LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122223\
Data File : BF136681.D
Acq On : 22 Dec 2023 12:22
Operator : CG\JU
Sample : PB157641BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB157641BL

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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136681.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.157	6	12	20	rVB	644448	1385363	51.45%	8.567%
2	5.028	494	500	511	rBV	786030	1014807	37.69%	6.275%
3	5.434	564	569	572	rBV	1431860	1386193	51.48%	8.572%
4	5.598	593	597	607	rBV2	70042	74428	2.76%	0.460%
5	6.039	668	672	682	rBV	117524	102635	3.81%	0.635%
6	6.428	733	738	741	rBV	1436090	1396809	51.87%	8.638%
7	6.781	794	798	802	rBV	514872	411658	15.29%	2.546%
8	6.934	821	824	839	rVB	104164	109539	4.07%	0.677%
9	7.345	888	894	897	rBV	1348394	1314863	48.83%	8.131%
10	8.057	1011	1015	1019	rBV	620642	547787	20.34%	3.387%
11	9.139	1193	1199	1202	rBV	2785884	2506765	93.09%	15.501%
12	9.816	1309	1314	1317	rBV	776430	627009	23.28%	3.877%
13	10.610	1445	1449	1452	rBV	1139326	990683	36.79%	6.126%
14	11.310	1564	1568	1571	rBV	818096	696578	25.87%	4.308%
15	12.910	1835	1840	1843	rBV	2814826	2692781	100.00%	16.652%
16	13.963	2015	2019	2025	rVB	536843	514015	19.09%	3.179%
17	15.439	2265	2270	2274	rBV	306201	399207	14.83%	2.469%

