LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016667.D
Acq On : 02 Oct 2021 11:44
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDCCC0.4

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: BN016667.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.244	16	18	20	rBV	6413	9077	1.65%	0.110%
2	3.281	20	22	43	rVB	5333	25274	4.60%	0.307%
3	3.595	51	56	77	rVB	6406	29832	5.43%	0.362%
4	5.264	231	237	253	rVB	14765	56748	10.33%	0.689%
5	6.822	401	406	417	rBV	24581	62540	11.38%	0.759%
6	6.979	418	423	429	rVV	14357	31681	5.77%	0.384%
7	7.080	429	434	440	rVV	34678	71805	13.07%	0.871%
8	7.200	440	447	460	rVB	12337	32614	5.93%	0.396%
9	7.523	478	482	489	rVB	6692	14529	2.64%	0.176%
10	7.643	490	495	508	rVB2	47912	117929	21.46%	1.431%
11	7.956	524	529	537	rVB2	45883	105716	19.24%	1.283%
12	8.168	547	552	557	rBV	3015	7289	1.33%	0.088%
13	8.430	571	577	591	rBV3	23121	52800	9.61%	0.641%
14	8.696	594	598	601	rBV	4595	8787	1.60%	0.107%
15	8.785	601	605	606	rBV	33782	67486	12.28%	0.819%
16	8.823	606	608	616	rVB	28547	53226	9.69%	0.646%
17	9.342	645	649	652	rBV	49562	84685	15.41%	1.028%
18	9.520	660	663	666	rBV	3537	6685	1.22%	0.081%
19	9.596	666	669	680	rVB	8760	16429	2.99%	0.199%
20	9.837	684	688	702	rBV	15483	28495	5.19%	0.346%
21	10.052	702	705	715	rVB	4341	9304	1.69%	0.113%
22	10.407	729	733	735	rBV	103862	196463	35.75%	2.384%
23	10.458	735	737	740	rVV	101753	171857	31.27%	2.086%
24	10.572	743	746	756	rVV	26174	56339	10.25%	0.684%
25	10.749	756	760	763	rVB	30577	55566	10.11%	0.674%
26	11.307	801	804	813	rBV	2173	5853	1.07%	0.071%
27	11.705	852	864	889	rBV	14288	26956	4.91%	0.327%
28	12.003	920	931	939	rBV2	56093	92782	16.88%	1.126%
29	12.074	939	947	972	rVV	129403	207223	37.71%	2.515%
30	12.296	987	997	1019	rVV	125849	199673	36.33%	2.423%
31	12.696	1056	1059	1062	rBV	18195	30869	5.62%	0.375%
32	12.759	1062	1064	1071	rVB	13395	26737	4.87%	0.324%
33	12.886	1071	1074	1078	rBV	125859	197130	35.87%	2.392%
34	13.140	1090	1094	1097	rBV	72190	127485	23.20%	1.547%
35	13.736	1138	1141	1143	rBV	11936	17626	3.21%	0.214%
36	13.850	1147	1150	1153	rVB	20868	30427	5.54%	0.369%

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Misc :
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Instrument : BNA_N
LabSampleId : SSTDCCC0.4

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	13.939	1154	1157	1158	rBV	5813	9194	1.67%	0.112%
38	13.990	1158	1161	1164	rVB	90541	160997	29.30%	1.954%
39	14.269	1180	1183	1185	rBV	137867	197350	35.91%	2.395%
40	14.332	1185	1188	1191	rVB	164880	244747	44.54%	2.970%
41	14.637	1209	1212	1220	rBV3	19264	46345	8.43%	0.562%
42	14.814	1223	1226	1230	rVV	6451	10713	1.95%	0.130%
43	14.903	1230	1233	1246	rVB	8313	14227	2.59%	0.173%
44	15.106	1246	1249	1252	rBV	9252	11906	2.17%	0.144%
45	15.322	1263	1266	1269	rBV2	238418	356149	64.81%	4.322%
46	15.411	1269	1273	1280	rVB2	2845	7823	1.42%	0.095%
47	15.538	1280	1283	1287	rBV	41489	64955	11.82%	0.788%
48	15.614	1287	1289	1292	rVB2	45915	65281	11.88%	0.792%
49	15.766	1298	1301	1311	rVB2	14434	24562	4.47%	0.298%
50	16.227	1334	1338	1341	rBV2	54064	93858	17.08%	1.139%
51	16.324	1343	1346	1349	rVV	49151	72473	13.19%	0.880%
52	16.494	1357	1360	1372	rBV	24076	39234	7.14%	0.476%
53	16.677	1372	1375	1384	rBV	22497	40290	7.33%	0.489%
54	17.018	1400	1403	1405	rBV	104995	166482	30.30%	2.020%
55	17.066	1405	1407	1410	rVV	143800	217542	39.59%	2.640%
56	17.152	1411	1414	1434	rVB	125775	192280	34.99%	2.334%
57	17.432	1434	1437	1453	rBV	90219	148069	26.94%	1.797%
58	18.016	1482	1485	1498	rVB7	6413	8126	1.48%	0.099%
59	19.063	1684	1696	1699	rBV	124496	177546	32.31%	2.155%
60	19.093	1699	1702	1742	rVB	199771	262674	47.80%	3.188%
61	19.460	1766	1776	1808	rBV	193293	269398	49.02%	3.269%
62	19.679	1813	1820	1856	rVV	112680	147551	26.85%	1.791%
63	20.378	1918	1921	1924	rBV	66782	76956	14.00%	0.934%
64	21.164	1993	1995	1997	rBV	64094	88276	16.06%	1.071%
65	21.217	1997	2000	2003	rVV2	224353	449238	81.75%	5.452%
66	21.270	2003	2005	2017	rVB	212663	283818	51.65%	3.444%
67	22.056	2076	2079	2089	rVB	98219	124888	22.73%	1.516%
68	22.321	2101	2104	2108	rBV	4144	6741	1.23%	0.082%
69	22.807	2217	2229	2235	rBV	141831	229773	41.81%	2.789%
70	22.851	2235	2242	2294	rVB2	148749	274987	50.04%	3.337%
71	23.385	2385	2398	2416	rBV2	98423	222372	40.47%	2.699%
72	23.485	2416	2427	2465	rVB	105941	219232	39.89%	2.661%
73	24.087	2592	2603	2636	rBV	13878	28260	5.14%	0.343%
74	24.857	2816	2828	2852	rBV	14246	33116	6.03%	0.402%
75	25.771	3066	3095	3186	rBV3	142456	549535	100.00%	6.669%
76	26.456	3271	3295	3356	rBV	74924	247845	45.10%	3.008%

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Misc :
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Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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77	26.819	3386	3401	3435	rVB2	3452	11462	2.09%	0.139%
78	28.085	3750	3771	3799	rBV	1960	7567	1.38%	0.092%

Sum of corrected areas: 8239755

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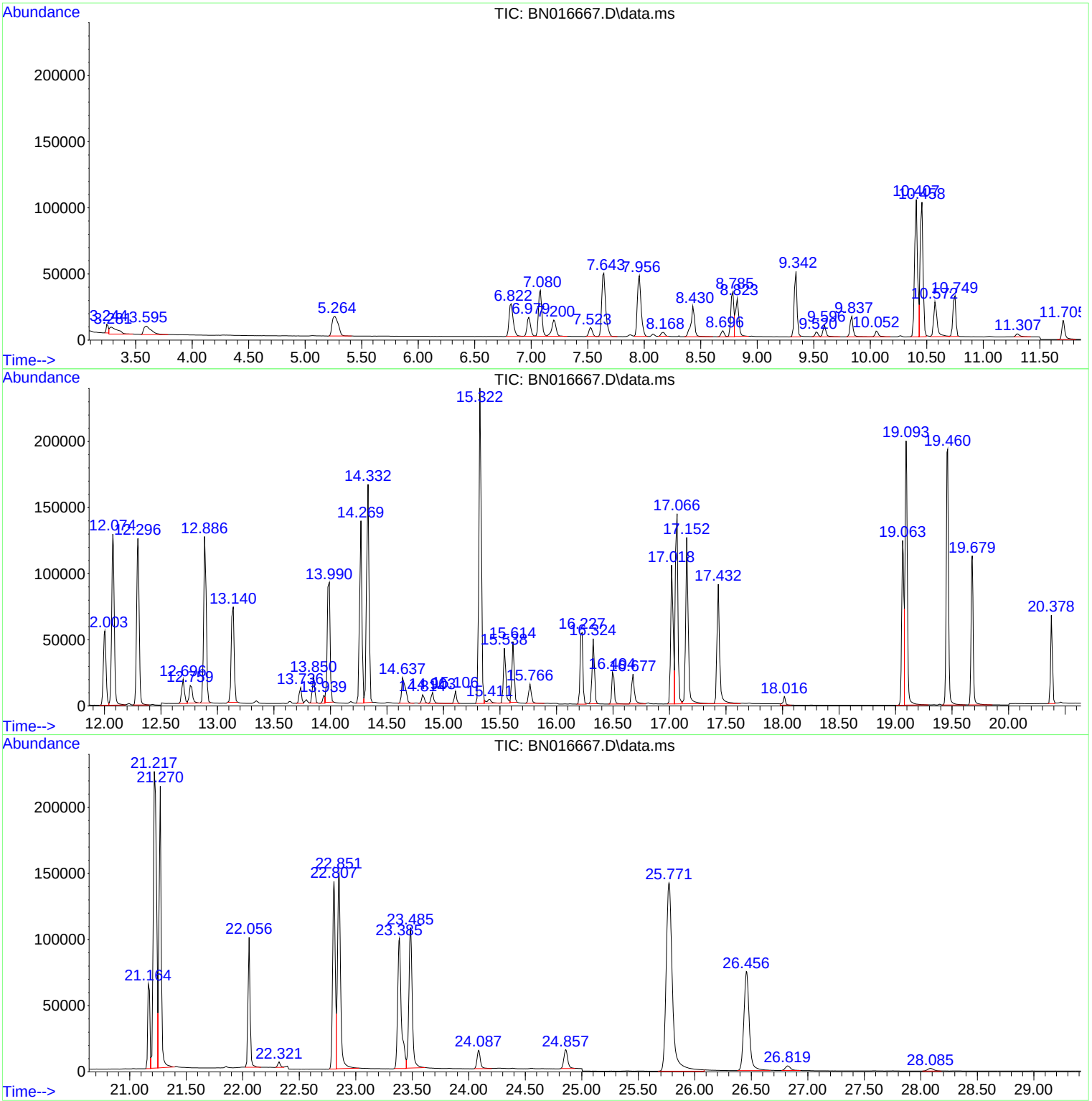
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

