LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016603.D
Acq On : 30 Sep 2021 16:44
Operator : CG/JU
Sample : SSTDICC3.2
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDICC3.2

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: BN016603.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	15	19	20	rBV	53439	75761	2.14%	0.148%
2	3.281	20	22	46	rVB	32701	154626	4.37%	0.301%
3	3.576	50	54	86	rBV2	50543	221525	6.26%	0.431%
4	5.254	231	236	263	rBV2	114269	425172	12.01%	0.828%
5	6.822	401	406	418	rBV	197006	481813	13.61%	0.938%
6	6.978	418	423	429	rVV	137827	296222	8.36%	0.577%
7	7.080	429	434	440	rVV	260595	509213	14.38%	0.992%
8	7.200	440	447	468	rVB	90675	242863	6.86%	0.473%
9	7.532	477	483	489	rVB	46792	104364	2.95%	0.203%
10	7.670	490	498	512	rVB2	54214	195562	5.52%	0.381%
11	7.956	524	529	538	rVB2	324266	724124	20.45%	1.410%
12	8.168	547	552	557	rBV	20688	51113	1.44%	0.100%
13	8.442	571	578	581	rBV2	167322	413920	11.69%	0.806%
14	8.696	594	598	601	rBV	32105	60333	1.70%	0.117%
15	8.784	601	605	607	rBV	325576	662438	18.71%	1.290%
16	8.822	607	608	612	rVB	255691	362198	10.23%	0.705%
17	9.342	646	649	653	rBV	432141	687345	19.41%	1.339%
18	9.532	660	664	666	rBV	35243	63804	1.80%	0.124%
19	9.596	666	669	673	rVB	77860	123325	3.48%	0.240%
20	9.836	685	688	691	rBV	135754	211360	5.97%	0.412%
21	10.052	702	705	709	rBV	37708	75821	2.14%	0.148%
22	10.407	729	733	734	rBV	85539	144853	4.09%	0.282%
23	10.457	734	737	741	rVV	775546	1293218	36.52%	2.518%
24	10.571	743	746	756	rVV	284941	541061	15.28%	1.054%
25	10.749	757	760	763	rVB	237299	379077	10.70%	0.738%
26	11.306	801	804	814	rBV	27845	59720	1.69%	0.116%
27	11.709	853	865	905	rBV	143211	232232	6.56%	0.452%
28	12.007	920	932	940	rBV	406890	658689	18.60%	1.283%
29	12.078	940	948	971	rVV	881149	1391138	39.28%	2.709%
30	12.301	988	998	1020	rVV	861098	1356140	38.29%	2.641%
31	12.695	1056	1059	1062	rBV	157724	257029	7.26%	0.501%
32	12.772	1062	1065	1068	rVV	129096	234530	6.62%	0.457%
33	12.898	1071	1075	1078	rBV	795218	1353904	38.23%	2.637%
34	13.140	1091	1094	1097	rVB	612797	920999	26.01%	1.794%
35	13.736	1138	1141	1143	rVV	96495	135999	3.84%	0.265%
36	13.787	1143	1145	1147	rVV	30595	41898	1.18%	0.082%

LSC Area Percent Report

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Sample : SSTDICC3.2
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDICC3.2

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	1147	1150	1154	rVB2	209249	337451	9.53%	0.657%
38	13.990	1158	1161	1164	rVB	876819	1297133	36.63%	2.526%
39	14.269	1180	1183	1185	rBV	106617	156591	4.42%	0.305%
40	14.332	1185	1188	1191	rVV	1177147	1721040	48.60%	3.351%
41	14.383	1191	1192	1198	rVV	24301	40558	1.15%	0.079%
42	14.649	1209	1213	1218	rBV2	235165	486585	13.74%	0.948%
43	14.827	1223	1227	1230	rBV	53236	93394	2.64%	0.182%
44	14.903	1230	1233	1236	rBV	78068	108532	3.06%	0.211%
45	15.106	1247	1249	1252	rBV	64549	92217	2.60%	0.180%
46	15.322	1263	1266	1270	rBV2	1492079	2479867	70.02%	4.829%
47	15.411	1270	1273	1276	rVV2	80153	132082	3.73%	0.257%
48	15.550	1280	1284	1287	rVV2	284475	499963	14.12%	0.974%
49	15.614	1287	1289	1293	rVB2	360881	612767	17.30%	1.193%
50	15.766	1298	1301	1304	rBV2	129516	204583	5.78%	0.398%
51	16.226	1335	1338	1341	rBV2	482511	676555	19.10%	1.318%
52	16.324	1343	1346	1350	rVV	282563	486116	13.73%	0.947%
53	16.506	1358	1361	1364	rBV	264757	331456	9.36%	0.645%
54	16.677	1372	1375	1378	rBV	264598	384044	10.84%	0.748%
55	17.030	1400	1404	1405	rBV2	74342	148789	4.20%	0.290%
56	17.066	1405	1407	1410	rVB	1108797	1477040	41.71%	2.876%
57	17.151	1411	1414	1418	rBV	849142	1385363	39.12%	2.698%
58	17.431	1434	1437	1440	rBV	698902	967739	27.33%	1.885%
59	18.020	1483	1486	1507	rVB	57938	72521	2.05%	0.141%
60	19.068	1686	1697	1700	rBV	902836	1276960	36.06%	2.487%
61	19.098	1700	1703	1739	rVB	1338744	1667386	47.08%	3.247%
62	19.460	1766	1776	1813	rBV	1378582	1829611	51.66%	3.563%
63	19.678	1813	1820	1852	rVB	821398	1004229	28.36%	1.956%
64	20.388	1919	1922	1924	rBV	466983	657197	18.56%	1.280%
65	21.174	1993	1996	1998	rBV	663642	801804	22.64%	1.561%
66	21.217	1998	2000	2003	rVV	1445514	1949527	55.05%	3.796%
67	21.270	2003	2005	2008	rVB	1491122	1754716	49.55%	3.417%
68	22.056	2076	2079	2096	rVB	794072	1089263	30.76%	2.121%
69	22.810	2216	2230	2236	rBV	945389	1562666	44.13%	3.043%
70	22.855	2236	2243	2300	rVB	938627	1591192	44.93%	3.099%
71	23.385	2384	2398	2417	rBV	761533	1412661	39.89%	2.751%
72	23.484	2418	2427	2479	rVB	77021	169055	4.77%	0.329%
73	25.778	3062	3097	3202	rBV3	1006286	3541417	100.00%	6.896%
74	26.462	3273	3297	3386	rBV	539454	1707897	48.23%	3.326%

Sum of corrected areas: 51351356

Instrument :
BNA_N
LabSampleId :
SSTDICC3.2

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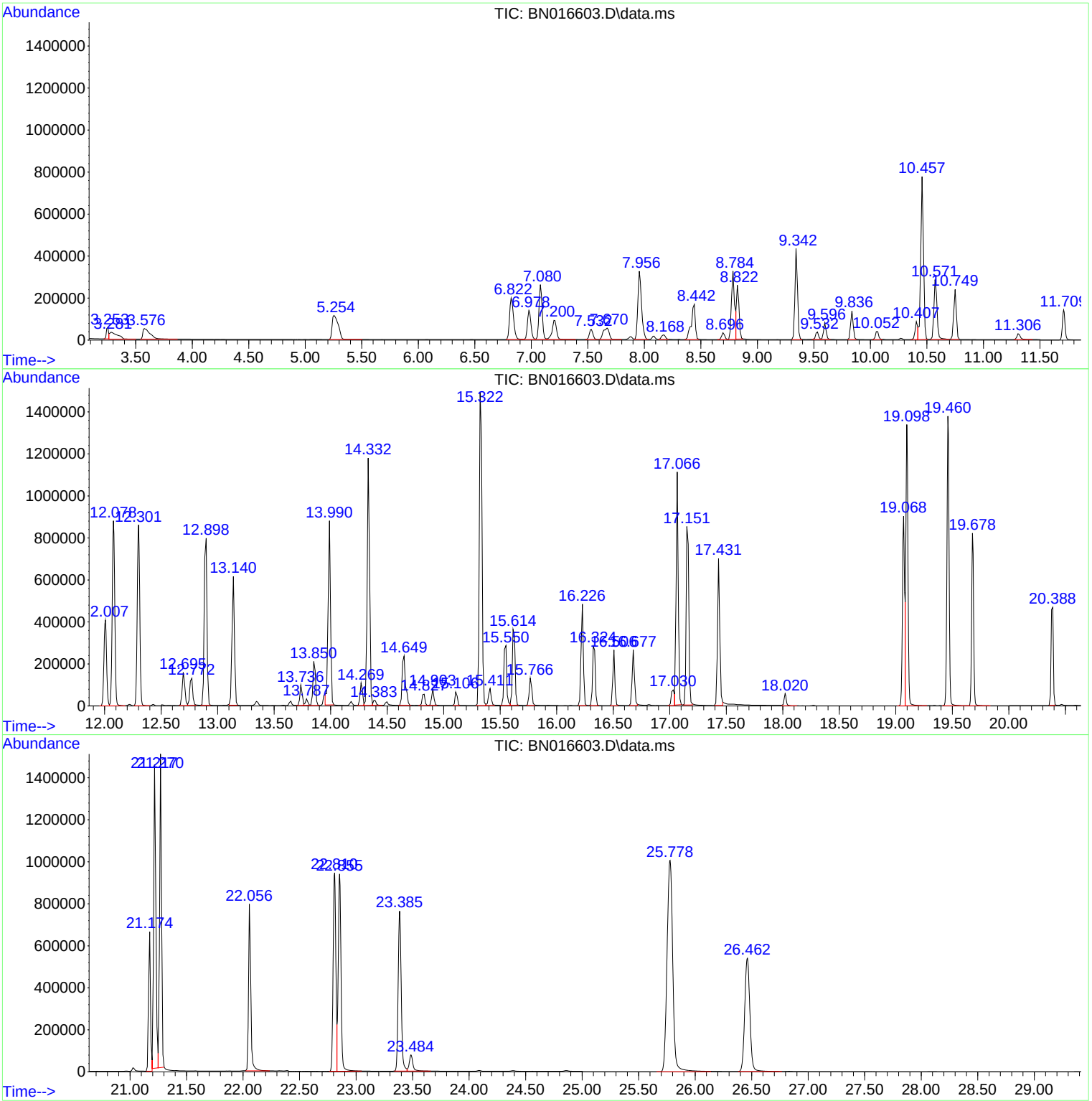
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC3.2

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



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Data File : BN016603.D
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Operator : CG/JU
Sample : SSTDICC3.2
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC3.2

