LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016647.D
Acq On : 01 Oct 2021 21:59
Operator : CG/JU
Sample : M3833-12
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : DUP03-20210920

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: BN016647.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.152	6	8	11	rBV	60296	74871	21.81%	3.204%
2	3.253	16	19	44	rVB	84613	343269	100.00%	14.691%
3	3.815	76	80	97	rVB	11794	49783	14.50%	2.131%
4	4.820	185	189	203	rVB	34742	80921	23.57%	3.463%
5	5.272	234	238	245	rVB	7501	20303	5.91%	0.869%
6	6.646	384	387	391	rBV	2465	4976	1.45%	0.213%
7	6.840	403	408	419	rVB2	6151	20897	6.09%	0.894%
8	7.264	451	454	460	rVB	6665	13836	4.03%	0.592%
9	7.642	490	495	500	rBV	44098	90918	26.49%	3.891%
10	7.863	516	519	526	rVB	4449	8878	2.59%	0.380%
11	8.168	549	552	560	rVB	2306	6022	1.75%	0.258%
12	8.306	565	567	569	rVB	6842	6800	1.98%	0.291%
13	8.784	601	605	612	rBV	26525	51341	14.96%	2.197%
14	10.191	713	716	721	rBV	14297	26450	7.71%	1.132%
15	10.406	729	733	737	rBV	93572	161117	46.94%	6.895%
16	11.205	793	796	802	rBV2	2814	6230	1.81%	0.267%
17	12.002	920	931	943	rBV	47201	76520	22.29%	3.275%
18	12.885	1071	1074	1078	rBV	85822	160847	46.86%	6.884%
19	14.268	1180	1183	1192	rBV	122672	181911	52.99%	7.785%
20	15.765	1299	1301	1305	rVB2	11218	18348	5.35%	0.785%
21	17.017	1400	1403	1410	rBV	86915	150121	43.73%	6.425%
22	19.068	1689	1697	1727	rBV	128354	183403	53.43%	7.849%
23	19.678	1813	1820	1851	rBV	131361	159306	46.41%	6.818%
24	20.972	1974	1977	1980	rBV	4838	8523	2.48%	0.365%