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 : BN016667.D
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Instrument :
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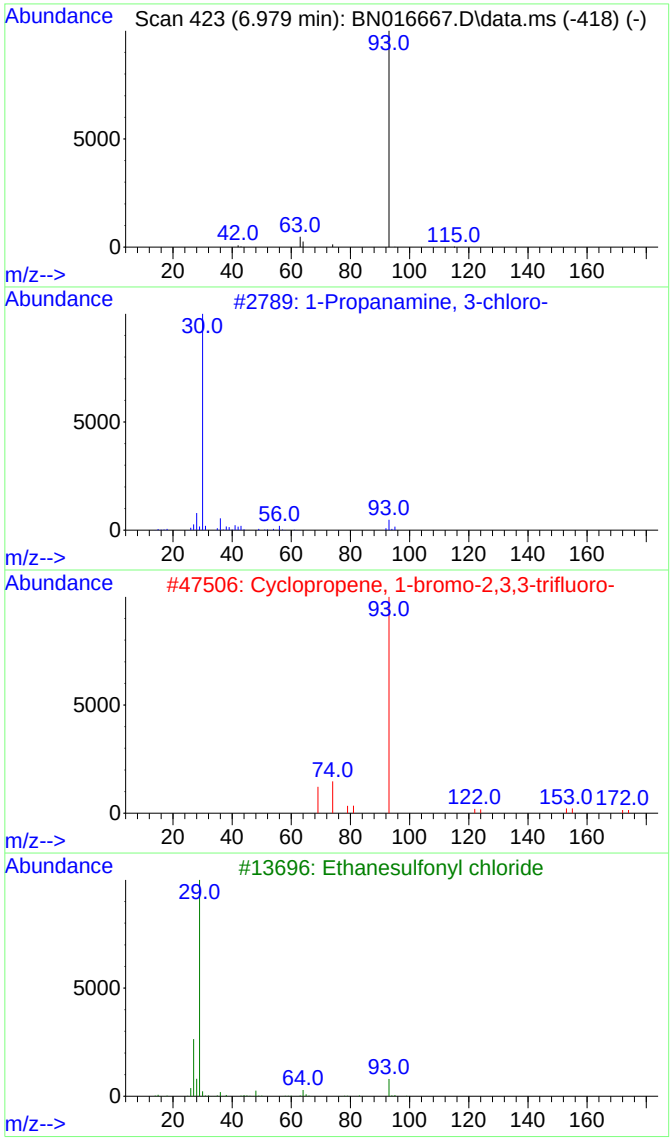
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

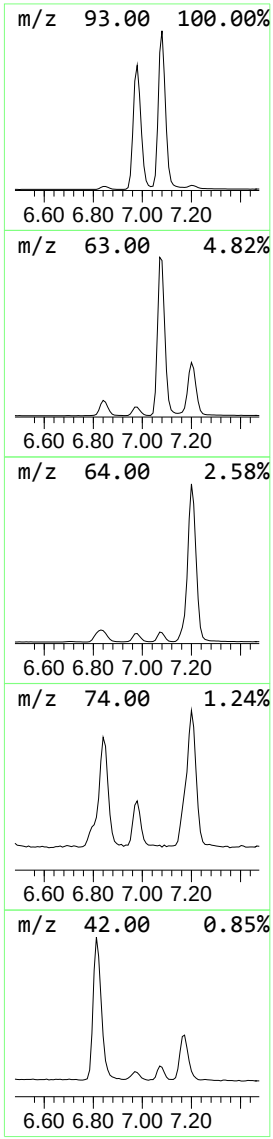
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1-Propanamine, 3-chloro- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.979	0.11 ng	31681	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\
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Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 35 Sample Multiplier: 1

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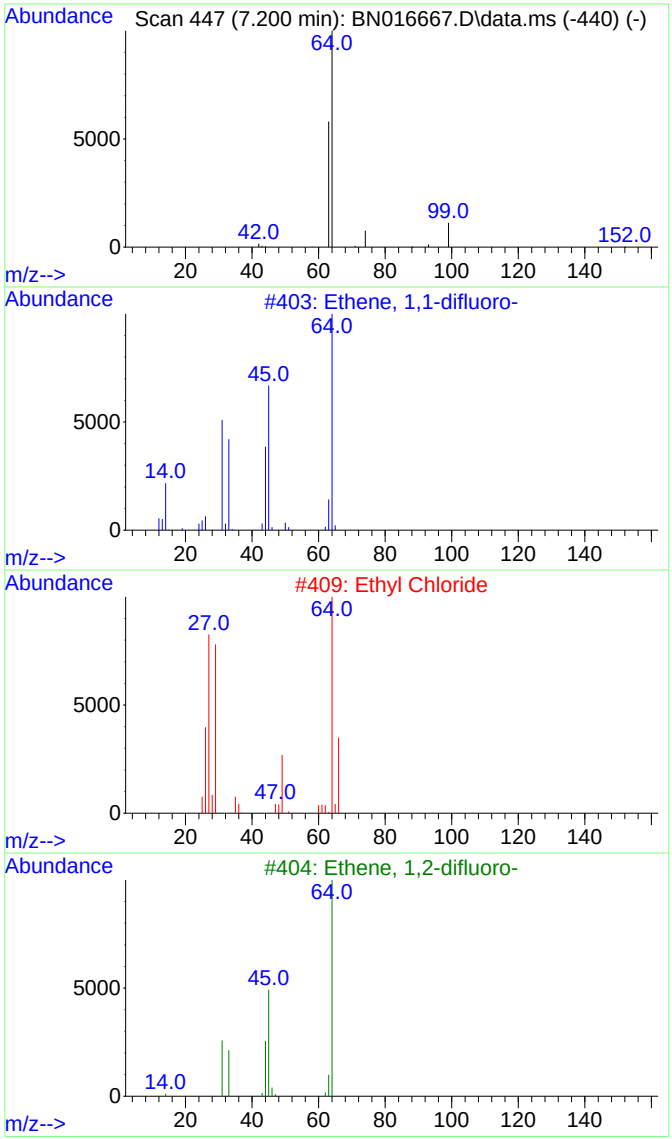
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

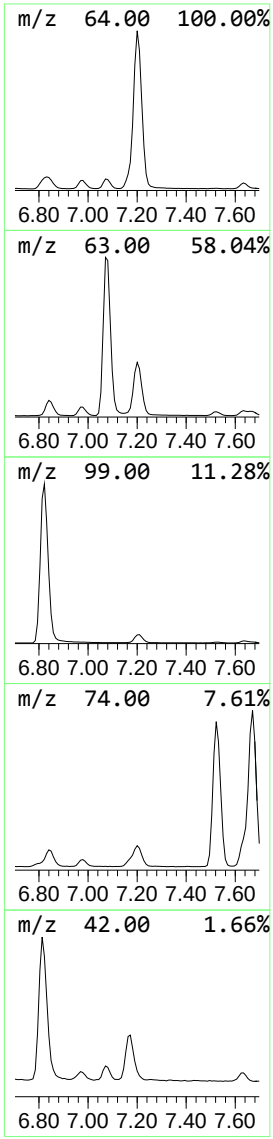
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethene, 1,1-difluoro- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.200	0.11 ng	32614	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	Ethyl Chloride	64	C2H5Cl	000075-00-3	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 : BN016667.D
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Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

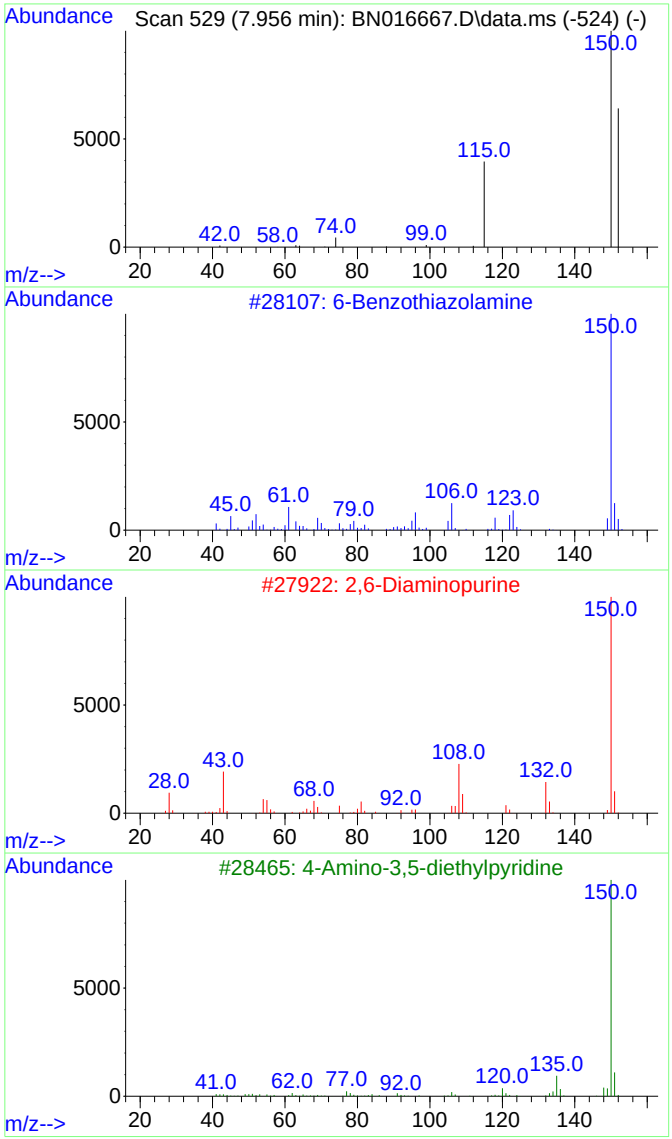
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

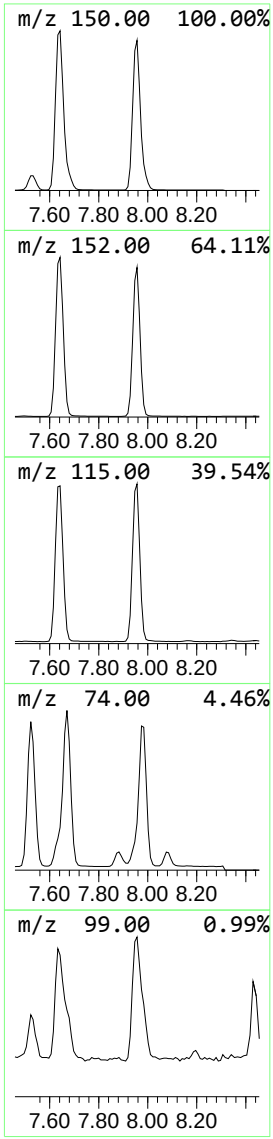
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 6-Benzothiazolamine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.956	0.36 ng	105716	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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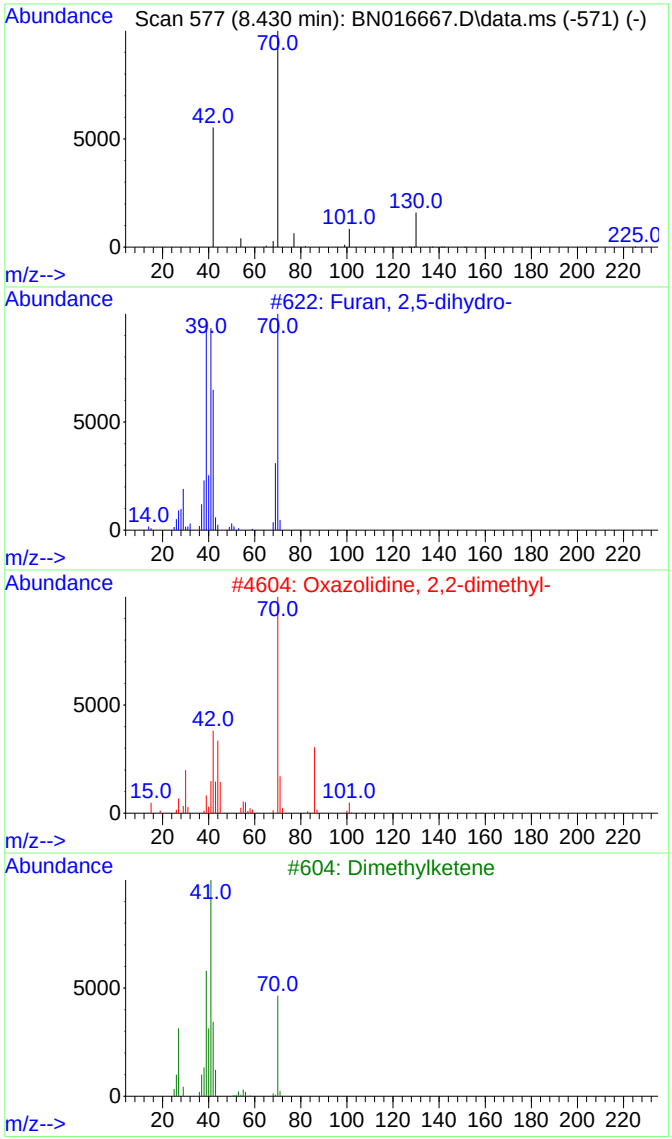
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

