

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102924\
 Data File : BF140110.D
 Acq On : 29 Oct 2024 14:16
 Operator : RC/JU
 Sample : P4578-05
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WB-305-BOT

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: BF140110.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	10	18	26	rVB	1269523	2020418	65.93%	8.537%
2	5.504	574	580	586	rBV	1833415	2533761	82.68%	10.706%
3	6.510	744	751	774	rVB	1793140	2685380	87.63%	11.346%
4	6.887	810	815	820	rBV	610280	741977	24.21%	3.135%
5	7.446	902	910	915	rBV	1292894	1691908	55.21%	7.149%
6	7.698	947	953	960	rVB2	79814	104509	3.41%	0.442%
7	8.169	1024	1033	1041	rBV	778342	1017598	33.21%	4.300%
8	8.381	1065	1069	1077	rBV	29395	39402	1.29%	0.166%
9	9.239	1209	1215	1225	rBV	2267904	3064468	100.00%	12.948%
10	9.322	1225	1229	1238	rVB	27662	46175	1.51%	0.195%
11	9.922	1326	1331	1336	rBV	893536	1120838	36.58%	4.736%
12	10.634	1447	1452	1459	rBV	571886	749452	24.46%	3.167%
13	10.710	1459	1465	1480	rVV	1474510	1933513	63.09%	8.170%
14	10.945	1501	1505	1510	rVB	37265	46017	1.50%	0.194%
15	11.410	1579	1584	1592	rBV	897493	1143972	37.33%	4.834%
16	11.481	1592	1596	1600	rVB3	37179	50038	1.63%	0.211%
17	11.933	1665	1673	1685	rBV	292080	472834	15.43%	1.998%
18	12.022	1685	1688	1698	rVB2	15010	37249	1.22%	0.157%
19	12.716	1802	1806	1820	rBV	32920	63656	2.08%	0.269%
20	12.998	1848	1854	1859	rBV	1974499	2551951	83.28%	10.783%
21	13.898	2001	2007	2027	rBV	63097	189551	6.19%	0.801%
22	14.057	2028	2034	2043	rVB	454752	638333	20.83%	2.697%
23	15.551	2282	2288	2301	rBV	444863	724454	23.64%	3.061%

