LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071024\
Data File : BF138497.D
Acq On : 10 Jul 2024 12:54
Operator : CG\JU
Sample : PB161493BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB161493BL

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-BF070924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138497.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.269	3	31	37	rVB	1060574	3842989	97.01%	14.251%
2	4.222	360	363	374	rBV	25203	59813	1.51%	0.222%
3	5.098	506	512	520	rBV	1384118	1802554	45.50%	6.684%
4	5.498	576	580	583	rBV	2318765	2131139	53.80%	7.903%
5	5.669	606	609	618	rVB2	133189	134382	3.39%	0.498%
6	6.116	682	685	688	rBV	244820	191719	4.84%	0.711%
7	6.498	745	750	753	rBV	2450820	2251640	56.84%	8.350%
8	6.863	808	812	816	rBV	816194	635375	16.04%	2.356%
9	6.963	824	829	834	rBV	50521	50305	1.27%	0.187%
10	7.016	834	838	849	rVB	240228	220491	5.57%	0.818%
11	7.428	902	908	911	rBV	2139877	2200684	55.55%	8.161%
12	7.775	963	967	973	rBV	41390	40257	1.02%	0.149%
13	8.145	1025	1030	1033	rBV	954172	859162	21.69%	3.186%
14	9.222	1207	1213	1216	rBV	4006180	3762781	94.99%	13.953%
15	9.898	1323	1328	1331	rBV	1198097	975995	24.64%	3.619%
16	10.686	1458	1462	1465	rBV	1700561	1431974	36.15%	5.310%
17	11.386	1577	1581	1584	rBV	1120496	1043704	26.35%	3.870%
18	12.974	1845	1851	1854	rBV	3809244	3961375	100.00%	14.690%
19	14.021	2025	2029	2032	rBV	809403	764308	19.29%	2.834%
20	15.480	2272	2277	2287	rBV	420661	564014	14.24%	2.091%
21	16.451	2436	2442	2448	rVB2	25434	42549	1.07%	0.158%

