LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082824\
Data File : BF139203.D
Acq On : 28 Aug 2024 12:09
Operator : RC/JU
Sample : PB163034BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB163034BL

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-BF082724.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139203.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.310	7	37	44	rBV	796399	3323514	85.79%	12.870%
2	4.228	358	363	378	rBV	23640	65079	1.68%	0.252%
3	5.122	507	515	521	rBV	939456	1499827	38.71%	5.808%
4	5.516	576	582	587	rBV	1612085	2140588	55.25%	8.289%
5	5.692	607	612	622	rVB2	84301	128338	3.31%	0.497%
6	6.140	683	688	698	rVB	148325	190657	4.92%	0.738%
7	6.516	745	752	757	rBV	1562219	2253644	58.17%	8.727%
8	6.892	810	816	820	rBV	505775	641022	16.55%	2.482%
9	6.987	827	832	836	rVV	37638	50654	1.31%	0.196%
10	7.045	836	842	847	rVB2	141138	201905	5.21%	0.782%
11	7.451	904	911	916	rBV	1546119	2193588	56.62%	8.495%
12	7.781	963	967	975	rVB	36744	45638	1.18%	0.177%
13	8.169	1028	1033	1038	rBV	645615	834073	21.53%	3.230%
14	9.245	1209	1216	1221	rBV	2897467	3874064	100.00%	15.002%
15	9.922	1325	1331	1336	rBV	756616	955470	24.66%	3.700%
16	10.710	1459	1465	1483	rVB	1174509	1482916	38.28%	5.743%
17	11.410	1578	1584	1589	rBV	812413	1019237	26.31%	3.947%
18	12.998	1848	1854	1859	rBV	2982281	3869464	99.88%	14.984%
19	14.045	2026	2032	2037	rBV	496630	626800	16.18%	2.427%
20	15.515	2276	2282	2287	rBV	283546	426749	11.02%	1.653%

