LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121423\
Data File : BF136567.D
Acq On : 14 Dec 2023 14:31
Operator : CG\JU
Sample : PB157494BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB157494BL

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-BF120523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136567.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	10	17	23	rVB	874442	1924372	41.87%	7.721%
2	5.034	495	501	510	rBV	955152	1274222	27.72%	5.112%
3	5.434	565	569	572	rBV	2266071	2023941	44.03%	8.120%
4	5.598	594	597	603	rBV2	107911	107901	2.35%	0.433%
5	6.040	669	672	676	rBV	158849	126897	2.76%	0.509%
6	6.428	733	738	741	rBV	2053280	1998802	43.49%	8.019%
7	6.787	795	799	802	rBV	720830	626435	13.63%	2.513%
8	6.940	821	825	834	rBV	169430	162432	3.53%	0.652%
9	7.351	888	895	897	rBV	1655296	1927536	41.93%	7.733%
10	8.063	1011	1016	1019	rBV	982583	862036	18.75%	3.458%
11	9.145	1193	1200	1203	rBV	4385860	4014729	87.34%	16.107%
12	9.822	1309	1315	1318	rBV	1162994	1033258	22.48%	4.145%
13	10.610	1445	1449	1453	rBV	1790604	1645143	35.79%	6.600%
14	11.310	1564	1568	1572	rBV	1380119	1130999	24.61%	4.538%
15	12.910	1835	1840	1843	rBV	4270218	4596499	100.00%	18.441%
16	13.963	2015	2019	2022	rBV	901884	821662	17.88%	3.297%
17	15.439	2264	2270	2275	rBV	540269	648316	14.10%	2.601%

