

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052324\
 Data File : BM045752.D
 Acq On : 23 May 2024 14:08
 Operator : MA/JU
 Sample : PB161074BL
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PB161074BL

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_M\Methods\8270-BM052224.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM045752.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.781	282	288	310	rVB	2487023	4278253	25.19%	5.388%
2	5.251	361	368	386	rVB	4248368	6197716	36.49%	7.805%
3	5.551	412	419	431	rBV4	152965	325770	1.92%	0.410%
4	6.269	534	541	548	rBV	264223	473629	2.79%	0.596%
5	6.834	630	637	648	rBV	4025685	6644199	39.12%	8.367%
6	7.569	753	762	772	rBV	1156569	1802401	10.61%	2.270%
7	7.910	814	820	836	rBV2	268883	535792	3.15%	0.675%
8	8.734	951	960	974	rBV	3706522	6370544	37.51%	8.023%
9	10.339	1226	1233	1244	rVB	1470737	2527318	14.88%	3.183%
10	12.821	1647	1655	1664	rBV	8279012	12558178	73.94%	15.815%
11	14.198	1882	1889	1899	rBV	2273506	3208744	18.89%	4.041%
12	15.698	2137	2144	2158	rBV	4439634	6045236	35.59%	7.613%
13	16.945	2350	2356	2362	rBV	2663636	3713742	21.86%	4.677%
14	19.586	2799	2805	2810	rBV	14062078	16984903	100.00%	21.390%
15	21.156	3067	3072	3079	rBV	2831264	3802855	22.39%	4.789%
16	23.950	3540	3547	3558	rVB	1717478	3935922	23.17%	4.957%

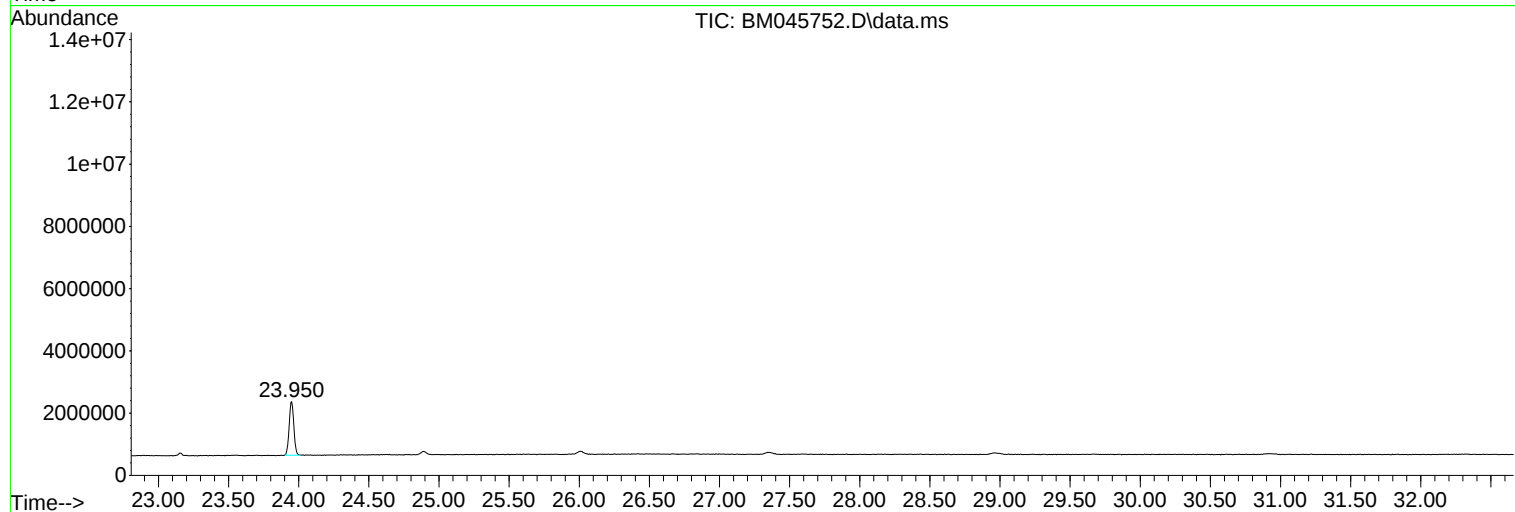
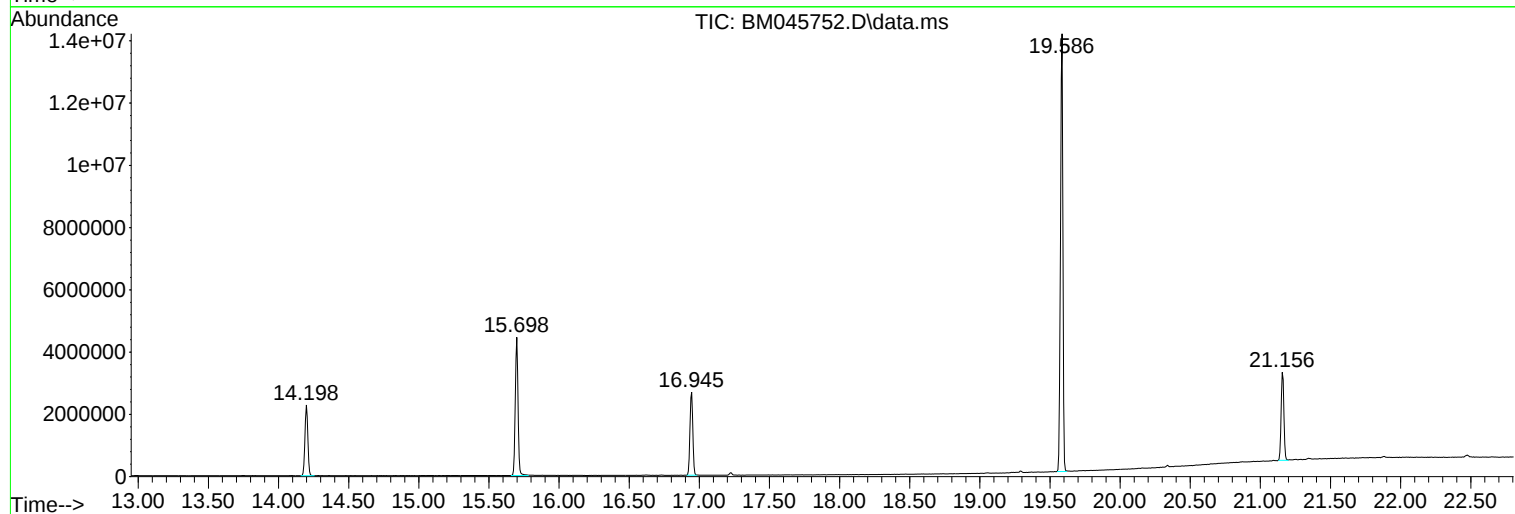
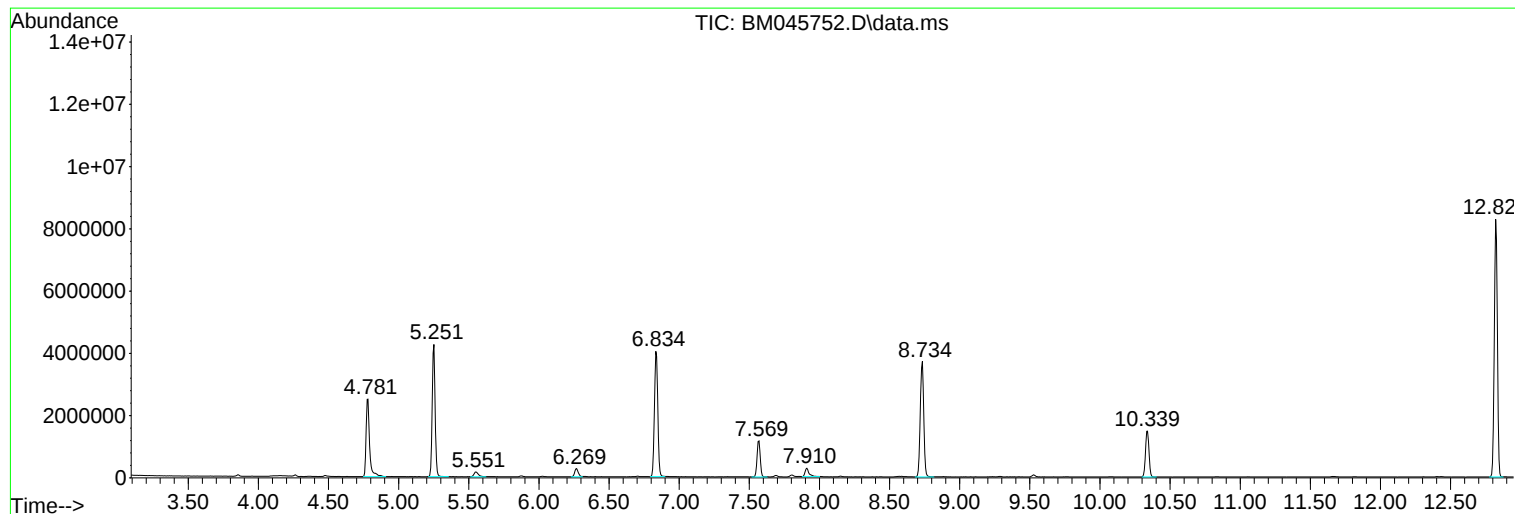
Sum of corrected areas: 79405202

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052324\
Data File : BM045752.D
Acq On : 23 May 2024 14:08
Operator : MA/JU
Sample : PB161074BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB161074BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052224.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_M\Data\BM052324\
