LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016600.D
Acq On : 30 Sep 2021 14:55
Operator : CG/JU
Sample : SSTDICCC0.4
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDICCC0.4

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: BN016600.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	9491	12362	3.08%	0.177%
2	3.585	51	55	76	rVB2	6005	27707	6.89%	0.396%
3	5.254	231	236	253	rVB2	14991	55623	13.84%	0.795%
4	6.821	401	406	418	rBV	23076	59227	14.74%	0.847%
5	6.978	419	423	429	rVV	15197	34477	8.58%	0.493%
6	7.080	430	434	441	rVV	32982	68635	17.08%	0.981%
7	7.200	441	447	460	rVB	11407	31086	7.73%	0.444%
8	7.531	478	483	490	rVB	6370	14277	3.55%	0.204%
9	7.642	490	495	506	rVB2	47112	114080	28.38%	1.631%
10	7.854	514	518	524	rBV2	4947	10831	2.69%	0.155%
11	7.956	524	529	537	rVV2	45580	102738	25.56%	1.469%
12	8.168	548	552	557	rVB	3110	7446	1.85%	0.106%
13	8.442	572	578	594	rVB2	19424	50146	12.48%	0.717%
14	8.695	595	598	601	rBV	4534	8744	2.18%	0.125%
15	8.784	601	605	607	rBV	33514	68663	17.08%	0.982%
16	8.822	607	608	612	rVB	24507	37818	9.41%	0.541%
17	9.342	646	649	653	rBV	47007	77960	19.40%	1.115%
18	9.532	661	664	666	rBV	3694	6742	1.68%	0.096%
19	9.595	666	669	678	rVB	8691	15589	3.88%	0.223%
20	9.836	685	688	700	rBV	15539	27308	6.79%	0.390%
21	10.064	703	706	708	rBV	4113	8002	1.99%	0.114%
22	10.406	730	733	735	rBV	99805	180715	44.96%	2.584%
23	10.457	735	737	741	rVV	108483	178214	44.34%	2.548%
24	10.584	743	747	756	rVV	25291	57401	14.28%	0.821%
25	10.749	757	760	763	rVB	32140	52454	13.05%	0.750%
26	11.306	801	804	815	rBV	2069	5422	1.35%	0.078%
27	11.709	854	865	891	rBV	13329	24892	6.19%	0.356%
28	12.007	920	932	940	rBV	54897	88836	22.10%	1.270%
29	12.078	940	948	973	rVB	122075	196560	48.90%	2.810%
30	12.300	988	998	1021	rBV	120382	190958	47.51%	2.730%
31	12.518	1043	1045	1048	rBV3	1586	4688	1.17%	0.067%
32	12.695	1056	1059	1062	rBV	15587	27448	6.83%	0.392%
33	12.771	1062	1065	1071	rVB	13029	23869	5.94%	0.341%
34	12.898	1071	1075	1078	rBV	112221	183974	45.77%	2.630%
35	13.139	1091	1094	1097	rVB	79386	120342	29.94%	1.721%
36	13.736	1138	1141	1143	rBV	11013	15544	3.87%	0.222%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016600.D
Acq On : 30 Sep 2021 14:55
Operator : CG/JU
Sample : SSTDICCC0.4
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDICCC0.4

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	13.850	1147	1150	1155	rVB	16654	26257	6.53%	0.375%
38	13.989	1158	1161	1164	rVB	99762	148270	36.89%	2.120%
39	14.268	1180	1183	1186	rBV	126429	186066	46.29%	2.660%
40	14.332	1186	1188	1191	rVB	160429	225724	56.16%	3.227%
41	14.649	1209	1213	1220	rBV3	15794	40525	10.08%	0.579%
42	14.827	1224	1227	1230	rBV	5275	9164	2.28%	0.131%
43	14.903	1230	1233	1243	rVB	7455	11838	2.95%	0.169%
44	15.106	1246	1249	1252	rBV	7601	10410	2.59%	0.149%
45	15.322	1263	1266	1270	rBV2	186213	320619	79.77%	4.584%
46	15.410	1270	1273	1280	rVV2	4839	9946	2.47%	0.142%
47	15.550	1280	1284	1287	rVV2	30869	56006	13.93%	0.801%
48	15.613	1287	1289	1293	rVB2	34603	58588	14.58%	0.838%
49	15.766	1298	1301	1312	rVB2	12471	20995	5.22%	0.300%
50	16.226	1335	1338	1341	rBV2	57727	82173	20.44%	1.175%
51	16.324	1343	1346	1350	rVB	38760	64911	16.15%	0.928%
52	16.506	1358	1361	1372	rBV	21225	31387	7.81%	0.449%
53	16.677	1372	1375	1384	rBV	18973	32595	8.11%	0.466%
54	17.029	1400	1404	1405	rBV	79605	140501	34.96%	2.009%
55	17.066	1405	1407	1410	rVV	140513	195939	48.75%	2.802%
56	17.151	1411	1414	1434	rVB	91655	167330	41.63%	2.393%
57	17.431	1434	1437	1453	rBV	73185	122709	30.53%	1.755%
58	18.020	1483	1486	1498	rVB	5054	6993	1.74%	0.100%
59	19.068	1686	1697	1699	rBV	103088	134727	33.52%	1.926%
60	19.097	1699	1703	1738	rVB	163452	235896	58.69%	3.373%
61	19.460	1767	1776	1813	rBV	160996	224233	55.79%	3.206%
62	19.678	1813	1820	1859	rVB	96121	123132	30.64%	1.761%
63	20.378	1918	1921	1925	rBV	38107	54926	13.67%	0.785%
64	21.025	1979	1982	1993	rBV	16008	30563	7.60%	0.437%
65	21.174	1993	1996	1998	rBV	55485	68396	17.02%	0.978%
66	21.227	1998	2001	2003	rVV2	178677	357833	89.03%	5.116%
67	21.270	2003	2005	2017	rVB	176133	234689	58.39%	3.356%
68	22.056	2076	2079	2090	rVB	65806	86668	21.56%	1.239%
69	22.810	2218	2230	2236	rBV	111707	181141	45.07%	2.590%
70	22.854	2236	2243	2281	rVB	111819	192045	47.78%	2.746%
71	23.388	2386	2399	2415	rBV	77801	152982	38.06%	2.187%
72	23.488	2416	2428	2475	rVB	75502	158822	39.52%	2.271%
73	25.778	3066	3097	3189	rBV4	104723	401923	100.00%	5.747%
74	26.459	3273	3296	3335	rBV	59753	196204	48.82%	2.805%

Sum of corrected areas: 6993904

Instrument :
BNA_N
LabSampleId :
SSTDICCC0.4

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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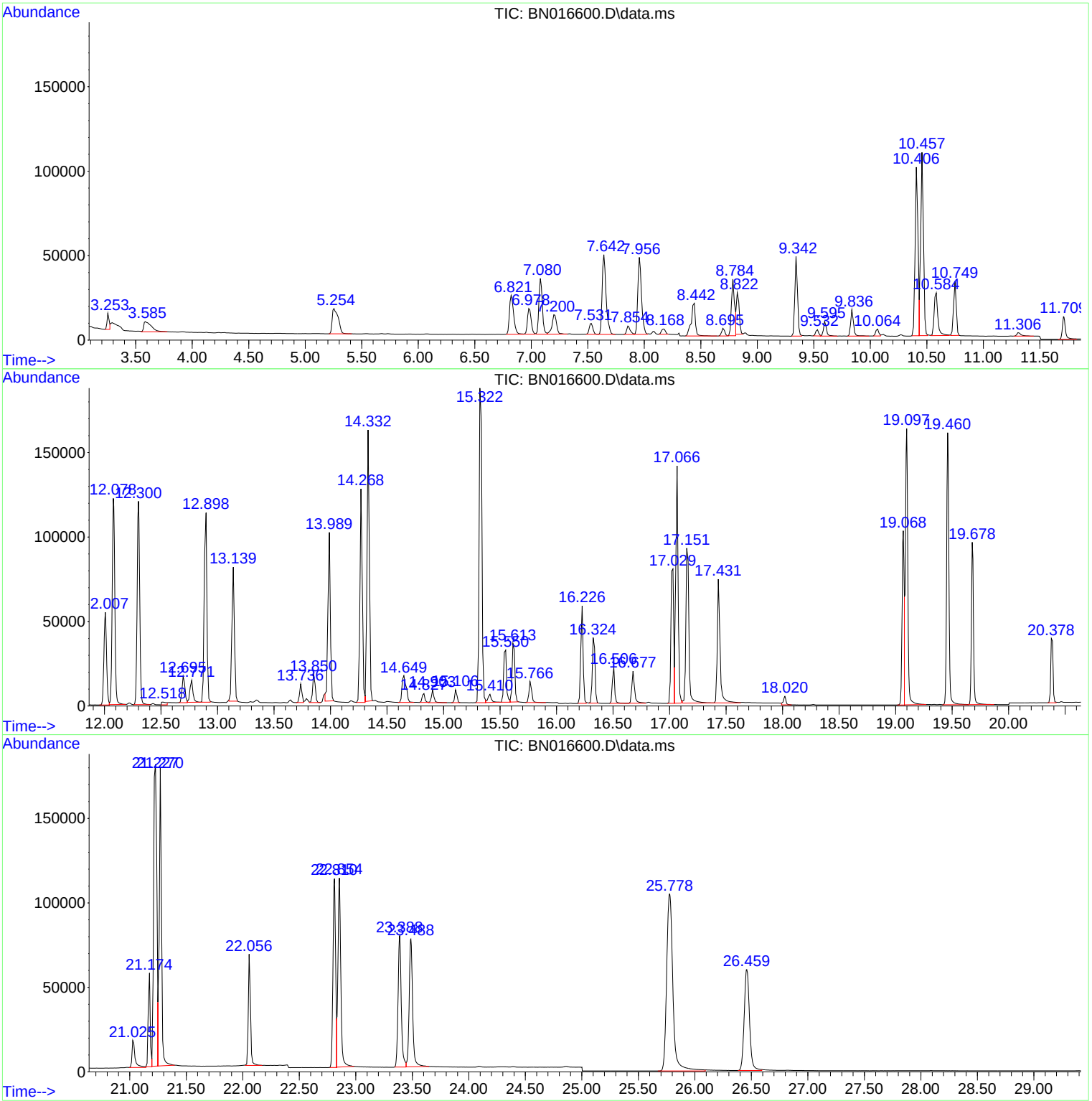
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICCC0.4

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 : BN016600.D
Acq On : 30 Sep 2021 14:55
Operator : CG/JU
Sample : SSTDICCC0.4
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICCC0.4

