

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072723\
 Data File : BP016406.D
 Acq On : 27 Jul 2023 18:30
 Operator : MA/JU
 Sample : 03706-10
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 FB02

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_P\Methods\8270E-BP072723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP016406.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.775	79	83	93	rVB	530692	705709	3.21%	0.702%
2	5.599	386	393	406	rBV	2429631	3705318	16.86%	3.687%
3	7.222	659	669	681	rVB	1470105	2435454	11.08%	2.423%
4	8.093	808	817	820	rBV	1152385	1866828	8.49%	1.857%
5	8.122	820	822	831	rVB	429762	542393	2.47%	0.540%
6	9.287	1011	1020	1034	rBV	3772622	6153757	28.00%	6.123%
7	10.922	1291	1298	1306	rBV	1528625	2523859	11.48%	2.511%
8	11.422	1373	1383	1388	rBV	1269914	1997458	9.09%	1.987%
9	11.487	1388	1394	1406	rVB	1656143	2671316	12.15%	2.658%
10	11.810	1444	1449	1457	rVB	202776	310735	1.41%	0.309%
11	12.757	1604	1610	1629	rVB	522305	755885	3.44%	0.752%
12	13.363	1701	1713	1721	rBV	9535927	13907558	63.28%	13.838%
13	13.598	1745	1753	1768	rBV	8352347	13398439	60.96%	13.331%
14	14.734	1937	1946	1953	rBV	2303035	3326357	15.13%	3.310%
15	16.222	2191	2199	2214	rBV	6781811	10132329	46.10%	10.081%
16	17.498	2408	2416	2428	rBV	2899233	4115378	18.72%	4.095%
17	17.604	2428	2434	2439	rBV3	159931	235706	1.07%	0.235%
18	20.039	2842	2848	2854	rBV	17016804	21978909	100.00%	21.868%
19	21.586	3106	3111	3123	rBV	3543004	4662138	21.21%	4.639%
20	24.180	3545	3552	3565	rVB2	2338627	5079692	23.11%	5.054%

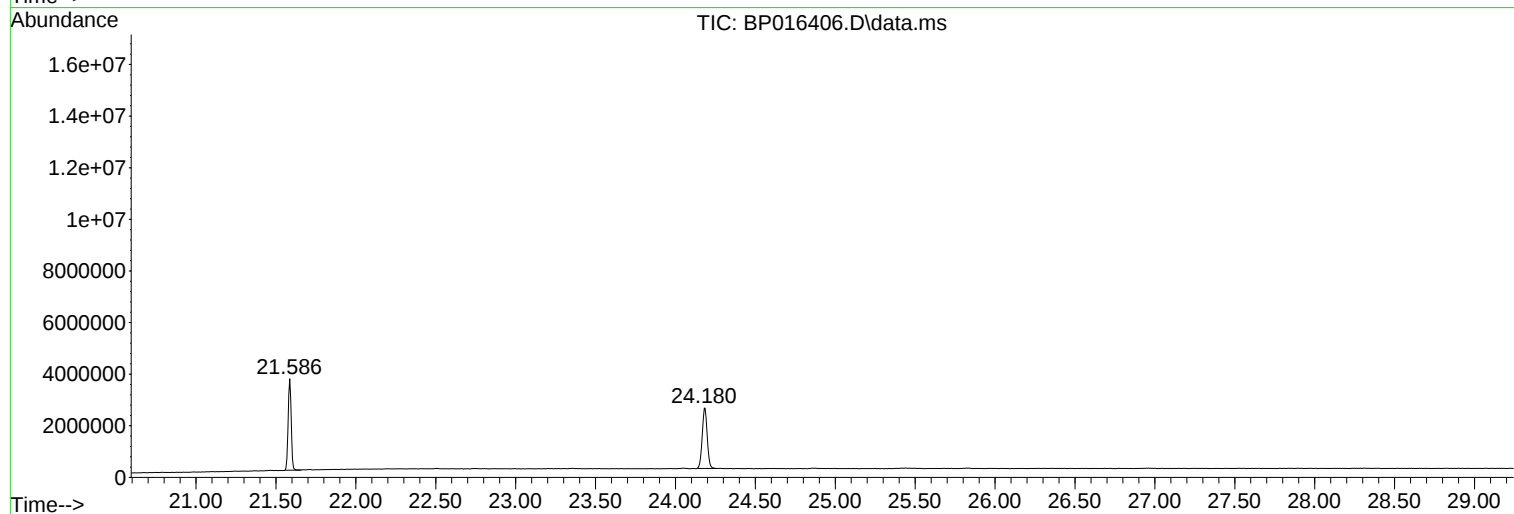
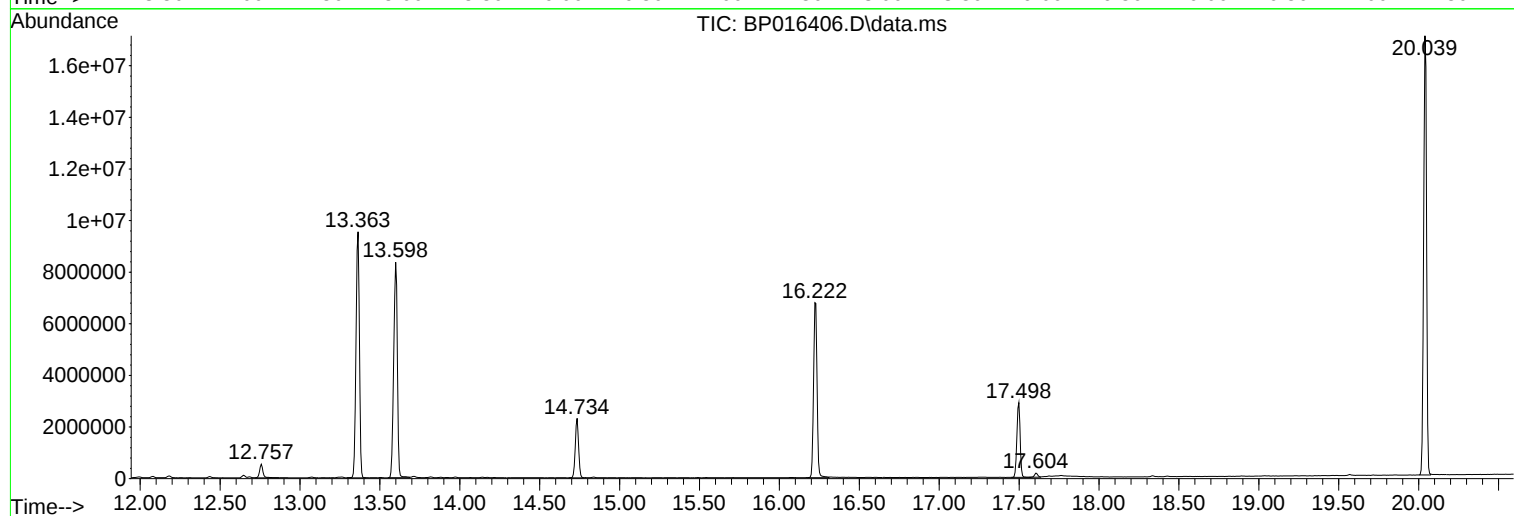
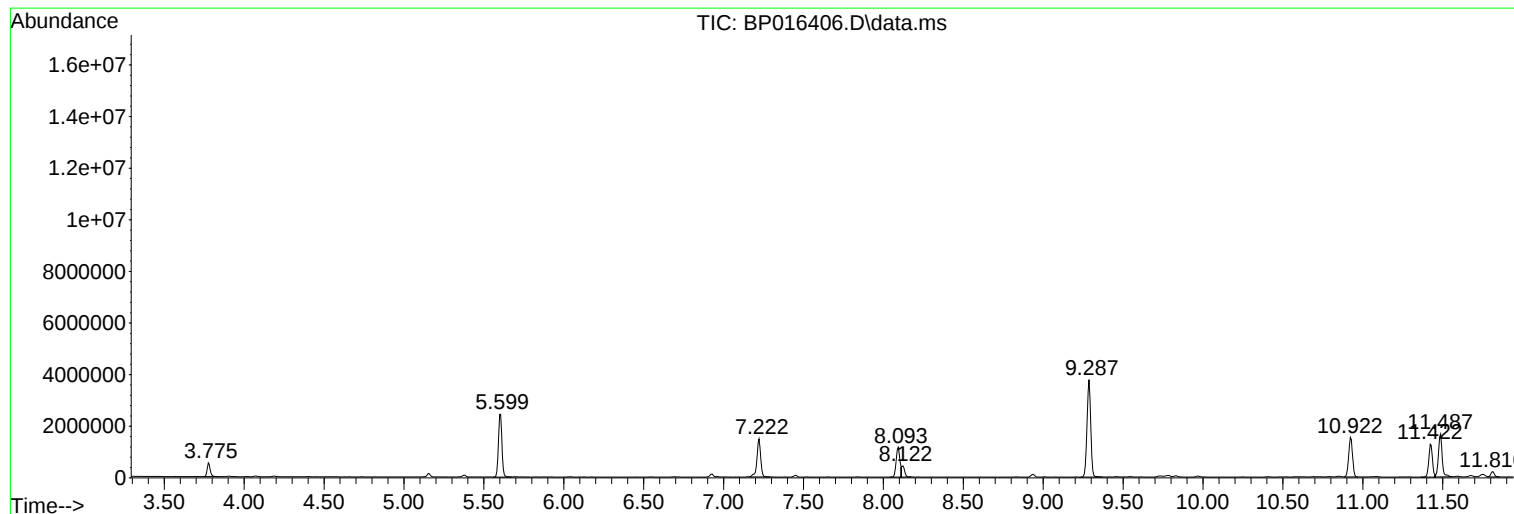
Sum of corrected areas: 100505218

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072723\
Data File : BP016406.D
Acq On : 27 Jul 2023 18:30
Operator : MA/JU
Sample : 03706-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP072723.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_P\Data\BP072723\