25	21.163	1993	1995	1998	rBV	25609	37327	10.87%	1.598%
26	21.227	1998	2001	2011	rVB	110511	176767	51.50%	7.565%
27	22.108	2081	2084	2089	rBV2	6641	9058	2.64%	0.388%
28	22.321	2100	2104	2108	rBV2	2576	5631	1.64%	0.241%
29	23.422	2402	2409	2415	rBV	2835	4319	1.26%	0.185%
30	23.484	2415	2427	2470	rVB	93352	184881	53.86%	7.912%
31	24.087	2595	2603	2618	rVB	3248	6201	1.81%	0.265%
32	24.857	2820	2828	2844	rVB	3093	6806	1.98%	0.291%

Sum of corrected areas: 2336581

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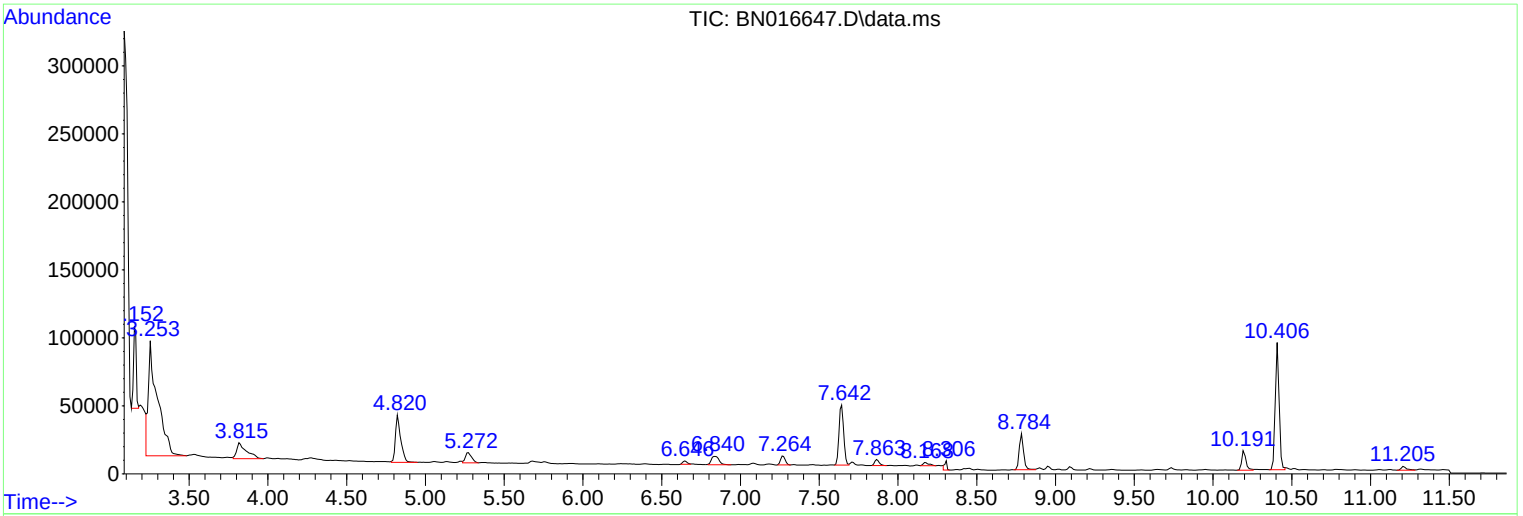
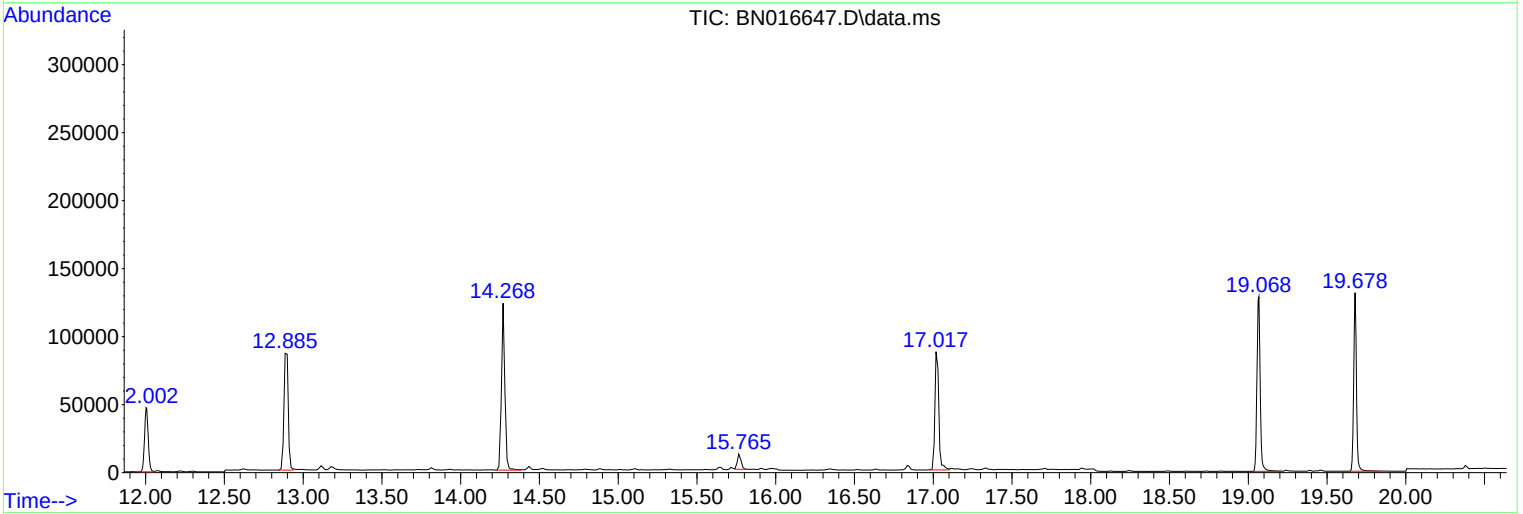
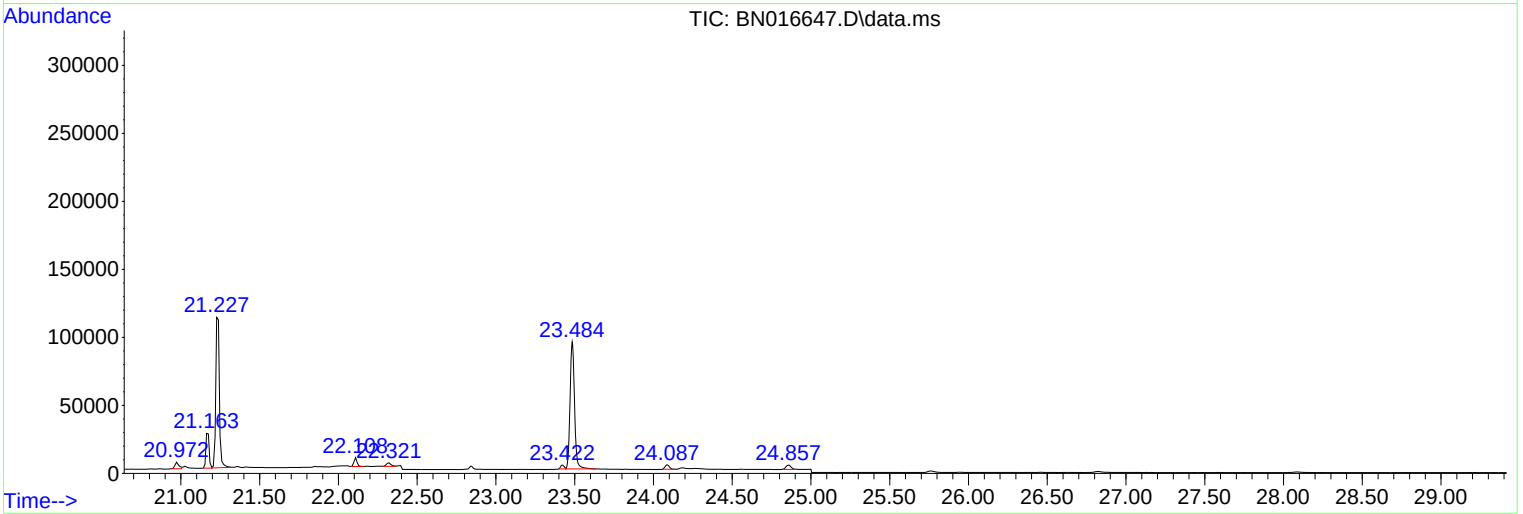
Instrument :
BNA_N
ClientSampleId :
DUP03-20210920

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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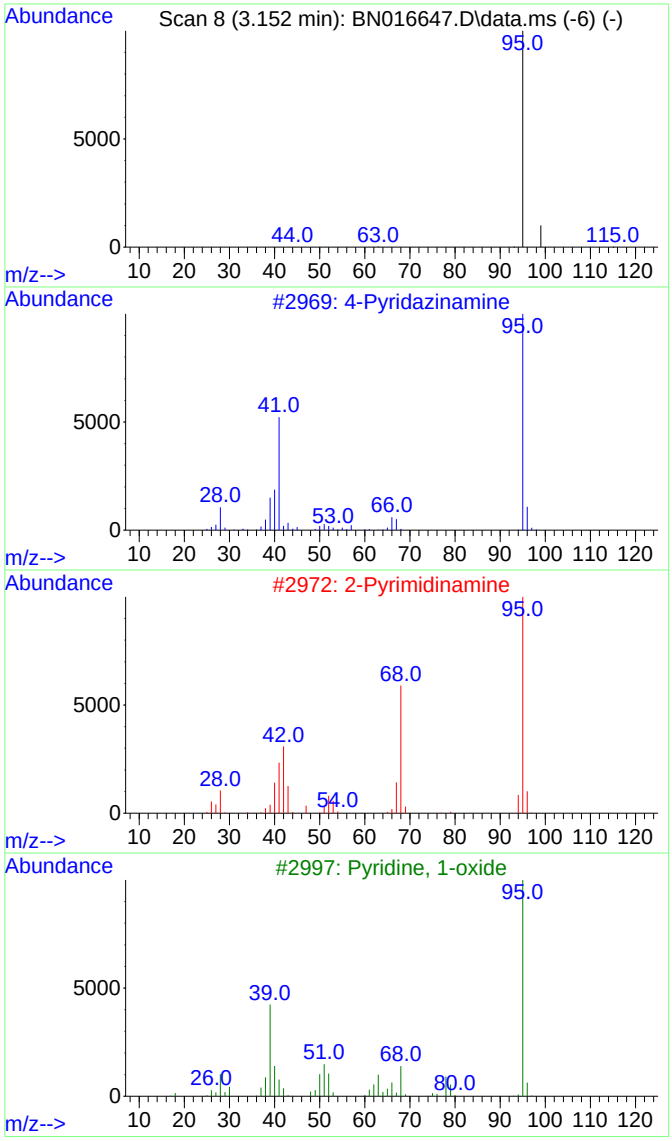