Sum of corrected areas: 24925180

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ClientSampleId :
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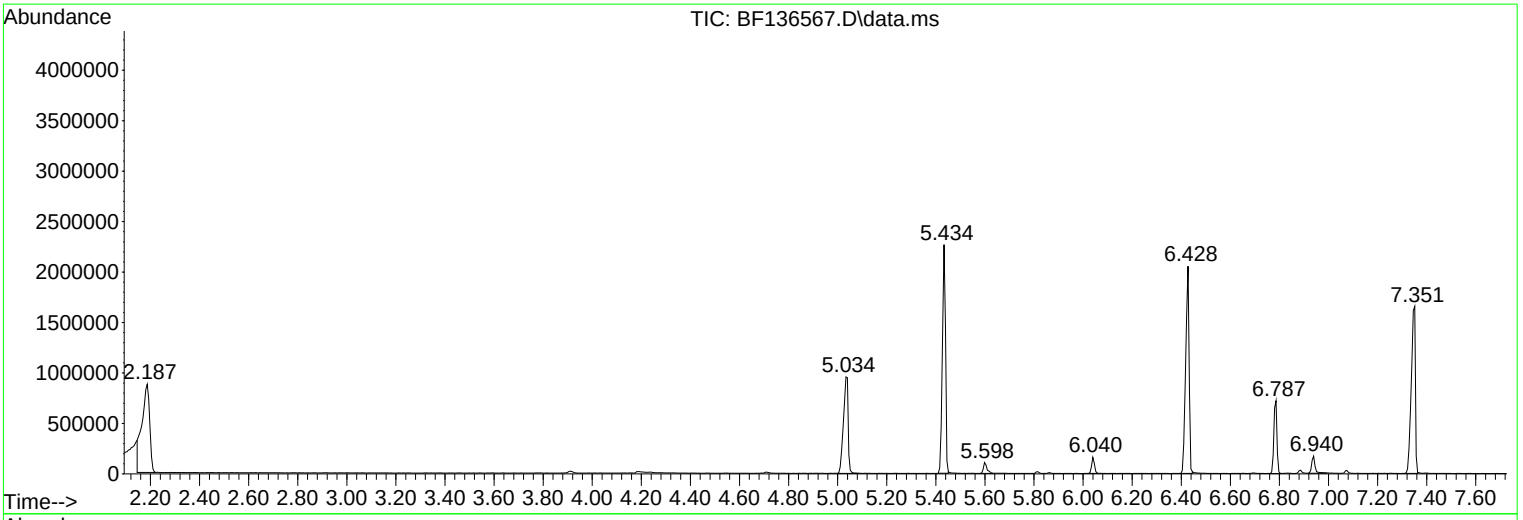
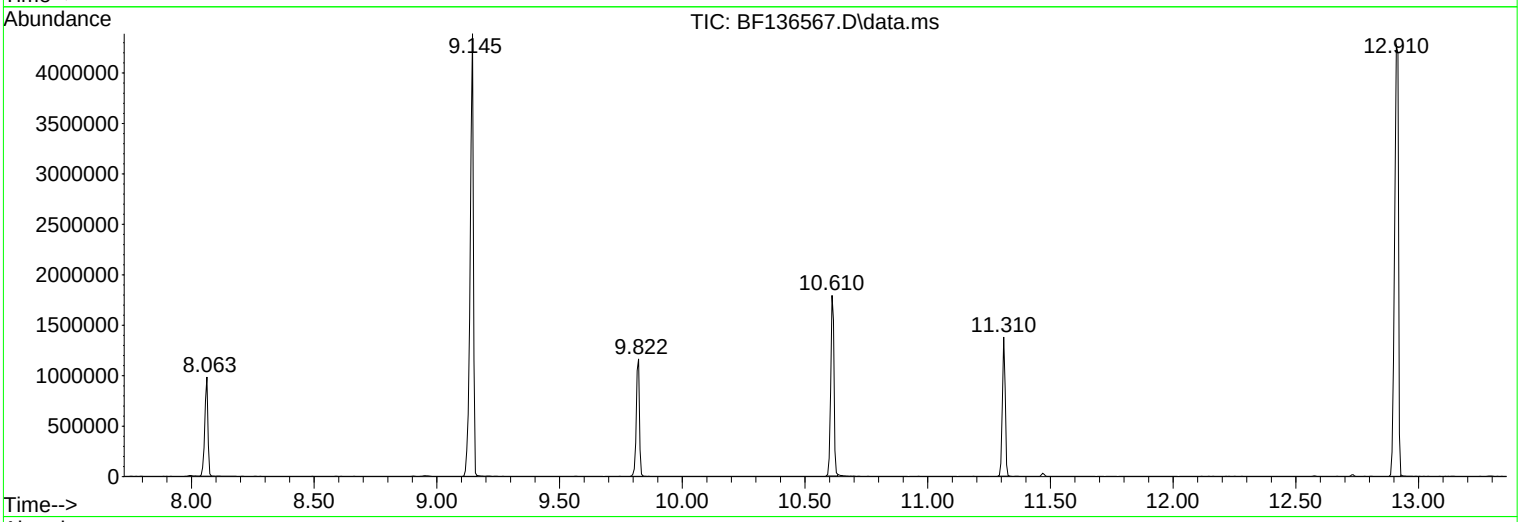
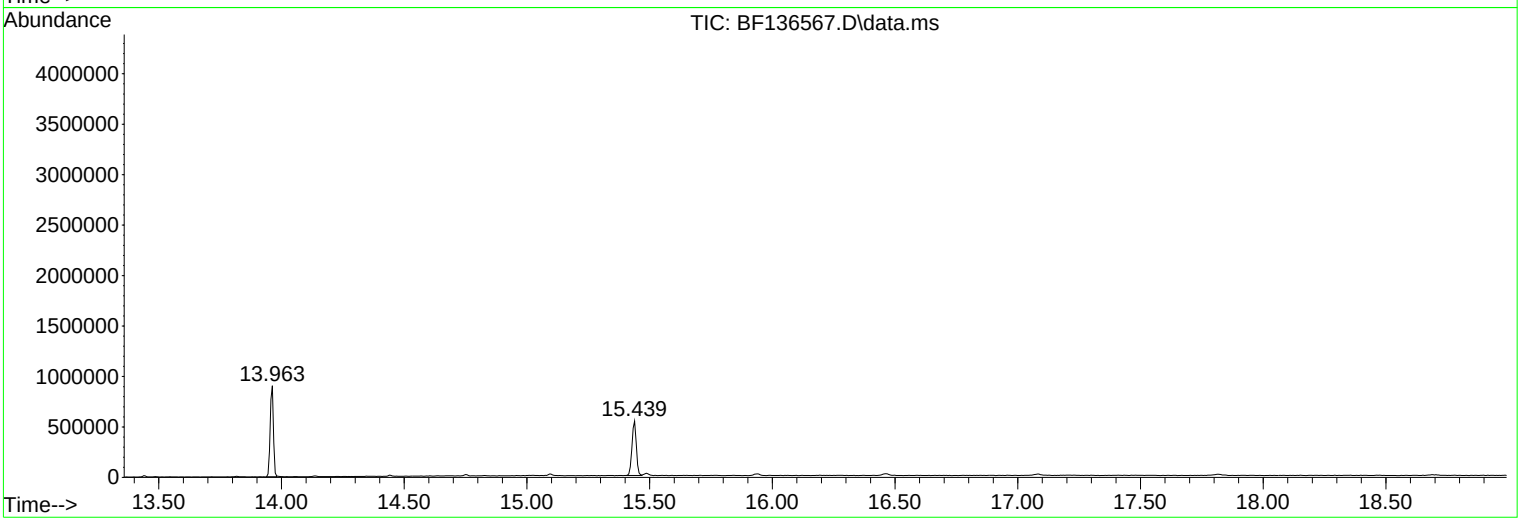
