LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120123\
Data File : BF136339.D
Acq On : 01 Dec 2023 15:53
Operator : CG\JU
Sample : PB157396BL
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB157396BL

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-BF112723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136339.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	15	21	28	rVB	1084714	2212281	48.02%	8.431%
2	5.057	499	505	512	rBV	1220646	1519662	32.98%	5.792%
3	5.451	567	572	575	rBV	2676319	2366882	51.37%	9.021%
4	5.622	597	601	612	rBV2	124650	134760	2.92%	0.514%
5	6.063	672	676	680	rBV	214026	172659	3.75%	0.658%
6	6.439	735	740	743	rBV	2467035	2312767	50.20%	8.814%
7	6.804	798	802	805	rBV	924405	707751	15.36%	2.697%
8	6.957	824	828	838	rBV	152042	157958	3.43%	0.602%
9	7.369	892	898	901	rBV	2065237	2239798	48.62%	8.536%
10	8.080	1014	1019	1023	rBV	1118150	958465	20.80%	3.653%
11	9.163	1197	1203	1206	rBV	5272941	4607211	100.00%	17.559%
12	9.839	1312	1318	1321	rBV	1322901	1117872	24.26%	4.260%
13	10.627	1448	1452	1467	rBV	1679101	1636316	35.52%	6.236%
14	11.333	1568	1572	1575	rBV	1260260	1109667	24.09%	4.229%
15	12.933	1839	1844	1847	rBV	3781203	3845126	83.46%	14.655%
16	13.980	2018	2022	2033	rBV	589934	587503	12.75%	2.239%
17	15.468	2269	2275	2282	rBV	373202	551815	11.98%	2.103%

