LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016636.D
Acq On : 01 Oct 2021 15:19
Operator : CG/JU
Sample : M3990-07MSD
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : S-836-K1-SO-1-1.5-092921MSD

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: BN016636.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.281	20	22	25	rBV	12683	16541	3.32%	0.183%
2	3.530	46	49	53	rBV	28177	50587	10.14%	0.561%
3	3.594	53	56	64	rVB	15362	30054	6.02%	0.333%
4	3.843	80	83	96	rVB	14655	38991	7.81%	0.432%
5	4.129	112	114	122	rVB	4220	9154	1.83%	0.101%
6	4.249	125	127	130	rBV	11249	16455	3.30%	0.182%
7	4.830	186	190	204	rVB	205805	320815	64.30%	3.557%
8	5.051	211	214	221	rBV	4494	9484	1.90%	0.105%
9	5.291	236	240	249	rVB	26050	45923	9.20%	0.509%
10	5.761	288	291	300	rVB	4774	9873	1.98%	0.109%
11	6.665	385	389	396	rVB	7444	14664	2.94%	0.163%
12	6.831	404	407	418	rVB2	29141	66648	13.36%	0.739%
13	6.988	420	424	430	rBV	13168	25872	5.19%	0.287%
14	7.080	430	434	443	rVB	39364	65315	13.09%	0.724%
15	7.209	445	448	450	rBV	12338	21808	4.37%	0.242%
16	7.532	480	483	490	rVB2	7262	14243	2.85%	0.158%
17	7.642	491	495	500	rBV	55611	103940	20.83%	1.152%
18	7.873	517	520	525	rVB2	3519	7554	1.51%	0.084%
19	7.983	529	532	540	rVB	6952	13833	2.77%	0.153%
20	8.177	549	553	559	rVB	4139	10442	2.09%	0.116%
21	8.306	565	567	569	rVB	8713	8739	1.75%	0.097%
22	8.442	569	578	582	rBV2	40378	98093	19.66%	1.087%
23	8.696	595	598	602	rBV	4433	7810	1.57%	0.087%
24	8.784	602	605	607	rVV	33993	67484	13.53%	0.748%
25	8.822	607	608	613	rVV	28703	41615	8.34%	0.461%
26	8.911	613	615	617	rVV	3515	7379	1.48%	0.082%
27	8.949	617	618	622	rVB	6956	9797	1.96%	0.109%
28	9.342	646	649	656	rVB	50176	80177	16.07%	0.889%
29	9.532	660	664	667	rBV	4004	8653	1.73%	0.096%
30	9.595	667	669	672	rVV	10053	19808	3.97%	0.220%
31	9.646	672	673	678	rVB	4624	7861	1.58%	0.087%
32	9.836	685	688	691	rBV	19032	29448	5.90%	0.326%
33	10.064	703	706	713	rBV2	5490	13304	2.67%	0.147%
34	10.204	713	717	720	rBV	238208	388009	77.77%	4.302%
35	10.407	730	733	735	rBV	98825	172256	34.53%	1.910%
36	10.457	735	737	740	rVV	99676	160761	32.22%	1.782%

LSC Area Percent Report

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Sample : M3990-07MSD
Misc :
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Instrument : BNA_N
ClientSampleId : S-836-K1-SO-1-1.5-092921MSD