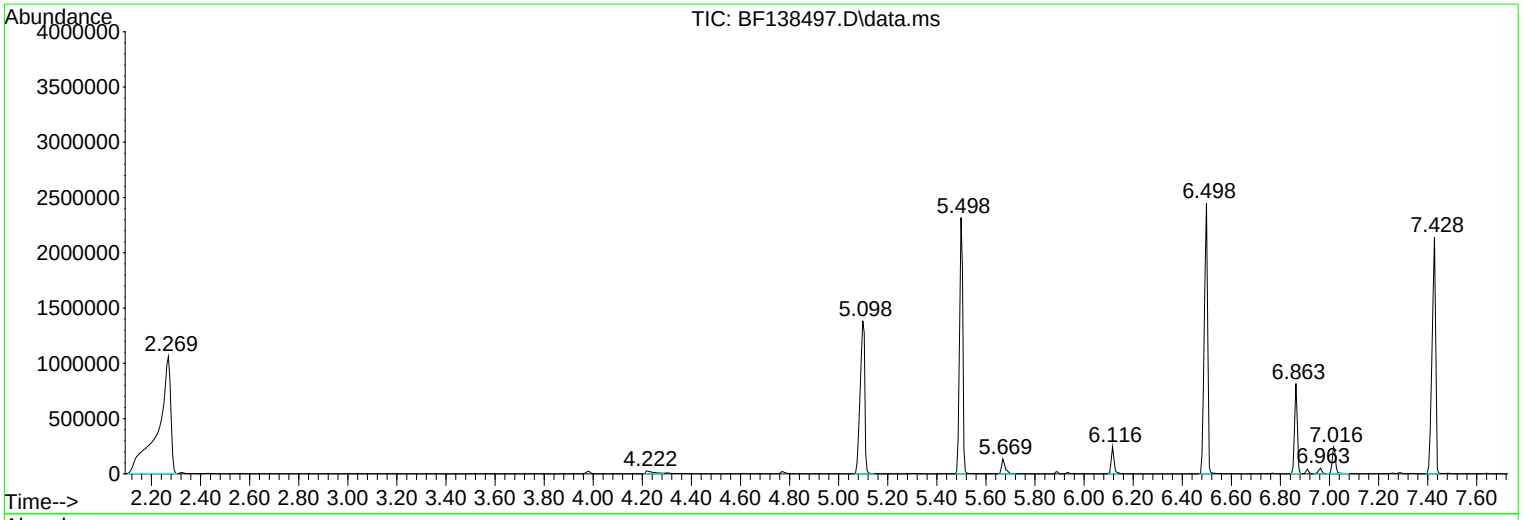
Sum of corrected areas: 26967210

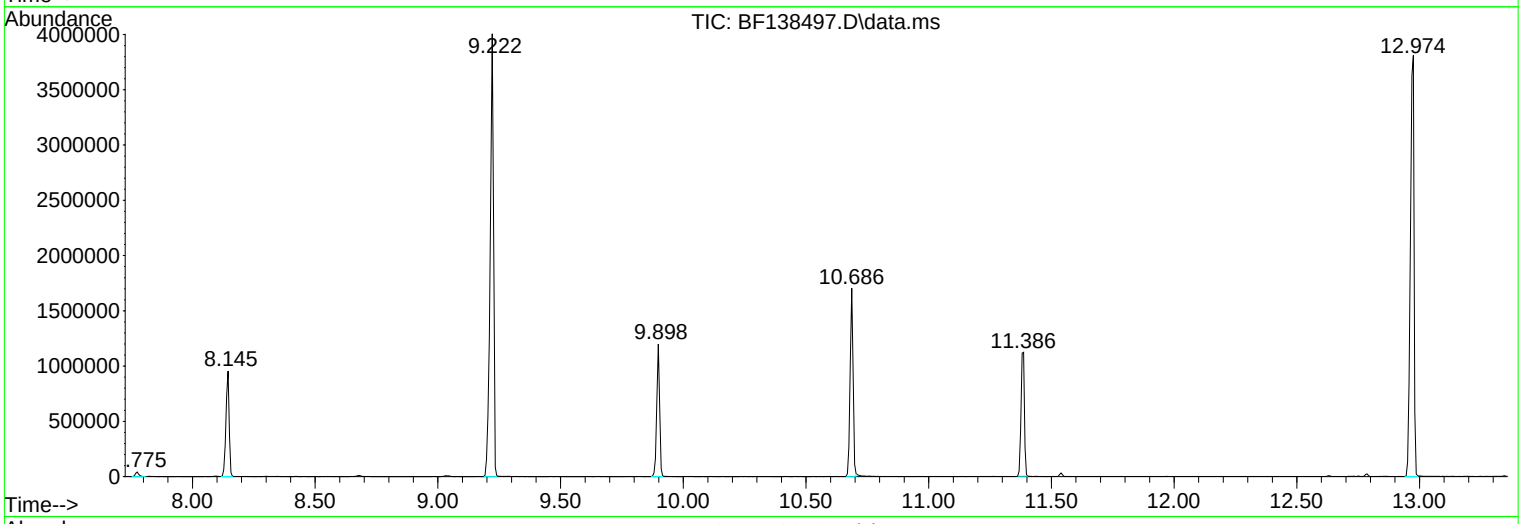
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071024\
Data File : BF138497.D
Acq On : 10 Jul 2024 12:54
Operator : CG\JU
Sample : PB161493BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