Sum of corrected areas: 26238493

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ClientSampleId :
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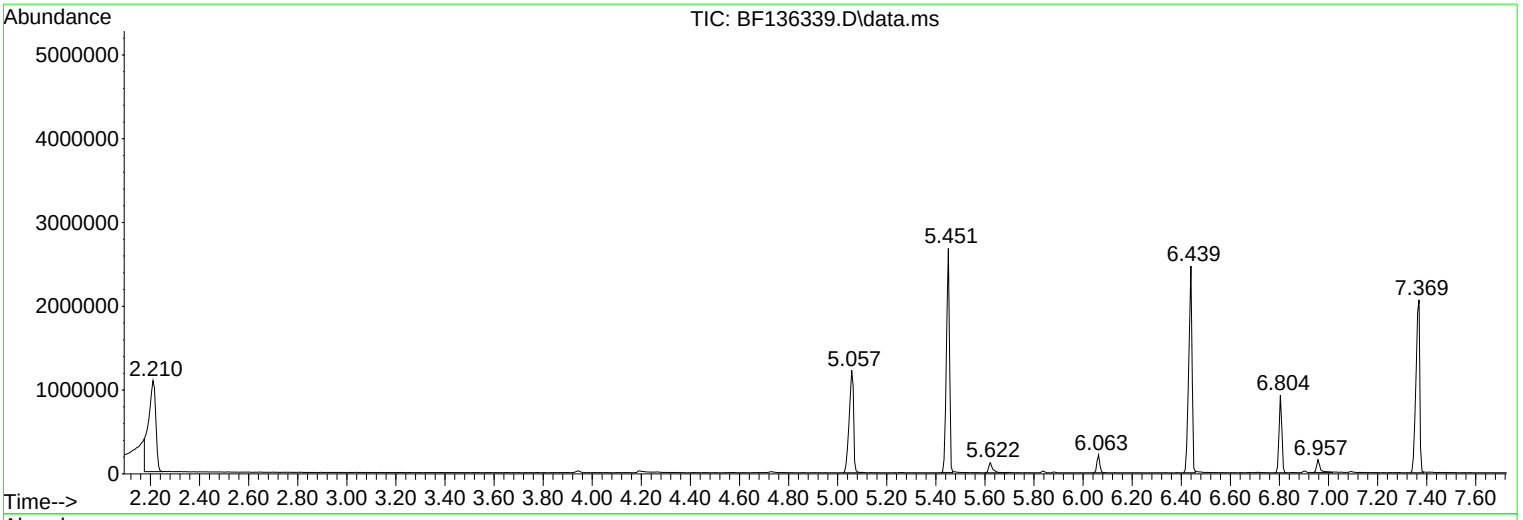
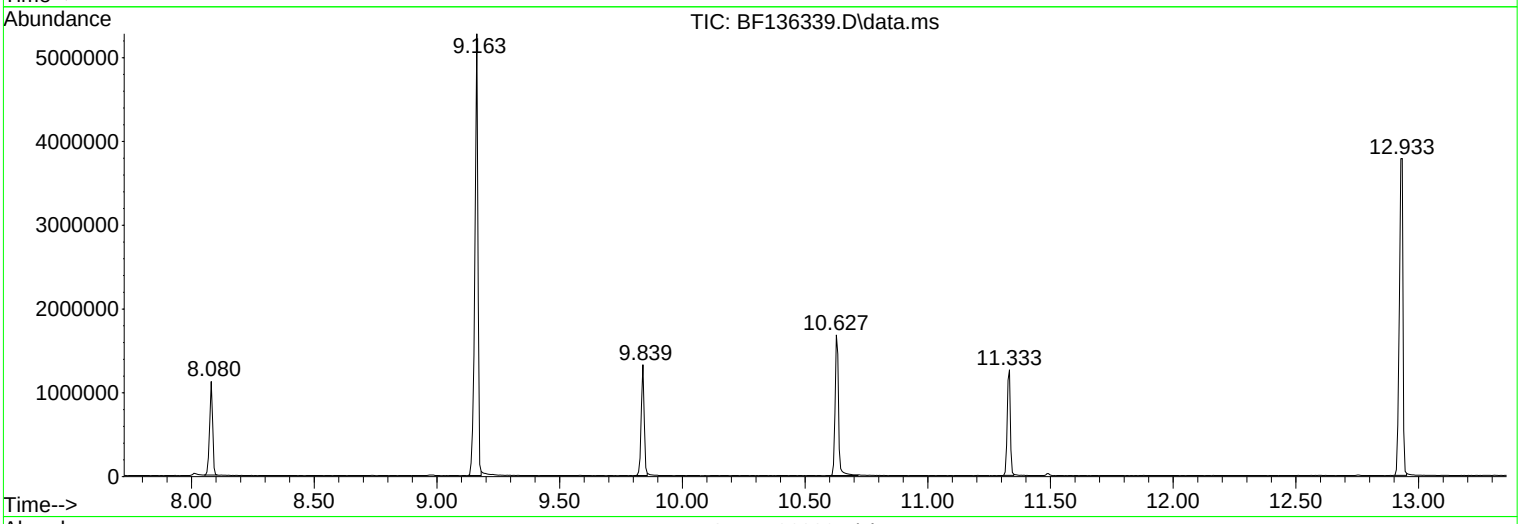
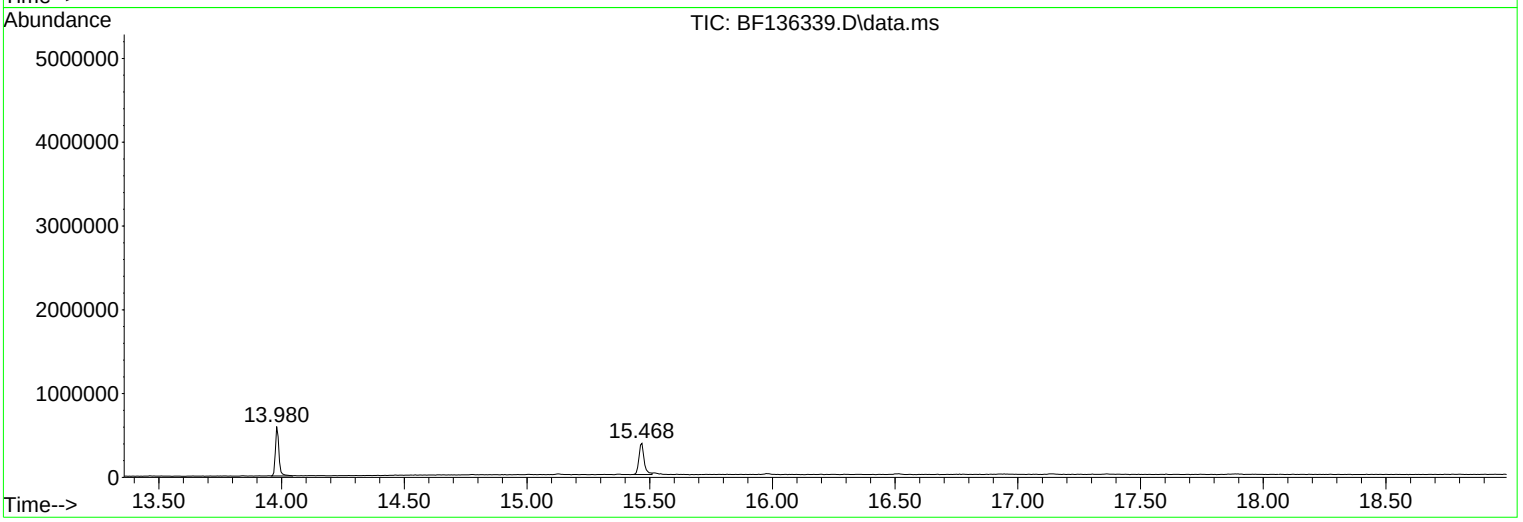
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120123\
Data File : BF136339.D
Acq On : 01 Dec 2023 15:53
Operator : CG\JU
Sample : PB157396BL
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB157396BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