Sum of corrected areas: 16171120

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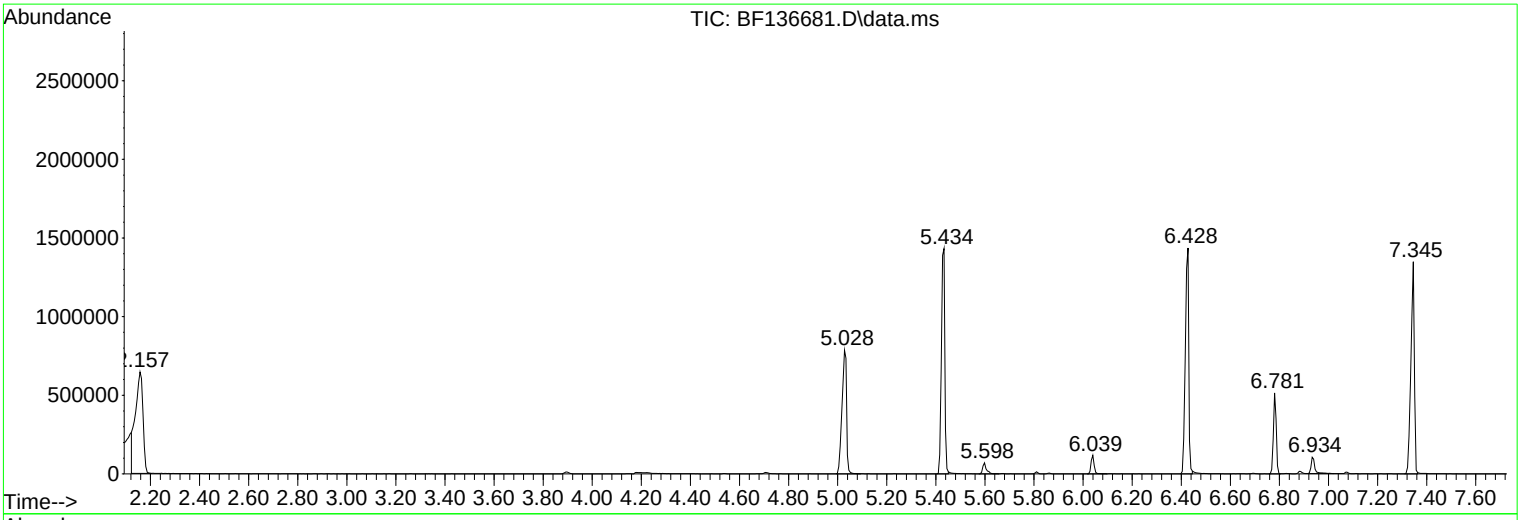
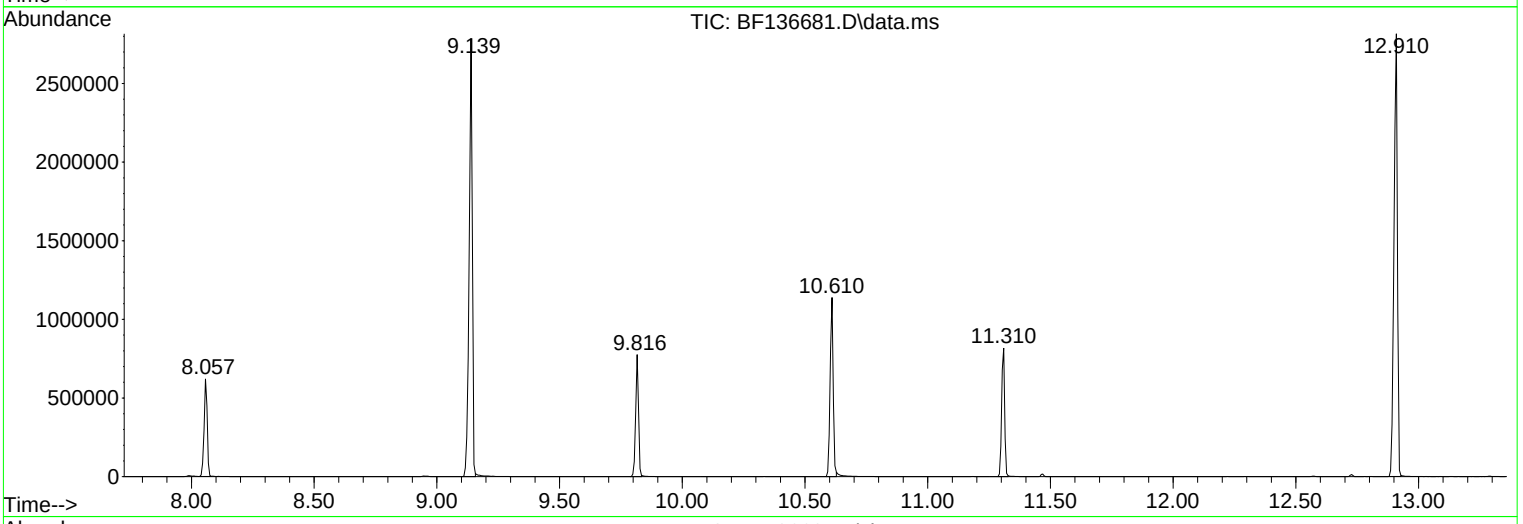
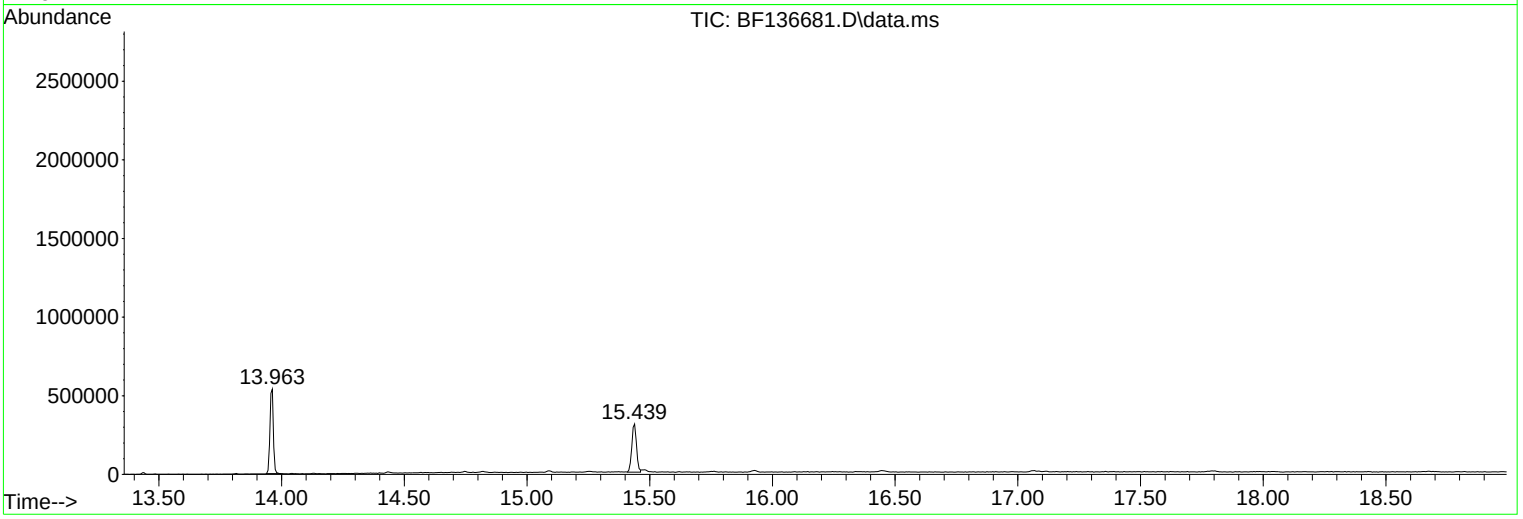
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Instrument :
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ClientSampleId :
PB157641BL

