LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016619.D
Acq On : 01 Oct 2021 04:12
Operator : CG/JU
Sample : PB139494BSD
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : PB139494BSD

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: BN016619.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	7589	10857	2.19%	0.144%
2	3.585	51	55	79	rVB2	6091	29902	6.03%	0.397%
3	5.254	231	236	251	rBV2	14496	56030	11.29%	0.745%
4	6.822	401	406	418	rBV	23248	60252	12.14%	0.801%
5	6.978	418	423	429	rVV	16565	37381	7.53%	0.497%
6	7.080	429	434	440	rVV	35163	73806	14.88%	0.981%
7	7.200	440	447	459	rVB	12125	32526	6.56%	0.432%
8	7.522	478	482	489	rVB	6950	15353	3.09%	0.204%
9	7.642	490	495	508	rVB2	49436	121981	24.59%	1.621%
10	7.956	524	529	538	rVB2	48429	109790	22.13%	1.459%
11	8.168	547	552	557	rBV	3335	7894	1.59%	0.105%
12	8.429	571	577	594	rBV3	20697	49844	10.05%	0.662%
13	8.696	595	598	601	rBV	5030	9357	1.89%	0.124%
14	8.784	601	605	607	rBV	32281	72353	14.58%	0.962%
15	8.822	607	608	616	rVB	26359	38613	7.78%	0.513%
16	9.342	645	649	656	rBV	46509	78317	15.78%	1.041%
17	9.532	660	664	666	rVV	3262	6767	1.36%	0.090%
18	9.595	666	669	679	rVB	8551	15504	3.12%	0.206%
19	9.836	685	688	702	rVB	15845	27693	5.58%	0.368%
20	10.052	702	705	709	rBV	3689	8089	1.63%	0.107%
21	10.406	729	733	735	rBV	107509	195473	39.40%	2.598%
22	10.457	735	737	741	rVV	110914	181831	36.65%	2.416%
23	10.571	743	746	756	rVV	25955	60183	12.13%	0.800%
24	10.749	756	760	763	rVB	33731	56825	11.45%	0.755%
25	11.306	801	804	818	rVB	2009	5130	1.03%	0.068%
26	11.709	853	865	890	rBV	12745	23852	4.81%	0.317%
27	12.003	921	931	940	rBV	56809	93149	18.77%	1.238%
28	12.078	940	948	973	rVV	128066	208066	41.94%	2.765%
29	12.296	988	997	1021	rVV	127835	200853	40.48%	2.669%
30	12.695	1056	1059	1062	rBV	15827	26880	5.42%	0.357%
31	12.771	1062	1065	1071	rVB	11245	23215	4.68%	0.309%
32	12.886	1071	1074	1078	rBV	111380	196527	39.61%	2.612%
33	13.139	1089	1094	1097	rBV	80254	132403	26.69%	1.760%
34	13.736	1138	1141	1143	rBV	11476	16210	3.27%	0.215%
35	13.850	1147	1150	1153	rVB	17489	25985	5.24%	0.345%
36	13.989	1158	1161	1164	rVB	95446	150252	30.28%	1.997%

LSC Area Percent Report

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Acq On : 01 Oct 2021 04:12
Operator : CG/JU
Sample : PB139494BSD
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : PB139494BSD

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	14.269	1180	1183	1186	rBV	135863	197662	39.84%	2.627%
38	14.332	1186	1188	1191	rVB	167353	235346	47.43%	3.128%
39	14.649	1209	1213	1220	rBV3	14916	40805	8.22%	0.542%
40	14.814	1224	1226	1230	rVV	4685	8470	1.71%	0.113%
41	14.903	1230	1233	1244	rVB	7073	11670	2.35%	0.155%
42	15.106	1246	1249	1252	rBV	8083	10648	2.15%	0.142%
43	15.322	1263	1266	1270	rBV2	213321	342288	68.99%	4.549%
44	15.410	1270	1273	1280	rVV2	3584	9418	1.90%	0.125%
45	15.537	1280	1283	1287	rVV	33194	59877	12.07%	0.796%
46	15.613	1287	1289	1298	rVV2	39377	62646	12.63%	0.833%
47	15.766	1298	1301	1311	rVB2	12427	20957	4.22%	0.278%
48	16.226	1335	1338	1341	rBV2	58747	87824	17.70%	1.167%
49	16.324	1343	1346	1350	rVB	45968	70821	14.27%	0.941%
50	16.506	1358	1361	1372	rBV	19269	31385	6.33%	0.417%
51	16.677	1372	1375	1384	rBV	17763	31292	6.31%	0.416%
52	17.017	1400	1403	1405	rBV	89314	150604	30.35%	2.001%
53	17.066	1405	1407	1410	rVV	144759	209122	42.15%	2.779%
54	17.151	1411	1414	1434	rVB	101757	176785	35.63%	2.349%
55	17.431	1434	1437	1453	rBV	75283	127902	25.78%	1.700%
56	18.020	1482	1486	1508	rVB	5062	7545	1.52%	0.100%
57	19.063	1686	1696	1699	rBV	110408	152528	30.74%	2.027%
58	19.093	1699	1702	1741	rVB	173104	248414	50.07%	3.301%
59	19.460	1767	1776	1813	rBV	174200	241759	48.73%	3.213%
60	19.678	1813	1820	1850	rVV	102796	133079	26.82%	1.768%
61	20.378	1918	1921	1924	rBV	44846	52593	10.60%	0.699%
62	21.164	1992	1995	1997	rBV	51227	57770	11.64%	0.768%
63	21.217	1997	2000	2003	rVV2	197843	395797	79.77%	5.260%
64	21.270	2003	2005	2017	rVB	168007	246885	49.76%	3.281%
65	22.056	2075	2079	2082	rBV	57011	79739	16.07%	1.060%
66	22.800	2216	2227	2234	rBV	120231	200329	40.38%	2.662%
67	22.848	2234	2241	2291	rVB	128104	234677	47.30%	3.119%
68	23.378	2384	2396	2414	rBV	83446	180087	36.30%	2.393%
69	23.477	2414	2425	2478	rVB	90988	194476	39.20%	2.584%
70	24.083	2592	2602	2621	rBV	6525	12448	2.51%	0.165%
71	24.853	2816	2827	2852	rVB	6857	15414	3.11%	0.205%
72	25.767	3067	3094	3174	rBV4	129122	496154	100.00%	6.593%
73	26.448	3271	3293	3352	rBV	71470	230637	46.48%	3.065%

Sum of corrected areas: 7524996

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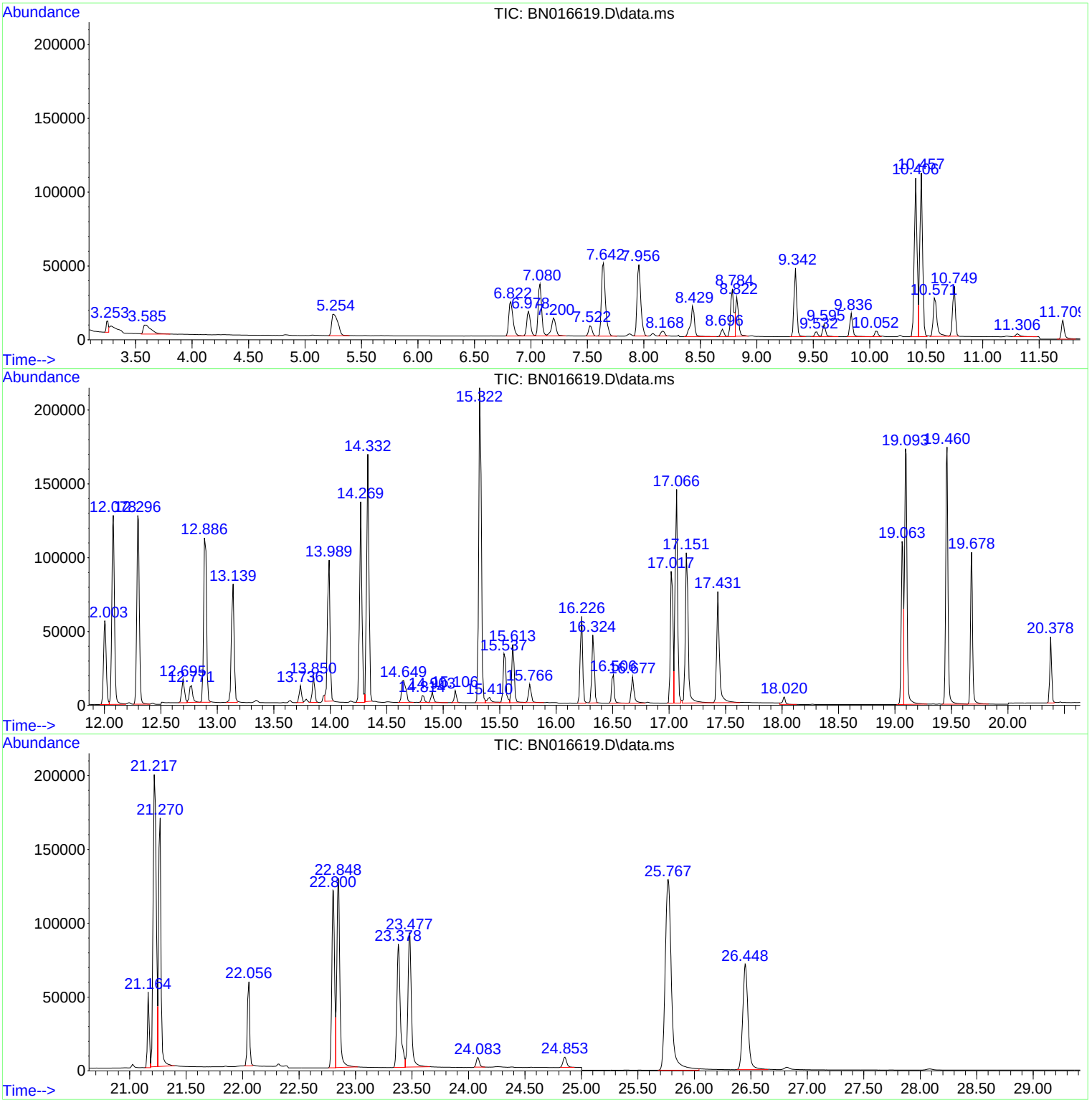
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139494BSD

