LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016657.D
Acq On : 02 Oct 2021 05:46
Operator : CG/JU
Sample : M3829-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : RE108D1-20210917

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: BN016657.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	6	9	12	rBV	103904	126052	59.61%	5.217%
2	3.253	17	19	30	rVB	83697	211456	100.00%	8.752%
3	3.816	77	80	98	rVB	8786	34696	16.41%	1.436%
4	4.821	185	189	202	rVB	43633	96695	45.73%	4.002%
5	5.263	234	237	245	rVB	6661	16467	7.79%	0.682%
6	5.678	279	282	288	rBV	1648	4491	2.12%	0.186%
7	6.637	383	386	400	rVB2	4304	11243	5.32%	0.465%
8	6.822	403	406	418	rVB3	4465	15656	7.40%	0.648%
9	7.181	441	445	450	rVB2	3236	8736	4.13%	0.362%
10	7.264	450	454	460	rVB2	6903	15288	7.23%	0.633%
11	7.633	489	494	500	rVB2	54494	110844	52.42%	4.588%
12	7.864	515	519	526	rBV	18308	37178	17.58%	1.539%
13	8.113	543	546	549	rBV	3415	7093	3.35%	0.294%
14	8.168	549	552	562	rVV	12357	34231	16.19%	1.417%
15	8.306	563	567	569	rVB	15180	19811	9.37%	0.820%
16	8.506	580	583	591	rVB	2990	6771	3.20%	0.280%
17	8.784	601	605	610	rBV	21100	43819	20.72%	1.814%
18	10.191	713	716	726	rBV	19477	36897	17.45%	1.527%
19	10.407	729	733	739	rBV	104506	185599	87.77%	7.681%
20	12.003	920	931	943	rBV	42864	70676	33.42%	2.925%
21	12.886	1071	1074	1078	rBV	87921	147052	69.54%	6.086%
22	14.269	1180	1183	1186	rBV	132445	194540	92.00%	8.051%
23	15.766	1299	1301	1308	rVB2	9694	16195	7.66%	0.670%
24	17.018	1400	1403	1410	rBV	98050	157417	74.44%	6.515%
25	18.003	1482	1484	1496	rVB7	1569	3084	1.46%	0.128%
26	19.063	1688	1696	1727	rBV	118469	165794	78.41%	6.862%
27	19.673	1813	1819	1846	rBV	112990	148687	70.32%	6.154%
28	21.164	1992	1995	1998	rBV	23525	28226	13.35%	1.168%
29	21.227	1998	2001	2011	rVV	126207	179302	84.79%	7.421%
30	22.109	2081	2084	2088	rBV2	3131	4959	2.35%	0.205%
31	22.321	2100	2104	2108	rBV	3494	6918	3.27%	0.286%
32	22.838	2231	2238	2255	rVB	5617	8806	4.16%	0.364%
33	23.419	2399	2408	2414	rBV	8455	13900	6.57%	0.575%
34	23.481	2414	2426	2470	rVB	95888	194302	91.89%	8.042%
35	24.083	2592	2602	2622	rBV2	8711	17177	8.12%	0.711%
36	24.854	2815	2827	2846	rBV	7981	18510	8.75%	0.766%

LSC Area Percent Report

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Misc :
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Instrument : BNA_N
ClientSampleId : RE108D1-20210917

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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	25.750	3072	3089	3118	rBV	2517	7568	3.58%	0.313%
38	26.818	3383	3401	3425	rBV	1845	6353	3.00%	0.263%
39	28.078	3749	3769	3794	rBV2	972	3721	1.76%	0.154%

