LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016631.D
Acq On : 01 Oct 2021 11:22
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 34 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: BN016631.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.253	16	19	20	rBV	7497	10511	1.84%	0.126%
2	3.281	20	22	45	rVB	5509	27566	4.81%	0.331%
3	3.594	51	56	77	rVB	6569	31097	5.43%	0.373%
4	5.254	231	236	249	rBV	15495	60090	10.49%	0.722%
5	6.821	401	406	418	rBV	25975	65926	11.51%	0.792%
6	6.978	418	423	429	rVV	18598	41306	7.21%	0.496%
7	7.080	429	434	440	rVV	37721	77141	13.47%	0.926%
8	7.200	440	447	460	rVB	12868	34792	6.08%	0.418%
9	7.522	478	482	489	rVB	6946	15673	2.74%	0.188%
10	7.642	490	495	512	rVB2	52063	127030	22.18%	1.525%
11	7.956	524	529	539	rVB2	50864	113621	19.84%	1.364%
12	8.168	547	552	557	rBV	3321	8047	1.41%	0.097%
13	8.429	571	577	587	rBV3	22076	54151	9.46%	0.650%
14	8.695	595	598	601	rBV	4953	9124	1.59%	0.110%
15	8.784	601	605	607	rBV	36938	79831	13.94%	0.959%
16	8.822	607	608	616	rVB	29344	43493	7.60%	0.522%
17	9.342	646	649	660	rBV	53022	86759	15.15%	1.042%
18	9.532	660	664	666	rVV	3652	7305	1.28%	0.088%
19	9.595	666	669	679	rVB	9440	16840	2.94%	0.202%
20	9.836	685	688	700	rVB	17406	29329	5.12%	0.352%
21	10.064	702	706	709	rBV	4227	8775	1.53%	0.105%
22	10.406	729	733	735	rBV	113497	202663	35.39%	2.434%
23	10.457	735	737	741	rVV	117214	190558	33.28%	2.288%
24	10.571	743	746	756	rVV	29690	67477	11.78%	0.810%
25	10.749	756	760	763	rVB	35431	59279	10.35%	0.712%
26	11.306	801	804	814	rVB	2471	5781	1.01%	0.069%
27	11.709	853	865	889	rBV	14793	27394	4.78%	0.329%
28	12.002	921	931	940	rBV	59275	97726	17.07%	1.174%
29	12.078	940	948	972	rVV	136037	217754	38.03%	2.615%
30	12.300	988	998	1021	rVV	132595	210191	36.71%	2.524%
31	12.695	1056	1059	1062	rBV	18866	31428	5.49%	0.377%
32	12.771	1062	1065	1071	rVB	14158	27615	4.82%	0.332%
33	12.886	1071	1074	1078	rBV	116506	206777	36.11%	2.483%
34	13.139	1091	1094	1097	rVB	85282	132289	23.10%	1.589%
35	13.736	1138	1141	1143	rBV	12861	17879	3.12%	0.215%
36	13.850	1147	1150	1153	rVB	20435	30301	5.29%	0.364%

LSC Area Percent Report

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Acq On : 01 Oct 2021 11:22
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Sample : SSTDCCC0.4
Misc :
ALS Vial : 34 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	103890	164907	28.80%	1.980%
38	14.268	1180	1183	1186	rBV	145314	211039	36.85%	2.534%
39	14.332	1186	1188	1191	rVB	178278	250066	43.67%	3.003%
40	14.636	1209	1212	1220	rBV3	17795	46844	8.18%	0.563%
41	14.814	1224	1226	1230	rBV	5929	10622	1.85%	0.128%
42	14.903	1230	1233	1236	rBV	8666	12599	2.20%	0.151%
43	15.106	1246	1249	1252	rBV	9632	12178	2.13%	0.146%
44	15.322	1263	1266	1270	rBV2	234304	367196	64.12%	4.409%
45	15.410	1270	1273	1280	rVV2	3618	9337	1.63%	0.112%
46	15.537	1280	1283	1287	rVV	37231	66437	11.60%	0.798%
47	15.613	1287	1289	1298	rVV2	44717	70266	12.27%	0.844%
48	15.766	1298	1301	1311	rVB2	14810	24940	4.36%	0.299%
49	16.226	1334	1338	1341	rBV2	62783	94991	16.59%	1.141%
50	16.324	1343	1346	1350	rVB	48822	75514	13.19%	0.907%
51	16.506	1358	1361	1372	rBV	24517	38216	6.67%	0.459%
52	16.677	1372	1375	1384	rBV	25100	43150	7.54%	0.518%
53	17.017	1400	1403	1405	rBV	100073	164572	28.74%	1.976%
54	17.066	1405	1407	1410	rVV	156773	227052	39.65%	2.726%
55	17.151	1411	1414	1434	rVV	118215	194753	34.01%	2.339%
56	17.431	1434	1437	1453	rVV	92976	148302	25.90%	1.781%
57	18.015	1482	1485	1498	rVB	6116	8830	1.54%	0.106%
58	19.063	1686	1696	1699	rBV	121423	168752	29.47%	2.026%
59	19.092	1699	1702	1738	rVB	196387	270264	47.20%	3.245%
60	19.460	1767	1776	1813	rBV	195823	268172	46.83%	3.220%
61	19.678	1813	1820	1858	rVB	113117	148229	25.89%	1.780%
62	20.378	1918	1921	1924	rBV	56903	69187	12.08%	0.831%
63	21.163	1993	1995	1997	rBV	56085	79317	13.85%	0.952%
64	21.217	1997	2000	2003	rVV2	215701	440773	76.97%	5.293%
65	21.270	2003	2005	2017	rVB	216351	284249	49.64%	3.413%
66	22.056	2076	2079	2082	rBV	79971	99847	17.44%	1.199%
67	22.806	2217	2229	2235	rBV	136802	226479	39.55%	2.720%
68	22.851	2235	2242	2280	rVB	151135	262113	45.77%	3.148%
69	23.381	2385	2397	2416	rBV	97132	207198	36.18%	2.488%
70	23.484	2416	2427	2482	rVB	105678	220285	38.47%	2.645%
71	24.087	2593	2603	2623	rBV	7041	13940	2.43%	0.167%
72	24.857	2817	2828	2850	rVB	7424	16591	2.90%	0.199%
73	25.771	3067	3095	3196	rBV3	150770	572628	100.00%	6.876%
74	26.452	3272	3294	3346	rBV	81651	264288	46.15%	3.174%

Sum of corrected areas: 8327642

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

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Misc :
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Instrument :
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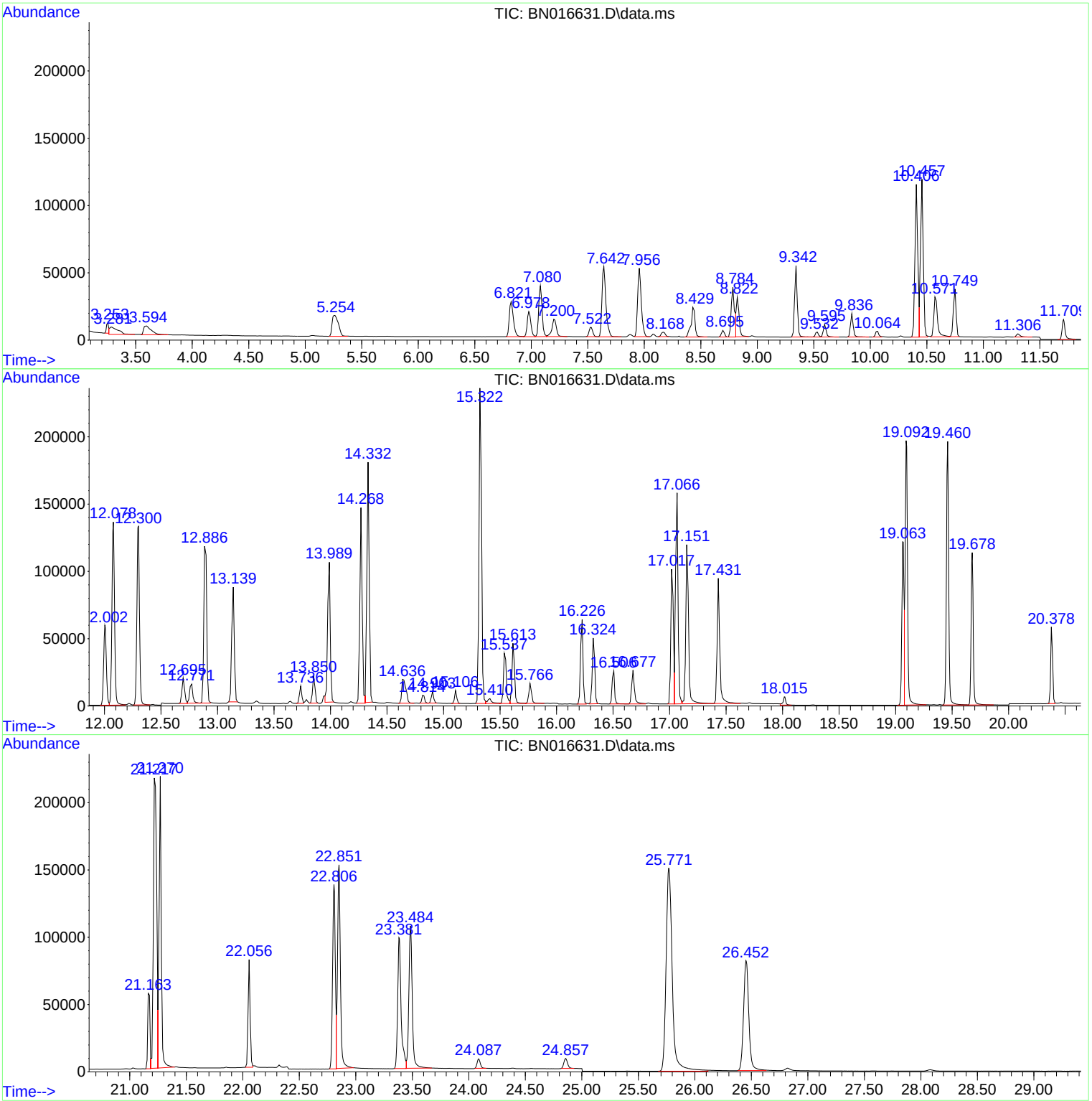
LabSampleId :
SSTDCCC0.4