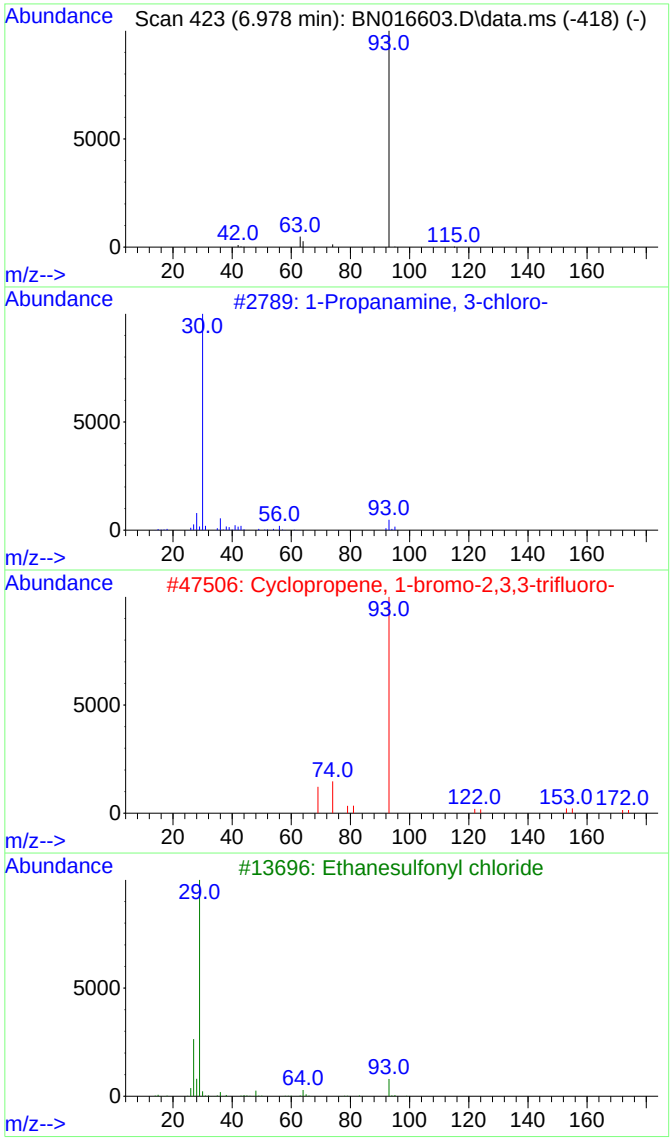
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

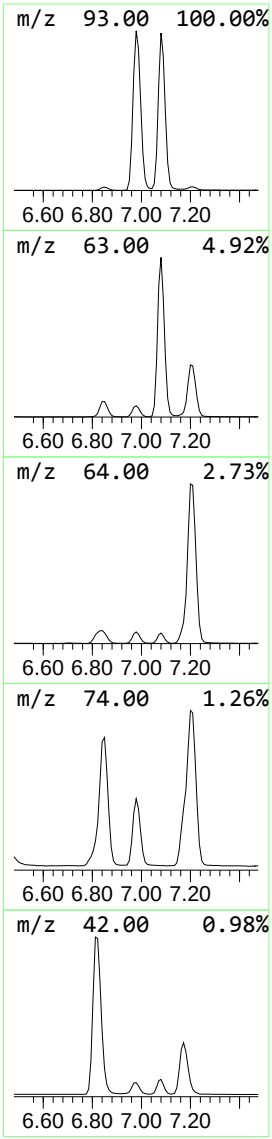
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1-Propanamine, 3-chloro- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.978	0.61 ng	296222	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





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016603.D
Acq On : 30 Sep 2021 16:44
Operator : CG/JU
Sample : SSTDICC3.2
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC3.2

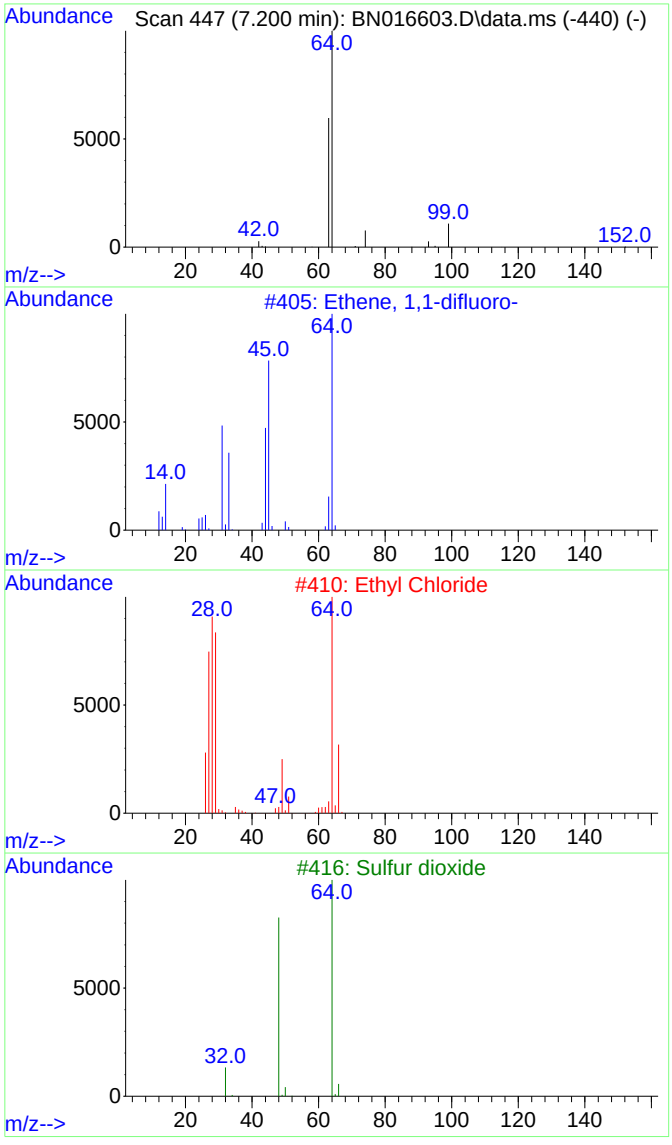
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

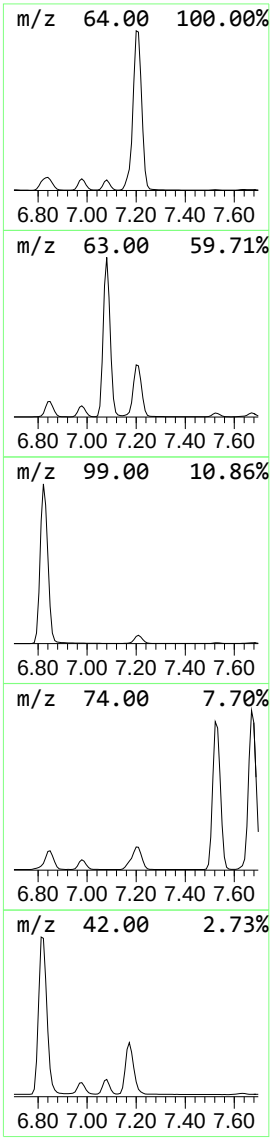
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethene, 1,1-difluoro- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.200	0.50 ng	242863	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	3
2	Ethyl Chloride	64	C2H5Cl	000075-00-3	3
3	Sulfur dioxide	64	O2S	007446-09-5	3
4	Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	3
5	(S)-(-)-2-Chloropropionic acid	108	C3H5ClO2	029617-66-1	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016603.D
Acq On : 30 Sep 2021 16:44
Operator : CG/JU
Sample : SSTDICC3.2
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC3.2

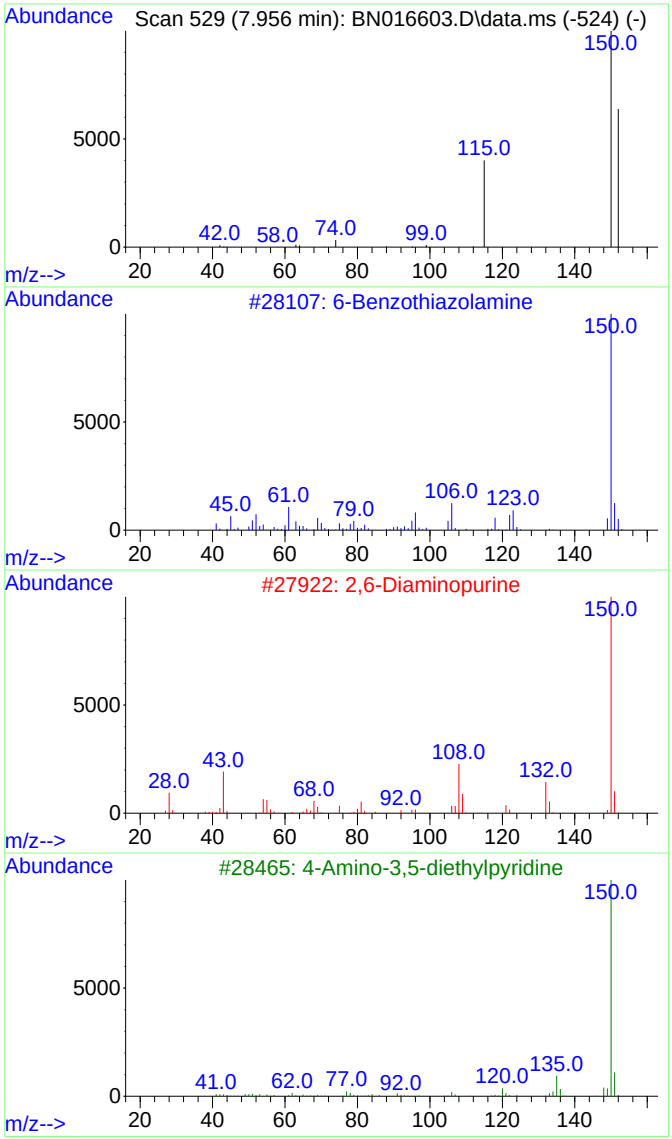
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

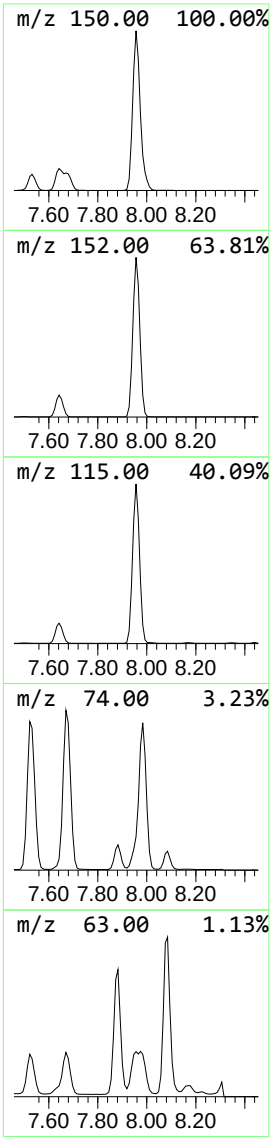
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 6-Benzothiazolamine Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.956	1.48 ng	724124	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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Operator : CG/JU
Sample : SSTDICC3.2
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC3.2

