LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016604.D
Acq On : 30 Sep 2021 17:20
Operator : CG/JU
Sample : SSTDICC5.0
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDICC5.0

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: BN016604.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	21	rBV	129343	164970	2.74%	0.190%
2	3.290	21	23	38	rVB	51444	233746	3.88%	0.270%
3	3.576	51	54	87	rBV	113573	400922	6.66%	0.463%
4	5.254	231	236	263	rVB2	223207	756637	12.57%	0.874%
5	6.821	401	406	418	rBV	351270	851262	14.15%	0.983%
6	6.978	418	423	429	rVV	221145	485808	8.07%	0.561%
7	7.080	429	434	440	rVV	450461	875518	14.55%	1.011%
8	7.209	440	448	460	rVB	158912	414792	6.89%	0.479%
9	7.531	476	483	490	rVB	81503	181496	3.02%	0.210%
10	7.670	490	498	513	rVB2	92168	293642	4.88%	0.339%
11	7.956	524	529	538	rVB2	561643	1249797	20.77%	1.443%
12	8.168	547	552	557	rBV	35080	86560	1.44%	0.100%
13	8.442	571	578	581	rBV2	316316	743066	12.35%	0.858%
14	8.695	594	598	601	rBV	54352	102339	1.70%	0.118%
15	8.784	601	605	607	rBV	605980	1200944	19.96%	1.387%
16	8.822	607	608	612	rVB	459452	662246	11.00%	0.765%
17	9.342	646	649	653	rBV	776222	1229212	20.43%	1.419%
18	9.532	661	664	666	rVV	64600	112561	1.87%	0.130%
19	9.595	666	669	673	rVB	137511	216254	3.59%	0.250%
20	9.836	685	688	691	rBV	236889	368235	6.12%	0.425%
21	10.052	702	705	709	rBV	68016	134534	2.24%	0.155%
22	10.406	729	733	734	rBV	100760	172726	2.87%	0.199%
23	10.457	734	737	741	rVV	1307229	2206111	36.66%	2.547%
24	10.571	743	746	756	rVV	449601	892006	14.82%	1.030%
25	10.749	757	760	763	rVB	407475	654046	10.87%	0.755%
26	11.319	801	805	814	rBV	55767	113357	1.88%	0.131%
27	11.709	851	865	903	rBV	254747	407777	6.78%	0.471%
28	12.007	920	932	940	rBV	680769	1108845	18.43%	1.280%
29	12.078	940	948	971	rVV	1463240	2326809	38.67%	2.687%
30	12.300	988	998	1019	rVV	1445672	2297807	38.18%	2.653%
31	12.695	1056	1059	1062	rBV	284742	455959	7.58%	0.526%
32	12.771	1062	1065	1068	rVV	231720	411386	6.84%	0.475%
33	12.898	1071	1075	1078	rVV	1356697	2280864	37.90%	2.634%
34	13.139	1091	1094	1097	rVB	1000725	1561857	25.95%	1.803%
35	13.342	1107	1110	1114	rVB2	37287	67354	1.12%	0.078%
36	13.647	1131	1134	1136	rBV	39126	60862	1.01%	0.070%

LSC Area Percent Report

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Operator : CG/JU
Sample : SSTDICC5.0
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDICC5.0

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	13.736	1138	1141	1143	rVV	160576	233626	3.88%	0.270%
38	13.786	1143	1145	1148	rVV	53958	77063	1.28%	0.089%
39	13.850	1148	1150	1154	rVB2	350604	602415	10.01%	0.696%
40	13.951	1155	1158	1159	rBV	103645	211409	3.51%	0.244%
41	13.989	1159	1161	1164	rVB	1496364	2139911	35.56%	2.471%
42	14.268	1180	1183	1185	rVV	121397	179191	2.98%	0.207%
43	14.332	1185	1188	1191	rVV	1964950	2880106	47.86%	3.325%
44	14.383	1191	1192	1198	rVV	54598	88602	1.47%	0.102%
45	14.497	1198	1201	1209	rVV	34873	63325	1.05%	0.073%
46	14.649	1209	1213	1218	rVV	460198	881178	14.64%	1.017%
47	14.827	1224	1227	1230	rBV	96484	162931	2.71%	0.188%
48	14.903	1230	1233	1236	rVV	132248	185147	3.08%	0.214%
49	15.106	1247	1249	1252	rBV	103089	158864	2.64%	0.183%
50	15.322	1263	1266	1270	rBV2	2376005	4078443	67.77%	4.709%
51	15.410	1270	1273	1276	rVV2	164695	262617	4.36%	0.303%
52	15.550	1280	1284	1287	rVV2	500342	840674	13.97%	0.971%
53	15.613	1287	1289	1293	rVB2	609581	1050000	17.45%	1.212%
54	15.766	1298	1301	1304	rBV2	224805	358503	5.96%	0.414%
55	16.226	1335	1338	1341	rBV2	821980	1140897	18.96%	1.317%
56	16.324	1343	1346	1350	rVV	466448	806668	13.40%	0.931%
57	16.506	1358	1361	1364	rBV	460971	571577	9.50%	0.660%
58	16.677	1372	1375	1378	rBV	491643	698374	11.61%	0.806%
59	17.029	1400	1404	1405	rBV	85674	172770	2.87%	0.199%
60	17.066	1405	1407	1410	rVV	1806293	2447190	40.67%	2.826%
61	17.151	1411	1414	1418	rBV	1433713	2316602	38.50%	2.675%
62	17.431	1434	1437	1440	rBV	1002054	1400383	23.27%	1.617%
63	18.020	1483	1486	1498	rVB	100371	129782	2.16%	0.150%
64	19.068	1685	1697	1700	rBV	1470062	2093997	34.80%	2.418%
65	19.097	1700	1703	1739	rVB	2173717	2701716	44.90%	3.119%
66	19.460	1767	1776	1811	rBV	2305817	3010006	50.02%	3.475%
67	19.678	1813	1820	1853	rVB	1319415	1621234	26.94%	1.872%
68	20.388	1919	1922	1924	rBV	882248	1187947	19.74%	1.372%
69	21.174	1993	1996	1998	rBV	1205972	1426616	23.71%	1.647%
70	21.217	1998	2000	2003	rVV	2341572	3120977	51.86%	3.604%
71	21.270	2003	2005	2008	rVB	2355861	2840411	47.20%	3.280%
72	22.056	2076	2079	2096	rVB	1313686	1930146	32.07%	2.229%
73	22.810	2216	2230	2237	rBV	1524506	2617588	43.50%	3.022%
74	22.854	2237	2243	2304	rVB	1558499	2610981	43.39%	3.015%
75	23.388	2384	2399	2418	rBV	1239985	2402383	39.92%	2.774%
76	23.488	2419	2428	2472	rVB	92551	201555	3.35%	0.233%

LSC Area Percent Report

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Data File : BN016604.D
Acq On : 30 Sep 2021 17:20
Operator : CG/JU
Sample : SSTDICC5.0
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC5.0

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

77	25.781	3066	3098	3186	rBV3	1670578	6017775	100.00%	6.948%
78	26.466	3272	3298	3373	rBV	908792	2903827	48.25%	3.353%

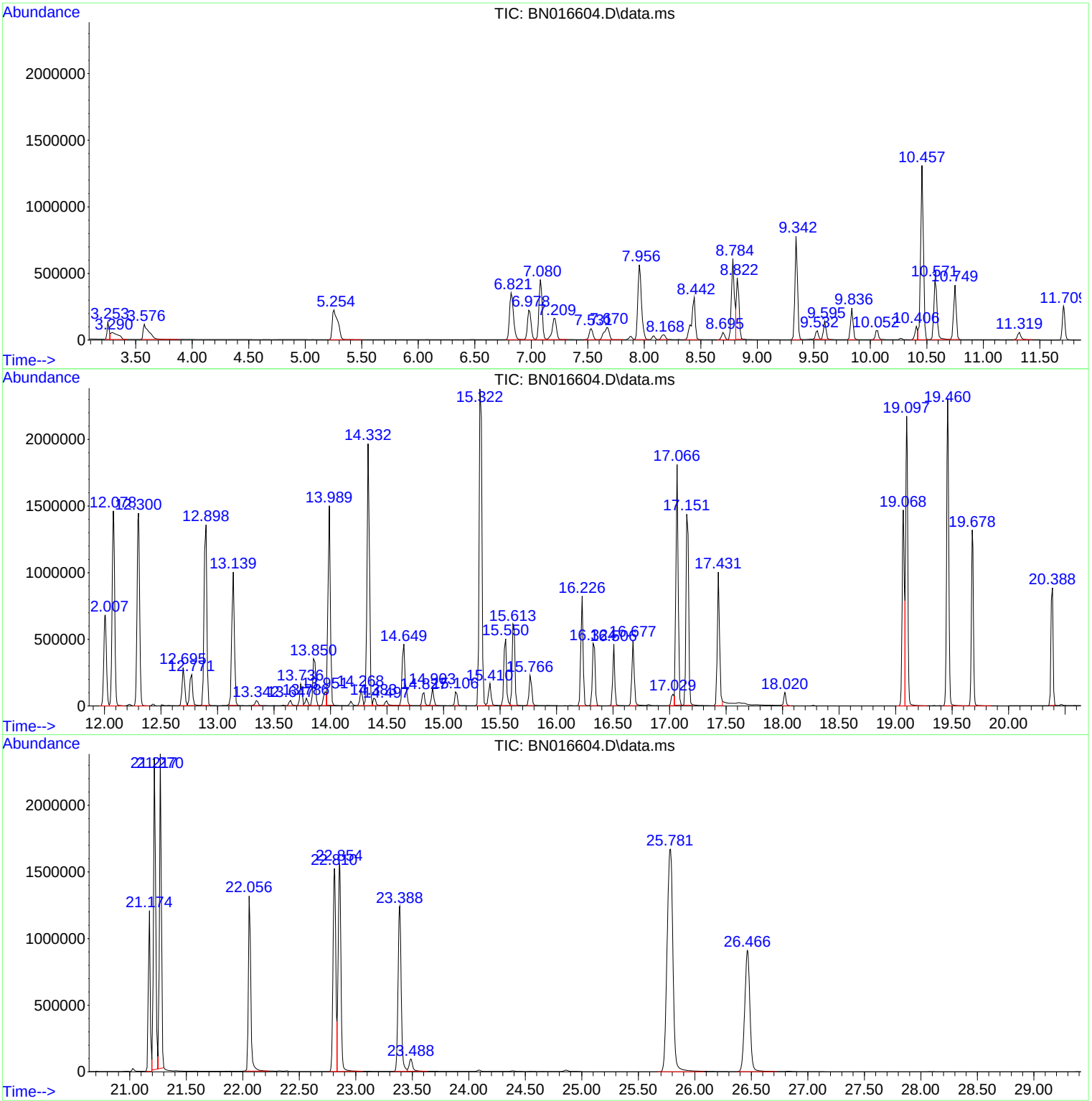
Sum of corrected areas: 86607714

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016604.D
Acq On : 30 Sep 2021 17:20
Operator : CG/JU
Sample : SSTDICC5.0
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC5.0

