

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101824\
 Data File : BF139861.D
 Acq On : 18 Oct 2024 18:41
 Operator : RC/JU
 Sample : P4425-07
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-4

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-BF101824.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139861.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	5	12	20	rVB	1692623	2670715	100.00%	14.539%
2	5.099	504	511	517	rBV	152767	220486	8.26%	1.200%
3	5.498	573	579	584	rBV	1637859	2094153	78.41%	11.400%
4	6.498	743	749	762	rVB	1605672	2097024	78.52%	11.416%
5	6.887	810	815	821	rVB	609331	776067	29.06%	4.225%
6	7.445	904	910	915	rBV	968204	1170355	43.82%	6.371%
7	7.698	949	953	958	rVB	69165	80484	3.01%	0.438%
8	8.169	1028	1033	1038	rBV	711126	862681	32.30%	4.696%
9	9.245	1210	1216	1221	rBV	1425430	1744448	65.32%	9.497%
10	9.922	1326	1331	1337	rVB	611292	761397	28.51%	4.145%
11	10.633	1447	1452	1457	rBV	280671	342875	12.84%	1.867%
12	10.710	1459	1465	1473	rBV	733128	922155	34.53%	5.020%
13	11.410	1579	1584	1589	rBV	672552	811497	30.39%	4.418%
14	11.933	1668	1673	1685	rBV2	67443	112314	4.21%	0.611%
15	12.716	1802	1806	1815	rBV4	19474	35384	1.32%	0.193%
16	12.998	1848	1854	1859	rBV	1602730	2040713	76.41%	11.110%
17	13.892	2001	2006	2018	rBV	112186	208141	7.79%	1.133%
18	14.051	2027	2033	2040	rBV	623189	838843	31.41%	4.567%
19	14.910	2176	2179	2189	rVB	24573	38942	1.46%	0.212%
20	15.527	2278	2284	2289	rBV	357796	540355	20.23%	2.942%

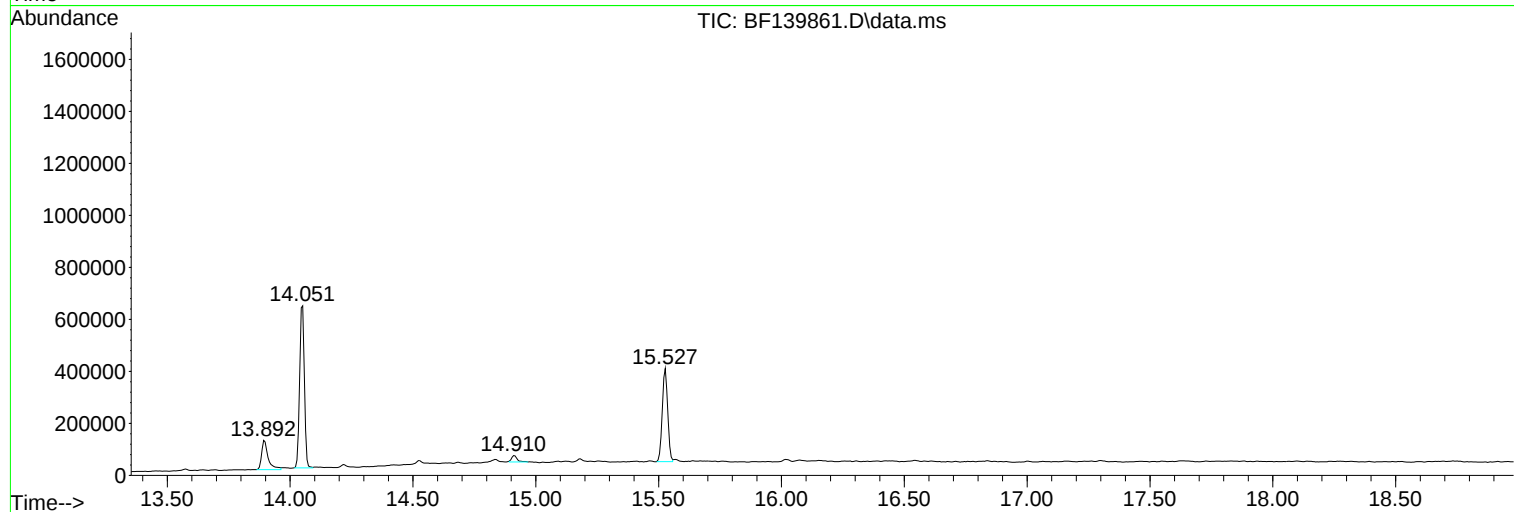
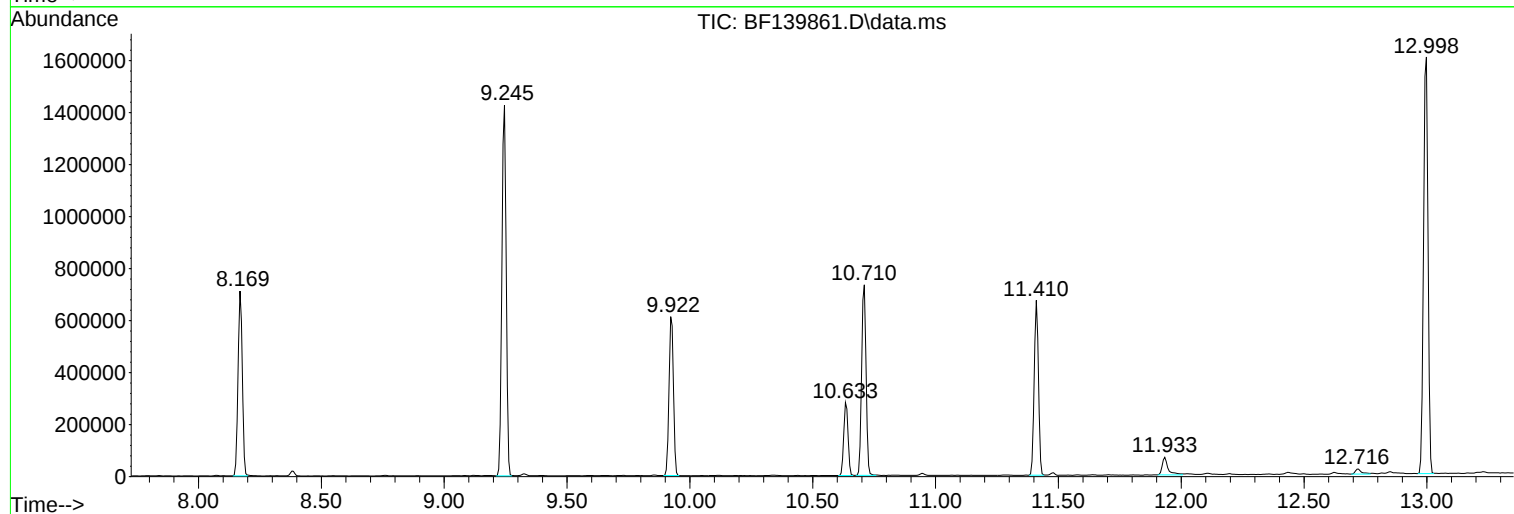
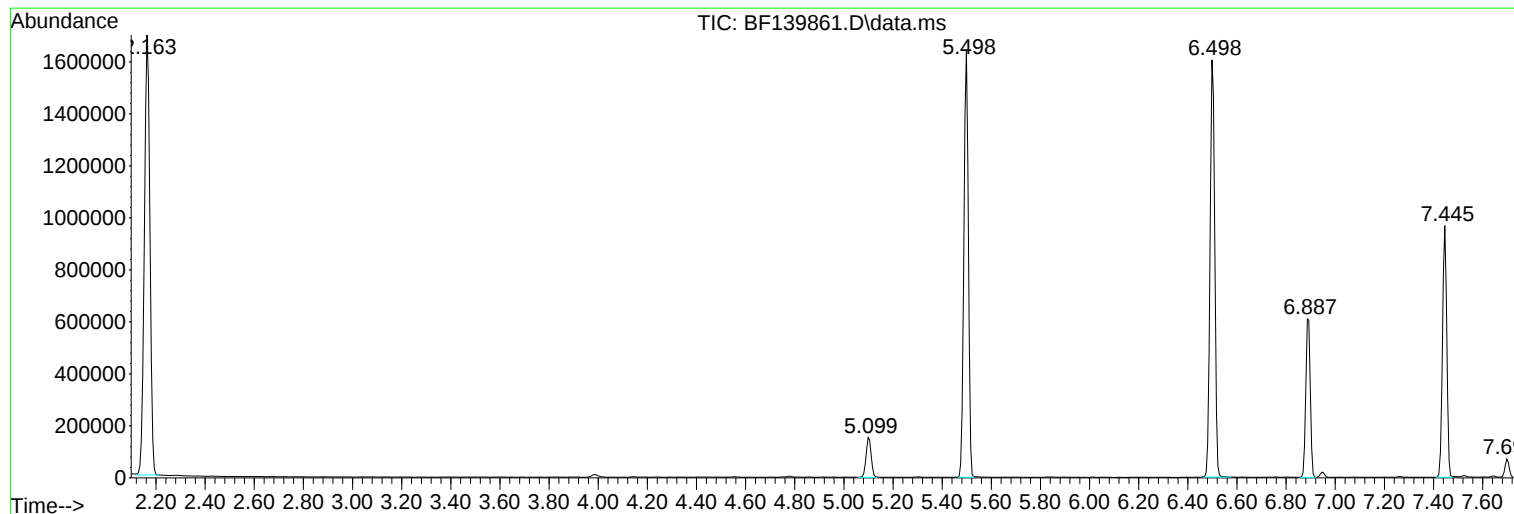
Sum of corrected areas: 18369029

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101824\
Data File : BF139861.D
Acq On : 18 Oct 2024 18:41
Operator : RC/JU
