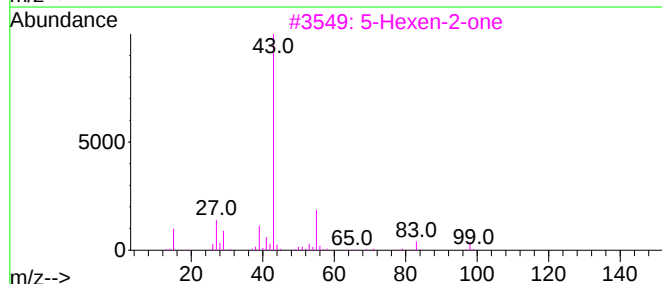
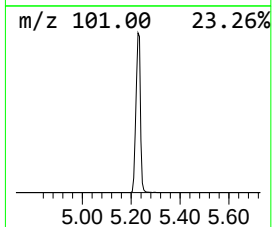
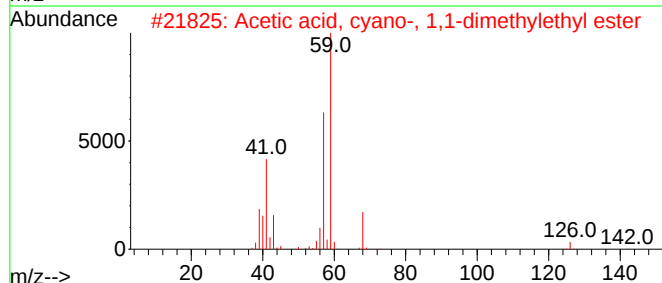
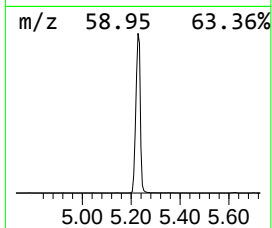
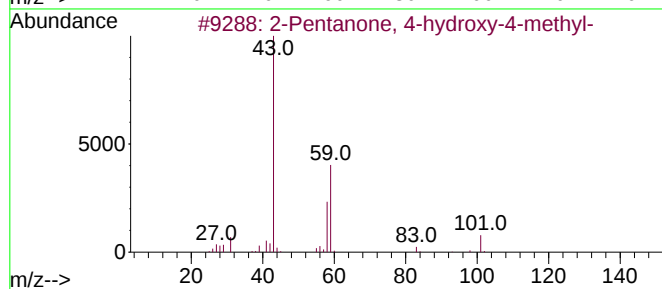
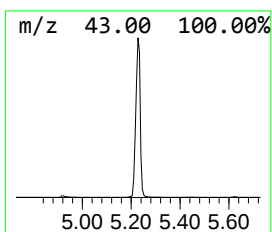
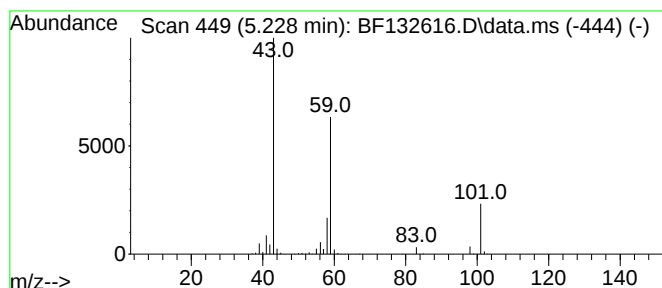
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.228	31.63 ng	1929590	1,4-Dichlorobenzene-d4	6.998

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	5-Hexen-2-one	98	C6H10O	000109-49-9	9		
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		
5	Guanidine	59	CH5N3	000113-00-8	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030223\
Data File : BF132616.D
Acq On : 02 Mar 2023 19:46
Operator : CG\JU
Sample : 01749-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CF-13

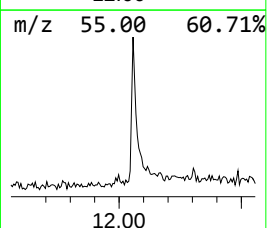
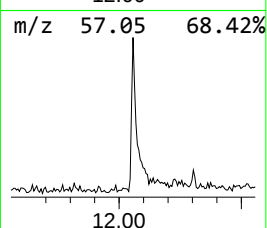
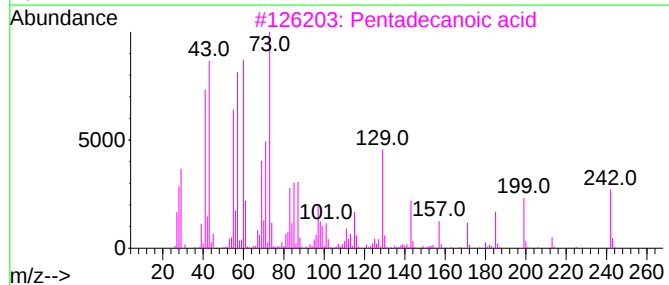
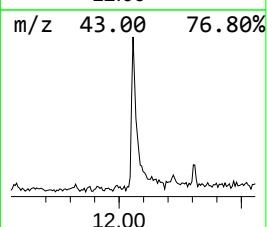