Data File : BM045752.D
Acq On : 23 May 2024 14:08
Operator : MA/JU
Sample : PB161074BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

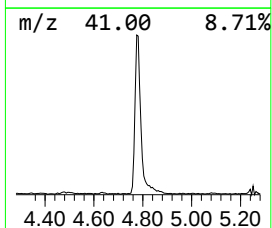
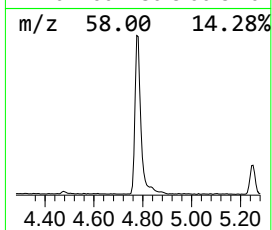
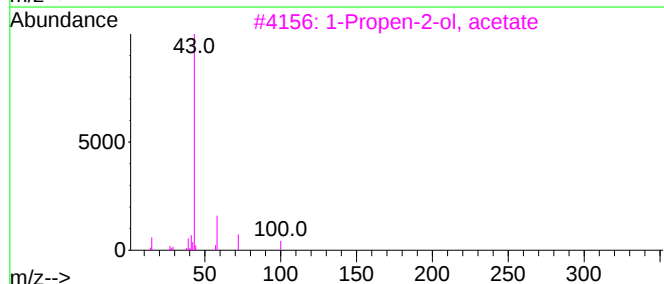
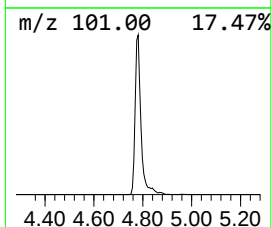
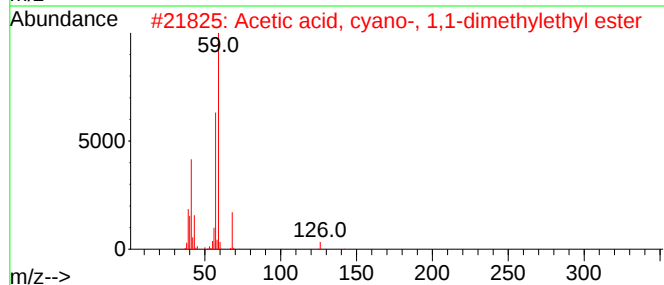
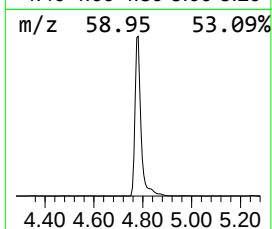
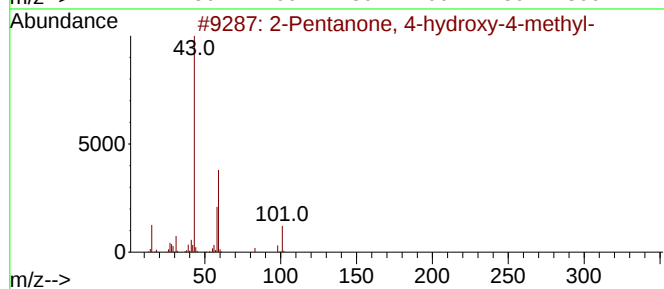
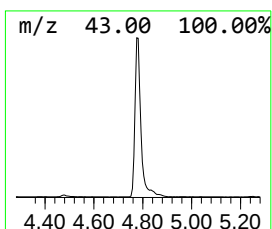
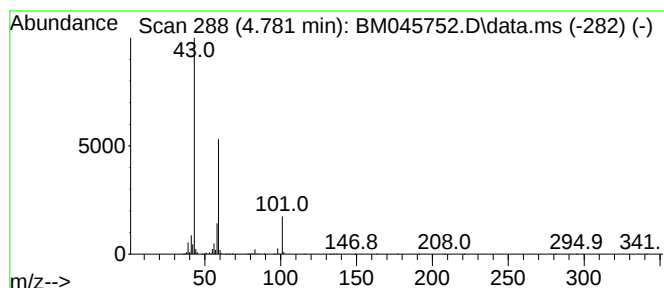
Instrument :
BNA_M
ClientSampleId :
PB161074BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052224.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 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.781	47.47 ng	4278250	1,4-Dichlorobenzene-d4	7.569	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052324\
Data File : BM045752.D
Acq On : 23 May 2024 14:08