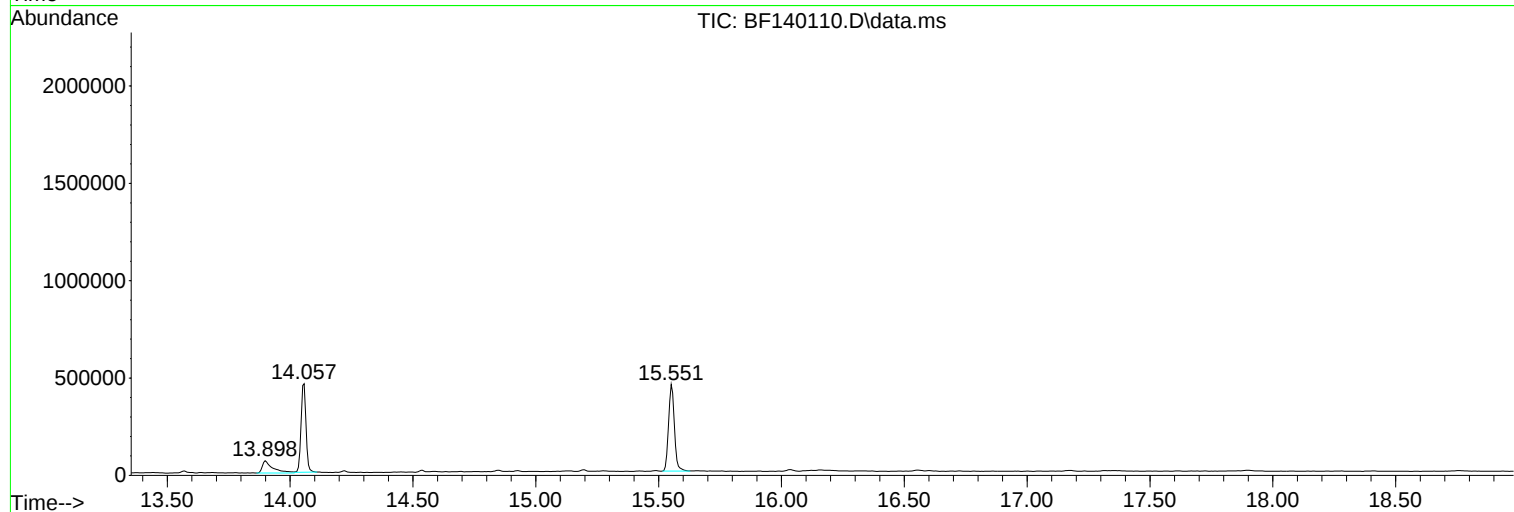
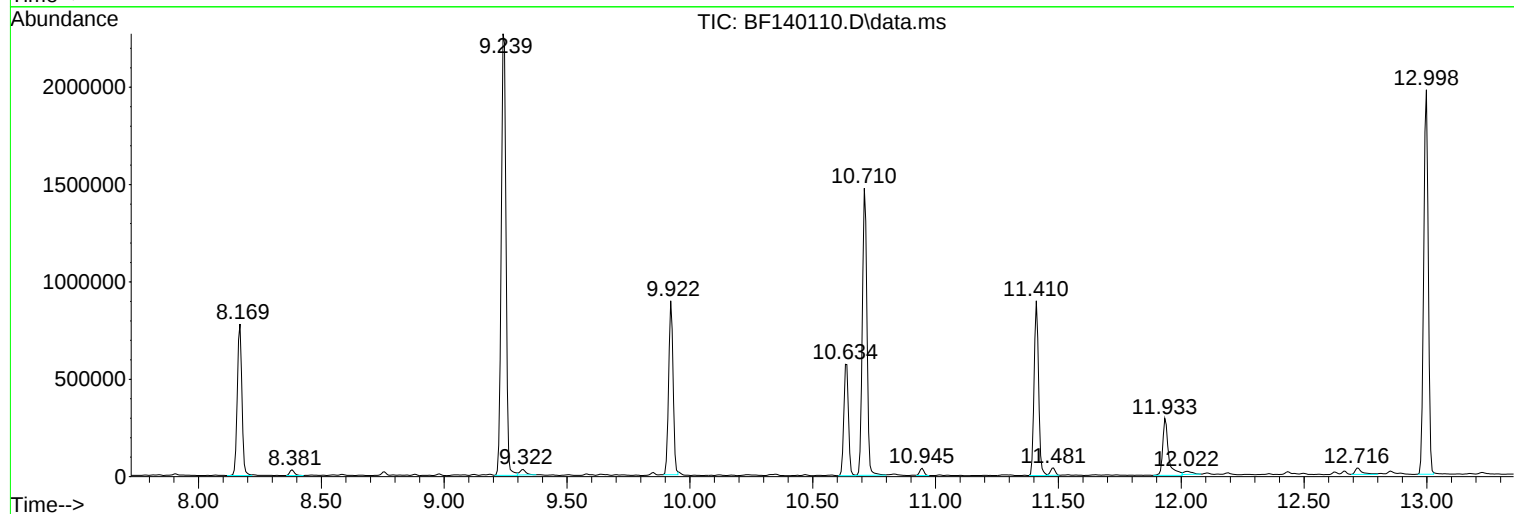
