

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016629.D
 Acq On : 01 Oct 2021 10:10
 Operator : CG/JU
 Sample : M3833-18
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 RE126D3-20210920

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: BN016629.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.825	77	81	97	rVB	7870	33054	18.86%	1.835%
2	4.821	185	189	211	rVB	47510	105159	60.02%	5.836%
3	5.273	234	238	245	rVB	5112	13079	7.46%	0.726%
4	6.831	403	407	419	rVB3	3739	11705	6.68%	0.650%
5	7.264	451	454	460	rVB	5720	11894	6.79%	0.660%
6	7.642	490	495	500	rBV	44127	89287	50.96%	4.956%
7	7.864	516	519	526	rVB	3736	7446	4.25%	0.413%
8	8.306	565	567	569	rVB	6084	6091	3.48%	0.338%
9	8.784	601	605	612	rBV	19714	38880	22.19%	2.158%
10	10.191	713	716	725	rBV	41333	68025	38.82%	3.775%
11	10.407	729	733	737	rBV	93087	162110	92.52%	8.997%
12	12.003	922	931	942	rBV	38749	63994	36.52%	3.552%
13	12.898	1071	1075	1078	rBV	67663	126049	71.94%	6.996%
14	13.178	1094	1097	1105	rBV	26914	43428	24.78%	2.410%
15	14.269	1180	1183	1186	rBV	120951	175221	100.00%	9.725%
16	15.766	1299	1301	1307	rVB2	9372	14890	8.50%	0.826%
17	15.969	1315	1317	1321	rVB2	3463	7058	4.03%	0.392%
18	17.017	1400	1403	1406	rBV	87361	142960	81.59%	7.935%
19	17.711	1455	1460	1468	rBV3	2414	6054	3.46%	0.336%
20	18.015	1483	1485	1497	rVB2	2821	3979	2.27%	0.221%
21	18.909	1661	1665	1681	rVB	8499	10152	5.79%	0.563%
22	19.063	1687	1696	1720	rBV	115884	166056	94.77%	9.216%
23	19.430	1765	1770	1774	rBV	2558	3651	2.08%	0.203%