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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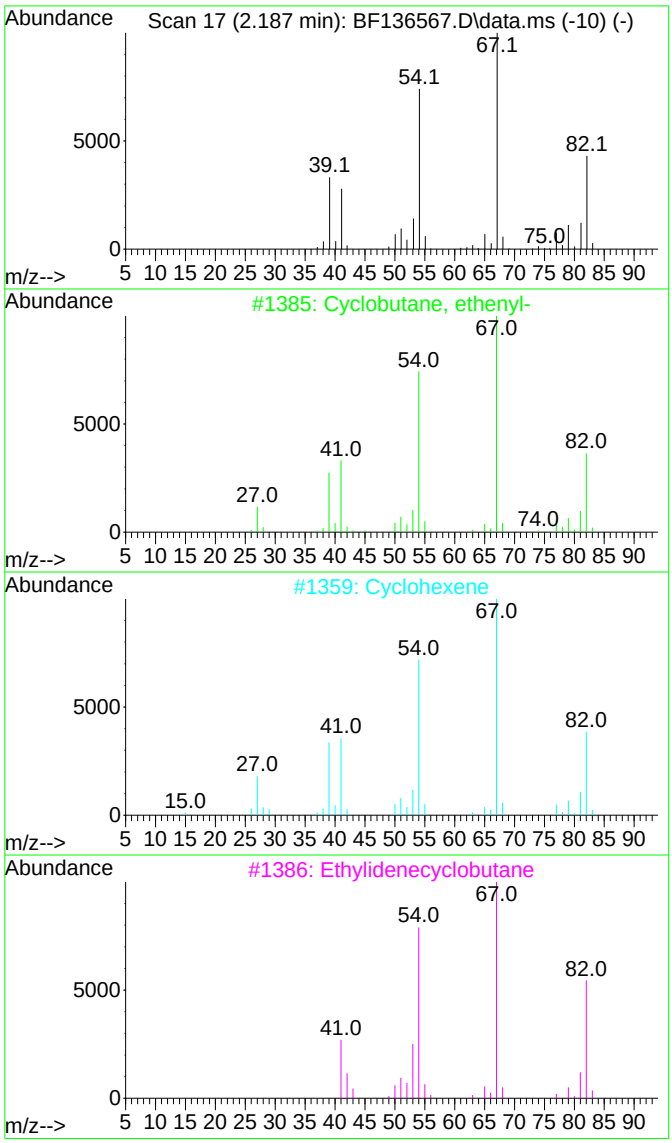
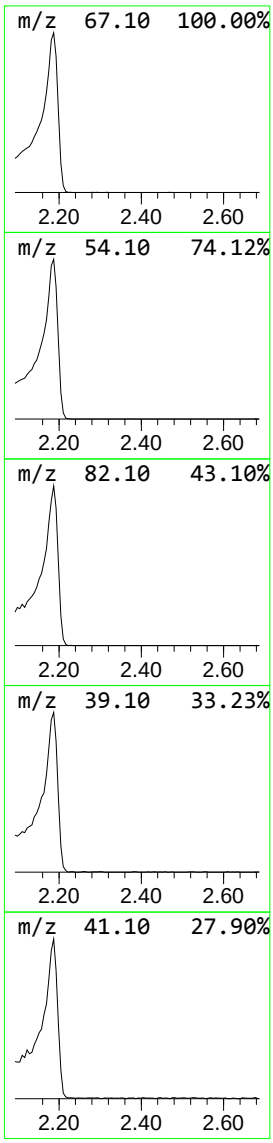
Peak Number 1 Cyclobutane, ethenyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	61.44 ng	1924370	1,4-Dichlorobenzene-d4	6.787

