LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016598.D
Acq On : 30 Sep 2021 13:42
Operator : CG/JU
Sample : SSTDICC0.1
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDICC0.1

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: BN016598.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.253	16	19	22	rBV	3305	5007	2.61%	0.203%
2	3.585	52	55	71	rVB3	1759	7320	3.81%	0.297%
3	5.245	231	235	248	rVB2	4279	15703	8.18%	0.637%
4	6.822	402	406	415	rVB	5566	14241	7.42%	0.578%
5	6.978	419	423	429	rBV	3495	7916	4.12%	0.321%
6	7.080	430	434	441	rBV	8276	16988	8.85%	0.689%
7	7.200	444	447	452	rVB	2718	6218	3.24%	0.252%
8	7.522	479	482	487	rVB	1587	3511	1.83%	0.142%
9	7.642	490	495	514	rVB	43318	96944	50.51%	3.933%
10	7.854	514	518	524	rBV	5228	9478	4.94%	0.384%
11	7.956	525	529	536	rVB2	12248	27054	14.10%	1.097%
12	8.306	565	567	569	rVB2	2138	2027	1.06%	0.082%
13	8.442	572	578	586	rVB2	5034	13117	6.83%	0.532%
14	8.696	595	598	602	rBV	1136	2255	1.18%	0.091%
15	8.784	602	605	607	rVV	8893	18313	9.54%	0.743%
16	8.822	607	608	612	rVV	6165	10696	5.57%	0.434%
17	8.886	612	613	617	rVB2	1555	2575	1.34%	0.104%
18	9.342	646	649	653	rBV	12133	19971	10.41%	0.810%
19	9.595	666	669	677	rVB	2054	3950	2.06%	0.160%
20	9.836	685	688	692	rBV	4022	6937	3.61%	0.281%
21	10.407	730	733	735	rBV	94005	163770	85.34%	6.643%
22	10.457	735	737	741	rVV	28362	47663	24.84%	1.933%
23	10.584	743	747	754	rVV	5784	13041	6.80%	0.529%
24	10.749	757	760	767	rVB	8663	14035	7.31%	0.569%
25	11.709	853	865	884	rBV	3308	6150	3.20%	0.249%
26	12.007	922	932	940	rBV2	13428	22088	11.51%	0.896%
27	12.078	940	948	971	rVB	30269	49441	25.76%	2.006%
28	12.301	988	998	1017	rBV	30481	48487	25.27%	1.967%
29	12.518	1043	1045	1049	rBV4	1673	6266	3.27%	0.254%
30	12.695	1057	1059	1062	rVB	3876	6383	3.33%	0.259%
31	12.772	1062	1065	1071	rVB	3132	5560	2.90%	0.226%
32	12.898	1071	1075	1078	rBV	30134	49235	25.65%	1.997%
33	13.139	1091	1094	1097	rVB	19153	28916	15.07%	1.173%
34	13.292	1103	1106	1109	rBV	1551	2575	1.34%	0.104%
35	13.736	1138	1141	1144	rBV	2676	4018	2.09%	0.163%
36	13.850	1147	1150	1155	rVB2	3640	6143	3.20%	0.249%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016598.D
Acq On : 30 Sep 2021 13:42
Operator : CG/JU
Sample : SSTDICC0.1
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDICC0.1

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	13.990	1158	1161	1164	rVB	23057	34132	17.79%	1.385%
38	14.269	1180	1183	1186	rBV	116674	173329	90.32%	7.031%
39	14.332	1186	1188	1191	rVB	38826	55847	29.10%	2.265%
40	14.649	1210	1213	1219	rVB3	3444	8802	4.59%	0.357%
41	14.827	1224	1227	1231	rBV2	1270	2804	1.46%	0.114%
42	15.106	1246	1249	1252	rBV	2468	3533	1.84%	0.143%
43	15.322	1263	1266	1270	rBV2	43449	76486	39.85%	3.103%
44	15.550	1281	1284	1287	rBV2	6891	12469	6.50%	0.506%
45	15.614	1287	1289	1297	rVV2	7321	14012	7.30%	0.568%
46	15.766	1298	1301	1306	rVB2	2847	4881	2.54%	0.198%
47	16.226	1335	1338	1341	rBV2	13692	19895	10.37%	0.807%
48	16.324	1344	1346	1350	rVB	9270	15718	8.19%	0.638%
49	16.506	1358	1361	1366	rBV	5548	8001	4.17%	0.325%
50	16.677	1372	1375	1384	rVB	4901	7855	4.09%	0.319%
51	17.030	1400	1404	1406	rBV	77194	138568	72.20%	5.621%
52	17.066	1406	1407	1410	rVV	35033	37560	19.57%	1.524%
53	17.163	1411	1415	1432	rVB	20579	40513	21.11%	1.643%
54	17.431	1434	1437	1445	rBV	15105	26588	13.85%	1.079%
55	19.068	1688	1697	1700	rBV	23591	35063	18.27%	1.422%
56	19.098	1700	1703	1728	rVB	37100	49560	25.82%	2.010%
57	19.460	1767	1776	1797	rBV	37253	52063	27.13%	2.112%
58	19.678	1814	1820	1837	rBV	23389	29998	15.63%	1.217%
59	20.378	1918	1921	1925	rBV	10205	14890	7.76%	0.604%
60	21.026	1979	1982	1993	rVB	95402	131818	68.69%	5.347%
61	21.174	1993	1996	1998	rBV	16655	19349	10.08%	0.785%
62	21.238	1998	2002	2004	rVV3	105570	191912	100.00%	7.785%
63	21.270	2004	2005	2011	rVB	41147	43182	22.50%	1.752%
64	22.056	2076	2079	2083	rBV	15171	20180	10.52%	0.819%
65	22.321	2102	2104	2108	rBV	1183	1992	1.04%	0.081%
66	22.810	2220	2230	2236	rBV	24411	40259	20.98%	1.633%
67	22.855	2237	2243	2267	rVB2	27368	47700	24.86%	1.935%
68	23.389	2388	2399	2407	rBV	16560	33441	17.43%	1.357%
69	23.488	2417	2428	2460	rVB	71562	140908	73.42%	5.716%
70	24.090	2596	2604	2617	rVB2	4237	7873	4.10%	0.319%
71	24.860	2821	2829	2846	rVB	4148	8923	4.65%	0.362%
72	25.778	3074	3097	3146	rBV4	25550	99562	51.88%	4.039%
73	26.459	3275	3296	3339	rBV	14174	46474	24.22%	1.885%
74	26.832	3390	3405	3428	rVB	964	3021	1.57%	0.123%
75	28.095	3755	3774	3795	rBV	545	2015	1.05%	0.082%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016598.D
Acq On : 30 Sep 2021 13:42
Operator : CG/JU
Sample : SSTDICC0.1
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.1