Sum of corrected areas: 2416210

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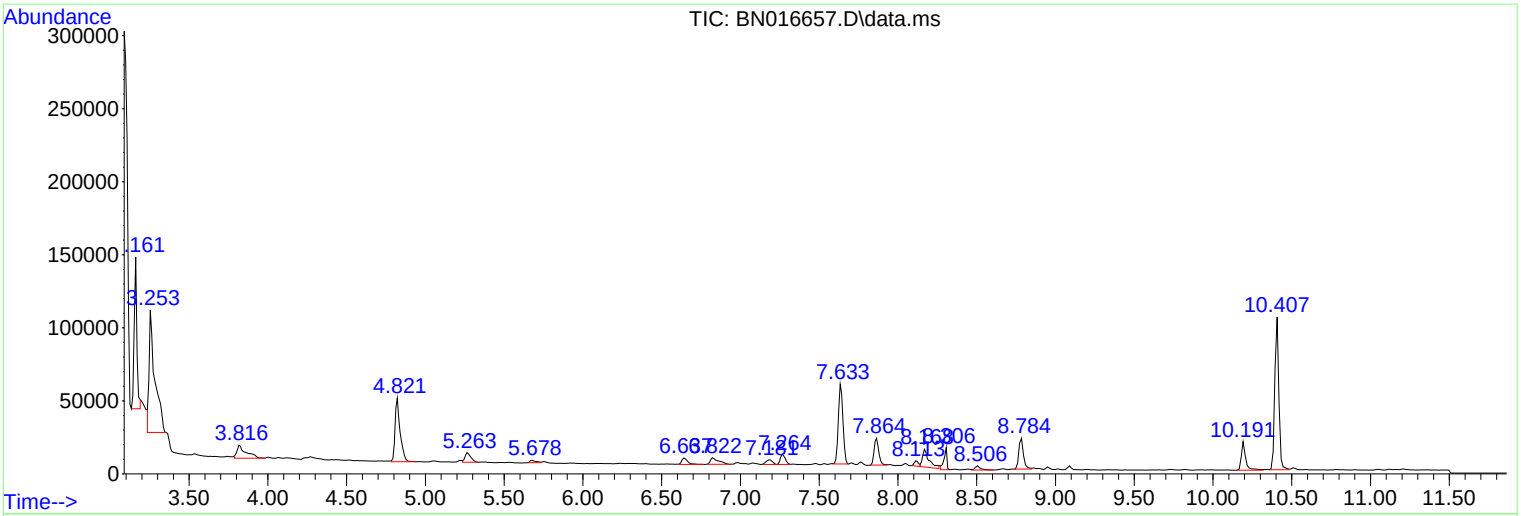
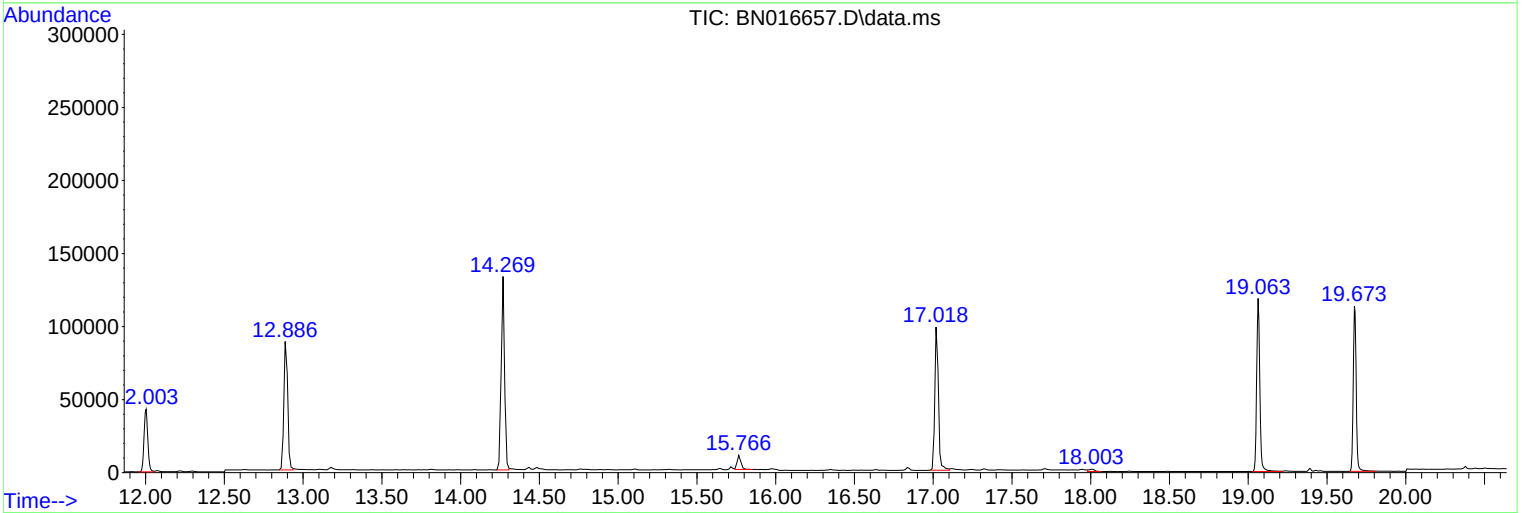
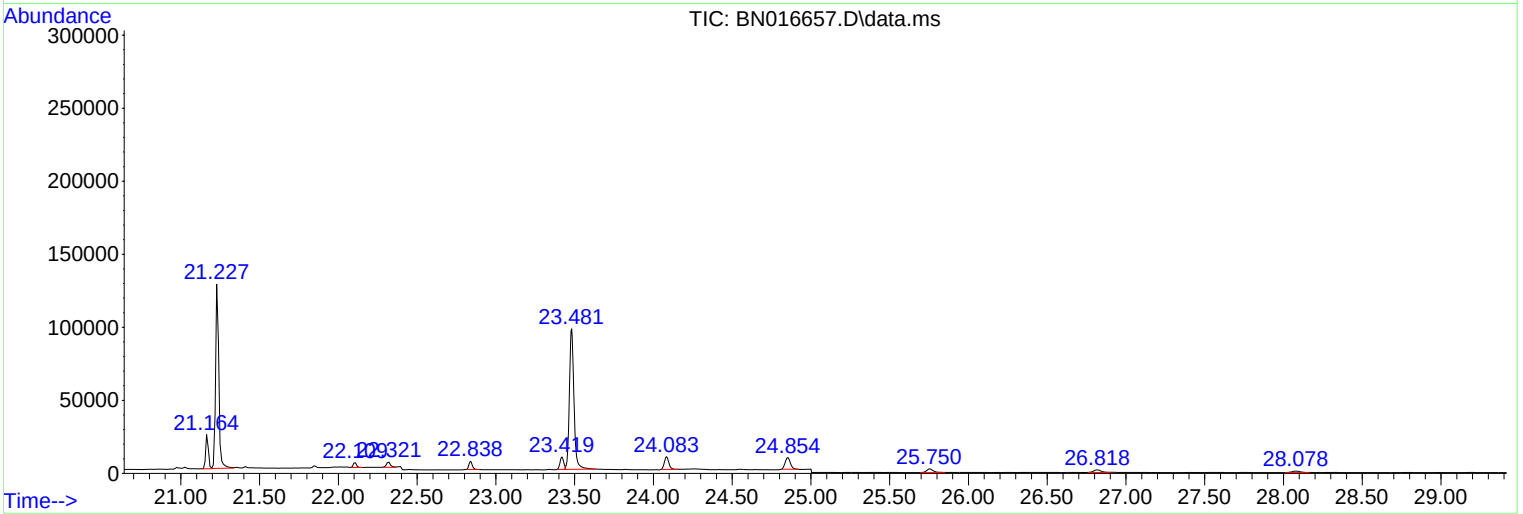
RE108D1-20210917