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, ethenyl-	82	C6H10	002597-49-1	94
2	Cyclohexene	82	C6H10	000110-83-8	94
3	Ethylidenecyclobutane	82	C6H10	001528-21-8	91
4	2,4-Hexadiene, (E,E)-	82	C6H10	005194-51-4	35
5	C2H5CH=CHCH=CH2	82	C6H10	000592-48-3	35





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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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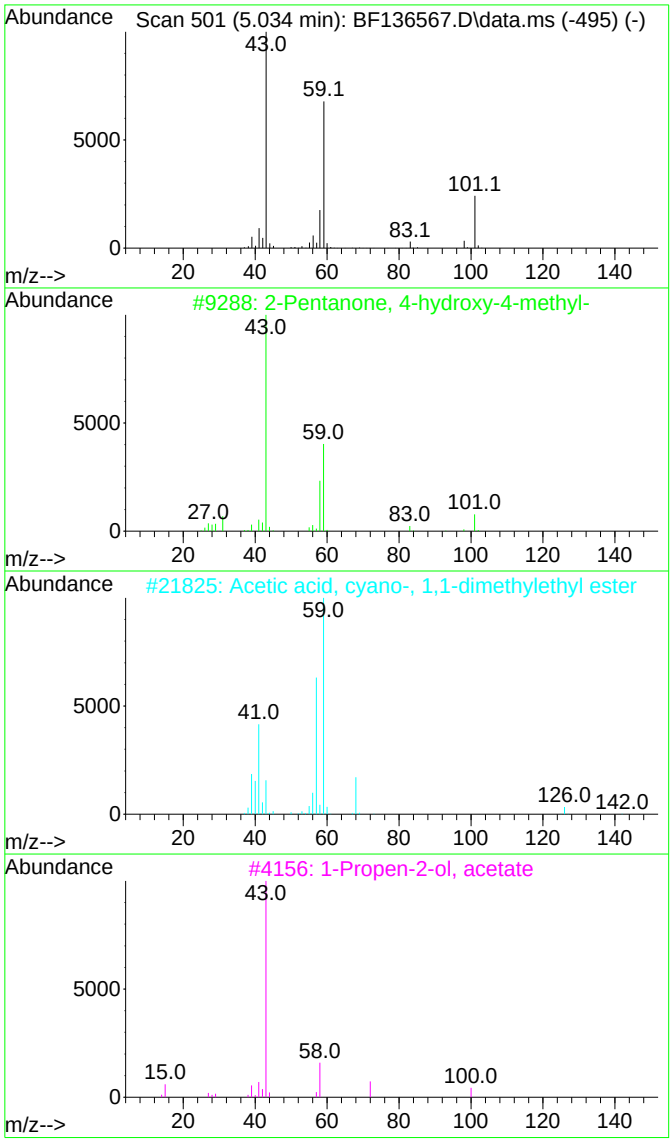
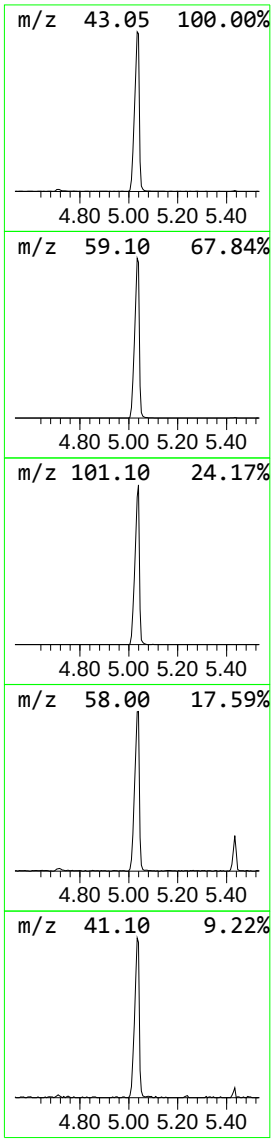
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.034	40.68 ng	1274220	1,4-Dichlorobenzene-d4	6.787