Sum of corrected areas: 25823227

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Misc :
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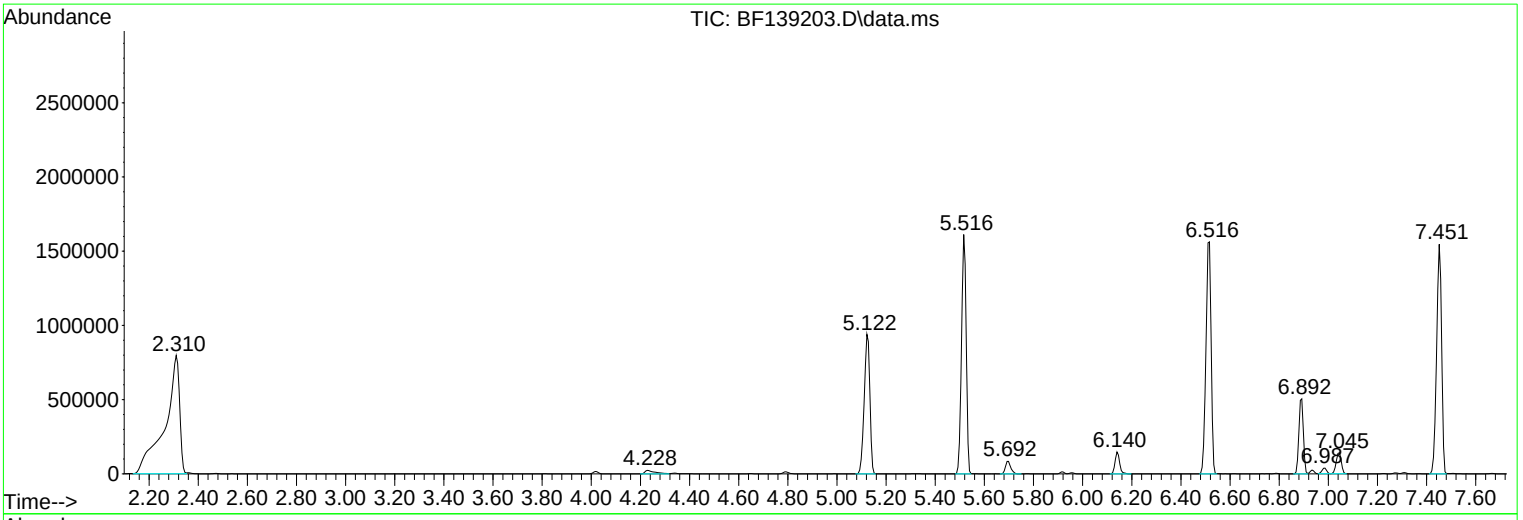
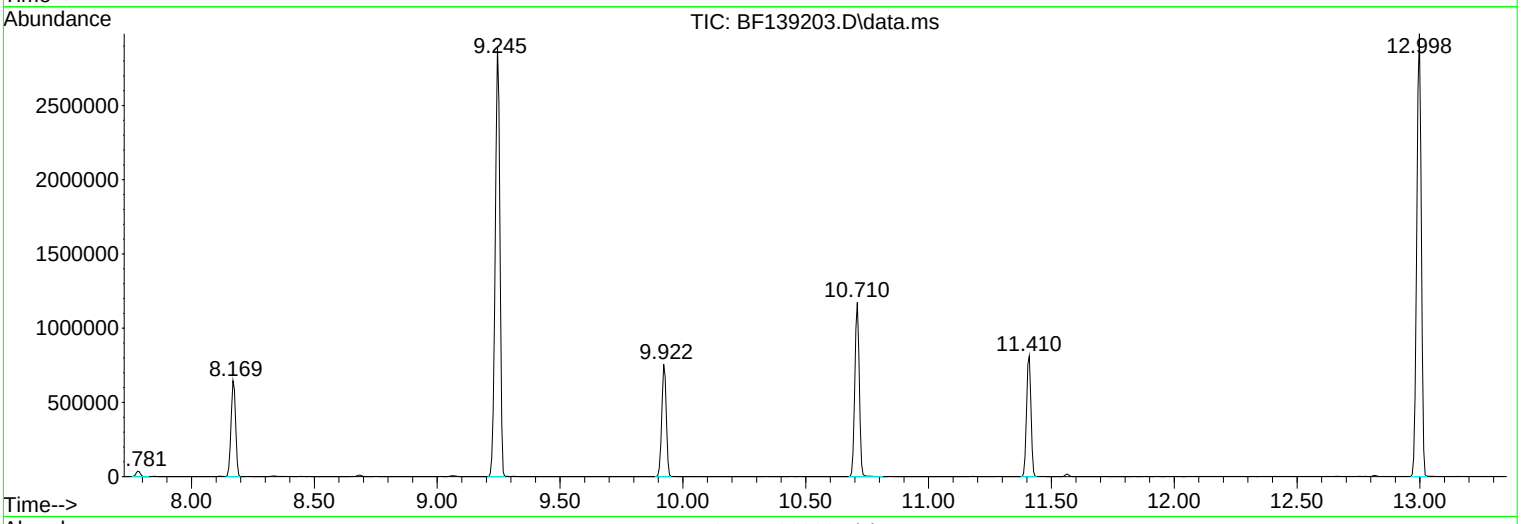
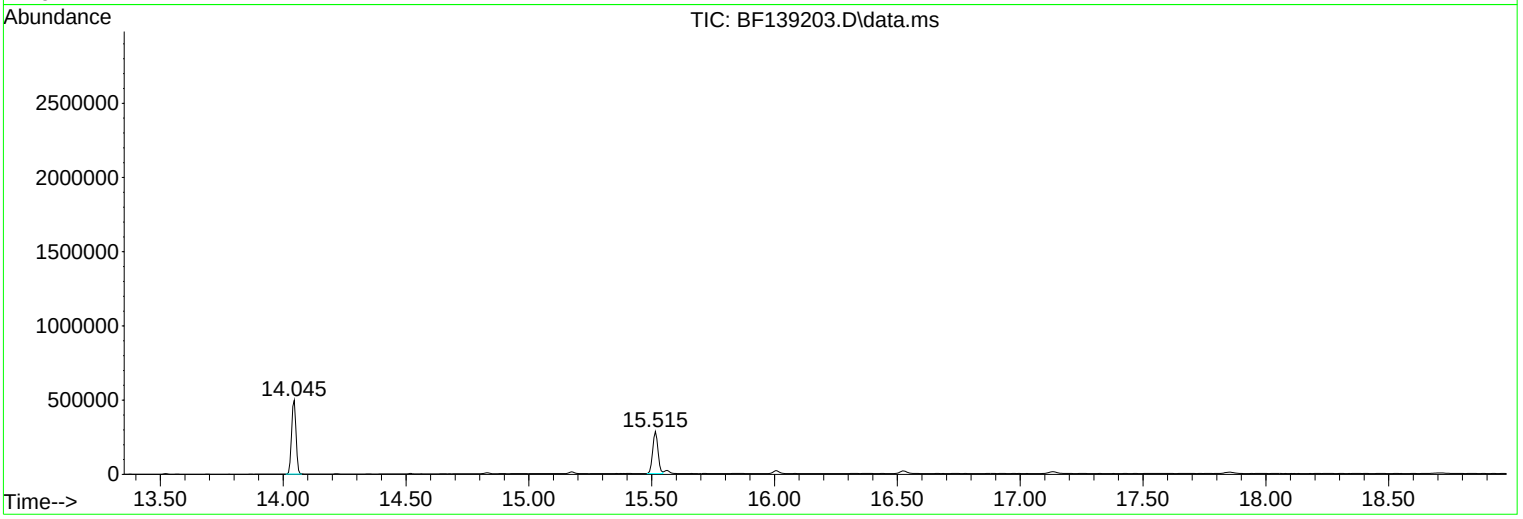
Instrument :
BNA_F
ClientSampleId :
PB163034BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.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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Operator : RC/JU
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

