

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010923\
 Data File : BF131975.D
 Acq On : 09 Jan 2023 21:36
 Operator : CG\JU
 Sample : 01043-04
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-202

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-BF010923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131975.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	14	rVB	39385	48256	2.26%	0.326%
2	4.987	488	493	504	rVB	573247	754847	35.37%	5.106%
3	5.398	559	563	566	rBV	1902149	1704450	79.86%	11.530%
4	6.422	732	737	740	rBV	1795909	1743558	81.70%	11.795%
5	6.781	795	798	802	rBV	546603	445599	20.88%	3.014%
6	7.357	890	896	899	rBV	1170412	1163605	54.52%	7.871%
7	8.069	1013	1017	1021	rBV	603161	570530	26.73%	3.859%
8	9.151	1196	1201	1204	rBV	2321397	2134183	100.00%	14.437%
9	9.833	1312	1317	1320	rBV	855417	689867	32.32%	4.667%
10	9.969	1338	1340	1347	rBV	47817	48329	2.26%	0.327%
11	10.551	1435	1439	1443	rVB	107083	82448	3.86%	0.558%
12	10.628	1447	1452	1455	rBV	1711414	1437875	67.37%	9.727%
13	11.322	1567	1570	1574	rBV	802345	728965	34.16%	4.931%
14	12.104	1700	1703	1706	rBV	59574	46651	2.19%	0.316%
15	12.916	1837	1841	1844	rBV	2325916	2069017	96.95%	13.996%
16	13.810	1990	1993	2005	rBV	136040	194416	9.11%	1.315%
17	13.974	2017	2021	2025	rVB	519298	444227	20.81%	3.005%
18	14.439	2097	2100	2109	rBV4	15011	30707	1.44%	0.208%
19	14.739	2147	2151	2155	rBV5	14345	23949	1.12%	0.162%
20	15.439	2265	2270	2276	rBV	318640	385672	18.07%	2.609%
21	15.951	2352	2357	2364	rBV8	14946	35605	1.67%	0.241%