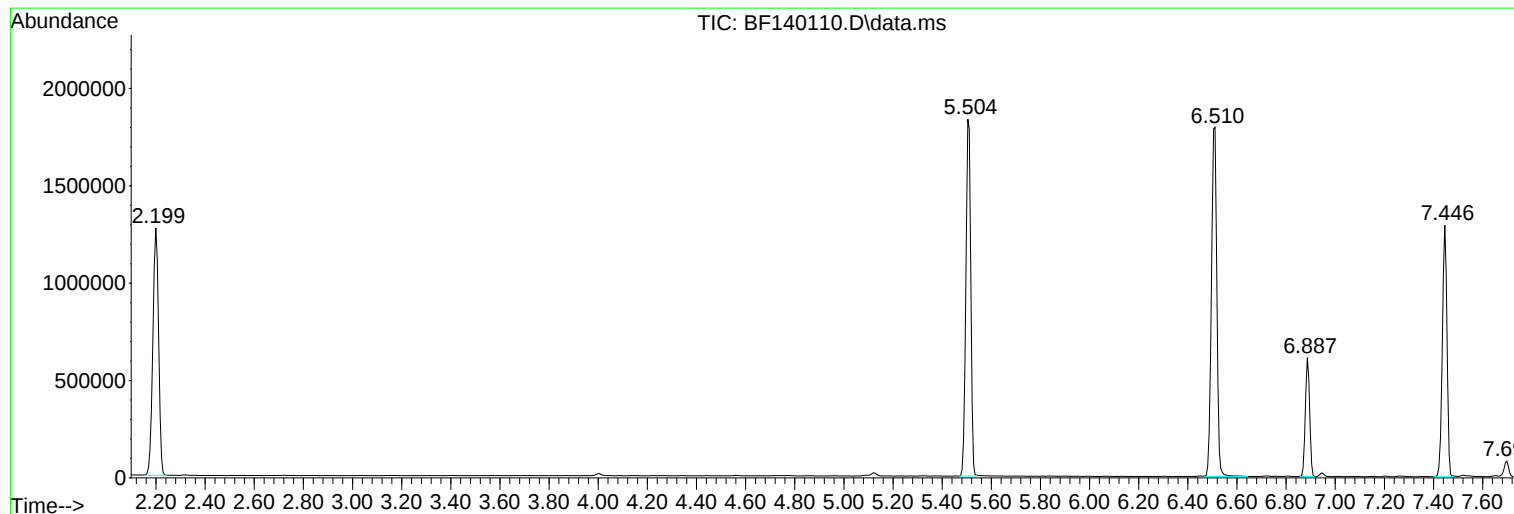
Sum of corrected areas: 23667454