Data File : BP016406.D
Acq On : 27 Jul 2023 18:30
Operator : MA/JU
Sample : 03706-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FB02

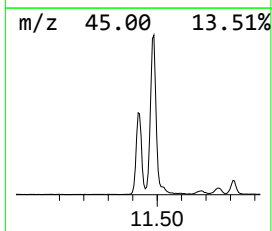
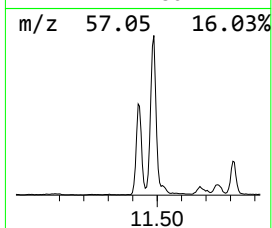
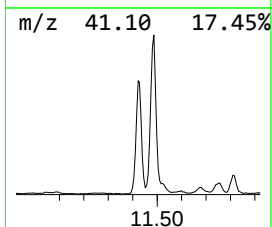
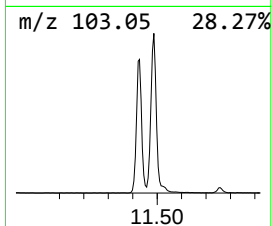
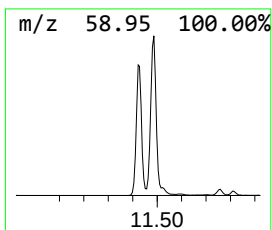
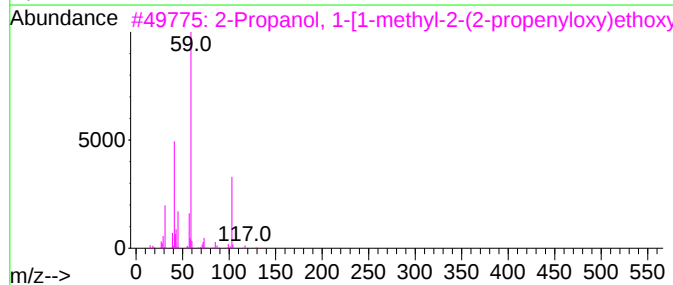
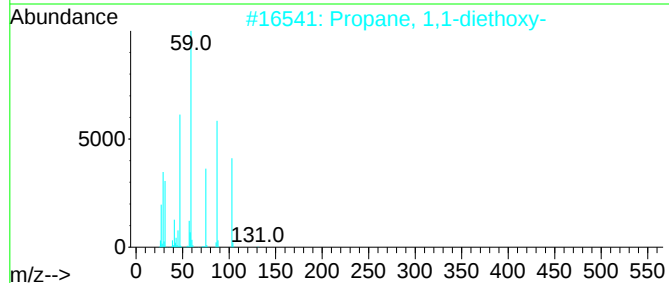
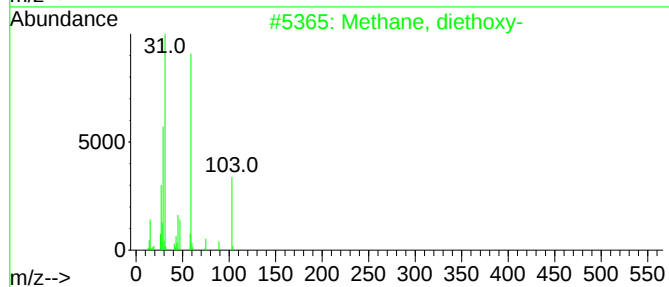
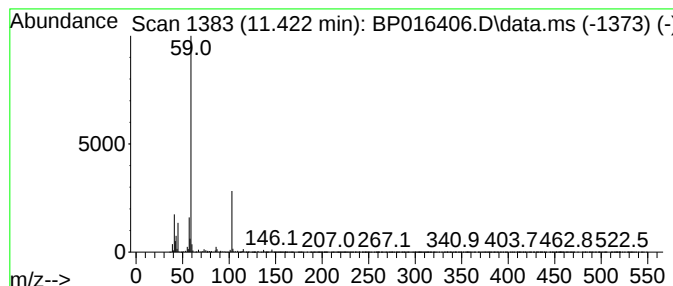
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP072723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Methane, diethoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.422	15.83 ng	1997460	Naphthalene-d8	10.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane, diethoxy-	104	C5H12O2	000462-95-3	80
2			Propane, 1,1-diethoxy-	132	C7H16O2	004744-08-5	78
3			2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	78
4			2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	74