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



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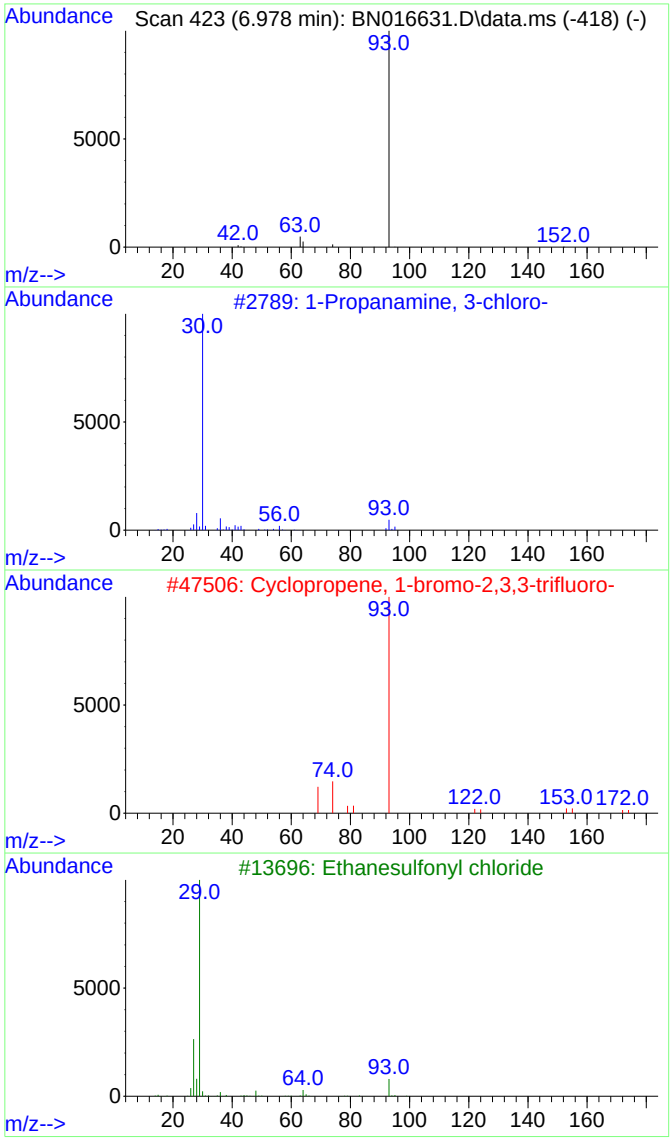
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

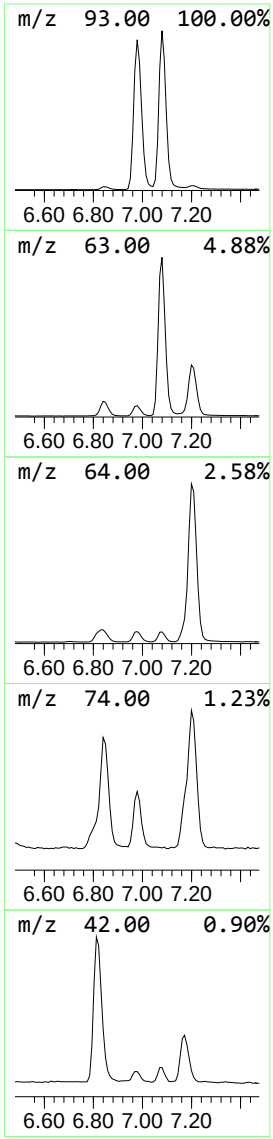
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1-Propanamine, 3-chloro- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.978	0.13 ng	41306	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 : BN016631.D
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Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

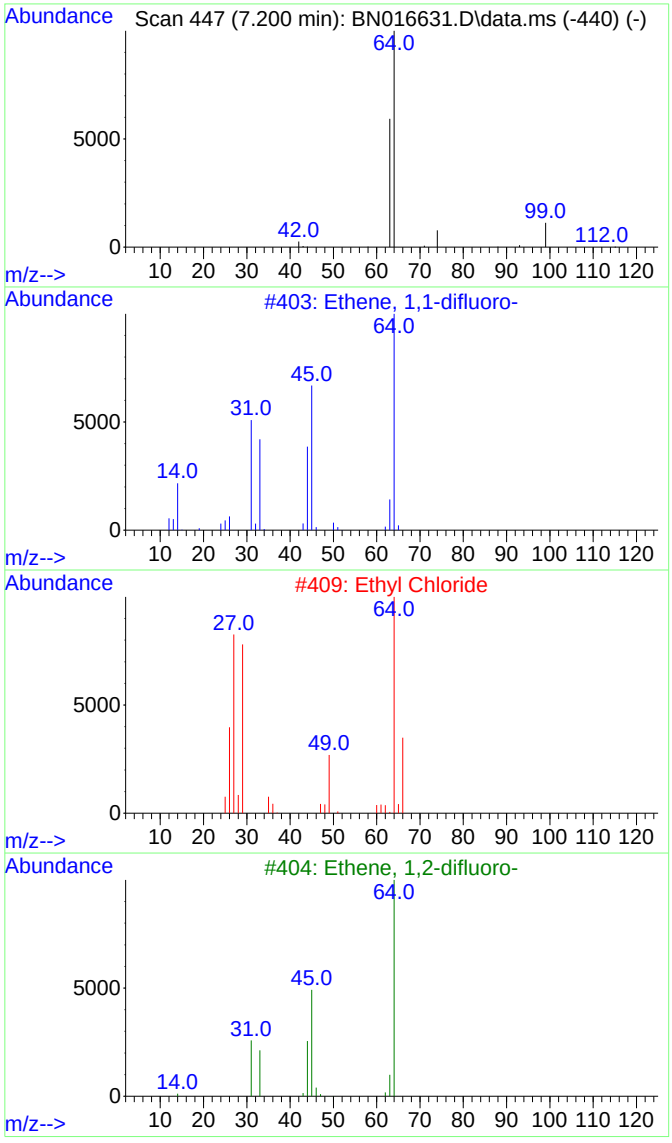
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

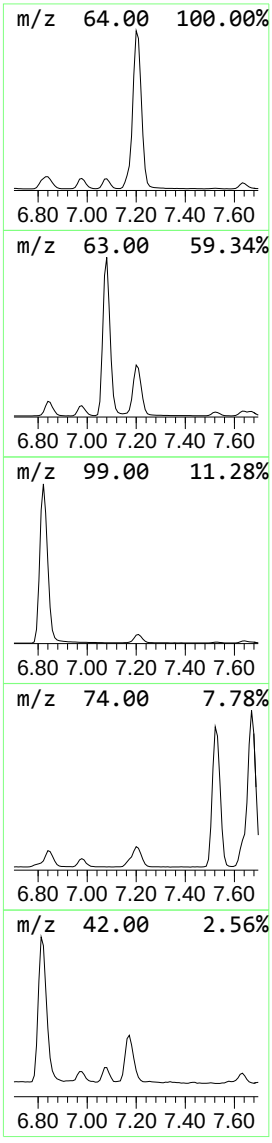
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.200	0.11 ng	34792	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\
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Misc :
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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

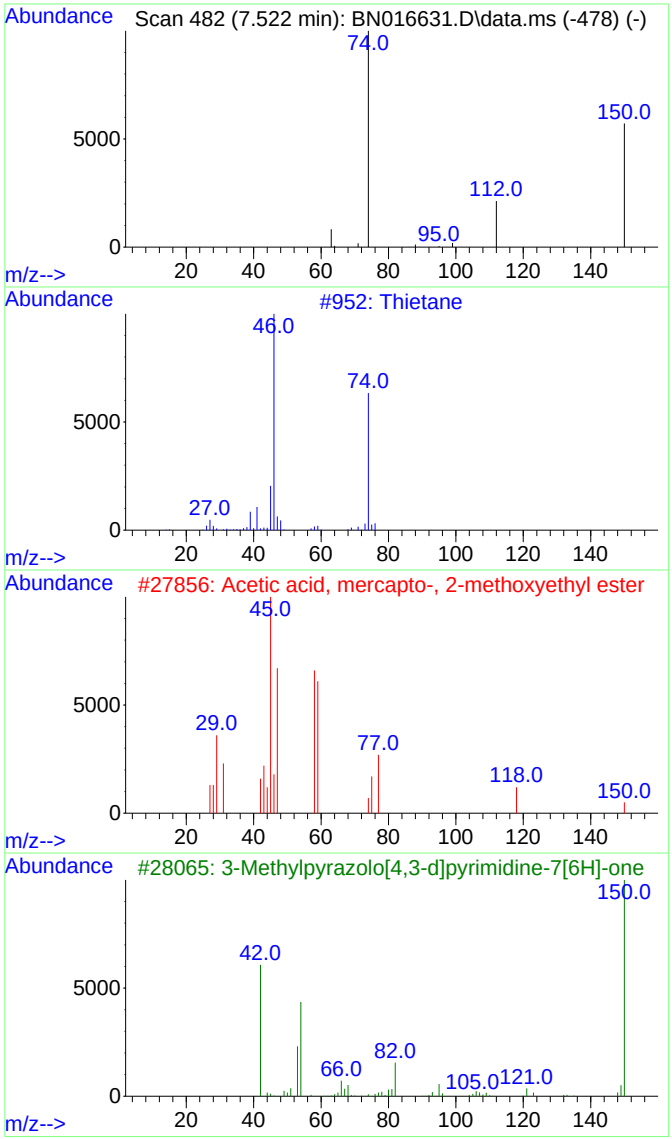
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

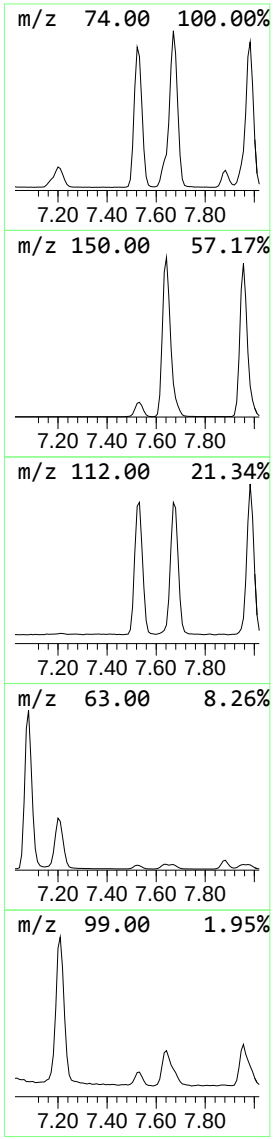
****

Peak Number 3 Thietane Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.522	0.05 ng	15673	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





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Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

