

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
 Data File : BF139975.D
 Acq On : 23 Oct 2024 20:22
 Operator : RC/JU
 Sample : P4397-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WB-301-SW

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: BF139975.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	8	18	25	rVB	5193508	9482581	100.00%	29.069%
2	5.110	505	513	521	rVB	74064	113426	1.20%	0.348%
3	5.504	574	580	585	rBV	1637936	2128310	22.44%	6.524%
4	6.504	744	750	764	rBV	1135868	1525513	16.09%	4.676%
5	6.887	810	815	821	rBV	712057	895974	9.45%	2.747%
6	7.451	904	911	916	rBV	2036614	2821277	29.75%	8.649%
7	8.169	1028	1033	1038	rBV	904722	1118375	11.79%	3.428%
8	9.245	1210	1216	1221	rBV	3608402	4641242	48.94%	14.228%
9	9.922	1326	1331	1341	rBV	879459	1147142	12.10%	3.517%
10	10.634	1447	1452	1459	rVB	109546	142989	1.51%	0.438%
11	10.710	1459	1465	1479	rBV	1649776	2163165	22.81%	6.631%
12	11.410	1579	1584	1592	rBV	770201	963887	10.16%	2.955%
13	11.933	1667	1673	1688	rBV3	42912	99209	1.05%	0.304%
14	12.998	1848	1854	1859	rBV	2809282	3601174	37.98%	11.039%
15	14.051	2027	2033	2040	rBV	705842	941026	9.92%	2.885%
16	15.527	2278	2284	2300	rBV	516363	835896	8.82%	2.562%

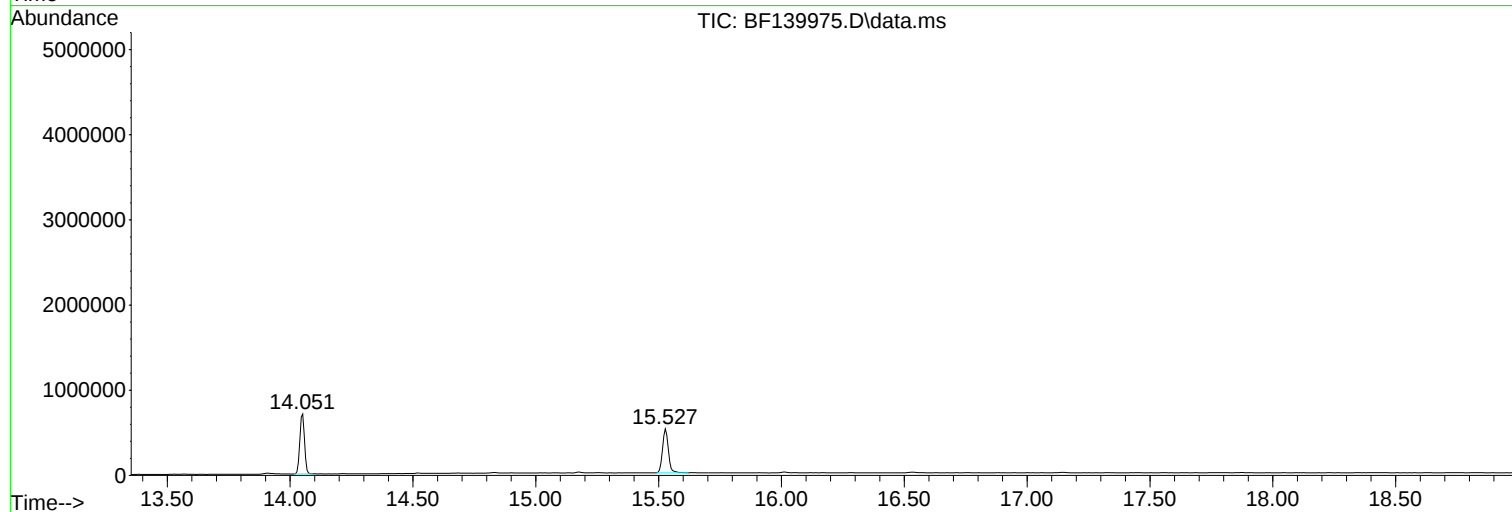
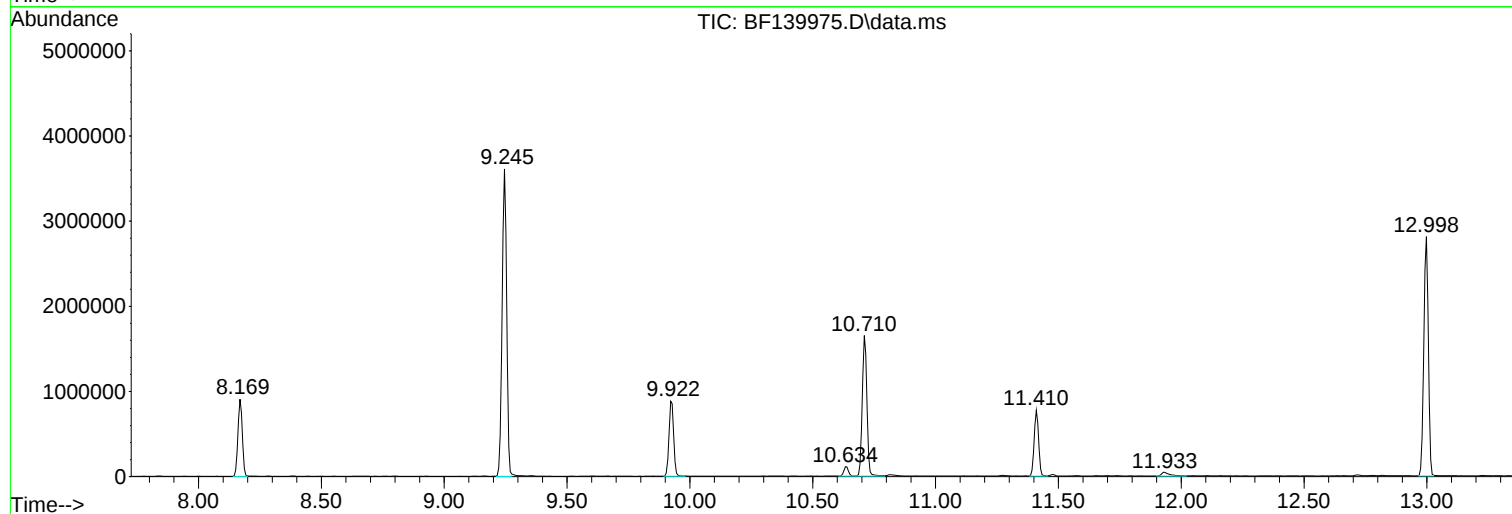
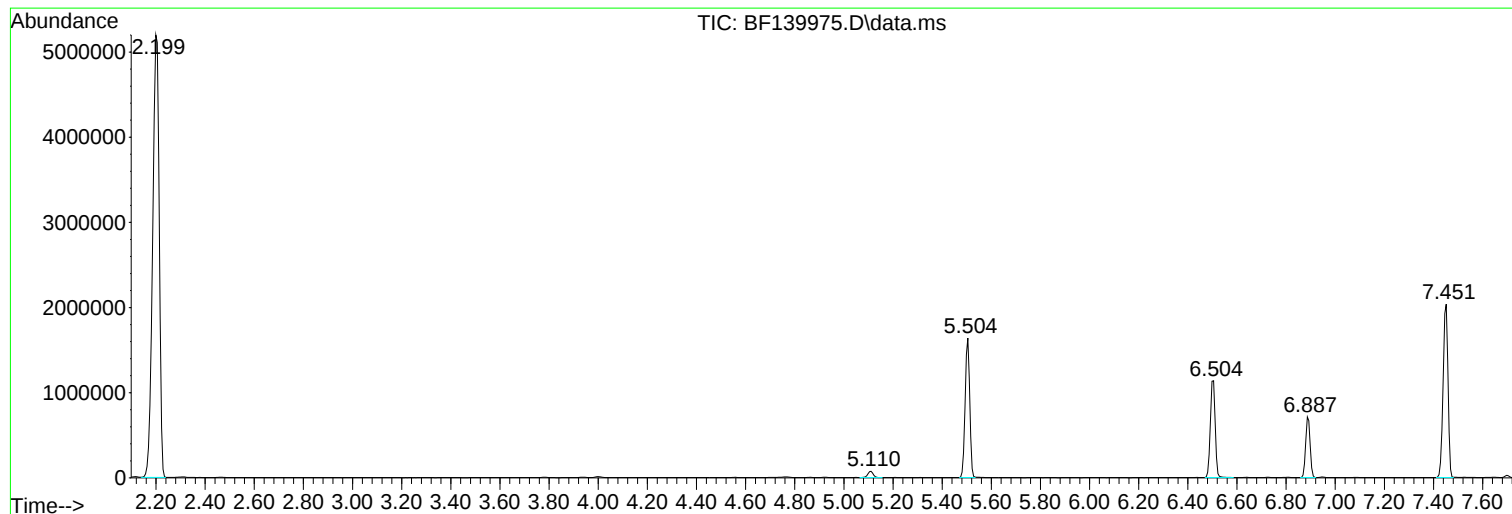
Sum of corrected areas: 32621186

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
Data File : BF139975.D
Acq On : 23 Oct 2024 20:22
Operator : RC/JU
Sample : P4397-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WB-301-SW

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\BF102324\
Data File : BF139975.D