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 : BN016604.D
Acq On : 30 Sep 2021 17:20
Operator : CG/JU
Sample : SSTDICC5.0
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC5.0

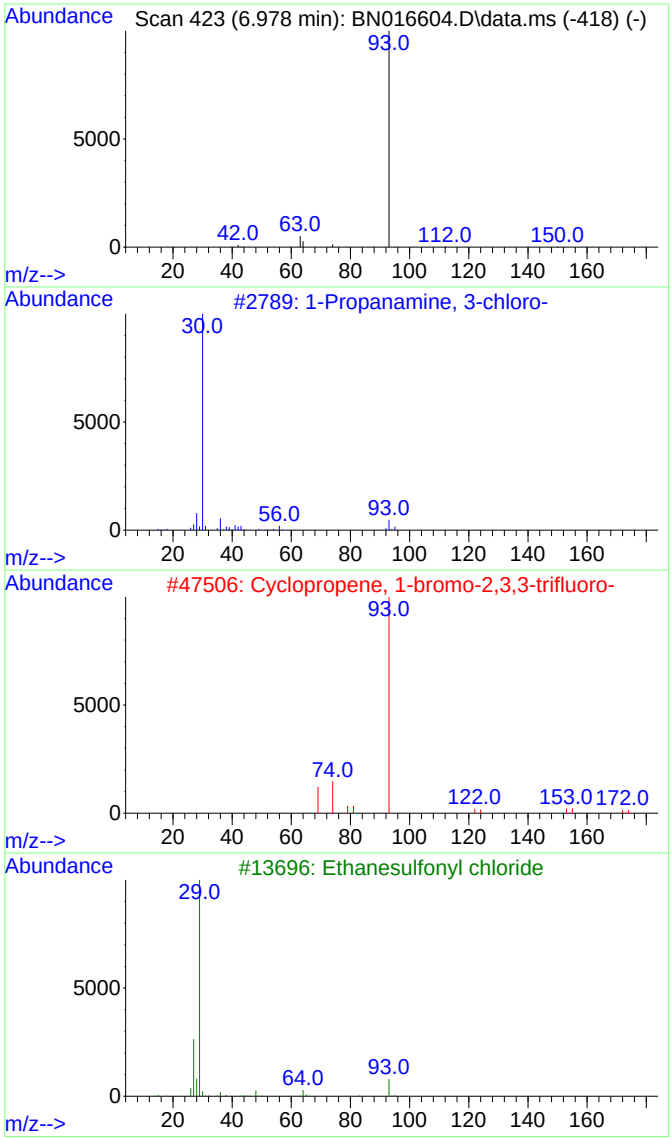
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

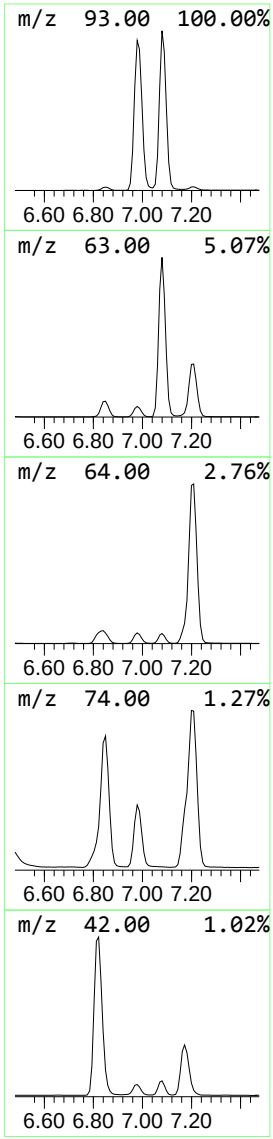
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1-Propanamine, 3-chloro- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.978	0.66 ng	485808	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 : BN016604.D
Acq On : 30 Sep 2021 17:20
Operator : CG/JU
Sample : SSTDICC5.0
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC5.0

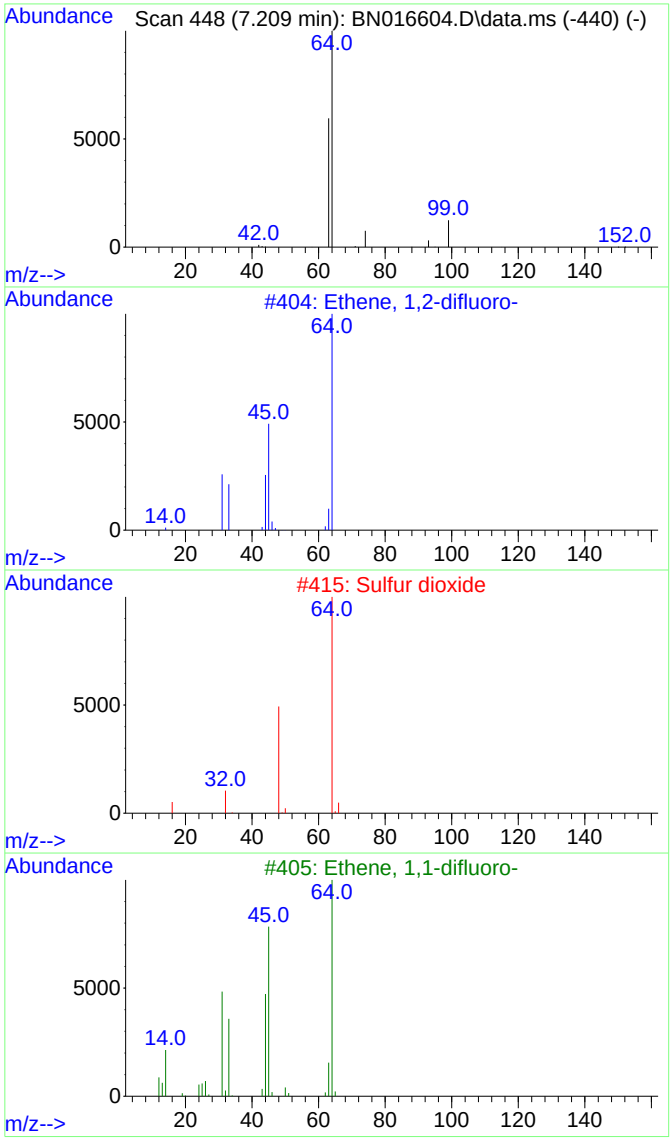
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

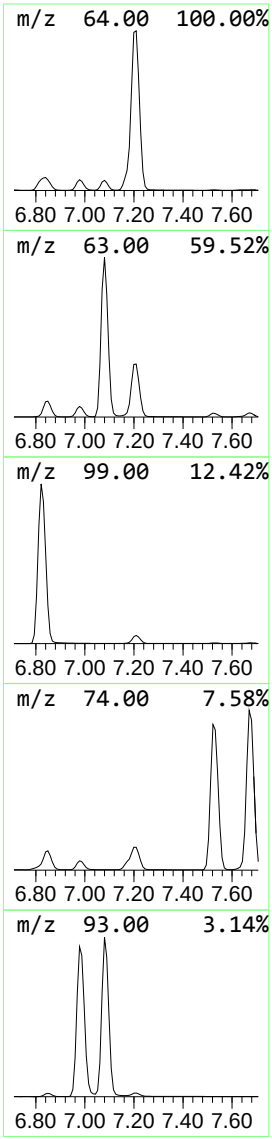
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethene, 1,2-difluoro- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.209	0.57 ng	414792	1,4-Dichlorobenzene-d4	7.642

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





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016604.D
Acq On : 30 Sep 2021 17:20
Operator : CG/JU
Sample : SSTDICC5.0
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC5.0

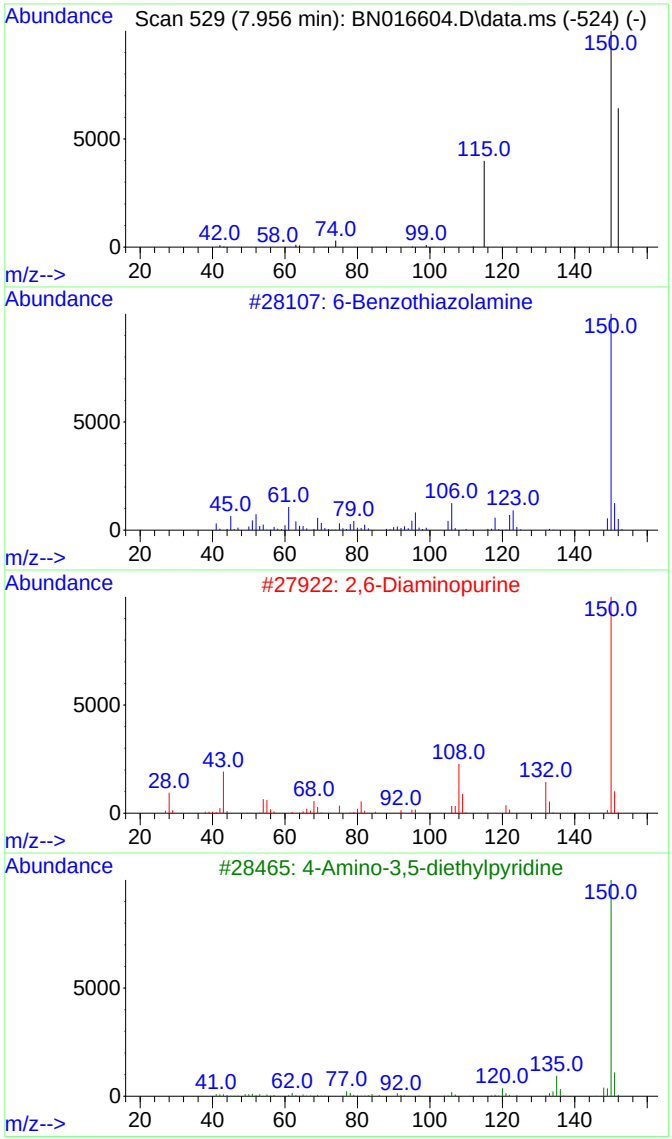
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

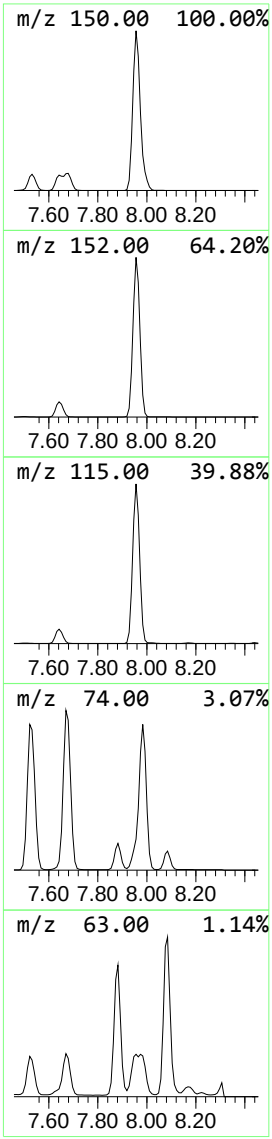
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 6-Benzothiazolamine Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.956	1.70 ng	1249800	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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Sample : SSTDICC5.0
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC5.0