Operator : MA/JU
Sample : PB161074BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB161074BL

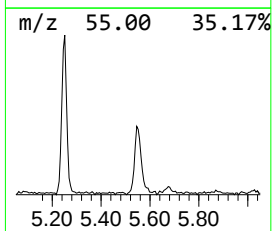
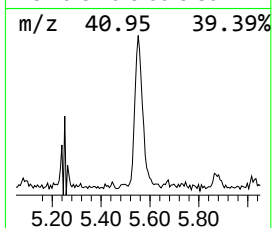
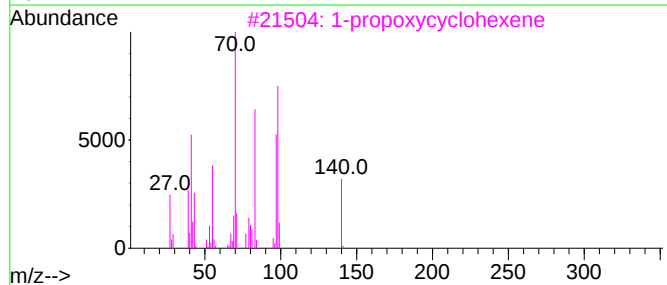
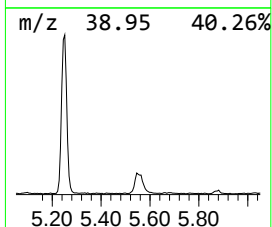
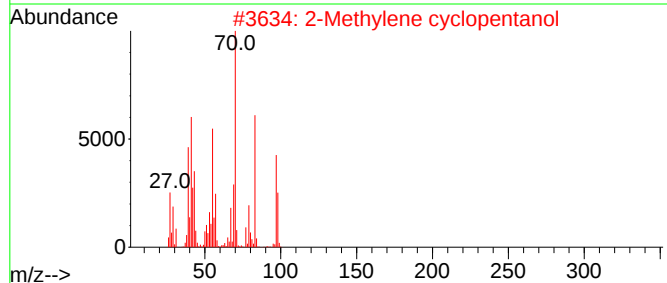
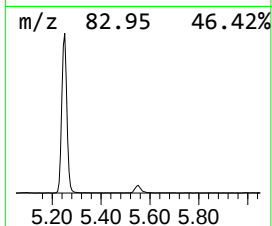
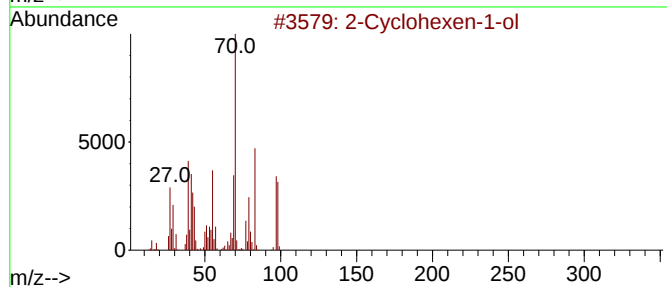
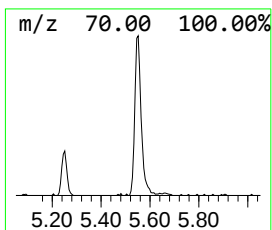
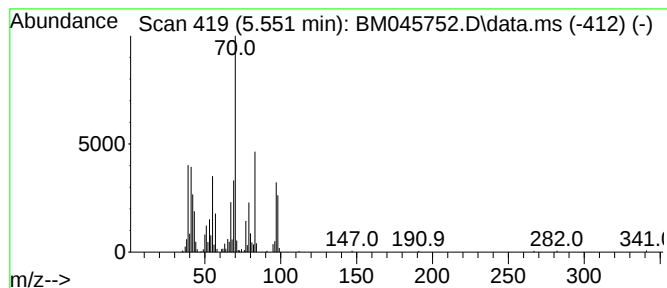
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Cyclohexen-1-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.551	3.61 ng	325770	1,4-Dichlorobenzene-d4	7.569

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	95
2			2-Methylene cyclopentanol	98	C6H10O	020461-31-8	72
3			1-propoxycyclohexene	140	C9H16O	061382-76-1	37
4			1-butoxycyclohexene	154	C10H18O	024159-57-7	32
