LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016599.D
Acq On : 30 Sep 2021 14:18
Operator : CG/JU
Sample : SSTDICC0.2
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDICC0.2

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: BN016599.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	21	rBV	2805	4630	1.77%	0.119%
2	3.604	52	57	73	rVB	2780	12642	4.84%	0.324%
3	5.061	212	215	229	rVB	833	2694	1.03%	0.069%
4	5.263	232	237	248	rVB	6936	25185	9.65%	0.645%
5	6.822	402	406	418	rVB	10437	26065	9.98%	0.668%
6	6.978	419	423	430	rVV	7493	16396	6.28%	0.420%
7	7.080	430	434	441	rVV	14847	30717	11.76%	0.787%
8	7.209	444	448	458	rVB	5195	12412	4.75%	0.318%
9	7.532	479	483	488	rVB	3009	6406	2.45%	0.164%
10	7.642	490	495	509	rVB	40716	90876	34.81%	2.328%
11	7.854	514	518	524	rBV	3663	7512	2.88%	0.192%
12	7.956	524	529	537	rBV2	22405	49470	18.95%	1.267%
13	8.168	548	552	562	rVB2	1623	4342	1.66%	0.111%
14	8.442	572	578	590	rBV2	8718	22191	8.50%	0.569%
15	8.696	595	598	601	rBV	2190	4150	1.59%	0.106%
16	8.784	601	605	607	rBV	15584	31434	12.04%	0.805%
17	8.822	607	608	612	rVB	9875	16084	6.16%	0.412%
18	9.342	646	649	656	rBV	21072	35112	13.45%	0.900%
19	9.532	661	664	667	rVV	1764	3377	1.29%	0.087%
20	9.596	667	669	678	rVB	3550	6661	2.55%	0.171%
21	9.836	685	688	694	rBV	6571	11832	4.53%	0.303%
22	10.064	703	706	708	rBV	1772	3473	1.33%	0.089%
23	10.407	730	733	735	rBV	85040	150277	57.56%	3.850%
24	10.457	735	737	741	rVV	49722	83126	31.84%	2.130%
25	10.584	743	747	757	rVV	11273	26625	10.20%	0.682%
26	10.749	757	760	764	rVB	15201	24406	9.35%	0.625%
27	11.714	854	866	891	rBV	5600	11160	4.27%	0.286%
28	12.007	922	932	940	rBV2	24444	39950	15.30%	1.023%
29	12.078	940	948	972	rVB	53738	89756	34.38%	2.299%
30	12.301	988	998	1022	rBV	55857	87865	33.65%	2.251%
31	12.518	1043	1045	1048	rBV3	1384	4316	1.65%	0.111%
32	12.695	1056	1059	1062	rBV	6857	12402	4.75%	0.318%
33	12.772	1062	1065	1071	rVB	5478	10383	3.98%	0.266%
34	12.898	1071	1075	1078	rBV	54155	90936	34.83%	2.330%
35	13.140	1091	1094	1097	rVB	36121	53662	20.55%	1.375%
36	13.736	1138	1141	1144	rBV	5022	7395	2.83%	0.189%

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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDICC0.2

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	13.850	1148	1150	1155	rVB	6871	11246	4.31%	0.288%
38	13.990	1158	1161	1164	rVB	42780	64239	24.60%	1.646%
39	14.269	1180	1183	1186	rBV	104910	161471	61.84%	4.137%
40	14.332	1186	1188	1191	rVB	72053	103719	39.72%	2.657%
41	14.649	1210	1213	1220	rBV3	6944	17652	6.76%	0.452%
42	14.827	1224	1227	1231	rBV	2451	4357	1.67%	0.112%
43	14.903	1231	1233	1237	rVB	3122	4667	1.79%	0.120%
44	15.106	1247	1249	1252	rBV	3535	4964	1.90%	0.127%
45	15.322	1263	1266	1270	rBV2	83020	150805	57.76%	3.864%
46	15.411	1270	1273	1278	rVV2	2227	5264	2.02%	0.135%
47	15.550	1281	1284	1287	rVV2	14857	25995	9.96%	0.666%
48	15.614	1287	1289	1298	rVV2	14721	27000	10.34%	0.692%
49	15.766	1298	1301	1311	rVB2	5574	9991	3.83%	0.256%
50	16.227	1335	1338	1341	rBV2	26947	39344	15.07%	1.008%
51	16.324	1343	1346	1350	rVB	18145	31728	12.15%	0.813%
52	16.506	1358	1361	1367	rBV	10773	15597	5.97%	0.400%
53	16.677	1372	1375	1384	rBV	9115	16241	6.22%	0.416%
54	17.030	1400	1404	1405	rBV2	78019	128245	49.12%	3.286%
55	17.066	1405	1407	1410	rVV	70750	101346	38.82%	2.596%
56	17.164	1412	1415	1434	rVB	43378	81246	31.12%	2.081%
57	17.431	1434	1437	1453	rBV	31515	58783	22.51%	1.506%
58	18.020	1483	1486	1498	rVB	2569	3735	1.43%	0.096%
59	19.068	1687	1697	1699	rBV	52553	68079	26.07%	1.744%
60	19.098	1699	1703	1732	rVB	81575	118152	45.25%	3.027%
61	19.460	1767	1776	1805	rBV	80498	114866	43.99%	2.943%
62	19.678	1813	1820	1843	rBV	53539	67816	25.97%	1.737%
63	20.378	1918	1921	1924	rBV	22561	30117	11.53%	0.772%
64	21.026	1979	1982	1993	rBV	17937	31193	11.95%	0.799%
65	21.174	1993	1996	1998	rVV	29600	39124	14.98%	1.002%
66	21.227	1998	2001	2003	rVV3	133990	261094	100.00%	6.689%
67	21.270	2003	2005	2017	rVB	95762	127914	48.99%	3.277%
68	22.056	2076	2079	2083	rBV	38112	47448	18.17%	1.216%
69	22.810	2218	2230	2236	rBV	57876	97337	37.28%	2.494%
70	22.851	2236	2242	2278	rVB	61963	109584	41.97%	2.807%
71	23.385	2386	2398	2416	rBV	40932	88490	33.89%	2.267%
72	23.484	2416	2427	2461	rVB	83296	166120	63.62%	4.256%
73	24.090	2596	2604	2618	rVB2	3616	6791	2.60%	0.174%
74	24.860	2820	2829	2850	rVB	3670	8072	3.09%	0.207%
75	25.774	3071	3096	3160	rBV4	59244	230378	88.24%	5.902%
76	26.459	3274	3296	3333	rBV2	33019	107190	41.05%	2.746%

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Acq On : 30 Sep 2021 14:18
Operator : CG/JU
Sample : SSTDICC0.2
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.2