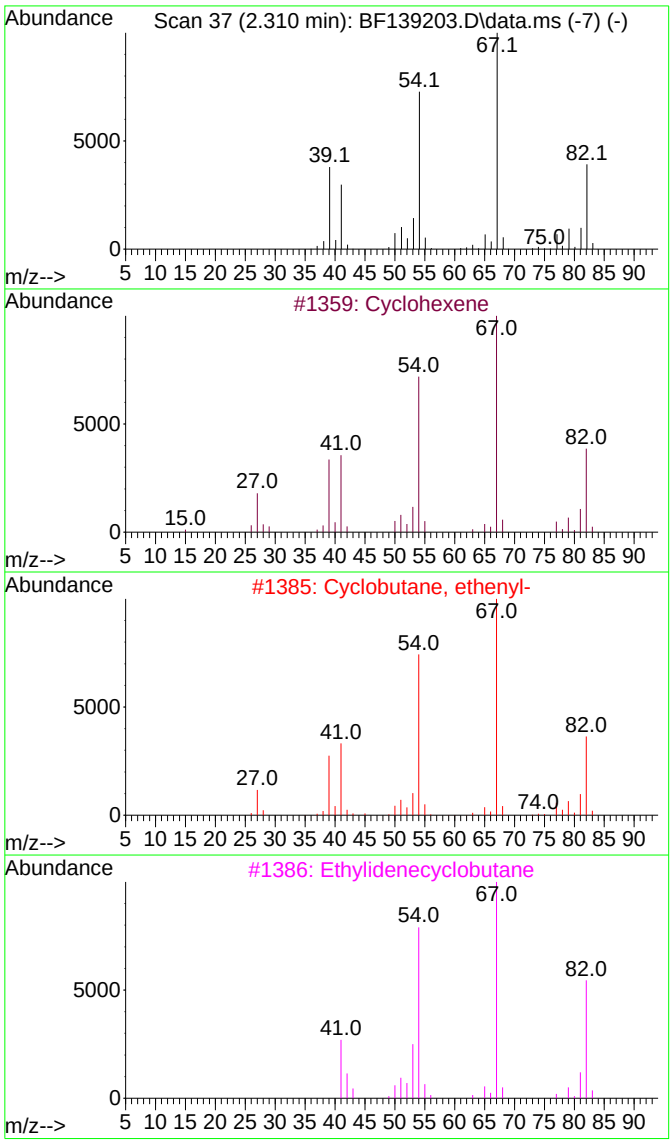
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