5			1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072723\
Data File : BP016406.D
Acq On : 27 Jul 2023 18:30
Operator : MA/JU
Sample : 03706-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

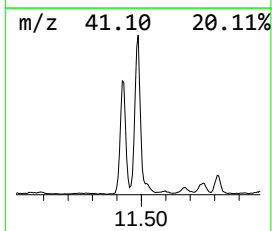
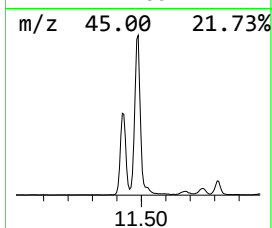
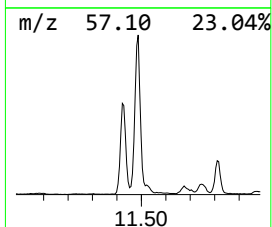
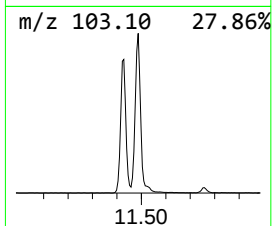
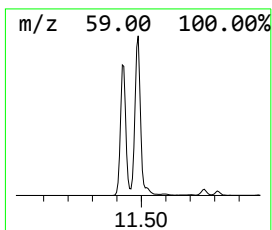
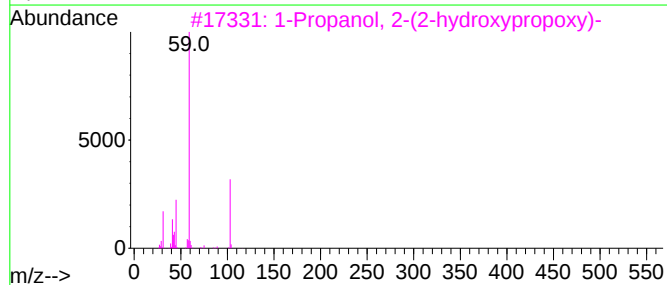
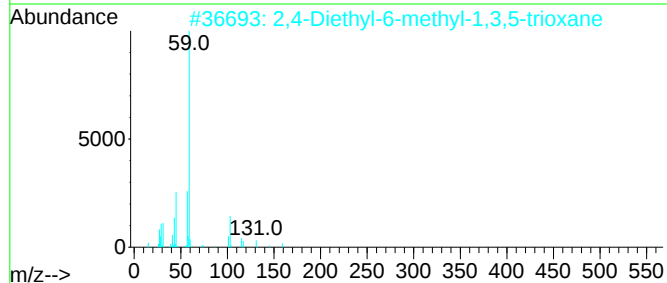
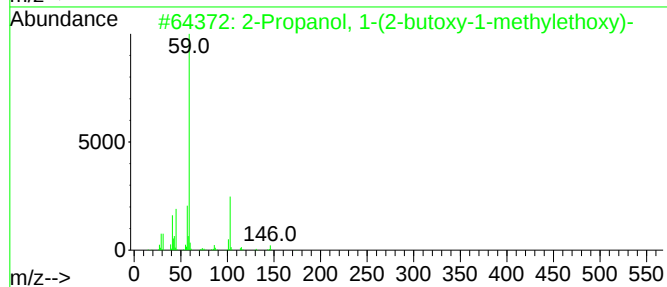
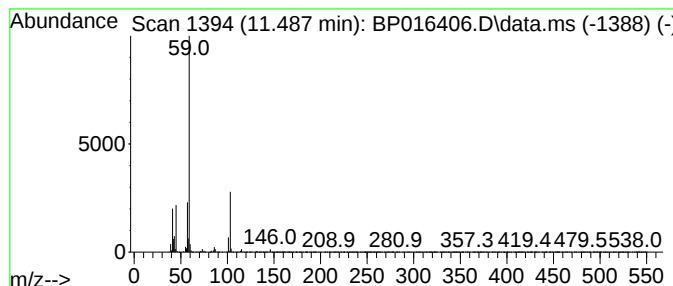
Instrument :
BNA_P
ClientSampleId :
FB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP072723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Propanol, 1-(2-butoxy-1-m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.487	21.17 ng	2671320	Naphthalene-d8	10.922	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	90
2	2,4-Diethyl-6-methyl-1,3,5-trioxane	160	C8H16O3	117888-04-7	78