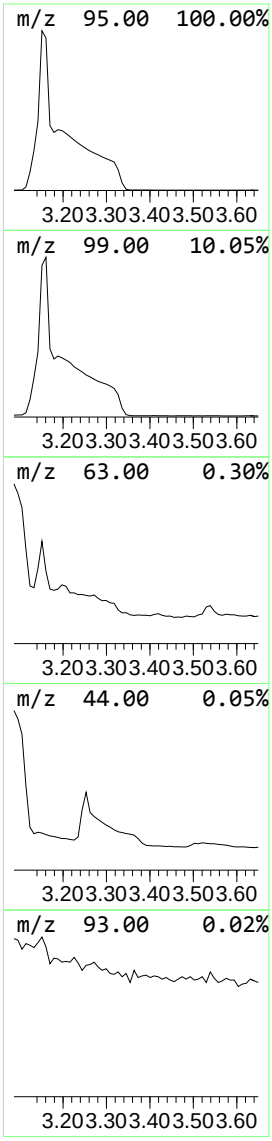
Peak Number 1 4-Pyridazinamine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.152	0.33 ng	74871	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Pyridazinamine	95	C4H5N3	020744-39-2	2
2	2-Pyrimidinamine	95	C4H5N3	000109-12-6	2
3	Pyridine, 1-oxide	95	C5H5NO	000694-59-7	2
4	3-Pyridinol	95	C5H5NO	000109-00-2	2
5	4-Pyridinol	95	C5H5NO	000626-64-2	2





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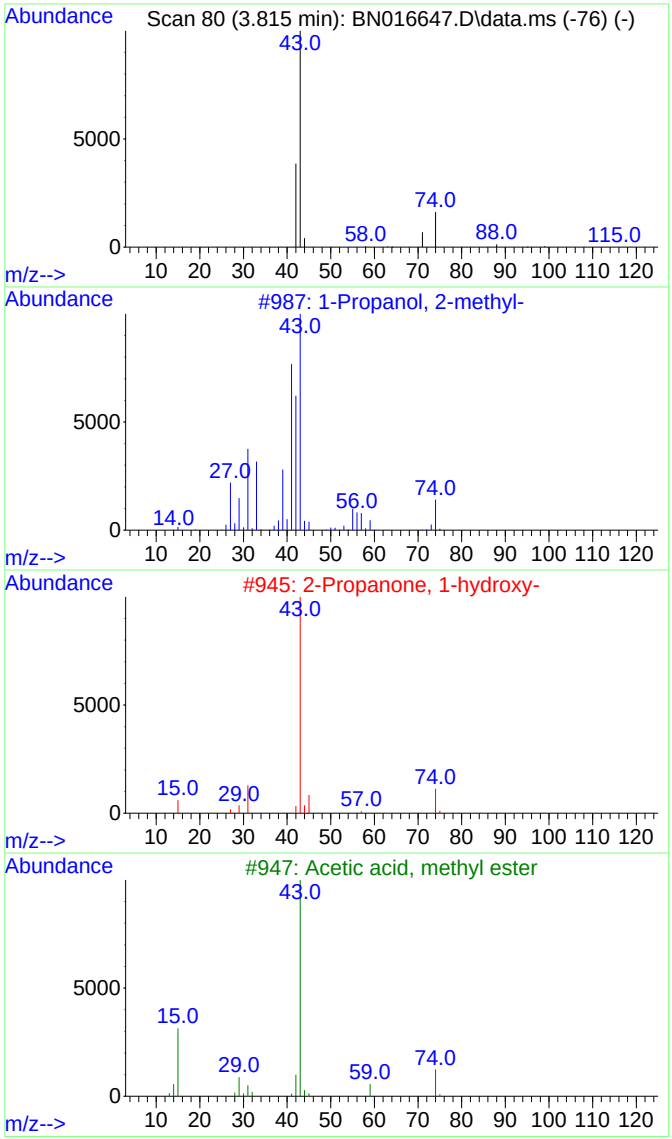
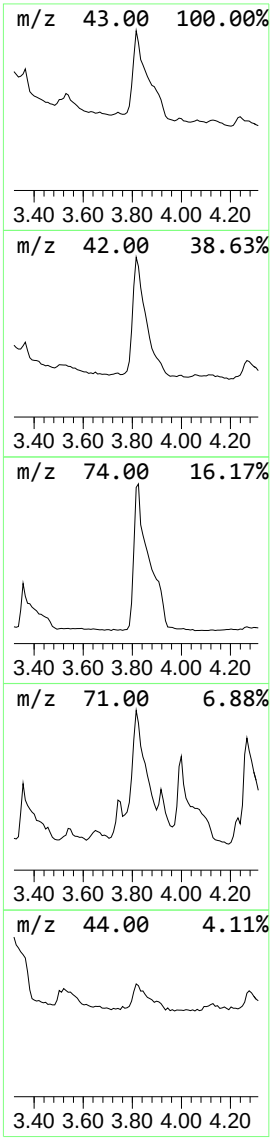
Peak Number 2 1-Propanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.815	0.22 ng	49783	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	5
2	2-Propanone, 1-hydroxy-	74	C3H6O2	000116-09-6	4