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	10.571	744	746	754	rVB	13968	30628	6.14%	0.340%
38	10.749	757	760	764	rVB	29498	47394	9.50%	0.525%
39	11.306	801	804	808	rBV	4147	8600	1.72%	0.095%
40	11.709	856	865	888	rBV	15603	26439	5.30%	0.293%
41	12.003	917	931	940	rBV	48854	81933	16.42%	0.908%
42	12.078	940	948	973	rVB	119452	187555	37.59%	2.079%
43	12.301	986	998	1020	rVB	109435	175595	35.19%	1.947%
44	12.695	1056	1059	1062	rBV	17094	27445	5.50%	0.304%
45	12.772	1062	1065	1071	rVB	13359	24505	4.91%	0.272%
46	12.886	1071	1074	1078	rBV2	82122	154080	30.88%	1.708%
47	13.101	1088	1091	1092	rBV	123337	182474	36.57%	2.023%
48	13.139	1092	1094	1096	rVV	78896	133129	26.68%	1.476%
49	13.178	1096	1097	1106	rVV	43239	58936	11.81%	0.653%
50	13.736	1138	1141	1143	rVB	12248	16505	3.31%	0.183%
51	13.850	1148	1150	1153	rVB	18848	28271	5.67%	0.313%
52	13.990	1158	1161	1164	rVB	97912	151532	30.37%	1.680%
53	14.269	1180	1183	1186	rBV	125938	186177	37.32%	2.064%
54	14.332	1186	1188	1191	rVV	151490	214209	42.93%	2.375%
55	14.434	1194	1196	1200	rVV	12268	19506	3.91%	0.216%
56	14.522	1200	1203	1206	rVV3	3246	8049	1.61%	0.089%
57	14.637	1210	1212	1219	rVV2	16792	44643	8.95%	0.495%
58	14.814	1222	1226	1229	rVV2	4767	11881	2.38%	0.132%
59	14.903	1229	1233	1239	rVB3	7056	15867	3.18%	0.176%
60	15.106	1246	1249	1255	rVB	10189	15327	3.07%	0.170%
61	15.322	1263	1266	1270	rBV2	196484	317101	63.56%	3.515%
62	15.537	1280	1283	1287	rVV	32175	56993	11.42%	0.632%
63	15.614	1287	1289	1295	rVV2	38456	69322	13.89%	0.769%
64	15.715	1295	1297	1299	rVV	14033	22082	4.43%	0.245%
65	15.766	1299	1301	1305	rVB2	12272	19637	3.94%	0.218%
66	15.969	1315	1317	1322	rVB2	3931	9823	1.97%	0.109%
67	16.226	1334	1338	1343	rBV2	59985	90946	18.23%	1.008%
68	16.324	1343	1346	1353	rVB	40123	69203	13.87%	0.767%
69	16.506	1358	1361	1364	rBV	30802	43223	8.66%	0.479%
70	16.677	1372	1375	1384	rVB	33811	52243	10.47%	0.579%
71	16.835	1384	1388	1392	rVB2	5560	10948	2.19%	0.121%
72	17.017	1400	1403	1405	rBV	91608	154908	31.05%	1.717%
73	17.066	1405	1407	1410	rVV	140424	197563	39.60%	2.190%
74	17.151	1411	1414	1419	rVV	116327	186742	37.43%	2.070%
75	17.431	1434	1437	1446	rBV	89982	135231	27.10%	1.499%
76	18.020	1483	1486	1503	rVB	10094	13081	2.62%	0.145%

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Instrument : BNA_N
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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : OFF Filtering: 5
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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	18.909	1661	1665	1671	rVB	10104	10977	2.20%	0.122%
78	19.063	1687	1696	1699	rBV	108012	154131	30.89%	1.709%
79	19.098	1699	1703	1725	rVV	183588	248206	49.75%	2.752%
80	19.460	1766	1776	1798	rVB	192337	256057	51.32%	2.839%
81	19.678	1813	1820	1837	rBV	85942	108922	21.83%	1.208%
82	20.378	1918	1921	1924	rBV	94569	108965	21.84%	1.208%
83	20.962	1974	1976	1980	rVV	18839	29984	6.01%	0.332%
84	21.164	1992	1995	1998	rBV	148767	204784	41.04%	2.270%
85	21.217	1998	2000	2003	rVV2	224898	424329	85.05%	4.704%
86	21.270	2003	2005	2008	rVB	176977	231658	46.43%	2.568%
87	21.854	2057	2060	2067	rBV2	5508	15272	3.06%	0.169%
88	22.056	2076	2079	2082	rBV	120294	167758	33.62%	1.860%
89	22.109	2082	2084	2089	rVB	24041	34513	6.92%	0.383%
90	22.311	2100	2103	2107	rBV	8229	20714	4.15%	0.230%
91	22.396	2108	2111	2112	rVB2	7570	12812	2.57%	0.142%
92	22.803	2217	2228	2235	rBV	129707	221490	44.39%	2.455%
93	22.848	2235	2241	2271	rVB2	139009	238012	47.70%	2.639%
94	23.382	2385	2397	2415	rBV	104344	208221	41.73%	2.308%
95	23.481	2415	2426	2464	rVB	97726	204522	40.99%	2.267%
96	24.083	2593	2602	2615	rBV	6897	13085	2.62%	0.145%
97	24.172	2618	2628	2650	rBV	14681	37901	7.60%	0.420%
98	24.857	2819	2828	2847	rVB	5525	12341	2.47%	0.137%
99	25.767	3071	3094	3127	rBV4	139027	498927	100.00%	5.531%
100	26.452	3272	3294	3329	rBV	75930	243472	48.80%	2.699%