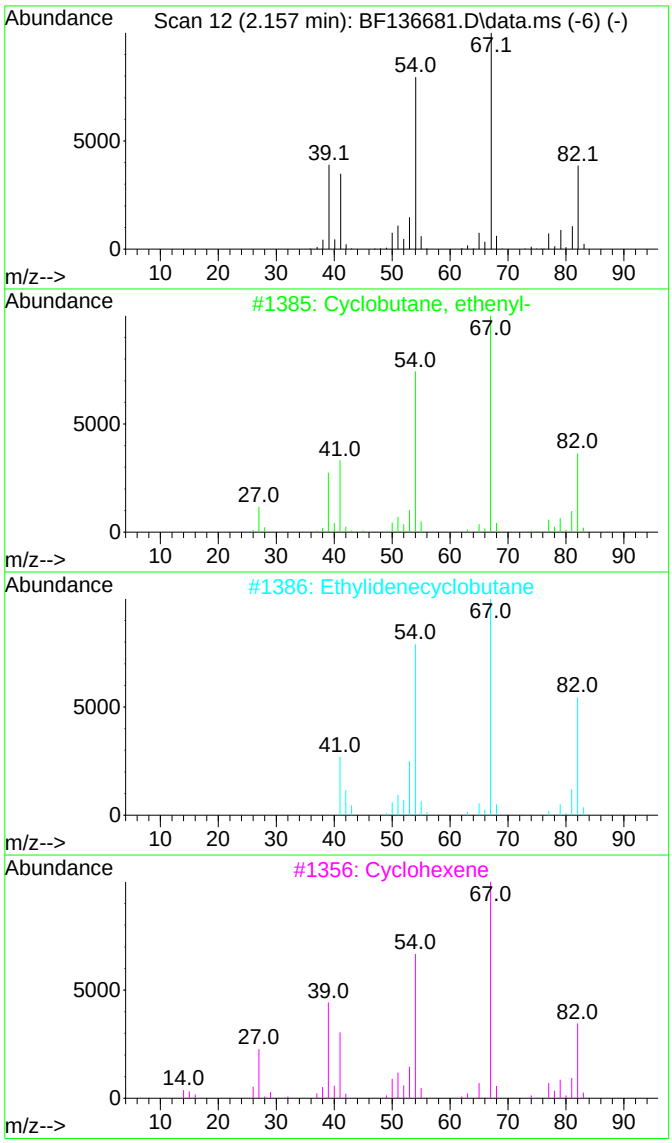
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