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

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Peak separation: 5

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

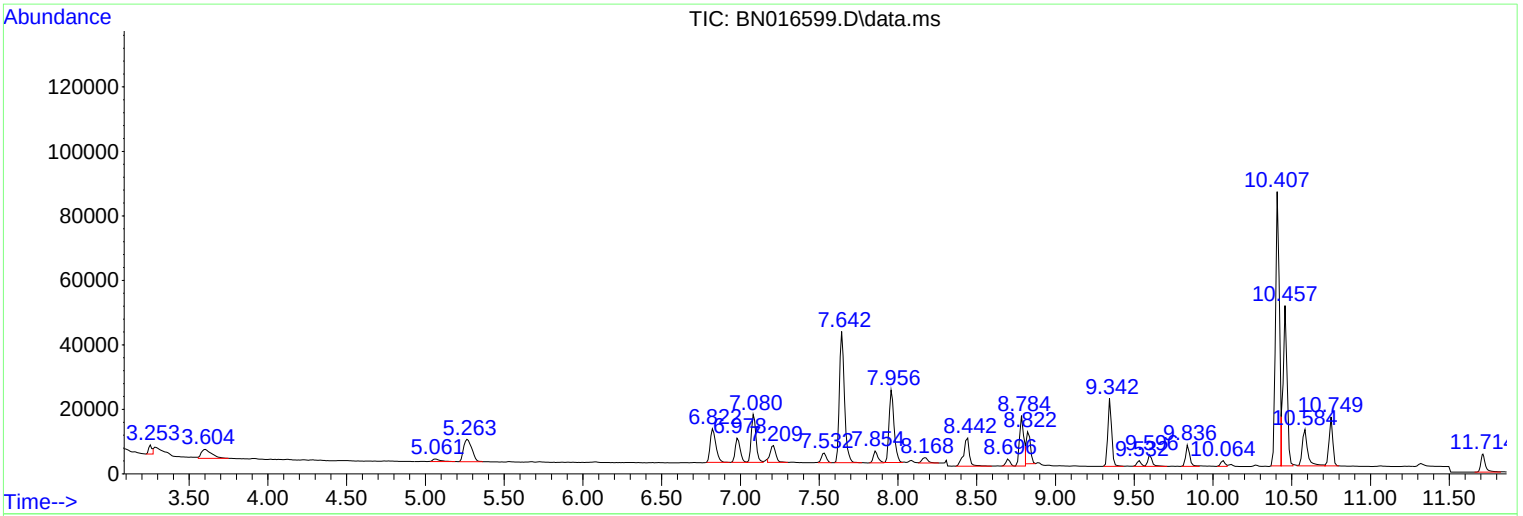
Sum of corrected areas: 3903320

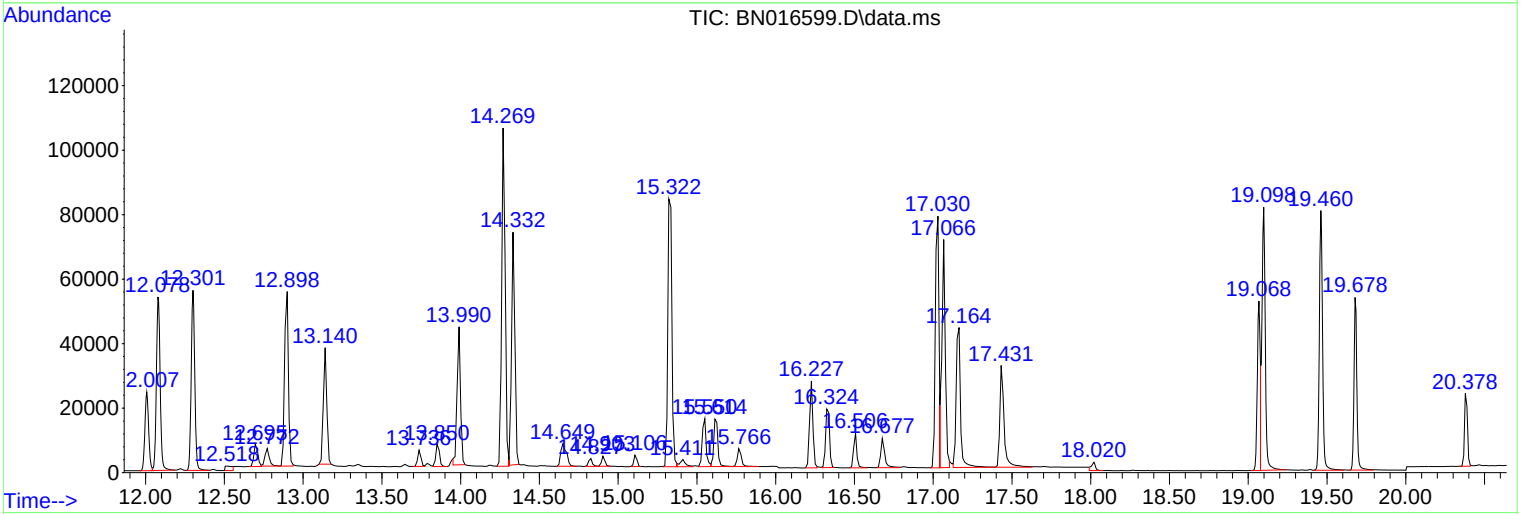
Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016599.D
Acq On : 30 Sep 2021 14:18
Operator : CG/JU
Sample : SSTDICC0.2
Misc :
ALS Vial : 3 Sample Multiplier: 1

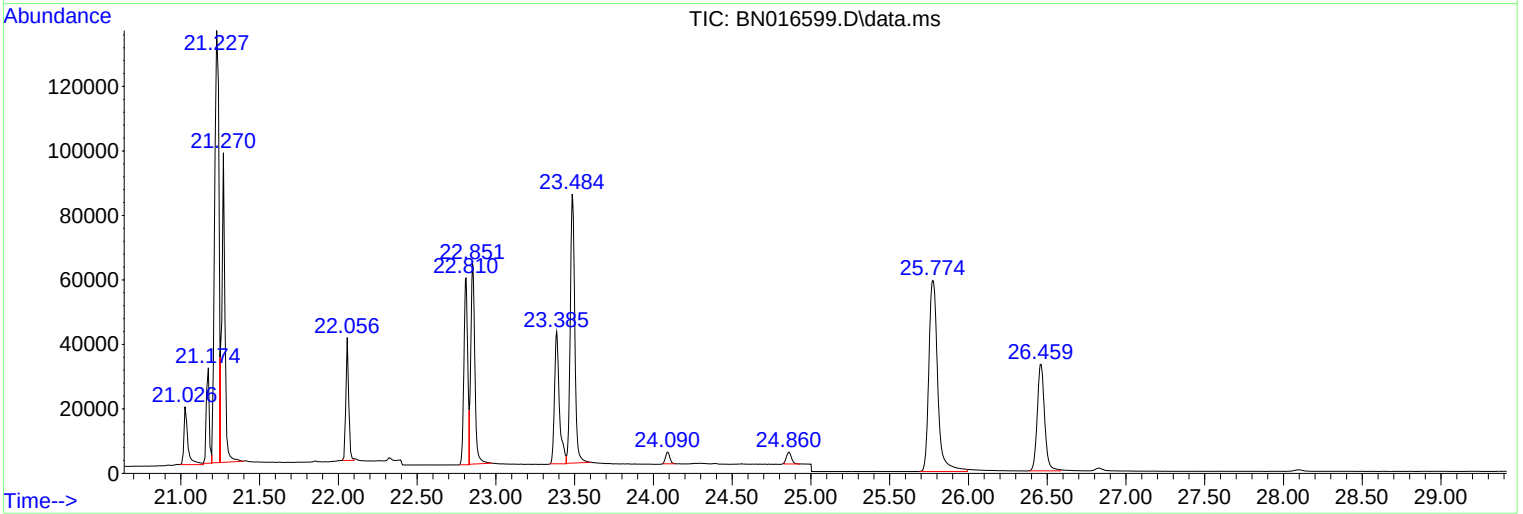
Instrument :
BNA_N
LabSampleId :
SSTDICC0.2

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 : BN016599.D
Acq On : 30 Sep 2021 14:18
Operator : CG/JU
Sample : SSTDICC0.2
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.2

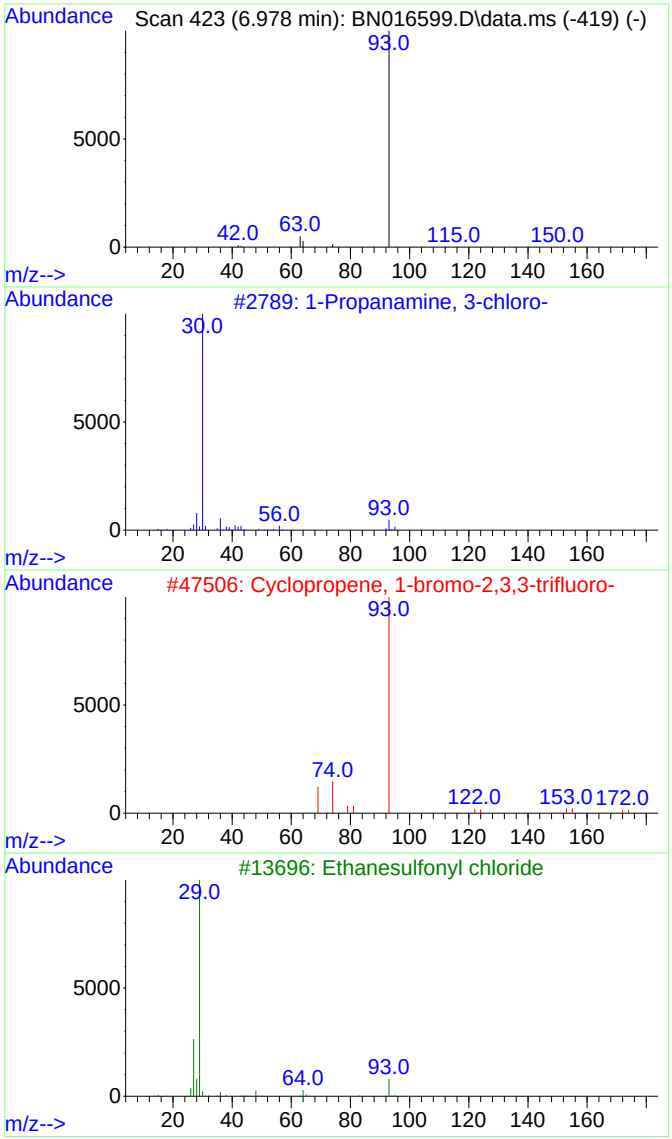
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

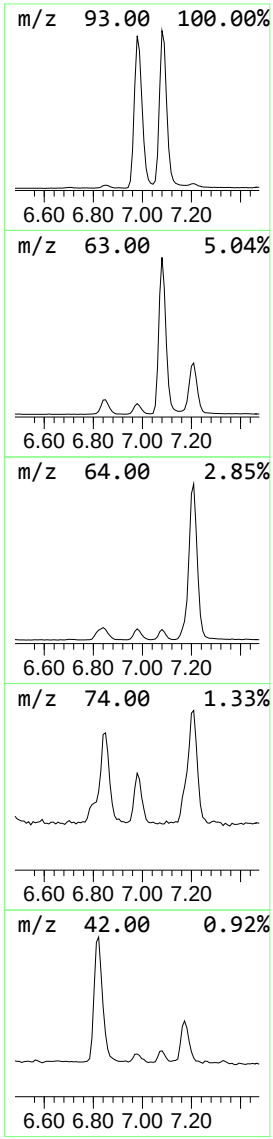
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1-Propanamine, 3-chloro- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.978	0.07 ng	16396	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanamine, 3-chloro-	93	C3H8ClN	014753-26-5	1
2	Cyclopropene, 1-bromo-2,3,3-trif...	172	C3BrF3	029777-44-4	1
3	Ethanesulfonyl chloride	128	C2H5ClO2S	000594-44-5	1
4	Carbonochloridic acid, ethyl ester	108	C3H5ClO2	000541-41-3	1
5	Ethenesulfonyl chloride	126	C2H3ClO2S	006608-47-5	1





