

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102922\
 Data File : BF130853.D
 Acq On : 29 Oct 2022 13:11
 Operator : CG\JU
 Sample : N5267-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP1-1024

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-BF102722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130853.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.281	27	33	44	rVB	840807	1082000	45.85%	6.122%
2	2.393	46	52	58	rBV	43210	53274	2.26%	0.301%
3	3.140	172	179	187	rBV	46818	80207	3.40%	0.454%
4	4.075	334	338	343	rVB	64444	77259	3.27%	0.437%
5	5.175	519	525	532	rVB	253074	306046	12.97%	1.732%
6	5.557	584	590	593	rBV	2203716	2105140	89.22%	11.911%
7	5.798	628	631	634	rBV	33144	30096	1.28%	0.170%
8	6.392	726	732	738	rBV3	45265	88592	3.75%	0.501%
9	6.469	742	745	747	rBV	33650	33568	1.42%	0.190%
10	6.498	747	750	752	rVB2	28289	27175	1.15%	0.154%
11	6.557	754	760	763	rBV	2040832	2094610	88.77%	11.851%
12	6.669	774	779	786	rBV4	22790	35767	1.52%	0.202%
13	6.769	792	796	800	rVB2	57235	55486	2.35%	0.314%
14	6.939	822	825	829	rBV	714353	582970	24.71%	3.298%
15	7.504	916	921	924	rBV	1423309	1264001	53.57%	7.152%
16	7.963	997	999	1003	rBV2	30557	27861	1.18%	0.158%
17	8.228	1040	1044	1047	rBV	853657	717398	30.40%	4.059%
