LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016644.D
Acq On : 01 Oct 2021 20:10
Operator : CG/JU
Sample : M3833-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : MW201D1-20210919

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: BN016644.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.502	43	46	59	rVB	7514	30723	11.22%	1.173%
2	3.825	77	81	88	rBV	9299	28961	10.58%	1.106%
3	4.821	185	189	205	rVB	44654	103899	37.94%	3.967%
4	5.272	234	238	246	rVB	7652	19124	6.98%	0.730%
5	6.646	383	387	397	rBV	7001	15982	5.84%	0.610%
6	6.849	403	409	419	rVB2	8807	28142	10.28%	1.074%
7	7.264	449	454	460	rVB3	7607	21001	7.67%	0.802%
8	7.642	490	495	500	rBV	48996	98019	35.80%	3.742%
9	7.707	500	502	506	rVB	3429	5307	1.94%	0.203%
10	7.863	515	519	525	rBV	8978	18900	6.90%	0.722%
11	8.177	549	553	555	rBV	4634	9752	3.56%	0.372%
12	8.306	564	567	569	rVB	8780	10255	3.75%	0.392%
13	8.784	602	605	610	rBV	30445	55751	20.36%	2.129%
14	8.898	611	614	616	rVV2	4237	8557	3.13%	0.327%
15	8.949	616	618	622	rVB	5948	9838	3.59%	0.376%
16	9.747	678	681	685	rBV	3882	7459	2.72%	0.285%
17	10.204	713	717	720	rBV	148239	273820	100.00%	10.454%
18	10.406	730	733	737	rBV	100476	173654	63.42%	6.630%
19	11.217	793	797	802	rBV2	5961	13831	5.05%	0.528%
20	11.306	802	804	814	rVB	2673	6729	2.46%	0.257%
21	12.007	920	932	943	rBV	46677	76986	28.12%	2.939%
22	12.885	1071	1074	1078	rBV2	90149	170391	62.23%	6.505%
23	13.114	1089	1092	1095	rBV	4759	7575	2.77%	0.289%
24	13.177	1095	1097	1107	rVB2	10666	21787	7.96%	0.832%
25	14.268	1180	1183	1193	rBV	131114	199039	72.69%	7.599%
26	14.433	1193	1196	1199	rBV	8810	13221	4.83%	0.505%
27	15.715	1295	1297	1299	rBV	11289	17264	6.30%	0.659%
28	15.766	1299	1301	1305	rVB2	13788	22416	8.19%	0.856%
29	15.969	1315	1317	1323	rVB5	2638	7445	2.72%	0.284%
30	16.835	1385	1388	1394	rVB	5593	9340	3.41%	0.357%
31	17.017	1400	1403	1410	rBV	97743	164419	60.05%	6.277%
32	17.954	1477	1480	1483	rBV	3870	8251	3.01%	0.315%
33	18.015	1483	1485	1499	rVB3	3255	5245	1.92%	0.200%
34	18.909	1661	1665	1671	rVB	8007	9088	3.32%	0.347%
35	19.063	1688	1696	1721	rBV	142113	200802	73.33%	7.667%
36	19.241	1728	1732	1745	rBV	3195	5189	1.90%	0.198%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016644.D
Acq On : 01 Oct 2021 20:10
Operator : CG/JU
Sample : M3833-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : MW201D1-20210919

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

37	19.678	1813	1820	1838	rBV	138597	168607	61.58%	6.437%
38	20.006	1885	1886	1888	rBV	3088	4588	1.68%	0.175%
39	20.972	1975	1977	1980	rBV	6175	9204	3.36%	0.351%
40	21.163	1993	1995	1998	rBV	44537	60224	21.99%	2.299%
41	21.227	1998	2001	2010	rVB	128716	195809	71.51%	7.476%
42	22.109	2081	2084	2089	rBV	14276	19649	7.18%	0.750%
43	22.321	2100	2104	2108	rBV2	4542	9452	3.45%	0.361%
44	22.841	2232	2239	2250	rVB	5061	7535	2.75%	0.288%
45	23.419	2400	2408	2415	rBV	6867	11201	4.09%	0.428%
46	23.481	2415	2426	2457	rVB	104705	205710	75.13%	7.854%
47	24.083	2593	2602	2617	rVB	7762	14856	5.43%	0.567%
48	24.853	2817	2827	2846	rVB	7405	16646	6.08%	0.636%
49	25.753	3076	3090	3116	rBV	2531	7463	2.73%	0.285%
50	26.818	3385	3401	3428	rBV	1813	6359	2.32%	0.243%
51	28.088	3753	3772	3795	rVB2	1029	3743	1.37%	0.143%

Sum of corrected areas: 2619208

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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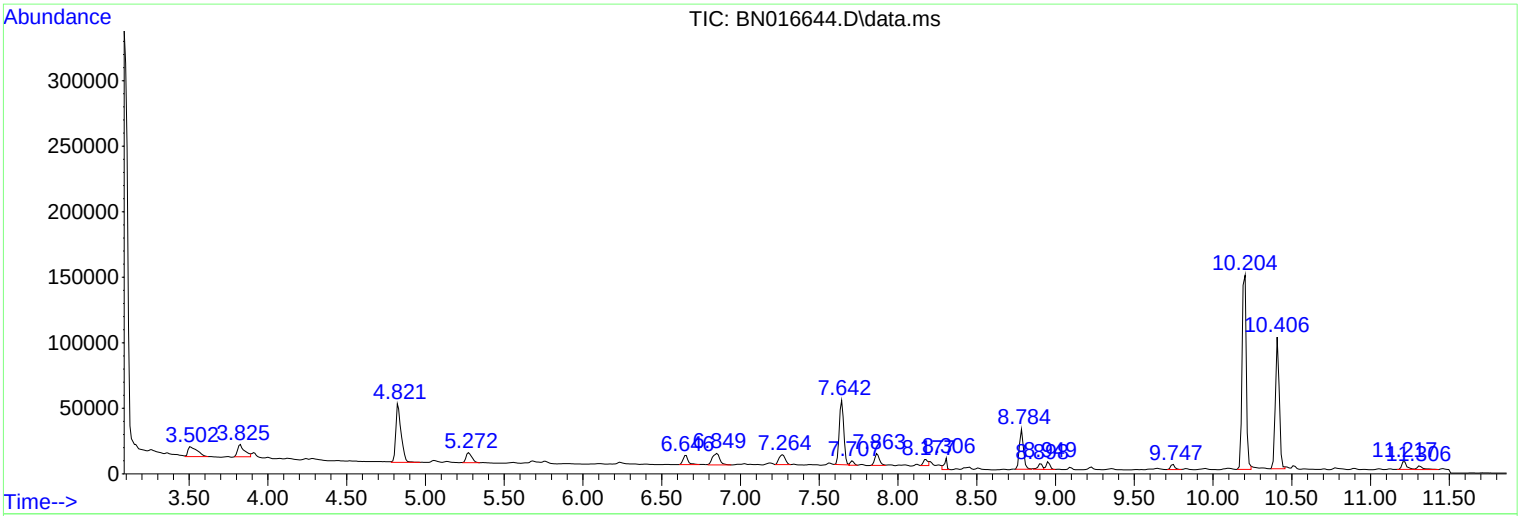
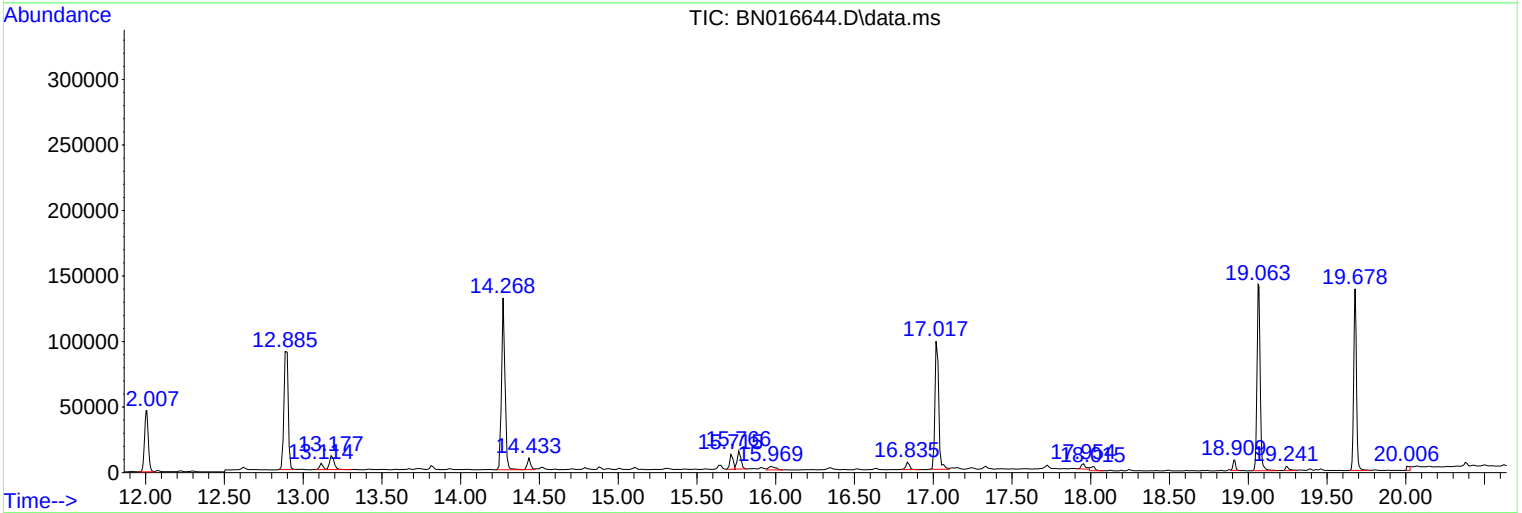
Misc :
ALS Vial : 13 Sample Multiplier: 1