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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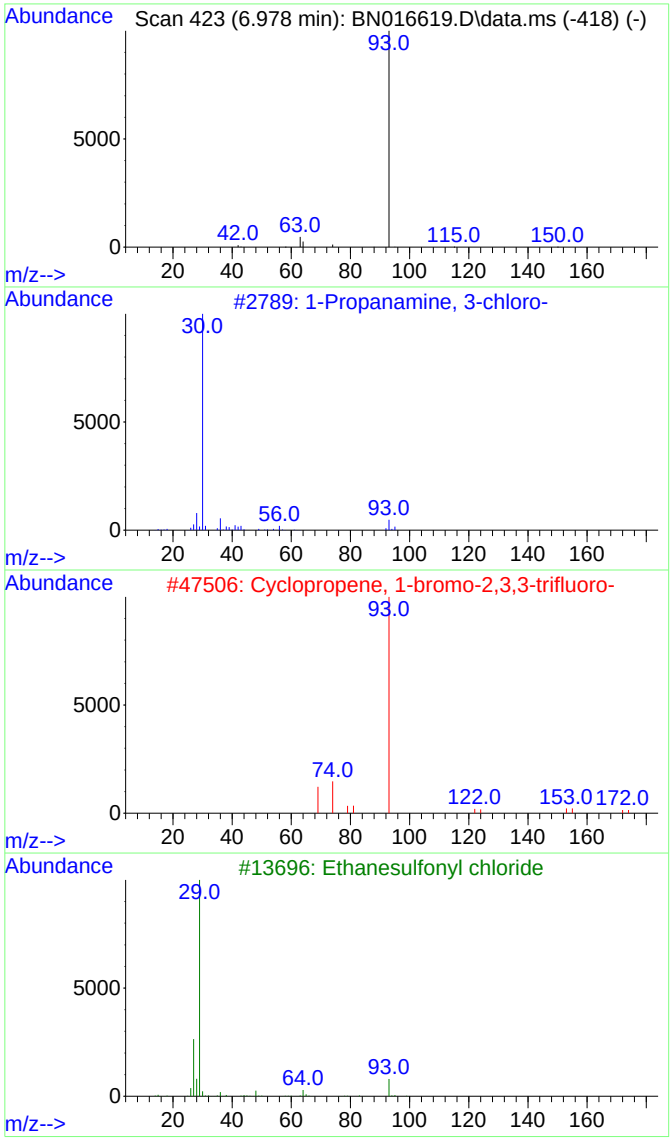
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

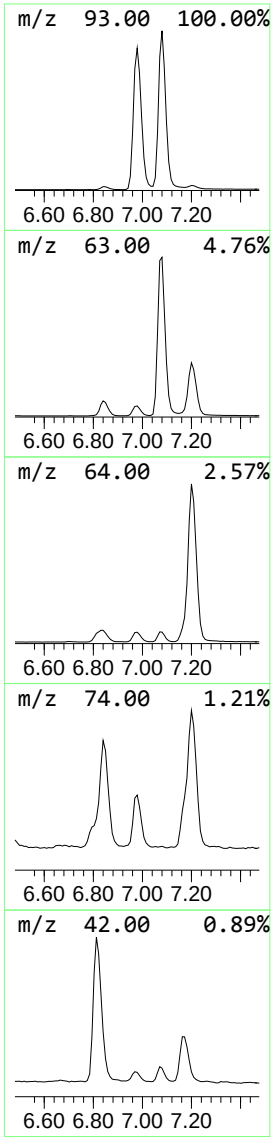
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.978	0.12 ng	37381	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 : BN016619.D
Acq On : 01 Oct 2021 04:12
Operator : CG/JU
Sample : PB139494BSD
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139494BSD

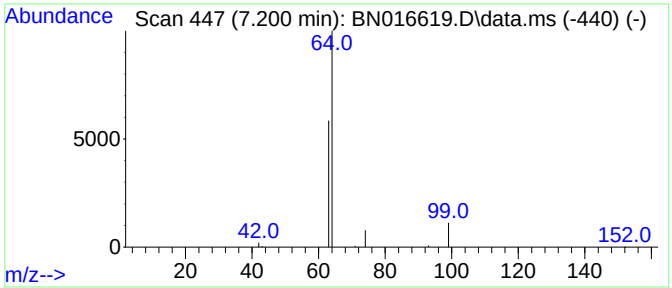
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

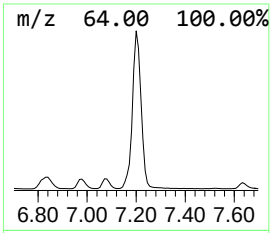
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

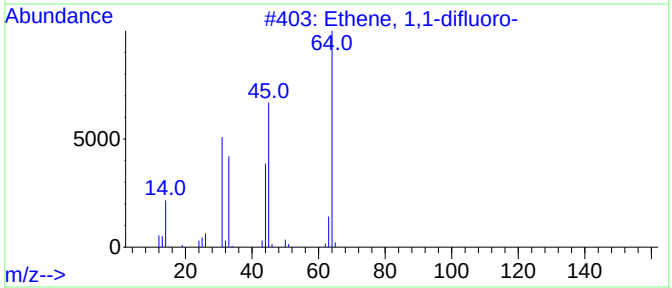
****
Peak Number 2 Ethene, 1,1-difluoro- Concentration Rank 11

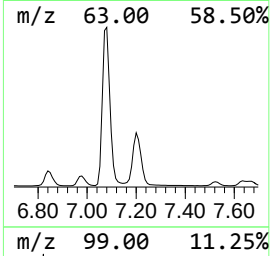
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.200	0.11 ng	32526	1,4-Dichlorobenzene-d4	7.642

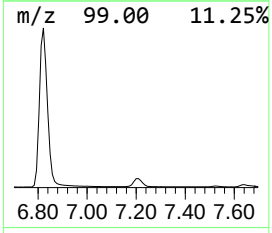
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	3
2	Ethyl Chloride	64	C2H5Cl	000075-00-3	3
3	Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	3
4	Sulfur dioxide	64	O2S	007446-09-5	3
5	(S)-(-)-2-Chloropropionic acid	108	C3H5ClO2	029617-66-1	2

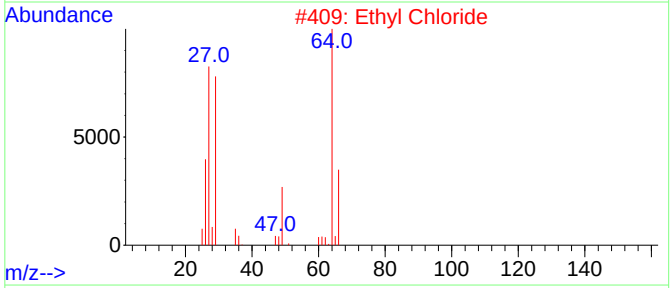


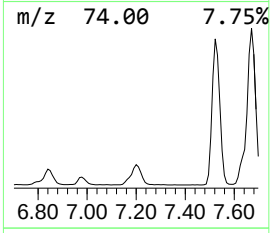


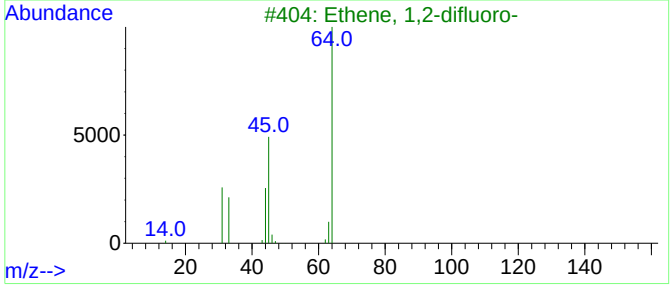


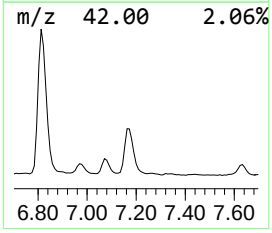












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Data File : BN016619.D
Acq On : 01 Oct 2021 04:12
Operator : CG/JU
Sample : PB139494BSD
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139494BSD

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

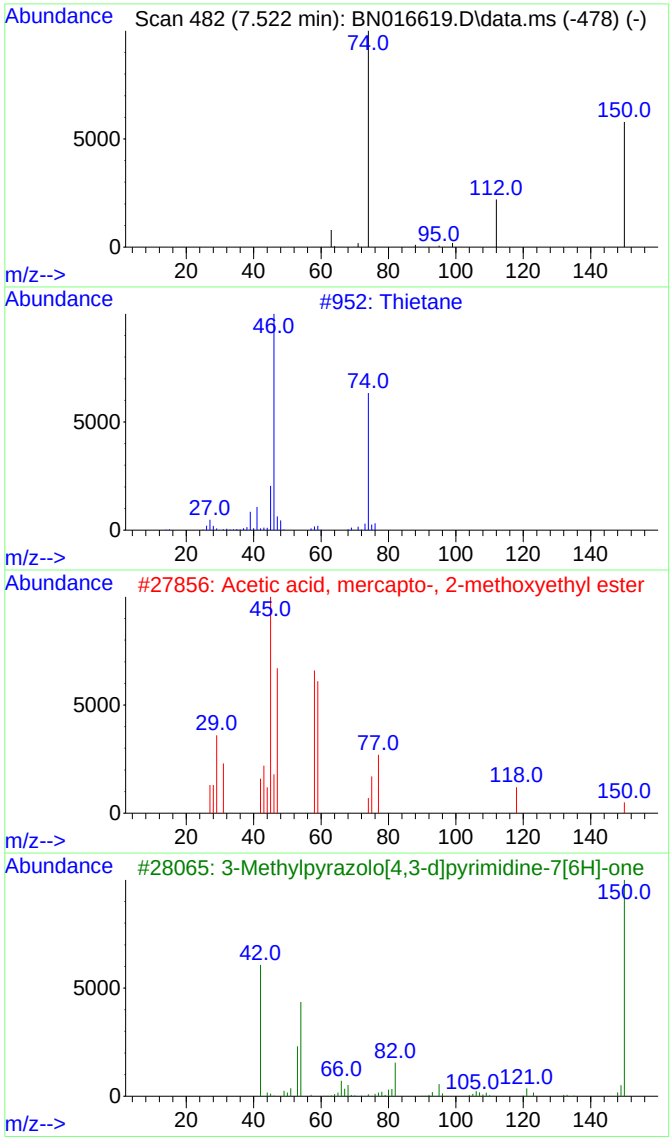
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

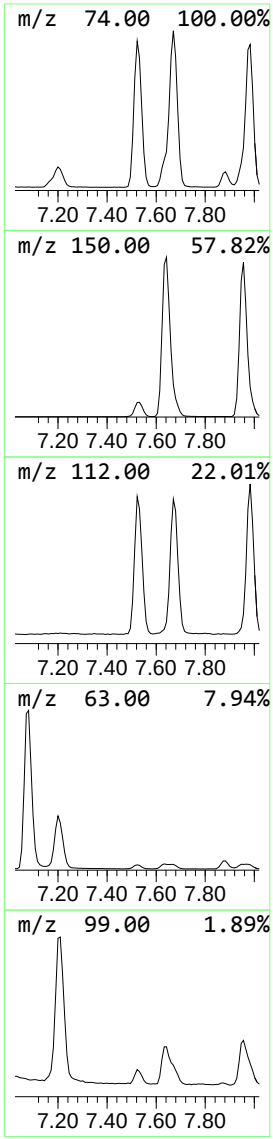
****

Peak Number 3 Thietane Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.522	0.05 ng	15353	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 :
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ClientSampleId :
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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