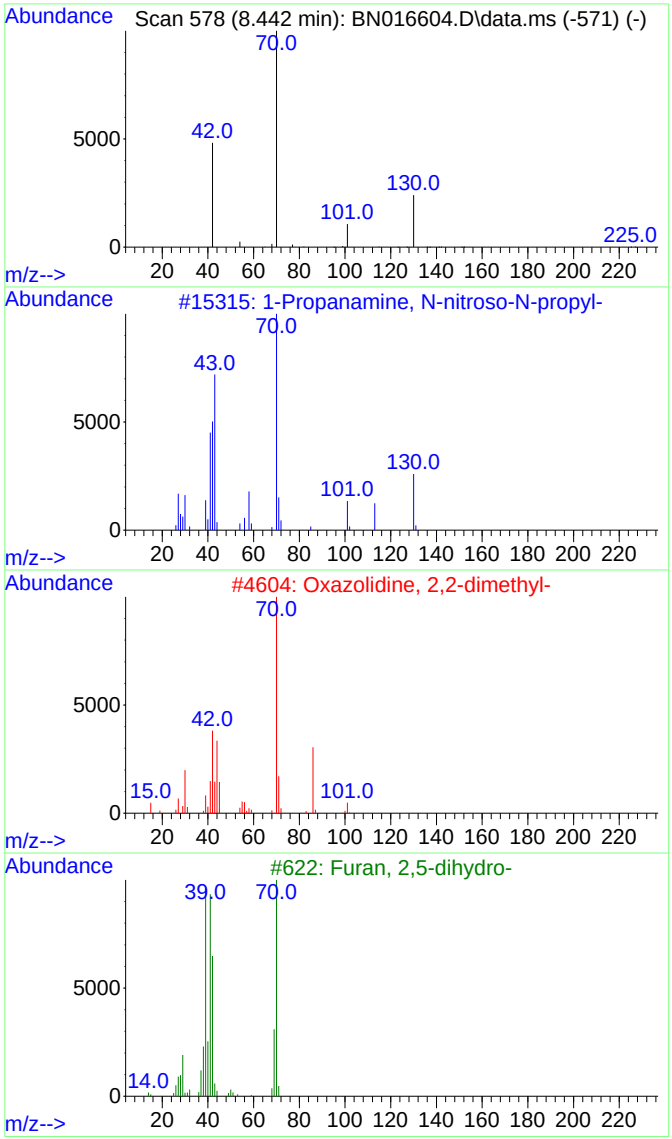
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

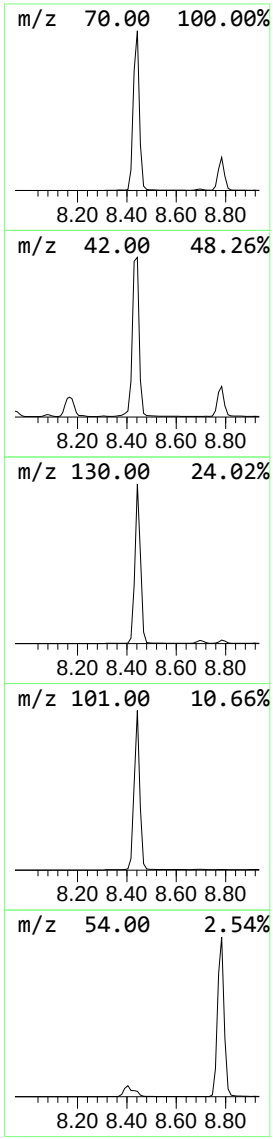
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Propanamine, N-nitroso-N-... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.442	1.01 ng	743066	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanamine, N-nitroso-N-propyl-	130	C6H14N2O	000621-64-7	78
2	Oxazolidine, 2,2-dimethyl-	101	C5H11NO	020515-62-2	7
3	Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	4
4	1-Oxa-3,4-diazacyclopentadiene	70	C2H2N2O	000288-99-3	4
5	2-Butenal, (E)-	70	C4H6O	000123-73-9	4





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Operator : CG/JU
Sample : SSTDICC5.0
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC5.0

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

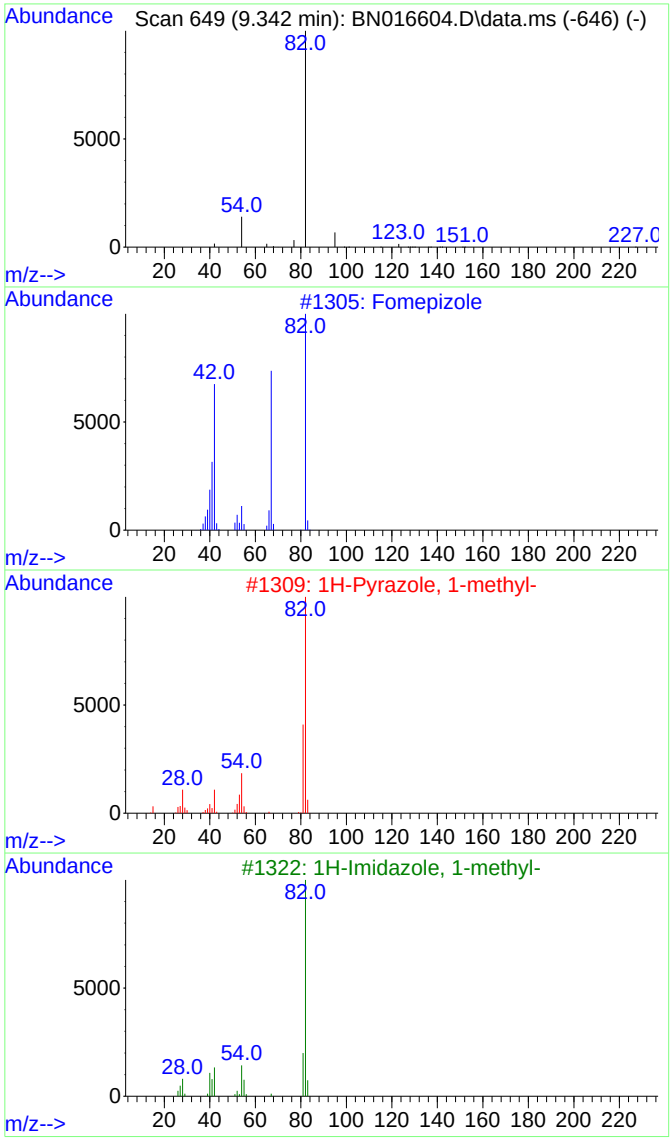
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

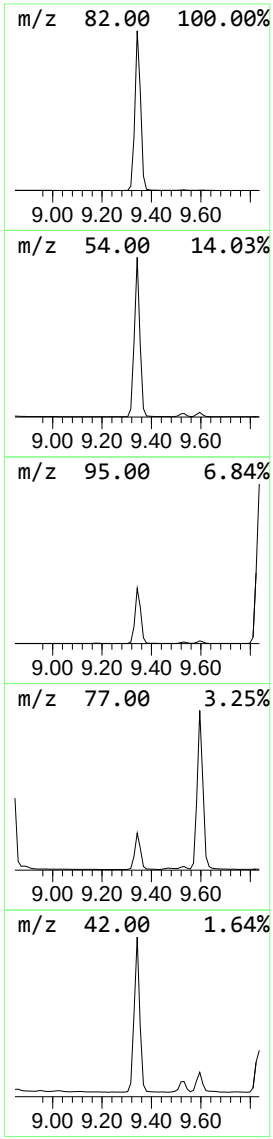
****

Peak Number 5 Fomepizole Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.342	2.85 ng	1229210	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 : BN016604.D
Acq On : 30 Sep 2021 17:20
Operator : CG/JU
Sample : SSTDICC5.0
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC5.0

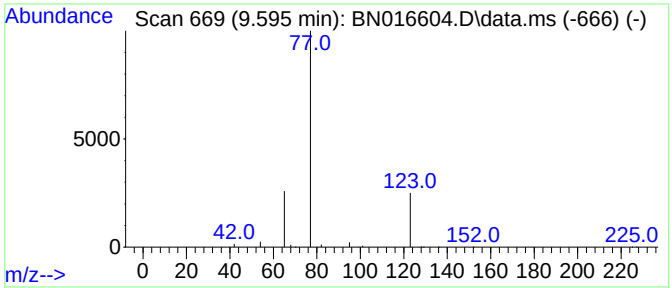
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

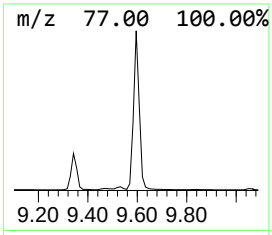
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

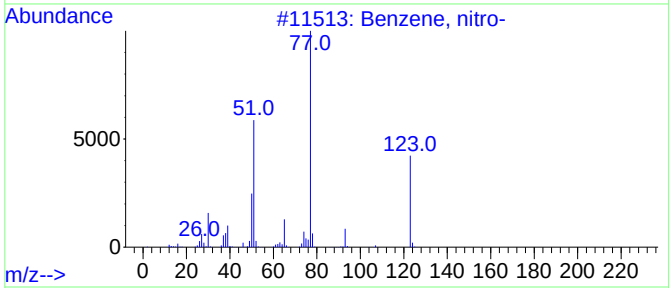
****
Peak Number 6 Benzene, nitro- Concentration Rank 20

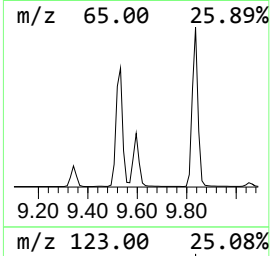
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.595	0.50 ng	216254	Naphthalene-d8	10.406

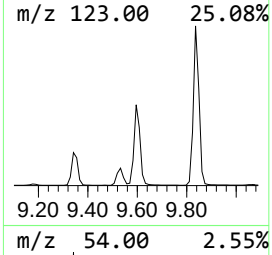
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, nitro-	123	C6H5NO2	000098-95-3	2
2	Cyclopropane, 1,1'-ethenylidenebis-	108	C8H12	000822-93-5	1
3	1,5-Hexadiene, 3,3,4,4-tetrafluoro-	154	C6H6F4	001763-21-9	1
4	Silanamine, N-silyl-	77	H7NSi2	005702-11-4	1
5	Cystamine	152	C4H12N2S2	000051-85-4	1

