

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102723\
 Data File : BM042484.D
 Acq On : 27 Oct 2023 22:14
 Operator : MA/JU
 Sample : PB156526BL
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PB156526BL

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-BM102123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM042484.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.328	191	194	203	rBV	29391	64172	1.22%	0.227%
2	5.092	318	324	340	rBV	1465890	1966335	37.26%	6.963%
3	5.528	392	398	413	rBV	1869171	2760023	52.29%	9.774%
4	5.887	453	459	464	rBV	95484	150488	2.85%	0.533%
5	6.657	584	590	602	rBV	133414	229219	4.34%	0.812%
6	7.157	668	675	691	rBV	1690216	2736511	51.85%	9.691%
7	7.981	809	815	825	rBV	505616	785456	14.88%	2.782%
8	8.333	867	875	886	rVV2	125257	244927	4.64%	0.867%
9	9.186	1012	1020	1040	rBV	1499006	2577792	48.84%	9.129%
10	10.804	1288	1295	1314	rBV	551451	1001682	18.98%	3.547%
11	13.251	1704	1711	1733	rBV	3445282	5139564	97.38%	18.201%
12	14.627	1938	1945	1960	rBV	765165	1201802	22.77%	4.256%
13	16.121	2192	2199	2215	rBV	1466605	2189630	41.49%	7.754%
14	17.380	2406	2413	2422	rBV	731526	1155742	21.90%	4.093%
15	18.233	2554	2558	2565	rBV4	49547	107192	2.03%	0.380%
16	19.986	2851	2856	2866	rBV	3995003	5277874	100.00%	18.691%
17	21.556	3120	3123	3134	rBV	426138	649508	12.31%	2.300%

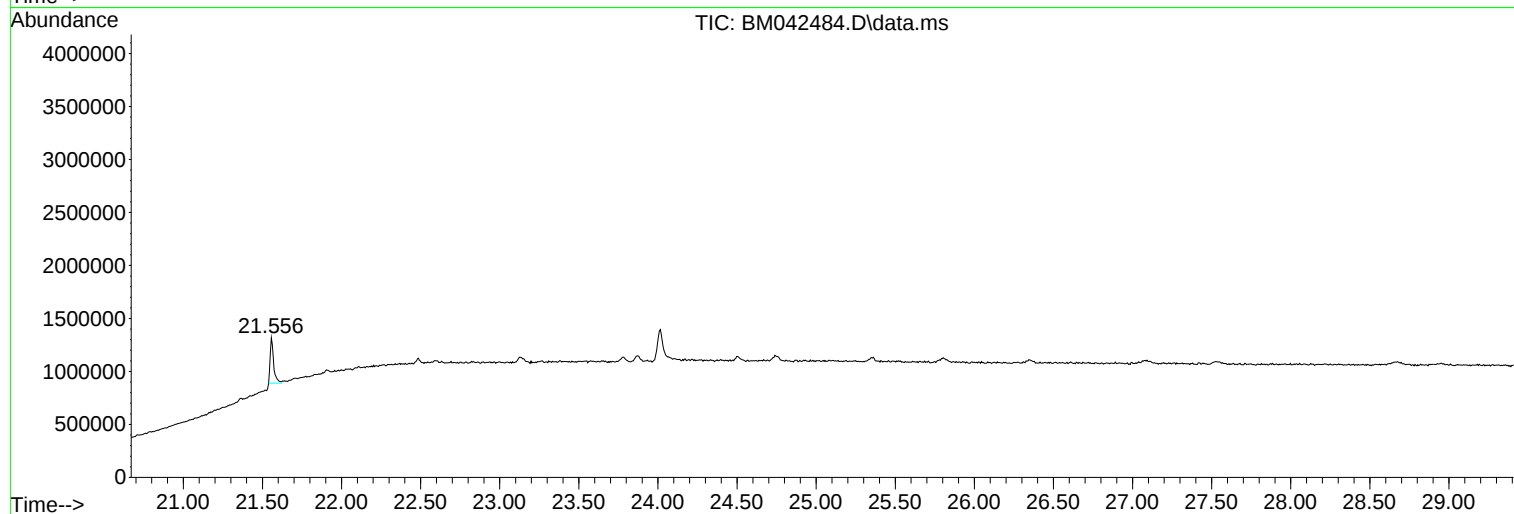
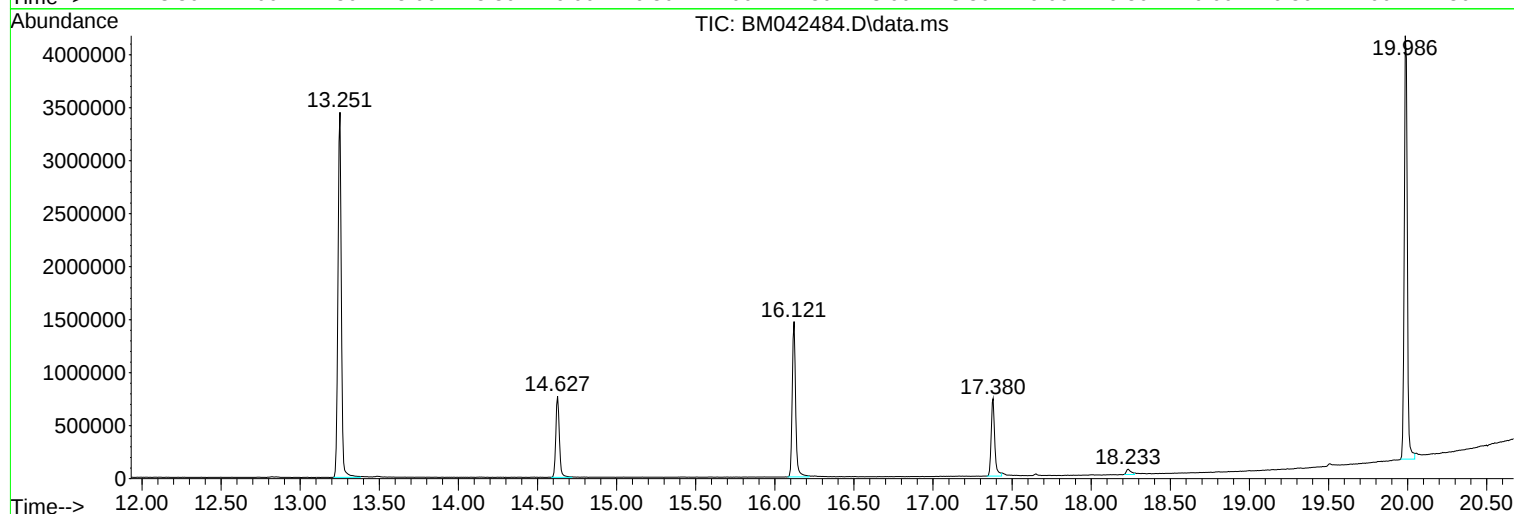
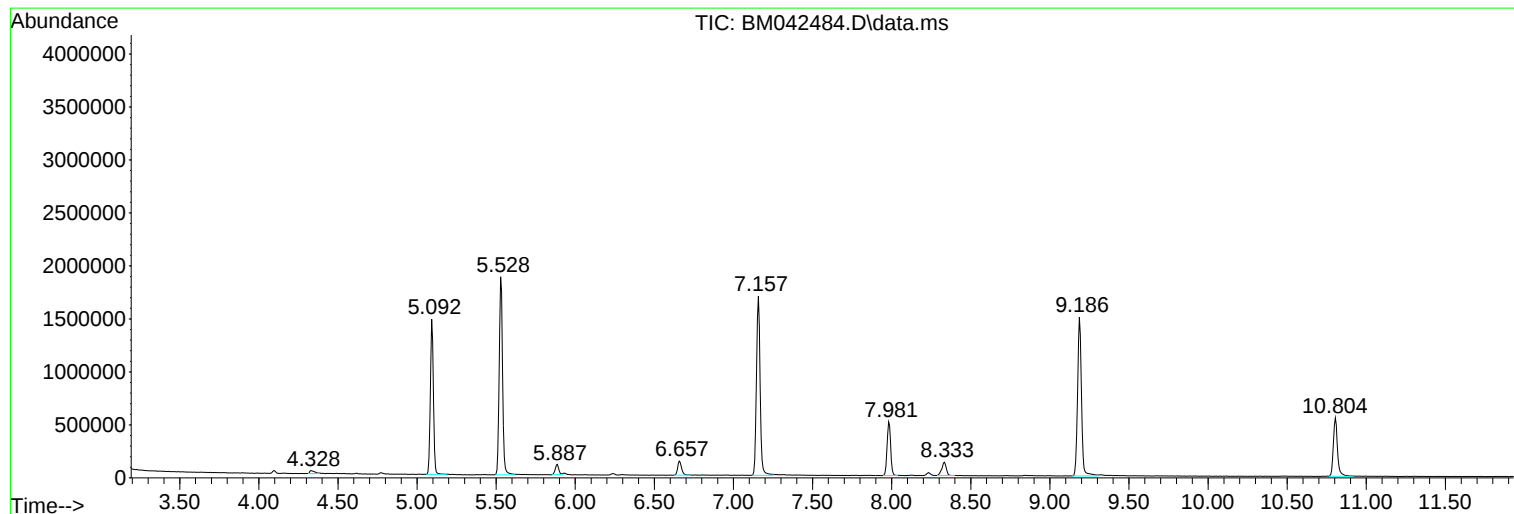
Sum of corrected areas: 28237917

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102723\
Data File : BM042484.D
Acq On : 27 Oct 2023 22:14
Operator : MA/JU
Sample : PB156526BL
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB156526BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.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\BM102723\