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

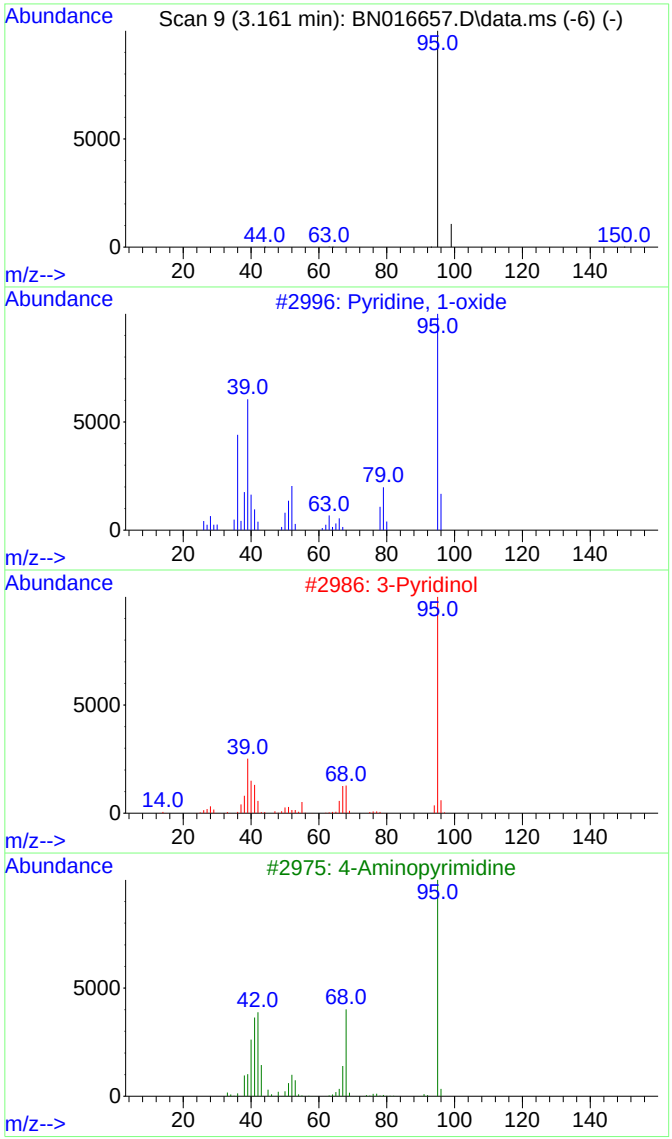
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

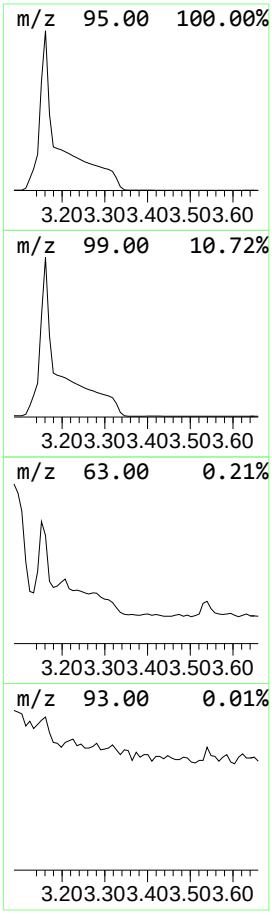
****

Peak Number 1 Pyridine, 1-oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.161	0.45 ng	126052	1,4-Dichlorobenzene-d4	7.633

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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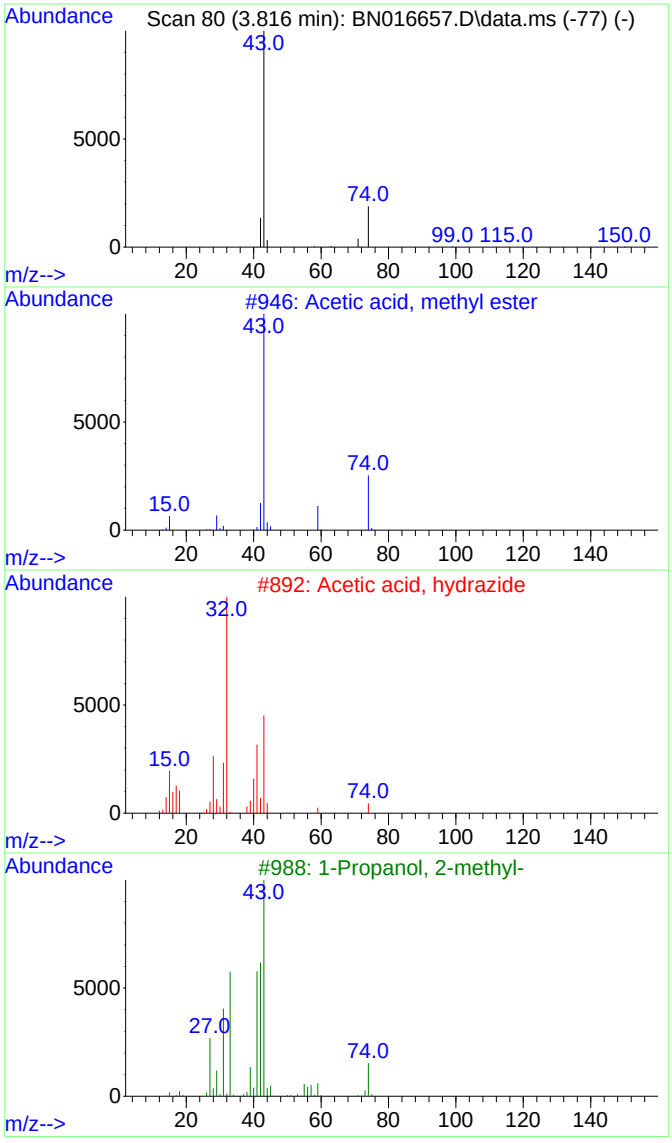
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

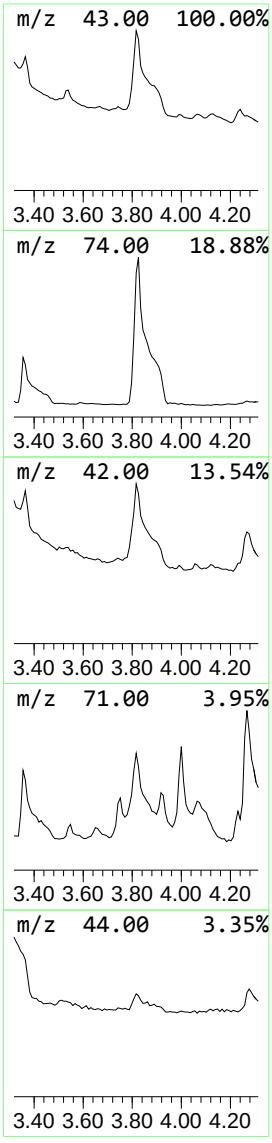
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.13 ng	34696	1,4-Dichlorobenzene-d4	7.633

