LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016602.D
Acq On : 30 Sep 2021 16:07
Operator : CG/JU
Sample : SSTDICC1.6
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDICC1.6

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: BN016602.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	28301	39918	1.98%	0.143%
2	3.281	20	22	42	rVB	17154	81552	4.04%	0.293%
3	3.576	50	54	82	rVB	25434	111456	5.53%	0.400%
4	5.254	231	236	253	rBV2	57794	218537	10.84%	0.784%
5	6.822	401	406	418	rBV	97693	243025	12.05%	0.872%
6	6.979	418	423	429	rVV	69728	149060	7.39%	0.535%
7	7.080	429	434	440	rVV	134919	267417	13.26%	0.960%
8	7.200	440	447	458	rVB	47354	124233	6.16%	0.446%
9	7.532	478	483	490	rVB	24107	54742	2.71%	0.196%
10	7.643	490	495	511	rVB2	41606	141857	7.04%	0.509%
11	7.956	524	529	538	rVB2	171469	386255	19.16%	1.386%
12	8.168	547	552	557	rBV	11163	27278	1.35%	0.098%
13	8.442	571	578	581	rBV2	79983	204959	10.16%	0.735%
14	8.696	594	598	601	rBV	16935	32133	1.59%	0.115%
15	8.785	601	605	607	rBV	153098	317708	15.76%	1.140%
16	8.823	607	608	612	rVB	123292	173839	8.62%	0.624%
17	9.342	646	649	653	rBV	212297	336792	16.70%	1.208%
18	9.532	660	664	666	rBV	16432	29804	1.48%	0.107%
19	9.596	666	669	673	rVB	37954	61444	3.05%	0.220%
20	9.836	685	688	700	rBV	68935	109434	5.43%	0.393%
21	10.065	702	706	709	rBV	18076	36974	1.83%	0.133%
22	10.407	729	733	735	rBV	85371	170681	8.46%	0.612%
23	10.457	735	737	741	rVV	405496	662951	32.88%	2.379%
24	10.572	743	746	756	rVV	132318	265181	13.15%	0.952%
25	10.749	757	760	763	rVB	123647	199284	9.88%	0.715%
26	11.307	801	804	814	rBV	12329	26517	1.32%	0.095%
27	11.709	852	865	900	rBV	66562	111684	5.54%	0.401%
28	12.007	921	932	940	rBV	210972	345571	17.14%	1.240%
29	12.078	940	948	971	rVV	472345	743665	36.88%	2.668%
30	12.301	988	998	1020	rVV	461737	717441	35.58%	2.574%
31	12.696	1056	1059	1062	rBV	75885	123384	6.12%	0.443%
32	12.772	1062	1065	1071	rVB	59475	112225	5.57%	0.403%
33	12.899	1071	1075	1078	rBV	412344	710350	35.23%	2.549%
34	13.140	1091	1094	1097	rVB	316195	476477	23.63%	1.710%
35	13.736	1138	1141	1143	rBV	50016	68319	3.39%	0.245%
36	13.850	1147	1150	1153	rVB	98225	150378	7.46%	0.540%

LSC Area Percent Report

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Sample : SSTDICC1.6
Misc :
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Instrument : BNA_N
LabSampleId : SSTDICC1.6

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	433086	651637	32.32%	2.338%
38	14.269	1180	1183	1185	rBV	105787	155316	7.70%	0.557%
39	14.332	1185	1188	1191	rVB	637313	890549	44.16%	3.195%
40	14.649	1209	1213	1218	rBV2	98160	218585	10.84%	0.784%
41	14.827	1223	1227	1230	rBV	24790	44217	2.19%	0.159%
42	14.903	1230	1233	1236	rBV	37107	51577	2.56%	0.185%
43	15.106	1246	1249	1252	rBV	33503	45957	2.28%	0.165%
44	15.322	1263	1266	1270	rBV2	787339	1289195	63.93%	4.626%
45	15.411	1270	1273	1280	rVV2	31512	57017	2.83%	0.205%
46	15.550	1280	1284	1287	rVV2	140120	251126	12.45%	0.901%
47	15.614	1287	1289	1293	rVB2	189150	297626	14.76%	1.068%
48	15.766	1298	1301	1304	rBV2	60582	96523	4.79%	0.346%
49	16.227	1335	1338	1341	rBV2	237782	342369	16.98%	1.228%
50	16.324	1343	1346	1350	rVB	155186	254668	12.63%	0.914%
51	16.507	1358	1361	1364	rBV	122758	161846	8.03%	0.581%
52	16.677	1372	1375	1384	rBV	111480	174521	8.65%	0.626%
53	17.018	1400	1403	1405	rBV	69250	137602	6.82%	0.494%
54	17.066	1405	1407	1410	rVV	562826	774782	38.42%	2.780%
55	17.152	1411	1414	1434	rVB	443594	727554	36.08%	2.611%
56	17.431	1434	1437	1457	rBV	378549	555997	27.57%	1.995%
57	18.021	1483	1486	1498	rVB	27376	34429	1.71%	0.124%
58	19.068	1686	1697	1699	rBV	459857	595785	29.55%	2.138%
59	19.098	1699	1703	1739	rVB	715561	957816	47.50%	3.437%
60	19.460	1765	1776	1813	rVV	745497	983542	48.78%	3.529%
61	19.679	1813	1820	1854	rVB	428228	517915	25.68%	1.858%
62	20.389	1919	1922	1924	rBV	229478	324954	16.12%	1.166%
63	21.026	1979	1982	1989	rBV	18220	28712	1.42%	0.103%
64	21.174	1993	1996	1998	rBV	325815	411464	20.41%	1.476%
65	21.217	1998	2000	2003	rVV2	853747	1306516	64.79%	4.688%
66	21.270	2003	2005	2008	rVB	830596	1002647	49.72%	3.598%
67	22.056	2076	2079	2096	rVB	408788	556937	27.62%	1.998%
68	22.810	2216	2230	2236	rBV	552594	894021	44.34%	3.208%
69	22.855	2236	2243	2292	rVB	529269	909037	45.08%	3.262%
70	23.344	2374	2386	2388	rBV	28970	44487	2.21%	0.160%
71	23.385	2388	2398	2416	rVV	423948	798621	39.61%	2.866%
72	23.485	2416	2427	2469	rVB	146698	305650	15.16%	1.097%
73	25.774	3065	3096	3185	rBV4	556276	2016438	100.00%	7.235%
74	26.459	3272	3296	3375	rBV	305614	969251	48.07%	3.478%

Sum of corrected areas: 27869411

Instrument :
BNA_N
LabSampleId :
SSTDICC1.6

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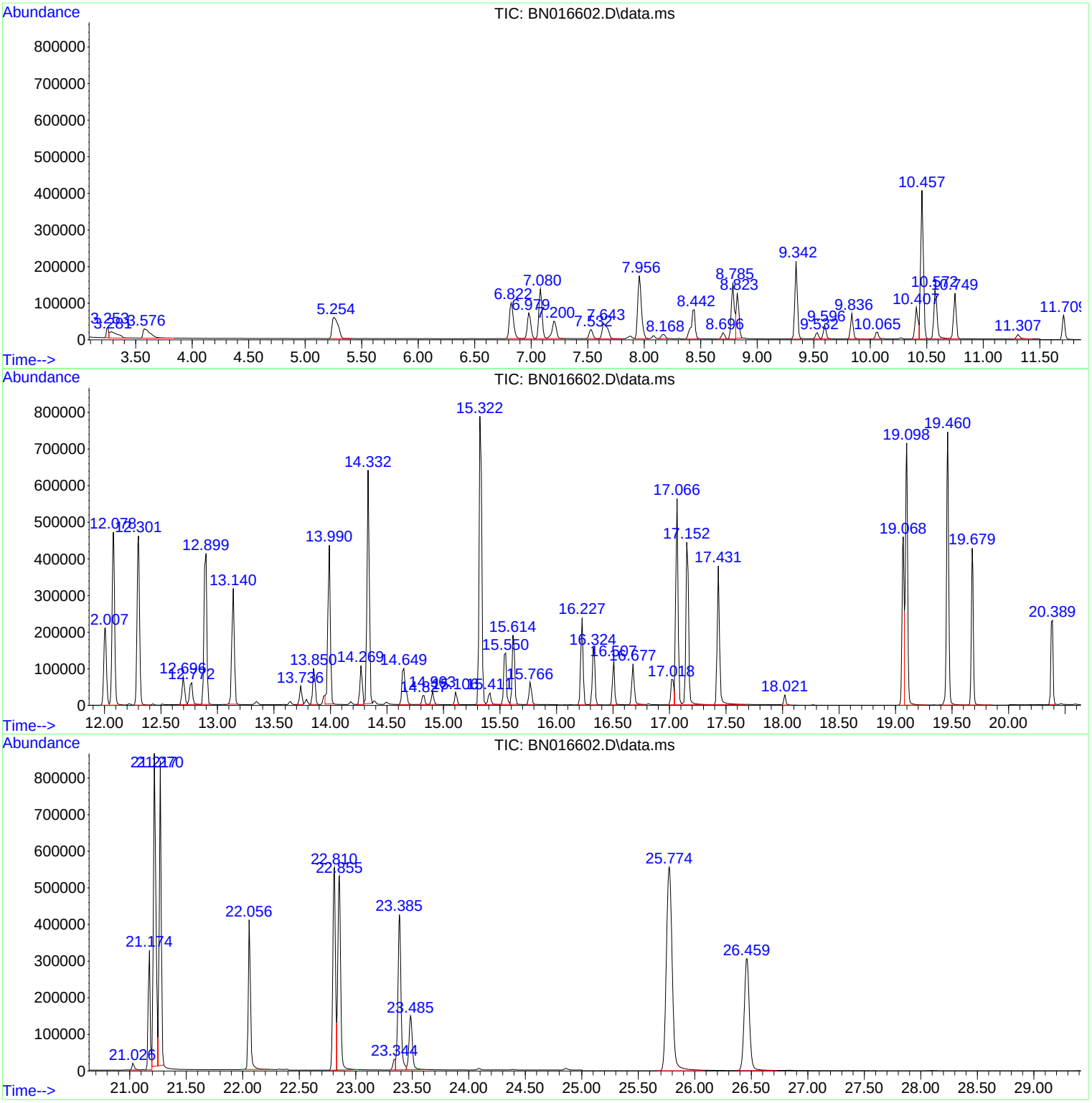
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC1.6

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 : BN016602.D
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Operator : CG/JU
Sample : SSTDICC1.6
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC1.6