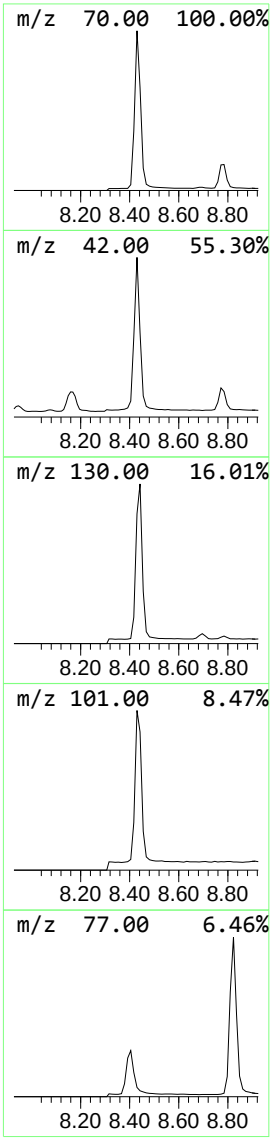
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Furan, 2,5-dihydro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.430	0.18 ng	52800	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	Oxazolidine, 2,2-dimethyl-	101	C5H11NO	020515-62-2	7
3	Dimethylketene	70	C4H6O	000598-26-5	5
4	Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	5
5	1-Oxa-3,4-diazacyclopentadiene	70	C2H2N2O	000288-99-3	4





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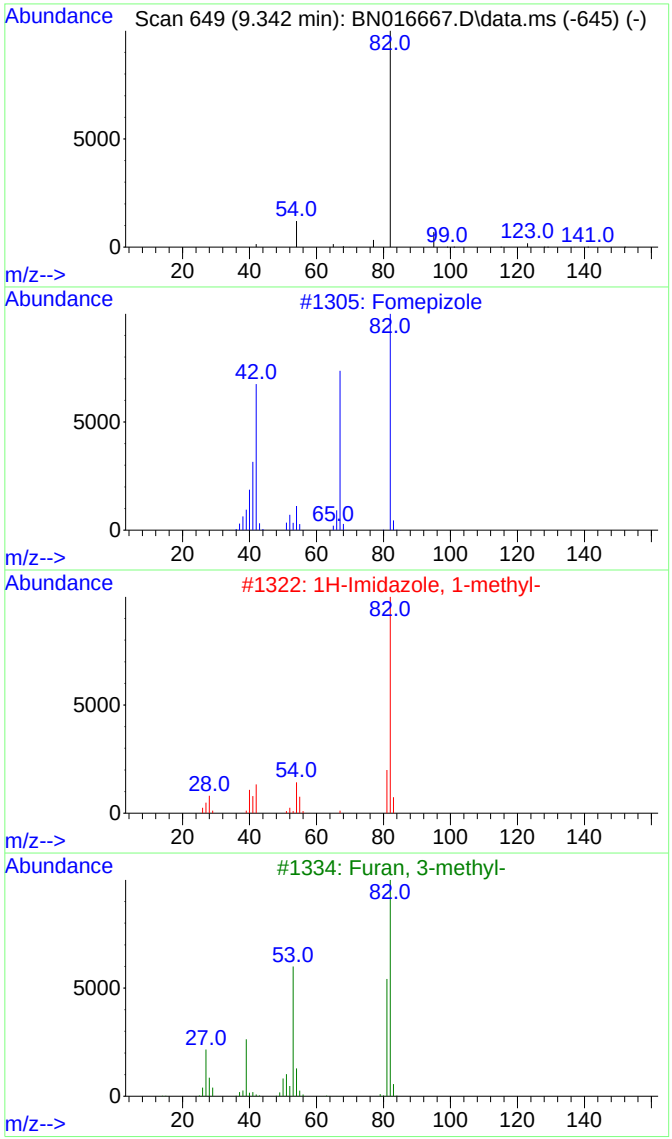
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

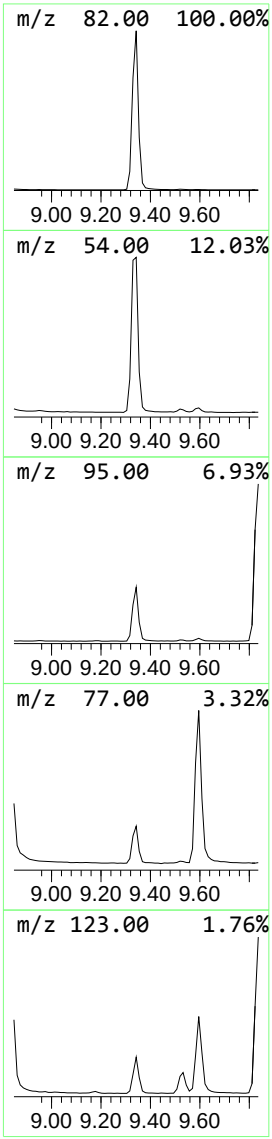
****

Peak Number 5 Fomepizole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.342	0.17 ng	84685	Naphthalene-d8	10.407

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





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Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

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

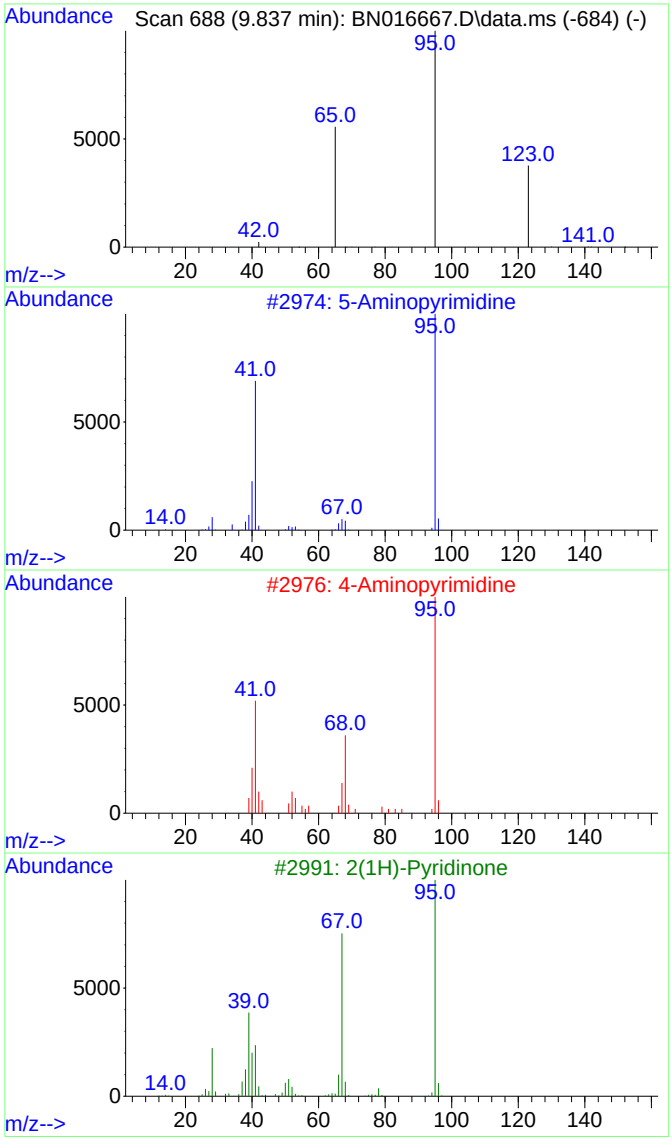
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

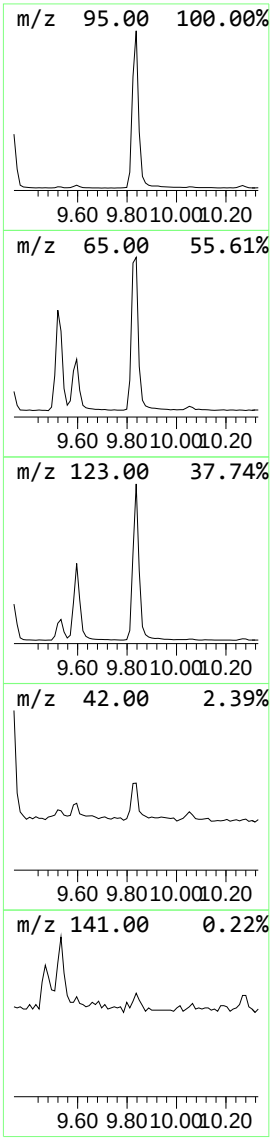
****

Peak Number 6 5-Aminopyrimidine Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.837	0.06 ng	28495	Naphthalene-d8	10.407

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminopyrimidine	95	C4H5N3	000591-55-9	3
2	4-Aminopyrimidine	95	C4H5N3	000591-54-8	2
3	2(1H)-Pyridinone	95	C5H5NO	000142-08-5	2
4	2-Pyrimidinamine	95	C4H5N3	000109-12-6	2
5	Pyridine, 1-oxide	95	C5H5NO	000694-59-7	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016667.D
Acq On : 02 Oct 2021 11:44
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 35 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