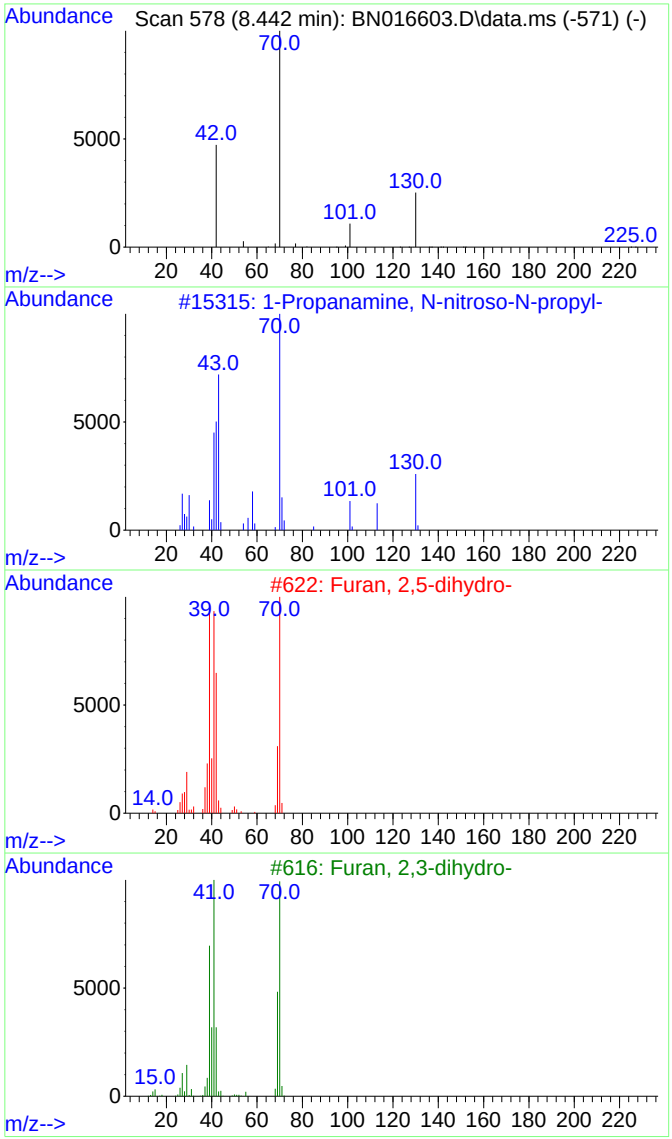
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

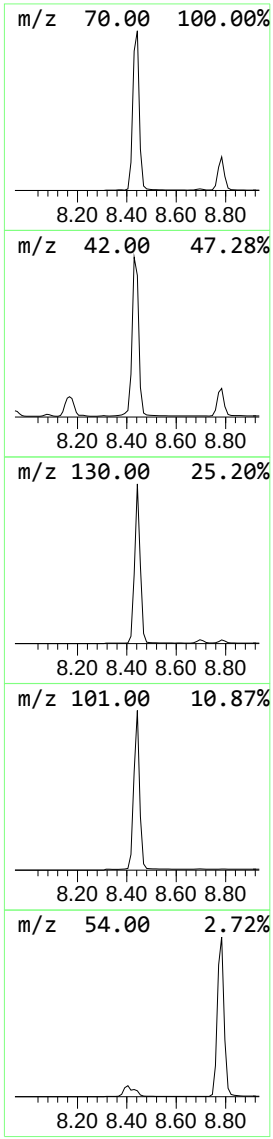
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Propanamine, N-nitroso-N-... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.442	0.85 ng	413920	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	78
2	Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	4
3	Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	4
4	2-Butenal, (E)-	70	C4H6O	000123-73-9	4
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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Operator : CG/JU
Sample : SSTDICC3.2
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC3.2

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

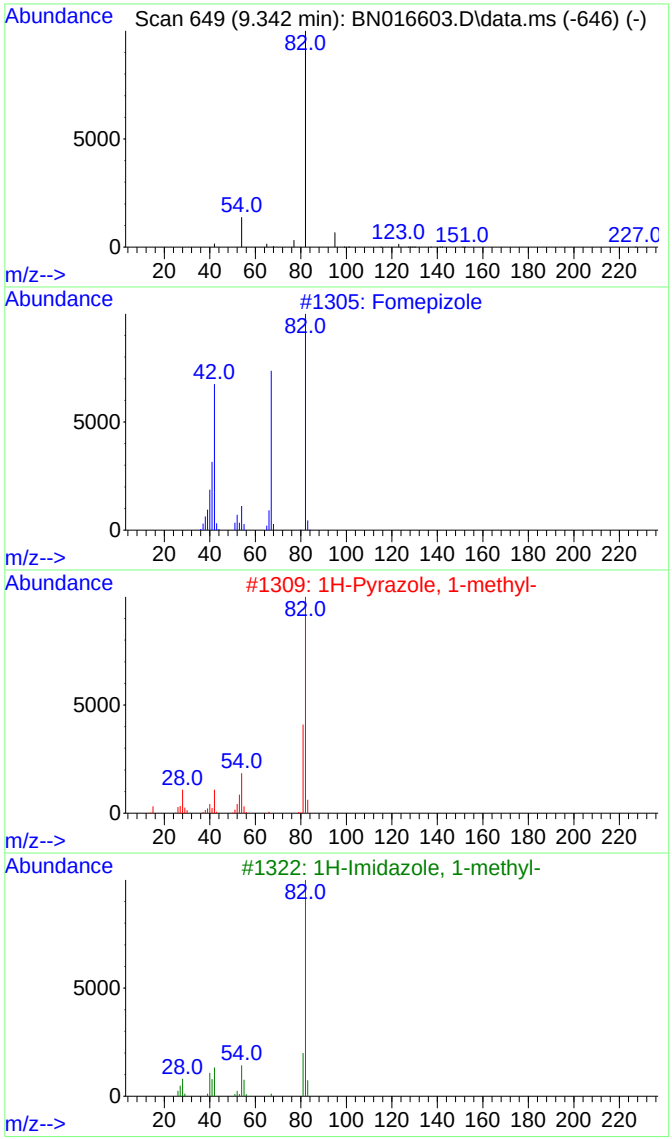
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

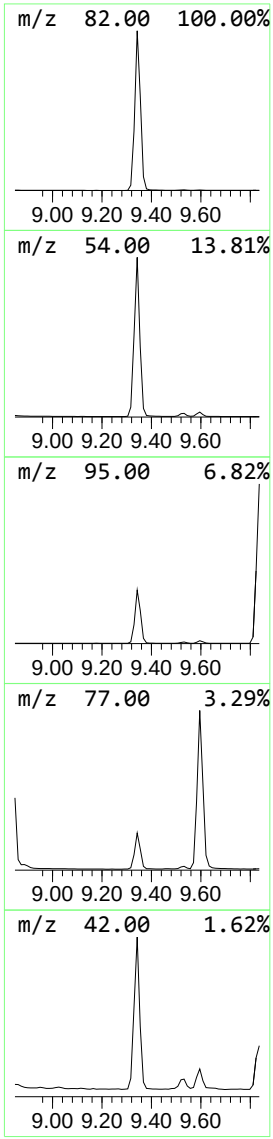
****

Peak Number 5 Fomepizole Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.342	1.90 ng	687345	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	1H-Imidazole, 1-methyl-	82	C4H6N2	000616-47-7	4
4	Furan, 3-methyl-	82	C5H6O	000930-27-8	4
5	Furan, 2-methyl-	82	C5H6O	000534-22-5	4





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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC3.2

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

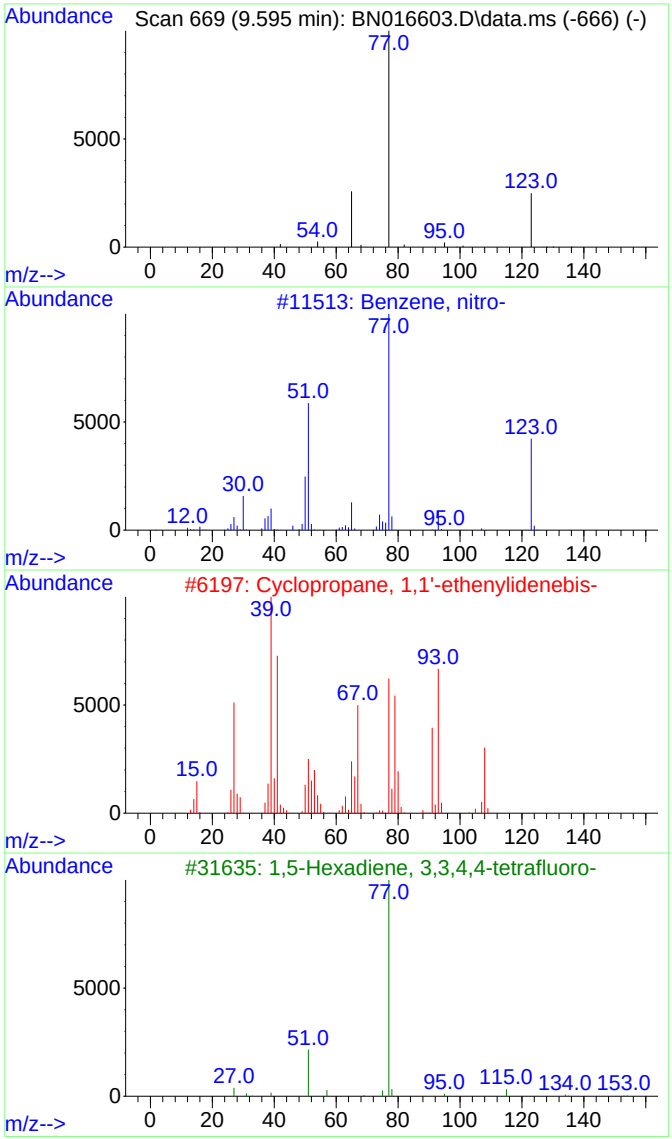
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

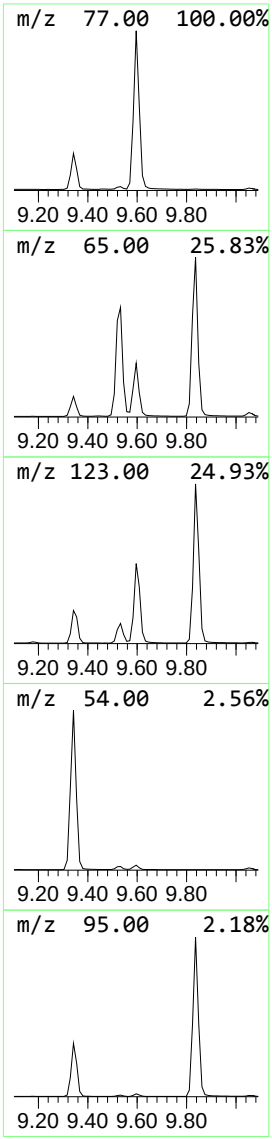
****

Peak Number 6 Benzene, nitro- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.595	0.34 ng	123325	Naphthalene-d8	10.407

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, nitro-	123	C6H5NO2	000098-95-3	2
2	Cyclopropane, 1,1'-ethenylidenebis-	108	C8H12	000822-93-5	1
3	1,5-Hexadiene, 3,3,4,4-tetrafluoro-	154	C6H6F4	001763-21-9	1
4	Silanamine, N-silyl-	77	H7NSi2	005702-11-4	1
5	Cystamine	152	C4H12N2S2	000051-85-4	1





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016603.D
Acq On : 30 Sep 2021 16:44
Operator : CG/JU
Sample : SSTDICC3.2
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC3.2