Data File : BM042484.D
Acq On : 27 Oct 2023 22:14
Operator : MA/JU
Sample : PB156526BL
Misc :
ALS Vial : 8 Sample Multiplier: 1

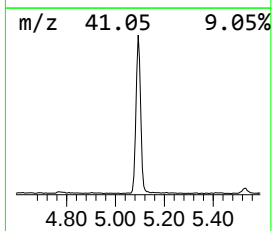
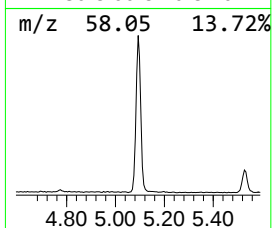
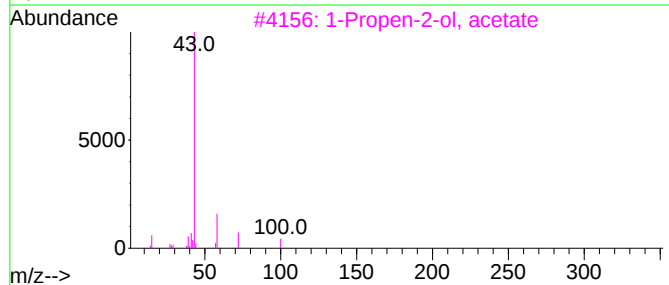
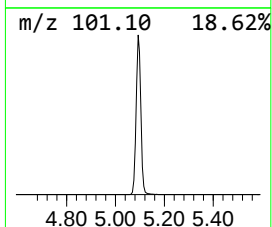
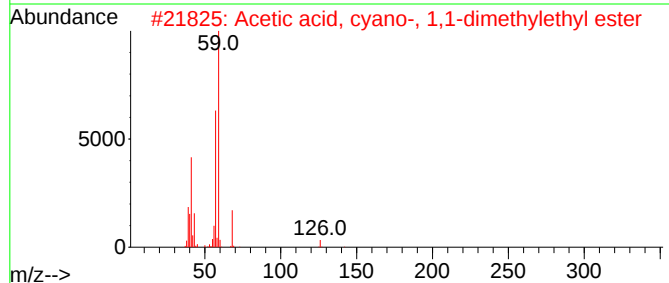
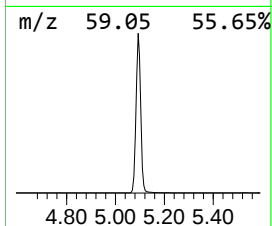
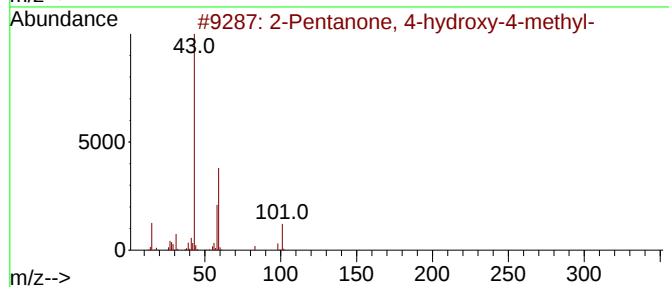
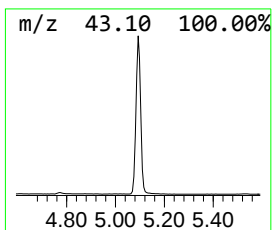
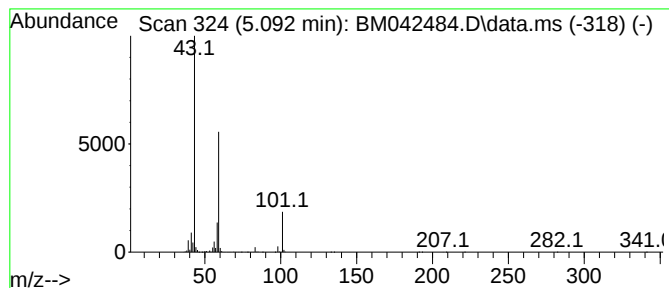
Instrument :
BNA_M
ClientSampleId :
PB156526BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.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.
5.092	50.07 ng	1966340	1,4-Dichlorobenzene-d4			7.981
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, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-		101	C5H11NO	000109-02-4	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102723\