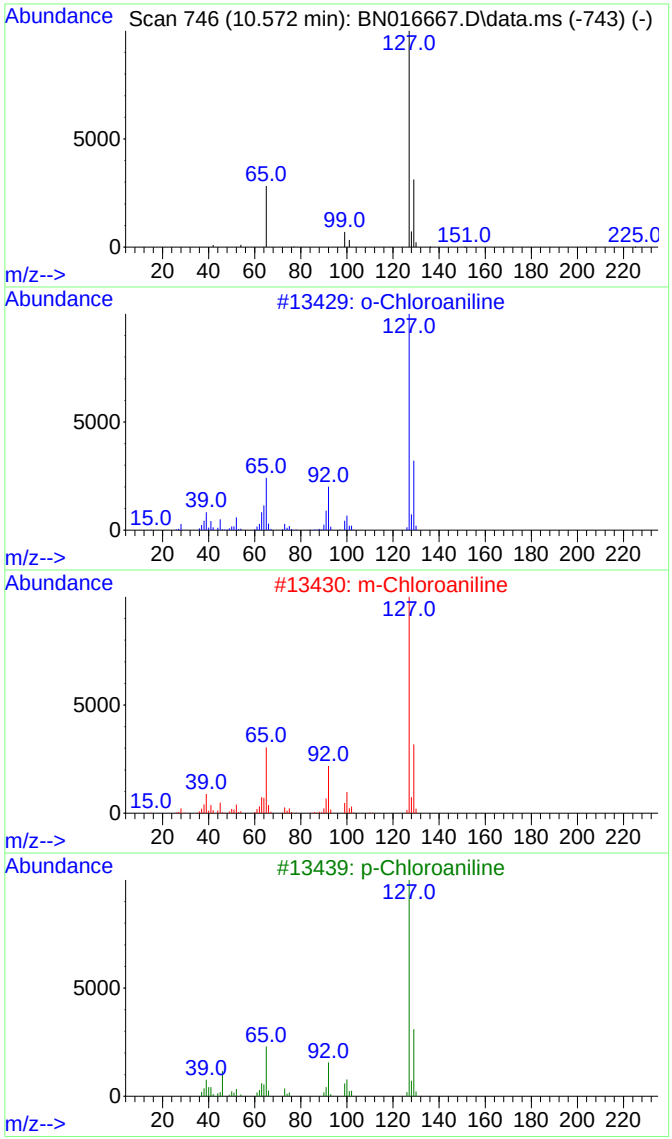
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

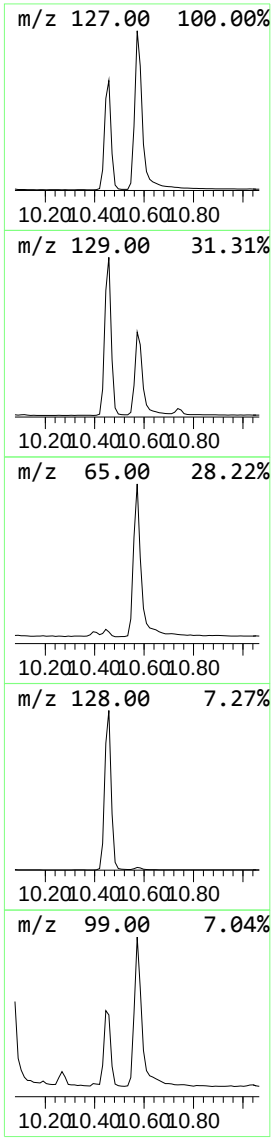
****

Peak Number 7 o-Chloroaniline Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.572	0.11 ng	56339	Naphthalene-d8	10.407

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





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Misc :
ALS Vial : 35 Sample Multiplier: 1

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

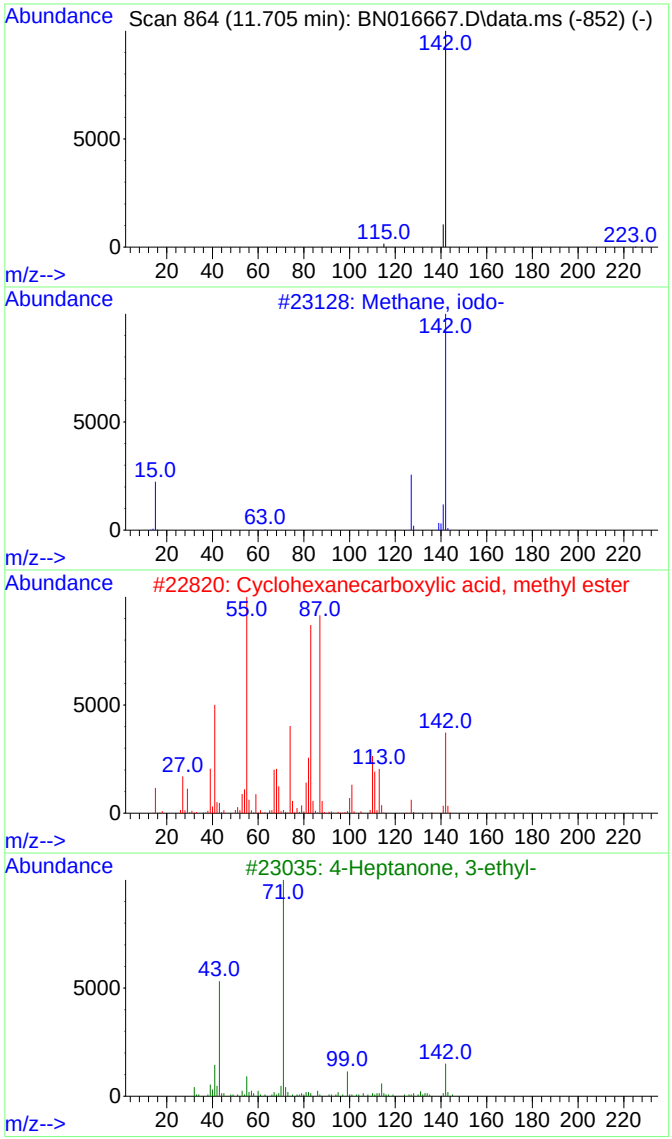
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

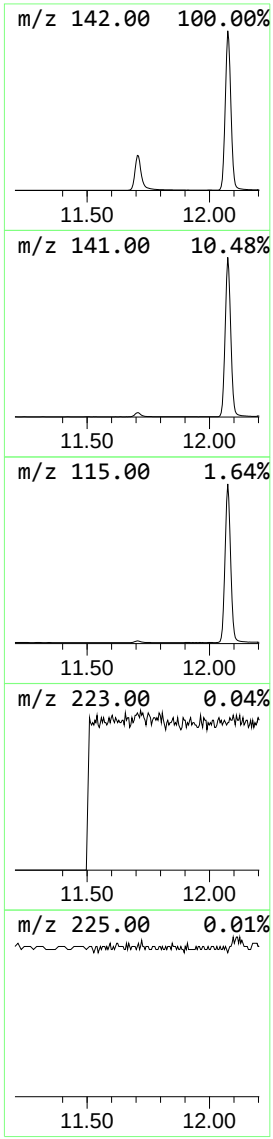
****

Peak Number 8 Methane, iodo- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.705	0.05 ng	26956	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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Acq On : 02 Oct 2021 11:44
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Sample : SSTDCCC0.4
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDCCC0.4

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

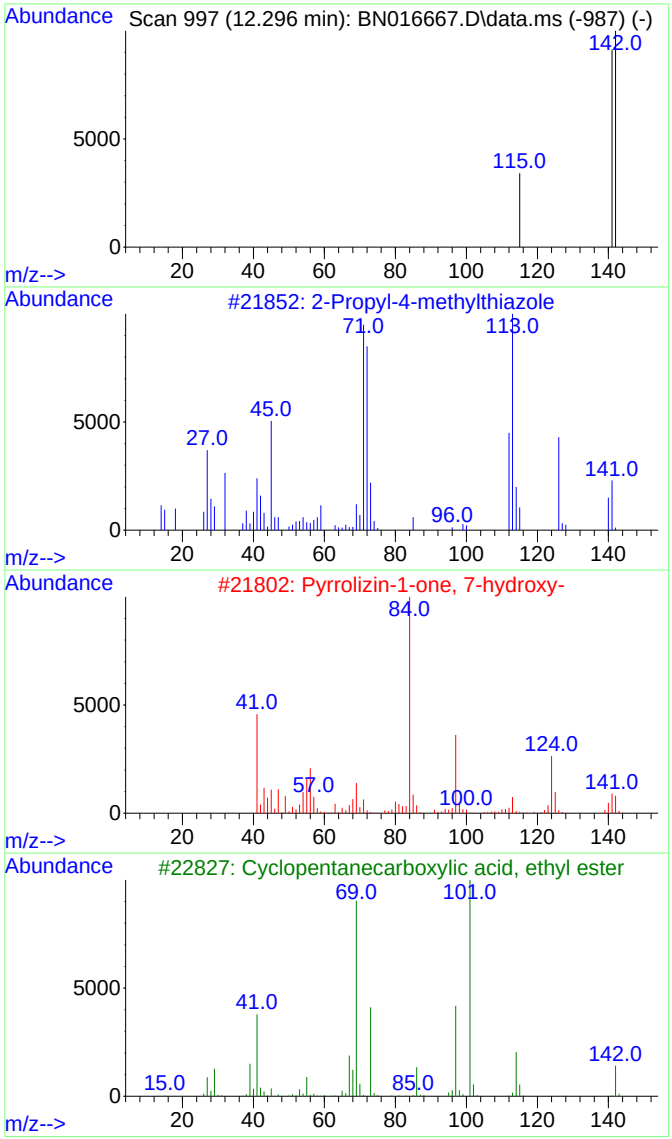
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

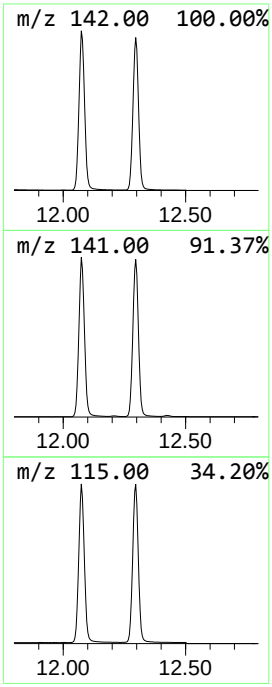
****

Peak Number 9 2-Propyl-4-methylthiazole Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.296	0.41 ng	199673	Naphthalene-d8	10.407

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





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Acq On : 02 Oct 2021 11:44
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

