

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060823\
 Data File : BF133637.D
 Acq On : 08 Jun 2023 12:27
 Operator : CG\JU
 Sample : 03016-04
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB29

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-BF052523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133637.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.110	3	4	11	rVB	525366	480972	16.48%	2.250%
2	5.057	499	505	512	rVB	34639	46298	1.59%	0.217%
3	5.451	567	572	575	rBV	2570538	2480006	84.96%	11.599%
4	6.463	738	744	747	rBV	2455821	2545554	87.21%	11.906%
5	6.834	803	807	810	rBV	1085657	827863	28.36%	3.872%
6	7.398	898	903	906	rBV	1894818	1655735	56.72%	7.744%
7	8.116	1022	1025	1029	rBV	1361749	1082191	37.07%	5.062%
8	9.192	1204	1208	1212	rBV	3168284	2918944	100.00%	13.652%
9	9.875	1320	1324	1327	rBV	1459021	1165455	39.93%	5.451%
10	10.586	1442	1445	1449	rBV	449369	351899	12.06%	1.646%
11	10.663	1454	1458	1461	rBV	2121836	1863203	63.83%	8.715%
12	11.363	1573	1577	1580	rBV	1476586	1200246	41.12%	5.614%
13	11.886	1663	1666	1679	rBV	195484	215266	7.37%	1.007%
14	12.951	1843	1847	1850	rBV	2855830	2545490	87.21%	11.906%
15	13.898	2003	2008	2019	rBV4	58044	177671	6.09%	0.831%
16	14.004	2022	2026	2030	rVB	848815	789239	27.04%	3.691%
17	14.480	2104	2107	2112	rBV	34267	35695	1.22%	0.167%
18	14.639	2130	2134	2138	rBV	93788	87922	3.01%	0.411%
19	14.863	2168	2172	2176	rVB	50331	53303	1.83%	0.249%
20	15.121	2214	2216	2221	rVB	42795	47202	1.62%	0.221%
21	15.468	2270	2275	2279	rBV	627239	765883	26.24%	3.582%
22	15.939	2352	2355	2361	rVB3	27007	44367	1.52%	0.208%

