LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016678.D
Acq On : 02 Oct 2021 19:33
Operator : CG/JU
Sample : M3829-21
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : MW202D-20210918

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: BN016678.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	rVB	53540	66571	15.48%	1.995%
2	3.816	76	80	86	rBV	10016	31132	7.24%	0.933%
3	3.908	86	90	105	rVB	122165	430114	100.00%	12.887%
4	4.821	185	189	204	rVB	33540	79995	18.60%	2.397%
5	5.273	234	238	245	rVB	7019	18611	4.33%	0.558%
6	5.678	279	282	298	rVB	2465	9615	2.24%	0.288%
7	6.647	383	387	392	rBV	3268	7889	1.83%	0.236%
8	6.822	403	406	419	rVB	5400	14913	3.47%	0.447%
9	7.264	450	454	460	rBV2	8283	18786	4.37%	0.563%
10	7.633	490	494	500	rVB	49174	103229	24.00%	3.093%
11	7.864	515	519	525	rBV	9104	19032	4.42%	0.570%
12	8.168	549	552	560	rVV	5413	16708	3.88%	0.501%
13	8.306	564	567	569	rVB2	9213	11521	2.68%	0.345%
14	8.784	601	605	610	rBV	22513	45020	10.47%	1.349%
15	9.583	665	668	671	rBV	4472	8210	1.91%	0.246%
16	10.191	713	716	729	rBV	124929	218533	50.81%	6.548%
17	10.407	729	733	736	rBV	106165	183536	42.67%	5.499%
18	12.003	920	931	941	rBV	44372	70599	16.41%	2.115%
19	12.886	1071	1074	1078	rBV	88162	149400	34.73%	4.476%
20	13.178	1094	1097	1100	rBV	199343	300052	69.76%	8.990%
21	13.812	1144	1147	1154	rBV	8152	16324	3.80%	0.489%
22	14.269	1180	1183	1186	rBV	138806	196195	45.61%	5.878%
23	14.459	1193	1198	1201	rBV2	6602	17494	4.07%	0.524%
24	14.675	1213	1215	1220	rBV2	4723	8532	1.98%	0.256%
25	15.246	1257	1260	1262	rBV	3471	6574	1.53%	0.197%
26	15.715	1294	1297	1299	rBV	9632	14129	3.28%	0.423%
27	15.766	1299	1301	1305	rVB2	12800	20185	4.69%	0.605%
28	15.969	1314	1317	1322	rVB2	2462	7018	1.63%	0.210%
29	17.018	1400	1403	1409	rBV	105739	167059	38.84%	5.005%
30	17.723	1457	1461	1467	rBV2	3242	6509	1.51%	0.195%
31	17.955	1477	1480	1483	rBV	8076	13057	3.04%	0.391%
32	18.909	1660	1665	1670	rVB	9674	10201	2.37%	0.306%
33	19.063	1687	1696	1710	rBV2	140570	211730	49.23%	6.344%
34	19.247	1728	1733	1747	rBV	9655	14995	3.49%	0.449%
35	19.678	1813	1820	1831	rBV	132747	164332	38.21%	4.924%
36	20.006	1885	1886	1888	rBV	4070	6131	1.43%	0.184%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016678.D
Acq On : 02 Oct 2021 19:33
Operator : CG/JU
Sample : M3829-21
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : MW202D-20210918

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	20.080	1890	1893	1897	rVV	11030	22651	5.27%	0.679%
38	20.155	1897	1900	1903	rVV	9124	16369	3.81%	0.490%
39	20.261	1907	1910	1912	rVV	5450	8251	1.92%	0.247%
40	20.314	1912	1915	1919	rVV2	7675	15939	3.71%	0.478%
41	20.378	1919	1921	1925	rBV	12085	19344	4.50%	0.580%
42	20.941	1971	1974	1976	rBV	4649	5660	1.32%	0.170%
43	21.026	1976	1982	1985	rBV2	3948	11225	2.61%	0.336%
44	21.164	1993	1995	1998	rBV	34137	46988	10.92%	1.408%
45	21.227	1998	2001	2009	rVV	129812	202697	47.13%	6.073%
46	21.334	2009	2011	2016	rVB	10549	16263	3.78%	0.487%
47	22.109	2081	2084	2089	rVB	5617	8002	1.86%	0.240%
48	22.321	2101	2104	2108	rBV2	4195	8123	1.89%	0.243%
49	22.841	2232	2239	2257	rVB	5356	8524	1.98%	0.255%
50	23.423	2400	2409	2415	rBV	7608	12353	2.87%	0.370%
51	23.484	2415	2427	2471	rVB	102896	206944	48.11%	6.200%
52	24.083	2593	2602	2622	rBV	7379	14829	3.45%	0.444%
53	24.854	2816	2827	2854	rBV2	7128	17140	3.98%	0.514%
54	25.761	3076	3092	3116	rBV2	2226	6847	1.59%	0.205%
55	26.822	3385	3402	3422	rBV	1607	5518	1.28%	0.165%