24	19.678	1813	1820	1840	rBV	98290	123001	70.20%	6.827%
25	21.174	1993	1996	1998	rBV	15517	22328	12.74%	1.239%
26	21.238	1998	2002	2010	rVV2	105751	169173	96.55%	9.389%
27	22.311	2100	2103	2109	rBV	4007	8398	4.79%	0.466%
28	23.484	2415	2427	2462	rVB	85404	165257	94.31%	9.172%
29	25.771	3076	3095	3119	rBV6	812	3371	1.92%	0.187%

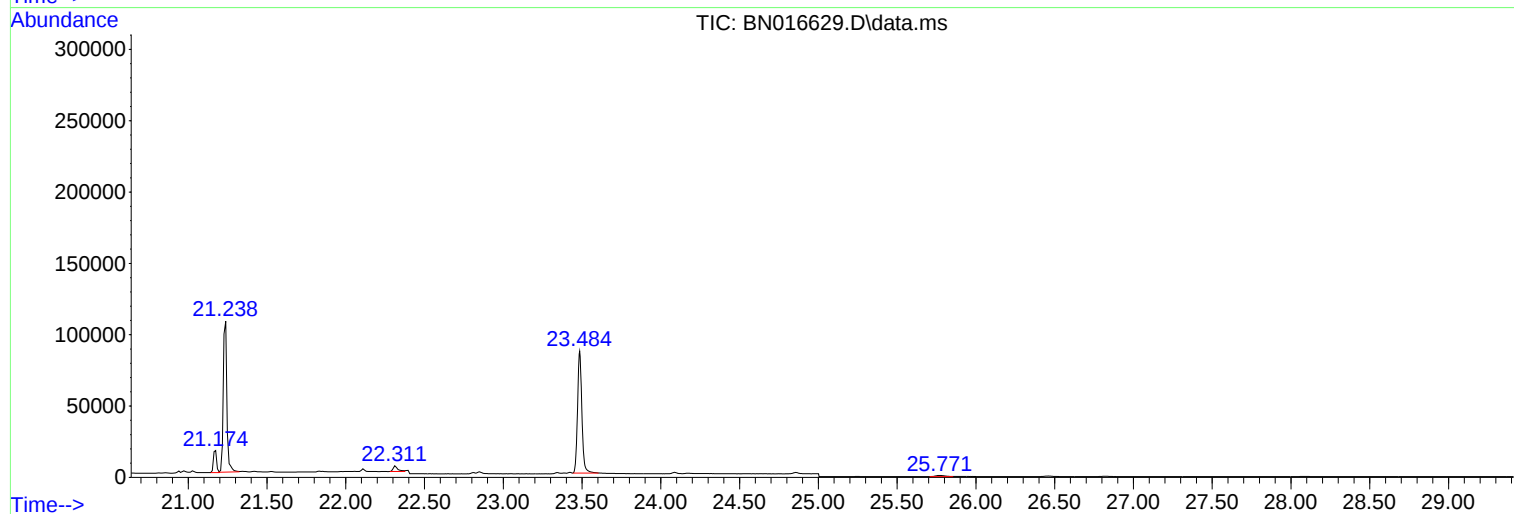
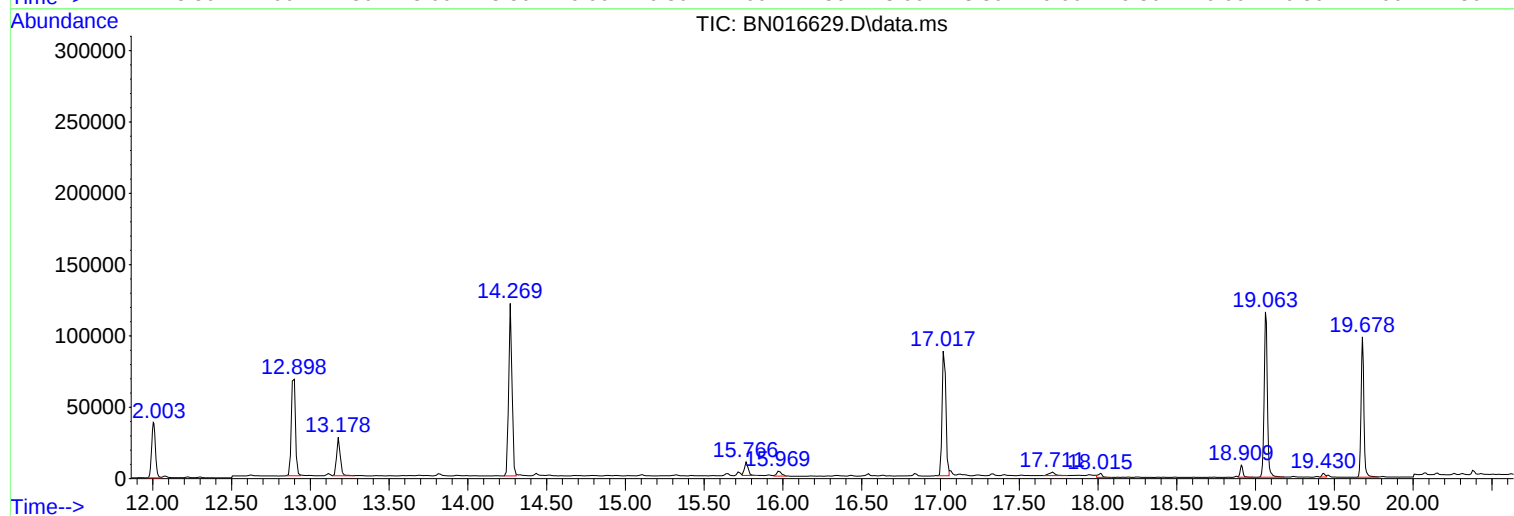
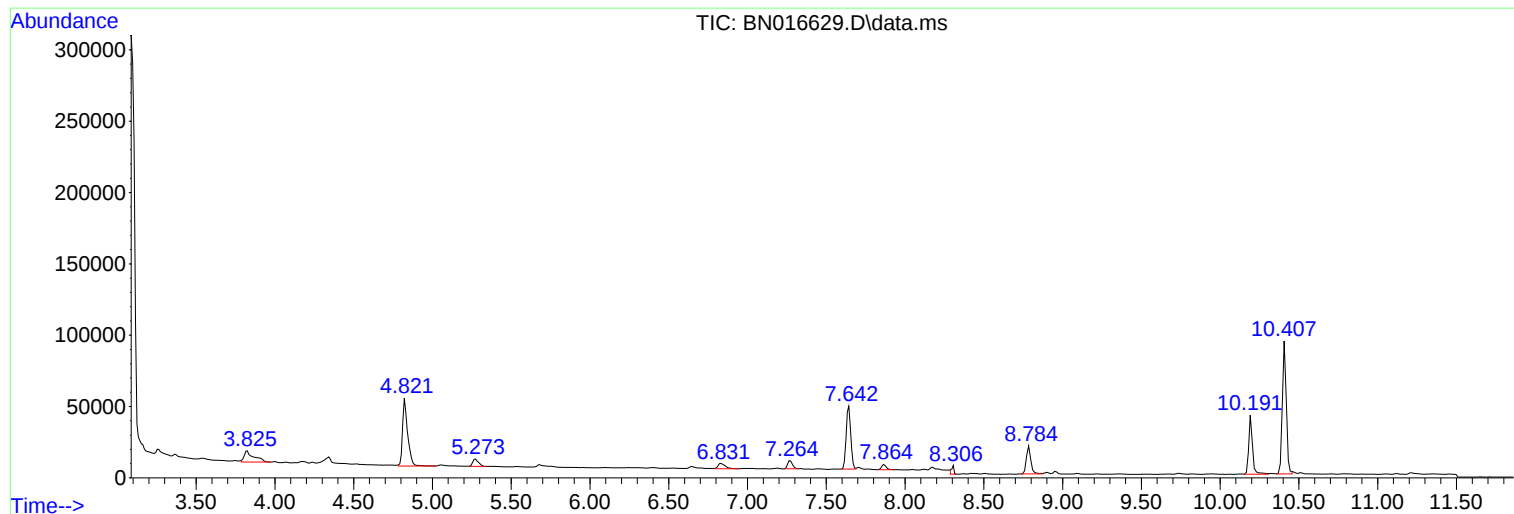
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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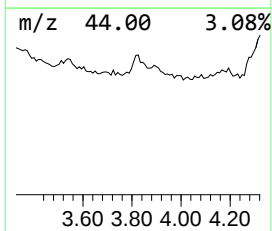
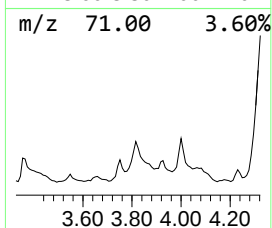
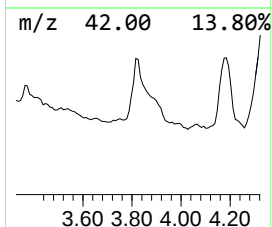
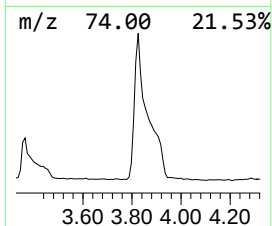
