

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
 Data File : BF127095.D
 Acq On : 28 Feb 2022 12:59
 Operator : CG\JU
 Sample : N1664-22
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-8

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-BF021622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127095.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.134	480	484	490	rVB	37503	45282	1.36%	0.208%
2	5.528	546	551	554	rBV	2730349	2698775	81.28%	12.388%
3	6.528	716	721	730	rVB	2569798	2854254	85.96%	13.101%
4	6.898	781	784	788	rBV	750335	619863	18.67%	2.845%
5	7.463	875	880	883	rBV	1919562	1906248	57.41%	8.750%
6	8.081	981	985	998	rBV	206068	224746	6.77%	1.032%
7	8.181	999	1002	1006	rBV	920122	829382	24.98%	3.807%
8	9.263	1180	1186	1189	rBV	3670126	3320398	100.00%	15.241%
9	9.369	1200	1204	1207	rBV	116409	107416	3.24%	0.493%
10	9.745	1264	1268	1275	rBV4	19864	39349	1.19%	0.181%
11	9.939	1298	1301	1305	rVB	1061391	919953	27.71%	4.223%
12	10.733	1432	1436	1439	rBV	2632209	2210197	66.56%	10.145%
13	11.433	1551	1555	1558	rBV	1156406	944466	28.44%	4.335%
14	11.816	1616	1620	1623	rBV	150264	125005	3.76%	0.574%
15	11.945	1639	1642	1647	rBV	117021	98413	2.96%	0.452%
16	12.198	1682	1685	1688	rBV	49772	37314	1.12%	0.171%
17	12.522	1737	1740	1743	rVB	199922	138910	4.18%	0.638%
18	12.610	1752	1755	1758	rVB	47399	40098	1.21%	0.184%
19	13.021	1820	1825	1828	rBV	3751891	3229537	97.26%	14.824%
20	13.916	1965	1977	1992	rBV5	102800	307276	9.25%	1.410%
21	14.074	2001	2004	2008	rBV	603374	577528	17.39%	2.651%
22	15.574	2254	2259	2264	rBV	424949	511374	15.40%	2.347%

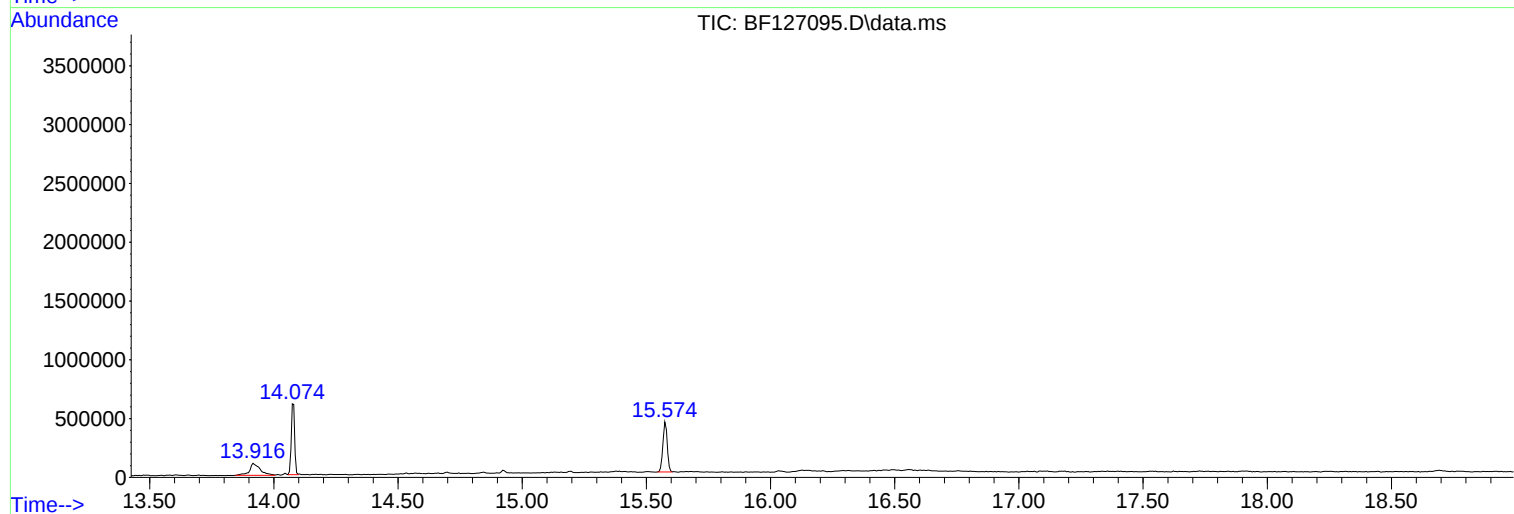
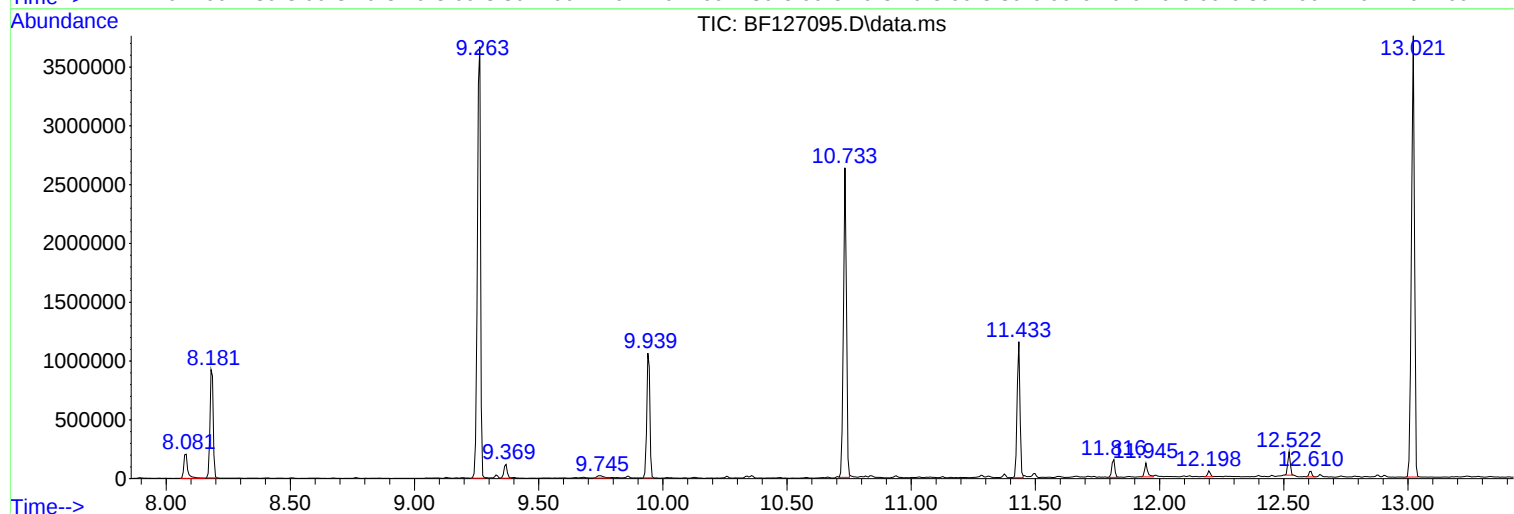
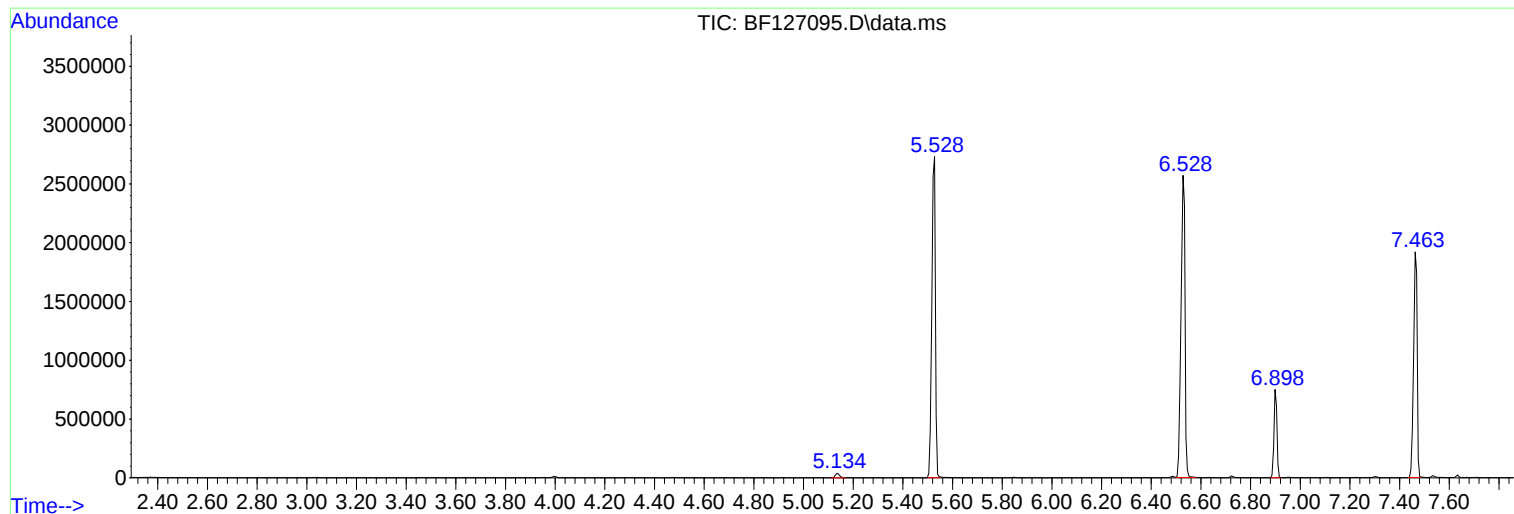
Sum of corrected areas: 21785784

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127095.D
Acq On : 28 Feb 2022 12:59
Operator : CG\JU
Sample : N1664-22