Sum of corrected areas: 9020169

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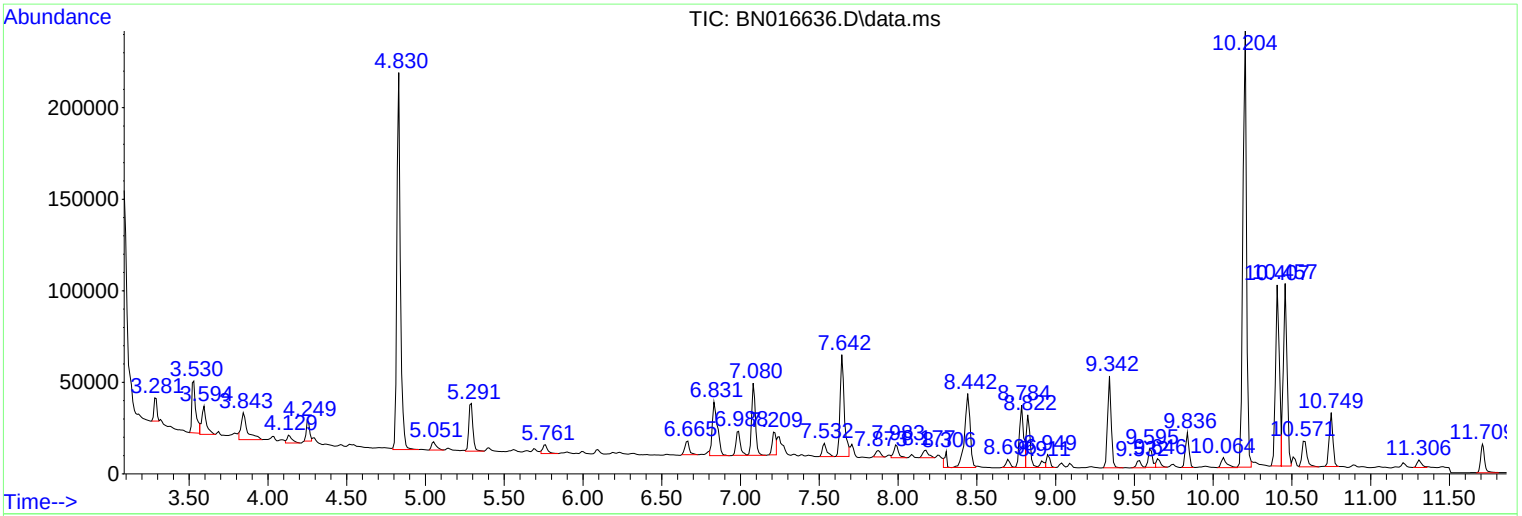
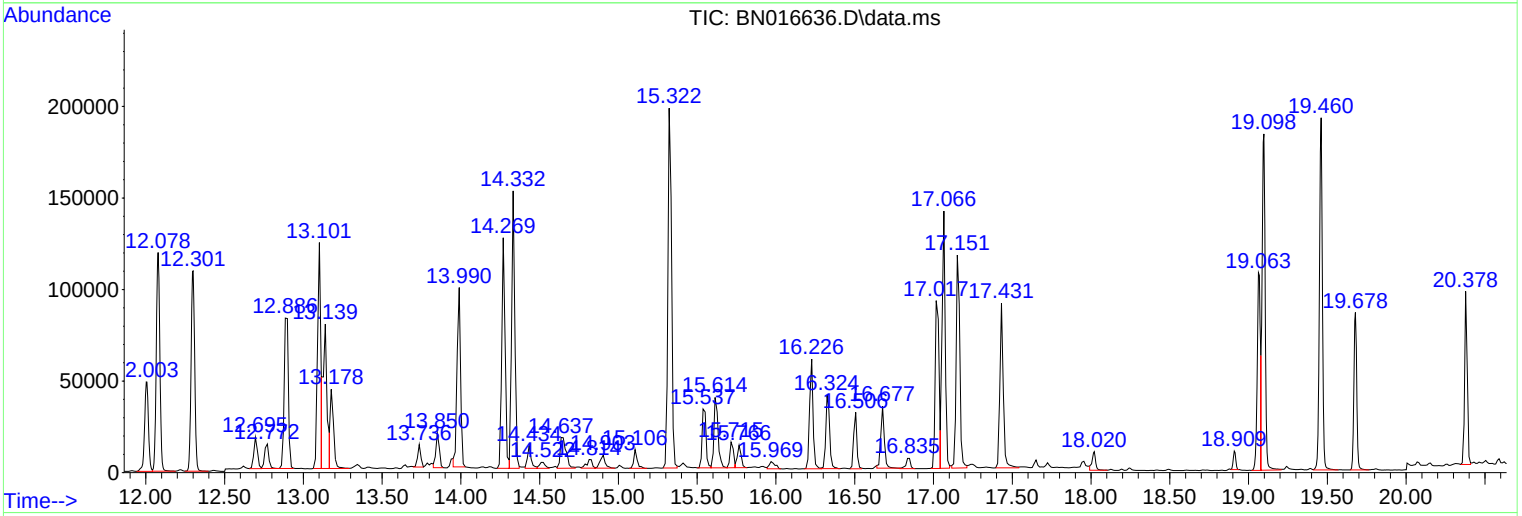
Misc :
ALS Vial : 5 Sample Multiplier: 1