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

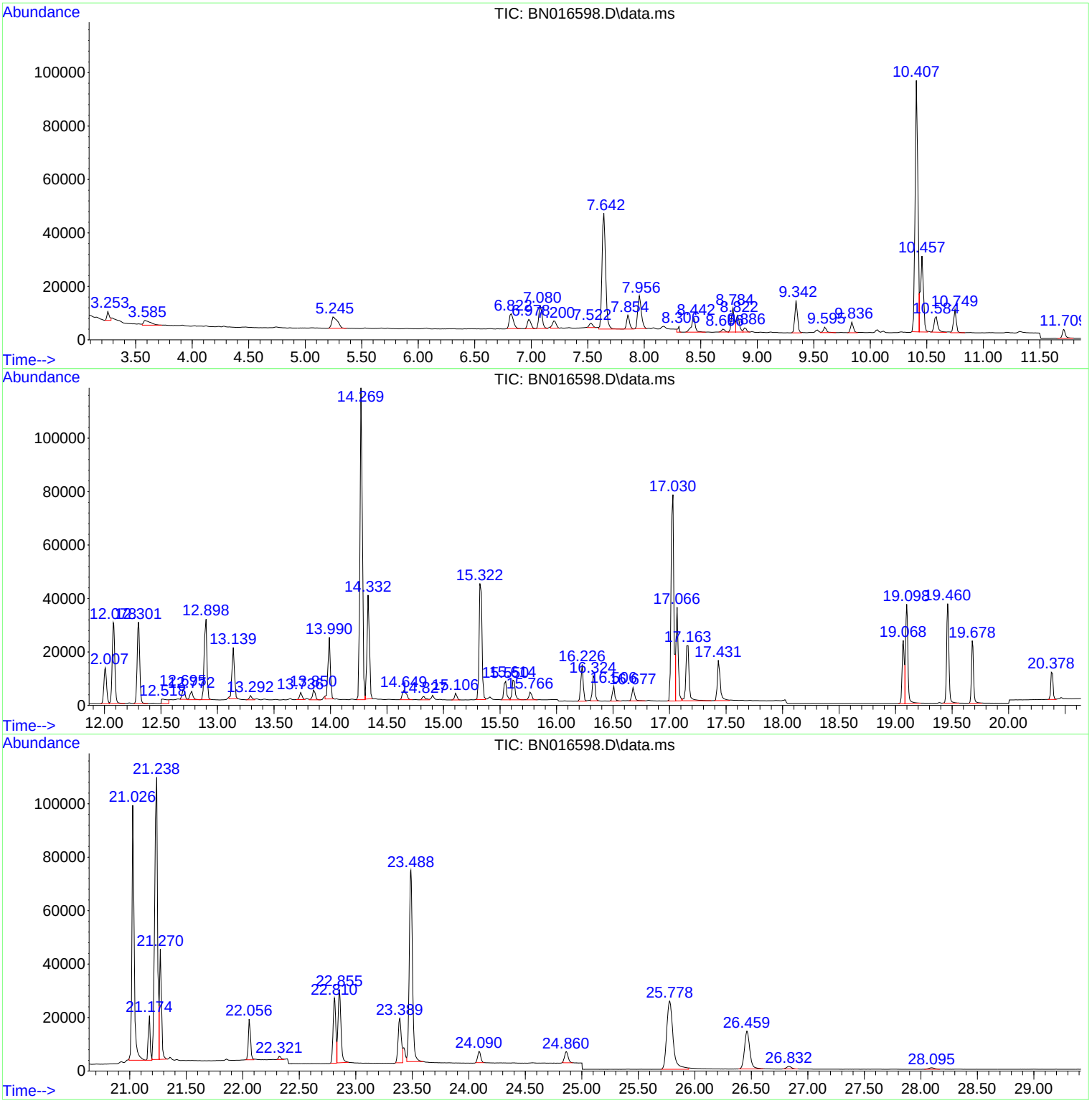
Sum of corrected areas: 2465168

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016598.D
Acq On : 30 Sep 2021 13:42
Operator : CG/JU
Sample : SSTDICC0.1
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.1

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 : BN016598.D
Acq On : 30 Sep 2021 13:42
Operator : CG/JU
Sample : SSTDICC0.1
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.1