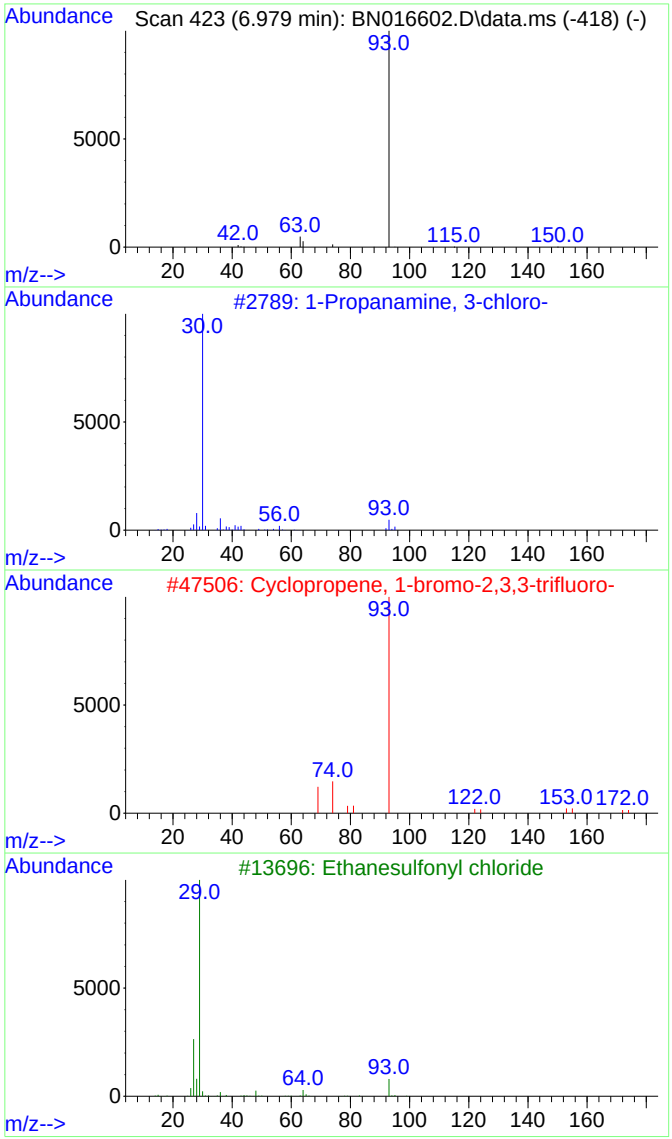
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

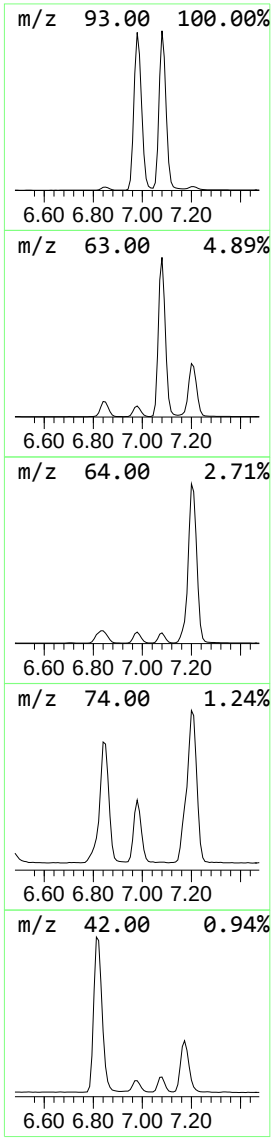
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1-Propanamine, 3-chloro- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.979	0.42 ng	149060	1,4-Dichlorobenzene-d4	7.643

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 : BN016602.D
Acq On : 30 Sep 2021 16:07
Operator : CG/JU
Sample : SSTDICC1.6
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC1.6

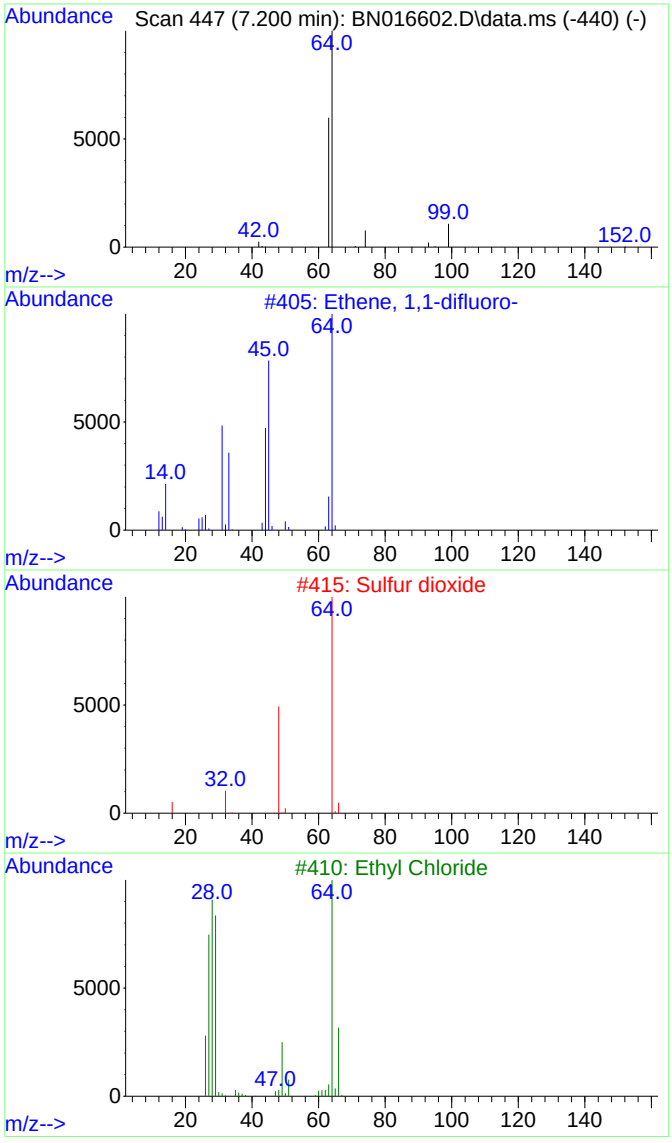
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

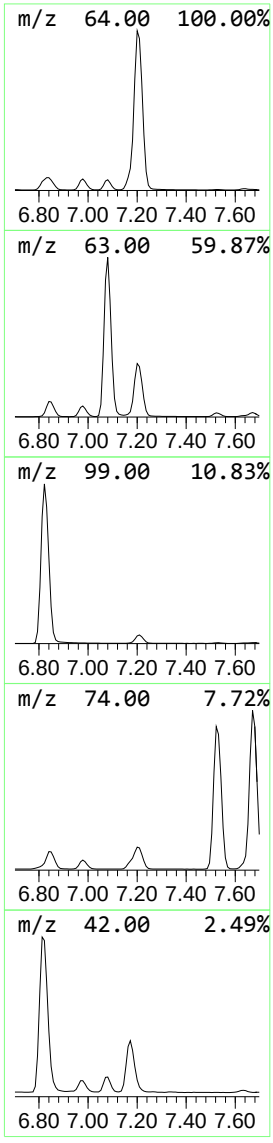
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethene, 1,1-difluoro- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.200	0.35 ng	124233	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	3
2	Sulfur dioxide	64	O2S	007446-09-5	3
3	Ethyl Chloride	64	C2H5Cl	000075-00-3	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 : BN016602.D
Acq On : 30 Sep 2021 16:07
Operator : CG/JU
Sample : SSTDICC1.6
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC1.6

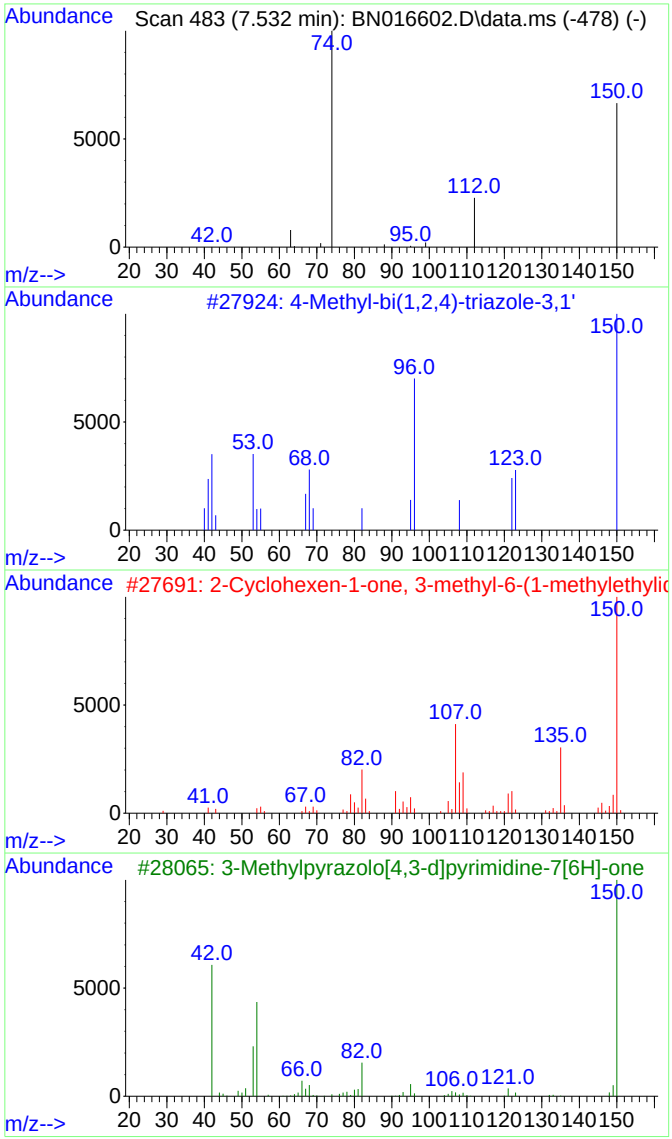
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

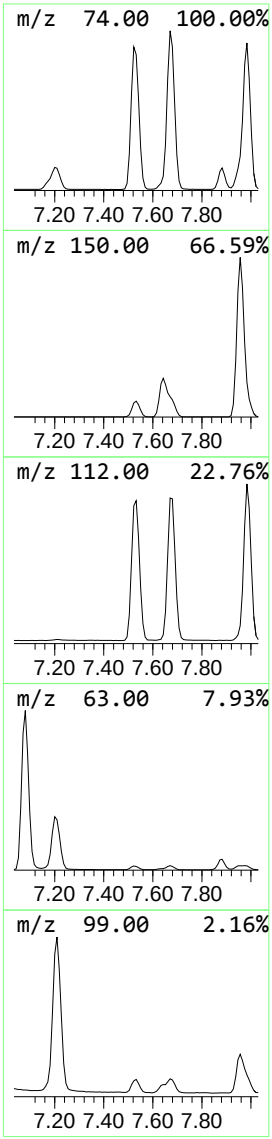
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 4-Methyl-bi(1,2,4)-triazole... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.532	0.15 ng	54742	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methyl-bi(1,2,4)-triazole-3,1'	150	C5H6N6	063523-89-7	2
2	2-Cyclohexen-1-one, 3-methyl-6-(...	150	C10H14O	000491-09-8	2
3	3-Methylpyrazolo[4,3-d]pyrimidin...	150	C6H6N4O	005399-94-0	2
4	3-Cyano-2,6-dihydroxy-4-methylpy...	150	C7H6N2O2	005444-02-0	2
5	N-Nitrosodimethylamine	74	C2H6N2O	000062-75-9	2