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Sample : SSTDICC0.2
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.2

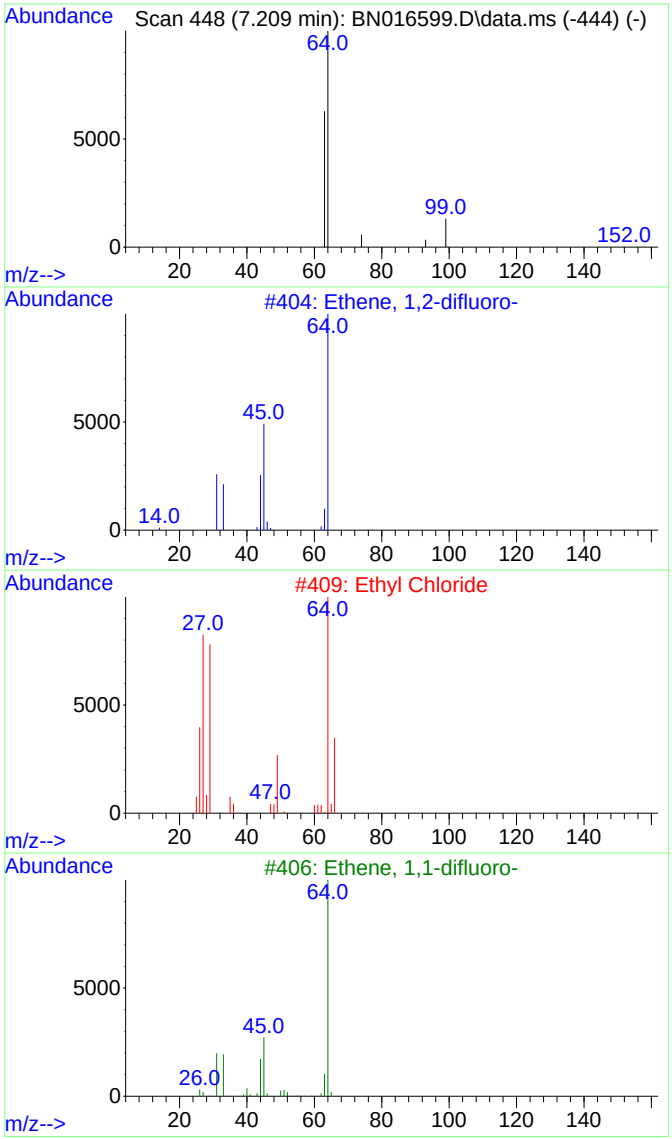
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

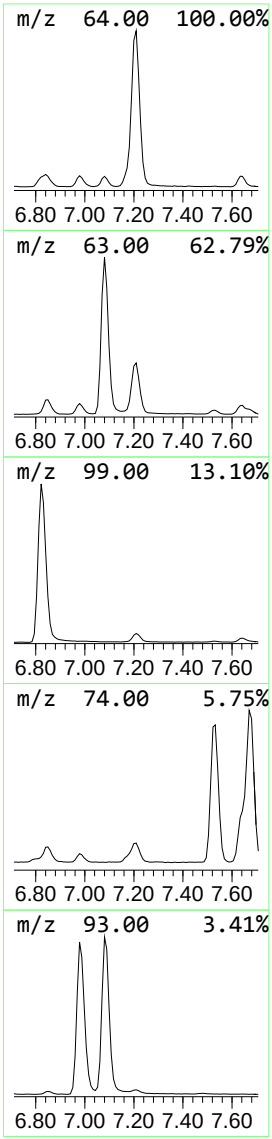
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethene, 1,2-difluoro- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.209	0.05 ng	12412	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	3
2	Ethyl Chloride	64	C2H5Cl	000075-00-3	3
3	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	3
4	Sulfur dioxide	64	O2S	007446-09-5	3
5	Pentaborane(9)	64	B5H9	019624-22-7	3





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Acq On : 30 Sep 2021 14:18
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Sample : SSTDICC0.2
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDICC0.2

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

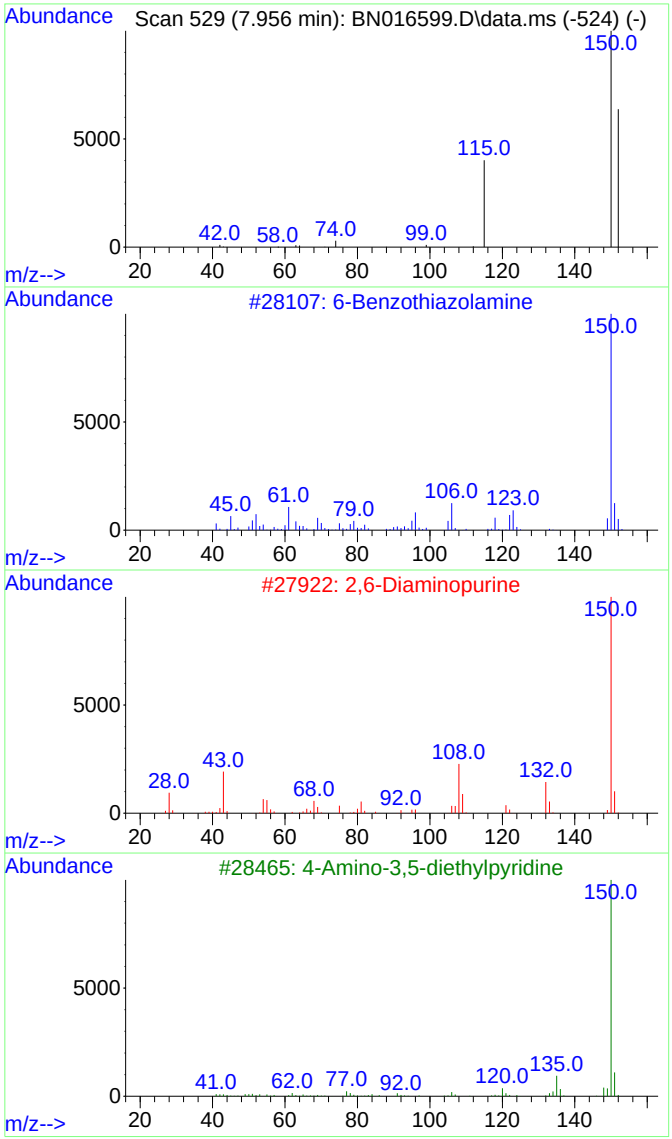
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

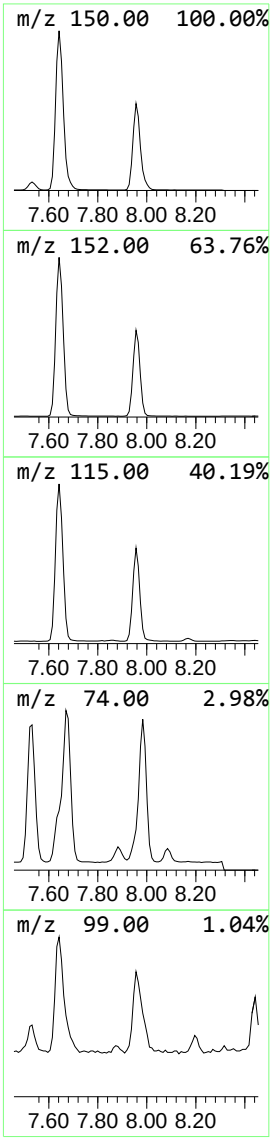
****

Peak Number 3 6-Benzothiazolamine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.956	0.22 ng	49470	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	2,6-Diaminopurine	150	C5H6N6	001904-98-9	2
3	4-Amino-3,5-diethylpyridine	150	C9H14N2	1000128-75-1	2
4	Benzene, 1,2,3,4-tetrafluoro-	150	C6H2F4	000551-62-2	2
5	2-Benzimidazolethiol	150	C7H6N2S	000583-39-1	2





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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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LabSampleId :
SSTDICC0.2

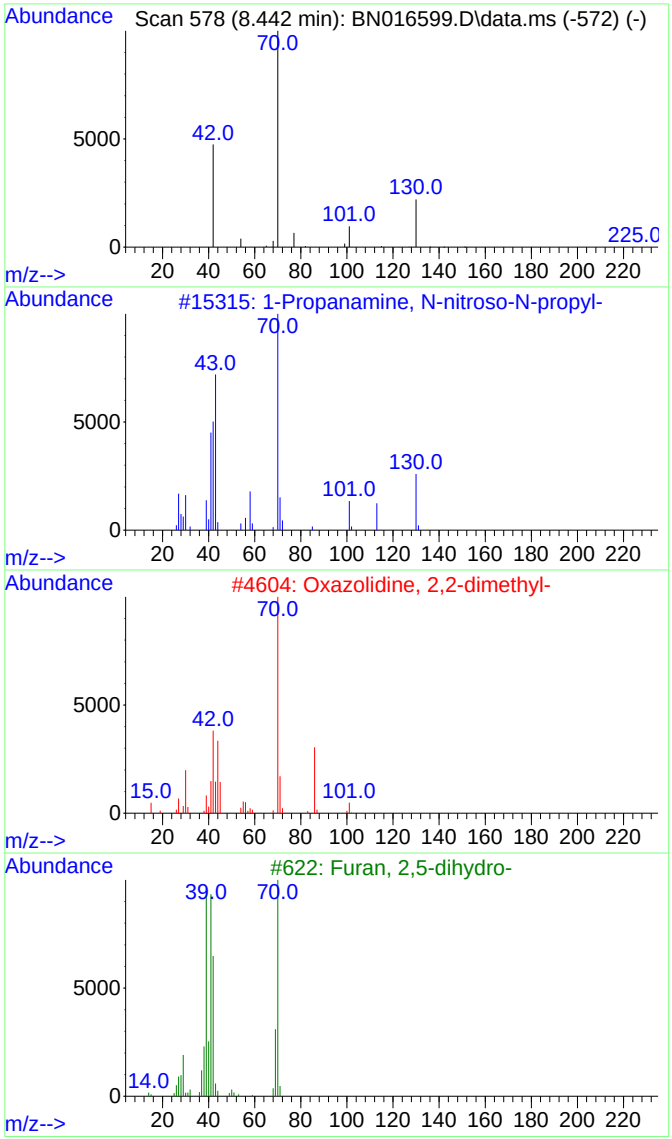
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