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Guanidine	59	CH5N3	000113-00-8	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Operator : CG\JU
Sample : PB157494BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB157494BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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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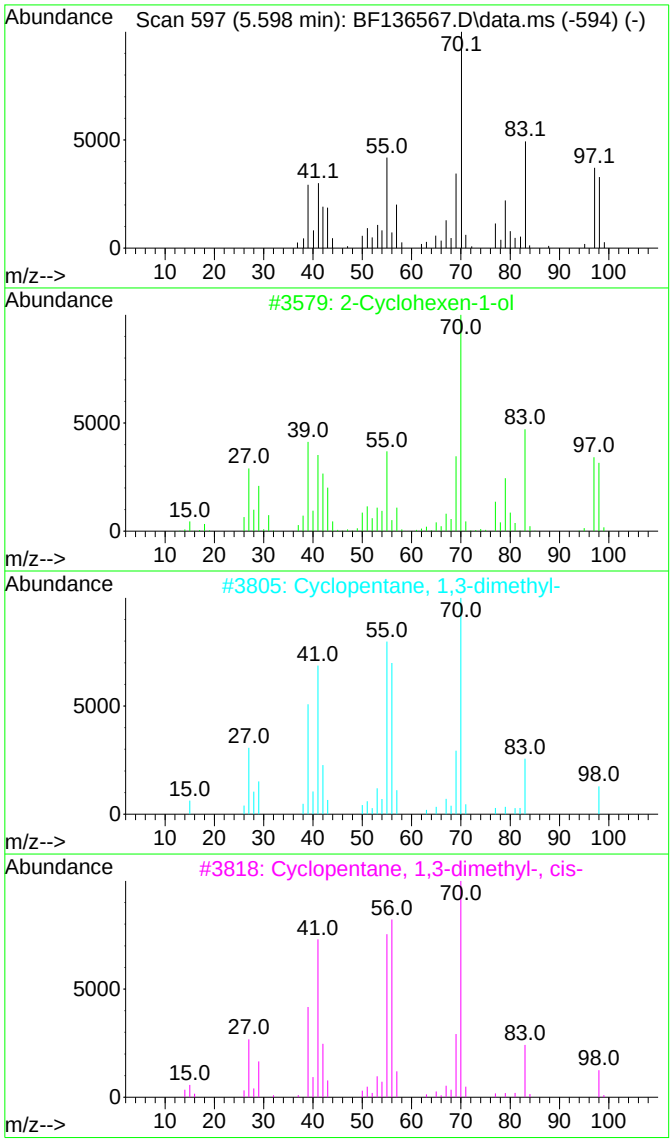
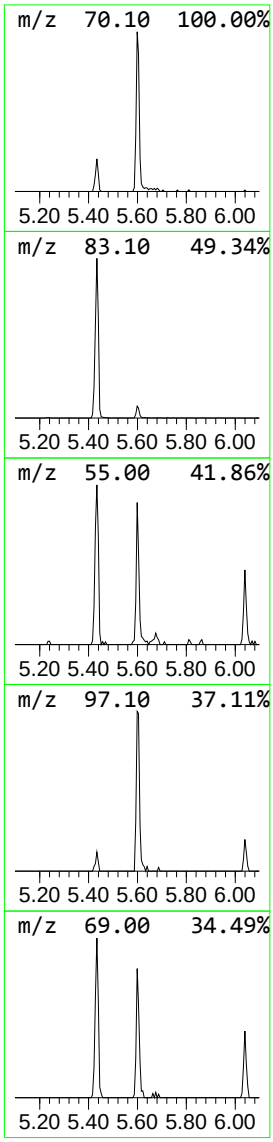
Peak Number 3 2-Cyclohexen-1-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.598	3.44 ng	107901	1,4-Dichlorobenzene-d4	6.787

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	93
2	Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	53
3	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	52
4	2-Methylene cyclopentanol	98	C6H10O	020461-31-8	37
5	2-Butenal, (Z)-	70	C4H6O	015798-64-8	25