Data File : BM042484.D
Acq On : 27 Oct 2023 22:14
Operator : MA/JU
Sample : PB156526BL
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB156526BL

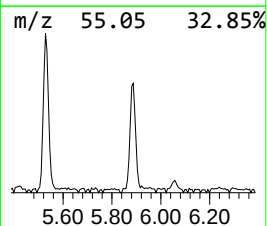
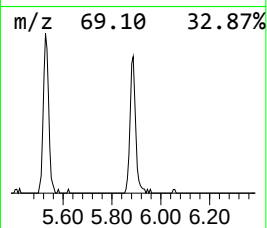
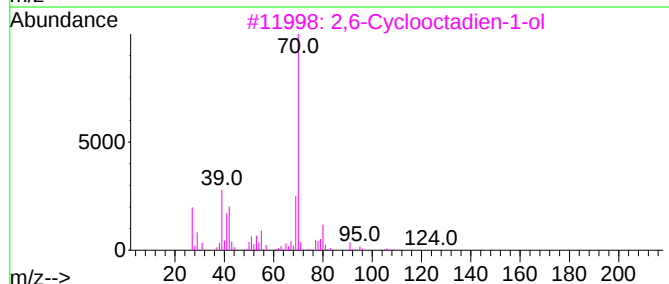
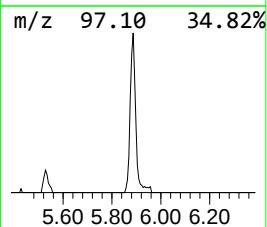
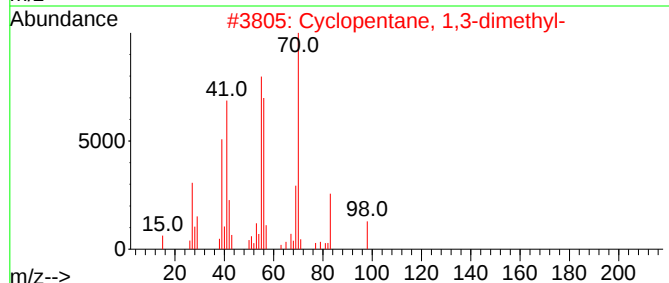
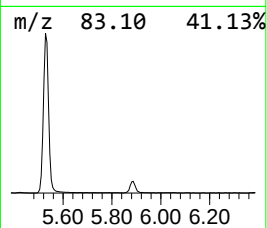
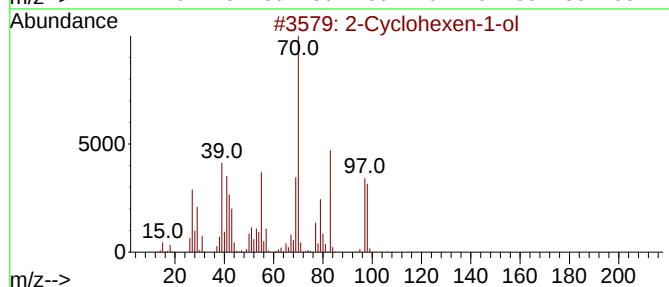
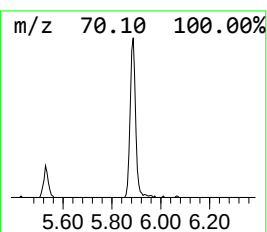
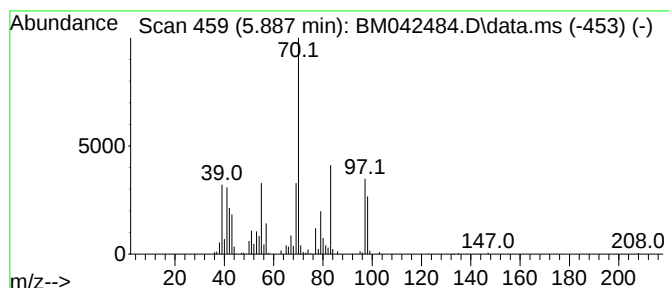
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.887	3.83 ng	150488	1,4-Dichlorobenzene-d4	7.981

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	96
2			Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	50
3			2,6-Cyclooctadien-1-ol	124	C8H12O	010017-18-2	38