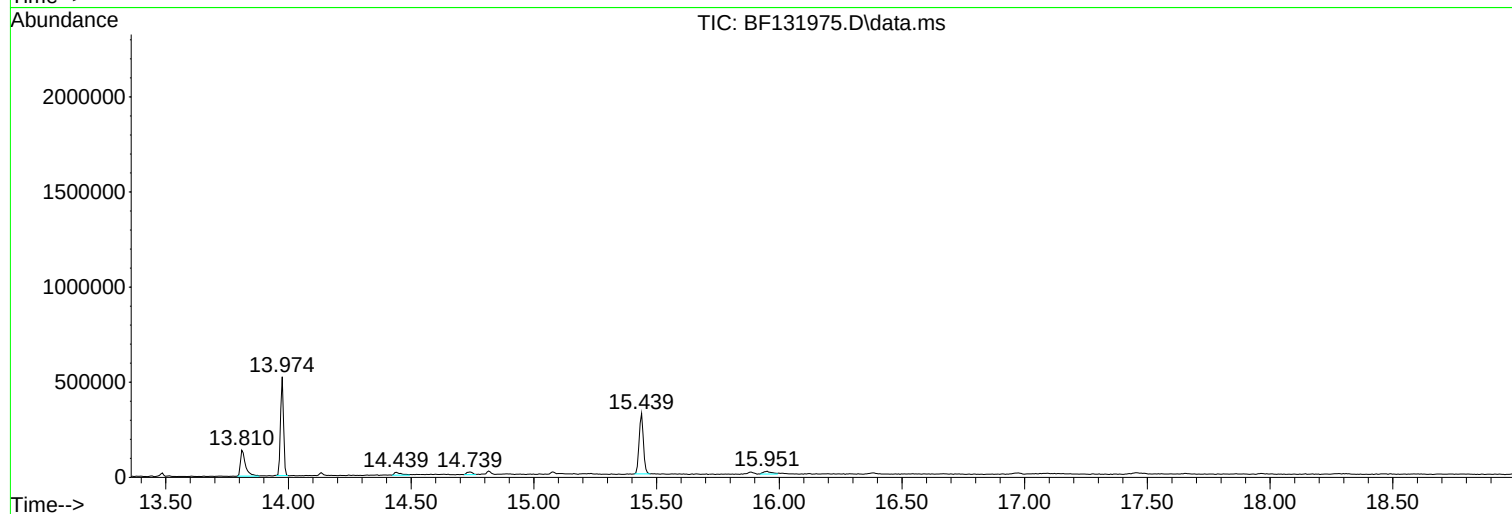
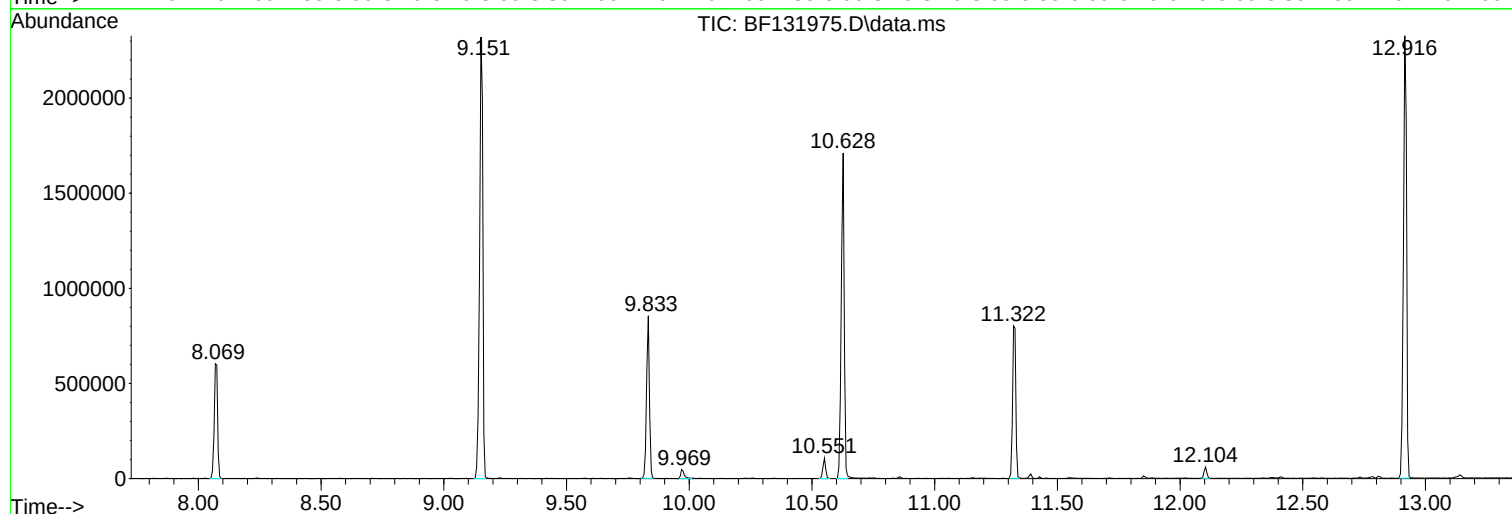