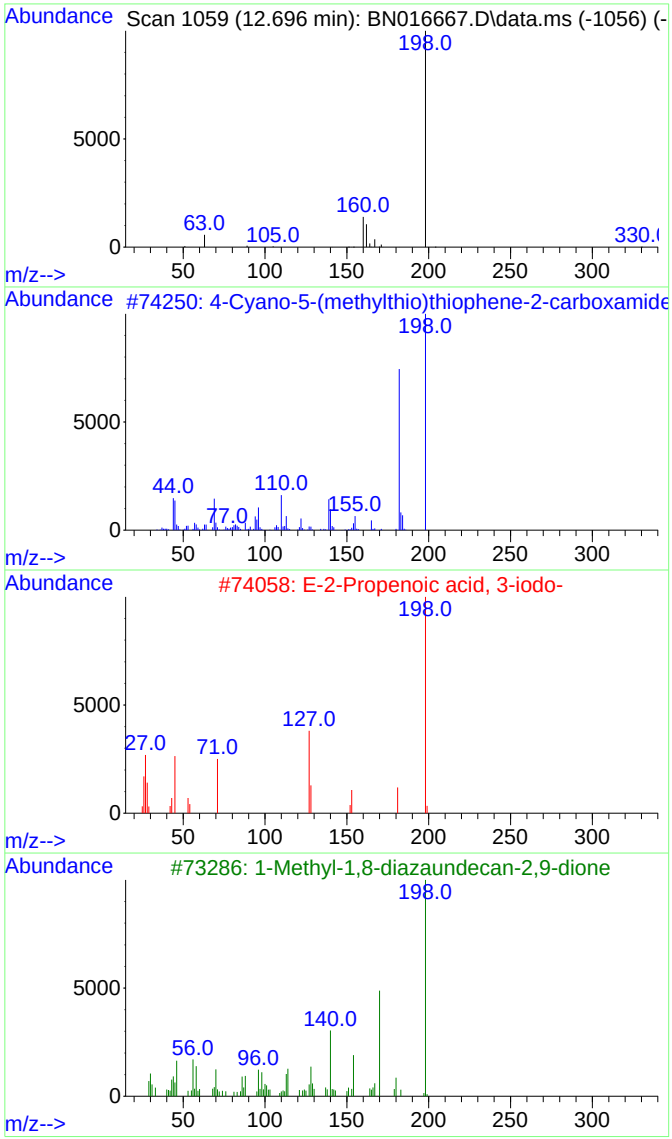
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

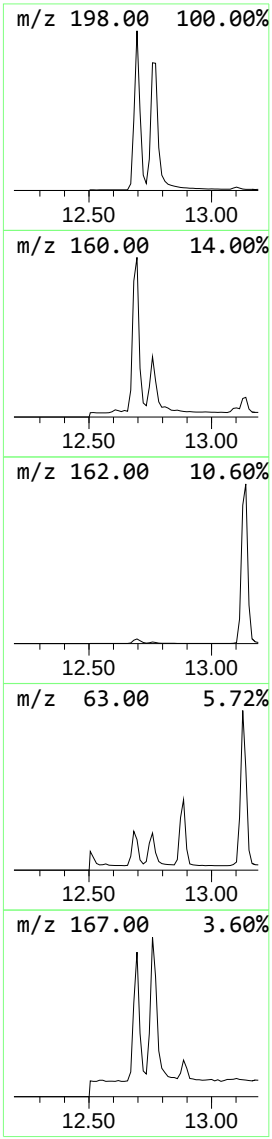
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 4-Cyano-5-(methylthio)thiop... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.696	0.06 ng	30869	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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Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 35 Sample Multiplier: 1

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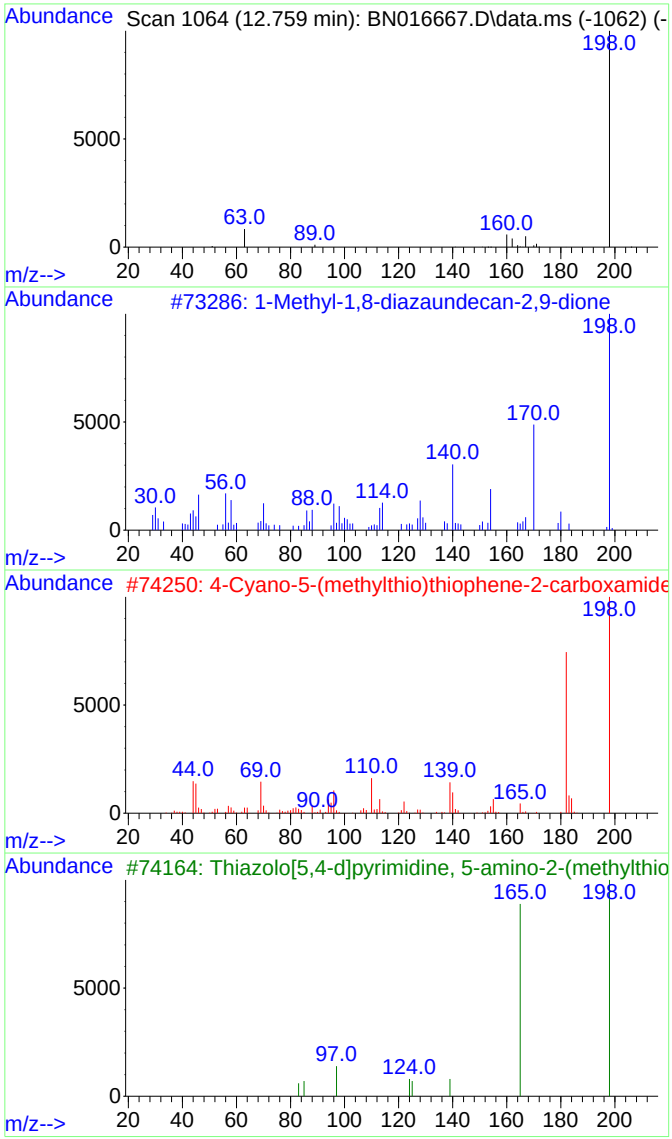
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

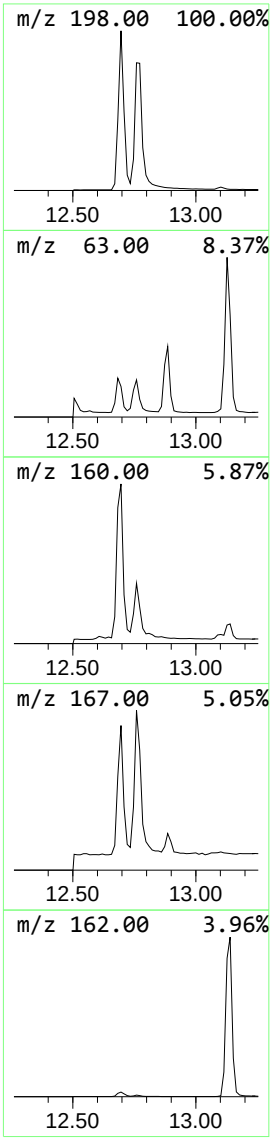
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 1-Methyl-1,8-diazaundecan-2... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.759	0.05 ng	26737	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyl-1,8-diazaundecan-2,9-dione	198	C10H18N2O2	1000298-94-5	4
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	E-2-Propenoic acid, 3-iodo-	198	C3H3IO2	1000308-86-7	3
5	Z-2-Propenoic acid, 3-iodo-	198	C3H3IO2	1000308-86-8	3





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Sample : SSTDCCC0.4
Misc :
ALS Vial : 35 Sample Multiplier: 1

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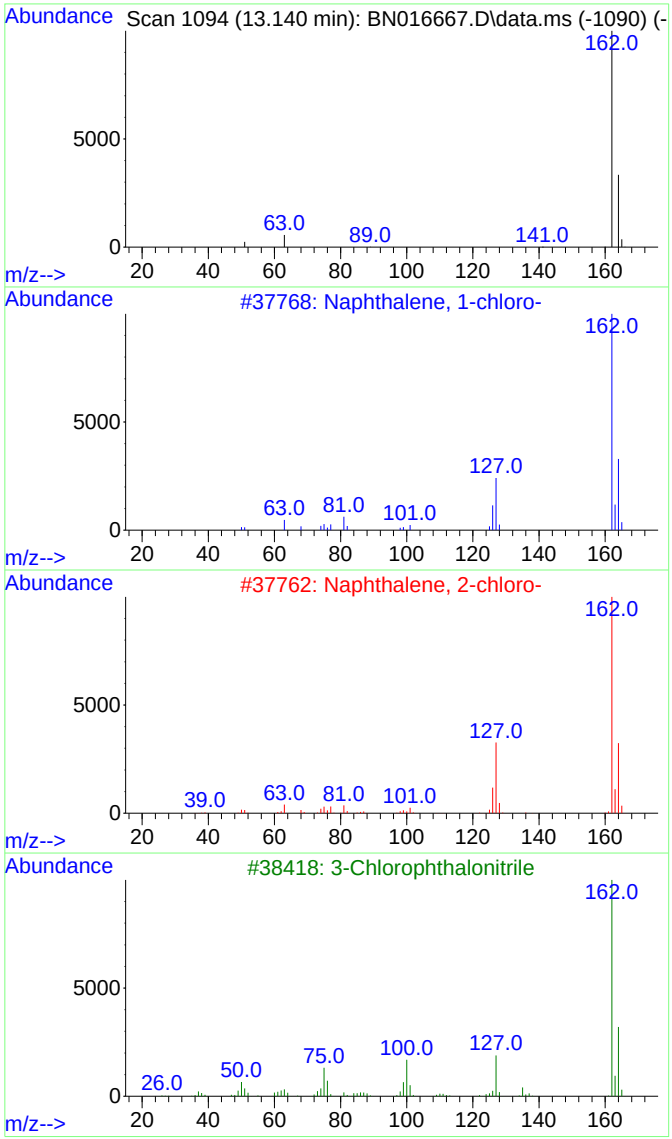
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

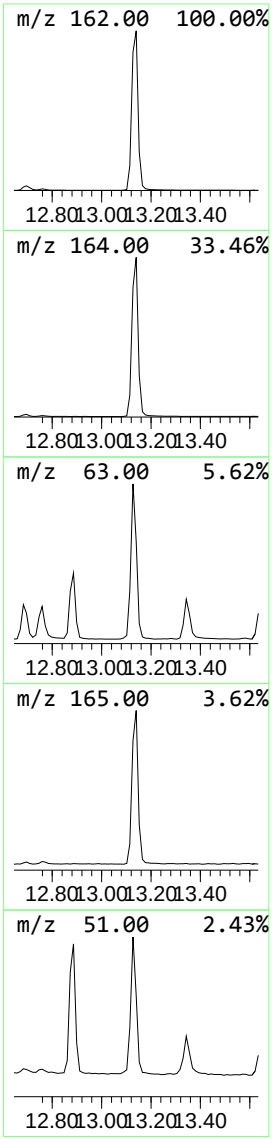
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Naphthalene, 1-chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.140	0.26 ng	127485	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	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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Sample : SSTDCCC0.4
Misc :
ALS Vial : 35 Sample Multiplier: 1

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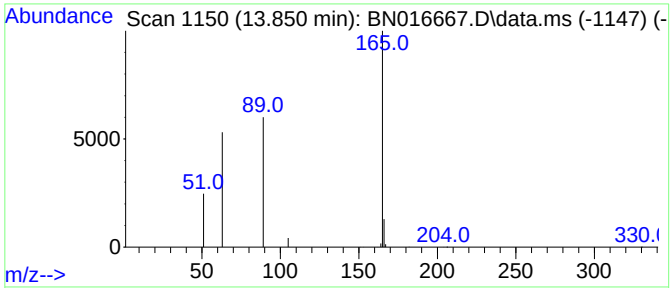
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

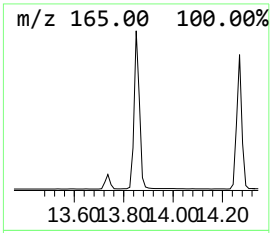
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