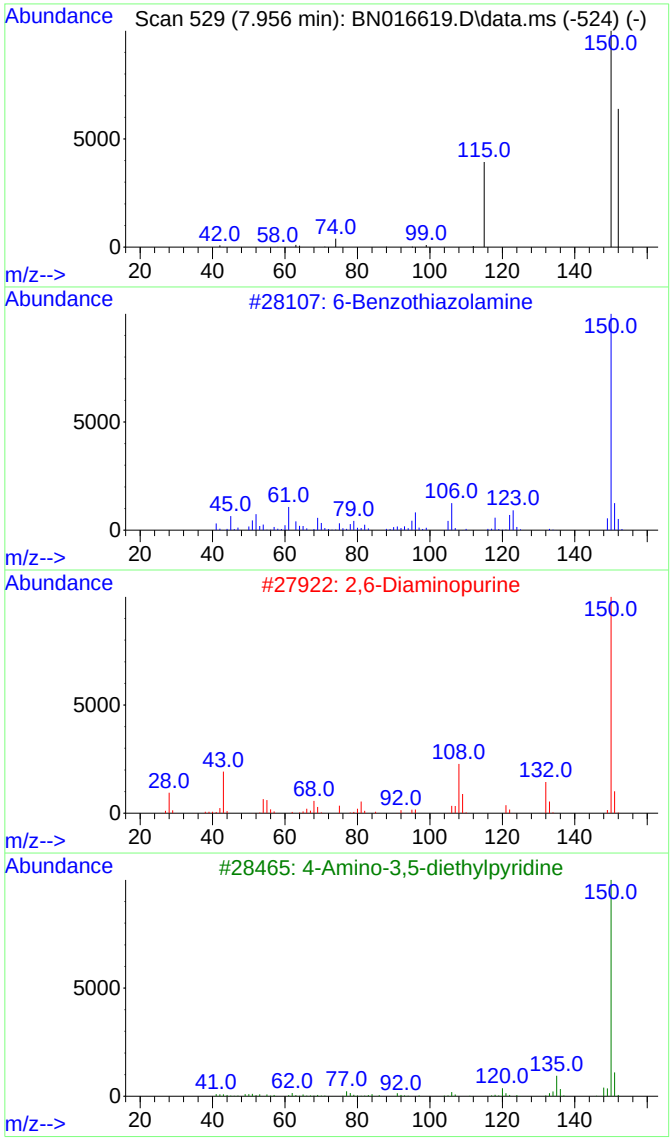
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

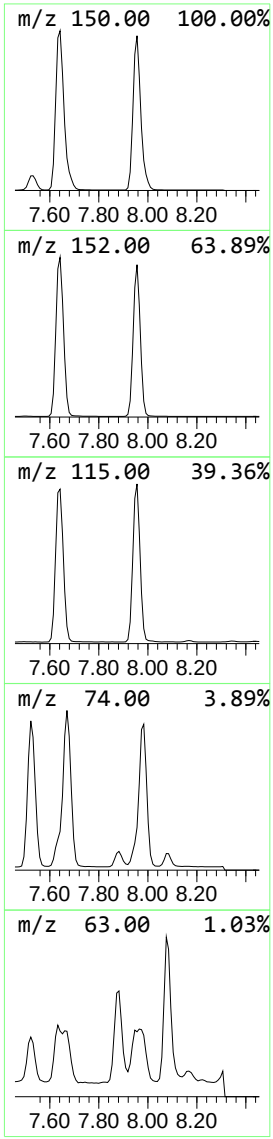
****

Peak Number 4 6-Benzothiazolamine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.956	0.36 ng	109790	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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Instrument :
BNA_N
ClientSampleId :
PB139494BSD

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

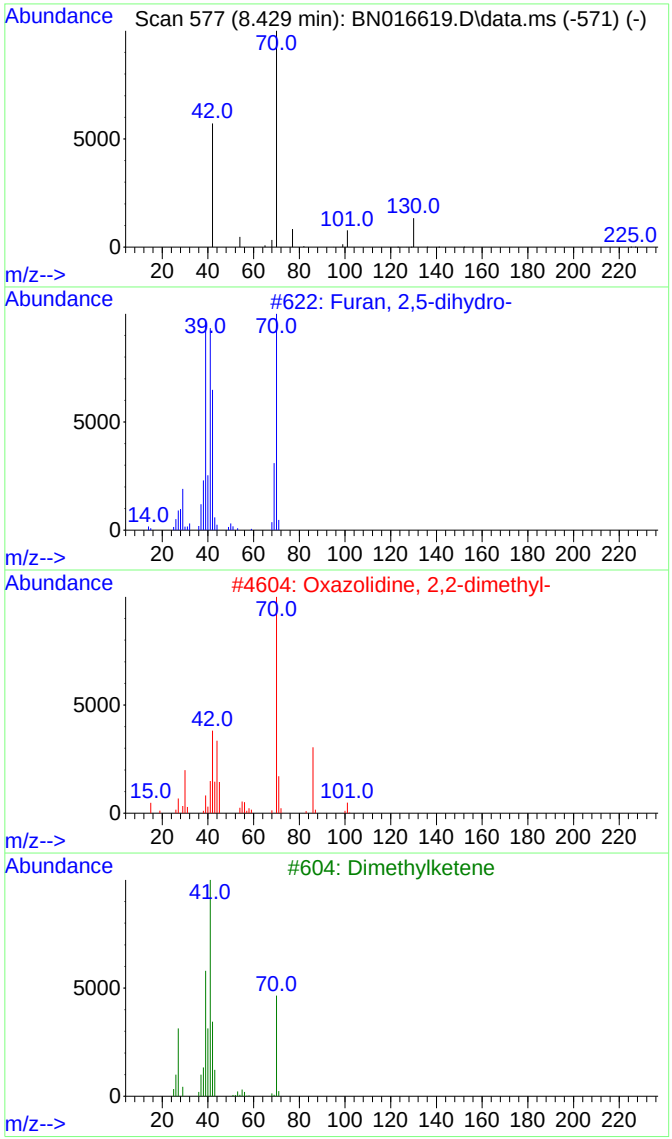
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

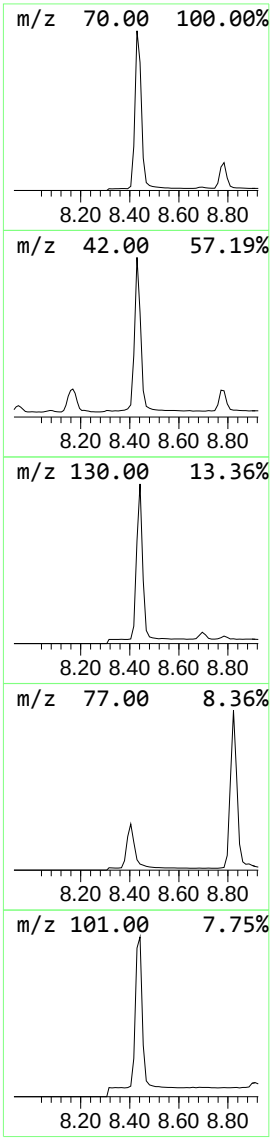
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.429	0.16 ng	49844	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	7
2	Oxazolidine, 2,2-dimethyl-	101	C5H11NO	020515-62-2	7
3	Dimethylketene	70	C4H6O	000598-26-5	5
4	Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	5
5	1-Propanamine, N-nitroso-N-propyl-	130	C6H14N2O	000621-64-7	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016619.D
Acq On : 01 Oct 2021 04:12
Operator : CG/JU
Sample : PB139494BSD
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139494BSD

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

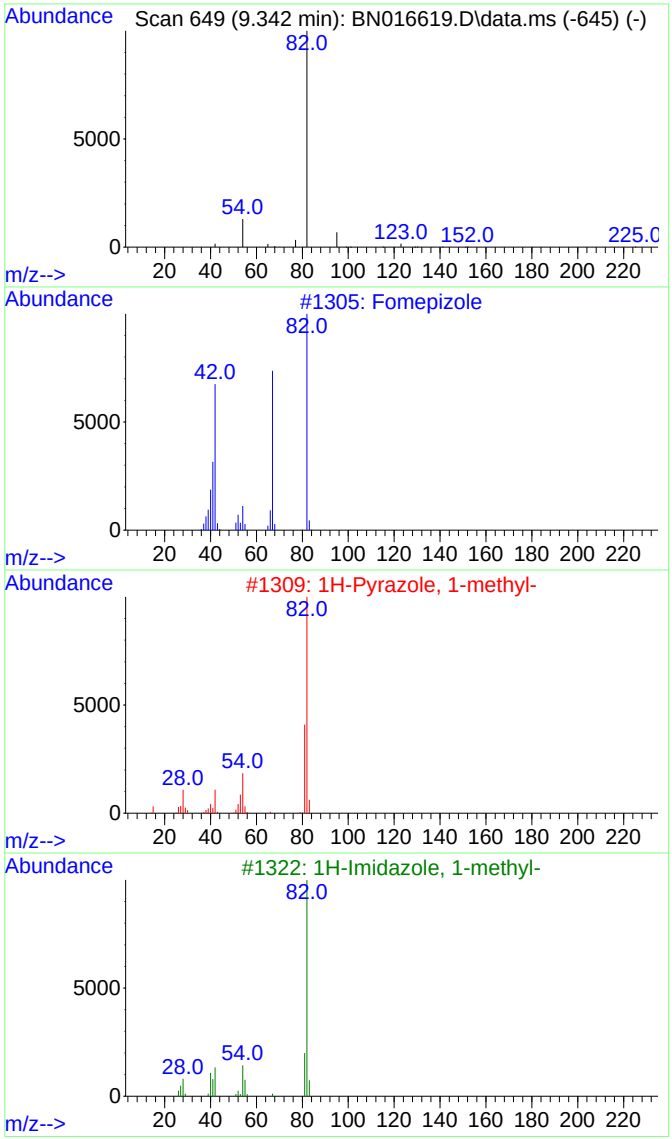
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