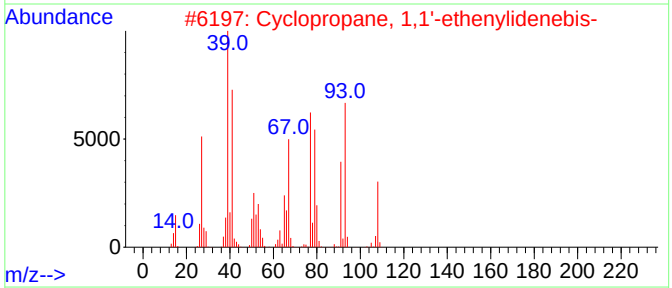


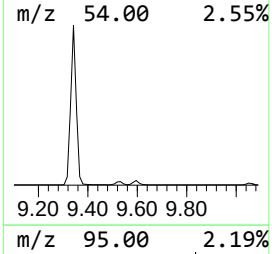


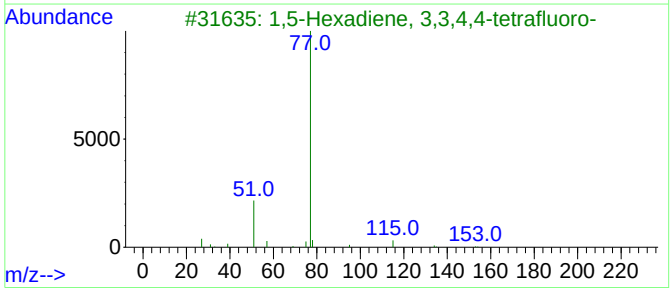


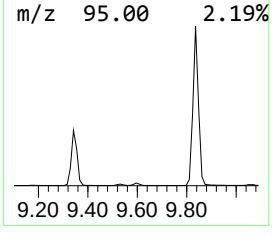












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Acq On : 30 Sep 2021 17:20
Operator : CG/JU
Sample : SSTDICC5.0
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC5.0

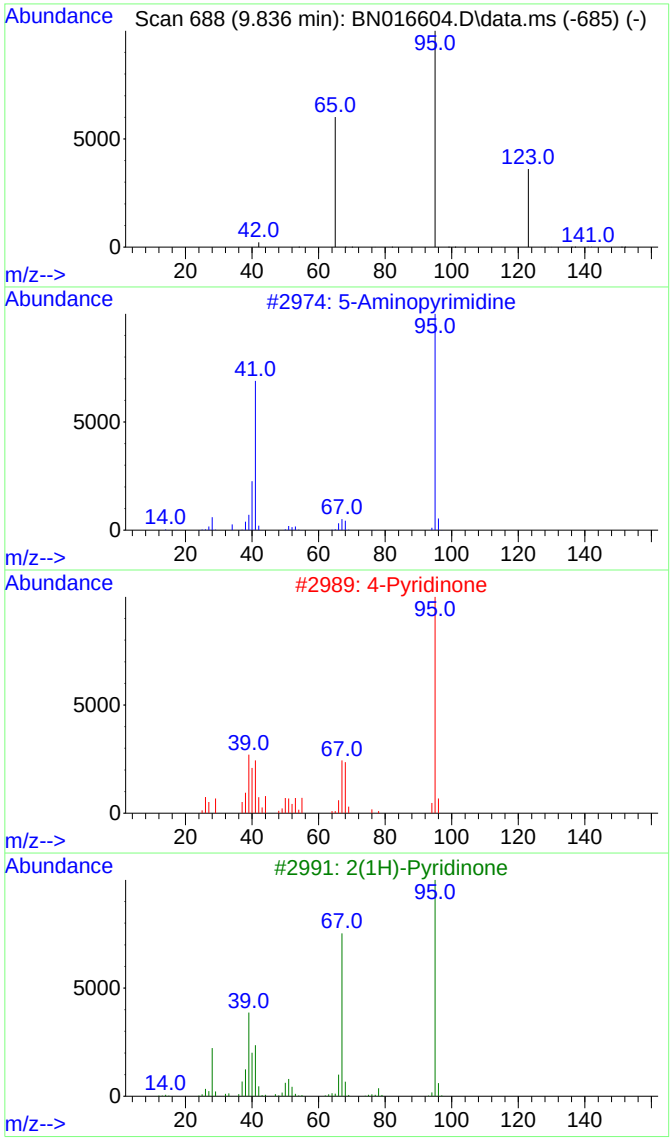
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

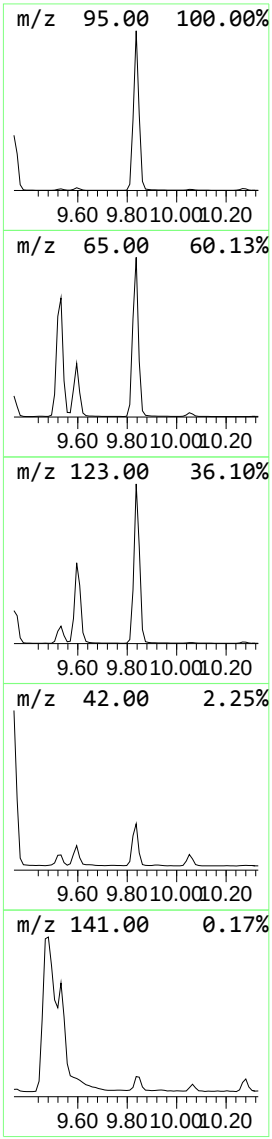
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 5-Aminopyrimidine Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.836	0.85 ng	368235	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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Sample : SSTDICC5.0
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC5.0

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

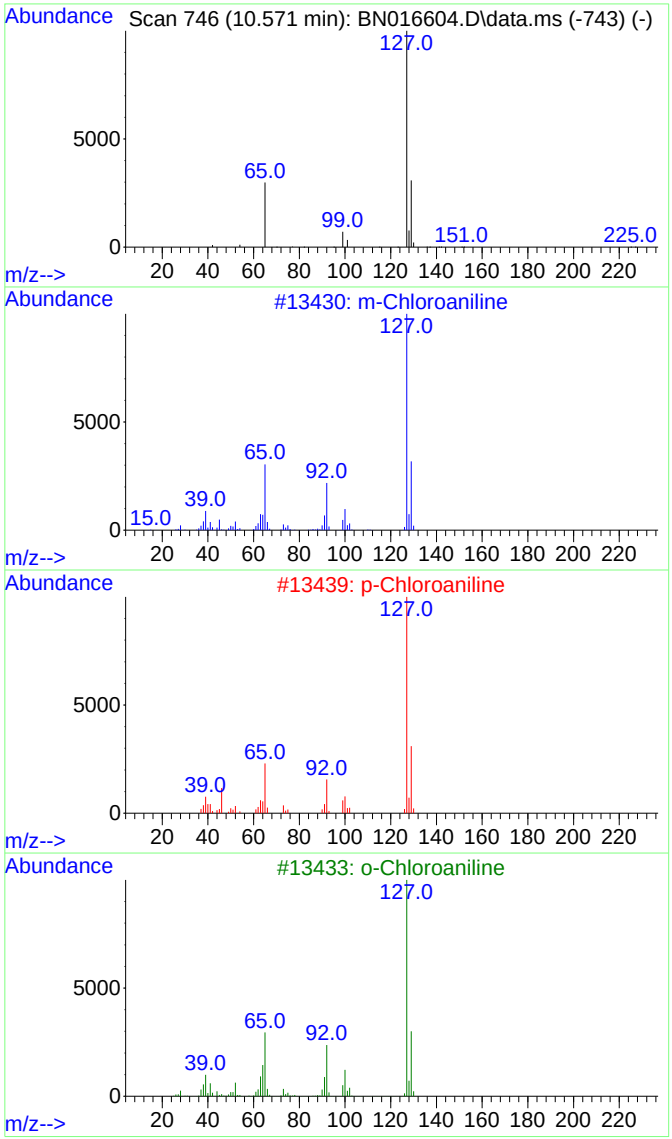
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

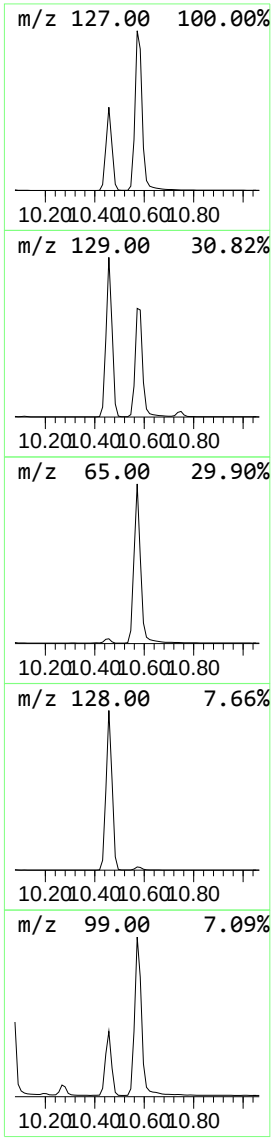
****

Peak Number 8 m-Chloroaniline Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.571	2.07 ng	892006	Naphthalene-d8	10.406

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





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Sample : SSTDICC5.0
Misc :
ALS Vial : 8 Sample Multiplier: 1

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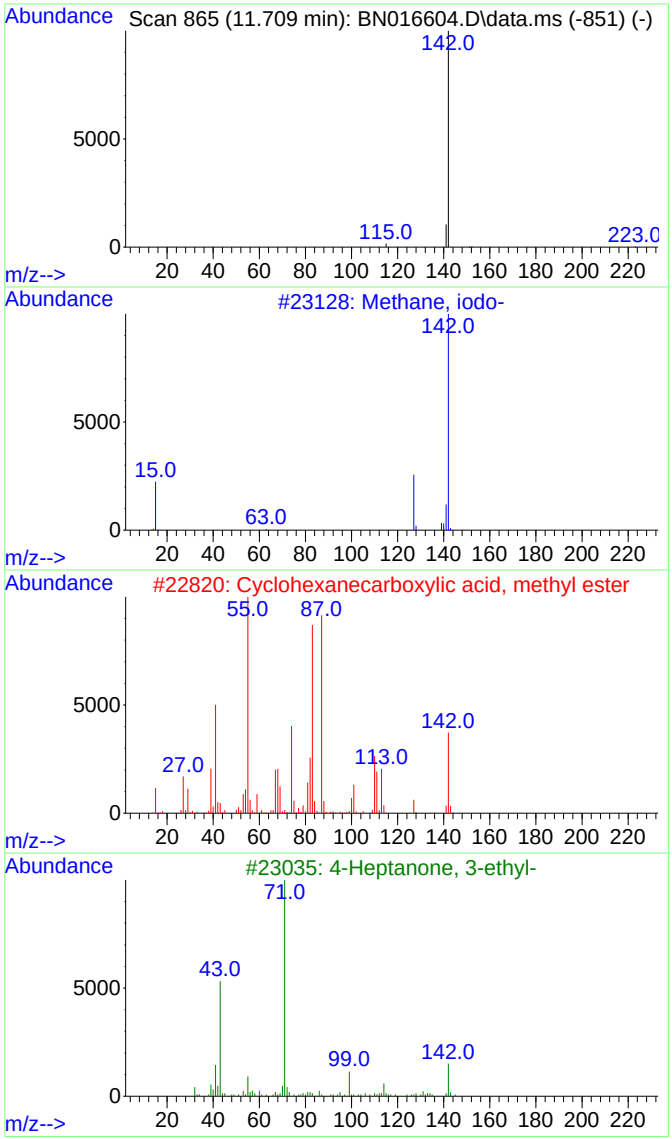
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

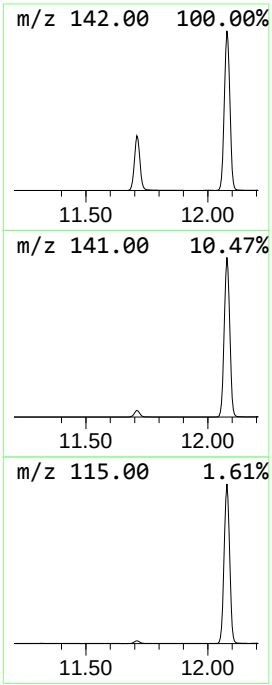
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Methane, iodo- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.709	0.94 ng	407777	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 : SSTDICC5.0
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDICC5.0