Sum of corrected areas: 3337598

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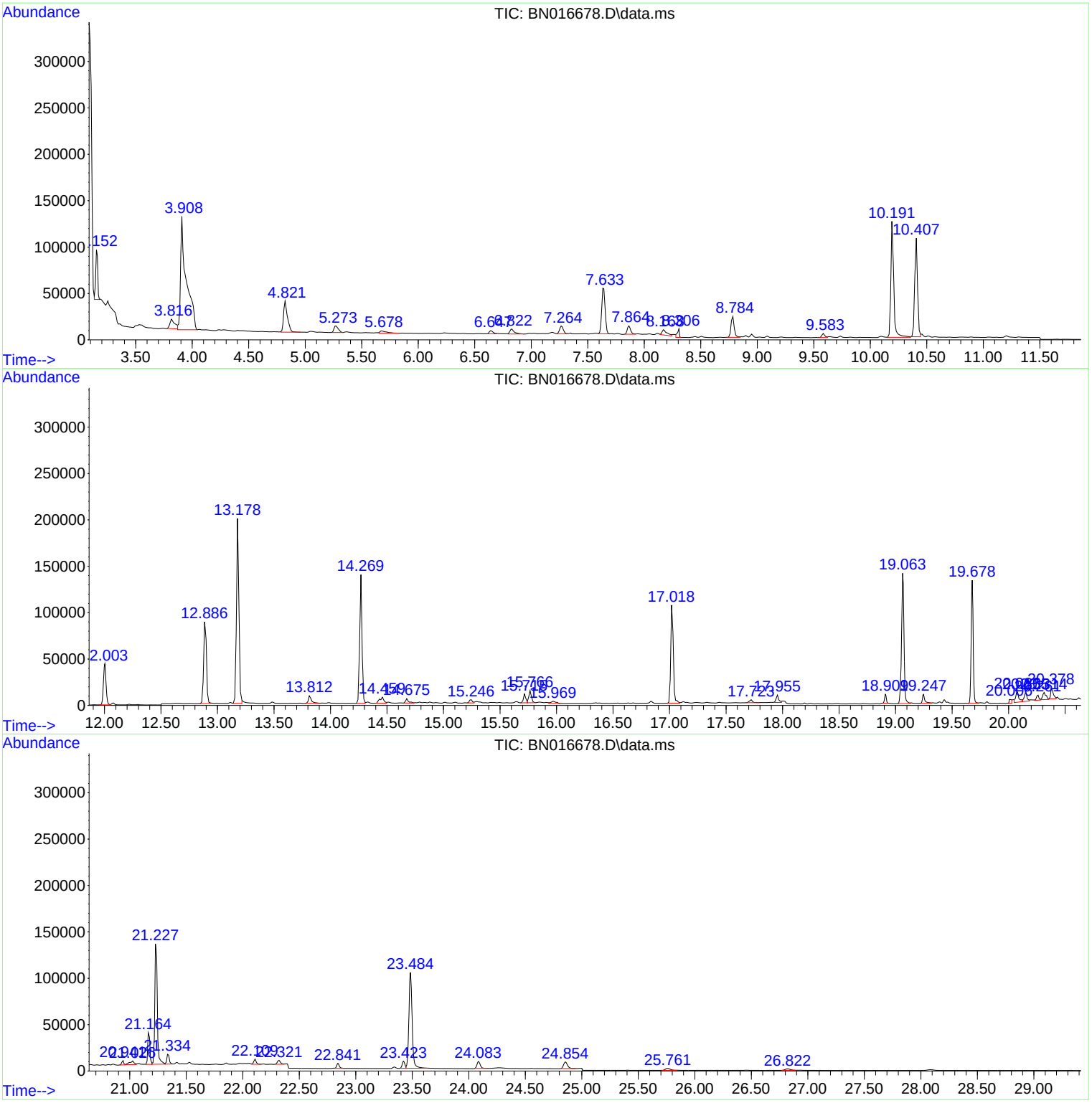
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW202D-20210918

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 : BN016678.D
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Operator : CG/JU
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Misc :
ALS Vial : 46 Sample Multiplier: 1

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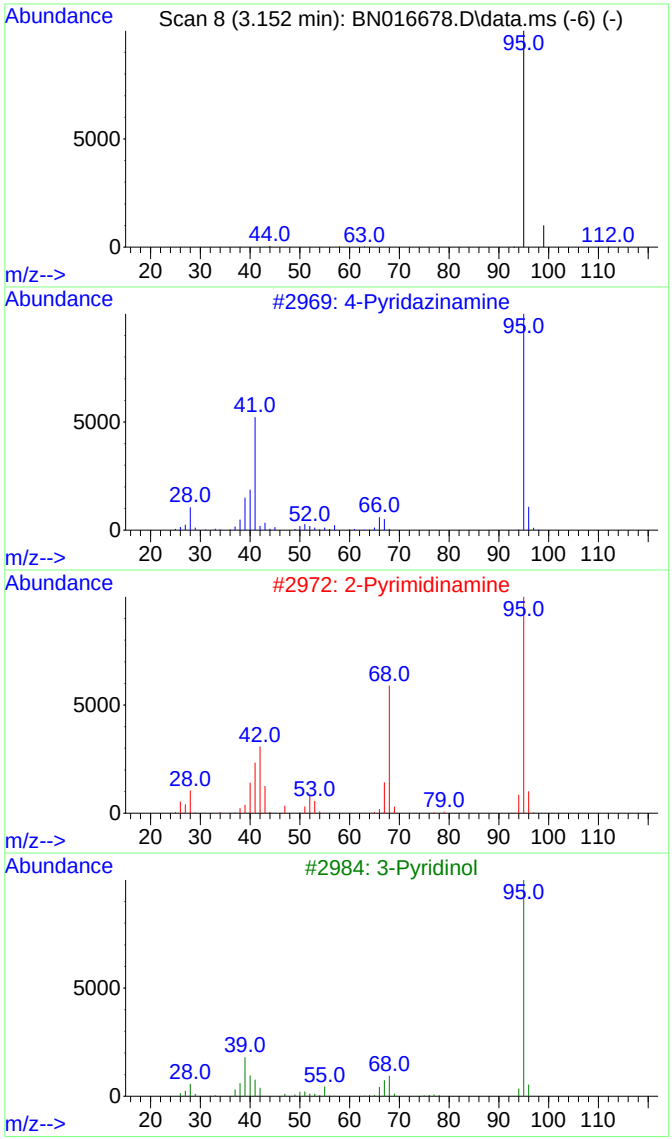
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

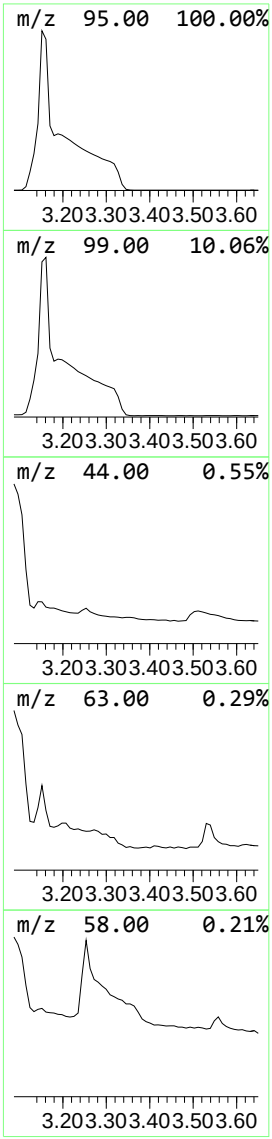
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 4-Pyridazinamine Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.152	0.26 ng	66571	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	3-Pyridinol	95	C5H5NO	000109-00-2	2
4	Pyridine, 1-oxide	95	C5H5NO	000694-59-7	2
5	2(1H)-Pyridinone	95	C5H5NO	000142-08-5	2





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Data File : BN016678.D
Acq On : 02 Oct 2021 19:33
Operator : CG/JU
Sample : M3829-21
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW202D-20210918

