

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021422\
 Data File : BP009141.D
 Acq On : 14 Feb 2022 18:54
 Operator : CG/JU
 Sample : N1443-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TP-1-SOUTH-COMP

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-BP020722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP009141.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.916	323	328	341	rVB	314831	491177	5.18%	0.911%
2	5.393	402	409	435	rBV	2922056	5040808	53.13%	9.348%
3	6.987	673	680	701	rBV	2731978	5118622	53.95%	9.492%
4	7.793	808	817	827	rBV	737139	1269017	13.37%	2.353%
5	8.957	1006	1015	1036	rBV	1884269	3532272	37.23%	6.550%
6	10.410	1249	1262	1277	rBV4	25021	107481	1.13%	0.199%
7	10.587	1284	1292	1309	rBV	809270	1577994	16.63%	2.926%
8	13.057	1704	1712	1737	rBV	4913065	7934521	83.63%	14.714%
9	13.339	1754	1760	1769	rVB	121505	202939	2.14%	0.376%
10	14.334	1921	1929	1937	rBV3	37275	112779	1.19%	0.209%
11	14.434	1940	1946	1964	rVB	1112594	1873074	19.74%	3.473%
12	15.939	2195	2202	2223	rBV	2811672	4961583	52.29%	9.201%
13	16.169	2236	2241	2253	rVB2	37326	115053	1.21%	0.213%
14	17.192	2409	2415	2430	rBV	1237940	2118578	22.33%	3.929%
15	17.869	2526	2530	2535	rVB	80503	99966	1.05%	0.185%
16	18.092	2561	2568	2576	rBV4	69426	189346	2.00%	0.351%
17	18.998	2719	2722	2730	rVB3	204258	240566	2.54%	0.446%
18	19.127	2741	2744	2751	rVB2	89001	121133	1.28%	0.225%
19	19.210	2754	2758	2765	rVV	99819	164224	1.73%	0.305%
20	19.563	2815	2818	2827	rVB	148467	222816	2.35%	0.413%
21	19.757	2846	2851	2861	rBV	7881324	9488164	100.00%	17.595%
22	20.380	2954	2957	2961	rVB2	87199	100259	1.06%	0.186%
23	20.539	2982	2984	2988	rVB2	121756	124442	1.31%	0.231%
24	20.998	3058	3062	3082	rVB4	572891	1610656	16.98%	2.987%
25	21.292	3107	3112	3116	rBV	1968150	2668657	28.13%	4.949%
26	22.380	3293	3297	3306	rBV	901322	1345758	14.18%	2.496%
27	23.686	3513	3519	3531	rVB2	1509223	3094420	32.61%	5.738%

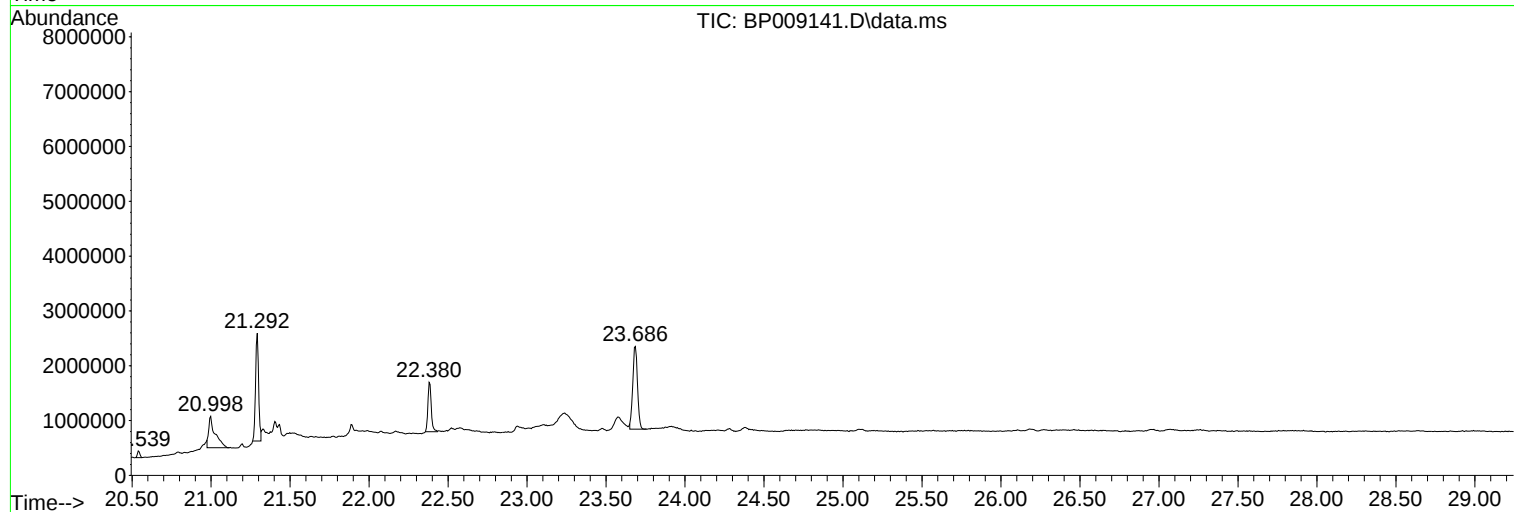