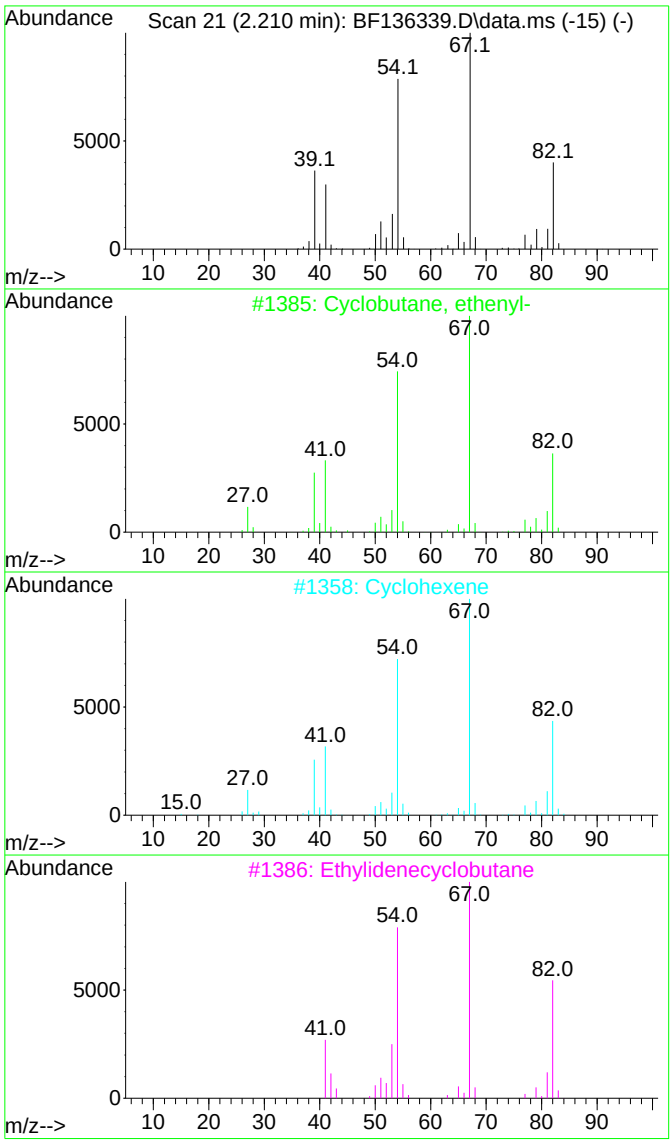
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