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102924\
Data File : BF140110.D
Acq On : 29 Oct 2024 14:16
Operator : RC/JU
Sample : P4578-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WB-305-BOT

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\BF102924\
Data File : BF140110.D
Acq On : 29 Oct 2024 14:16
Operator : RC/JU
Sample : P4578-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WB-305-BOT

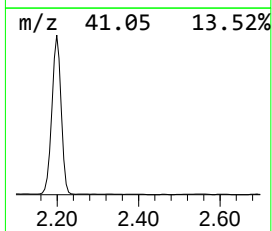
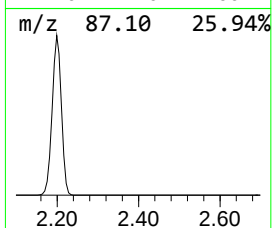
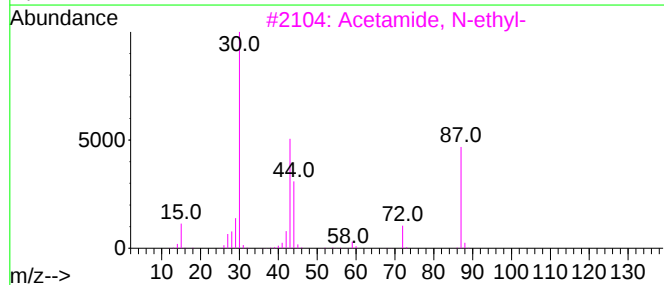
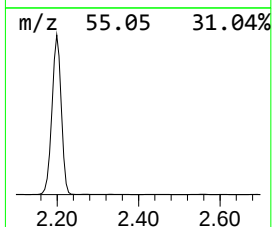
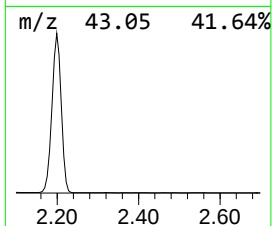
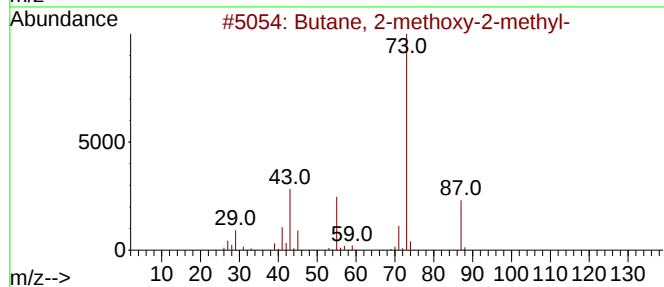
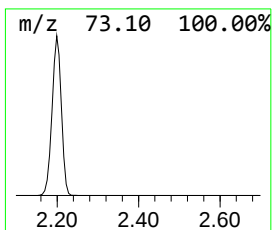
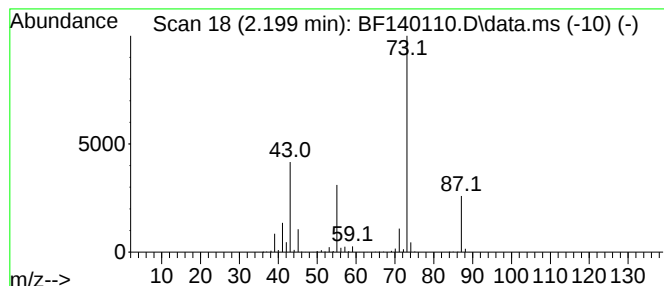
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.199	54.46 ng	2020420	1,4-Dichlorobenzene-d4	6.887

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			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102924\
Data File : BF140110.D
Acq On : 29 Oct 2024 14:16
Operator : RC/JU
Sample : P4578-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WB-305-BOT