3	Acetic acid, methyl ester	74	C3H6O2	000079-20-9	4
4	Acetic acid, hydrazide	74	C2H6N2O	001068-57-1	4
5	Hydrogen isocyanate	43	CHNO	000075-13-8	3





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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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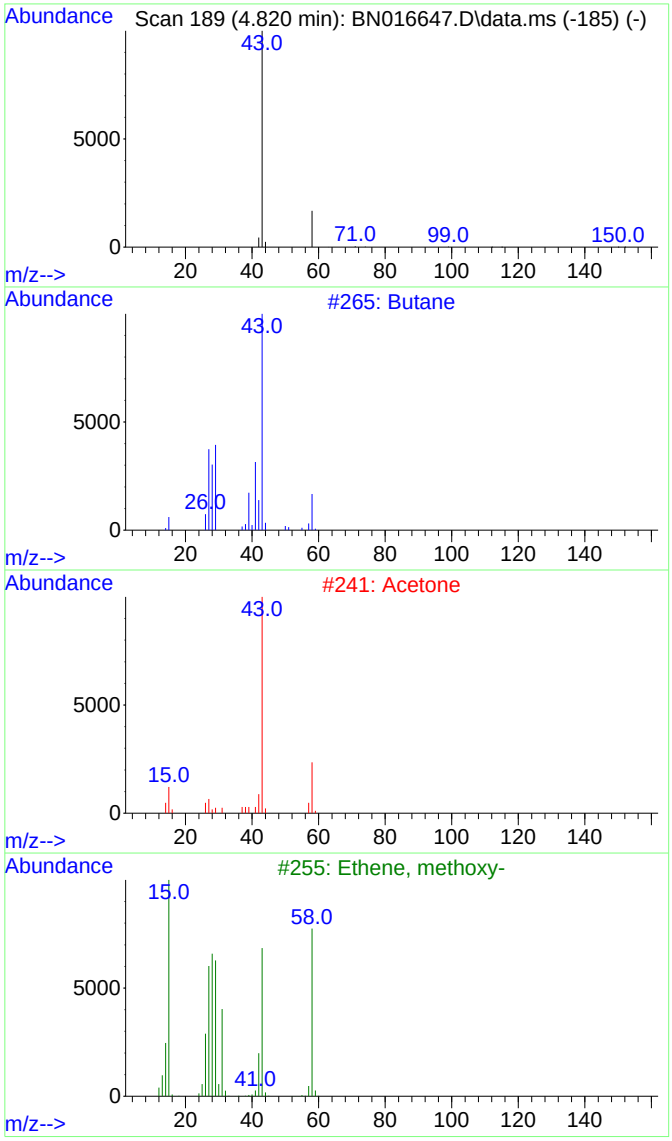
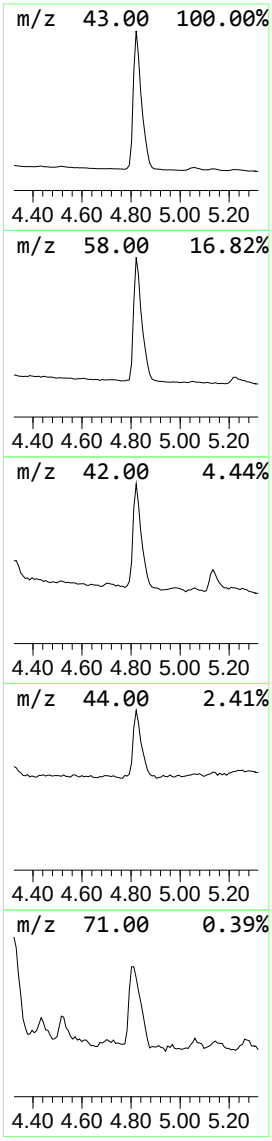
Peak Number 3 Butane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.820	0.36 ng	80921	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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Sample : M3833-12
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Instrument :
BNA_N
ClientSampleId :
DUP03-20210920