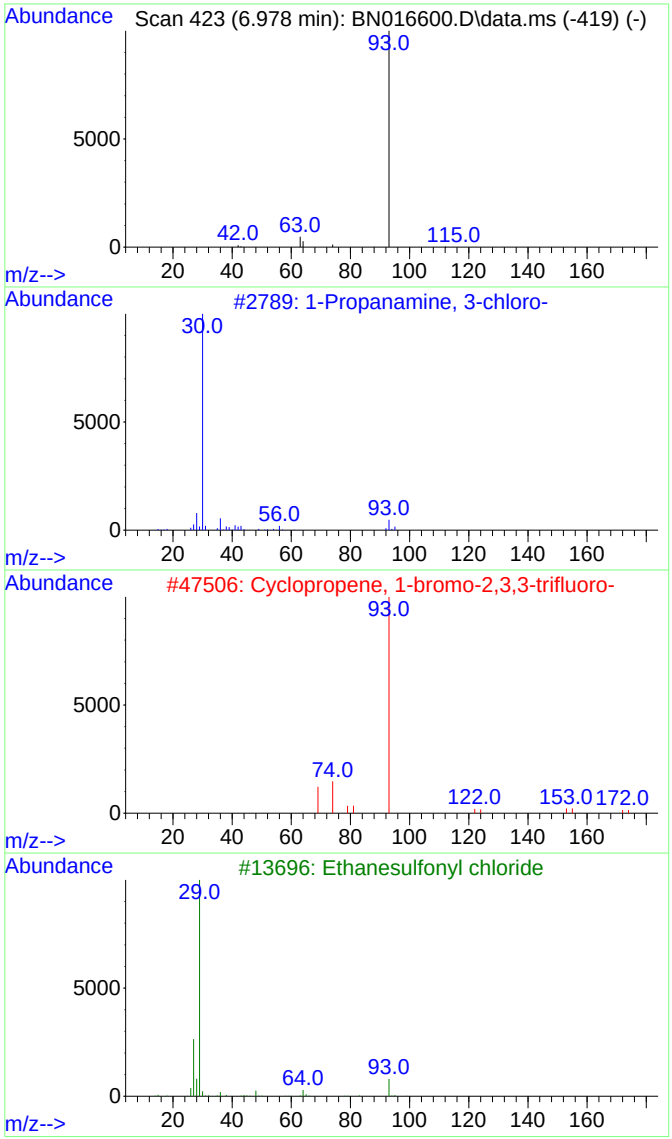
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

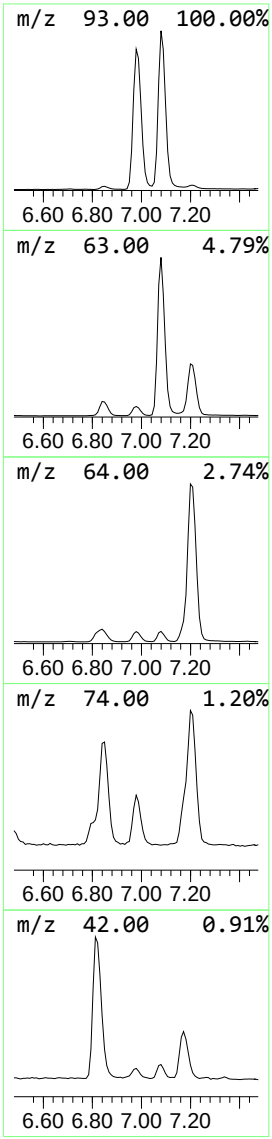
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.978	0.12 ng	34477	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 : BN016600.D
Acq On : 30 Sep 2021 14:55
Operator : CG/JU
Sample : SSTDICCC0.4
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICCC0.4

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

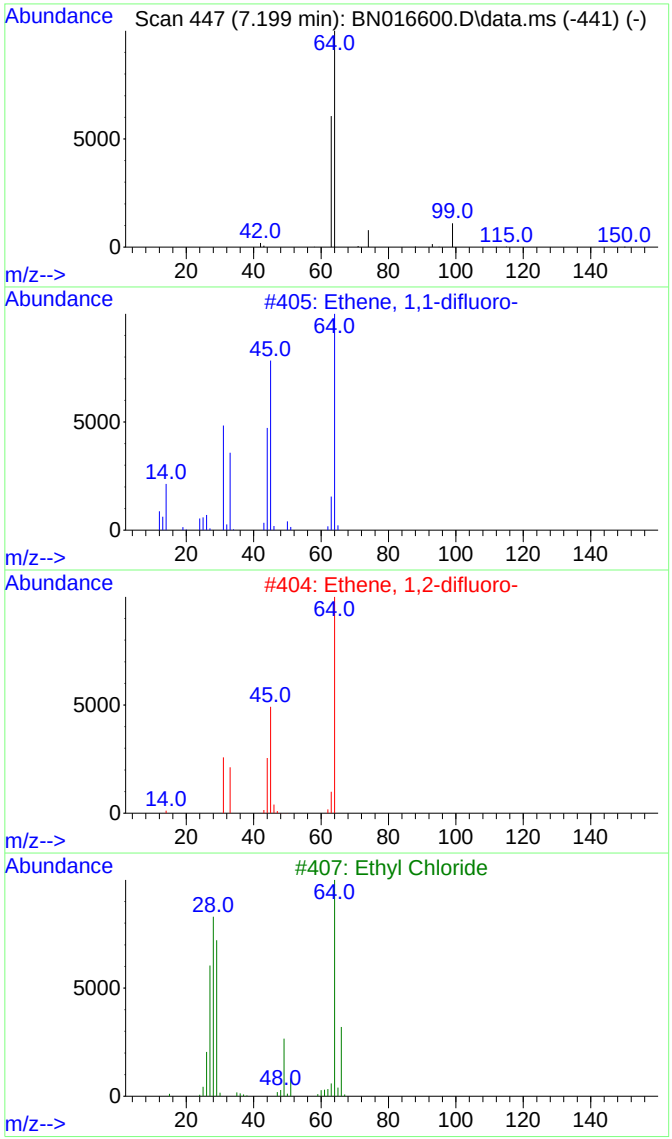
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

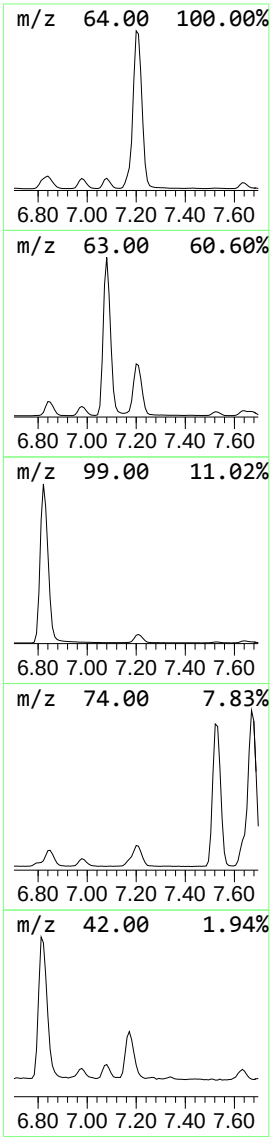
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.199	0.11 ng	31086	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	Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	3
3	Ethyl Chloride	64	C2H5Cl	000075-00-3	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 : BN016600.D
Acq On : 30 Sep 2021 14:55
Operator : CG/JU
Sample : SSTDICCC0.4
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICCC0.4

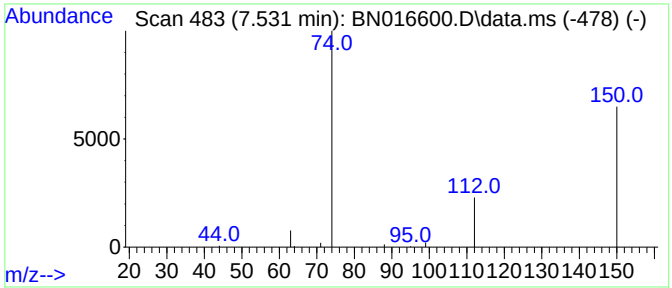
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

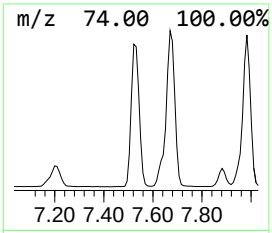
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

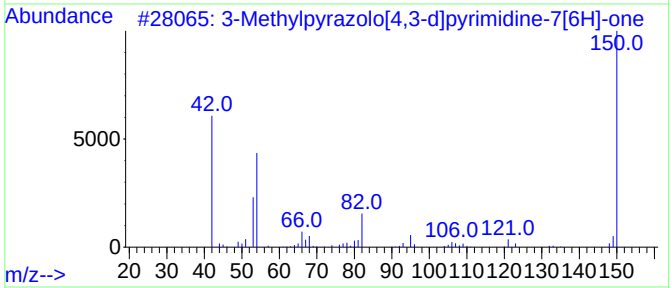
****
Peak Number 3 3-Methylpyrazolo[4,3-d]pyri... Concentration Rank 20

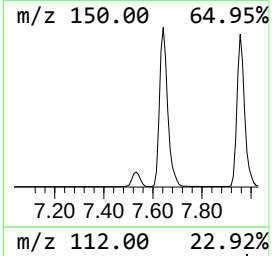
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.531	0.05 ng	14277	1,4-Dichlorobenzene-d4	7.642

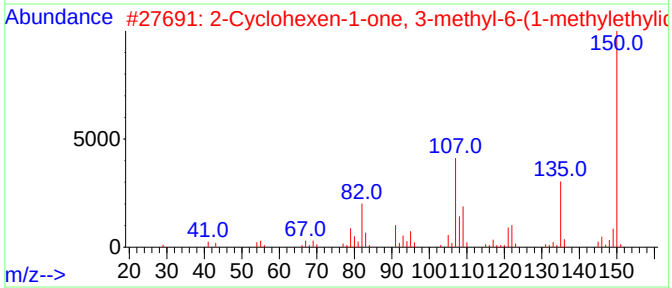
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methylpyrazolo[4,3-d]pyrimidin...	150	C6H6N4O	005399-94-0	2
2	2-Cyclohexen-1-one, 3-methyl-6-(...	150	C10H14O	000491-09-8	2
3	4-Methyl-bi(1,2,4)-triazole-3,1'	150	C5H6N6	063523-89-7	2
4	N-Nitrosodimethylamine	74	C2H6N2O	000062-75-9	2
5	Propanoic acid	74	C3H6O2	000079-09-4	2

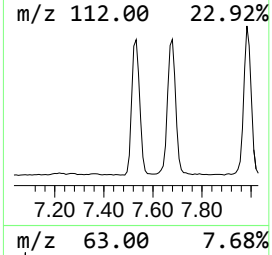


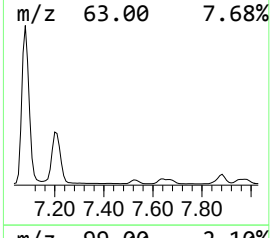


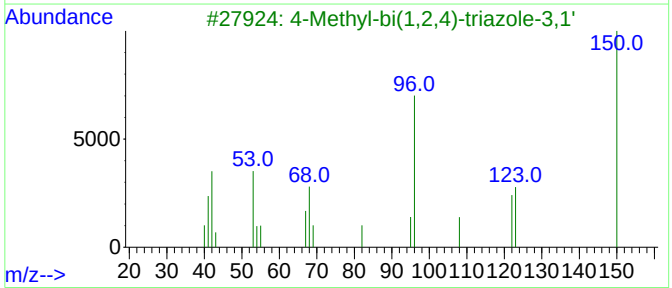


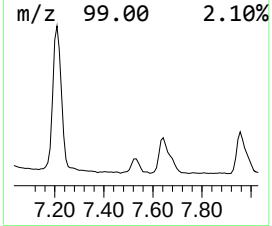












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Acq On : 30 Sep 2021 14:55
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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICCC0.4