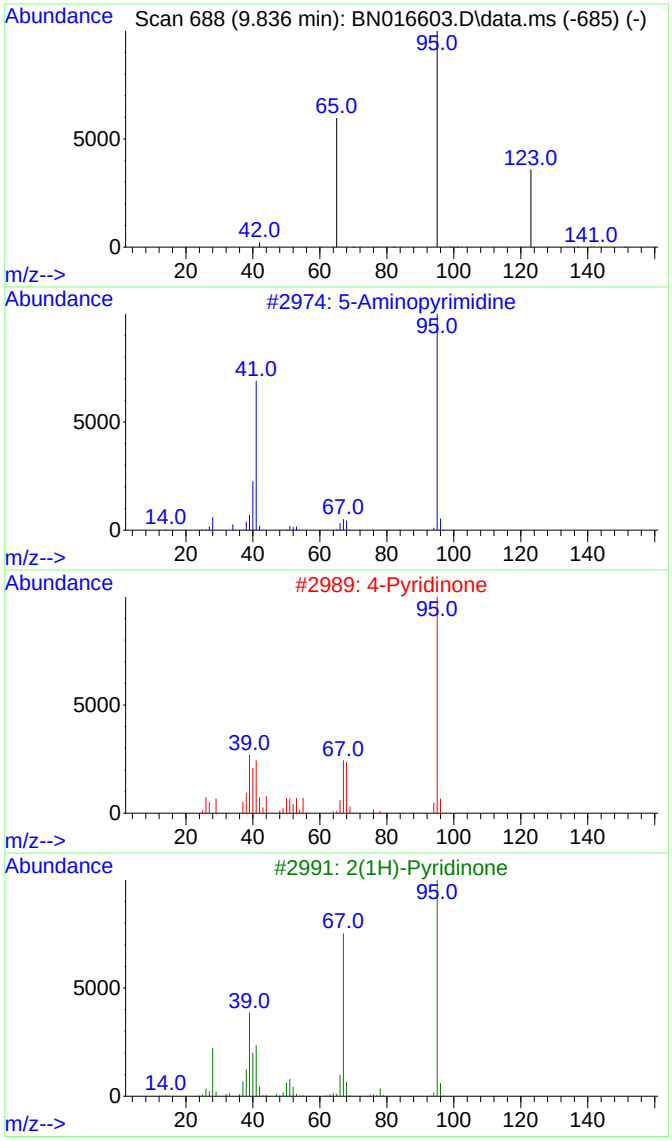
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

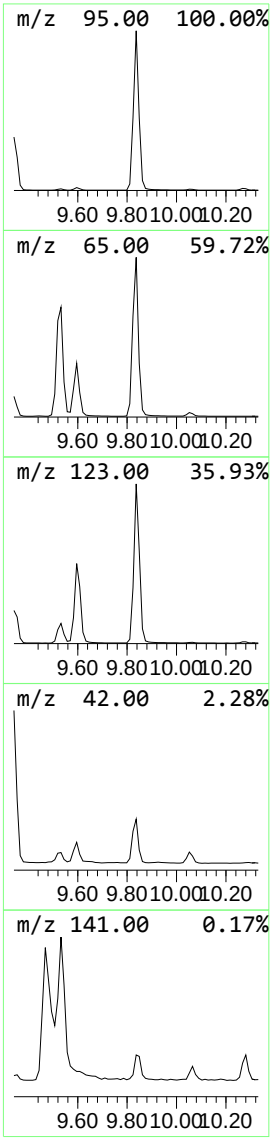
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 5-Aminopyrimidine Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.836	0.58 ng	211360	Naphthalene-d8	10.407

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminopyrimidine	95	C4H5N3	000591-55-9	3
2	4-Pyridinone	95	C5H5NO	1000433-50-4	2
3	2(1H)-Pyridinone	95	C5H5NO	000142-08-5	2
4	4(1H)-Pyridone	95	C5H5NO	000108-96-3	2
5	3-Pyridinol	95	C5H5NO	000109-00-2	2





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Acq On : 30 Sep 2021 16:44
Operator : CG/JU
Sample : SSTDICC3.2
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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LabSampleId :
SSTDICC3.2

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

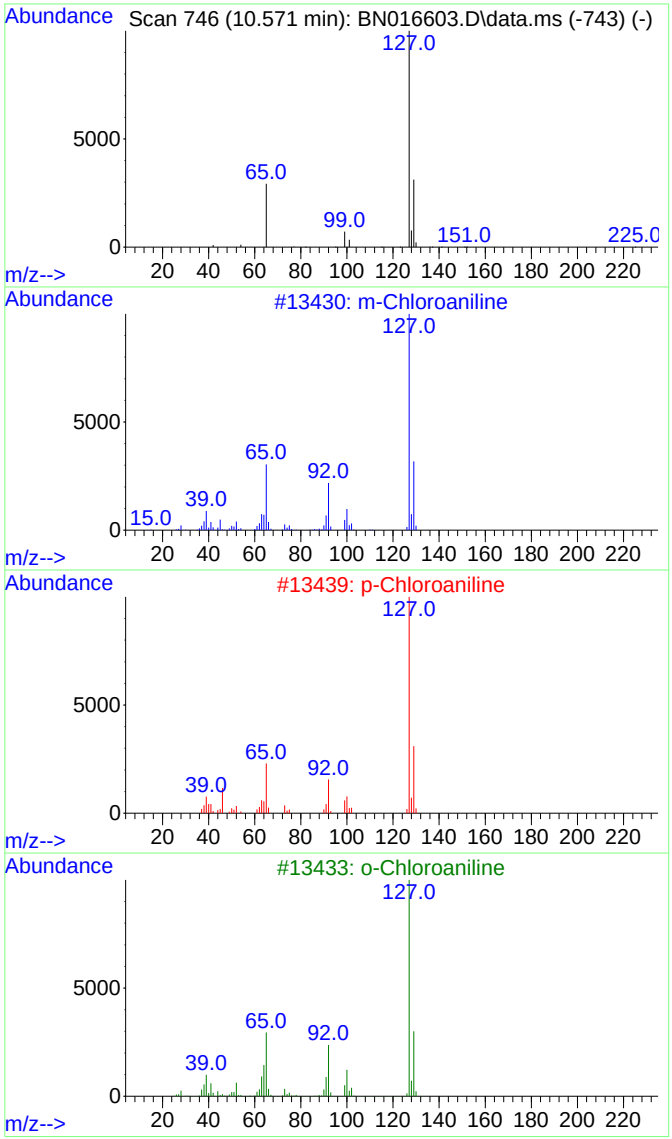
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

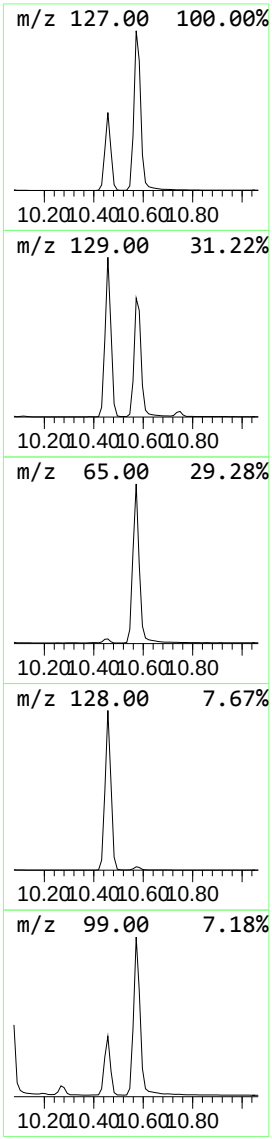
****

Peak Number 8 m-Chloroaniline Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.571	1.49 ng	541061	Naphthalene-d8	10.407

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	m-Chloroaniline	127	C6H6ClN	000108-42-9	90
2	p-Chloroaniline	127	C6H6ClN	000106-47-8	90
3	o-Chloroaniline	127	C6H6ClN	000095-51-2	90
4	Picloxydine	474	C20H24Cl2N10	005636-92-0	83
5	4-(Chloromethyl)pyridine	127	C6H6ClN	010445-91-7	80





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Sample : SSTDICC3.2
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC3.2

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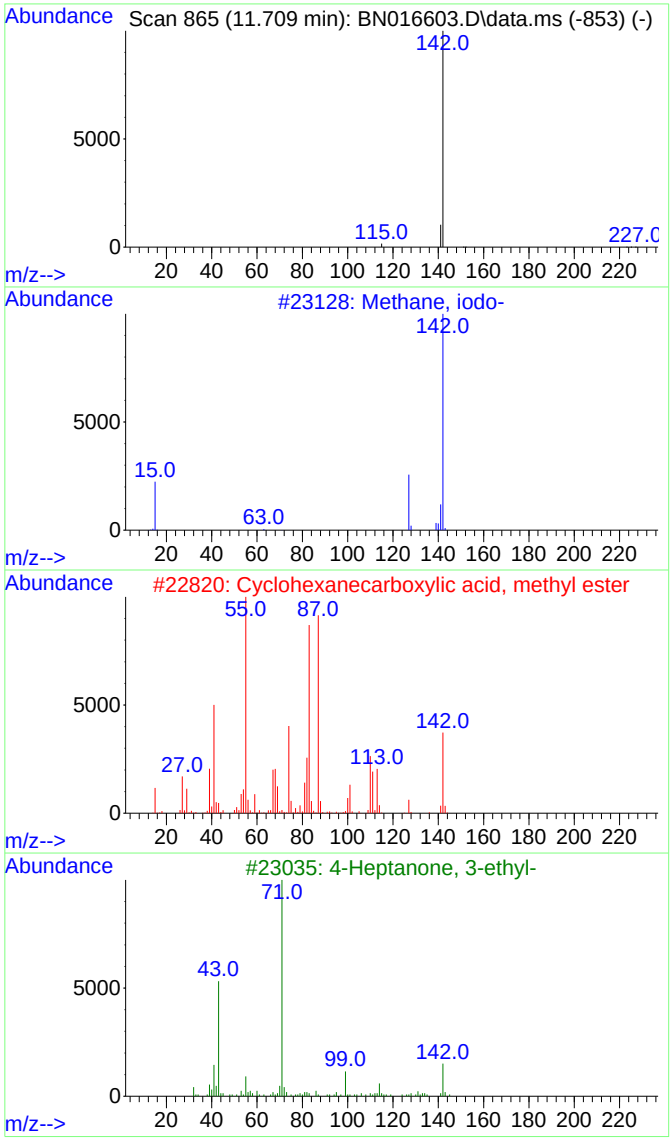
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

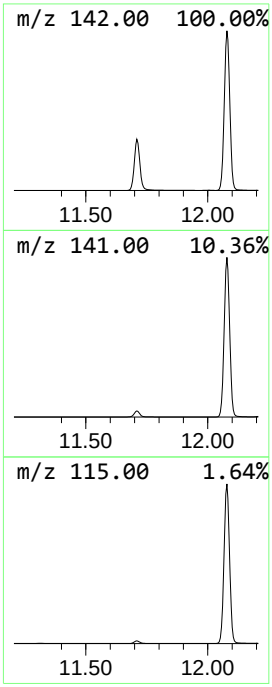
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Methane, iodo- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.709	0.64 ng	232232	Naphthalene-d8	10.407

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methane, iodo-	142	CH3I	000074-88-4	4
2	Cyclohexanecarboxylic acid, meth...	142	C8H14O2	004630-82-4	4
3	4-Heptanone, 3-ethyl-	142	C9H18O	001528-25-2	3
4	Cyclohexane carboxylic acid hydr...	142	C7H14N2O	038941-47-8	3
5	2-Butanone, diethylhydrazone	142	C8H18N2	028236-94-4	3





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Sample : SSTDICC3.2
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC3.2