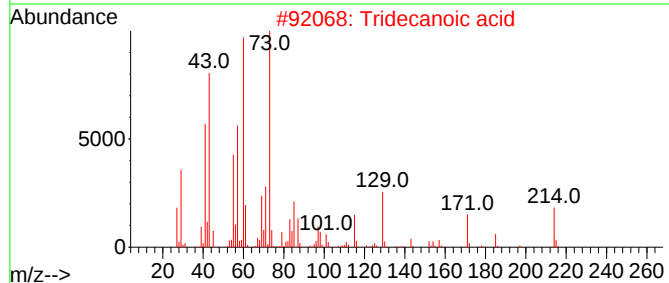
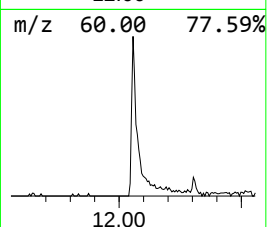
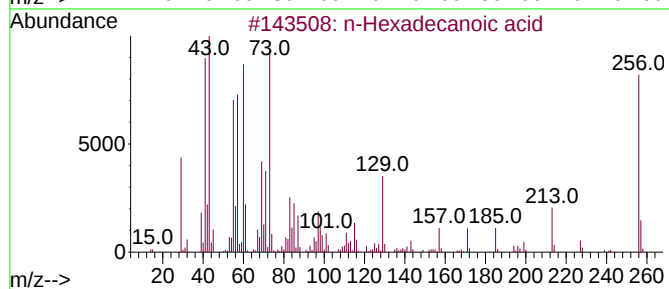
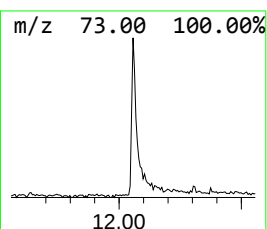
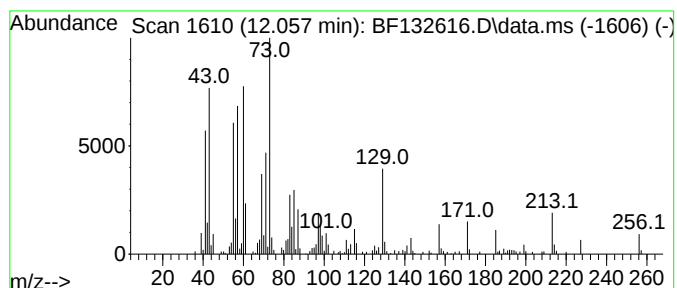
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.057	4.47 ng	283068	Phenanthrene-d10	11.545

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	74
4			n-Decanoic acid	172	C10H20O2	000334-48-5	68
5			Nonanoic acid	158	C9H18O2	000112-05-0	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030223\
Data File : BF132616.D
Acq On : 02 Mar 2023 19:46
Operator : CG\JU
Sample : 01749-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CF-13

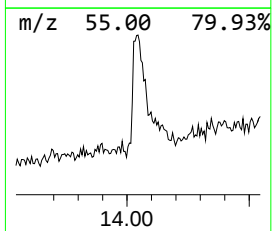
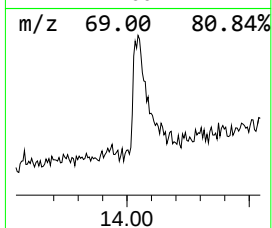
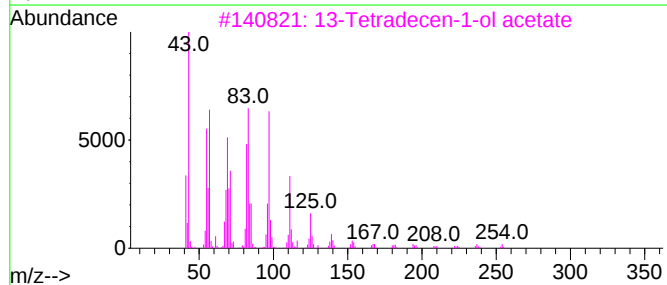
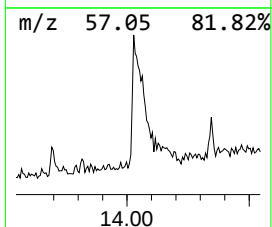
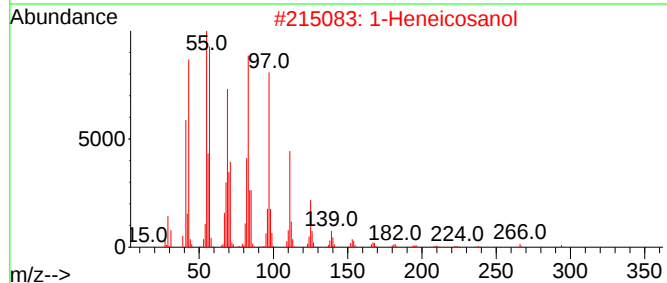
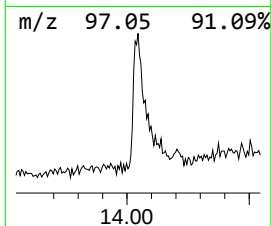