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	78
4	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	72
5	Hexaethylene glycol dimethyl ether	310	C14H30O7	001072-40-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072723\
Data File : BP016406.D
Acq On : 27 Jul 2023 18:30
Operator : MA/JU
Sample : 03706-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FB02

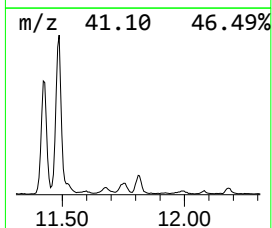
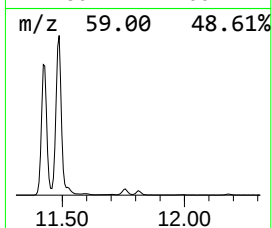
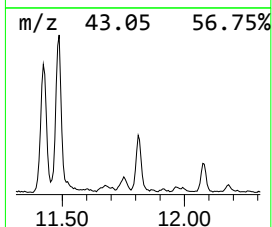
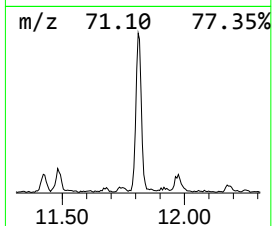
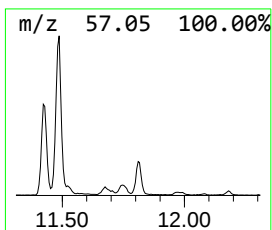
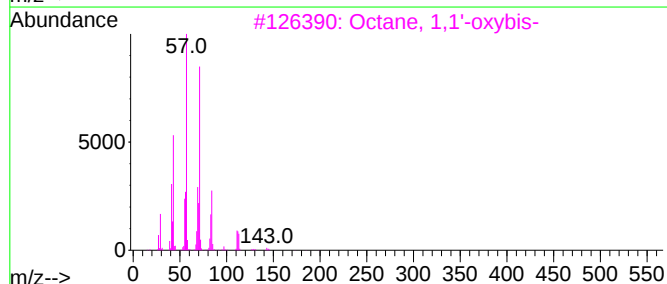
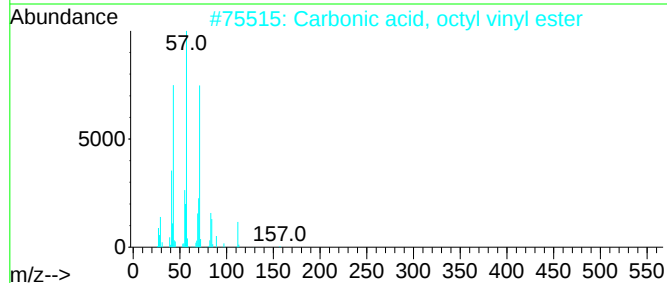
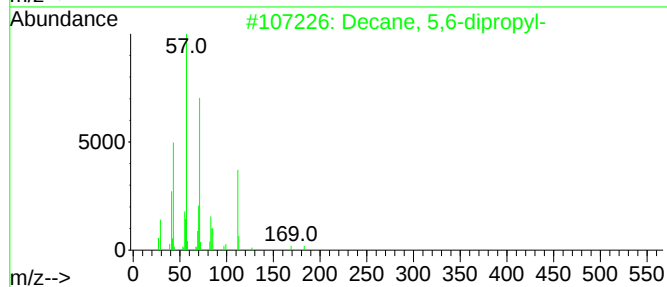
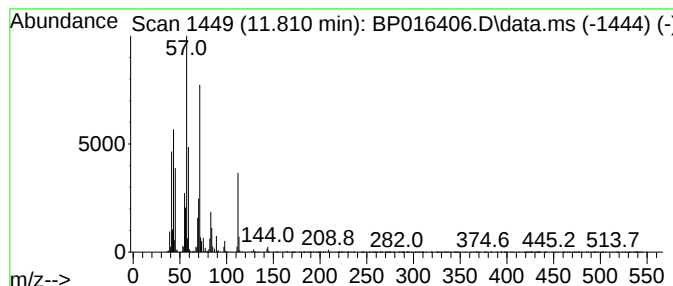
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP072723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Decane, 5,6-dipropyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.810	2.46 ng	310735	Naphthalene-d8	10.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 5,6-dipropyl-	226	C16H34	119209-20-0	52