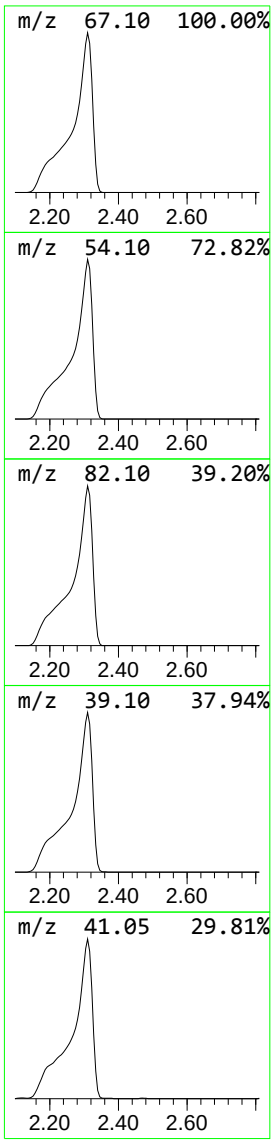
****

Peak Number 1 Cyclohexene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.310	103.69 ng	3323510	1,4-Dichlorobenzene-d4	6.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene	82	C6H10	000110-83-8	94
2	Cyclobutane, ethenyl-	82	C6H10	002597-49-1	90
3	Ethylidenecyclobutane	82	C6H10	001528-21-8	90
4	2,4-Hexadiene, (E,Z)-	82	C6H10	005194-50-3	76
5	1,3-Pentadiene, 2-methyl-, (E)-	82	C6H10	000926-54-5	76





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Operator : RC/JU
Sample : PB163034BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB163034BL

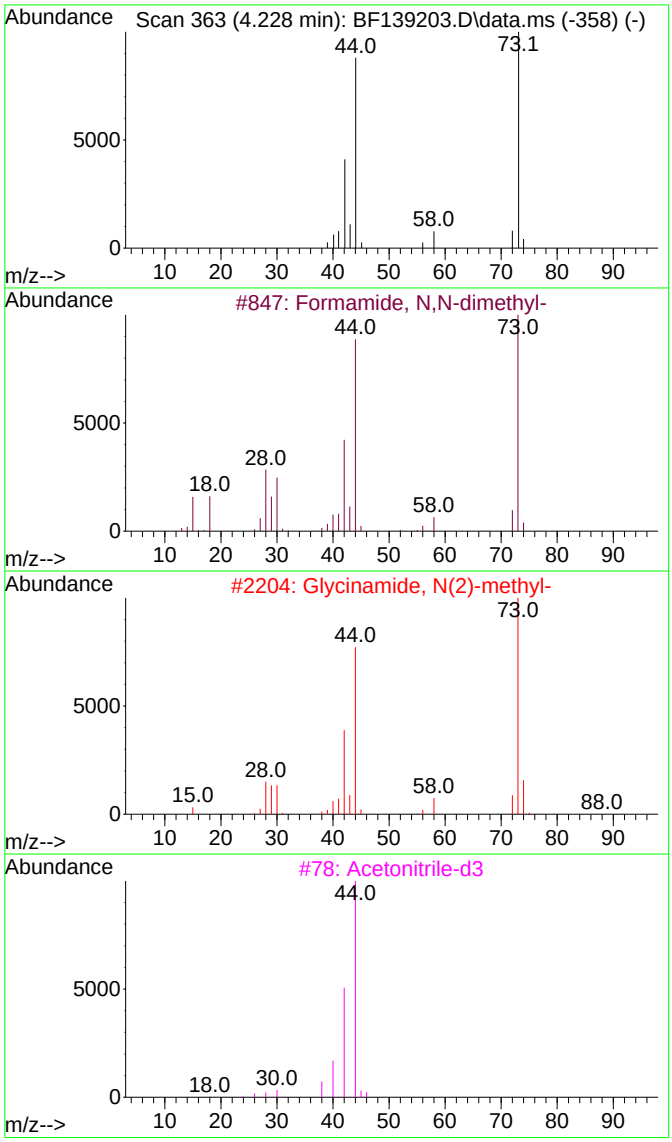
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

