LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016601.D
Acq On : 30 Sep 2021 15:31
Operator : CG/JU
Sample : SSTDICC0.8
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDICC0.8

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: BN016601.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.254	16	19	20	rBV	12669	17923	2.00%	0.138%
2	3.281	20	22	43	rVB	9226	44654	4.97%	0.343%
3	3.595	51	56	79	rVB	10997	52318	5.83%	0.402%
4	5.254	231	236	255	rVB	26314	103651	11.54%	0.796%
5	6.822	401	406	418	rBV	45235	113209	12.61%	0.869%
6	6.979	418	423	429	rVV	31939	69704	7.76%	0.535%
7	7.080	429	434	440	rVV	63490	128677	14.33%	0.988%
8	7.200	440	447	458	rVB	22043	59075	6.58%	0.454%
9	7.532	478	483	489	rVB	11784	26668	2.97%	0.205%
10	7.643	490	495	508	rVB2	41168	112416	12.52%	0.863%
11	7.864	515	519	524	rBV2	3538	10413	1.16%	0.080%
12	7.956	524	529	538	rVV2	83592	188830	21.03%	1.450%
13	8.168	547	552	557	rBV	5684	13767	1.53%	0.106%
14	8.430	571	577	591	rBV3	36469	94361	10.51%	0.725%
15	8.696	595	598	601	rBV	8569	15916	1.77%	0.122%
16	8.785	601	605	607	rBV	66215	139202	15.50%	1.069%
17	8.823	607	608	612	rVB	51809	74617	8.31%	0.573%
18	9.342	646	649	653	rBV	94271	150951	16.81%	1.159%
19	9.532	660	664	666	rBV	7116	13440	1.50%	0.103%
20	9.596	666	669	678	rVB	17694	30149	3.36%	0.232%
21	9.836	685	688	702	rBV	31201	51584	5.75%	0.396%
22	10.065	702	706	708	rBV	8016	16065	1.79%	0.123%
23	10.407	729	733	735	rBV	86337	160613	17.89%	1.234%
24	10.458	735	737	741	rVV	199051	322456	35.91%	2.477%
25	10.572	743	746	756	rVV	55521	119573	13.32%	0.918%
26	10.749	757	760	763	rVB	60452	97050	10.81%	0.745%
27	11.307	801	804	814	rBV	4876	11375	1.27%	0.087%
28	11.709	853	865	902	rBV	28184	50190	5.59%	0.385%
29	12.007	921	932	940	rBV	101540	166517	18.55%	1.279%
30	12.079	940	948	971	rVV	228145	366657	40.84%	2.816%
31	12.301	988	998	1020	rVV	222521	351744	39.17%	2.701%
32	12.696	1056	1059	1062	rBV	33223	55202	6.15%	0.424%
33	12.772	1062	1065	1071	rVB	25817	49690	5.53%	0.382%
34	12.899	1071	1075	1078	rBV	197650	348085	38.77%	2.673%
35	13.140	1091	1094	1097	rVB	147210	227553	25.34%	1.748%
36	13.736	1138	1141	1143	rBV	22721	31171	3.47%	0.239%

LSC Area Percent Report

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Acq On : 30 Sep 2021 15:31
Operator : CG/JU
Sample : SSTDICC0.8
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDICC0.8

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	1153	rVB	38082	58004	6.46%	0.445%
38	13.990	1158	1161	1164	rVB	196334	297539	33.14%	2.285%
39	14.269	1180	1183	1185	rBV	110911	158758	17.68%	1.219%
40	14.332	1185	1188	1191	rVB	300947	430038	47.89%	3.303%
41	14.650	1209	1213	1220	rBV2	37130	89112	9.92%	0.684%
42	14.827	1224	1227	1230	rBV	10500	19353	2.16%	0.149%
43	14.903	1230	1233	1236	rBV	16156	22569	2.51%	0.173%
44	15.106	1246	1249	1252	rBV	15903	21080	2.35%	0.162%
45	15.322	1263	1266	1270	rBV2	381827	624639	69.57%	4.797%
46	15.411	1270	1273	1280	rVV2	10491	20727	2.31%	0.159%
47	15.538	1280	1283	1287	rVV	65213	116002	12.92%	0.891%
48	15.614	1287	1289	1293	rVB2	81661	128508	14.31%	0.987%
49	15.766	1298	1301	1311	rVB2	26434	44021	4.90%	0.338%
50	16.227	1335	1338	1341	rBV2	114108	162464	18.09%	1.248%
51	16.324	1343	1346	1350	rVB	76438	124614	13.88%	0.957%
52	16.507	1358	1361	1364	rBV	48097	67632	7.53%	0.519%
53	16.677	1372	1375	1384	rBV	44736	73374	8.17%	0.564%
54	17.018	1400	1403	1405	rBV	68737	128219	14.28%	0.985%
55	17.066	1405	1407	1410	rVV	275381	380419	42.37%	2.922%
56	17.152	1411	1414	1434	rVV	199315	335287	37.34%	2.575%
57	17.431	1434	1437	1457	rVV	177013	260861	29.05%	2.003%
58	18.021	1483	1486	1498	rVB	10722	14140	1.57%	0.109%
59	19.068	1686	1697	1699	rBV	213764	276051	30.74%	2.120%
60	19.098	1699	1703	1741	rVB	341354	469233	52.26%	3.604%
61	19.460	1767	1776	1806	rBV	335728	453057	50.46%	3.480%
62	19.679	1813	1820	1854	rVB	203036	251366	28.00%	1.931%
63	20.378	1918	1921	1924	rBV	84041	120788	13.45%	0.928%
64	21.026	1979	1982	1993	rBV	16851	29929	3.33%	0.230%
65	21.174	1993	1996	1998	rBV	124125	148944	16.59%	1.144%
66	21.217	1998	2000	2003	rVV2	351900	567066	63.16%	4.355%
67	21.270	2003	2005	2008	rVB	357386	440167	49.02%	3.381%
68	22.056	2076	2079	2096	rVB	141123	185702	20.68%	1.426%
69	22.810	2217	2230	2236	rBV	236444	385673	42.95%	2.962%
70	22.855	2236	2243	2292	rVB	236865	410873	45.76%	3.156%
71	23.389	2385	2399	2416	rBV	169815	335969	37.42%	2.580%
72	23.488	2417	2428	2470	rVB	75619	159212	17.73%	1.223%
73	25.778	3067	3097	3191	rBV4	237666	897887	100.00%	6.896%
74	26.459	3273	3296	3364	rBV	130446	425794	47.42%	3.270%

Sum of corrected areas: 13020537

Instrument :
BNA_N
LabSampleId :
SSTDICC0.8

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Acq On : 30 Sep 2021 15:31
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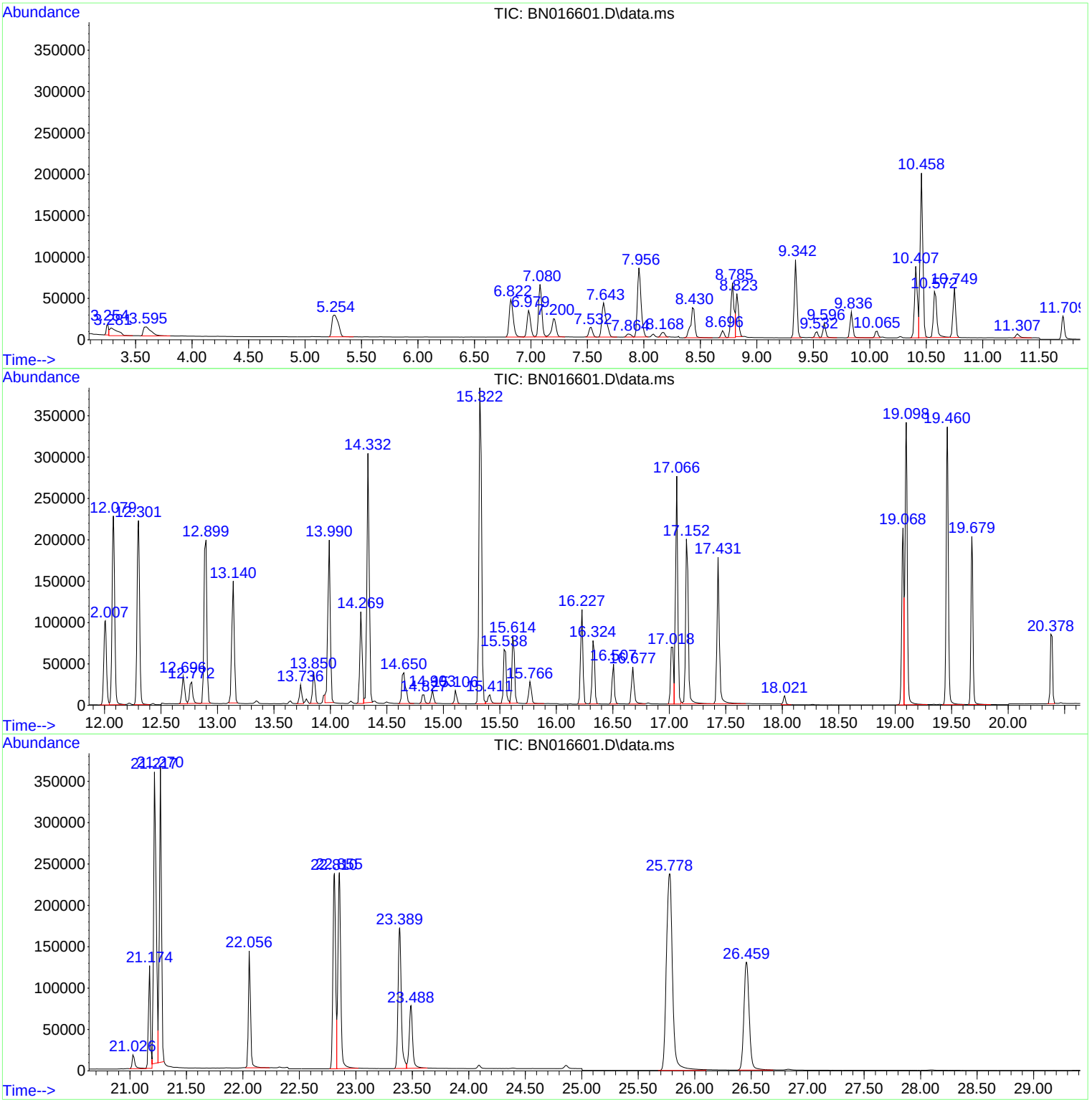
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.8

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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Operator : CG/JU
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BNA_N
LabSampleId :
SSTDICC0.8