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Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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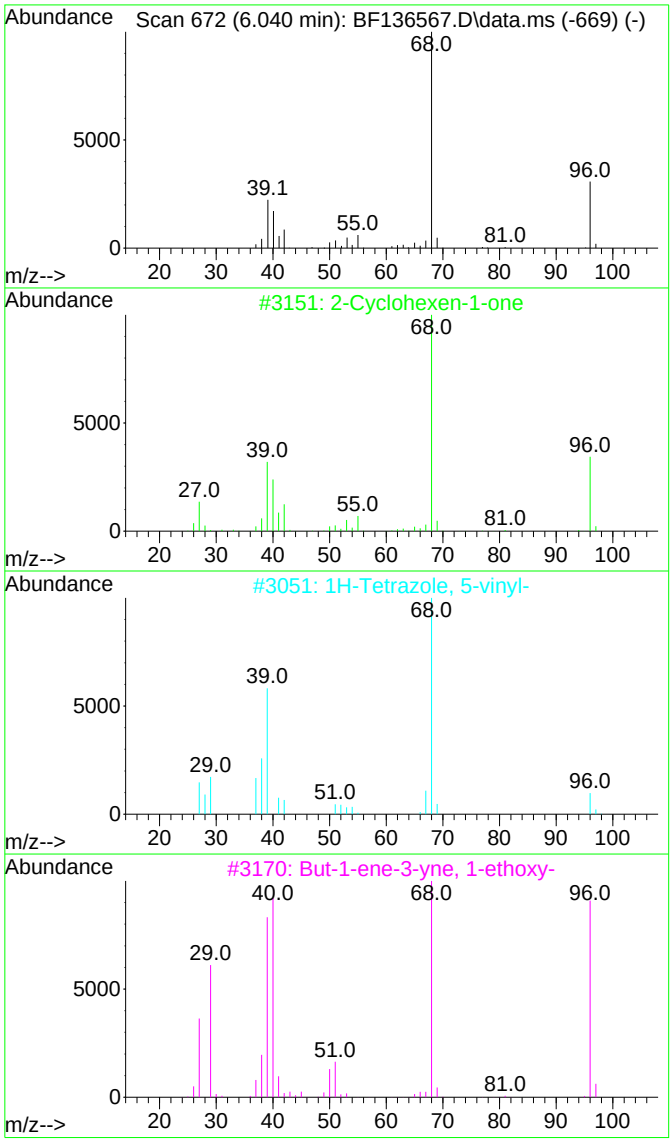
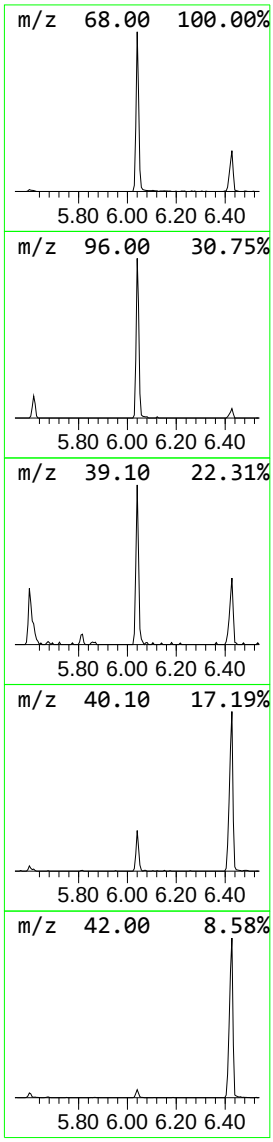
Peak Number 4 2-Cyclohexen-1-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.040	4.05 ng	126897	1,4-Dichlorobenzene-d4	6.787

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	91
2	1H-Tetrazole, 5-vinyl-	96	C3H4N4	018755-47-0	56
3	But-1-ene-3-yne, 1-ethoxy-	96	C6H8O	002806-41-9	50
4	Ethyl cyanoacetate	113	C5H7NO2	000105-56-6	33
5	2,5-Dihydro-3-methyl-thiophene 1...	132	C5H8O2S	001193-10-8	12