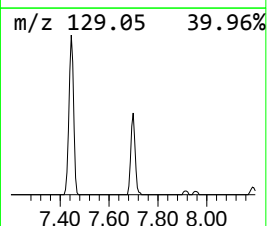
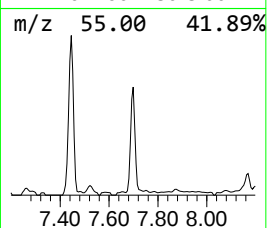
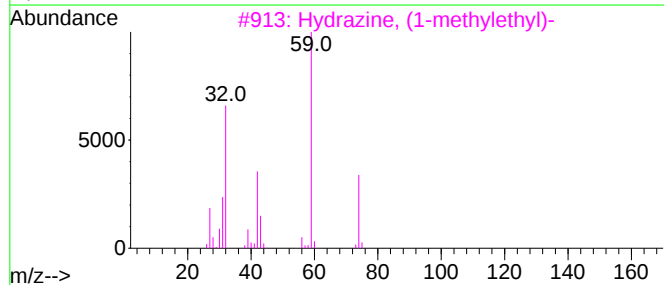
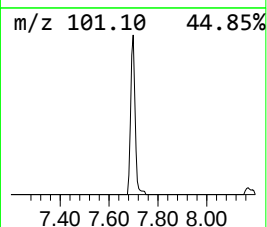
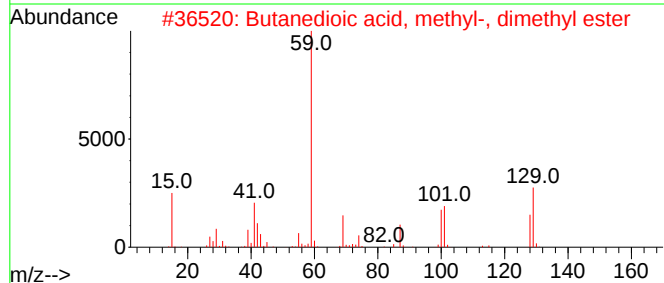
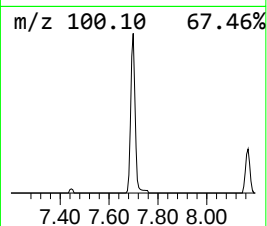
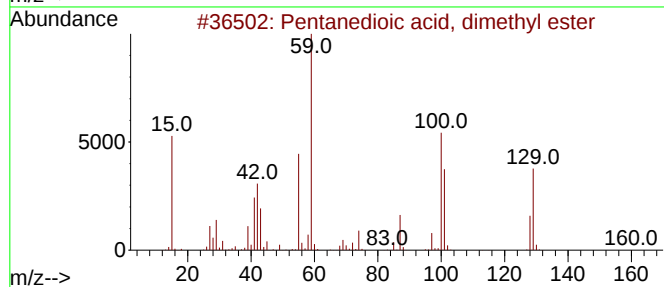
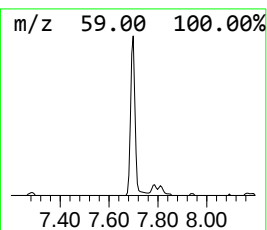
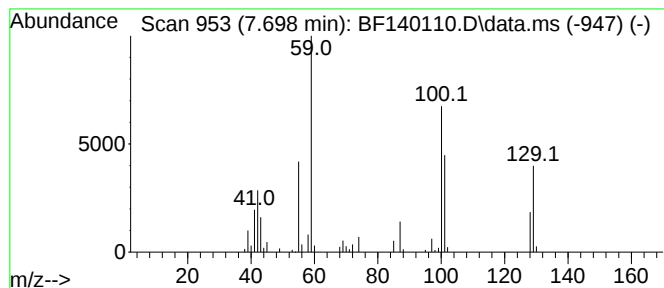
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Pentanedioic acid, dimethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.698	2.05 ng	104509	Naphthalene-d8	8.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	83
2			Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	53
3			Hydrazine, (1-methylethyl)-	74	C3H10N2	002257-52-5	30
4			Hydrazine, trimethyl-	74	C3H10N2	001741-01-1	27
5			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102924\
Data File : BF140110.D
Acq On : 29 Oct 2024 14:16
Operator : RC/JU
Sample : P4578-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