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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\BF022822\
Data File : BF127095.D
Acq On : 28 Feb 2022 12:59
Operator : CG\JU
Sample : N1664-22
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-8

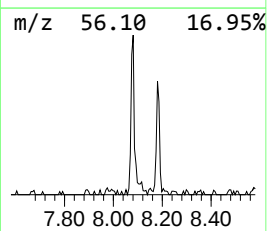
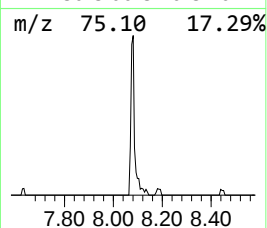
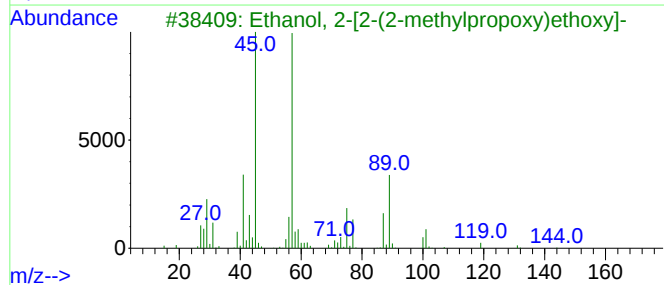
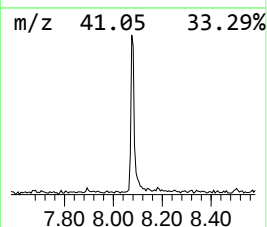
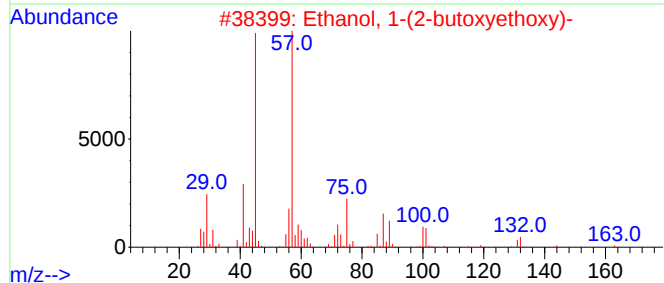
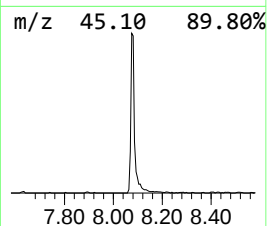
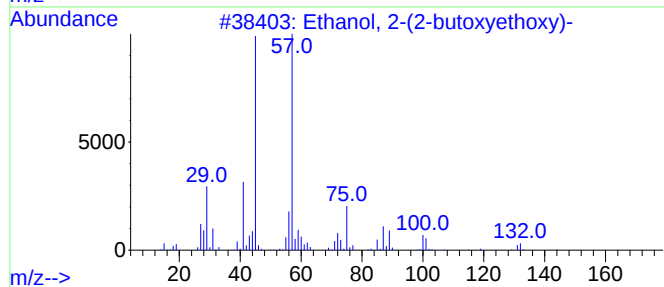
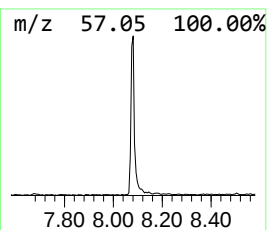
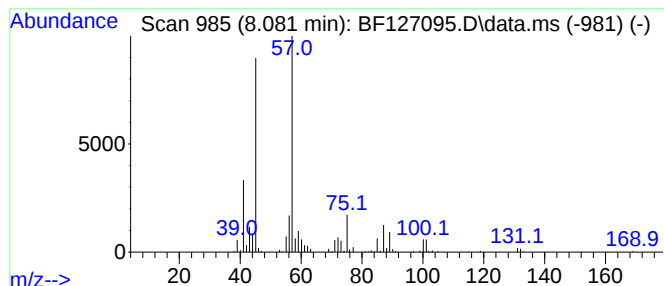
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.081	5.42 ng	224746	Naphthalene-d8	8.181

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	78
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	53
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127095.D
Acq On : 28 Feb 2022 12:59
Operator : CG\JU
Sample : N1664-22
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-8