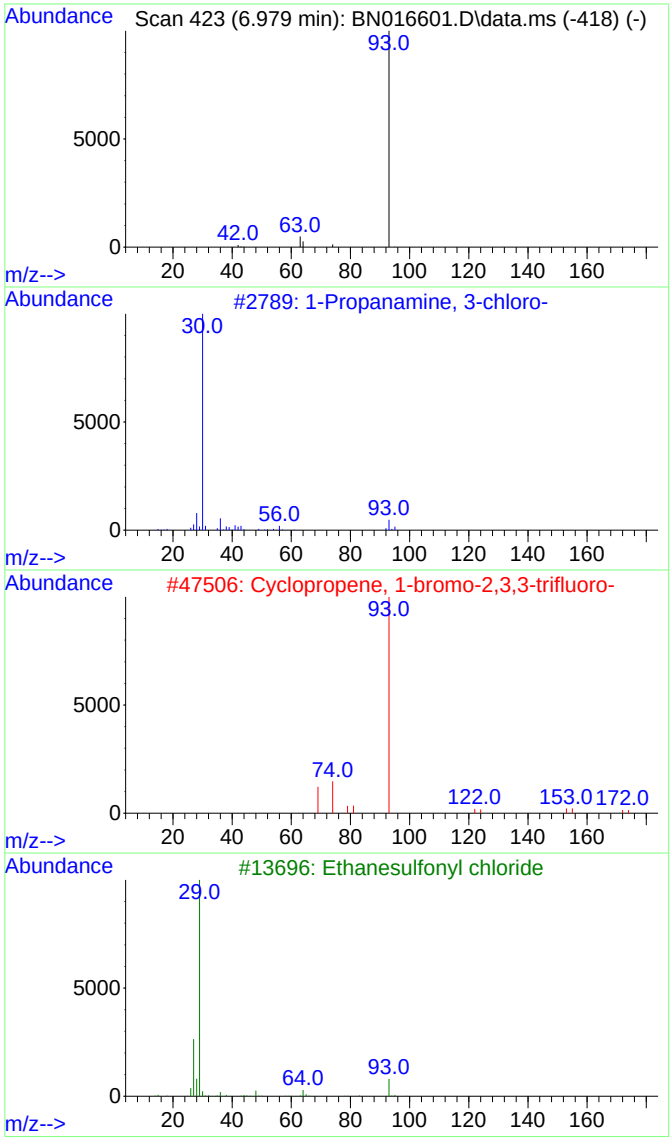
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

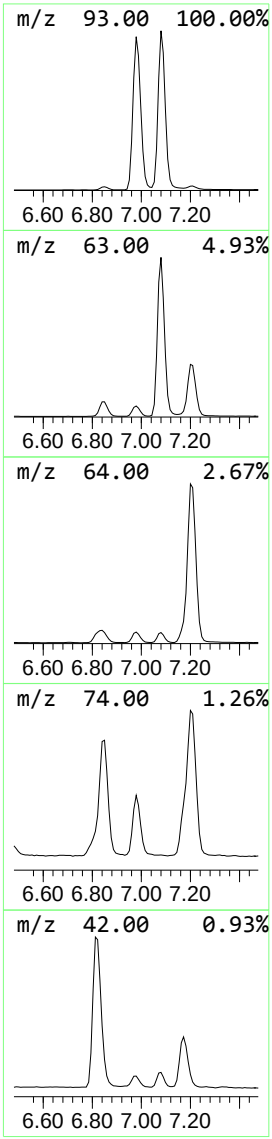
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1-Propanamine, 3-chloro- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.979	0.25 ng	69704	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 : BN016601.D
Acq On : 30 Sep 2021 15:31
Operator : CG/JU
Sample : SSTDICC0.8
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.8

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

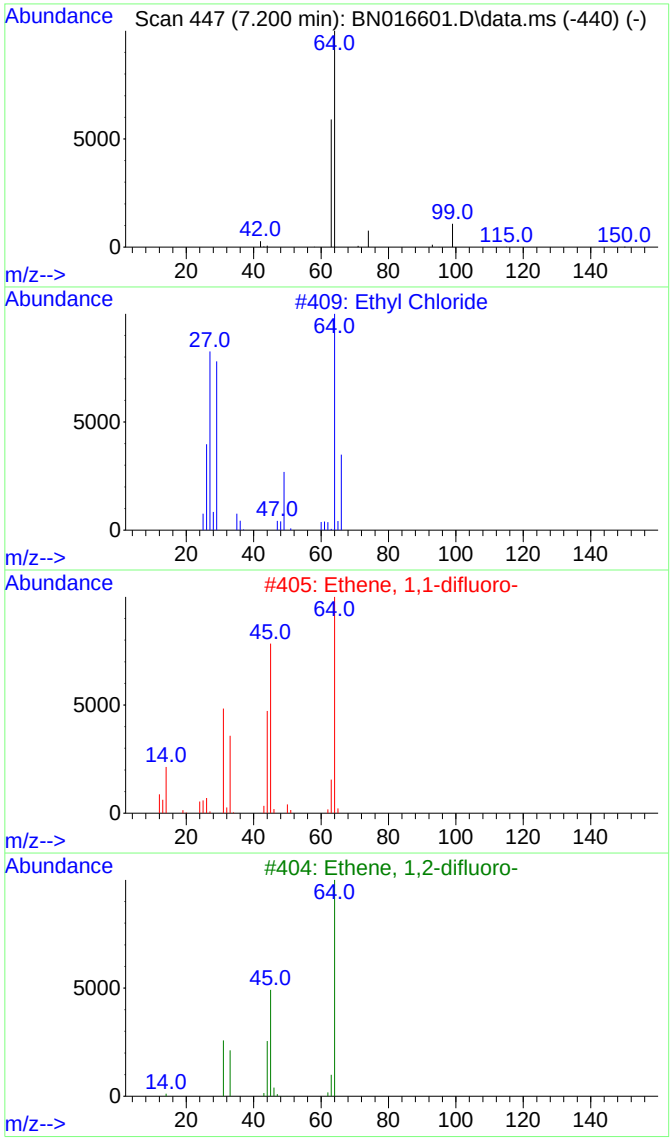
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

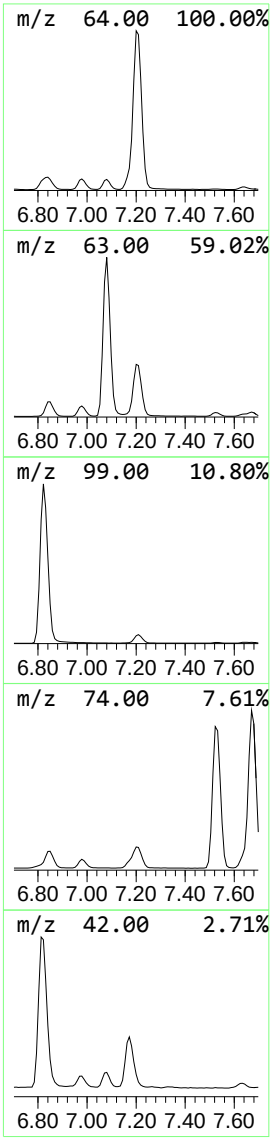
****

Peak Number 2 Ethyl Chloride Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.200	0.21 ng	59075	1,4-Dichlorobenzene-d4	7.643

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





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016601.D
Acq On : 30 Sep 2021 15:31
Operator : CG/JU
Sample : SSTDICC0.8
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.8

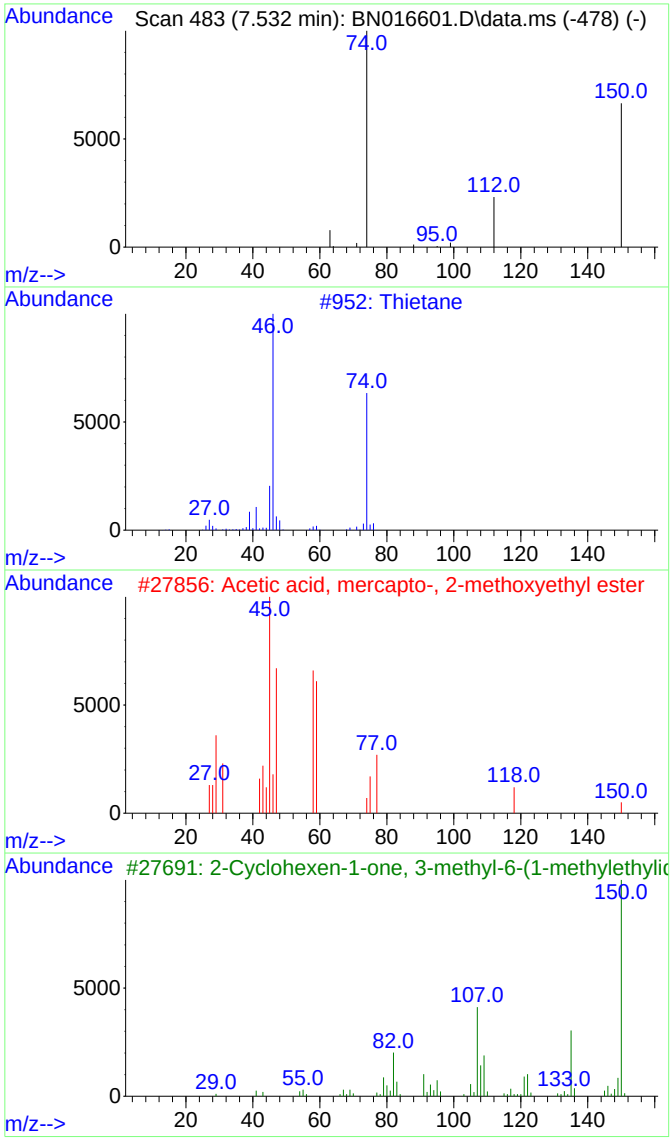
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

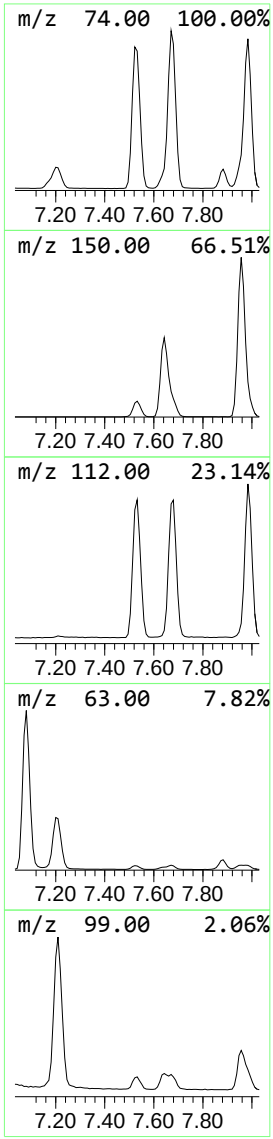
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Thietane Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.532	0.09 ng	26668	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thietane	74	C3H6S	000287-27-4	3
2	Acetic acid, mercapto-, 2-methox...	150	C5H10O3S	019788-48-8	3
3	2-Cyclohexen-1-one, 3-methyl-6-(...	150	C10H14O	000491-09-8	2
4	3-Methylpyrazolo[4,3-d]pyrimidin...	150	C6H6N4O	005399-94-0	2
5	3-Cyano-2,6-dihydroxy-4-methylpy...	150	C7H6N2O2	005444-02-0	2