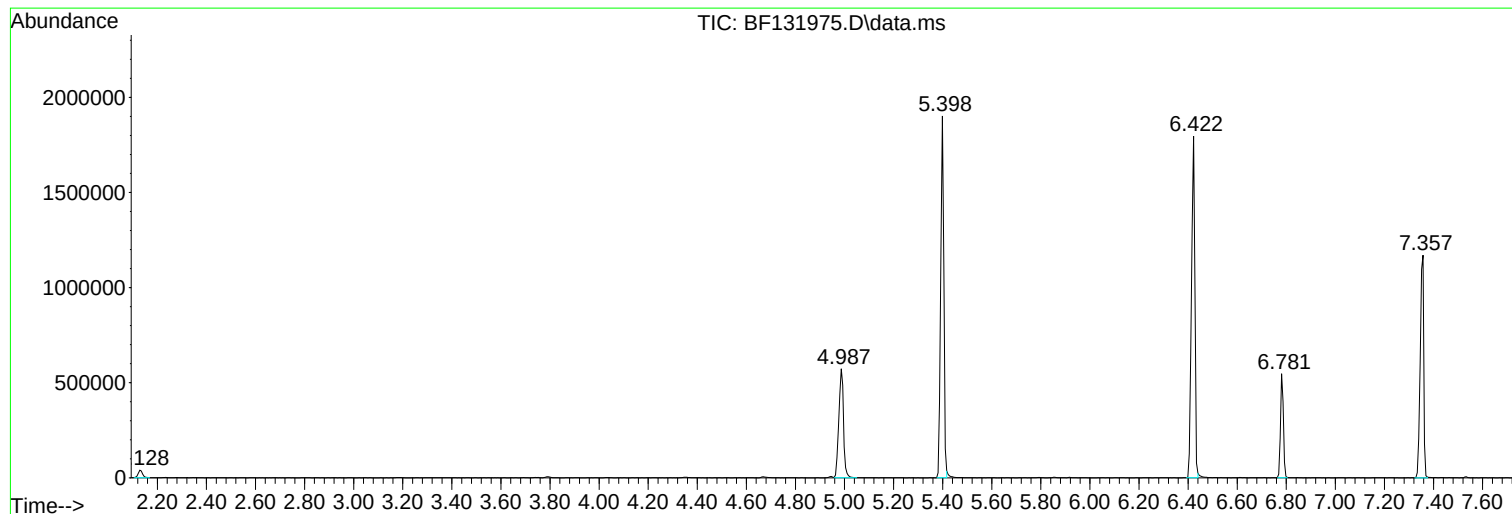
Sum of corrected areas: 14782756