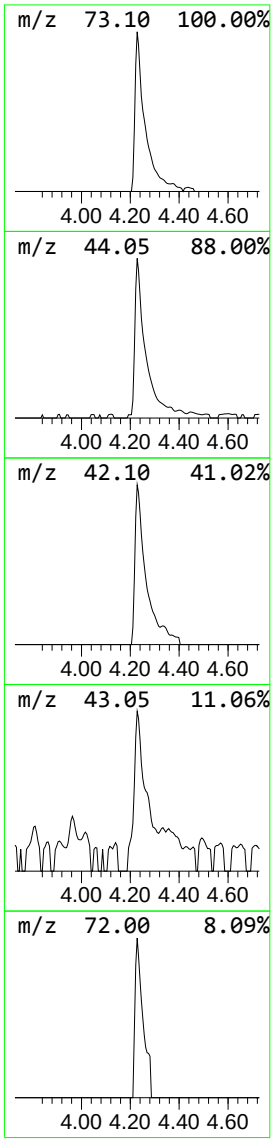
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Formamide, N,N-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.228	2.03 ng	65079	1,4-Dichlorobenzene-d4	6.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Formamide, N,N-dimethyl-	73	C3H7NO	000068-12-2	90
2	Glycinamide, N(2)-methyl-	88	C3H8N2O	1000452-55-9	74
3	Acetonitrile-d3	44	C2D3N	002206-26-0	7
4	N-Ethylformamide	73	C3H7NO	000627-45-2	5
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	5





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Acq On : 28 Aug 2024 12:09
Operator : RC/JU
Sample : PB163034BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB163034BL

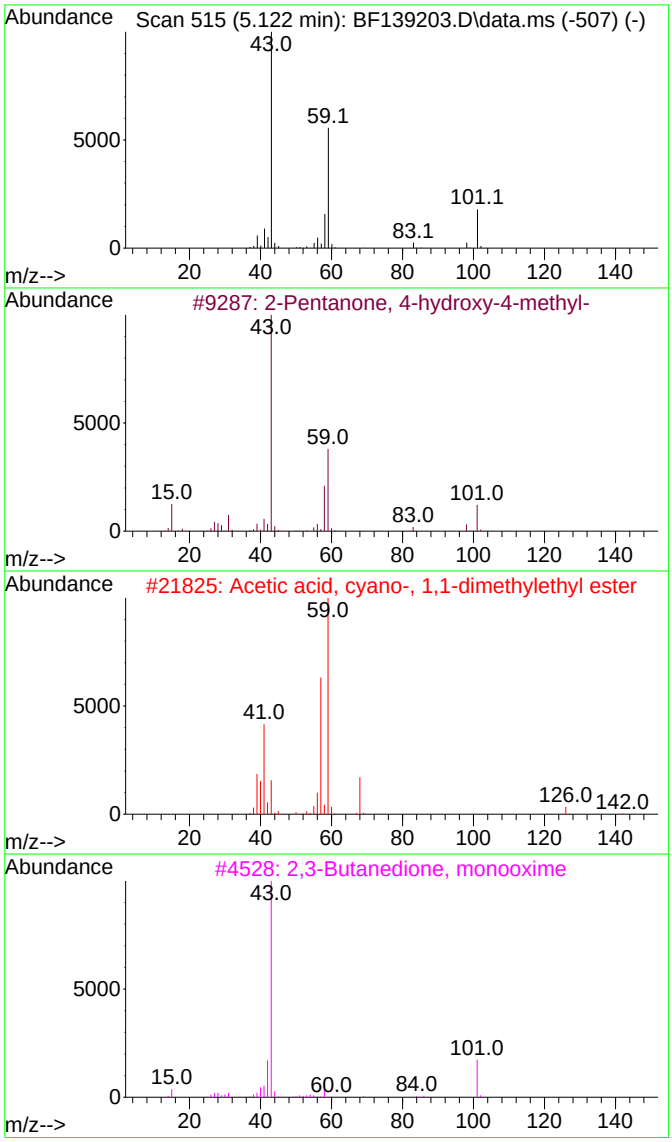
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

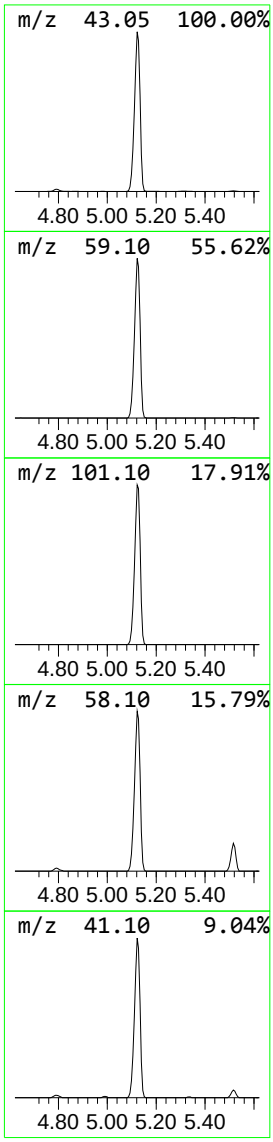
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.122	46.79 ng	1499830	1,4-Dichlorobenzene-d4	6.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	Acetone	58	C3H6O	000067-64-1	12