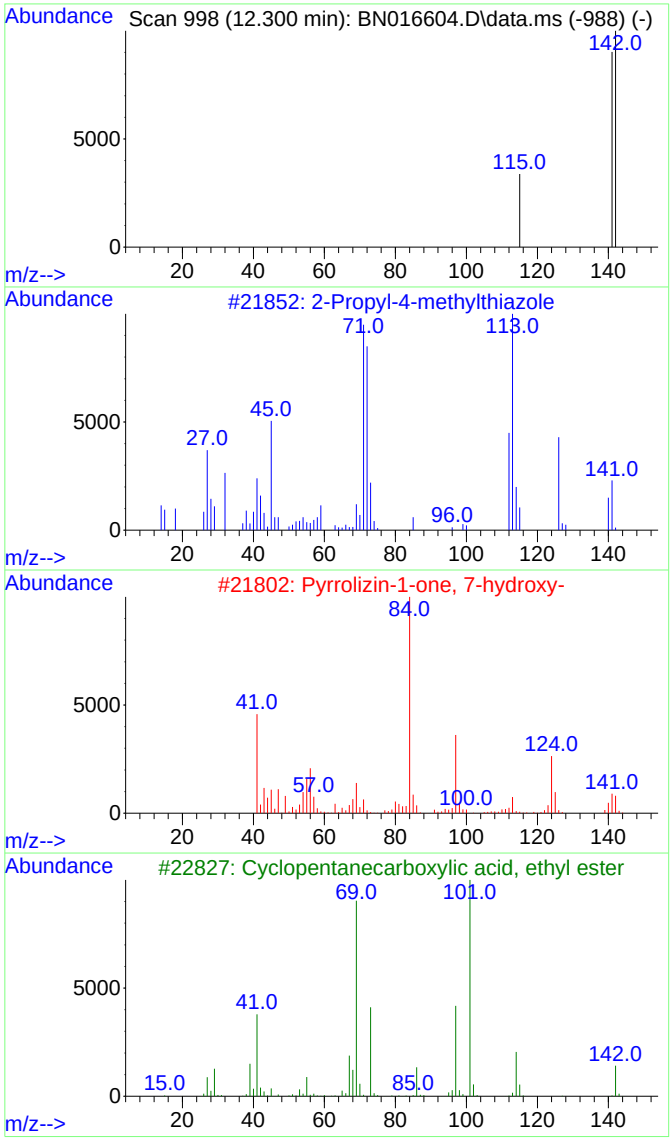
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

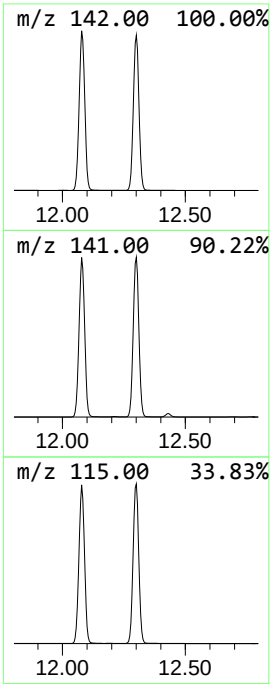
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.300	5.32 ng	2297810	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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Operator : CG/JU
Sample : SSTDICC5.0
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ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC5.0

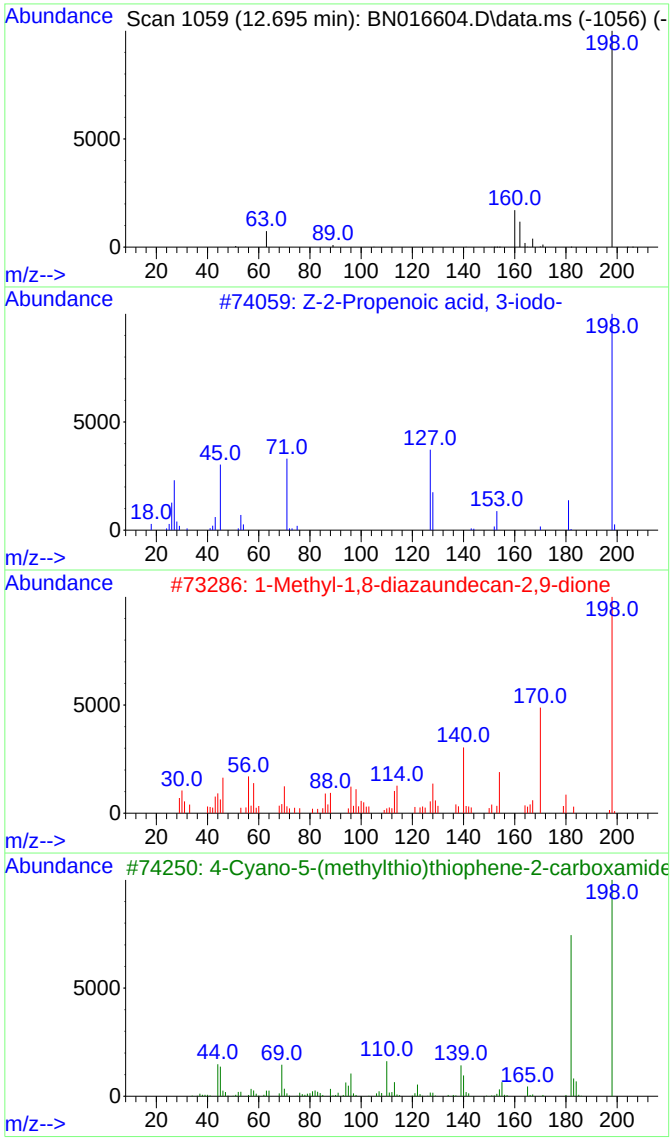
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

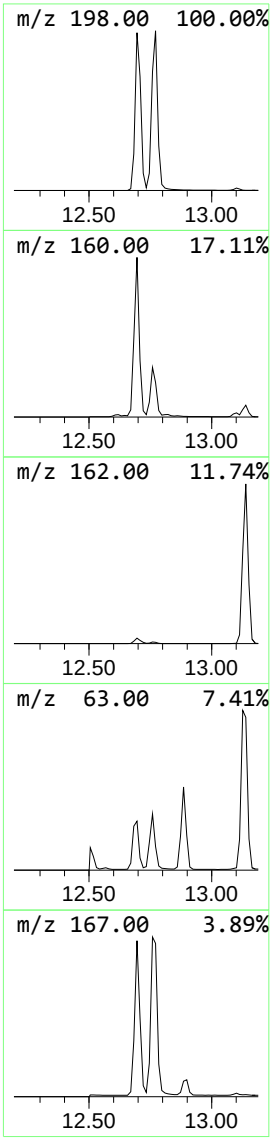
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Z-2-Propenoic acid, 3-iodo- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.695	1.02 ng	455959	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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Operator : CG/JU
Sample : SSTDICC5.0
Misc :
ALS Vial : 8 Sample Multiplier: 1

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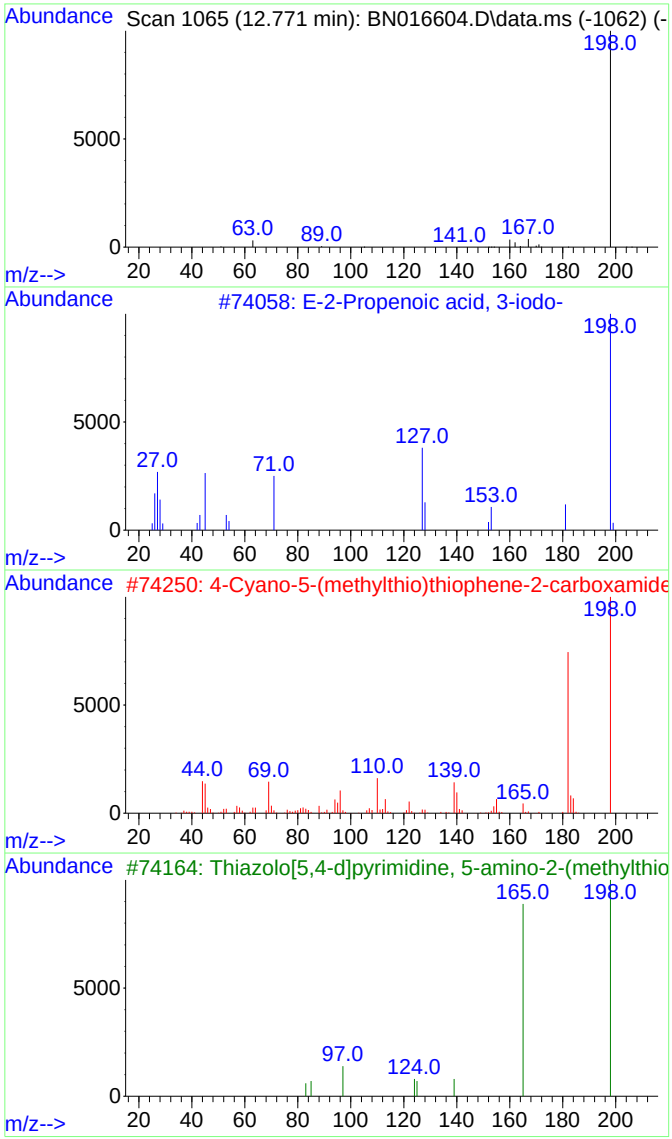
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

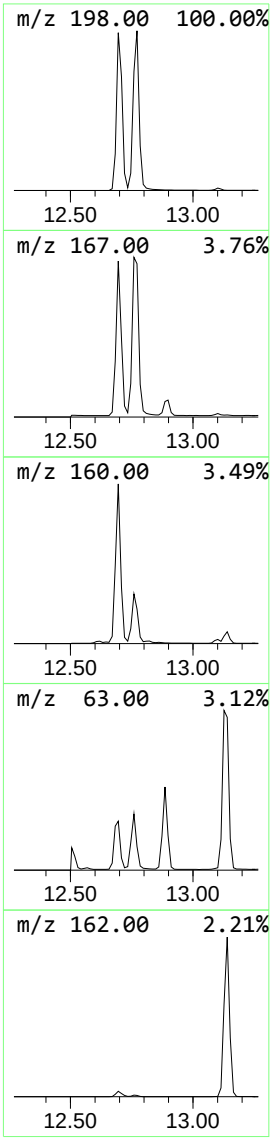
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.771	0.92 ng	411386	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 : SSTDICC5.0
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDICC5.0