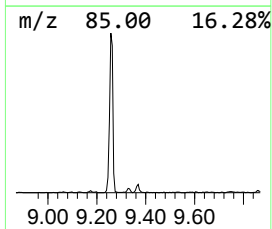
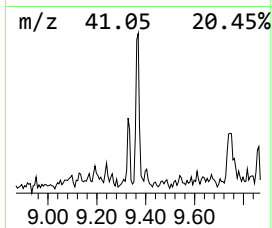
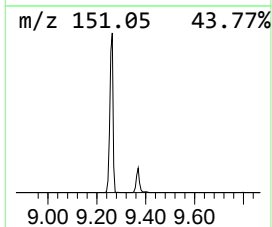
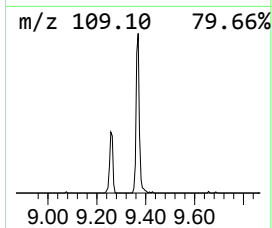
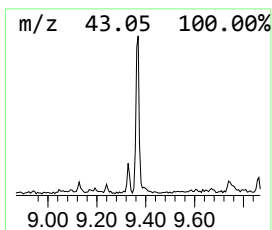
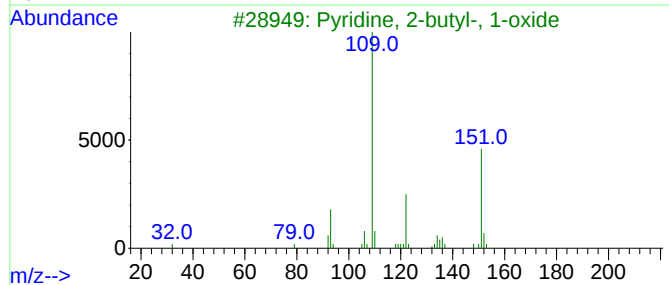
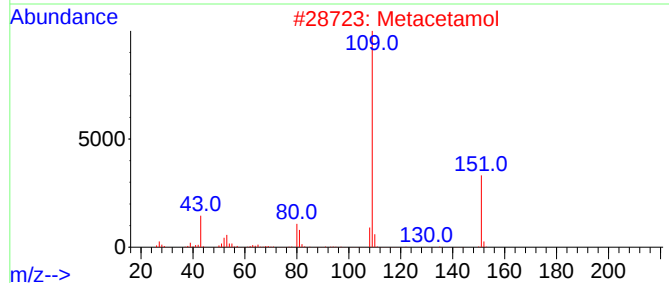
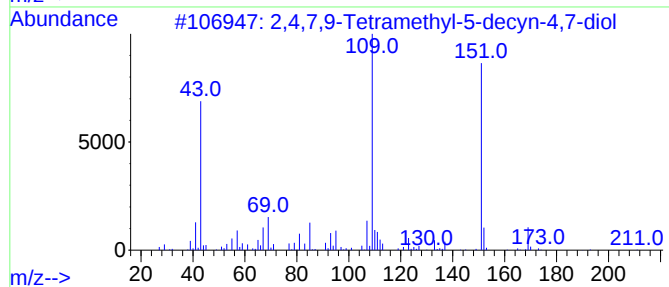
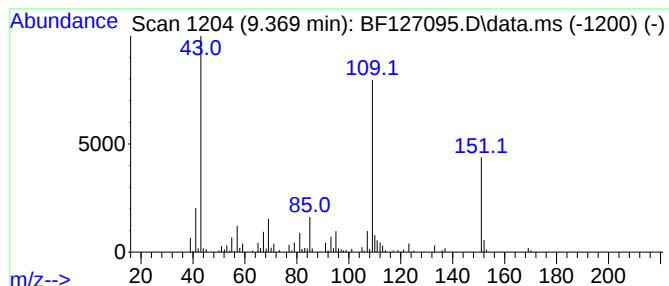
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.369	2.34 ng	107416	Acenaphthene-d10	9.939

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	90	
2	Metacetamol	151	C8H9NO2	000621-42-1	59	
3	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59	
4	Acetaminophen	151	C8H9NO2	000103-90-2	59	
5	Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O	000116-02-9	47	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127095.D
Acq On : 28 Feb 2022 12:59
Operator : CG\JU
Sample : N1664-22
Misc :
ALS Vial : 7 Sample Multiplier: 1

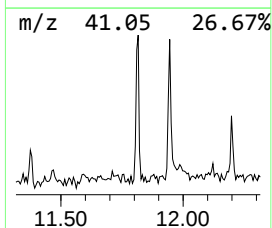