Acq On : 23 Oct 2024 20:22
Operator : RC/JU
Sample : P4397-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WB-301-SW

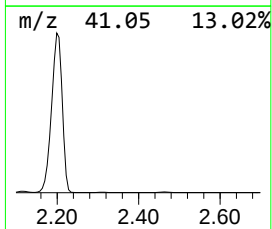
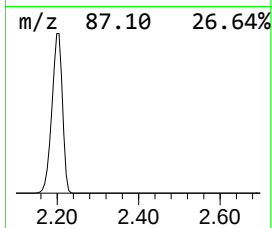
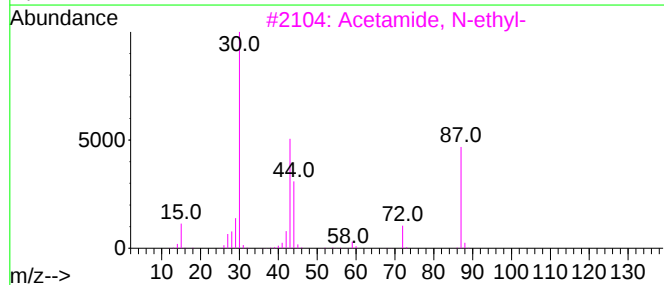
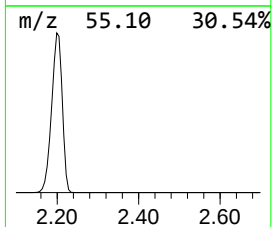
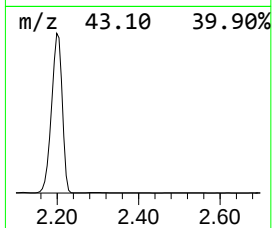
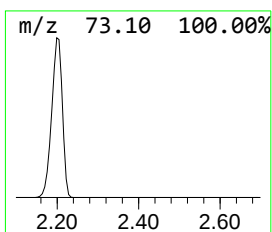
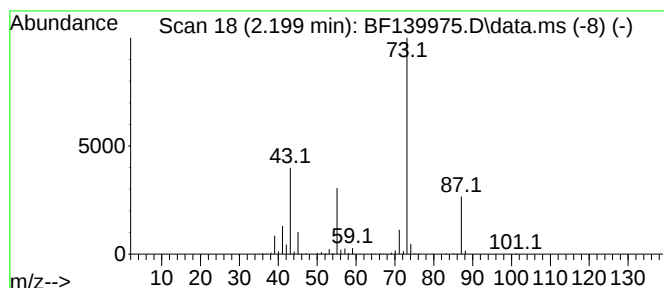
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	211.67 ng	9482580	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			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
Data File : BF139975.D
Acq On : 23 Oct 2024 20:22
Operator : RC/JU
Sample : P4397-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WB-301-SW

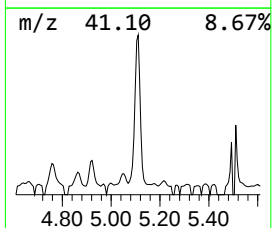
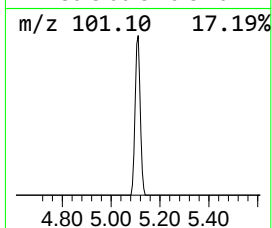