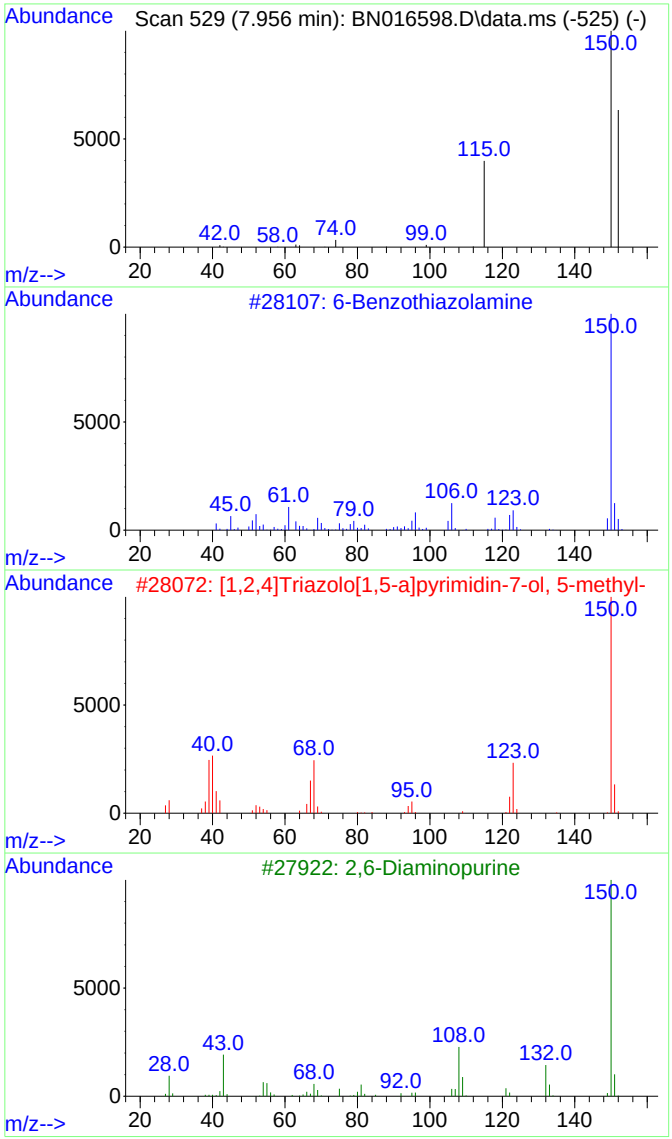
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

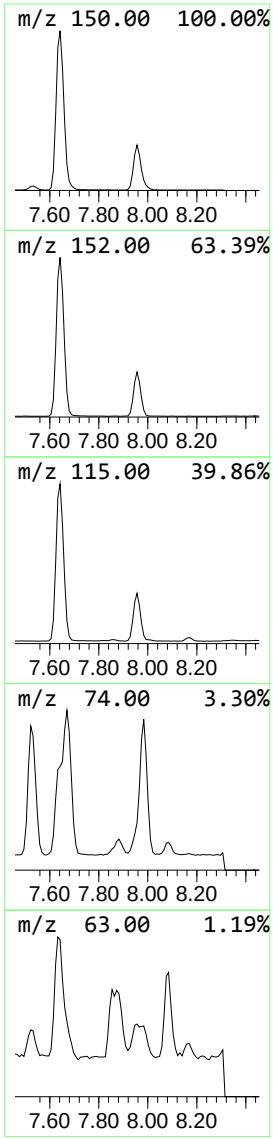
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 6-Benzothiazolamine Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.956	0.11 ng	27054	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Benzothiazolamine	150	C7H6N2S	000533-30-2	4
2	[1,2,4]Triazolo[1,5-a]pyrimidin-...	150	C6H6N4O	002503-56-2	4
3	2,6-Diaminopurine	150	C5H6N6	001904-98-9	2
4	4-Amino-3,5-diethylpyridine	150	C9H14N2	1000128-75-1	2
5	Benzene, 1,2,3,4-tetrafluoro-	150	C6H2F4	000551-62-2	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016598.D
Acq On : 30 Sep 2021 13:42
Operator : CG/JU
Sample : SSTDICC0.1
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.1

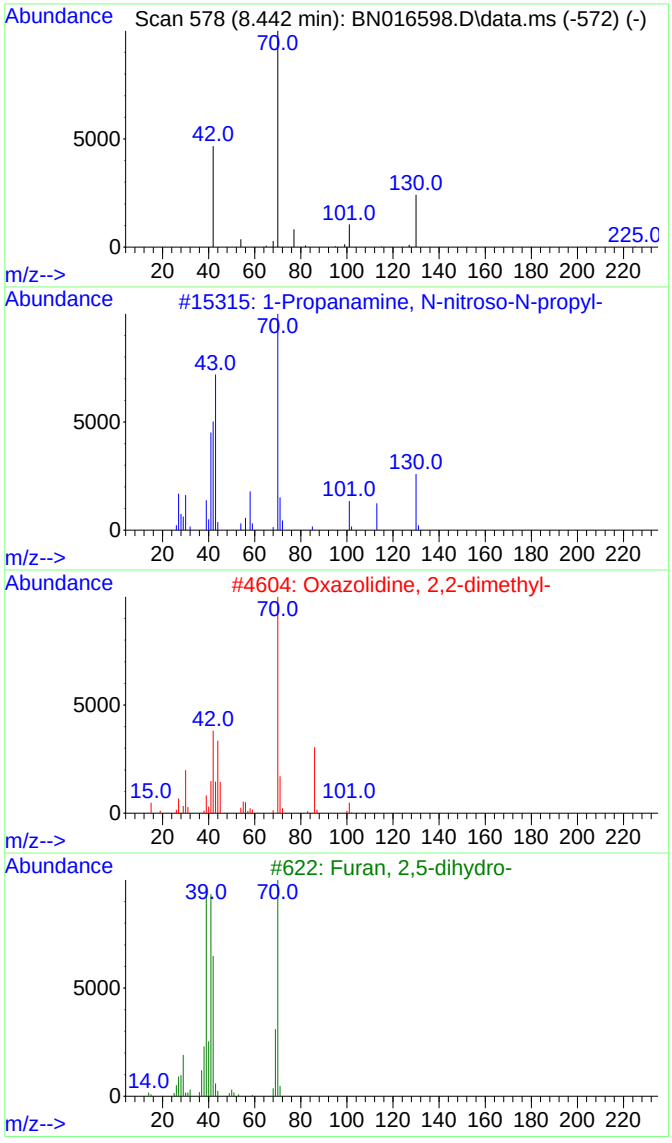
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