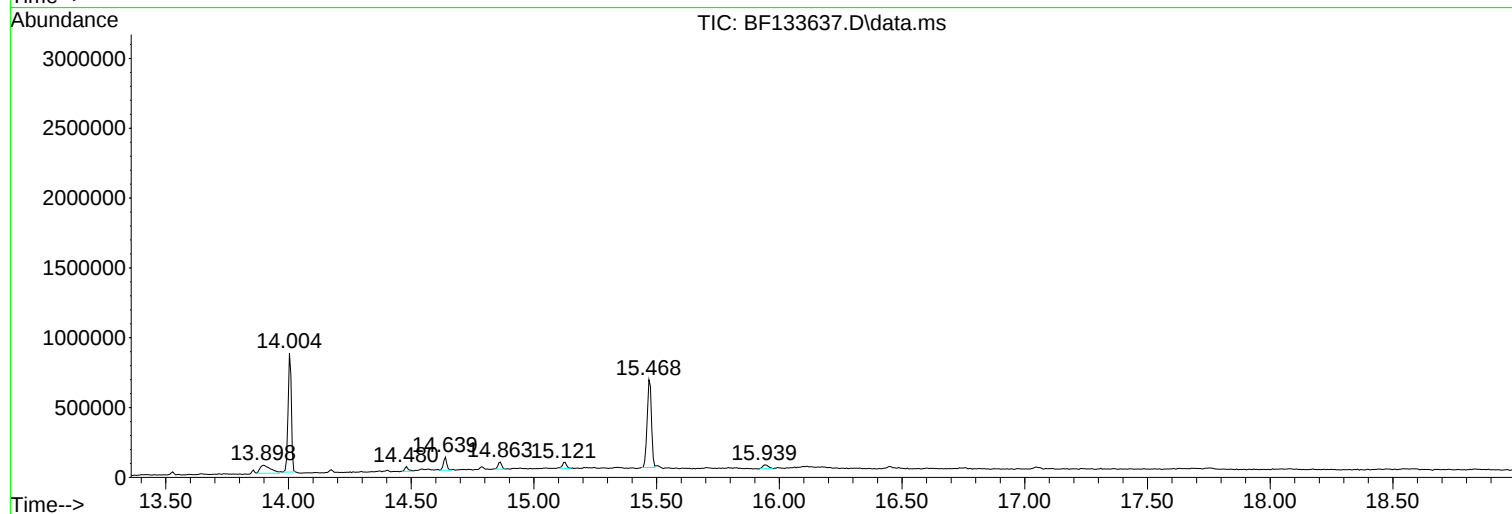
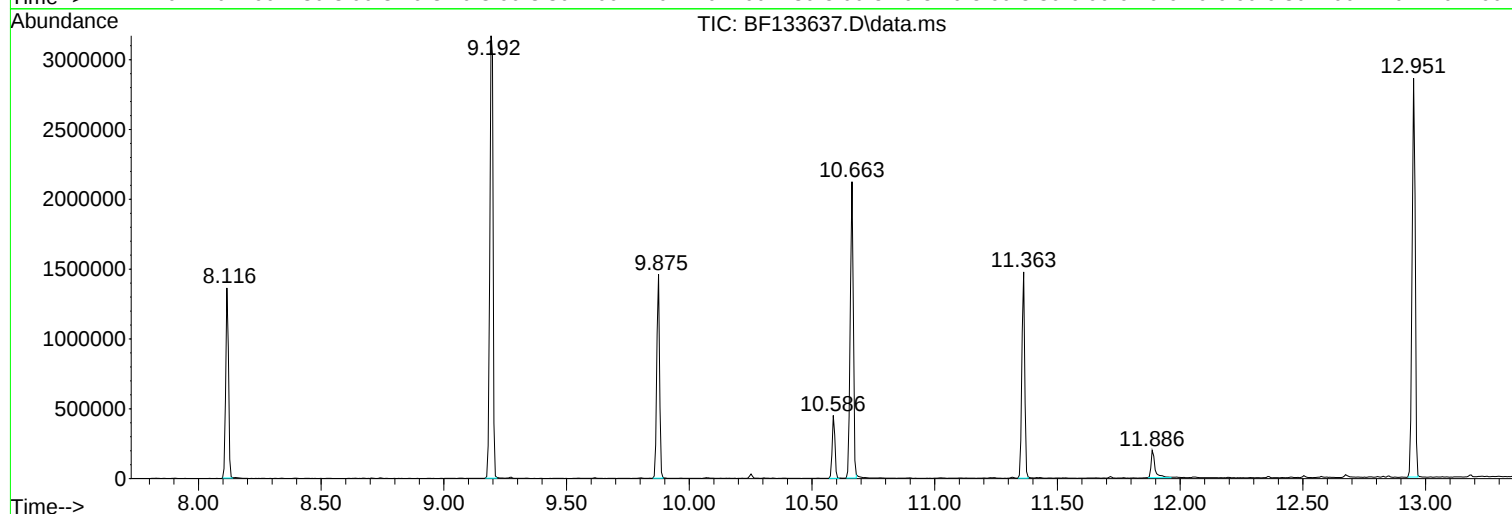
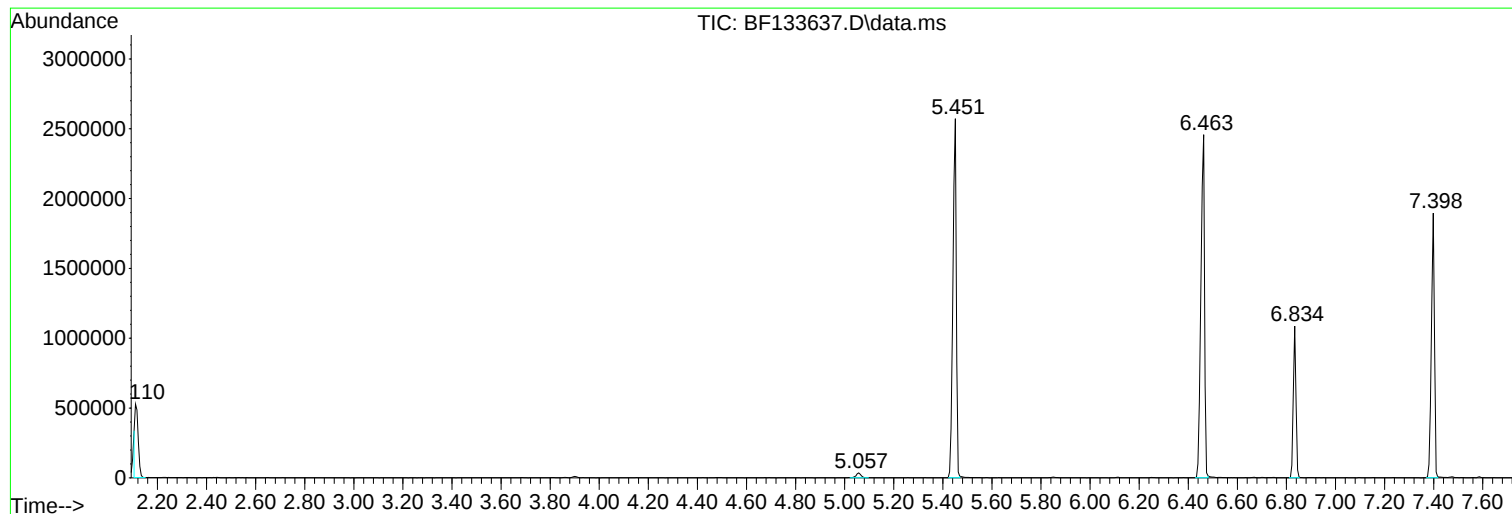
Sum of corrected areas: 21380404