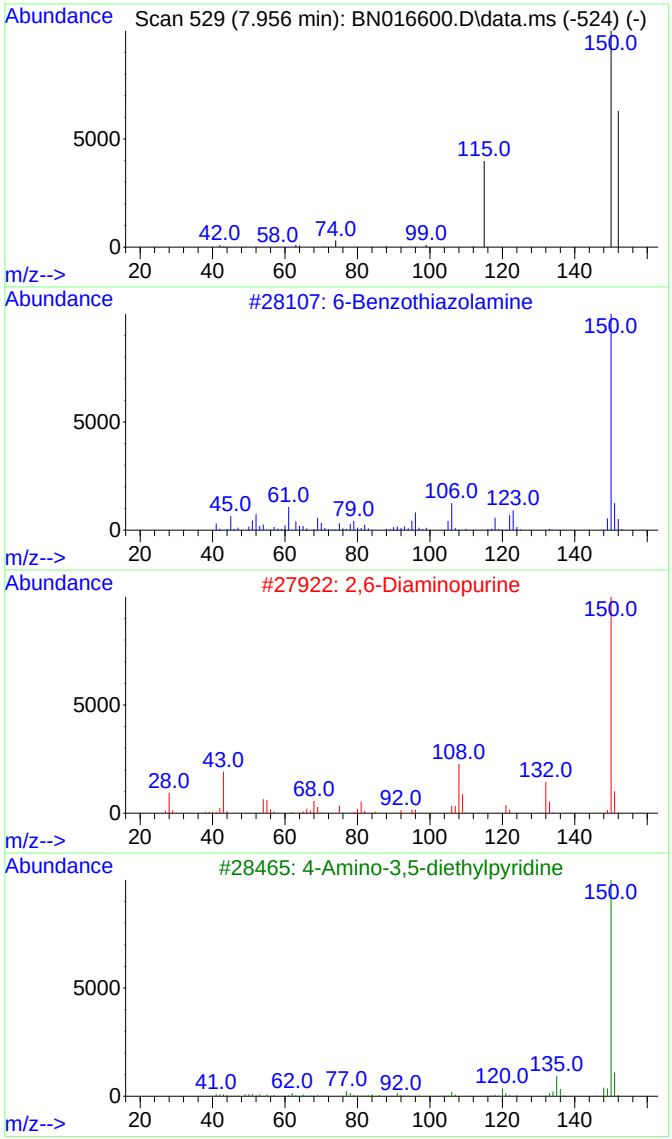
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

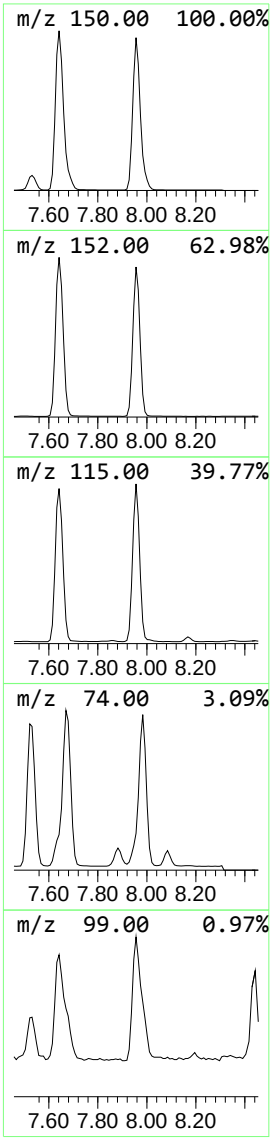
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.956	0.36 ng	102738	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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Data File : BN016600.D
Acq On : 30 Sep 2021 14:55
Operator : CG/JU
Sample : SSTDICCC0.4
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICCC0.4

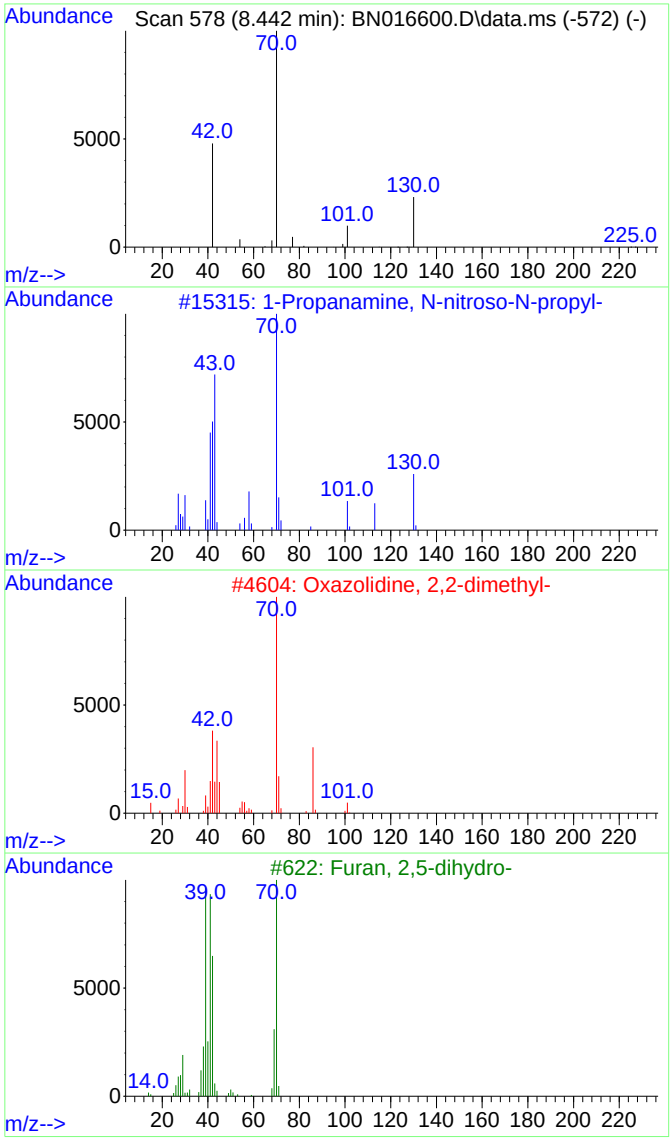
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

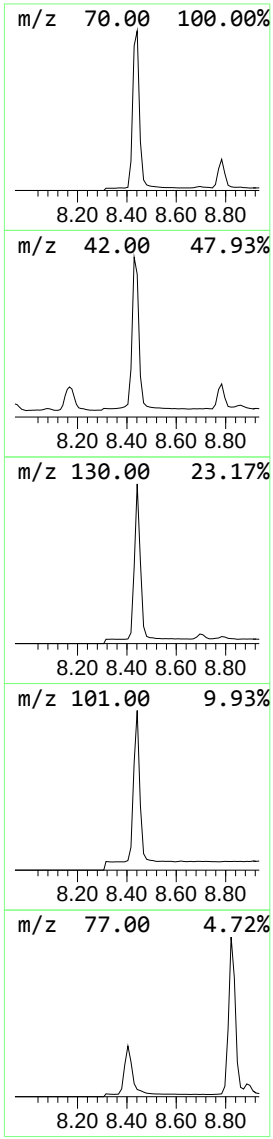
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Propanamine, N-nitroso-N-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.442	0.18 ng	50146	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	72
2	Oxazolidine, 2,2-dimethyl-	101	C5H11NO	020515-62-2	7
3	Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	7
4	Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	5
5	1-Oxa-3,4-diazacyclopentadiene	70	C2H2N2O	000288-99-3	4





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ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICCC0.4

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

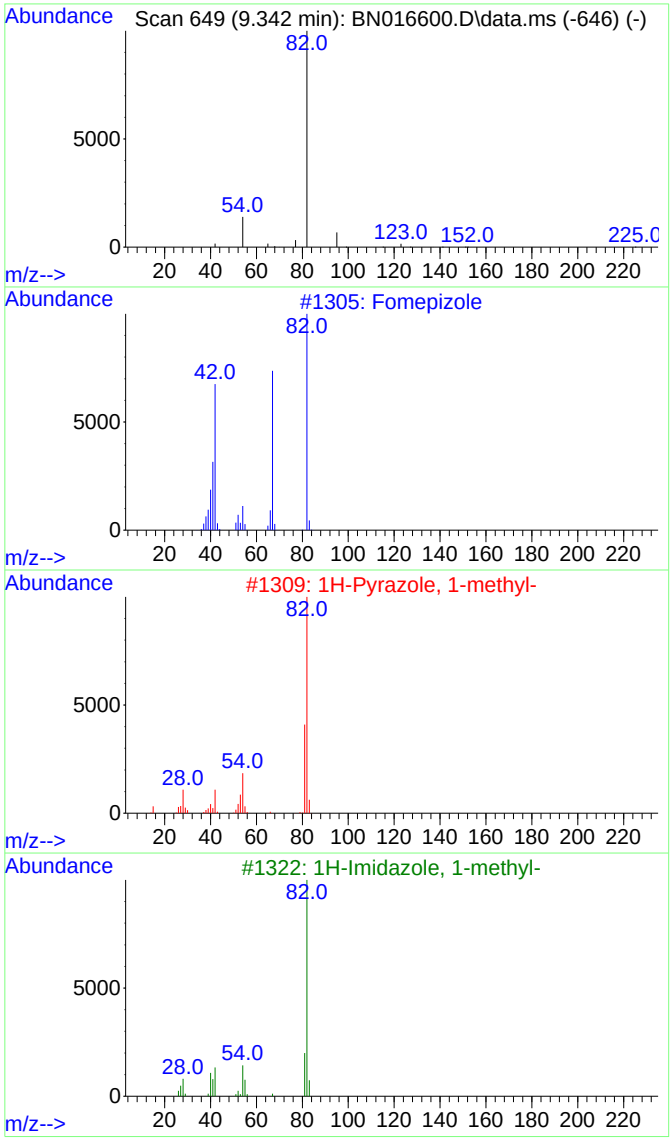
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

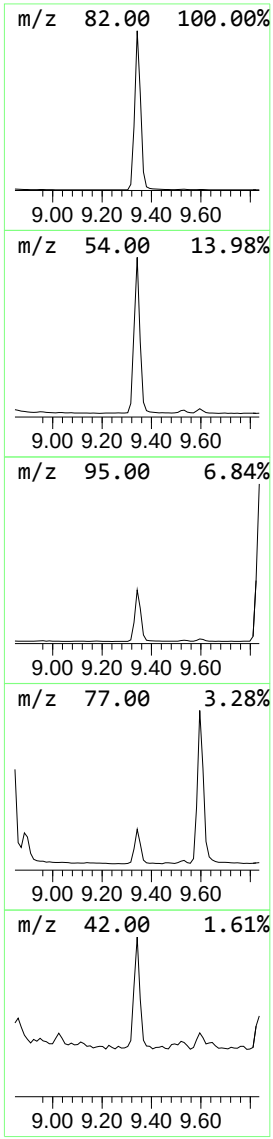
****

Peak Number 6 Fomepizole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.342	0.17 ng	77960	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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Sample : SSTDICCC0.4
Misc :
ALS Vial : 4 Sample Multiplier: 1