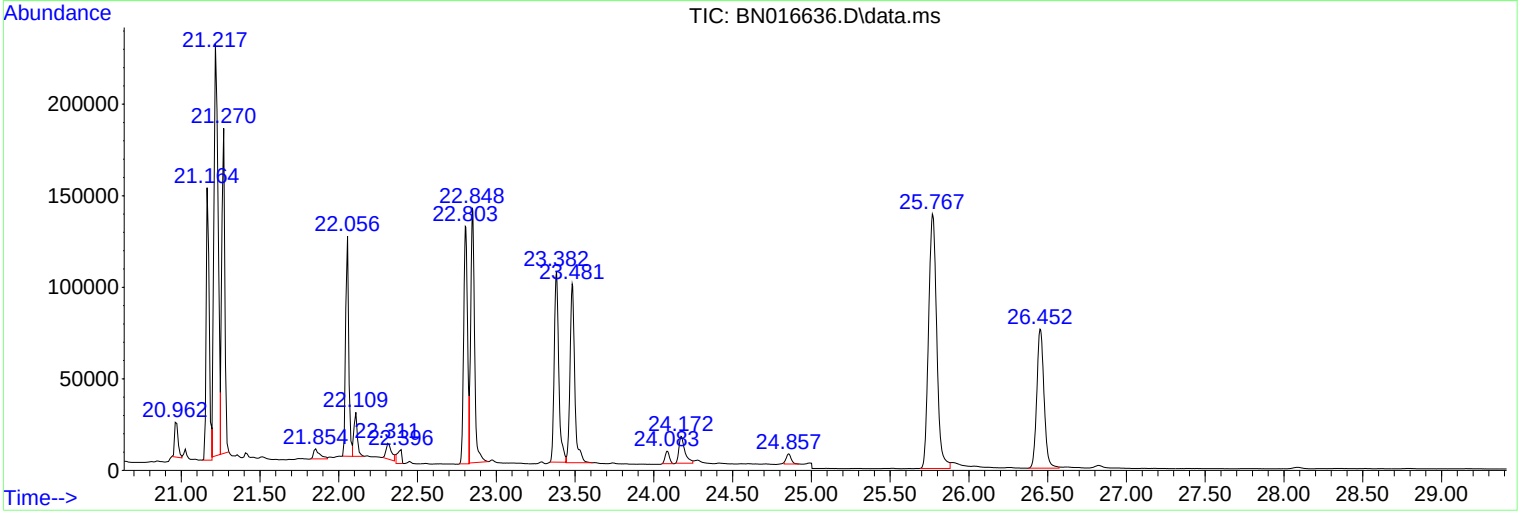
Instrument :
BNA_N
ClientSampleId :
S-836-K1-SO-1-1.5-092921MSD