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

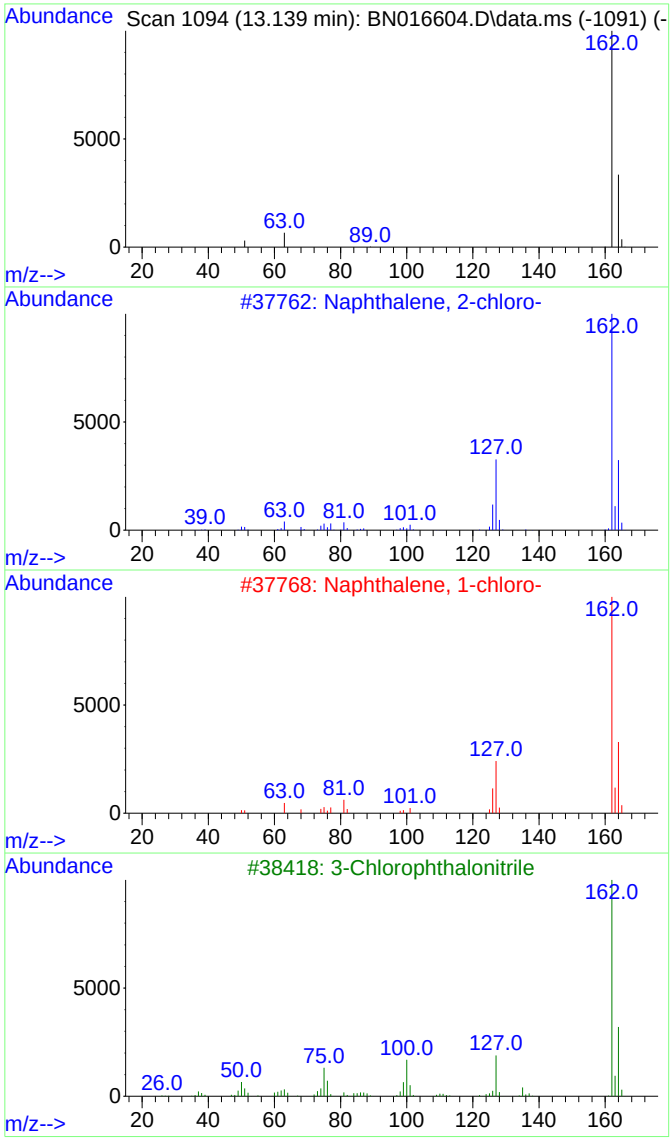
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

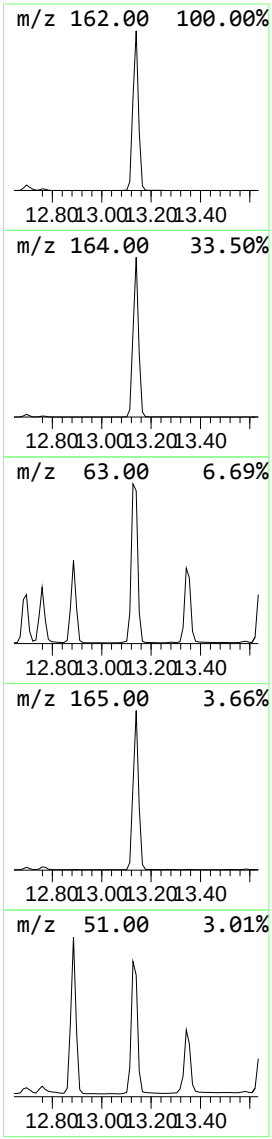
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.139	3.49 ng	1561860	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	3-Chloro-4-fluorothiophenol	162	C6H4ClFS	060811-23-6	5





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Sample : SSTDICC5.0
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDICC5.0

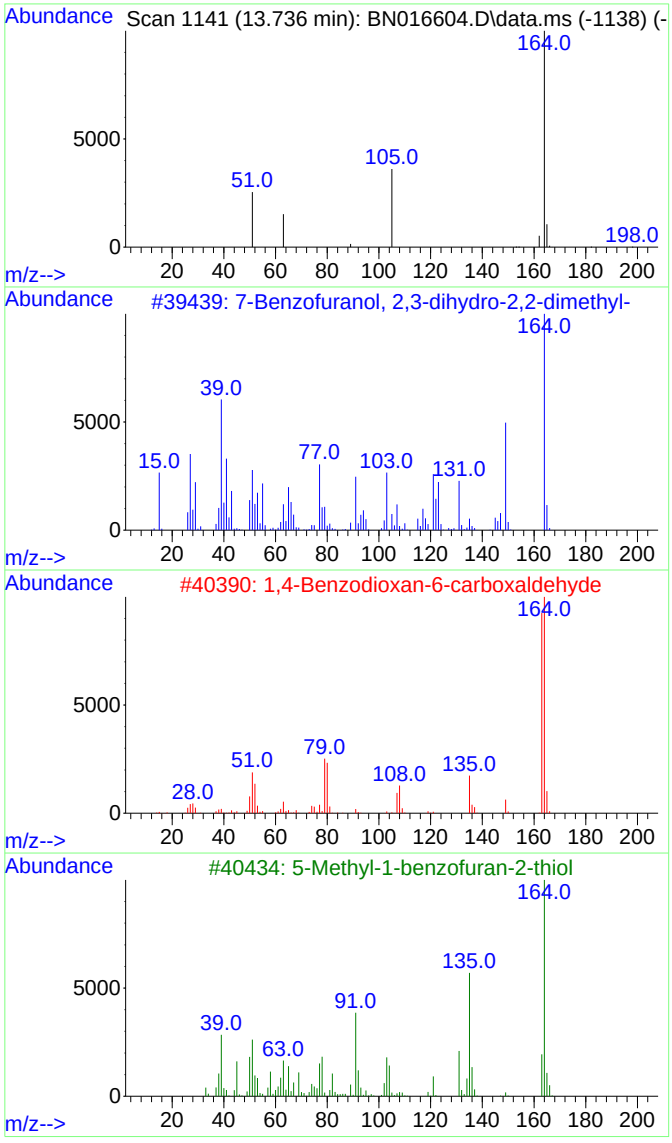
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

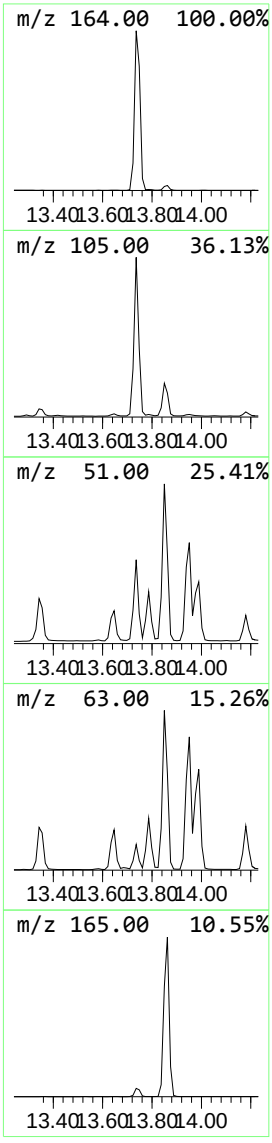
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 7-Benzofuranol, 2,3-dihydro... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.736	0.52 ng	233626	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Benzofuranol, 2,3-dihydro-2,2-...	164	C10H12O2	001563-38-8	9
2	1,4-Benzodioxan-6-carboxaldehyde	164	C9H8O3	029668-44-8	9
3	5-Methyl-1-benzofuran-2-thiol	164	C9H8OS	1000410-59-6	9
4	4,5-Dimethyl-2-sulfanylpyridine-...	164	C8H8N2S	1000435-16-1	9
5	4,6-Dimethyl-2-mercaptopyridine-...	164	C8H8N2S	054585-47-6	9





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Sample : SSTDICC5.0
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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LabSampleId :
SSTDICC5.0

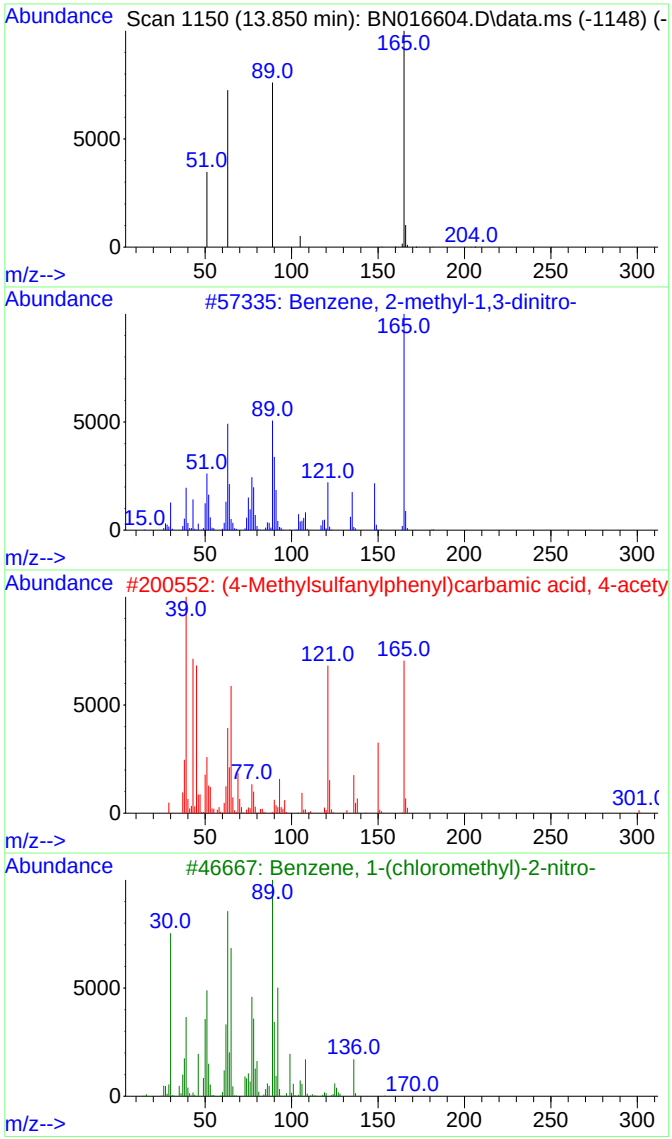
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

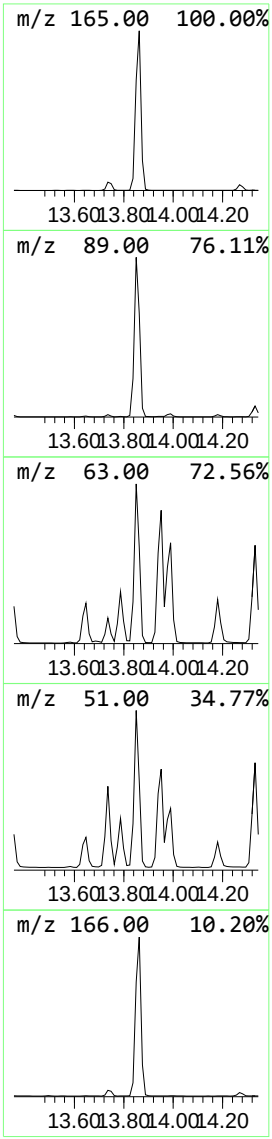
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 Benzene, 2-methyl-1,3-dinitro- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.850	1.34 ng	602415	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	23
2	(4-Methylsulfanylphenyl)carbamic...	301	C16H15NO3S	1000305-20-0	17
3	Benzene, 1-(chloromethyl)-2-nitro-	171	C7H6ClNO2	000612-23-7	9
4	2-Butanone, 3-[(2-chloroethyl)th...	166	C6H11ClOS	117239-10-8	4
5	Thiazole, tetrahydro-	89	C3H7NS	000504-78-9	3