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Data File : BN016601.D
Acq On : 30 Sep 2021 15:31
Operator : CG/JU
Sample : SSTDICC0.8
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.8

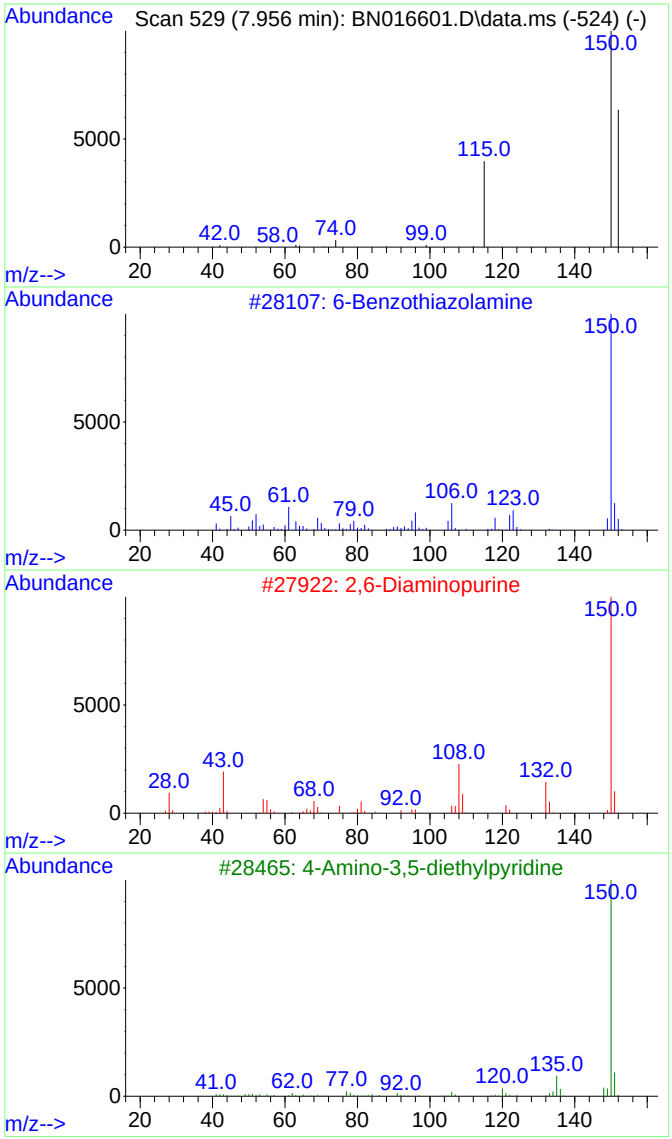
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

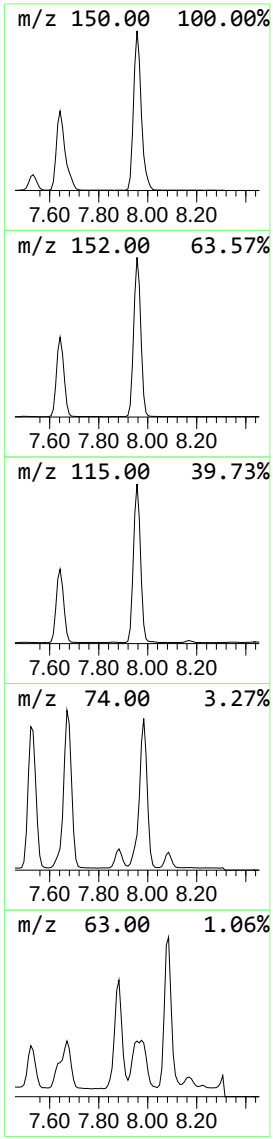
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 6-Benzothiazolamine Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.956	0.67 ng	188830	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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Operator : CG/JU
Sample : SSTDICC0.8
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.8

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

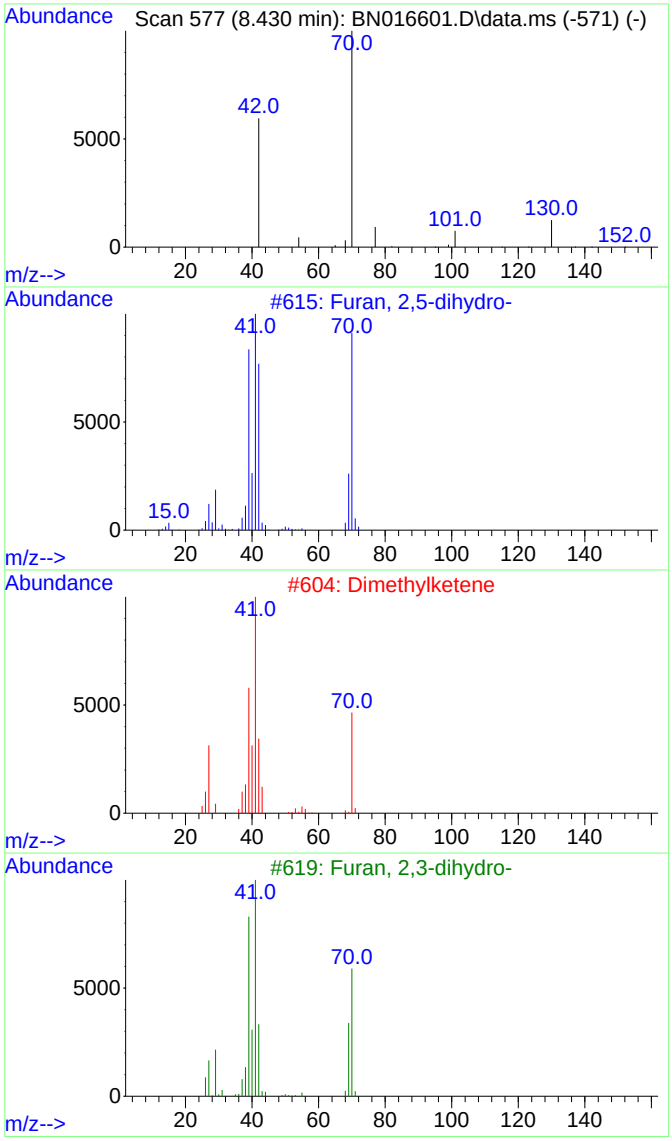
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

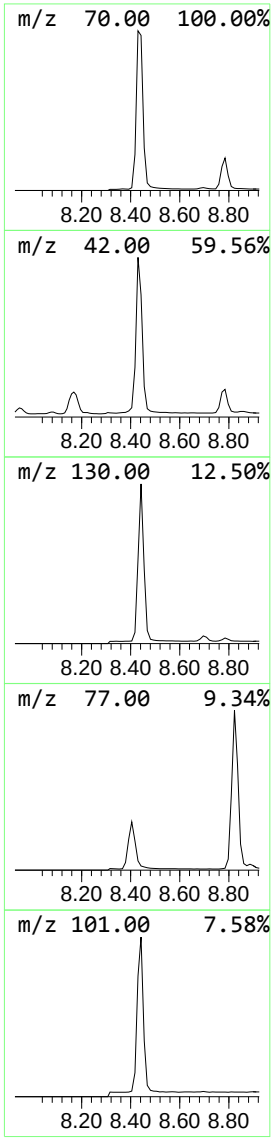
****

Peak Number 5 Furan, 2,5-dihydro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.430	0.34 ng	94361	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	7
2	Dimethylketene	70	C4H6O	000598-26-5	5
3	Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	5
4	1-Propanamine, N-nitroso-N-propyl-	130	C6H14N2O	000621-64-7	4
5	Ethoxyacetylene	70	C4H6O	000927-80-0	4





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Data File : BN016601.D
Acq On : 30 Sep 2021 15:31
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.8

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

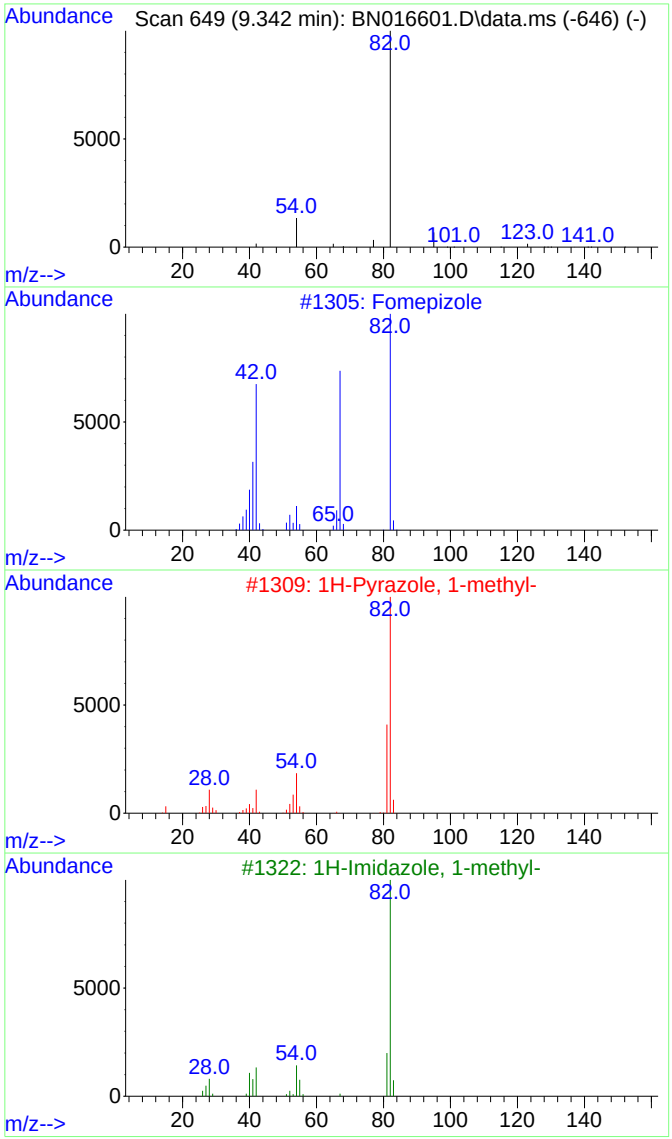
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

