LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016651.D
Acq On : 02 Oct 2021 01:36
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 2 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: BN016651.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	6736	9959	1.85%	0.125%
2	3.281	20	22	40	rVB	5276	24993	4.65%	0.314%
3	3.594	51	56	80	rVB	6339	30212	5.62%	0.379%
4	5.263	231	237	251	rBV	14514	56029	10.42%	0.703%
5	6.822	401	406	418	rBV	23999	60631	11.28%	0.761%
6	6.978	418	423	429	rVV	15945	34614	6.44%	0.434%
7	7.080	429	434	440	rVV	35224	72611	13.51%	0.911%
8	7.200	440	447	459	rVB	12311	32334	6.02%	0.406%
9	7.522	478	482	489	rVB	6861	15027	2.80%	0.189%
10	7.642	490	495	510	rVB2	49680	121041	22.52%	1.519%
11	7.956	524	529	539	rVB2	47683	108049	20.10%	1.356%
12	8.168	547	552	557	rBV	3131	7529	1.40%	0.094%
13	8.429	571	577	591	rBV3	21050	49724	9.25%	0.624%
14	8.696	595	598	601	rVB	4754	8716	1.62%	0.109%
15	8.784	601	605	606	rBV	33269	62325	11.60%	0.782%
16	8.822	606	608	617	rVB	27333	51583	9.60%	0.647%
17	9.342	645	649	652	rBV	46481	76529	14.24%	0.960%
18	9.532	660	664	666	rBV	3159	6429	1.20%	0.081%
19	9.595	666	669	679	rVB	8710	15483	2.88%	0.194%
20	9.836	685	688	702	rVB	15658	28103	5.23%	0.353%
21	10.052	702	705	714	rBV	4046	8900	1.66%	0.112%
22	10.406	729	733	735	rBV	107596	193787	36.06%	2.432%
23	10.457	735	737	741	rVV	108683	178416	33.20%	2.239%
24	10.571	743	746	756	rVV	26522	58682	10.92%	0.736%
25	10.749	756	760	763	rVB	32561	56027	10.42%	0.703%
26	11.709	855	865	892	rBV	13645	25565	4.76%	0.321%
27	12.003	921	931	939	rBV	57300	92748	17.26%	1.164%
28	12.074	939	947	972	rVV	123778	206958	38.51%	2.597%
29	12.296	987	997	1021	rVV	125983	199342	37.09%	2.501%
30	12.695	1056	1059	1062	rBV	17333	29126	5.42%	0.365%
31	12.759	1062	1064	1071	rVB	12340	25549	4.75%	0.321%
32	12.886	1071	1074	1078	rBV	119515	197403	36.73%	2.477%
33	13.139	1089	1094	1097	rBV	78577	132849	24.72%	1.667%
34	13.736	1138	1141	1143	rBV	12045	16934	3.15%	0.212%
35	13.850	1147	1150	1153	rVB	19541	28394	5.28%	0.356%
36	13.939	1155	1157	1158	rBV	5368	8685	1.62%	0.109%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Acq On : 02 Oct 2021 01:36
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 2 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

37	13.989	1158	1161	1164	rVB	93472	154862	28.81%	1.943%
38	14.269	1180	1183	1185	rBV	138776	195918	36.45%	2.458%
39	14.332	1185	1188	1191	rVB	167787	242707	45.16%	3.046%
40	14.637	1209	1212	1220	rBV3	16791	43874	8.16%	0.551%
41	14.814	1224	1226	1230	rBV	5526	9547	1.78%	0.120%
42	14.903	1230	1233	1236	rBV	7723	11532	2.15%	0.145%
43	15.106	1246	1249	1252	rBV	9072	11455	2.13%	0.144%
44	15.322	1263	1266	1270	rBV2	229645	354864	66.03%	4.453%
45	15.410	1270	1273	1280	rVV2	2829	7669	1.43%	0.096%
46	15.537	1280	1283	1287	rVV	36745	62739	11.67%	0.787%
47	15.613	1287	1289	1298	rVV2	41781	65201	12.13%	0.818%
48	15.766	1298	1301	1311	rVB2	13689	22933	4.27%	0.288%
49	16.226	1334	1338	1341	rBV2	57851	92324	17.18%	1.158%
50	16.324	1343	1346	1349	rVV	47695	73146	13.61%	0.918%
51	16.506	1358	1361	1372	rBV	21236	34755	6.47%	0.436%
52	16.677	1372	1375	1384	rBV	21222	37152	6.91%	0.466%
53	17.017	1400	1403	1405	rBV	97307	161155	29.98%	2.022%
54	17.066	1405	1407	1410	rVV	152185	218995	40.75%	2.748%
55	17.151	1411	1414	1434	rVV	116405	189848	35.32%	2.382%
56	17.431	1434	1437	1452	rVV	89079	140115	26.07%	1.758%
57	18.015	1482	1485	1505	rVB9	5720	7476	1.39%	0.094%
58	19.063	1684	1696	1699	rBV	119417	165999	30.89%	2.083%
59	19.093	1699	1702	1745	rVB	197237	262020	48.75%	3.288%
60	19.460	1766	1776	1800	rBV	186337	258852	48.16%	3.248%
61	19.678	1813	1820	1853	rVB	107881	143151	26.63%	1.796%
62	20.378	1918	1921	1924	rBV	57453	63195	11.76%	0.793%
63	21.164	1992	1995	1997	rBV	57890	66987	12.46%	0.841%
64	21.217	1997	2000	2003	rVV2	213539	434963	80.93%	5.458%
65	21.270	2003	2005	2016	rVB	181468	270951	50.41%	3.400%
66	22.056	2075	2079	2082	rBV	62084	88139	16.40%	1.106%
67	22.803	2216	2228	2234	rBV	135123	218877	40.72%	2.747%
68	22.848	2234	2241	2283	rVB	143429	264967	49.30%	3.325%
69	23.382	2384	2397	2415	rBV	90921	205027	38.15%	2.573%
70	23.481	2415	2426	2466	rVB	102171	214731	39.95%	2.694%
71	24.083	2592	2602	2624	rBV	10497	20816	3.87%	0.261%
72	24.853	2815	2827	2859	rBV	10834	25470	4.74%	0.320%
73	25.767	3066	3094	3167	rBV4	134472	537460	100.00%	6.744%
74	26.452	3271	3294	3350	rBV2	75892	243282	45.27%	3.053%
75	26.815	3385	3400	3436	rVB2	2695	9212	1.71%	0.116%
76	28.081	3747	3770	3792	rBV	1467	5619	1.05%	0.071%

LSC Area Percent Report

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Data File : BN016651.D
Acq On : 02 Oct 2021 01:36
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 2 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

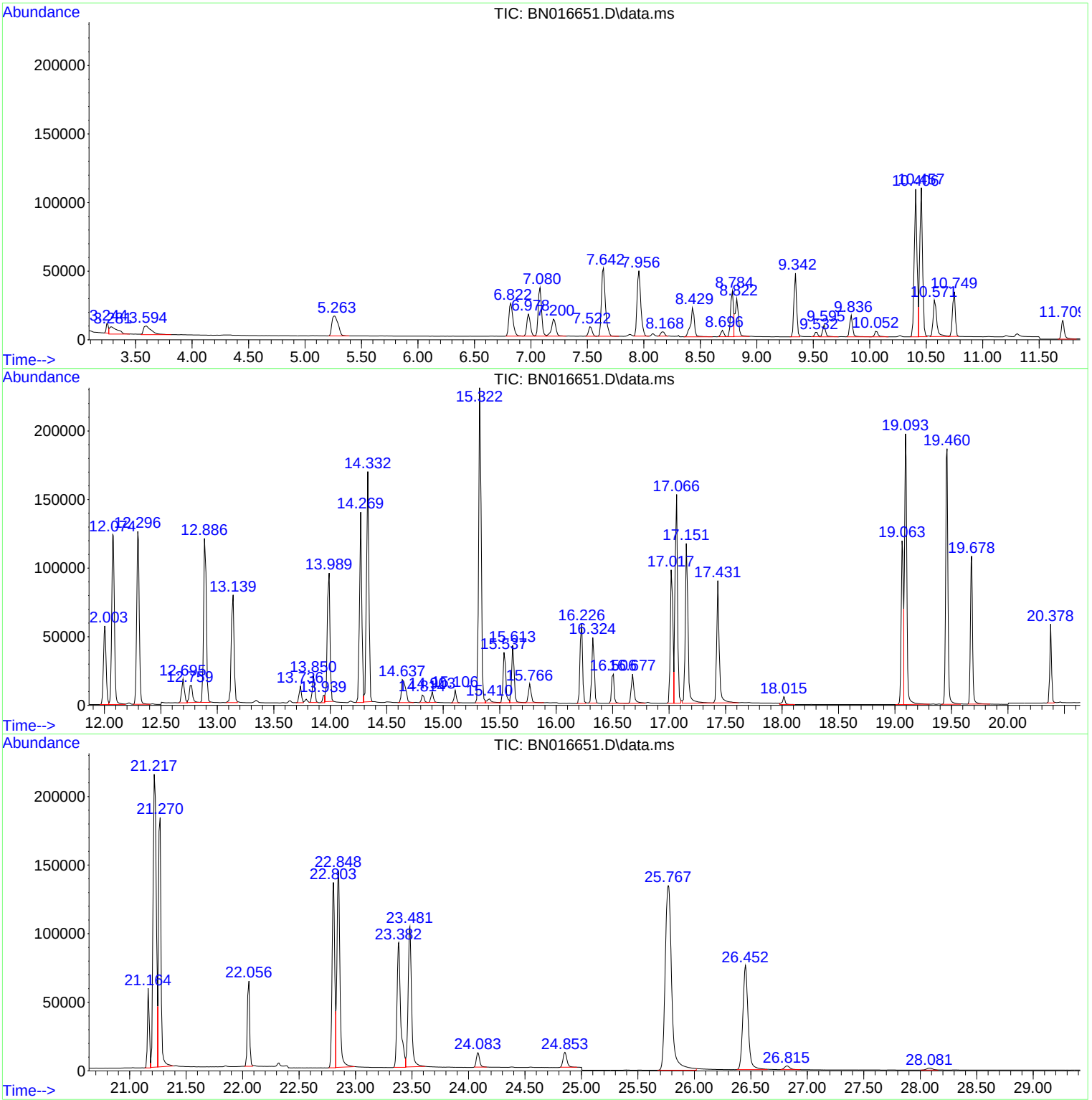
Sum of corrected areas: 7969271

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016651.D
Acq On : 02 Oct 2021 01:36
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 2 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 : BN016651.D
Acq On : 02 Oct 2021 01:36
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