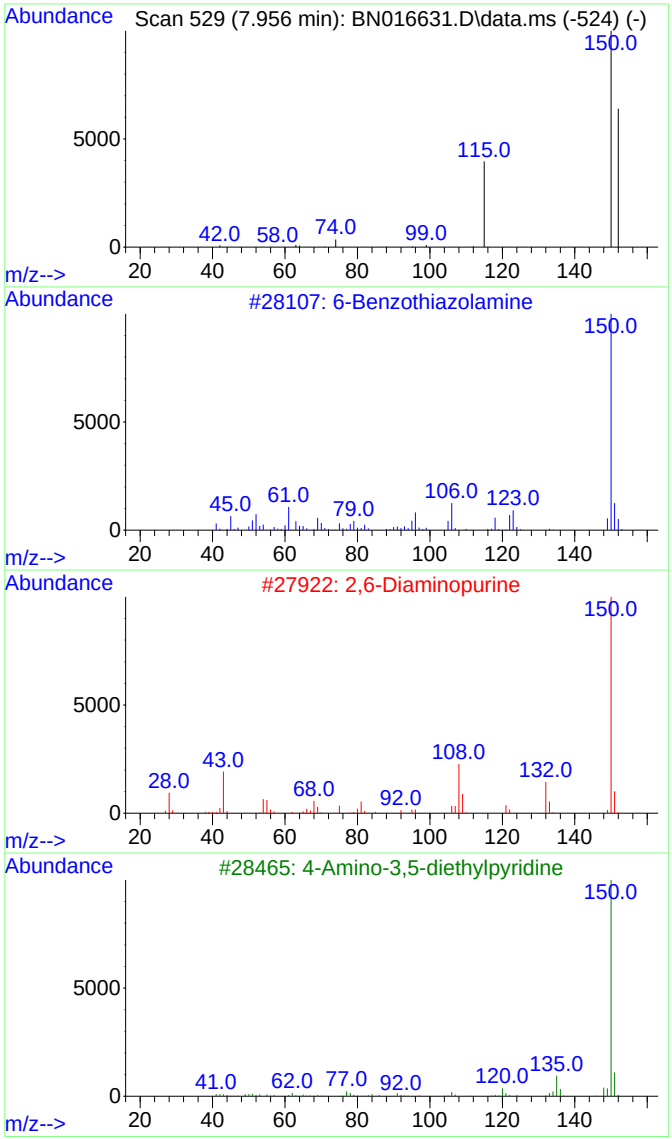
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

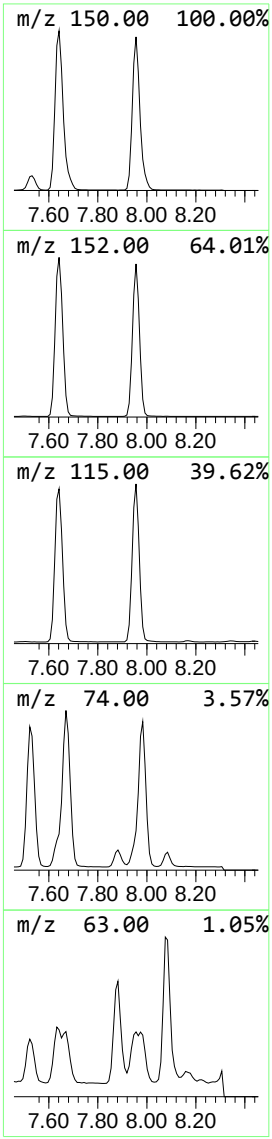
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.956	0.36 ng	113621	1,4-Dichlorobenzene-d4	7.642

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





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Misc :
ALS Vial : 34 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

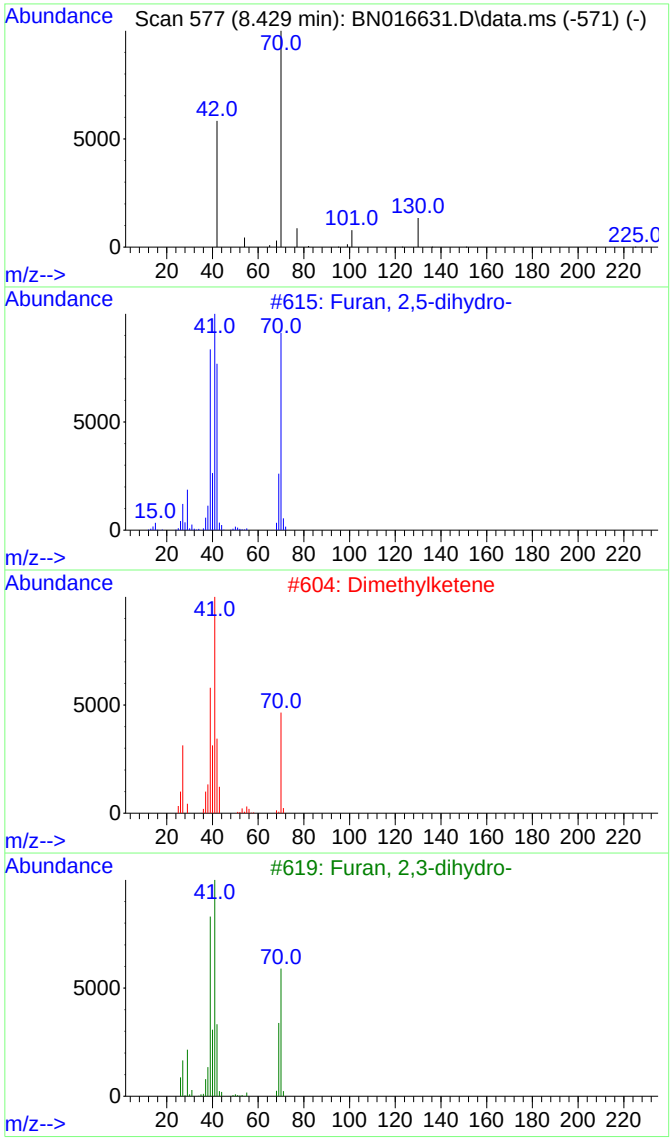
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

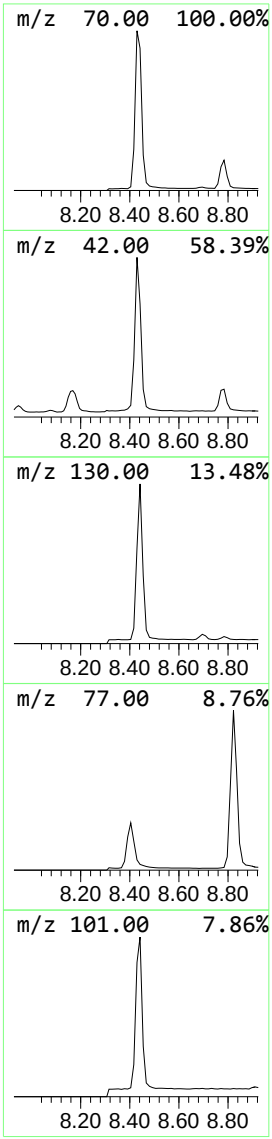
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.429	0.17 ng	54151	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	Dimethylketene	70	C4H6O	000598-26-5	5
3	Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	5
4	1-Oxa-3,4-diazacyclopentadiene	70	C2H2N2O	000288-99-3	4
5	1-Propanamine, N-nitroso-N-propyl-	130	C6H14N2O	000621-64-7	4





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ALS Vial : 34 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

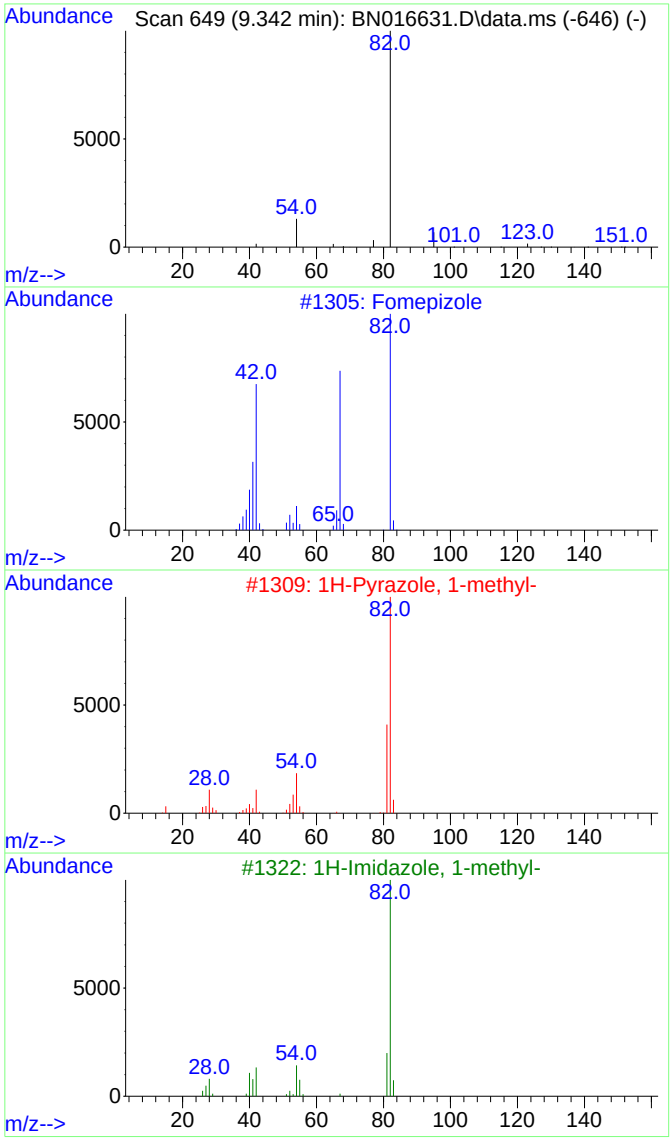
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

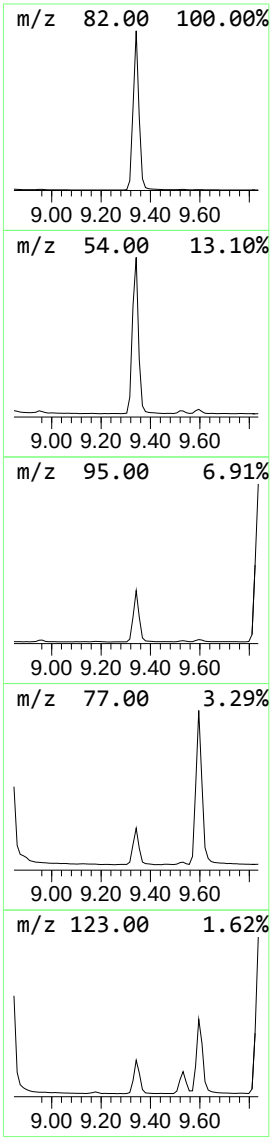
****

Peak Number 6 Fomepizole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.342	0.17 ng	86759	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





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016631.D
Acq On : 01 Oct 2021 11:22
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 34 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