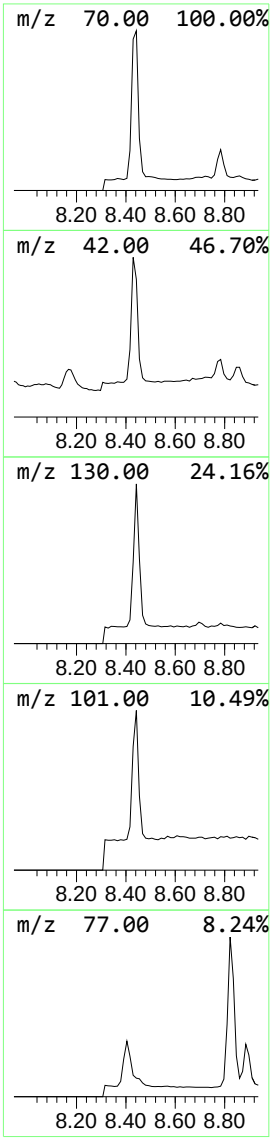
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-Propanamine, N-nitroso-N-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.442	0.05 ng	13117	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanamine, N-nitroso-N-propyl-	130	C6H14N2O	000621-64-7	72
2	Oxazolidine, 2,2-dimethyl-	101	C5H11NO	020515-62-2	7
3	Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	7
4	Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	4
5	2-Butenal, (E)-	70	C4H6O	000123-73-9	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016598.D
Acq On : 30 Sep 2021 13:42
Operator : CG/JU
Sample : SSTDICC0.1
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.1

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

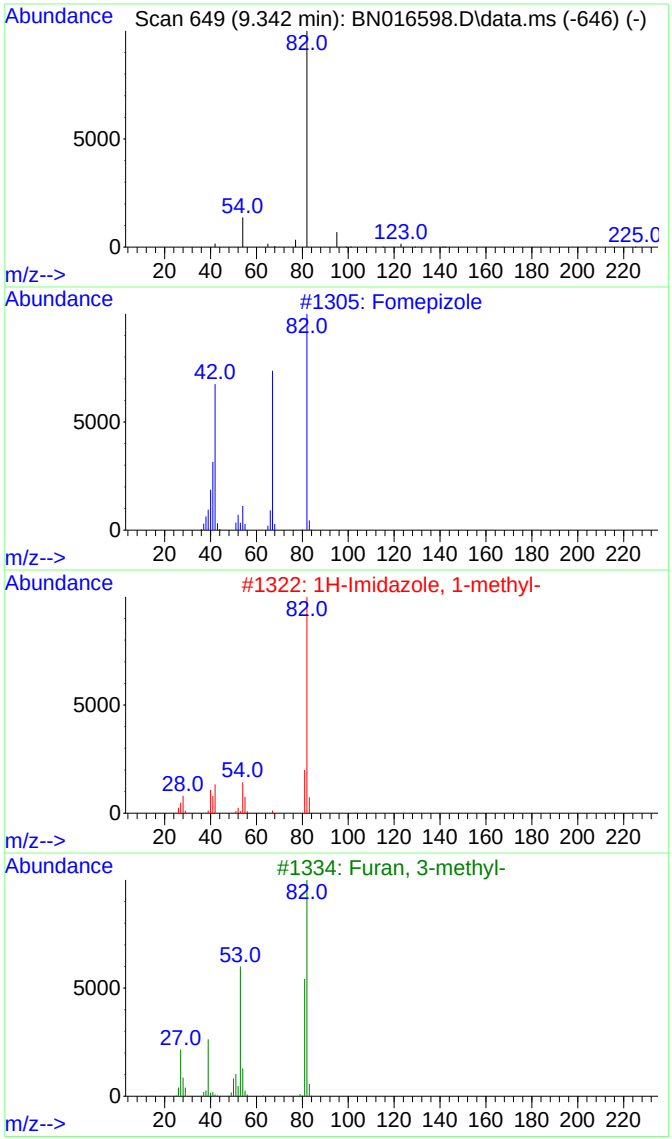
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

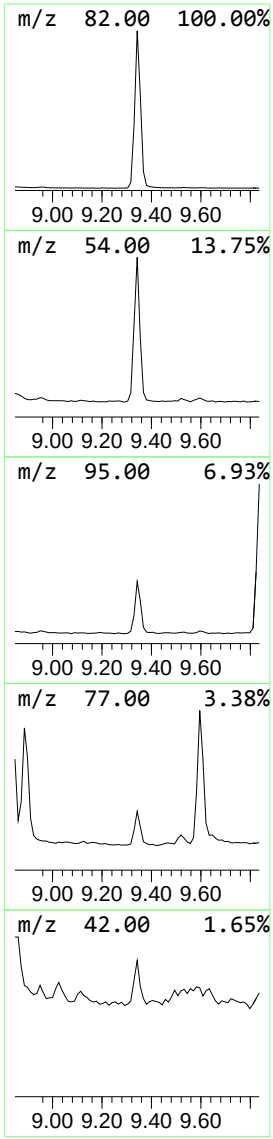
****

Peak Number 3 Fomepizole Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.342	0.05 ng	19971	Naphthalene-d8	10.406