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Data File : BN016602.D
Acq On : 30 Sep 2021 16:07
Operator : CG/JU
Sample : SSTDICC1.6
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC1.6

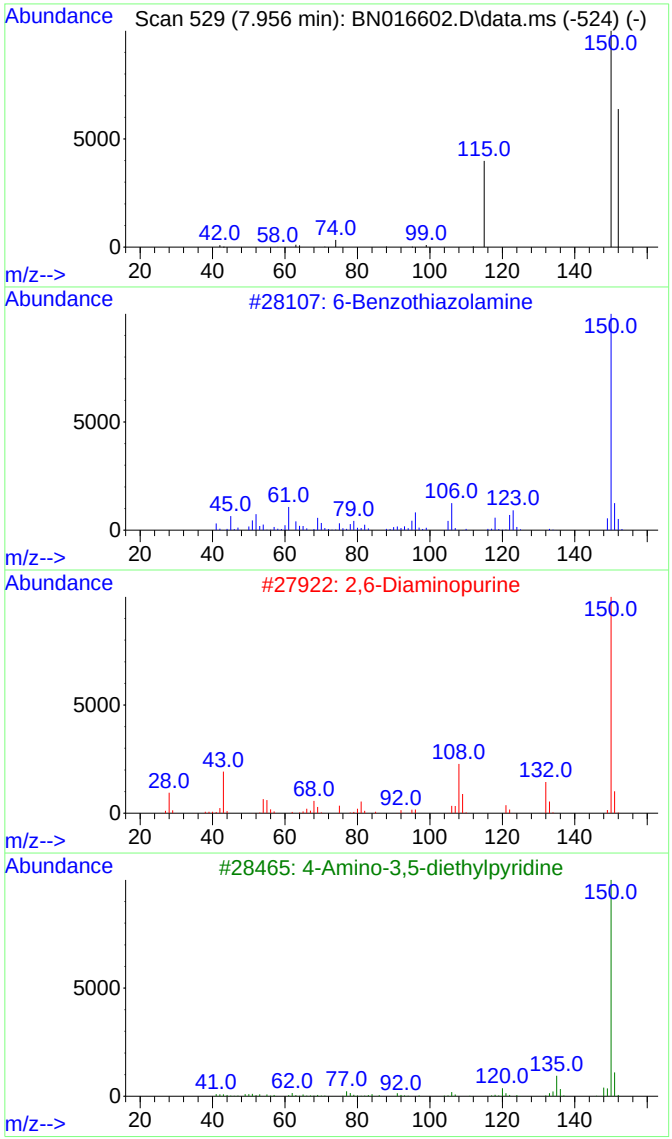
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

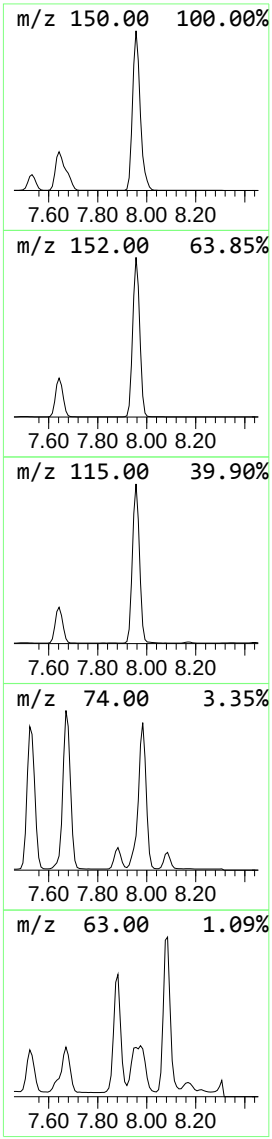
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 6-Benzothiazolamine Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.956	1.09 ng	386255	1,4-Dichlorobenzene-d4	7.643

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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Acq On : 30 Sep 2021 16:07
Operator : CG/JU
Sample : SSTDICC1.6
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC1.6

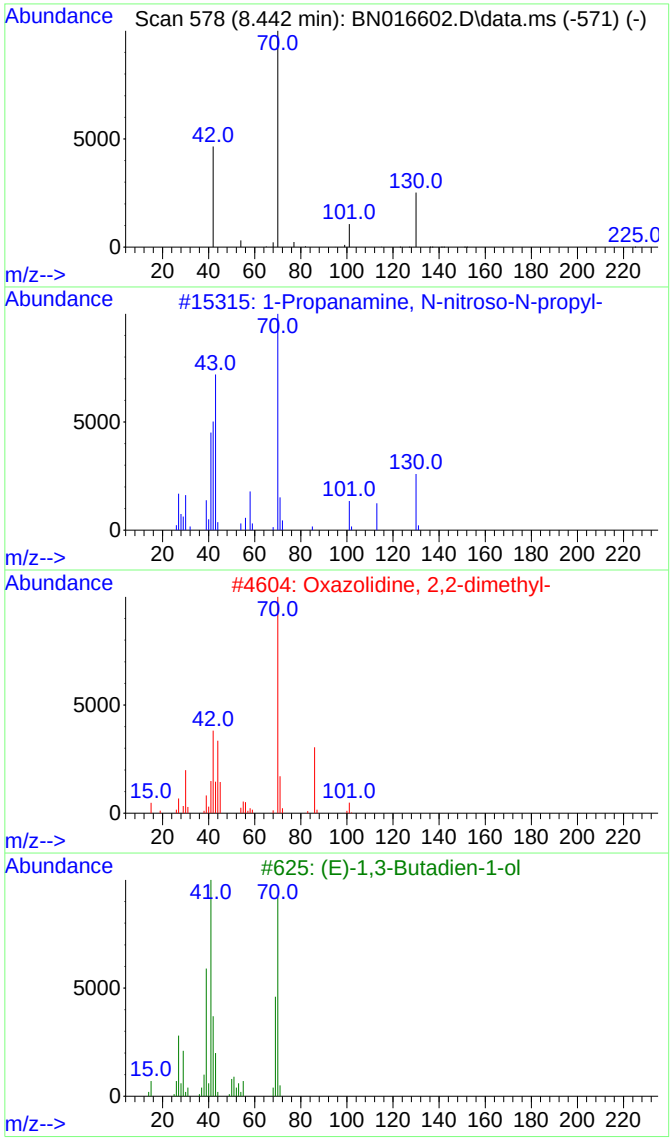
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

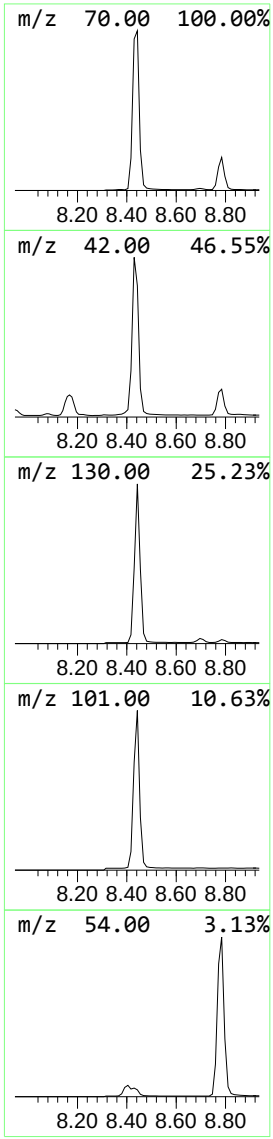
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Propanamine, N-nitroso-N-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.442	0.58 ng	204959	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanamine, N-nitroso-N-propyl-	130	C6H14N2O	000621-64-7	78
2	Oxazolidine, 2,2-dimethyl-	101	C5H11NO	020515-62-2	7
3	(E)-1,3-Butadien-1-ol	70	C4H6O	070411-98-2	4
4	2-Butenal, (E)-	70	C4H6O	000123-73-9	4
5	Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	4





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Data File : BN016602.D
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Sample : SSTDICC1.6
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC1.6

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

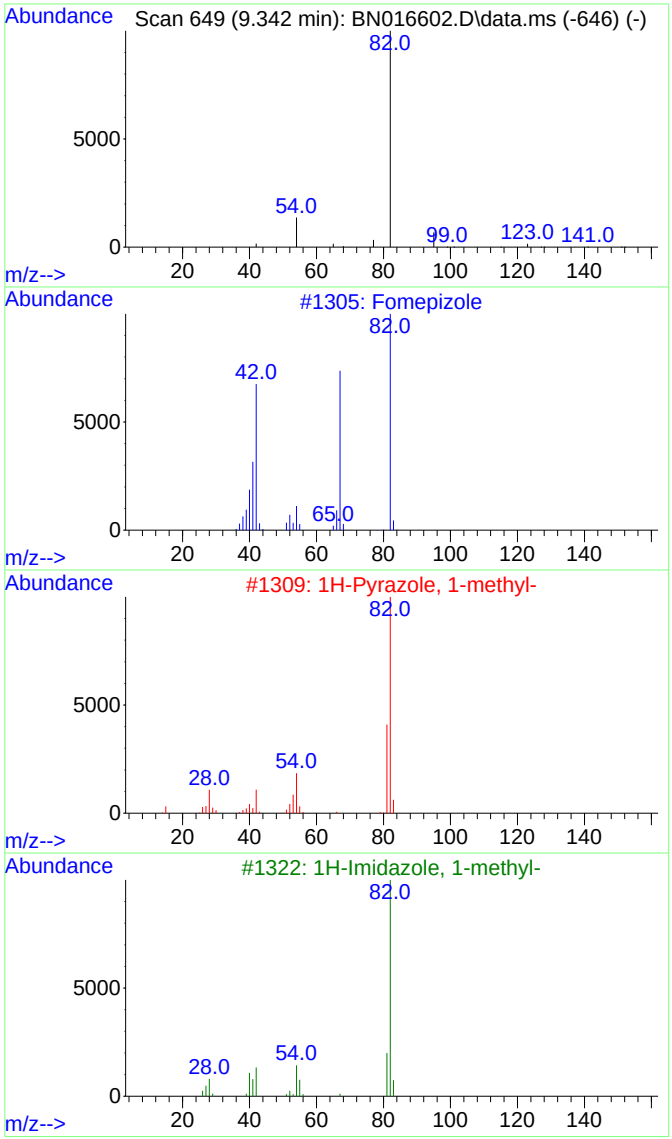
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

