LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016630.D
Acq On : 01 Oct 2021 10:46
Operator : CG/JU
Sample : M3833-17
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : RE126D2-20210920

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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_N\METHODS\8270-SIM-BN100121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BN016630.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.161	5	9	11	rBV	962095	1501324	100.00%	43.310%
2	3.816	77	80	97	rVB	8181	35295	2.35%	1.018%
3	4.821	185	189	199	rVB	48157	108397	7.22%	3.127%
4	6.840	403	408	420	rVB2	4589	15792	1.05%	0.456%
5	7.642	490	495	500	rBV	45780	95545	6.36%	2.756%
6	8.784	602	605	612	rBV	21897	42772	2.85%	1.234%
7	10.191	713	716	725	rBV	82978	133329	8.88%	3.846%
8	10.407	729	733	736	rBV	97795	168203	11.20%	4.852%
9	12.003	920	931	943	rBV2	43496	71990	4.80%	2.077%
10	12.886	1071	1074	1078	rBV	75922	141470	9.42%	4.081%
11	13.178	1094	1097	1100	rBV	67268	103160	6.87%	2.976%
12	14.269	1180	1183	1186	rBV	123449	181691	12.10%	5.241%
13	17.017	1400	1403	1406	rBV	94696	148965	9.92%	4.297%
14	18.909	1661	1665	1682	rVB	15050	17868	1.19%	0.515%
15	19.063	1687	1696	1722	rBV	126607	187728	12.50%	5.416%
16	19.678	1813	1820	1838	rBV	107560	138184	9.20%	3.986%
17	21.174	1993	1996	1998	rBV	21404	30309	2.02%	0.874%
18	21.238	1998	2002	2009	rVV2	105690	174362	11.61%	5.030%