18	8.939	1162	1165	1168	rVB	56290	43363	1.84%	0.245%
19	9.304	1222	1227	1230	rBV	2822753	2359621	100.00%	13.351%
20	9.563	1264	1271	1275	rBV	24947	34083	1.44%	0.193%
21	9.986	1336	1343	1346	rBV	1071859	839139	35.56%	4.748%
22	10.775	1473	1477	1480	rBV	1624261	1399536	59.31%	7.919%
23	10.898	1494	1498	1501	rBV2	32101	43180	1.83%	0.244%
24	11.480	1593	1597	1600	rBV	884171	803848	34.07%	4.548%
25	11.992	1680	1684	1689	rBV3	101943	137067	5.81%	0.776%
26	12.780	1816	1818	1822	rVB3	33567	31802	1.35%	0.180%
27	13.069	1862	1867	1870	rBV	2204665	1846875	78.27%	10.450%
28	13.621	1958	1961	1966	rBV2	53791	60129	2.55%	0.340%
29	14.063	2031	2036	2041	rBV5	34358	77546	3.29%	0.439%
30	14.121	2043	2046	2050	rVB	605651	506562	21.47%	2.866%
31	14.221	2058	2063	2069	rBV	153124	177651	7.53%	1.005%
32	14.592	2123	2126	2130	rVB	27292	28762	1.22%	0.163%
33	15.268	2238	2241	2249	rVB2	35368	49157	2.08%	0.278%
34	15.639	2298	2304	2308	rBV	375214	492006	20.85%	2.784%
35	15.674	2308	2310	2315	rVB3	33283	39084	1.66%	0.221%
36	16.139	2385	2389	2396	rVB2	28027	43201	1.83%	0.244%

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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-BF102722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