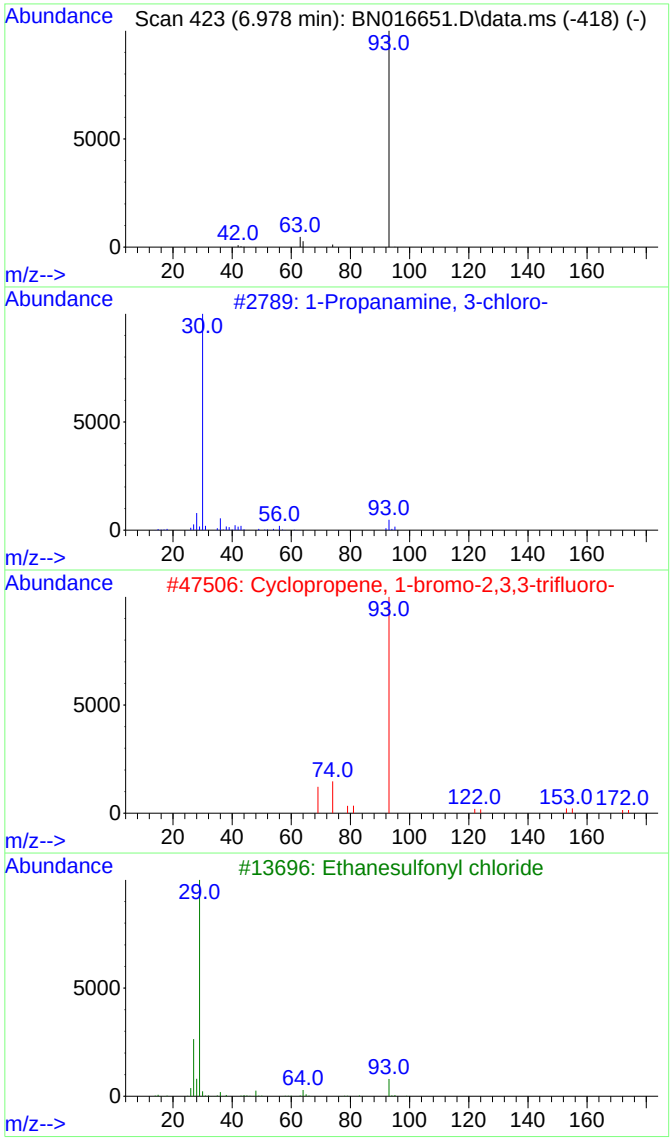
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

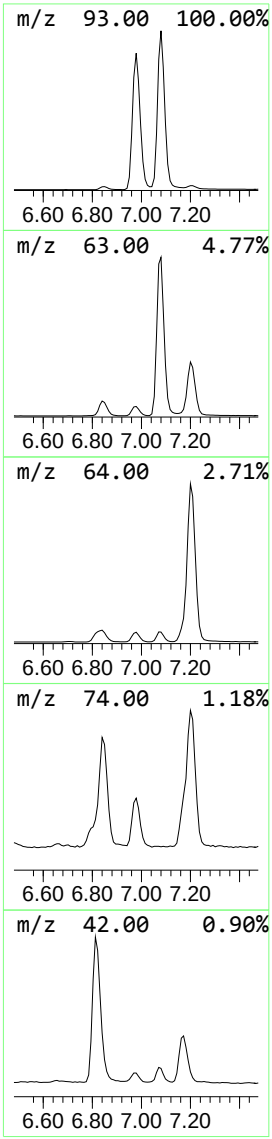
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.978	0.11 ng	34614	1,4-Dichlorobenzene-d4	7.642

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





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016651.D
Acq On : 02 Oct 2021 01:36
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

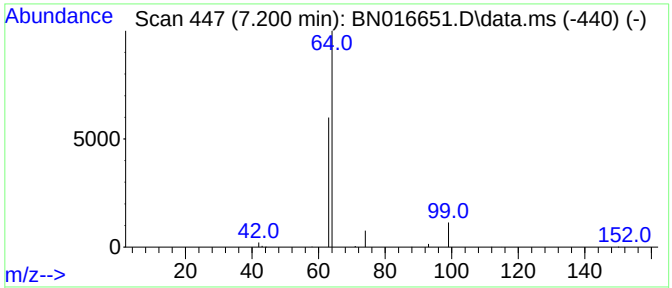
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

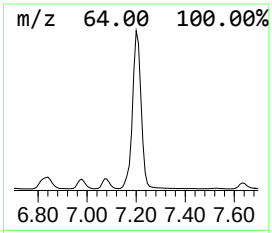
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

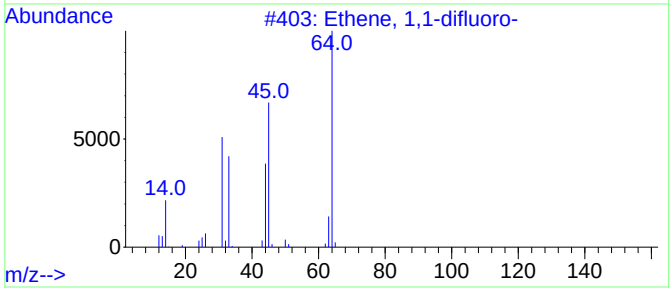
****
Peak Number 2 Ethene, 1,1-difluoro- Concentration Rank 11

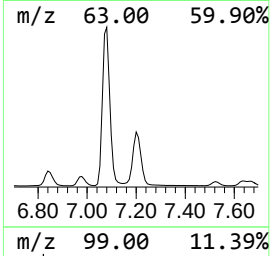
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.200	0.11 ng	32334	1,4-Dichlorobenzene-d4	7.642

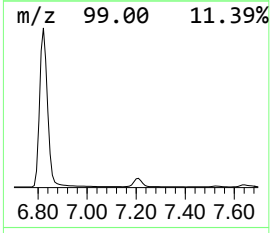
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	3
2	Ethyl Chloride	64	C2H5Cl	000075-00-3	3
3	Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	3
4	Sulfur dioxide	64	O2S	007446-09-5	3
5	(S)-(-)-2-Chloropropionic acid	108	C3H5ClO2	029617-66-1	2

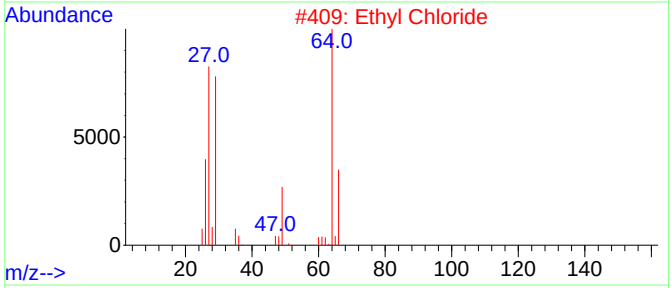


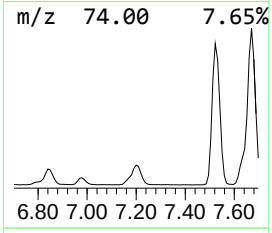


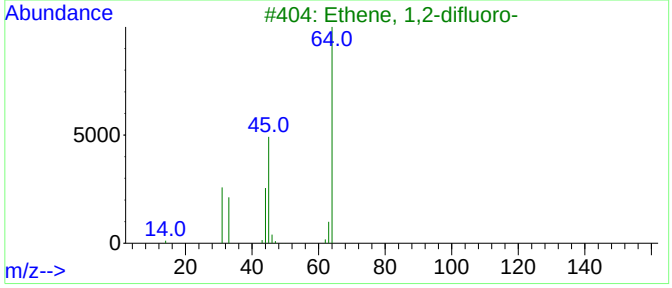


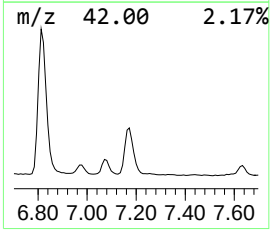












Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016651.D
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Misc :
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Instrument :
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LabSampleId :
SSTDCCC0.4

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

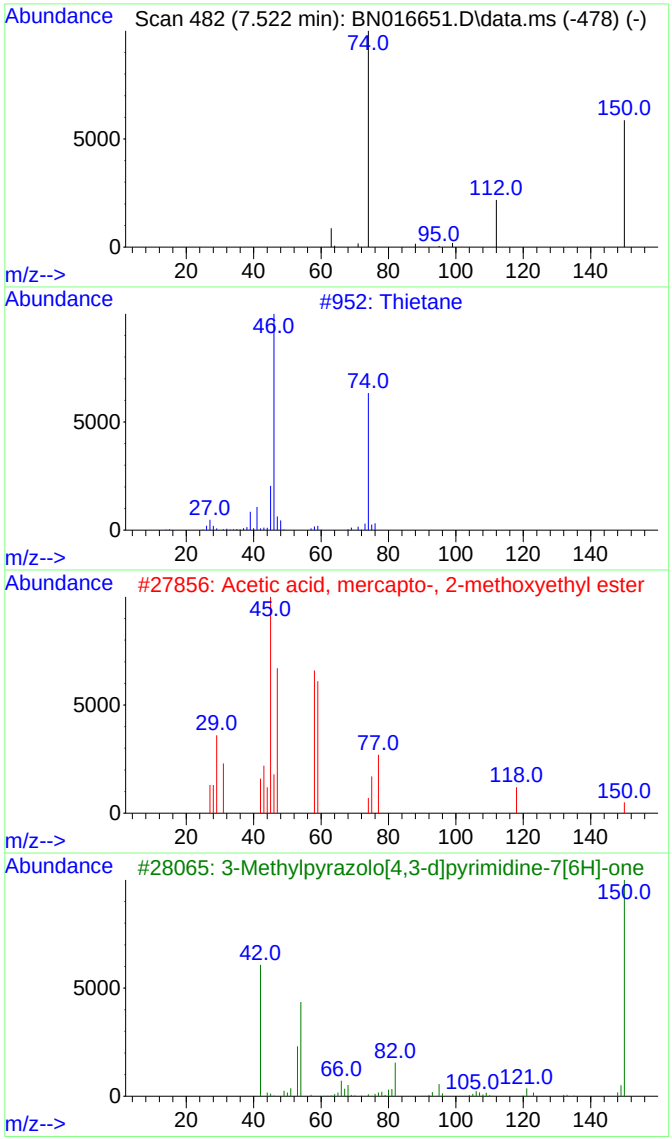
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

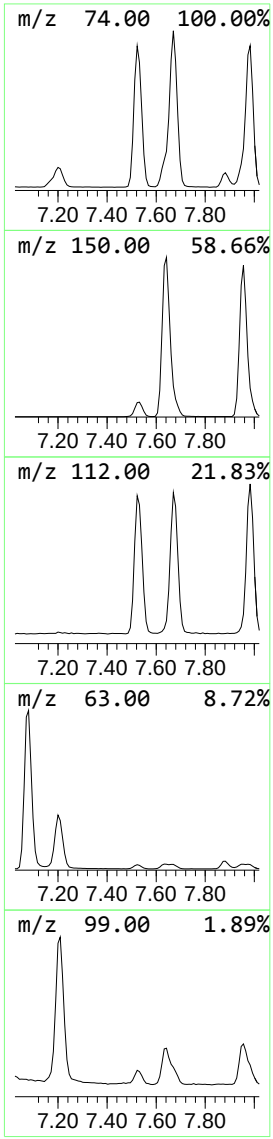
****

Peak Number 3 Thietane Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.522	0.05 ng	15027	1,4-Dichlorobenzene-d4	7.642

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	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	3-Methyl-4,4'-bi(1,2,4-triazole)	150	C5H6N6	063523-91-1	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016651.D
Acq On : 02 Oct 2021 01:36
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