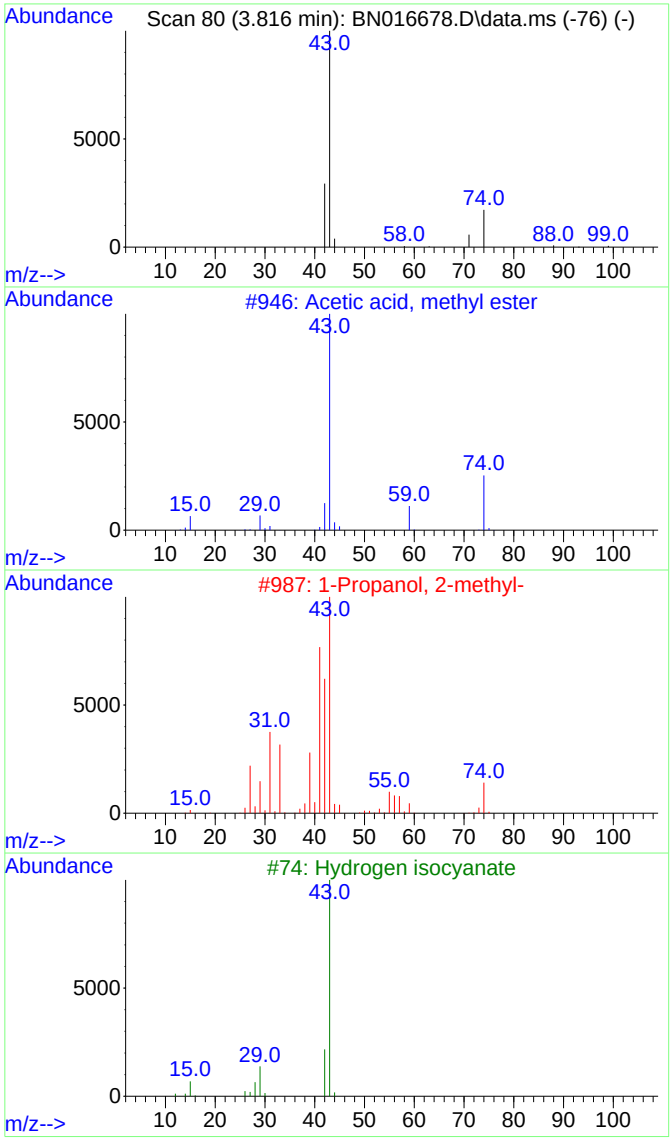
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

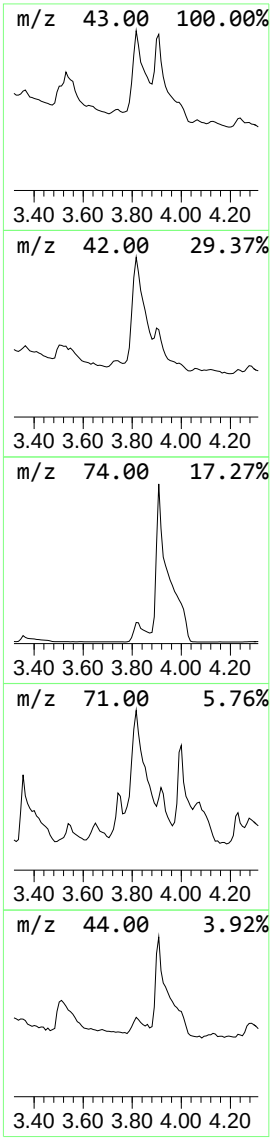
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Acetic acid, methyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.12 ng	31132	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	(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	3
5	Acetic acid, hydrazide	74	C2H6N2O	001068-57-1	3





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Operator : CG/JU
Sample : M3829-21
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW202D-20210918

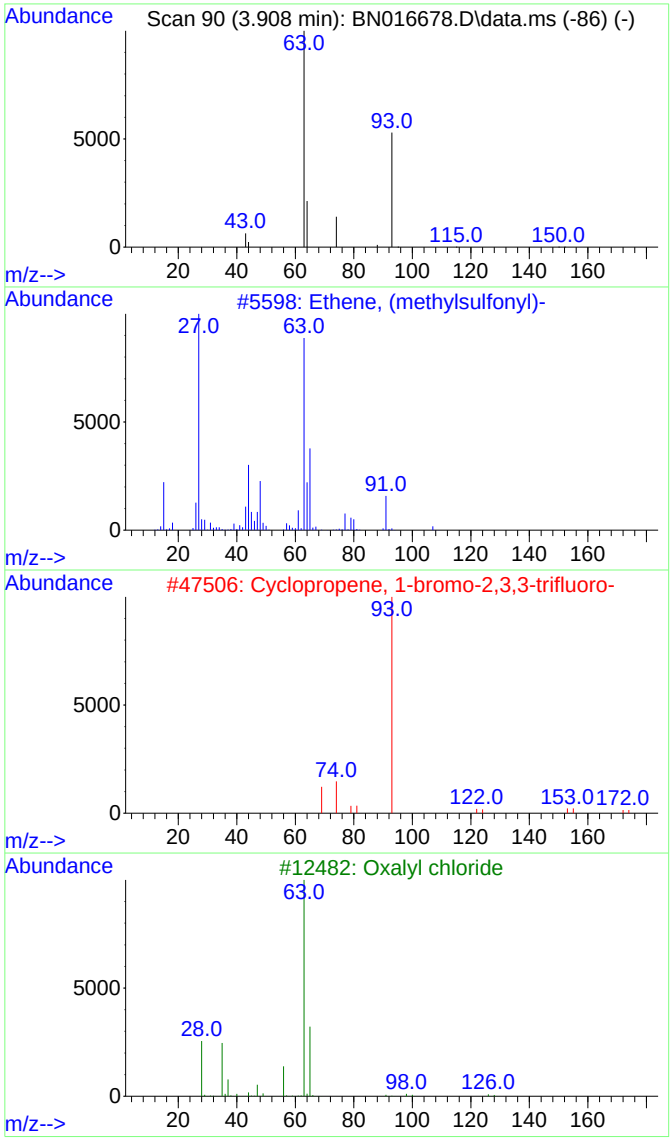
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

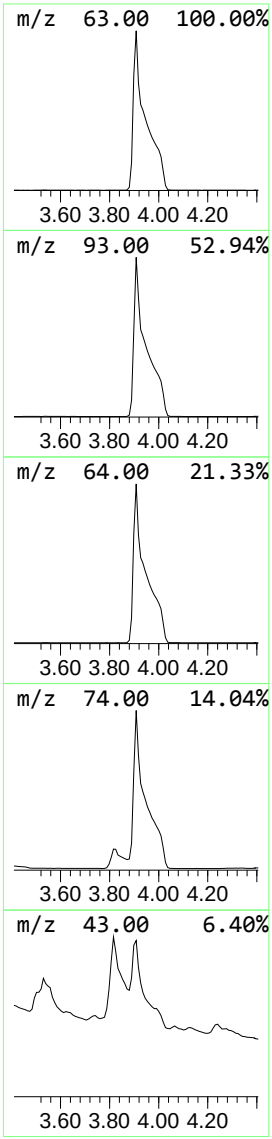
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethene, (methylsulfonyl)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.908	1.67 ng	430114	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethene, (methylsulfonyl)-	106	C3H6O2S	003680-02-2	2
2	Cyclopropene, 1-bromo-2,3,3-trif...	172	C3BrF3	029777-44-4	1
3	Oxalyl chloride	126	C2Cl2O2	000079-37-8	1
4	2-Propanol, 1-chloro-3-fluoro-	112	C3H6ClFO	189937-18-6	1
5	Ethene, trifluoro-	82	C2HF3	000359-11-5	1