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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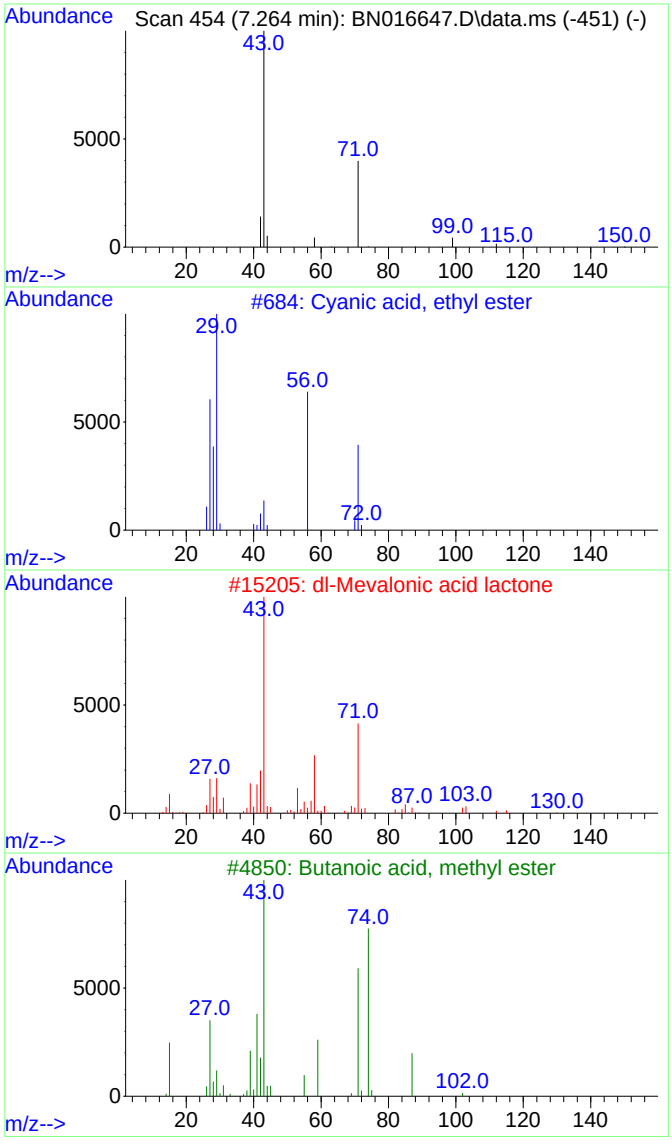
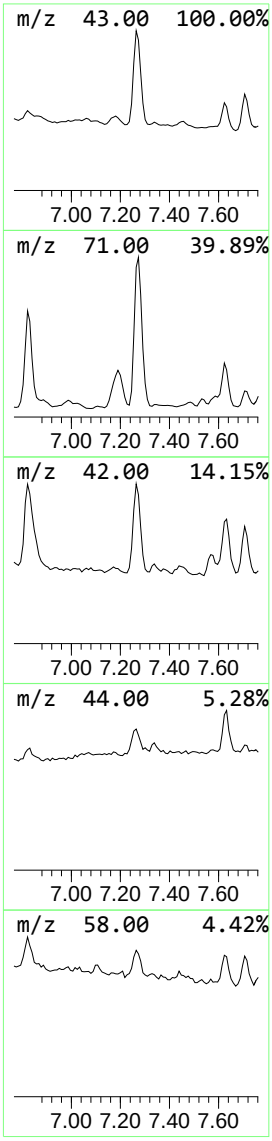
Peak Number 4 Cyanic acid, ethyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.264	0.06 ng	13836	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	4
2	dl-Mevalonic acid lactone	130	C6H10O3	000674-26-0	4
3	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	4
4	Isobutane	58	C4H10	000075-28-5	4
5	1,6-Heptadien-4-ol	112	C7H12O	002883-45-6	4





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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
DUP03-20210920

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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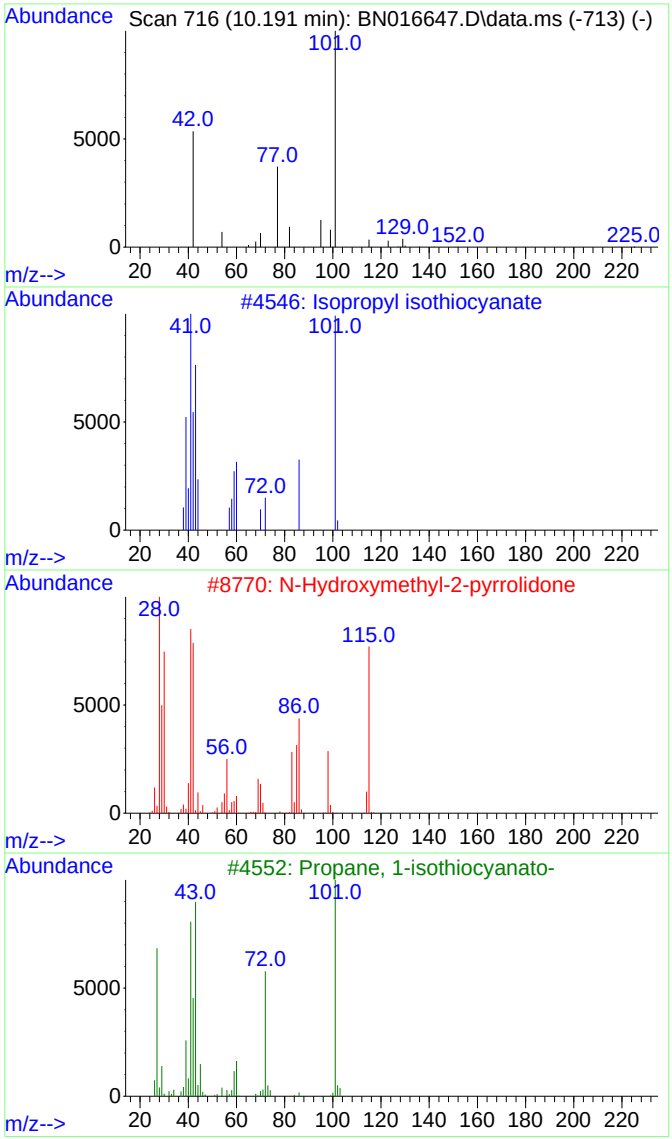