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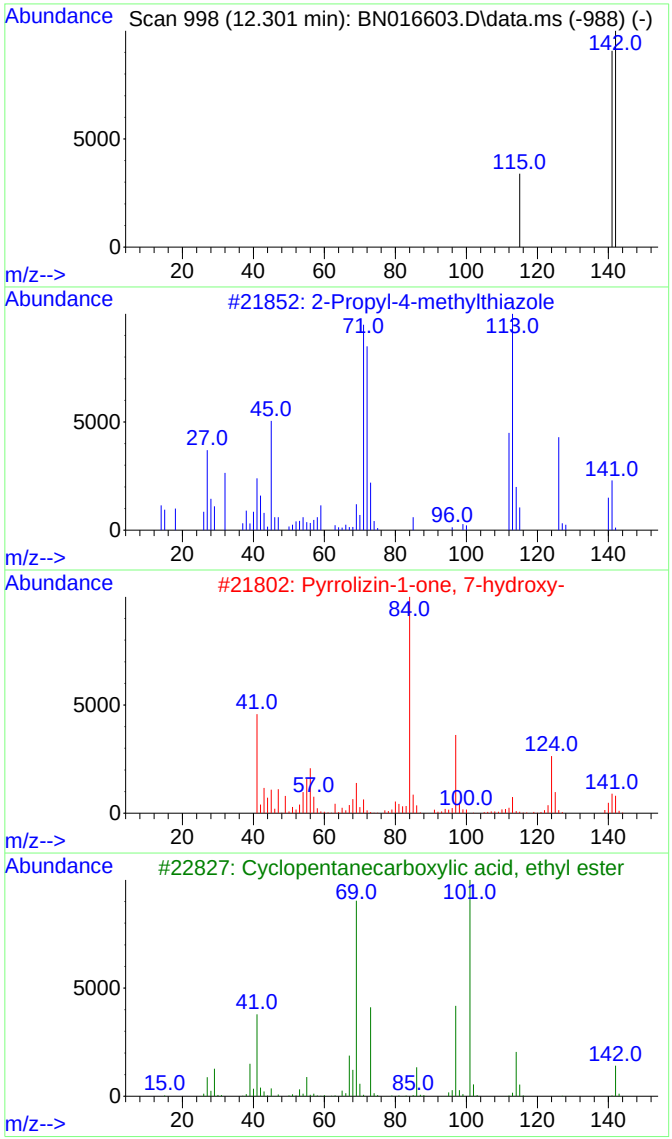
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

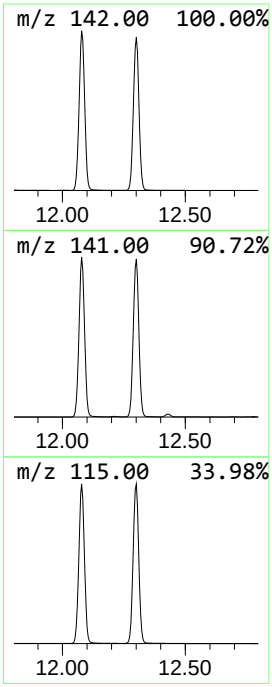
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2-Propyl-4-methylthiazole Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.301	3.74 ng	1356140	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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Sample : SSTDICC3.2
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC3.2

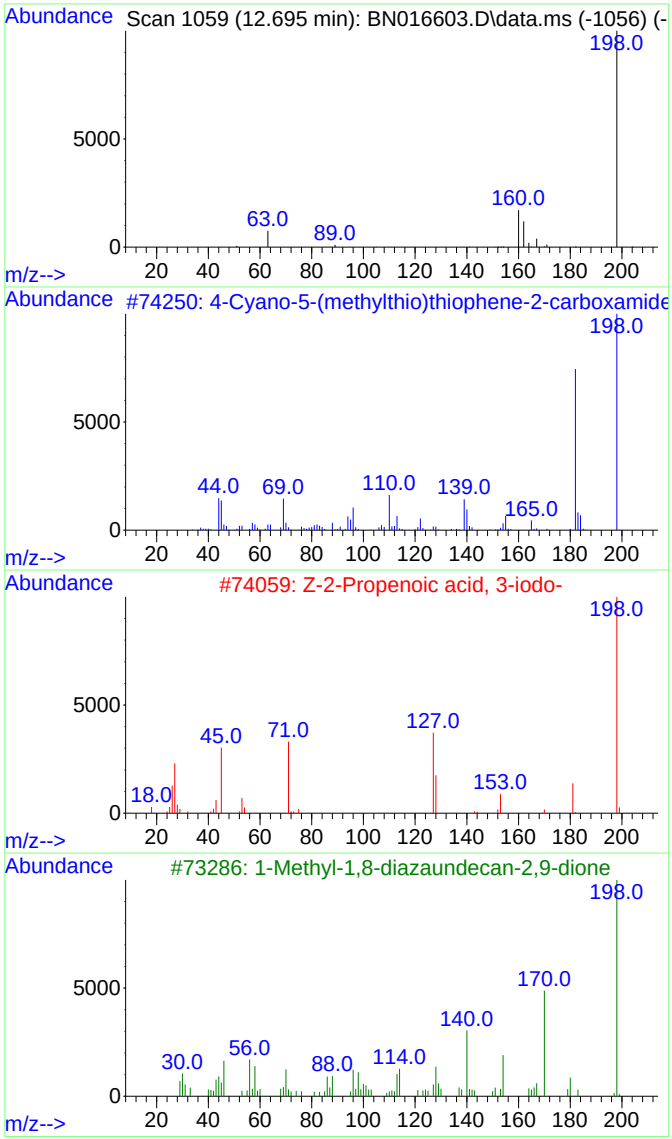
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

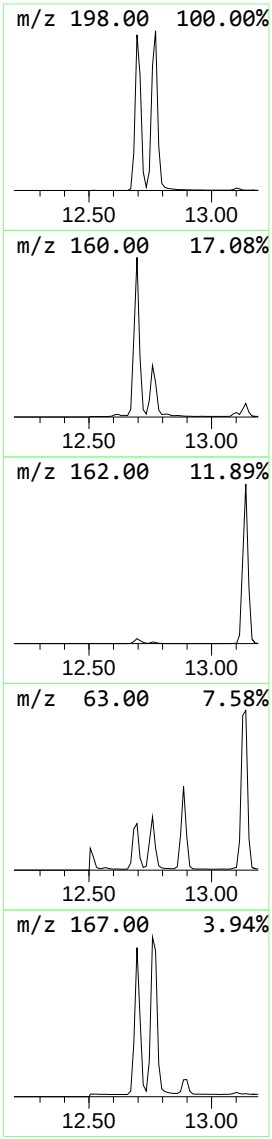
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 4-Cyano-5-(methylthio)thiop... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.695	0.66 ng	257029	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Cyano-5-(methylthio)thiophene-...	198	C7H6N2OS2	1000267-39-2	3
2	Z-2-Propenoic acid, 3-iodo-	198	C3H3IO2	1000308-86-8	3
3	1-Methyl-1,8-diazaundecan-2,9-dione	198	C10H18N2O2	1000298-94-5	3
4	Thiazolo[5,4-d]pyrimidine, 5-ami...	198	C6H6N4S2	019835-31-5	3
5	E-2-Propenoic acid, 3-iodo-	198	C3H3IO2	1000308-86-7	3





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Operator : CG/JU
Sample : SSTDICC3.2
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC3.2

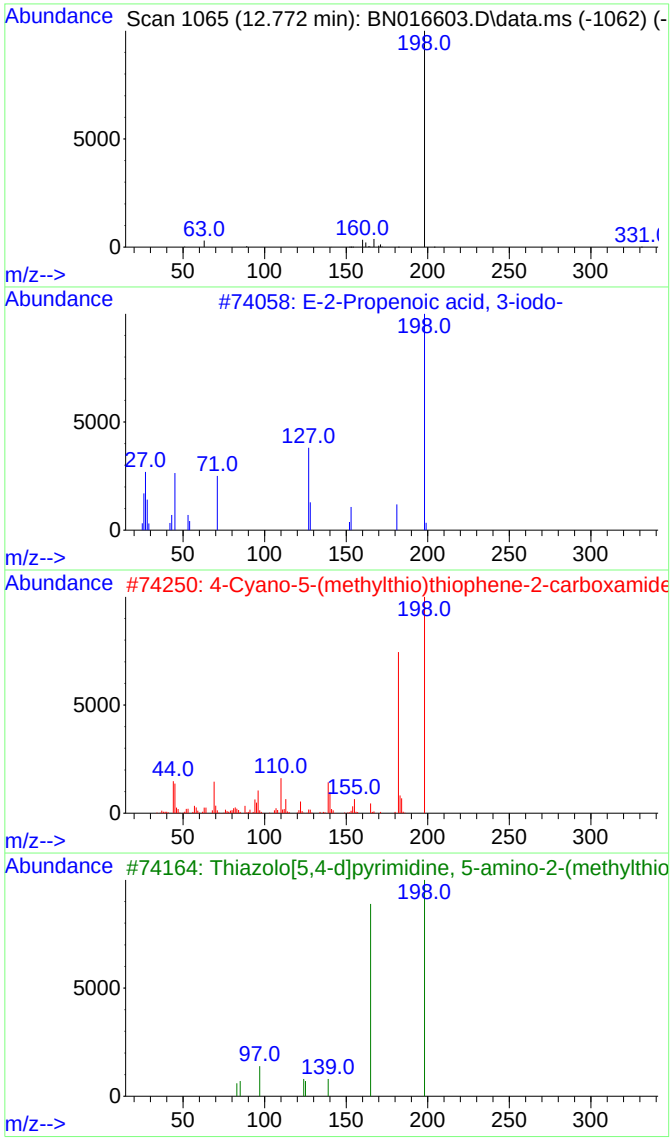
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

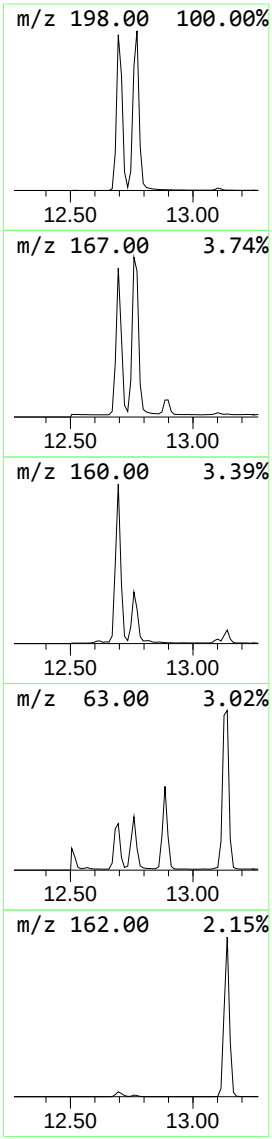
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 E-2-Propenoic acid, 3-iodo- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.772	0.60 ng	234530	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-2-Propenoic acid, 3-iodo-	198	C3H3IO2	1000308-86-7	3
2	4-Cyano-5-(methylthio)thiophene-...	198	C7H6N2OS2	1000267-39-2	3
3	Thiazolo[5,4-d]pyrimidine, 5-ami...	198	C6H6N4S2	019835-31-5	3
4	Z-2-Propenoic acid, 3-iodo-	198	C3H3IO2	1000308-86-8	3
5	Methyl 2-(dimethylhydrazono)-3,3...	198	C6H9F3N2O2	1000489-35-4	2





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Acq On : 30 Sep 2021 16:44
Operator : CG/JU
Sample : SSTDICC3.2
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC3.2