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010923\
Data File : BF131975.D
Acq On : 09 Jan 2023 21:36
Operator : CG\JU
Sample : 01043-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-202

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.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\BF010923\
Data File : BF131975.D
Acq On : 09 Jan 2023 21:36
Operator : CG\JU
Sample : 01043-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-202

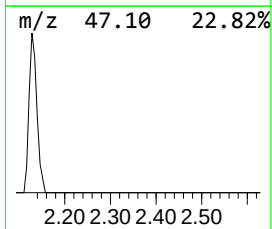
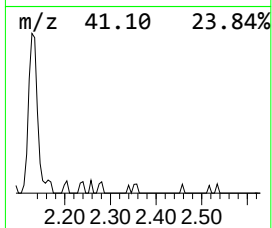
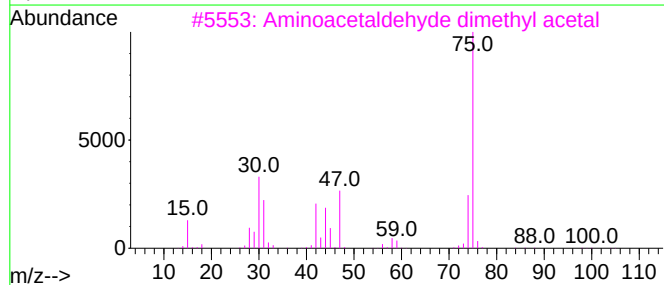
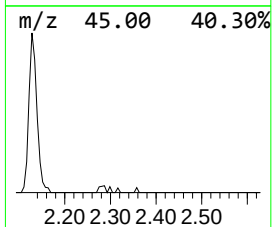
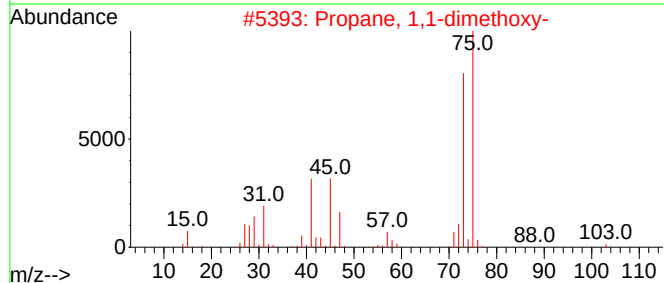
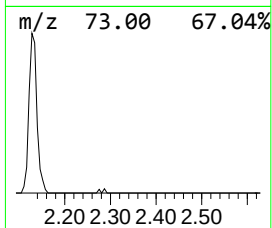
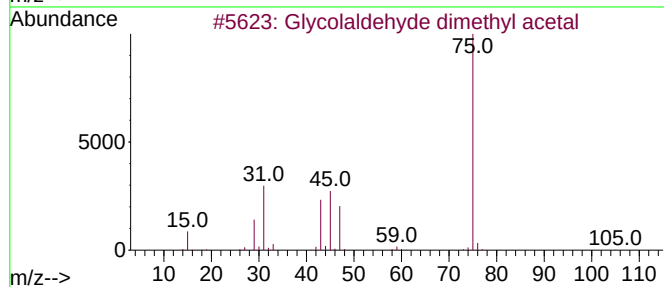
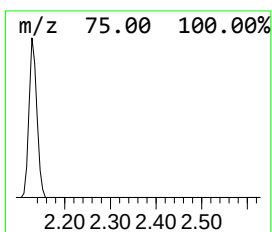
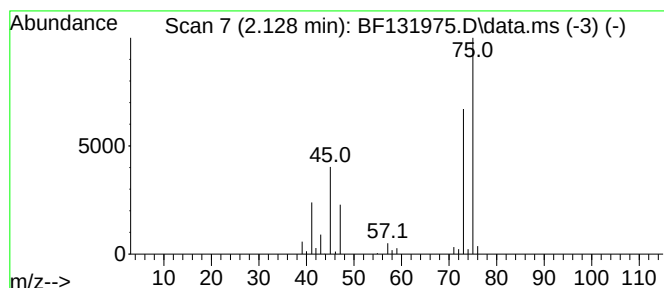
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Glycolaldehyde dimethyl acetal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	2.17 ng	48256	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	64
2			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
3			Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	9
4			Glycine	75	C2H5NO2	000056-40-6	7
5			Ethylamine	45	C2H7N	000075-04-7	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010923\
Data File : BF131975.D
Acq On : 09 Jan 2023 21:36
Operator : CG\JU
Sample : 01043-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-202

