LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016621.D
Acq On : 01 Oct 2021 05:24
Operator : CG/JU
Sample : M3986-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : SW-RR-01-(2.0)

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: BN016621.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.733	68	71	75	rBV	2500	6524	3.27%	0.280%
2	3.816	76	80	98	rVB	10408	46255	23.21%	1.985%
3	4.821	185	189	196	rBV	38837	84910	42.61%	3.643%
4	5.264	234	237	245	rVB	5253	13564	6.81%	0.582%
5	5.752	287	290	300	rVB	4053	10140	5.09%	0.435%
6	6.647	383	387	396	rBV2	5260	13529	6.79%	0.581%
7	6.850	403	409	419	rVB3	7745	24952	12.52%	1.071%
8	7.191	441	446	450	rBV2	2728	7626	3.83%	0.327%
9	7.264	451	454	460	rVB2	6485	14624	7.34%	0.628%
10	7.643	490	495	499	rBV	48595	102581	51.47%	4.402%
11	7.707	499	502	506	rVB	5755	9460	4.75%	0.406%
12	7.864	515	519	526	rBV	14723	29489	14.80%	1.265%
13	8.168	549	552	559	rVB	8039	17972	9.02%	0.771%
14	8.306	564	567	569	rVB	11915	13572	6.81%	0.582%
15	8.455	574	579	581	rBV	3797	9192	4.61%	0.394%
16	8.785	601	605	610	rBV	23520	43975	22.07%	1.887%
17	8.949	616	618	621	rVB	4891	7491	3.76%	0.321%
18	9.659	671	674	677	rVB2	4887	9085	4.56%	0.390%
19	10.191	713	716	721	rBV	16926	29976	15.04%	1.286%
20	10.407	729	733	736	rBV	103590	178189	89.41%	7.646%
21	12.003	921	931	942	rBV	45081	72697	36.48%	3.119%
22	12.886	1071	1074	1078	rBV	86911	148017	74.27%	6.351%
23	13.178	1094	1097	1104	rVB	6360	11043	5.54%	0.474%
24	14.269	1180	1183	1186	rBV	132968	193926	97.31%	8.321%
25	14.434	1193	1196	1200	rBV	6603	10292	5.16%	0.442%
26	14.738	1216	1220	1223	rBV	37622	77036	38.66%	3.306%
27	15.766	1299	1301	1305	rVB2	13984	21573	10.82%	0.926%
28	15.956	1314	1316	1322	rVB2	3185	9673	4.85%	0.415%
29	16.835	1383	1388	1391	rBV	8613	14049	7.05%	0.603%
30	17.018	1400	1403	1406	rBV	107705	164802	82.69%	7.071%
31	17.955	1477	1480	1497	rVB	9671	19345	9.71%	0.830%
32	19.063	1689	1696	1713	rBV	133949	189284	94.98%	8.122%
33	19.242	1727	1732	1754	rBV	8649	13578	6.81%	0.583%
34	19.430	1765	1770	1772	rBV2	2795	3526	1.77%	0.151%
35	19.455	1772	1775	1782	rVB	6700	8882	4.46%	0.381%
36	19.674	1813	1819	1838	rBV	120878	152712	76.63%	6.553%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016621.D
Acq On : 01 Oct 2021 05:24
Operator : CG/JU
Sample : M3986-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : SW-RR-01-(2.0)

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	20.006	1884	1886	1889	rBV2	4075	7670	3.85%	0.329%
38	20.973	1974	1977	1980	rBV	13928	25435	12.76%	1.091%
39	21.026	1980	1982	1990	rVB	3749	6490	3.26%	0.278%
40	21.164	1993	1995	1998	rBV	36098	44757	22.46%	1.920%
41	21.228	1998	2001	2004	rBV	145689	192473	96.58%	8.259%
42	22.109	2081	2084	2088	rBV	7818	12889	6.47%	0.553%
43	22.396	2109	2111	2112	rVB	10456	12717	6.38%	0.546%
44	22.803	2222	2228	2234	rBV	2520	4136	2.08%	0.177%
45	22.844	2236	2240	2251	rVB3	3542	5317	2.67%	0.228%
46	23.481	2414	2426	2455	rVB	100082	199289	100.00%	8.551%
47	24.176	2621	2629	2644	rBV	2756	6945	3.48%	0.298%
48	24.275	2650	2658	2681	rVB	7561	15601	7.83%	0.669%
49	25.764	3078	3093	3118	rBV4	2378	8719	4.38%	0.374%
50	26.456	3279	3295	3317	rVB2	1462	4538	2.28%	0.195%