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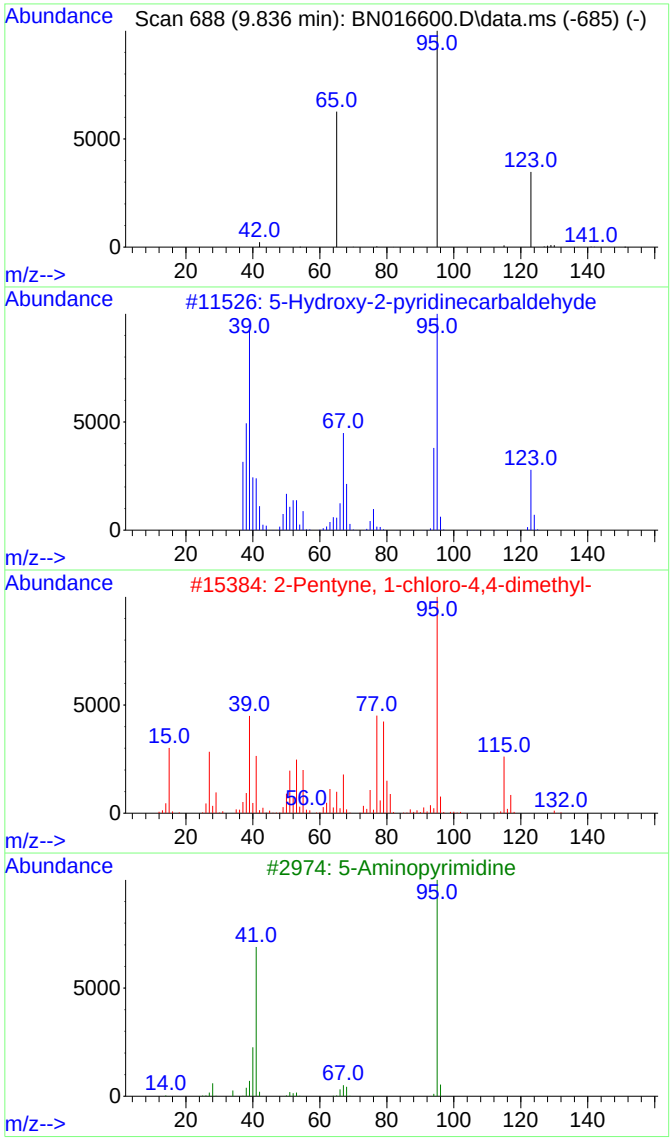
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

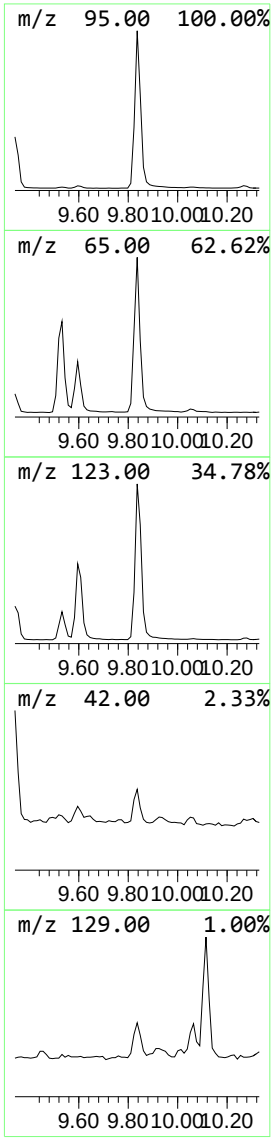
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 5-Hydroxy-2-pyridinecarbald... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.836	0.06 ng	27308	Naphthalene-d8	10.406

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Hydroxy-2-pyridinecarbaldehyde	123	C6H5NO2	031191-08-9	5
2	2-Pentyne, 1-chloro-4,4-dimethyl-	130	C7H11Cl	055683-00-6	4
3	5-Aminopyrimidine	95	C4H5N3	000591-55-9	3
4	2-Furanmethanethiol, 5-methyl-	128	C6H8OS	059303-05-8	3
5	4-Aminopyrimidine	95	C4H5N3	000591-54-8	2





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Misc :
ALS Vial : 4 Sample Multiplier: 1

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

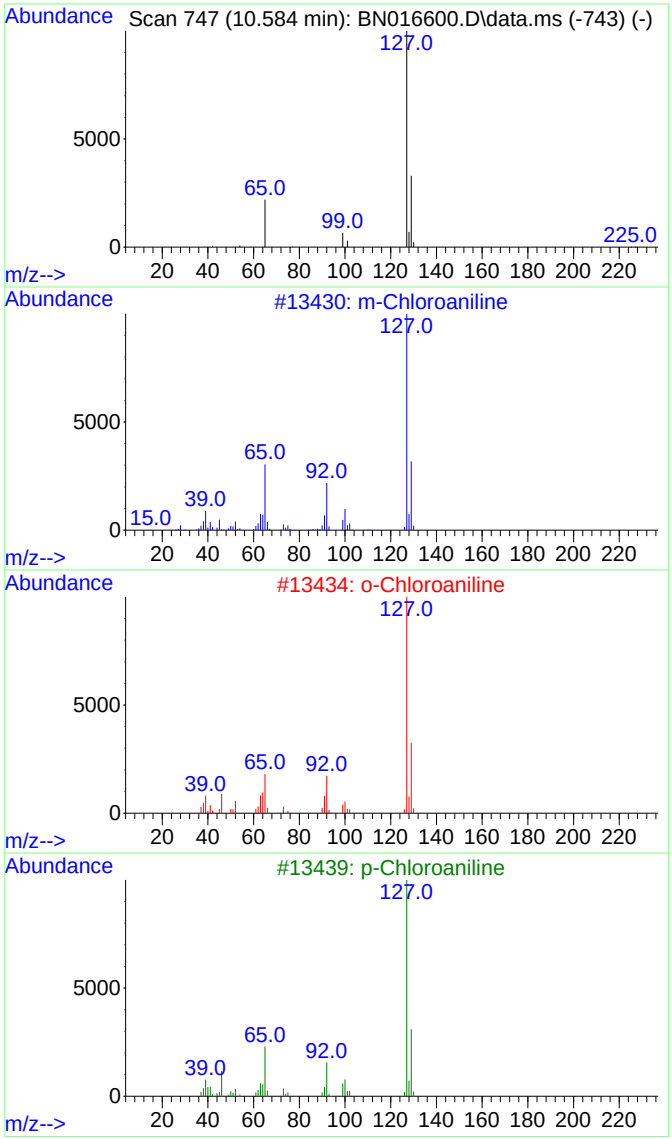
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

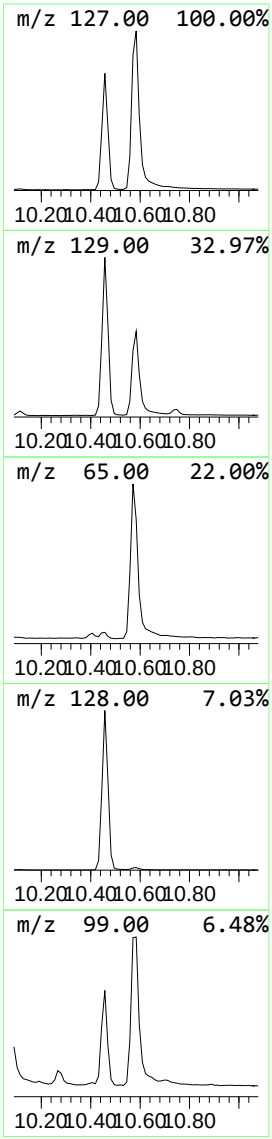
****

Peak Number 8 m-Chloroaniline Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.584	0.13 ng	57401	Naphthalene-d8	10.406

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	m-Chloroaniline	127	C6H6ClN	000108-42-9	90
2	o-Chloroaniline	127	C6H6ClN	000095-51-2	90
3	p-Chloroaniline	127	C6H6ClN	000106-47-8	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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Misc :
ALS Vial : 4 Sample Multiplier: 1

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

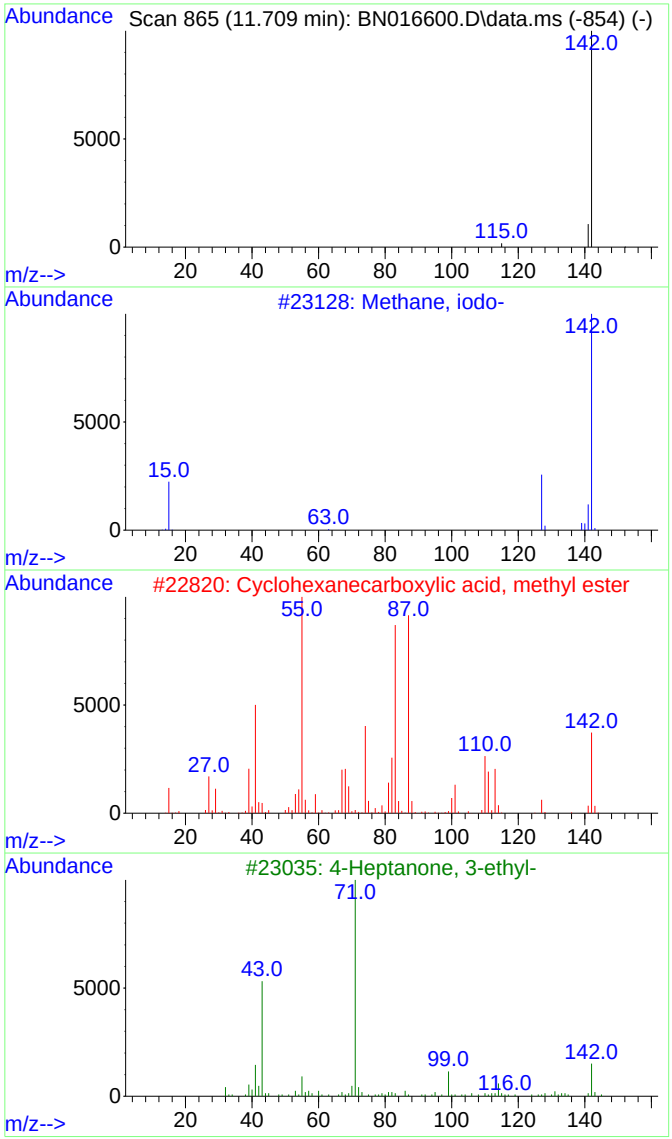
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