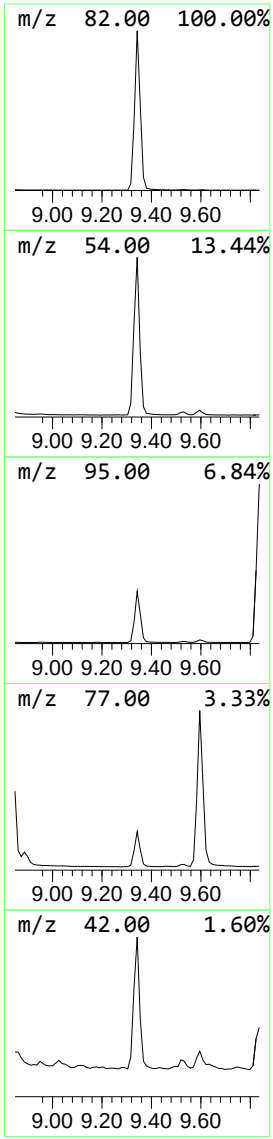
****

Peak Number 6 Fomepizole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.342	0.38 ng	150951	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 : BN016601.D
Acq On : 30 Sep 2021 15:31
Operator : CG/JU
Sample : SSTDICC0.8
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.8

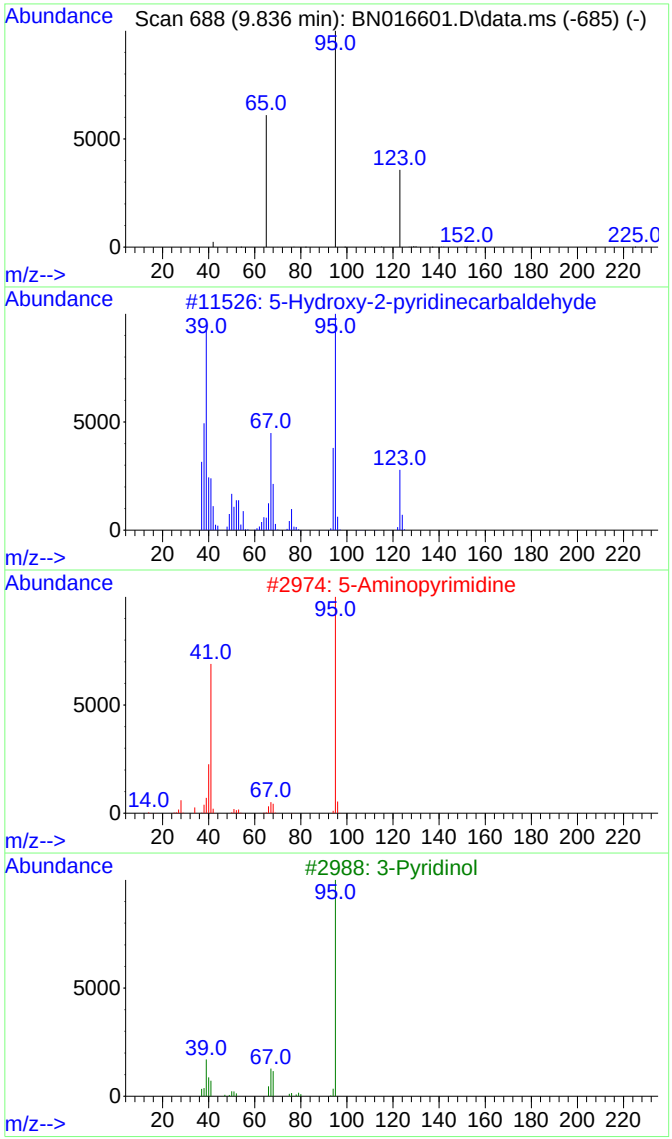
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

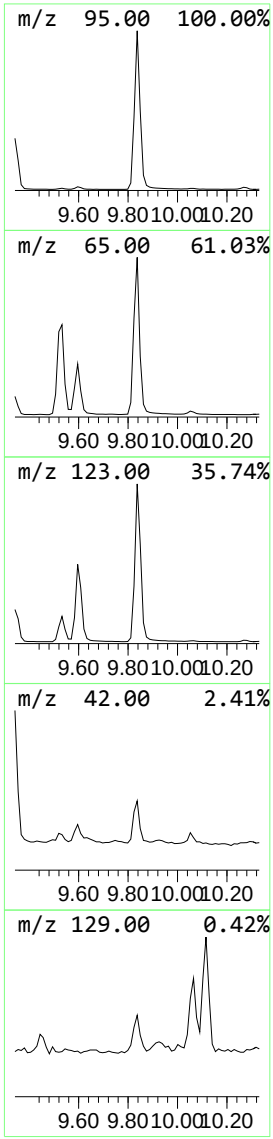
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 5-Hydroxy-2-pyridinecarbald... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.836	0.13 ng	51584	Naphthalene-d8	10.407

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Hydroxy-2-pyridinecarbaldehyde	123	C6H5NO2	031191-08-9	5
2	5-Aminopyrimidine	95	C4H5N3	000591-55-9	3
3	3-Pyridinol	95	C5H5NO	000109-00-2	2
4	2-Pyrimidinamine	95	C4H5N3	000109-12-6	2
5	4-Pyridinol	95	C5H5NO	000626-64-2	2





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Sample : SSTDICC0.8
Misc :
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LabSampleId :
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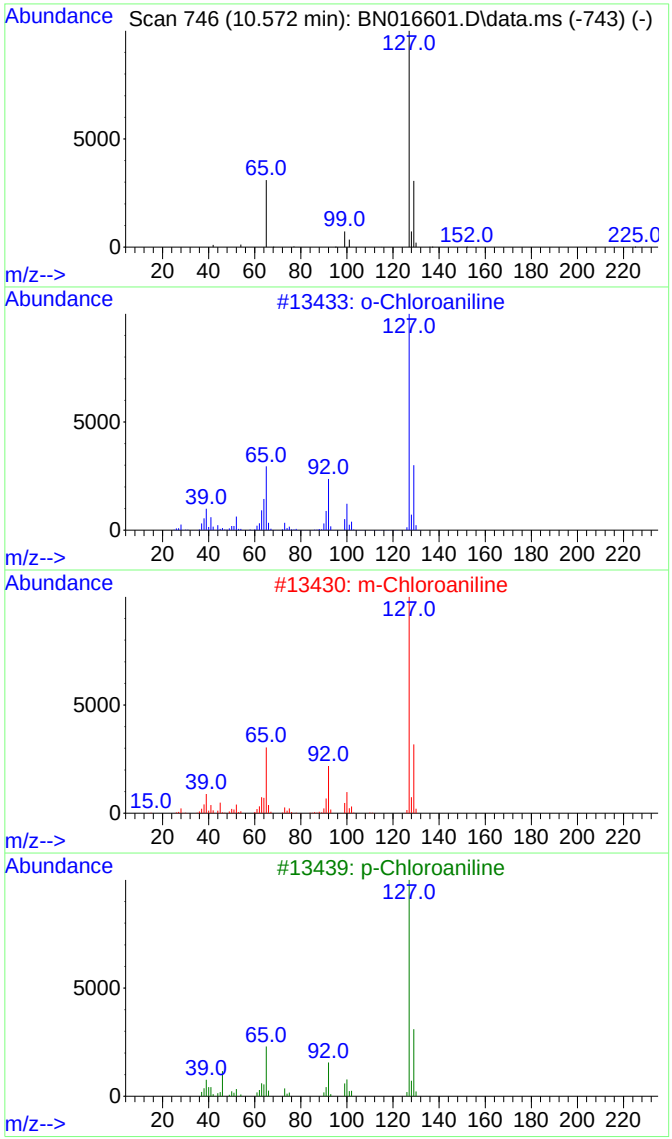
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

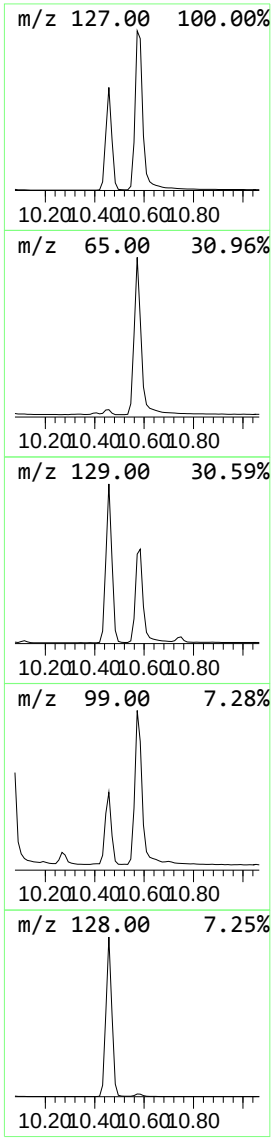
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 o-Chloroaniline Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.572	0.30 ng	119573	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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Misc :
ALS Vial : 5 Sample Multiplier: 1

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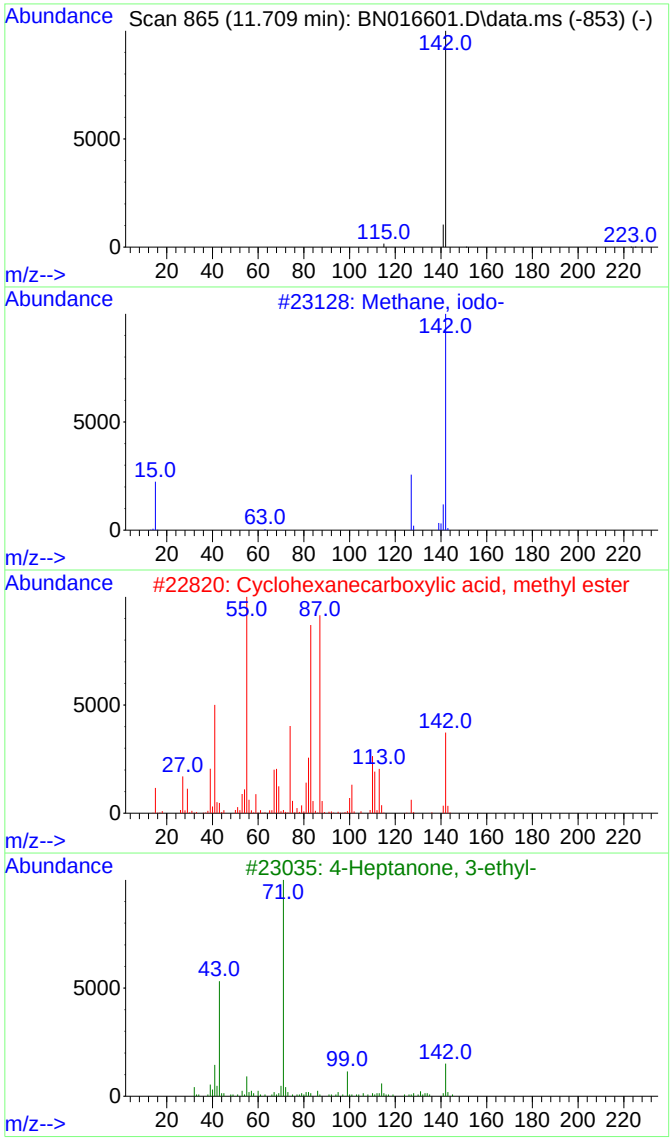
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