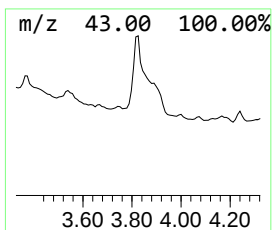
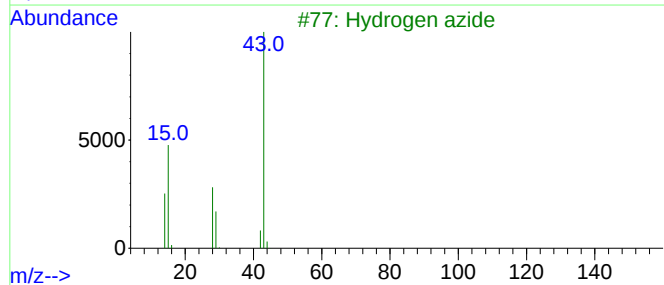
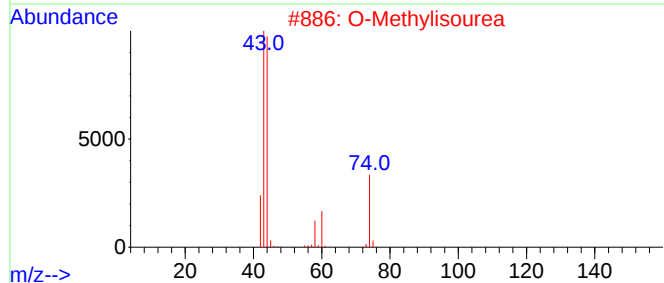
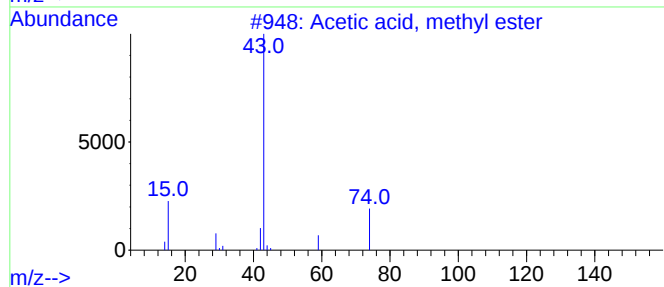
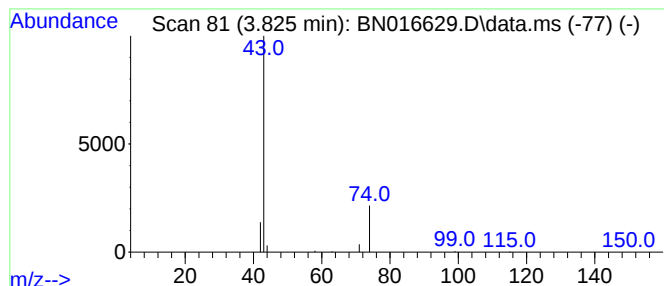
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Acetic acid, methyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.825	0.15 ng	33054	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			O-Methylisourea	74	C2H6N2O	002440-60-0	4
3			Hydrogen azide	43	HN3	007782-79-8	4
4			Urea, methyl-	74	C2H6N2O	000598-50-5	3
5			1-Ethyl-1-methylhydrazine	74	C3H10N2	004986-48-5	3



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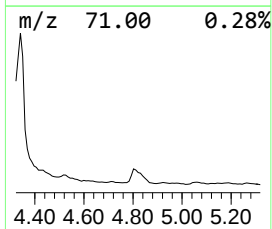
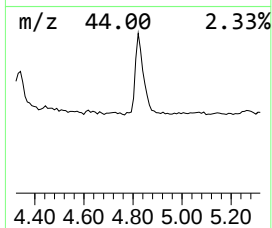
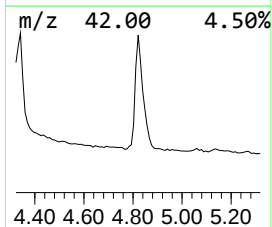