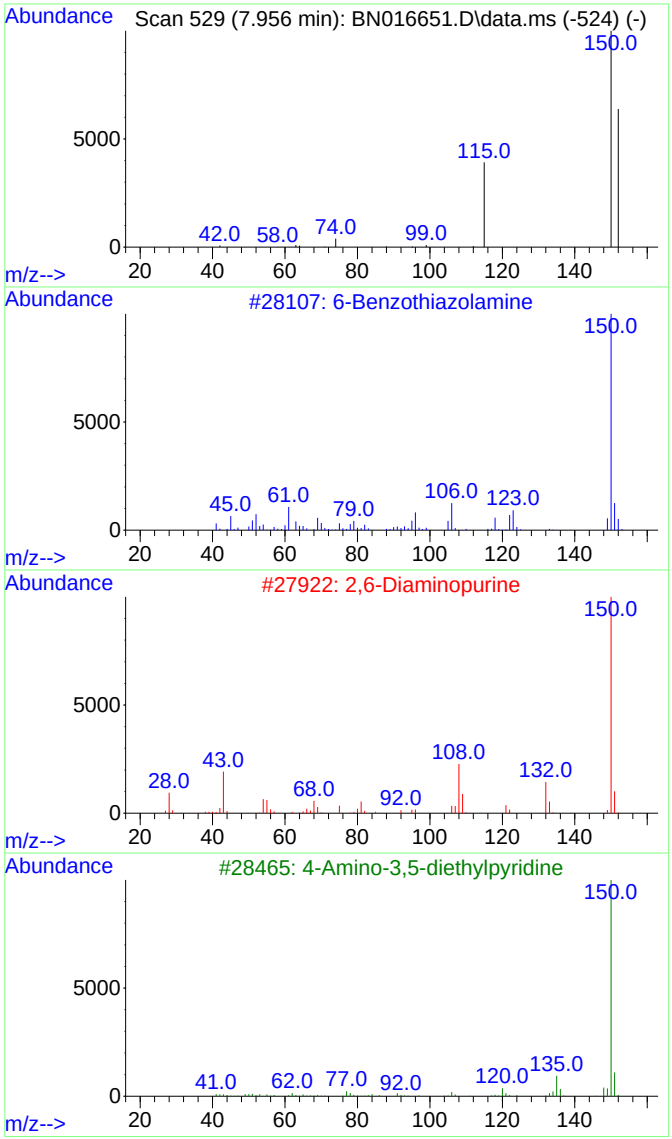
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

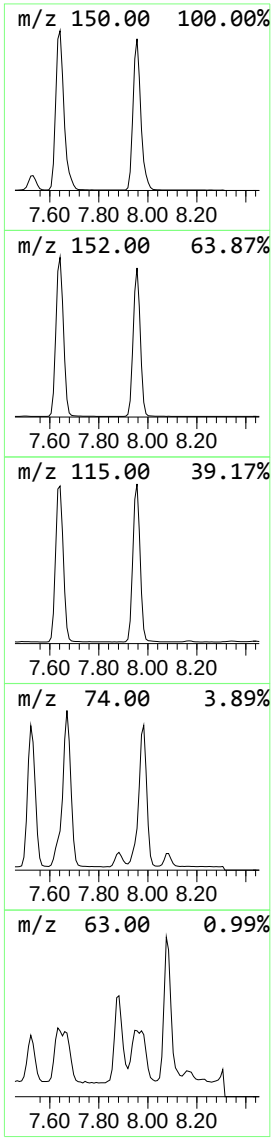
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 6-Benzothiazolamine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.956	0.36 ng	108049	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Benzothiazolamine	150	C7H6N2S	000533-30-2	4
2	2,6-Diaminopurine	150	C5H6N6	001904-98-9	2
3	4-Amino-3,5-diethylpyridine	150	C9H14N2	1000128-75-1	2
4	Benzene, 1,2,3,4-tetrafluoro-	150	C6H2F4	000551-62-2	2
5	2-Benzimidazolethiol	150	C7H6N2S	000583-39-1	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016651.D
Acq On : 02 Oct 2021 01:36
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

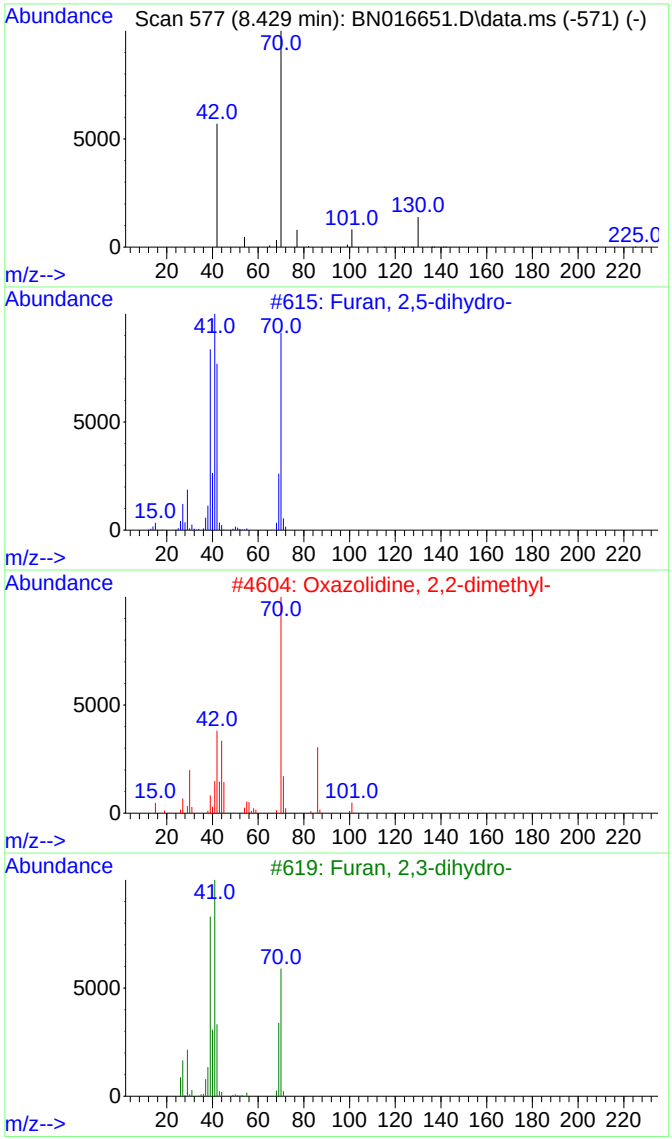
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

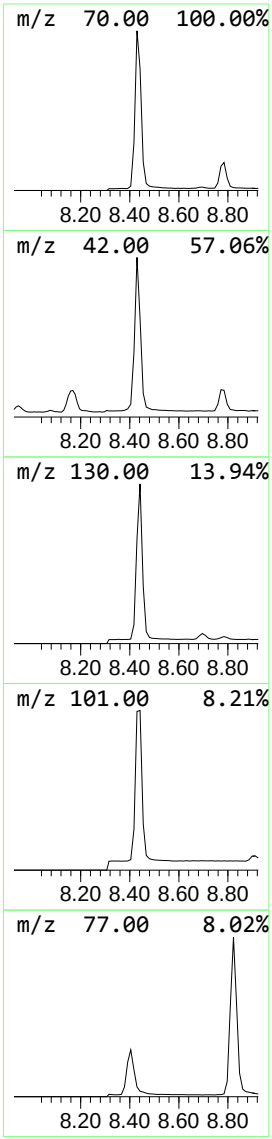
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.429	0.16 ng	49724	1,4-Dichlorobenzene-d4	7.642

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	Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	5
4	Dimethylketene	70	C4H6O	000598-26-5	5
5	1-Propanamine, N-nitroso-N-propyl-	130	C6H14N2O	000621-64-7	4





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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

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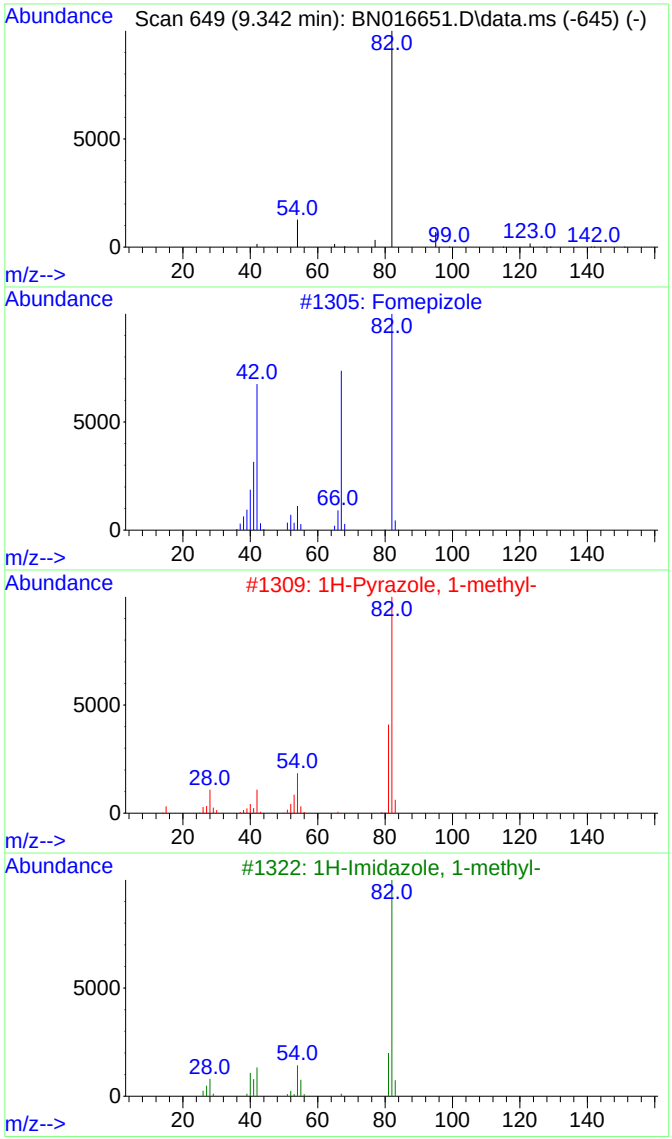
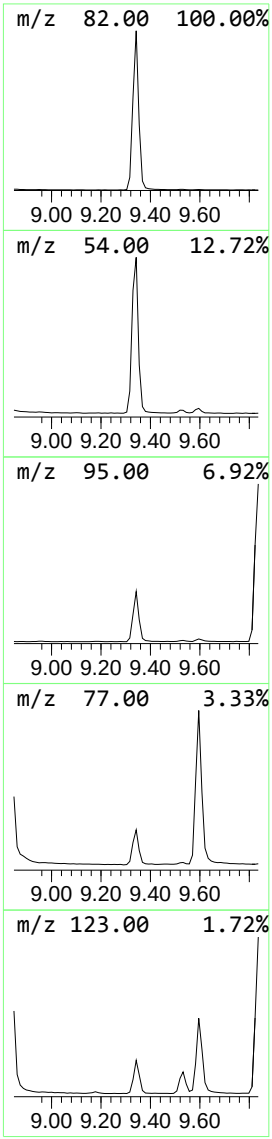
Peak Number 6 Fomepizole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.342	0.16 ng	76529	Naphthalene-d8	10.406