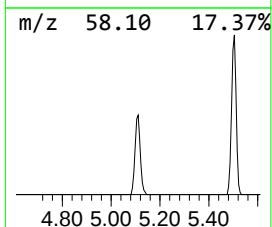
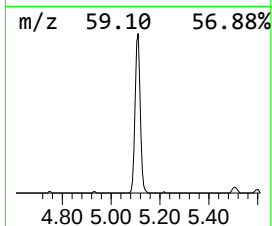
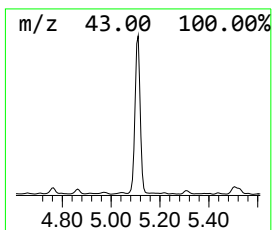
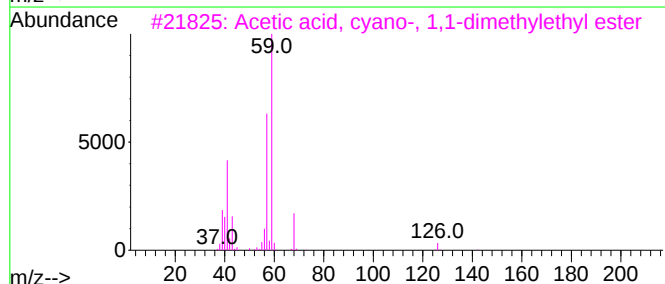
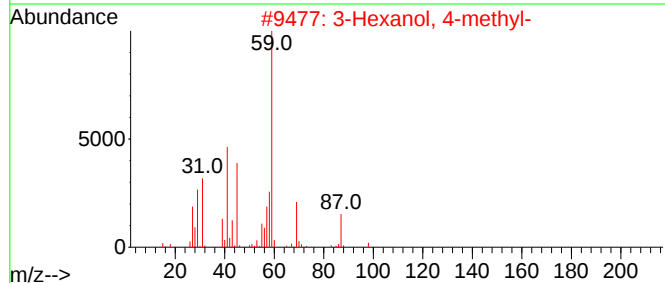
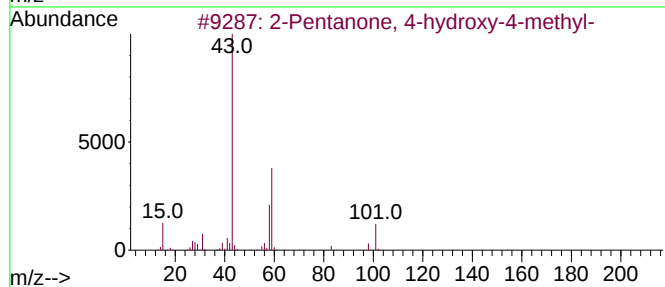
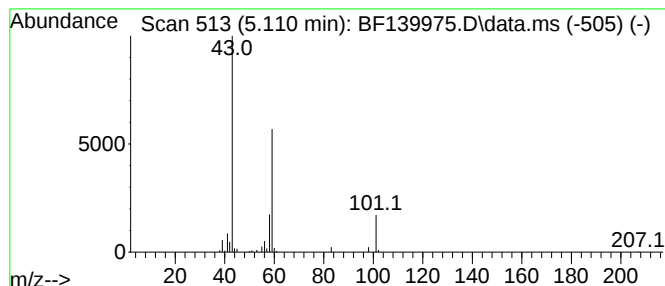
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	2.53 ng	113426	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23
5			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
Data File : BF139975.D
Acq On : 23 Oct 2024 20:22
Operator : RC/JU
Sample : P4397-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WB-301-SW

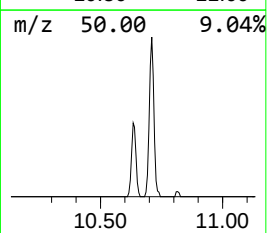
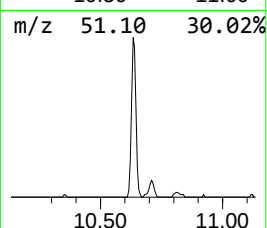
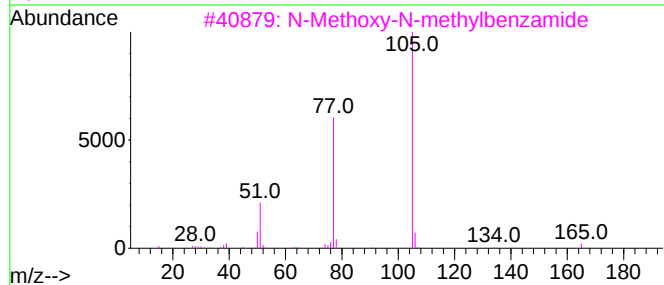
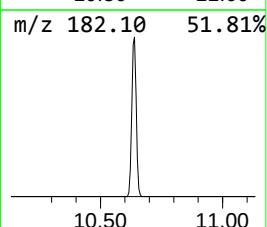
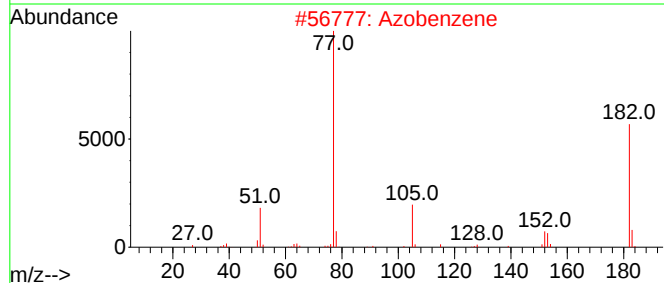