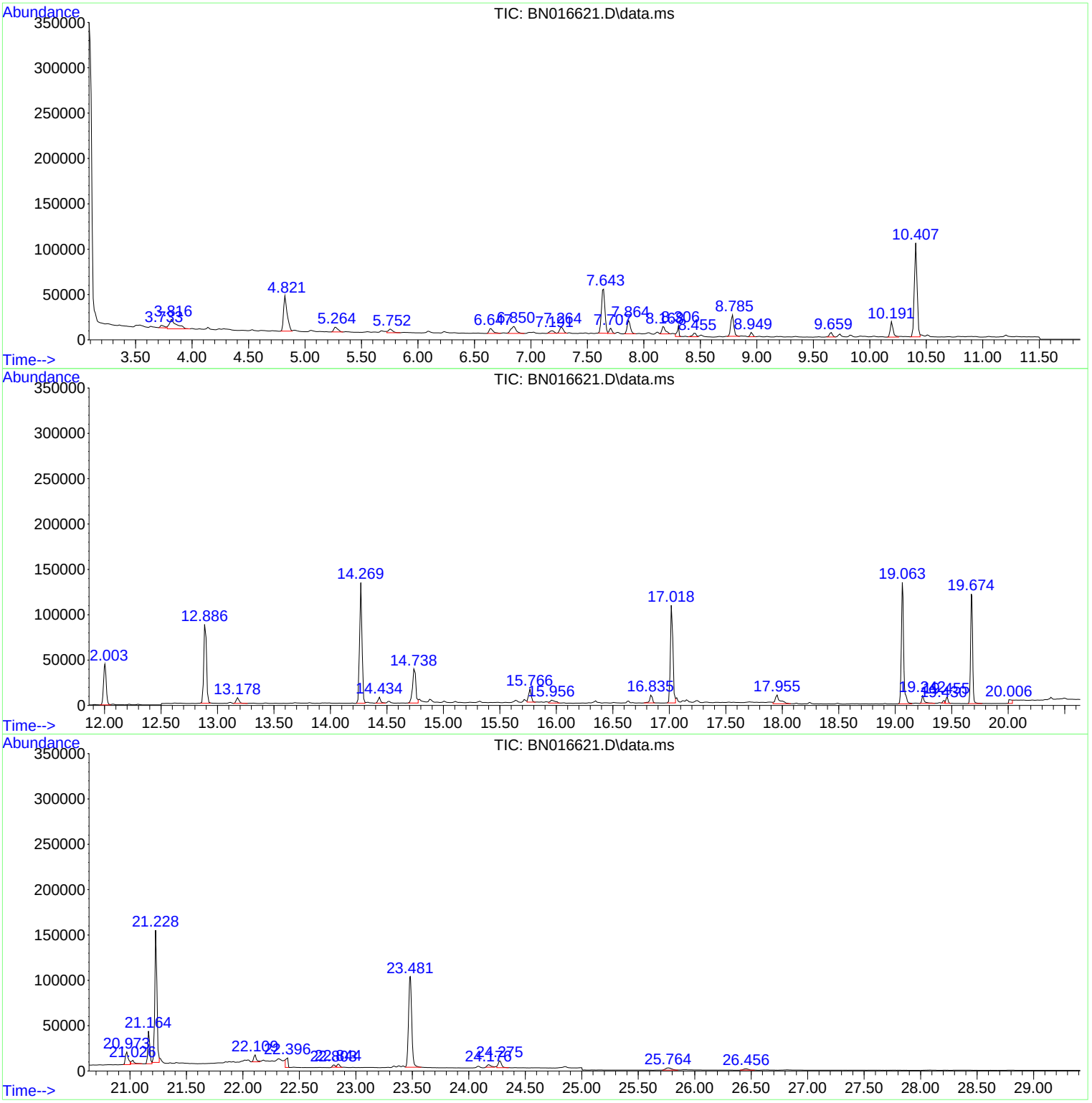
Sum of corrected areas: 2330517

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016621.D
Acq On : 01 Oct 2021 05:24
Operator : CG/JU
Sample : M3986-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
SW-RR-01-(2.0)

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 : BN016621.D
Acq On : 01 Oct 2021 05:24
Operator : CG/JU
Sample : M3986-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
SW-RR-01-(2.0)

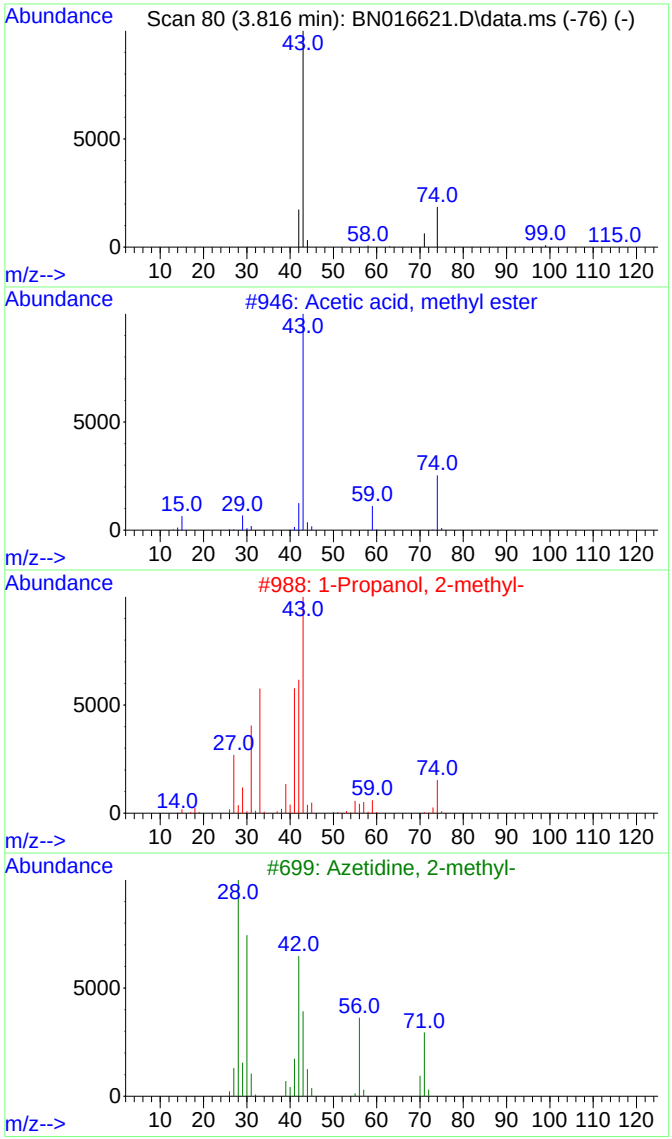
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

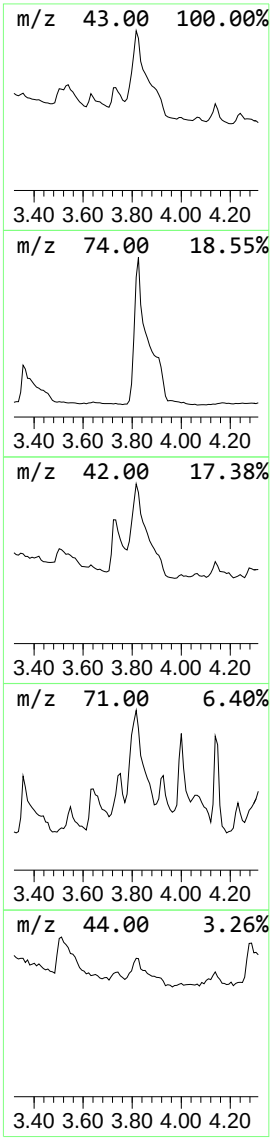
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Acetic acid, methyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.18 ng	46255	1,4-Dichlorobenzene-d4	7.643

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	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	4
4	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	4
5	Methoxyacetonitrile	71	C3H5NO	001738-36-9	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016621.D
Acq On : 01 Oct 2021 05:24
Operator : CG/JU
Sample : M3986-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
SW-RR-01-(2.0)