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fomepizole	82	C4H6N2	007554-65-6	5
2	1H-Imidazole, 1-methyl-	82	C4H6N2	000616-47-7	4
3	Furan, 3-methyl-	82	C5H6O	000930-27-8	4
4	Furan, 2-methyl-	82	C5H6O	000534-22-5	4
5	3-Aminocrotononitrile	82	C4H6N2	001118-61-2	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016598.D
Acq On : 30 Sep 2021 13:42
Operator : CG/JU
Sample : SSTDICC0.1
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.1

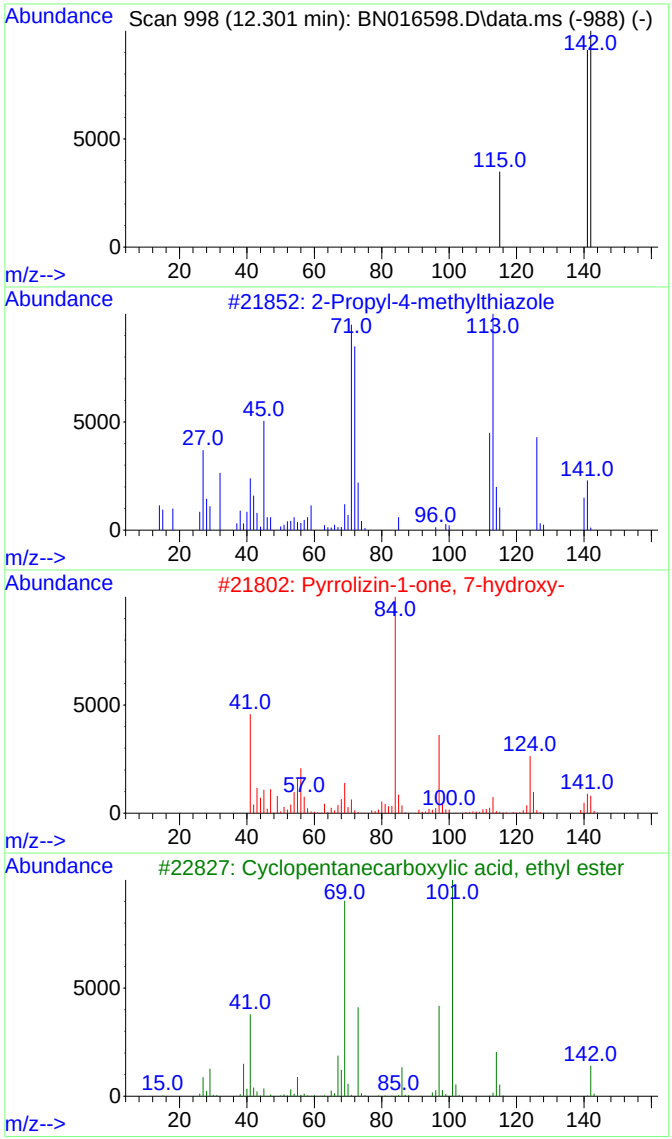
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

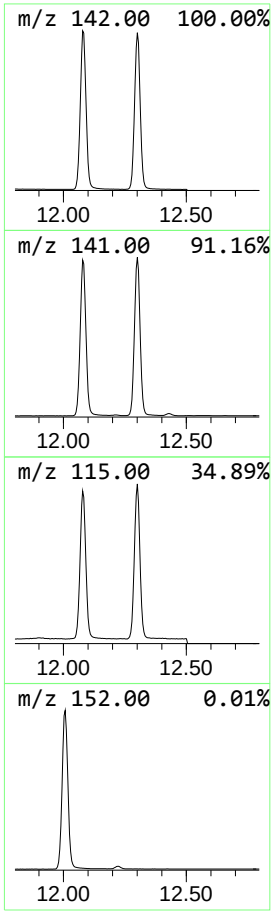
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Propyl-4-methylthiazole Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.301	0.12 ng	48487	Naphthalene-d8	10.406

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propyl-4-methylthiazole	141	C7H11NS	052414-87-6	4
2	Pyrrolizin-1-one, 7-hydroxy-	141	C7H11NO2	1000125-96-2	3
3	Cyclopentanecarboxylic acid, eth...	142	C8H14O2	1000375-86-4	3
4	2-Propionylthiazole	141	C6H7NOS	043039-98-1	3
5	2,4(1H,3H)-Pyrimidinedione, 6-am...	141	C5H7N3O2	002434-53-9	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016598.D
Acq On : 30 Sep 2021 13:42
Operator : CG/JU
Sample : SSTDICC0.1
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.1