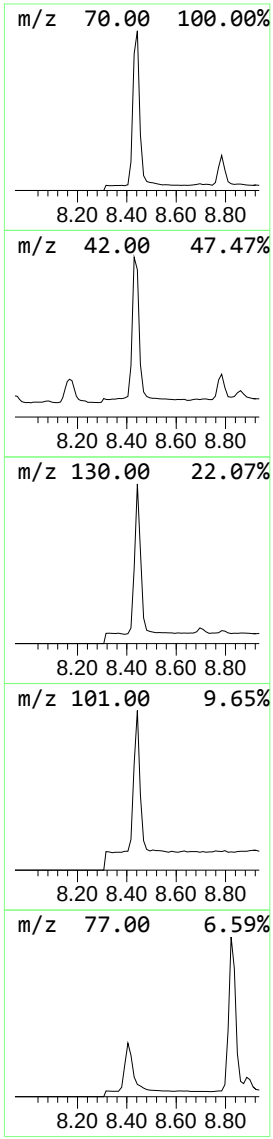
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Propanamine, N-nitroso-N-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.442	0.10 ng	22191	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	5
5	(E)-1,3-Butadien-1-ol	70	C4H6O	070411-98-2	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Sample : SSTDICC0.2
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.2

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

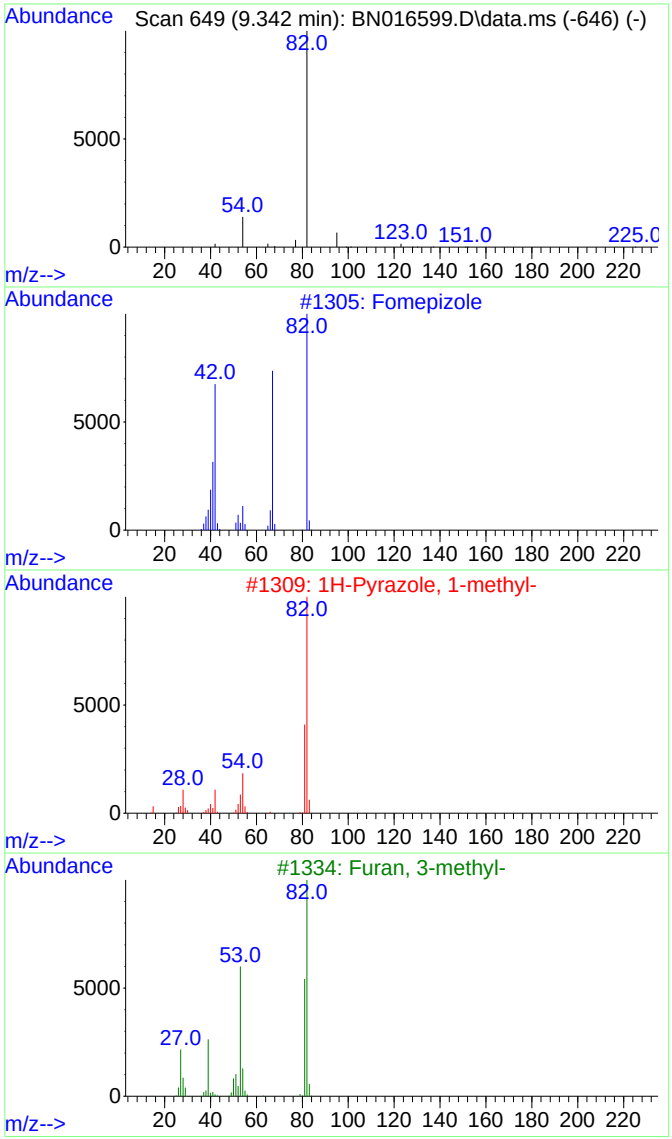
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

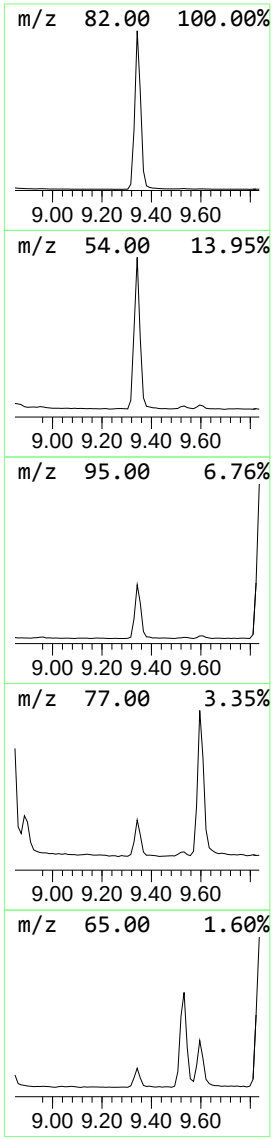
****

Peak Number 5 Fomepizole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.342	0.09 ng	35112	Naphthalene-d8	10.407

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fomepizole	82	C4H6N2	007554-65-6	5
2	1H-Pyrazole, 1-methyl-	82	C4H6N2	000930-36-9	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 : BN016599.D
Acq On : 30 Sep 2021 14:18
Operator : CG/JU
Sample : SSTDICC0.2
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.2

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

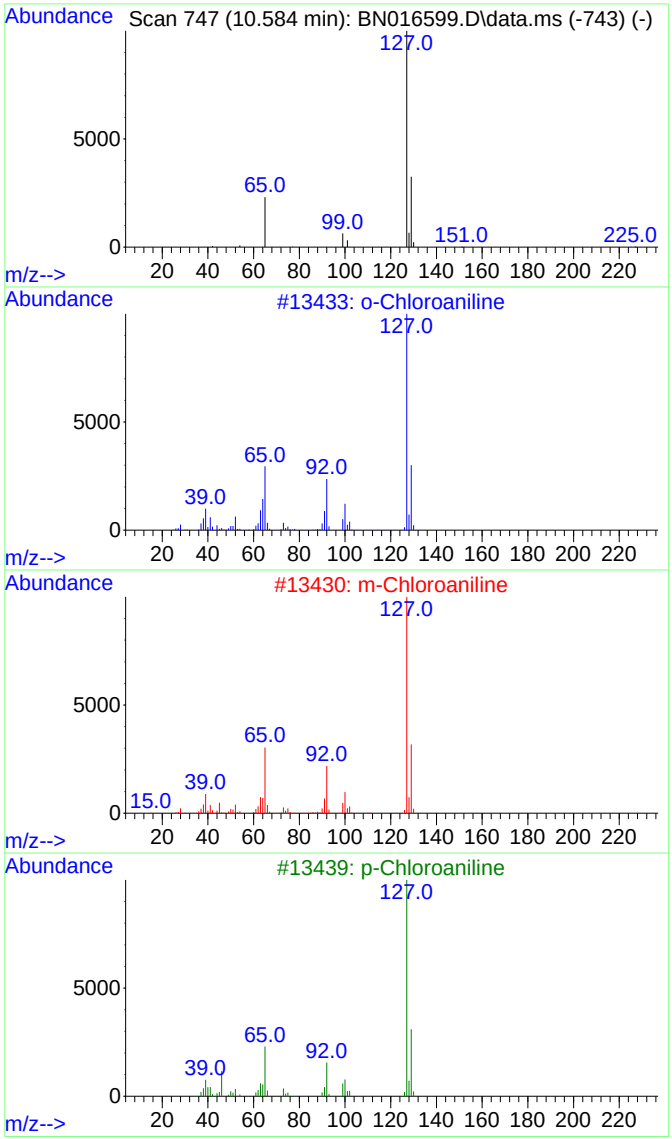
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

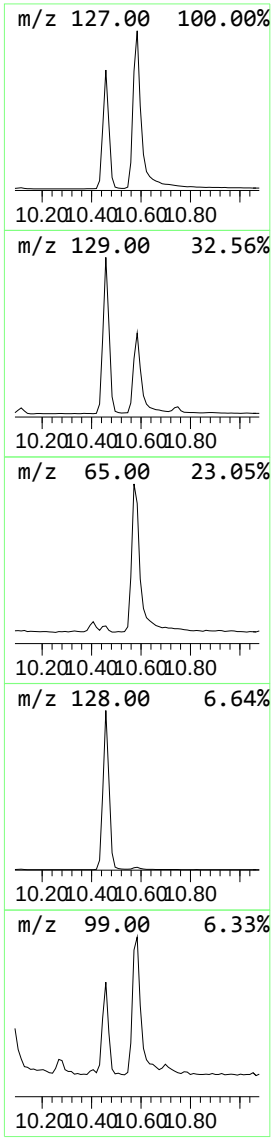
****

Peak Number 6 o-Chloroaniline Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.584	0.07 ng	26625	Naphthalene-d8	10.407