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

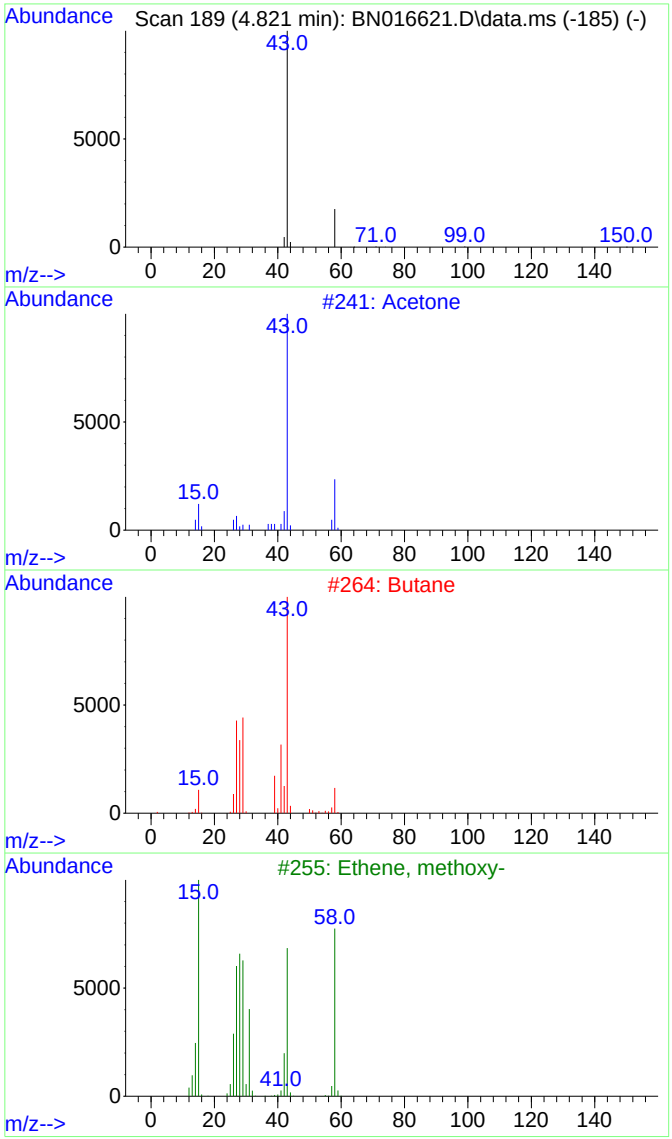
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

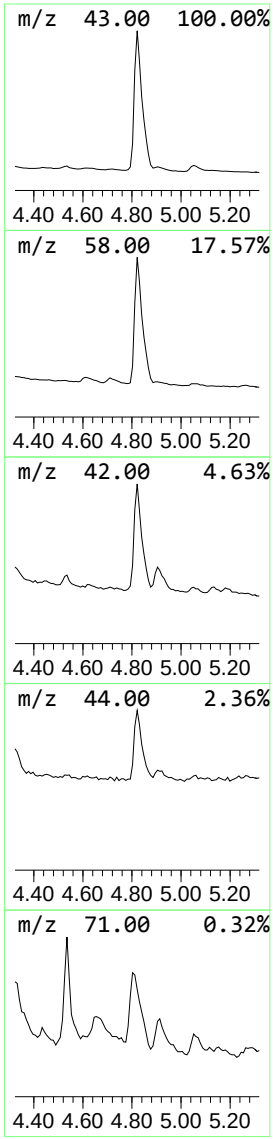
****

Peak Number 2 Acetone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.33 ng	84910	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetone	58	C3H6O	000067-64-1	4
2	Butane	58	C4H10	000106-97-8	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 : BN016621.D
Acq On : 01 Oct 2021 05:24
Operator : CG/JU
Sample : M3986-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : SW-RR-01-(2.0)

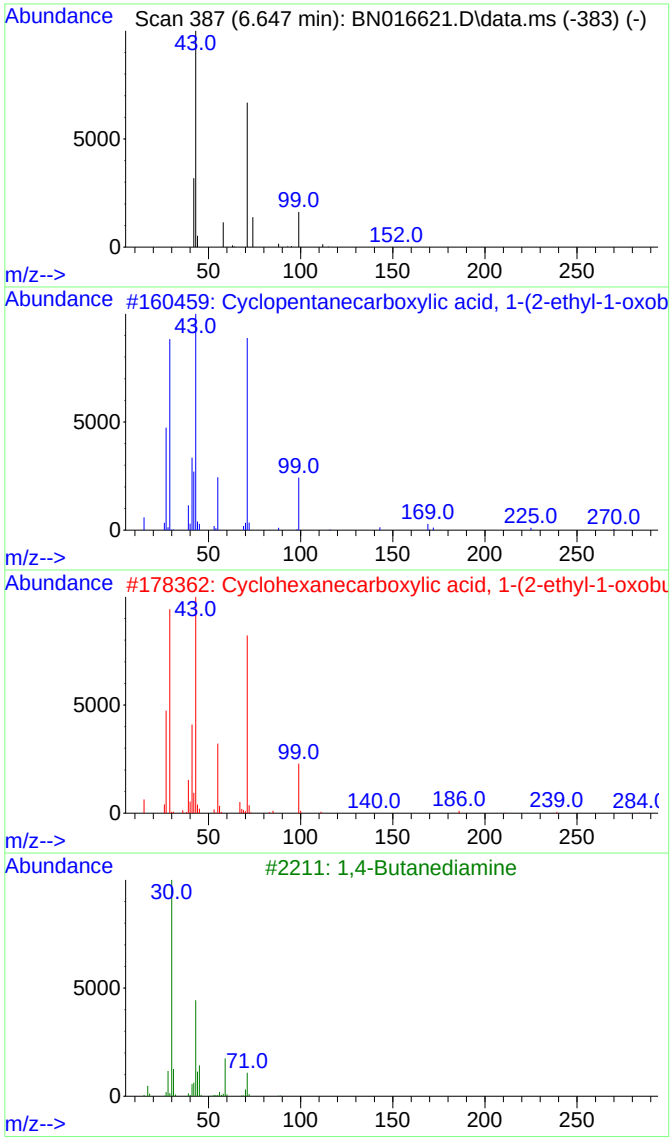
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

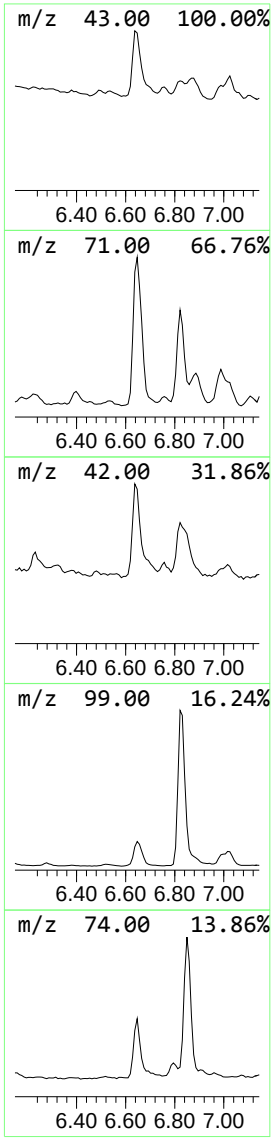
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopentanecarboxylic acid... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.647	0.05 ng	13529	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanecarboxylic acid, 1-(...	270	C14H22O5	1000460-66-4	36
2	Cyclohexanecarboxylic acid, 1-(2...	284	C15H24O5	1000460-66-2	9
3	1,4-Butanediamine	88	C4H12N2	000110-60-1	5
4	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	4
5	Acetic acid, hydrazide	74	C2H6N2O	001068-57-1	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016621.D
Acq On : 01 Oct 2021 05:24
Operator : CG/JU
Sample : M3986-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : SW-RR-01-(2.0)