5			Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052324\
Data File : BM045752.D
Acq On : 23 May 2024 14:08
Operator : MA/JU
Sample : PB161074BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB161074BL

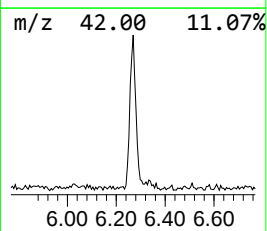
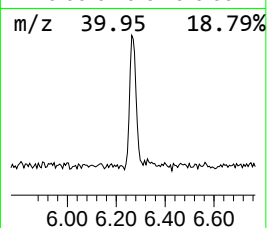
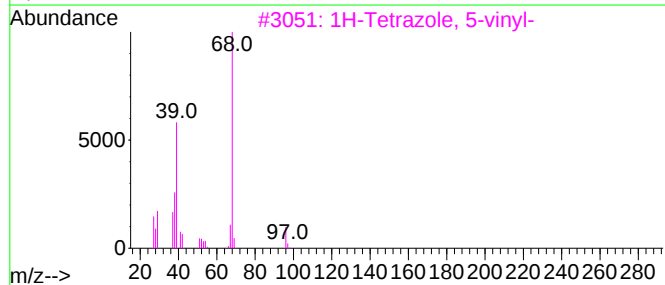
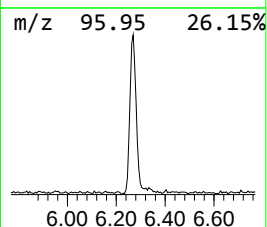
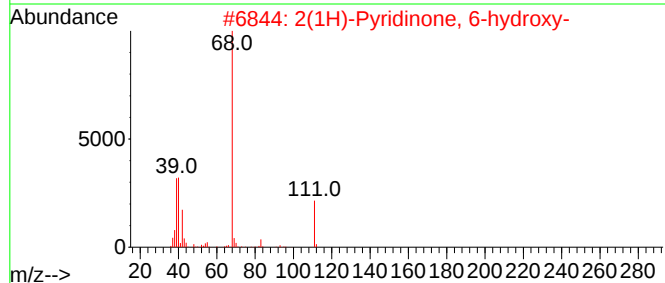
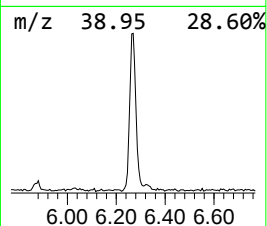
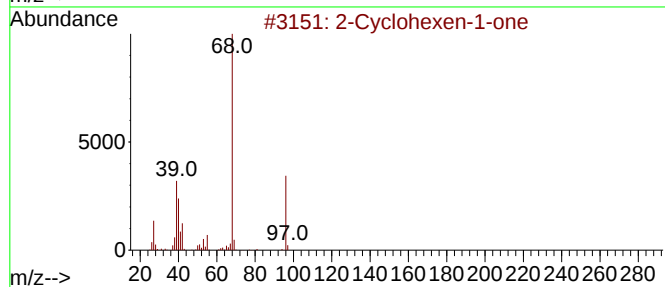
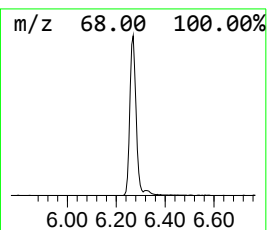
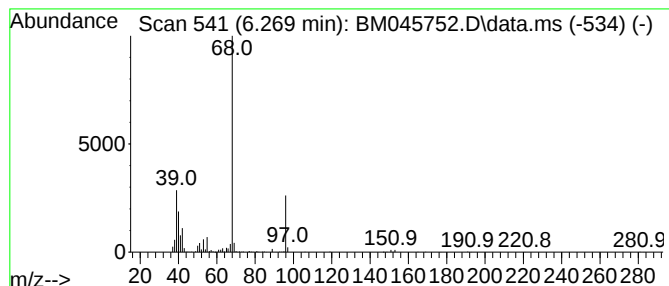
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Cyclohexen-1-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.269	5.26 ng	473629	1,4-Dichlorobenzene-d4	7.569

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyclohexen-1-one	96	C6H8O	000930-68-7	91
2			2(1H)-Pyridinone, 6-hydroxy-	111	C5H5NO2	000626-06-2	53