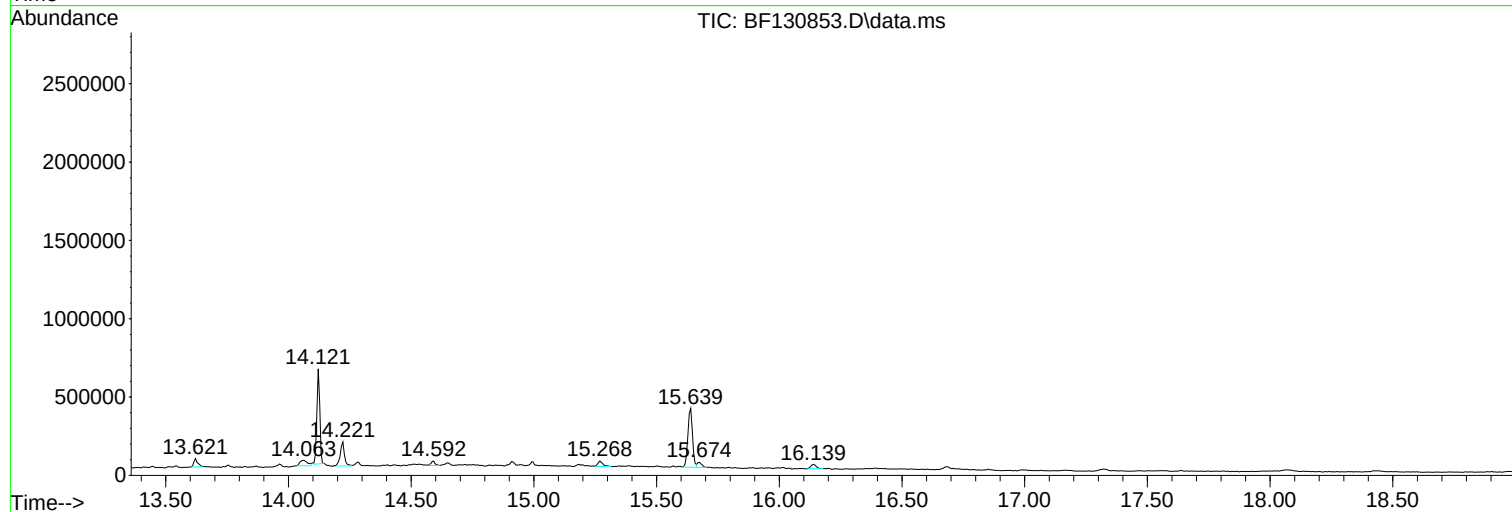
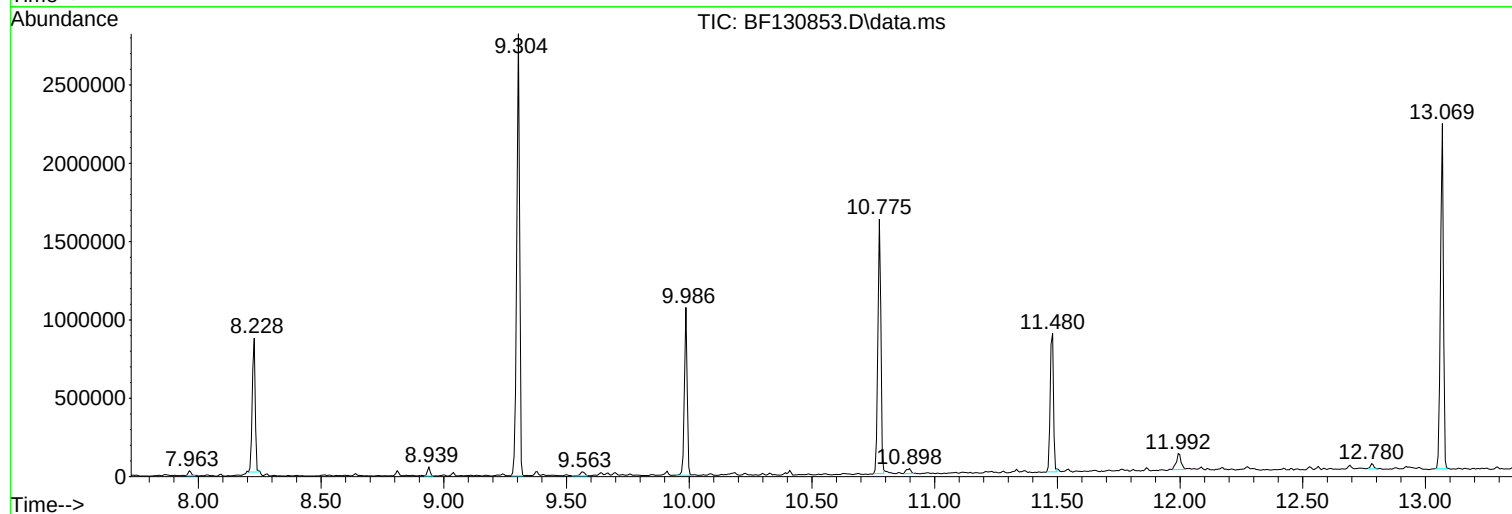
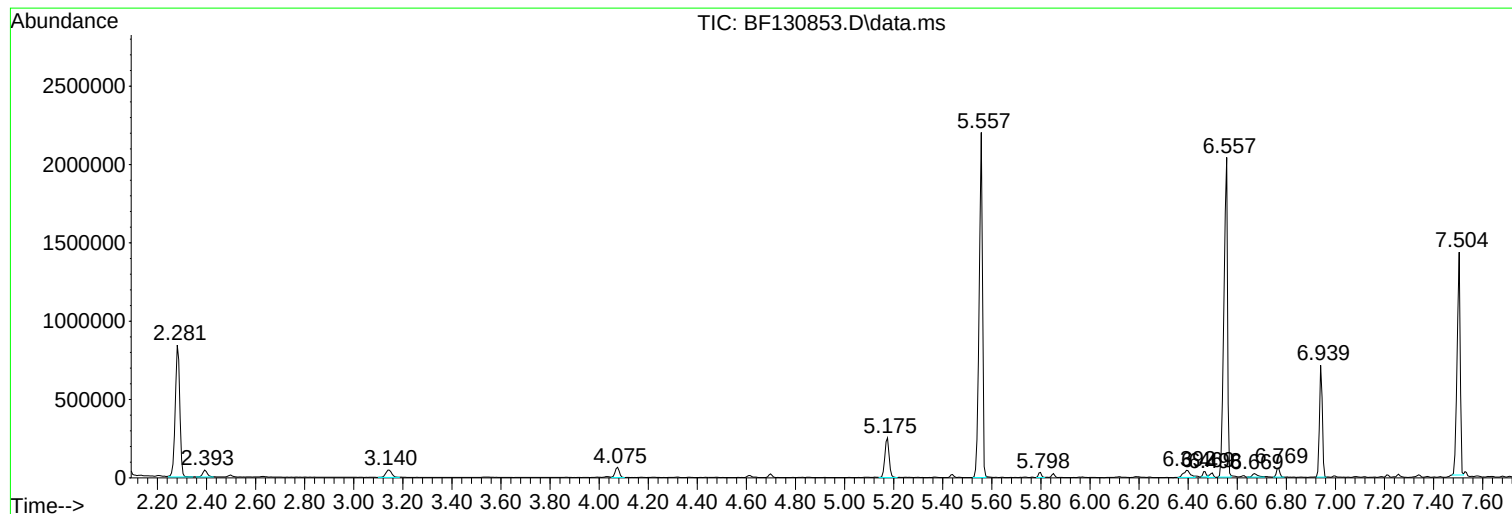
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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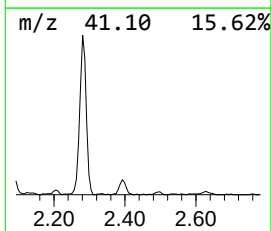
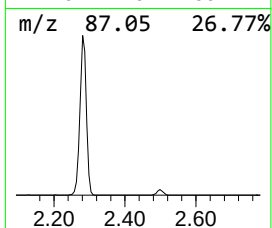
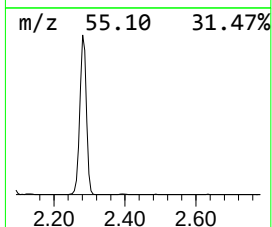
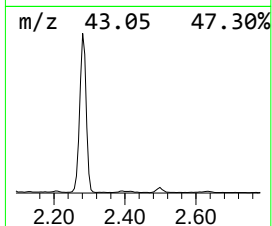
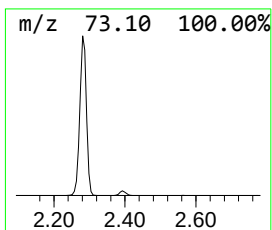
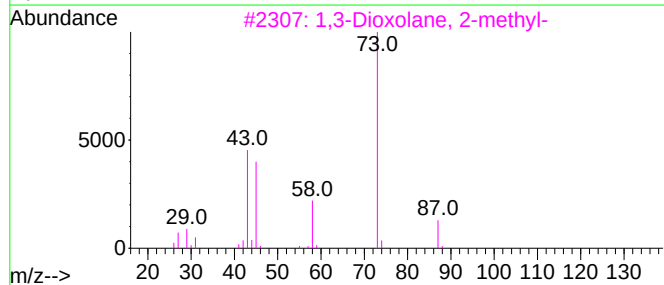
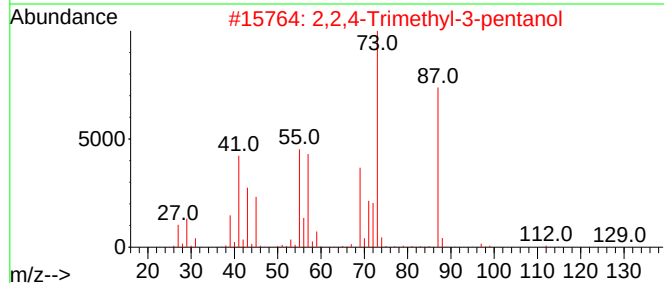
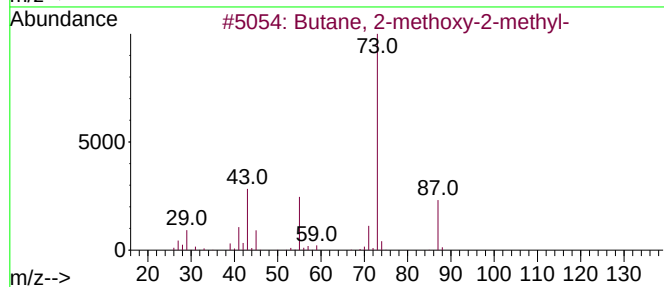
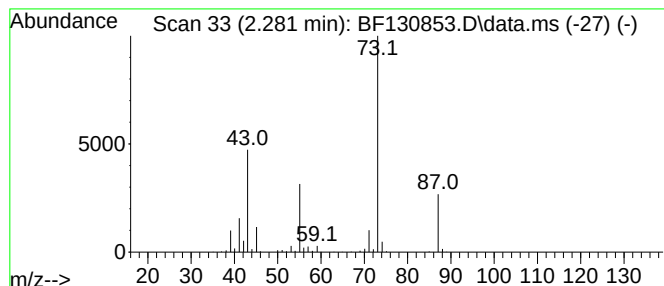
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.281	37.12 ng	1082000	1,4-Dichlorobenzene-d4	6.939

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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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Misc :
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Instrument :
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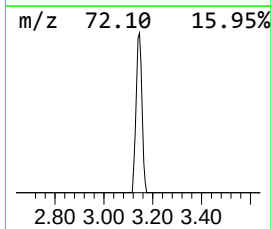
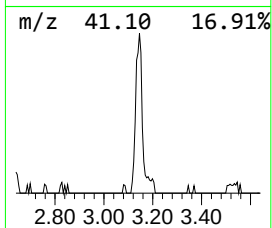
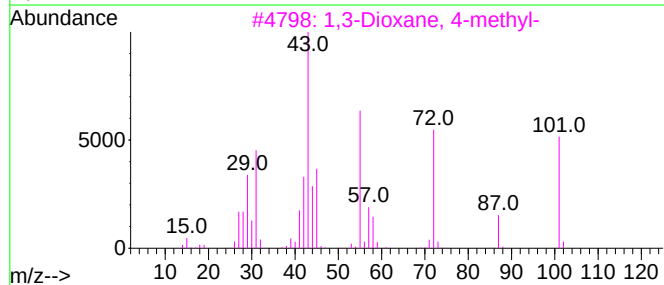
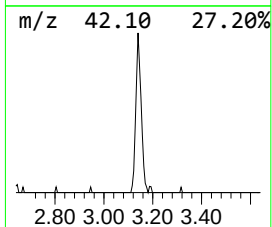
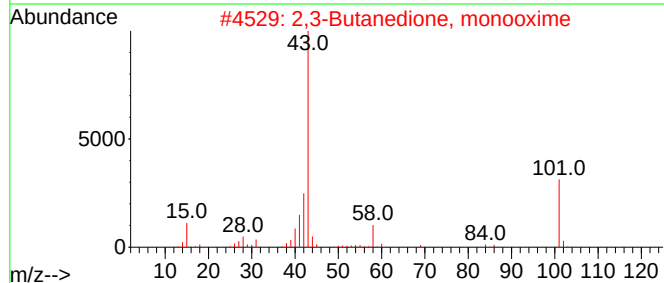
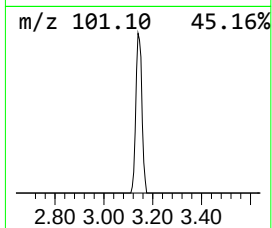