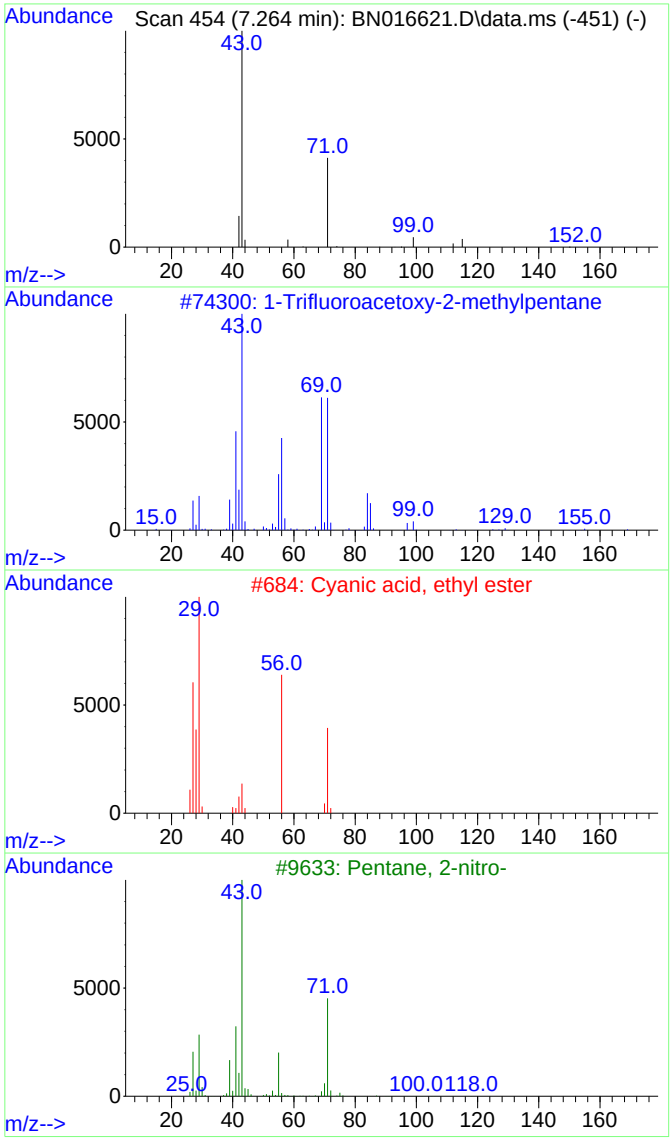
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

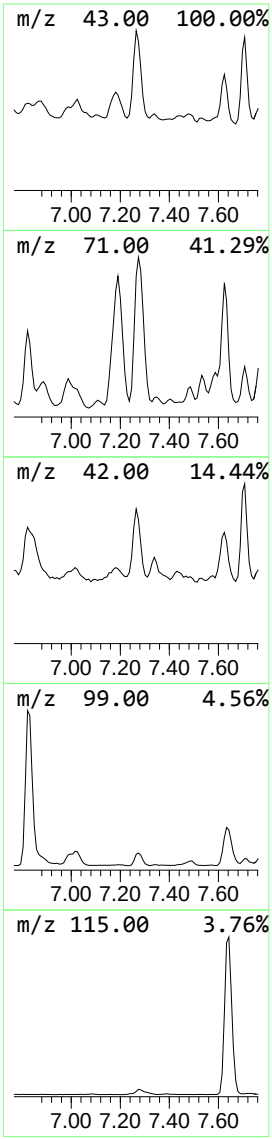
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Trifluoroacetoxy-2-methyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.264	0.06 ng	14624	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Trifluoroacetoxy-2-methylpentane	198	C8H13F3O2	155089-96-6	9
2	Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	4
3	Pentane, 2-nitro-	117	C5H11NO2	004609-89-6	4
4	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	4
5	Morpholine, 2,6-dimethyl-	115	C6H13NO	000141-91-3	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016621.D
Acq On : 01 Oct 2021 05:24
Operator : CG/JU
Sample : M3986-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : SW-RR-01-(2.0)

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

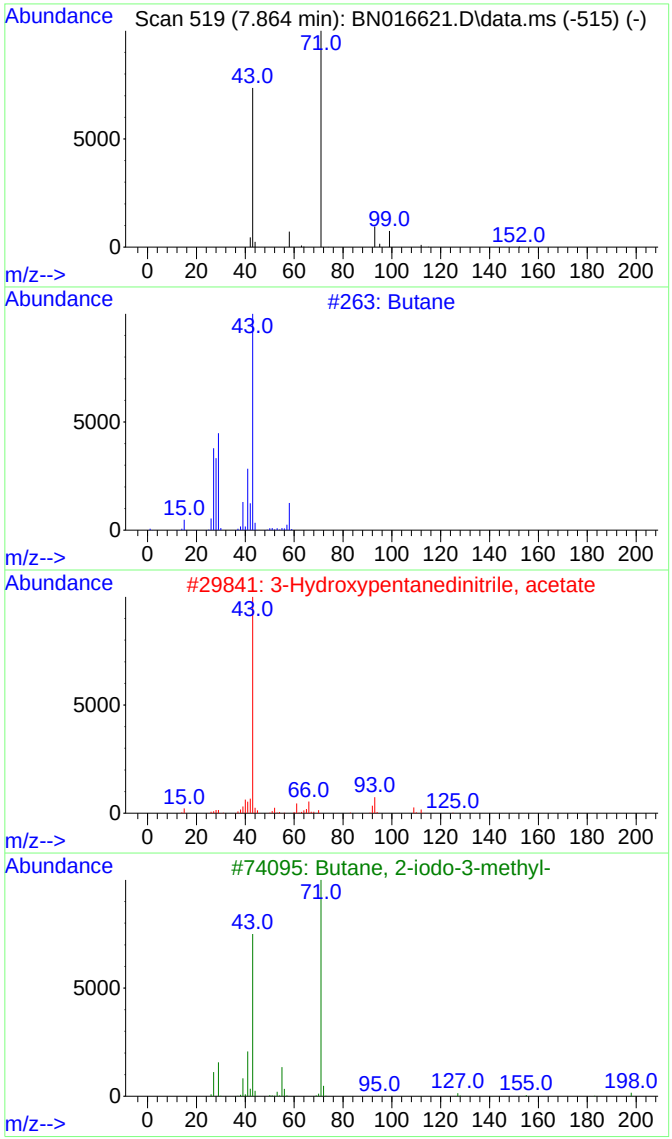
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