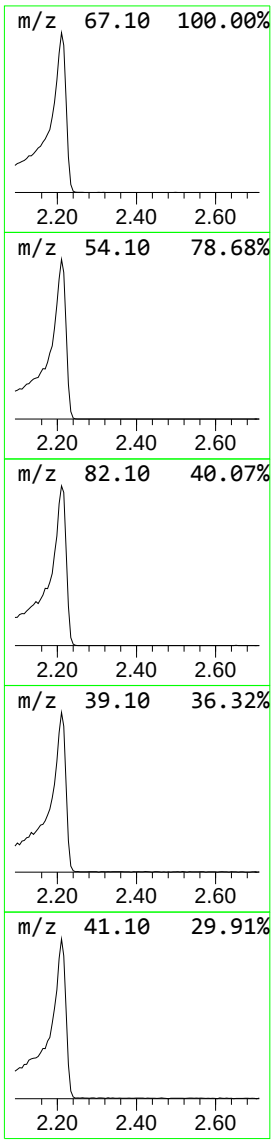
****

Peak Number 1 Cyclobutane, ethenyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.210	62.52 ng	2212280	1,4-Dichlorobenzene-d4	6.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, ethenyl-	82	C6H10	002597-49-1	91
2	Cyclohexene	82	C6H10	000110-83-8	91
3	Ethylidenecyclobutane	82	C6H10	001528-21-8	91
4	C2H5CH=CHCH=CH2	82	C6H10	000592-48-3	38
5	4-Methyl-1,3-pentadiene	82	C6H10	000926-56-7	35





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ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB157396BL

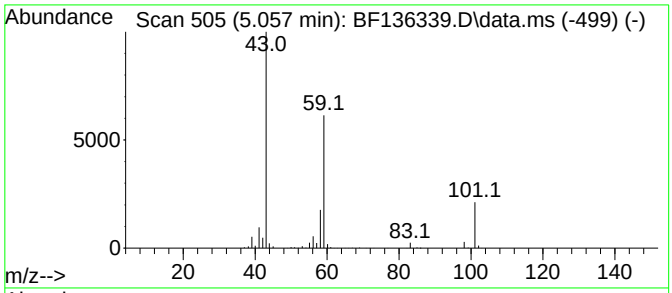
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

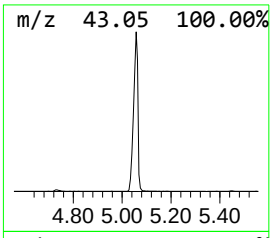
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

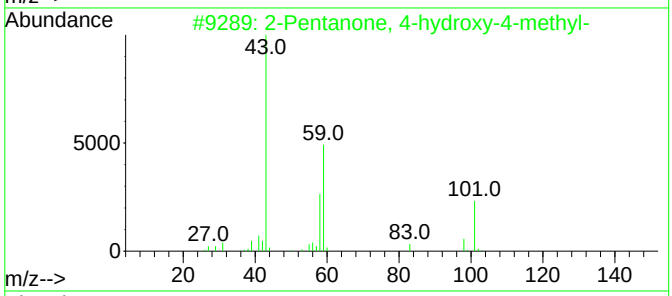
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

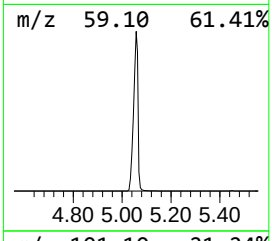
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	42.94 ng	1519660	1,4-Dichlorobenzene-d4	6.804

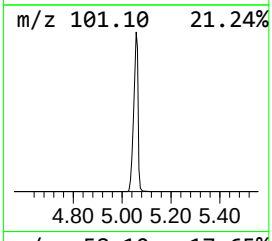
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9

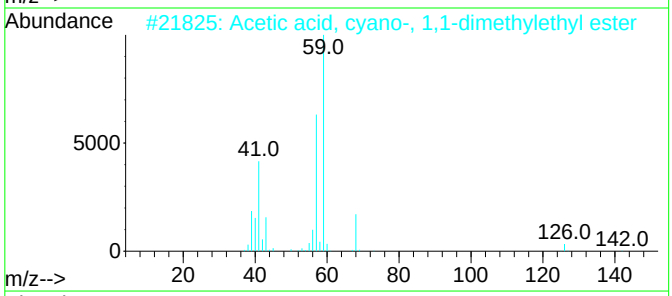


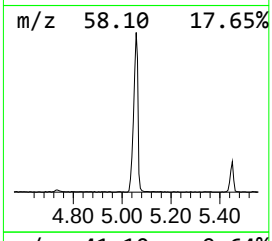


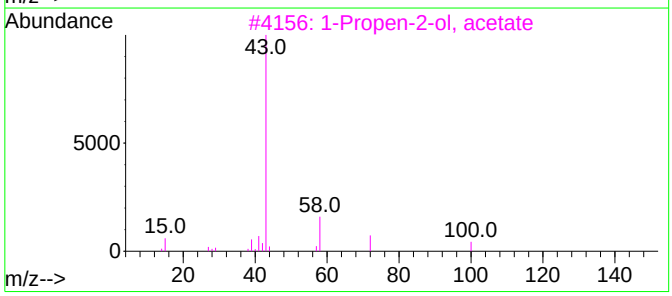


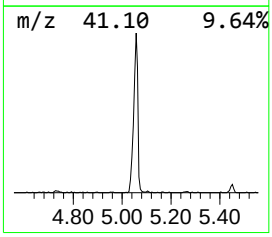












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ClientSampleId :
PB157396BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