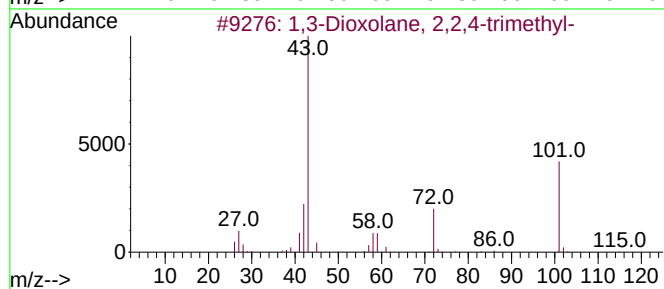
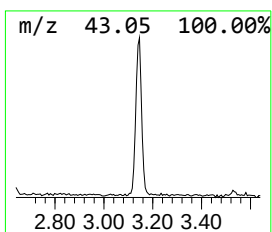
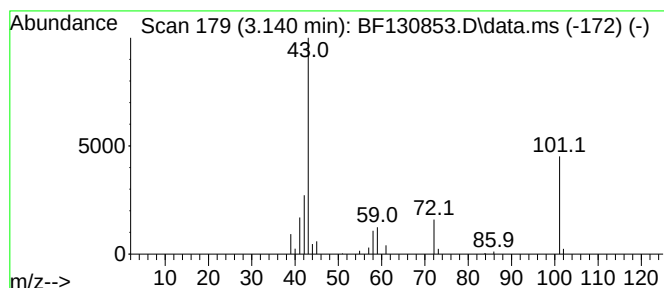
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.140	2.75 ng	80207	1,4-Dichlorobenzene-d4	6.939

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	86
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	59
3		1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	45
4		Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	42
5		1-Methoxy-2-propyl acetate	132	C6H12O3	000108-65-6	10



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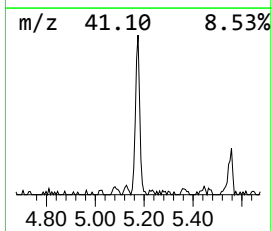
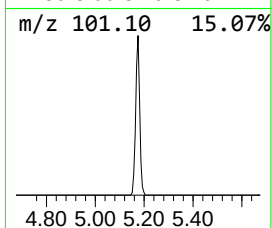
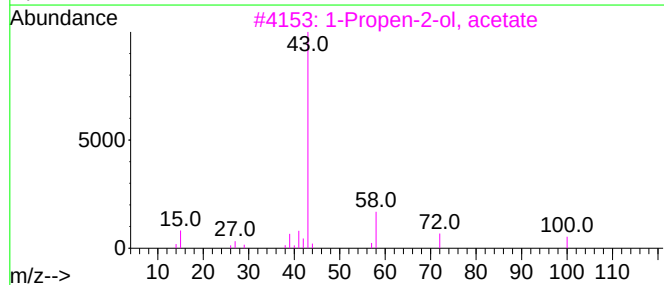
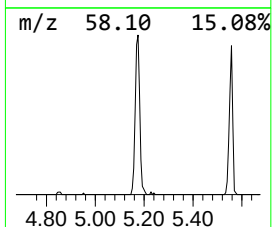
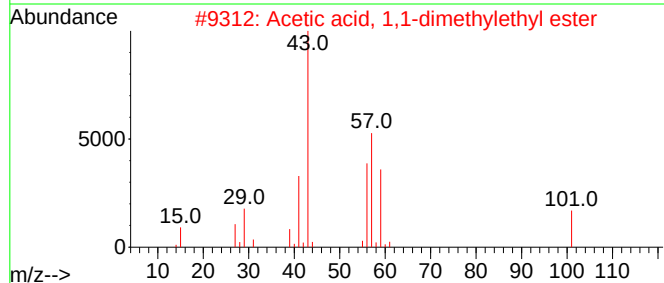
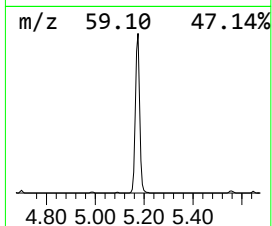
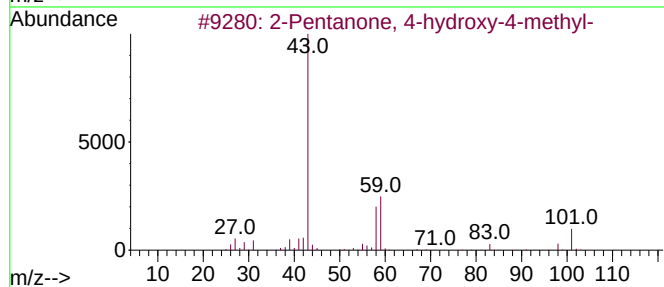
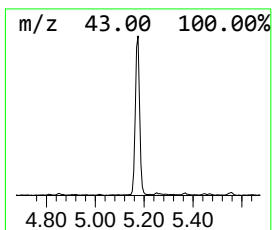
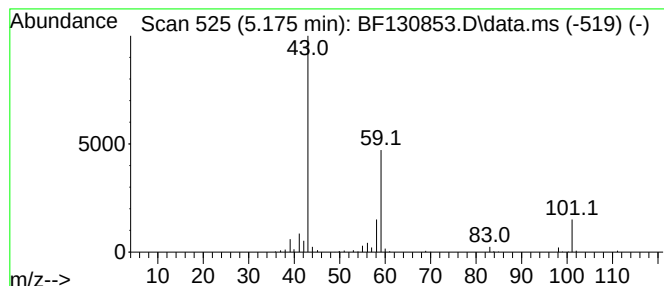
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.175	10.50 ng	306046	1,4-Dichlorobenzene-d4	6.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9



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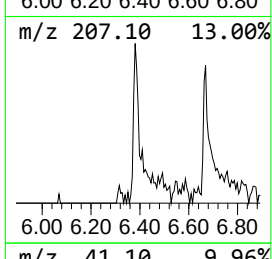
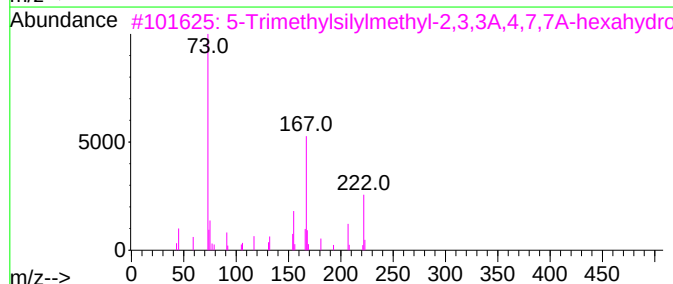