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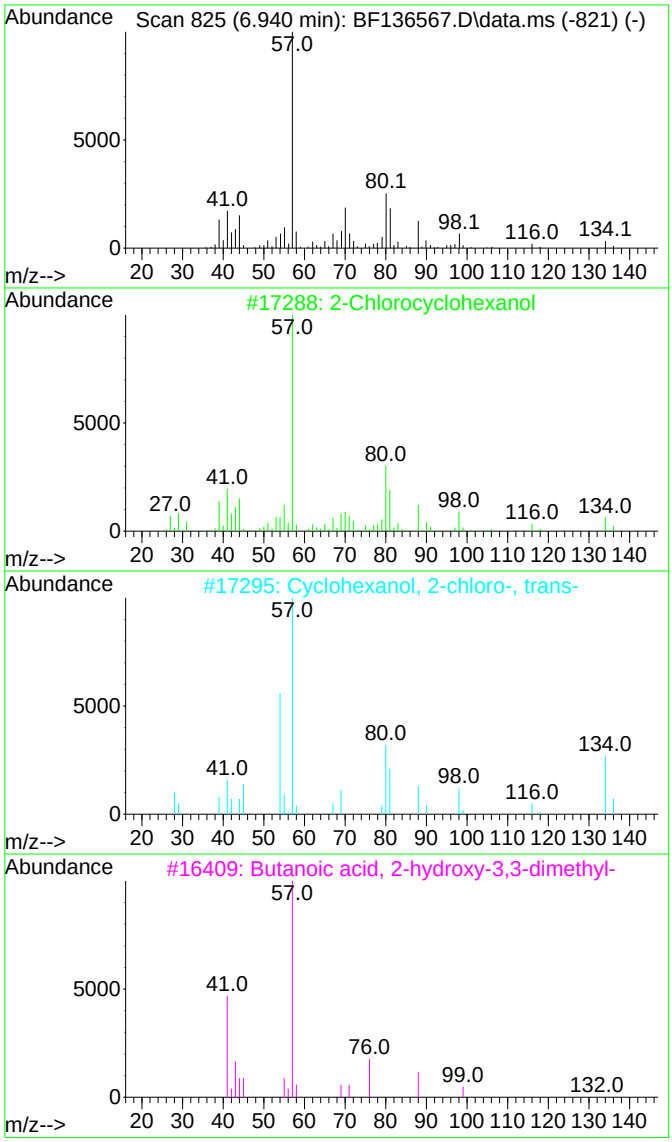
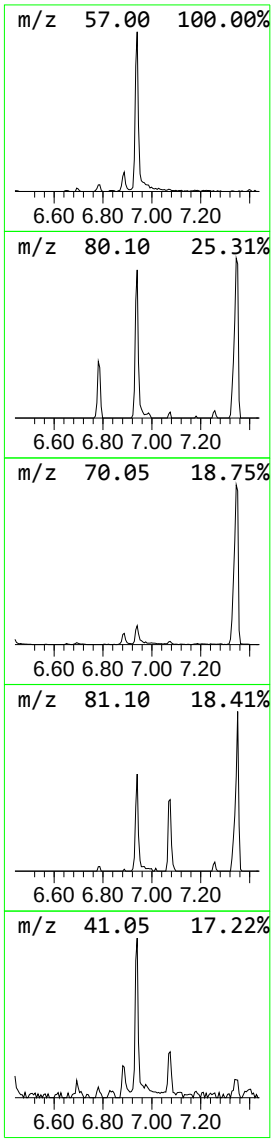
Peak Number 5 2-Chlorocyclohexanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.940	5.19 ng	162432	1,4-Dichlorobenzene-d4	6.787

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	38
3	Butanoic acid, 2-hydroxy-3,3-dim...	132	C6H12O3	004026-20-4	27
4	Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	22
5	Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	16





Tentatively Identified Compound (LSC) summary

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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...	2.187	61.4	ng	1924370	1	6.787	626435	20.0
2-Pentanone, 4-...	5.034	40.7	ng	1274220	1	6.787	626435	20.0
2-Cyclohexen-1-ol	5.598	3.4	ng	107901	1	6.787	626435	20.0
2-Cyclohexen-1-one	6.040	4.0	ng	126897	1	6.787	626435	20.0
2-Chlorocyclohe...	6.940	5.2	ng	162432	1	6.787	626435	20.0