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Acq On : 02 Oct 2021 19:33
Operator : CG/JU
Sample : M3829-21
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW202D-20210918

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

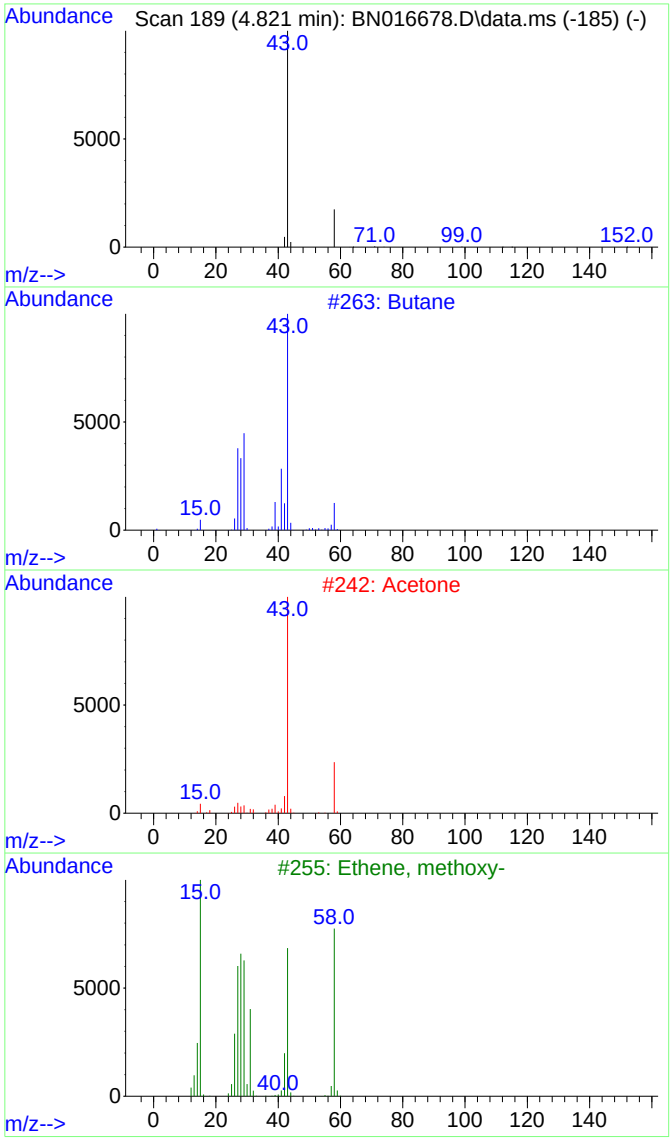
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

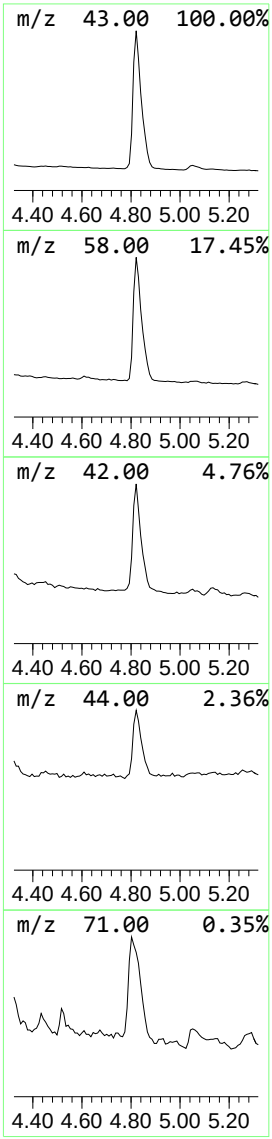
****

Peak Number 4 Butane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.31 ng	79995	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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Operator : CG/JU
Sample : M3829-21
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW202D-20210918

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

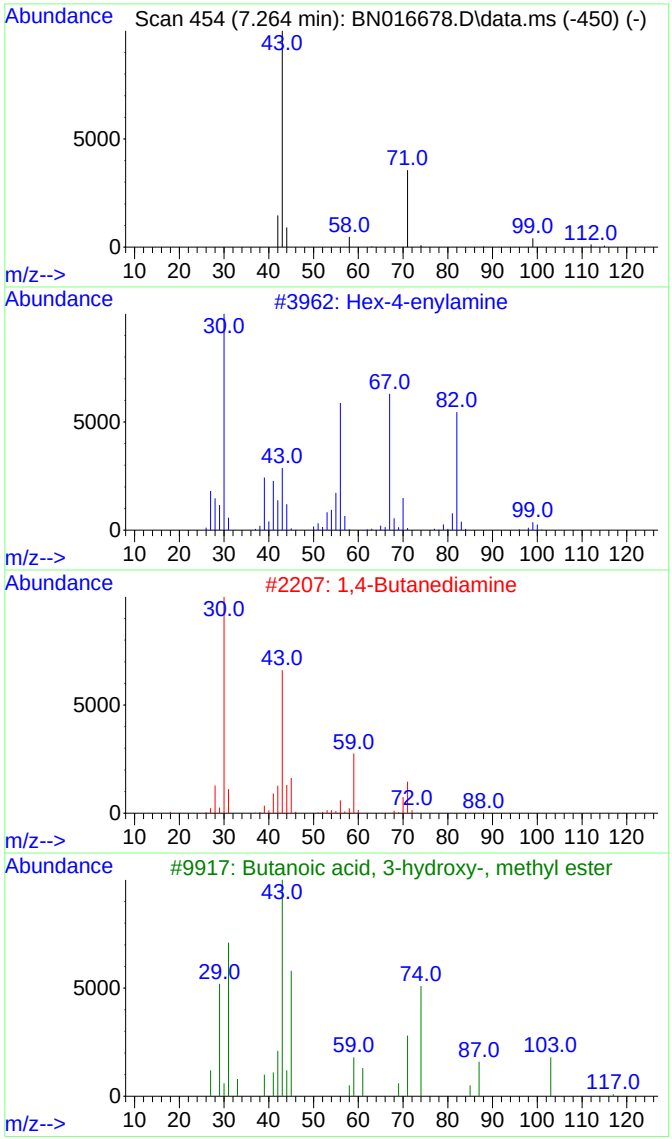
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