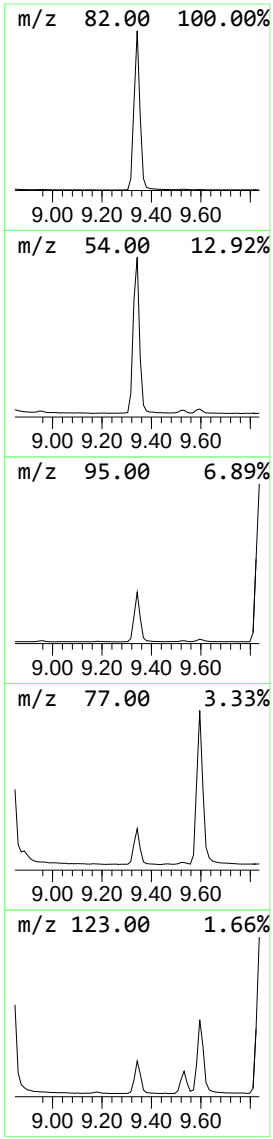
****

Peak Number 6 Fomepizole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.342	0.16 ng	78317	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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Operator : CG/JU
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Misc :
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ClientSampleId :
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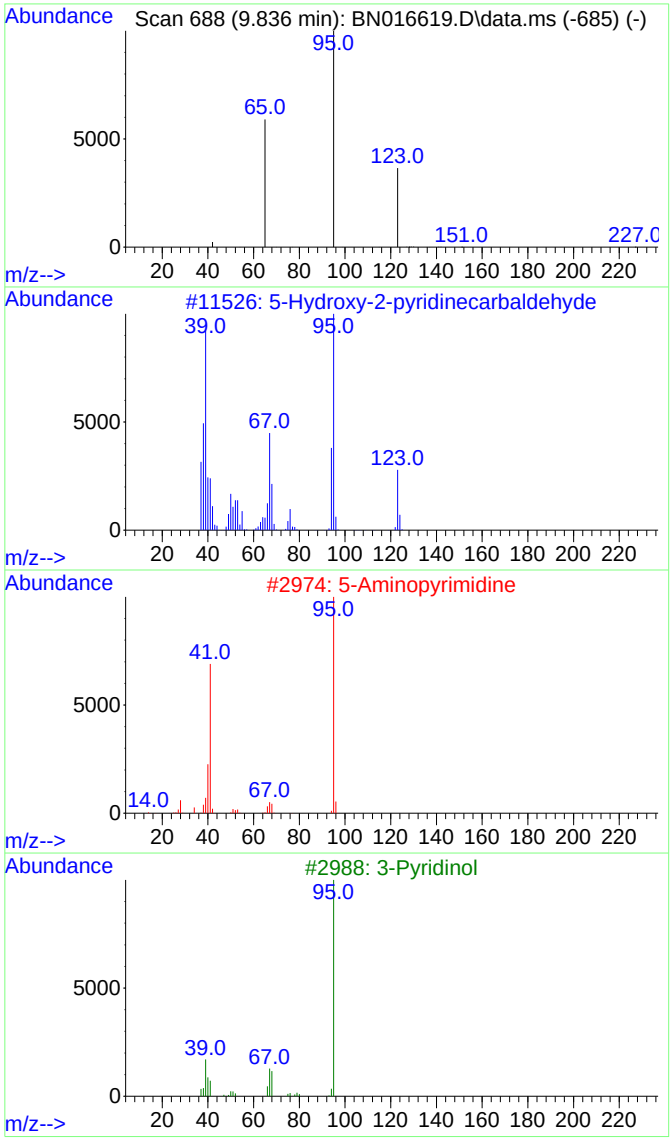
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

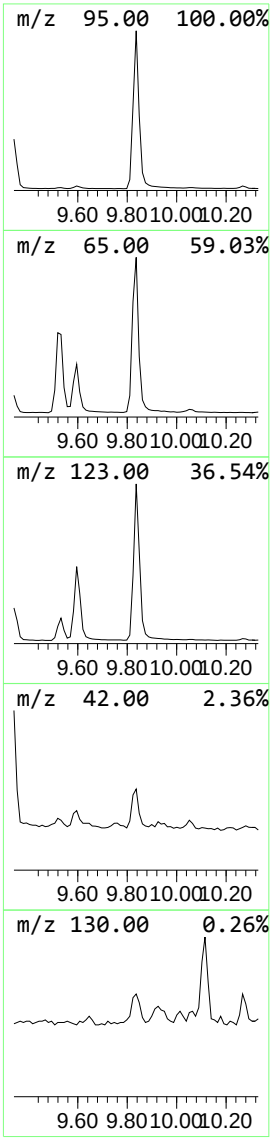
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 5-Hydroxy-2-pyridinecarbald... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.836	0.06 ng	27693	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	5-Aminopyrimidine	95	C4H5N3	000591-55-9	3
3	3-Pyridinol	95	C5H5NO	000109-00-2	2
4	2-Pyrimidinamine	95	C4H5N3	000109-12-6	2
5	4-Pyridinol	95	C5H5NO	000626-64-2	2





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

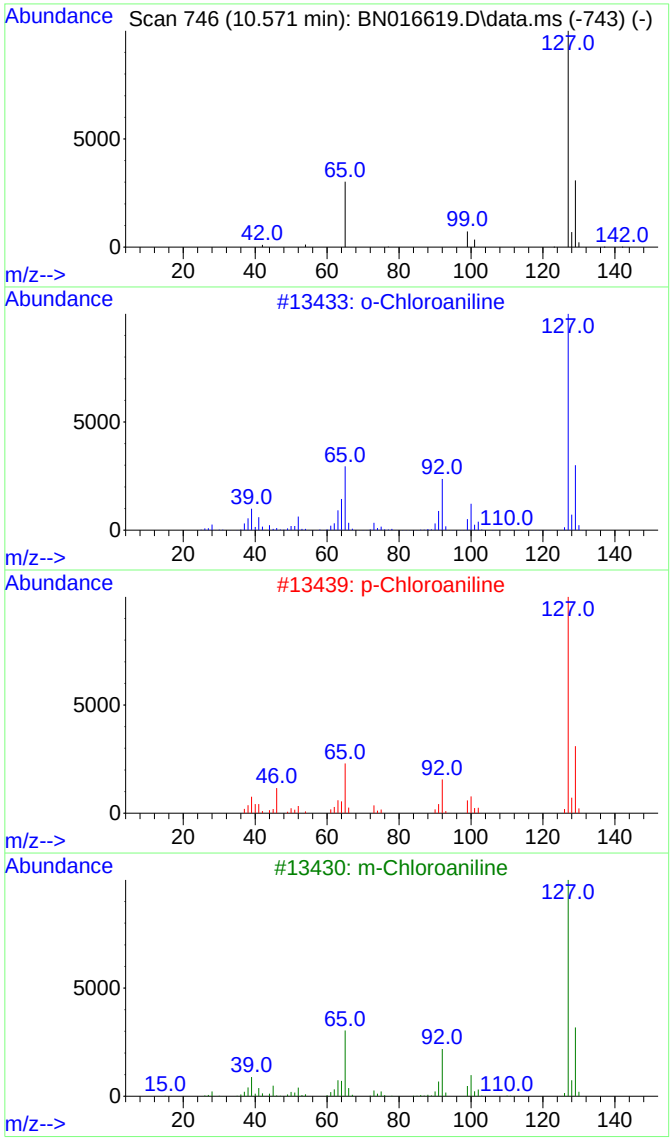
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

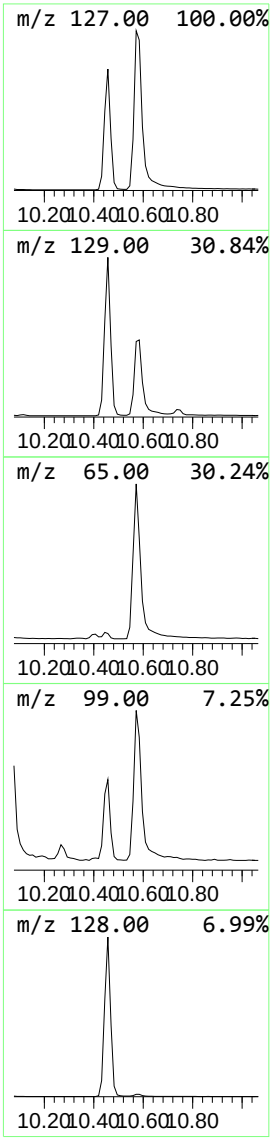
****

Peak Number 8 o-Chloroaniline Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.571	0.12 ng	60183	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	4-(Chloromethyl)pyridine	127	C6H6ClN	010445-91-7	86
5	Picloxydine	474	C20H24Cl2N10	005636-92-0	83





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

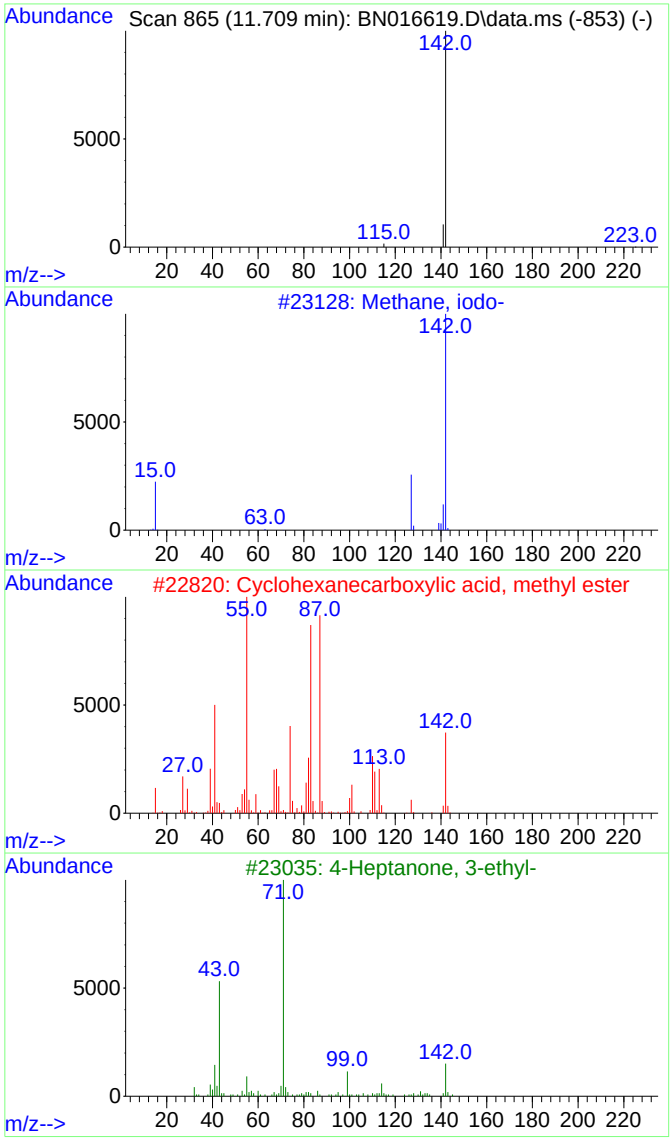
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

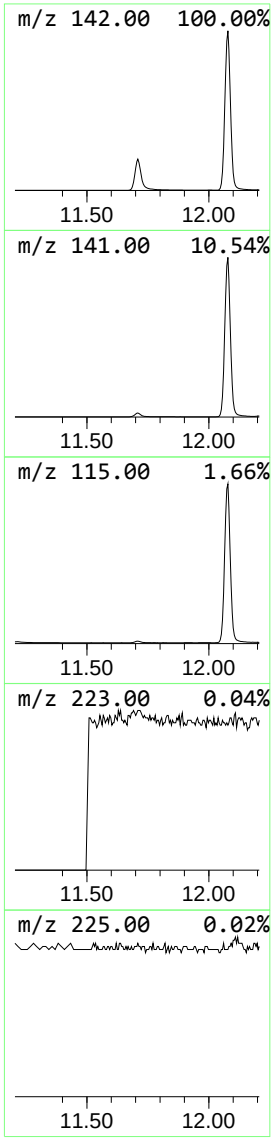
****

Peak Number 9 Methane, iodo- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.709	0.05 ng	23852	Naphthalene-d8	10.406