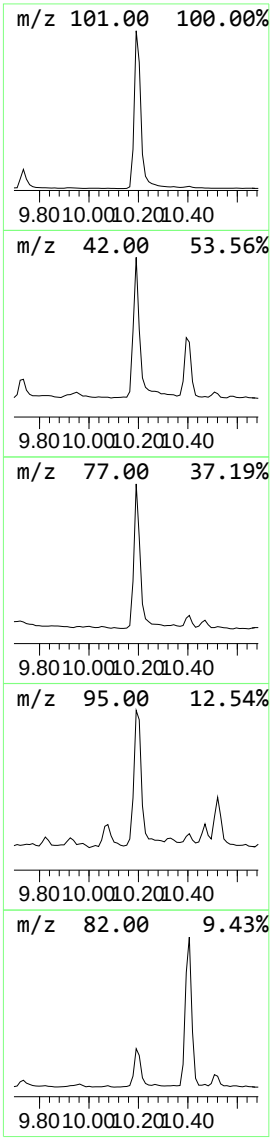
Peak Number 5 Isopropyl isothiocyanate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.07 ng	26450	Naphthalene-d8	10.406

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	9
2	N-Hydroxymethyl-2-pyrrolidone	115	C5H9NO2	1000426-51-3	7
3	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5
4	4-Methyl-1,2,5-oxadiazol-3-amine	99	C3H5N3O	1000411-31-0	5
5	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5





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
4-Pyridazinamine	3.152	0.3	ng	74871	1	7.642	90918	0.4
1-Propanol, 2-m...	3.815	0.2	ng	49783	1	7.642	90918	0.4
Butane	4.820	0.4	ng	80921	1	7.642	90918	0.4
Cyanic acid, et...	7.264	0.1	ng	13836	1	7.642	90918	0.4
Isopropyl isoth...	10.191	0.1	ng	26450	2	10.406	161117	0.4