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060823\
Data File : BF133637.D
Acq On : 08 Jun 2023 12:27
Operator : CG\JU
Sample : 03016-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB29

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.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\BF060823\
Data File : BF133637.D
Acq On : 08 Jun 2023 12:27
Operator : CG\JU
Sample : 03016-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB29

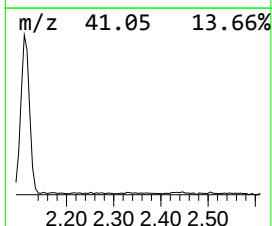
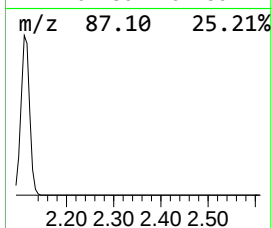
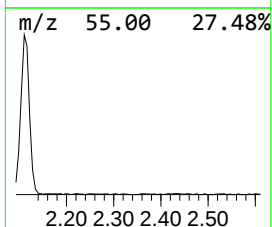
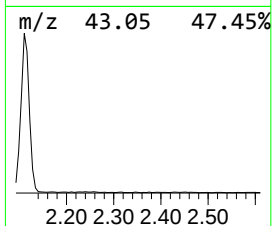
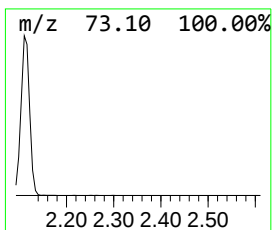
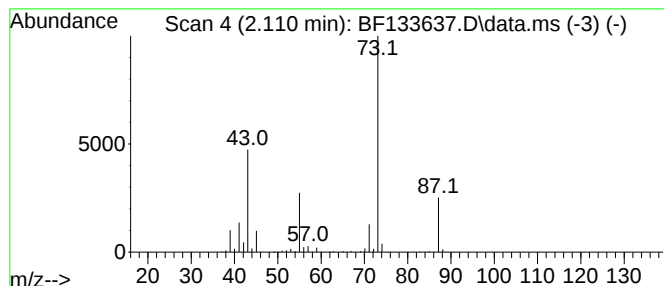
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.110	11.62 ng	480972	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060823\
Data File : BF133637.D
Acq On : 08 Jun 2023 12:27
Operator : CG\JU
Sample : 03016-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB29