Sample : P4425-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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\BF101824\
Data File : BF139861.D
Acq On : 18 Oct 2024 18:41
Operator : RC/JU
Sample : P4425-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

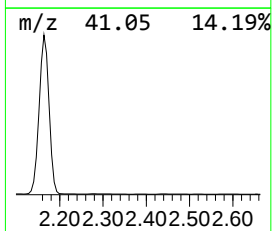
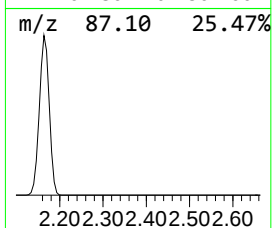
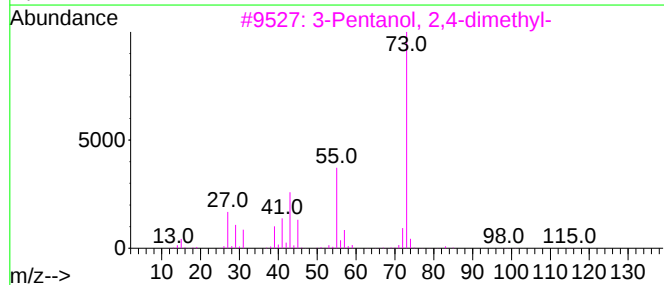
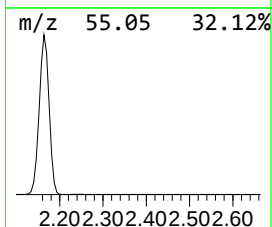
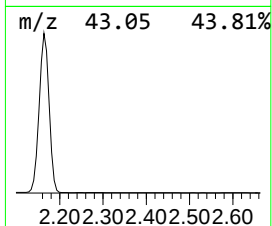
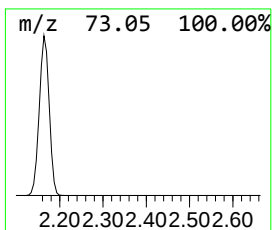
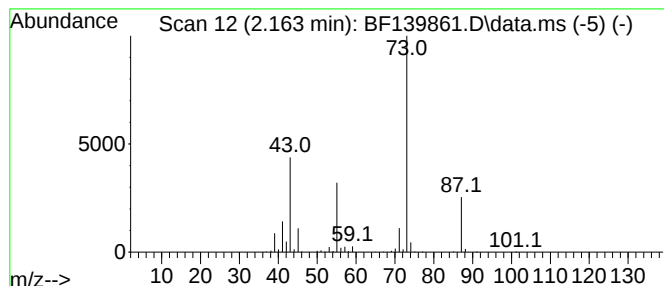
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.163	68.83 ng	2670720	1,4-Dichlorobenzene-d4	6.893

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	40
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101824\
Data File : BF139861.D
Acq On : 18 Oct 2024 18:41
Operator : RC/JU
Sample : P4425-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