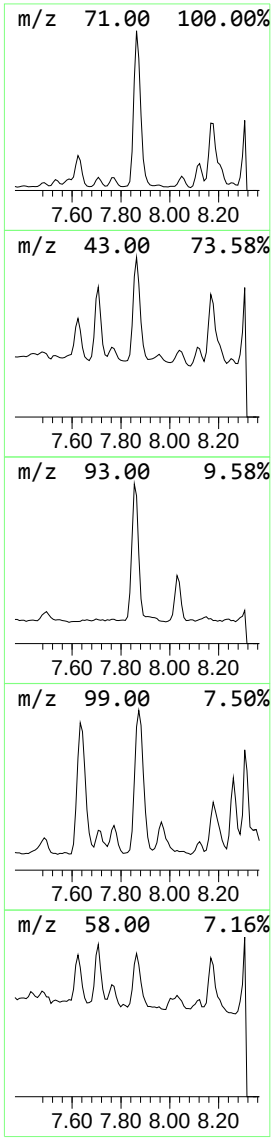
****

Peak Number 5 Butane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.864	0.11 ng	29489	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	4
2	3-Hydroxypentanedinitrile, acetate	152	C7H8N2O2	1000506-60-2	4
3	Butane, 2-iodo-3-methyl-	198	C5H11I	018295-27-7	4
4	3-Penten-2-ol	86	C5H10O	001569-50-2	4
5	Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016621.D
Acq On : 01 Oct 2021 05:24
Operator : CG/JU
Sample : M3986-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
SW-RR-01-(2.0)

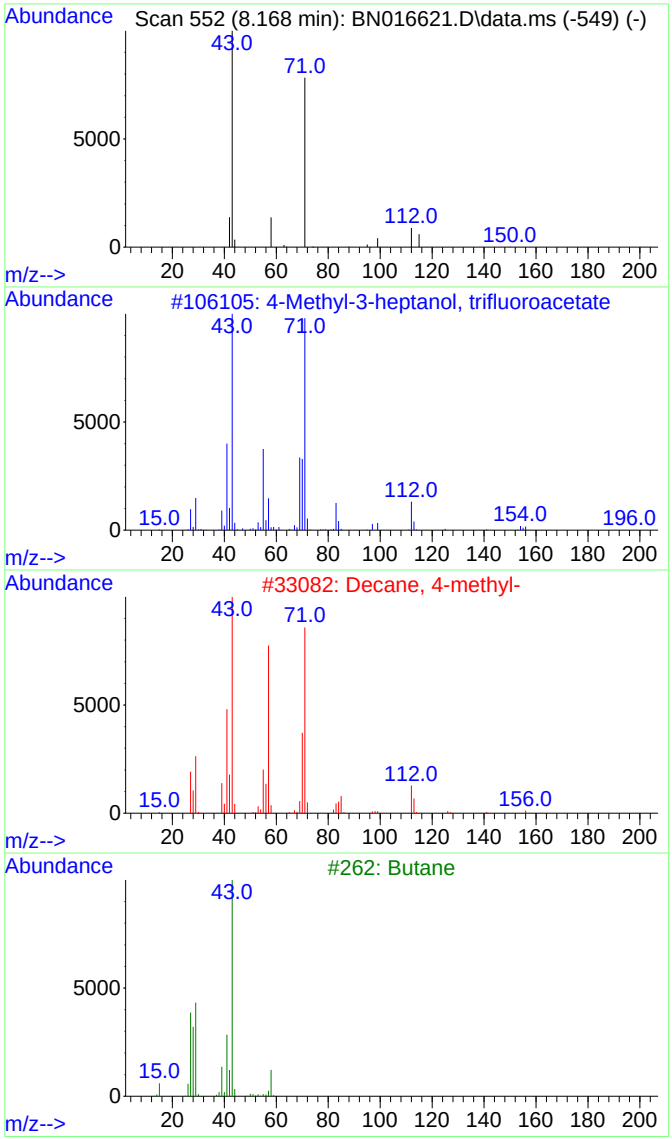
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

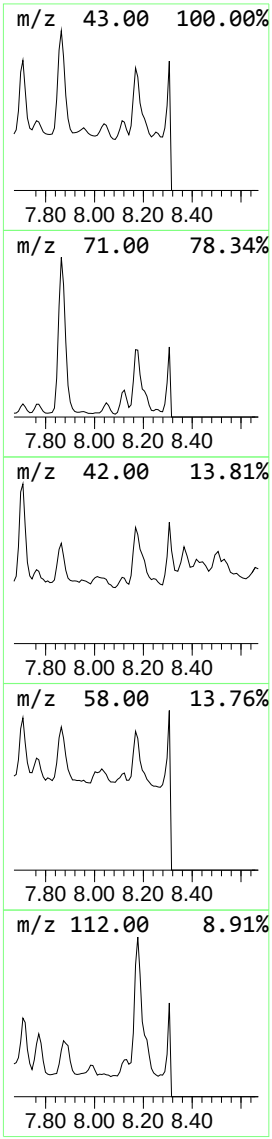
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 4-Methyl-3-heptanol, triflu... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.168	0.07 ng	17972	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methyl-3-heptanol, trifluoroac...	226	C10H17F3O2	1000365-51-8	9
2	Decane, 4-methyl-	156	C11H24	002847-72-5	9
3	Butane	58	C4H10	000106-97-8	7
4	Trifluoroacetamidine	112	C2H3F3N2	000354-37-0	7
5	1,3-Butadien-1-ol, acetate	112	C6H8O2	001515-76-0	7





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016621.D
Acq On : 01 Oct 2021 05:24
Operator : CG/JU
Sample : M3986-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
SW-RR-01-(2.0)

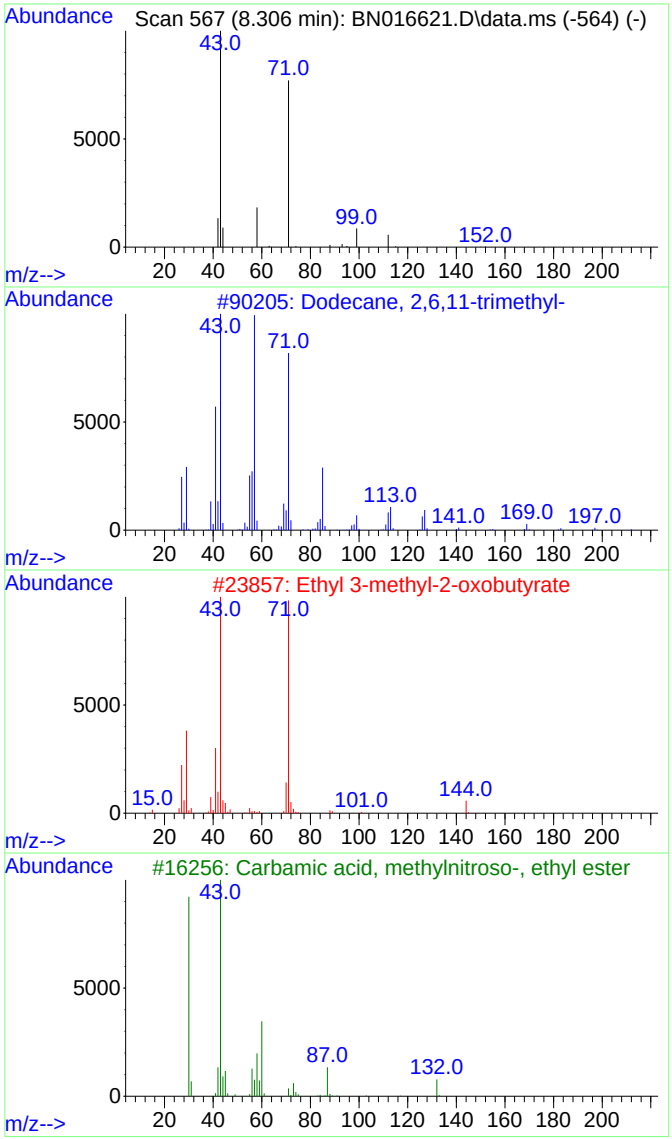
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