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, methyl ester	74	C3H6O2	000079-20-9	9
2	Acetic acid, hydrazide	74	C2H6N2O	001068-57-1	5
3	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	4
4	Hydrogen azide	43	HN3	007782-79-8	4
5	2-Propanone, 1-hydroxy-	74	C3H6O2	000116-09-6	4





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Acq On : 02 Oct 2021 05:46
Operator : CG/JU
Sample : M3829-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

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

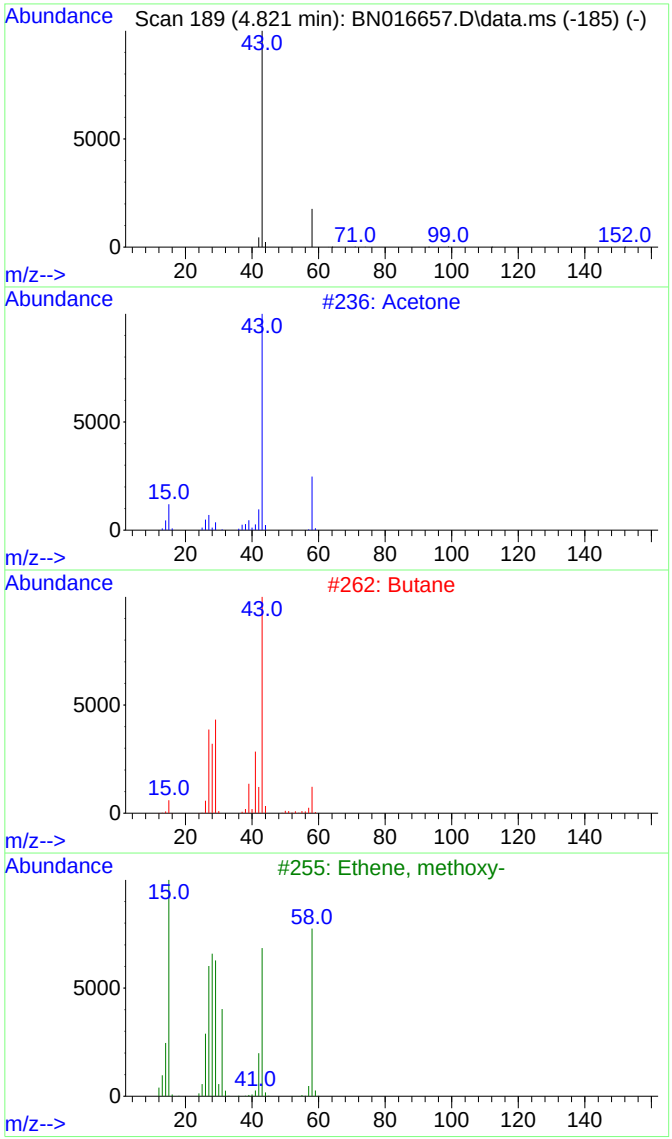
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

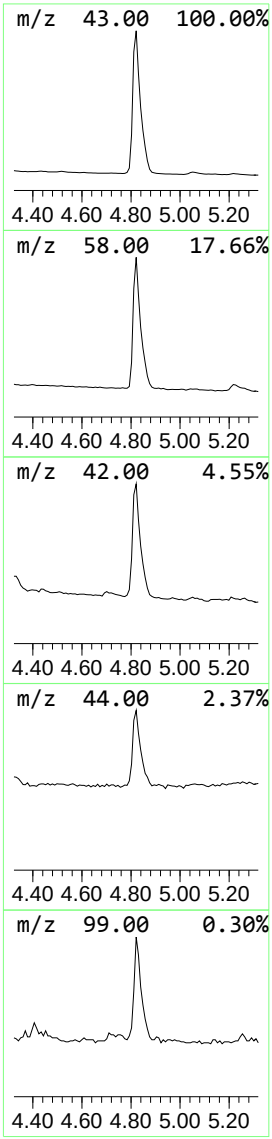
****

Peak Number 3 Acetone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.35 ng	96695	1,4-Dichlorobenzene-d4	7.633