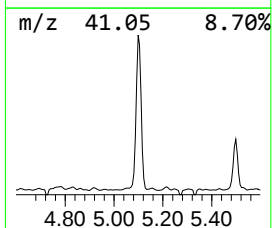
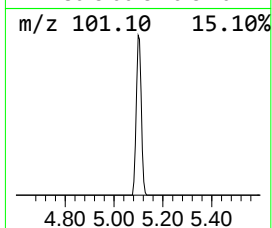
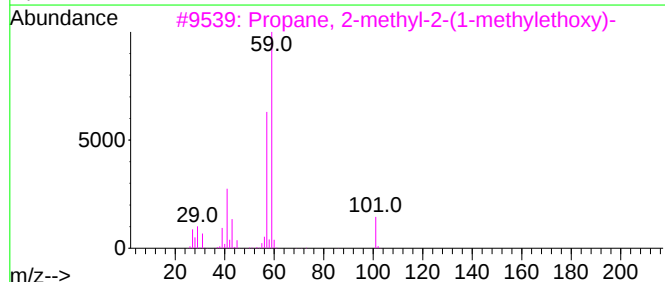
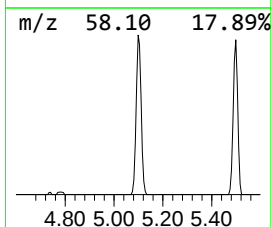
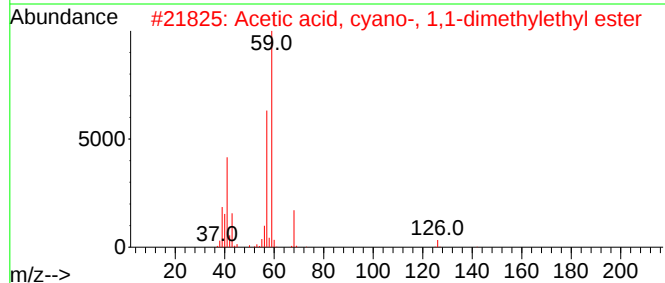
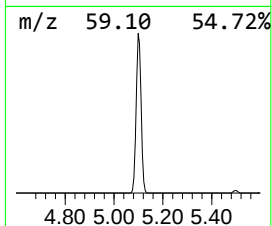
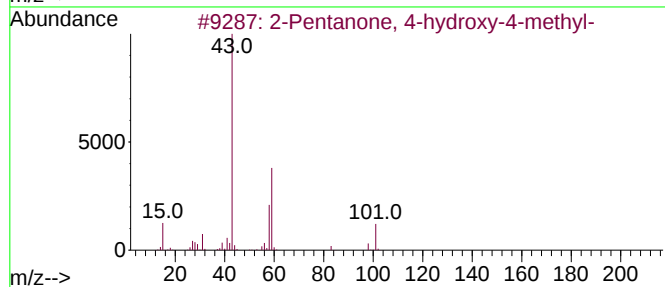
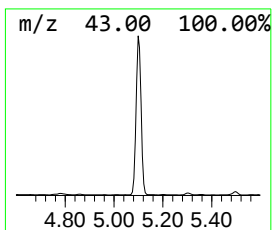
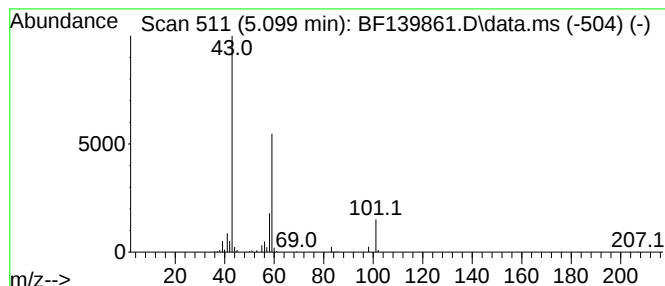
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.099	5.68 ng	220486	1,4-Dichlorobenzene-d4	6.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4			3-Octanol	130	C8H18O	000589-98-0	33
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101824\
Data File : BF139861.D
Acq On : 18 Oct 2024 18:41
Operator : RC/JU
Sample : P4425-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

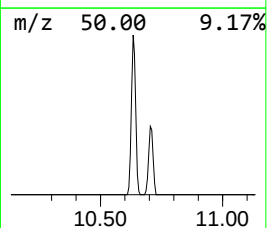
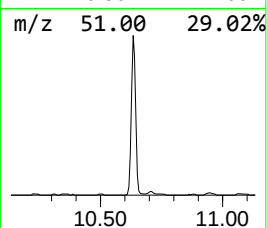
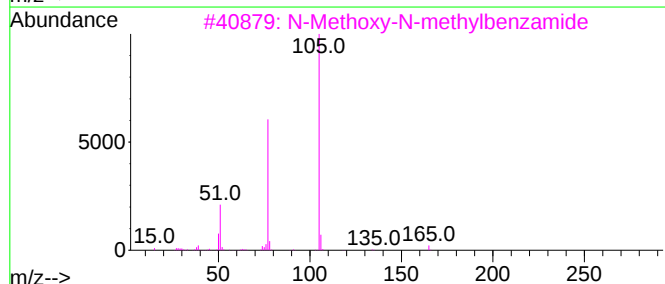