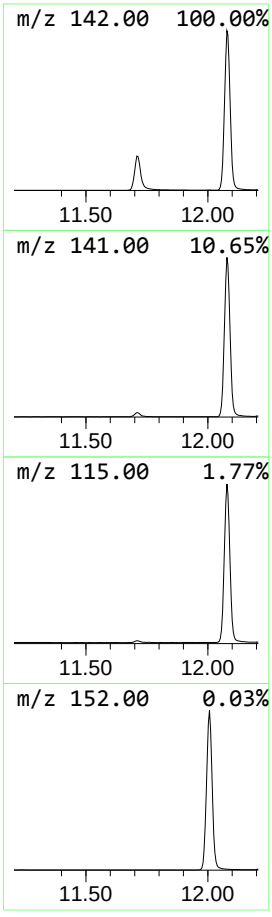
****

Peak Number 9 Methane, iodo- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.709	0.06 ng	24892	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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Sample : SSTDICCC0.4
Misc :
ALS Vial : 4 Sample Multiplier: 1

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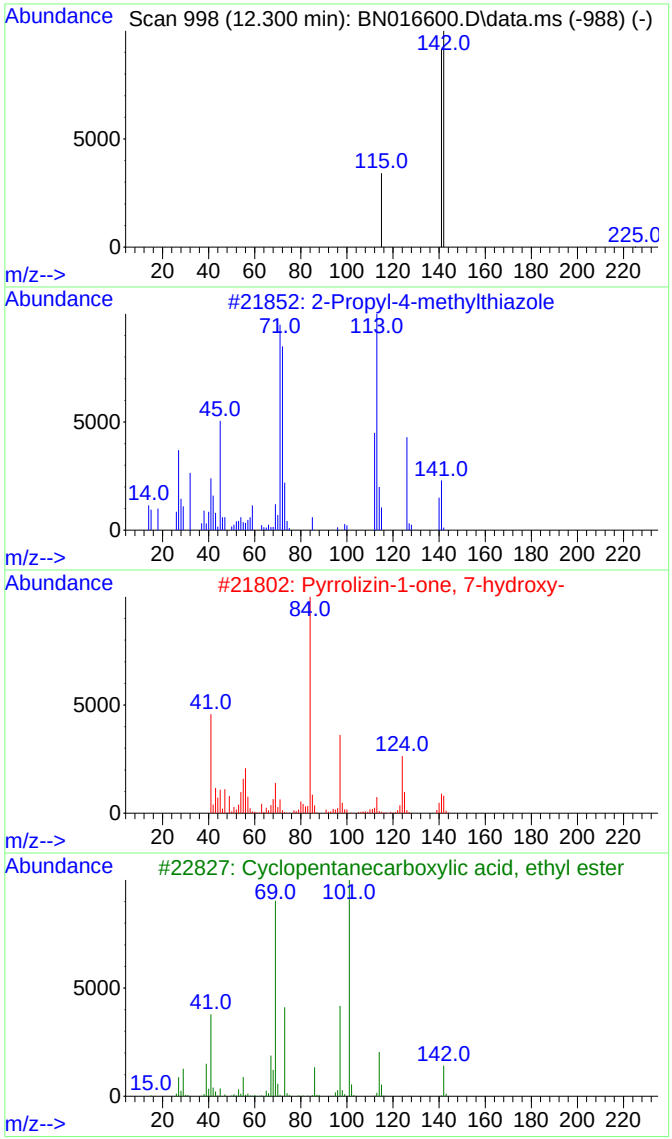
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

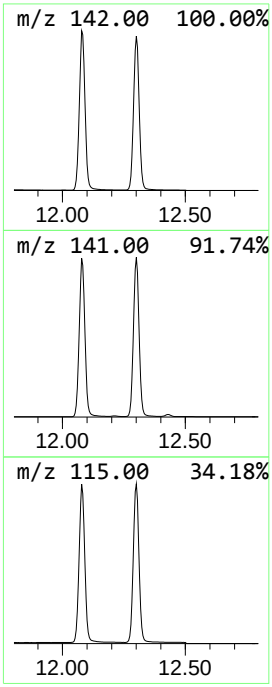
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.300	0.42 ng	190958	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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Misc :
ALS Vial : 4 Sample Multiplier: 1

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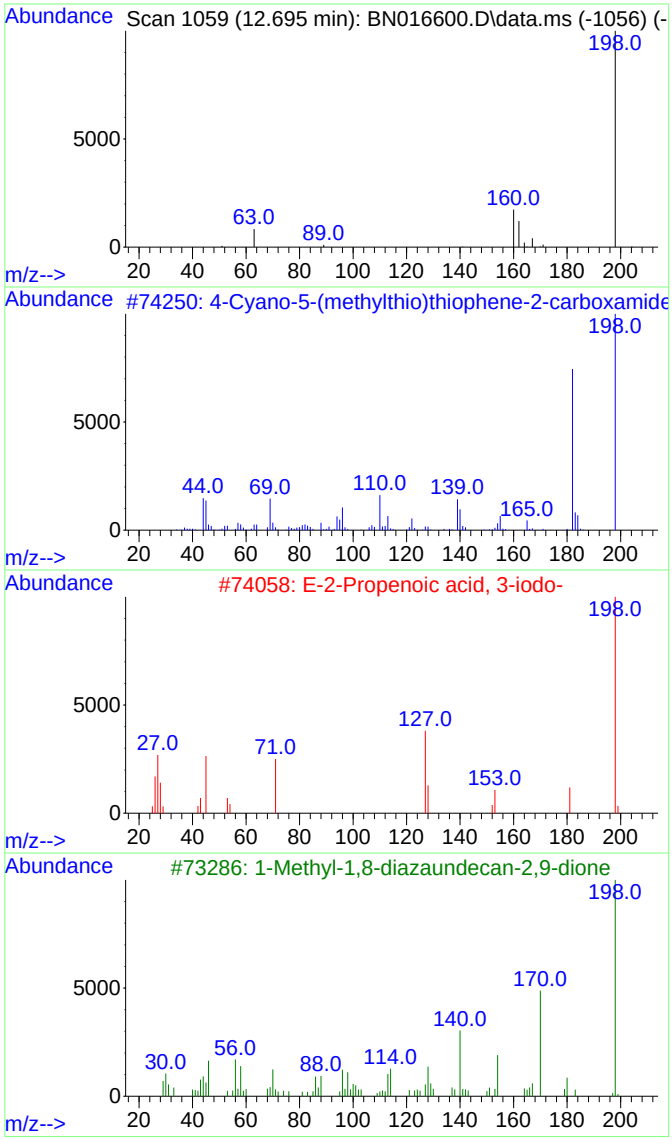
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

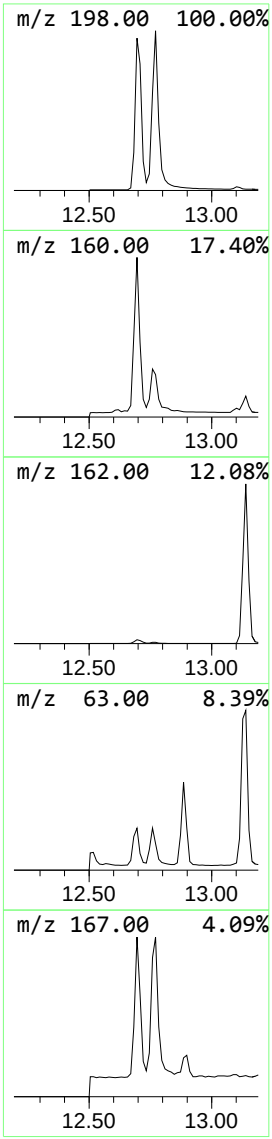
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 4-Cyano-5-(methylthio)thiop... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.695	0.06 ng	27448	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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Sample : SSTDICCC0.4
Misc :
ALS Vial : 4 Sample Multiplier: 1

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

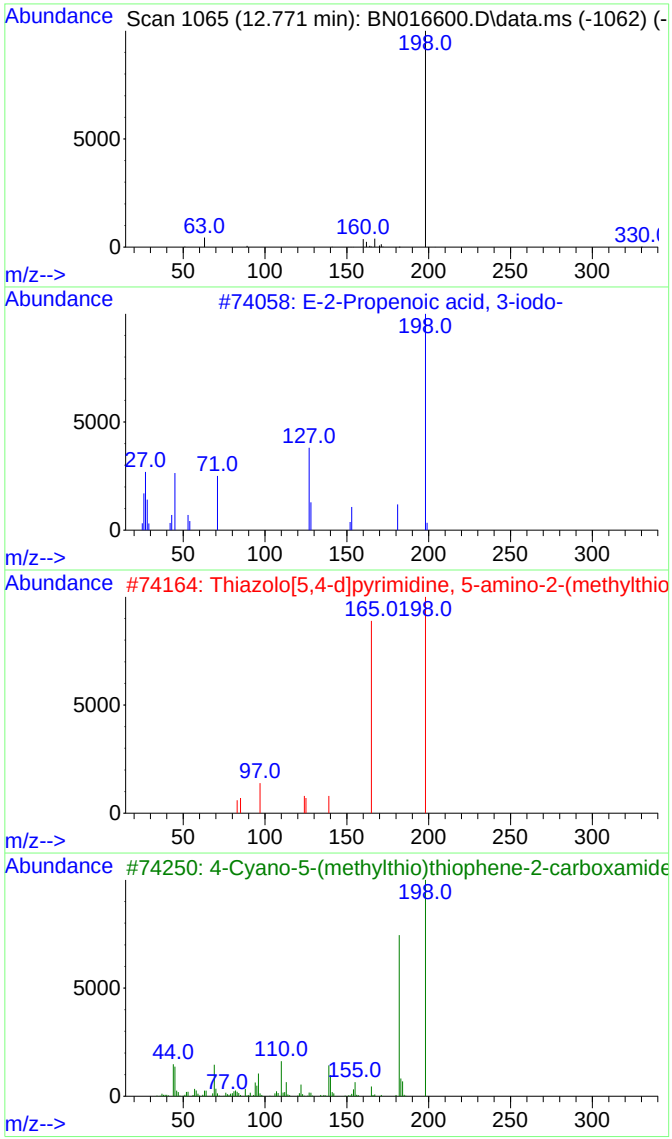
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

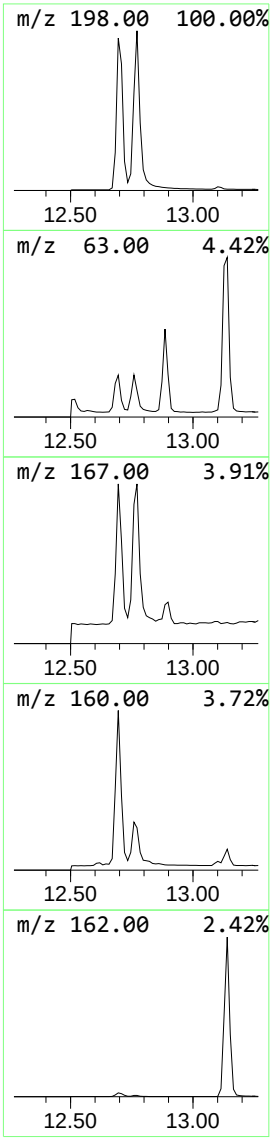
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.771	0.05 ng	23869	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	Thiazolo[5,4-d]pyrimidine, 5-ami...	198	C6H6N4S2	019835-31-5	3
3	4-Cyano-5-(methylthio)thiophene-...	198	C7H6N2OS2	1000267-39-2	3
4	Z-2-Propenoic acid, 3-iodo-	198	C3H3IO2	1000308-86-8	3
5	Imidazolidine-2,4,5-trione, 1,3-...	198	C7H6N2O5	115083-04-0	2