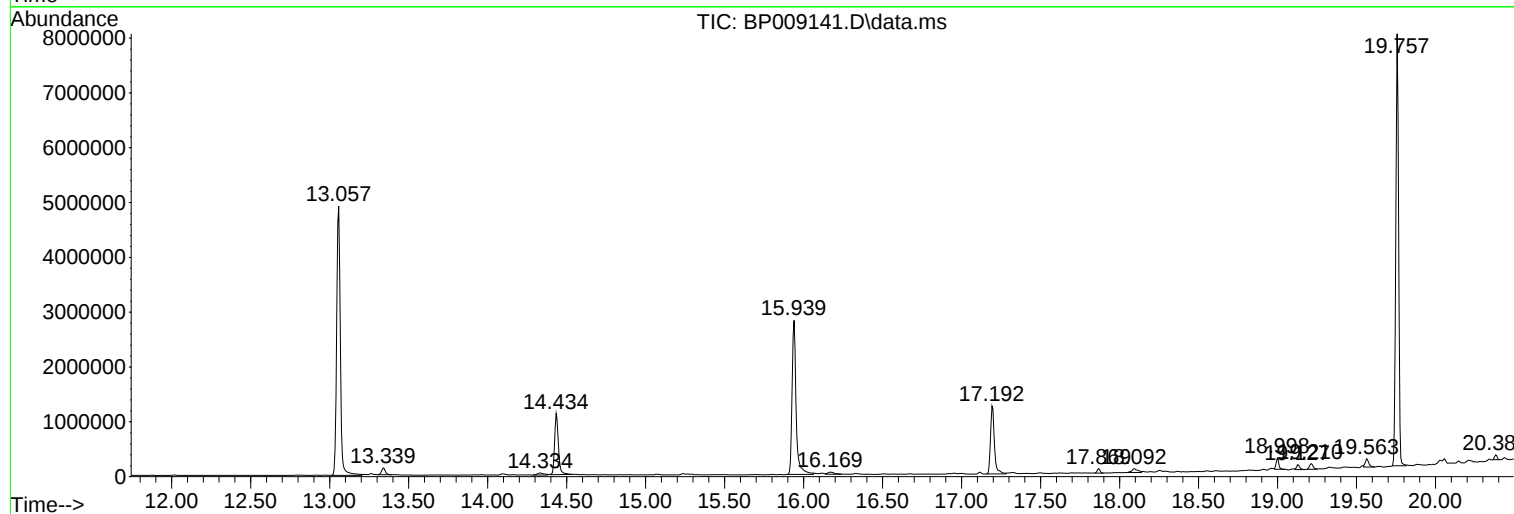
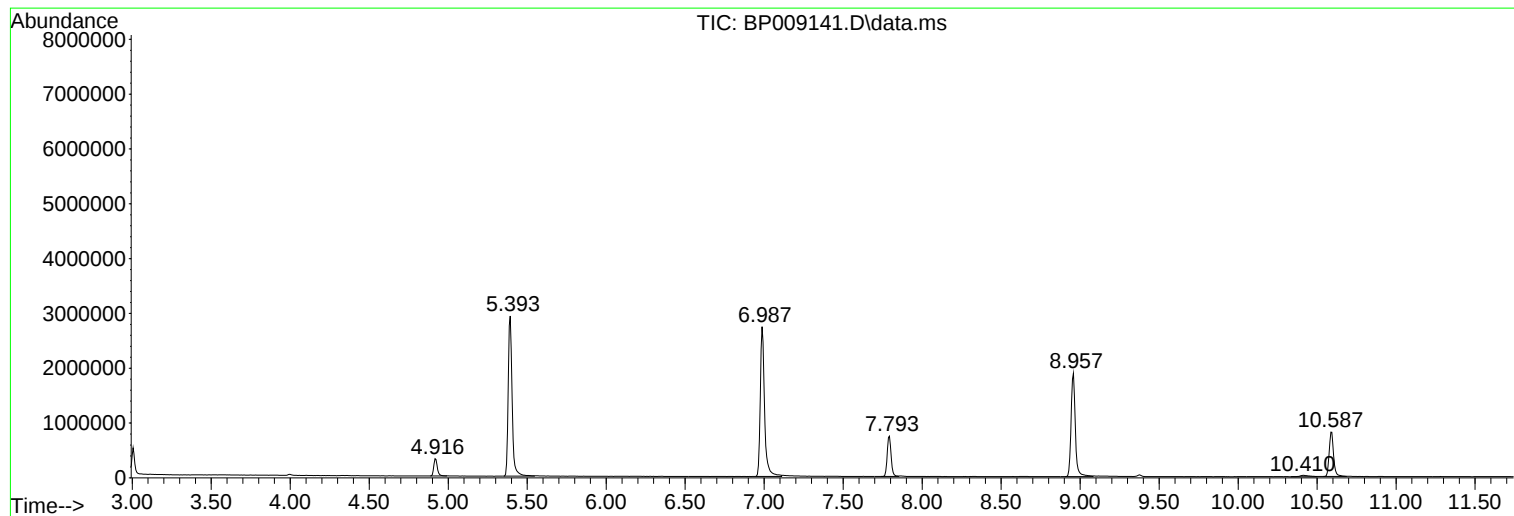
Sum of corrected areas: 53926305

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021422\
Data File : BP009141.D
Acq On : 14 Feb 2022 18:54
Operator : CG/JU
Sample : N1443-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-1-SOUTH-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.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\BP021422\
Data File : BP009141.D
Acq On : 14 Feb 2022 18:54
Operator : CG/JU
Sample : N1443-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-1-SOUTH-COMP

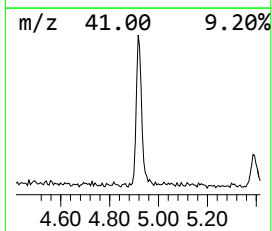
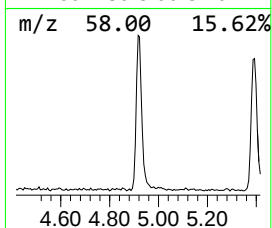
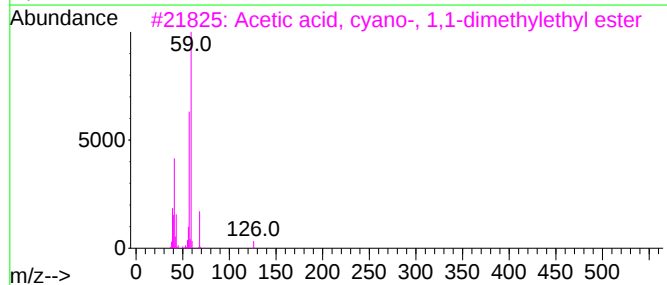
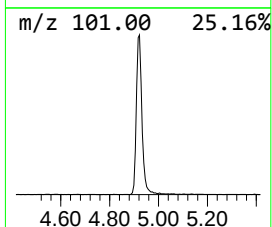
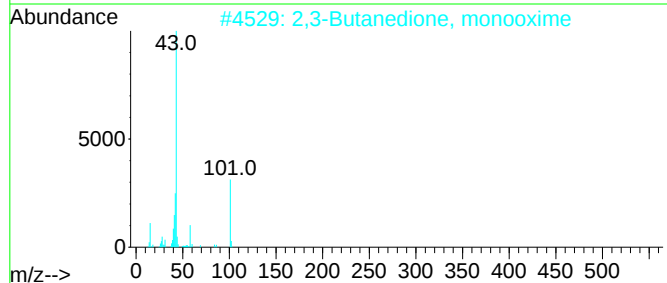
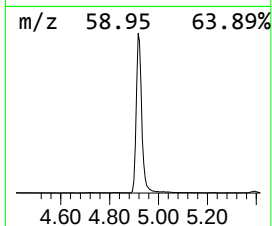
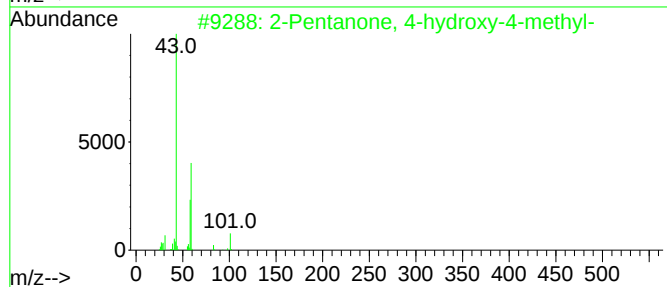
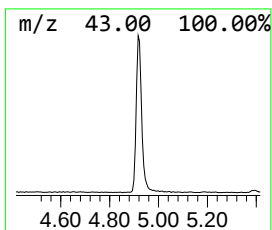
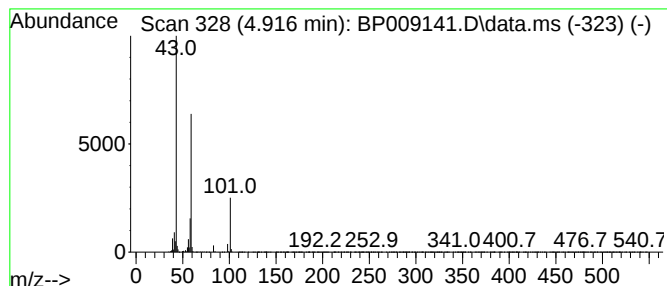