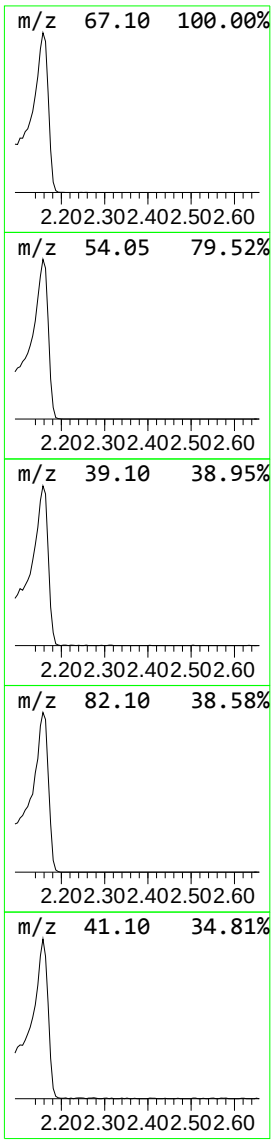
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Cyclobutane, ethenyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.157	67.31 ng	1385360	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, ethenyl-	82	C6H10	002597-49-1	93
2	Ethylidenecyclobutane	82	C6H10	001528-21-8	91
3	Cyclohexene	82	C6H10	000110-83-8	91
4	4-Methyl-1,3-pentadiene	82	C6H10	000926-56-7	35
5	1,3-Pentadiene, 2-methyl-	82	C6H10	001118-58-7	30





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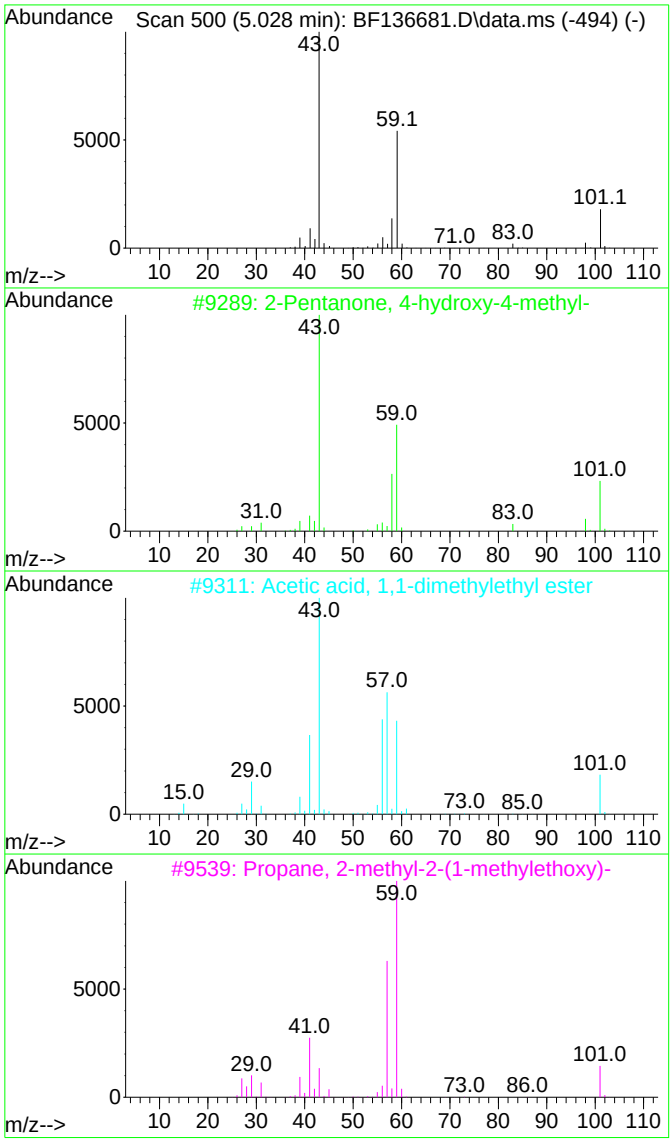
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