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.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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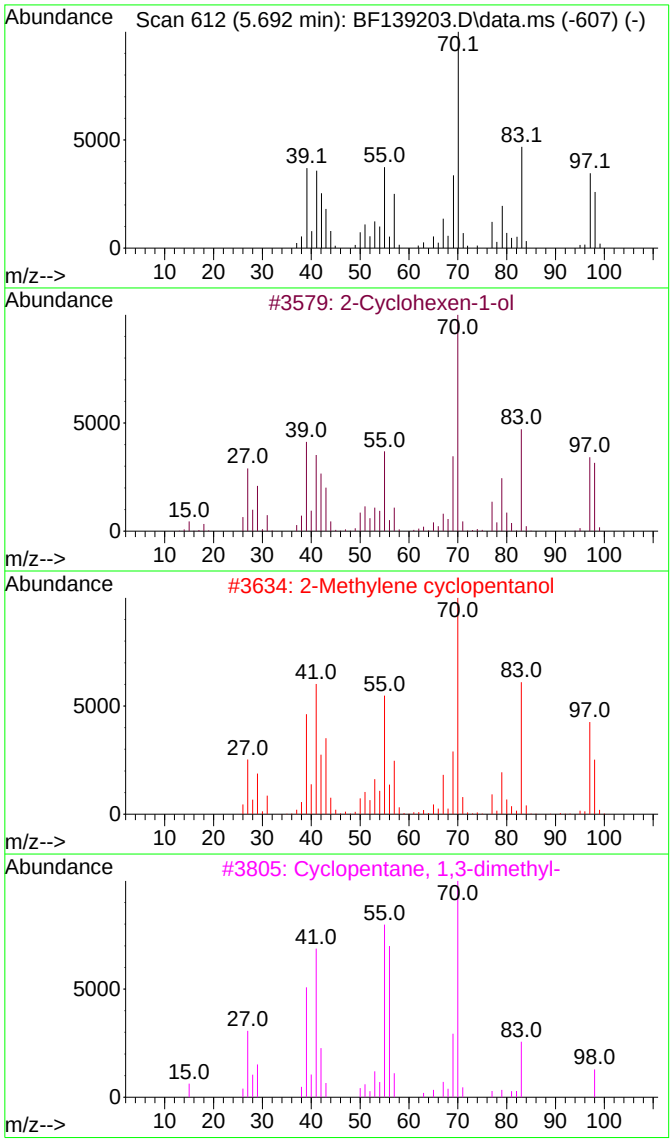
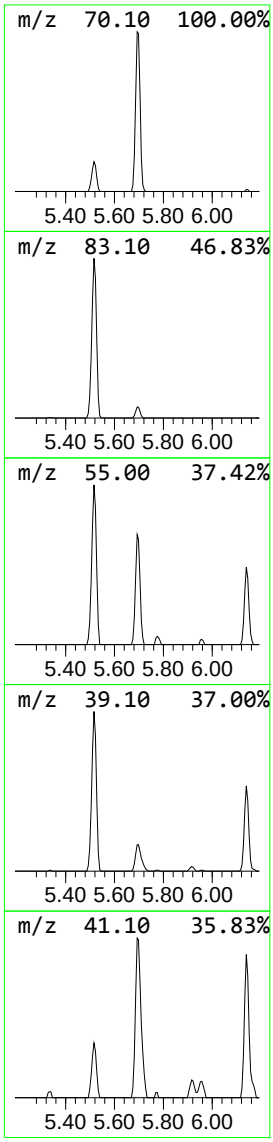
Peak Number 4 2-Cyclohexen-1-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.692	4.00 ng	128338	1,4-Dichlorobenzene-d4	6.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	96
2	2-Methylene cyclopentanol	98	C6H10O	020461-31-8	86
3	Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	38
4	2,6-Cyclooctadien-1-ol	124	C8H12O	010017-18-2	38
5	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	37





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ALS Vial : 6 Sample Multiplier: 1