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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC5.0

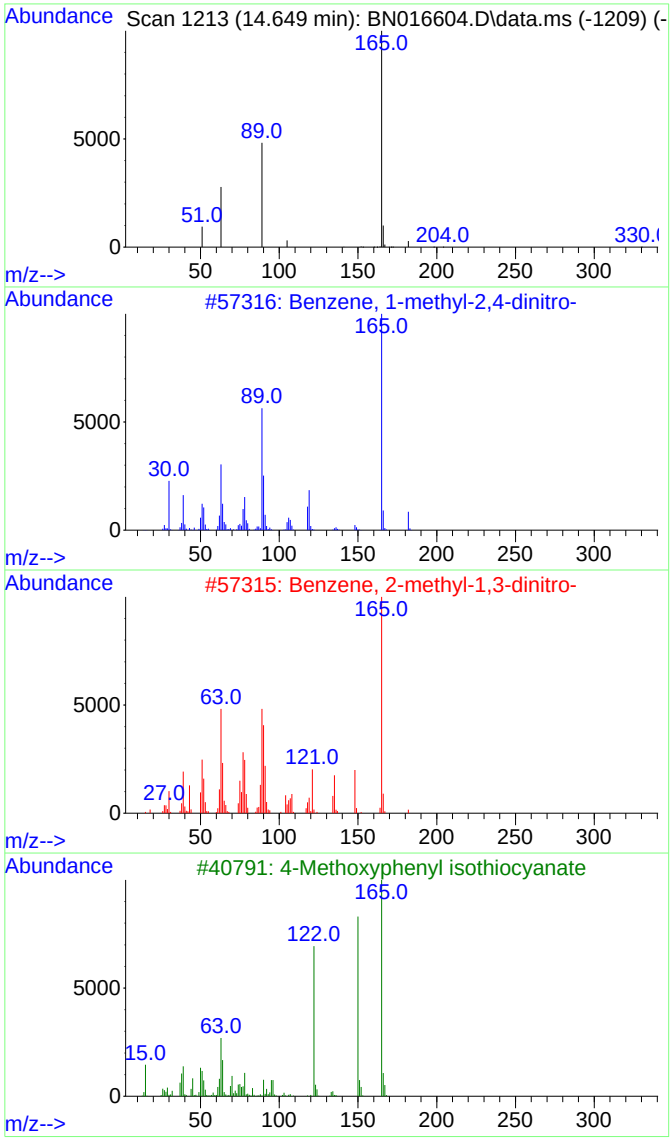
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

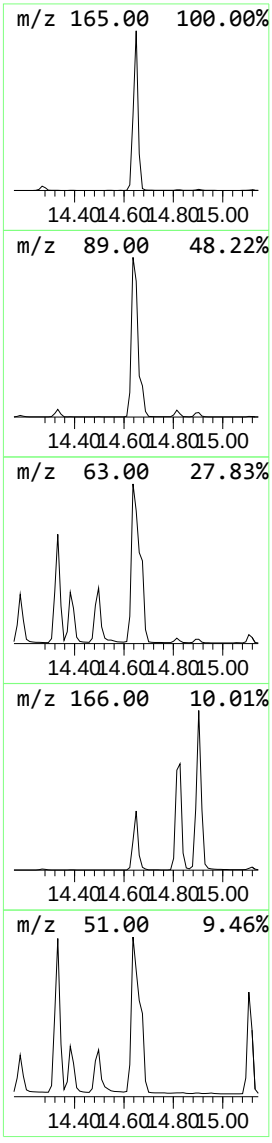
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 Benzene, 1-methyl-2,4-dinitro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.649	1.97 ng	881178	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-2,4-dinitro-	182	C7H6N2O4	000121-14-2	43
2	Benzene, 2-methyl-1,3-dinitro-	182	C7H6N2O4	000606-20-2	38
3	4-Methoxyphenyl isothiocyanate	165	C8H7NOS	002284-20-0	9
4	Benzamide, 3,4-dimethoxy-N-(2-ph...	439	C28H41NO3	1000491-47-7	9
5	2(3H)-Benzoxazolethione, 5-methyl-	165	C8H7NOS	022876-22-8	7





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Data File : BN016604.D
Acq On : 30 Sep 2021 17:20
Operator : CG/JU
Sample : SSTDICC5.0
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC5.0

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

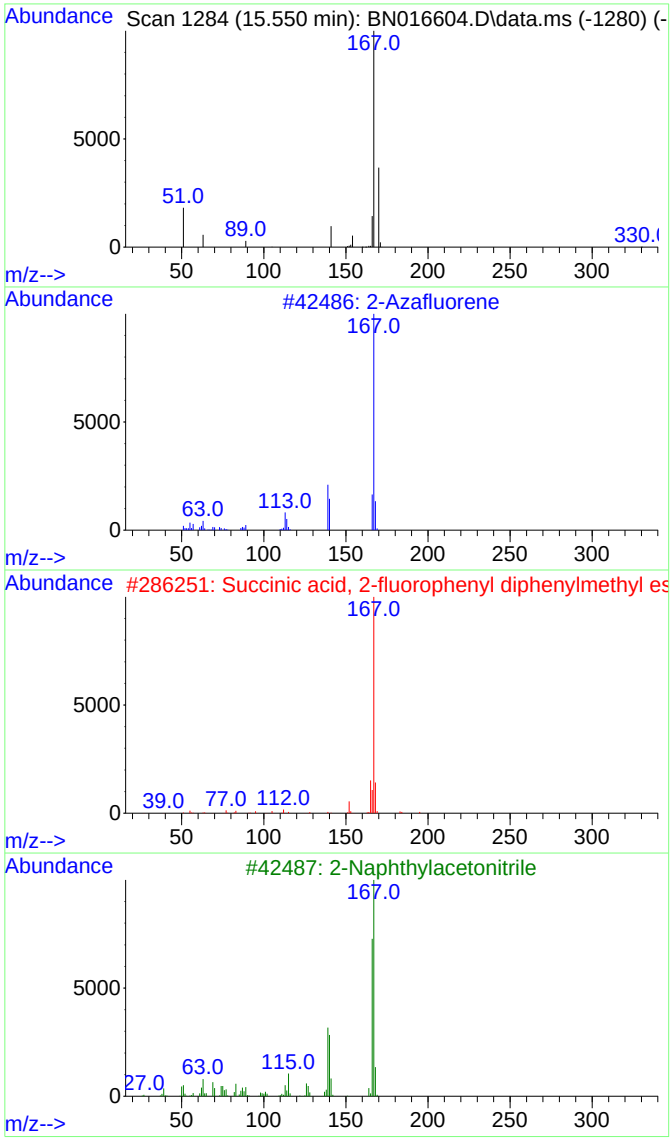
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

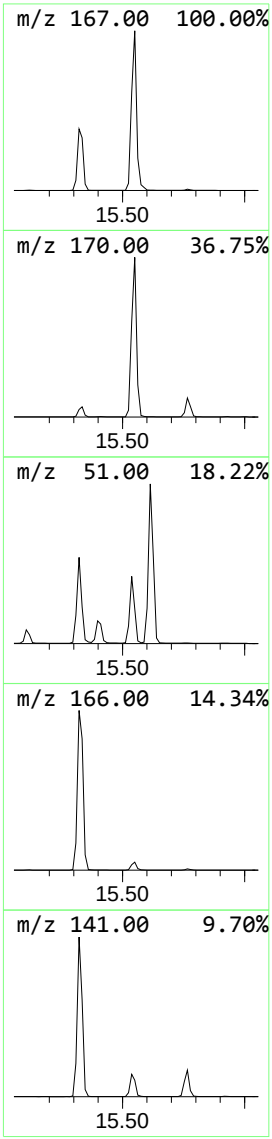
****

Peak Number 17 2-Azafluorene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.550	1.88 ng	840674	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Azafluorene	167	C12H9N	000244-40-6	9
2	Succinic acid, 2-fluorophenyl di...	378	C23H19FO4	1000390-17-0	9
3	2-Naphthylacetonitrile	167	C12H9N	007498-57-9	7
4	2,4(1H,3H)-Pyrimidinedione, 5-me...	170	C7H10N2O3	059264-10-7	5
5	Benzaldehyde, 2-hydroxy-5-nitro-	167	C7H5NO4	000097-51-8	5





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Data File : BN016604.D
Acq On : 30 Sep 2021 17:20
Operator : CG/JU
Sample : SSTDICC5.0
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC5.0

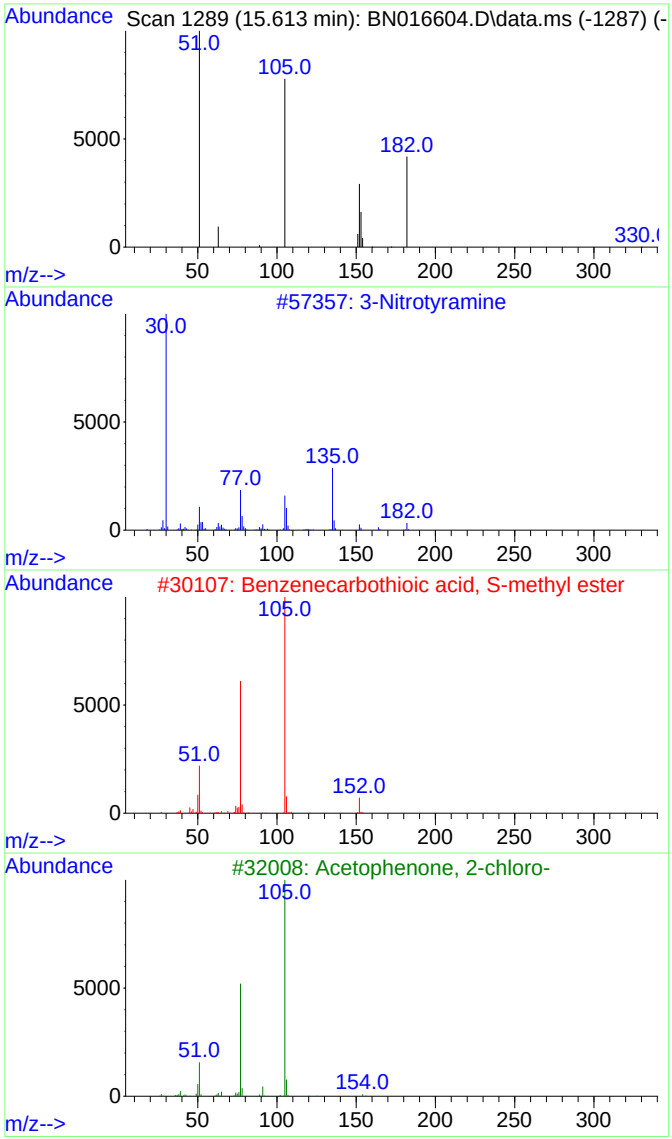
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