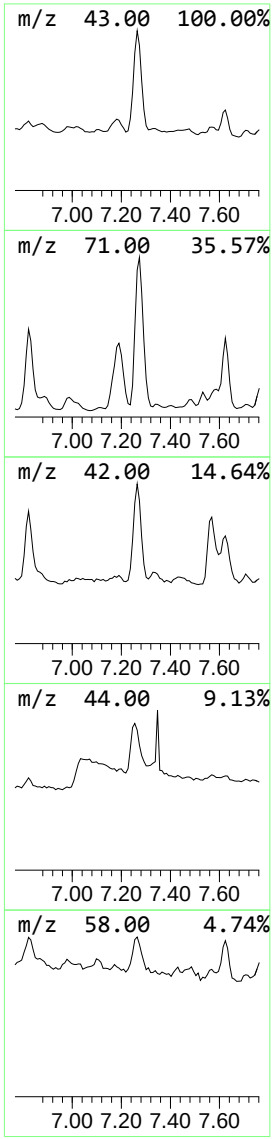
****

Peak Number 5 Hex-4-enylamine Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.264	0.07 ng	18786	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hex-4-enylamine	99	C6H13N	055108-01-5	5
2	1,4-Butanediamine	88	C4H12N2	000110-60-1	4
3	Butanoic acid, 3-hydroxy-, methy...	118	C5H10O3	001487-49-6	4
4	dl-Mevalonic acid lactone	130	C6H10O3	000674-26-0	4
5	Hydroxylamine, O-(3-methylbutyl)-	103	C5H13NO	019411-65-5	4





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ALS Vial : 46 Sample Multiplier: 1

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BNA_N
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MW202D-20210918

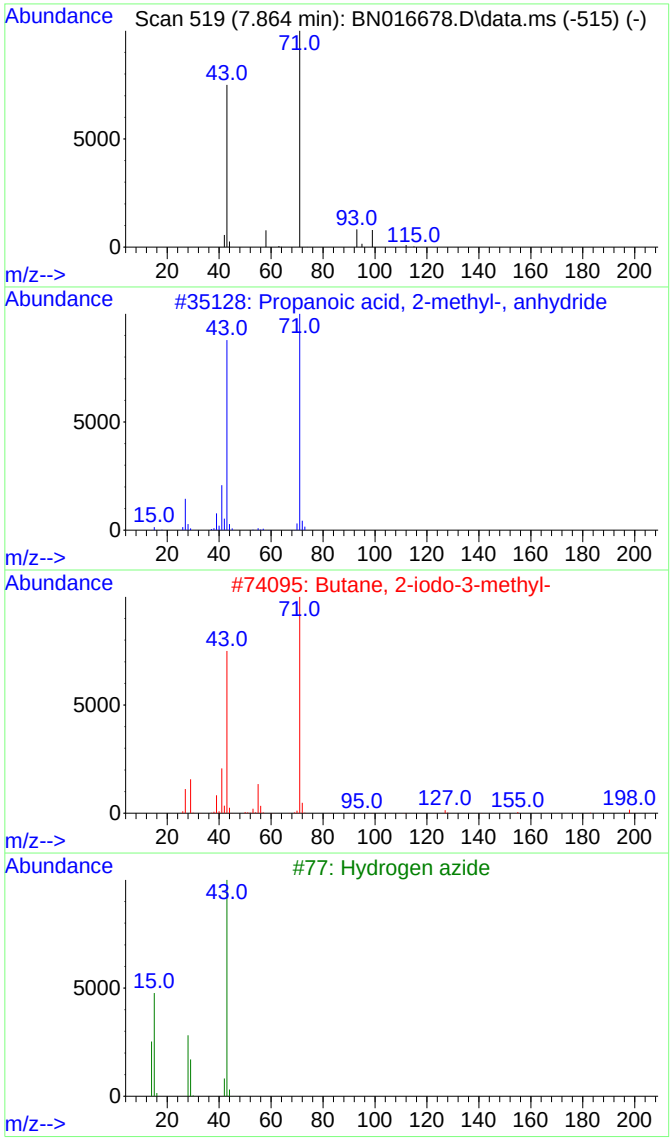
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

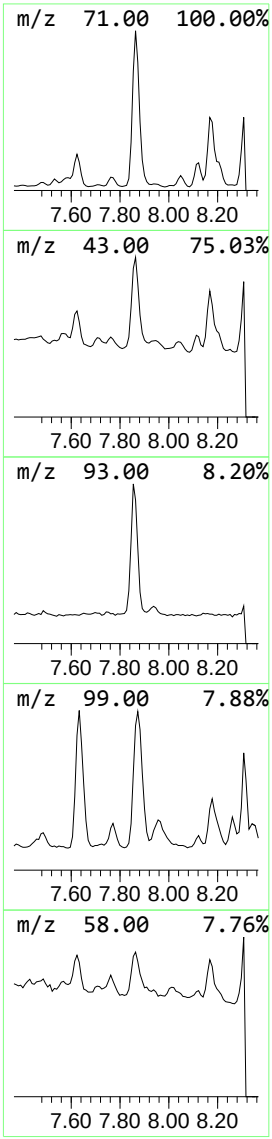
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Propanoic acid, 2-methyl-, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.864	0.07 ng	19032	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	4
2	Butane, 2-iodo-3-methyl-	198	C5H11I	018295-27-7	4
3	Hydrogen azide	43	HN3	007782-79-8	4
4	1-Hexene, 4,5-dimethyl-	112	C8H16	016106-59-5	4
5	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	4





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ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW202D-20210918