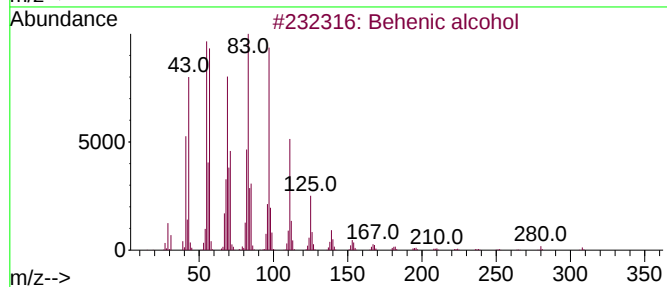
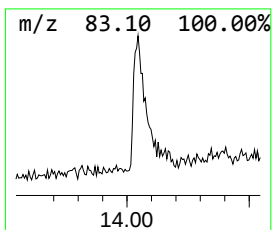
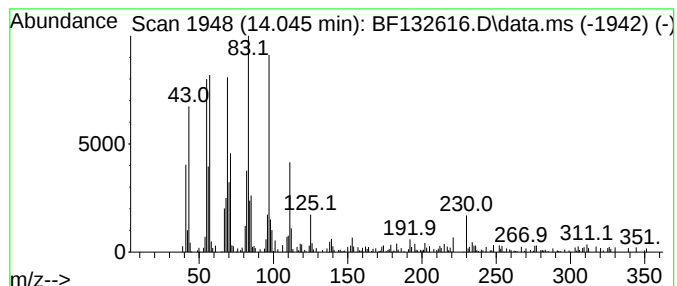
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Behenic alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.045	6.32 ng	364924	Chrysene-d12	14.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	91
2			1-Heneicosanol	312	C21H44O	015594-90-8	91
3			13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	89
4			Pentacos-1-ene	350	C25H50	016980-85-1	76
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030223\
Data File : BF132616.D
Acq On : 02 Mar 2023 19:46
Operator : CG\JU
Sample : 01749-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CF-13

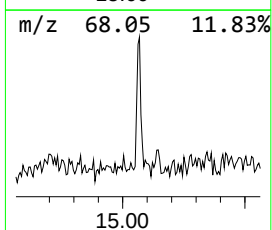
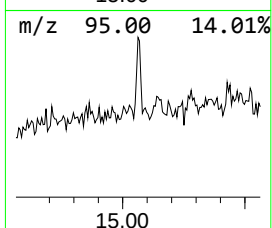
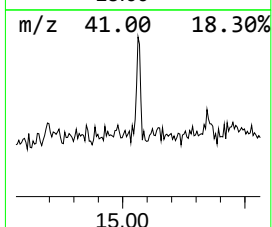
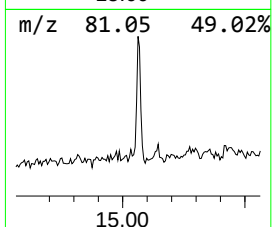
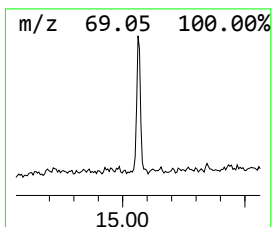
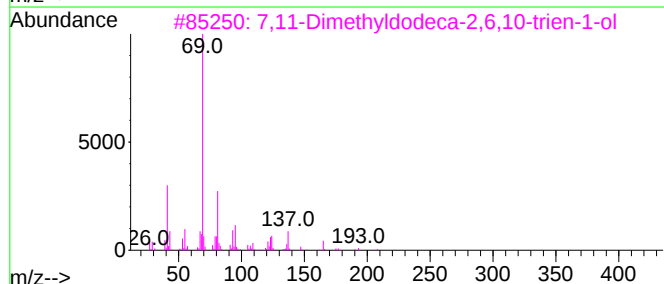