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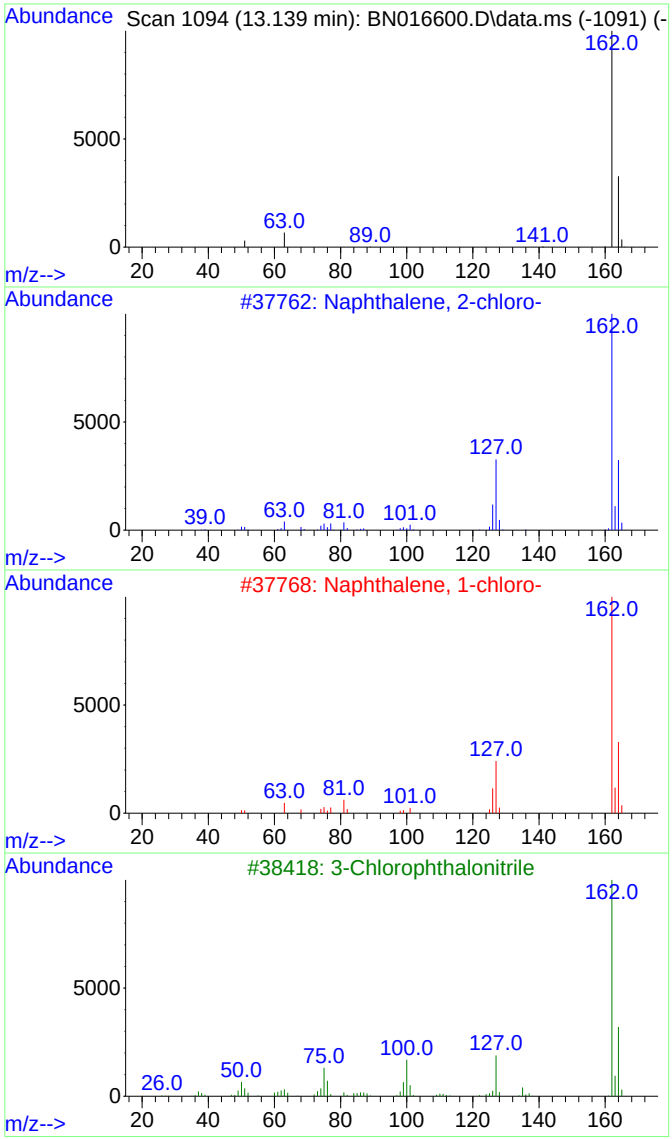
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

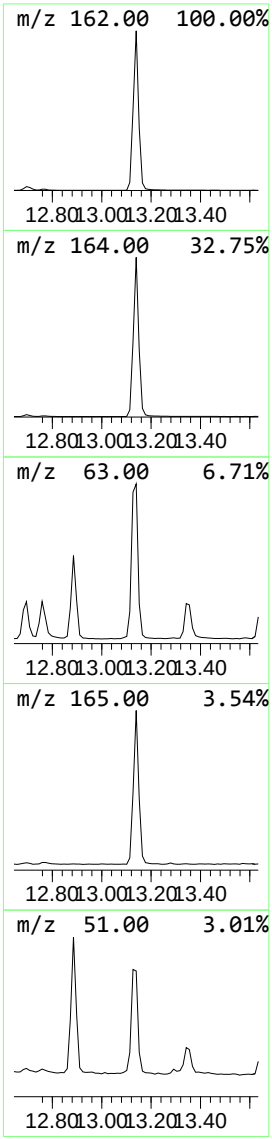
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.139	0.26 ng	120342	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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Instrument :
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LabSampleId :
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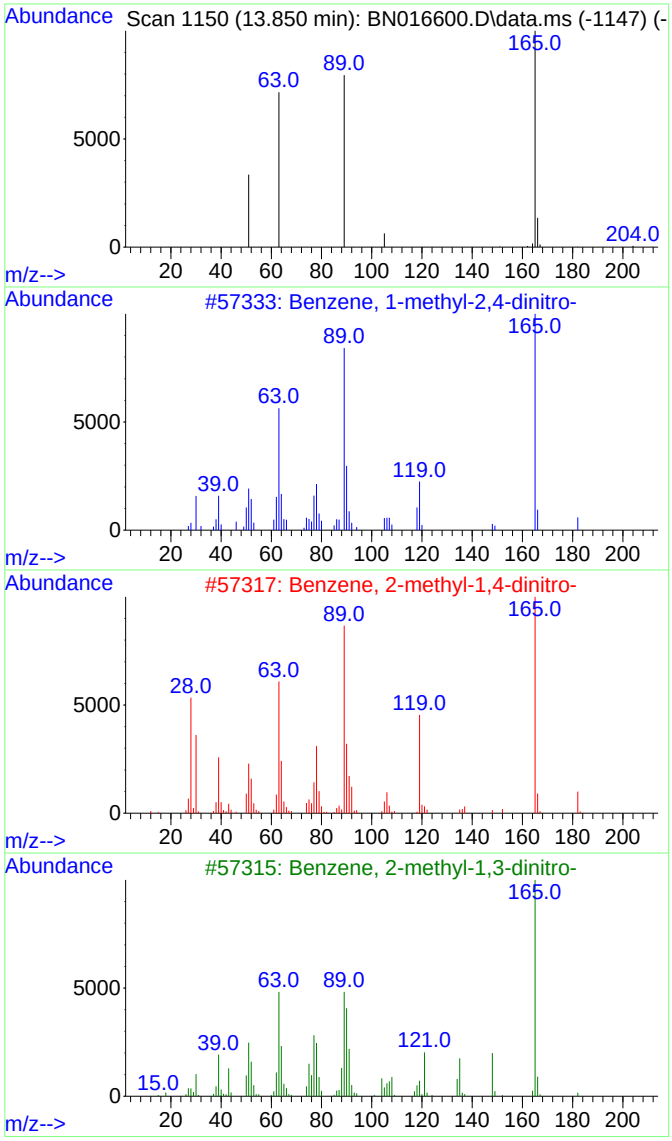
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

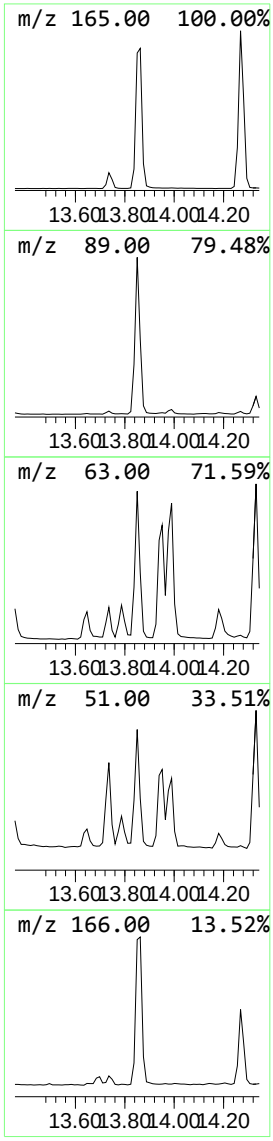
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 Benzene, 1-methyl-2,4-dinitro- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.850	0.06 ng	26257	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-1,4-dinitro-	182	C7H6N2O4	000619-15-8	74
3	Benzene, 2-methyl-1,3-dinitro-	182	C7H6N2O4	000606-20-2	40
4	Benzene, 1-(chloromethyl)-2-nitro-	171	C7H6ClNO2	000612-23-7	9
5	(4-Methylsulfanylphenyl)carbamic...	301	C16H15NO3S	1000305-20-0	9





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ALS Vial : 4 Sample Multiplier: 1

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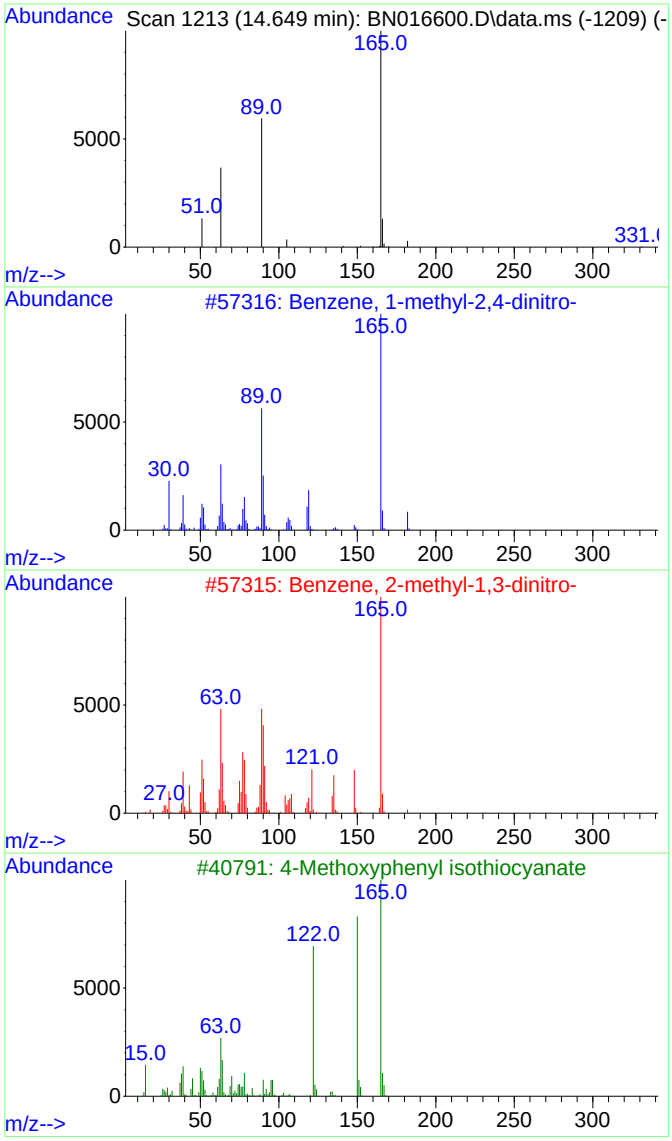
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