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fomepizole	82	C4H6N2	007554-65-6	5
2	1H-Pyrazole, 1-methyl-	82	C4H6N2	000930-36-9	4
3	1H-Imidazole, 1-methyl-	82	C4H6N2	000616-47-7	4
4	Furan, 3-methyl-	82	C5H6O	000930-27-8	4
5	Furan, 2-methyl-	82	C5H6O	000534-22-5	4





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Misc :
ALS Vial : 2 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

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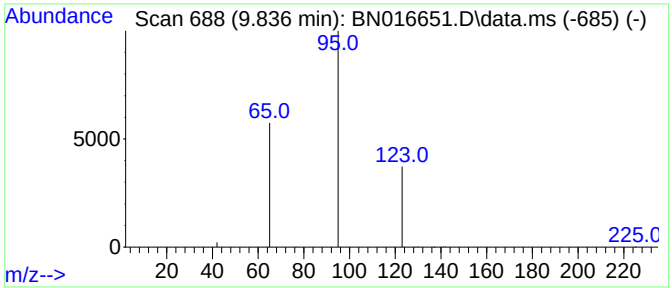
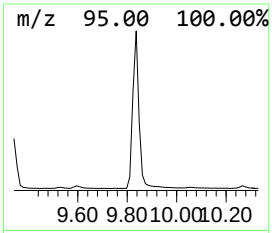
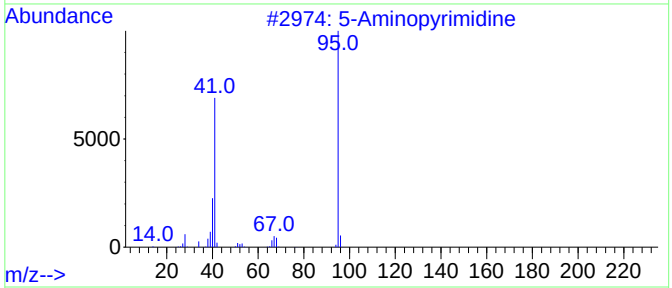
Peak Number 7 5-Aminopyrimidine Concentration Rank 16

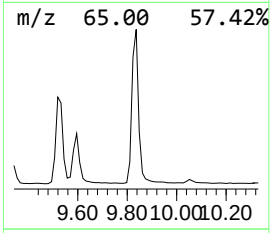
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.836	0.06 ng	28103	Naphthalene-d8	10.406

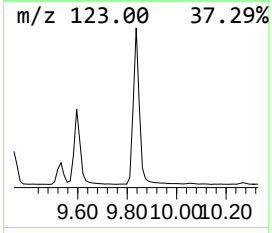
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminopyrimidine	95	C4H5N3	000591-55-9	3
2	4-Aminopyrimidine	95	C4H5N3	000591-54-8	2
3	2(1H)-Pyridinone	95	C5H5NO	000142-08-5	2
4	2-Pyrimidinamine	95	C4H5N3	000109-12-6	2
5	Pyridine, 1-oxide	95	C5H5NO	000694-59-7	2

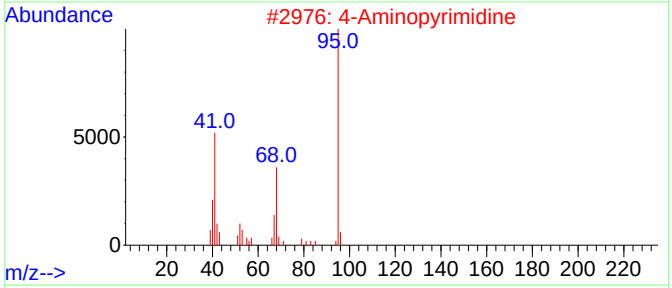


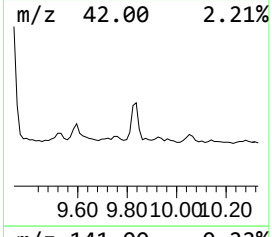


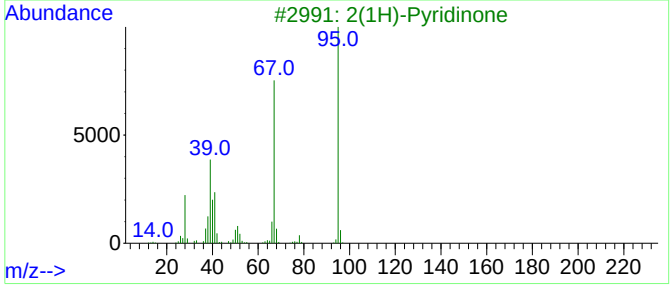


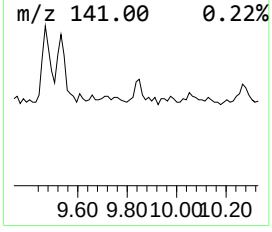












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Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 2 Sample Multiplier: 1

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

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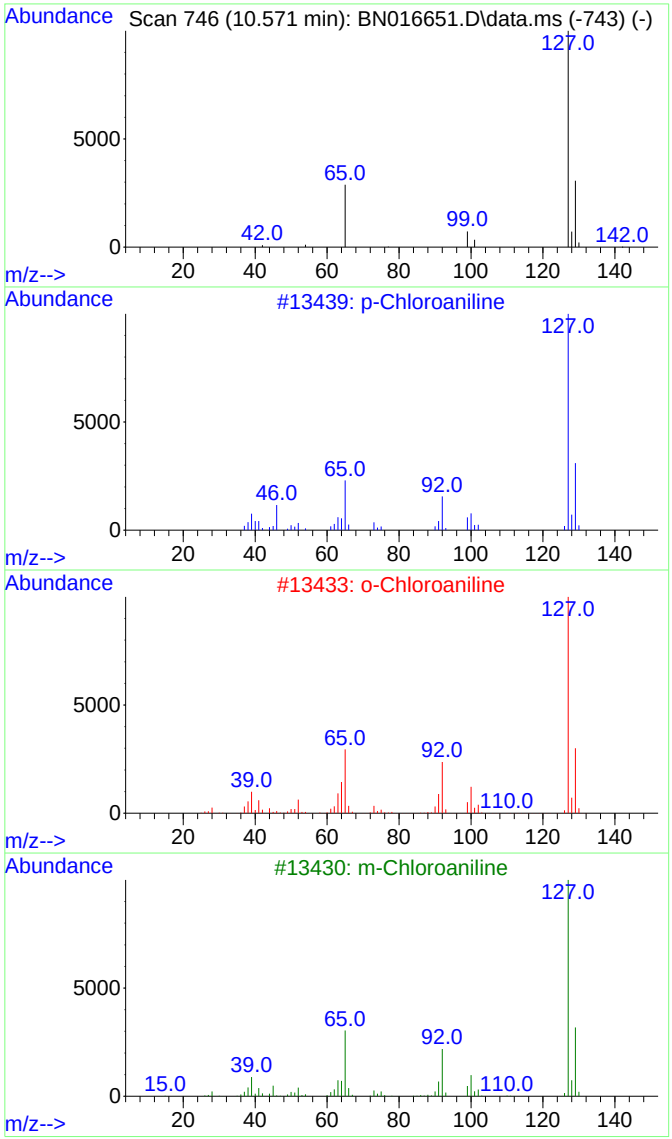
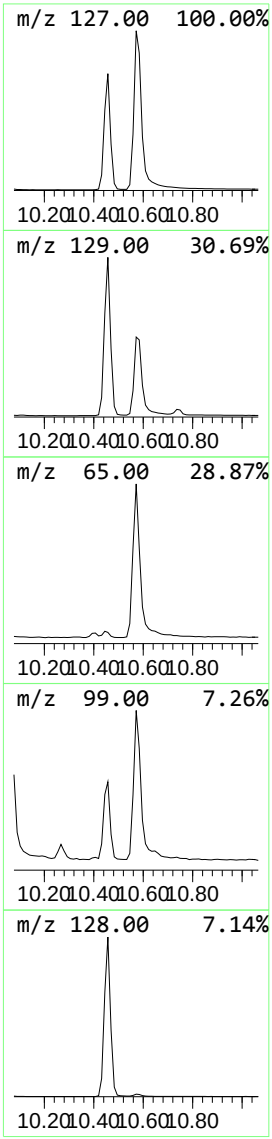
Peak Number 8 p-Chloroaniline Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.571	0.12 ng	58682	Naphthalene-d8	10.406

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Chloroaniline	127	C6H6ClN	000106-47-8	90
2	o-Chloroaniline	127	C6H6ClN	000095-51-2	90
3	m-Chloroaniline	127	C6H6ClN	000108-42-9	90
4	4-(Chloromethyl)pyridine	127	C6H6ClN	010445-91-7	86
5	Pyridine, 2-chloro-6-methyl-	127	C6H6ClN	018368-63-3	83





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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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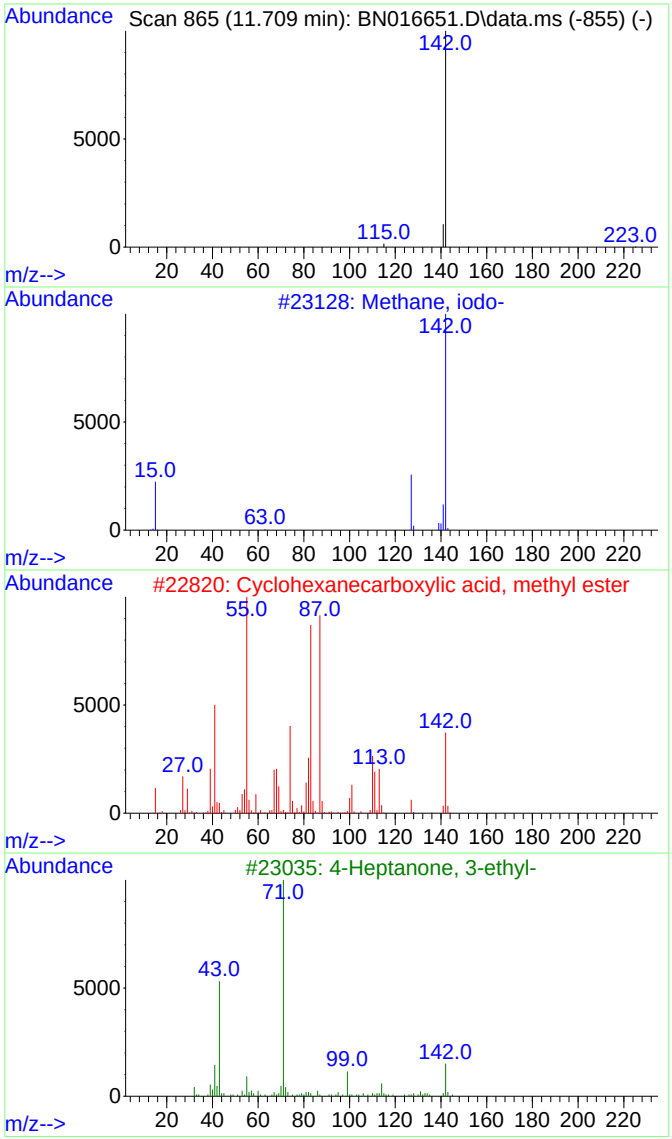
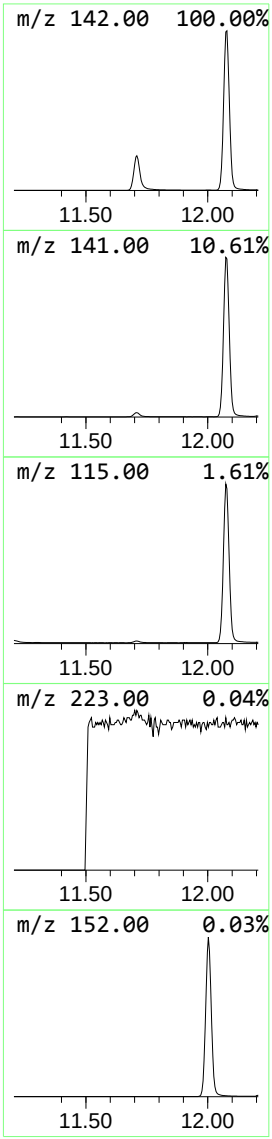
Peak Number 9 Methane, iodo- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.709	0.05 ng	25565	Naphthalene-d8	10.406