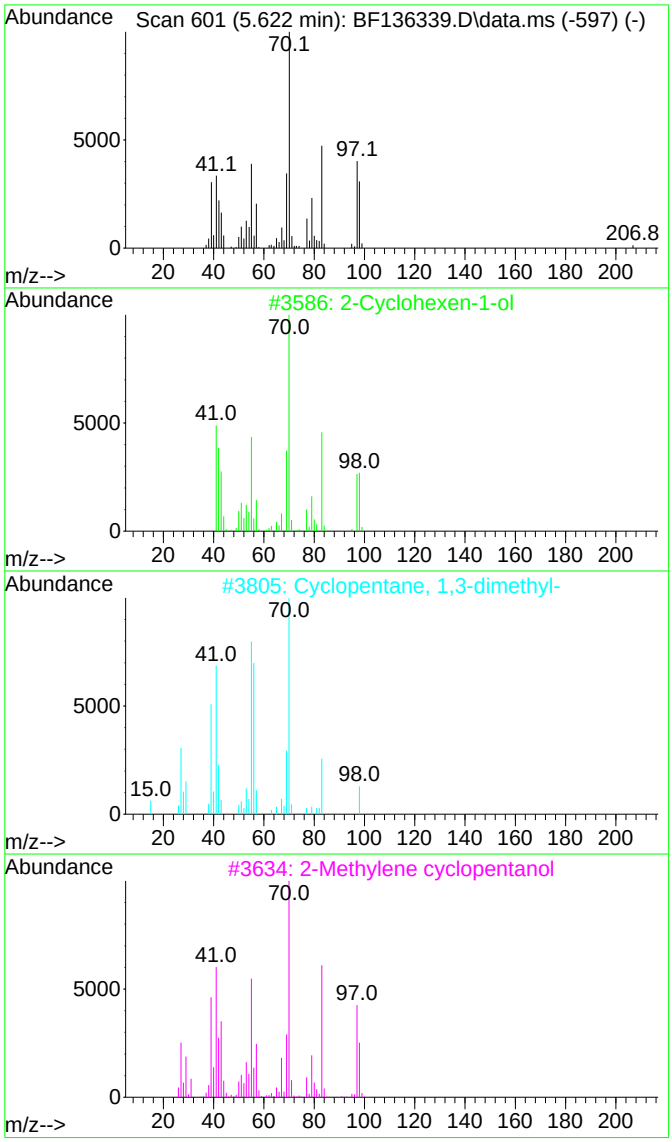
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

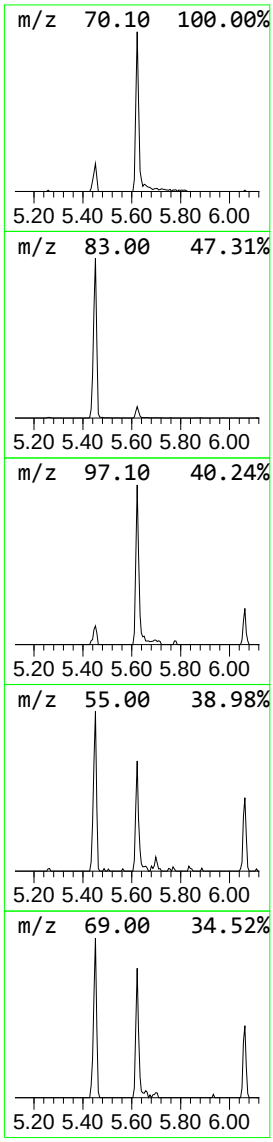
****

Peak Number 3 2-Cyclohexen-1-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.622	3.81 ng	134760	1,4-Dichlorobenzene-d4	6.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	90
2	Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	50
3	2-Methylene cyclopentanol	98	C6H10O	020461-31-8	42
4	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	38
5	Cyanoacetaldehyde diethylacetal	143	C7H13NO2	002032-34-0	25