3			1H-Tetrazole, 5-vinyl-	96	C3H4N4	018755-47-0	50
4			2H-Pyran-2-one, 5,6-dihydro-	98	C5H6O2	003393-45-1	42
5			1-Pentyn-3-amine, 3-methyl-	97	C6H11N	018369-96-5	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052324\
Data File : BM045752.D
Acq On : 23 May 2024 14:08
Operator : MA/JU
Sample : PB161074BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB161074BL

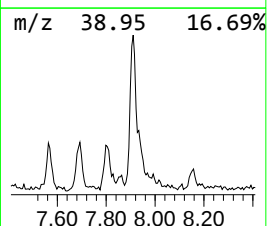
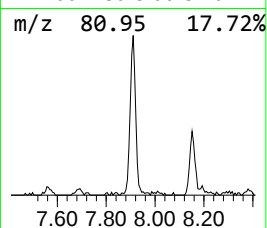
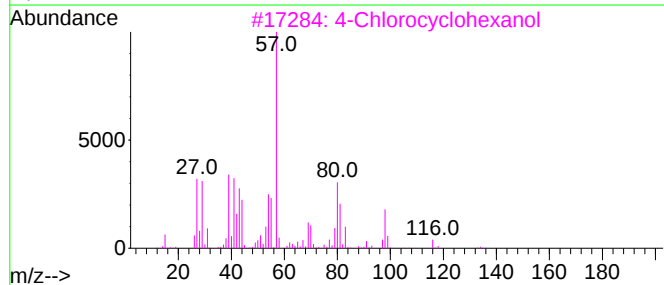
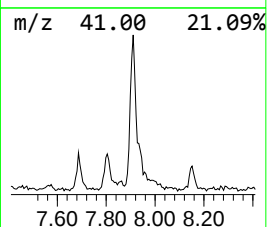
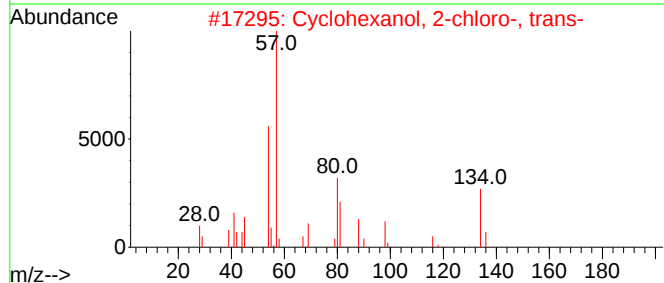
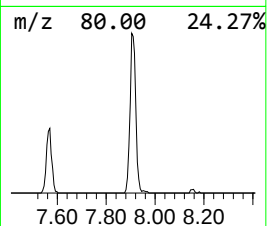
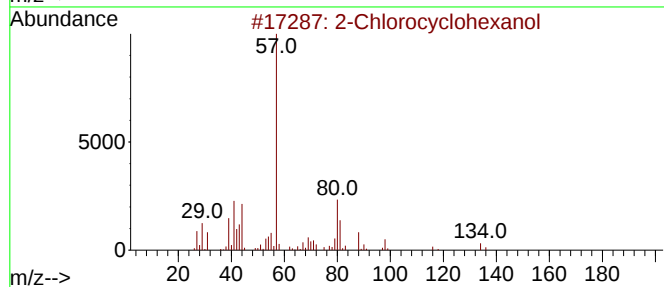
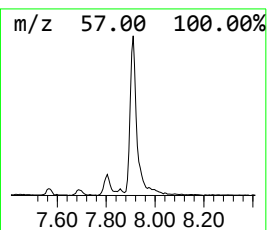
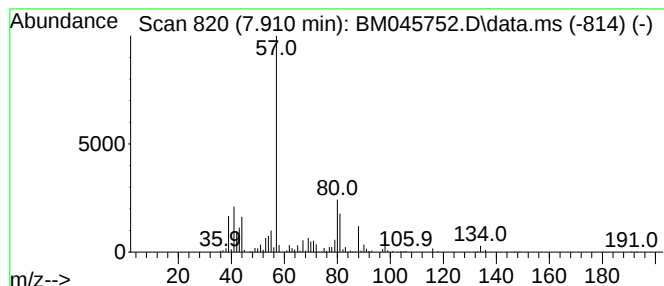
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 2-Chlorocyclohexanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.910	5.95 ng	535792	1,4-Dichlorobenzene-d4	7.569

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Chlorocyclohexanol	134	C6H11ClO	001561-86-0	94
2		Cyclohexanol, 2-chloro-, trans-	134	C6H11ClO	006628-80-4	40
3		4-Chlorocyclohexanol	134	C6H11ClO	030485-71-3	28
4		(S)-(+)-3-Hydroxytetrahydrofuran	88	C4H8O2	086087-23-2	17
5		Cyclohexanol, 4-chloro-, trans-	134	C6H11ClO	029538-77-0	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052324\
Data File : BM045752.D
Acq On : 23 May 2024 14:08
Operator : MA/JU
Sample : PB161074BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB161074BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052224.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-...	4.781	47.5	ng	4278250	1	7.569	1802400	20.0
2-Cyclohexen-1-ol	5.551	3.6	ng	325770	1	7.569	1802400	20.0
2-Cyclohexen-1-one	6.269	5.3	ng	473629	1	7.569	1802400	20.0
2-Chlorocyclohe...	7.910	6.0	ng	535792	1	7.569	1802400	20.0