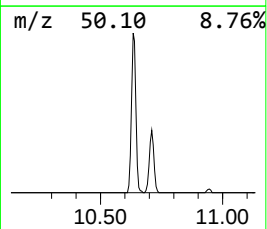
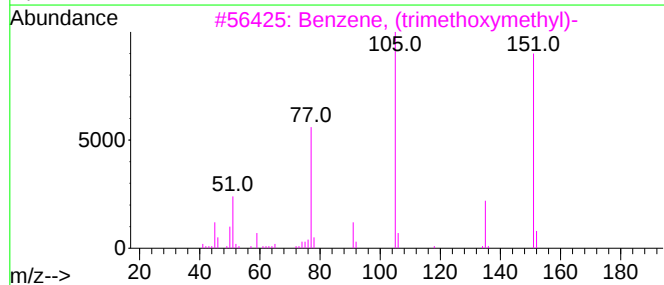
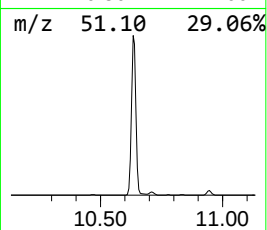
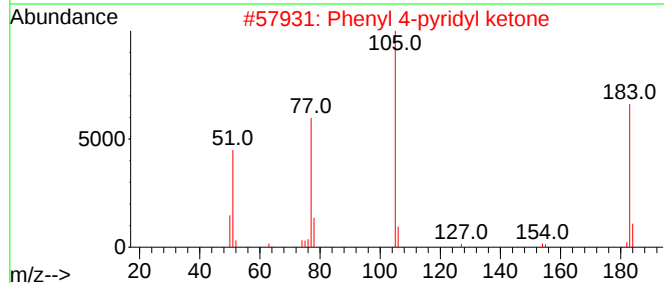
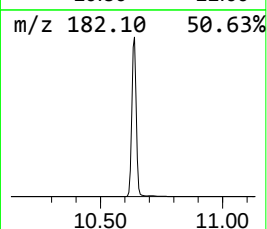
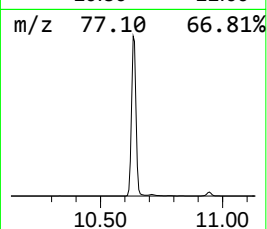
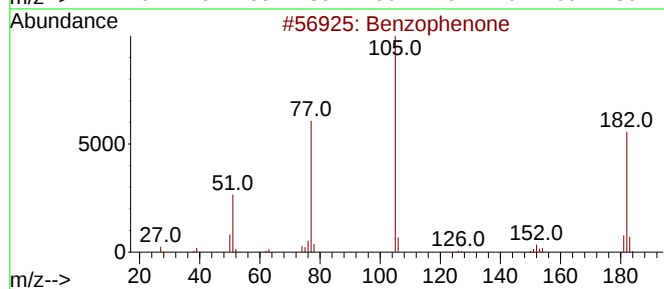
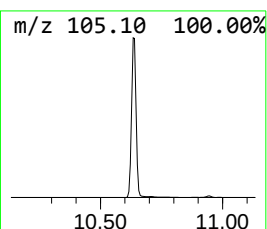
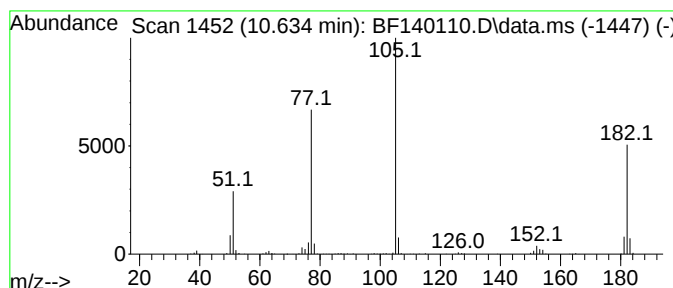
Instrument :
BNA_F
ClientSampleId :
WB-305-BOT

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	13.37 ng	749452	Acenaphthene-d10	9.922	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
3	Benzene, (trimethoxymethyl)-	182	C10H14O3	000707-07-3	47
4	N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47
5	Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102924\
Data File : BF140110.D
Acq On : 29 Oct 2024 14:16
Operator : RC/JU
Sample : P4578-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WB-305-BOT