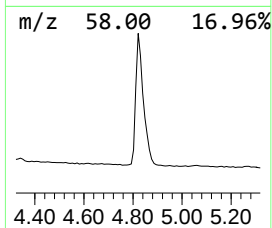
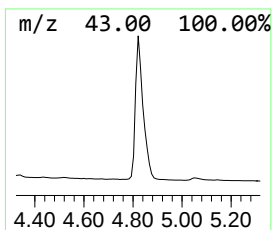
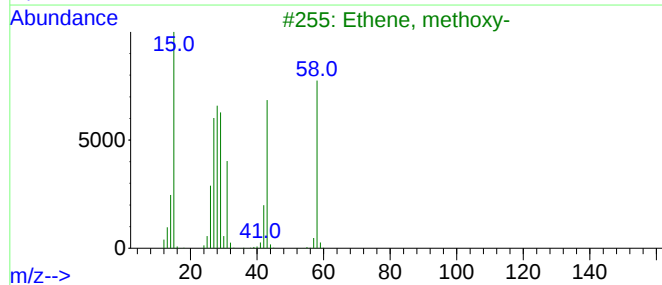
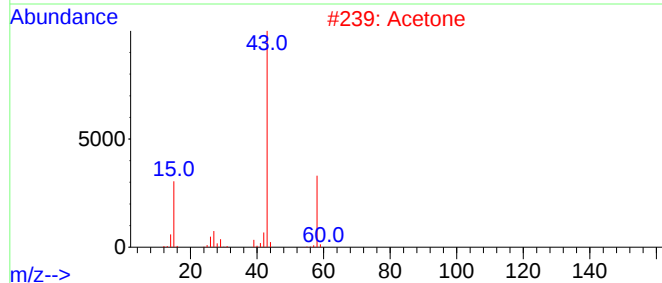
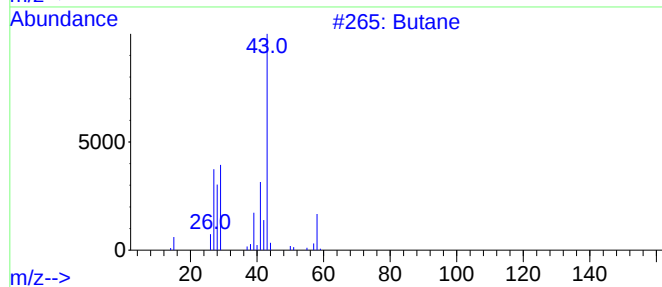
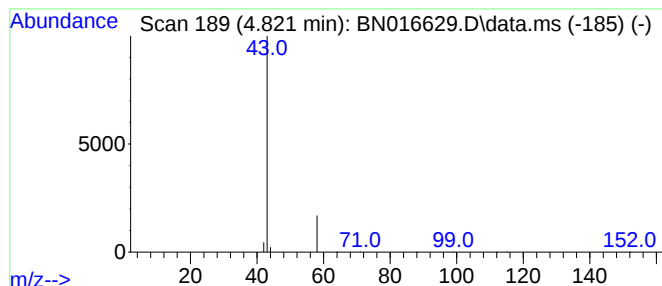
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 Butane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.47 ng	105159	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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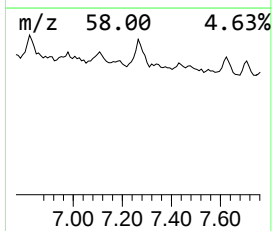
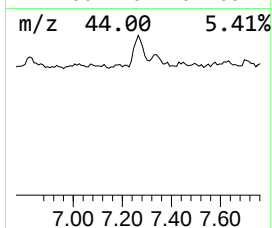
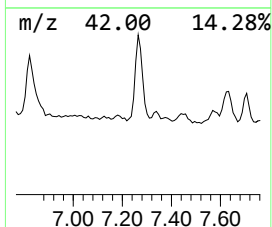
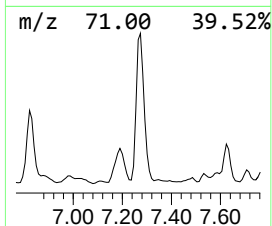
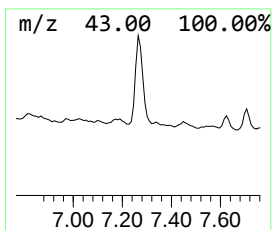
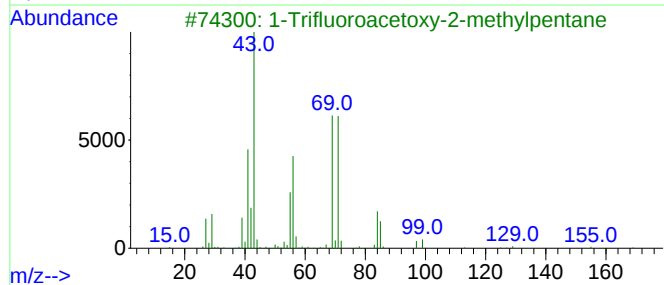