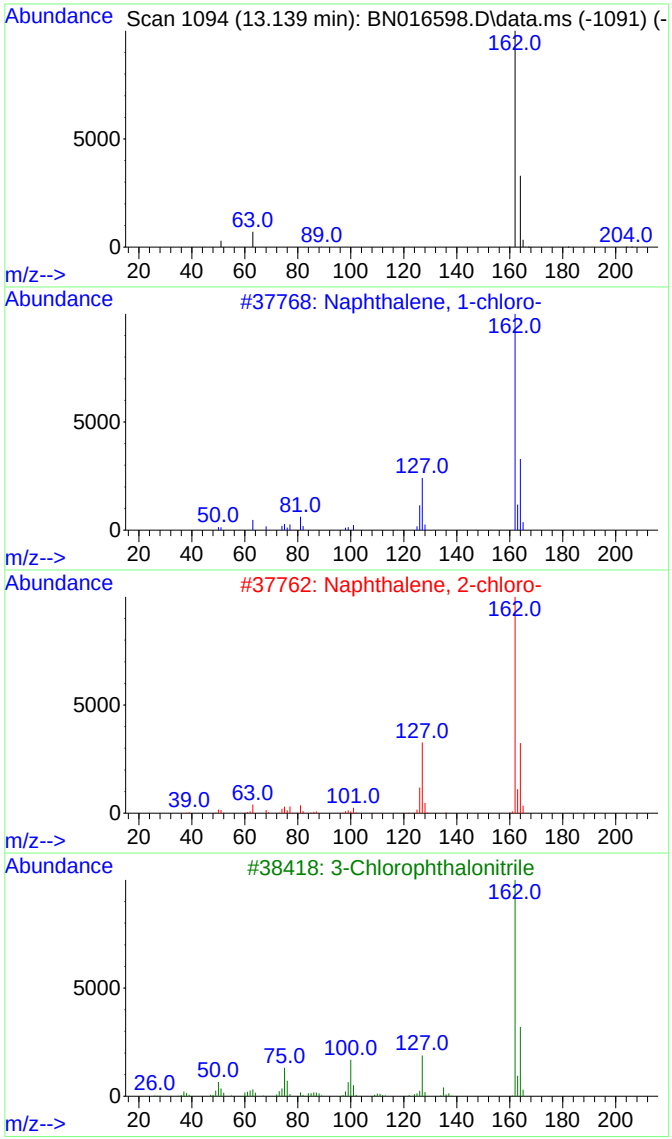
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

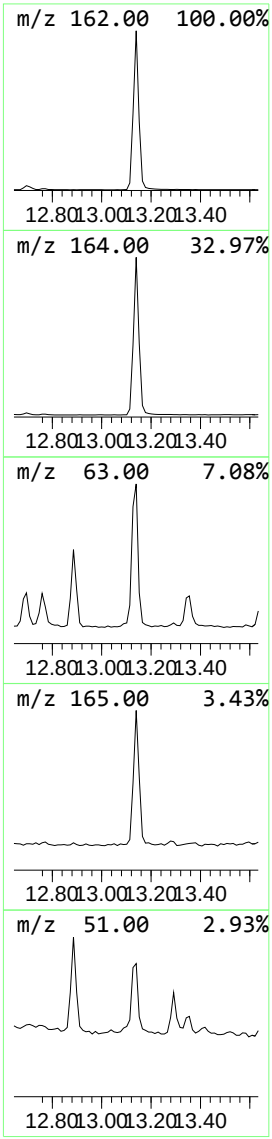
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Naphthalene, 1-chloro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.139	0.07 ng	28916	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-chloro-	162	C10H7Cl	000090-13-1	64
2	Naphthalene, 2-chloro-	162	C10H7Cl	000091-58-7	64
3	3-Chlorophthalonitrile	162	C8H3ClN2	076241-79-7	7
4	2-Chloroisophthalonitrile	162	C8H3ClN2	028442-78-6	7
5	2-Amino-4-chloro-1,3-thiazole-5-...	162	C4H3ClN2OS	076874-79-8	5





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016598.D
Acq On : 30 Sep 2021 13:42
Operator : CG/JU
Sample : SSTDICC0.1
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.1

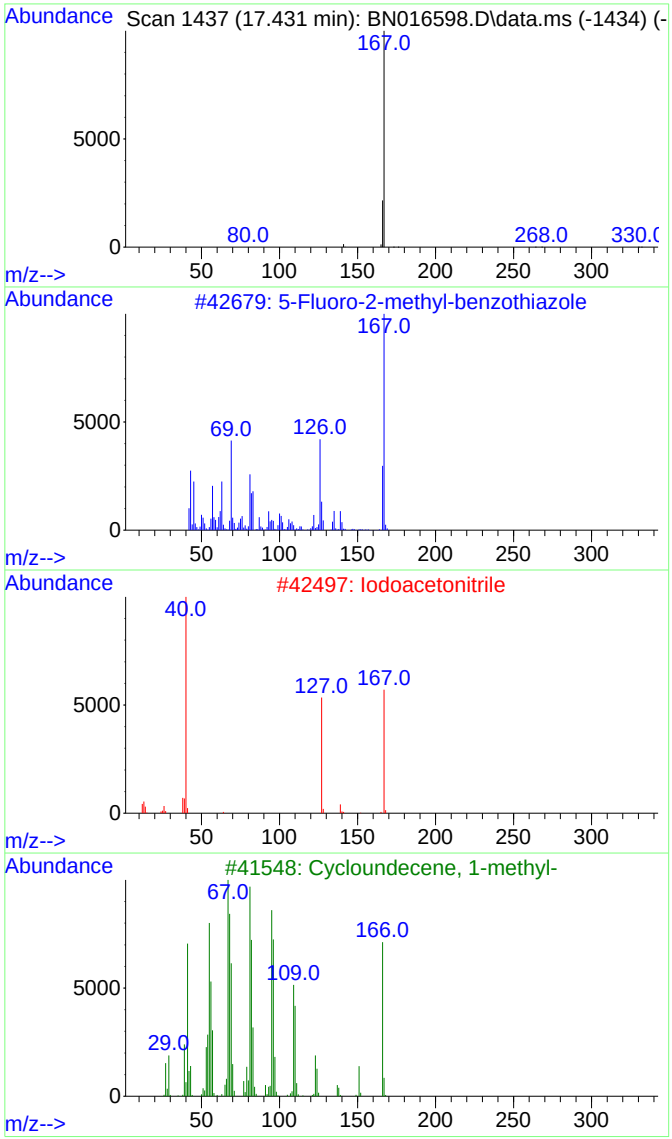
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