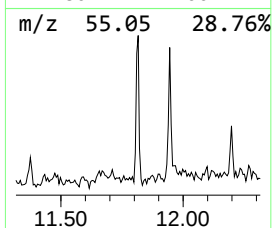
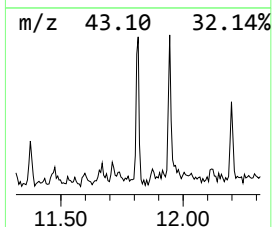
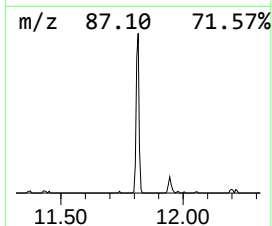
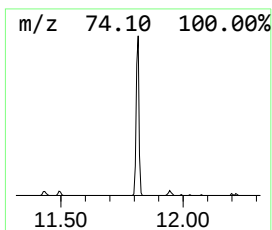
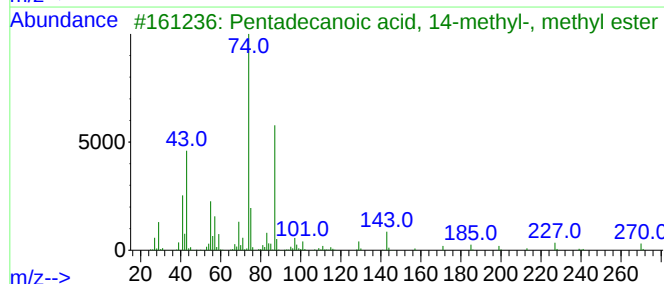
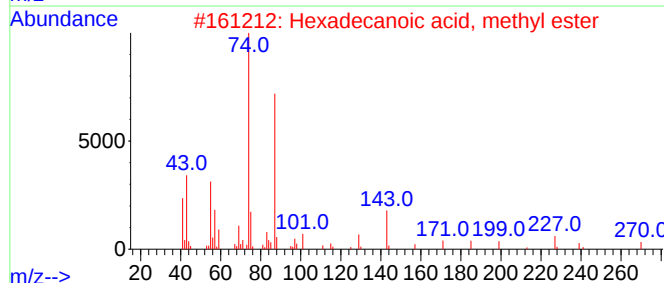
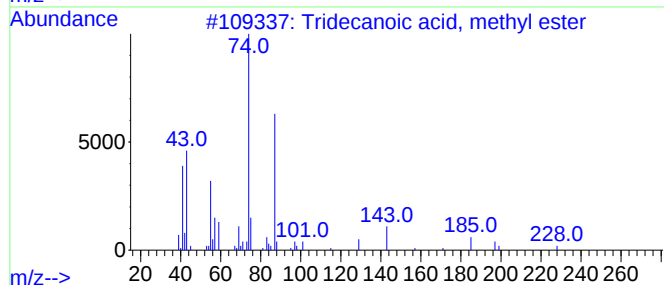
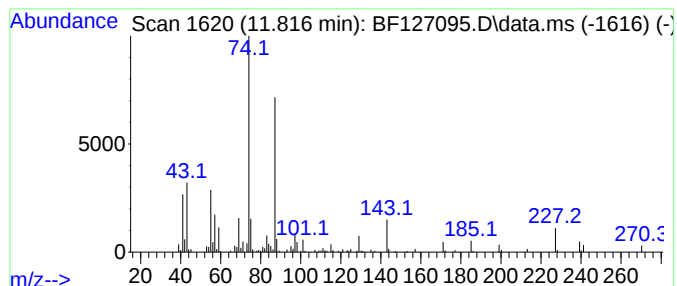
Instrument :
BNA_F
ClientSampleId :
TP-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Tridecanoic acid, methyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.816	2.65 ng	125005	Phenanthrene-d10		11.433	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Tridecanoic acid, methyl ester		228	C14H28O2	001731-88-0	94
2	Hexadecanoic acid, methyl ester		270	C17H34O2	000112-39-0	93
3	Pentadecanoic acid, 14-methyl-, ...		270	C17H34O2	005129-60-2	93
4	Pentadecanoic acid, methyl ester		256	C16H32O2	007132-64-1	86
5	Methyl 11-methyl-dodecanoate		228	C14H28O2	1000336-45-1	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127095.D