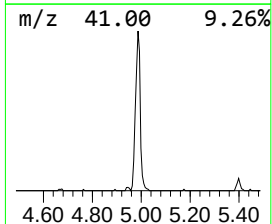
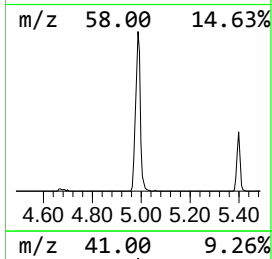
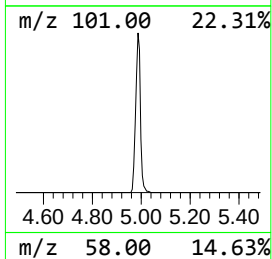
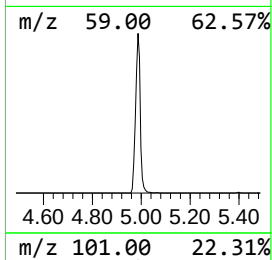
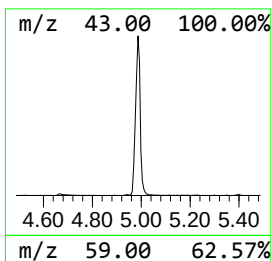
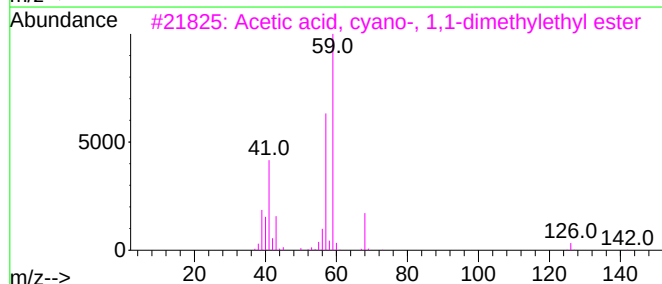
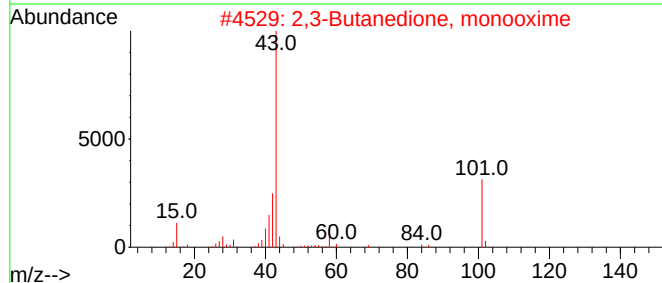
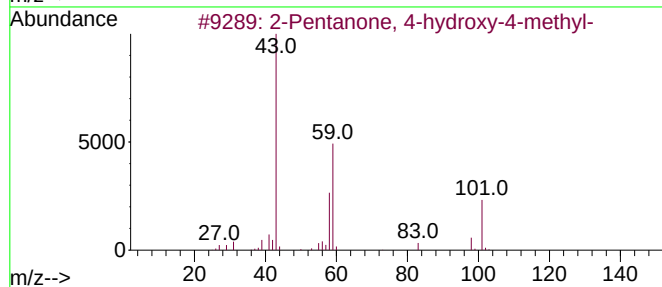
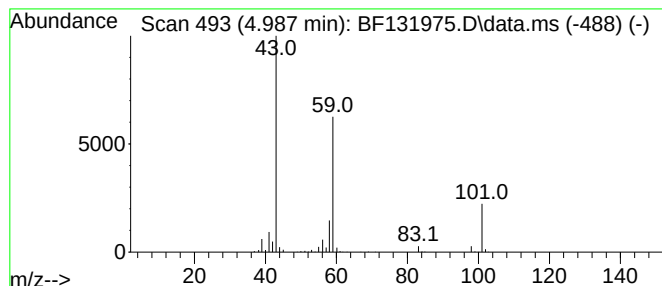
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	33.88 ng	754847	1,4-Dichlorobenzene-d4	6.781

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	23
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010923\
Data File : BF131975.D
Acq On : 09 Jan 2023 21:36
Operator : CG\JU
Sample : 01043-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-202