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methane, iodo-	142	CH3I	000074-88-4	4
2	Cyclohexanecarboxylic acid, meth...	142	C8H14O2	004630-82-4	4
3	4-Heptanone, 3-ethyl-	142	C9H18O	001528-25-2	3
4	Cyclohexane carboxylic acid hydr...	142	C7H14N2O	038941-47-8	3
5	2-Butanone, diethylhydrazone	142	C8H18N2	028236-94-4	3





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

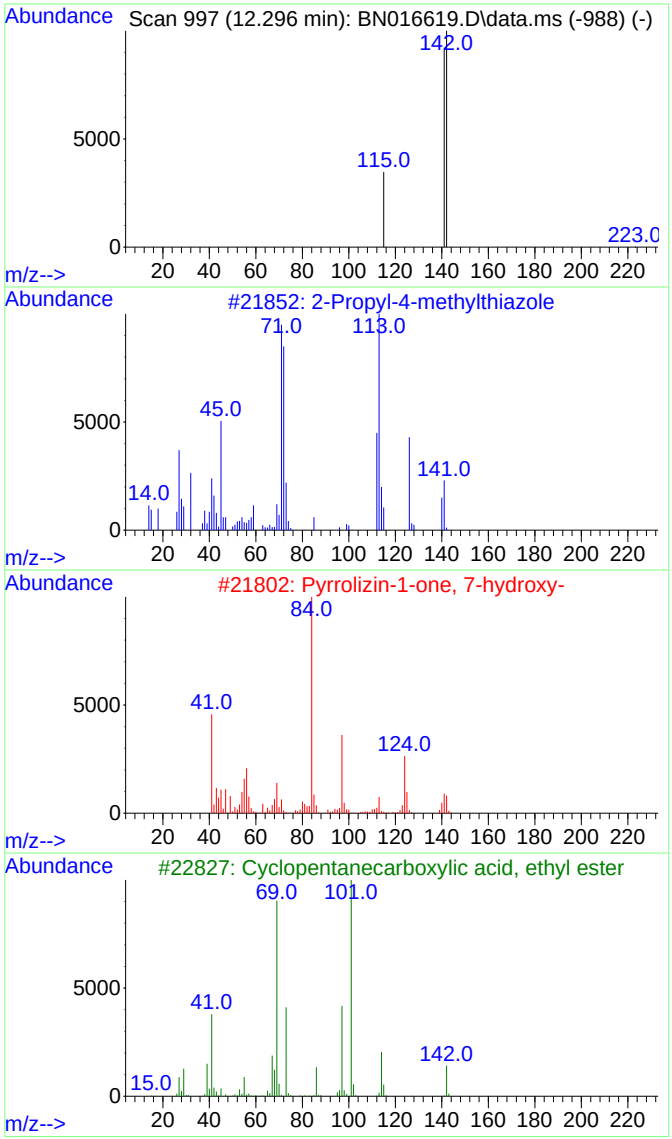
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

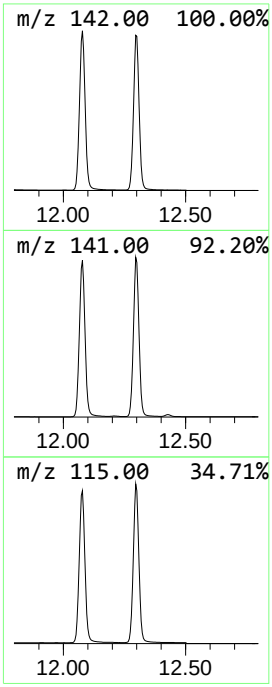
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.296	0.41 ng	200853	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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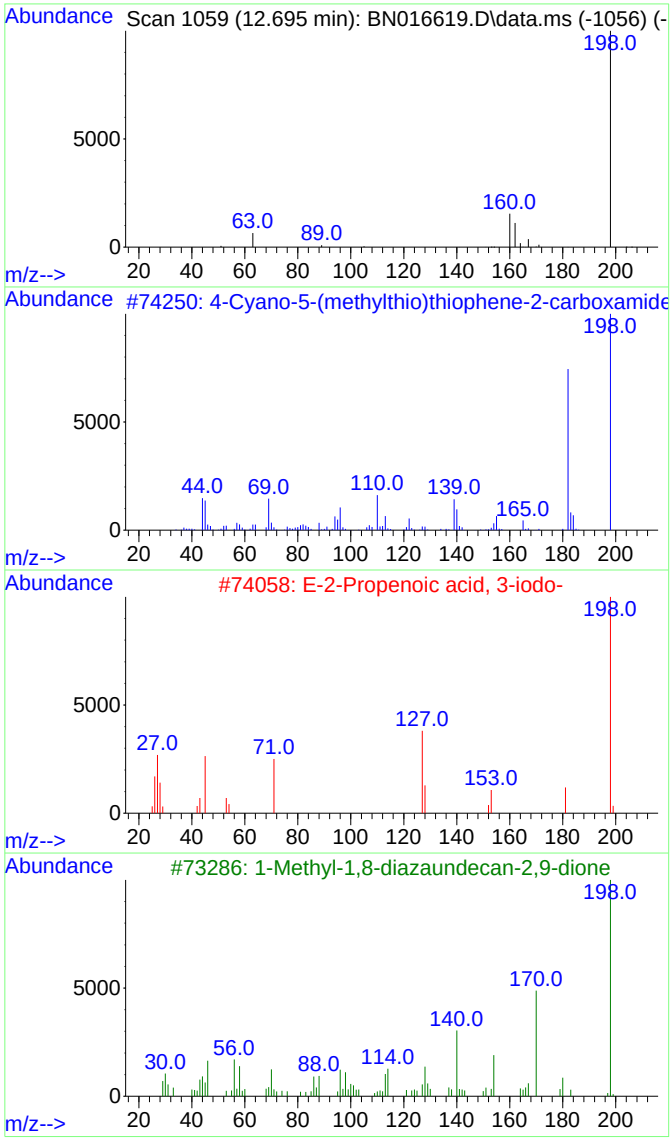
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

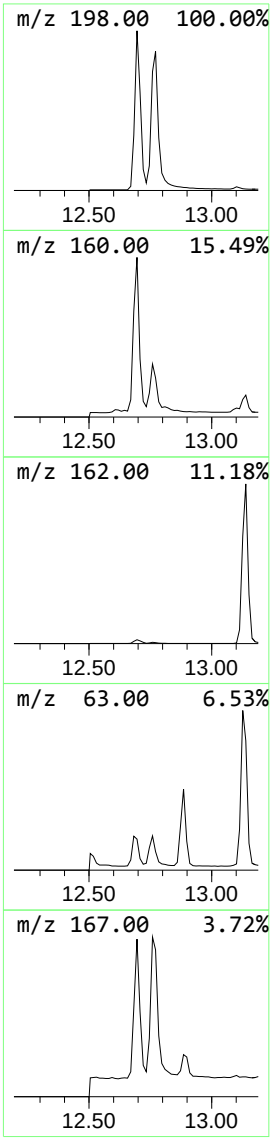
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 4-Cyano-5-(methylthio)thiop... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.695	0.05 ng	26880	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Cyano-5-(methylthio)thiophene-...	198	C7H6N2OS2	1000267-39-2	3
2	E-2-Propenoic acid, 3-iodo-	198	C3H3IO2	1000308-86-7	3
3	1-Methyl-1,8-diazaundecan-2,9-dione	198	C10H18N2O2	1000298-94-5	3
4	Z-2-Propenoic acid, 3-iodo-	198	C3H3IO2	1000308-86-8	3
5	Thiazolo[5,4-d]pyrimidine, 5-ami...	198	C6H6N4S2	019835-31-5	3





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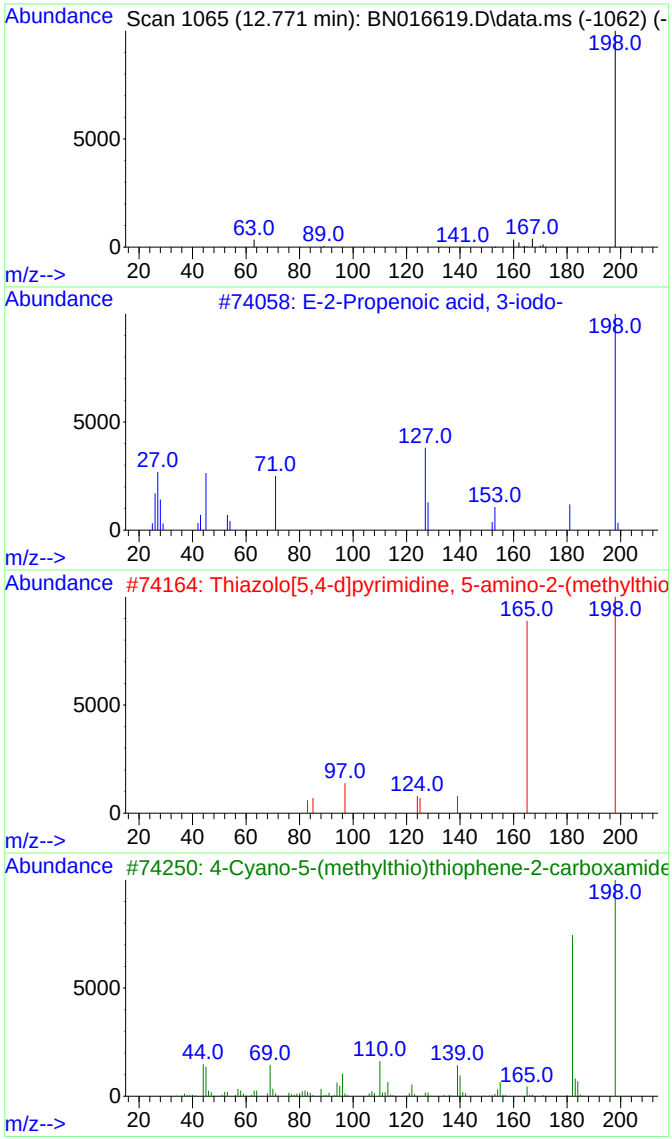
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