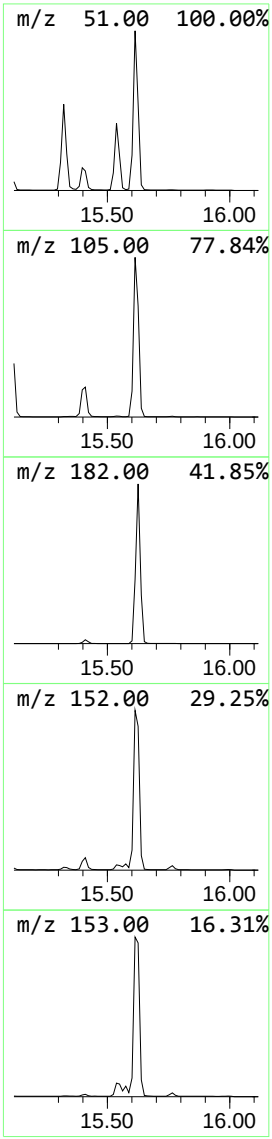
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 3-Nitrotyramine Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.613	2.34 ng	1050000	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Nitrotyramine	182	C8H10N2O3	049607-15-0	4
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	3
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	3
4	Propiolonitrile	51	C3HN	001070-71-9	3
5	Benzeneethanamine, 4-methoxy-	151	C9H13NO	000055-81-2	3





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Data File : BN016604.D
Acq On : 30 Sep 2021 17:20
Operator : CG/JU
Sample : SSTDICC5.0
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC5.0

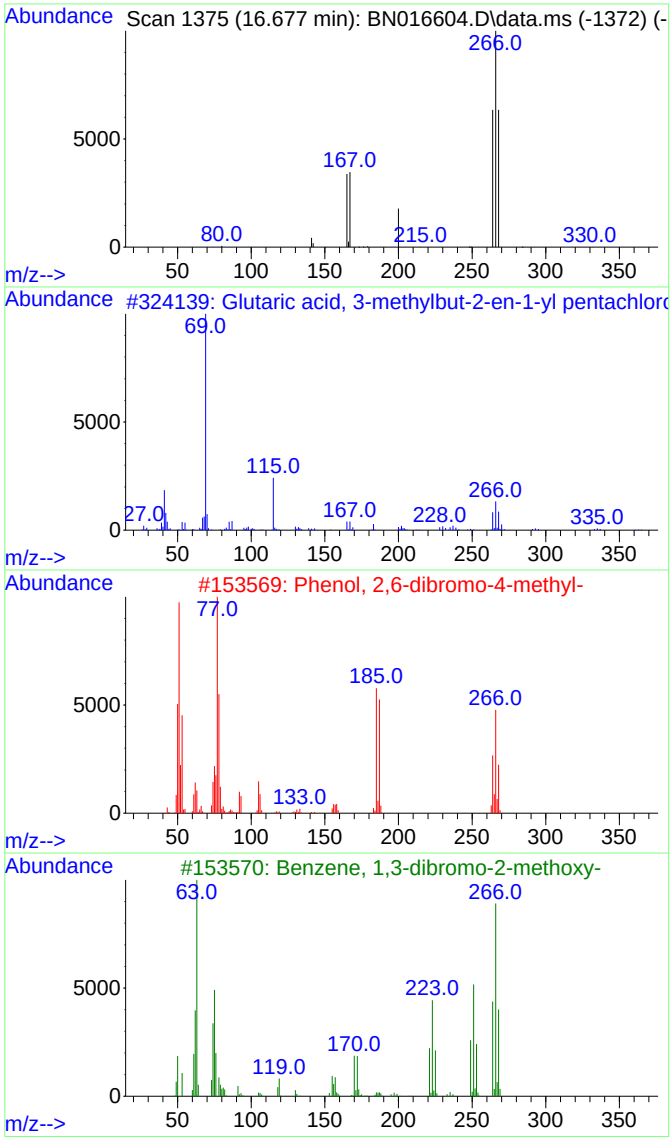
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

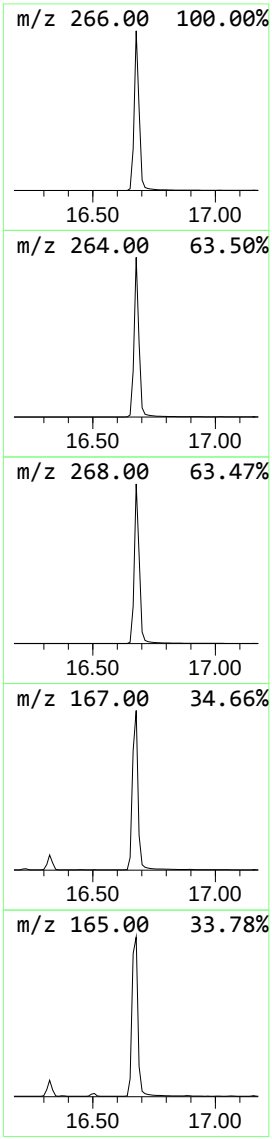
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 Glutaric acid, 3-methylbut-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.677	1.62 ng	698374	Phenanthrene-d10	17.029

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Glutaric acid, 3-methylbut-2-en-...	446	C16H15Cl5O4	1000392-32-9	64
2	Phenol, 2,6-dibromo-4-methyl-	264	C7H6Br2O	002432-14-6	42
3	Benzene, 1,3-dibromo-2-methoxy-	264	C7H6Br2O	038603-09-7	42
4	2-Amino-3,5-dibromo-6-methylpyri...	264	C6H6Br2N2	091872-10-5	42
5	o-Cresol, 4,6-dibromo-	264	C7H6Br2O	000609-22-3	42





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Data File : BN016604.D
Acq On : 30 Sep 2021 17:20
Operator : CG/JU
Sample : SSTDICC5.0
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICC5.0

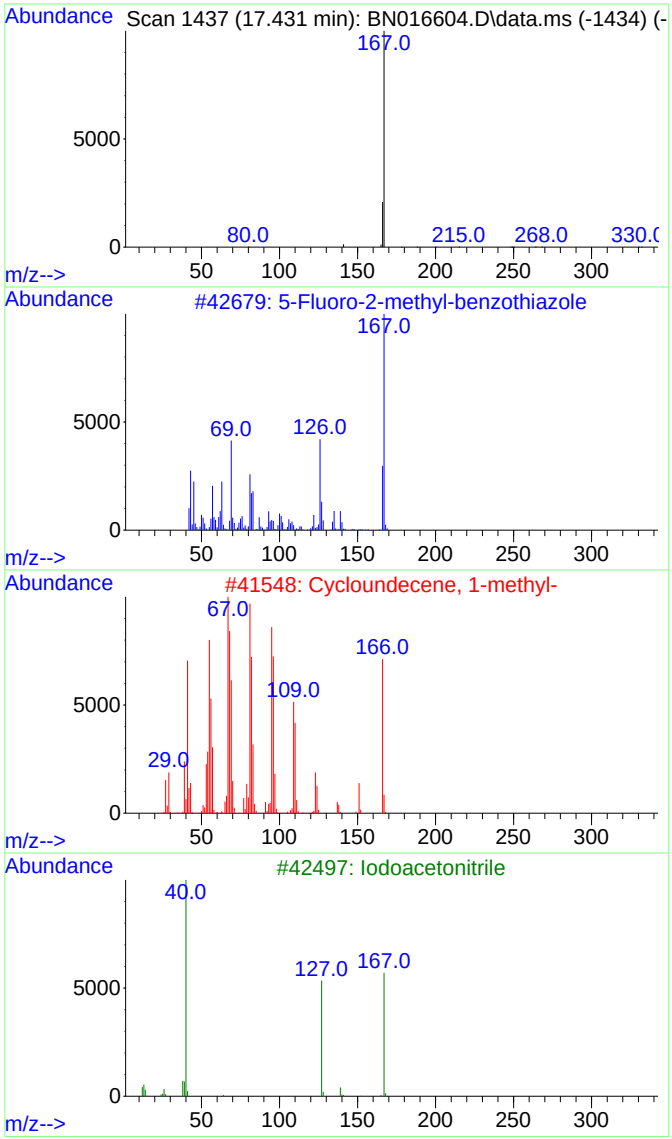
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

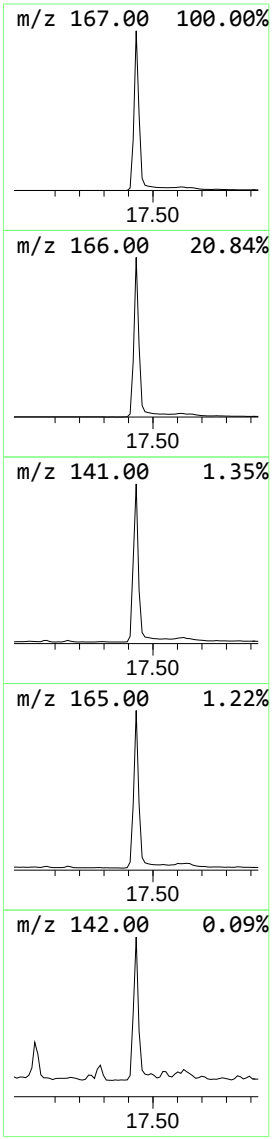
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 5-Fluoro-2-methyl-benzothia... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.431	3.24 ng	1400380	Phenanthrene-d10	17.029

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





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016604.D
Acq On : 30 Sep 2021 17:20
Operator : CG/JU
Sample : SSTDICC5.0
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDICC5.0

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	0.7	ng	485808	1	7.642	293642	0.4
Ethene, 1,2-dif...	7.209	0.6	ng	414792	1	7.642	293642	0.4
6-Benzothiazola...	7.956	1.7	ng	1249800	1	7.642	293642	0.4
1-Propanamine, ...	8.442	1.0	ng	743066	1	7.642	293642	0.4
Fomepizole	9.342	2.8	ng	1229210	2	10.406	172726	0.4
Benzene, nitro-	9.595	0.5	ng	216254	2	10.406	172726	0.4
5-Aminopyrimidine	9.836	0.9	ng	368235	2	10.406	172726	0.4
m-Chloroaniline	10.571	2.1	ng	892006	2	10.406	172726	0.4
Methane, iodo-	11.709	0.9	ng	407777	2	10.406	172726	0.4
2-Propyl-4-meth...	12.300	5.3	ng	2297810	2	10.406	172726	0.4
Z-2-Propenoic a...	12.695	1.0	ng	455959	3	14.269	179191	0.4
E-2-Propenoic a...	12.771	0.9	ng	411386	3	14.269	179191	0.4
Naphthalene, 2-...	13.139	3.5	ng	1561860	3	14.269	179191	0.4
7-Benzofuranol,...	13.736	0.5	ng	233626	3	14.269	179191	0.4
Benzene, 2-meth...	13.850	1.3	ng	602415	3	14.269	179191	0.4
Benzene, 1-meth...	14.649	2.0	ng	881178	3	14.269	179191	0.4
2-Azafluorene	15.550	1.9	ng	840674	3	14.269	179191	0.4
3-Nitrotyramine	15.613	2.3	ng	1050000	3	14.269	179191	0.4
Glutaric acid, ...	16.677	1.6	ng	698374	4	17.029	172770	0.4
5-Fluoro-2-meth...	17.431	3.2	ng	1400380	4	17.029	172770	0.4