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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

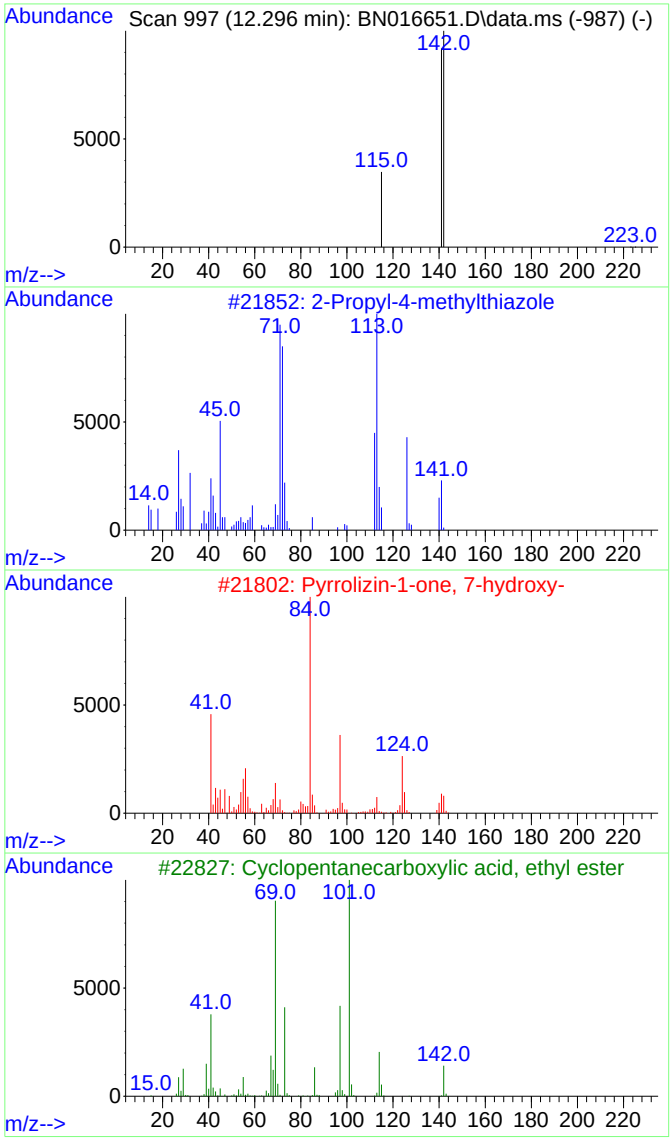
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

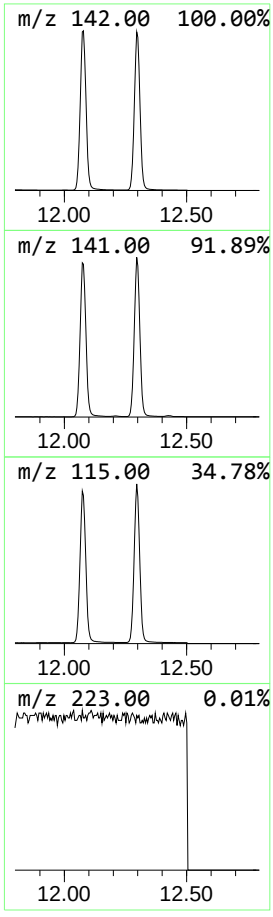
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.296	0.41 ng	199342	Naphthalene-d8	10.406

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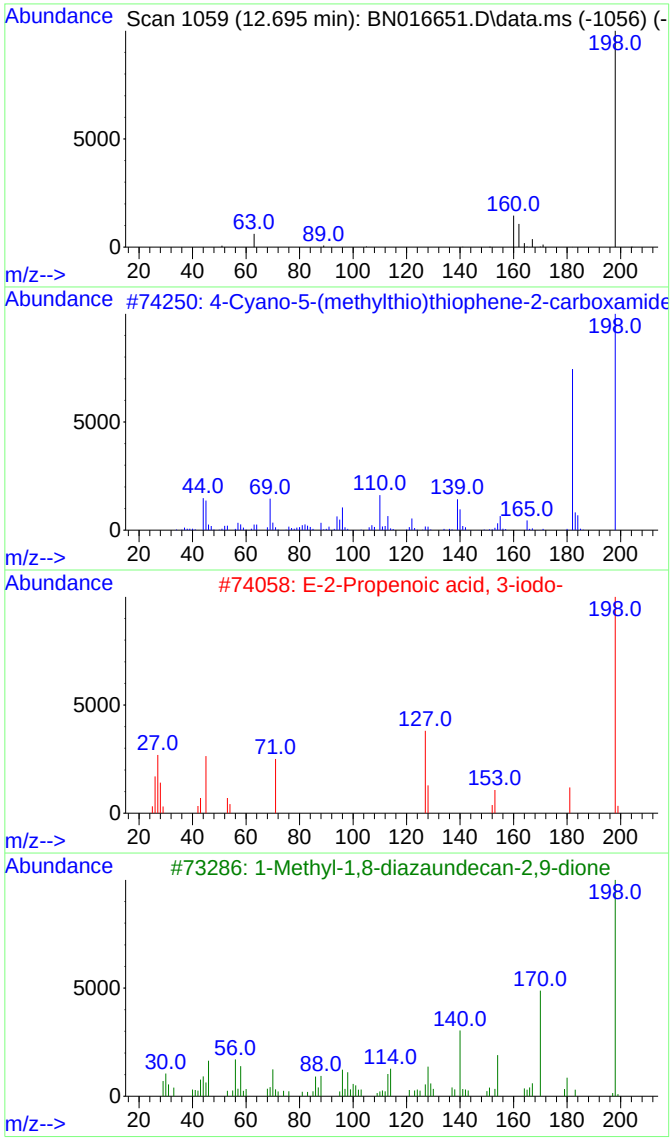
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

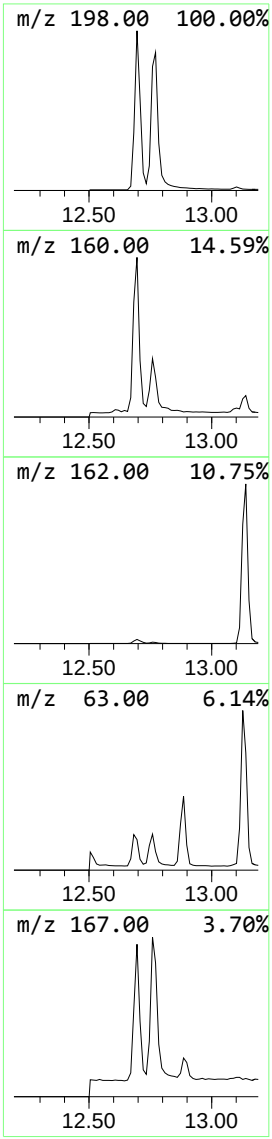
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.695	0.06 ng	29126	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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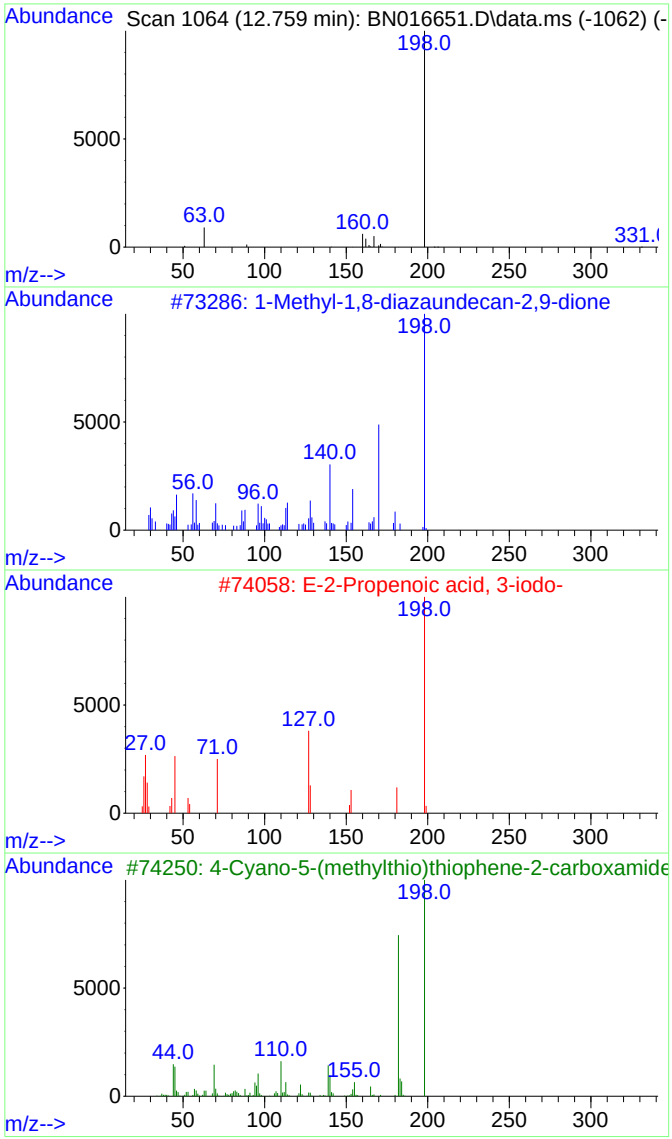
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