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.916	7.74 ng	491177	1,4-Dichlorobenzene-d4	7.793

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	Acetone	58	C3H6O	000067-64-1	10		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021422\
Data File : BP009141.D
Acq On : 14 Feb 2022 18:54
Operator : CG/JU
Sample : N1443-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-1-SOUTH-COMP

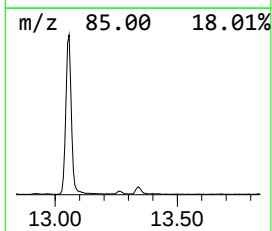
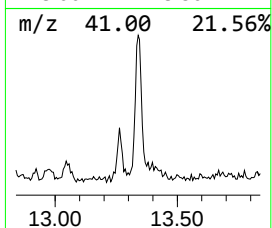
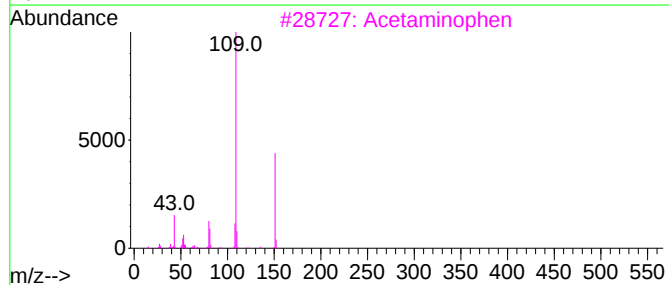
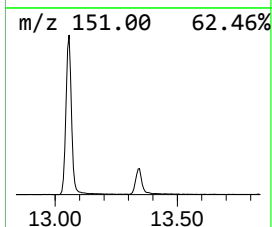
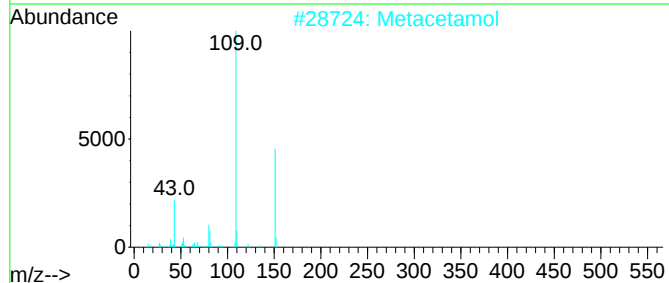
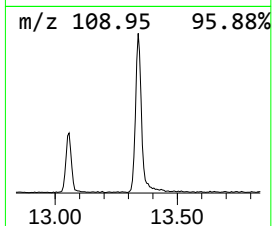
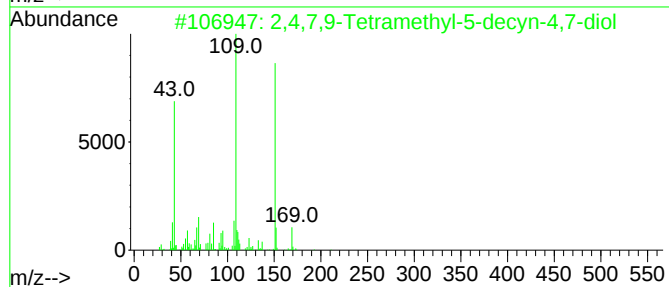
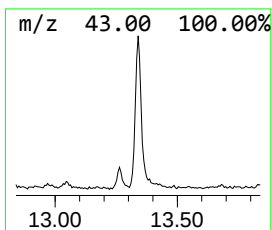
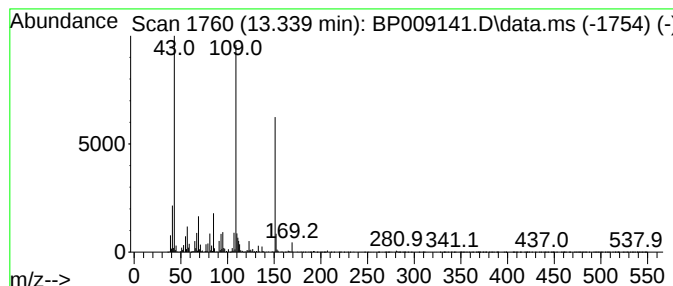
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
13.339	2.17 ng	202939	Acenaphthene-d10	14.434

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	87	
2	Metacetamol	151	C8H9NO2	000621-42-1	53	