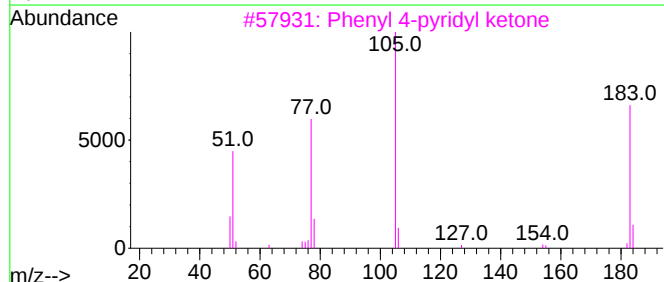
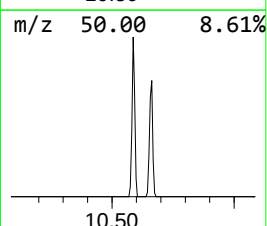
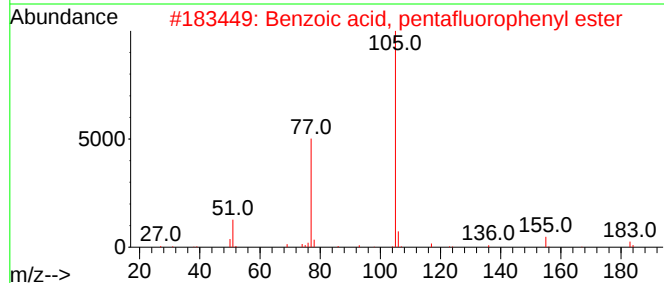
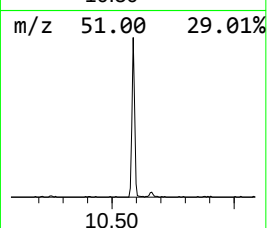
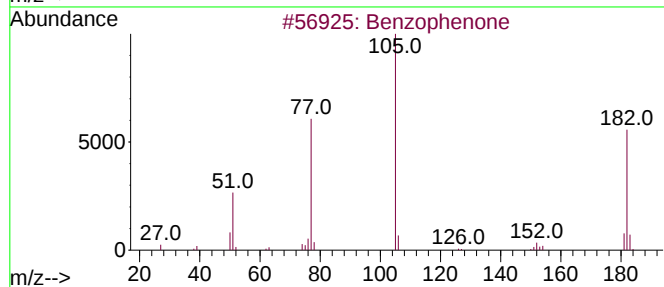
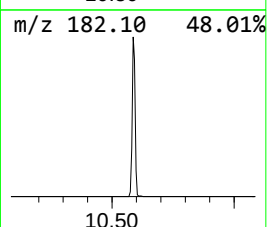
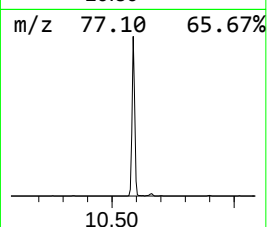
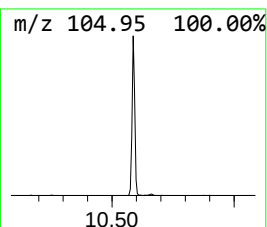
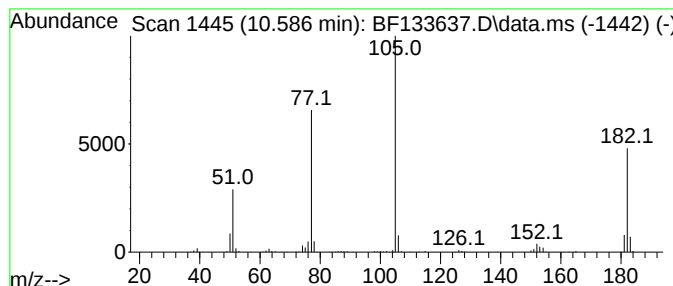
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.586	6.04 ng	351899	Acenaphthene-d10	9.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	50
3			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
4			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
5			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060823\
Data File : BF133637.D
Acq On : 08 Jun 2023 12:27
Operator : CG\JU
Sample : 03016-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB29