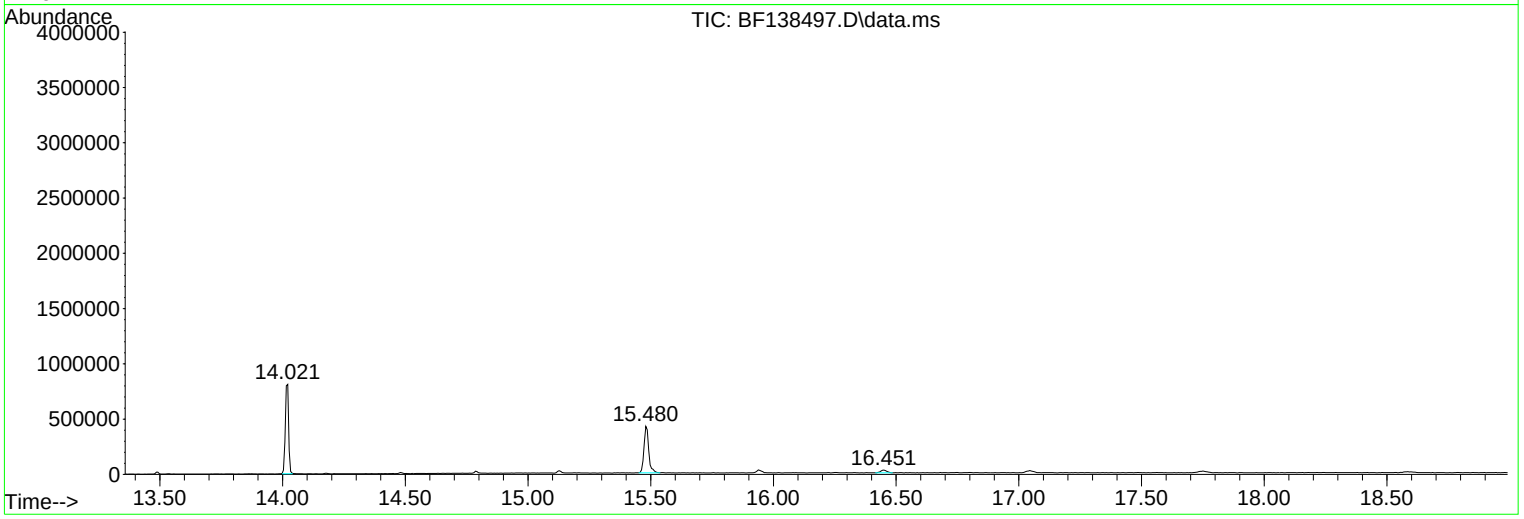
Instrument :
BNA_F
ClientSampleId :
PB161493BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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\BF071024\
Data File : BF138497.D
Acq On : 10 Jul 2024 12:54
Operator : CG\JU
Sample : PB161493BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB161493BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

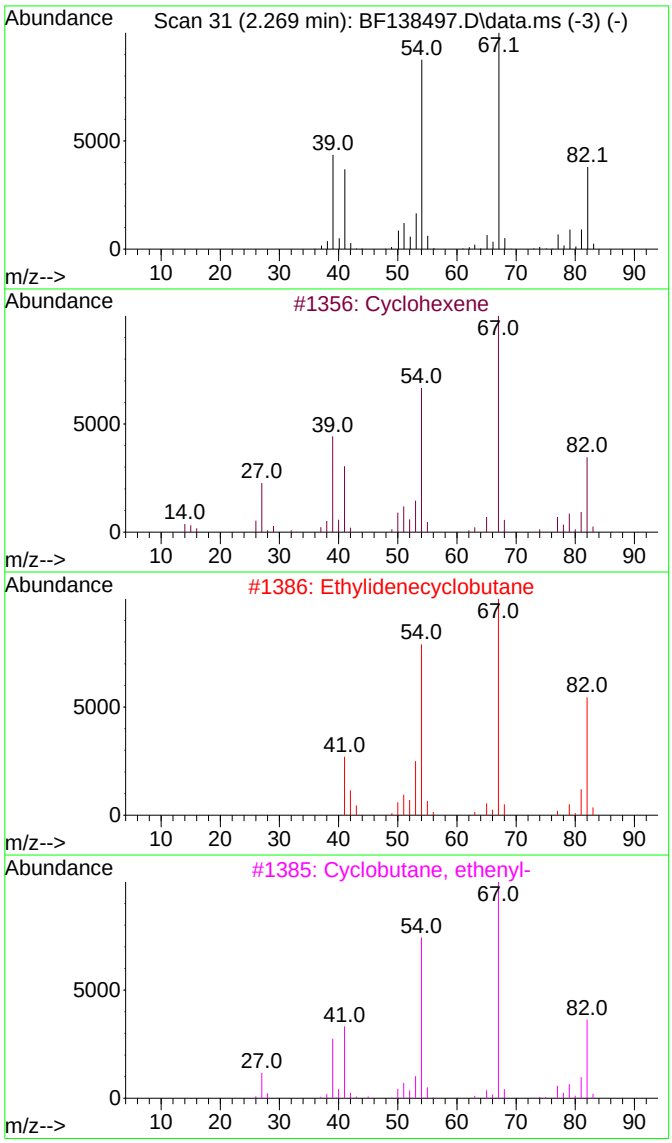
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