4			2-Methylene cyclopentanol	98	C6H10O	020461-31-8	38
5			Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102723\
Data File : BM042484.D
Acq On : 27 Oct 2023 22:14
Operator : MA/JU
Sample : PB156526BL
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB156526BL

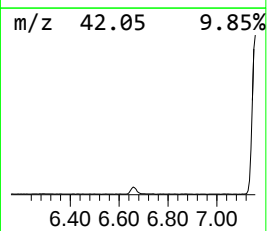
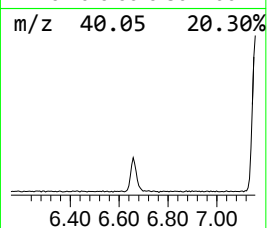
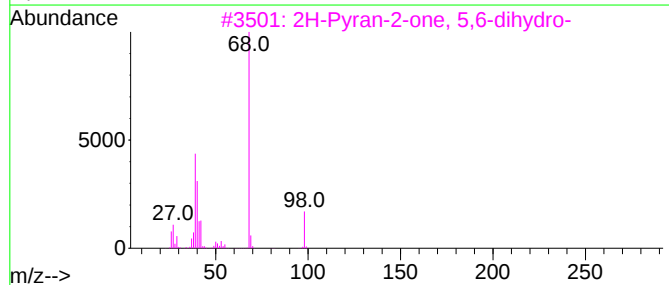
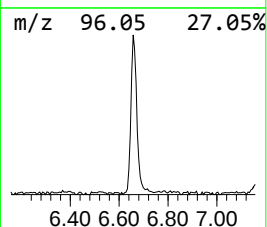
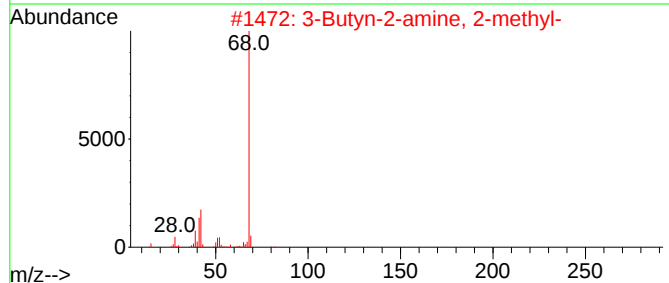
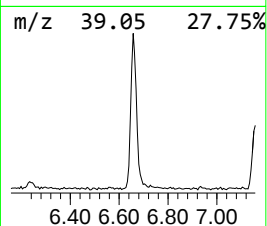
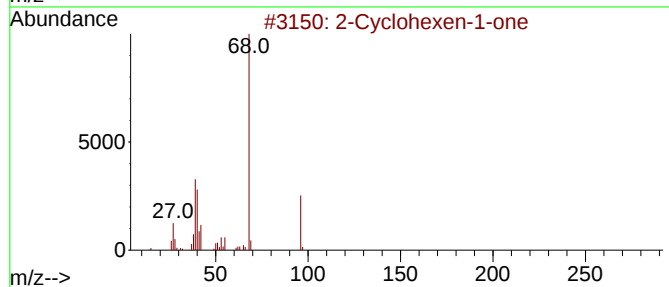
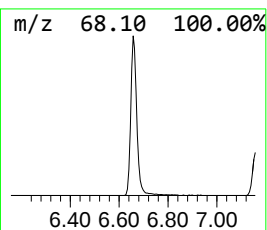
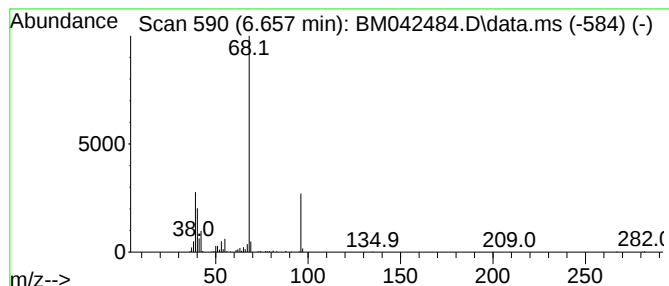
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
6.657	5.84 ng	229219	1,4-Dichlorobenzene-d4	7.981

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyclohexen-1-one	96	C6H8O	000930-68-7	91
2			3-Butyn-2-amine, 2-methyl-	83	C5H9N	002978-58-7	59