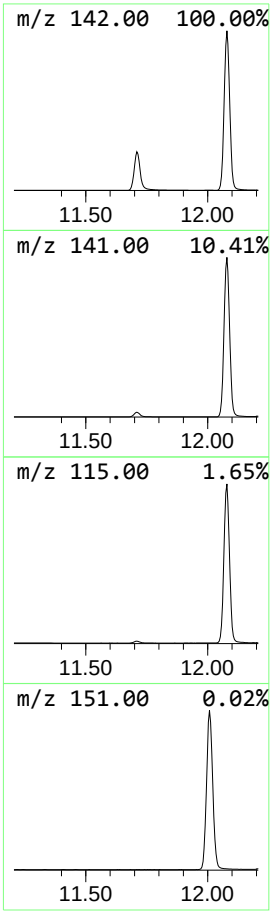
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Methane, iodo- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.710	0.12 ng	50190	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 :
ALS Vial : 5 Sample Multiplier: 1

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LabSampleId : SSTDICC0.8

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

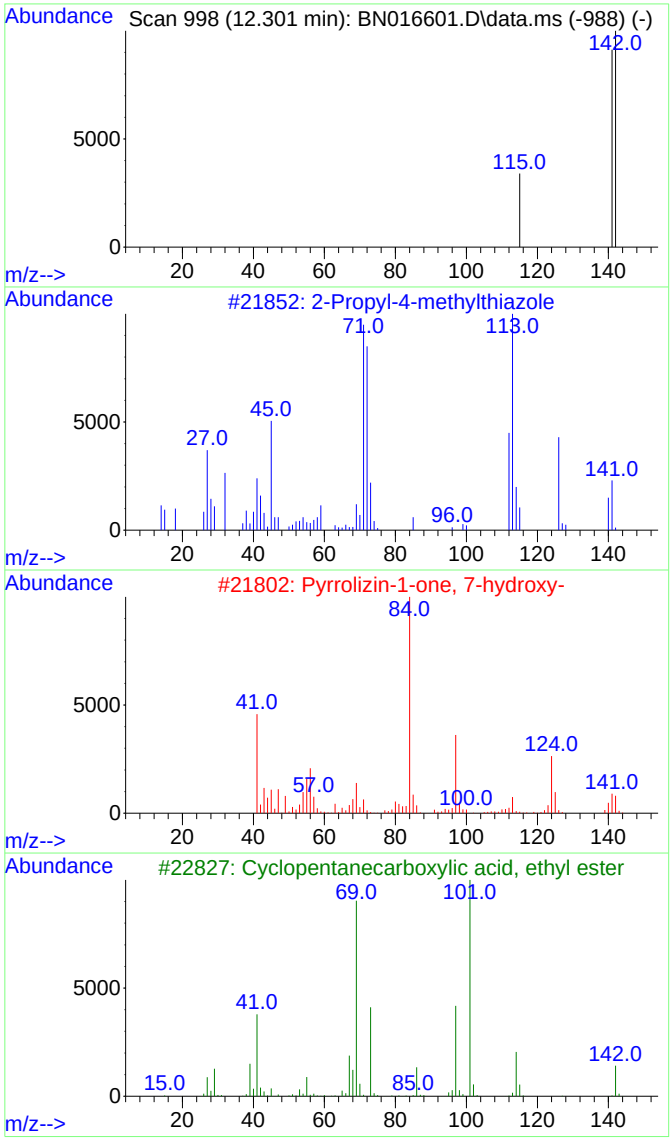
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

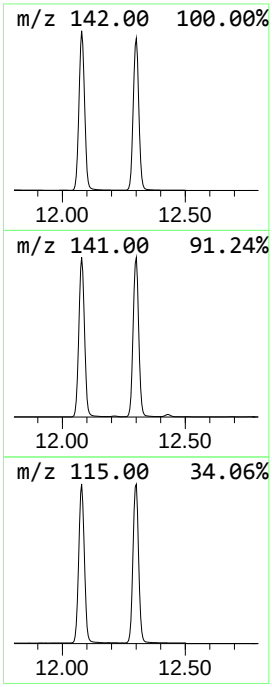
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.301	0.88 ng	351744	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 : 5 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDICC0.8

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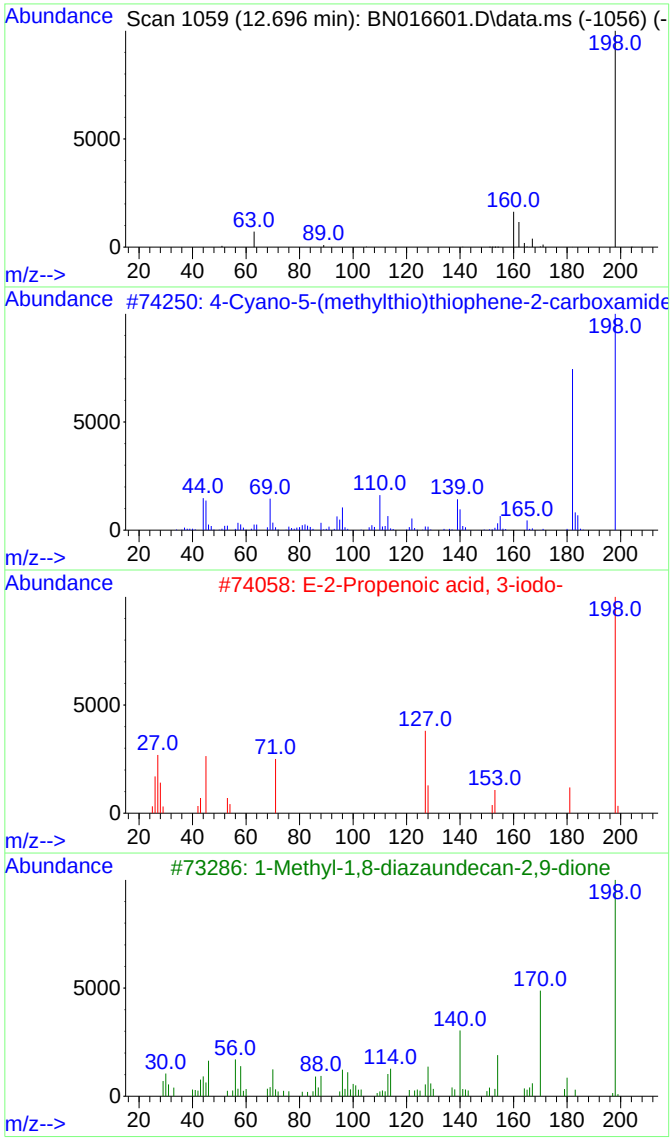
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

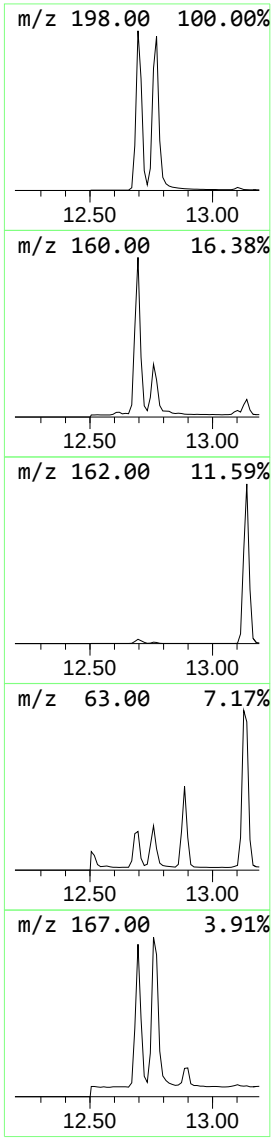
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.696	0.14 ng	55202	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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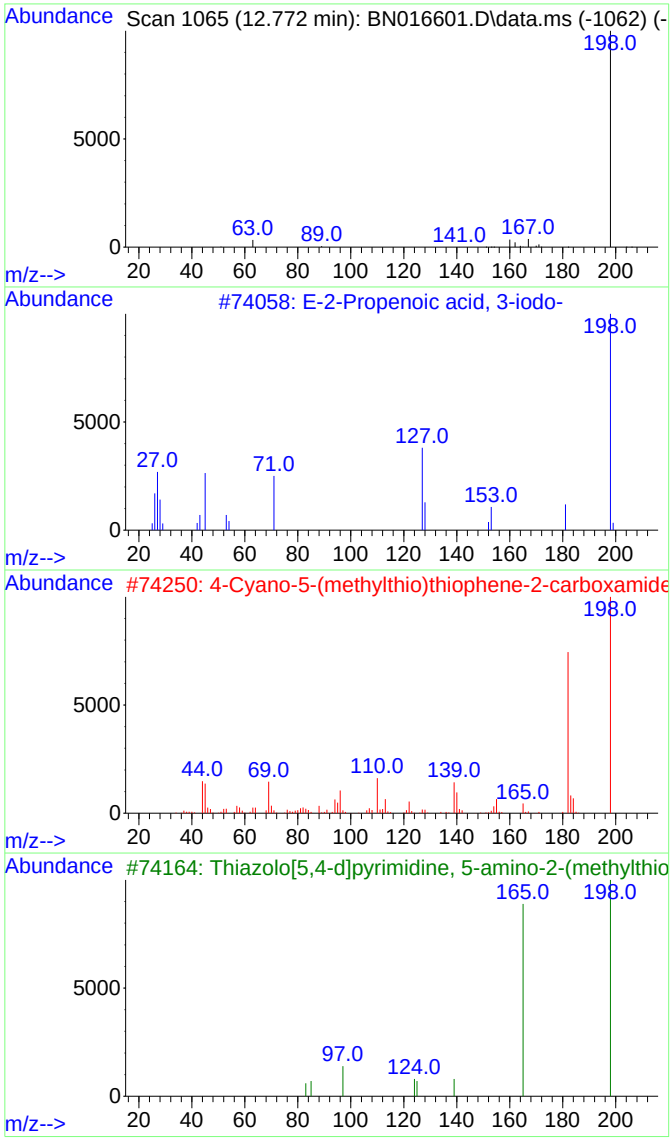
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

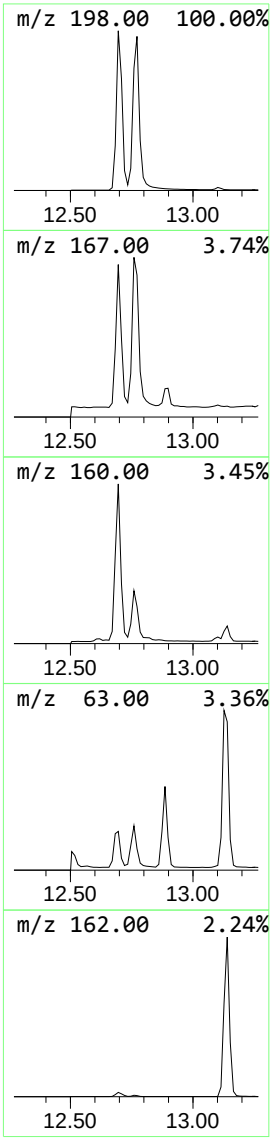
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 E-2-Propenoic acid, 3-iodo- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.772	0.13 ng	49690	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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Misc :
ALS Vial : 5 Sample Multiplier: 1