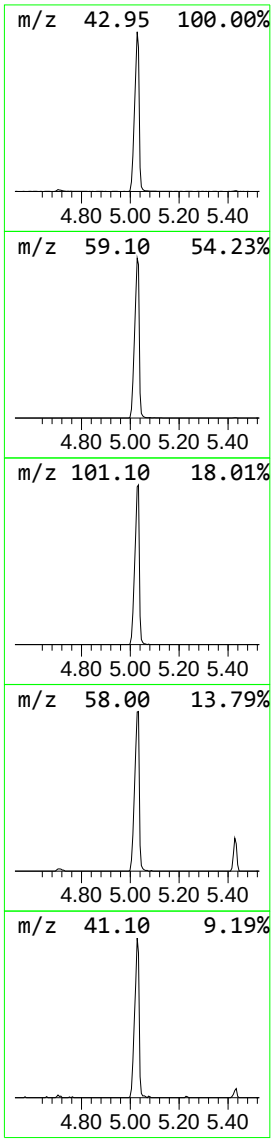
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.028	49.30 ng	1014810	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	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Data File : BF136681.D
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Operator : CG\JU
Sample : PB157641BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB157641BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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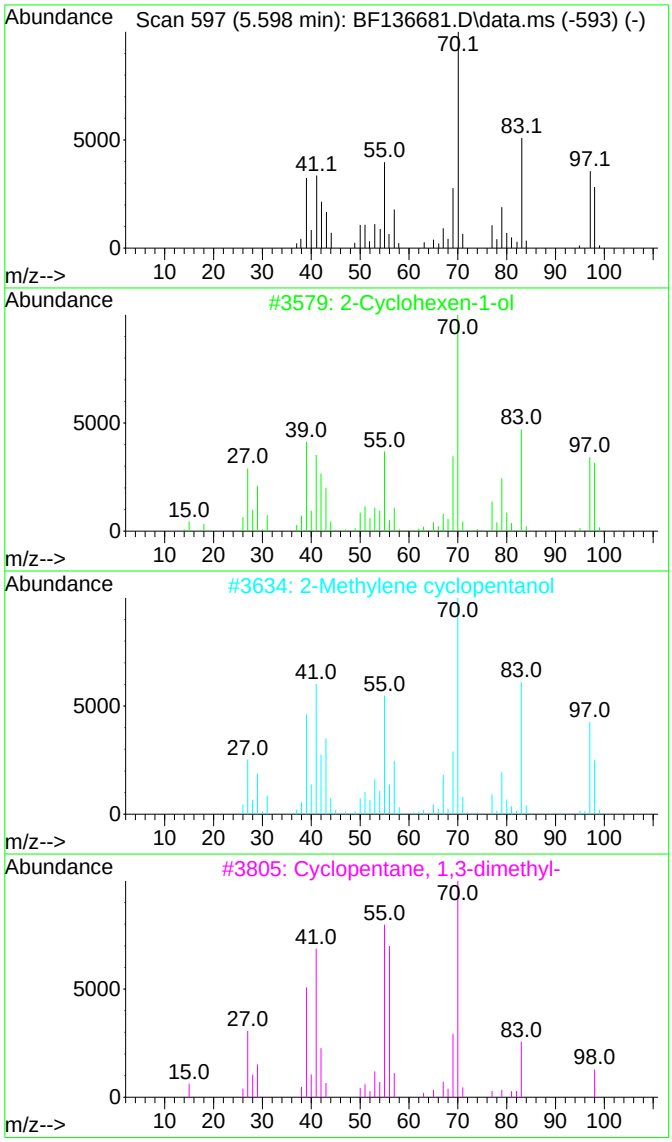
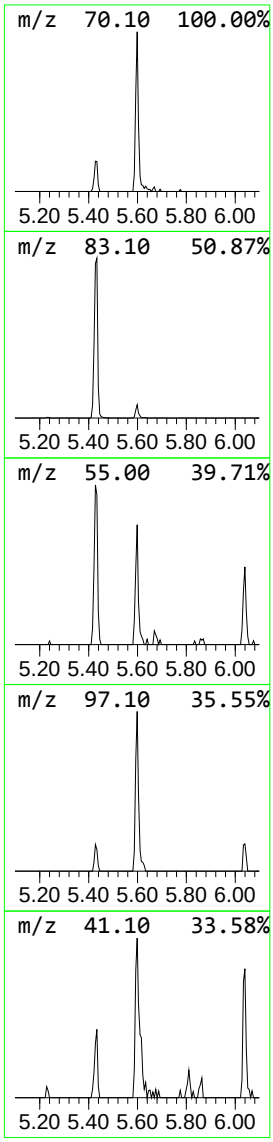
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.598	3.62 ng	74428	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	93
2	2-Methylene cyclopentanol	98	C6H10O	020461-31-8	56
3	Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	47
4	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	47
5	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	37