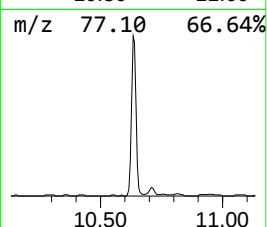
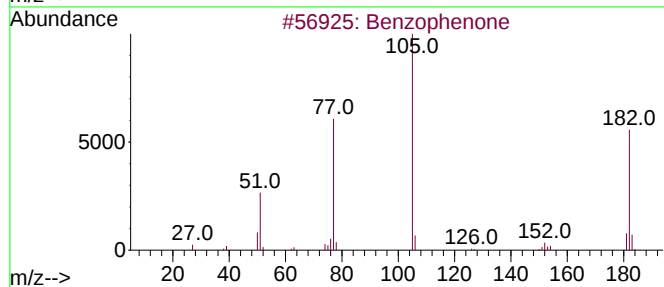
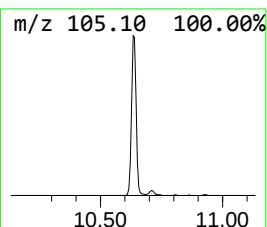
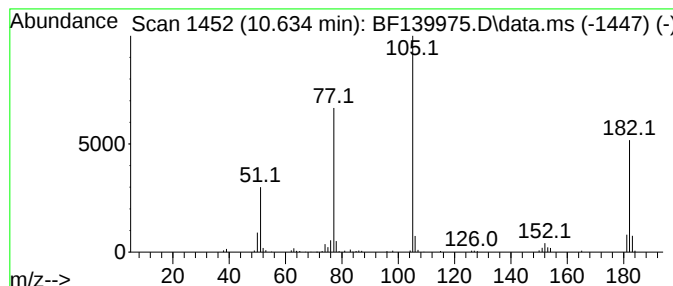
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.634	2.49 ng	142989	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	58
3			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	50
4			acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	50
5			Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
Data File : BF139975.D
Acq On : 23 Oct 2024 20:22
Operator : RC/JU
Sample : P4397-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WB-301-SW

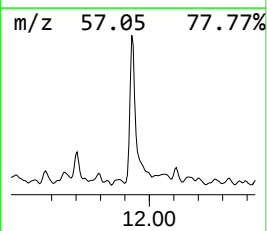
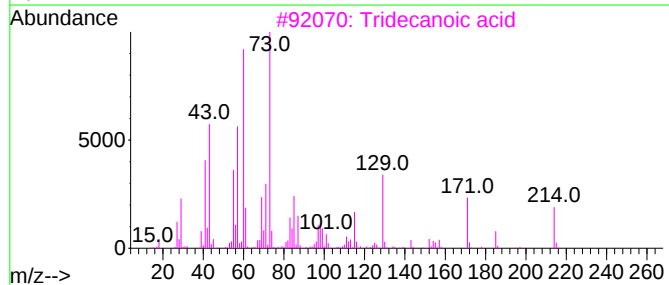
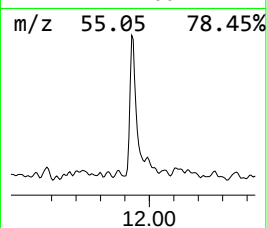
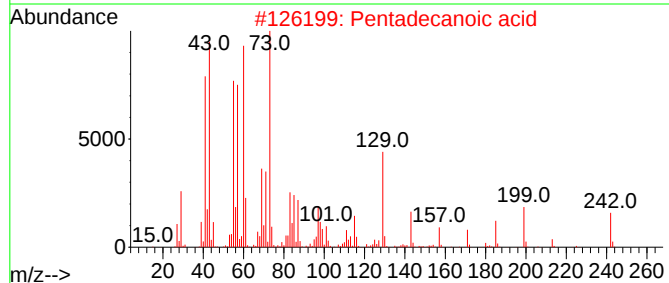
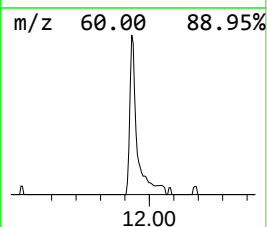