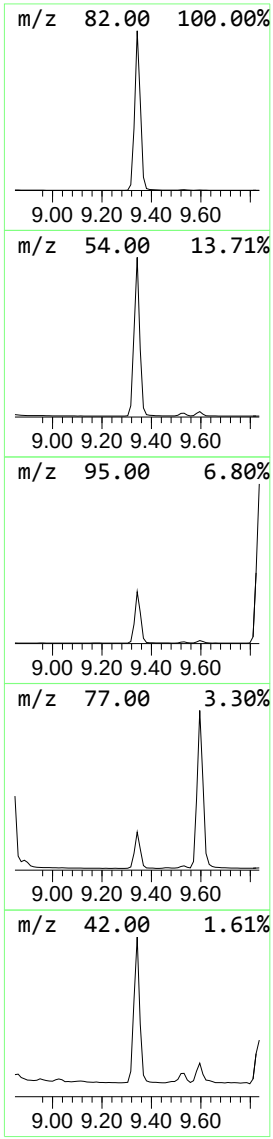
****

Peak Number 6 Fomepizole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.342	0.79 ng	336792	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





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016602.D
Acq On : 30 Sep 2021 16:07
Operator : CG/JU
Sample : SSTDICC1.6
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC1.6

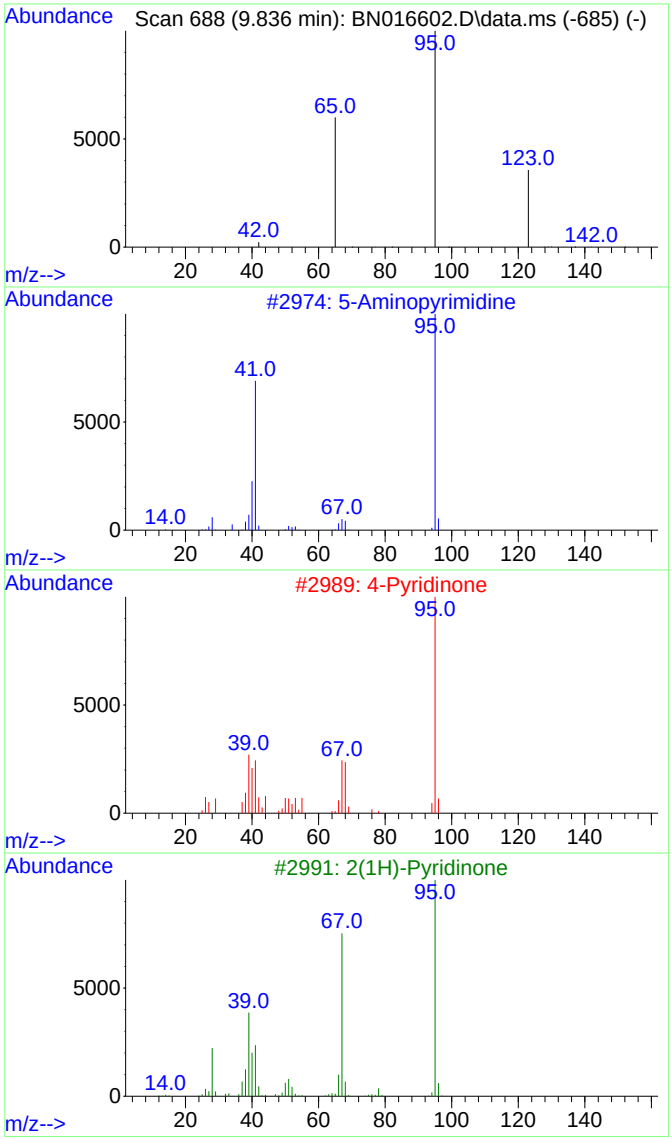
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

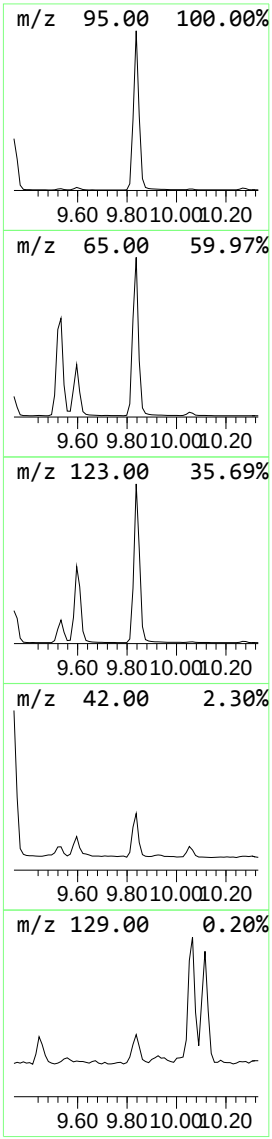
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.836	0.26 ng	109434	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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Sample : SSTDICC1.6
Misc :
ALS Vial : 6 Sample Multiplier: 1

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

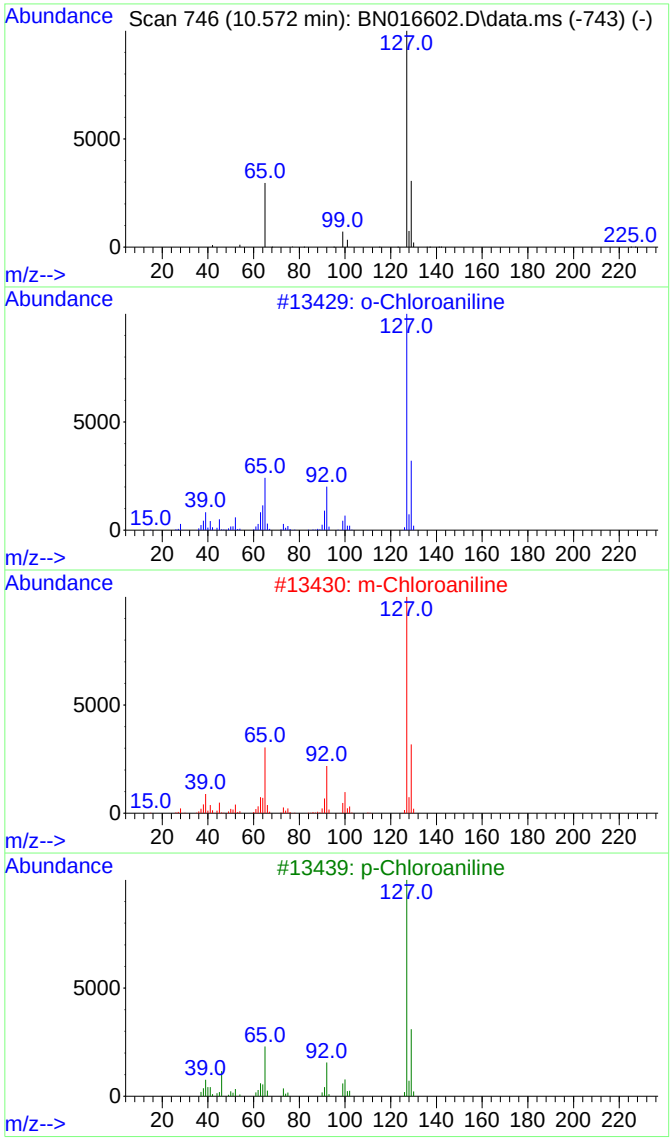
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

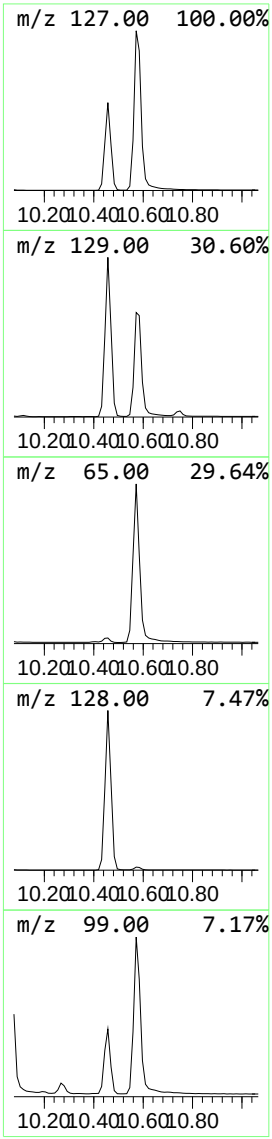
****

Peak Number 8 o-Chloroaniline Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.572	0.62 ng	265181	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	Picloxydine	474	C20H24Cl2N10	005636-92-0	83
5	4-(Chloromethyl)pyridine	127	C6H6ClN	010445-91-7	80





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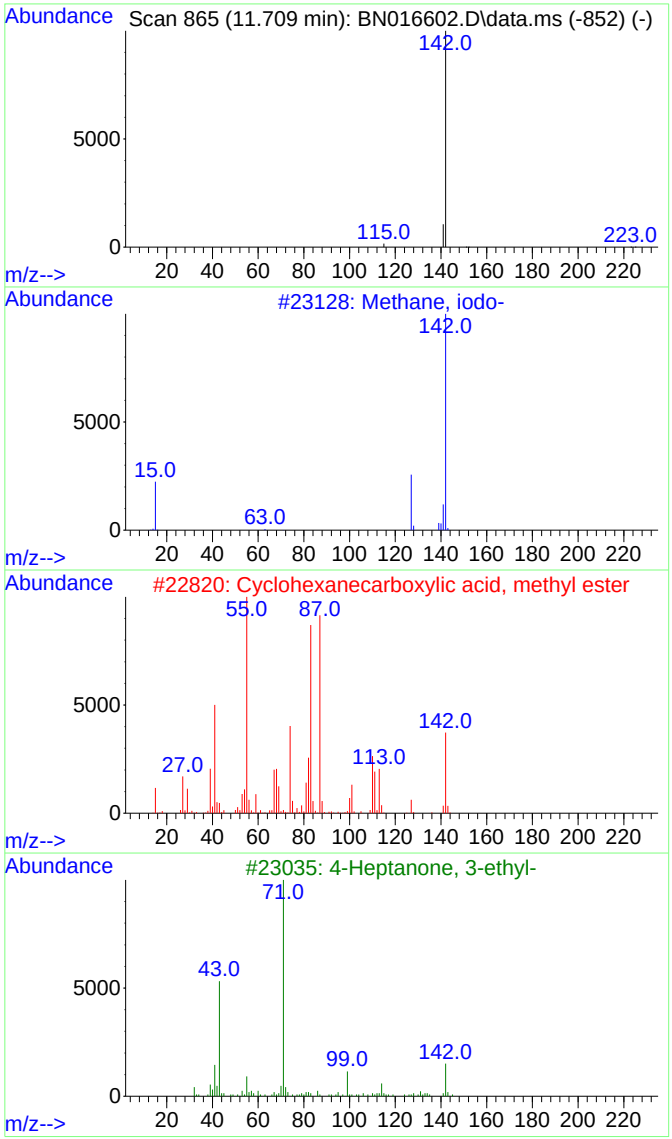
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