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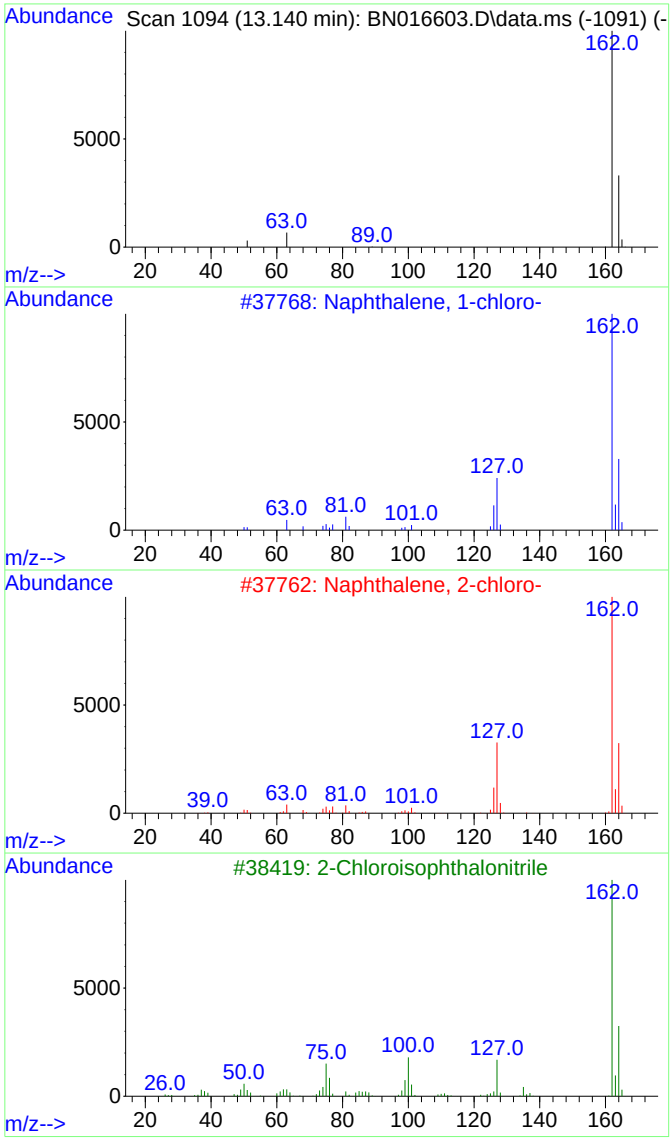
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

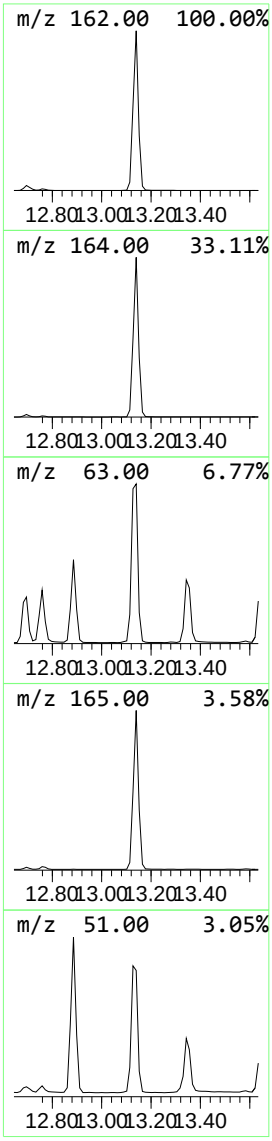
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Naphthalene, 1-chloro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.140	2.35 ng	920999	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-chloro-	162	C10H7Cl	000090-13-1	74
2	Naphthalene, 2-chloro-	162	C10H7Cl	000091-58-7	74
3	2-Chloroisophthalonitrile	162	C8H3ClN2	028442-78-6	7
4	3-Chlorophthalonitrile	162	C8H3ClN2	076241-79-7	7
5	3-Chloro-4-fluorothiophenol	162	C6H4ClFS	060811-23-6	5





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Misc :
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Instrument :
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LabSampleId :
SSTDICC3.2

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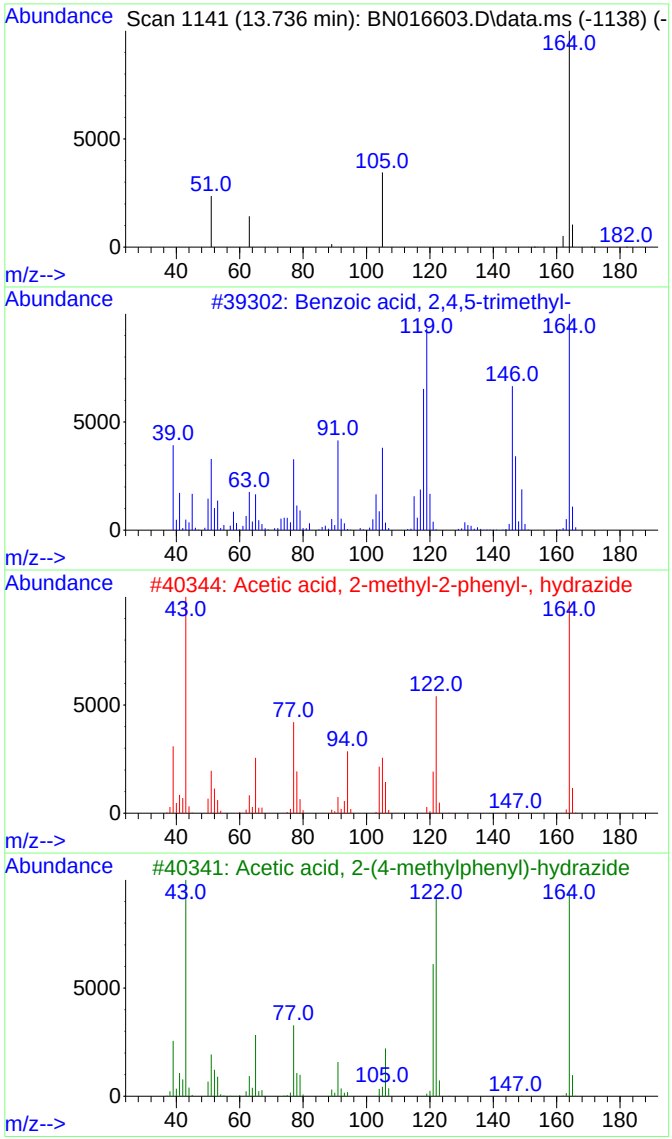
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

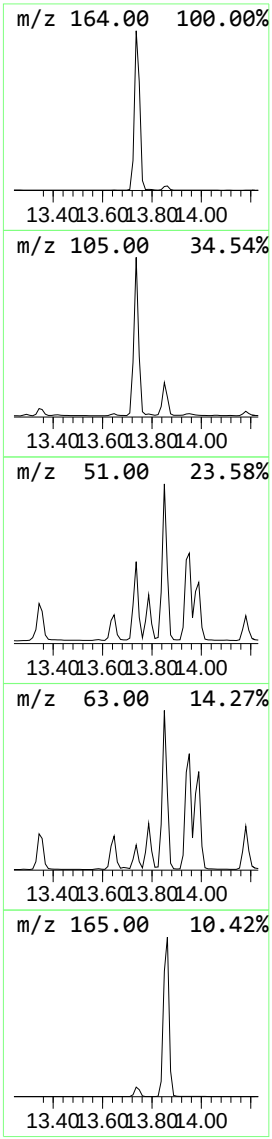
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 Benzoic acid, 2,4,5-trimethyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.736	0.35 ng	135999	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2,4,5-trimethyl-	164	C10H12O2	000528-90-5	9
2	Acetic acid, 2-methyl-2-phenyl-,...	164	C9H12N2O	038604-68-1	9
3	Acetic acid, 2-(4-methylphenyl)-...	164	C9H12N2O	061700-79-6	9
4	1,4-Benzodioxan-6-carboxaldehyde	164	C9H8O3	029668-44-8	9
5	Phenol, 2-methoxy-5-(1-propenyl)...	164	C10H12O2	019784-98-6	9





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Operator : CG/JU
Sample : SSTDICC3.2
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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LabSampleId :
SSTDICC3.2

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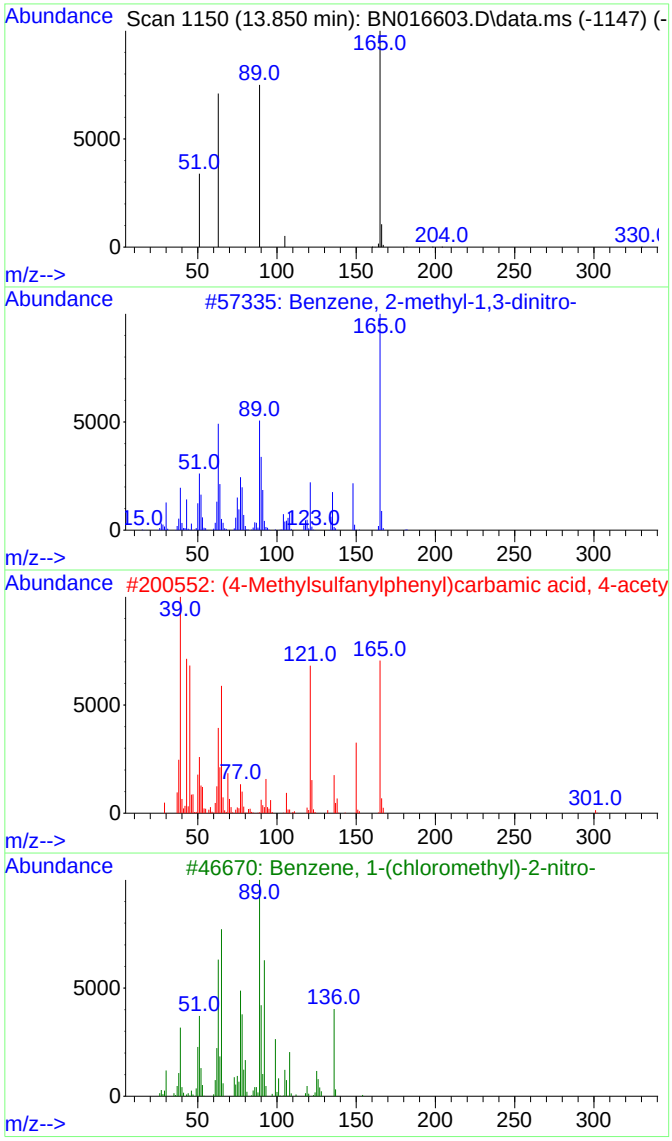
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