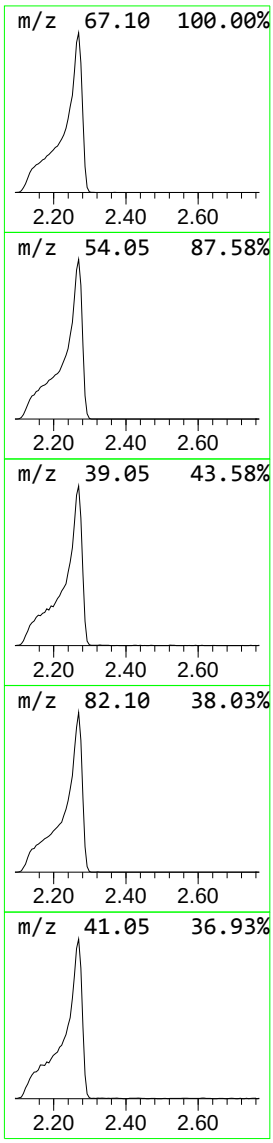
****

Peak Number 1 Cyclohexene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.269	120.97 ng	3842990	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene	82	C6H10	000110-83-8	94
2	Ethylidenecyclobutane	82	C6H10	001528-21-8	91
3	Cyclobutane, ethenyl-	82	C6H10	002597-49-1	90
4	1,3-Pentadiene, 2-methyl-, (E)-	82	C6H10	000926-54-5	38
5	Cyclopropane, (1-methylethylidene)-	82	C6H10	004741-86-0	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071024\
Data File : BF138497.D
Acq On : 10 Jul 2024 12:54
Operator : CG\JU
Sample : PB161493BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB161493BL