Acq On : 28 Feb 2022 12:59
Operator : CG\JU
Sample : N1664-22
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-8

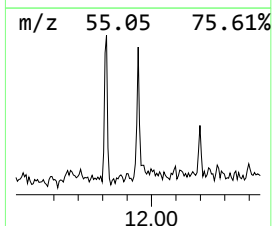
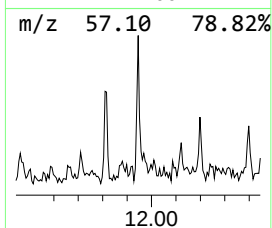
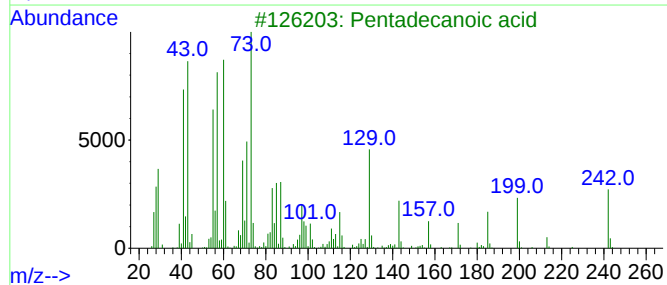
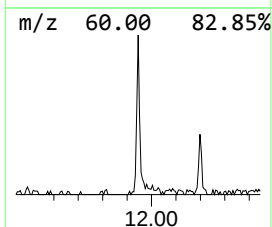
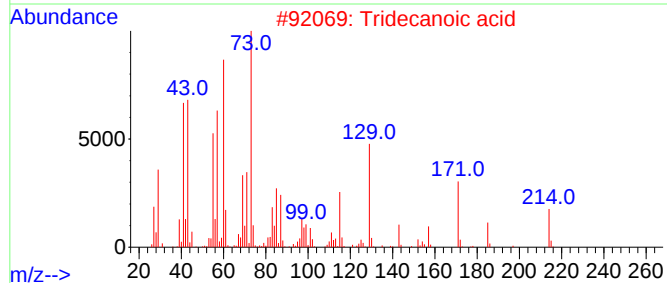
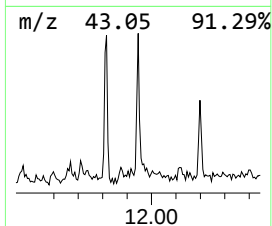
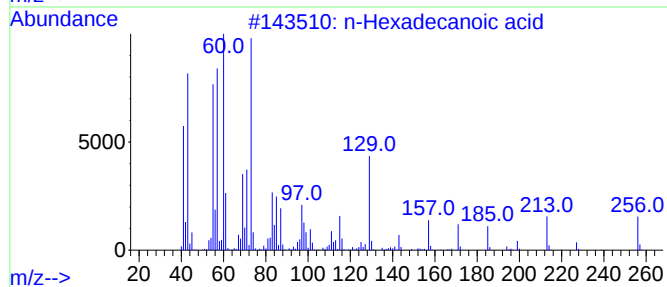
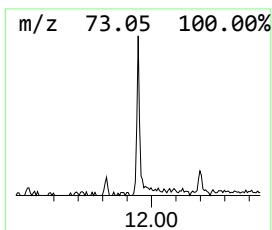
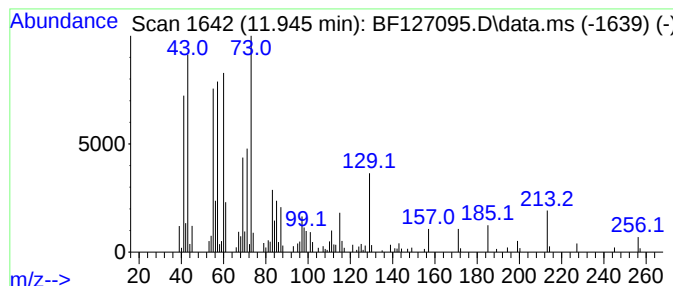
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	2.08 ng	98413	Phenanthrene-d10	11.433

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	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127095.D
Acq On : 28 Feb 2022 12:59
Operator : CG\JU
Sample : N1664-22
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-8

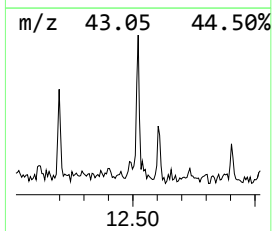
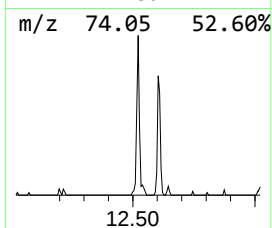
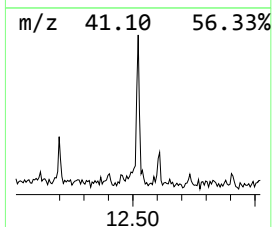