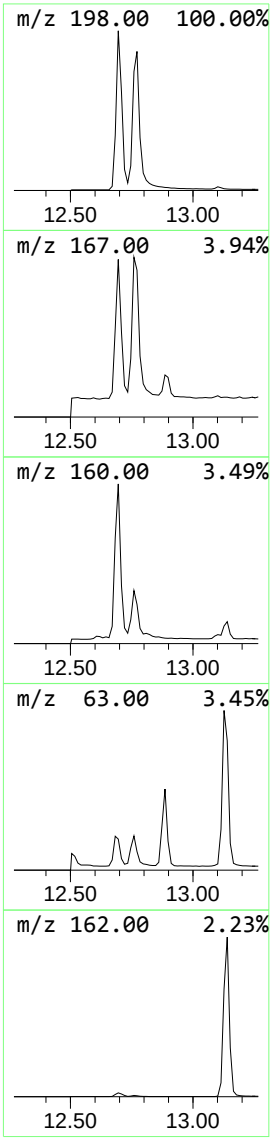
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 E-2-Propenoic acid, 3-iodo- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.771	0.05 ng	23215	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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

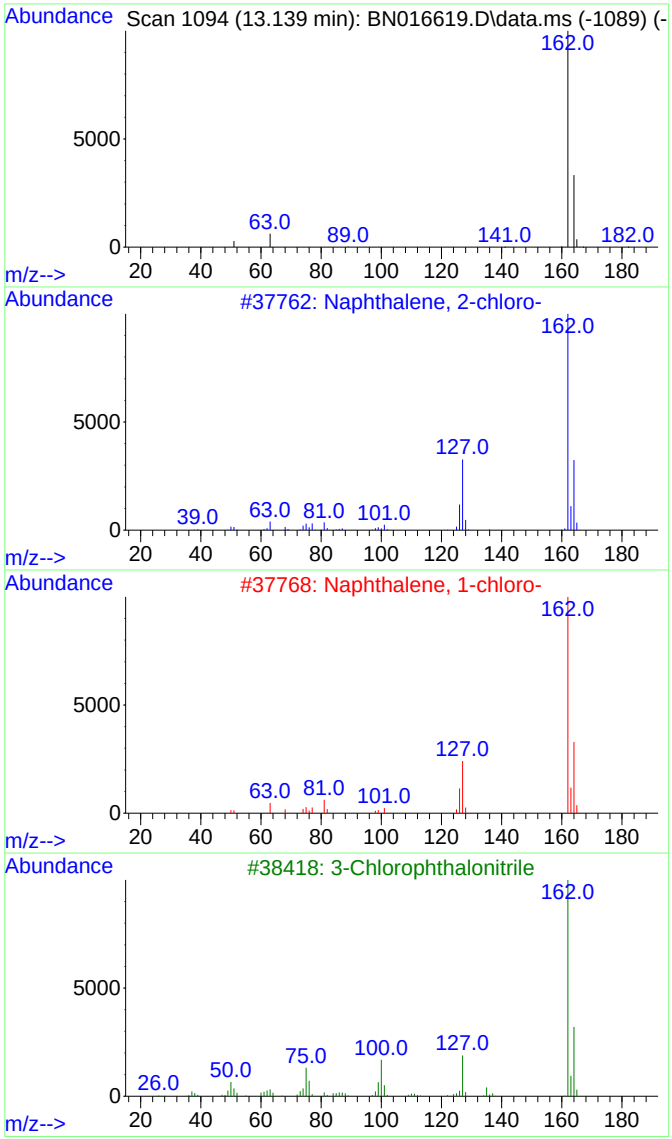
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

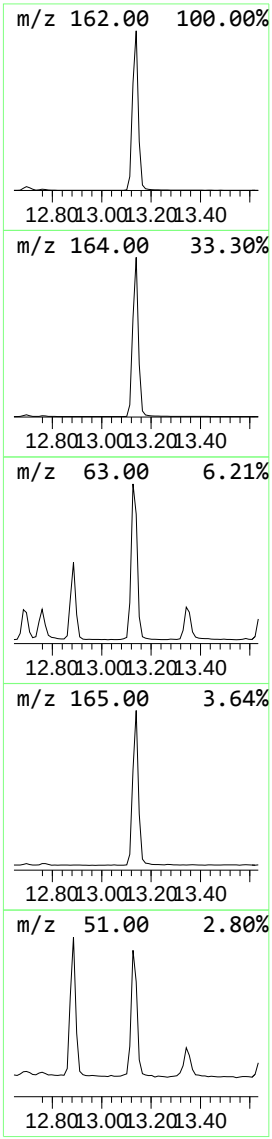
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.139	0.27 ng	132403	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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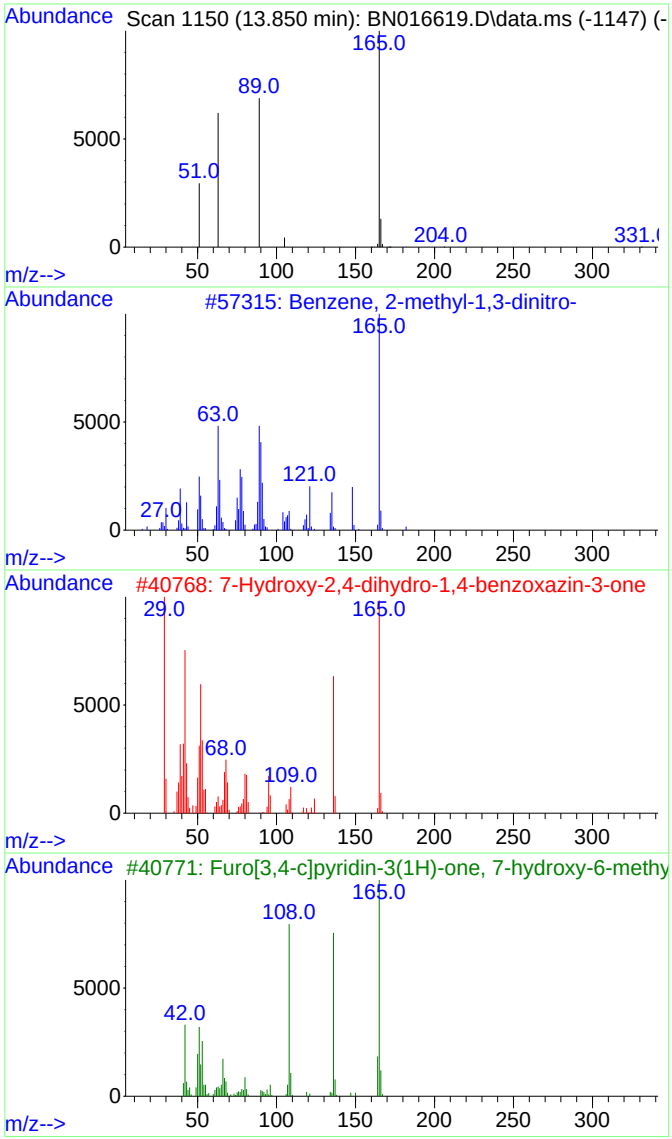
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

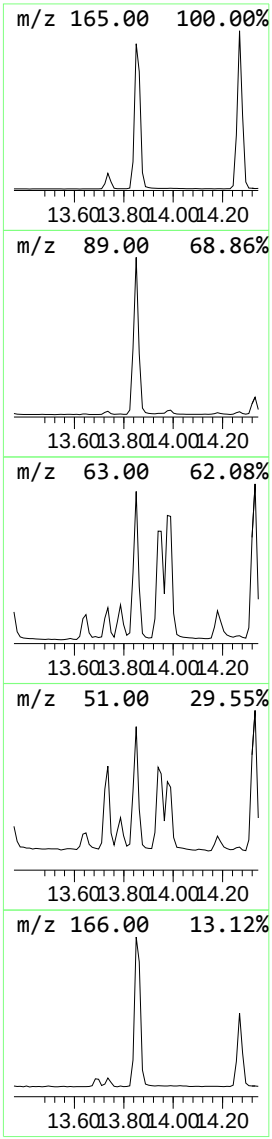
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.850	0.05 ng	25985	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	7-Hydroxy-2,4-dihydro-1,4-benzox...	165	C8H7NO3	067193-97-9	9
3	Furo[3,4-c]pyridin-3(1H)-one, 7-...	165	C8H7NO3	004543-56-0	9
4	6-Oxa-3-azabicyclo[3.2.1]octa-1,...	165	C8H7NO3	055255-96-4	9
5	Furo[3,4-c]pyridin-1(3H)-one, 7-...	165	C8H7NO3	004753-19-9	9





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TIC Library : C:\Database\NIST20.L
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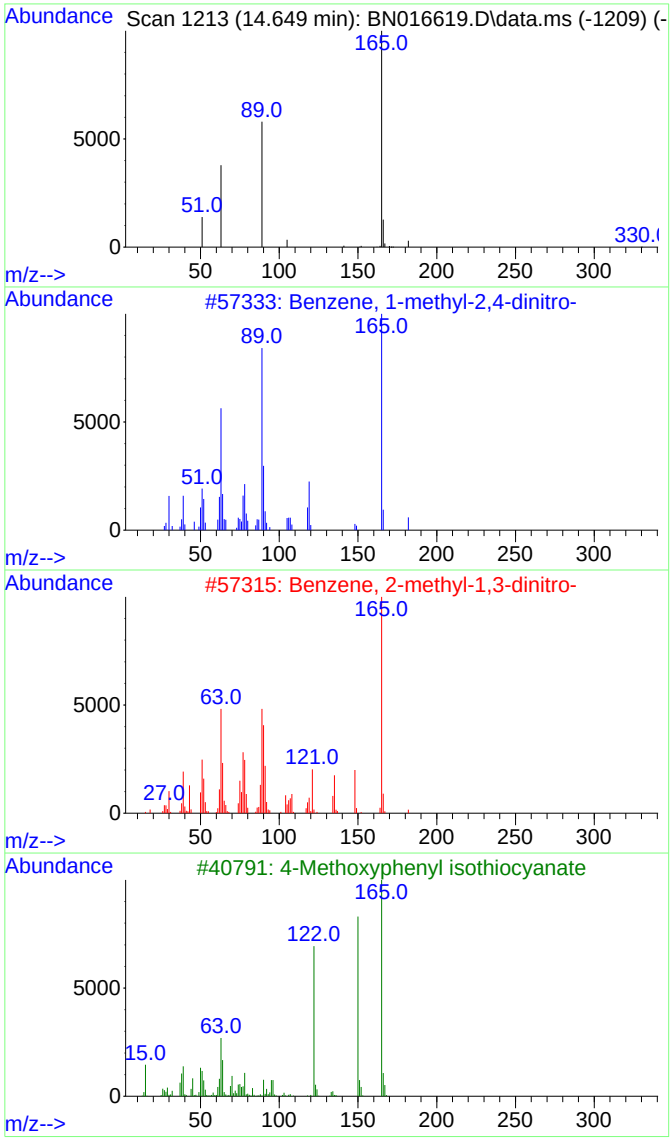
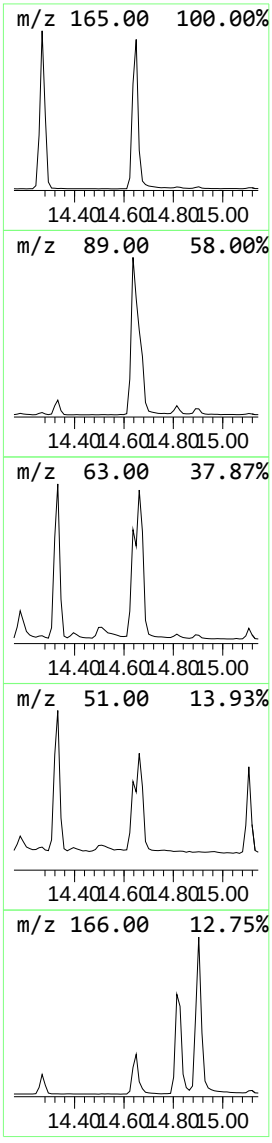
****
Peak Number 15 Benzene, 1-methyl-2,4-dinitro- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.649	0.08 ng	40805	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	50
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	Ethanol, 1-(4-nitrophenyl)-2-[1-...	304	C17H24N2O3	1000264-75-7	9