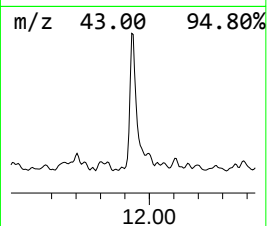
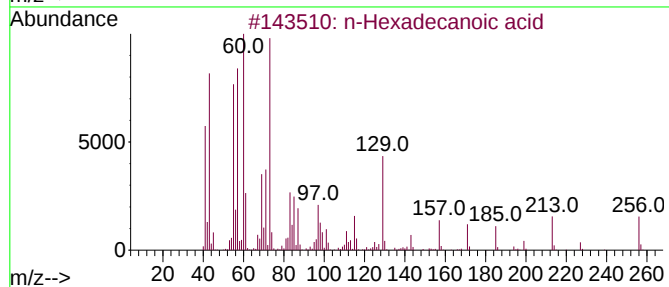
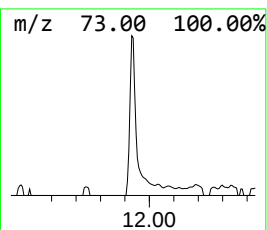
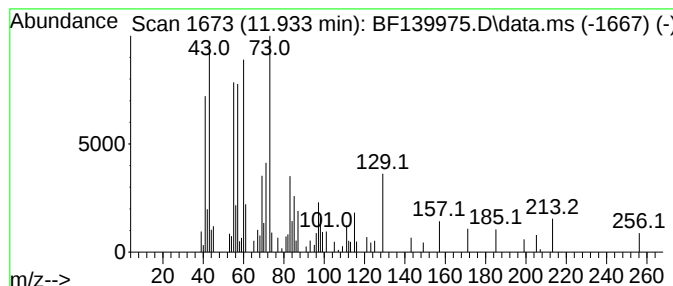
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	2.06 ng	99209	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	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	80
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\BF102324\
Data File : BF139975.D
Acq On : 23 Oct 2024 20:22
Operator : RC/JU
Sample : P4397-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WB-301-SW

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	211.7	ng	9482580	1	6.887	895974	20.0
2-Pentanone, 4-...	5.110	2.5	ng	113426	1	6.887	895974	20.0
Benzophenone	10.634	2.5	ng	142989	3	9.922	1147140	20.0
n-Hexadecanoic ...	11.933	2.1	ng	99209	4	11.410	963887	20.0