3			2H-Pyran-2-one, 5,6-dihydro-	98	C5H6O2	003393-45-1	53
4			2,5-Dihydro-3-methyl-thiophene 1...	132	C5H8O2S	001193-10-8	36
5			1H-Pyrazole	68	C3H4N2	000288-13-1	36



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102723\
Data File : BM042484.D
Acq On : 27 Oct 2023 22:14
Operator : MA/JU
Sample : PB156526BL
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB156526BL

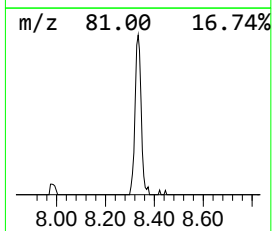
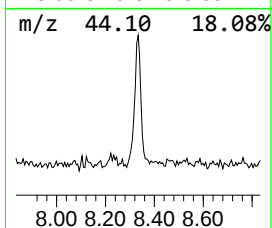
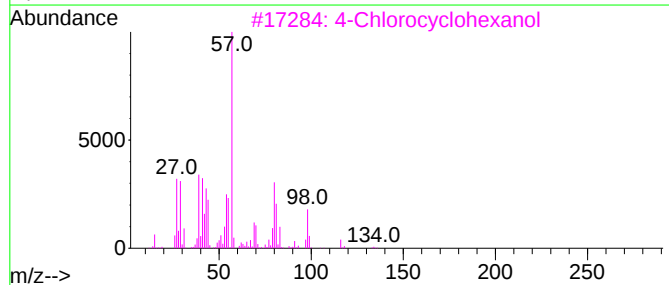
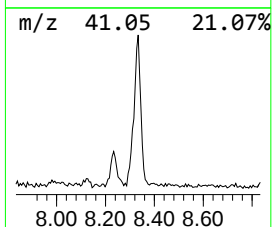
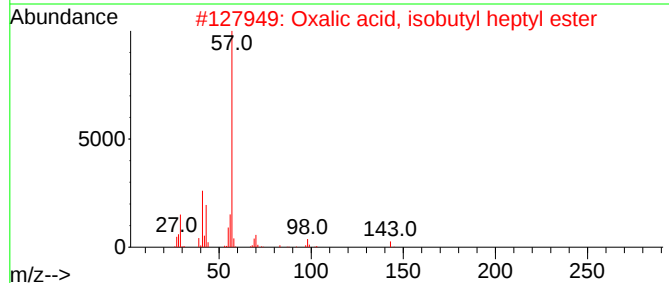
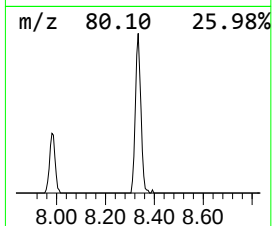
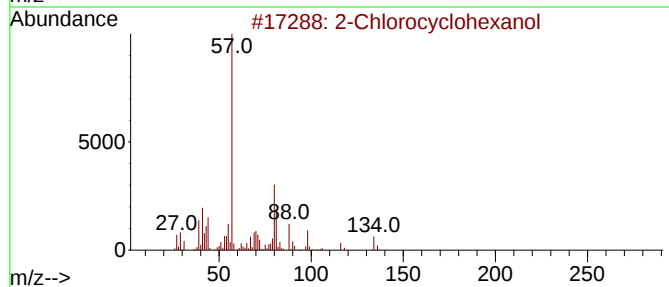
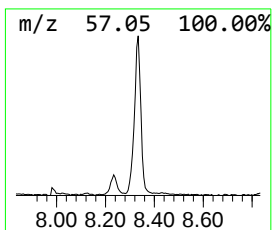
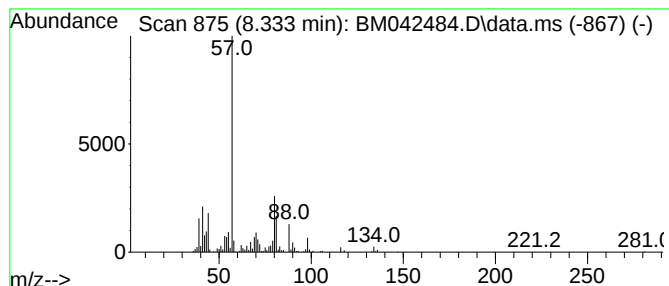
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
8.333	6.24 ng	244927	1,4-Dichlorobenzene-d4	7.981

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Chlorocyclohexanol	134	C6H11ClO	001561-86-0	93
2			Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	22
3			4-Chlorocyclohexanol	134	C6H11ClO	030485-71-3	17
4			1-Ethylhexyl propionate	186	C11H22O2	1010430-89-6	12
5			Hexanoic acid, 2-ethyl-, heptyl ...	242	C15H30O2	112445-68-8	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102723\
Data File : BM042484.D
Acq On : 27 Oct 2023 22:14
Operator : MA/JU
Sample : PB156526BL
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB156526BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.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-...	5.092	50.1	ng	1966340	1	7.981	785456	20.0
2-Cyclohexen-1-ol	5.887	3.8	ng	150488	1	7.981	785456	20.0
2-Cyclohexen-1-one	6.657	5.8	ng	229219	1	7.981	785456	20.0
2-Chlorocyclohe...	8.333	6.2	ng	244927	1	7.981	785456	20.0