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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BNA_N
ClientSampleId :
S-836-K1-SO-1-1.5-092921MSD

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

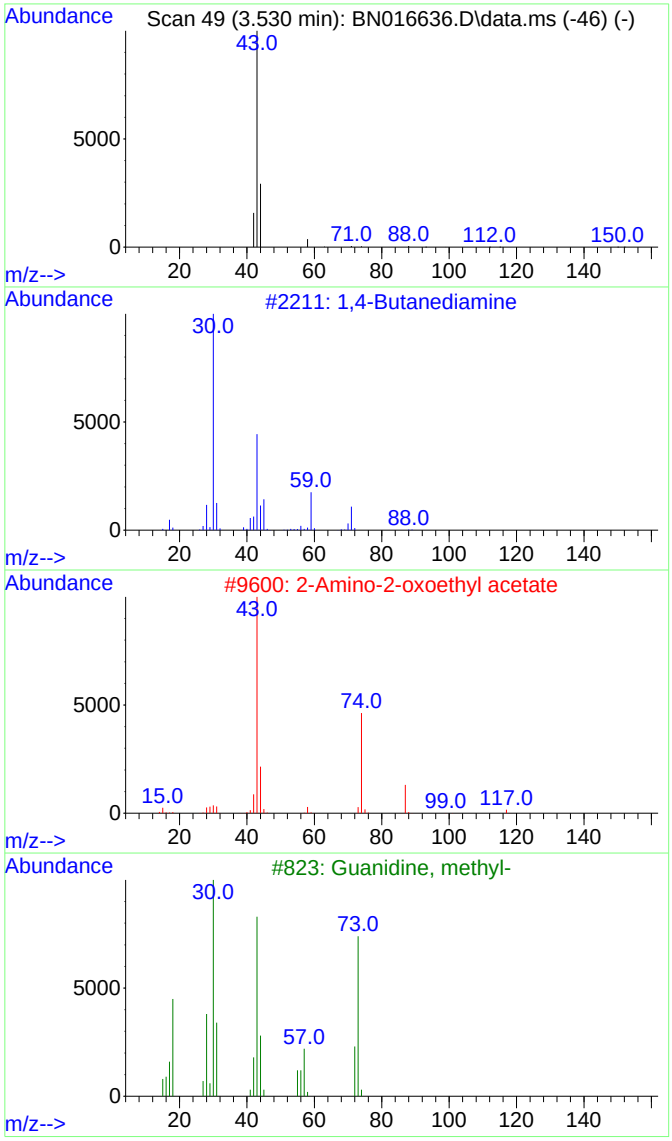
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