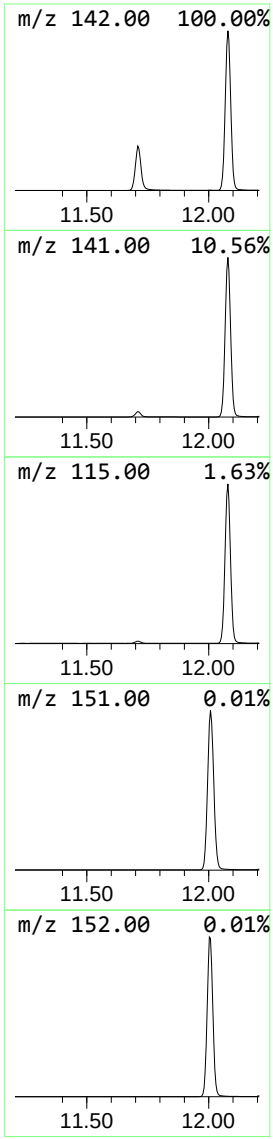
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Methane, iodo- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.710	0.26 ng	111684	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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Misc :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

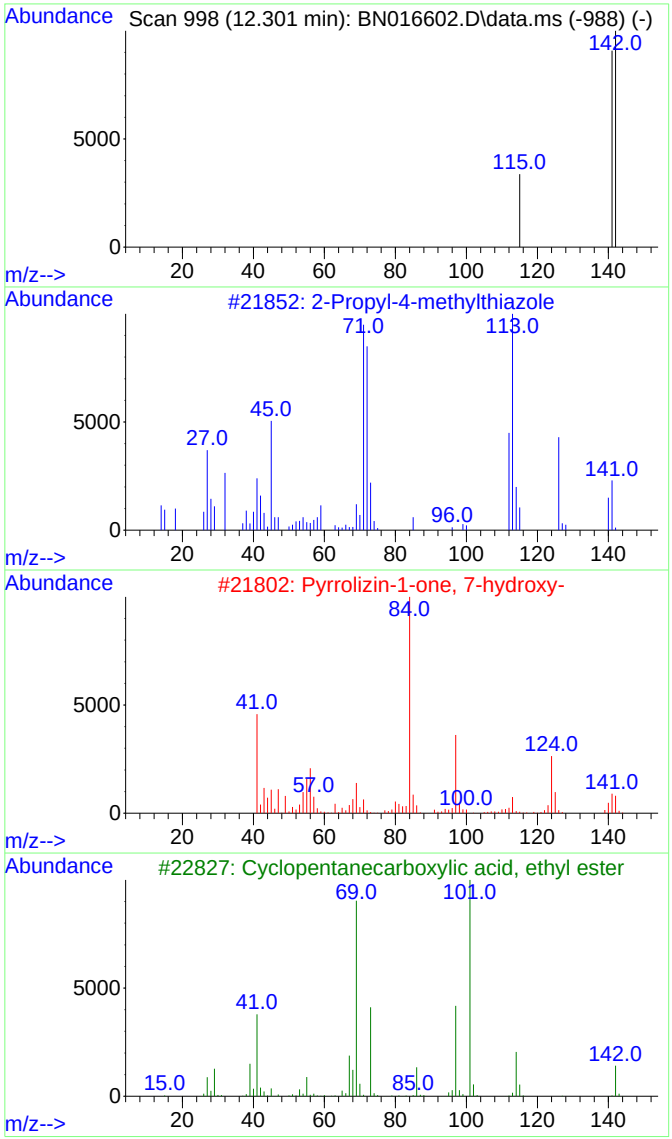
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

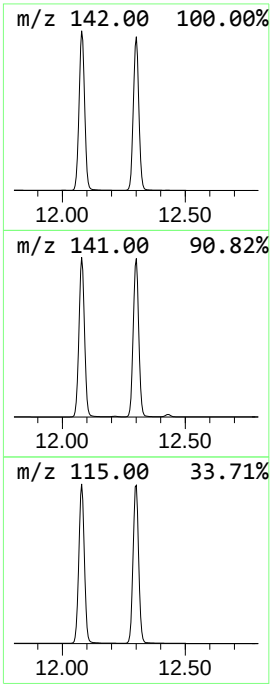
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.301	1.68 ng	717441	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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Misc :
ALS Vial : 6 Sample Multiplier: 1

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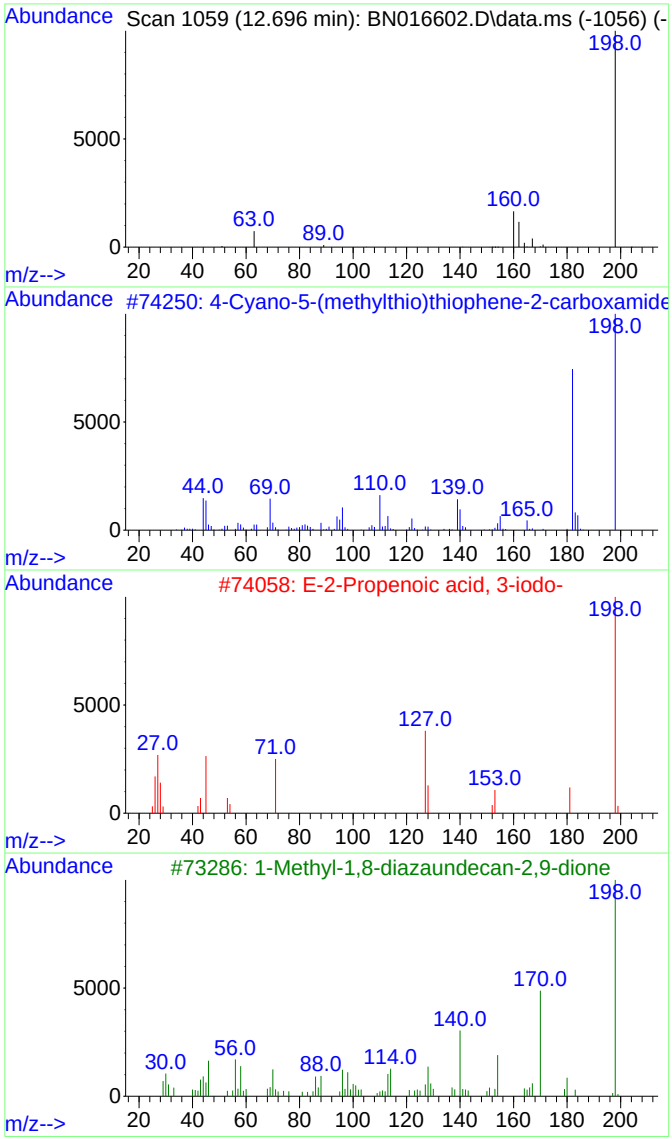
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

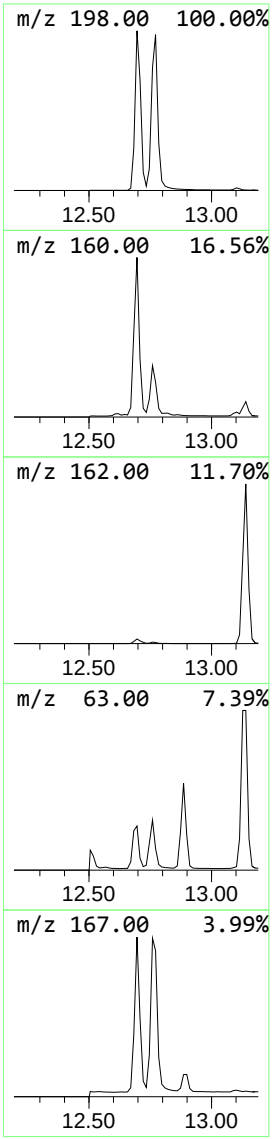
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 4-Cyano-5-(methylthio)thiop... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.696	0.32 ng	123384	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	E-2-Propenoic acid, 3-iodo-	198	C3H3IO2	1000308-86-7	3
3	1-Methyl-1,8-diazaundecan-2,9-dione	198	C10H18N2O2	1000298-94-5	3
4	Z-2-Propenoic acid, 3-iodo-	198	C3H3IO2	1000308-86-8	3
5	Thiazolo[5,4-d]pyrimidine, 5-ami...	198	C6H6N4S2	019835-31-5	3





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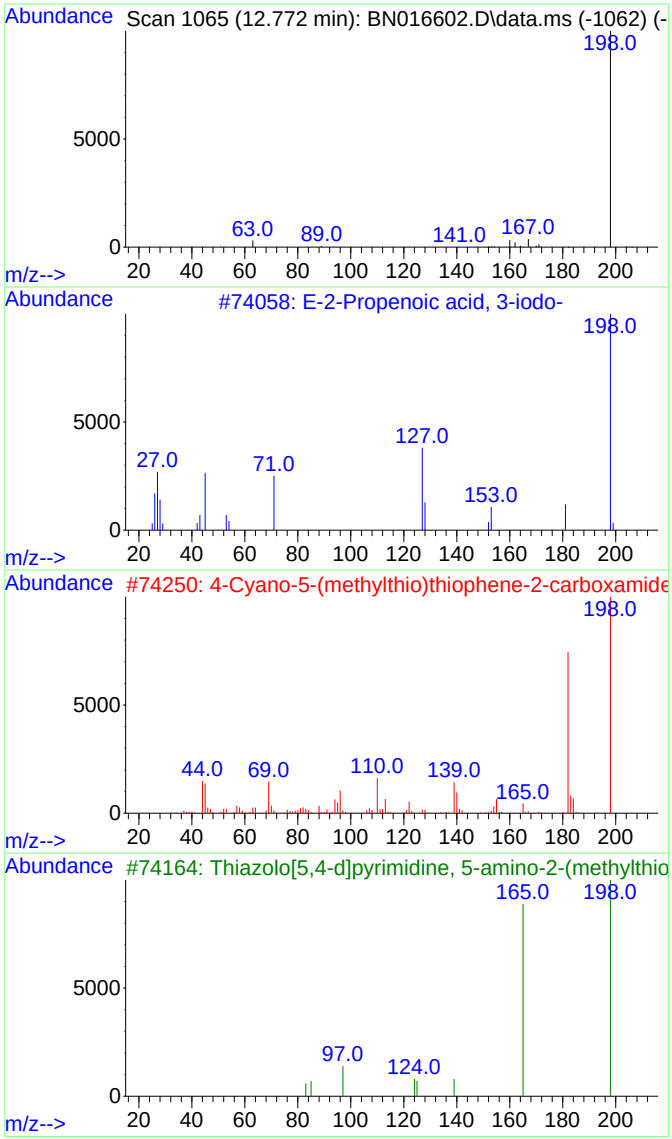
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