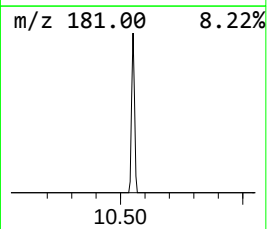
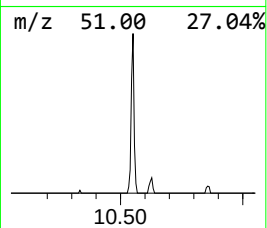
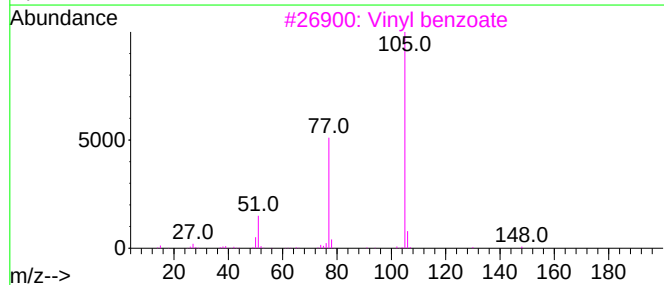
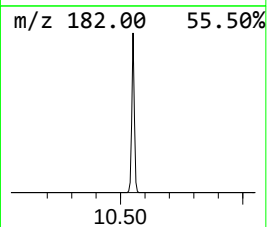
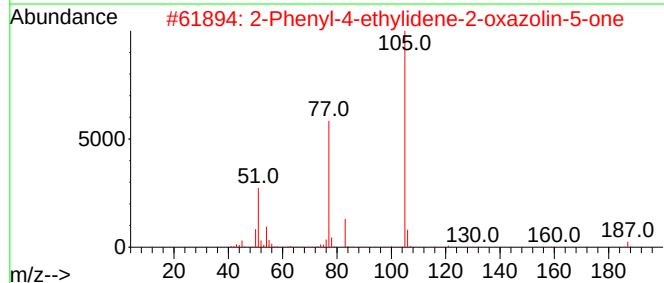
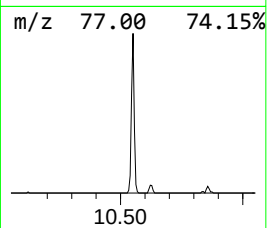
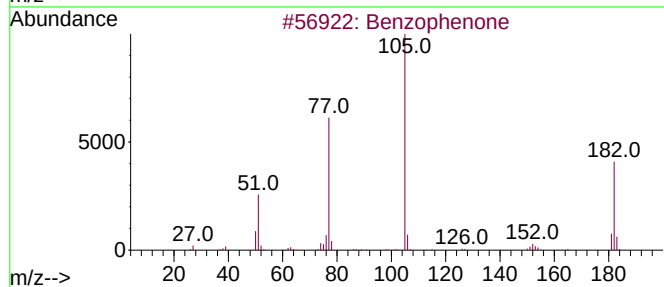
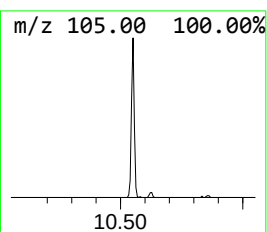
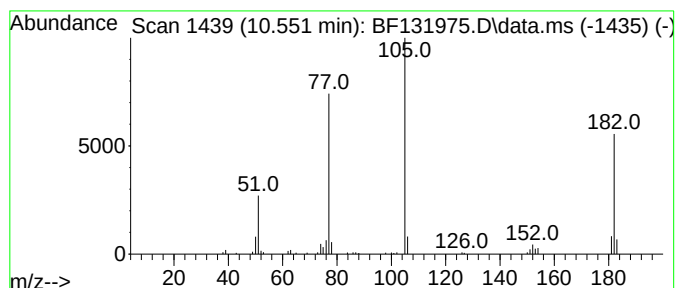
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
10.551	2.39 ng	82448	Acenaphthene-d10	9.833

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	53
3			Vinyl benzoate	148	C9H8O2	000769-78-8	53
4			1,2,4-Triazine-3,5(2H,4H)-dione,...	249	C10H7N3O3S	024168-34-1	53
5			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010923\
Data File : BF131975.D
Acq On : 09 Jan 2023 21:36
Operator : CG\JU
Sample : 01043-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