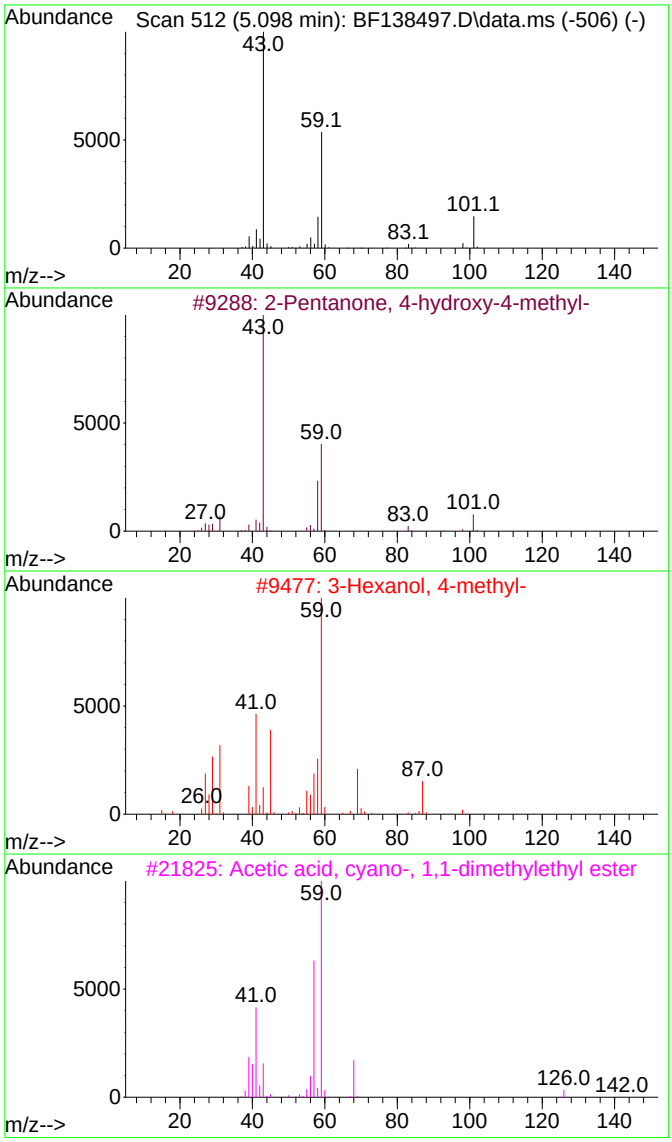
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

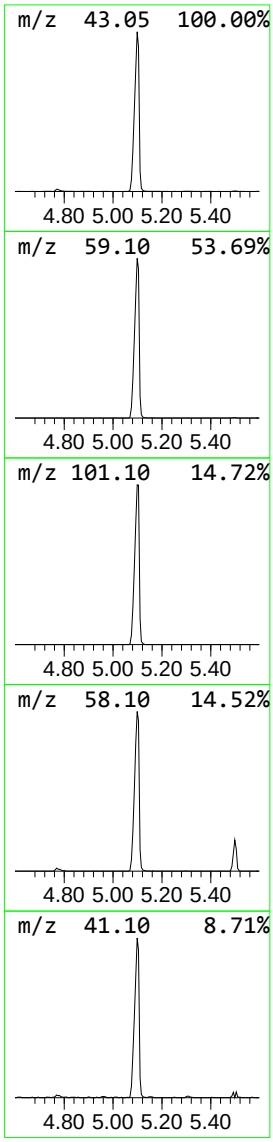
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	56.74 ng	1802550	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071024\
Data File : BF138497.D
Acq On : 10 Jul 2024 12:54
Operator : CG\JU
Sample : PB161493BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB161493BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