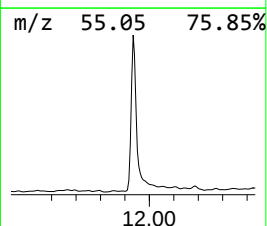
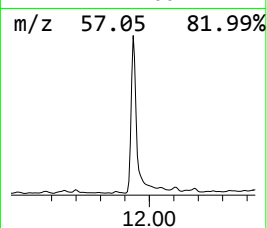
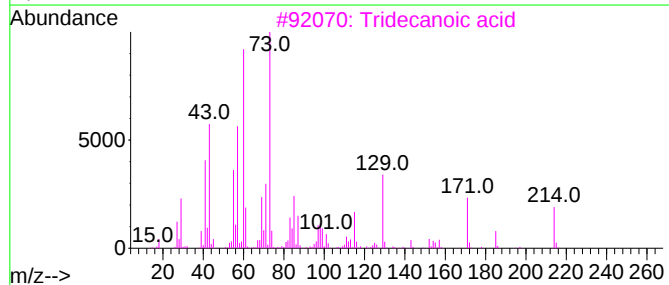
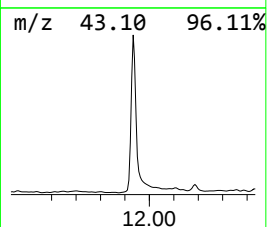
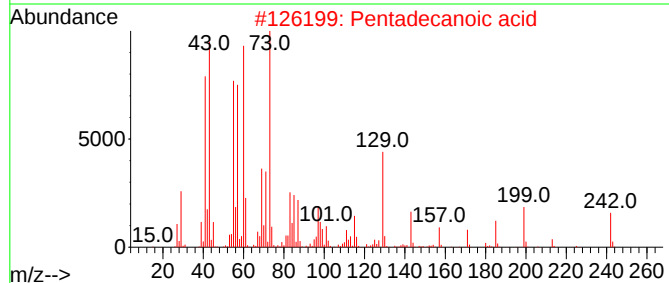
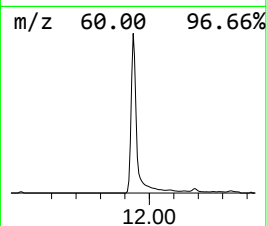
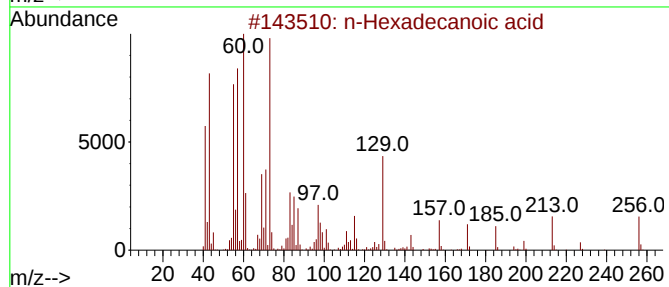
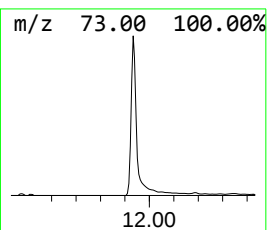
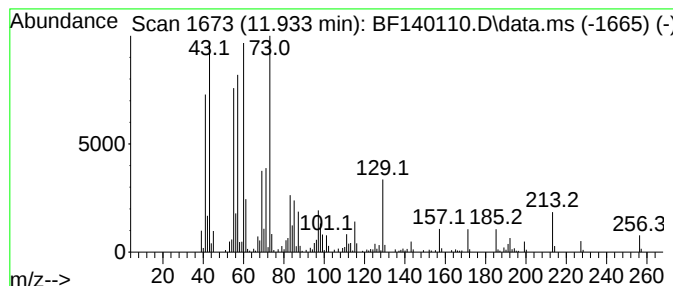
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.934	8.27 ng	472834	Phenanthrene-d10	11.410

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	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102924\
Data File : BF140110.D
Acq On : 29 Oct 2024 14:16
Operator : RC/JU
Sample : P4578-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