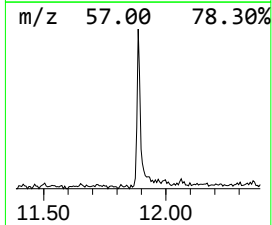
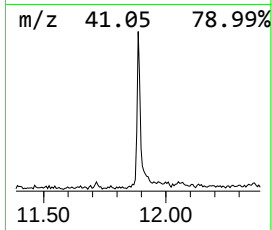
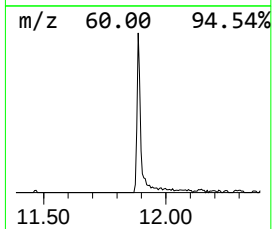
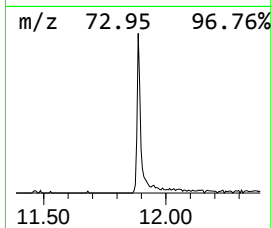
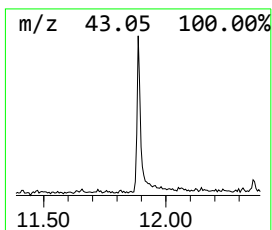
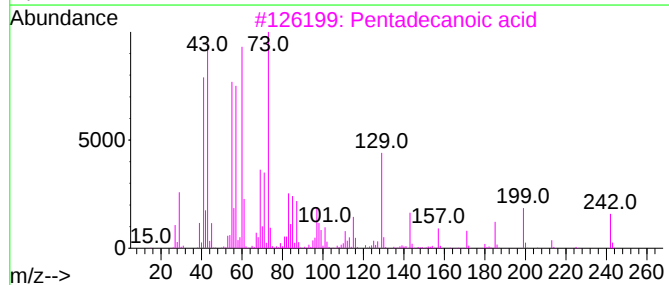
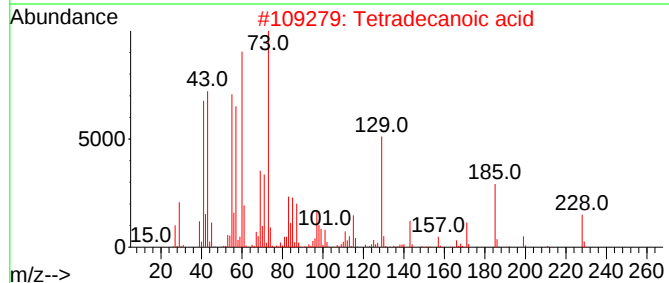
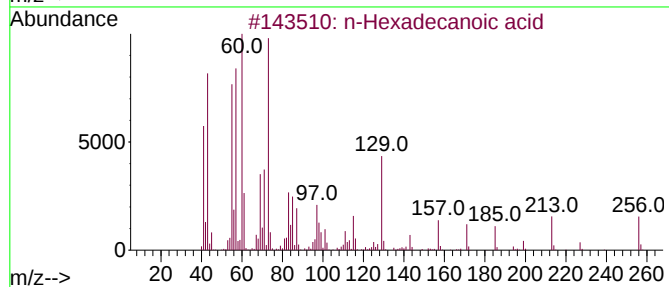
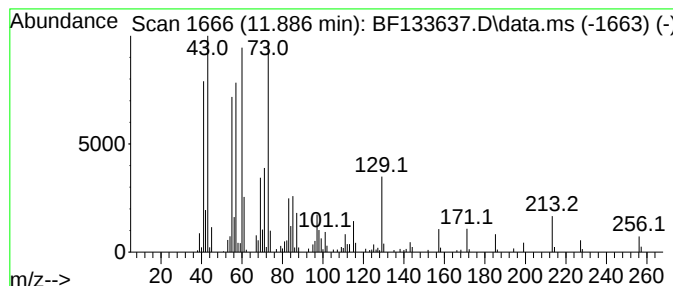
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
11.886	3.59 ng	215266	Phenanthrene-d10	11.363

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Undecanoic acid	186	C11H22O2	000112-37-8	80
5		Tridecanoic acid	214	C13H26O2	000638-53-9	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060823\
Data File : BF133637.D
Acq On : 08 Jun 2023 12:27
Operator : CG\JU
Sample : 03016-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB29