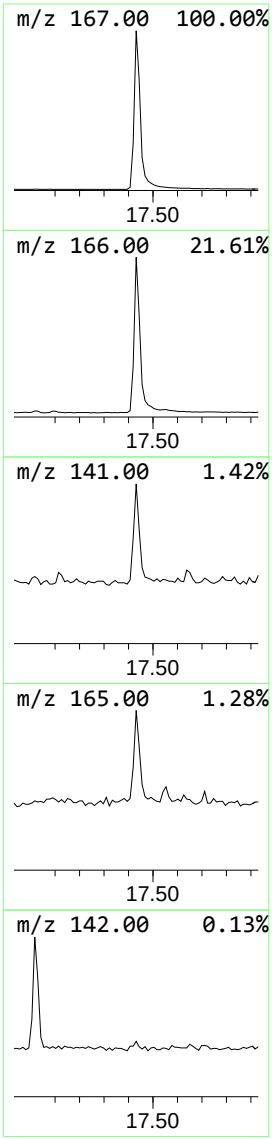
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 5-Fluoro-2-methyl-benzothia... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.431	0.08 ng	26588	Phenanthrene-d10	17.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	5
2	Iodoacetonitrile	167	C2H2IN	000624-75-9	4
3	Cycloundecene, 1-methyl-	166	C12H22	088828-82-4	4
4	1,3,5-Triazine-2,4-diamine, N,N'...	167	C7H13N5	004150-59-8	4
5	1-Cyclopropanecarbonylpiperidin-...	167	C9H13NO2	063463-43-4	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016598.D
Acq On : 30 Sep 2021 13:42
Operator : CG/JU
Sample : SSTDICC0.1
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.1

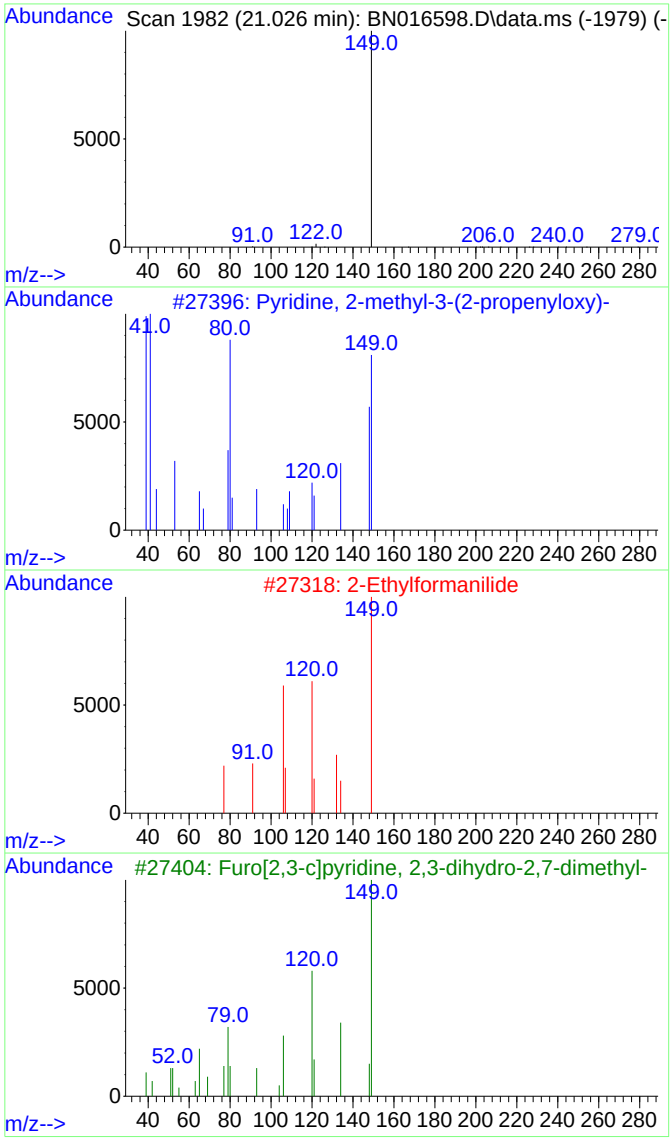
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

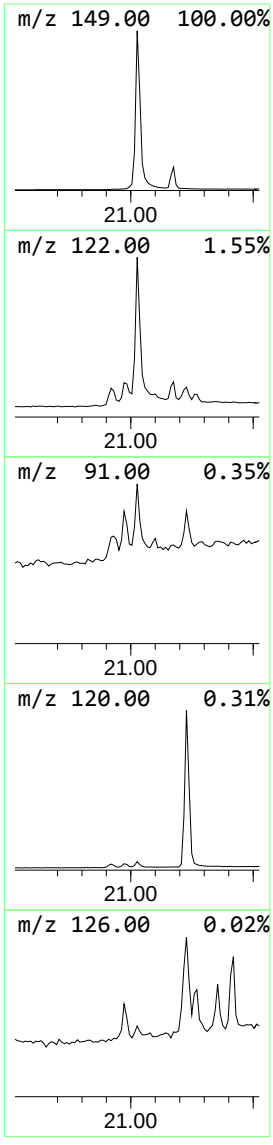
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Pyridine, 2-methyl-3-(2-pro... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.026	0.27 ng	131818	Chrysene-d12	21.238