19	23.484	2414	2427	2458	rBV	87302	170072	11.33%	4.906%

Sum of corrected areas: 3466456

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ClientSampleId :
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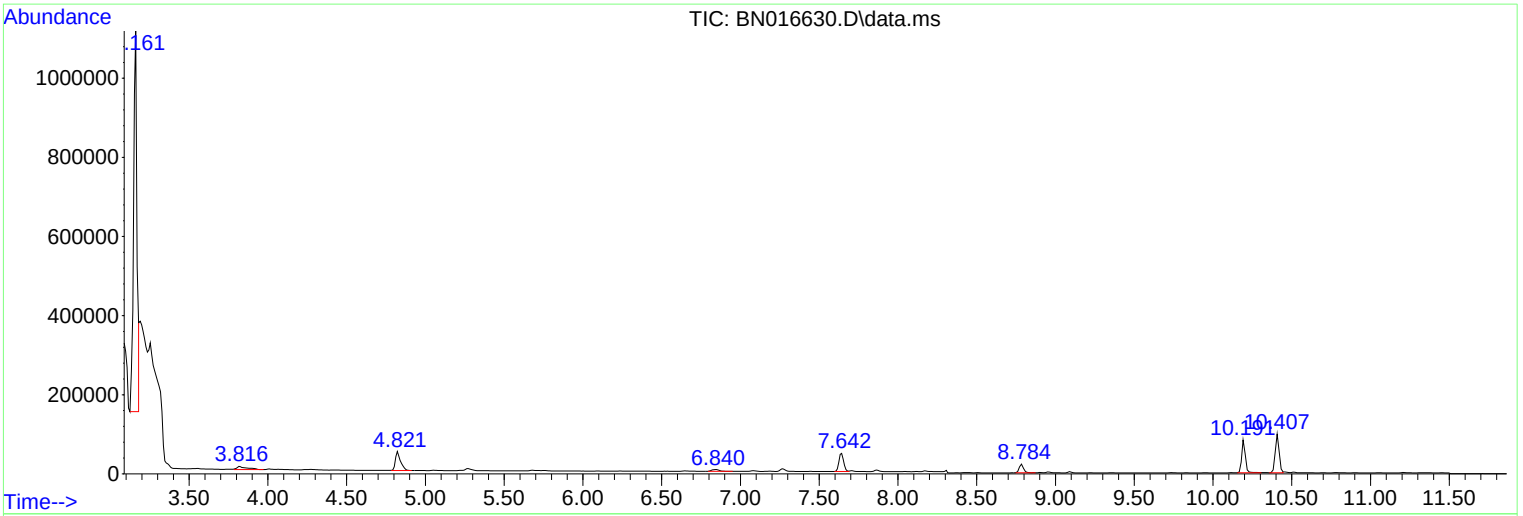
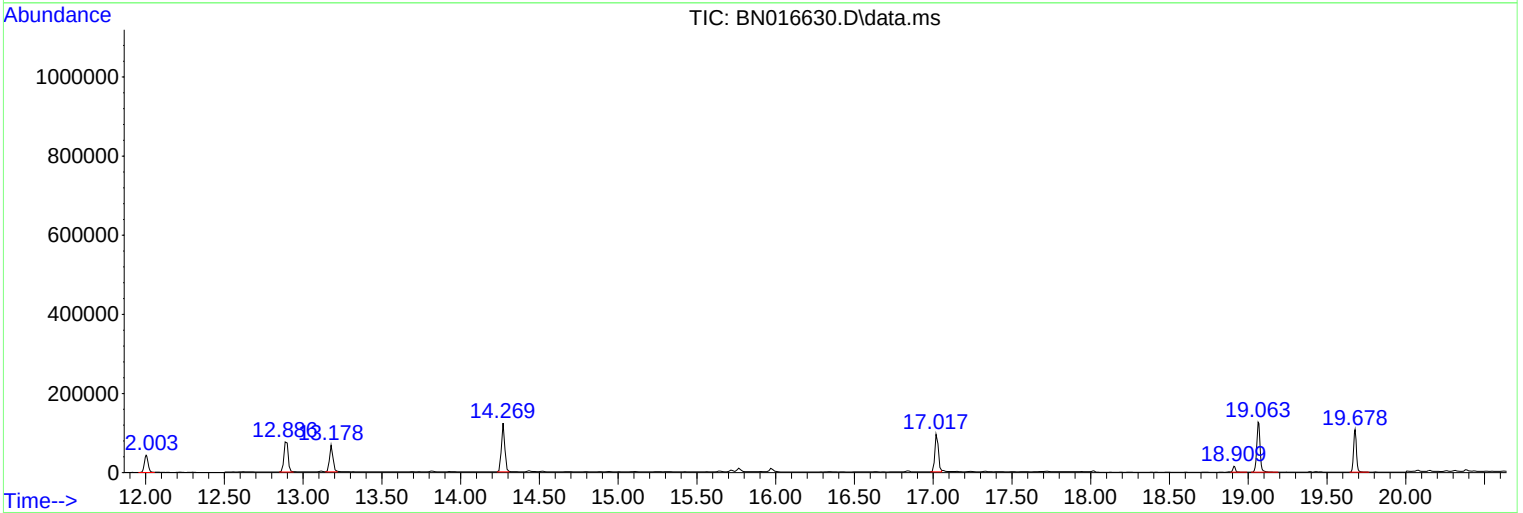
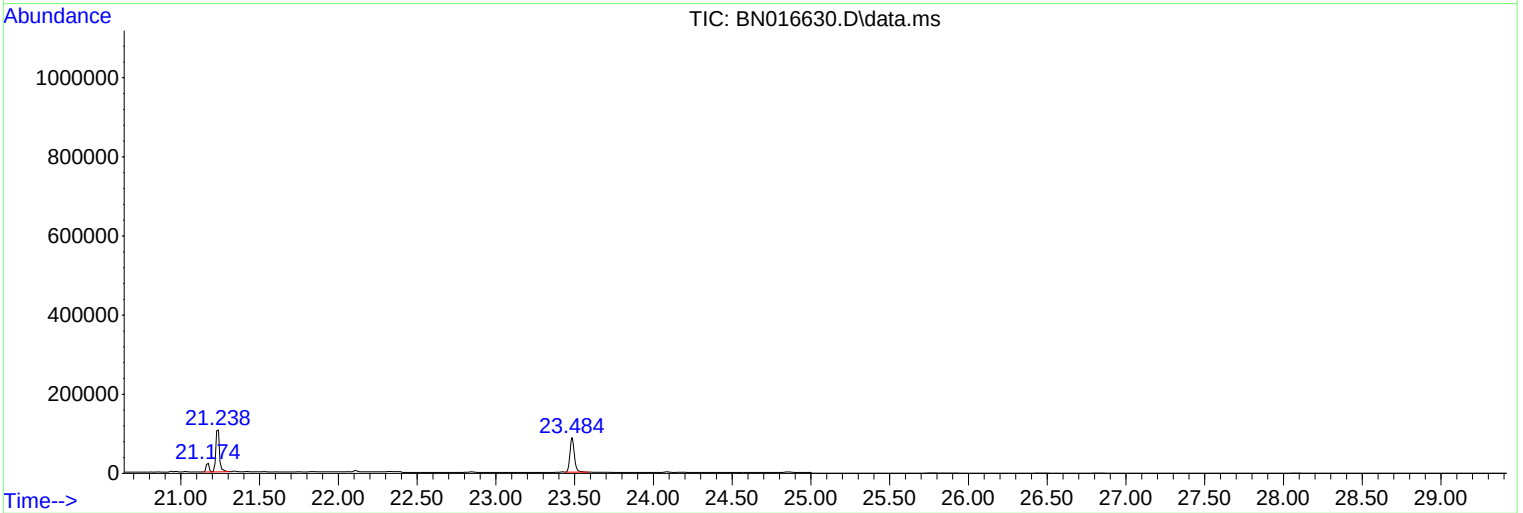
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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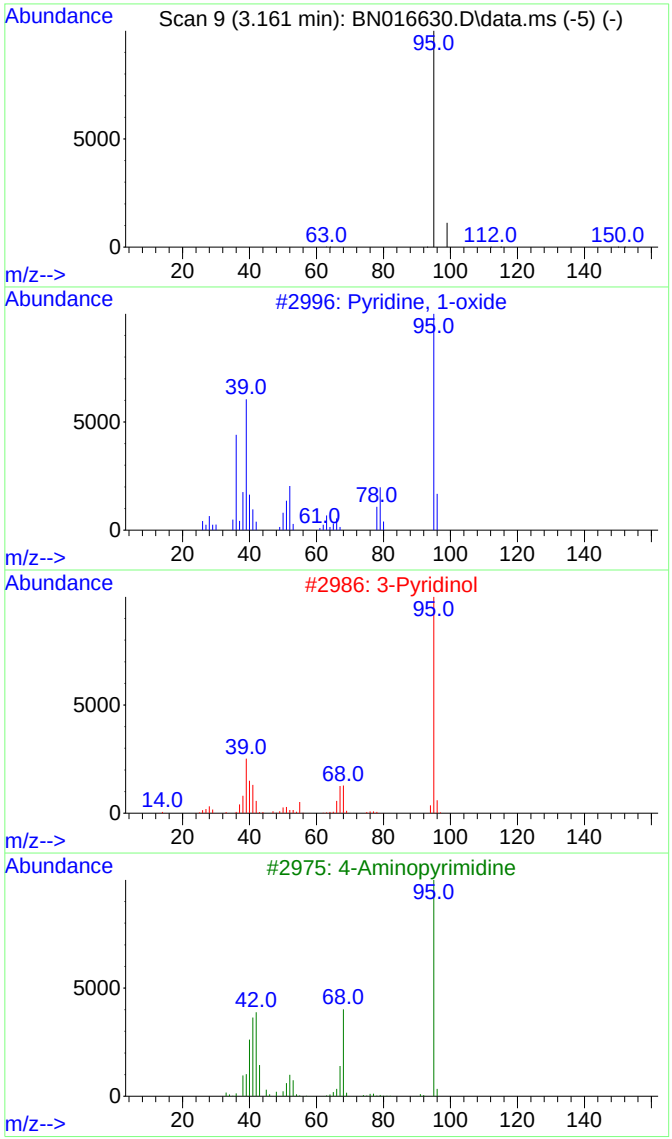
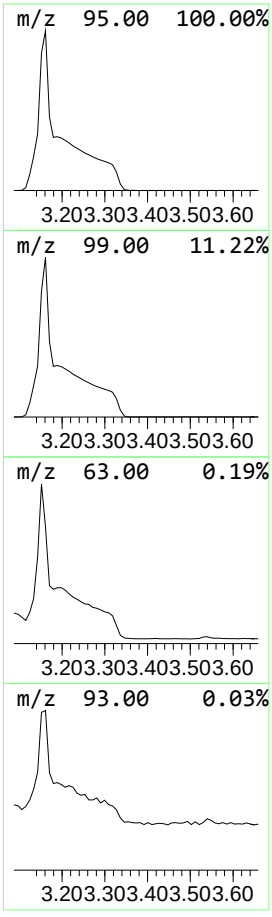
****
Peak Number 1 Pyridine, 1-oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.161	6.29 ng	1501320	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine, 1-oxide	95	C5H5NO	000694-59-7	2