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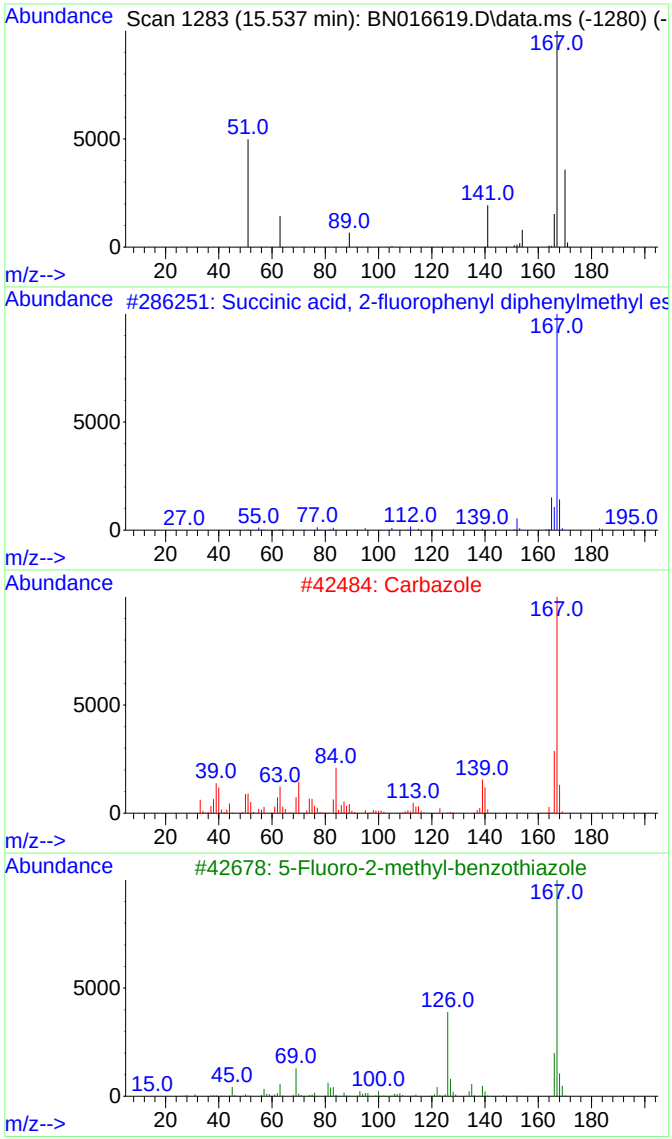
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

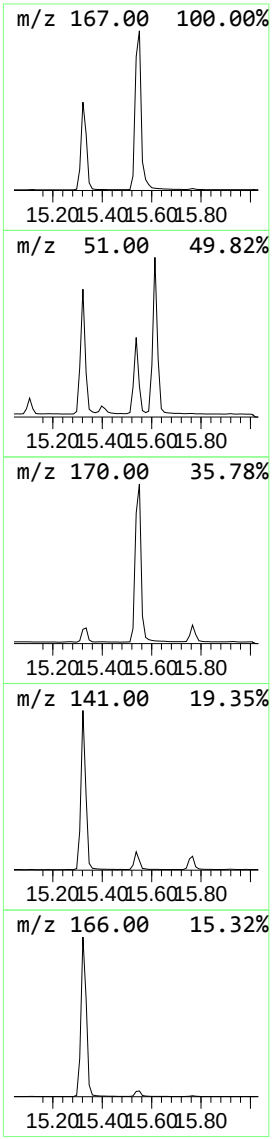
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.537	0.12 ng	59877	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	5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	5
4	Benzaldehyde, 2-hydroxy-5-nitro-	167	C7H5NO4	000097-51-8	5
5	2-Azafluorene	167	C12H9N	000244-40-6	4





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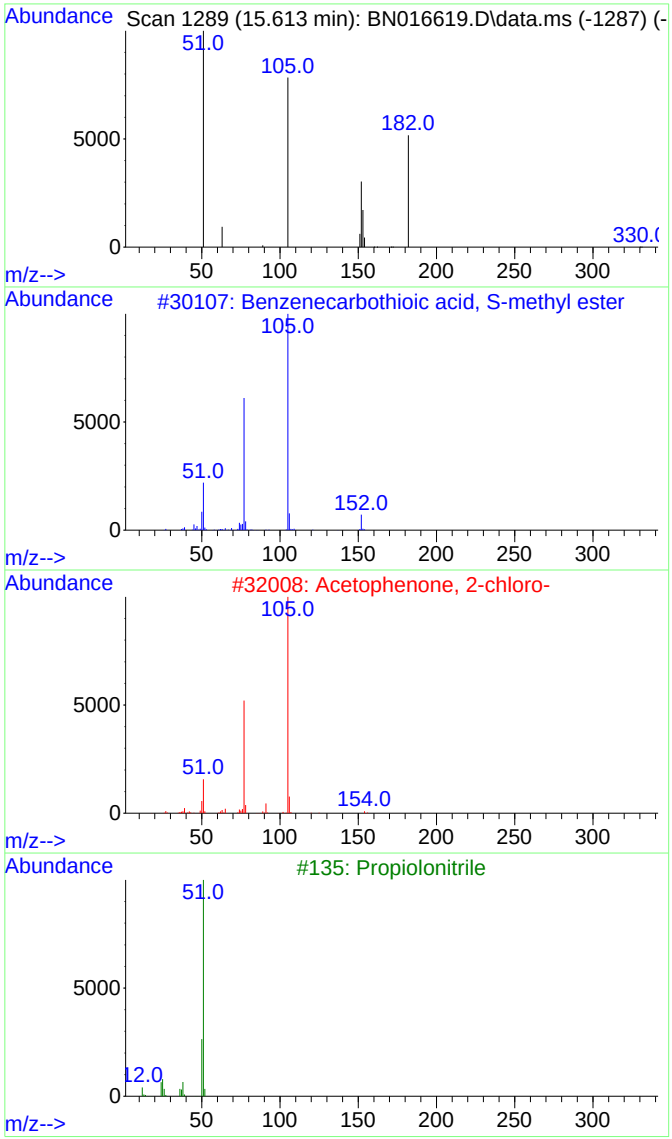
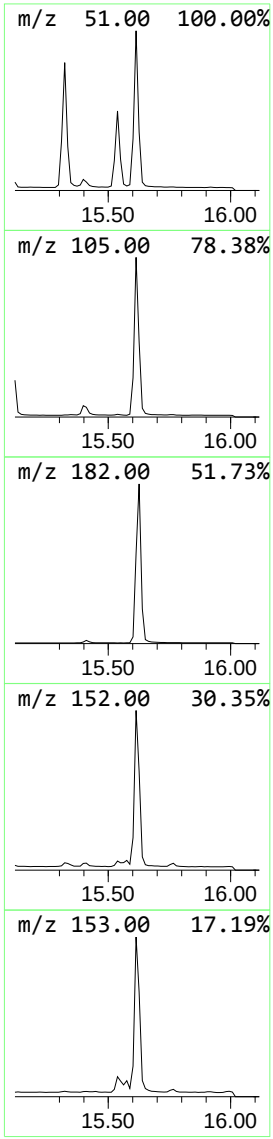
****
Peak Number 17 Benzenecarbothioic acid, S-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.613	0.13 ng	62646	Acenaphthene-d10	14.269

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





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Data File : BN016619.D
Acq On : 01 Oct 2021 04:12
Operator : CG/JU
Sample : PB139494BSD
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139494BSD

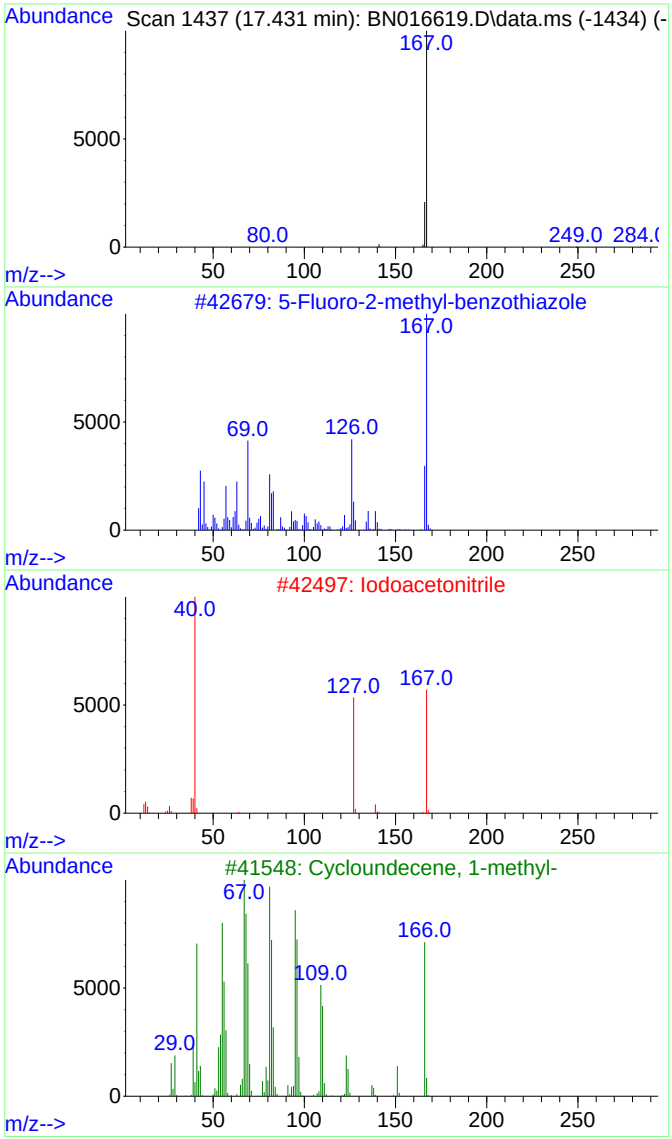
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