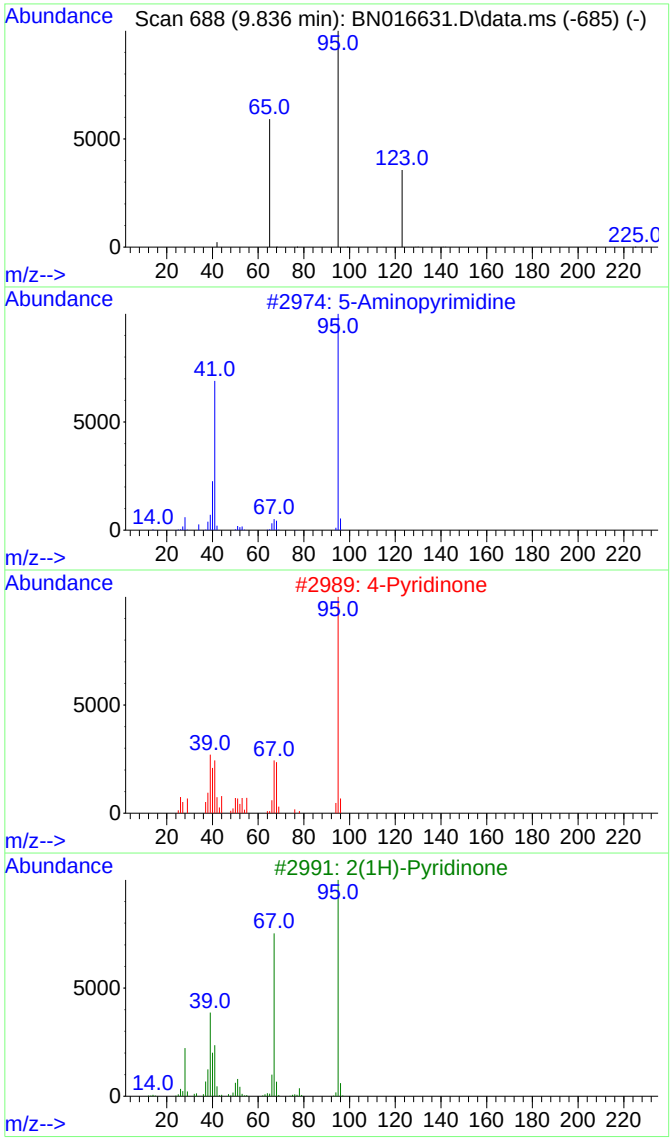
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

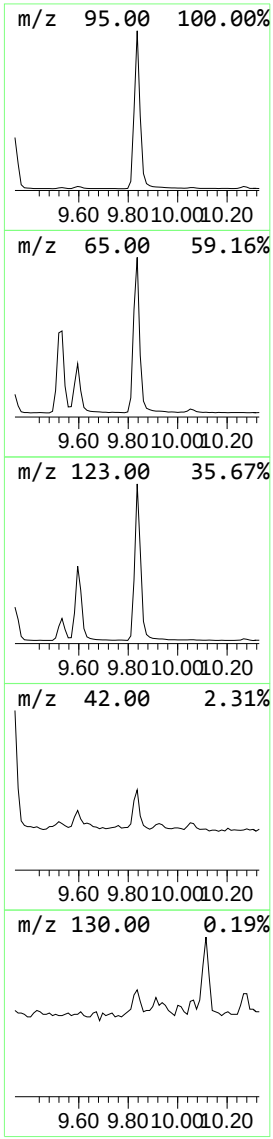
****

Peak Number 7 5-Aminopyrimidine Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.836	0.06 ng	29329	Naphthalene-d8	10.406

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





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Data File : BN016631.D
Acq On : 01 Oct 2021 11:22
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 34 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

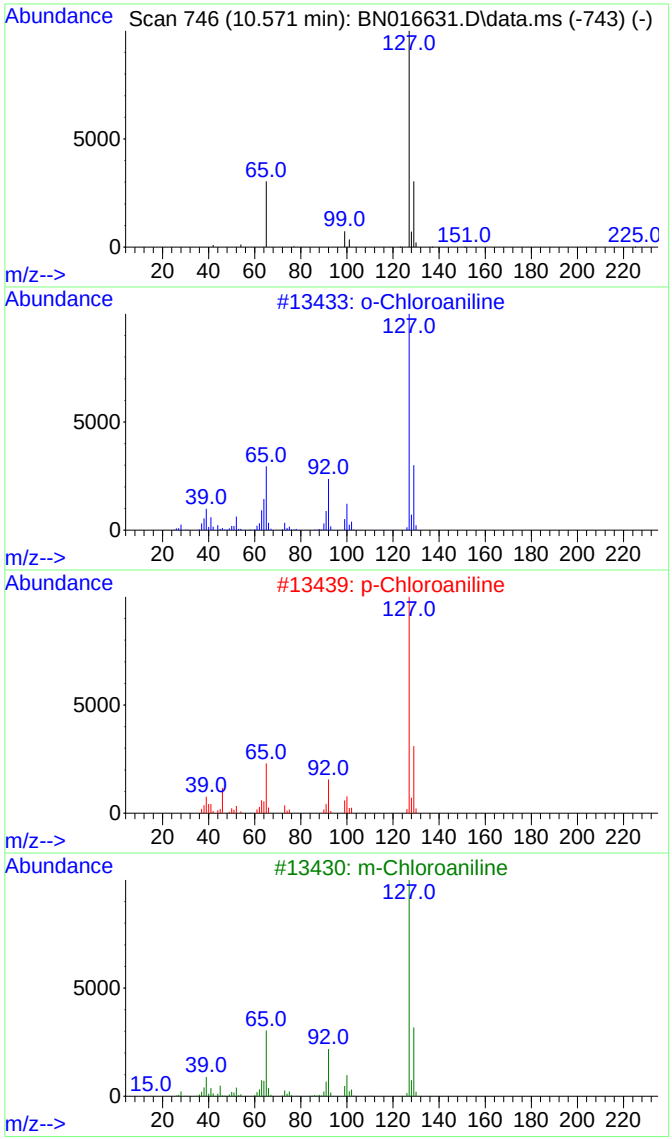
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

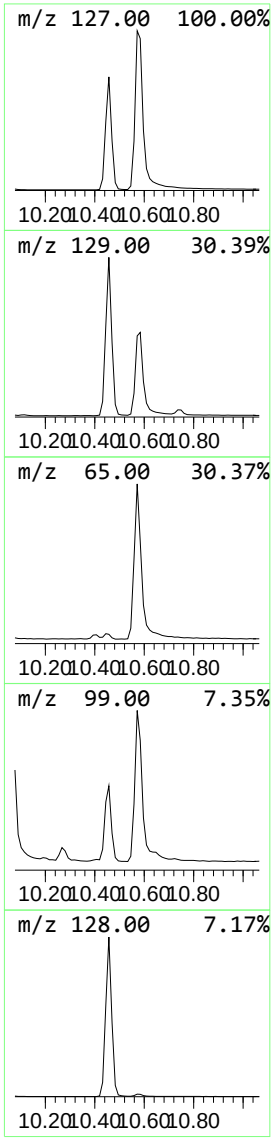
****

Peak Number 8 o-Chloroaniline Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.571	0.13 ng	67477	Naphthalene-d8	10.406

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





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Acq On : 01 Oct 2021 11:22
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

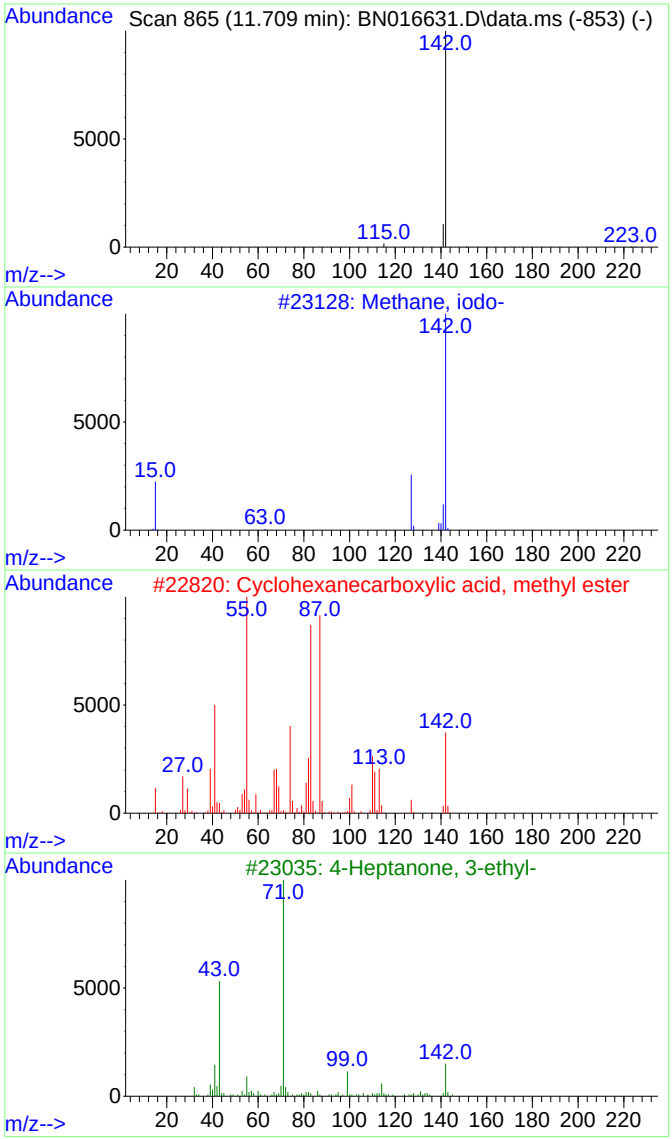
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

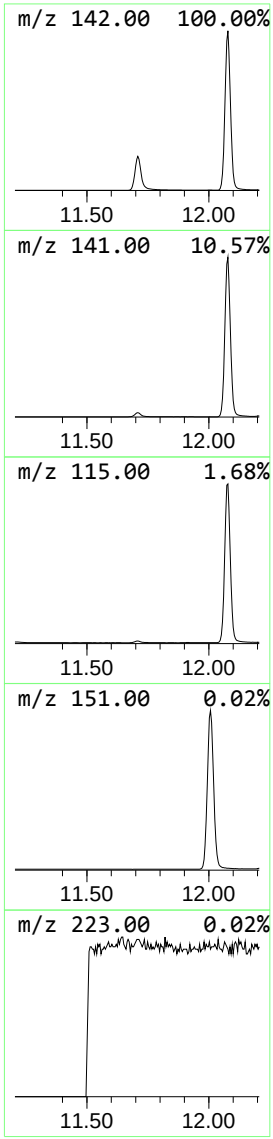
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.709	0.05 ng	27394	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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Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDCCC0.4