3	Acetaminophen	151	C8H9NO2	000103-90-2	53	
4	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	53	
5	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53	



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021422\
Data File : BP009141.D
Acq On : 14 Feb 2022 18:54
Operator : CG/JU
Sample : N1443-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-1-SOUTH-COMP

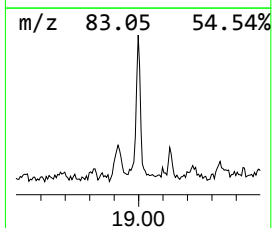
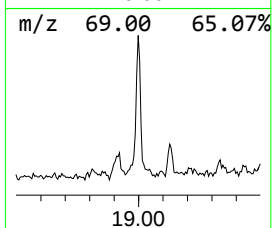
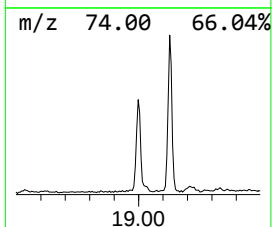
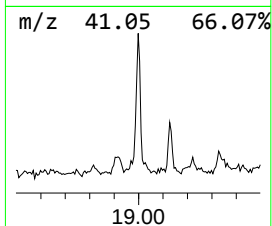
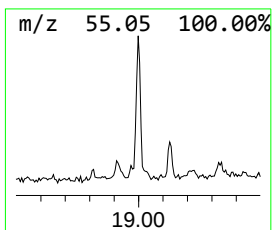
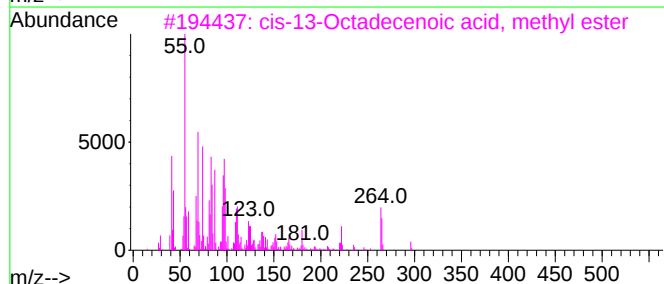
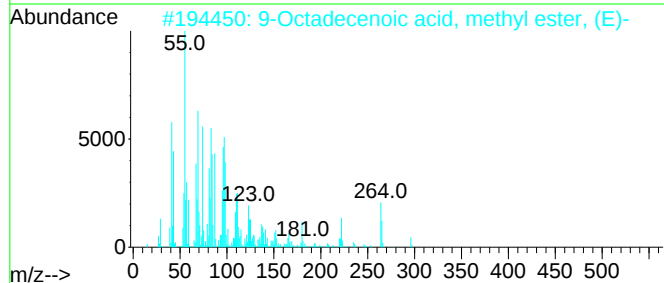
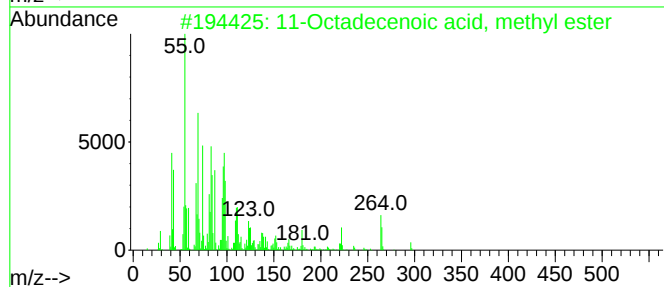
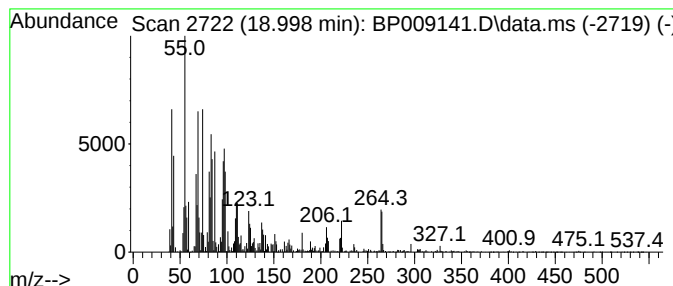
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 11-Octadecenoic acid, methyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.998	2.27 ng	240566	Phenanthrene-d10	17.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99