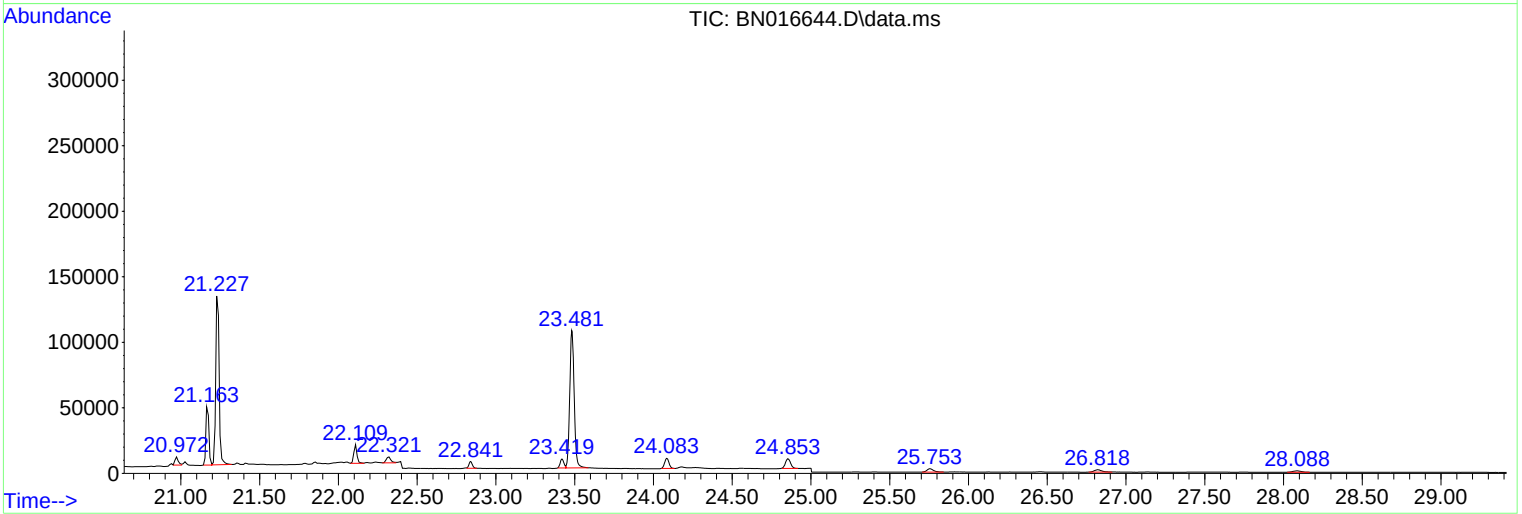
Instrument :
BNA_N
ClientSampleId :
MW201D1-20210919

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016644.D
Acq On : 01 Oct 2021 20:10
Operator : CG/JU
Sample : M3833-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW201D1-20210919

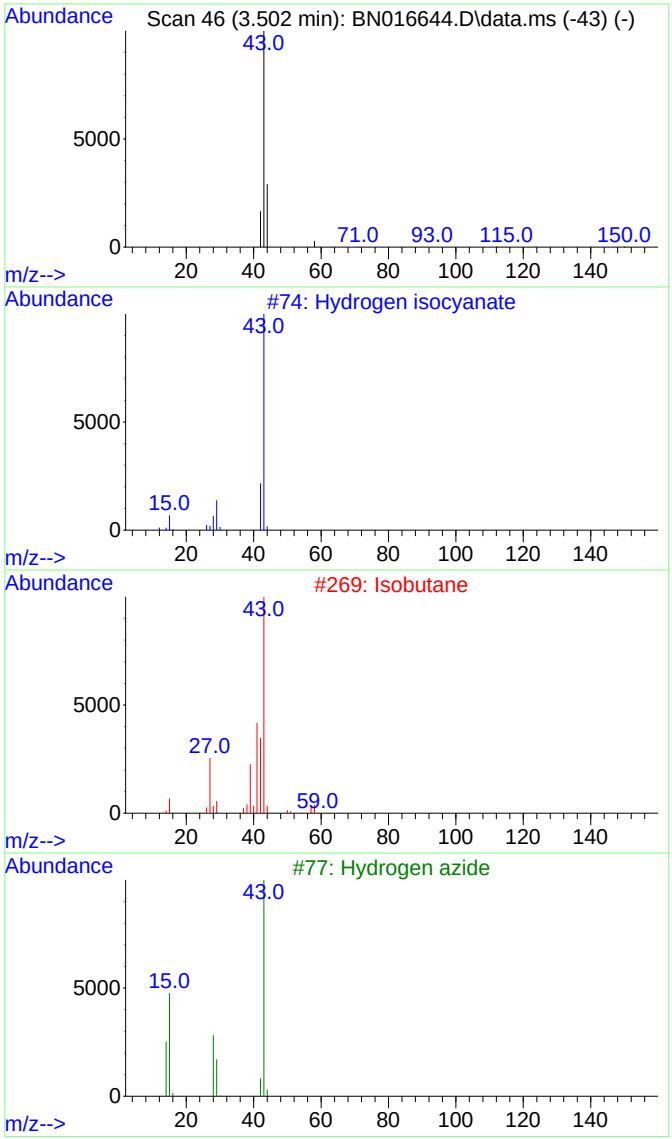
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