2	3-Pyridinol	95	C5H5NO	000109-00-2	2
3	4-Aminopyrimidine	95	C4H5N3	000591-54-8	2
4	4-Pyridinol	95	C5H5NO	000626-64-2	2
5	2-(Aminomethylene)aminoacrylontrile	95	C4H5N3	167320-31-2	2





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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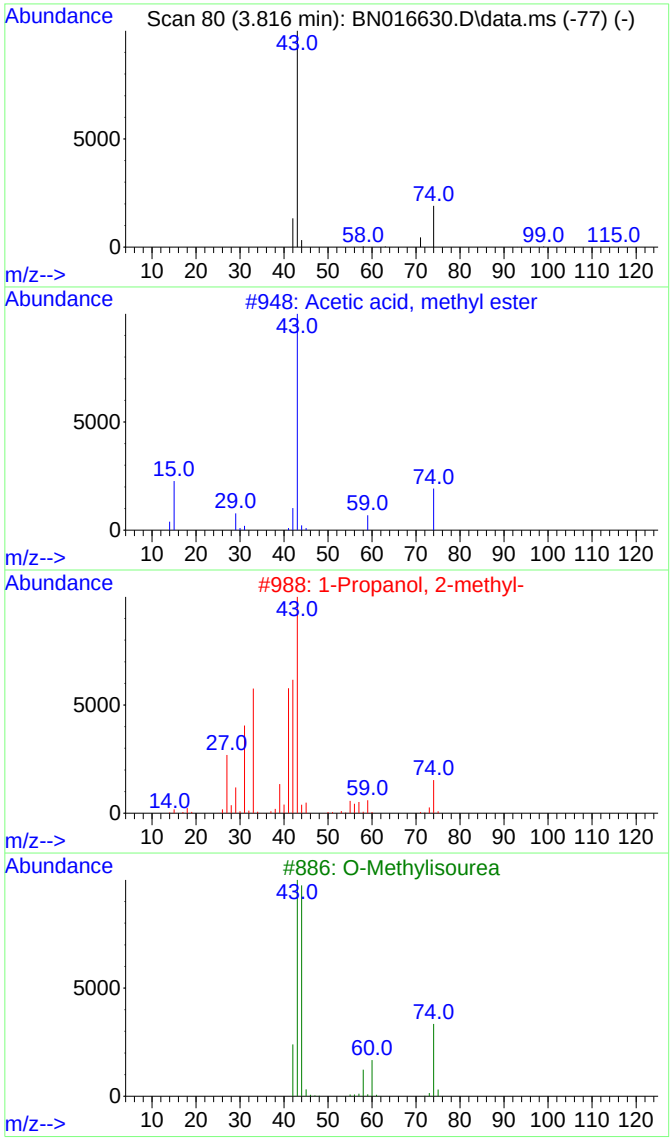
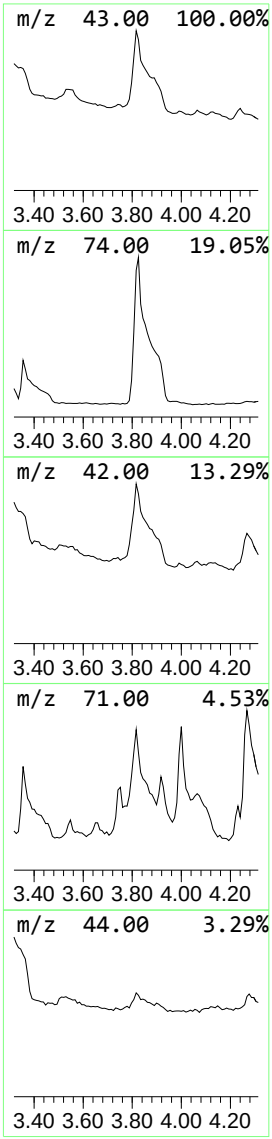
****
Peak Number 2 Acetic acid, methyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.15 ng	35295	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, methyl ester	74	C3H6O2	000079-20-9	9
2	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	4
3	O-Methylisourea	74	C2H6N2O	002440-60-0	4
4	Methoxyacetonitrile	71	C3H5NO	001738-36-9	4