2			9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
3			cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1010333-58-3	99
4			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
5			8-Octadecenoic acid, methyl este...	296	C19H36O2	026528-50-7	99



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021422\
Data File : BP009141.D
Acq On : 14 Feb 2022 18:54
Operator : CG/JU
Sample : N1443-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-1-SOUTH-COMP

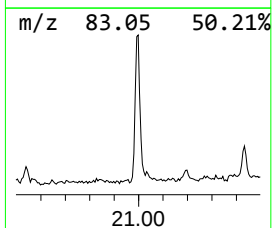
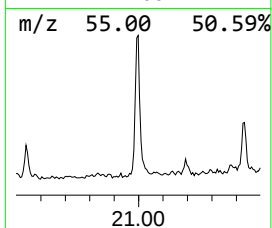
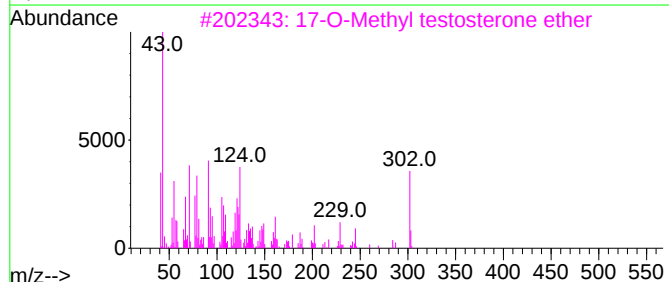
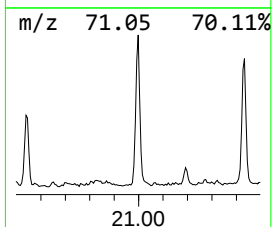
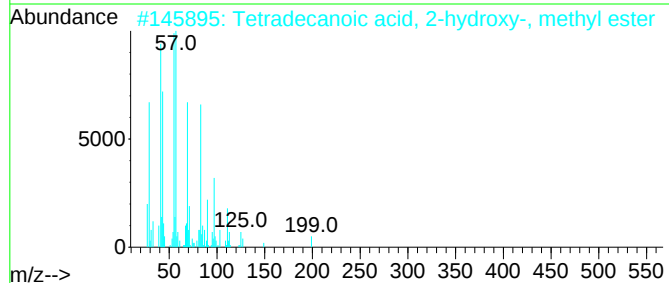
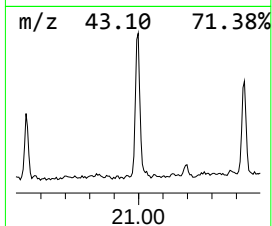
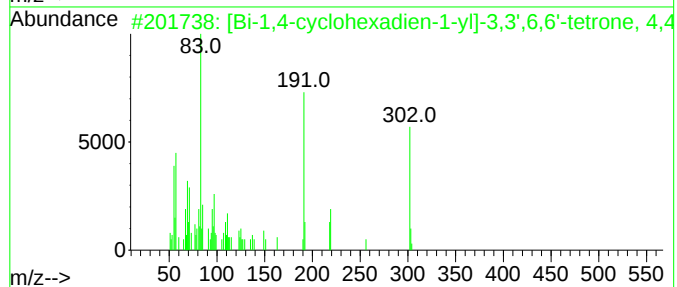
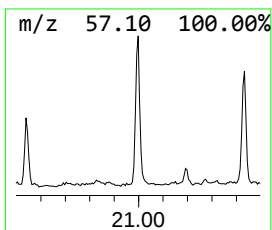
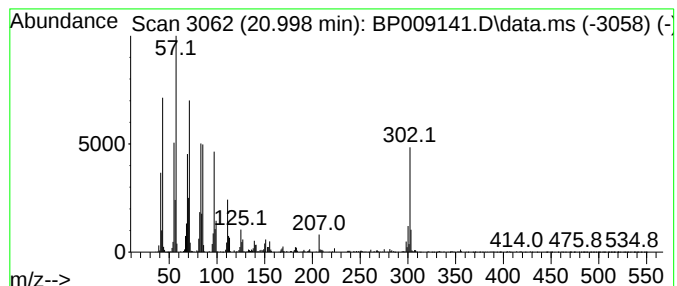