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

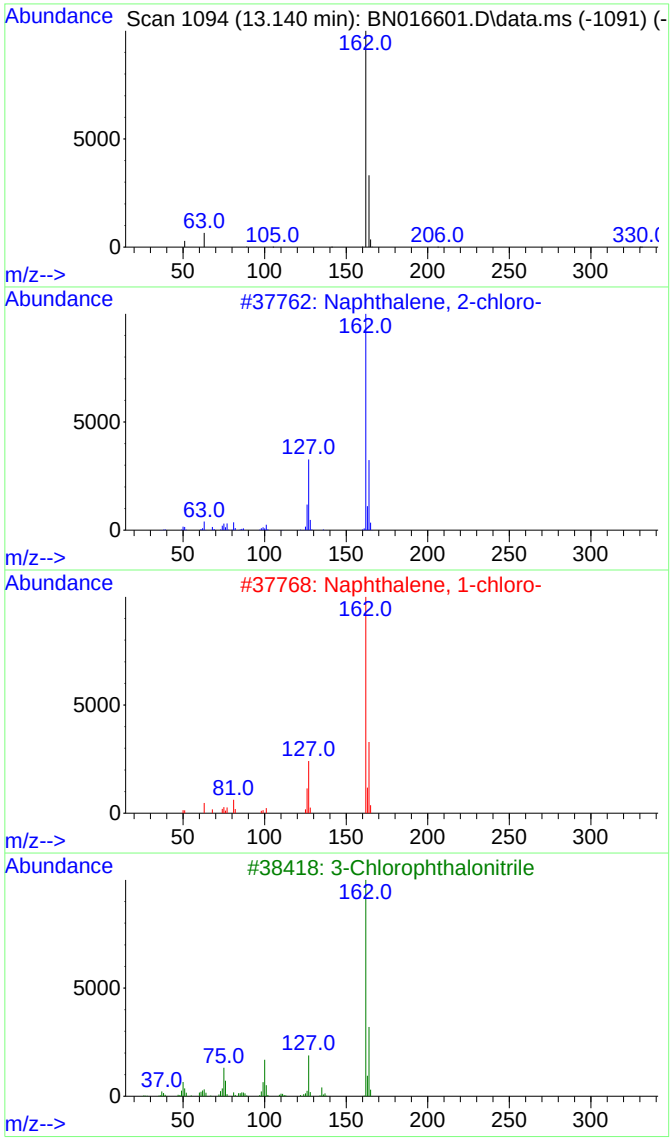
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

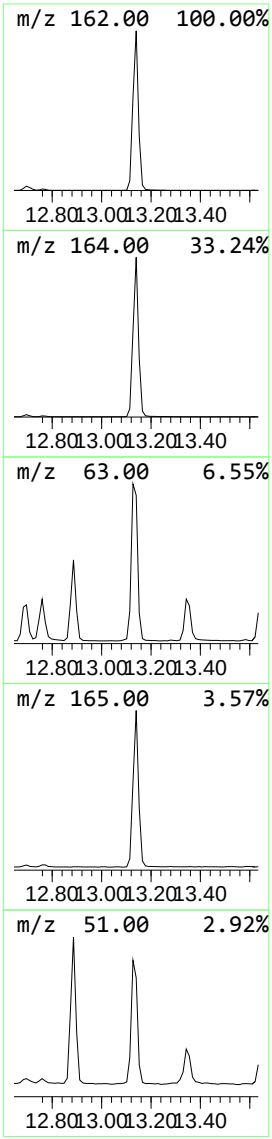
****

Peak Number 13 Naphthalene, 2-chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.140	0.57 ng	227553	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	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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Misc :
ALS Vial : 5 Sample Multiplier: 1

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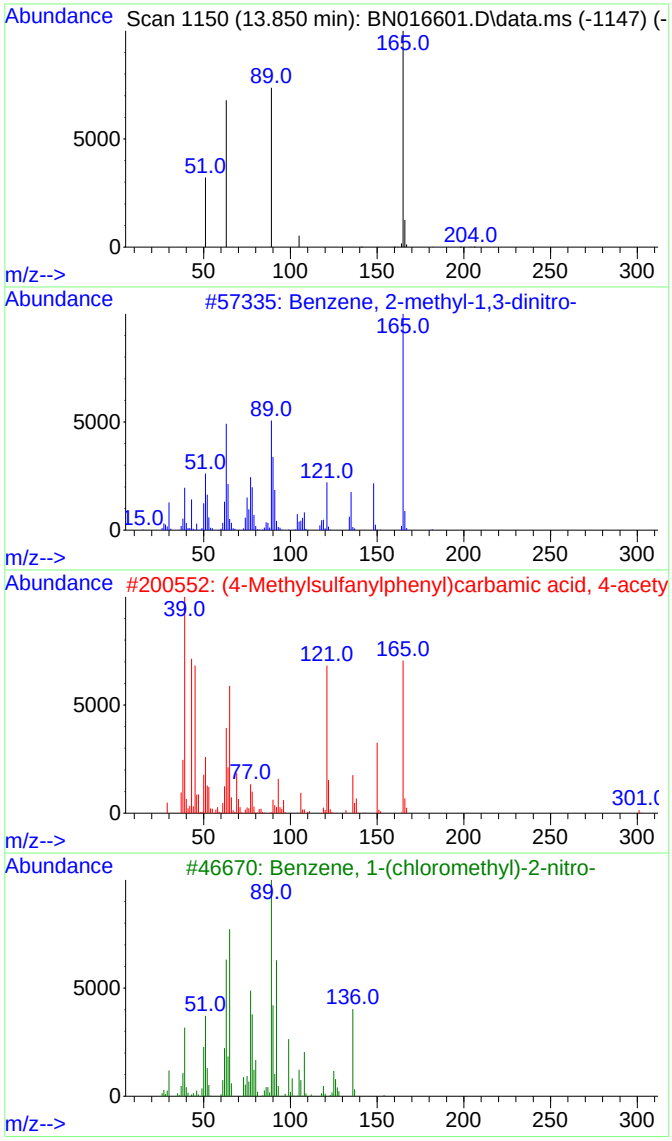
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

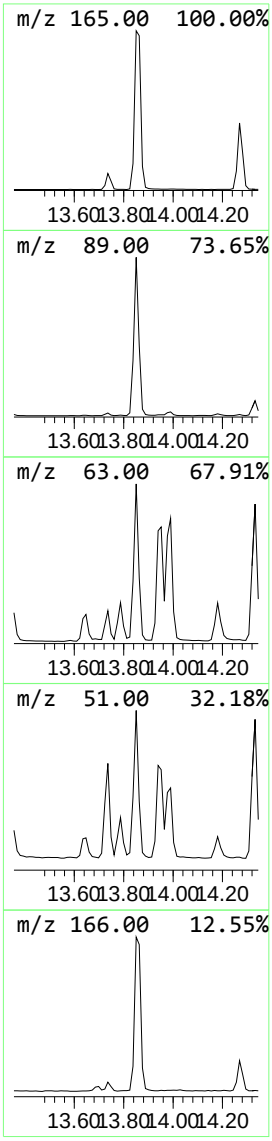
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 Benzene, 2-methyl-1,3-dinitro- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.850	0.15 ng	58004	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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Instrument :
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LabSampleId :
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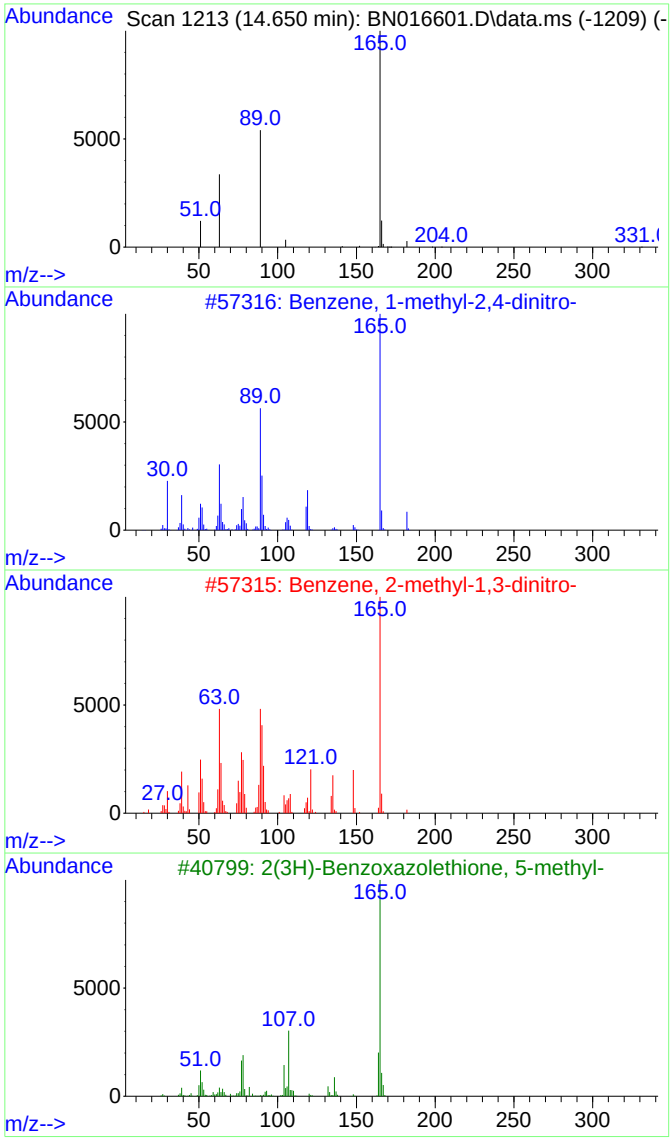
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