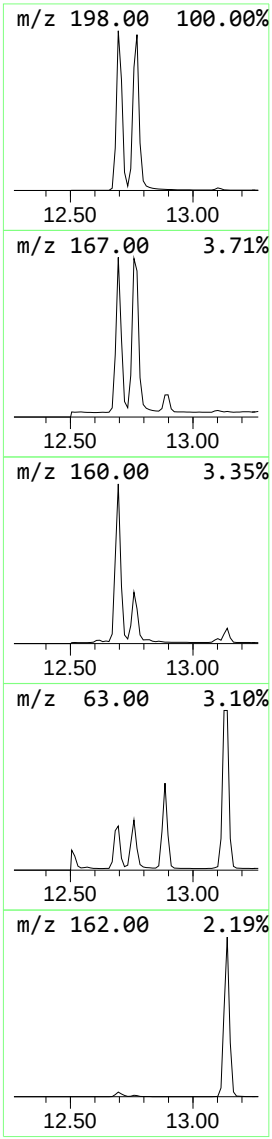
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 E-2-Propenoic acid, 3-iodo- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.772	0.29 ng	112225	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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LabSampleId :
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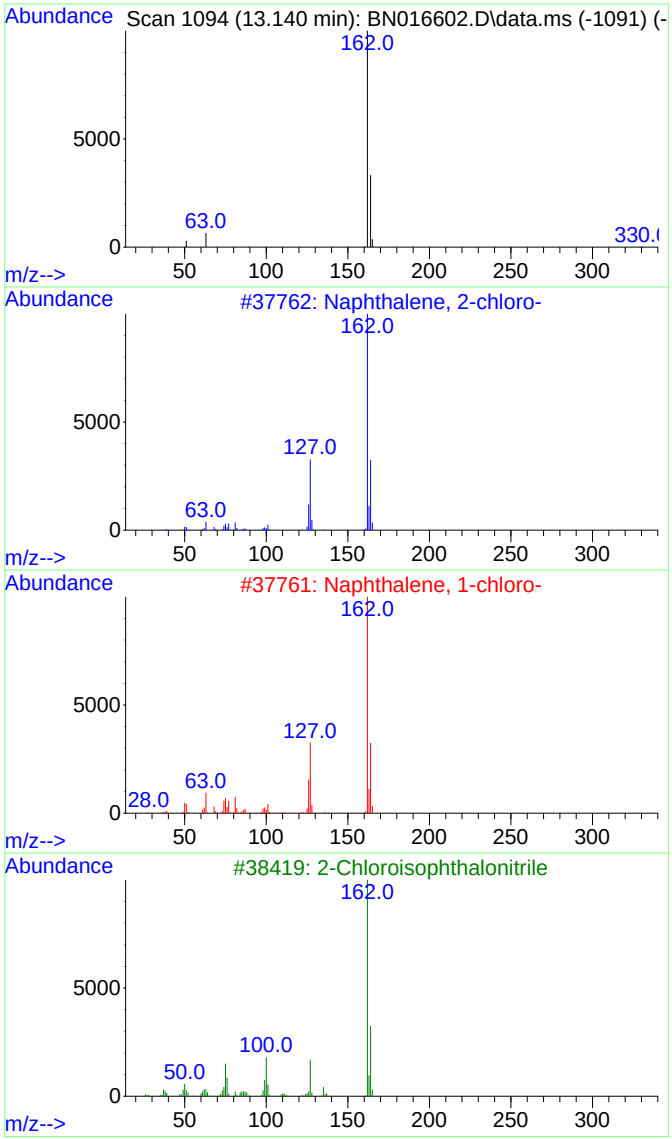
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

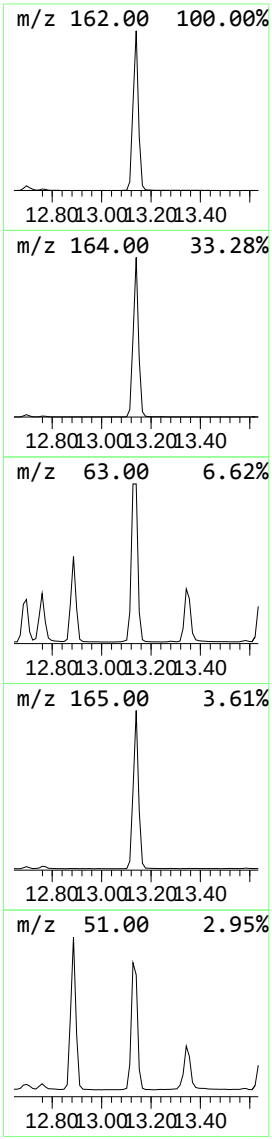
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Naphthalene, 2-chloro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.140	1.23 ng	476477	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-chloro-	162	C10H7Cl	000091-58-7	74
2	Naphthalene, 1-chloro-	162	C10H7Cl	000090-13-1	74
3	2-Chloroisophthalonitrile	162	C8H3ClN2	028442-78-6	7
4	3-Chlorophthalonitrile	162	C8H3ClN2	076241-79-7	7
5	2-Amino-4-chloro-1,3-thiazole-5-...	162	C4H3ClN2OS	076874-79-8	5





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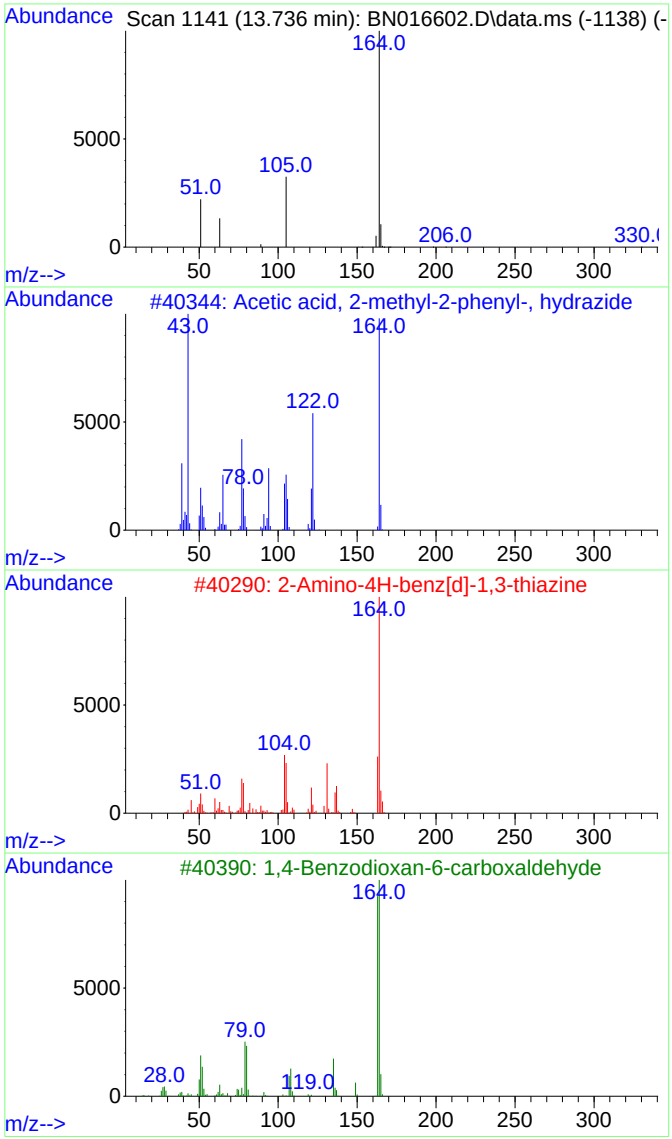
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

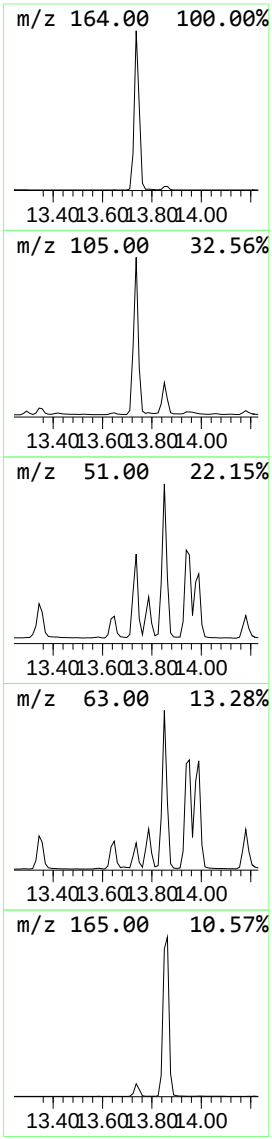
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 Acetic acid, 2-methyl-2-phe... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.736	0.18 ng	68319	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 2-methyl-2-phenyl-,...	164	C9H12N2O	038604-68-1	56
2	2-Amino-4H-benz[d]-1,3-thiazine	164	C8H8N2S	078959-46-3	9
3	1,4-Benzodioxan-6-carboxaldehyde	164	C9H8O3	029668-44-8	9
4	Benzoic acid, 2,4,5-trimethyl-	164	C10H12O2	000528-90-5	9
5	p-Phenylenediamine, N'-ethyl-N,N...	164	C10H16N2	024340-88-3	9





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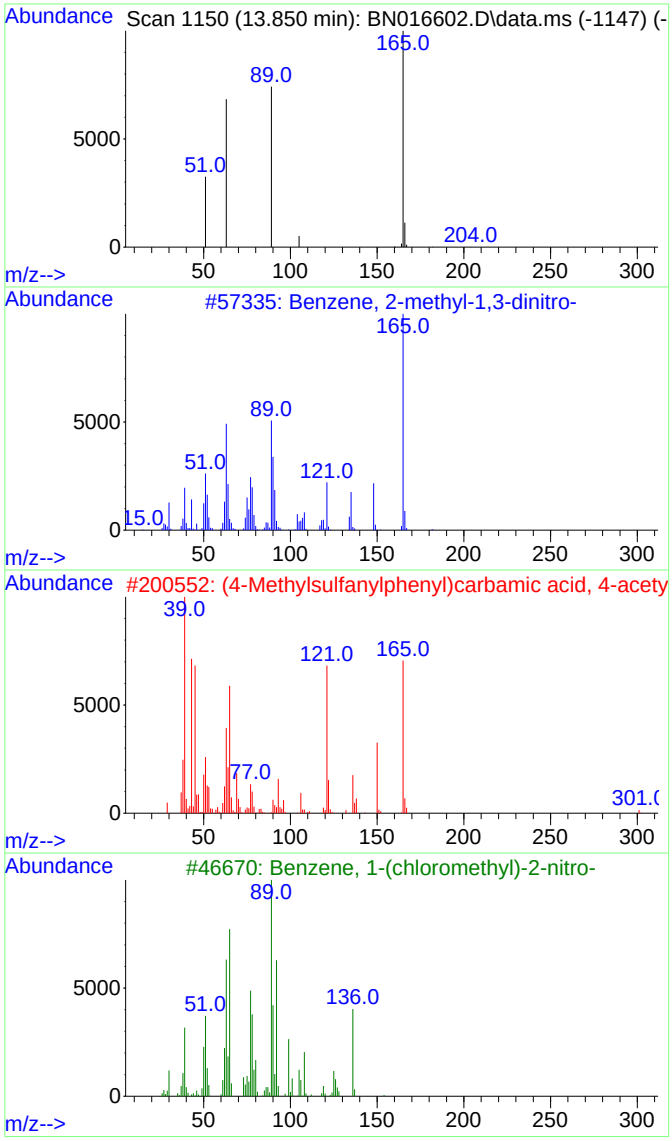
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