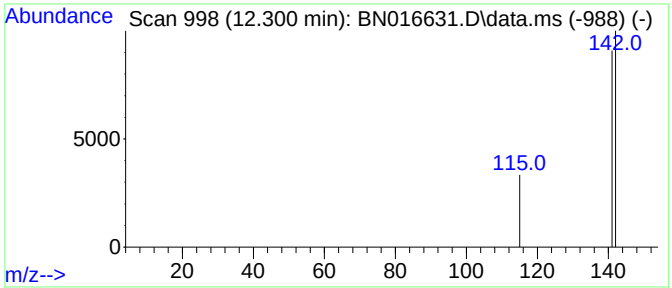
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

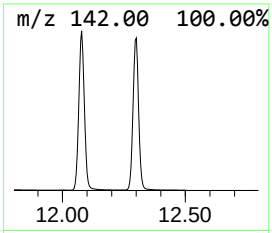
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

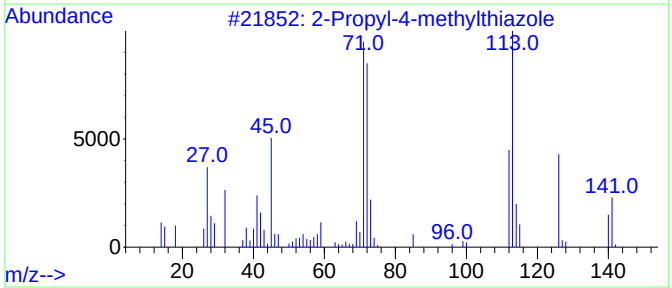
****
Peak Number 10 2-Propyl-4-methylthiazole Concentration Rank 1

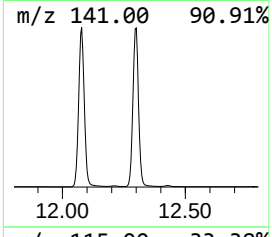
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.300	0.41 ng	210191	Naphthalene-d8	10.406

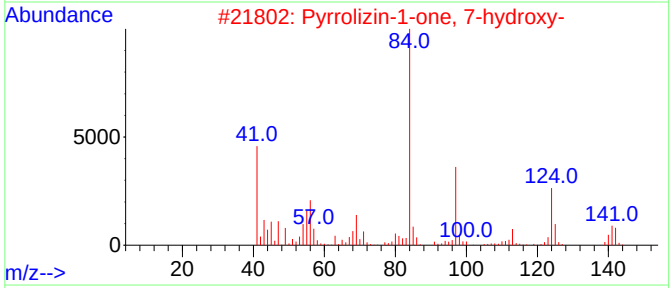
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propyl-4-methylthiazole	141	C7H11NS	052414-87-6	4
2	Pyrrolizin-1-one, 7-hydroxy-	141	C7H11NO2	1000125-96-2	3
3	Cyclopentanecarboxylic acid, eth...	142	C8H14O2	1000375-86-4	3
4	2-Propionylthiazole	141	C6H7NOS	043039-98-1	3
5	2,4(1H,3H)-Pyrimidinedione, 6-am...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

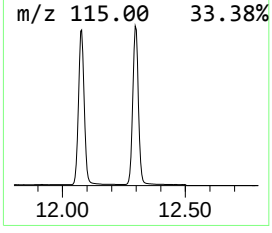


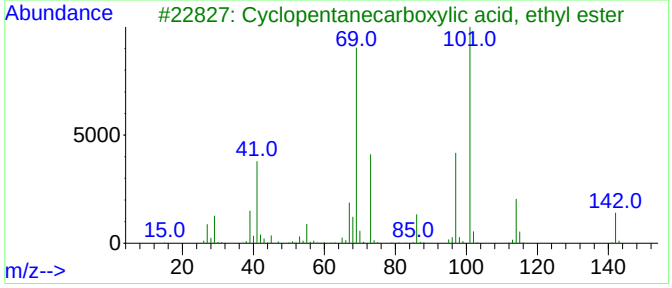












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Data File : BN016631.D
Acq On : 01 Oct 2021 11:22
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

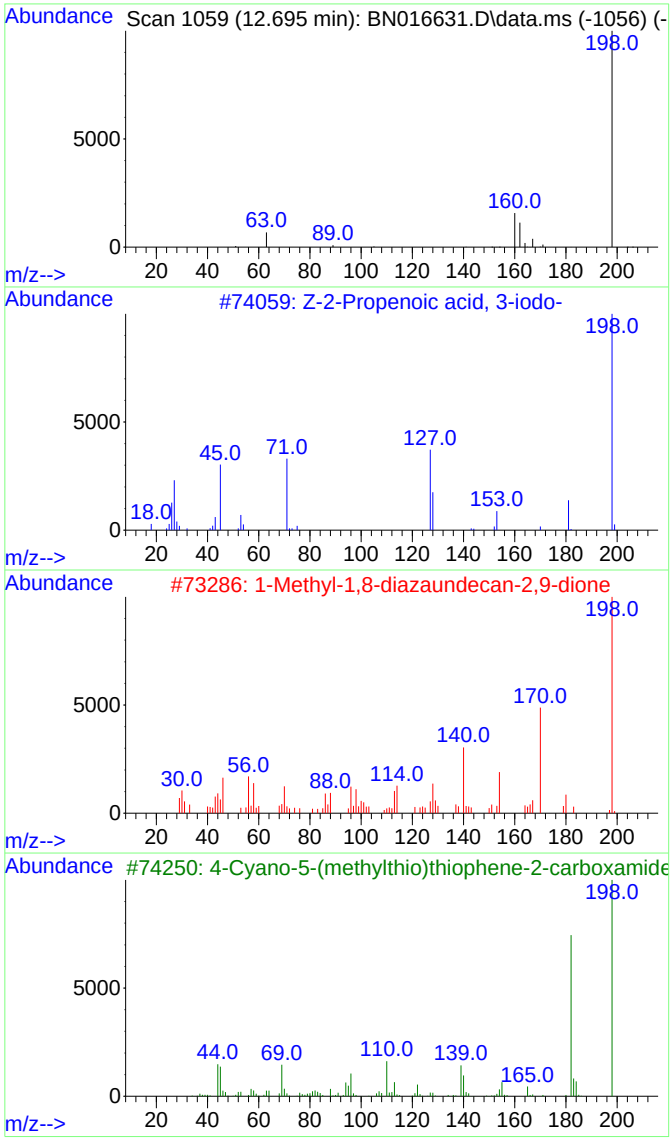
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

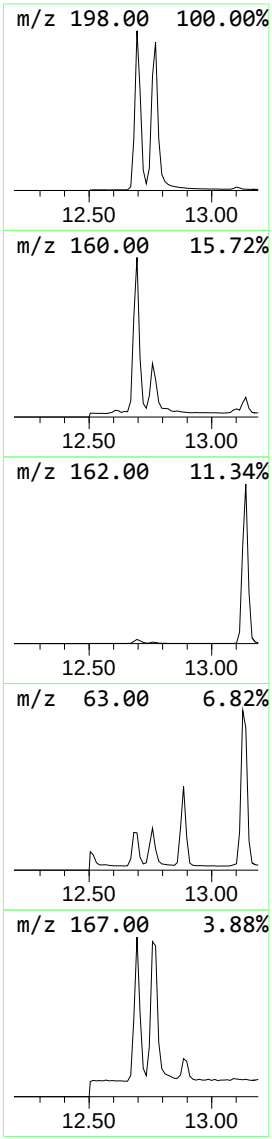
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Z-2-Propenoic acid, 3-iodo- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.695	0.06 ng	31428	Acenaphthene-d10	14.269

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





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Data File : BN016631.D
Acq On : 01 Oct 2021 11:22
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

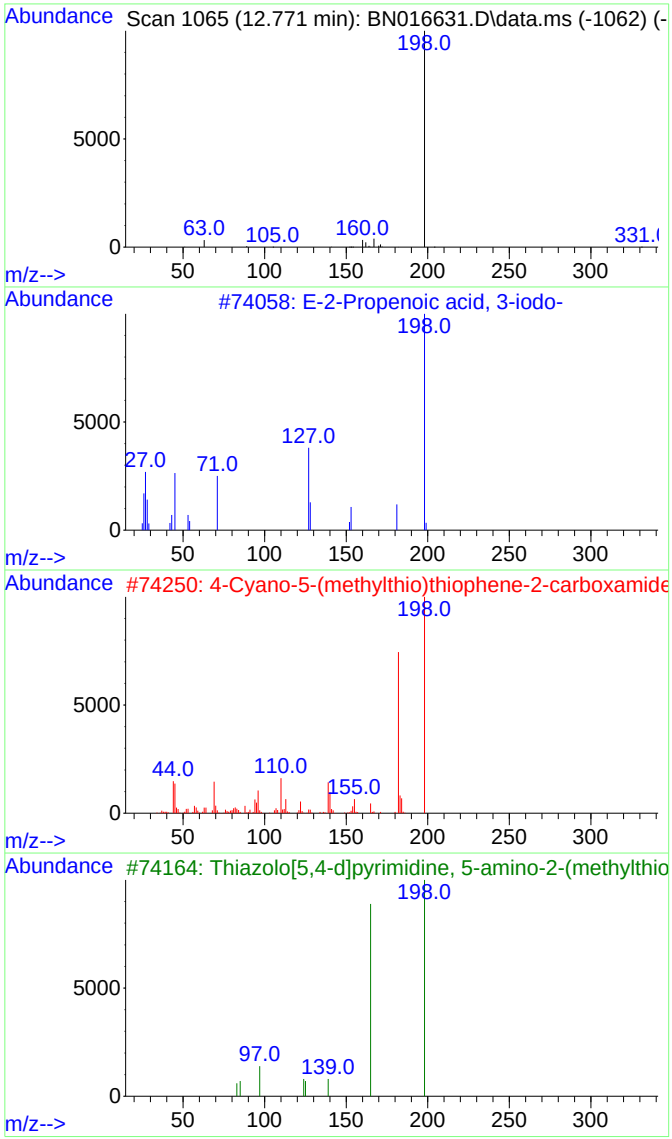
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

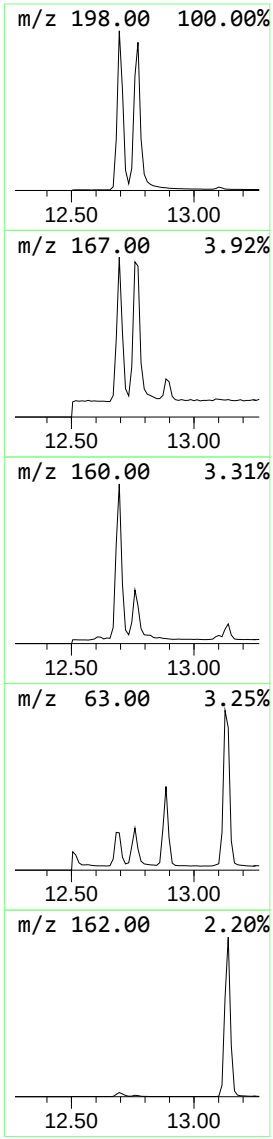
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 E-2-Propenoic acid, 3-iodo- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.771	0.05 ng	27615	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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Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