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Chloroaniline	127	C6H6ClN	000095-51-2	90
2	m-Chloroaniline	127	C6H6ClN	000108-42-9	90
3	p-Chloroaniline	127	C6H6ClN	000106-47-8	90
4	4-(Chloromethyl)pyridine	127	C6H6ClN	010445-91-7	86
5	Picloxydine	474	C20H24Cl2N10	005636-92-0	83





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Data File : BN016599.D
Acq On : 30 Sep 2021 14:18
Operator : CG/JU
Sample : SSTDICC0.2
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.2

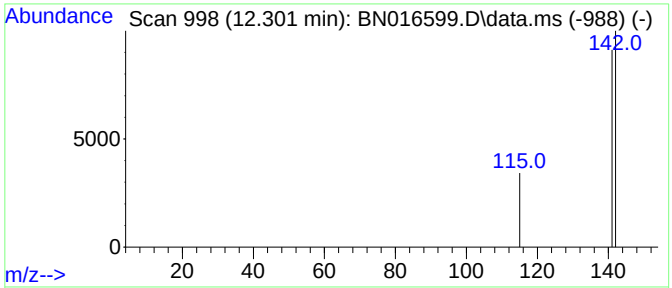
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

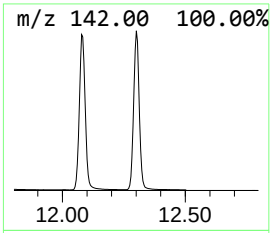
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

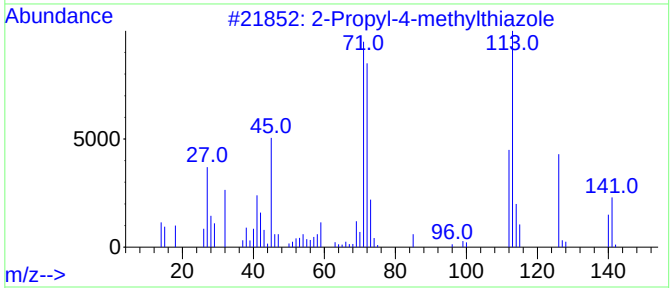
****
Peak Number 7 2-Propyl-4-methylthiazole Concentration Rank 1

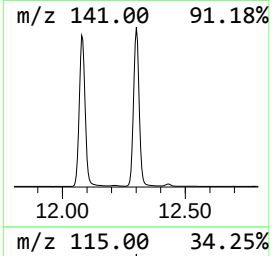
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.301	0.23 ng	87865	Naphthalene-d8	10.407

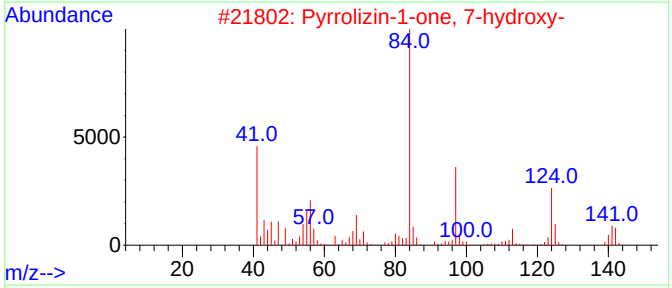
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propyl-4-methylthiazole	141	C7H11NS	052414-87-6	4
2	Pyrrolizin-1-one, 7-hydroxy-	141	C7H11NO2	1000125-96-2	3
3	Cyclopentanecarboxylic acid, eth...	142	C8H14O2	1000375-86-4	3
4	2-Propionylthiazole	141	C6H7NOS	043039-98-1	3
5	2,4(1H,3H)-Pyrimidinedione, 6-am...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

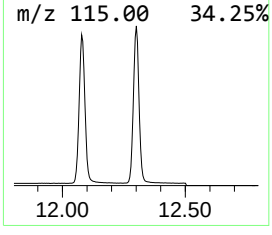


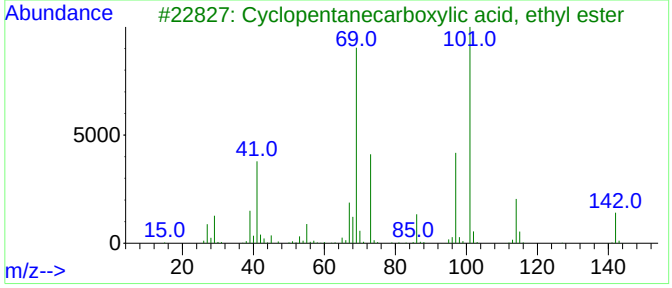












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Acq On : 30 Sep 2021 14:18
Operator : CG/JU
Sample : SSTDICC0.2
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.2

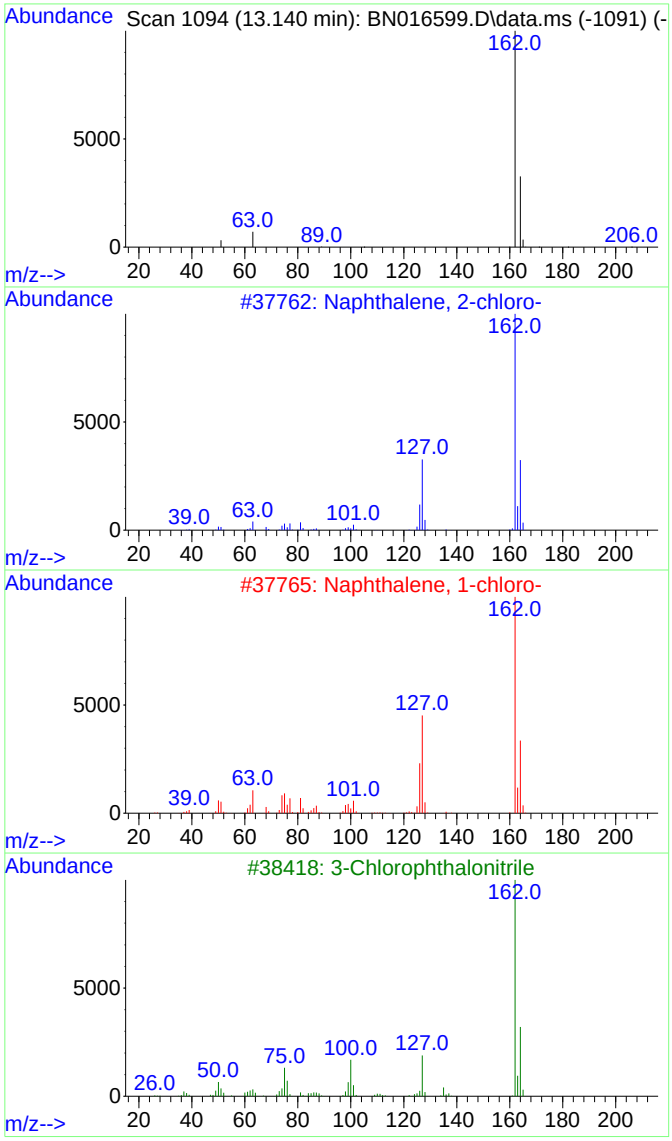
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

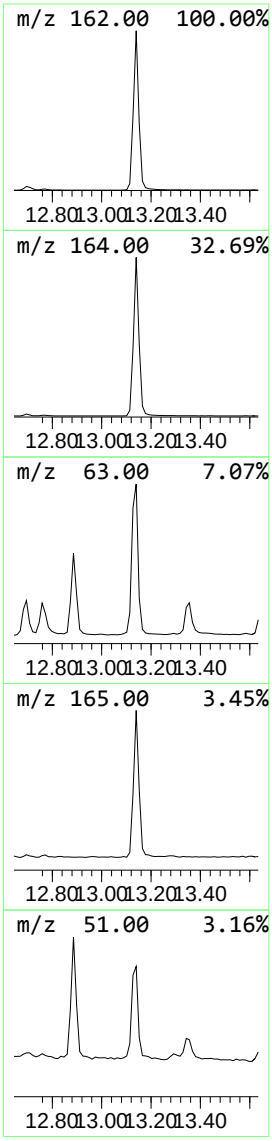
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Naphthalene, 2-chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.140	0.13 ng	53662	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-chloro-	162	C10H7Cl	000091-58-7	64
2	Naphthalene, 1-chloro-	162	C10H7Cl	000090-13-1	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





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Data File : BN016599.D
Acq On : 30 Sep 2021 14:18
Operator : CG/JU
Sample : SSTDICC0.2
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.2