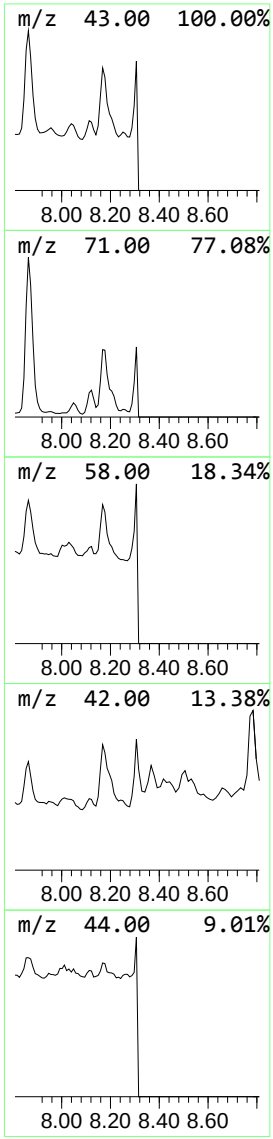
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Dodecane, 2,6,11-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.306	0.05 ng	13572	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	39
2	Ethyl 3-methyl-2-oxobutyrate	144	C7H12O3	020201-24-5	9
3	Carbamic acid, methylnitroso-, e...	132	C4H8N2O3	000615-53-2	9
4	Butane	58	C4H10	000106-97-8	5
5	Acetone	58	C3H6O	000067-64-1	5





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016621.D
Acq On : 01 Oct 2021 05:24
Operator : CG/JU
Sample : M3986-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
SW-RR-01-(2.0)

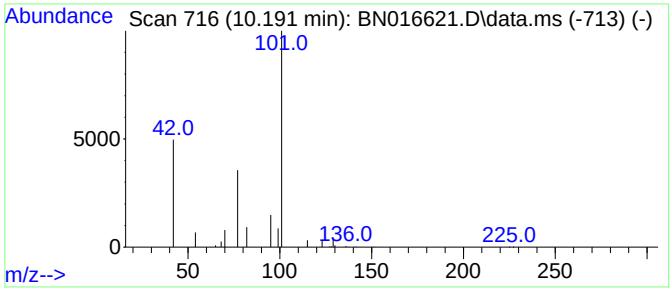
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

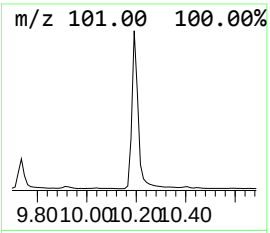
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

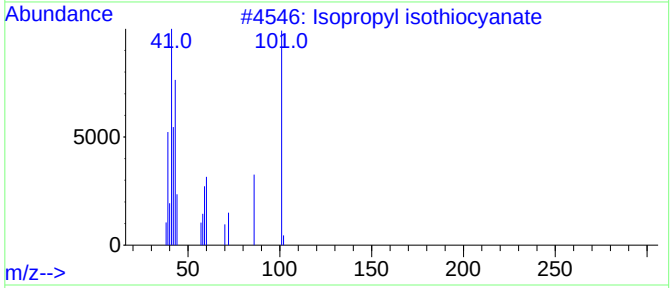
****
Peak Number 8 Isopropyl isothiocyanate Concentration Rank 6

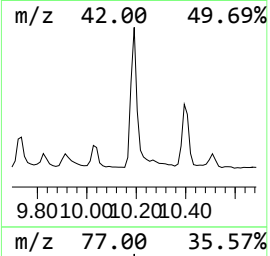
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.07 ng	29976	Naphthalene-d8	10.407

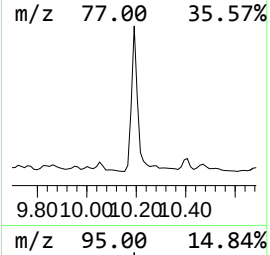
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	9
2	Succinic acid, tridec-2-yn-1-yl ...	380	C23H40O4	1000389-66-3	9
3	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
4	2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	5
5	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5

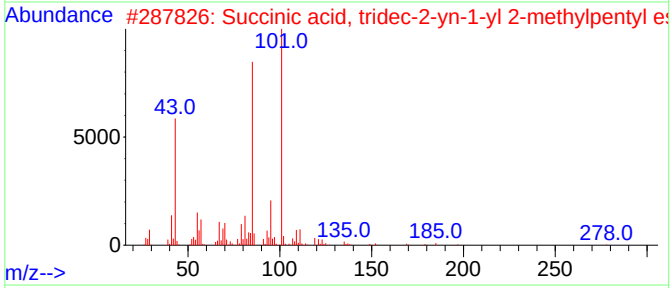


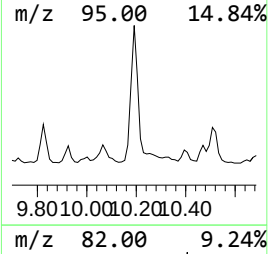


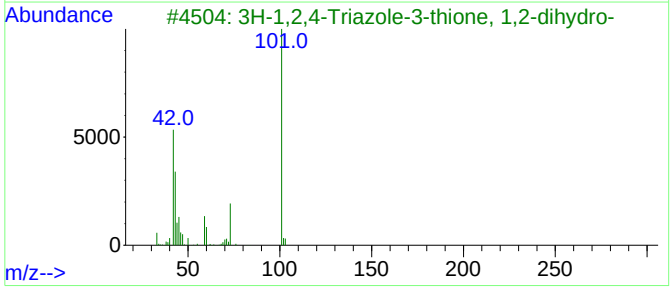


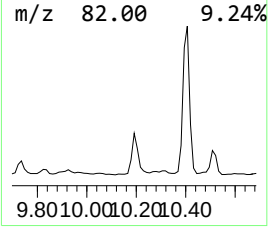












Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016621.D
Acq On : 01 Oct 2021 05:24
Operator : CG/JU
Sample : M3986-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
SW-RR-01-(2.0)