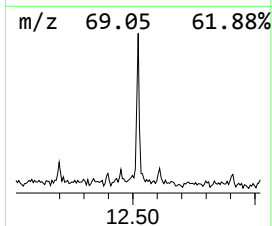
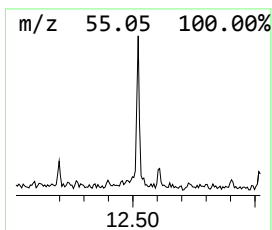
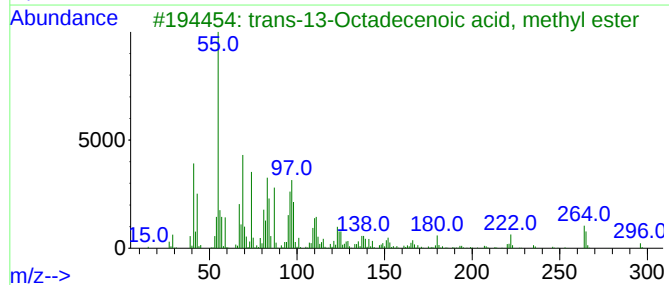
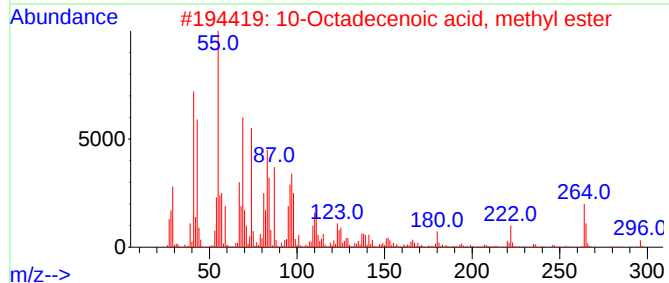
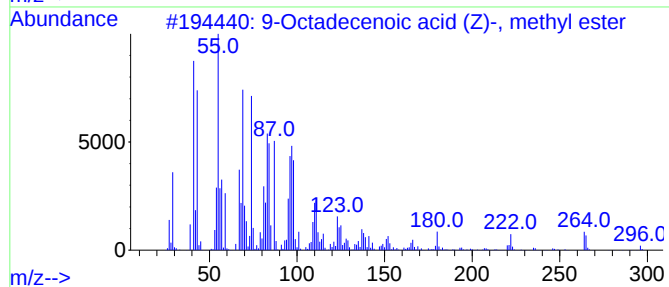
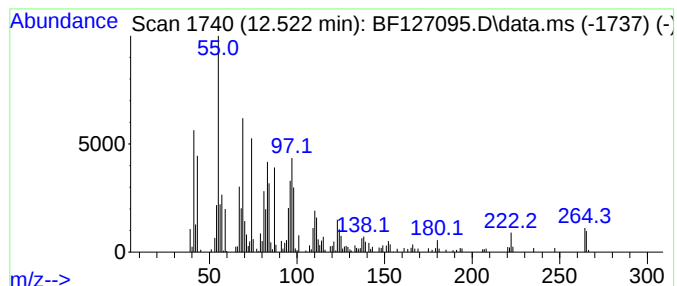
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.522	2.94 ng	138910	Phenanthrene-d10	11.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94
3			trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	94
4			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
5			(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127095.D
Acq On : 28 Feb 2022 12:59
Operator : CG\JU
Sample : N1664-22
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-8

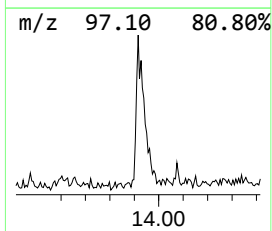
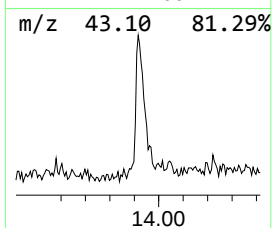
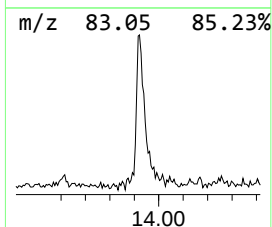
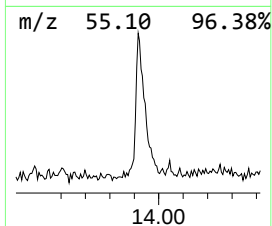
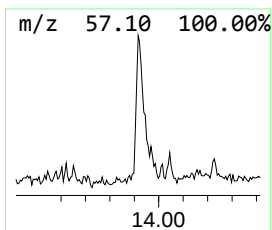
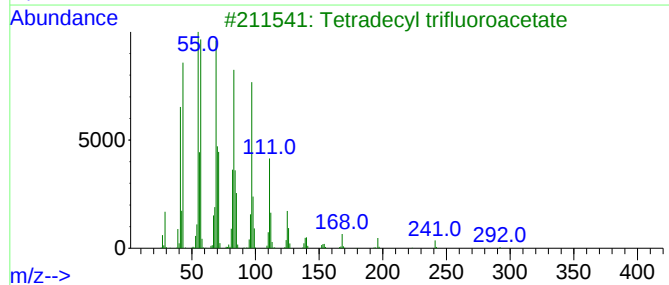
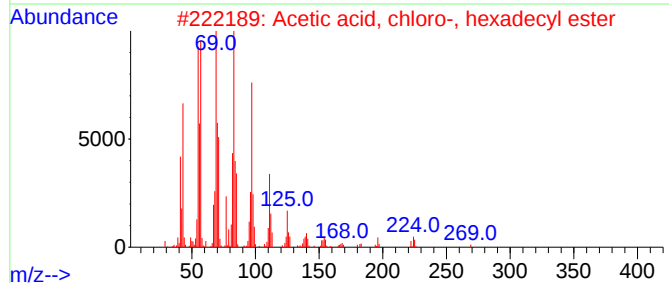