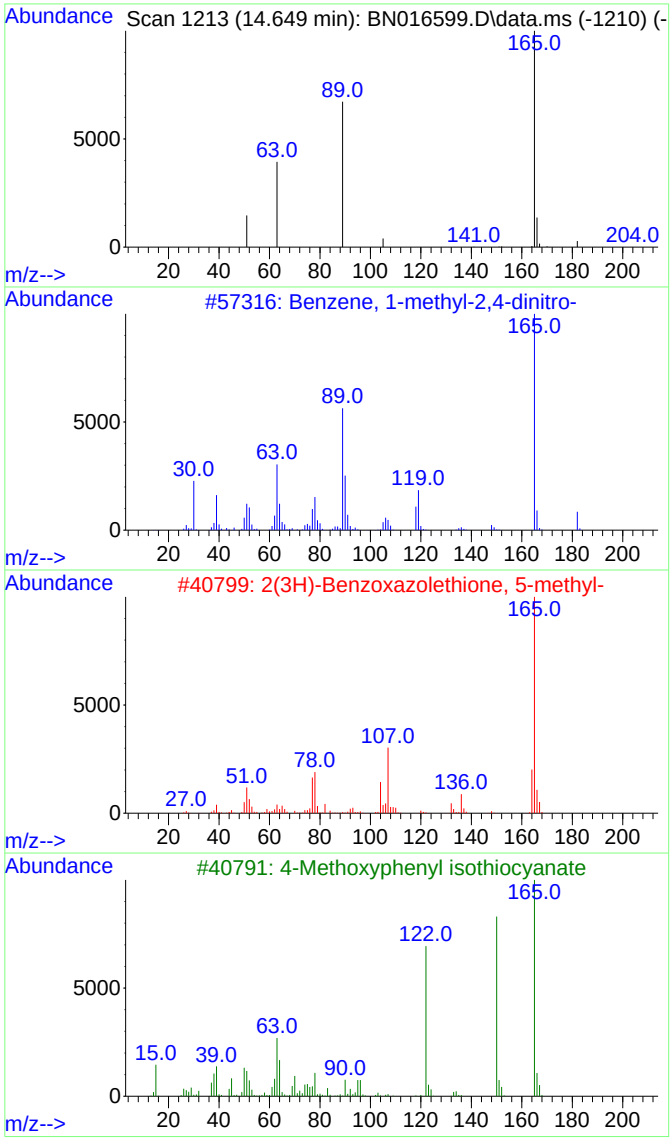
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

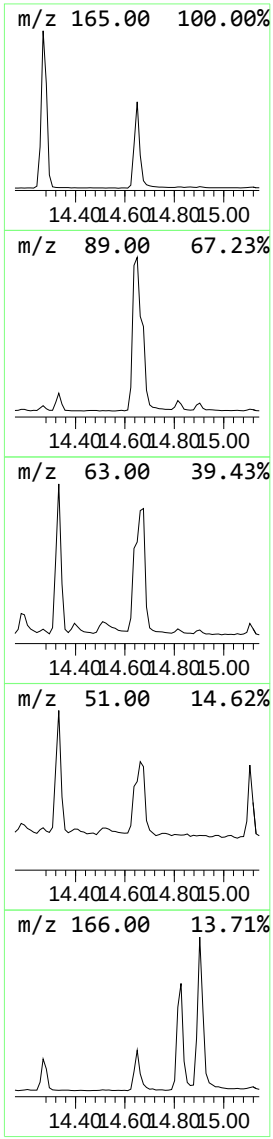
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-methyl-2,4-dinitro- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.649	0.04 ng	17652	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-2,4-dinitro-	182	C7H6N2O4	000121-14-2	64
2	2(3H)-Benzoxazolethione, 5-methyl-	165	C8H7NOS	022876-22-8	9
3	4-Methoxyphenyl isothiocyanate	165	C8H7NOS	002284-20-0	9
4	Benzene, 2-methyl-1,3-dinitro-	182	C7H6N2O4	000606-20-2	9
5	Ethanol, 1-(4-nitrophenyl)-2-[1-...	304	C17H24N2O3	1000264-75-7	9





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Sample : SSTDICC0.2
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.2

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

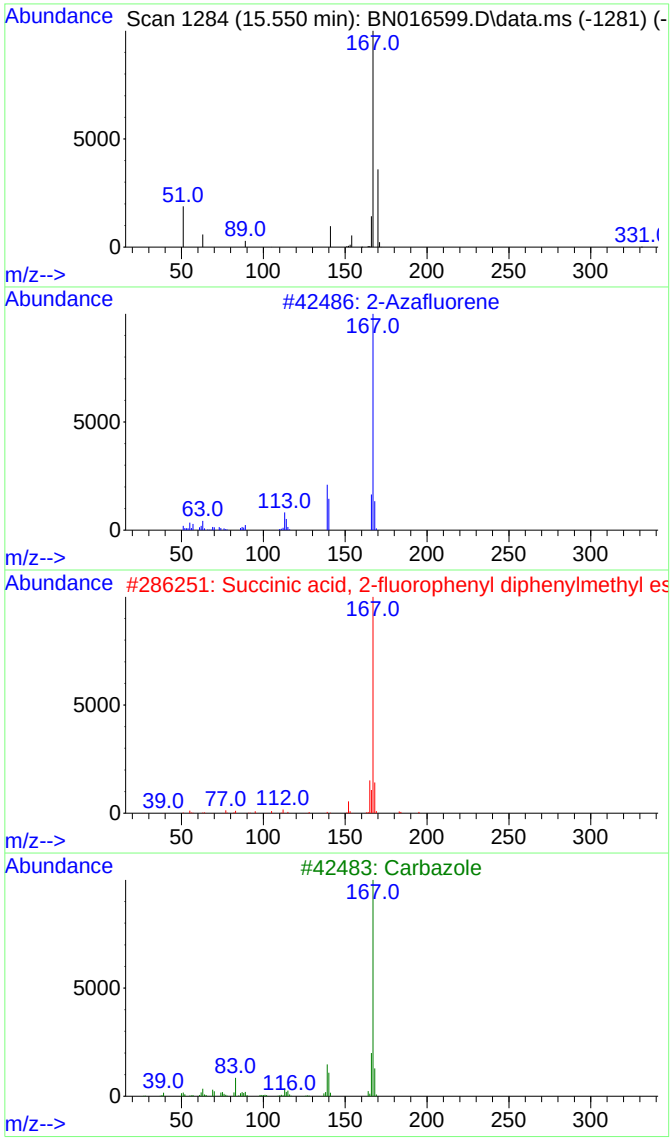
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

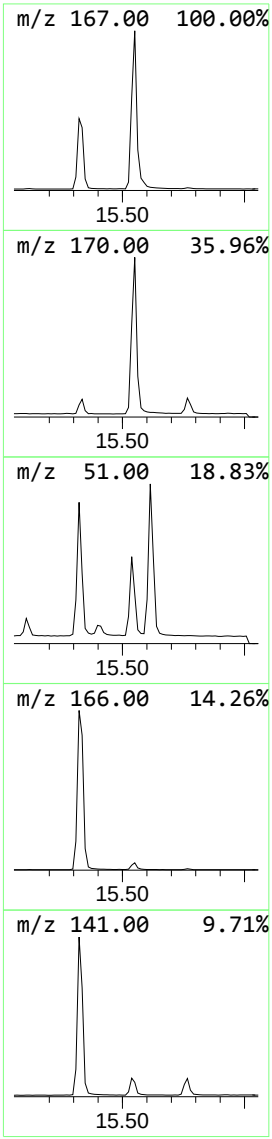
****

Peak Number 10 2-Azafluorene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.550	0.06 ng	25995	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Azafluorene	167	C12H9N	000244-40-6	9
2	Succinic acid, 2-fluorophenyl di...	378	C23H19FO4	1000390-17-0	9
3	Carbazole	167	C12H9N	000086-74-8	7
4	2-Naphthylacetonitrile	167	C12H9N	007498-57-9	7
5	2,4(1H,3H)-Pyrimidinedione, 5-me...	170	C7H10N2O3	059264-10-7	5





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Data File : BN016599.D
Acq On : 30 Sep 2021 14:18
Operator : CG/JU
Sample : SSTDICC0.2
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.2

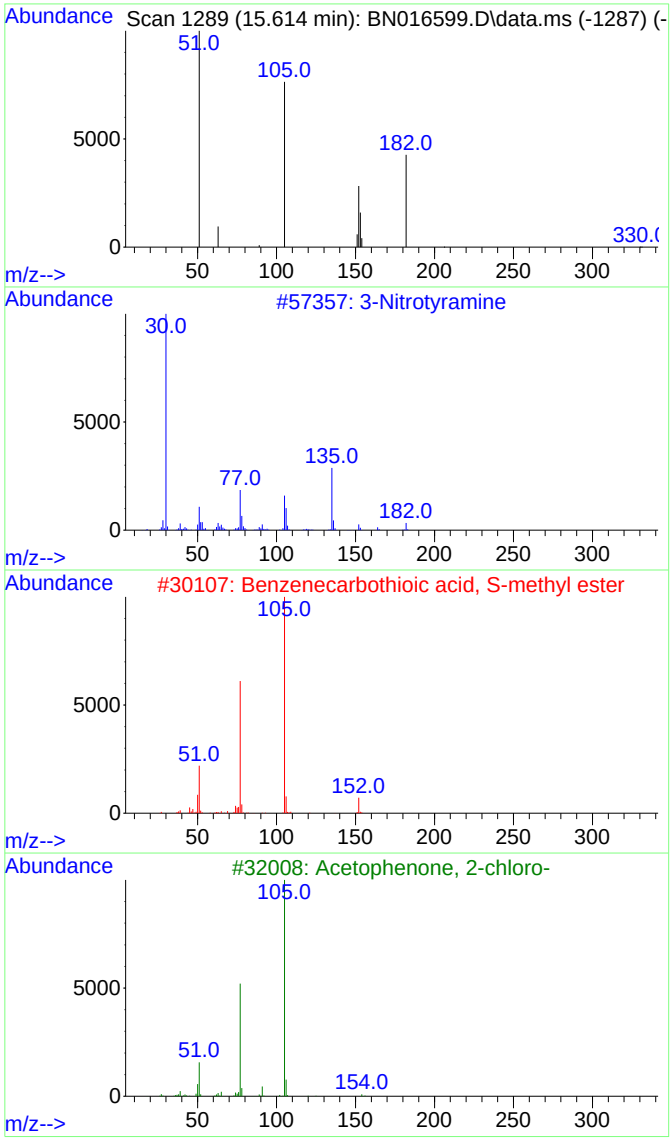
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