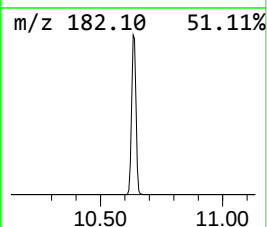
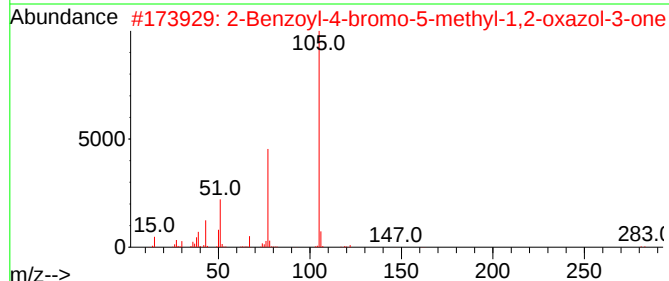
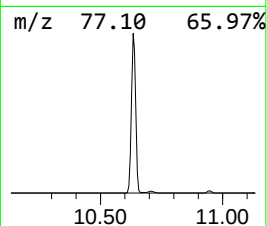
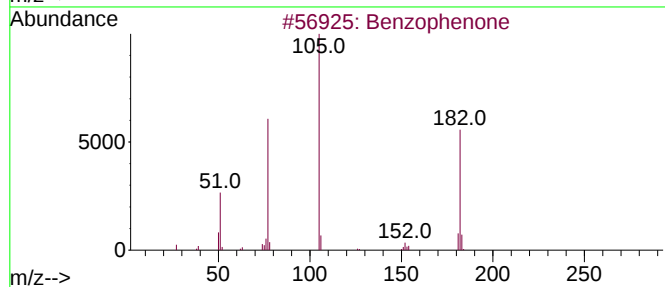
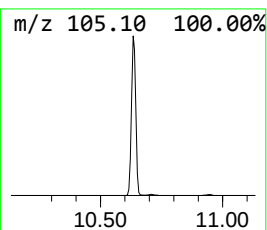
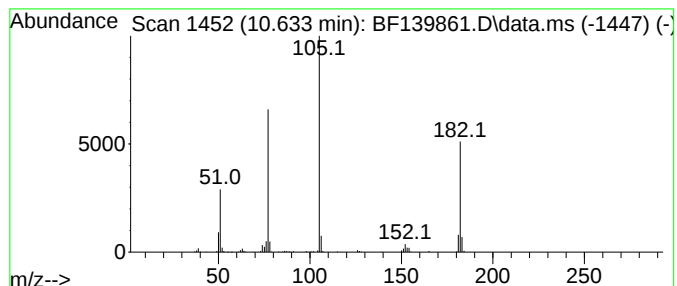
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.634	9.01 ng	342875	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	50
3			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	50
4			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50
5			Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101824\
Data File : BF139861.D
Acq On : 18 Oct 2024 18:41
Operator : RC/JU
Sample : P4425-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

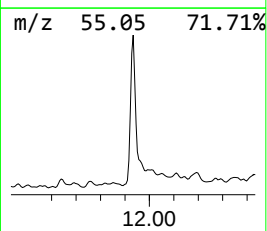
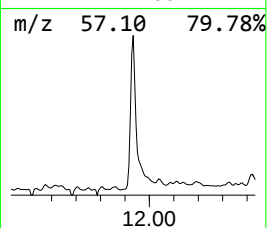
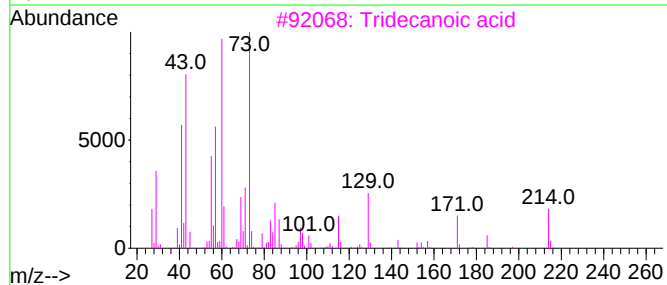
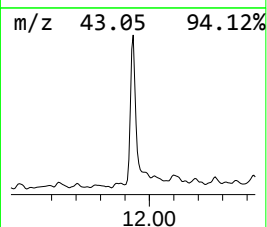