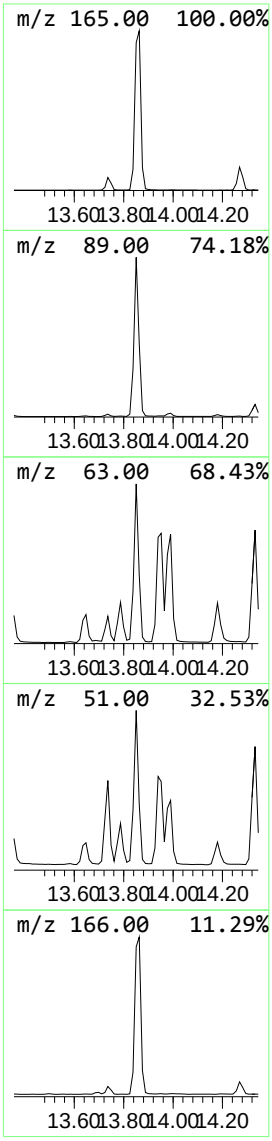
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 Benzene, 2-methyl-1,3-dinitro- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.850	0.39 ng	150378	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	9
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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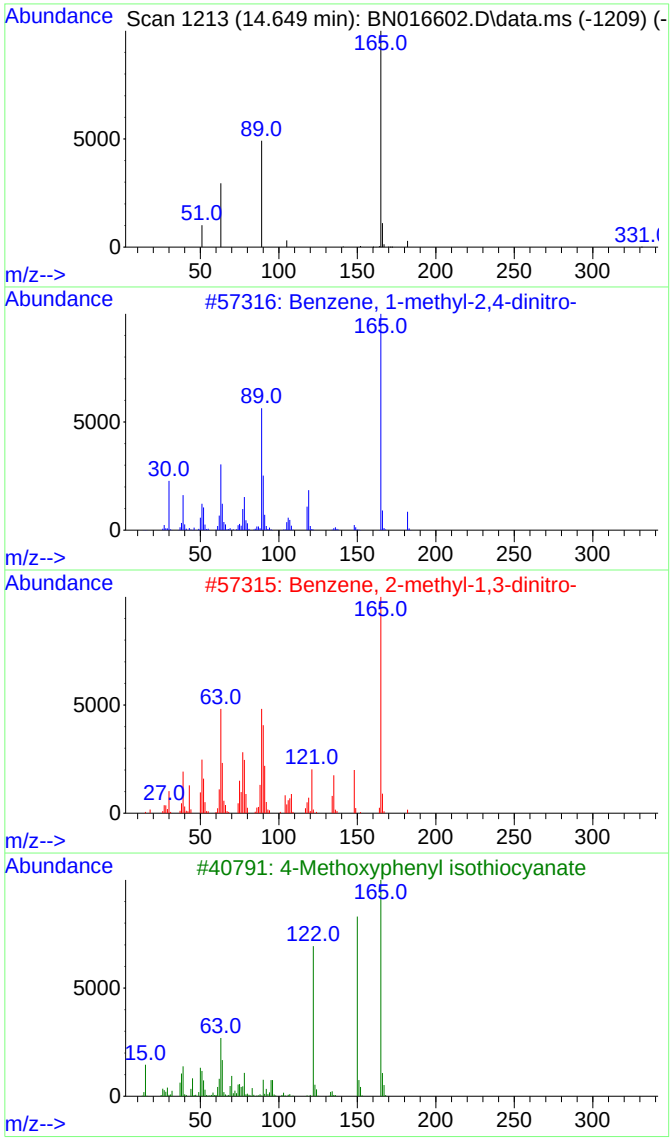
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

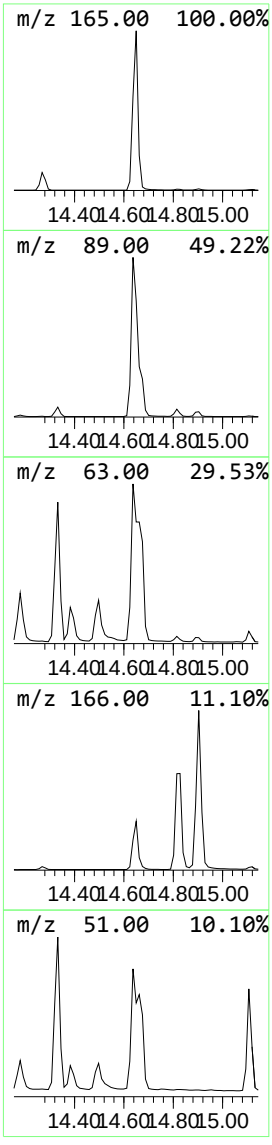
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 Benzene, 1-methyl-2,4-dinitro- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.650	0.56 ng	218585	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	2(3H)-Benzoxazolethione, 5-methyl-	165	C8H7NOS	022876-22-8	9
5	1H-1,2,4-Triazol-5-amine, 1-(3,4...	325	C16H15N5O3	1000319-98-0	9





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Instrument :
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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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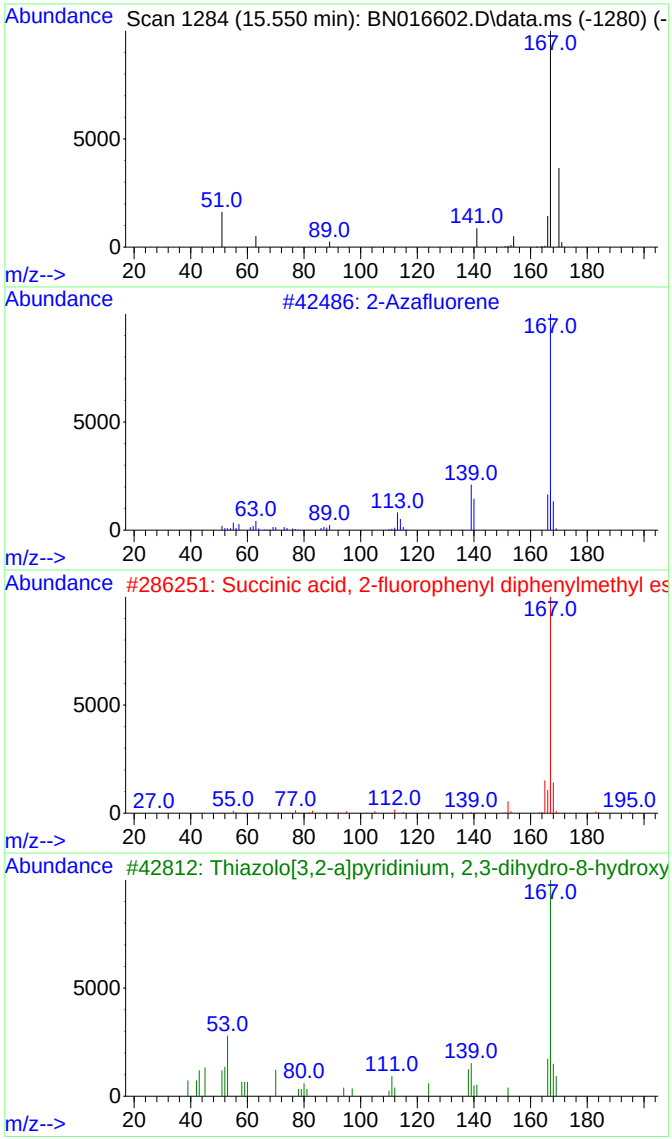
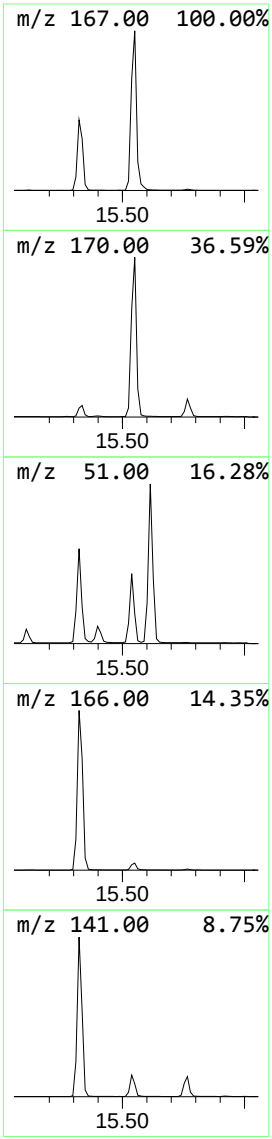
Peak Number 17 2-Azafluorene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.550	0.65 ng	251126	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	Carbazole	167	C12H9N	000086-74-8	7
5	2,4(1H,3H)-Pyrimidinedione, 5-me...	170	C7H10N2O3	059264-10-7	5





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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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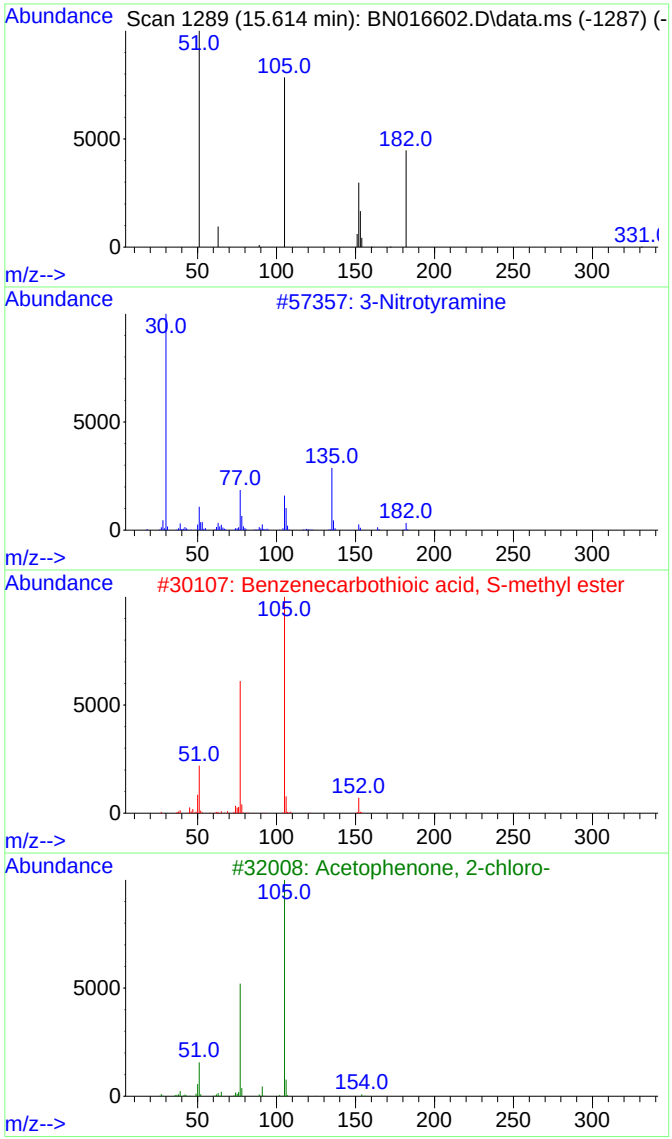
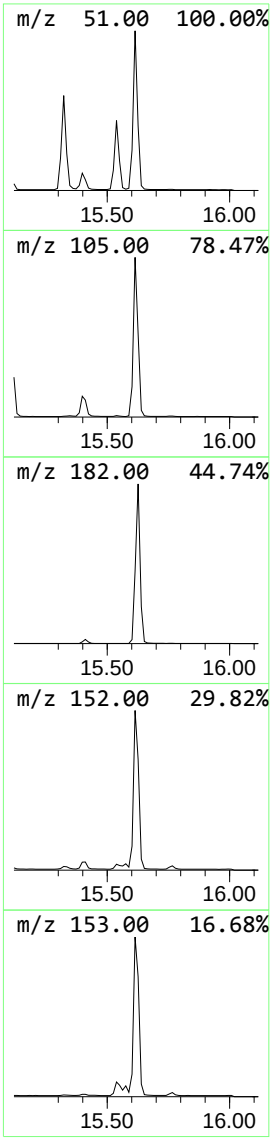
Peak Number 18 3-Nitrotyramine Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.614	0.77 ng	297626	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