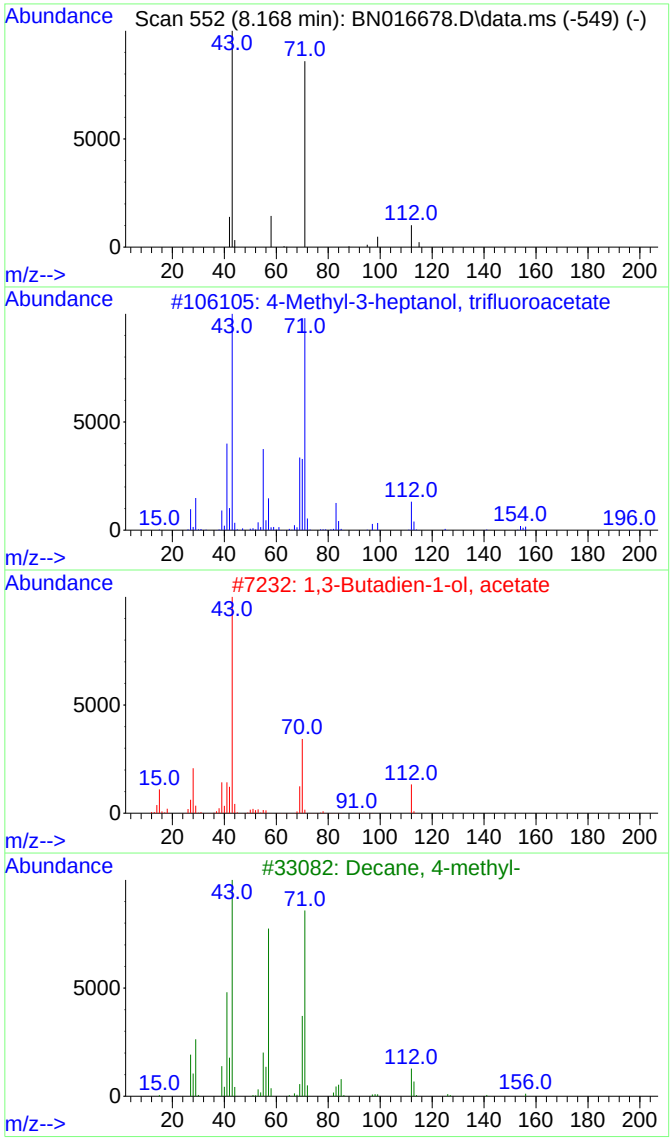
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

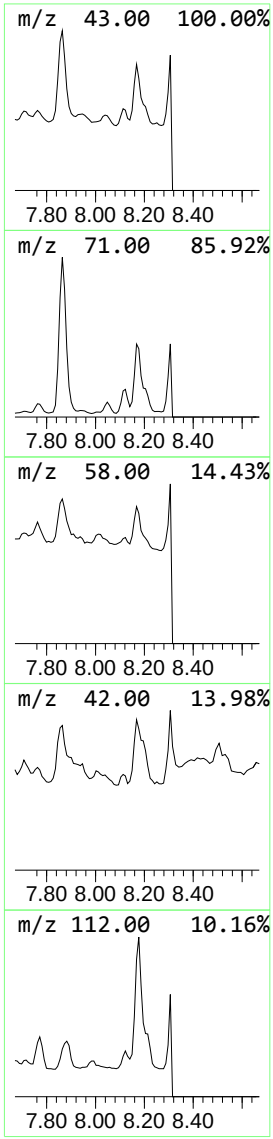
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 4-Methyl-3-heptanol, triflu... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.168	0.06 ng	16708	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methyl-3-heptanol, trifluoroac...	226	C10H17F3O2	1000365-51-8	43
2	1,3-Butadien-1-ol, acetate	112	C6H8O2	001515-76-0	9
3	Decane, 4-methyl-	156	C11H24	002847-72-5	9
4	Butane	58	C4H10	000106-97-8	7
5	Trifluoroacetamidine	112	C2H3F3N2	000354-37-0	7





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016678.D
Acq On : 02 Oct 2021 19:33
Operator : CG/JU
Sample : M3829-21
Misc :
ALS Vial : 46 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

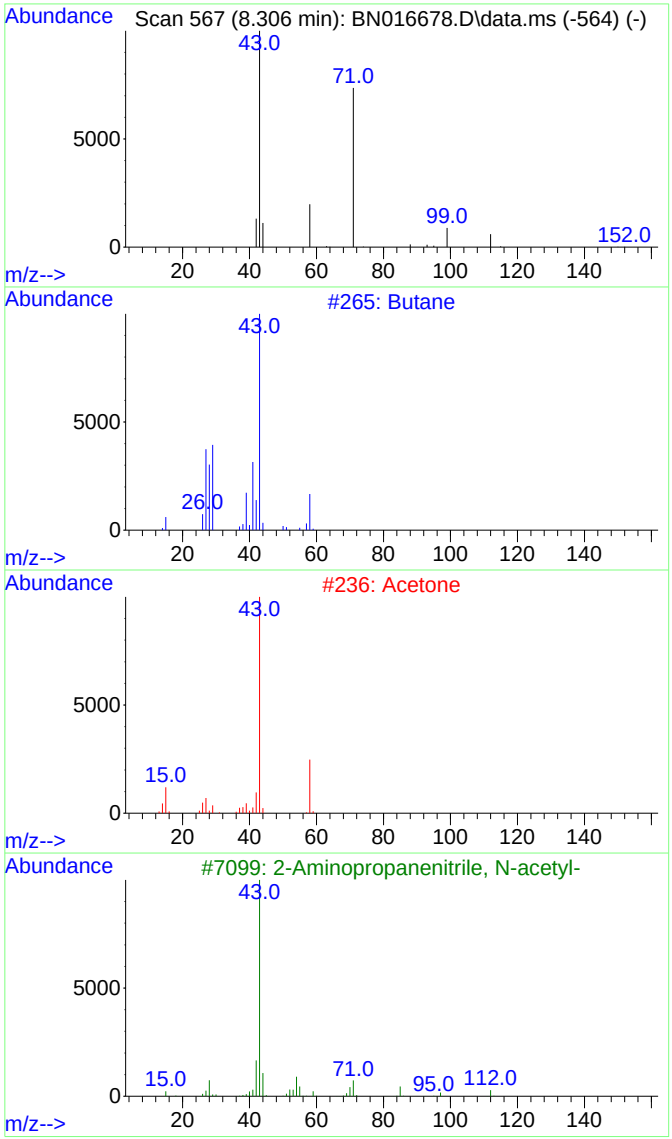
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

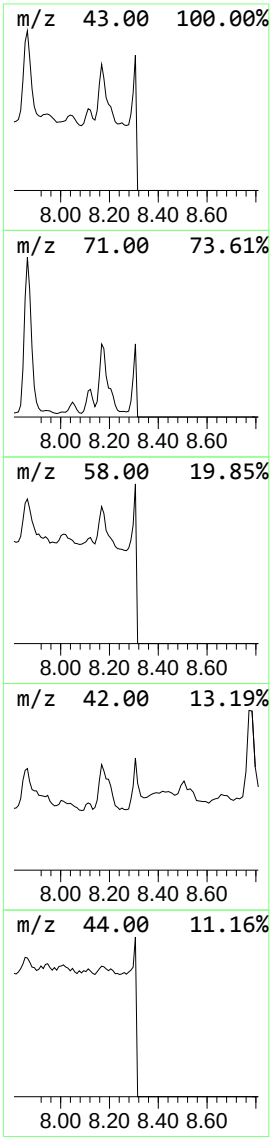
****

Peak Number 8 Butane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.306	0.04 ng	11521	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	5
2	Acetone	58	C3H6O	000067-64-1	5
3	2-Aminopropanenitrile, N-acetyl-	112	C5H8N2O	019861-71-3	4
4	Hexamethylenimine	99	C6H13N	000111-49-9	4
5	Sulfurous acid, octyl 2-propyl e...	236	C11H24O3S	1000309-11-9	4