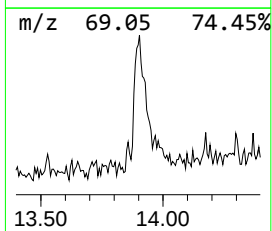
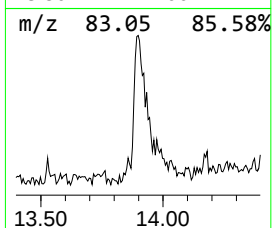
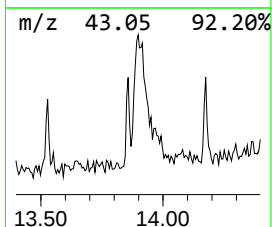
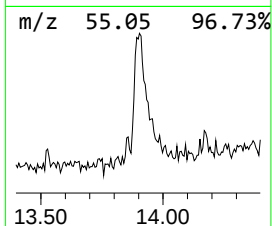
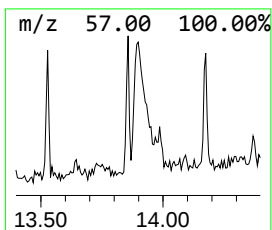
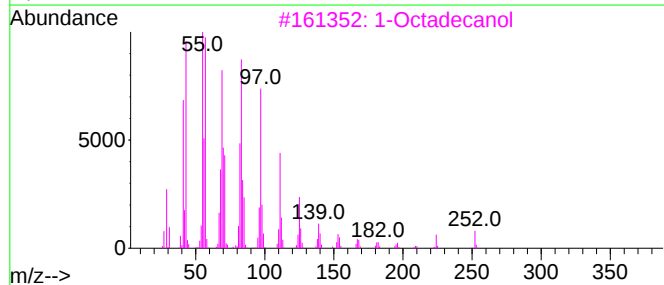
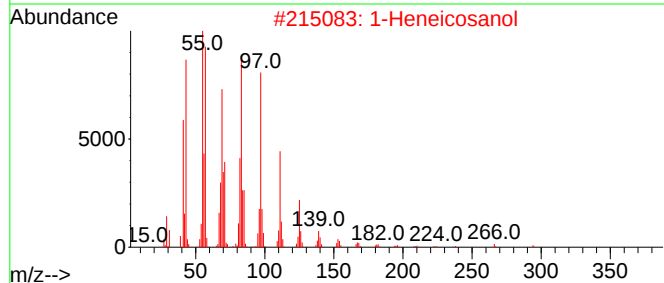
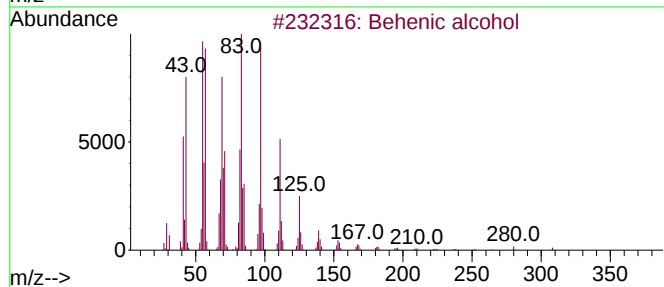
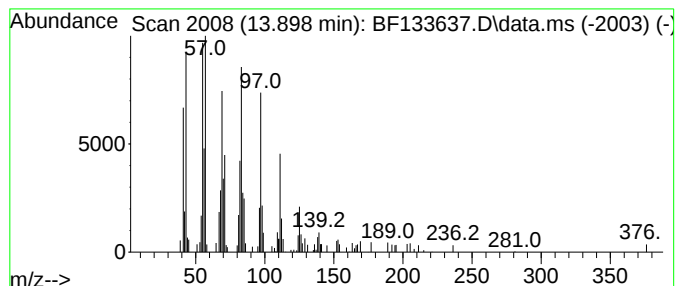
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Behenic alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	4.50 ng	177671	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	95
2			1-Heneicosanol	312	C21H44O	015594-90-8	95
3			1-Octadecanol	270	C18H38O	000112-92-5	95
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	95
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060823\
Data File : BF133637.D
Acq On : 08 Jun 2023 12:27
Operator : CG\JU
Sample : 03016-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