5	Hydrogen azide	43	HN3	007782-79-8	4





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ClientSampleId :
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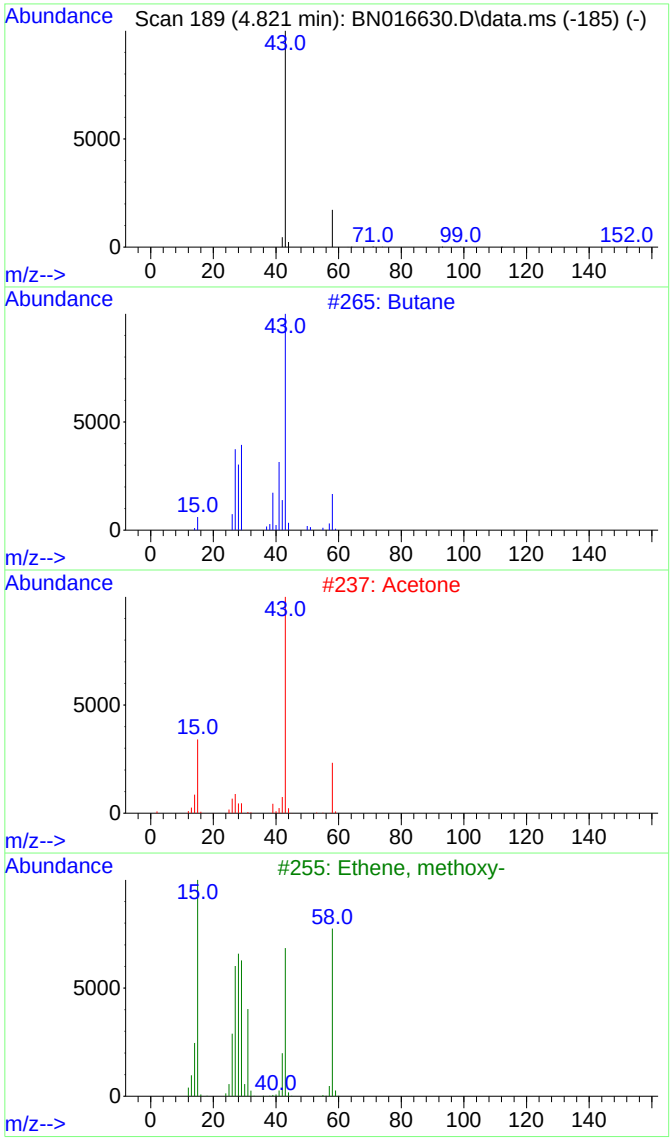
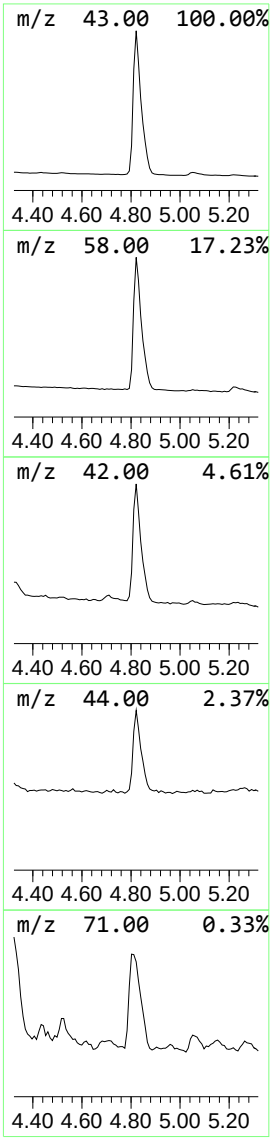
Peak Number 3 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.45 ng	108397	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	4
2	Acetone	58	C3H6O	000067-64-1	4
3	Ethene, methoxy-	58	C3H6O	000107-25-5	3
4	Diazene, dimethyl-	58	C2H6N2	000503-28-6	3
5	Hydrogen isocyanate	43	CHNO	000075-13-8	2





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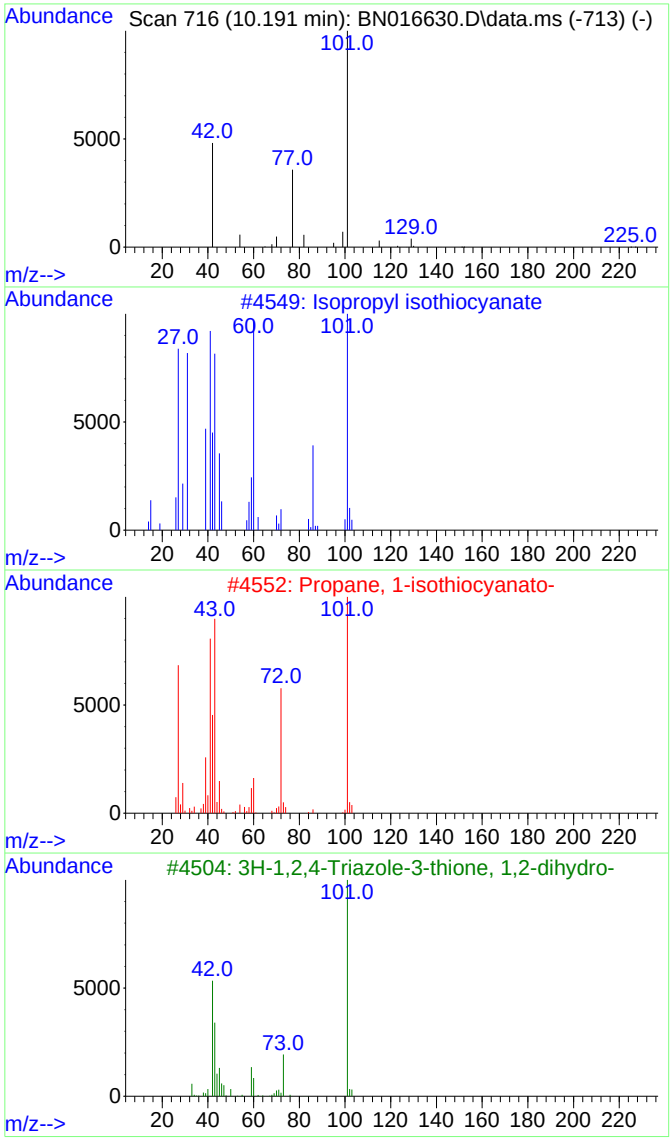
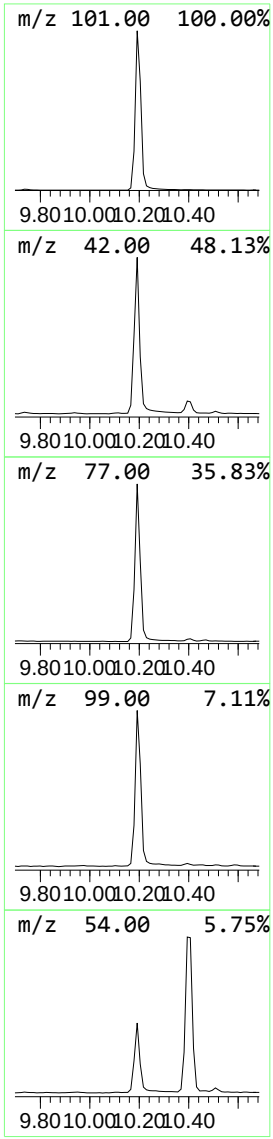