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

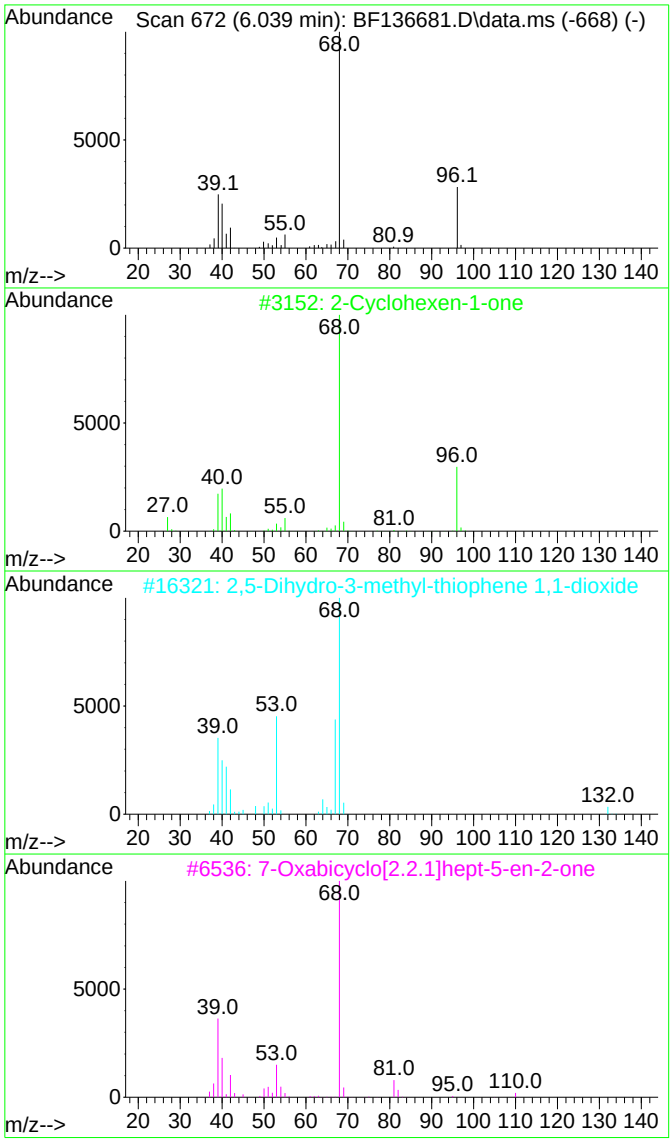
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

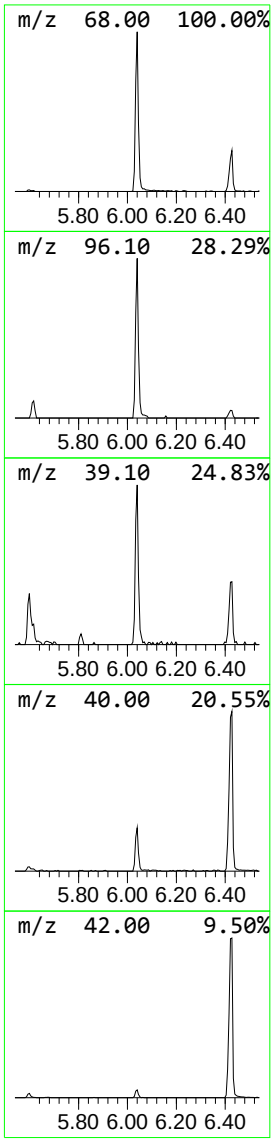
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.039	4.99 ng	102635	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	91
2	2,5-Dihydro-3-methyl-thiophene 1...	132	C5H8O2S	001193-10-8	42
3	7-Oxabicyclo[2.2.1]hept-5-en-2-one	110	C6H6O2	095530-78-2	38
4	1H-Pyrazole	68	C3H4N2	000288-13-1	36
5	But-1-ene-3-yne, 1-ethoxy-	96	C6H8O	002806-41-9	14





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ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