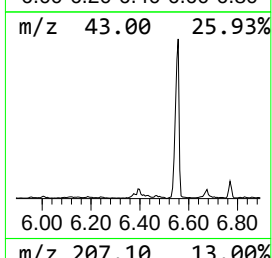
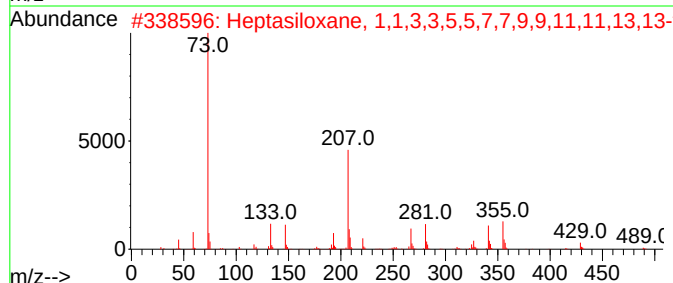
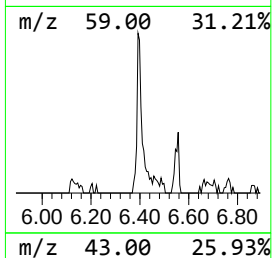
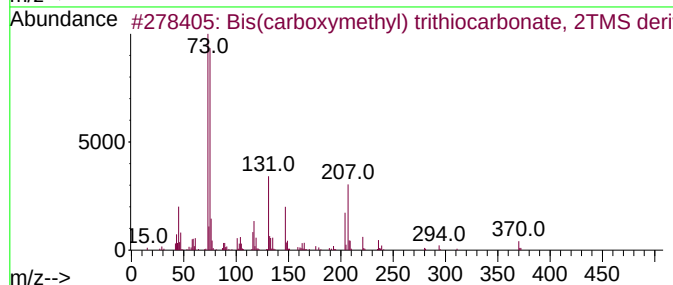
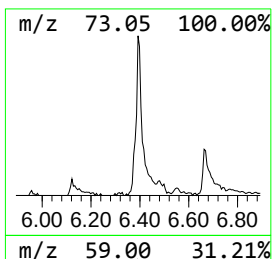
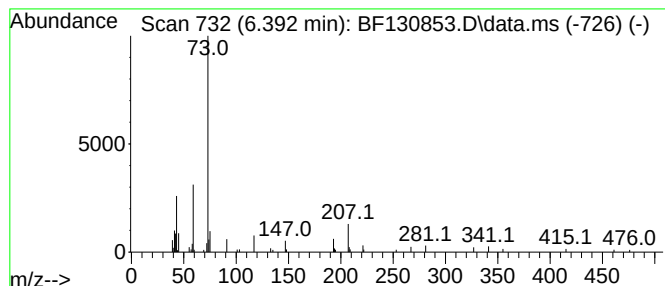
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown6.392 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.392	3.04 ng	88592	1,4-Dichlorobenzene-d4	6.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bis(carboxymethyl) trithiocarbon...	370	C11H22O4S3Si2	1000332-44-0	25
2			Heptasiloxane, 1,1,3,3,5,5,7,7,9...	504	C14H44O6Si7	019095-23-9	23
3			5-Trimethylsilylmethyl-2,3,3A,4,...	222	C13H22OSi	1000424-82-6	10
4			Trimethylsilyl-di(trimethylsiloxy...	280	C9H28O2Si4	139347-50-5	10
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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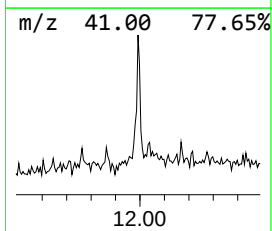
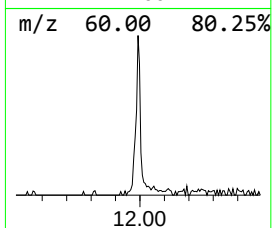
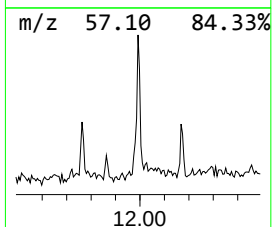
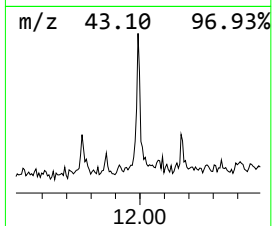
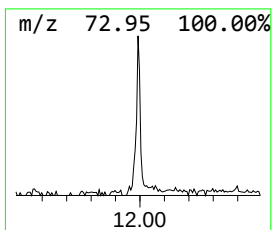
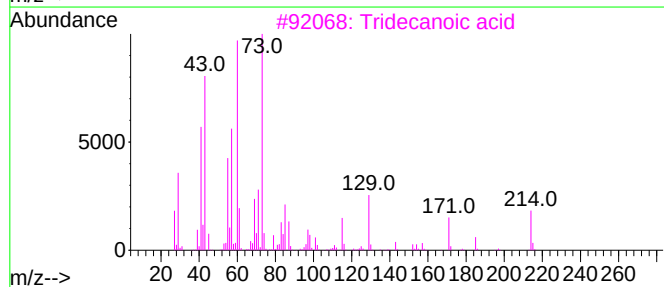
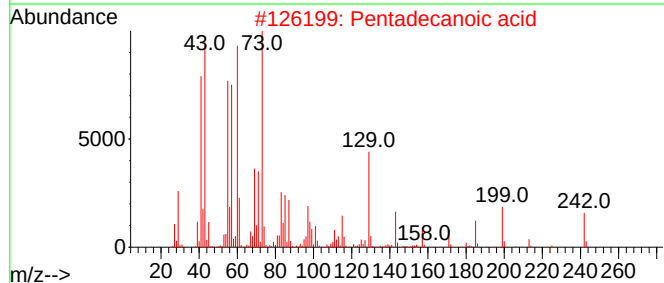
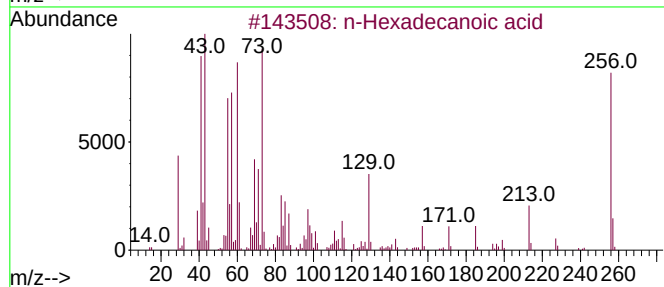
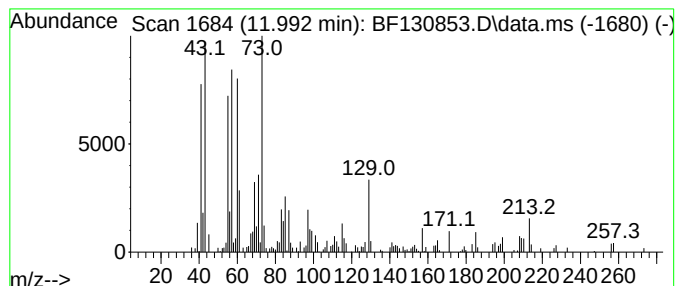
Instrument :
BNA_F
ClientSampleId :