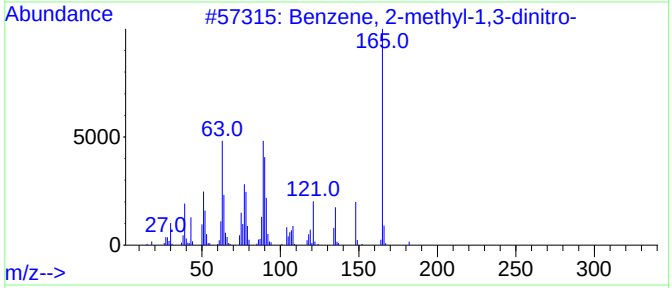
****
Peak Number 13 Benzene, 2-methyl-1,3-dinitro- Concentration Rank 16

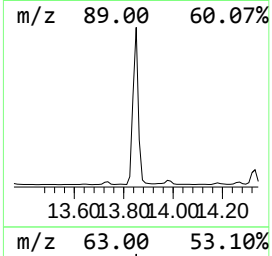
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.850	0.06 ng	30427	Acenaphthene-d10	14.269

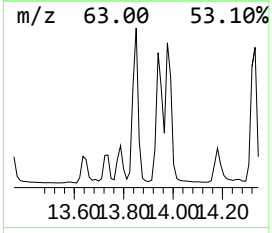
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-methyl-1,3-dinitro-	182	C7H6N2O4	000606-20-2	83
2	6-Oxa-3-azabicyclo[3.2.1]octa-1,...	165	C8H7NO3	055255-96-4	9
3	5,6-Dimethoxy-3-pyridazinecarbon...	165	C7H7N3O2	020552-46-9	9
4	Furo[3,4-c]pyridin-3(1H)-one, 7-...	165	C8H7NO3	004543-56-0	9
5	Furo[3,4-c]pyridin-1(3H)-one, 7-...	165	C8H7NO3	004753-19-9	9

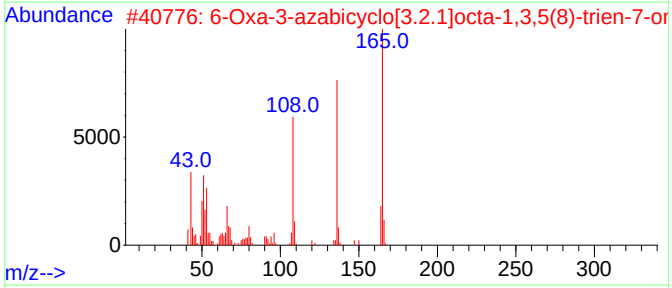


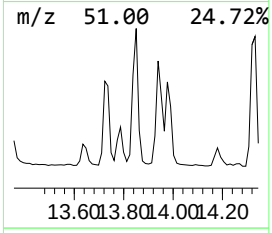


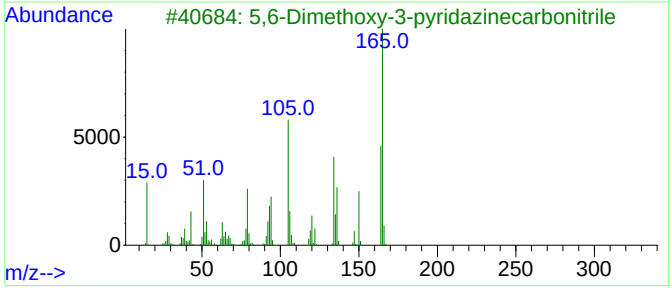


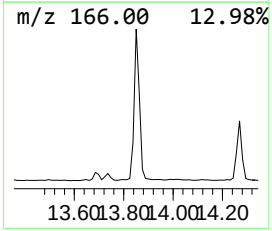












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Acq On : 02 Oct 2021 11:44
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDCCC0.4

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

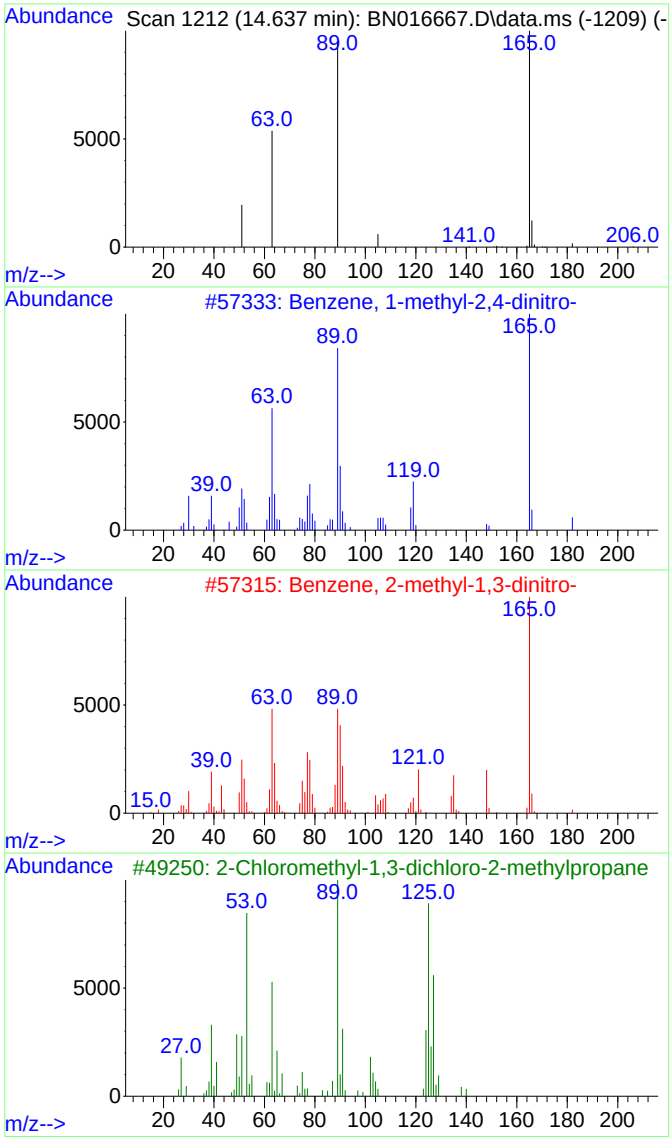
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

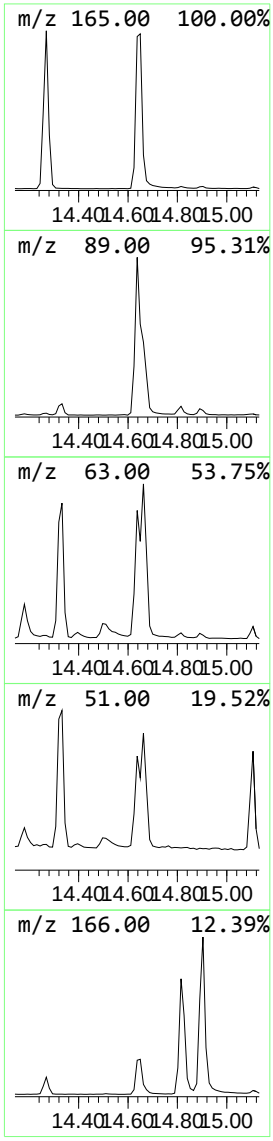
****

Peak Number 14 Benzene, 1-methyl-2,4-dinitro- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.637	0.09 ng	46345	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	83
2	Benzene, 2-methyl-1,3-dinitro-	182	C7H6N2O4	000606-20-2	38
3	2-Chloromethyl-1,3-dichloro-2-me...	174	C5H9Cl3	001067-09-0	9
4	5-[2-Chlorophenyl]tetraazole	180	C7H5ClN4	050907-46-5	9
5	Ethanol, 1-(4-nitrophenyl)-2-[1-...	304	C17H24N2O3	1000264-75-7	9





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Sample : SSTDCCC0.4
Misc :
ALS Vial : 35 Sample Multiplier: 1

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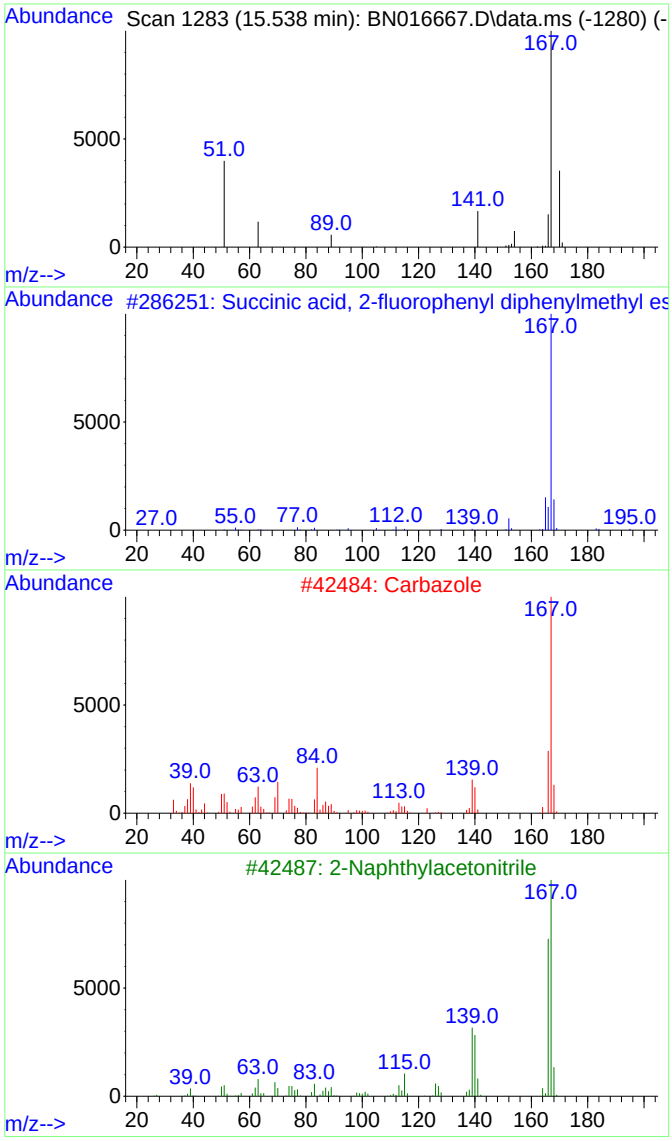
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

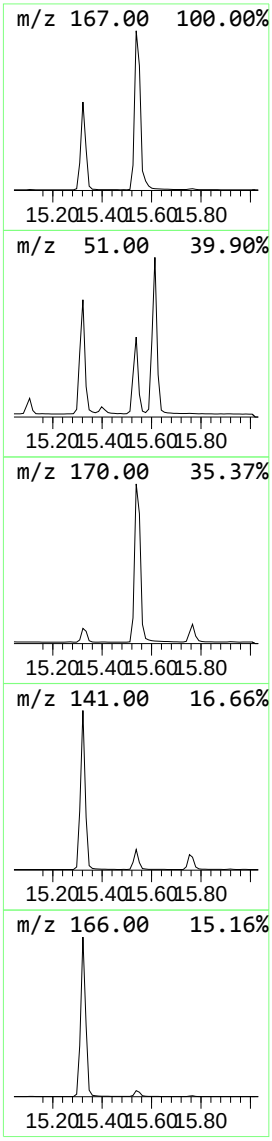
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 Succinic acid, 2-fluorophen... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.538	0.13 ng	64955	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	2-Naphthylacetonitrile	167	C12H9N	007498-57-9	7
4	5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	5
5	Benzaldehyde, 2-hydroxy-5-nitro-	167	C7H5NO4	000097-51-8	5