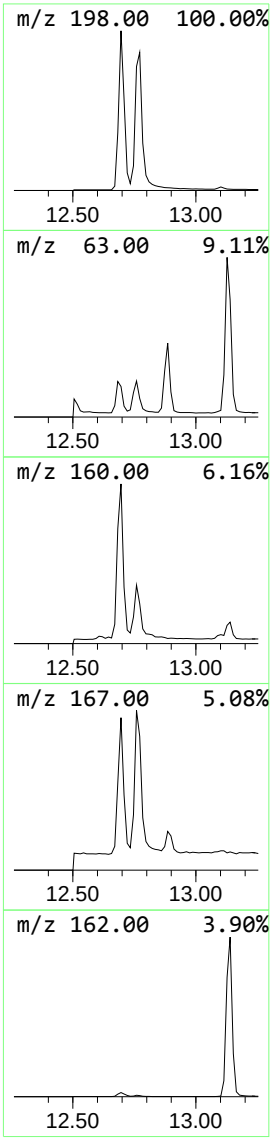
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 1-Methyl-1,8-diazaundecan-2... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.759	0.05 ng	25549	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	E-2-Propenoic acid, 3-iodo-	198	C3H3IO2	1000308-86-7	3
3	4-Cyano-5-(methylthio)thiophene-...	198	C7H6N2OS2	1000267-39-2	3
4	Thiazolo[5,4-d]pyrimidine, 5-ami...	198	C6H6N4S2	019835-31-5	3
5	Z-2-Propenoic acid, 3-iodo-	198	C3H3IO2	1000308-86-8	3





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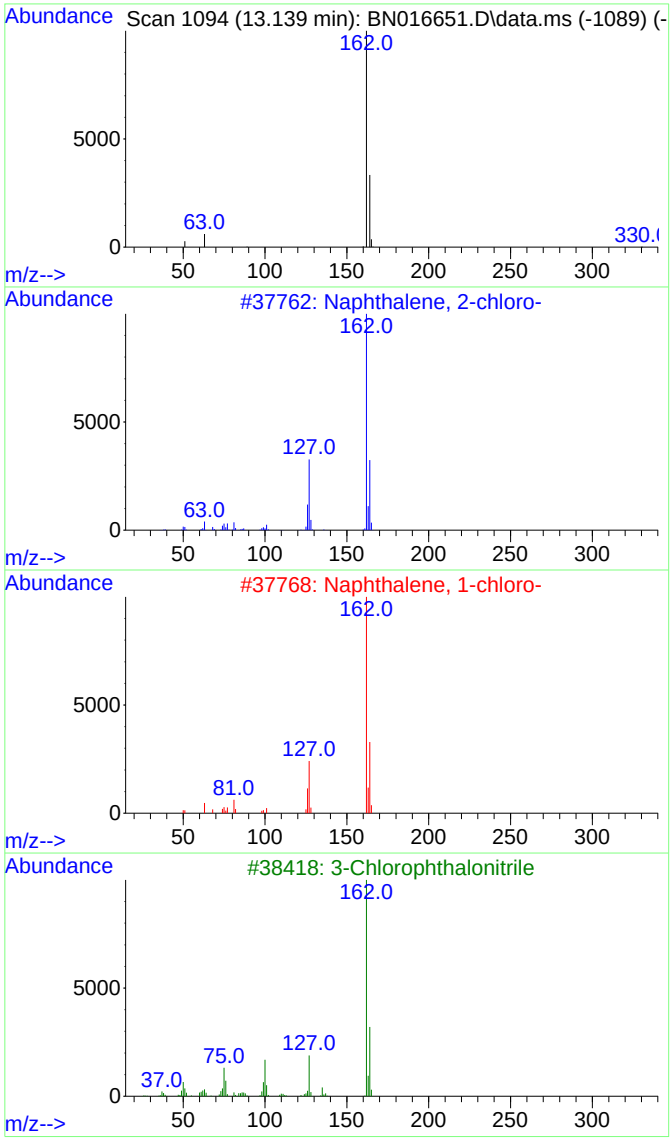
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

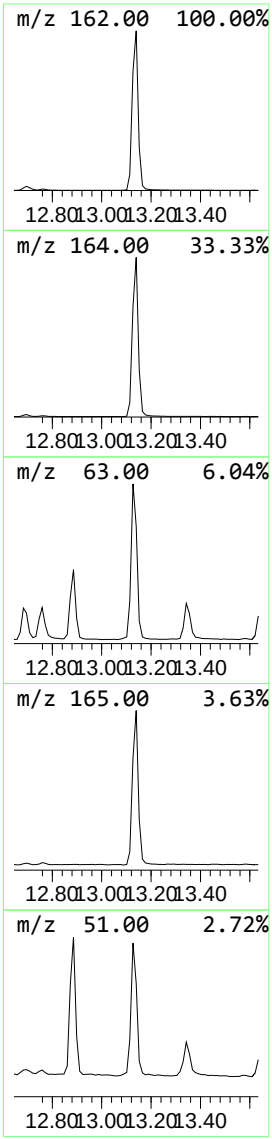
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.139	0.27 ng	132849	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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LabSampleId :
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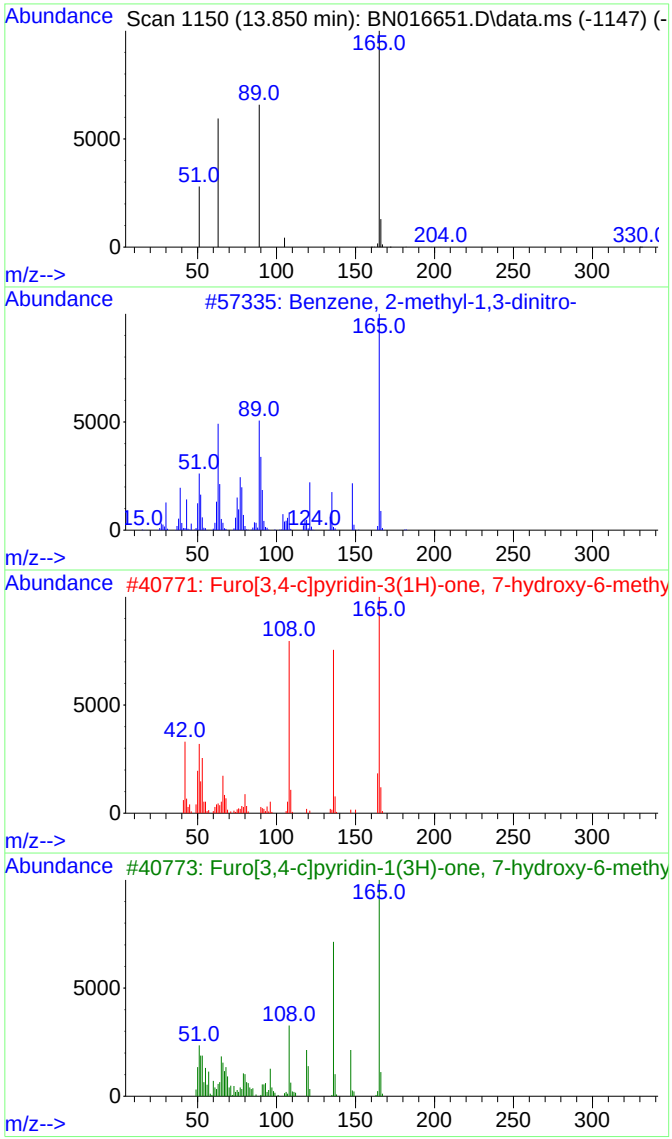
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

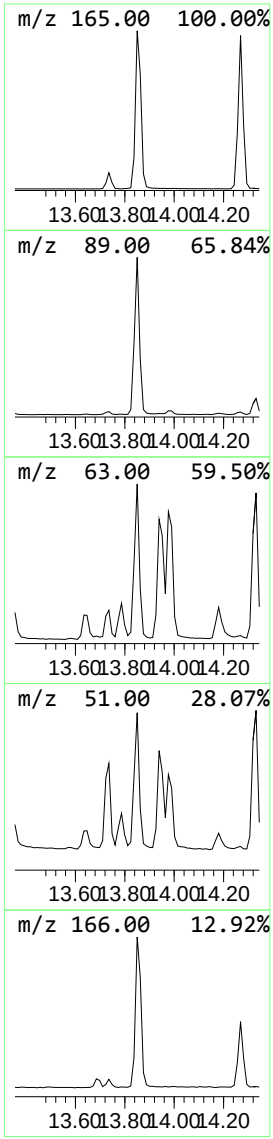
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 Benzene, 2-methyl-1,3-dinitro- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.850	0.06 ng	28394	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	Furo[3,4-c]pyridin-3(1H)-one, 7-...	165	C8H7NO3	004543-56-0	9
3	Furo[3,4-c]pyridin-1(3H)-one, 7-...	165	C8H7NO3	004753-19-9	9
4	6-Oxa-3-azabicyclo[3.2.1]octa-1,...	165	C8H7NO3	055255-96-4	9
5	5,6-Dimethoxy-3-pyridazinecarbon...	165	C7H7N3O2	020552-46-9	9





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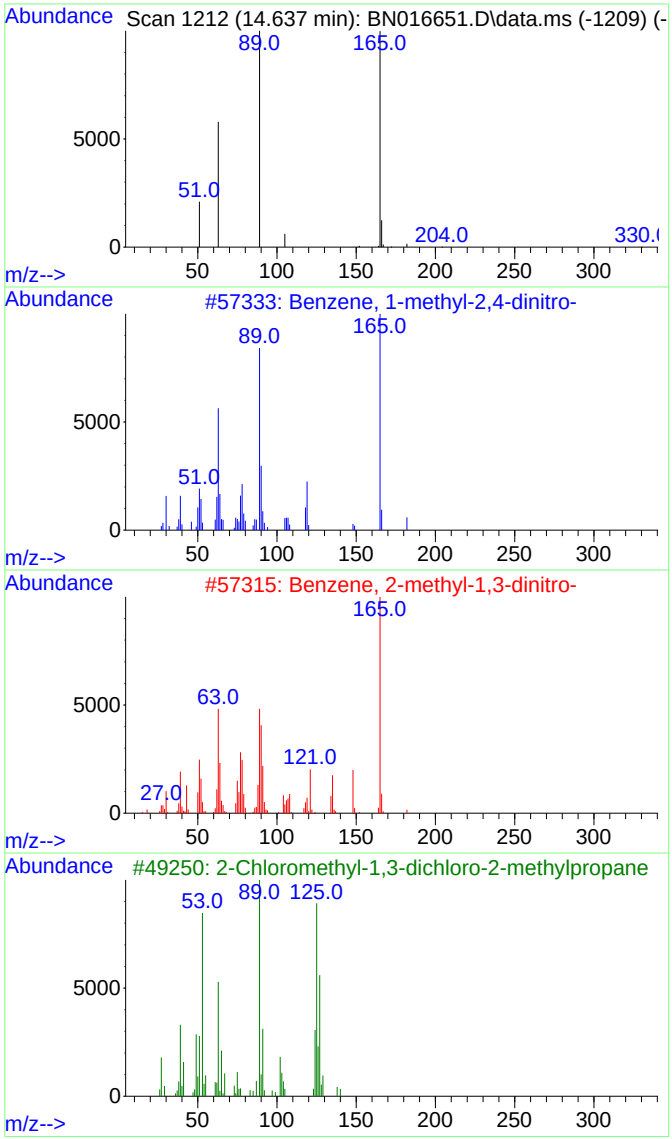
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