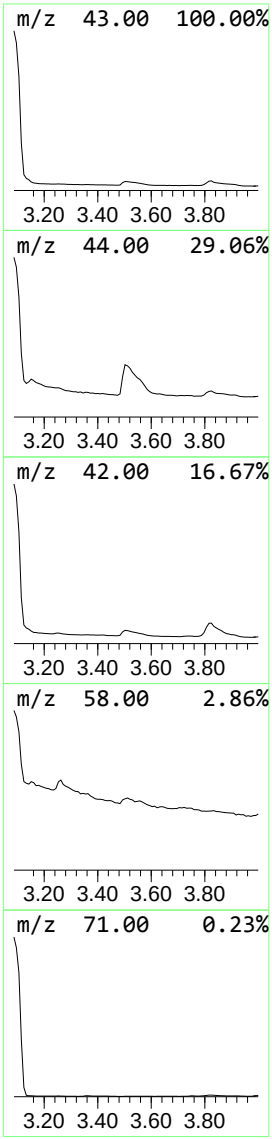
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Hydrogen isocyanate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.502	0.13 ng	30723	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrogen isocyanate	43	CHNO	000075-13-8	3
2	Isobutane	58	C4H10	000075-28-5	3
3	Hydrogen azide	43	HN3	007782-79-8	3
4	Ethylene oxide	44	C2H4O	000075-21-8	2
5	Acetaldehyde	44	C2H4O	000075-07-0	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016644.D
Acq On : 01 Oct 2021 20:10
Operator : CG/JU
Sample : M3833-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW201D1-20210919

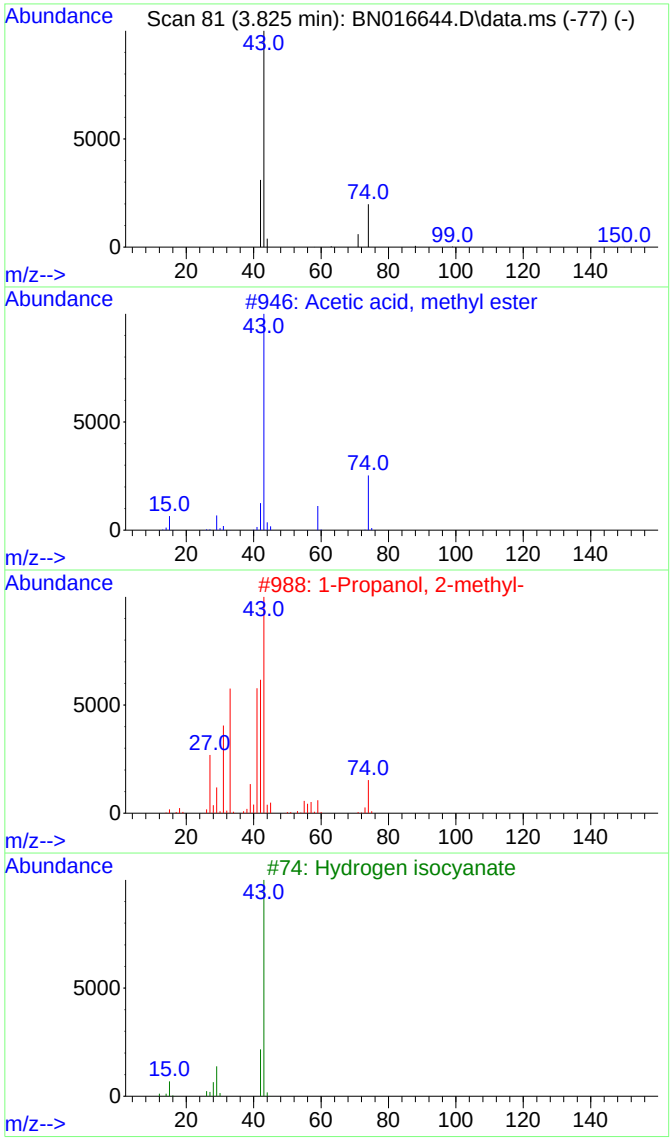
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

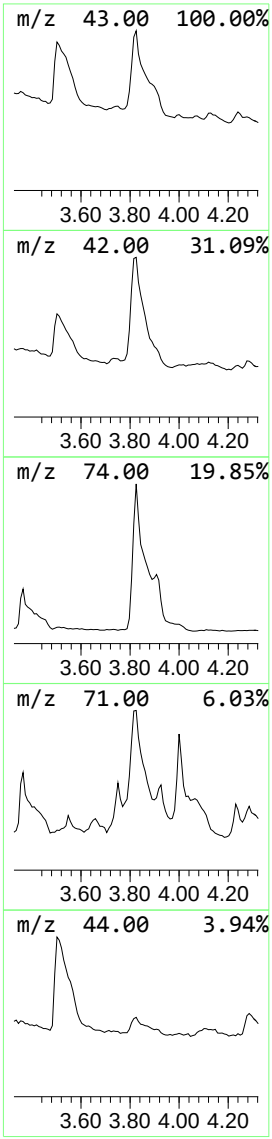
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Acetic acid, methyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.825	0.12 ng	28961	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	5
2	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	4
3	Hydrogen isocyanate	43	CHNO	000075-13-8	3
4	Acetic acid, hydrazide	74	C2H6N2O	001068-57-1	3
5	(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	3





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016644.D
Acq On : 01 Oct 2021 20:10
Operator : CG/JU
Sample : M3833-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW201D1-20210919

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

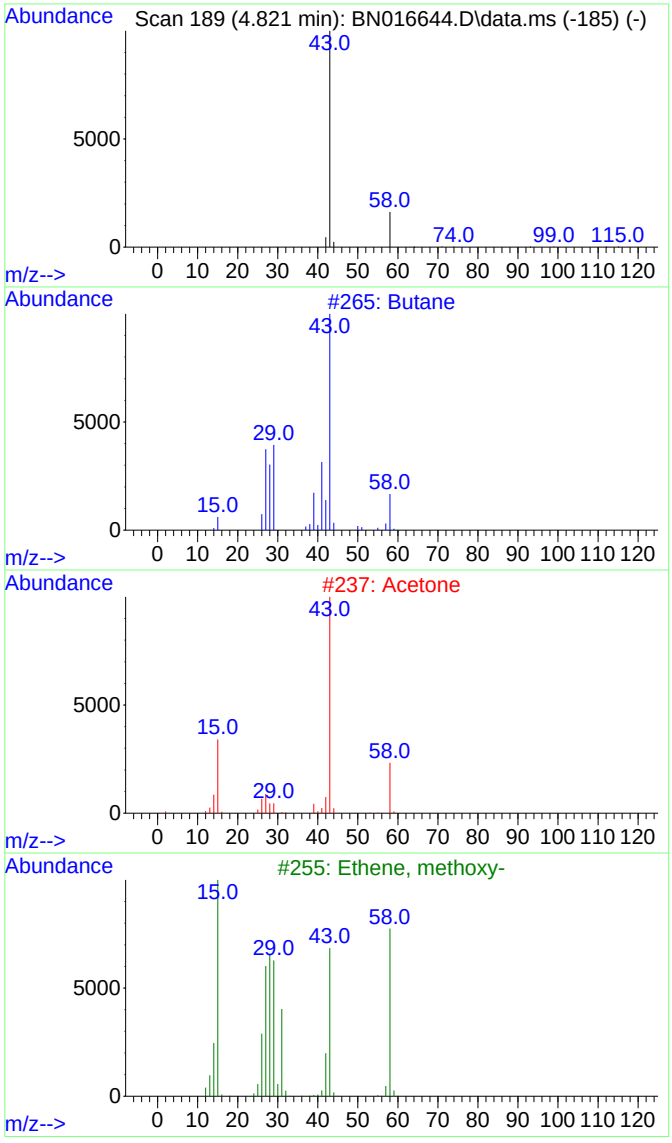
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