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

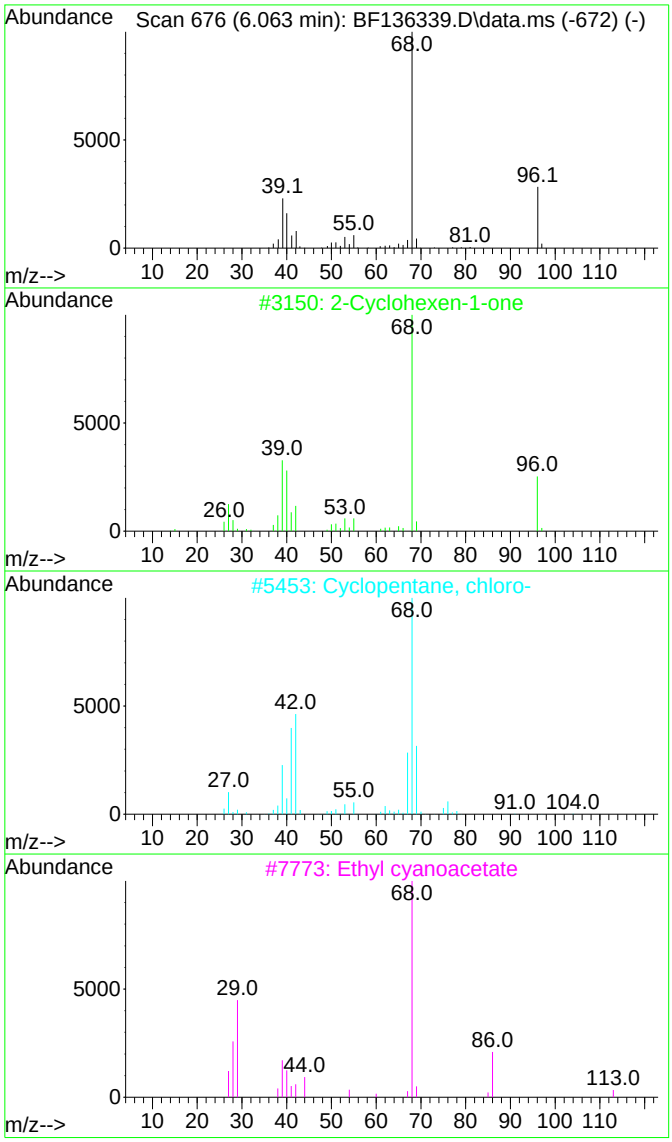
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

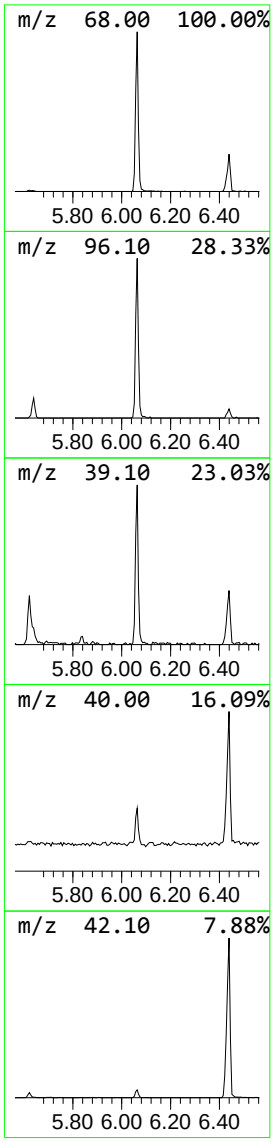
****

Peak Number 4 2-Cyclohexen-1-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.063	4.88 ng	172659	1,4-Dichlorobenzene-d4	6.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	91
2	Cyclopentane, chloro-	104	C5H9Cl	000930-28-9	36
3	Ethyl cyanoacetate	113	C5H7NO2	000105-56-6	36
4	Bicyclo[3.1.0]hexan-2-one	96	C6H8O	004160-49-0	22
5	But-1-ene-3-yne, 1-ethoxy-	96	C6H8O	002806-41-9	12





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Sample : PB157396BL
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB157396BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