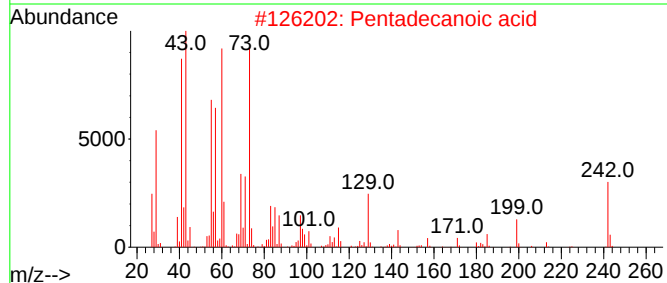
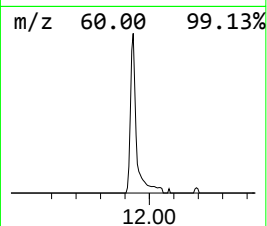
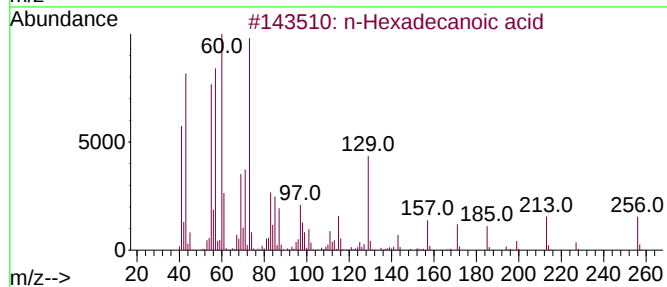
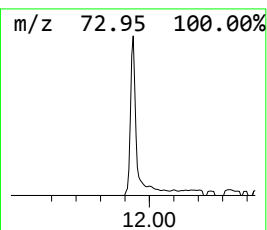
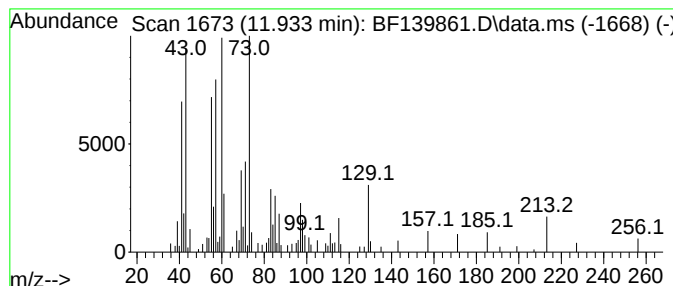
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
11.933	2.77 ng	112314	Phenanthrene-d10	11.410

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3		Tridecanoic acid	214	C13H26O2	000638-53-9	83
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101824\
Data File : BF139861.D
Acq On : 18 Oct 2024 18:41
Operator : RC/JU
Sample : P4425-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

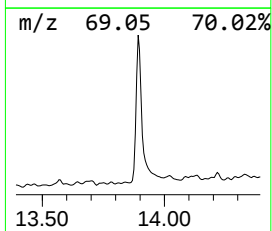
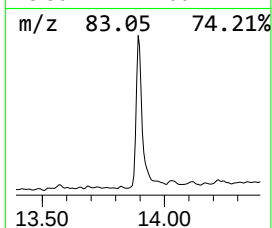
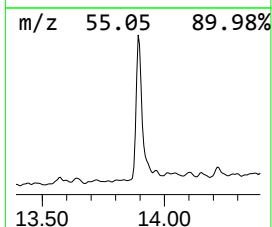
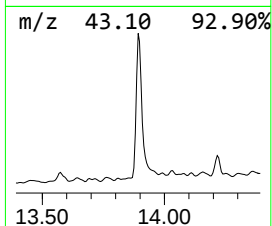
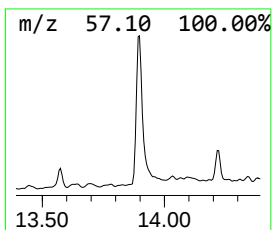
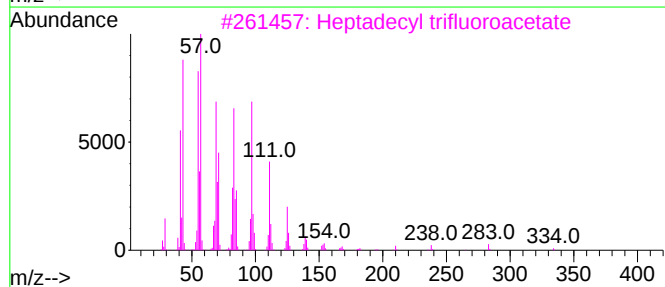
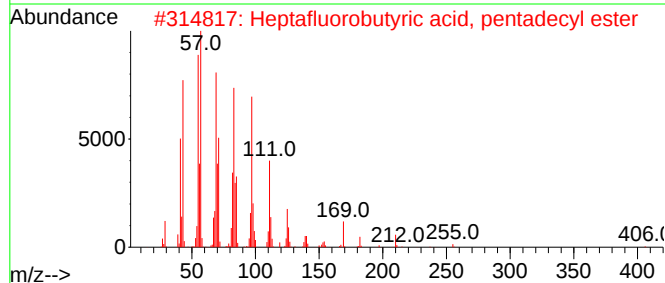