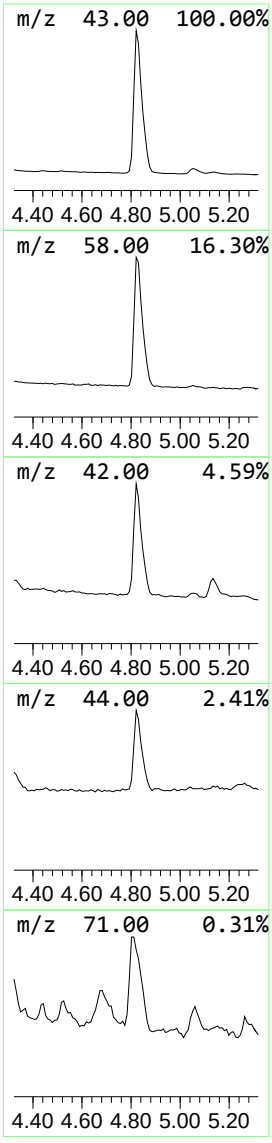
****

Peak Number 3 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.42 ng	103899	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





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016644.D
Acq On : 01 Oct 2021 20:10
Operator : CG/JU
Sample : M3833-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW201D1-20210919

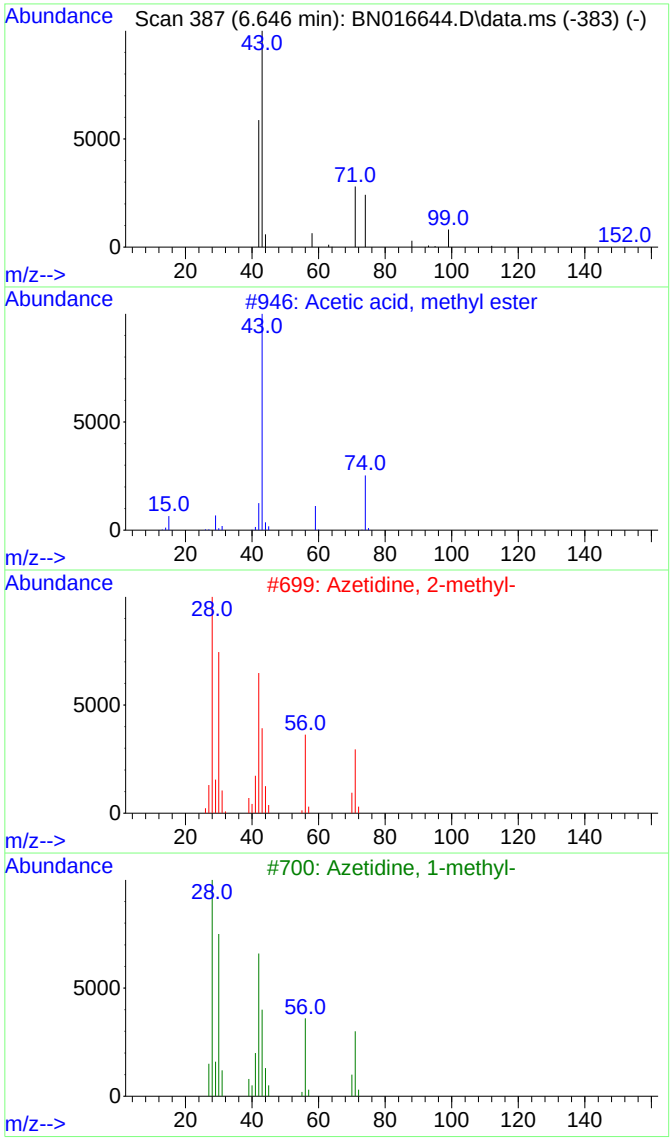
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

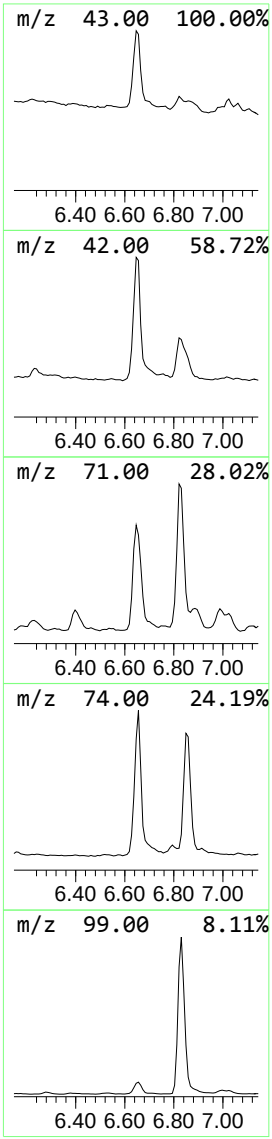
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Acetic acid, methyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.646	0.07 ng	15982	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	5
2	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	4
3	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	4
4	Butanal, 3-hydroxy-	88	C4H8O2	000107-89-1	4
5	Isobutane	58	C4H10	000075-28-5	4





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Data File : BN016644.D
Acq On : 01 Oct 2021 20:10
Operator : CG/JU
Sample : M3833-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW201D1-20210919

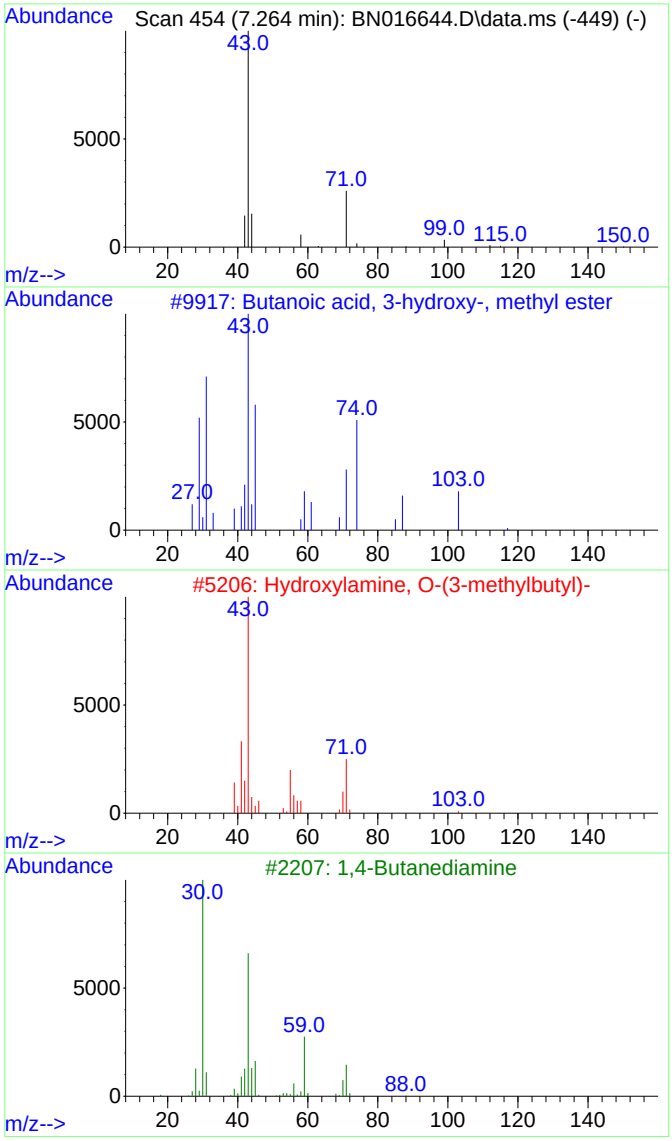
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