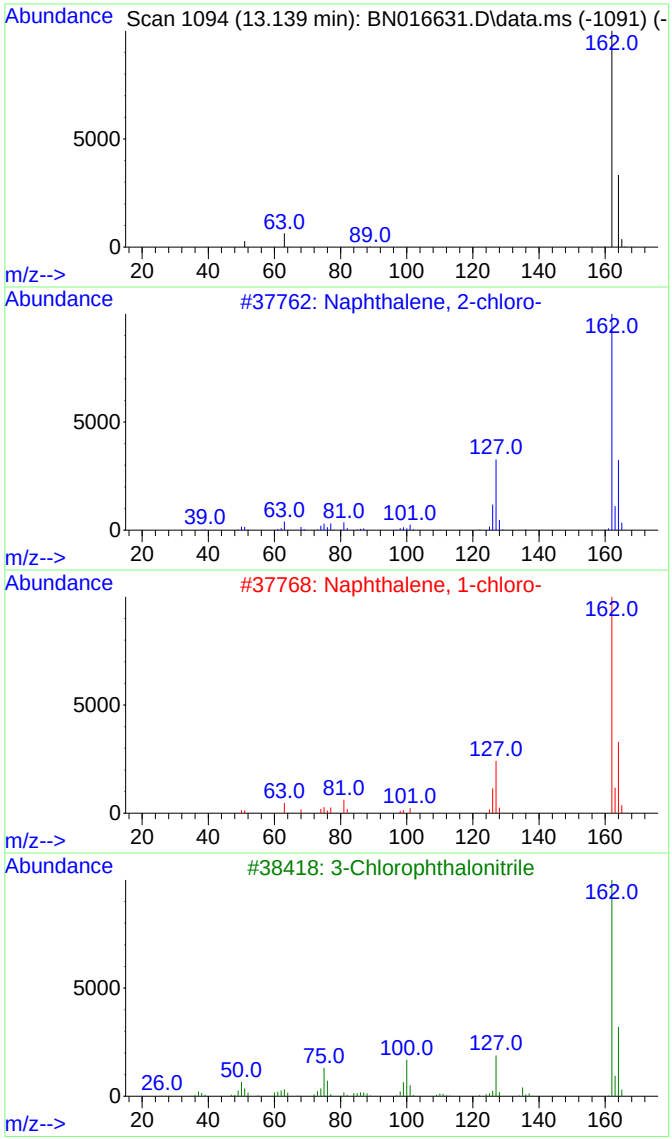
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

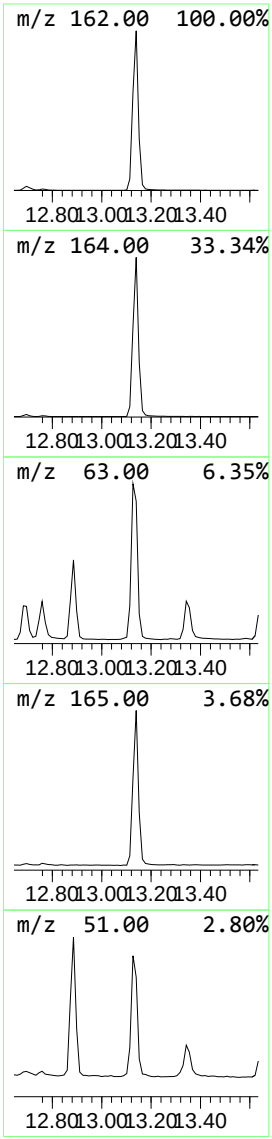
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.139	0.25 ng	132289	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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Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 34 Sample Multiplier: 1

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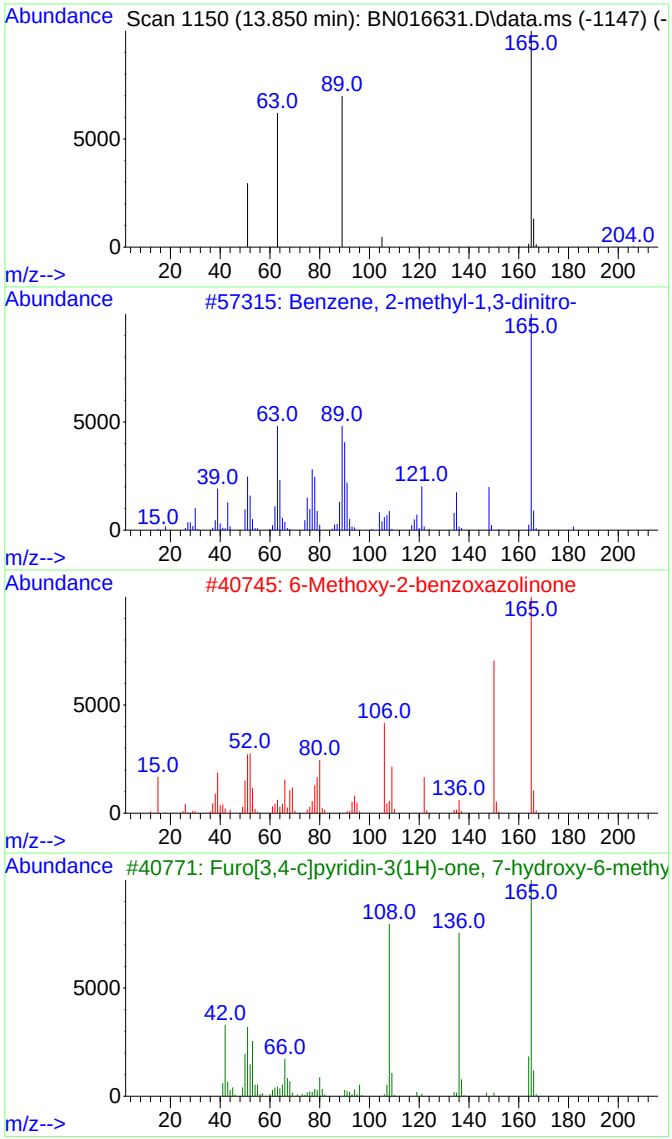
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

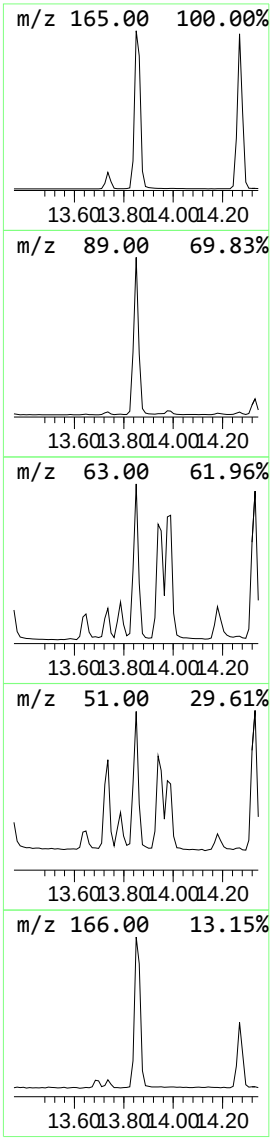
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.850	0.06 ng	30301	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-Methoxy-2-benzoxazolinone	165	C8H7NO3	000532-91-2	9
3	Furo[3,4-c]pyridin-3(1H)-one, 7-...	165	C8H7NO3	004543-56-0	9
4	7-Hydroxy-2,4-dihydro-1,4-benzox...	165	C8H7NO3	067193-97-9	9
5	Furo[3,4-c]pyridin-1(3H)-one, 7-...	165	C8H7NO3	004753-19-9	9





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Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

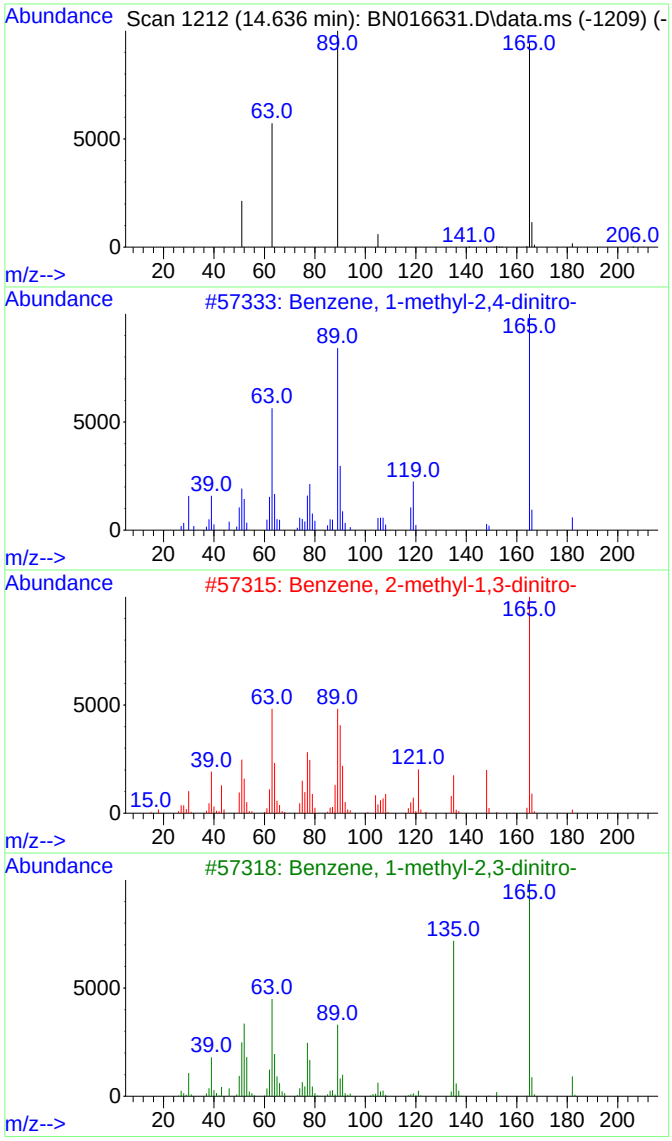
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

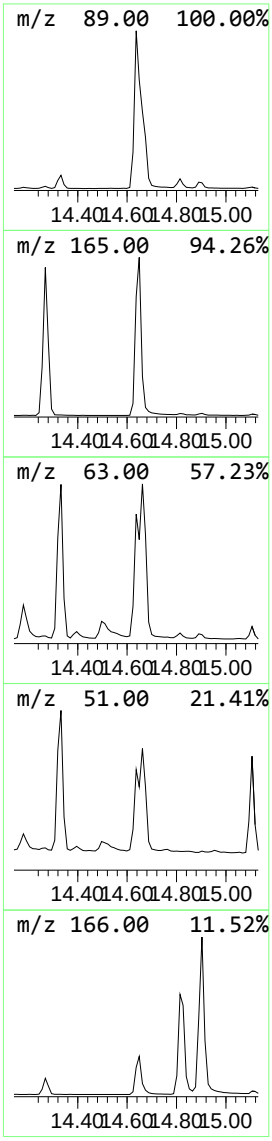
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 Benzene, 1-methyl-2,4-dinitro- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.636	0.09 ng	46844	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	Benzene, 1-methyl-2,3-dinitro-	182	C7H6N2O4	000602-01-7	17
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 : 34 Sample Multiplier: 1