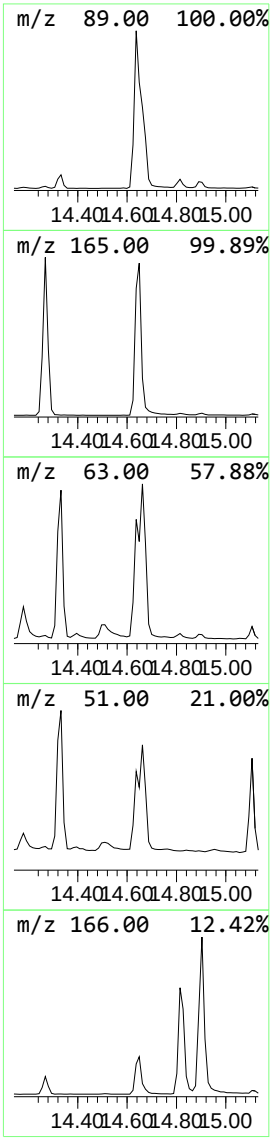
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 Benzene, 1-methyl-2,4-dinitro- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.637	0.09 ng	43874	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	74
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	6-Nitro-m-tolunitrile	162	C8H6N2O2	064113-86-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016651.D
Acq On : 02 Oct 2021 01:36
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

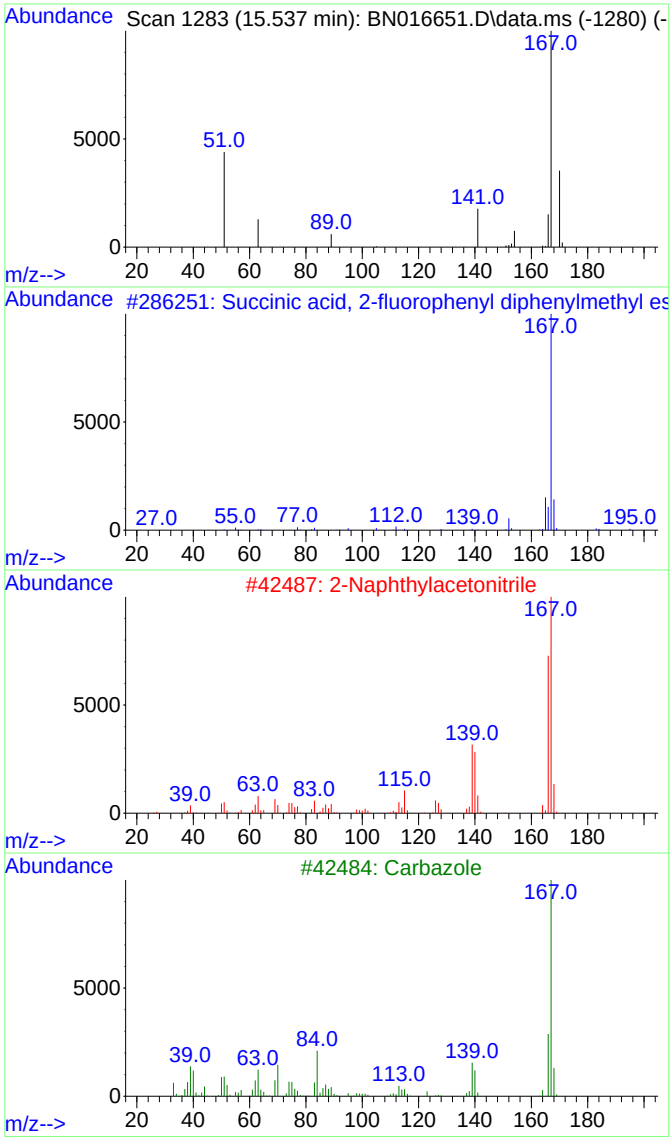
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

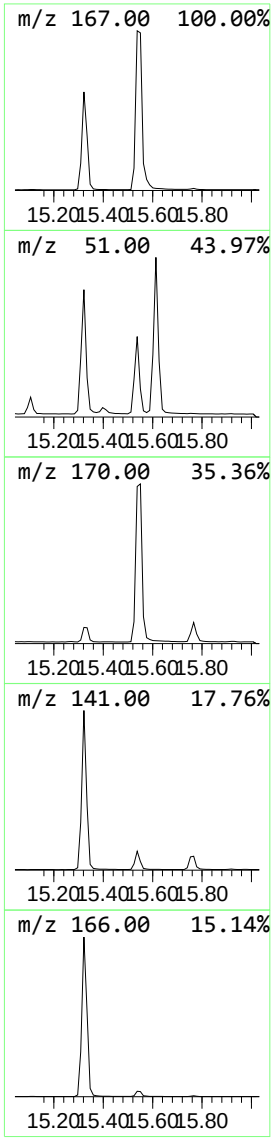
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 Succinic acid, 2-fluorophen... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.537	0.13 ng	62739	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	2-Naphthylacetonitrile	167	C12H9N	007498-57-9	7
3	Carbazole	167	C12H9N	000086-74-8	7
4	Benzaldehyde, 2-hydroxy-5-nitro-	167	C7H5NO4	000097-51-8	5
5	5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	5





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016651.D
Acq On : 02 Oct 2021 01:36
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

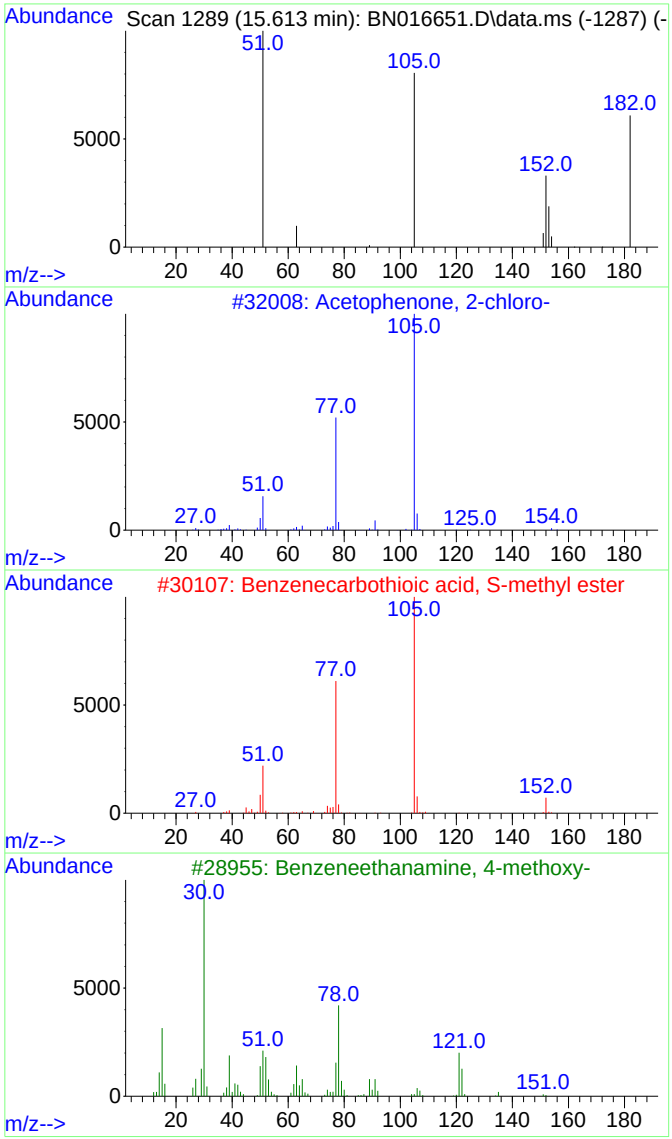
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

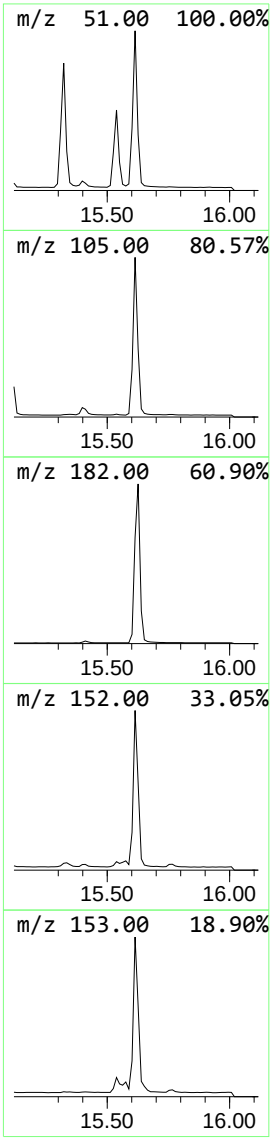
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 Acetophenone, 2-chloro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.614	0.13 ng	65201	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	3
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	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





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016651.D
Acq On : 02 Oct 2021 01:36
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

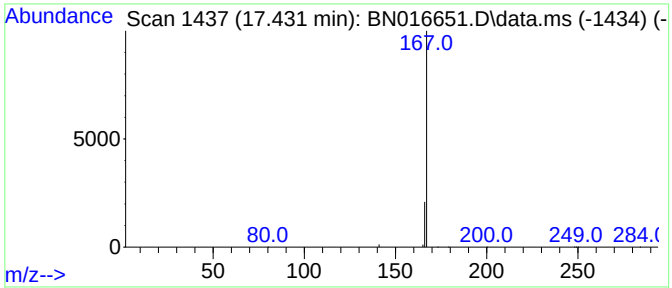
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

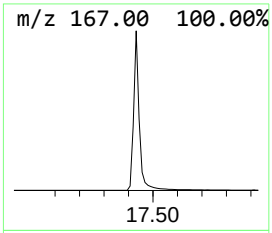
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

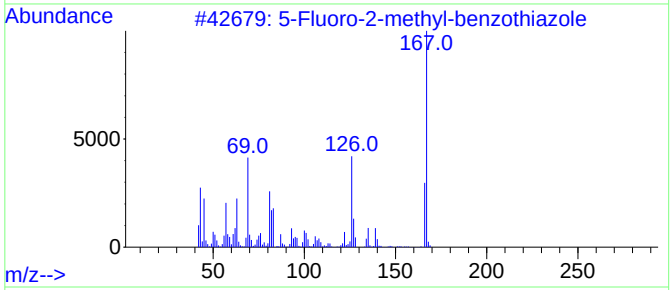
****
Peak Number 18 5-Fluoro-2-methyl-benzothia... Concentration Rank 3

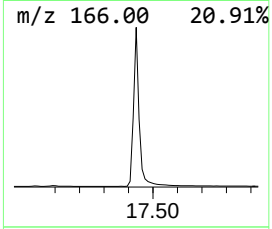
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.431	0.35 ng	140115	Phenanthrene-d10	17.017

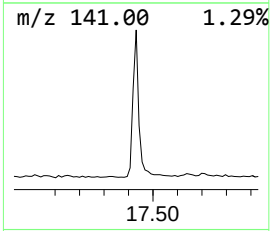
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	5
2	Iodoacetonitrile	167	C2H2IN	000624-75-9	4
3	Cycloundecene, 1-methyl-	166	C12H22	088828-82-4	4
4	1-Cyclopropanecarbonylpiperidin-...	167	C9H13NO2	063463-43-4	4
5	1,3,5-Triazine-2,4-diamine, N,N'...	167	C7H13N5	004150-59-8	4