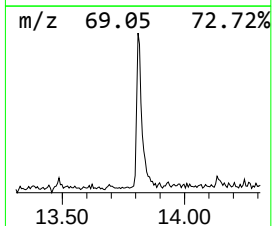
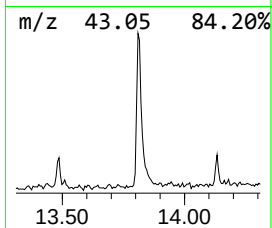
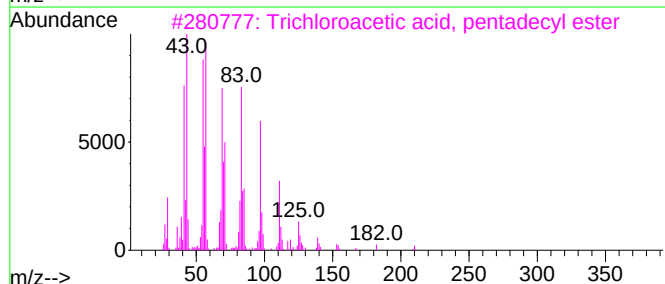
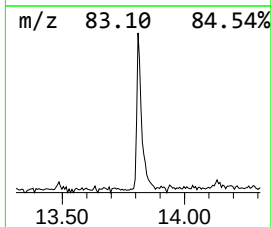
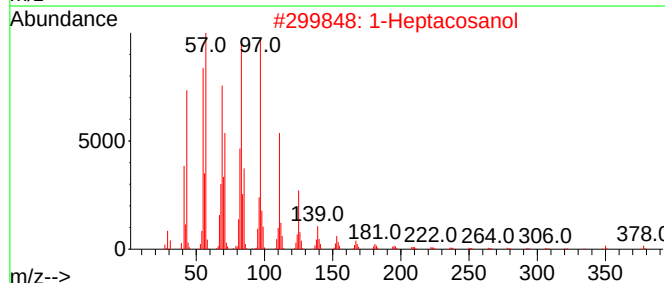
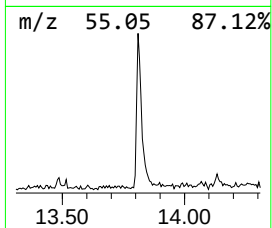
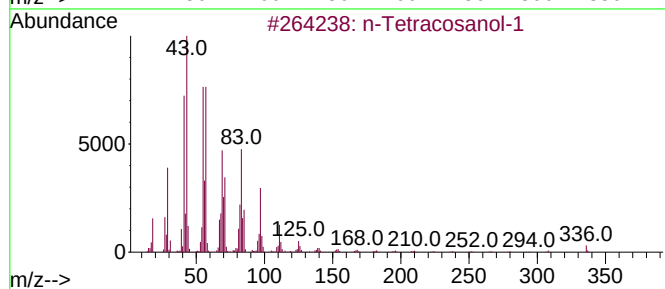
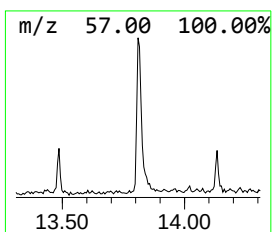
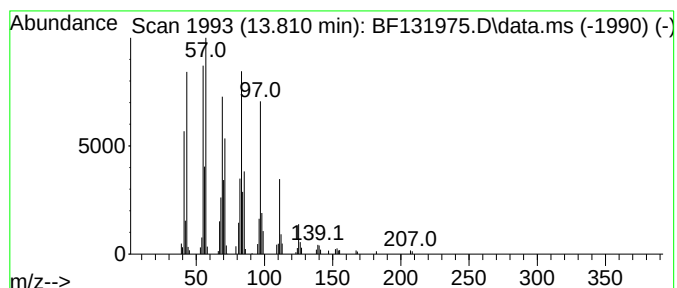
Instrument :
BNA_F
ClientSampleId :
TP-202

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.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-Tetracosanol-1 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.810	8.75 ng	194416	Chrysene-d12	13.974	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2	1-Heptacosanol	396	C27H56O	002004-39-9	91
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
4	Behenic alcohol	326	C22H46O	000661-19-8	90
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010923\
Data File : BF131975.D
Acq On : 09 Jan 2023 21:36
Operator : CG\JU
Sample : 01043-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-202

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.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
Glycolaldehyde ...	2.128	2.2	ng	48256	1	6.781	445599	20.0
2-Pentanone, 4-...	4.987	33.9	ng	754847	1	6.781	445599	20.0
Benzophenone	10.551	2.4	ng	82448	3	9.833	689867	20.0
n-Tetracosanol-1	13.810	8.8	ng	194416	5	13.974	444227	20.0