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
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TIC Library : C:\Database\NIST20.L
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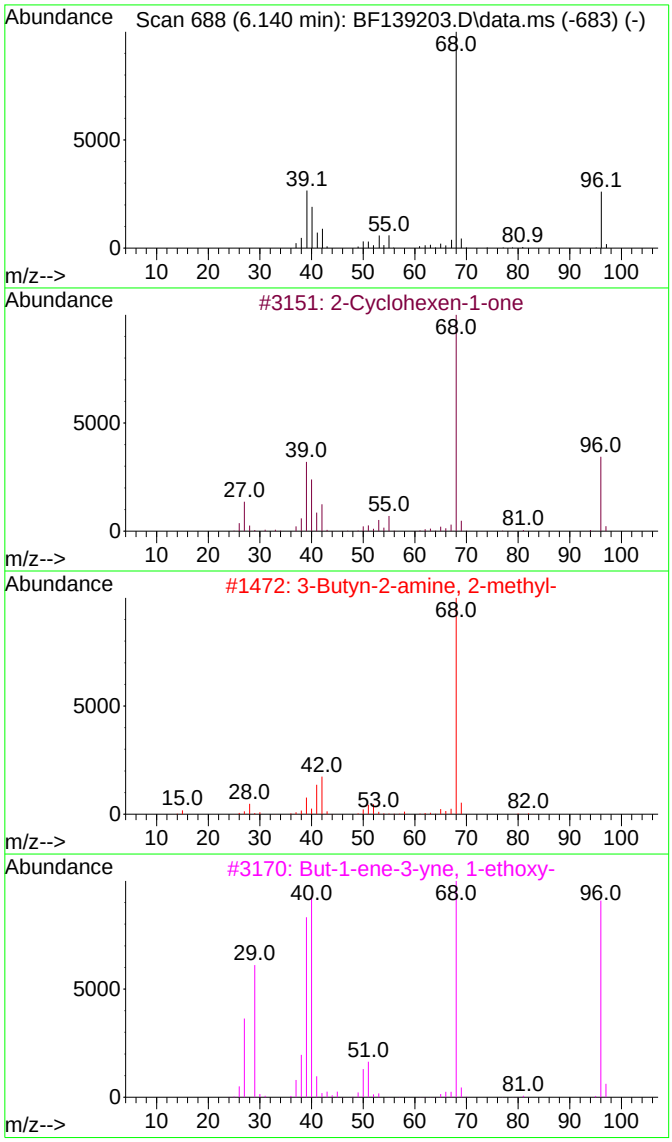
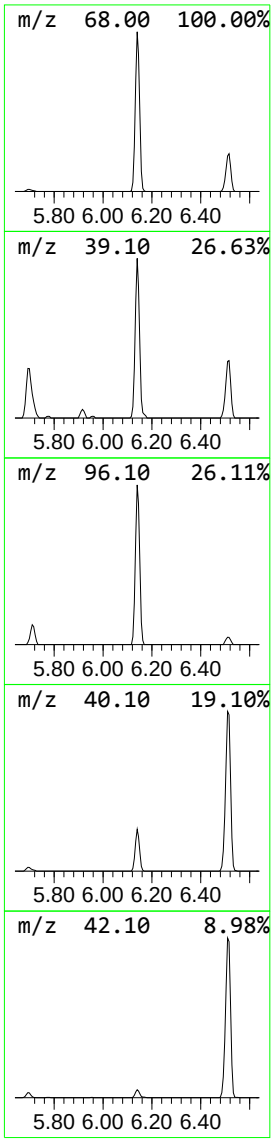
Peak Number 5 2-Cyclohexen-1-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.140	5.95 ng	190657	1,4-Dichlorobenzene-d4	6.892

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	42
3	But-1-ene-3-yne, 1-ethoxy-	96	C6H8O	002806-41-9	39
4	7-Oxabicyclo[2.2.1]hept-5-en-2-one	110	C6H6O2	095530-78-2	36
5	1,5-Cyclooctadien-4-one	122	C8H10O	001460-21-5	12