TP1-1024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.992	3.41 ng	137067	Phenanthrene-d10	11.480	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102922\
Data File : BF130853.D
Acq On : 29 Oct 2022 13:11
Operator : CG\JU
Sample : N5267-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-1024

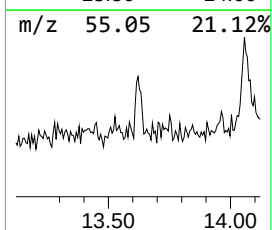
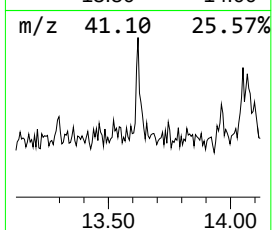
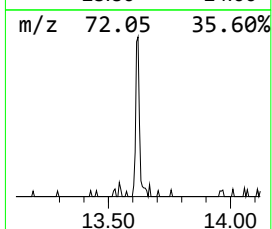
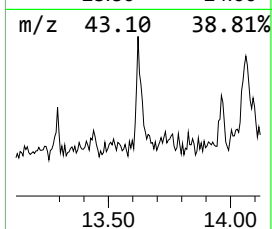
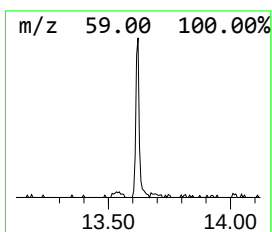
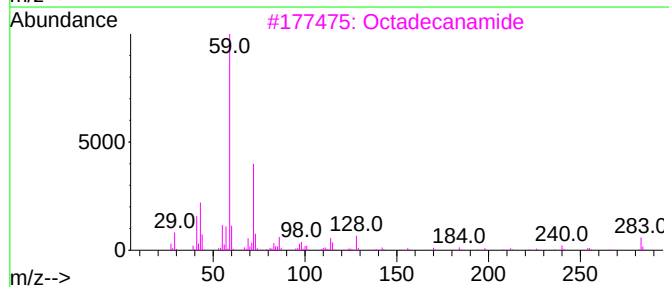
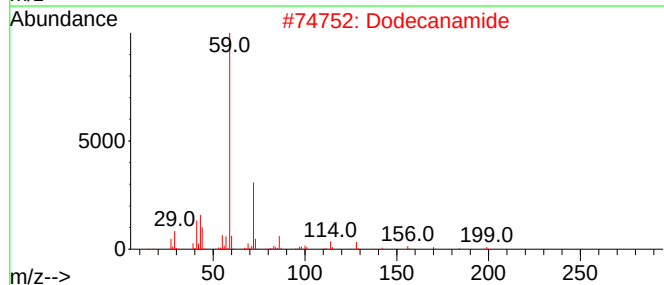
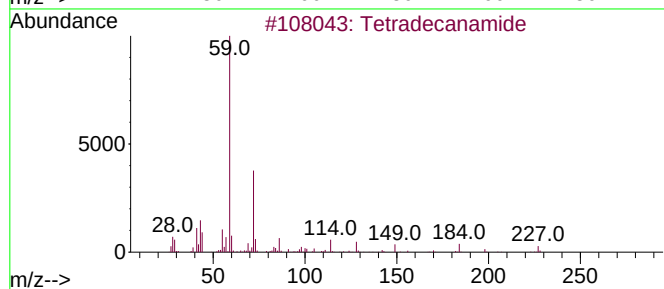
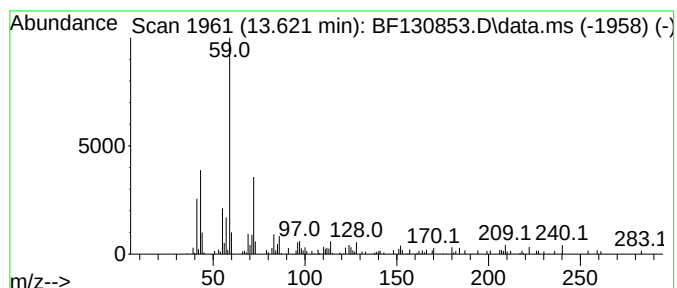
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetradecanamide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.621	2.37 ng	60129	Chrysene-d12	14.121

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecanamide	227	C14H29NO	000638-58-4	93
2		Dodecanamide	199	C12H25NO	001120-16-7	87
3		Octadecanamide	283	C18H37NO	000124-26-5	80
4		Hexadecanamide	255	C16H33NO	000629-54-9	80
5		Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102922\
Data File : BF130853.D
Acq On : 29 Oct 2022 13:11
Operator : CG\JU
Sample : N5267-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