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





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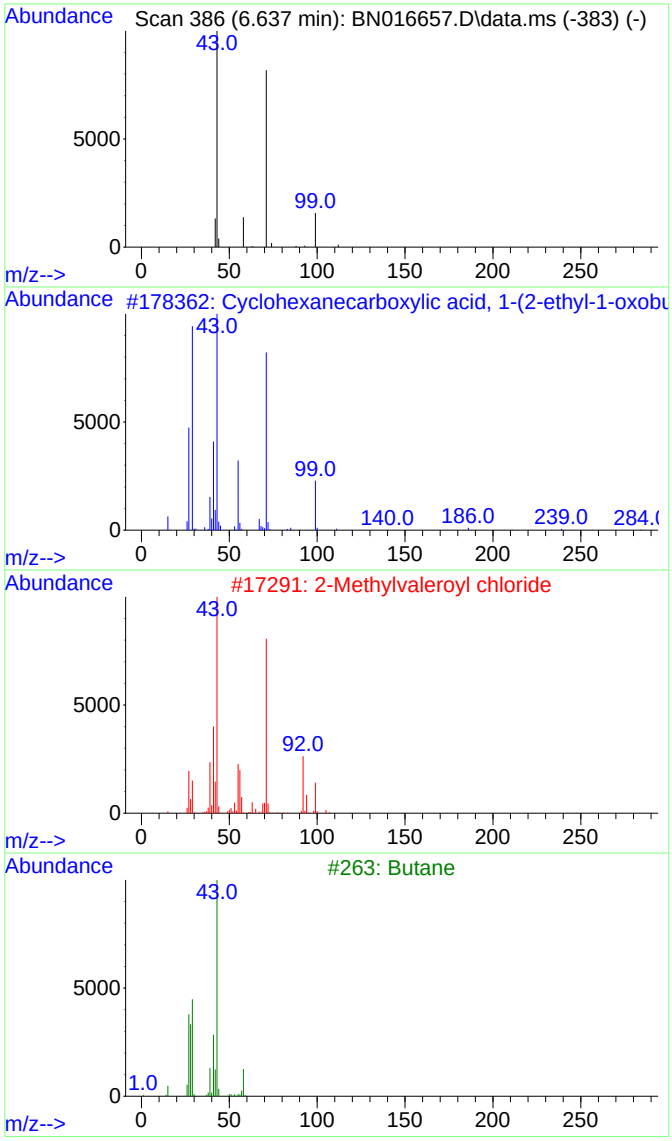
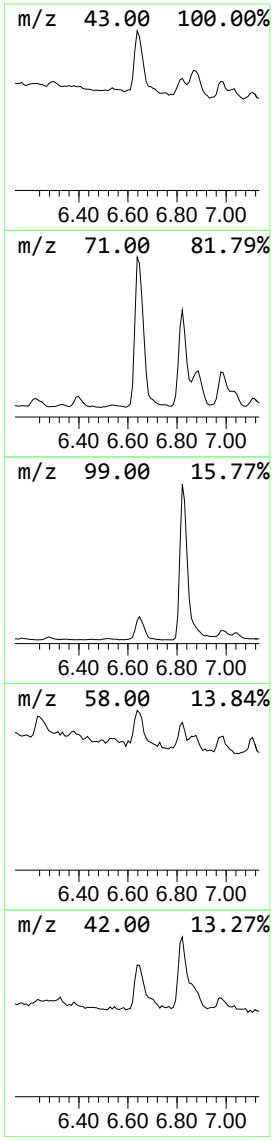
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclohexanecarboxylic acid,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.637	0.04 ng	11243	1,4-Dichlorobenzene-d4	7.633

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanecarboxylic acid, 1-(2...	284	C15H24O5	1000460-66-2	43
2	2-Methylvaleroyl chloride	134	C6H11ClO	005238-27-7	9
3	Butane	58	C4H10	000106-97-8	7
4	1H-1,2,3,4-Tetrazol-5-ylmethanamine	99	C2H5N5	031602-63-8	4
5	Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	4





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Misc :
ALS Vial : 25 Sample Multiplier: 1

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
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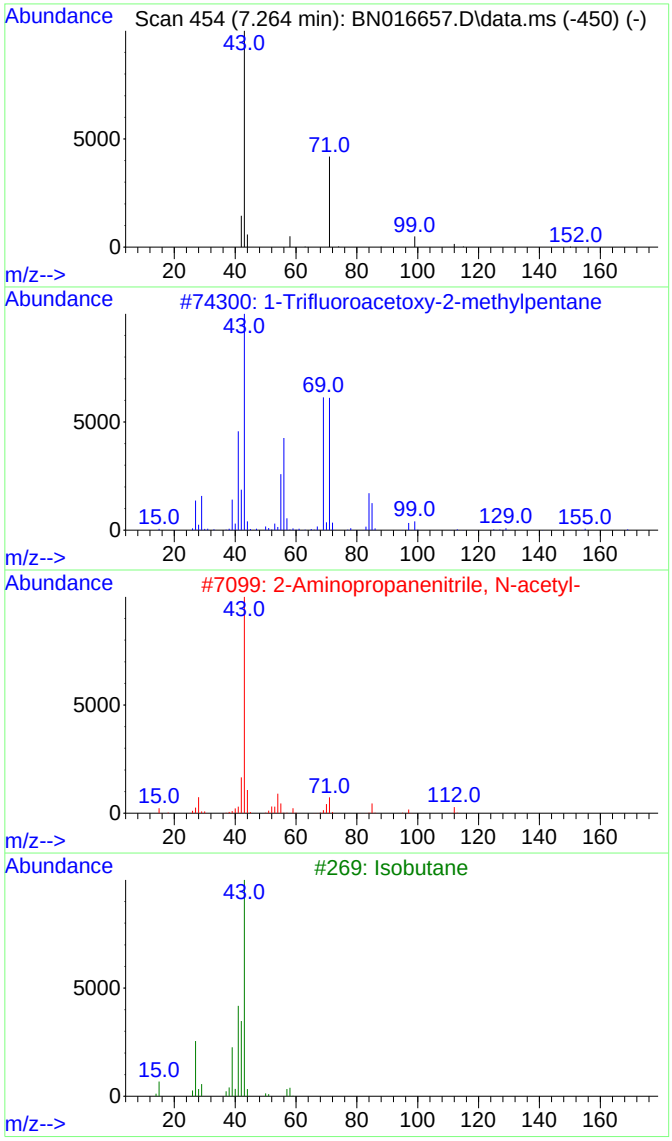
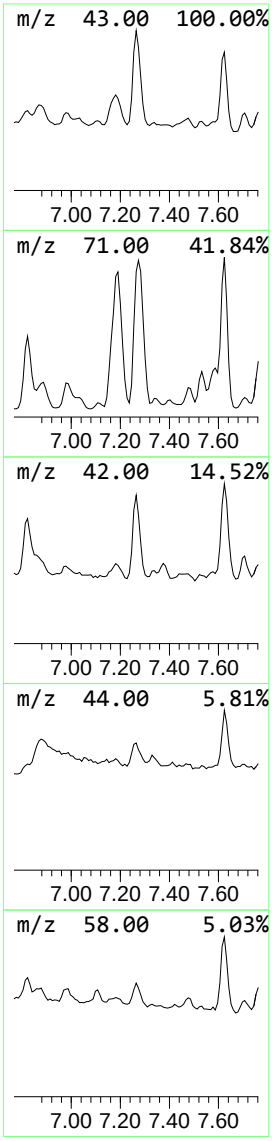
****
Peak Number 5 1-Trifluoroacetoxy-2-methyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.264	0.06 ng	15288	1,4-Dichlorobenzene-d4	7.633