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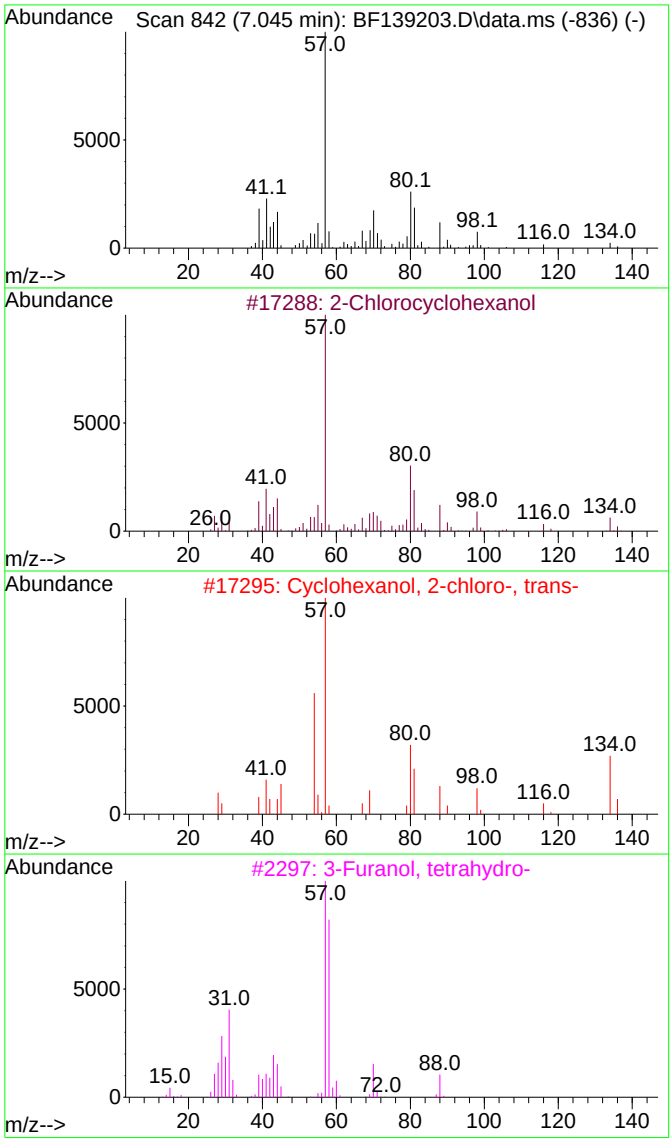
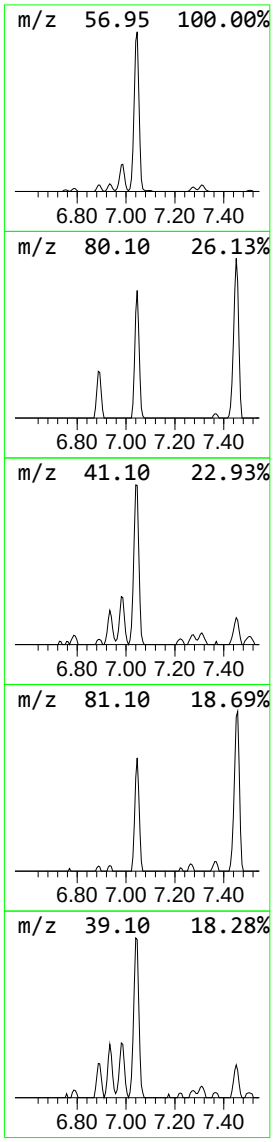
Peak Number 6 2-Chlorocyclohexanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.045	6.30 ng	201905	1,4-Dichlorobenzene-d4	6.892

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	3-Furanol, tetrahydro-	88	C4H8O2	000453-20-3	38
4	(S)-(+)-3-Hydroxytetrahydrofuran	88	C4H8O2	086087-23-2	32
5	4-Chlorocyclohexanol	134	C6H11ClO	030485-71-3	23





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclohexene	2.310	103.7	ng	3323510	1	6.892	641022	20.0
Formamide, N,N-...	4.228	2.0	ng	65079	1	6.892	641022	20.0
2-Pentanone, 4-...	5.122	46.8	ng	1499830	1	6.892	641022	20.0
2-Cyclohexen-1-ol	5.692	4.0	ng	128338	1	6.892	641022	20.0
2-Cyclohexen-1-one	6.140	6.0	ng	190657	1	6.892	641022	20.0
2-Chlorocyclohe...	7.045	6.3	ng	201905	1	6.892	641022	20.0