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine, 2-methyl-3-(2-propenyl...	149	C9H11NO	069022-75-9	2
2	2-Ethylformanilide	149	C9H11NO	002860-30-2	2
3	Furo[2,3-c]pyridine, 2,3-dihydro...	149	C9H11NO	069022-82-8	2
4	6,7-Dimethyl-triazolo(4,3-b)(1,2...	149	C6H7N5	061139-73-9	2
5	Carbamodithioic acid, dimethyl-,...	149	C5H11NS2	000617-38-9	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016598.D
Acq On : 30 Sep 2021 13:42
Operator : CG/JU
Sample : SSTDICC0.1
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.1

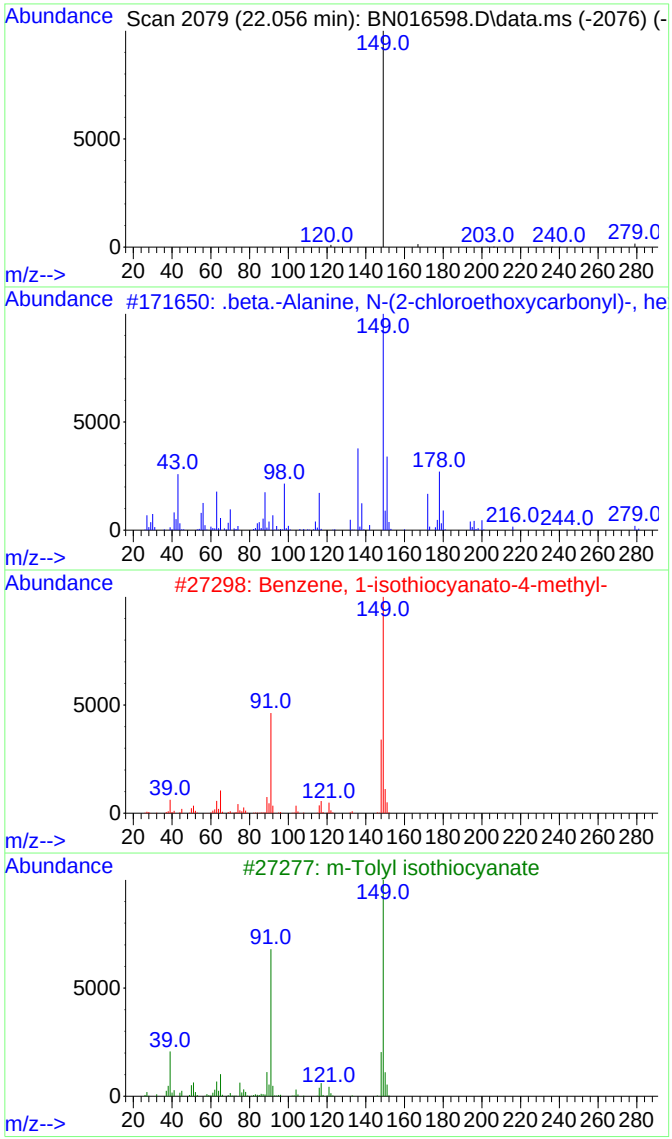
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

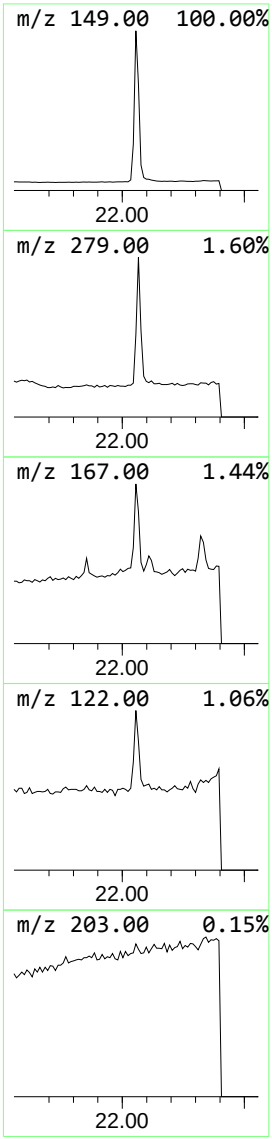
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 .beta.-Alanine, N-(2-chloro... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.056	0.04 ng	20180	Chrysene-d12	21.238

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Alanine, N-(2-chloroethox...	279	C12H22ClNO4	1010328-58-4	4
2	Benzene, 1-isothiocyanato-4-methyl-	149	C8H7NS	000622-59-3	4
3	m-Tolyl isothiocyanate	149	C8H7NS	000621-30-7	4
4	Benzothiazole, 2-methyl-	149	C8H7NS	000120-75-2	4
5	Pyridine, pentamethyl-	149	C10H15N	003748-83-2	4





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016598.D
Acq On : 30 Sep 2021 13:42
Operator : CG/JU
Sample : SSTDICC0.1
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDICC0.1

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
6-Benzothiazola...	7.956	0.1	ng	27054	1	7.642	96944	0.4
1-Propanamine, ...	8.442	0.1	ng	13117	1	7.642	96944	0.4
Fomepizole	9.342	0.0	ng	19971	2	10.406	163770	0.4
2-Propyl-4-meth...	12.301	0.1	ng	48487	2	10.406	163770	0.4
Naphthalene, 1-...	13.139	0.1	ng	28916	3	14.269	173329	0.4
5-Fluoro-2-meth...	17.431	0.1	ng	26588	4	17.030	138568	0.4
Pyridine, 2-met...	21.026	0.3	ng	131818	5	21.238	191912	0.4
.beta.-Alanine,...	22.056	0.0	ng	20180	5	21.238	191912	0.4