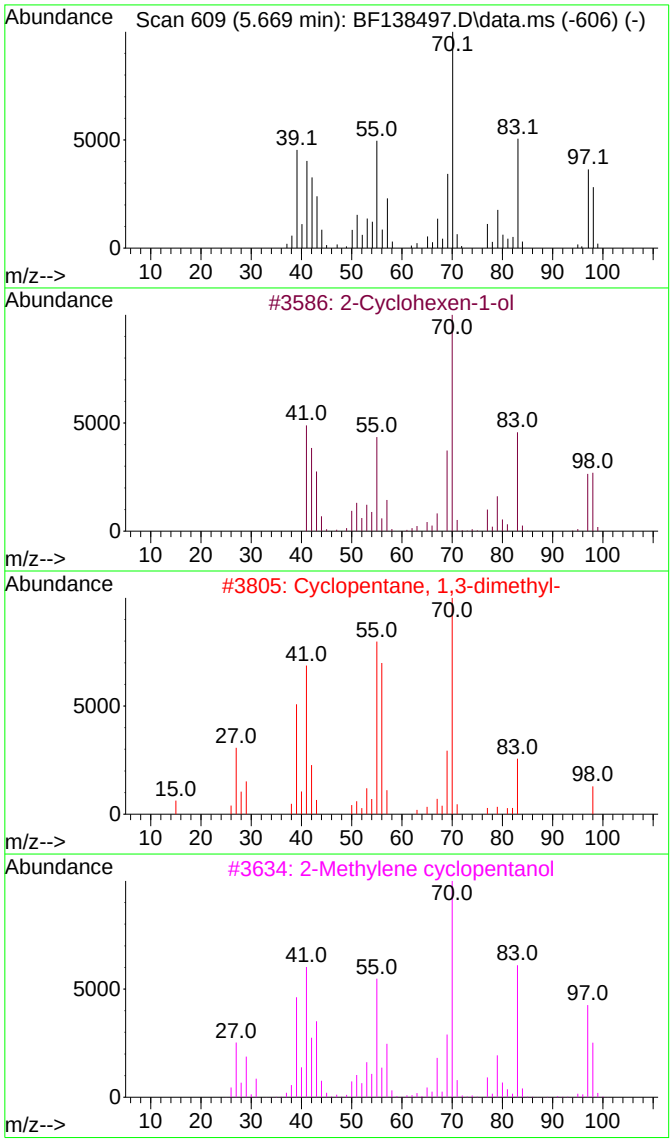
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

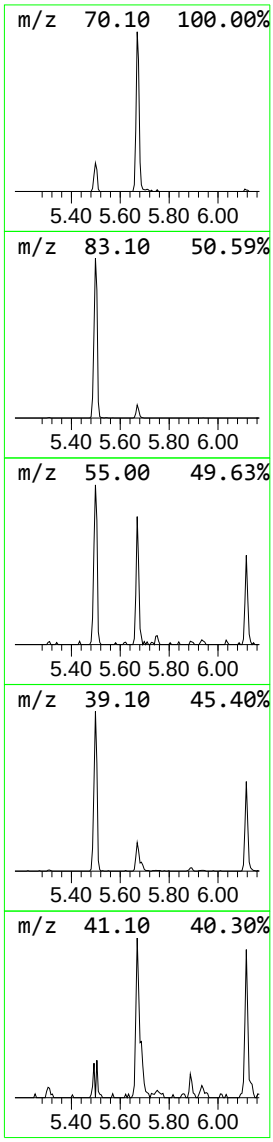
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.669	4.23 ng	134382	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	81
2	Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	47
3	2-Methylene cyclopentanol	98	C6H10O	020461-31-8	43
4	Furan, 2,5-dihydro-2,5-dimethyl-	98	C6H10O	059242-27-2	41
5	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071024\
Data File : BF138497.D
Acq On : 10 Jul 2024 12:54
Operator : CG\JU
Sample : PB161493BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB161493BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