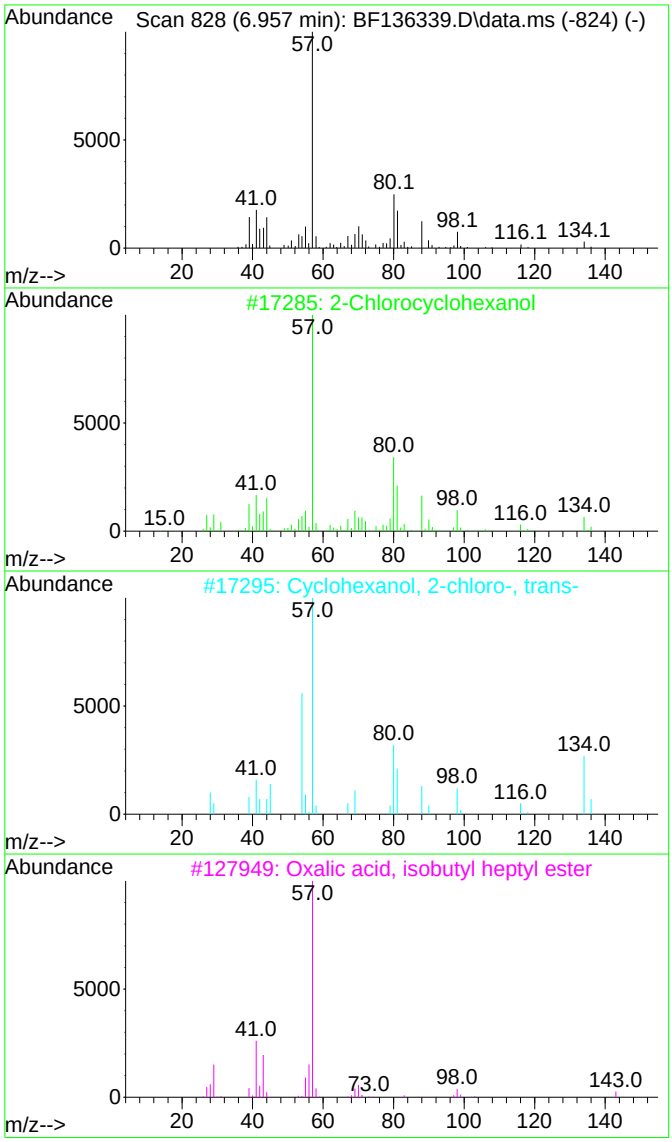
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

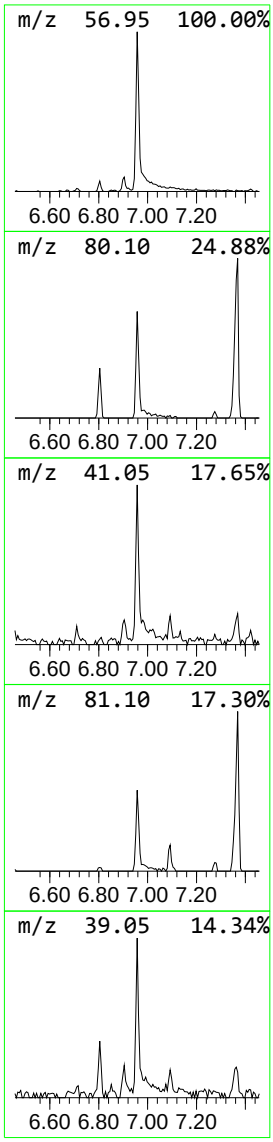
****

Peak Number 5 2-Chlorocyclohexanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.957	4.46 ng	157958	1,4-Dichlorobenzene-d4	6.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chlorocyclohexanol	134	C6H11ClO	001561-86-0	93
2	Cyclohexanol, 2-chloro-, trans-	134	C6H11ClO	006628-80-4	38
3	Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	22
4	Cyclohexanol, 4-chloro-, trans-	134	C6H11ClO	029538-77-0	17
5	3-Furanol, tetrahydro-	88	C4H8O2	000453-20-3	16





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclobutane, et...	2.210	62.5	ng	2212280	1	6.804	707751	20.0
2-Pentanone, 4-...	5.057	42.9	ng	1519660	1	6.804	707751	20.0
2-Cyclohexen-1-ol	5.622	3.8	ng	134760	1	6.804	707751	20.0
2-Cyclohexen-1-one	6.063	4.9	ng	172659	1	6.804	707751	20.0
2-Chlorocyclohe...	6.957	4.5	ng	157958	1	6.804	707751	20.0