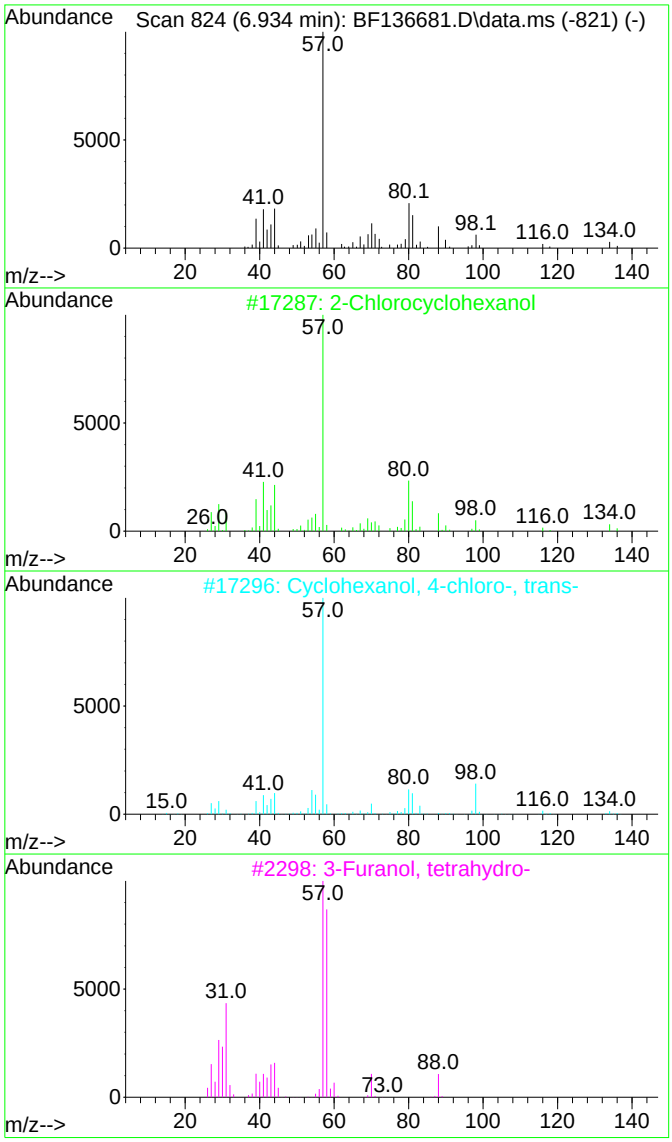
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

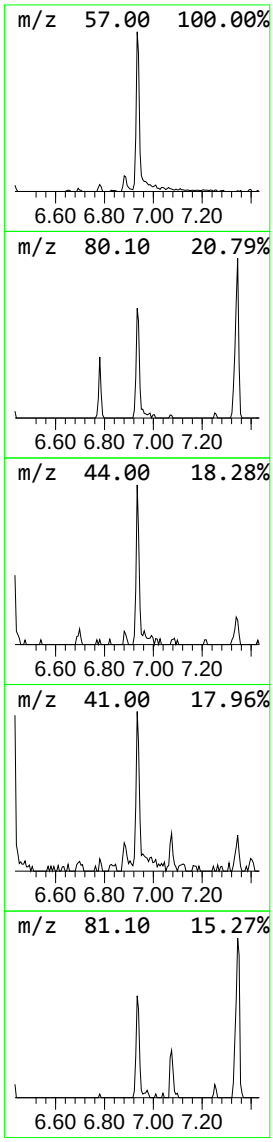
****

Peak Number 5 2-Chlorocyclohexanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.934	5.32 ng	109539	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chlorocyclohexanol	134	C6H11ClO	001561-86-0	94
2	Cyclohexanol, 4-chloro-, trans-	134	C6H11ClO	029538-77-0	43
3	3-Furanol, tetrahydro-	88	C4H8O2	000453-20-3	38
4	Cyclohexanol, 2-chloro-, trans-	134	C6H11ClO	006628-80-4	28
5	Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	22





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...	2.157	67.3	ng	1385360	1	6.781	411658	20.0
2-Pentanone, 4-...	5.028	49.3	ng	1014810	1	6.781	411658	20.0
2-Cyclohexen-1-ol	5.598	3.6	ng	74428	1	6.781	411658	20.0
2-Cyclohexen-1-one	6.039	5.0	ng	102635	1	6.781	411658	20.0
2-Chlorocyclohe...	6.934	5.3	ng	109539	1	6.781	411658	20.0