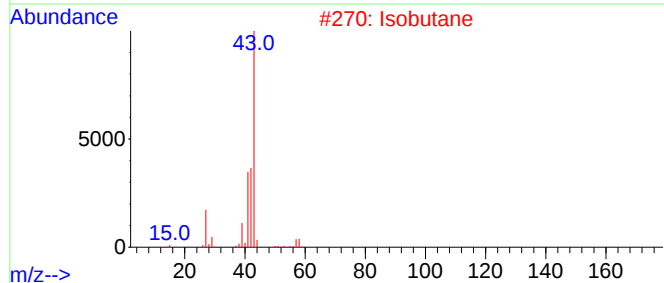
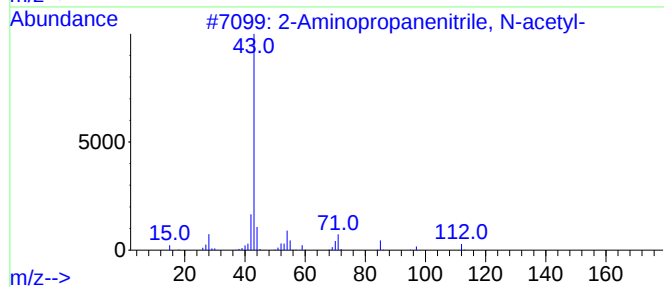
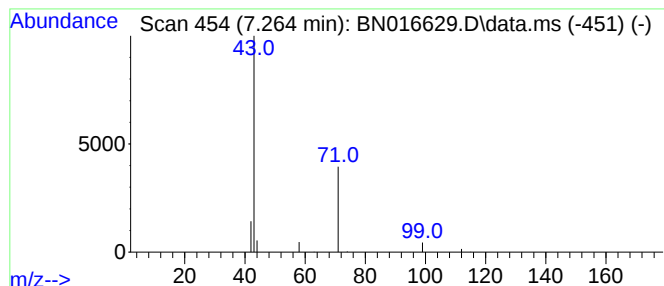
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Aminopropanenitrile, N-ac... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.264	0.05 ng	11894	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Aminopropanenitrile, N-acetyl-	112	C5H8N2O	019861-71-3	4
2	Isobutane	58	C4H10	000075-28-5	4
3	1-Trifluoroacetoxy-2-methylpentane	198	C8H13F3O2	155089-96-6	4
4	1,6-Heptadien-4-ol	112	C7H12O	002883-45-6	4
5	dl-Mevalonic acid lactone	130	C6H10O3	000674-26-0	4



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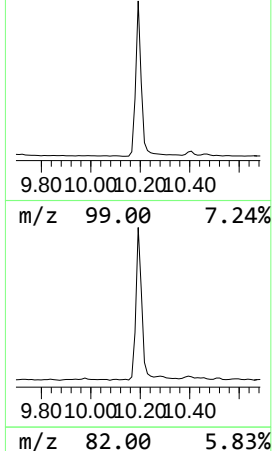
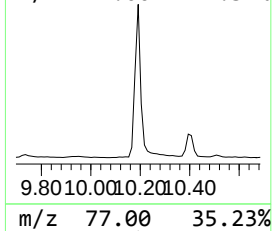