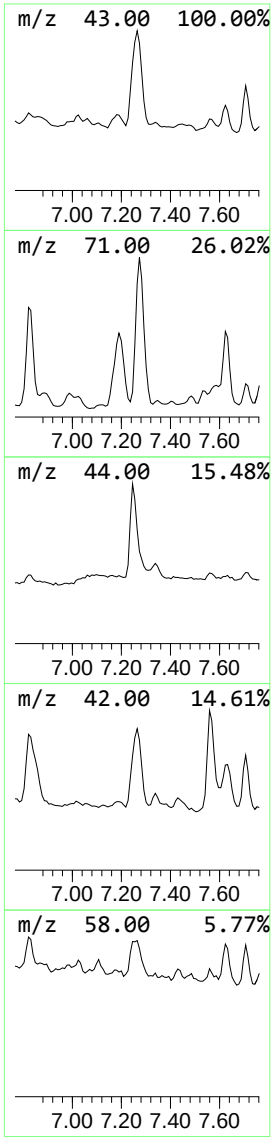
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Butanoic acid, 3-hydroxy-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.264	0.09 ng	21001	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-hydroxy-, methy...	118	C5H10O3	001487-49-6	9
2	Hydroxylamine, O-(3-methylbutyl)-	103	C5H13NO	019411-65-5	9
3	1,4-Butanediamine	88	C4H12N2	000110-60-1	7
4	Hex-4-enylamine	99	C6H13N	055108-01-5	5
5	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	4





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Acq On : 01 Oct 2021 20:10
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Sample : M3833-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : MW201D1-20210919

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

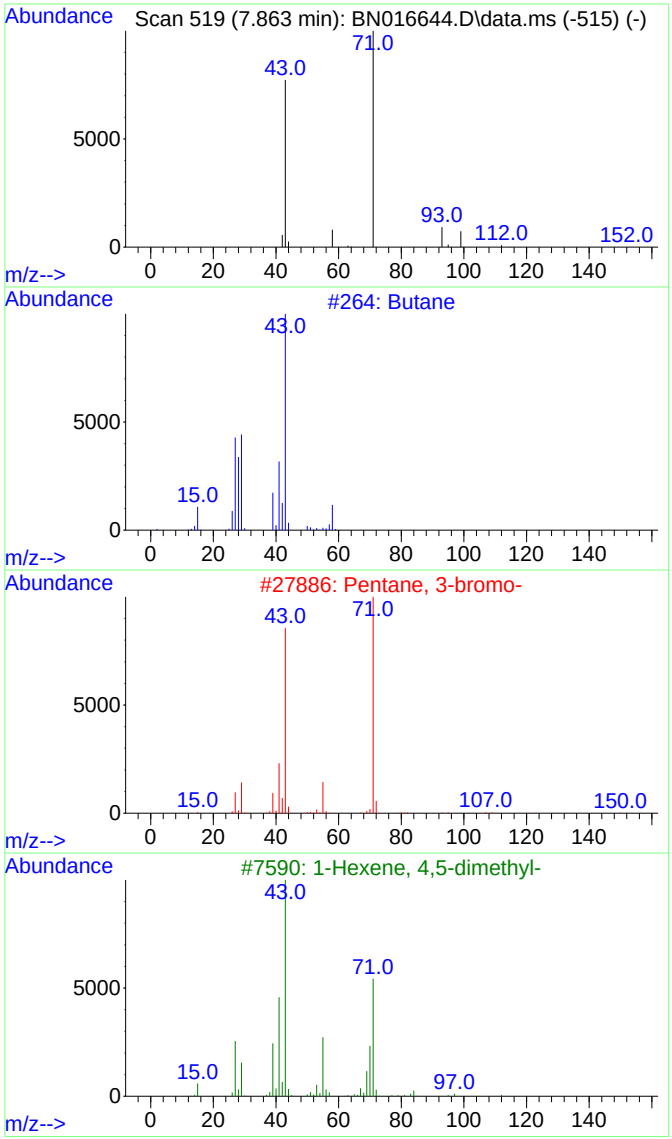
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

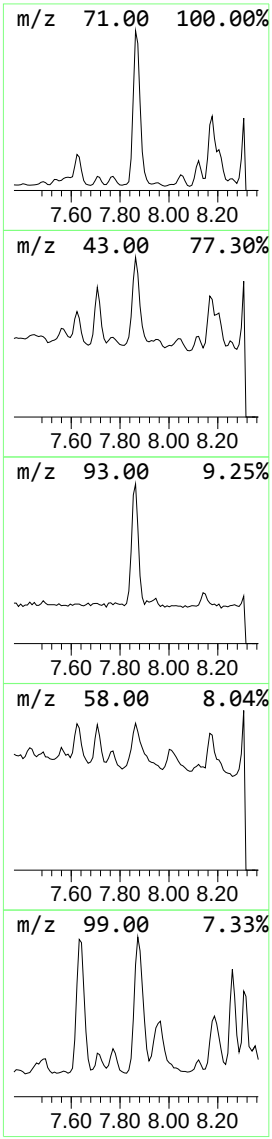
****

Peak Number 6 Butane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.863	0.08 ng	18900	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	4
2	Pentane, 3-bromo-	150	C5H11Br	001809-10-5	4
3	1-Hexene, 4,5-dimethyl-	112	C8H16	016106-59-5	4
4	Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	4
5	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	4





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Data File : BN016644.D
Acq On : 01 Oct 2021 20:10
Operator : CG/JU
Sample : M3833-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW201D1-20210919

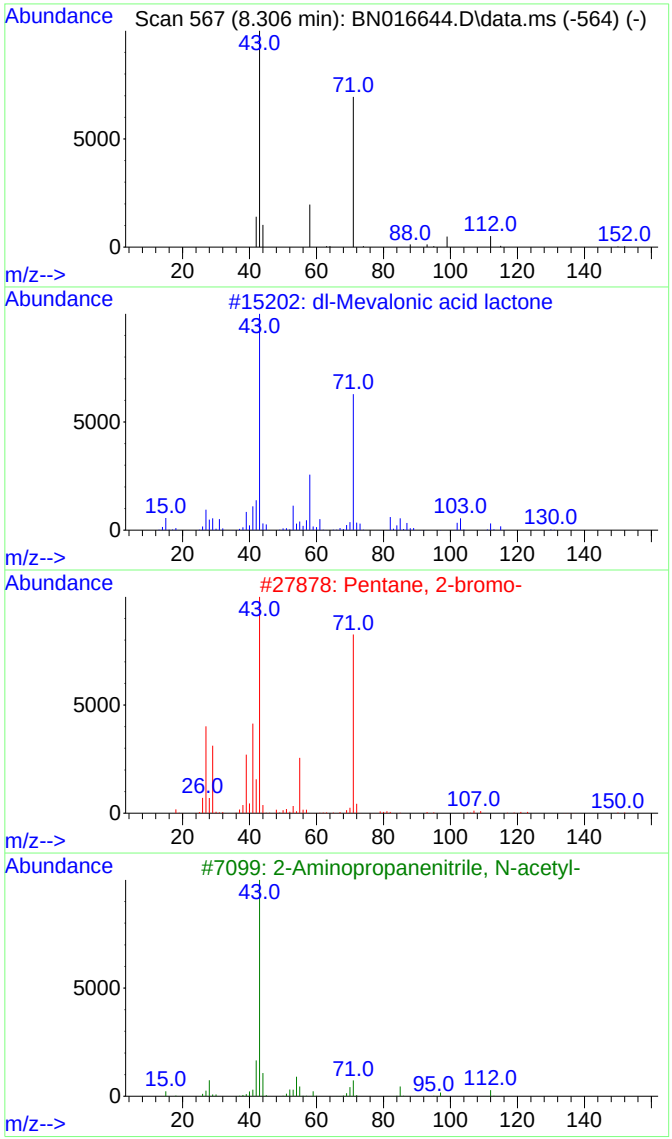
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