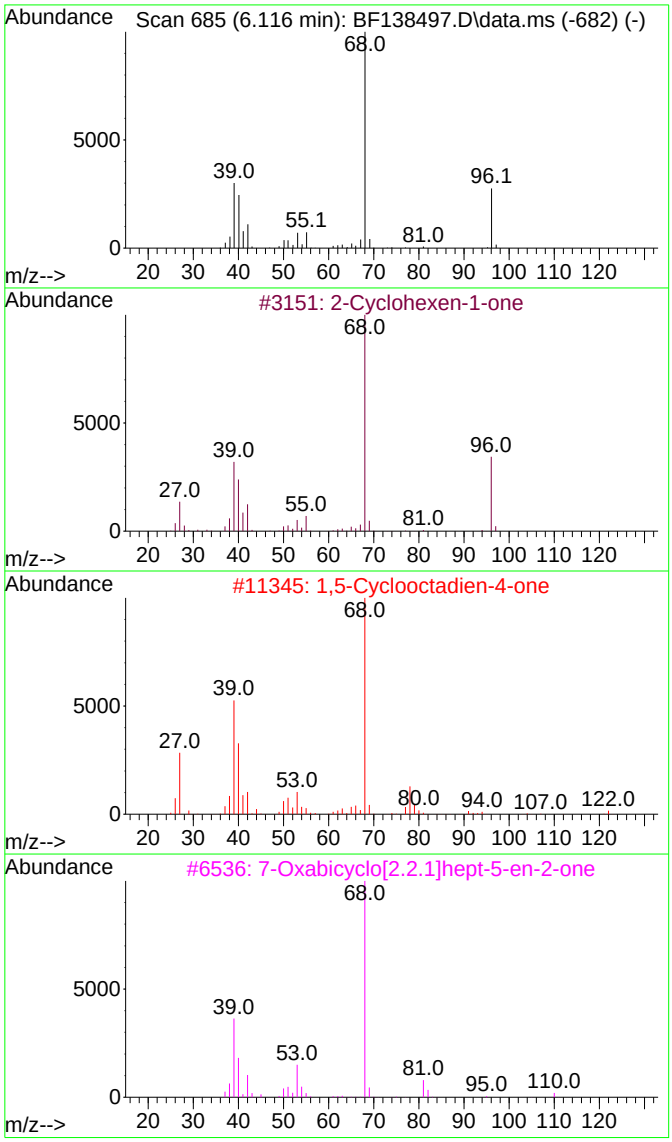
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

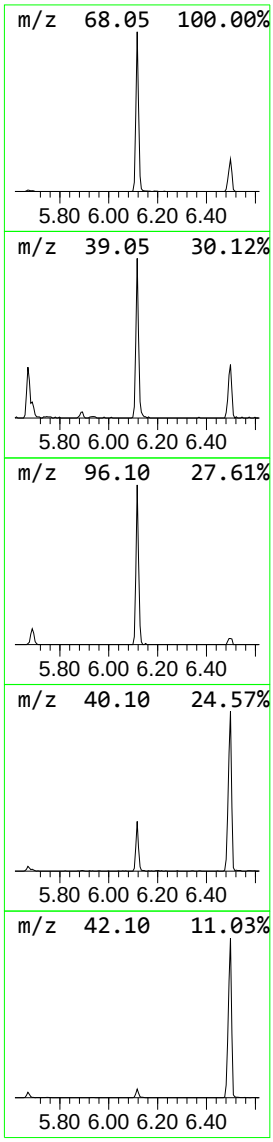
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.116	6.03 ng	191719	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	91
2	1,5-Cyclooctadien-4-one	122	C8H10O	001460-21-5	53
3	7-Oxabicyclo[2.2.1]hept-5-en-2-one	110	C6H6O2	095530-78-2	42
4	1H-Pyrazole	68	C3H4N2	000288-13-1	36
5	2,5-Dihydro-3-methyl-thiophene 1...	132	C5H8O2S	001193-10-8	36





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071024\
Data File : BF138497.D
Acq On : 10 Jul 2024 12:54
Operator : CG\JU
Sample : PB161493BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB161493BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