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016602.D
Acq On : 30 Sep 2021 16:07
Operator : CG/JU
Sample : SSTDICC1.6
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC1.6

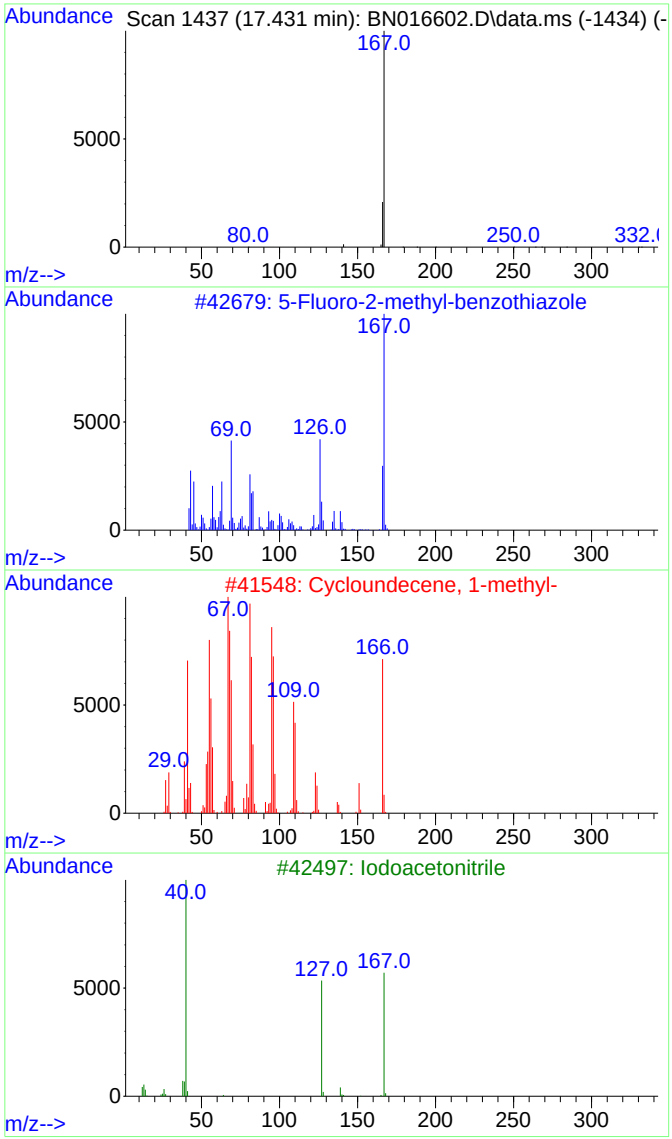
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

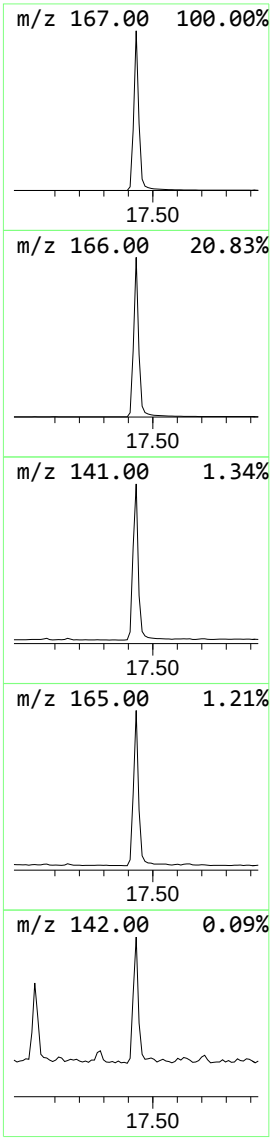
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 5-Fluoro-2-methyl-benzothia... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.432	1.62 ng	555997	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





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016602.D
Acq On : 30 Sep 2021 16:07
Operator : CG/JU
Sample : SSTDICC1.6
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDICC1.6

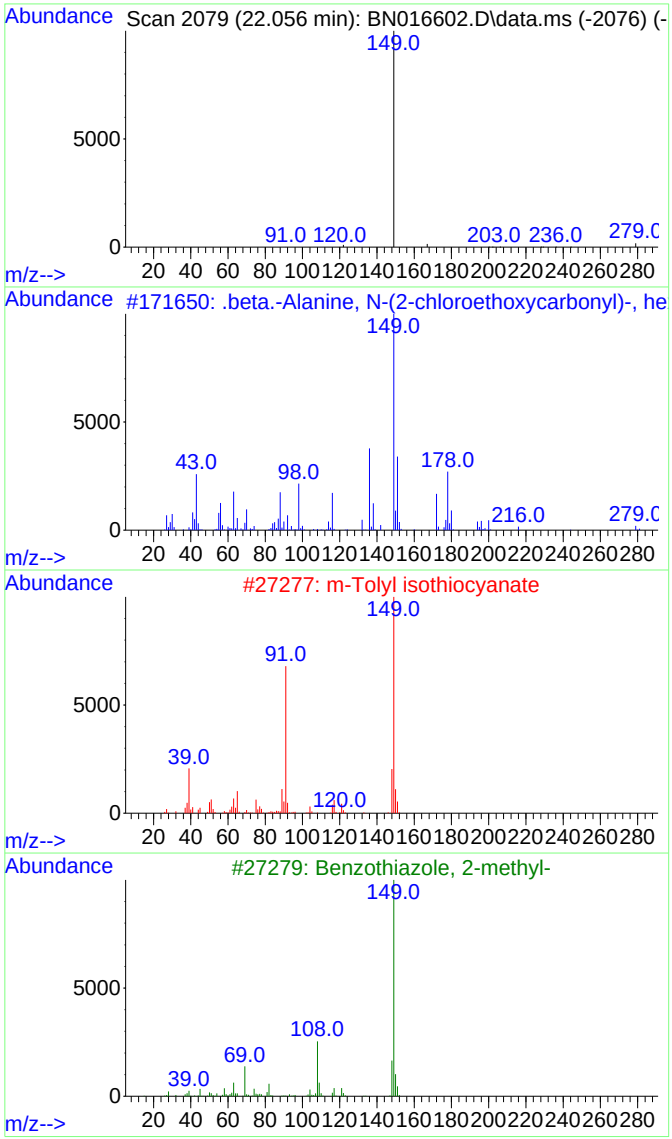
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

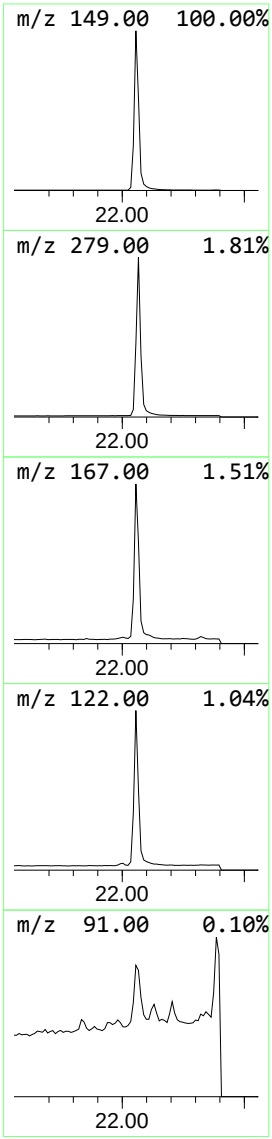
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 .beta.-Alanine, N-(2-chloro... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.056	0.17 ng	556937	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	m-Tolyl isothiocyanate	149	C8H7NS	000621-30-7	4
3	Benzothiazole, 2-methyl-	149	C8H7NS	000120-75-2	4
4	Benzene, 1-isothiocyanato-4-methyl-	149	C8H7NS	000622-59-3	4
5	3-Hydroxy-2-pyridin-3-yl-propenal	149	C8H7NO2	1000311-61-6	4





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016602.D
Acq On : 30 Sep 2021 16:07
Operator : CG/JU
Sample : SSTDICC1.6
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDICC1.6

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, ...	6.979	0.4	ng	149060	1	7.643	141857	0.4
Ethene, 1,1-dif...	7.200	0.4	ng	124233	1	7.643	141857	0.4
4-Methyl-bi(1,2...	7.532	0.2	ng	54742	1	7.643	141857	0.4
6-Benzothiazola...	7.956	1.1	ng	386255	1	7.643	141857	0.4
1-Propanamine, ...	8.442	0.6	ng	204959	1	7.643	141857	0.4
Fomepizole	9.342	0.8	ng	336792	2	10.407	170681	0.4
5-Aminopyrimidine	9.836	0.3	ng	109434	2	10.407	170681	0.4
o-Chloroaniline	10.572	0.6	ng	265181	2	10.407	170681	0.4
Methane, iodo-	11.710	0.3	ng	111684	2	10.407	170681	0.4
2-Propyl-4-meth...	12.301	1.7	ng	717441	2	10.407	170681	0.4
4-Cyano-5-(meth...	12.696	0.3	ng	123384	3	14.269	155316	0.4
E-2-Propenoic a...	12.772	0.3	ng	112225	3	14.269	155316	0.4
Naphthalene, 2-...	13.140	1.2	ng	476477	3	14.269	155316	0.4
Acetic acid, 2-...	13.736	0.2	ng	68319	3	14.269	155316	0.4
Benzene, 2-meth...	13.850	0.4	ng	150378	3	14.269	155316	0.4
Benzene, 1-meth...	14.650	0.6	ng	218585	3	14.269	155316	0.4
2-Azafluorene	15.550	0.6	ng	251126	3	14.269	155316	0.4
3-Nitrotyramine	15.614	0.8	ng	297626	3	14.269	155316	0.4
5-Fluoro-2-meth...	17.432	1.6	ng	555997	4	17.030	137602	0.4
.beta.-Alanine,...	22.056	0.2	ng	556937	5	21.238	1306520	0.4