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Data File : BN016678.D
Acq On : 02 Oct 2021 19:33
Operator : CG/JU
Sample : M3829-21
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW202D-20210918

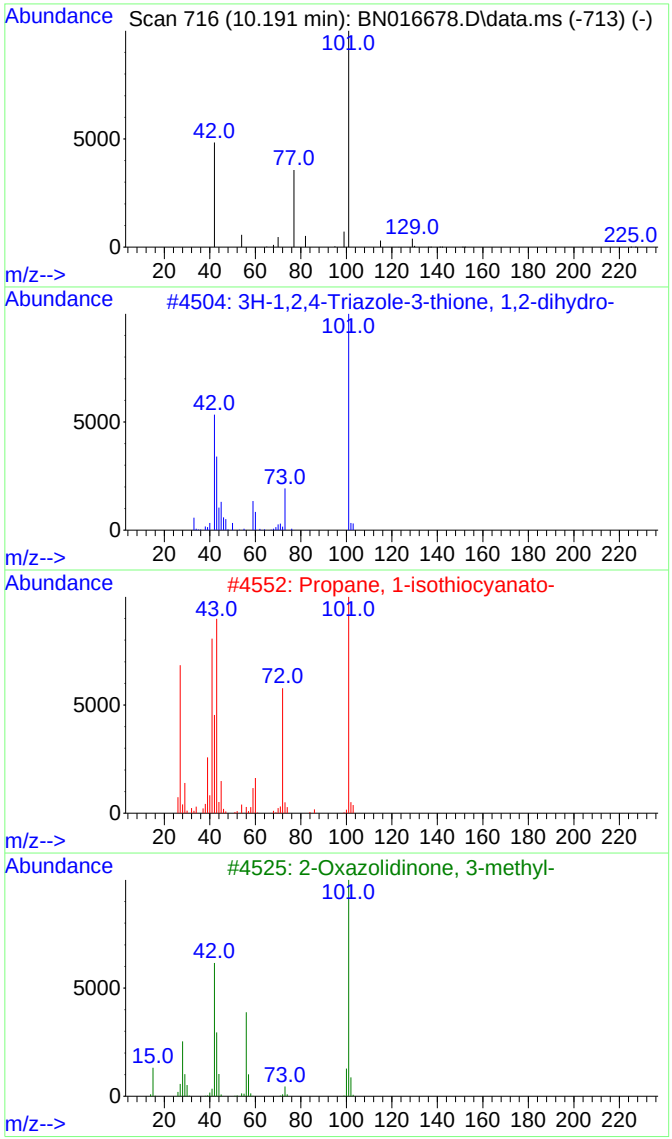
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

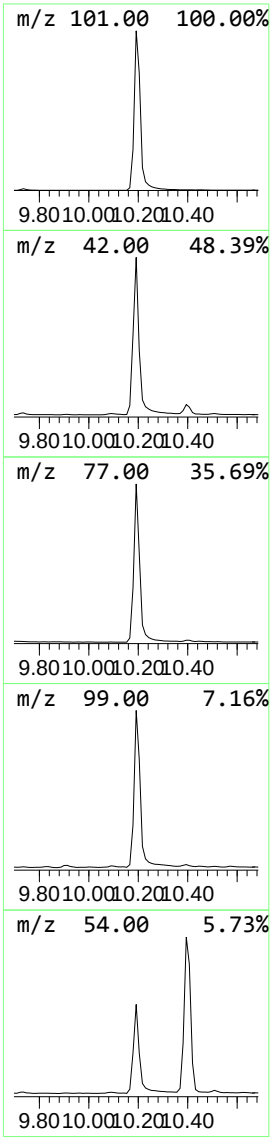
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.48 ng	218533	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	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5
3	2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	5
4	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	5
5	3-Aminopropionitrile	70	C3H6N2	000151-18-8	4





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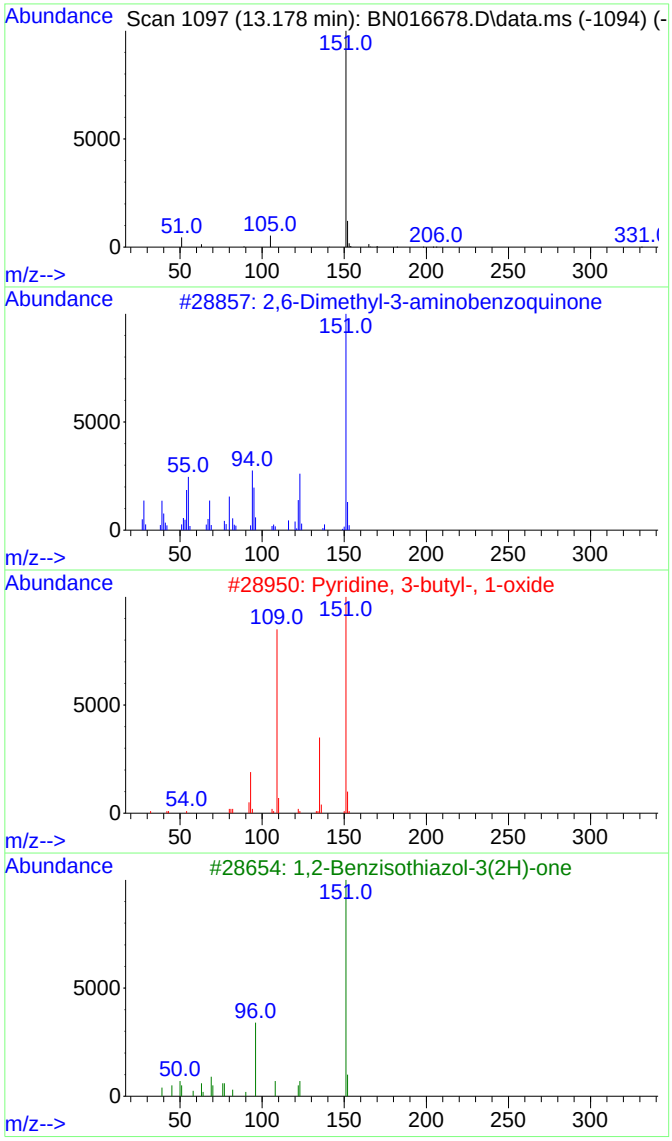
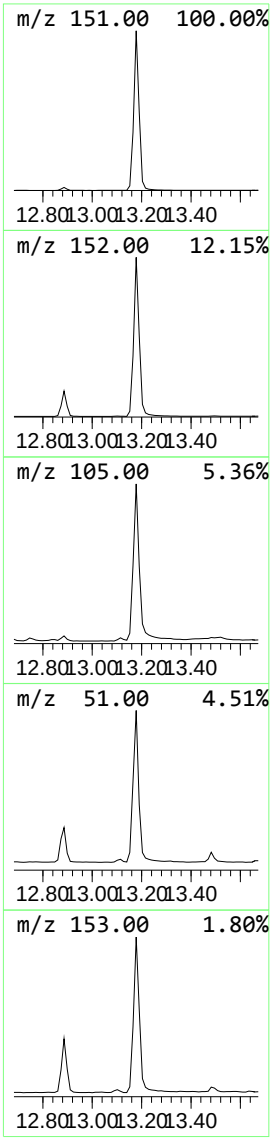
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2,6-Dimethyl-3-aminobenzoqu... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.178	0.61 ng	300052	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	Pyridine, 3-butyl-, 1-oxide	151	C9H13NO	031396-33-5	7
3	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	7
4	7-Methyl-7H-pyrazolo(3,4-d)-v-tr...	151	C5H5N5O	018213-76-8	7
5	Carbamic acid, phenyl-, methyl e...	151	C8H9NO2	002603-10-3	7