2			Carbonic acid, octyl vinyl ester	200	C11H20O3	1000383-25-5	49
3			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	46
4			Heptane, 3-[(ethenloxy)methyl]-	156	C10H20O	000103-44-6	43
5			Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072723\
Data File : BP016406.D
Acq On : 27 Jul 2023 18:30
Operator : MA/JU
Sample : 03706-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

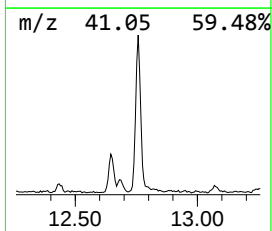
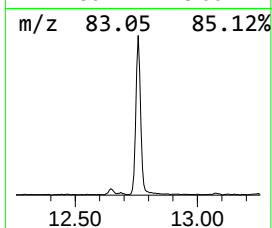
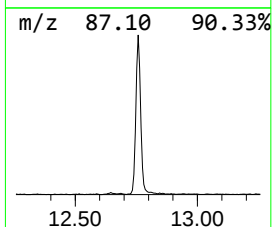
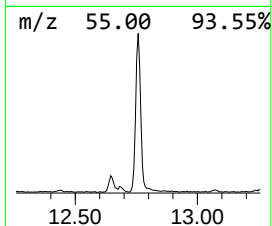
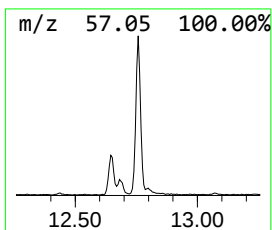
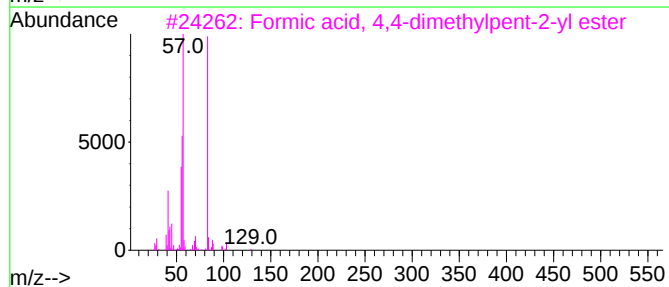
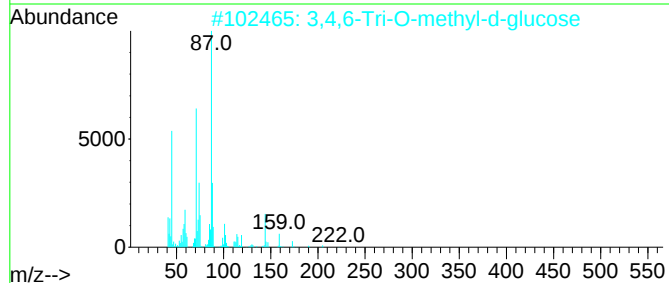
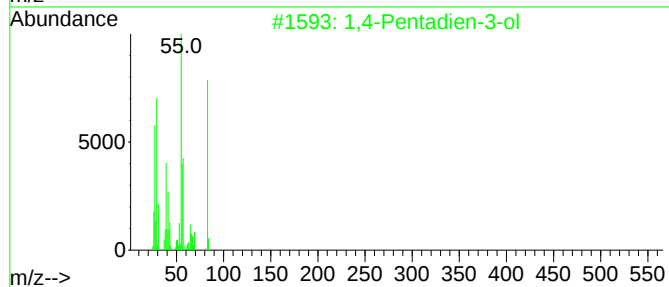
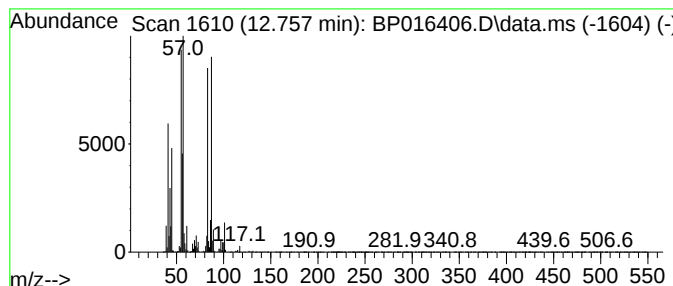
Instrument :
BNA_P
ClientSampleId :