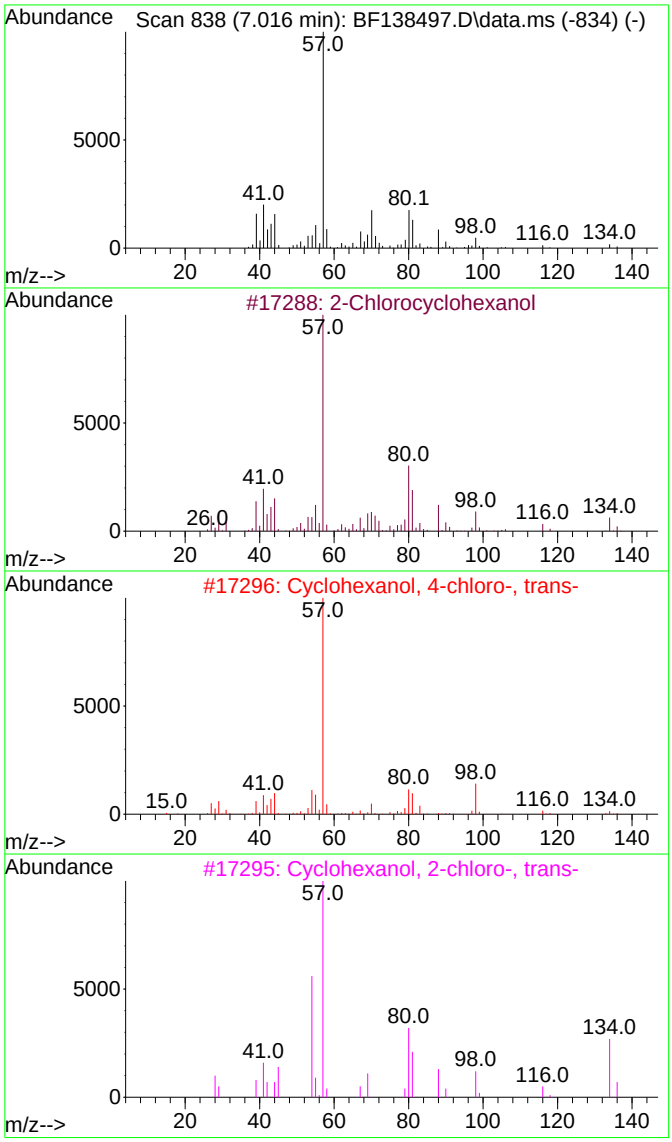
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

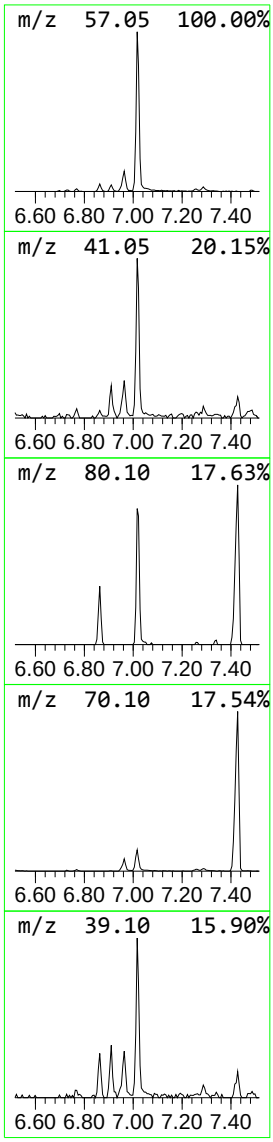
****

Peak Number 5 2-Chlorocyclohexanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.016	6.94 ng	220491	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chlorocyclohexanol	134	C6H11ClO	001561-86-0	81
2	Cyclohexanol, 4-chloro-, trans-	134	C6H11ClO	029538-77-0	45
3	Cyclohexanol, 2-chloro-, trans-	134	C6H11ClO	006628-80-4	43
4	3-Furanol, tetrahydro-	88	C4H8O2	000453-20-3	37
5	trans-2-tert-Butylcyclohexanol, ...	302	C13H19F5O2	1000467-24-5	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071024\
Data File : BF138497.D
Acq On : 10 Jul 2024 12:54
Operator : CG\JU
Sample : PB161493BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB161493BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
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
Cyclohexene	2.269	121.0	ng	3842990	1	6.863	635375	20.0
2-Pentanone, 4-...	5.098	56.7	ng	1802550	1	6.863	635375	20.0
2-Cyclohexen-1-ol	5.669	4.2	ng	134382	1	6.863	635375	20.0
2-Cyclohexen-1-one	6.116	6.0	ng	191719	1	6.863	635375	20.0
2-Chlorocyclohe...	7.016	6.9	ng	220491	1	6.863	635375	20.0