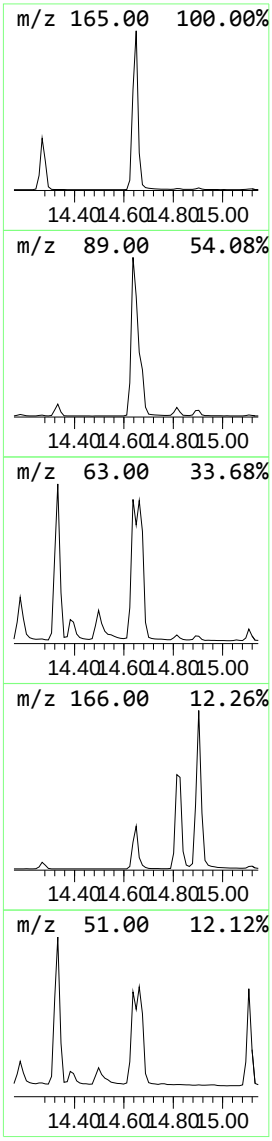
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 Benzene, 1-methyl-2,4-dinitro- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.650	0.22 ng	89112	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	2(3H)-Benzoxazolethione, 5-methyl-	165	C8H7NOS	022876-22-8	9
4	4-Methoxyphenyl isothiocyanate	165	C8H7NOS	002284-20-0	9
5	6-Nitro-m-tolunitrile	162	C8H6N2O2	064113-86-6	9





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ALS Vial : 5 Sample Multiplier: 1

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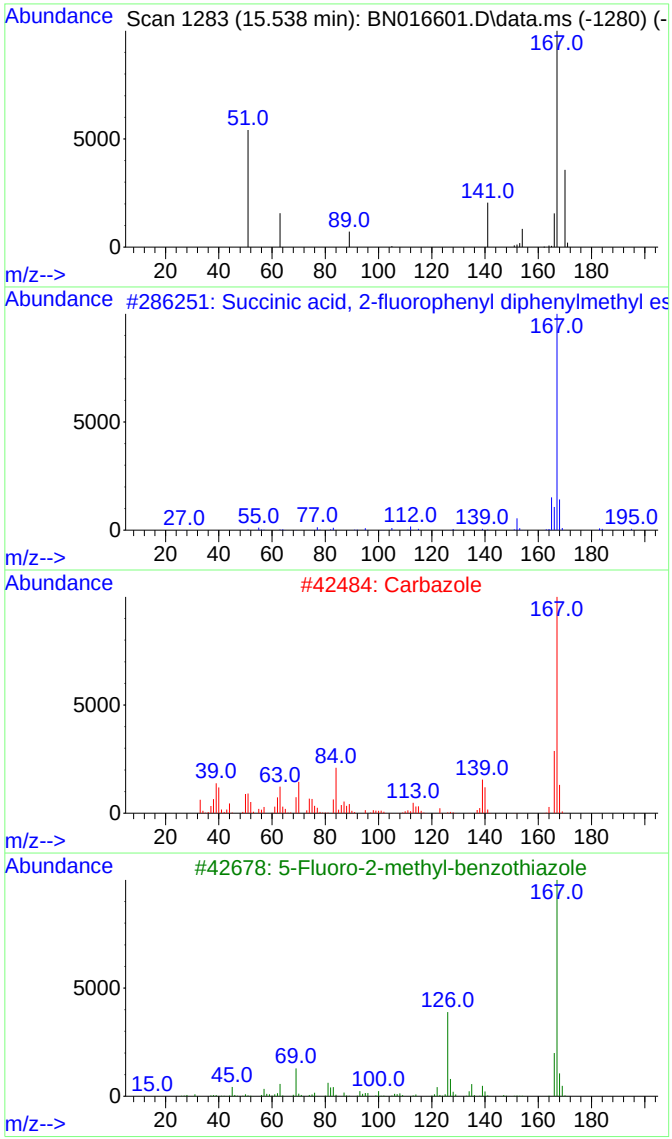
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

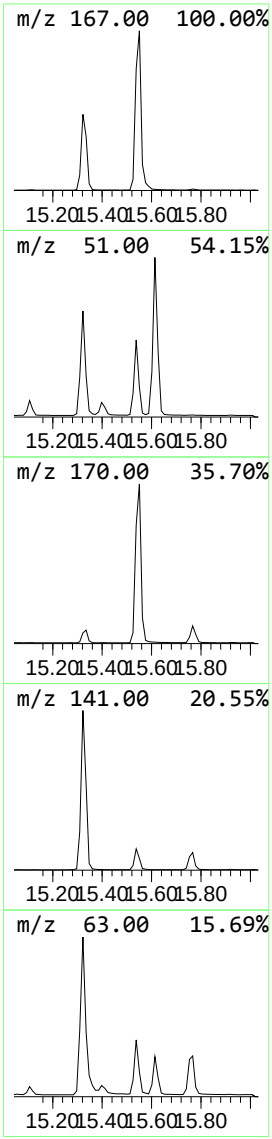
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 Succinic acid, 2-fluorophen... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.538	0.29 ng	116002	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Succinic acid, 2-fluorophenyl di...	378	C23H19FO4	1000390-17-0	9
2	Carbazole	167	C12H9N	000086-74-8	7
3	5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	5
4	Benzaldehyde, 2-hydroxy-5-nitro-	167	C7H5NO4	000097-51-8	5
5	3,5-Pyridinedicarboxylic acid	167	C7H5NO4	000499-81-0	4





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ALS Vial : 5 Sample Multiplier: 1

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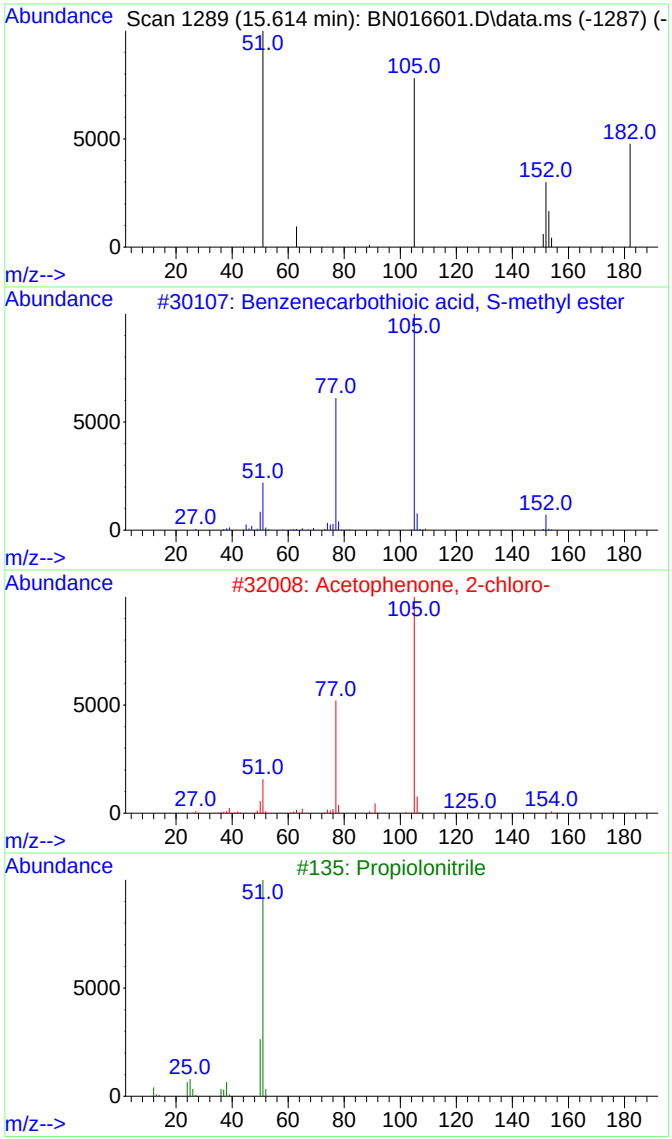
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

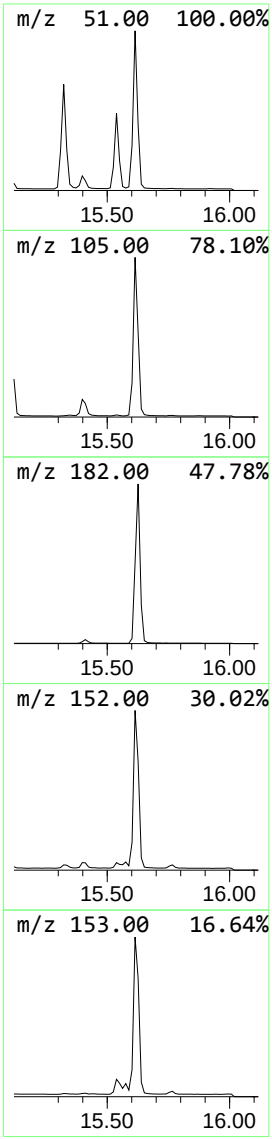
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 Benzenecarbothioic acid, S-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.614	0.32 ng	128508	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	3
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	3
3	Propiolonitrile	51	C3HN	001070-71-9	3
4	Benzeneethanamine, 4-methoxy-	151	C9H13NO	000055-81-2	3
5	Propanal, 2-(benzoyloxy)-, (R)-	178	C10H10O3	078871-04-2	2





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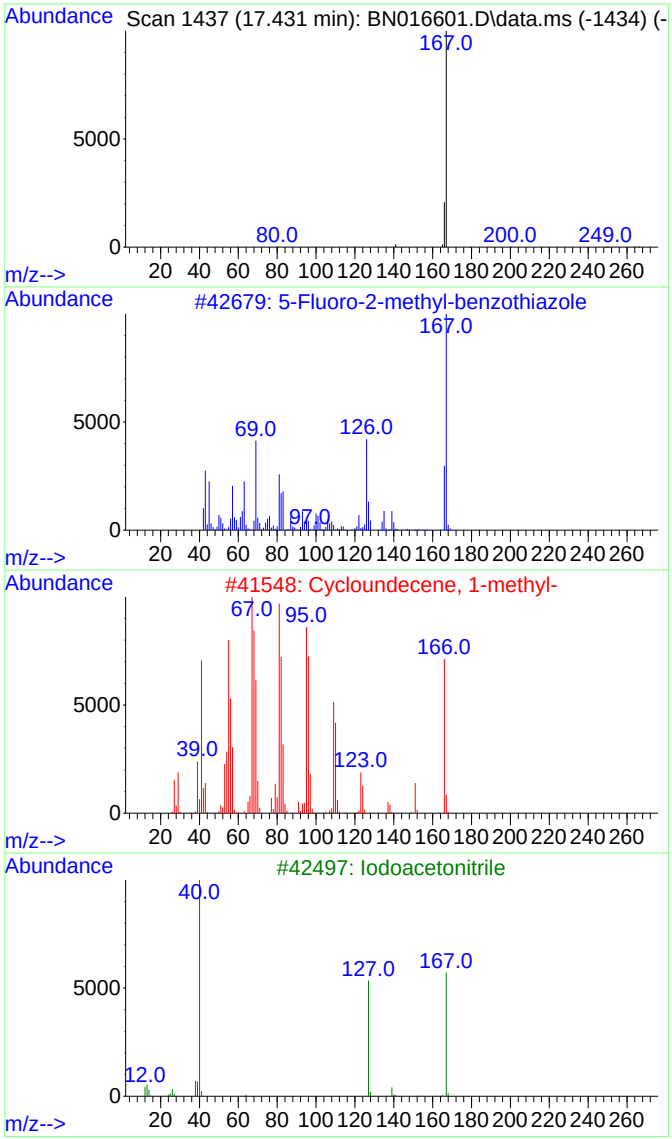
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