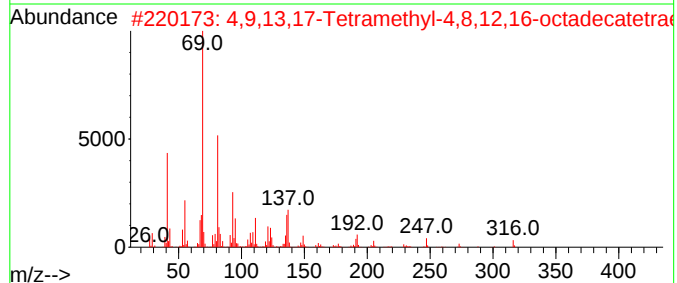
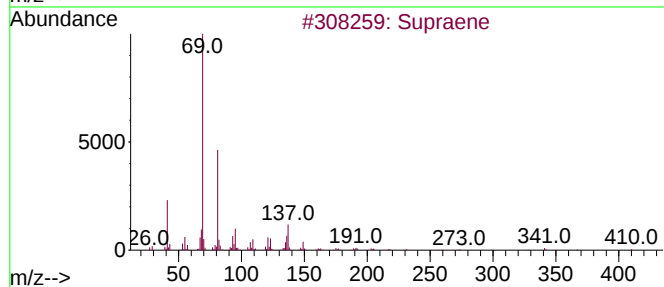
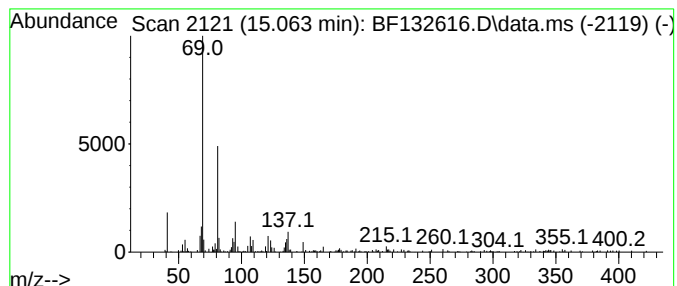
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.063	2.27 ng	105914	Perylene-d12	15.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	96
2			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	72
3			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4			(3E,7E)-4,8,12-Trimethyltrideca...	218	C16H26	062235-06-7	64
5			2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030223\
Data File : BF132616.D
Acq On : 02 Mar 2023 19:46
Operator : CG\JU
Sample : 01749-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CF-13

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-...	5.228	31.6	ng	1929590	1	6.998	1220240	20.0
n-Hexadecanoic ...	12.057	4.5	ng	283068	4	11.545	1265250	20.0
Behenic alcohol	14.045	6.3	ng	364924	5	14.204	1154130	20.0
Supraene	15.063	2.3	ng	105914	6	15.757	931242	20.0