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Sample : SSTDCCC0.4
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
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LabSampleId :
SSTDCCC0.4

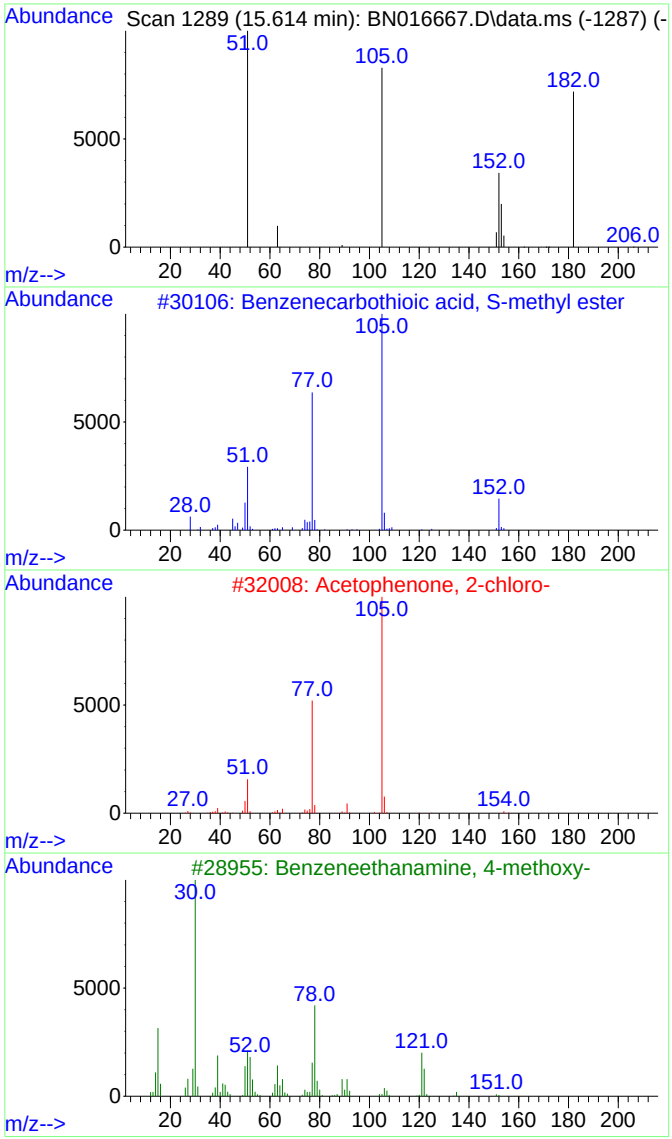
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

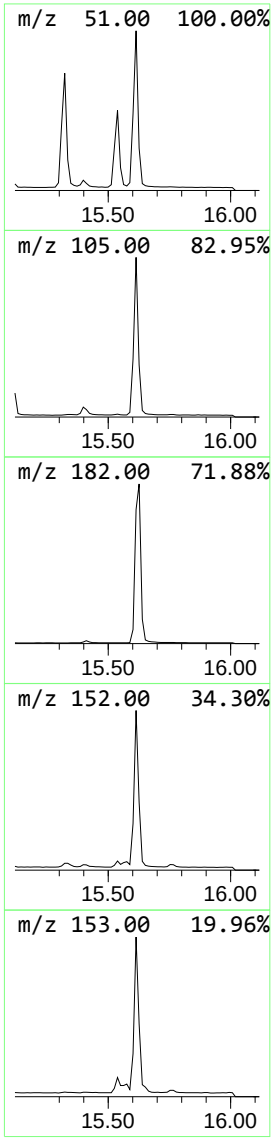
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 Benzenecarbothioic acid, S-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.614	0.13 ng	65281	Acenaphthene-d10	14.269

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





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Data File : BN016667.D
Acq On : 02 Oct 2021 11:44
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

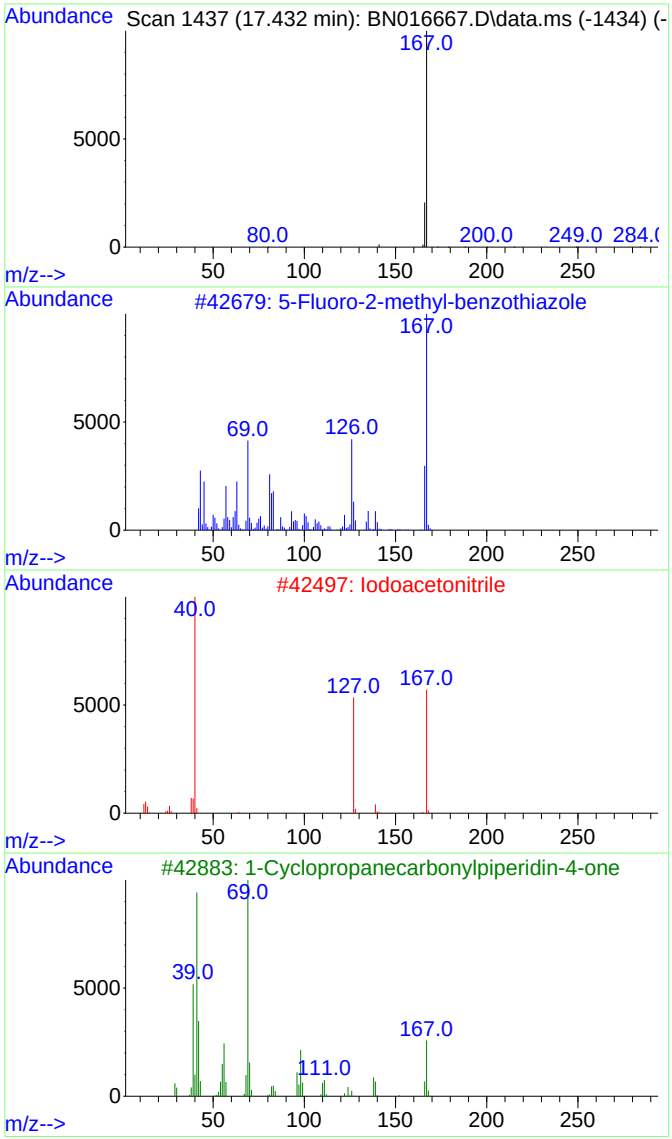
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

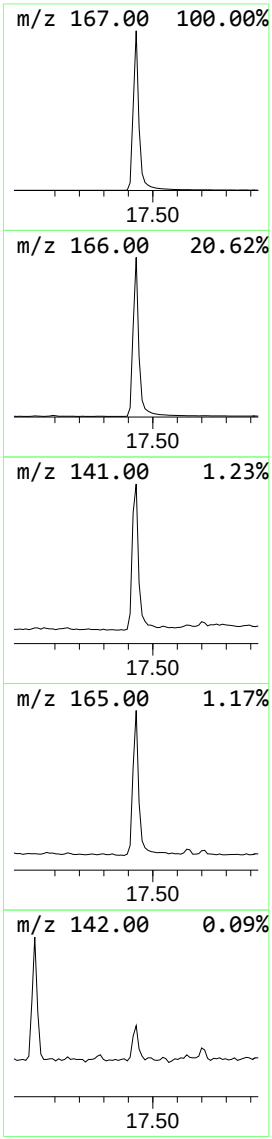
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 5-Fluoro-2-methyl-benzothia... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.432	0.36 ng	148069	Phenanthrene-d10	17.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	5
2	Iodoacetonitrile	167	C2H2IN	000624-75-9	4
3	1-Cyclopropanecarbonylpiperidin-...	167	C9H13NO2	063463-43-4	4
4	2(1H)-Pyrimidinone, 4-[(2-methyl...	167	C8H13N3O	119608-70-7	4
5	1,3,5-Triazine-2,4-diamine, N,N'...	167	C7H13N5	004150-59-8	4





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Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

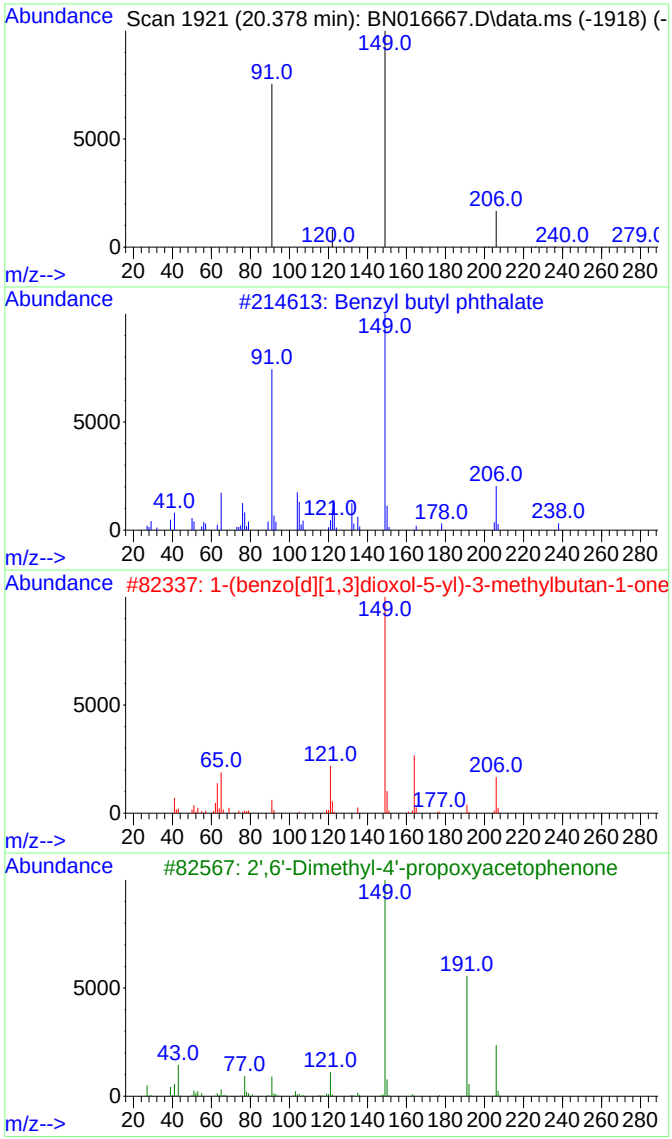
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