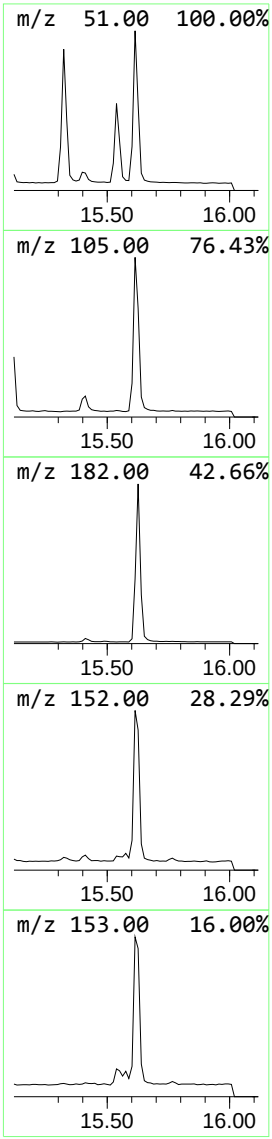
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 3-Nitrotyramine Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.614	0.07 ng	27000	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Nitrotyramine	182	C8H10N2O3	049607-15-0	4
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	3
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	3
4	Propiolonitrile	51	C3HN	001070-71-9	3
5	Benzeneethanamine, 4-methoxy-	151	C9H13NO	000055-81-2	3





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Data File : BN016599.D
Acq On : 30 Sep 2021 14:18
Operator : CG/JU
Sample : SSTDICC0.2
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.2

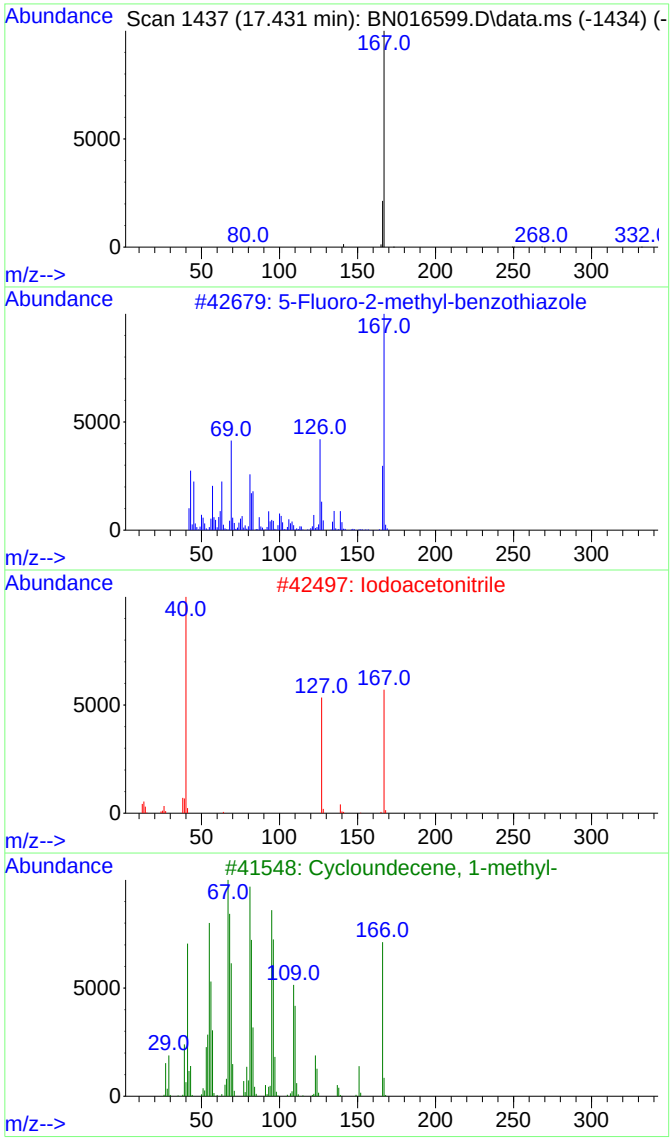
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

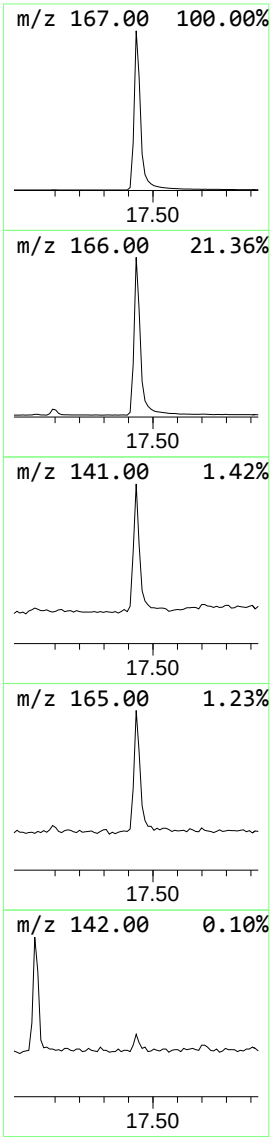
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 5-Fluoro-2-methyl-benzothia... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.431	0.18 ng	58783	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





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Sample : SSTDICC0.2
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.2

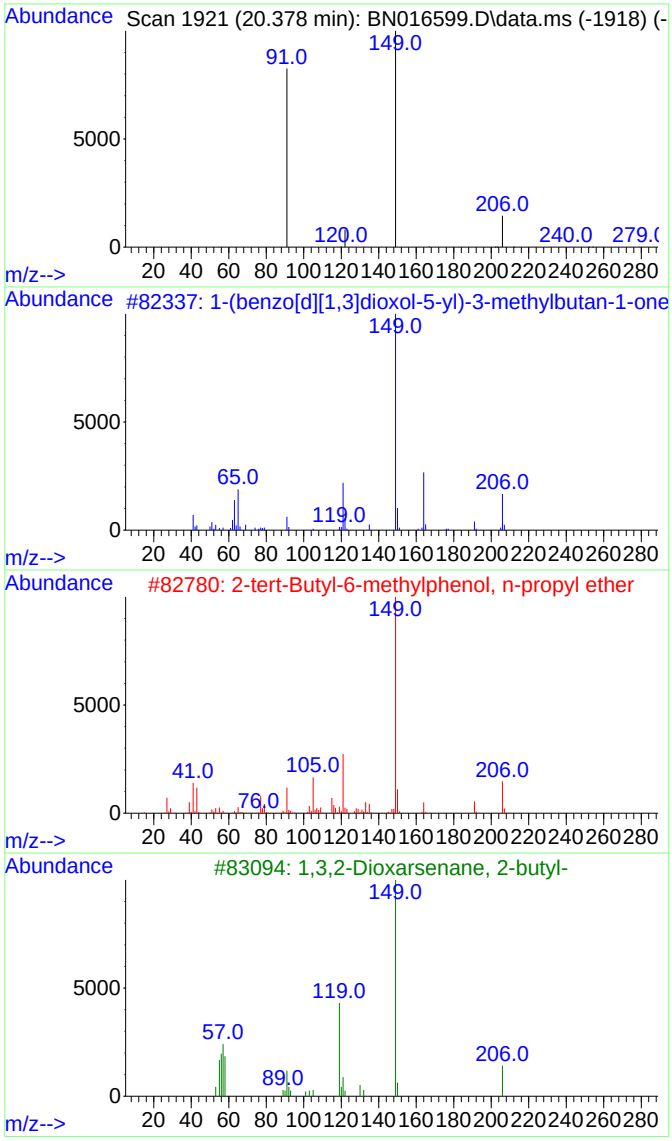
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

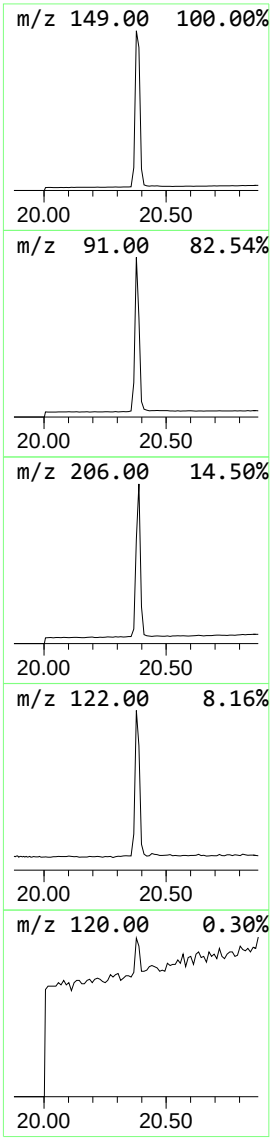
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 1-(benzo[d][1,3]dioxol-5-yl... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.378	0.05 ng	30117	Chrysene-d12	21.238

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(benzo[d][1,3]dioxol-5-yl)-3-m...	206	C12H14O3	1000456-66-2	9
2	2-tert-Butyl-6-methylphenol, n-p...	206	C14H22O	1000395-19-2	5
3	1,3,2-Dioxarsenane, 2-butyl-	206	C7H15AsO2	042541-33-3	5
4	2-Methyl-2-(4'-methoxyphenyl)pen...	206	C13H18O2	185700-49-6	5
5	Benzene, 1-isothiocyanato-4-methyl-	149	C8H7NS	000622-59-3	4