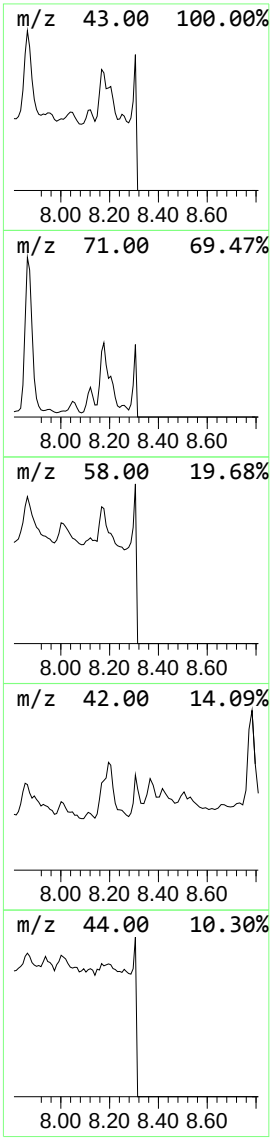
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 dl-Mevalonic acid lactone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.306	0.04 ng	10255	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	dl-Mevalonic acid lactone	130	C6H10O3	000674-26-0	39
2	Pentane, 2-bromo-	150	C5H11Br	000107-81-3	9
3	2-Aminopropanenitrile, N-acetyl-	112	C5H8N2O	019861-71-3	9
4	Pentane, 3-bromo-	150	C5H11Br	001809-10-5	9
5	Carbamic acid, methylnitroso-, e...	132	C4H8N2O3	000615-53-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016644.D
Acq On : 01 Oct 2021 20:10
Operator : CG/JU
Sample : M3833-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW201D1-20210919

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

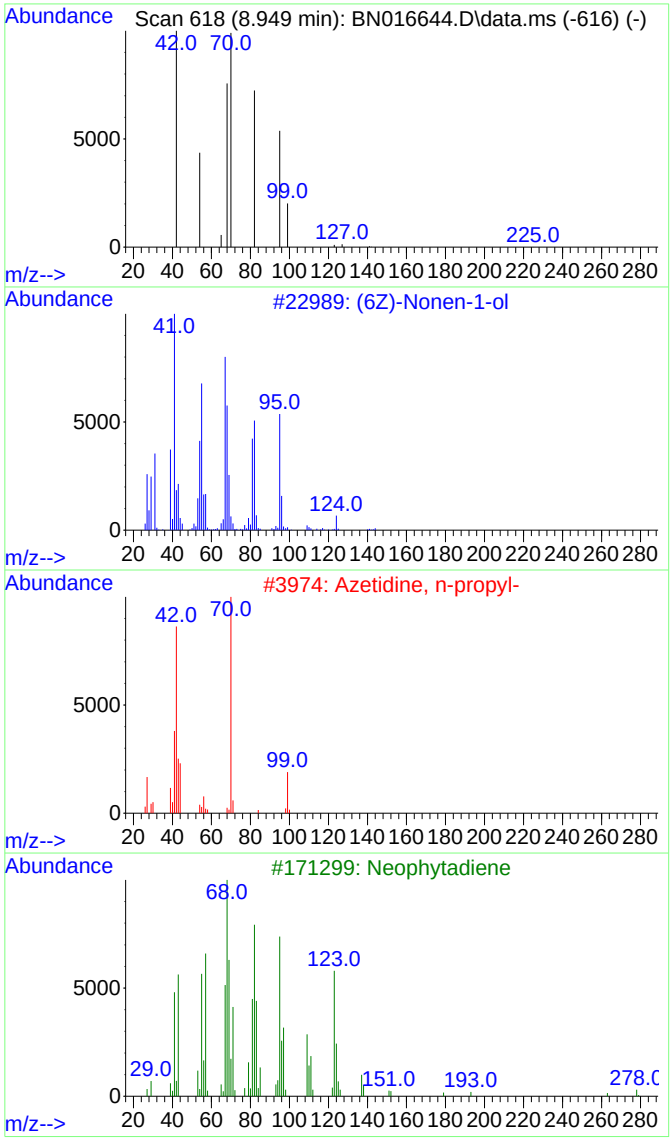
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

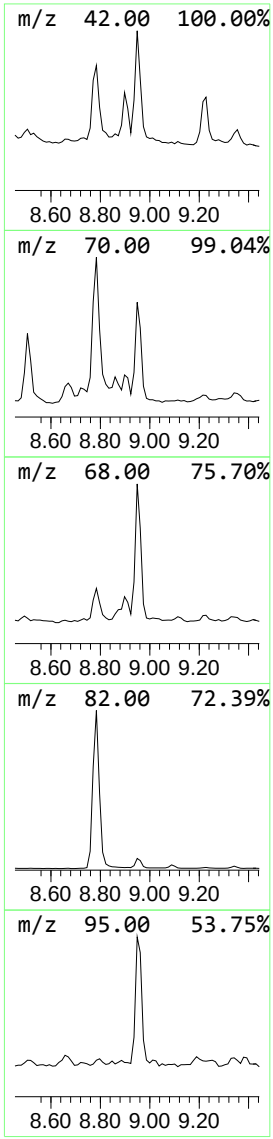
****

Peak Number 8 (6Z)-Nonen-1-ol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.949	0.04 ng	9838	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(6Z)-Nonen-1-ol	142	C9H18O	035854-86-5	23
2	Azetidine, n-propyl-	99	C6H13N	1000288-41-2	9
3	Neophytadiene	278	C20H38	000504-96-1	9
4	2-Octenoic acid, (E)-	142	C8H14O2	001871-67-6	9
5	2-Octenoic acid	142	C8H14O2	001470-50-4	9





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Acq On : 01 Oct 2021 20:10
Operator : CG/JU
Sample : M3833-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW201D1-20210919

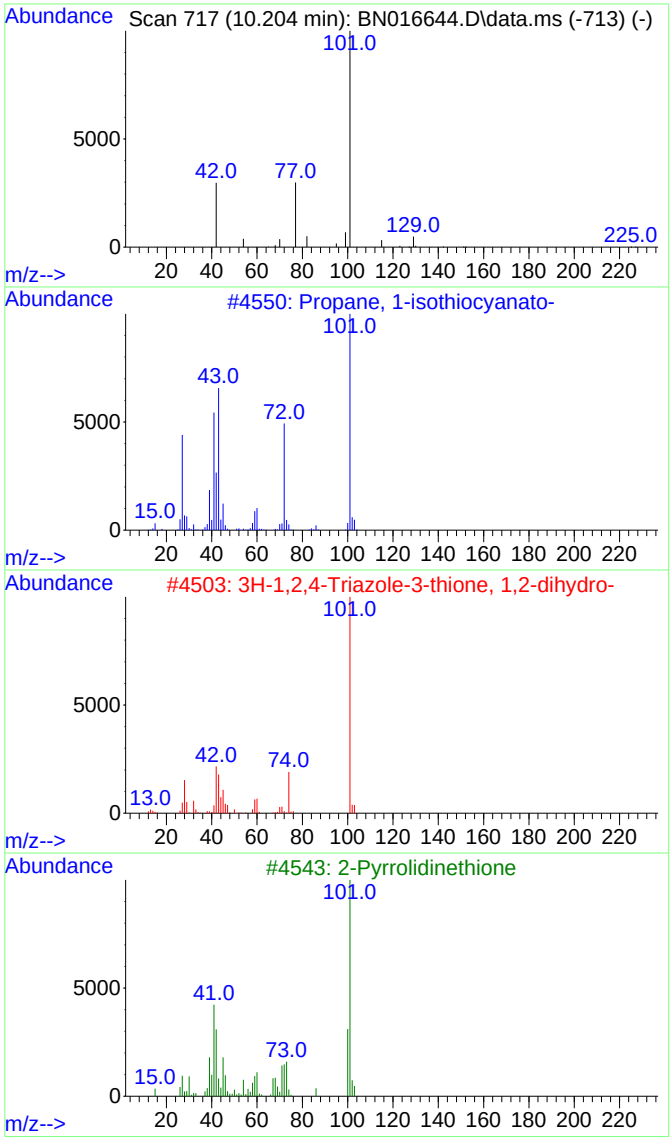
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