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Trifluoroacetoxy-2-methylpentane	198	C8H13F3O2	155089-96-6	9
2	2-Aminopropanenitrile, N-acetyl-	112	C5H8N2O	019861-71-3	4
3	Isobutane	58	C4H10	000075-28-5	4
4	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	4
5	Hydrogen azide	43	HN3	007782-79-8	4





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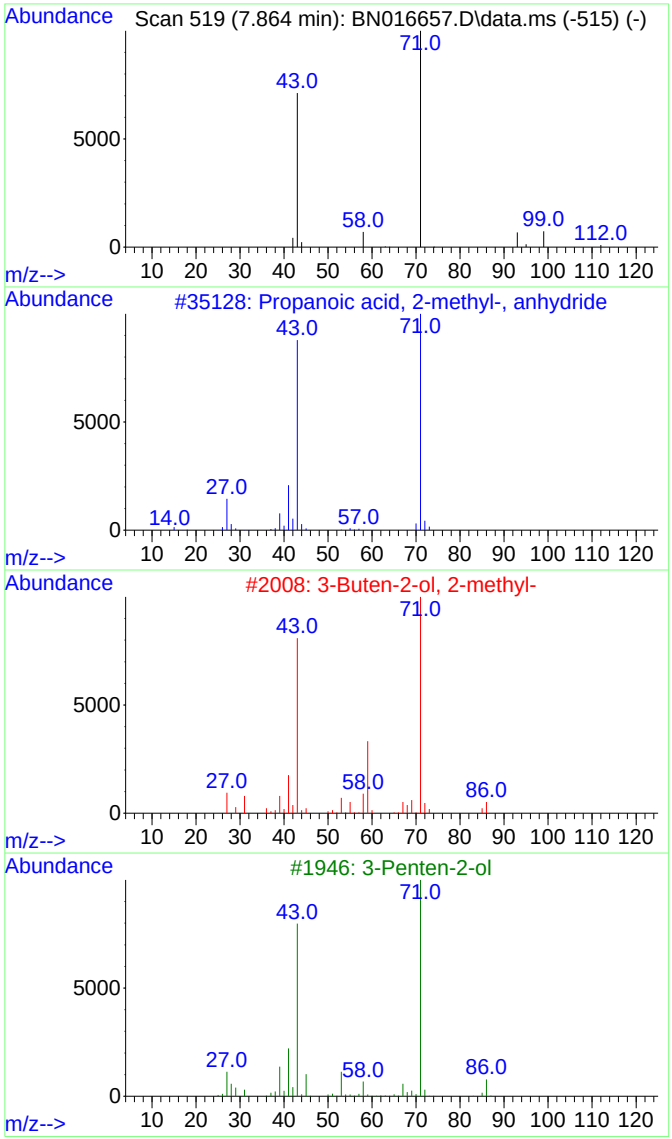
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

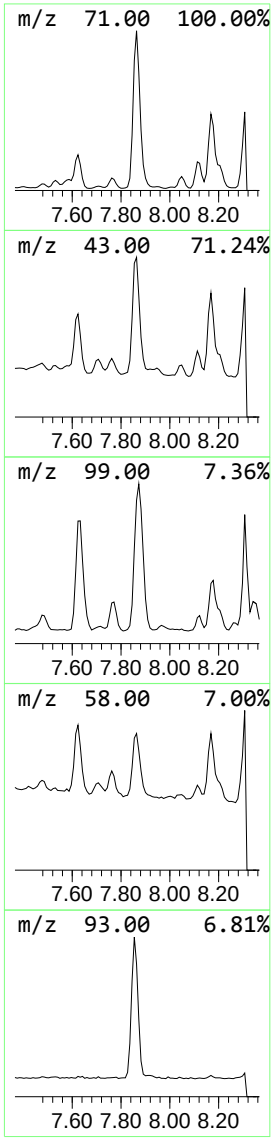
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Propanoic acid, 2-methyl-, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.864	0.13 ng	37178	1,4-Dichlorobenzene-d4	7.633

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	4
2	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	4
3	3-Penten-2-ol	86	C5H10O	001569-50-2	4
4	Butane, 2-iodo-3-methyl-	198	C5H11I	018295-27-7	4
5	3-Hydroxypentanedinitrile, acetate	152	C7H8N2O2	1000506-60-2	4