****

Peak Number 4 Isopropyl isothiocyanate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.32 ng	133329	Naphthalene-d8	10.407

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	5
2	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5
3	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
4	2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	5
5	3-Aminopropionitrile	70	C3H6N2	000151-18-8	4





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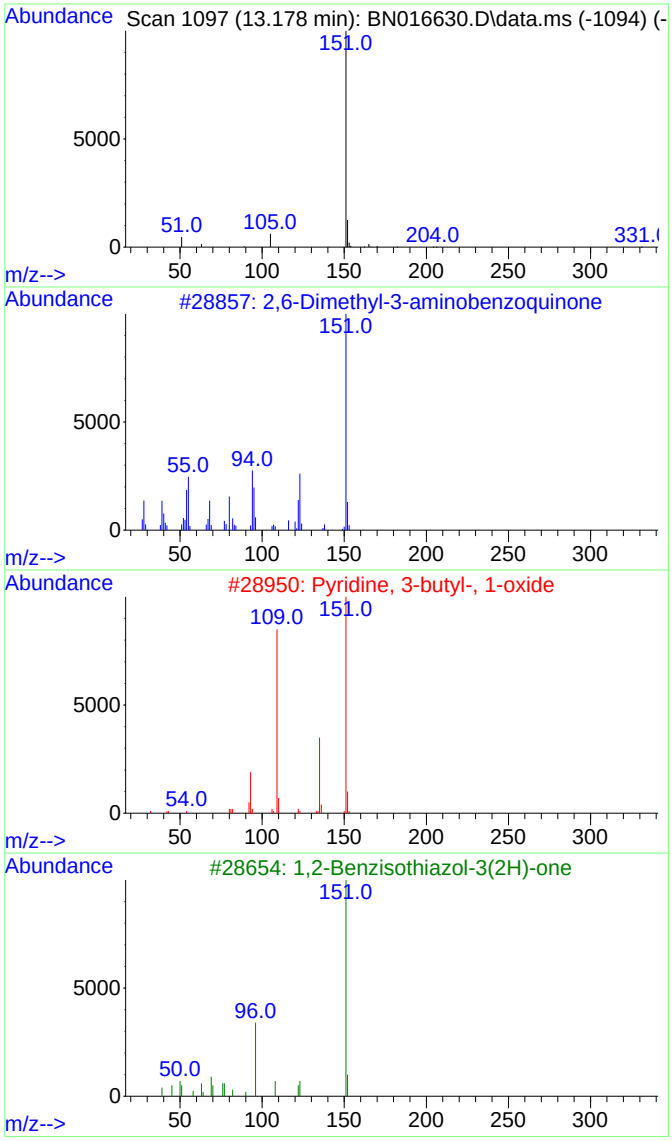
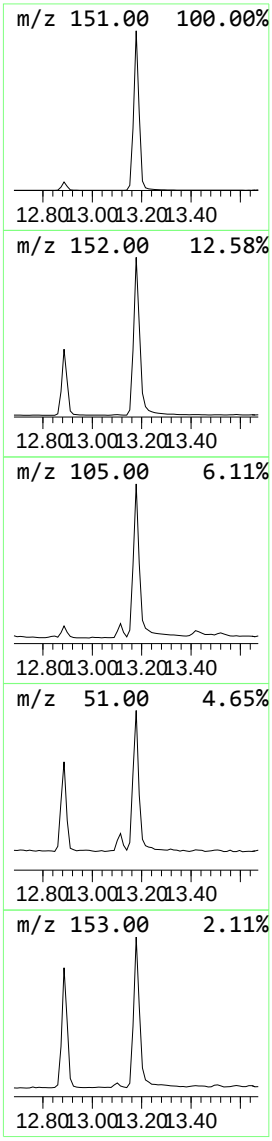
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2,6-Dimethyl-3-aminobenzoqu... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.178	0.23 ng	103160	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Dimethyl-3-aminobenzoquinone	151	C8H9NO2	090005-56-4	7