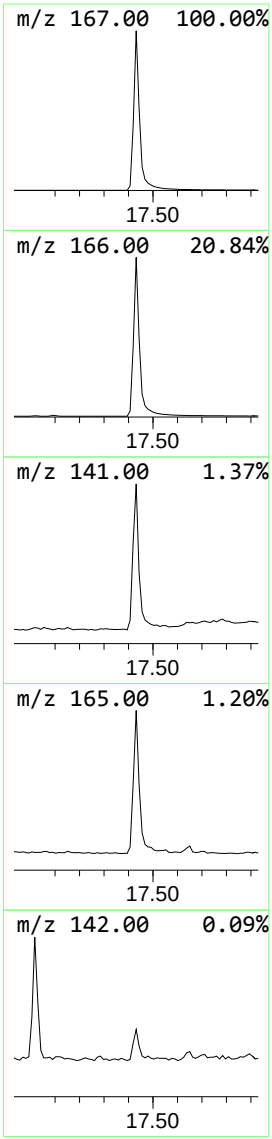
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.431	0.34 ng	127902	Phenanthrene-d10	17.017

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	5
2	Iodoacetonitrile	167	C2H2IN	000624-75-9	4
3	Cycloundecene, 1-methyl-	166	C12H22	088828-82-4	4
4	1,3,5-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 : BN016619.D
Acq On : 01 Oct 2021 04:12
Operator : CG/JU
Sample : PB139494BSD
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : PB139494BSD

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

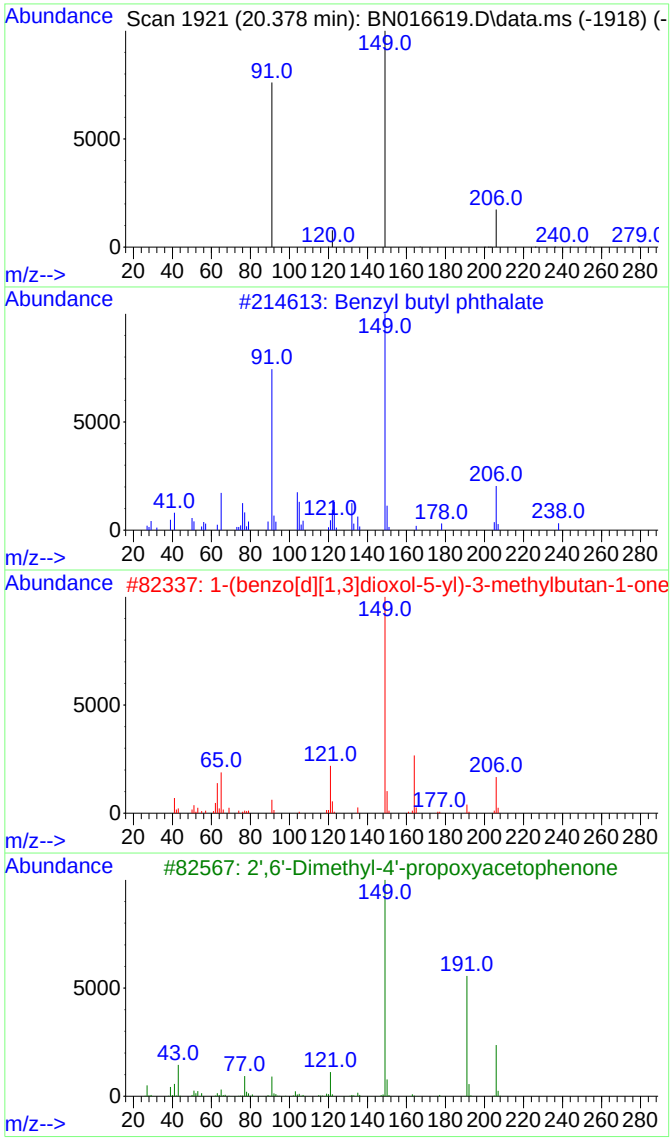
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

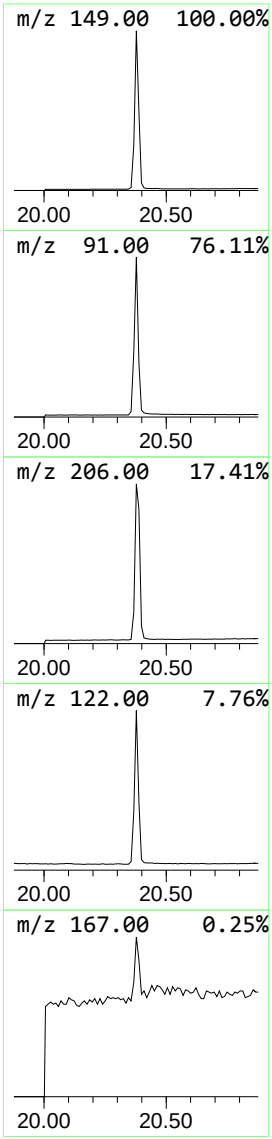
****

Peak Number 19 Benzyl butyl phthalate Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.378	0.05 ng	52593	Chrysene-d12	21.227

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 : BN016619.D
Acq On : 01 Oct 2021 04:12
Operator : CG/JU
Sample : PB139494BSD
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139494BSD

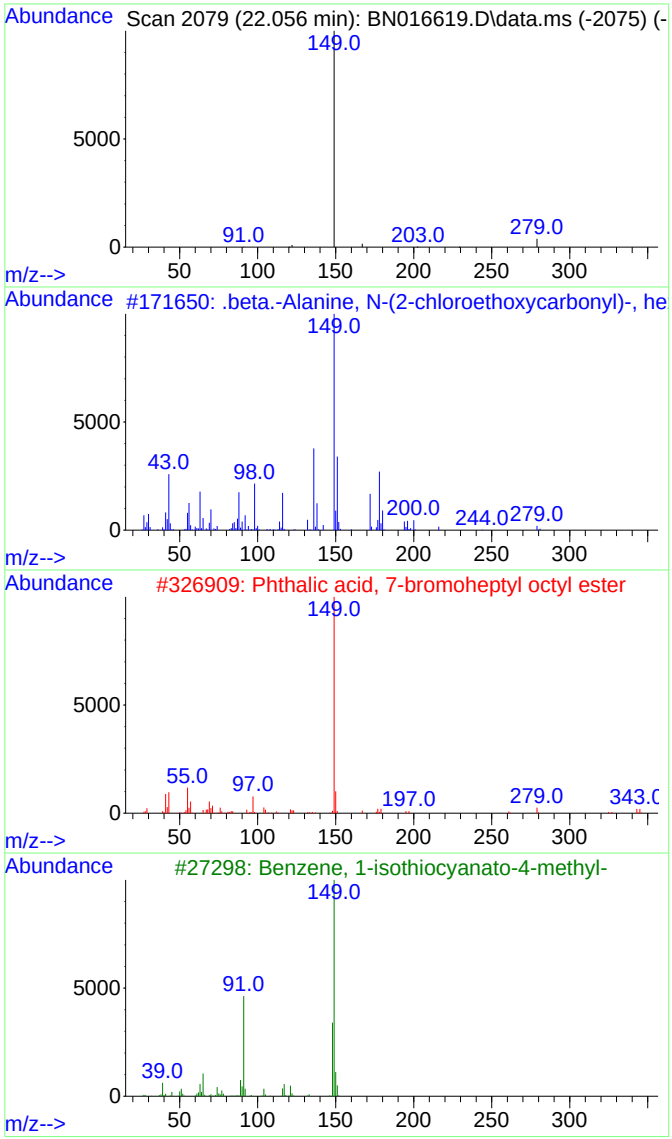
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

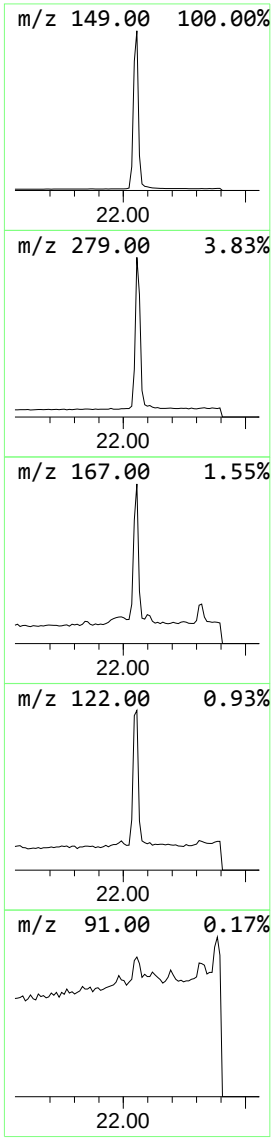
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.056	0.08 ng	79739	Chrysene-d12	21.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Alanine, N-(2-chloroethox...	279	C12H22ClNO4	1010328-58-4	4
2	Phthalic acid, 7-bromoheptyl oct...	454	C23H35BrO4	1000415-52-2	4
3	Benzene, 1-isothiocyanato-4-methyl-	149	C8H7NS	000622-59-3	4
4	3-Hydroxy-2-pyridin-3-yl-propenal	149	C8H7NO2	1000311-61-6	4
5	5-Methylthieno[3,2-b]pyridine	149	C8H7NS	001759-29-1	2





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016619.D
Acq On : 01 Oct 2021 04:12
Operator : CG/JU
Sample : PB139494BSD
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : PB139494BSD

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	37381	1	7.642	121981	0.4
Ethene, 1,1-dif...	7.200	0.1	ng	32526	1	7.642	121981	0.4
Thietane	7.522	0.1	ng	15353	1	7.642	121981	0.4
6-Benzothiazola...	7.956	0.4	ng	109790	1	7.642	121981	0.4
Furan, 2,5-dihy...	8.429	0.2	ng	49844	1	7.642	121981	0.4
Fomepizole	9.342	0.2	ng	78317	2	10.406	195473	0.4
5-Hydroxy-2-pyr...	9.836	0.1	ng	27693	2	10.406	195473	0.4
o-Chloroaniline	10.571	0.1	ng	60183	2	10.406	195473	0.4
Methane, iodo-	11.709	0.0	ng	23852	2	10.406	195473	0.4
2-Propyl-4-meth...	12.296	0.4	ng	200853	2	10.406	195473	0.4
4-Cyano-5-(meth...	12.695	0.1	ng	26880	3	14.269	197662	0.4
E-2-Propenoic a...	12.771	0.0	ng	23215	3	14.269	197662	0.4
Naphthalene, 2-...	13.139	0.3	ng	132403	3	14.269	197662	0.4
Benzene, 2-meth...	13.850	0.1	ng	25985	3	14.269	197662	0.4
Benzene, 1-meth...	14.649	0.1	ng	40805	3	14.269	197662	0.4
Succinic acid, ...	15.537	0.1	ng	59877	3	14.269	197662	0.4
Benzenecarbothi...	15.613	0.1	ng	62646	3	14.269	197662	0.4
5-Fluoro-2-meth...	17.431	0.3	ng	127902	4	17.017	150604	0.4
Benzyl butyl ph...	20.378	0.1	ng	52593	5	21.227	395797	0.4
.beta.-Alanine,...	22.056	0.1	ng	79739	5	21.227	395797	0.4