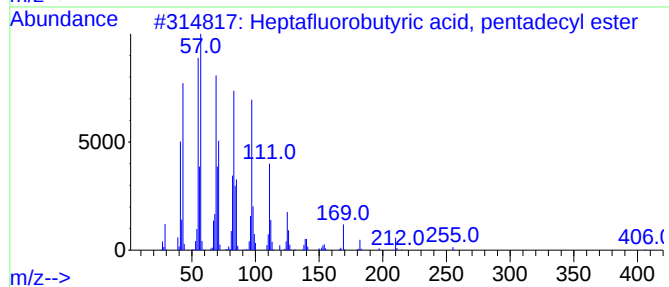
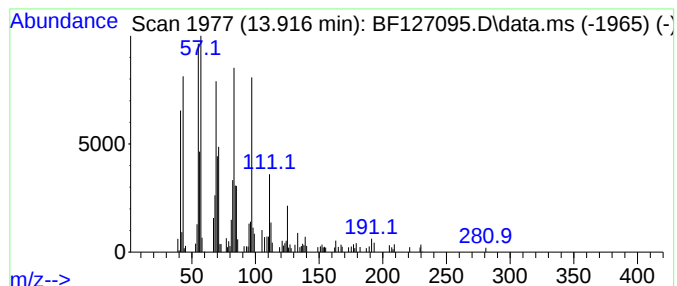
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptafluorobutyric acid, pe... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.916	10.64 ng	307276	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2			Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	94
3			Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	91
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127095.D
Acq On : 28 Feb 2022 12:59
Operator : CG\JU
Sample : N1664-22
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol, 2-(2-b...	8.081	5.4	ng	224746	2	8.181	829382	20.0
2,4,7,9-Tetrame...	9.369	2.3	ng	107416	3	9.939	919953	20.0
Tridecanoic aci...	11.816	2.6	ng	125005	4	11.433	944466	20.0
n-Hexadecanoic ...	11.945	2.1	ng	98413	4	11.433	944466	20.0
9-Octadecenoic ...	12.522	2.9	ng	138910	4	11.433	944466	20.0
Heptafluorobuty...	13.916	10.6	ng	307276	5	14.080	577528	20.0