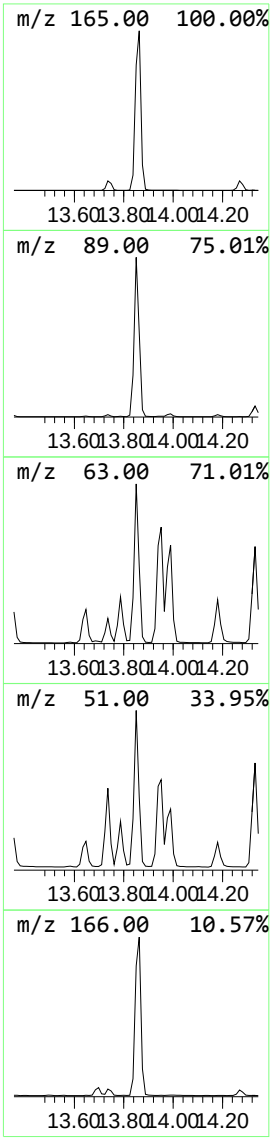
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 Benzene, 2-methyl-1,3-dinitro- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.850	0.86 ng	337451	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-methyl-1,3-dinitro-	182	C7H6N2O4	000606-20-2	83
2	(4-Methylsulfanylphenyl)carbamic...	301	C16H15NO3S	1000305-20-0	17
3	Benzene, 1-(chloromethyl)-2-nitro-	171	C7H6ClNO2	000612-23-7	9
4	2-Butanone, 3-[(2-chloroethyl)th...	166	C6H11ClOS	117239-10-8	4
5	Thiazole, tetrahydro-	89	C3H7NS	000504-78-9	3





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Operator : CG/JU
Sample : SSTDICC3.2
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC3.2

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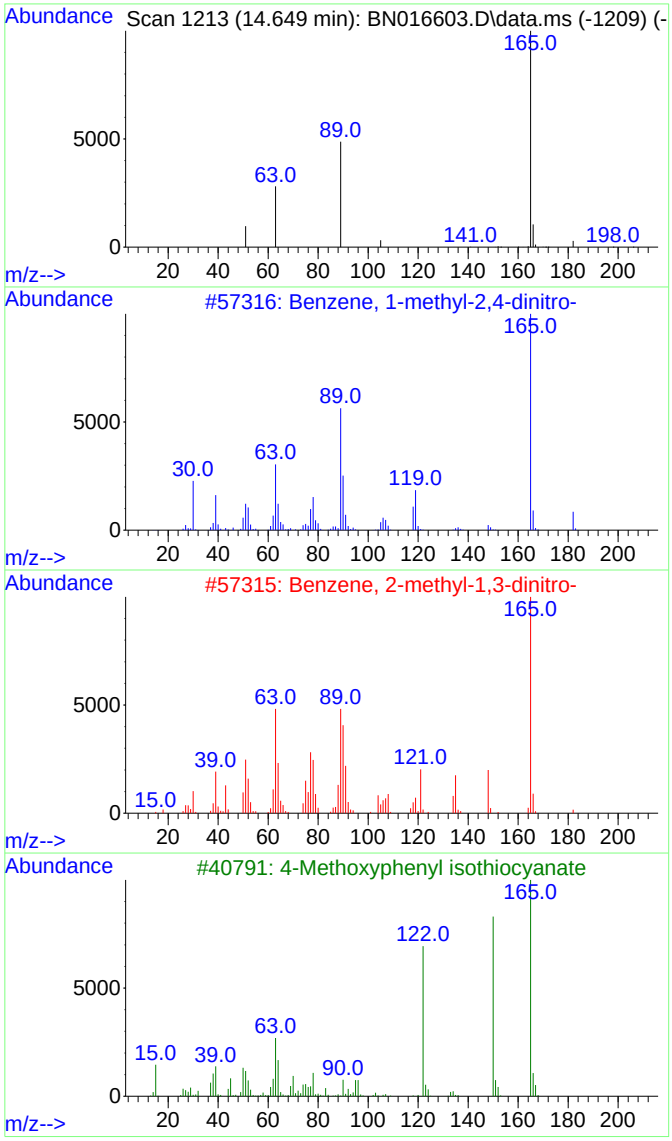
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

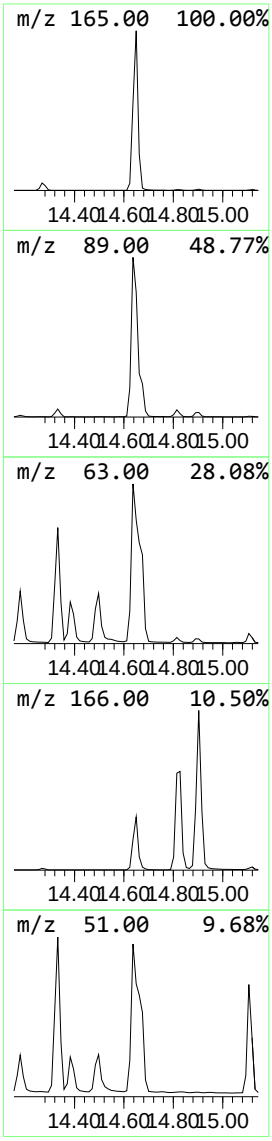
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 Benzene, 1-methyl-2,4-dinitro- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.649	1.24 ng	486585	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	43
2	Benzene, 2-methyl-1,3-dinitro-	182	C7H6N2O4	000606-20-2	38
3	4-Methoxyphenyl isothiocyanate	165	C8H7NOS	002284-20-0	9
4	Benzamide, 3,4-dimethoxy-N-(2-ph...	439	C28H41NO3	1000491-47-7	9
5	Furo[3,4-c]pyridine-3,4(1H,5H)-d...	165	C8H7NO3	007472-18-6	7





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Misc :
ALS Vial : 7 Sample Multiplier: 1

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BNA_N
LabSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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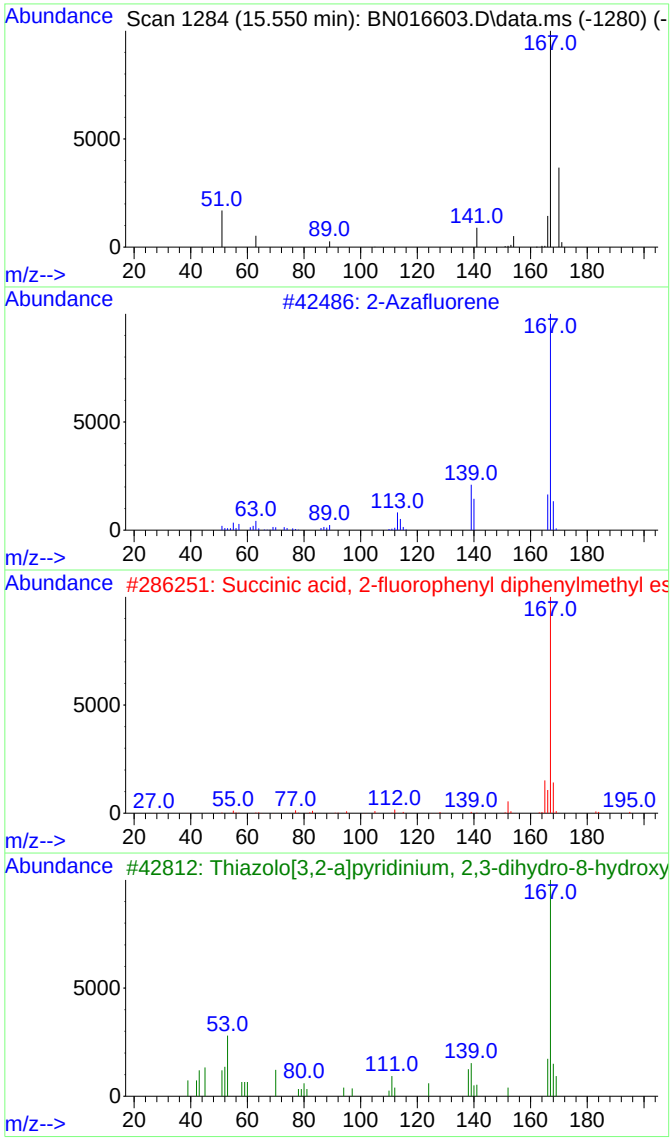
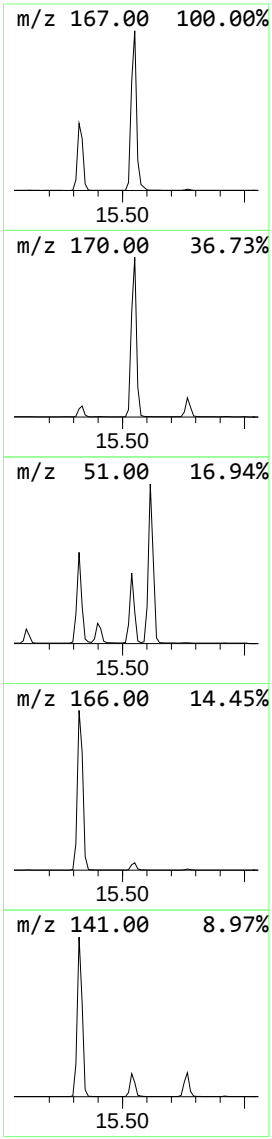
Peak Number 17 2-Azafluorene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.550	1.28 ng	499963	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	Thiazolo[3,2-a]pyridinium, 2,3-d...	167	C8H9NOS	023003-43-2	7
4	2,4(1H,3H)-Pyrimidinedione, 5-me...	170	C7H10N2O3	059264-10-7	5
5	Benzaldehyde, 2-hydroxy-5-nitro-	167	C7H5NO4	000097-51-8	5





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Instrument :
BNA_N
LabSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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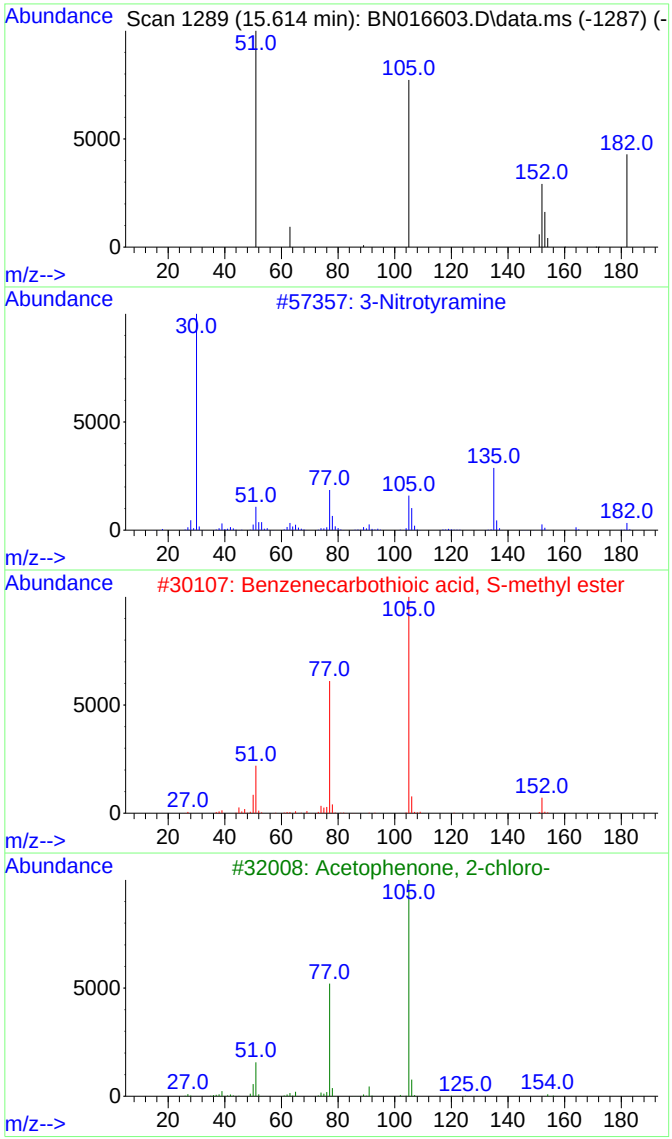
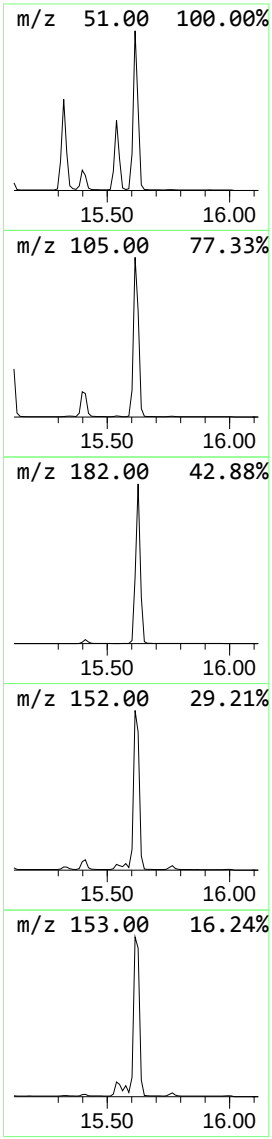
Peak Number 18 3-Nitrotyramine Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.614	1.57 ng	612767	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 : BN016603.D
Acq On : 30 Sep 2021 16:44
Operator : CG/JU
Sample : SSTDICC3.2
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC3.2