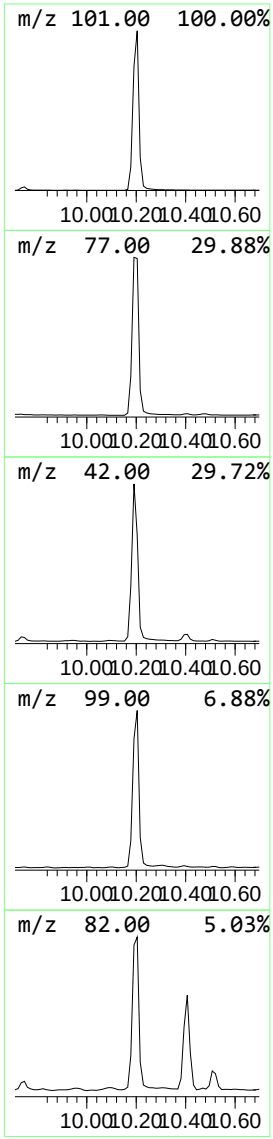
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Propane, 1-isothiocyanato- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.204	0.63 ng	273820	Naphthalene-d8	10.406

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	4
2	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	4
3	2-Pyrrolidinethione	101	C4H7NS	002295-35-4	4
4	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	4
5	1,3,4-Thiadiazol-2-amine	101	C2H3N3S	004005-51-0	4





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BNA_N
ClientSampleId :
MW201D1-20210919

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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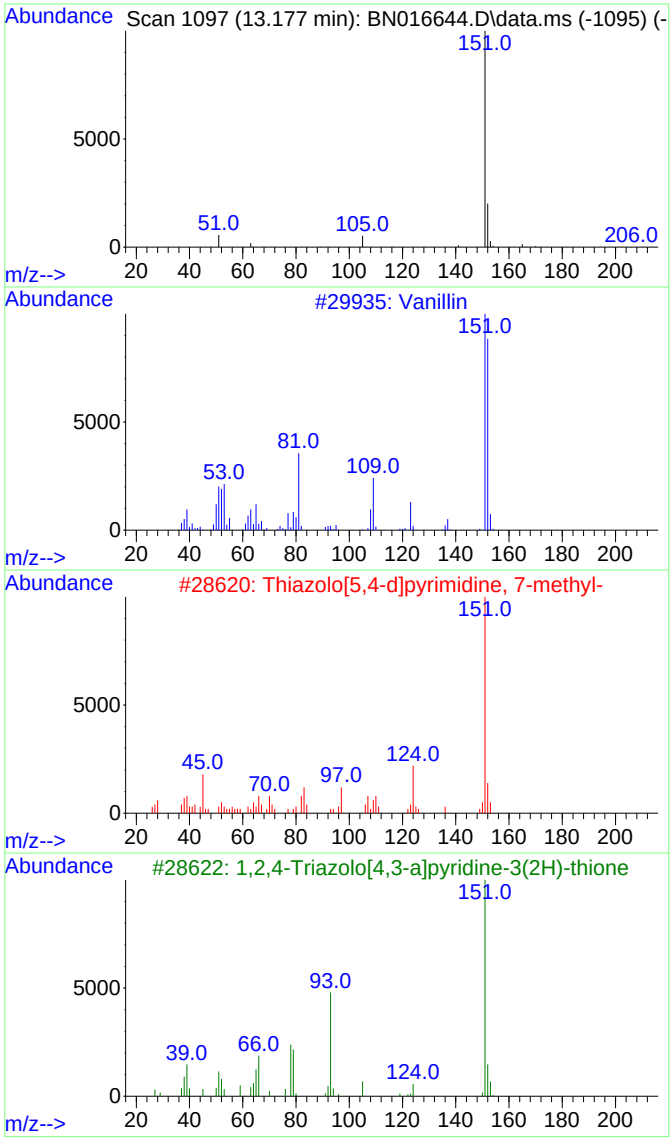
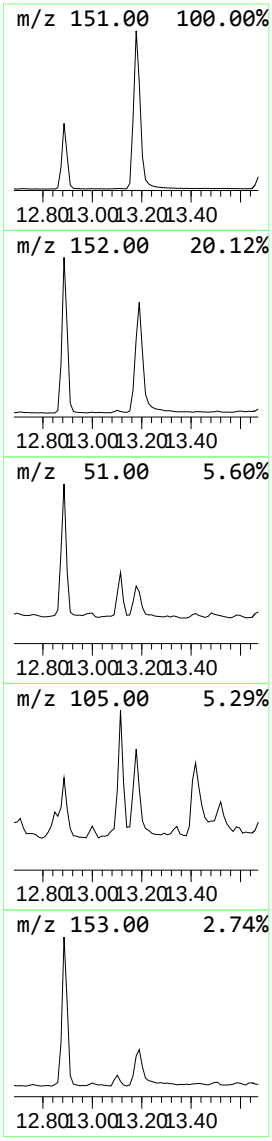
Peak Number 10 Vanillin Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.177	0.04 ng	21787	Acenaphthene-d10	14.268

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Vanillin	152	C8H8O3	000121-33-5	5
2	Thiazolo[5,4-d]pyrimidine, 7-met...	151	C6H5N3S	013316-06-8	4
3	1,2,4-Triazolo[4,3-a]pyridine-3(...	151	C6H5N3S	006952-68-7	4
4	Ethanethioamide, N-phenyl-	151	C8H9NS	000637-53-6	4
5	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	4





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Sample : M3833-05
Misc :
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BNA_N
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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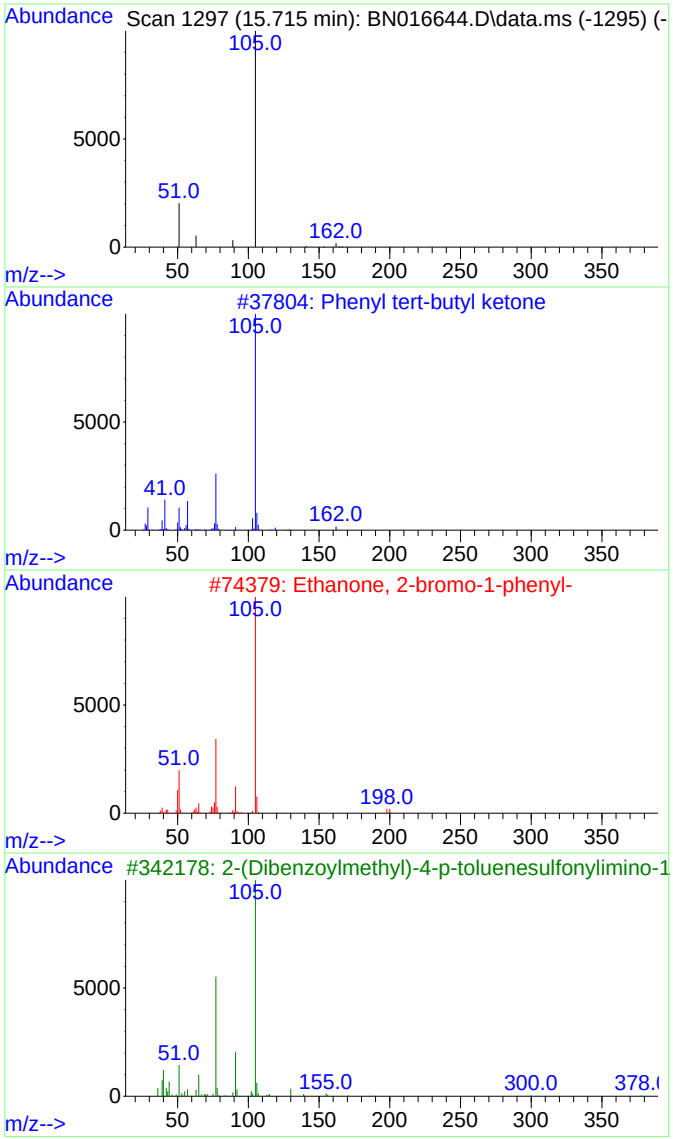
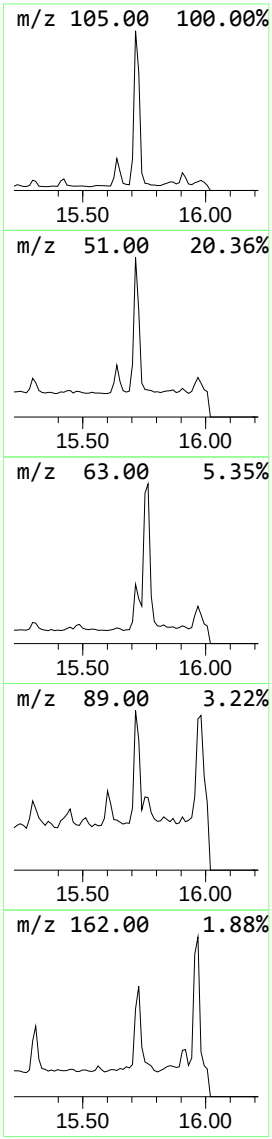
Peak Number 11 Phenyl tert-butyl ketone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.715	0.04 ng	17264	Phenanthrene-d10	17.017