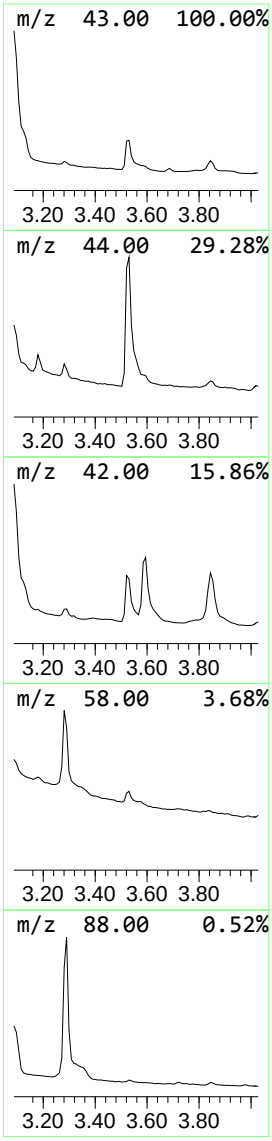
****

Peak Number 1 1,4-Butanediamine Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.530	0.19 ng	50587	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Butanediamine	88	C4H12N2	000110-60-1	9
2	2-Amino-2-oxoethyl acetate	117	C4H7NO3	1000500-76-5	4
3	Guanidine, methyl-	73	C2H7N3	000471-29-4	4
4	Hydrogen isocyanate	43	CHNO	000075-13-8	3
5	Hydrogen azide	43	HN3	007782-79-8	3





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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

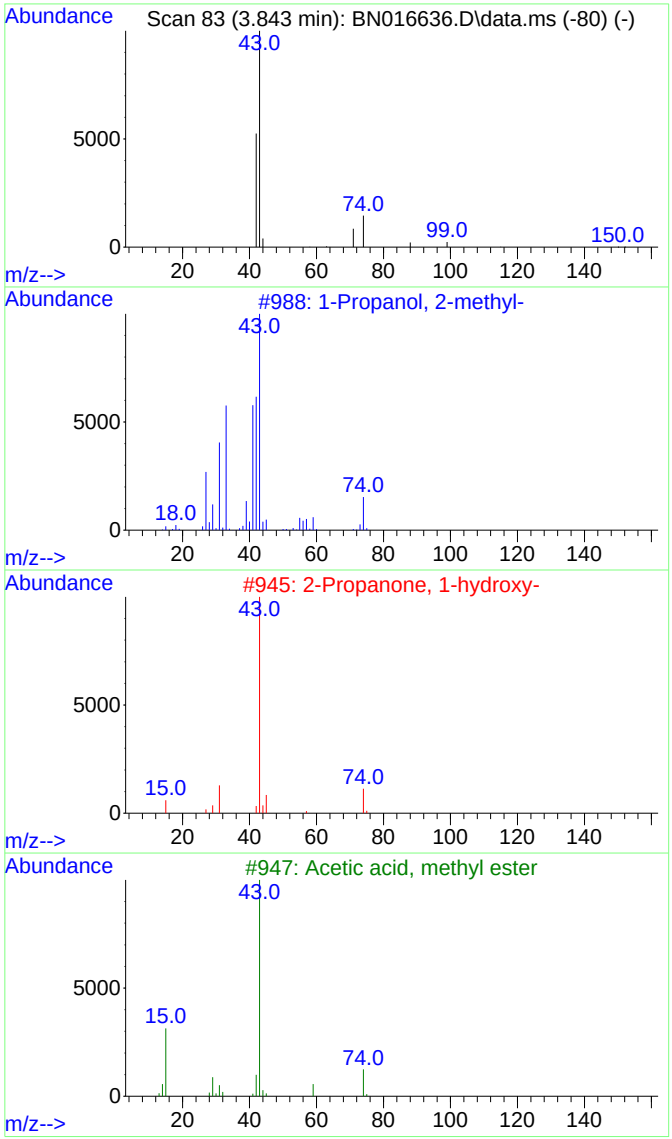
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