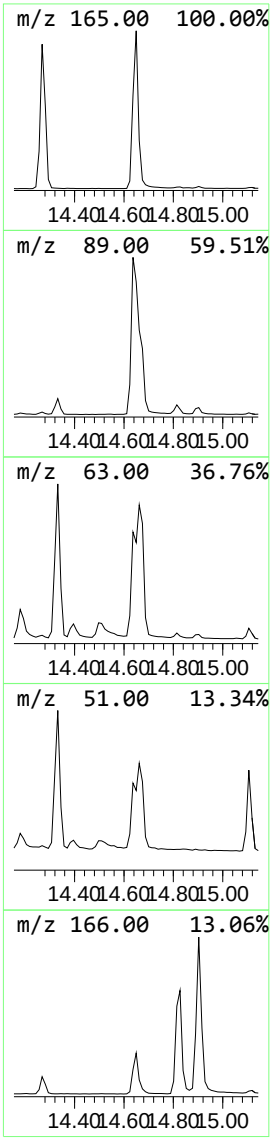
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.649	0.09 ng	40525	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	2(3H)-Benzoxazolethione, 5-methyl-	165	C8H7NOS	022876-22-8	9
5	6-Nitro-m-tolunitrile	162	C8H6N2O2	064113-86-6	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

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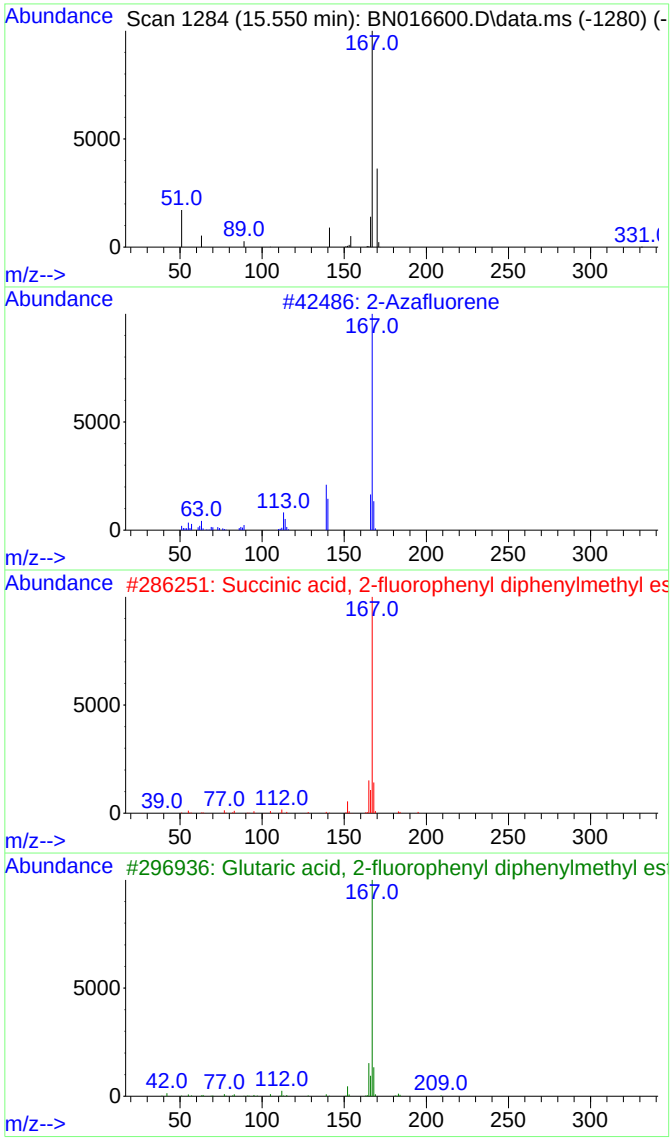
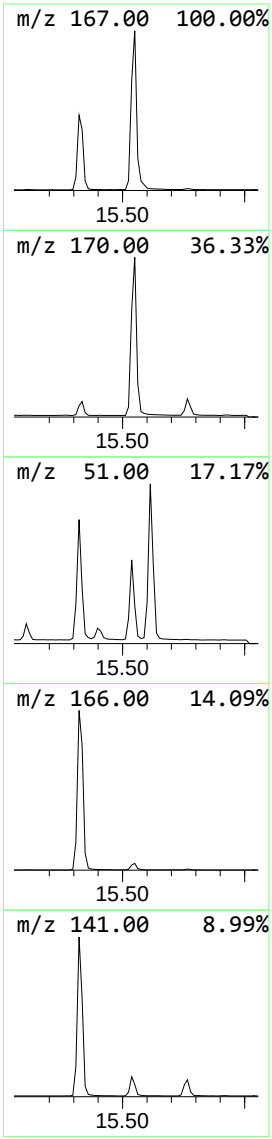
Peak Number 16 2-Azafluorene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.550	0.12 ng	56006	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	Glutaric acid, 2-fluorophenyl di...	392	C24H21FO4	1000393-34-5	9
4	Thiazolo[3,2-a]pyridinium, 2,3-d...	167	C8H9NOS	023003-43-2	7
5	Carbazole	167	C12H9N	000086-74-8	7





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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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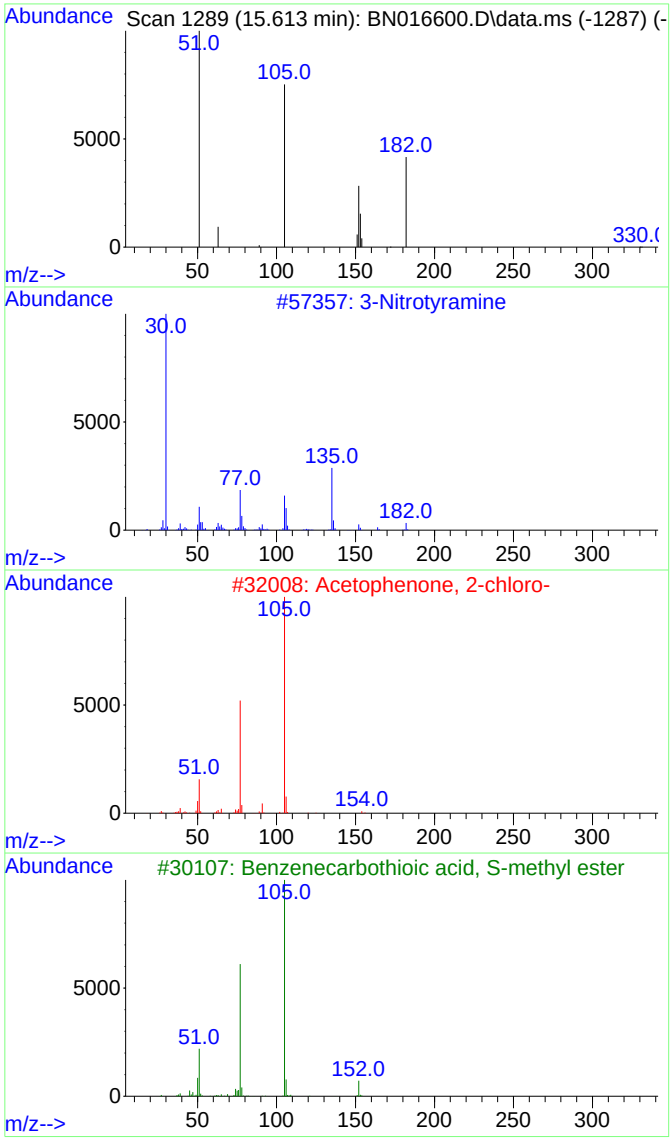
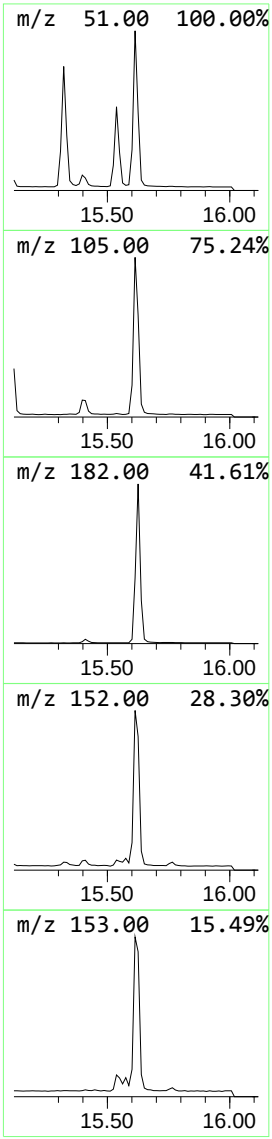
Peak Number 17 3-Nitrotyramine Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.613	0.13 ng	58588	Acenaphthene-d10	14.269

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





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Acq On : 30 Sep 2021 14:55
Operator : CG/JU
Sample : SSTDICCC0.4
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICCC0.4

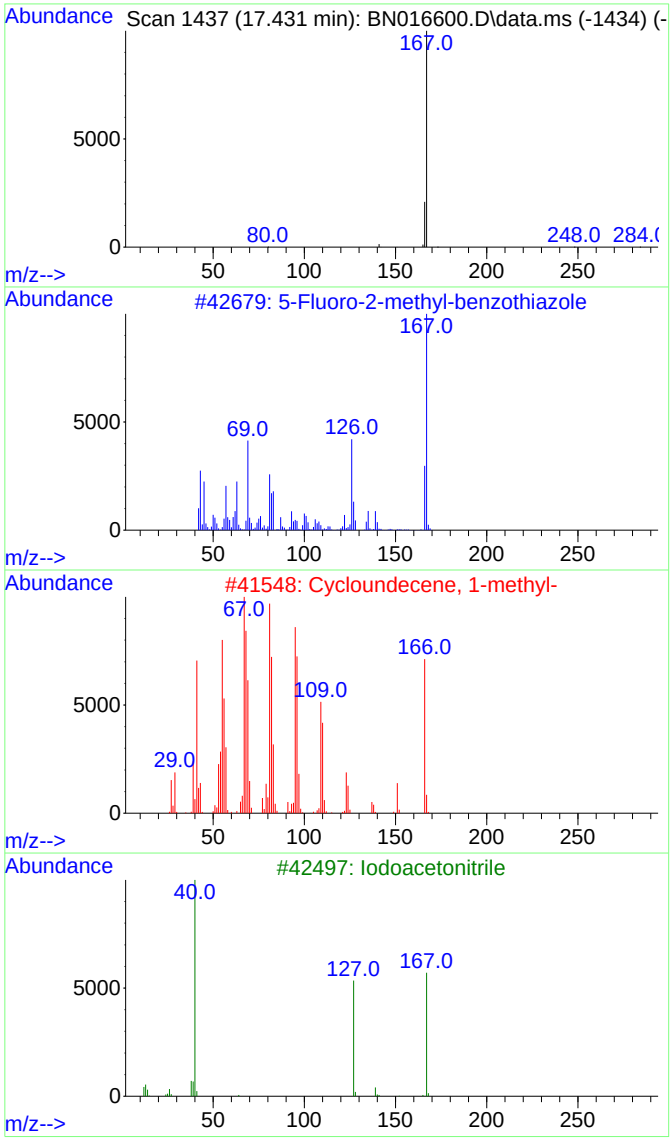
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