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenyl tert-butyl ketone	162	C11H14O	000938-16-9	3
2	Ethanone, 2-bromo-1-phenyl-	198	C8H7BrO	000070-11-1	2
3	2-(Dibenzoylmethyl)-4-p-toluenes...	533	C32H23NO5S	300360-29-6	2
4	Benzofurazan-5-carbohydrazide, N...	282	C14H10N4O3	1000272-94-4	2
5	.alpha.,.alpha.-Dichloroacetophe...	188	C8H6Cl2O	002648-61-5	2





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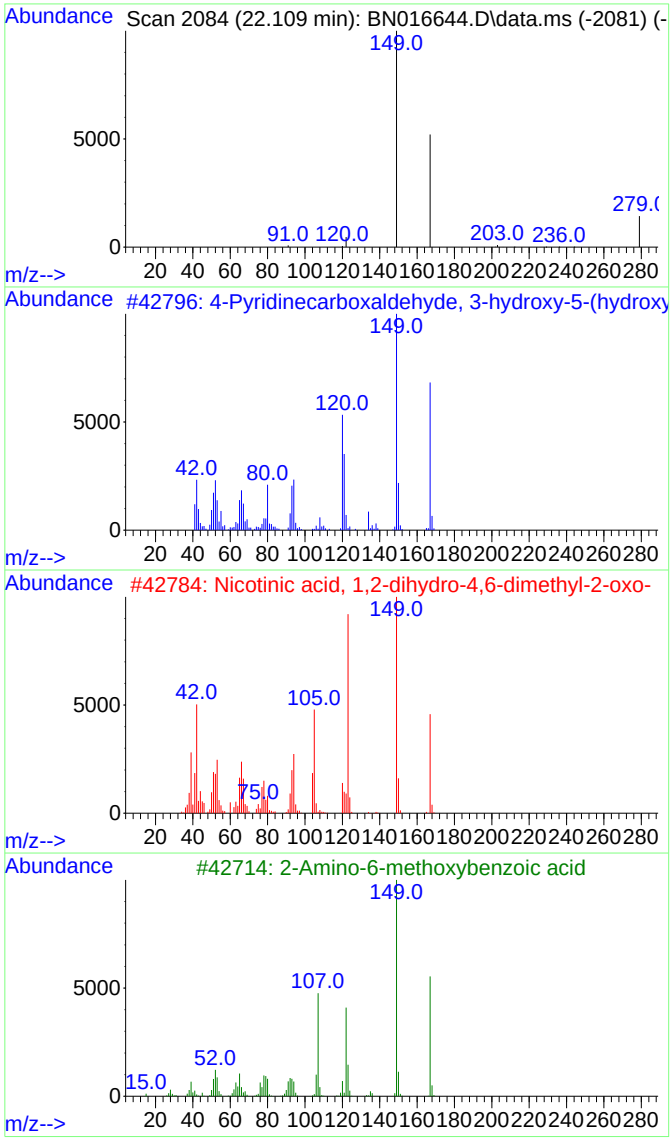
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

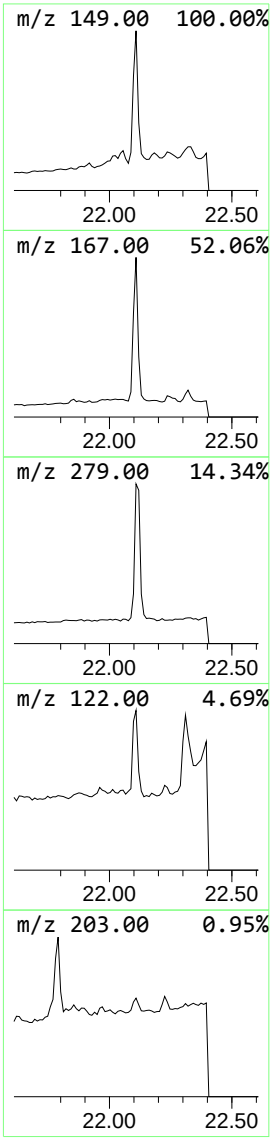
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 4-Pyridinecarboxaldehyde, 3... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.108	0.04 ng	19649	Chrysene-d12	21.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Pyridinecarboxaldehyde, 3-hydr...	167	C8H9NO3	000066-72-8	9
2	Nicotinic acid, 1,2-dihydro-4,6-...	167	C8H9NO3	024667-09-2	5
3	2-Amino-6-methoxybenzoic acid	167	C8H9NO3	1000496-75-6	5
4	6H-Thieno[2,3-b]pyrrole-5-carbox...	167	C7H5NO2S	051856-25-8	5
5	4-Methoxyanthranilic acid	167	C8H9NO3	004294-95-5	5





Tentatively Identified Compound (LSC) summary

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Data File : BN016644.D
Acq On : 01 Oct 2021 20:10
Operator : CG/JU
Sample : M3833-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW201D1-20210919

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Hydrogen isocya...	3.502	0.1	ng	30723	1	7.642	98019	0.4
Acetic acid, me...	3.825	0.1	ng	28961	1	7.642	98019	0.4
Butane	4.821	0.4	ng	103899	1	7.642	98019	0.4
Acetic acid, me...	6.646	0.1	ng	15982	1	7.642	98019	0.4
Butanoic acid, ...	7.264	0.1	ng	21001	1	7.642	98019	0.4
Butane	7.863	0.1	ng	18900	1	7.642	98019	0.4
dl-Mevalonic ac...	8.306	0.0	ng	10255	1	7.642	98019	0.4
(6Z)-Nonen-1-ol	8.949	0.0	ng	9838	1	7.642	98019	0.4
Propane, 1-isot...	10.204	0.6	ng	273820	2	10.406	173654	0.4
Vanillin	13.177	0.0	ng	21787	3	14.268	199039	0.4
Phenyl tert-but...	15.715	0.0	ng	17264	4	17.017	164419	0.4
4-Pyridinecarbo...	22.108	0.0	ng	19649	5	21.227	195809	0.4