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Sample : SSTDICC0.2
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.2

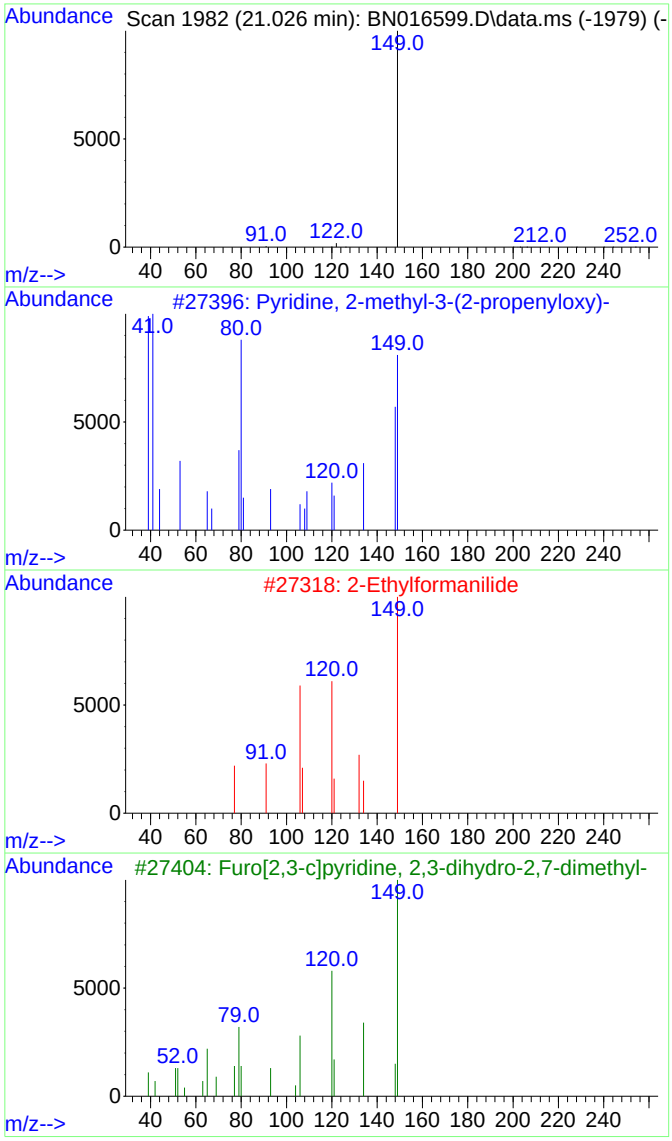
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

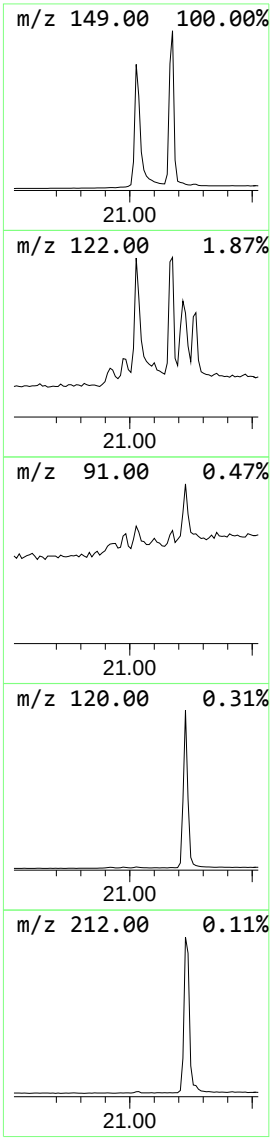
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 Pyridine, 2-methyl-3-(2-pro... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.026	0.05 ng	31193	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





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Sample : SSTDICC0.2
Misc :
ALS Vial : 3 Sample Multiplier: 1

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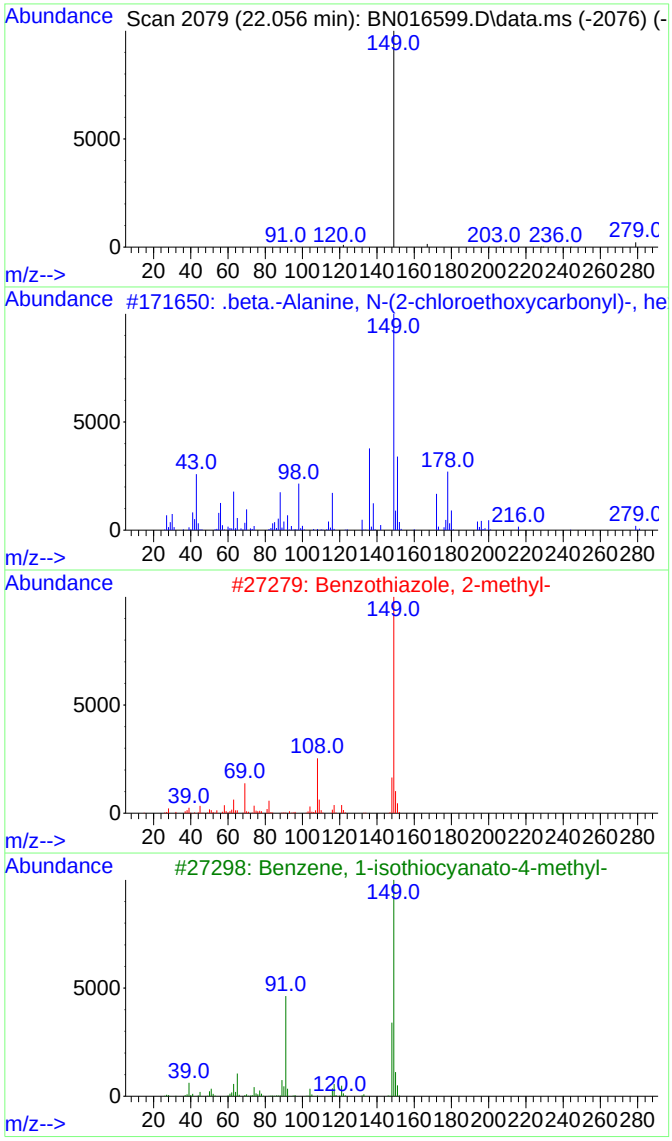
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

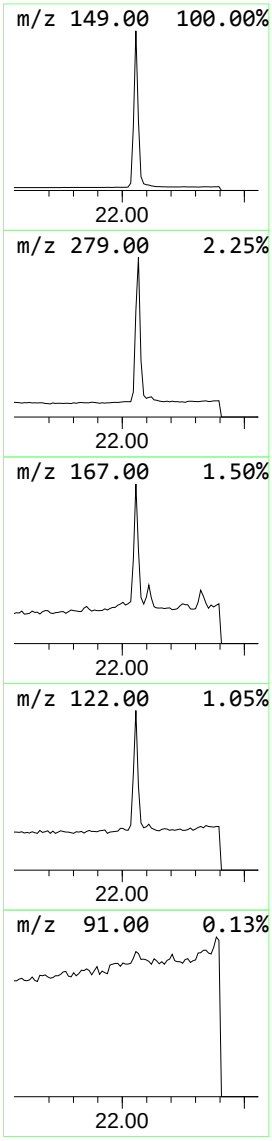
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 .beta.-Alanine, N-(2-chloro... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.056	0.07 ng	47448	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	Benzothiazole, 2-methyl-	149	C8H7NS	000120-75-2	4
3	Benzene, 1-isothiocyanato-4-methyl-	149	C8H7NS	000622-59-3	4
4	Phthalic acid, 7-bromoheptyl oct...	454	C23H35BrO4	1000415-52-2	4
5	Pyridine, pentamethyl-	149	C10H15N	003748-83-2	4





Tentatively Identified Compound (LSC) summary

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Data File : BN016599.D
Acq On : 30 Sep 2021 14:18
Operator : CG/JU
Sample : SSTDICC0.2
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ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDICC0.2

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
1-Propanamine, ...	6.978	0.1	ng	16396	1	7.642	90876	0.4
Ethene, 1,2-dif...	7.209	0.1	ng	12412	1	7.642	90876	0.4
6-Benzothiazola...	7.956	0.2	ng	49470	1	7.642	90876	0.4
1-Propanamine, ...	8.442	0.1	ng	22191	1	7.642	90876	0.4
Fomepizole	9.342	0.1	ng	35112	2	10.407	150277	0.4
o-Chloroaniline	10.584	0.1	ng	26625	2	10.407	150277	0.4
2-Propyl-4-meth...	12.301	0.2	ng	87865	2	10.407	150277	0.4
Naphthalene, 2-...	13.140	0.1	ng	53662	3	14.269	161471	0.4
Benzene, 1-meth...	14.649	0.0	ng	17652	3	14.269	161471	0.4
2-Azafluorene	15.550	0.1	ng	25995	3	14.269	161471	0.4
3-Nitrotyramine	15.614	0.1	ng	27000	3	14.269	161471	0.4
5-Fluoro-2-meth...	17.431	0.2	ng	58783	4	17.030	128245	0.4
1-(benzo[d][1,3...	20.378	0.0	ng	30117	5	21.238	261094	0.4
Pyridine, 2-met...	21.026	0.0	ng	31193	5	21.238	261094	0.4
.beta.-Alanine,...	22.056	0.1	ng	47448	5	21.238	261094	0.4