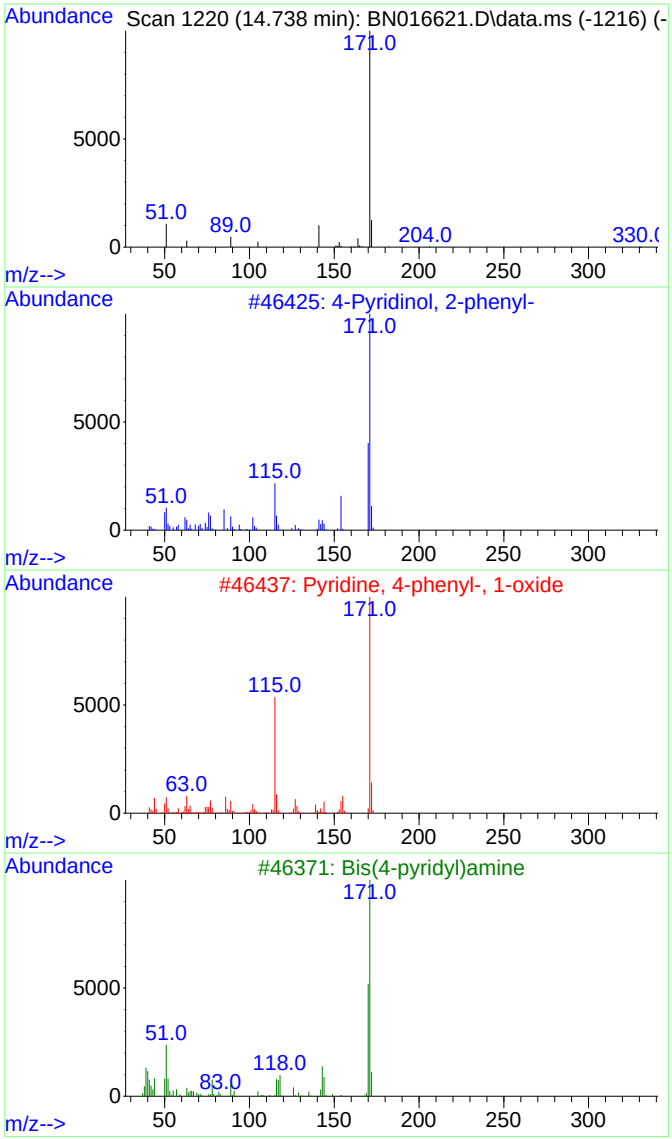
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

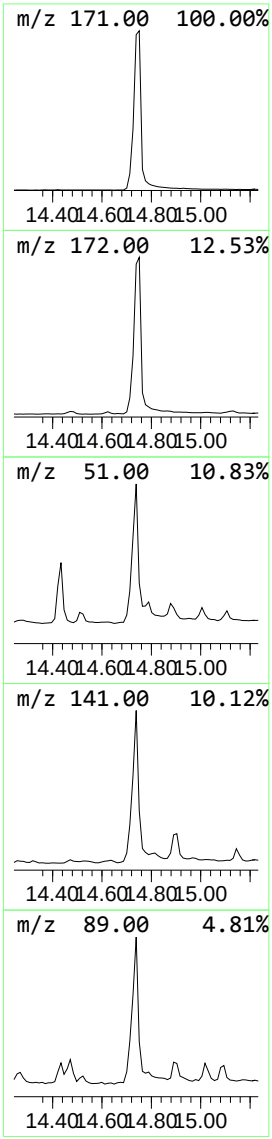
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 4-Pyridinol, 2-phenyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.738	0.16 ng	77036	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Pyridinol, 2-phenyl-	171	C11H9NO	1000253-54-5	56
2	Pyridine, 4-phenyl-, 1-oxide	171	C11H9NO	001131-61-9	9
3	Bis(4-pyridyl)amine	171	C10H9N3	001915-42-0	9
4	3,3'-Dipyridylamine	171	C10H9N3	001915-41-9	9
5	Benzonitrile, 4-(trifluoromethyl)-	171	C8H4F3N	000455-18-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016621.D
Acq On : 01 Oct 2021 05:24
Operator : CG/JU
Sample : M3986-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
SW-RR-01-(2.0)

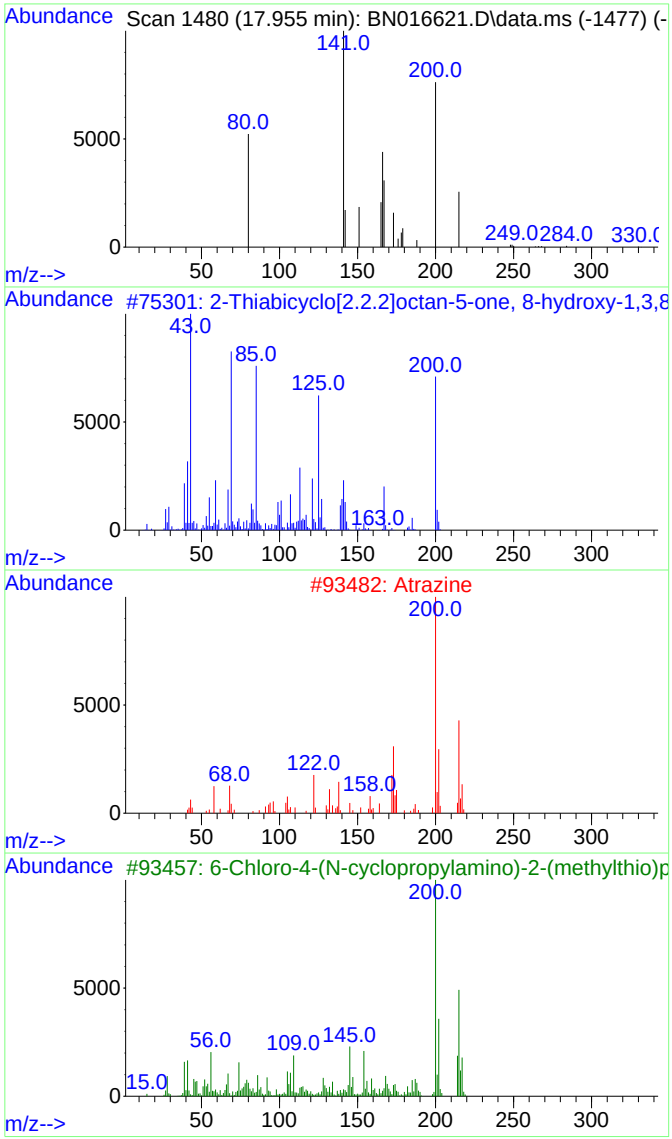
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