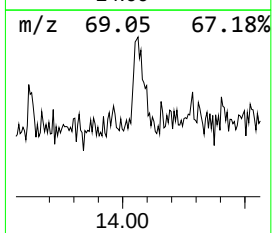
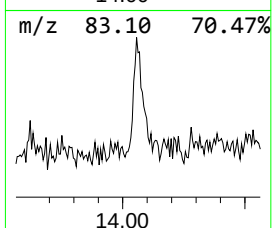
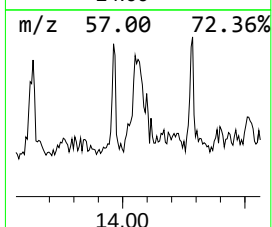
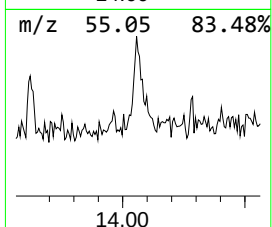
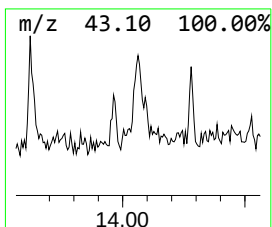
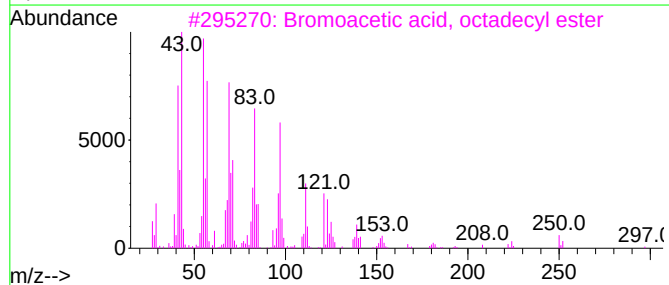
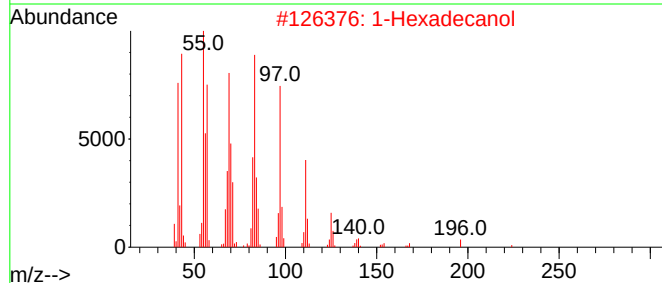
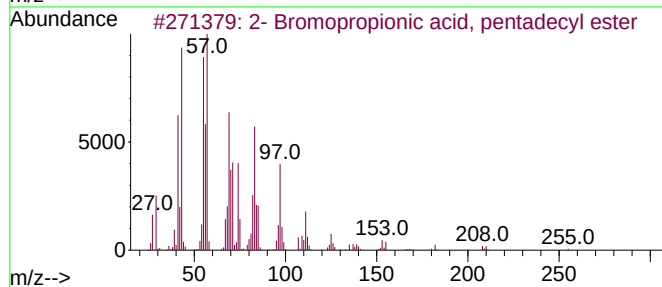
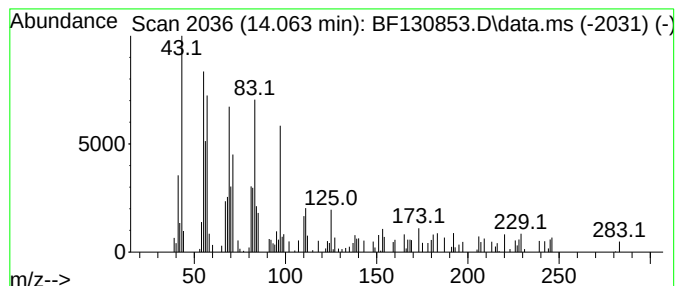
Instrument :
BNA_F
ClientSampleId :
TP1-1024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2- Bromopropionic acid, pen... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.063	3.06 ng	77546	Chrysene-d12	14.121	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	86
2	1-Hexadecanol	242	C16H34O	036653-82-4	68
3	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	64
4	Cyclohexadecane	224	C16H32	000295-65-8	64
5	Isoheptadecanol	256	C17H36O	057289-07-3	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102922\
Data File : BF130853.D
Acq On : 29 Oct 2022 13:11
Operator : CG\JU
Sample : N5267-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-1024

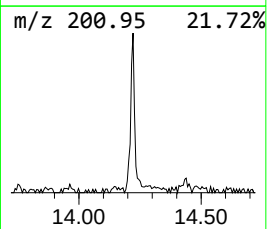
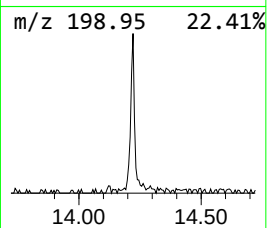
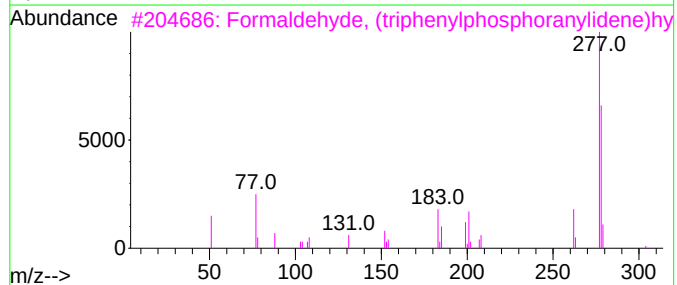
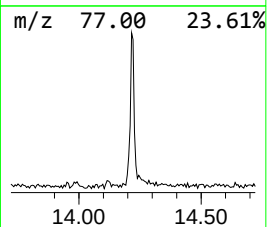