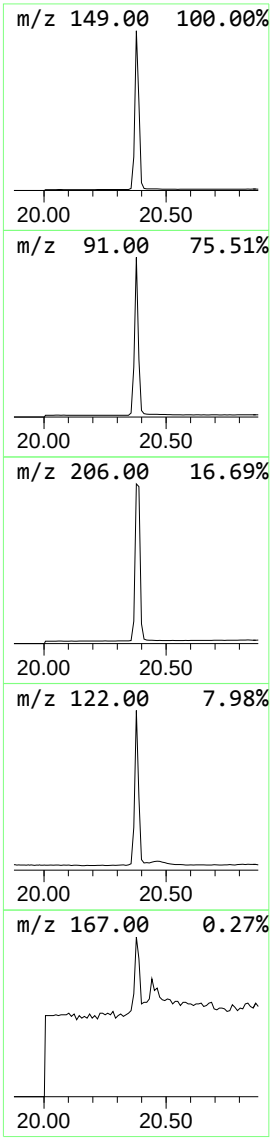
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 Benzyl butyl phthalate Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.378	0.07 ng	76956	Chrysene-d12	21.228

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzyl butyl phthalate	312	C19H20O4	000085-68-7	40
2	1-(benzo[d][1,3]dioxol-5-yl)-3-m...	206	C12H14O3	1000456-66-2	9
3	2',6'-Dimethyl-4'-propoxyacetoph...	206	C13H18O2	1010195-98-1	5
4	2-tert-Butyl-6-methylphenol, n-p...	206	C14H22O	1000395-19-2	5
5	1,3,2-Dioxarsenane, 2-butyl-	206	C7H15AsO2	042541-33-3	5





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Data File : BN016667.D
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Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

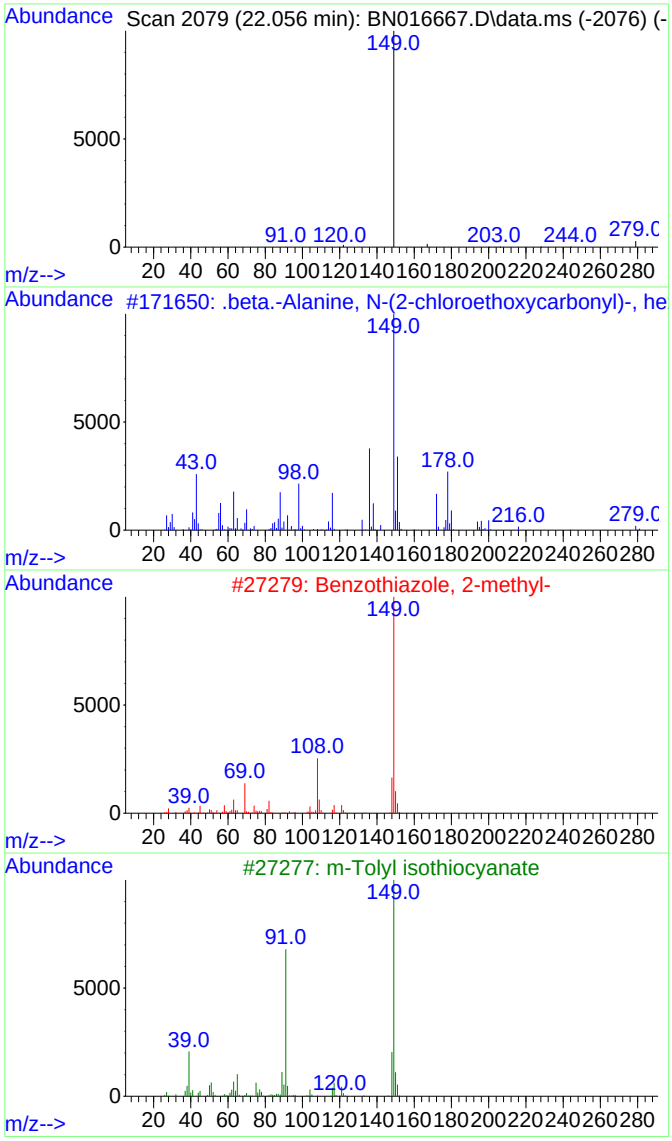
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

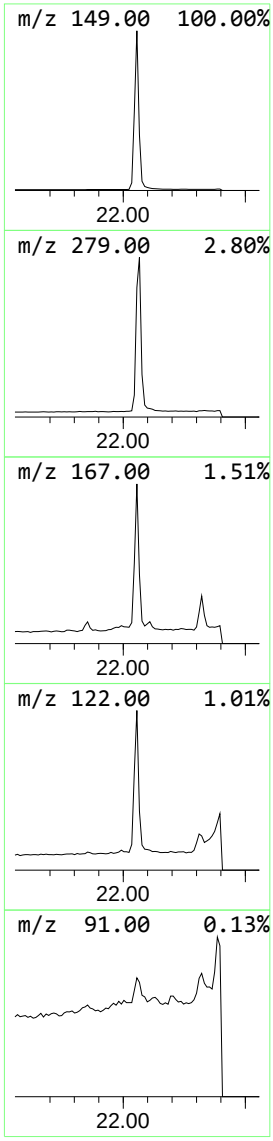
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 .beta.-Alanine, N-(2-chloro... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.056	0.11 ng	124888	Chrysene-d12	21.228

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	Pyridine, pentamethyl-	149	C10H15N	003748-83-2	4
5	Phthalic acid, 7-bromoheptyl oct...	454	C23H35BrO4	1000415-52-2	4





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Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

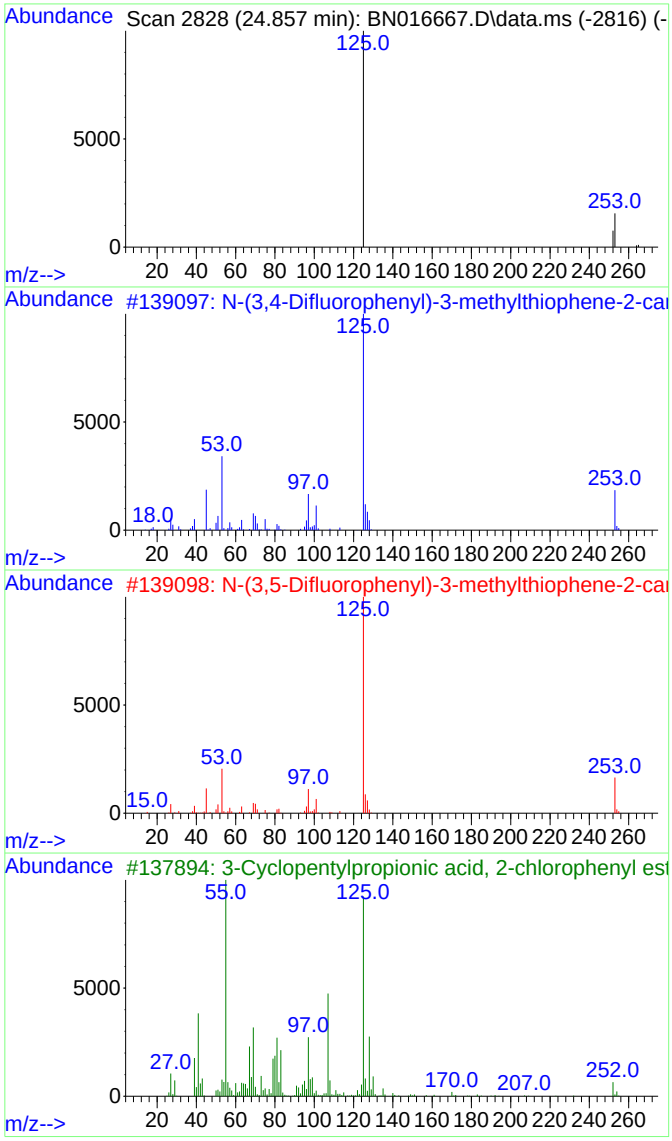
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

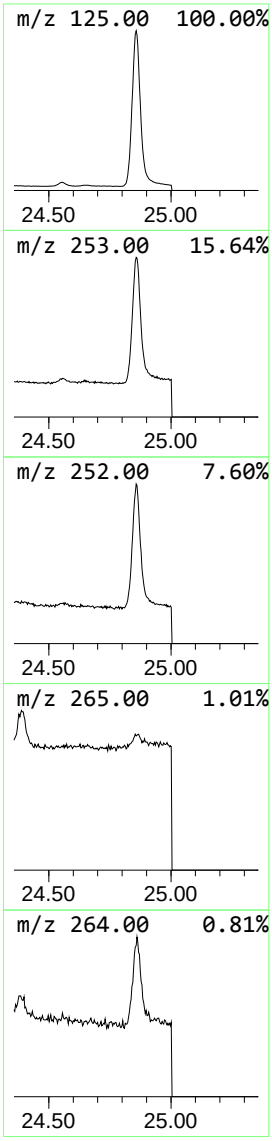
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 N-(3,4-Difluorophenyl)-3-me... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.857	0.06 ng	33116	Perylene-d12	23.485

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-(3,4-Difluorophenyl)-3-methylt...	253	C12H9F2NOS	1000436-25-1	4
2	N-(3,5-Difluorophenyl)-3-methylt...	253	C12H9F2NOS	1000436-25-2	4
3	3-Cyclopentylpropionic acid, 2-c...	252	C14H17ClO2	1000293-58-8	4
4	3-Cyclopentylpropionic acid, 3-c...	252	C14H17ClO2	1000325-52-2	4
5	Furane-2-carboxylic acid, 5-(4-c...	252	C12H9ClO4	074556-57-3	4





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016667.D
Acq On : 02 Oct 2021 11:44
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDCCC0.4

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	0.1	ng	31681	1	7.643	117929	0.4
Ethene, 1,1-dif...	7.200	0.1	ng	32614	1	7.643	117929	0.4
6-Benzothiazola...	7.956	0.4	ng	105716	1	7.643	117929	0.4
Furan, 2,5-dihy...	8.430	0.2	ng	52800	1	7.643	117929	0.4
Fomepizole	9.342	0.2	ng	84685	2	10.407	196463	0.4
5-Aminopyrimidine	9.837	0.1	ng	28495	2	10.407	196463	0.4
o-Chloroaniline	10.572	0.1	ng	56339	2	10.407	196463	0.4
Methane, iodo-	11.705	0.1	ng	26956	2	10.407	196463	0.4
2-Propyl-4-meth...	12.296	0.4	ng	199673	2	10.407	196463	0.4
4-Cyano-5-(meth...	12.696	0.1	ng	30869	3	14.269	197350	0.4
1-Methyl-1,8-di...	12.759	0.1	ng	26737	3	14.269	197350	0.4
Naphthalene, 1-...	13.140	0.3	ng	127485	3	14.269	197350	0.4
Benzene, 2-meth...	13.850	0.1	ng	30427	3	14.269	197350	0.4
Benzene, 1-meth...	14.637	0.1	ng	46345	3	14.269	197350	0.4
Succinic acid, ...	15.538	0.1	ng	64955	3	14.269	197350	0.4
Benzenecarbothi...	15.614	0.1	ng	65281	3	14.269	197350	0.4
5-Fluoro-2-meth...	17.432	0.4	ng	148069	4	17.018	166482	0.4
Benzyl butyl ph...	20.378	0.1	ng	76956	5	21.228	449238	0.4
.beta.-Alanine,...	22.056	0.1	ng	124888	5	21.228	449238	0.4
N-(3,4-Difluoro...	24.857	0.1	ng	33116	6	23.485	219232	0.4