2	Pyridine, 3-butyl-, 1-oxide	151	C9H13NO	031396-33-5	7
3	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	7
4	7-Methyl-7H-pyrazolo(3,4-d)-v-tr...	151	C5H5N5O	018213-76-8	7
5	Carbamic acid, phenyl-, methyl e...	151	C8H9NO2	002603-10-3	7





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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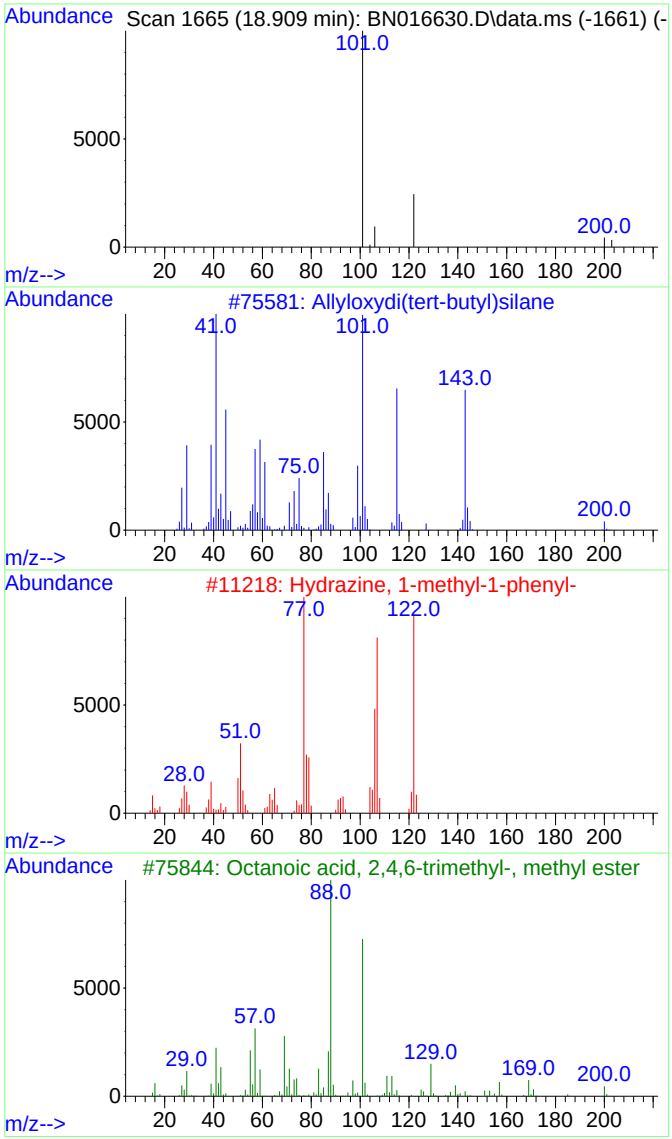
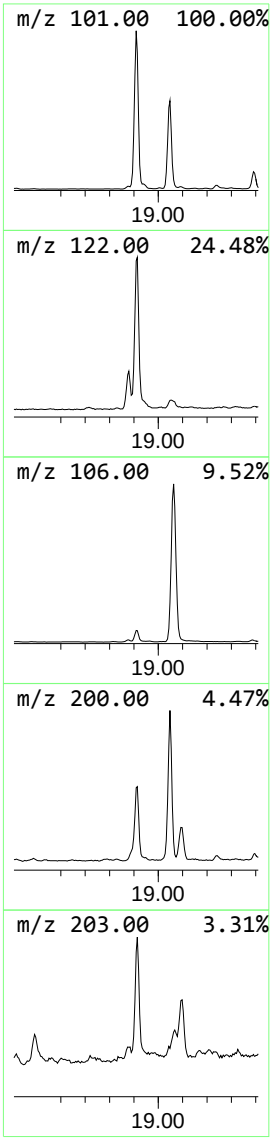
****

Peak Number 6 Allyloxydi(tert-butyl)silane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.909	0.05 ng	17868	Phenanthrene-d10	17.017

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Allyloxydi(tert-butyl)silane	200	C11H24OSi	1000279-09-4	4
2	Hydrazine, 1-methyl-1-phenyl-	122	C7H10N2	000618-40-6	4
3	Octanoic acid, 2,4,6-trimethyl-,...	200	C12H24O2	054984-07-5	4
4	Decanoic acid, ethyl ester	200	C12H24O2	000110-38-3	3
5	1,2-Propanediol, 3-(methylthio)-	122	C4H10O2S	022551-26-4	3





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
Pyridine, 1-oxide	3.161	6.3	ng	1501320	1	7.642	95545	0.4
Acetic acid, me...	3.816	0.1	ng	35295	1	7.642	95545	0.4
Butane	4.821	0.5	ng	108397	1	7.642	95545	0.4
Isopropyl isoth...	10.191	0.3	ng	133329	2	10.407	168203	0.4
2,6-Dimethyl-3-...	13.178	0.2	ng	103160	3	14.269	181691	0.4
Allyloxydi(tert...	18.909	0.0	ng	17868	4	17.017	148965	0.4