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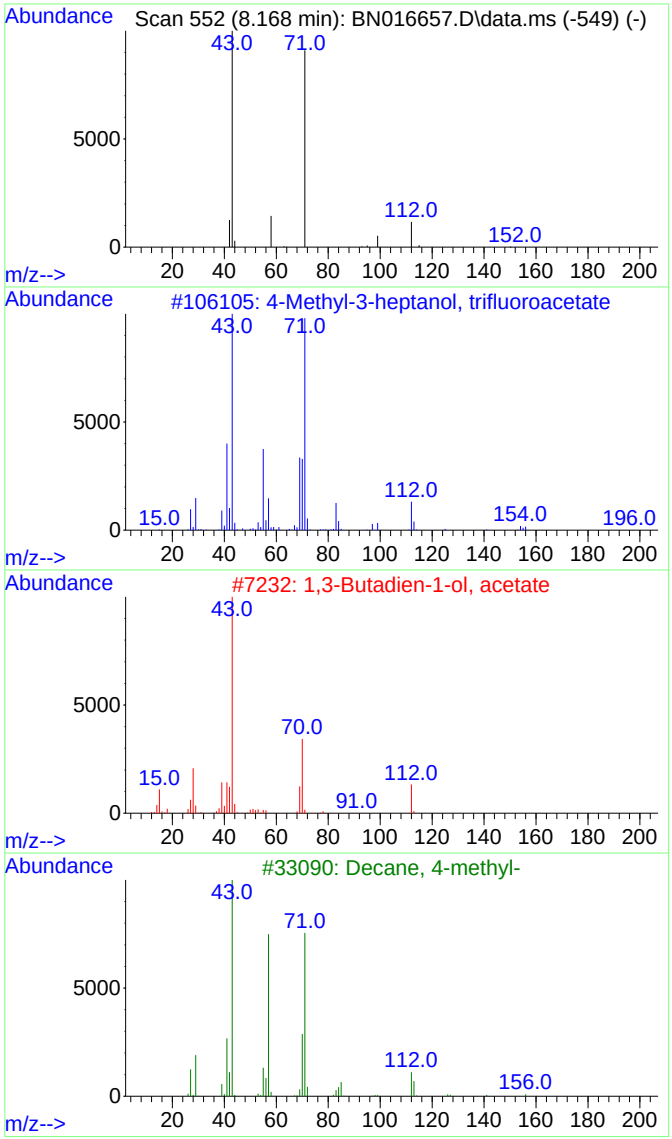
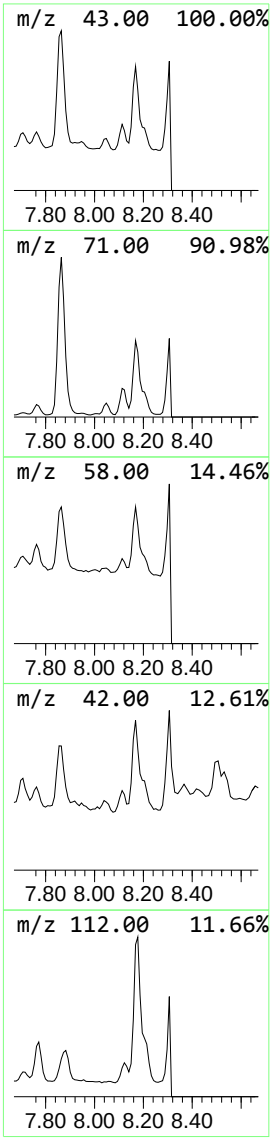
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 4-Methyl-3-heptanol, triflu... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.168	0.12 ng	34231	1,4-Dichlorobenzene-d4	7.633

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methyl-3-heptanol, trifluoroac...	226	C10H17F3O2	1000365-51-8	40
2	1,3-Butadien-1-ol, acetate	112	C6H8O2	001515-76-0	9
3	Decane, 4-methyl-	156	C11H24	002847-72-5	9
4	Heptane, 5-ethyl-2-methyl-	142	C10H22	013475-78-0	9
5	Octane, 3-ethyl-	142	C10H22	005881-17-4	9





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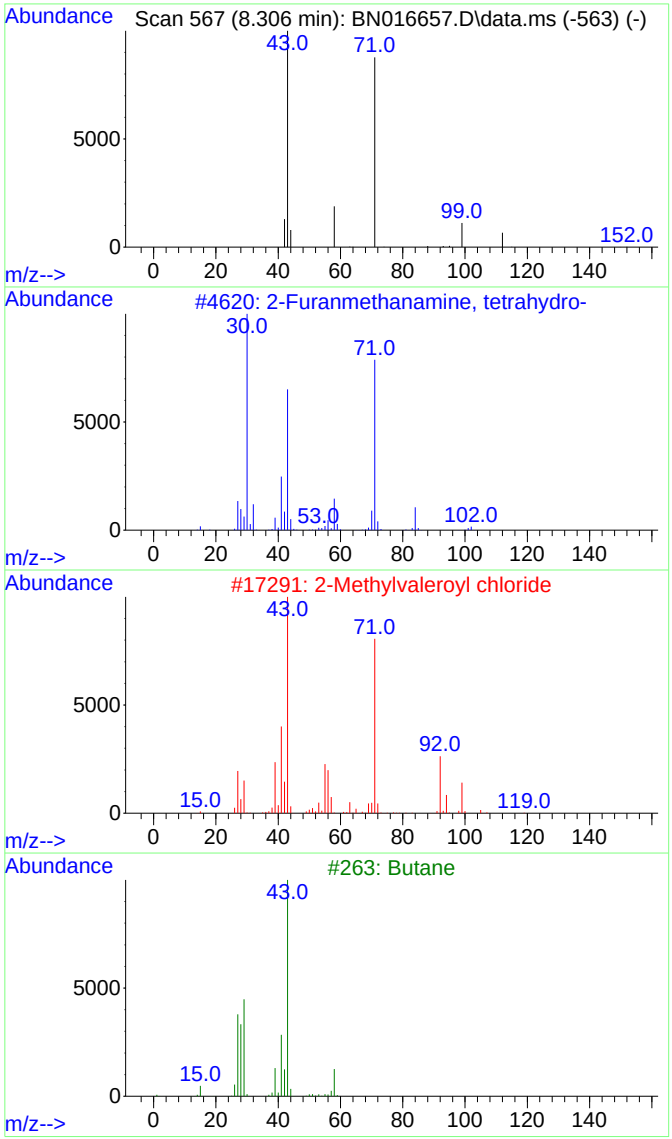
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

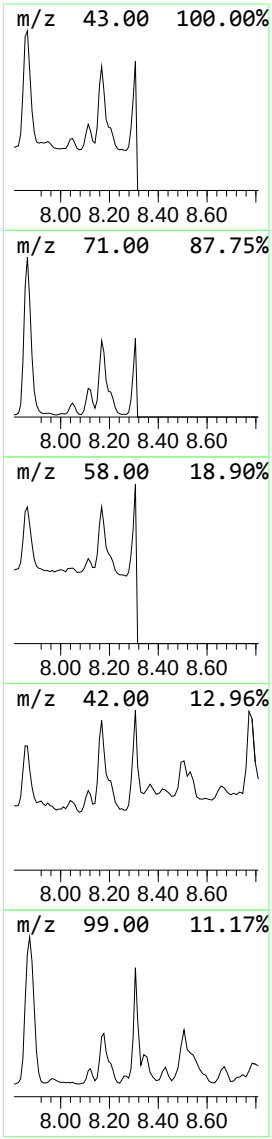
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2-Furanmethanamine, tetrahy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.306	0.07 ng	19811	1,4-Dichlorobenzene-d4	7.633