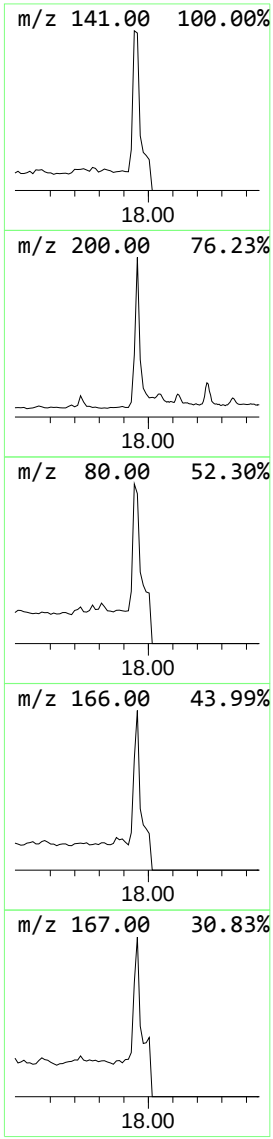
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2-Thiabicyclo[2.2.2]octan-5... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.955	0.05 ng	19345	Phenanthrene-d10	17.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Thiabicyclo[2.2.2]octan-5-one,...	200	C10H16O2S	057274-39-2	9
2	Atrazine	215	C8H14ClN5	001912-24-9	9
3	6-Chloro-4-(N-cyclopropylamino)-...	215	C8H10ClN3S	951884-05-2	9
4	2,3-Dichloro-7-methylenebicyclo[...	176	C8H10Cl2	1000210-21-0	9
5	Hydrazinecarboxamide, 2-cyclopen...	141	C6H11N3O	005459-00-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016621.D
Acq On : 01 Oct 2021 05:24
Operator : CG/JU
Sample : M3986-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
SW-RR-01-(2.0)

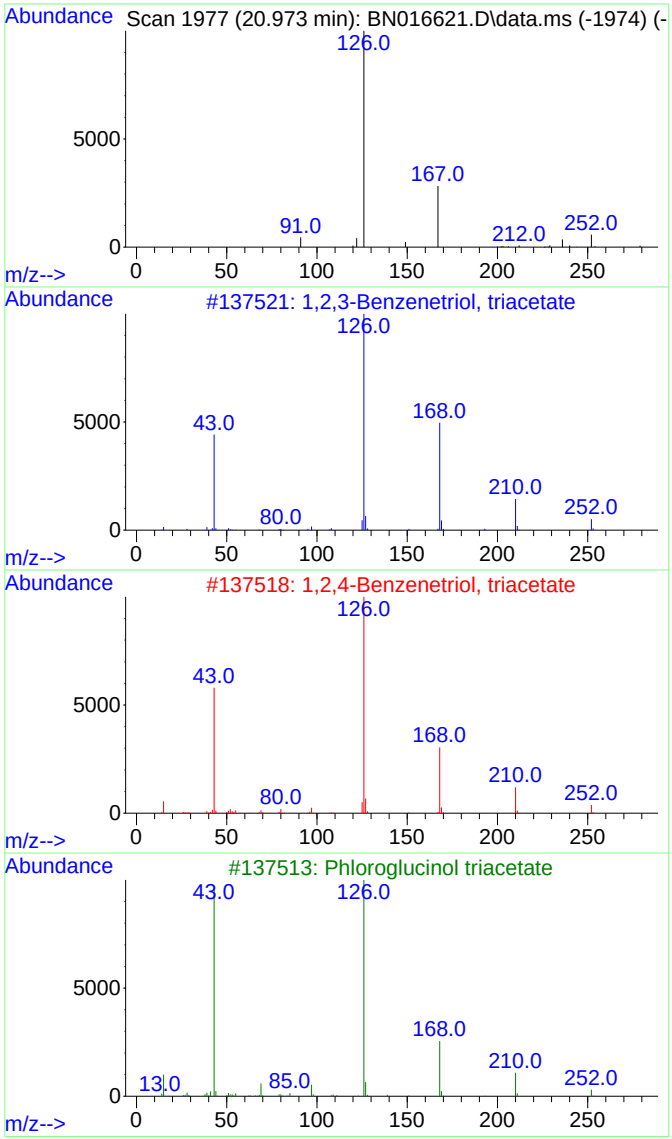
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

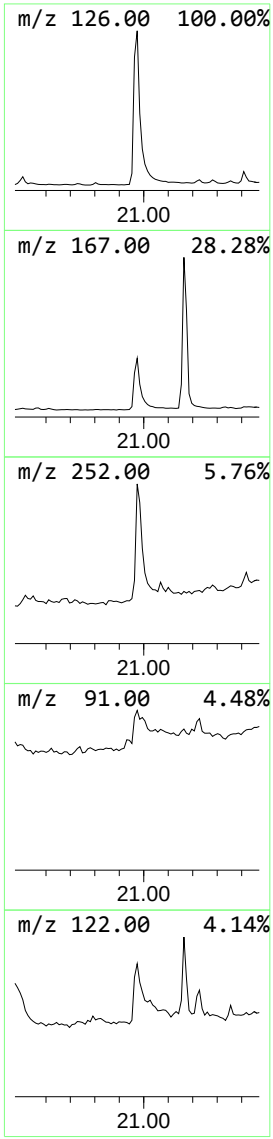
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 1,2,3-Benzenetriol, triacetate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.973	0.05 ng	25435	Chrysene-d12	21.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,3-Benzenetriol, triacetate	252	C12H12O6	000525-52-0	4
2	1,2,4-Benzenetriol, triacetate	252	C12H12O6	000613-03-6	4
3	Phloroglucinol triacetate	252	C12H12O6	002999-40-8	4
4	(6S,12aR,E)-2,2-Dimethyltetrahyd...	236	C14H24N2O	155975-43-2	4
5	Bicyclo[2.2.1]heptane-1,2-dicarb...	212	C11H16O4	1000191-44-2	4





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016621.D
Acq On : 01 Oct 2021 05:24
Operator : CG/JU
Sample : M3986-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : SW-RR-01-(2.0)

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
Acetic acid, me...	3.816	0.2	ng	46255	1	7.643	102581	0.4
Acetone	4.821	0.3	ng	84910	1	7.643	102581	0.4
Cyclopentanecar...	6.647	0.1	ng	13529	1	7.643	102581	0.4
1-Trifluoroacet...	7.264	0.1	ng	14624	1	7.643	102581	0.4
Butane	7.864	0.1	ng	29489	1	7.643	102581	0.4
4-Methyl-3-hept...	8.168	0.1	ng	17972	1	7.643	102581	0.4
Dodecane, 2,6,1...	8.306	0.1	ng	13572	1	7.643	102581	0.4
Isopropyl isoth...	10.191	0.1	ng	29976	2	10.407	178189	0.4
4-Pyridinol, 2-...	14.738	0.2	ng	77036	3	14.269	193926	0.4
2-Thiabicyclo[2...	17.955	0.0	ng	19345	4	17.018	164802	0.4
1,2,3-Benzenetr...	20.973	0.1	ng	25435	5	21.227	192473	0.4