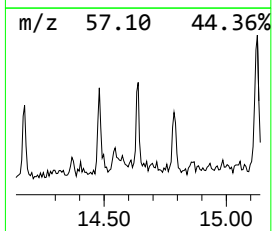
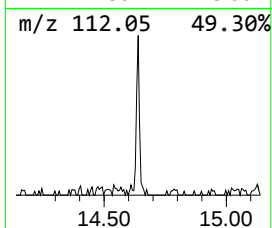
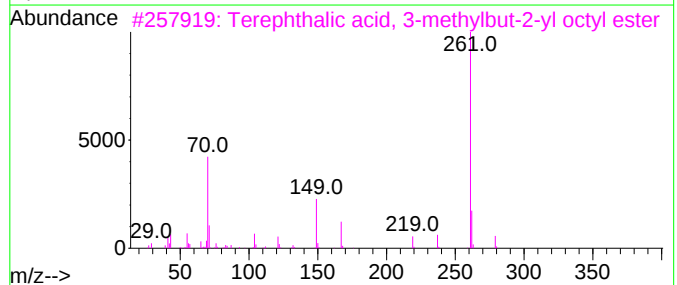
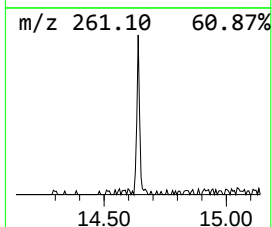
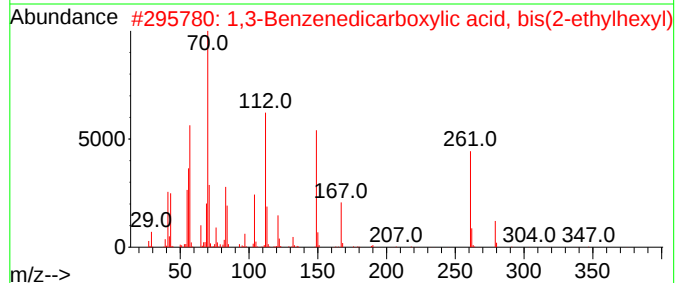
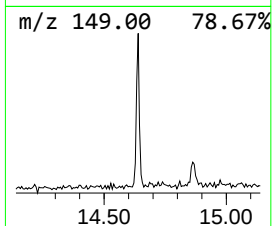
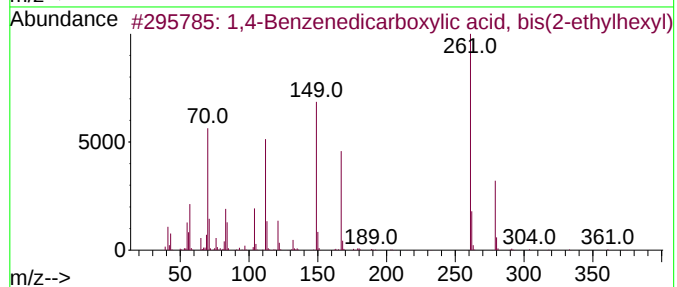
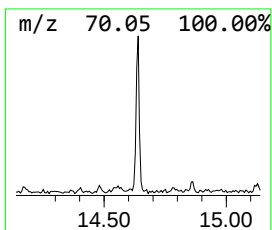
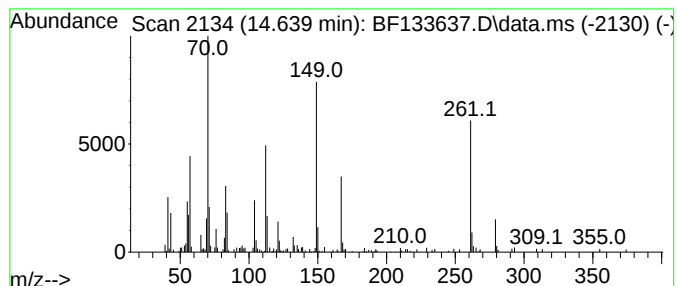
Instrument :
BNA_F
ClientSampleId :
SB29

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1,4-Benzenedicarboxylic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.639	2.23 ng	87922	Chrysene-d12	14.004	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	87
2	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	68
3	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	52
4	Terephthalic acid, but-2-enyl oc...	332	C20H28O4	1000356-31-6	38
5	Phthalic acid, 4-chloro-3-methyl...	402	C23H27ClO4	1000309-84-9	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060823\
Data File : BF133637.D
Acq On : 08 Jun 2023 12:27
Operator : CG\JU
Sample : 03016-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB29

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.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
Butane, 2-metho...	2.110	11.6	ng	480972	1	6.834	827863	20.0
Benzophenone	10.586	6.0	ng	351899	3	9.875	1165460	20.0
n-Hexadecanoic ...	11.886	3.6	ng	215266	4	11.363	1200250	20.0
Behenic alcohol	13.898	4.5	ng	177671	5	14.004	789239	20.0
1,4-Benzenedica...	14.639	2.2	ng	87922	5	14.004	789239	20.0