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Misc :
ALS Vial : 46 Sample Multiplier: 1

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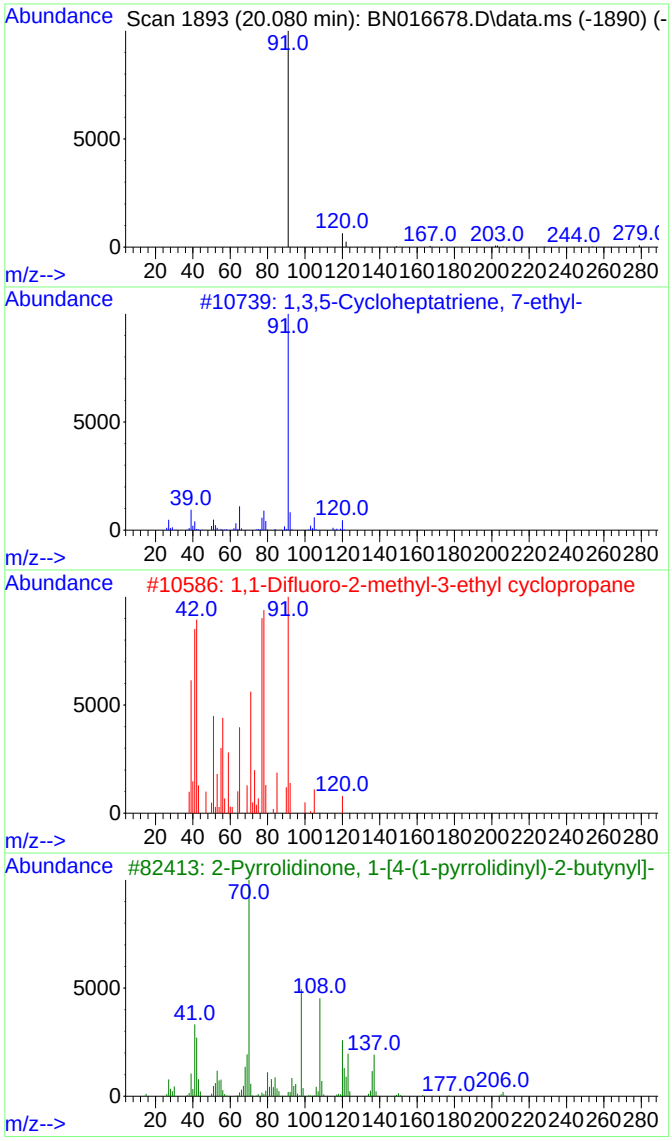
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

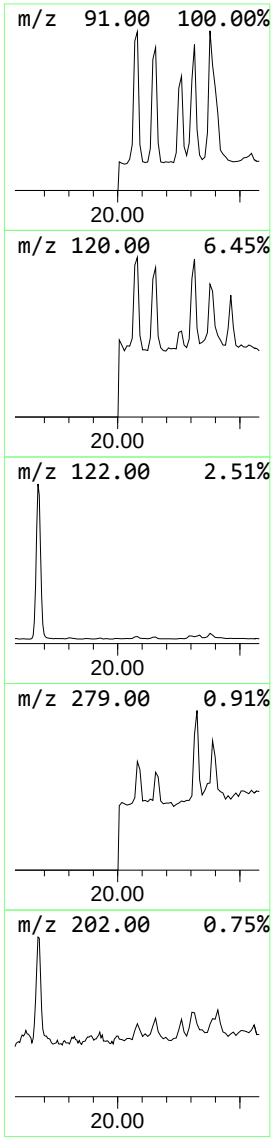
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 1,3,5-Cycloheptatriene, 7-e... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.081	0.04 ng	22651	Chrysene-d12	21.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Cycloheptatriene, 7-ethyl-	120	C9H12	017634-51-4	3
2	1,1-Difluoro-2-methyl-3-ethyl cy...	120	C6H10F2	1000144-82-1	3
3	2-Pyrrolidinone, 1-[4-(1-pyrroli...	206	C12H18N2O	000070-22-4	3
4	2-Benzylthio-4-chloronitrobenzene	279	C13H10ClNO2S	069741-45-3	3
5	2-Phenyl-5-(4-methoxyphenyl)-tet...	252	C14H12N4O	020433-10-7	2





Tentatively Identified Compound (LSC) summary

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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
4-Pyridazinamine	3.152	0.3	ng	66571	1	7.642	103229	0.4
Acetic acid, me...	3.816	0.1	ng	31132	1	7.642	103229	0.4
Ethene, (methyl...	3.908	1.7	ng	430114	1	7.642	103229	0.4
Butane	4.821	0.3	ng	79995	1	7.642	103229	0.4
Hex-4-enylamine	7.264	0.1	ng	18786	1	7.642	103229	0.4
Propanoic acid,...	7.864	0.1	ng	19032	1	7.642	103229	0.4
4-Methyl-3-hept...	8.168	0.1	ng	16708	1	7.642	103229	0.4
Butane	8.306	0.0	ng	11521	1	7.642	103229	0.4
3H-1,2,4-Triazo...	10.191	0.5	ng	218533	2	10.407	183536	0.4
2,6-Dimethyl-3-...	13.178	0.6	ng	300052	3	14.269	196195	0.4
1,3,5-Cyclohept...	20.081	0.0	ng	22651	5	21.227	202697	0.4