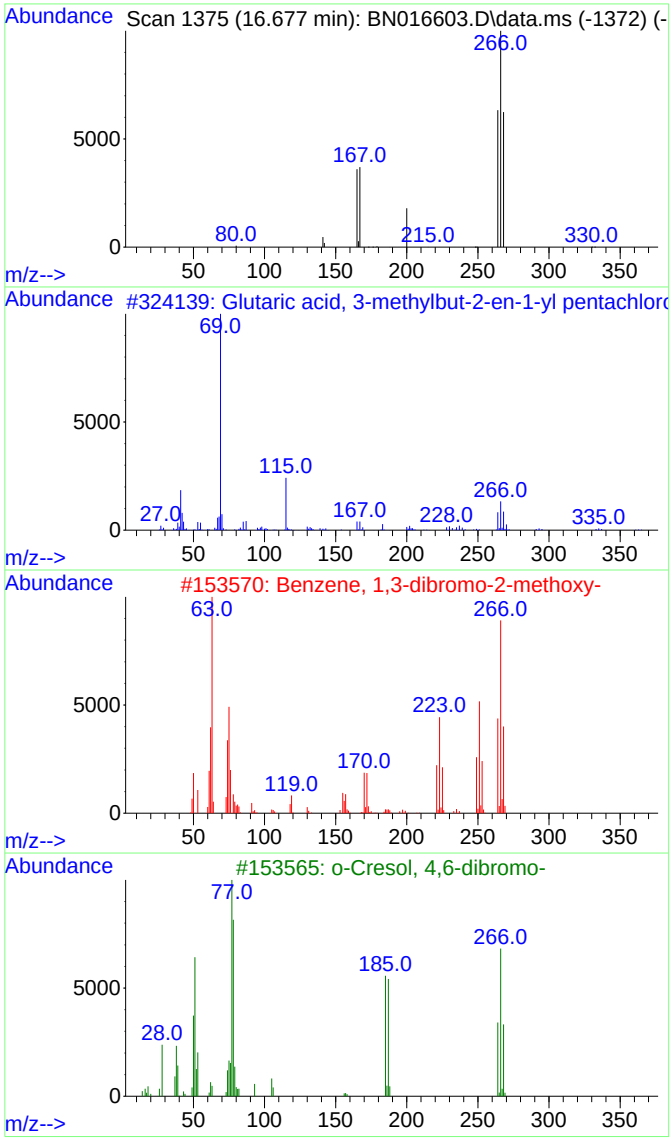
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

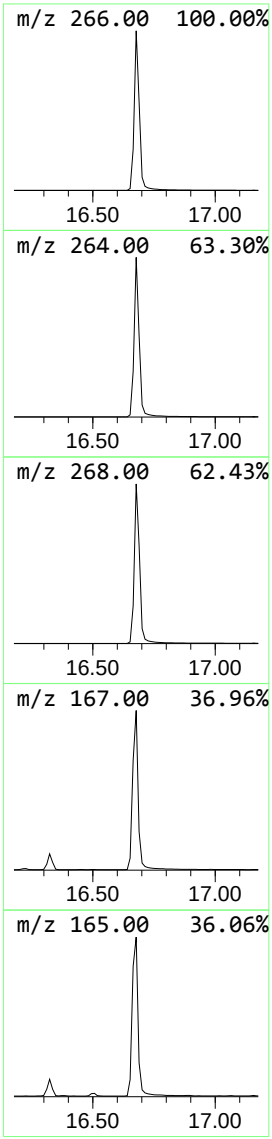
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 Glutaric acid, 3-methylbut-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.677	1.03 ng	384044	Phenanthrene-d10	17.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Glutaric acid, 3-methylbut-2-en-...	446	C16H15Cl5O4	1000392-32-9	64
2	Benzene, 1,3-dibromo-2-methoxy-	264	C7H6Br2O	038603-09-7	42
3	o-Cresol, 4,6-dibromo-	264	C7H6Br2O	000609-22-3	42
4	Benzene, 2,4-dibromo-1-methoxy-	264	C7H6Br2O	021702-84-1	42
5	Phenol, 2,6-dibromo-4-methyl-	264	C7H6Br2O	002432-14-6	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016603.D
Acq On : 30 Sep 2021 16:44
Operator : CG/JU
Sample : SSTDICC3.2
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC3.2

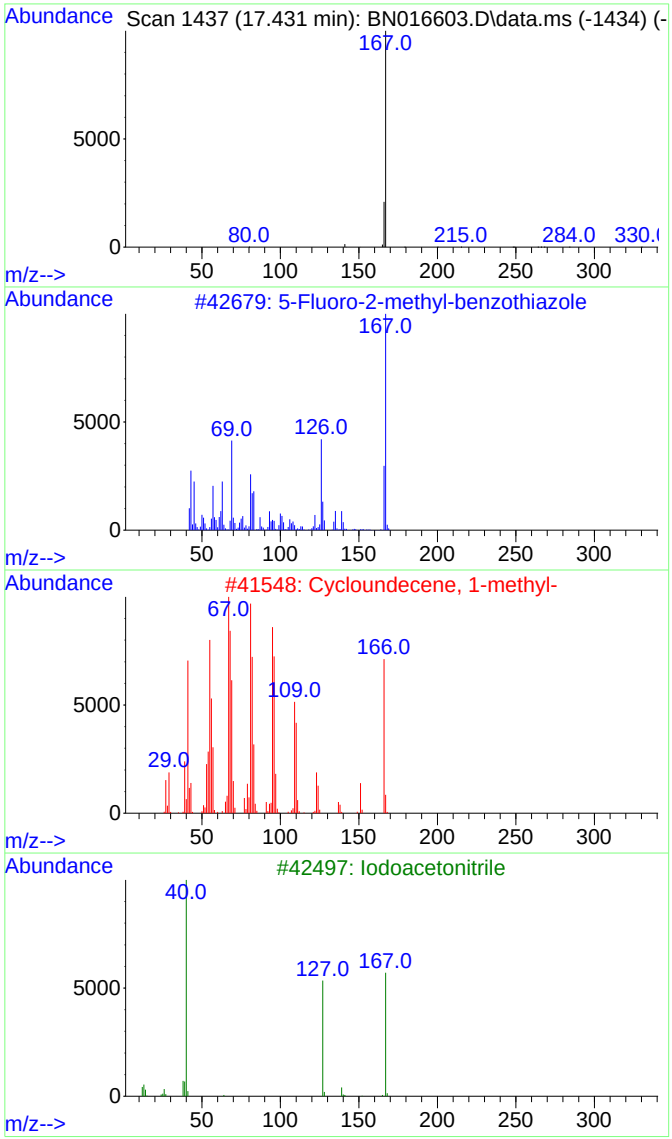
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

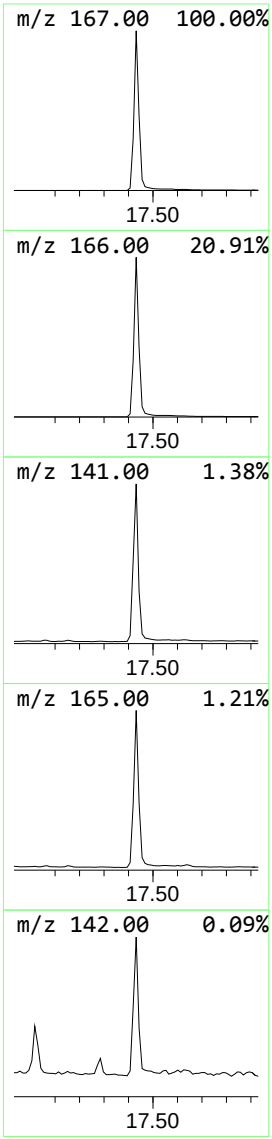
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 5-Fluoro-2-methyl-benzothia... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.431	2.60 ng	967739	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	Cycloundecene, 1-methyl-	166	C12H22	088828-82-4	4
3	Iodoacetonitrile	167	C2H2IN	000624-75-9	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





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016603.D
Acq On : 30 Sep 2021 16:44
Operator : CG/JU
Sample : SSTDICC3.2
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDICC3.2

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	0.6	ng	296222	1	7.642	195562	0.4
Ethene, 1,1-dif...	7.200	0.5	ng	242863	1	7.642	195562	0.4
6-Benzothiazola...	7.956	1.5	ng	724124	1	7.642	195562	0.4
1-Propanamine, ...	8.442	0.8	ng	413920	1	7.642	195562	0.4
Fomepizole	9.342	1.9	ng	687345	2	10.407	144853	0.4
Benzene, nitro-	9.595	0.3	ng	123325	2	10.407	144853	0.4
5-Aminopyrimidine	9.836	0.6	ng	211360	2	10.407	144853	0.4
m-Chloroaniline	10.571	1.5	ng	541061	2	10.407	144853	0.4
Methane, iodo-	11.709	0.6	ng	232232	2	10.407	144853	0.4
2-Propyl-4-meth...	12.301	3.7	ng	1356140	2	10.407	144853	0.4
4-Cyano-5-(meth...	12.695	0.7	ng	257029	3	14.269	156591	0.4
E-2-Propenoic a...	12.772	0.6	ng	234530	3	14.269	156591	0.4
Naphthalene, 1-...	13.140	2.4	ng	920999	3	14.269	156591	0.4
Benzoic acid, 2...	13.736	0.3	ng	135999	3	14.269	156591	0.4
Benzene, 2-meth...	13.850	0.9	ng	337451	3	14.269	156591	0.4
Benzene, 1-meth...	14.649	1.2	ng	486585	3	14.269	156591	0.4
2-Azafluorene	15.550	1.3	ng	499963	3	14.269	156591	0.4
3-Nitrotyramine	15.614	1.6	ng	612767	3	14.269	156591	0.4
Glutaric acid, ...	16.677	1.0	ng	384044	4	17.030	148789	0.4
5-Fluoro-2-meth...	17.431	2.6	ng	967739	4	17.030	148789	0.4