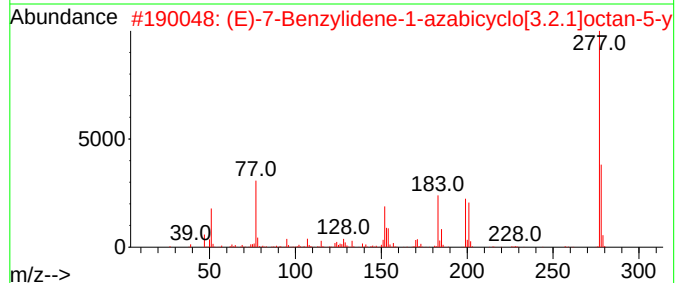
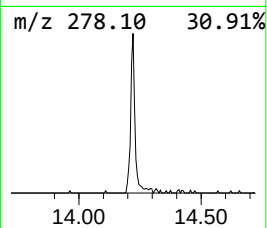
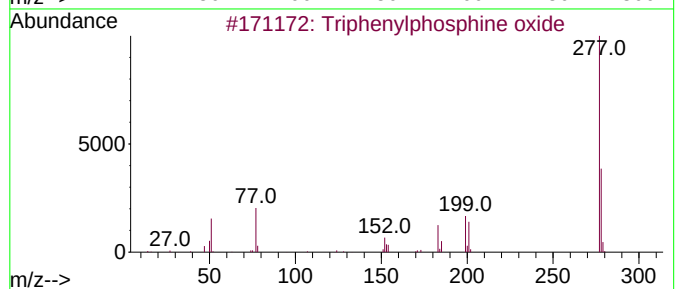
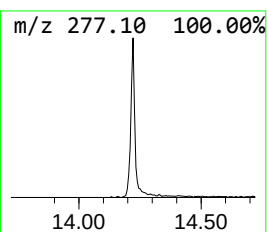
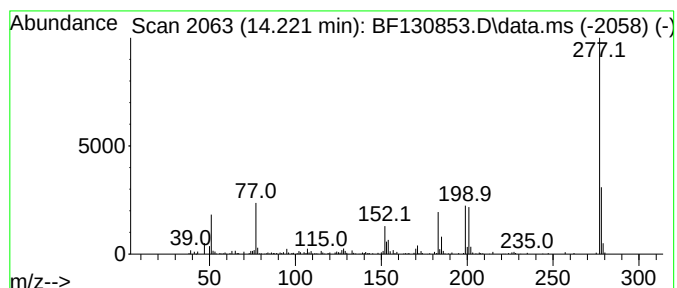
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.221	7.01 ng	177651	Chrysene-d12	14.121

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	62
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	50
4			Vanadium, cycloheptatrienyl-(pen...]	277	C17H22V	1000155-20-5	38
5			[1,2,4]Triazolo[1,5-a]pyrimidine...	278	C15H14N6	1000350-69-0	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102922\
Data File : BF130853.D
Acq On : 29 Oct 2022 13:11
Operator : CG\JU
Sample : N5267-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-1024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.281	37.1	ng	1082000	1	6.939	582970	20.0
1,3-Dioxolane, ...	3.140	2.8	ng	80207	1	6.939	582970	20.0
2-Pentanone, 4-...	5.175	10.5	ng	306046	1	6.939	582970	20.0
unknown6.392	6.392	3.0	ng	88592	1	6.939	582970	20.0
n-Hexadecanoic ...	11.992	3.4	ng	137067	4	11.480	803848	20.0
Tetradecanamide	13.621	2.4	ng	60129	5	14.121	506562	20.0
2- Bromopropion...	14.063	3.1	ng	77546	5	14.121	506562	20.0
Triphenylphosph...	14.221	7.0	ng	177651	5	14.121	506562	20.0