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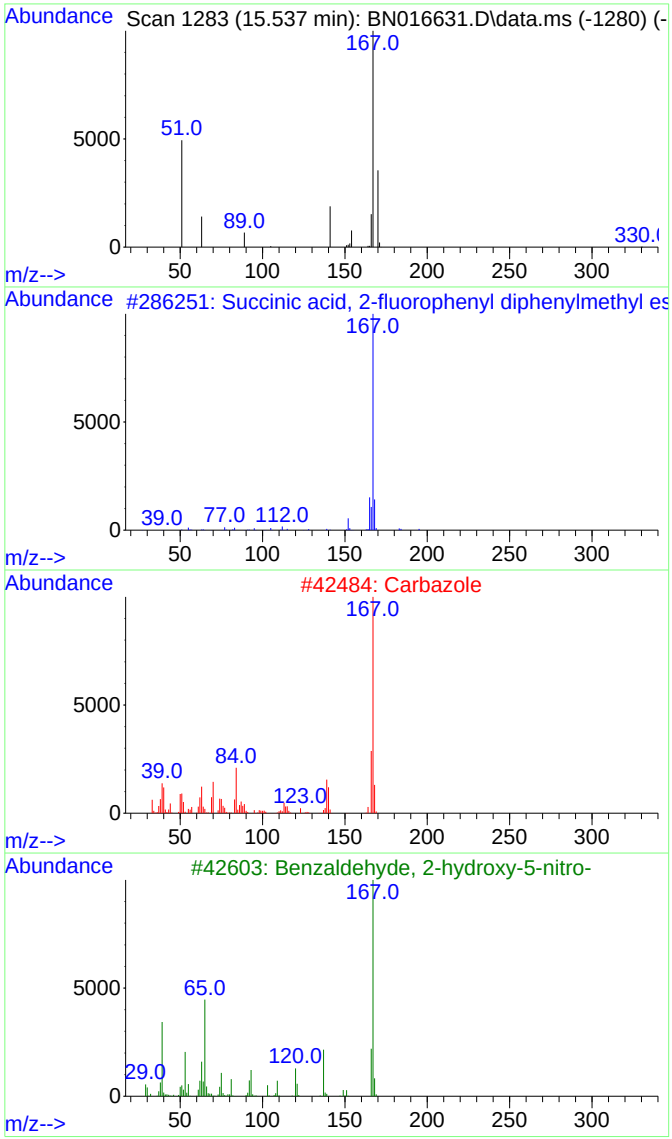
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

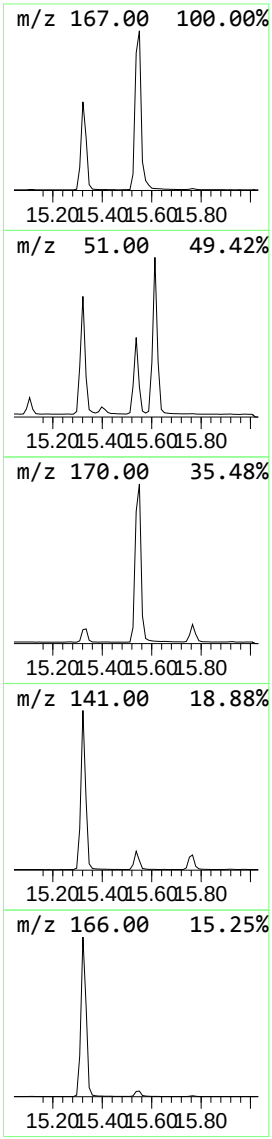
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 Succinic acid, 2-fluorophen... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.537	0.13 ng	66437	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	Benzaldehyde, 2-hydroxy-5-nitro-	167	C7H5NO4	000097-51-8	5
4	5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	5
5	2-Azafluorene	167	C12H9N	000244-40-6	4





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Sample : SSTDCCC0.4
Misc :
ALS Vial : 34 Sample Multiplier: 1

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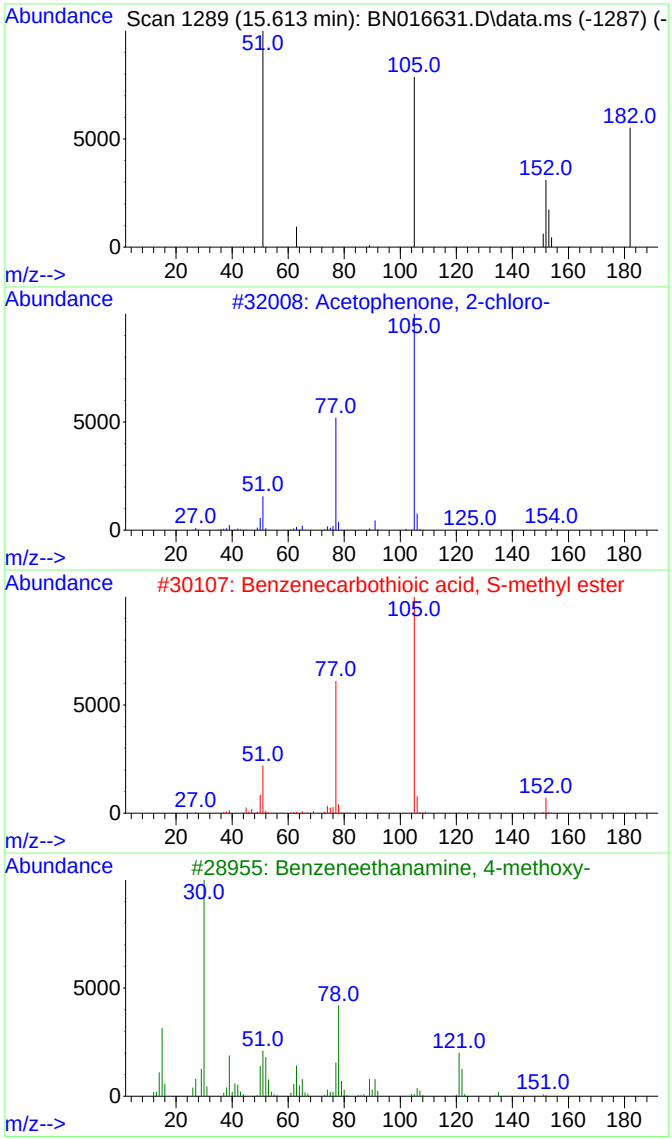
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

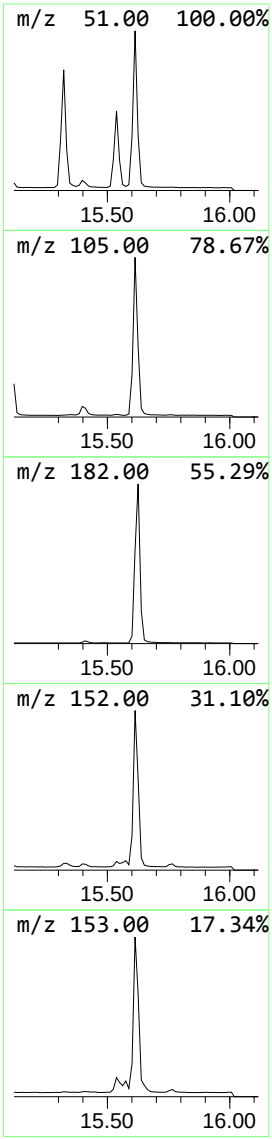
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.613	0.13 ng	70266	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





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Acq On : 01 Oct 2021 11:22
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

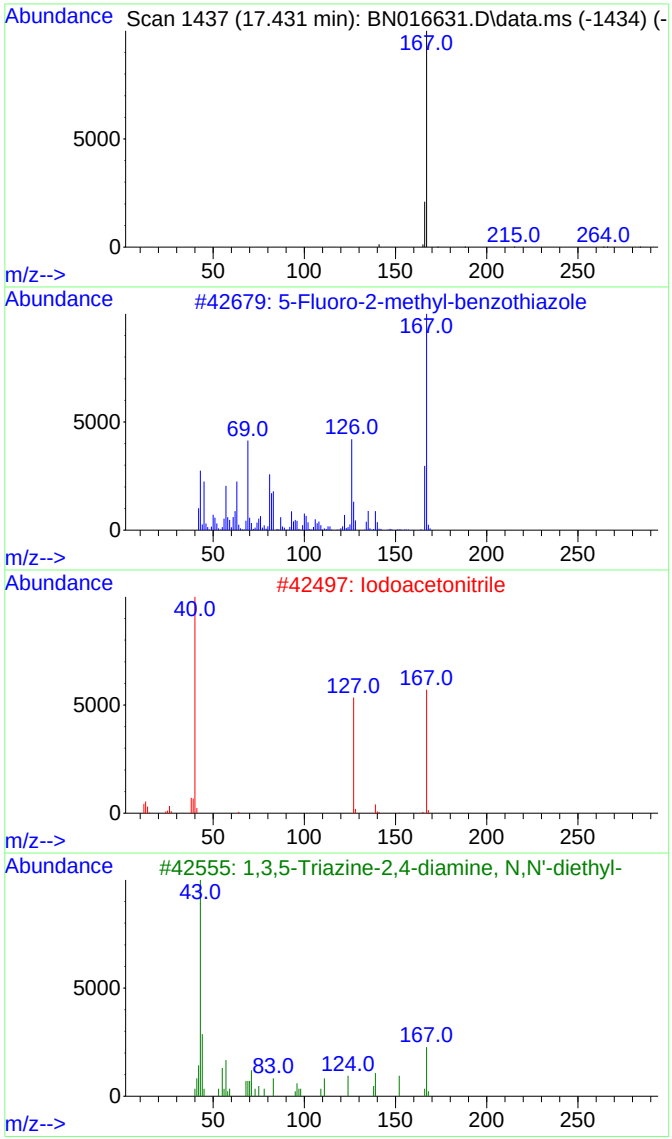
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