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown20.998 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.998	12.07 ng	1610660	Chrysene-d12	21.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			[Bi-1,4-cyclohexadien-1-yl]-3,3'...	302	C16H14O6	010493-51-3	16
2			Tetradecanoic acid, 2-hydroxy-, ...	258	C15H30O3	056009-40-6	12
3			17-O-Methyl testosterone ether	302	C20H30O2	013990-32-4	9
4			3-Amino-4-butyryl-5-phenyl-2,4-c...	302	C18H14N4O	1000326-93-7	9
5			1,22-Docosanediol	342	C22H46O2	022513-81-1	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021422\
Data File : BP009141.D
Acq On : 14 Feb 2022 18:54
Operator : CG/JU
Sample : N1443-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-1-SOUTH-COMP

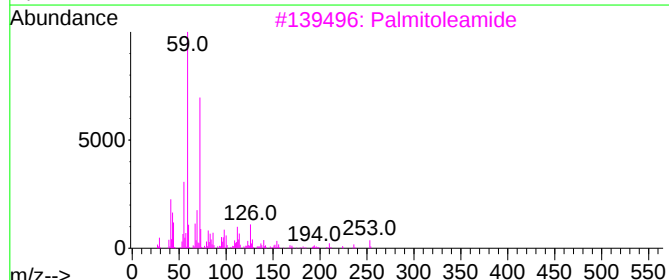
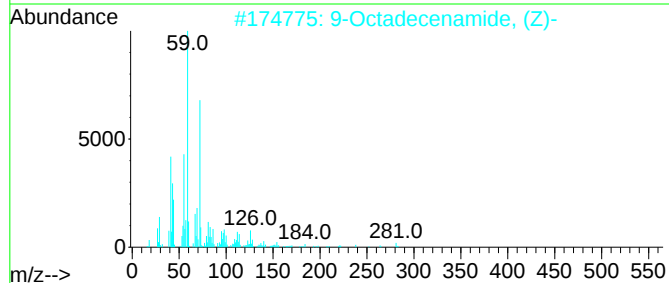
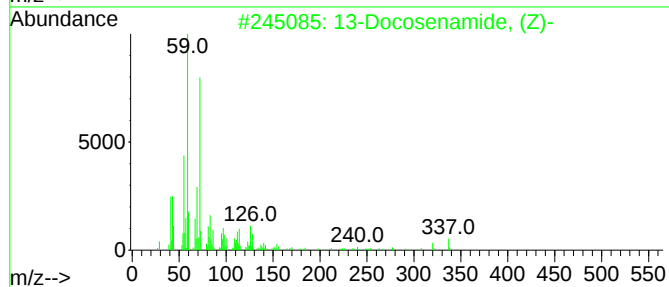
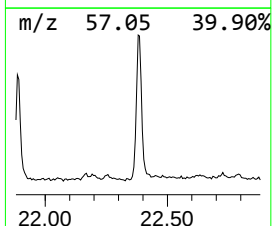
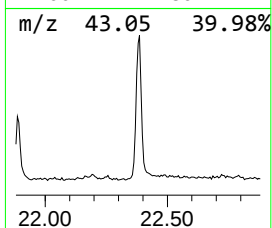
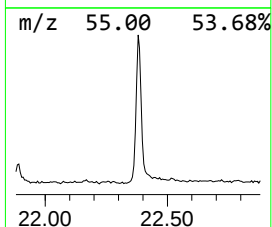
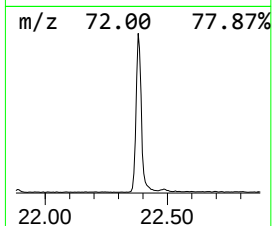
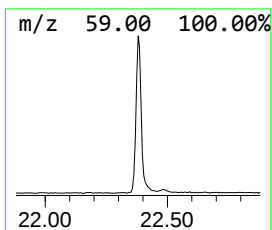
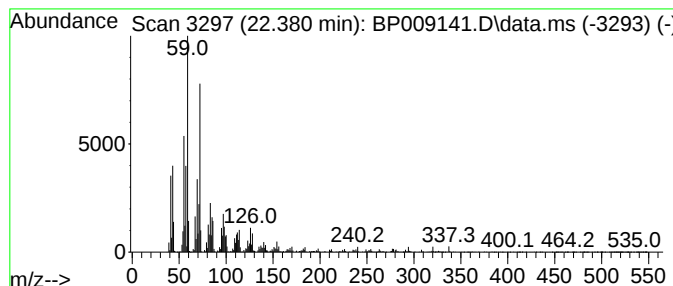
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 13-Docosenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.380	10.09 ng	1345760	Chrysene-d12	21.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	98
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
3			Palmitoleamide	253	C16H31NO	106010-22-4	80
4			Tetradecanamide	227	C14H29NO	000638-58-4	47
5			Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021422\
Data File : BP009141.D
Acq On : 14 Feb 2022 18:54
Operator : CG/JU
Sample : N1443-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-1-SOUTH-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.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
2-Pentanone, 4-...	4.916	7.7	ng	491177	1	7.793	1269020	20.0
2,4,7,9-Tetrame...	13.339	2.2	ng	202939	3	14.434	1873070	20.0
11-Octadecenoic...	18.998	2.3	ng	240566	4	17.192	2118580	20.0
unknown20.998	20.998	12.1	ng	1610660	5	21.292	2668660	20.0
13-Docosenamide...	22.380	10.1	ng	1345760	5	21.292	2668660	20.0