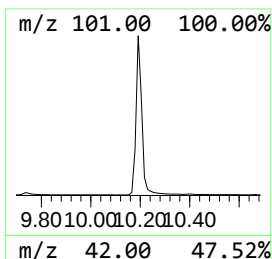
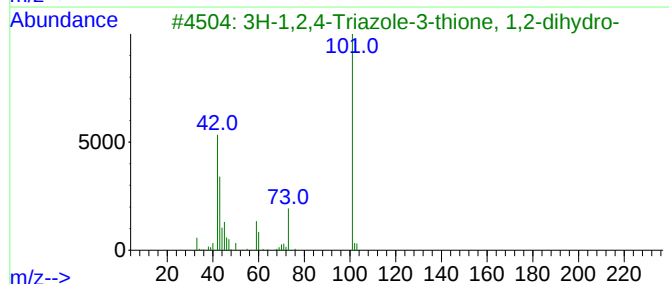
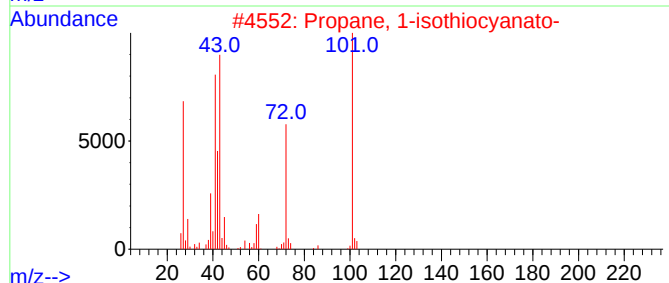
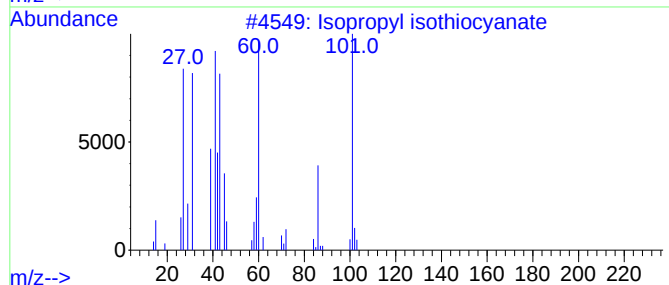
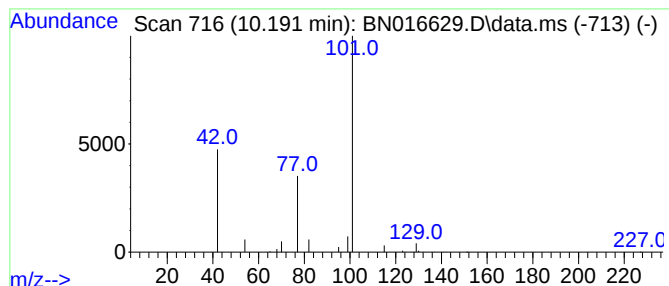
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Isopropyl isothiocyanate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.17 ng	68025	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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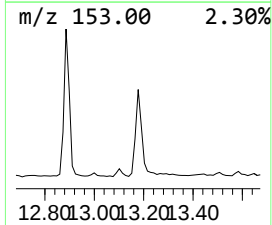
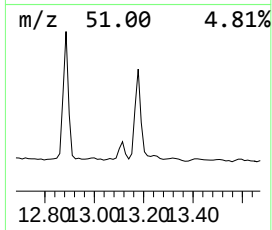
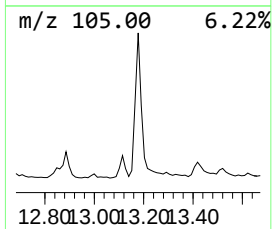
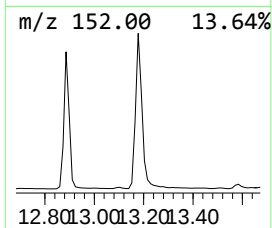
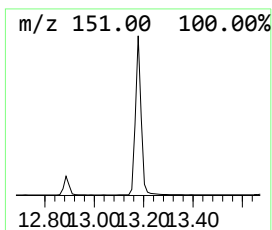
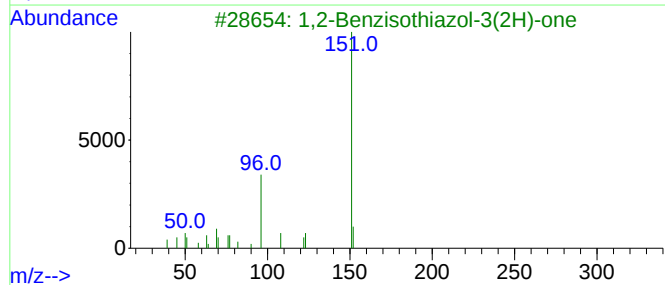
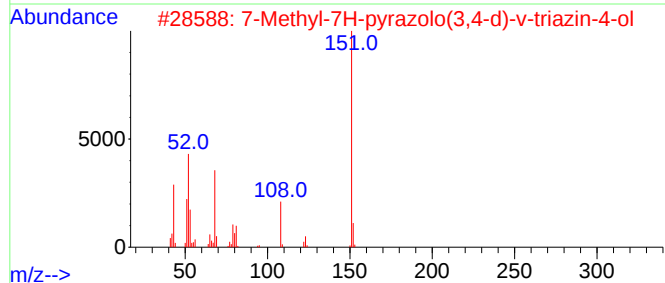
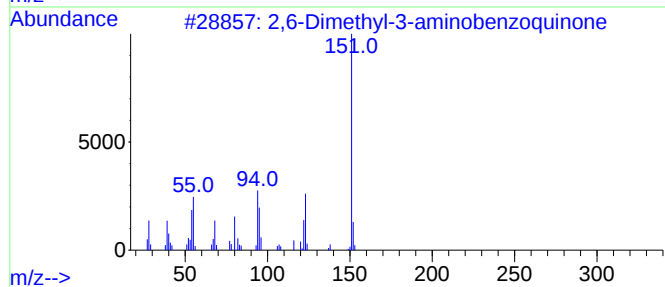