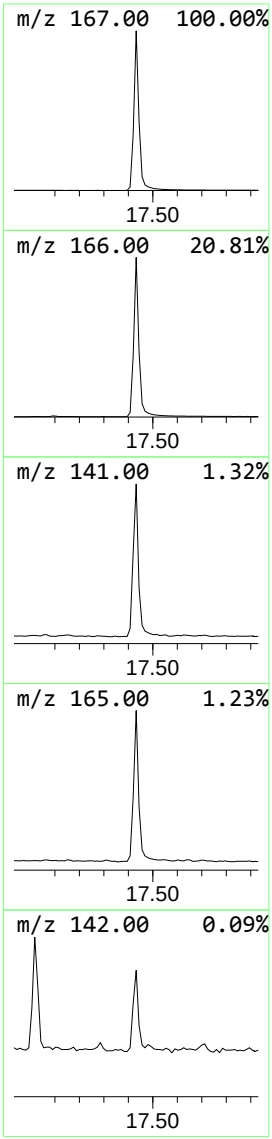
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 5-Fluoro-2-methyl-benzothia... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.432	0.81 ng	260861	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





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Acq On : 30 Sep 2021 15:31
Operator : CG/JU
Sample : SSTDICC0.8
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.8

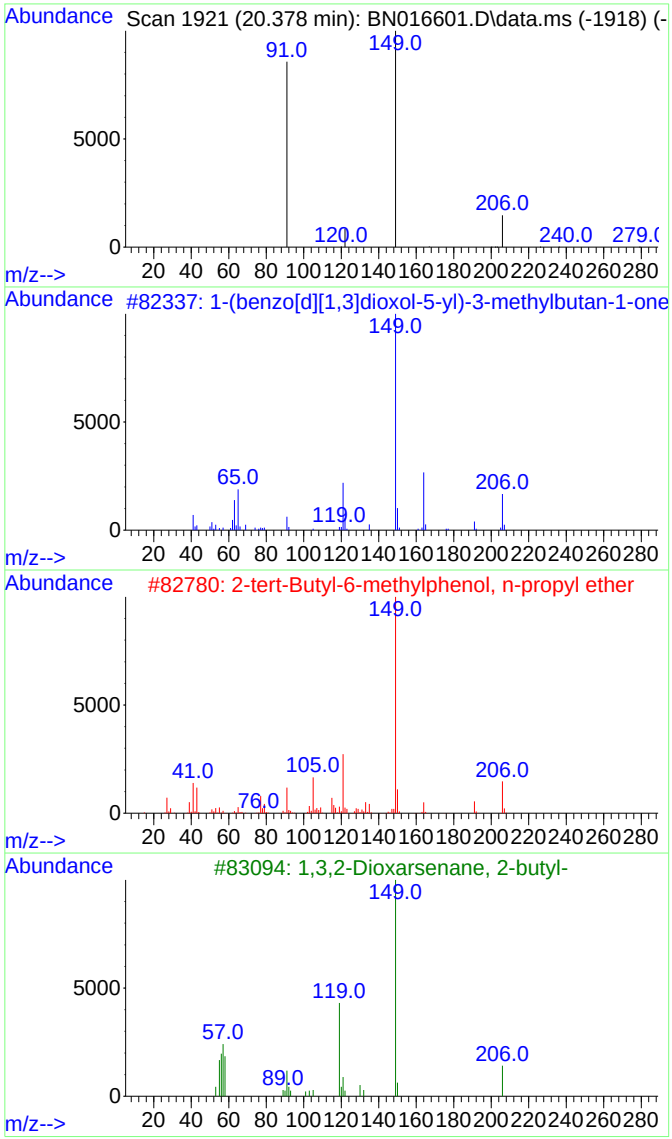
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

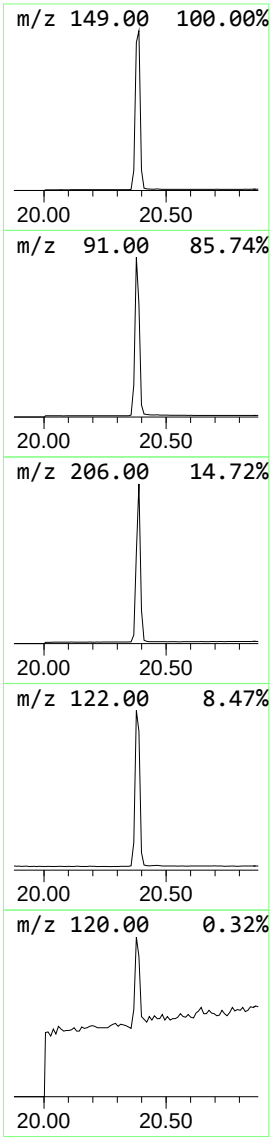
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 1-(benzo[d][1,3]dioxol-5-yl... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.378	0.09 ng	120788	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	Phenylpropanamide	149	C9H11NO	000102-93-2	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016601.D
Acq On : 30 Sep 2021 15:31
Operator : CG/JU
Sample : SSTDICC0.8
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC0.8

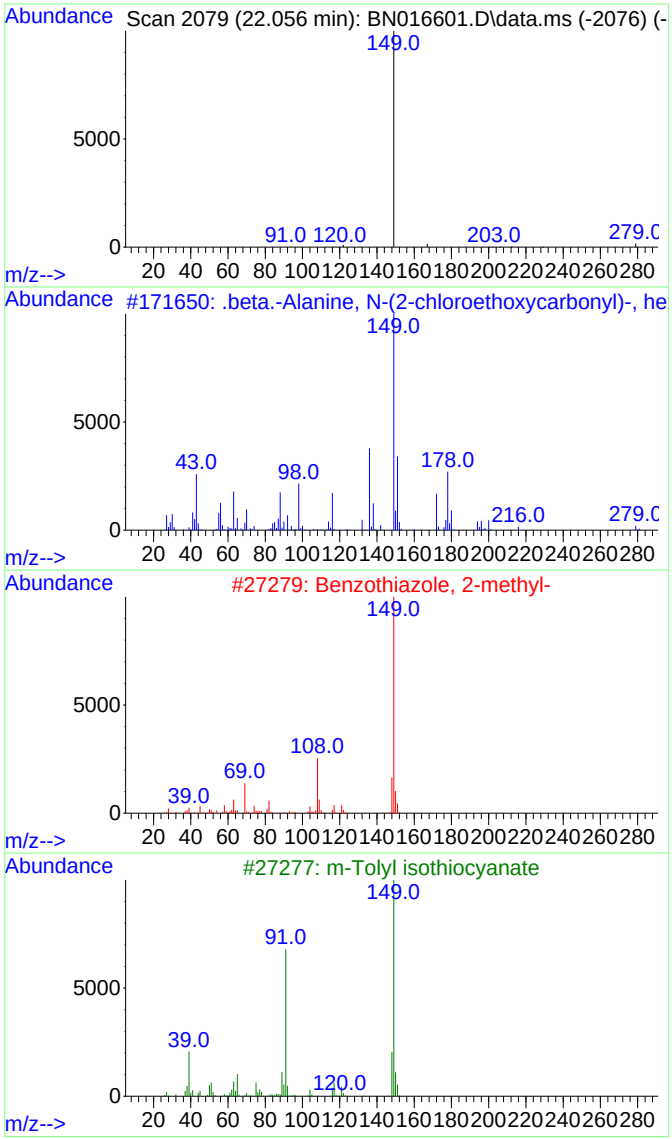
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

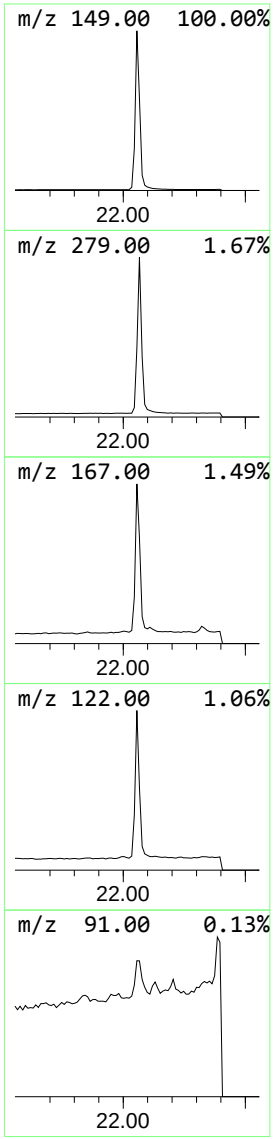
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 .beta.-Alanine, N-(2-chloro... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.056	0.13 ng	185702	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	m-Tolyl isothiocyanate	149	C8H7NS	000621-30-7	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 : BN016601.D
Acq On : 30 Sep 2021 15:31
Operator : CG/JU
Sample : SSTDICC0.8
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDICC0.8

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	0.2	ng	69704	1	7.643	112416	0.4
Ethyl Chloride	7.200	0.2	ng	59075	1	7.643	112416	0.4
Thietane	7.532	0.1	ng	26668	1	7.643	112416	0.4
6-Benzothiazola...	7.956	0.7	ng	188830	1	7.643	112416	0.4
Furan, 2,5-dihy...	8.430	0.3	ng	94361	1	7.643	112416	0.4
Fomepizole	9.342	0.4	ng	150951	2	10.407	160613	0.4
5-Hydroxy-2-pyr...	9.836	0.1	ng	51584	2	10.407	160613	0.4
o-Chloroaniline	10.572	0.3	ng	119573	2	10.407	160613	0.4
Methane, iodo-	11.710	0.1	ng	50190	2	10.407	160613	0.4
2-Propyl-4-meth...	12.301	0.9	ng	351744	2	10.407	160613	0.4
4-Cyano-5-(meth...	12.696	0.1	ng	55202	3	14.269	158758	0.4
E-2-Propenoic a...	12.772	0.1	ng	49690	3	14.269	158758	0.4
Naphthalene, 2-...	13.140	0.6	ng	227553	3	14.269	158758	0.4
Benzene, 2-meth...	13.850	0.1	ng	58004	3	14.269	158758	0.4
Benzene, 1-meth...	14.650	0.2	ng	89112	3	14.269	158758	0.4
Succinic acid, ...	15.538	0.3	ng	116002	3	14.269	158758	0.4
Benzenecarbothi...	15.614	0.3	ng	128508	3	14.269	158758	0.4
5-Fluoro-2-meth...	17.432	0.8	ng	260861	4	17.030	128219	0.4
1-(benzo[d][1,3...	20.378	0.1	ng	120788	5	21.238	567066	0.4
.beta.-Alanine,...	22.056	0.1	ng	185702	5	21.238	567066	0.4