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Furanmethanamine, tetrahydro-	101	C5H11NO	004795-29-3	9
2	2-Methylvaleroyl chloride	134	C6H11ClO	005238-27-7	9
3	Butane	58	C4H10	000106-97-8	5
4	Acetone	58	C3H6O	000067-64-1	5
5	1H-1,2,3,4-Tetrazol-5-ylmethanamine	99	C2H5N5	031602-63-8	4





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Instrument :
BNA_N
ClientSampleId :
RE108D1-20210917

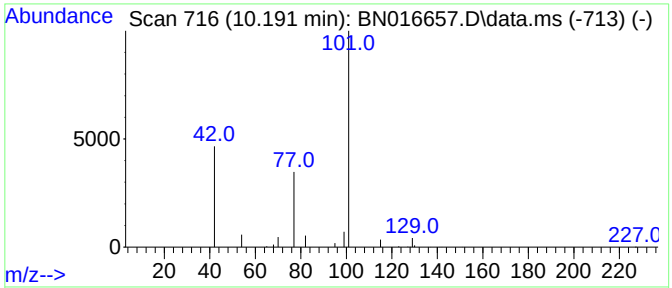
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

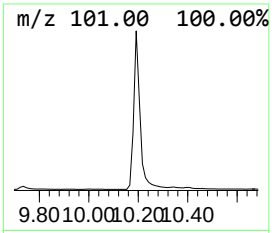
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

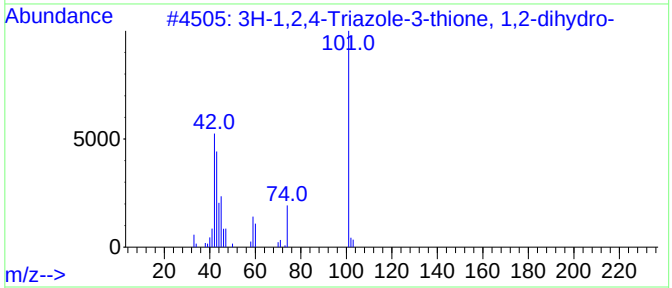
****
Peak Number 9 3H-1,2,4-Triazole-3-thione,... Concentration Rank 6

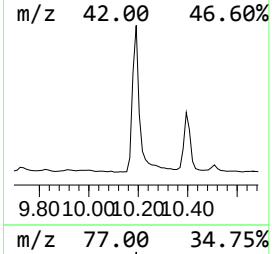
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.08 ng	36897	Naphthalene-d8	10.407

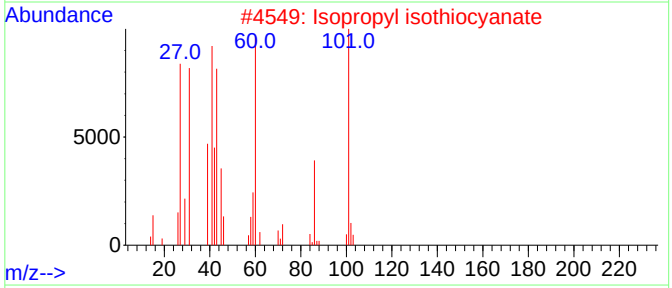
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
2	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	5
3	2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	5
4	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5
5	3-Aminopropionitrile	70	C3H6N2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

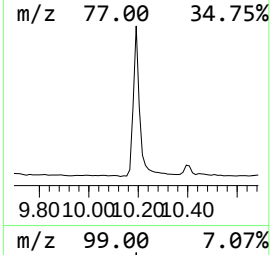


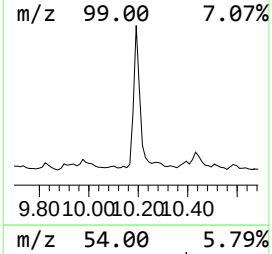


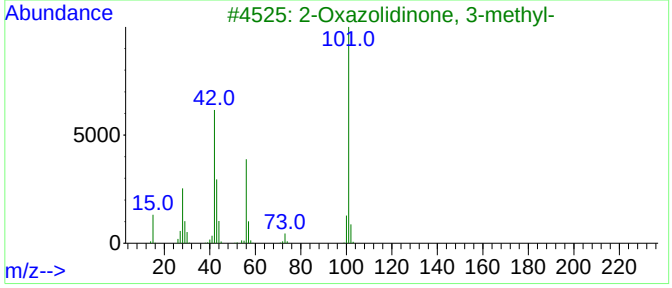


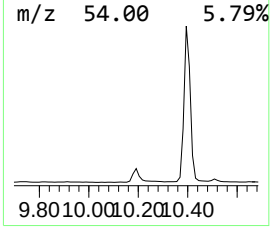












Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016657.D
Acq On : 02 Oct 2021 05:46
Operator : CG/JU
Sample : M3829-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE108D1-20210917

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
Pyridine, 1-oxide	3.161	0.5	ng	126052	1	7.633	110844	0.4
Acetic acid, me...	3.816	0.1	ng	34696	1	7.633	110844	0.4
Acetone	4.821	0.3	ng	96695	1	7.633	110844	0.4
Cyclohexanecarb...	6.637	0.0	ng	11243	1	7.633	110844	0.4
1-Trifluoroacet...	7.264	0.1	ng	15288	1	7.633	110844	0.4
Propanoic acid,...	7.864	0.1	ng	37178	1	7.633	110844	0.4
4-Methyl-3-hept...	8.168	0.1	ng	34231	1	7.633	110844	0.4
2-Furanmethanam...	8.306	0.1	ng	19811	1	7.633	110844	0.4
3H-1,2,4-Triazo...	10.191	0.1	ng	36897	2	10.407	185599	0.4