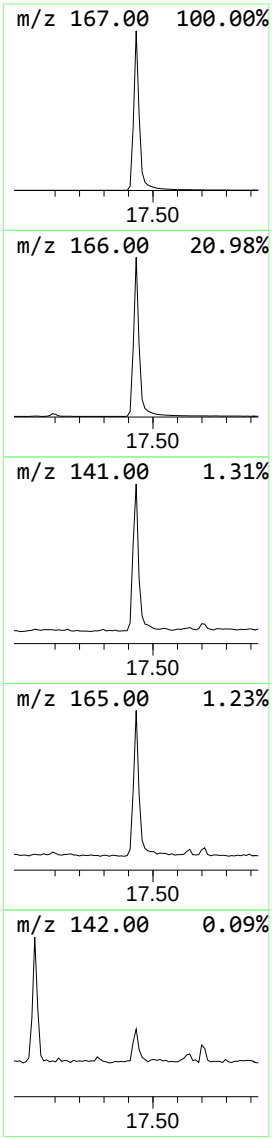
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.431	0.36 ng	148302	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	1,3,5-Triazine-2,4-diamine, N,N'...	167	C7H13N5	004150-59-8	4
4	1-Cyclopropanecarbonylpiperidin-...	167	C9H13NO2	063463-43-4	4
5	2(1H)-Pyrimidinone, 4-[(2-methyl...	167	C8H13N3O	119608-70-7	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016631.D
Acq On : 01 Oct 2021 11:22
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

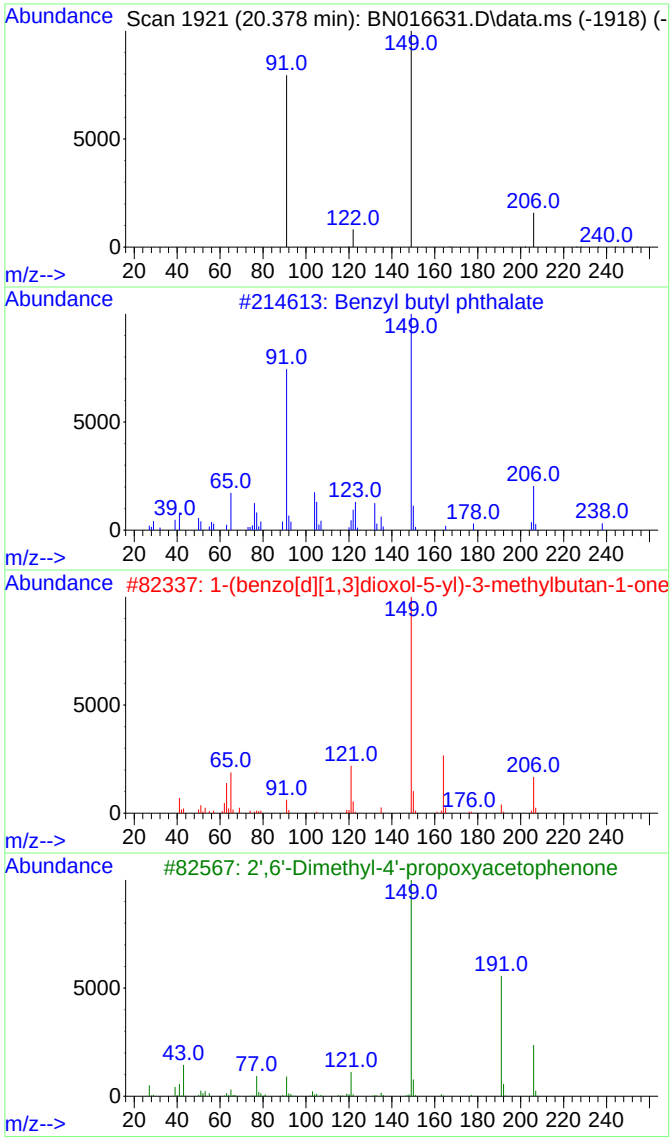
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

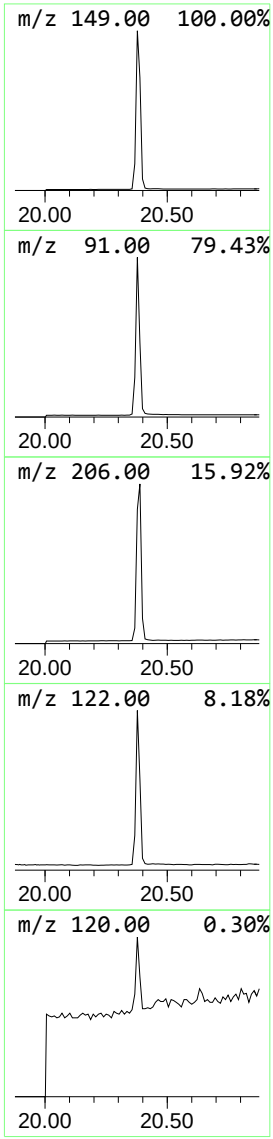
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 Benzyl butyl phthalate Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.378	0.06 ng	69187	Chrysene-d12	21.238

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzyl butyl phthalate	312	C19H20O4	000085-68-7	43
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	1,3,2-Dioxarsenane, 2-butyl-	206	C7H15AsO2	042541-33-3	5
5	2-Methyl-2-(4'-methoxyphenyl)pen...	206	C13H18O2	185700-49-6	5





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016631.D
Acq On : 01 Oct 2021 11:22
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDCCC0.4

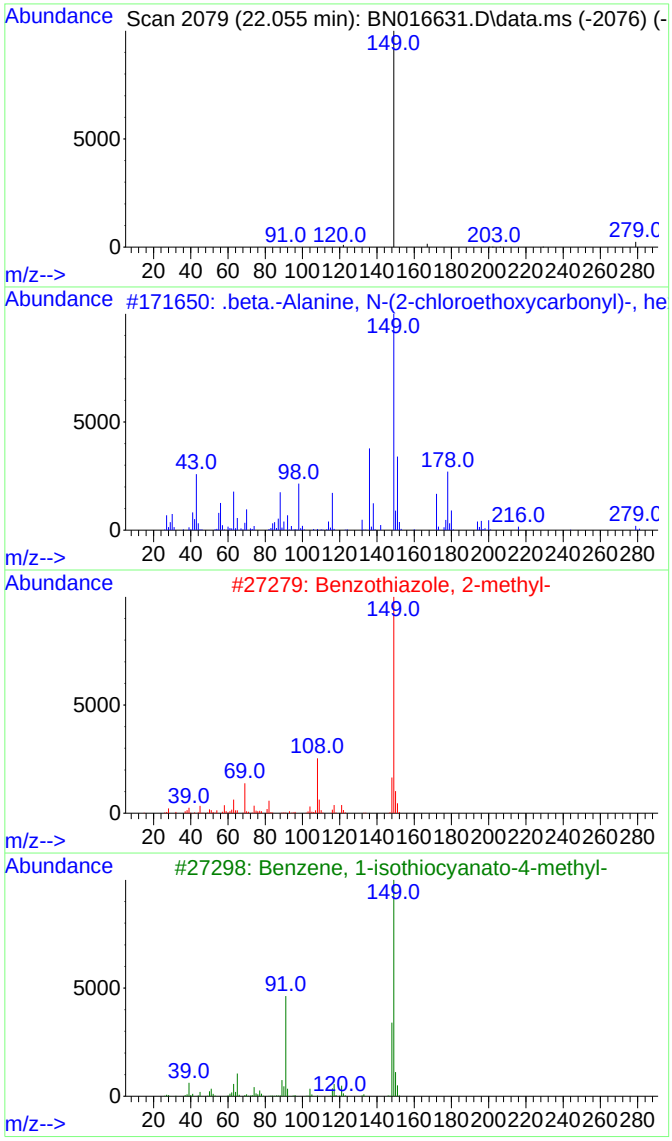
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

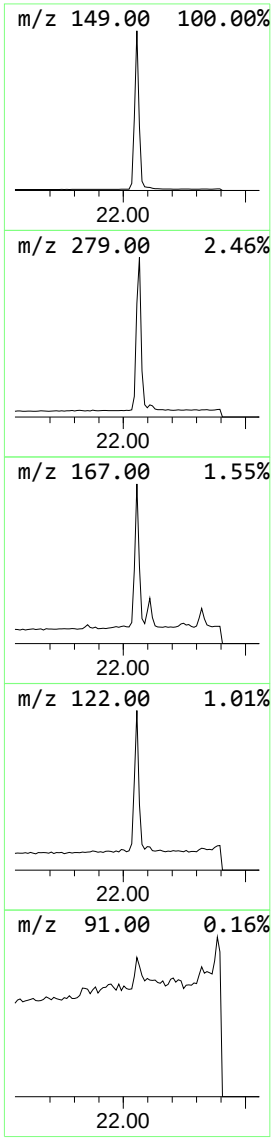
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 .beta.-Alanine, N-(2-chloro... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.055	0.09 ng	99847	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	Benzene, 1-isothiocyanato-4-methyl-	149	C8H7NS	000622-59-3	4
4	Phthalic acid, 7-bromoheptyl oct...	454	C23H35BrO4	1000415-52-2	4
5	Pyridine, pentamethyl-	149	C10H15N	003748-83-2	4





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016631.D
Acq On : 01 Oct 2021 11:22
Operator : CG/JU
Sample : SSTDCCC0.4
Misc :
ALS Vial : 34 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	41306	1	7.642	127030	0.4
Ethene, 1,1-dif...	7.200	0.1	ng	34792	1	7.642	127030	0.4
Thietane	7.522	0.0	ng	15673	1	7.642	127030	0.4
6-Benzothiazola...	7.956	0.4	ng	113621	1	7.642	127030	0.4
Furan, 2,5-dihy...	8.429	0.2	ng	54151	1	7.642	127030	0.4
Fomepizole	9.342	0.2	ng	86759	2	10.406	202663	0.4
5-Aminopyrimidine	9.836	0.1	ng	29329	2	10.406	202663	0.4
o-Chloroaniline	10.571	0.1	ng	67477	2	10.406	202663	0.4
Methane, iodo-	11.709	0.1	ng	27394	2	10.406	202663	0.4
2-Propyl-4-meth...	12.300	0.4	ng	210191	2	10.406	202663	0.4
Z-2-Propenoic a...	12.695	0.1	ng	31428	3	14.269	211039	0.4
E-2-Propenoic a...	12.771	0.1	ng	27615	3	14.269	211039	0.4
Naphthalene, 2-...	13.139	0.3	ng	132289	3	14.269	211039	0.4
Benzene, 2-meth...	13.850	0.1	ng	30301	3	14.269	211039	0.4
Benzene, 1-meth...	14.636	0.1	ng	46844	3	14.269	211039	0.4
Succinic acid, ...	15.537	0.1	ng	66437	3	14.269	211039	0.4
Acetophenone, 2...	15.613	0.1	ng	70266	3	14.269	211039	0.4
5-Fluoro-2-meth...	17.431	0.4	ng	148302	4	17.017	164572	0.4
Benzyl butyl ph...	20.378	0.1	ng	69187	5	21.238	440773	0.4
.beta.-Alanine,...	22.055	0.1	ng	99847	5	21.238	440773	0.4