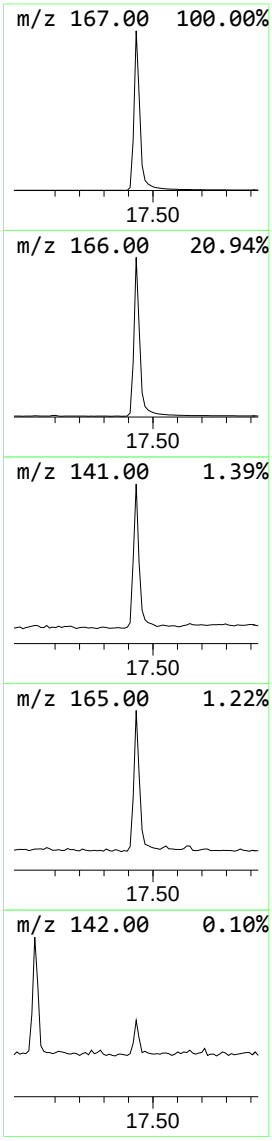
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
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	122709	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





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016600.D
Acq On : 30 Sep 2021 14:55
Operator : CG/JU
Sample : SSTDICCC0.4
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICCC0.4

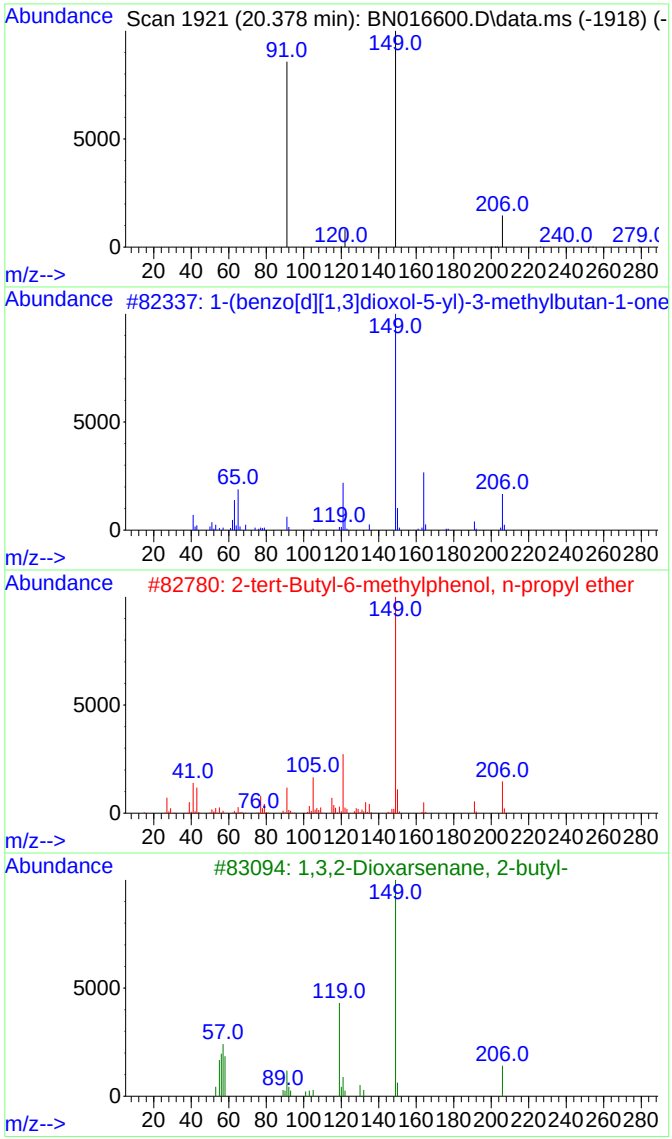
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

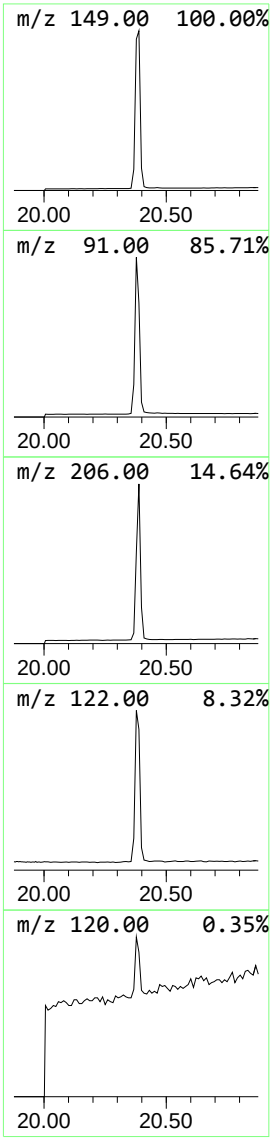
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 1-(benzo[d][1,3]dioxol-5-yl... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.378	0.06 ng	54926	Chrysene-d12	21.238

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(benzo[d][1,3]dioxol-5-yl)-3-m...	206	C12H14O3	1000456-66-2	9
2	2-tert-Butyl-6-methylphenol, n-p...	206	C14H22O	1000395-19-2	5
3	1,3,2-Dioxarsenane, 2-butyl-	206	C7H15AsO2	042541-33-3	5
4	2-Methyl-2-(4'-methoxyphenyl)pen...	206	C13H18O2	185700-49-6	5
5	Phenylpropanamide	149	C9H11NO	000102-93-2	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016600.D
Acq On : 30 Sep 2021 14:55
Operator : CG/JU
Sample : SSTDICCC0.4
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_N
LabSampleId :
SSTDICCC0.4

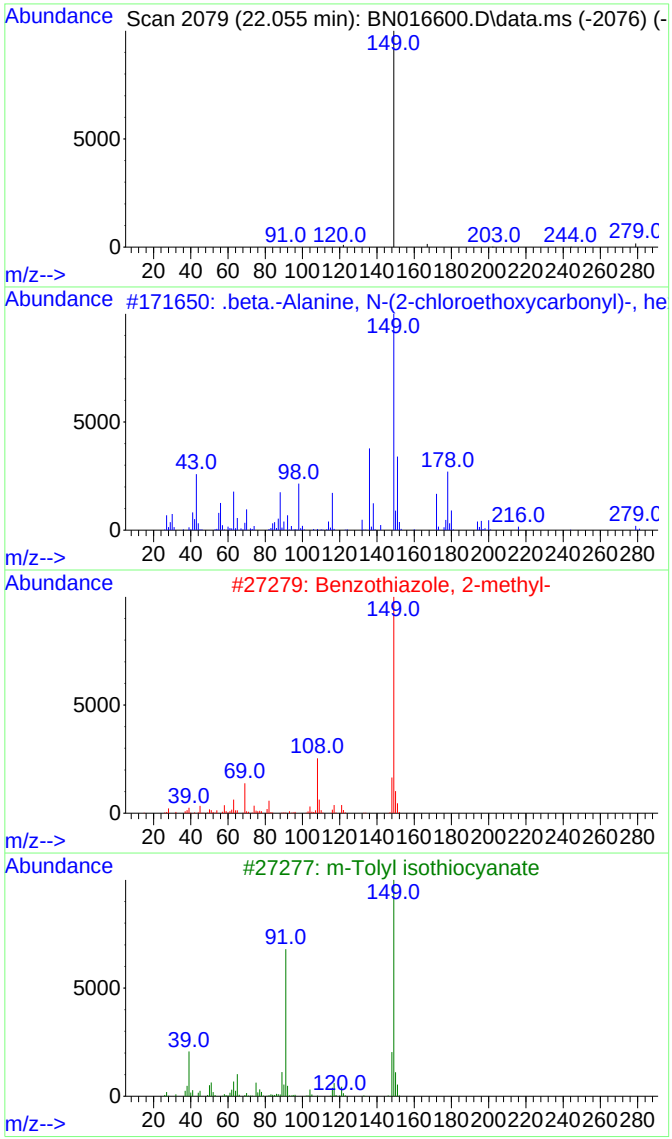
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

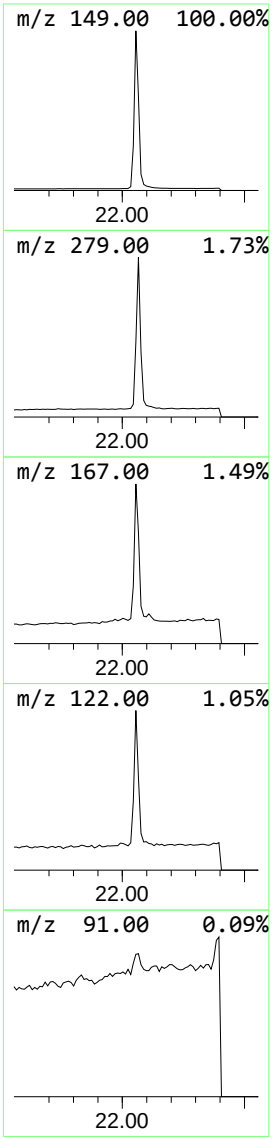
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.055	0.10 ng	86668	Chrysene-d12	21.238

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Alanine, N-(2-chloroethox...	279	C12H22ClNO4	1010328-58-4	4
2	Benzothiazole, 2-methyl-	149	C8H7NS	000120-75-2	4
3	m-Tolyl isothiocyanate	149	C8H7NS	000621-30-7	4
4	Benzene, 1-isothiocyanato-4-methyl-	149	C8H7NS	000622-59-3	4
5	3-Hydroxy-2-pyridin-3-yl-propenal	149	C8H7NO2	1000311-61-6	4





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016600.D
Acq On : 30 Sep 2021 14:55
Operator : CG/JU
Sample : SSTDICCC0.4
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_N
LabSampleId : SSTDICCC0.4

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	34477	1	7.642	114080	0.4
Ethene, 1,1-dif...	7.199	0.1	ng	31086	1	7.642	114080	0.4
3-Methylpyrazol...	7.531	0.1	ng	14277	1	7.642	114080	0.4
6-Benzothiazola...	7.956	0.4	ng	102738	1	7.642	114080	0.4
1-Propanamine, ...	8.442	0.2	ng	50146	1	7.642	114080	0.4
Fomepizole	9.342	0.2	ng	77960	2	10.406	180715	0.4
5-Hydroxy-2-pyr...	9.836	0.1	ng	27308	2	10.406	180715	0.4
m-Chloroaniline	10.584	0.1	ng	57401	2	10.406	180715	0.4
Methane, iodo-	11.709	0.1	ng	24892	2	10.406	180715	0.4
2-Propyl-4-meth...	12.300	0.4	ng	190958	2	10.406	180715	0.4
4-Cyano-5-(meth...	12.695	0.1	ng	27448	3	14.269	186066	0.4
E-2-Propenoic a...	12.771	0.1	ng	23869	3	14.269	186066	0.4
Naphthalene, 2-...	13.139	0.3	ng	120342	3	14.269	186066	0.4
Benzene, 1-meth...	13.850	0.1	ng	26257	3	14.269	186066	0.4
Benzene, 1-meth...	14.649	0.1	ng	40525	3	14.269	186066	0.4
2-Azafluorene	15.550	0.1	ng	56006	3	14.269	186066	0.4
3-Nitrotyramine	15.613	0.1	ng	58588	3	14.269	186066	0.4
5-Fluoro-2-meth...	17.431	0.3	ng	122709	4	17.029	140501	0.4
1-(benzo[d][1,3...	20.378	0.1	ng	54926	5	21.238	357833	0.4
.beta.-Alanine,...	22.055	0.1	ng	86668	5	21.238	357833	0.4