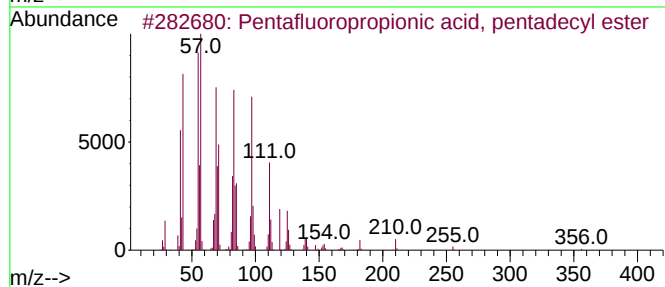
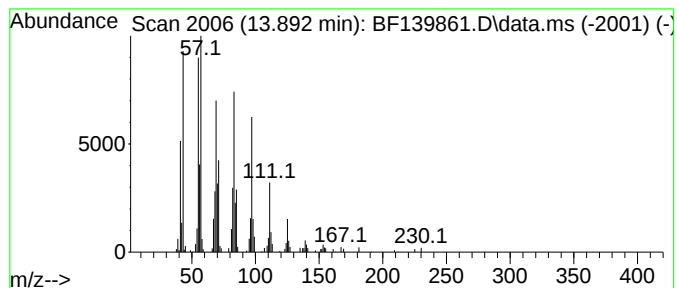
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	4.96 ng	208141	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
2			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
4			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
5			1-Heneicosanol	312	C21H44O	015594-90-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101824\
Data File : BF139861.D
Acq On : 18 Oct 2024 18:41
Operator : RC/JU
Sample : P4425-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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...	2.163	68.8	ng	2670720	1	6.893	776067	20.0
2-Pentanone, 4-...	5.099	5.7	ng	220486	1	6.893	776067	20.0
Benzophenone	10.634	9.0	ng	342875	3	9.922	761397	20.0
n-Hexadecanoic ...	11.933	2.8	ng	112314	4	11.410	811497	20.0
Pentafluoroprop...	13.892	5.0	ng	208141	5	14.051	838843	20.0