FB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP072723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown12.757 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.757	5.99 ng	755885	Naphthalene-d8	10.922	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Pentadien-3-ol	84	C5H8O	000922-65-6	38
2	3,4,6-Tri-O-methyl-d-glucose	222	C9H18O6	1000127-03-2	35
3	Formic acid, 4,4-dimethylpent-2-...	144	C8H16O2	1000368-69-9	32
4	1,2-Butanediol, 3,3-dimethyl-	118	C6H14O2	059562-82-2	32
5	4-Nonanol, 4-methyl-	158	C10H22O	023418-38-4	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072723\
Data File : BP016406.D
Acq On : 27 Jul 2023 18:30
Operator : MA/JU
Sample : 03706-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

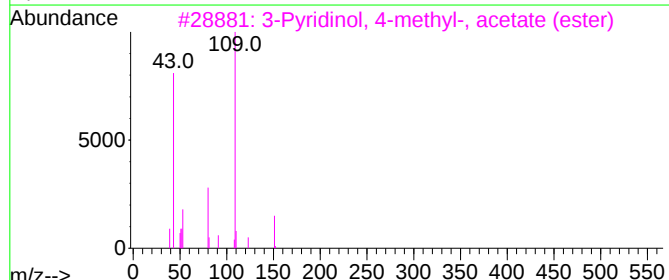
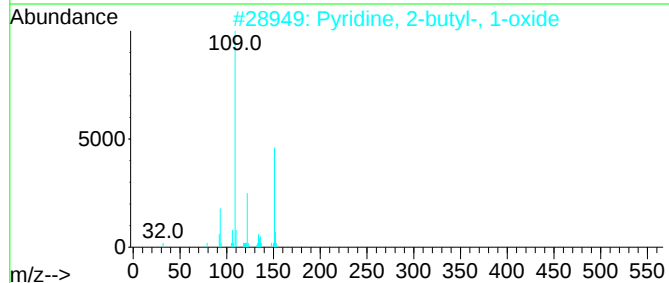
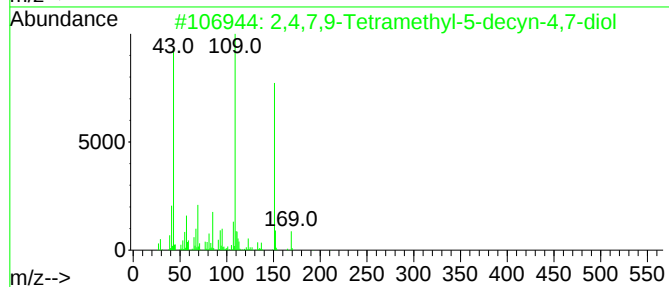
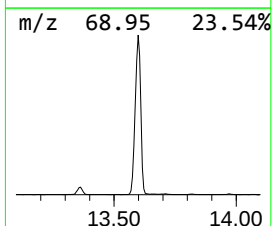
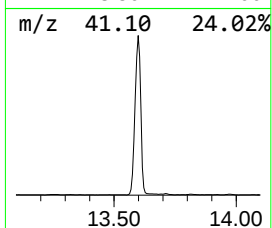
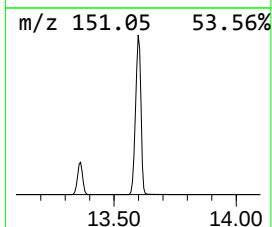
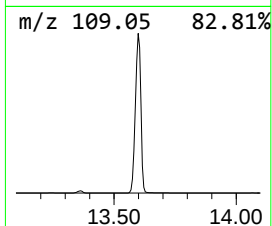
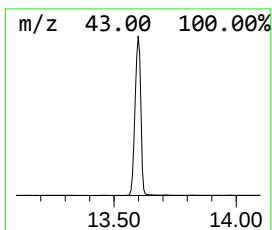
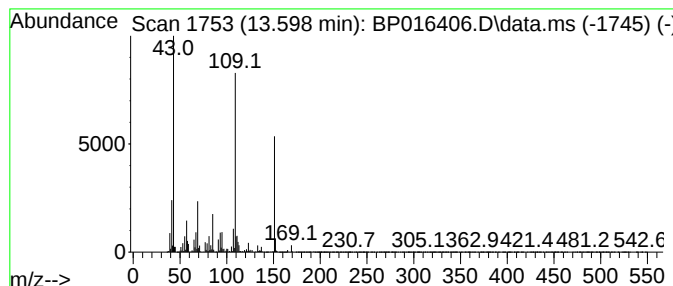
Instrument :
BNA_P
ClientSampleId :
FB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP072723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.598	80.56 ng	13398400	Acenaphthene-d10	14.734	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59
3	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	59
4	Metacetamol	151	C8H9NO2	000621-42-1	59
5	Cyclopentanol, 1-(methylenecyclo...	138	C9H14O	086951-58-8	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072723\
Data File : BP016406.D
Acq On : 27 Jul 2023 18:30
Operator : MA/JU
Sample : 03706-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP072723.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
Methane, diethoxy-	11.422	15.8	ng	1997460	2	10.922	2523860	20.0
2-Propanol, 1-(...	11.487	21.2	ng	2671320	2	10.922	2523860	20.0
Decane, 5,6-dip...	11.810	2.5	ng	310735	2	10.922	2523860	20.0
unknown12.757	12.757	6.0	ng	755885	2	10.922	2523860	20.0
2,4,7,9-Tetrame...	13.598	80.6	ng	13398400	3	14.734	3326360	20.0