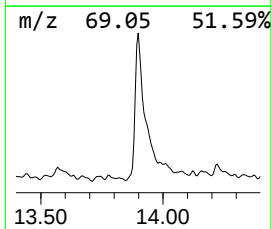
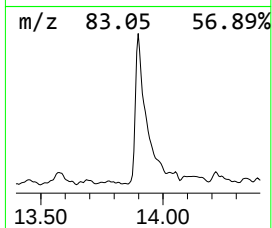
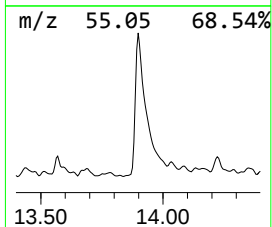
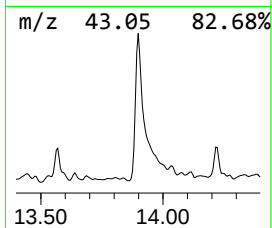
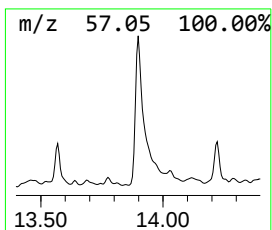
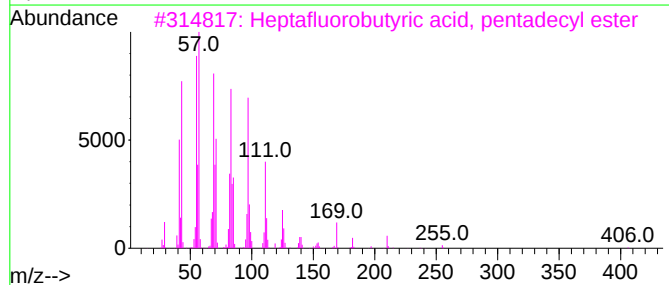
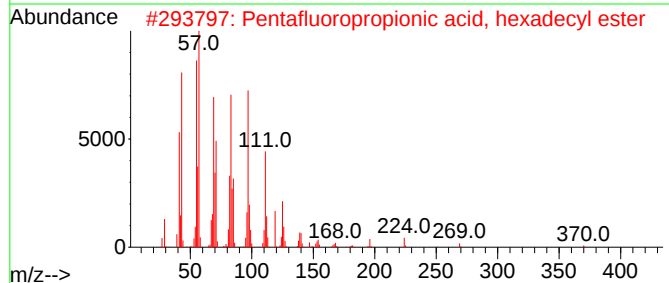
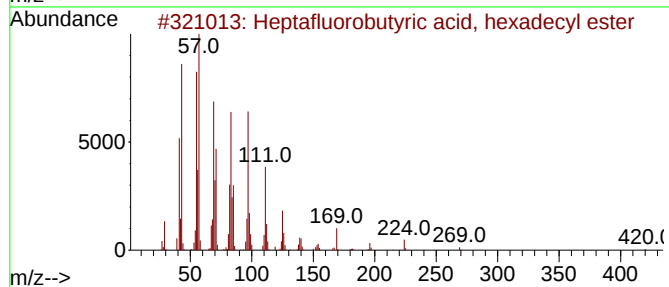
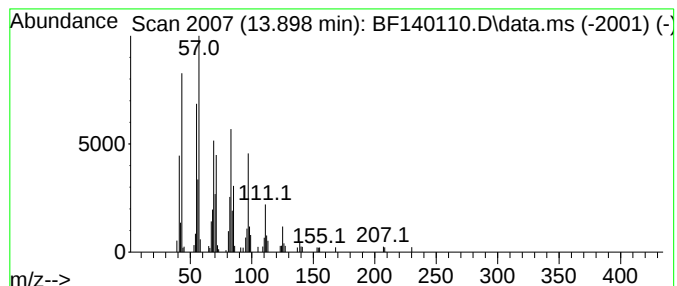
Instrument :
BNA_F
ClientSampleId :
WB-305-BOT

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 Heptafluorobutyric acid, he... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.898	5.94 ng	189551	Chrysene-d12	14.057	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
2	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102924\
Data File : BF140110.D
Acq On : 29 Oct 2024 14:16
Operator : RC/JU
Sample : P4578-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WB-305-BOT

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...	2.199	54.5	ng	2020420	1	6.887	741977	20.0
Pentanedioic ac...	7.698	2.0	ng	104509	2	8.169	1017600	20.0
Benzophenone	10.634	13.4	ng	749452	3	9.922	1120840	20.0
n-Hexadecanoic ...	11.934	8.3	ng	472834	4	11.410	1143970	20.0
Heptafluorobuty...	13.898	5.9	ng	189551	5	14.057	638333	20.0