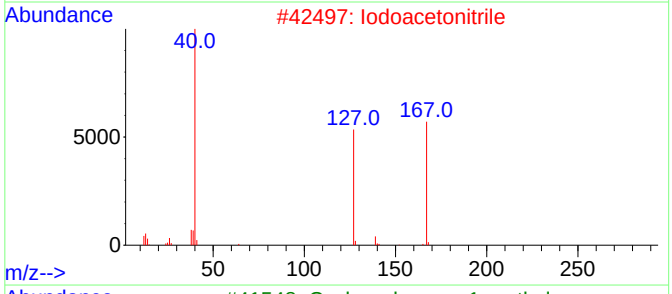


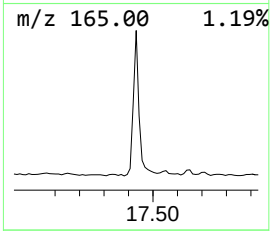


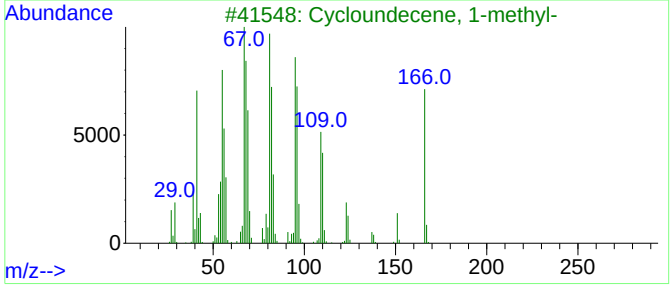


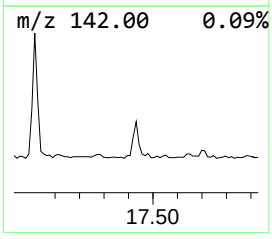












Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016651.D
Acq On : 02 Oct 2021 01:36
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

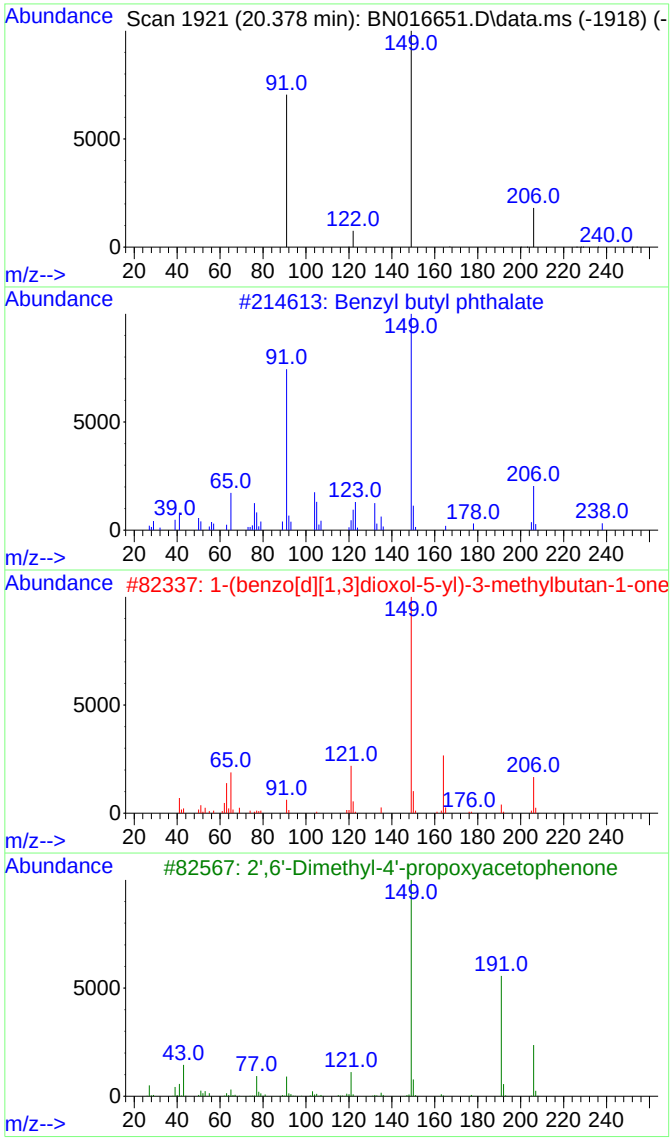
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

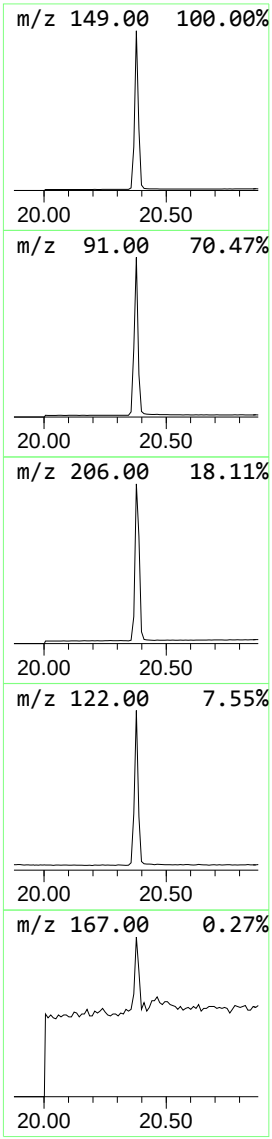
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 Benzyl butyl phthalate Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.378	0.06 ng	63195	Chrysene-d12	21.227

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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Sample : SSTDCCC0.4
Misc :
ALS Vial : 2 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

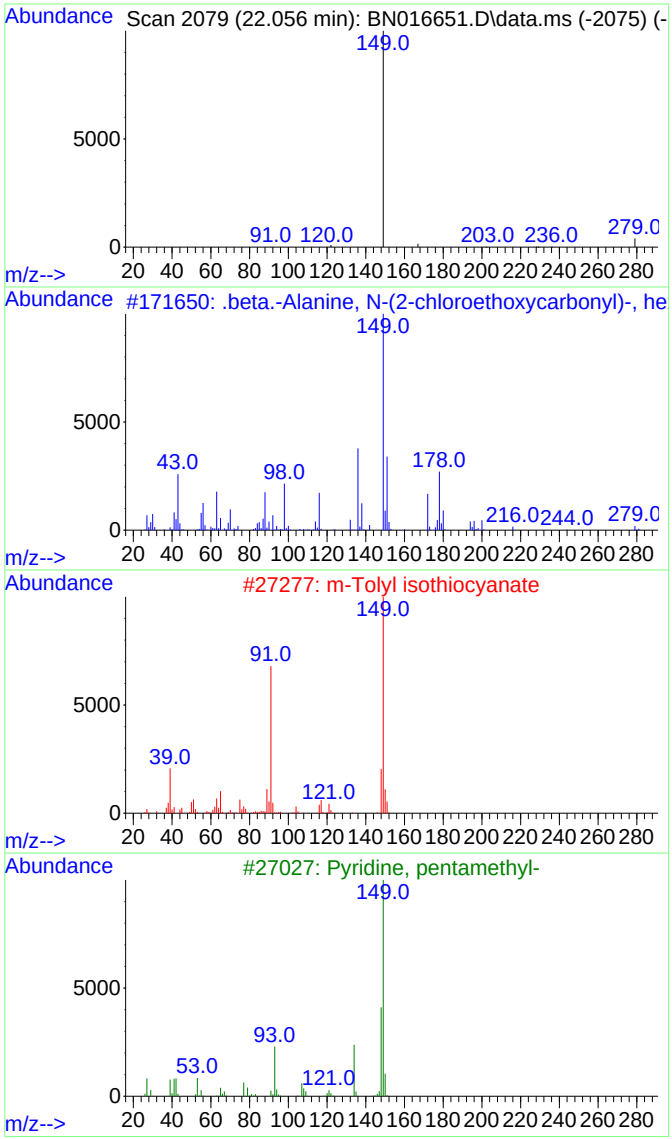
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

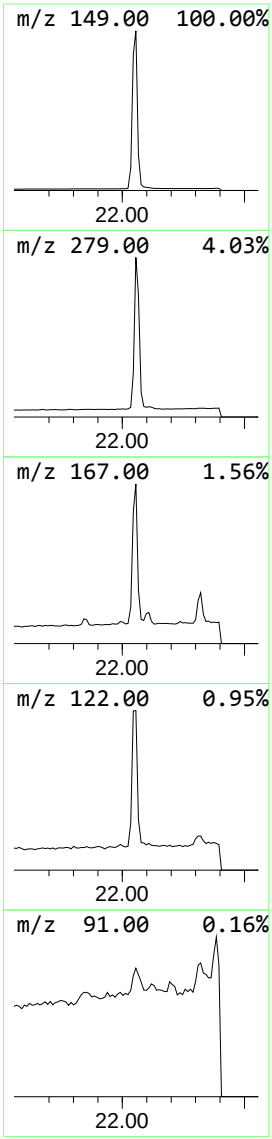
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 .beta.-Alanine, N-(2-chloro... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.056	0.08 ng	88139	Chrysene-d12	21.227

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	Pyridine, pentamethyl-	149	C10H15N	003748-83-2	4
4	Phthalic acid, 7-bromoheptyl oct...	454	C23H35BrO4	1000415-52-2	4
5	Benzene, 1-isothiocyanato-4-methyl-	149	C8H7NS	000622-59-3	4





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016651.D
Acq On : 02 Oct 2021 01:36
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 2 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, ...	6.978	0.1	ng	34614	1	7.642	121041	0.4
Ethene, 1,1-dif...	7.200	0.1	ng	32334	1	7.642	121041	0.4
Thietane	7.522	0.0	ng	15027	1	7.642	121041	0.4
6-Benzothiazola...	7.956	0.4	ng	108049	1	7.642	121041	0.4
Furan, 2,5-dihy...	8.429	0.2	ng	49724	1	7.642	121041	0.4
Fomepizole	9.342	0.2	ng	76529	2	10.406	193787	0.4
5-Aminopyrimidine	9.836	0.1	ng	28103	2	10.406	193787	0.4
p-Chloroaniline	10.571	0.1	ng	58682	2	10.406	193787	0.4
Methane, iodo-	11.709	0.1	ng	25565	2	10.406	193787	0.4
2-Propyl-4-meth...	12.296	0.4	ng	199342	2	10.406	193787	0.4
4-Cyano-5-(meth...	12.695	0.1	ng	29126	3	14.269	195918	0.4
1-Methyl-1,8-di...	12.759	0.1	ng	25549	3	14.269	195918	0.4
Naphthalene, 2-...	13.139	0.3	ng	132849	3	14.269	195918	0.4
Benzene, 2-meth...	13.850	0.1	ng	28394	3	14.269	195918	0.4
Benzene, 1-meth...	14.637	0.1	ng	43874	3	14.269	195918	0.4
Succinic acid, ...	15.537	0.1	ng	62739	3	14.269	195918	0.4
Acetophenone, 2...	15.614	0.1	ng	65201	3	14.269	195918	0.4
5-Fluoro-2-meth...	17.431	0.3	ng	140115	4	17.017	161155	0.4
Benzyl butyl ph...	20.378	0.1	ng	63195	5	21.227	434963	0.4
.beta.-Alanine,...	22.056	0.1	ng	88139	5	21.227	434963	0.4