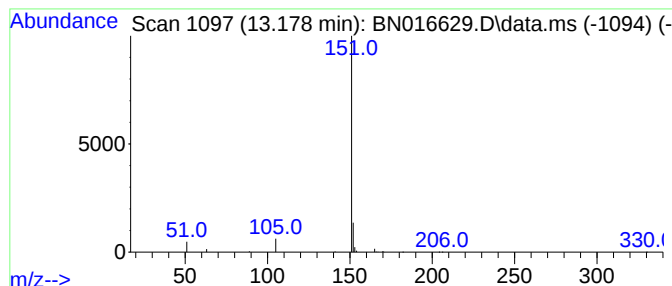
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.178	0.10 ng	43428	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			7-Methyl-7H-pyrazolo(3,4-d)-v-tr...	151	C5H5N5O	018213-76-8	7
3			1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	7
4			Vanillin	152	C8H8O3	000121-33-5	5
5			Butane-1,3-dione, 1-(pyrrol-2-yl)-	151	C8H9NO2	022441-25-4	5



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetic acid, me...	3.825	0.1	ng	33054	1	7.642	89287	0.4
Butane	4.821	0.5	ng	105159	1	7.642	89287	0.4
2-Aminopropanen...	7.264	0.1	ng	11894	1	7.642	89287	0.4
Isopropyl isoth...	10.191	0.2	ng	68025	2	10.407	162110	0.4
2,6-Dimethyl-3-...	13.178	0.1	ng	43428	3	14.269	175221	0.4