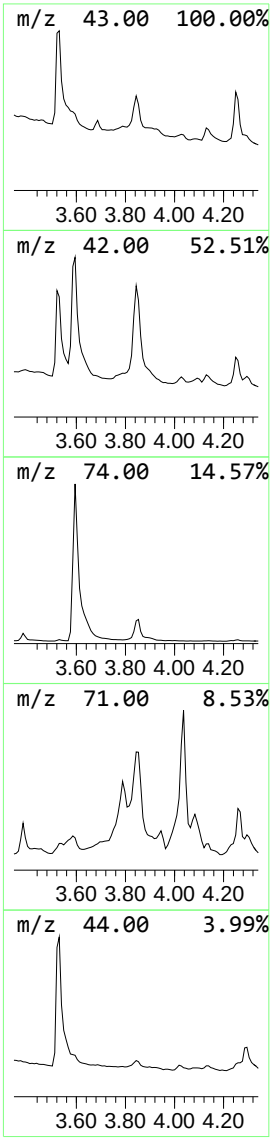
****

Peak Number 2 1-Propanol, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.843	0.15 ng	38991	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
2	2-Propanone, 1-hydroxy-	74	C3H6O2	000116-09-6	4
3	Acetic acid, methyl ester	74	C3H6O2	000079-20-9	4
4	Cyanamide	42	CH2N2	000420-04-2	3
5	Acetic acid, hydrazide	74	C2H6N2O	001068-57-1	3





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ALS Vial : 5 Sample Multiplier: 1

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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

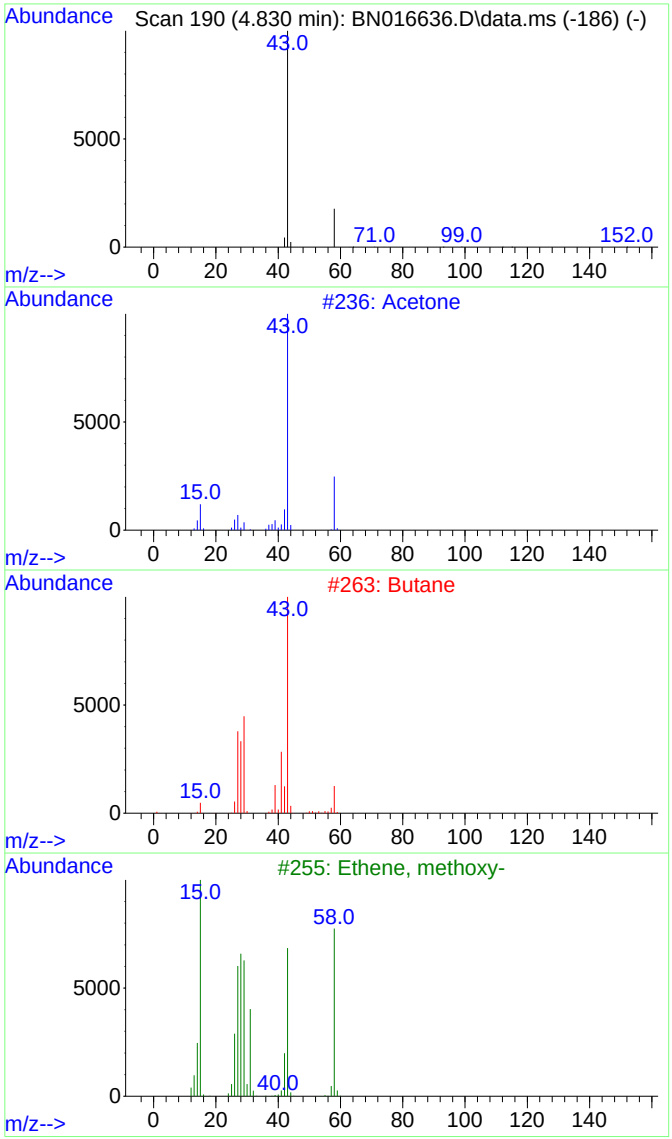
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

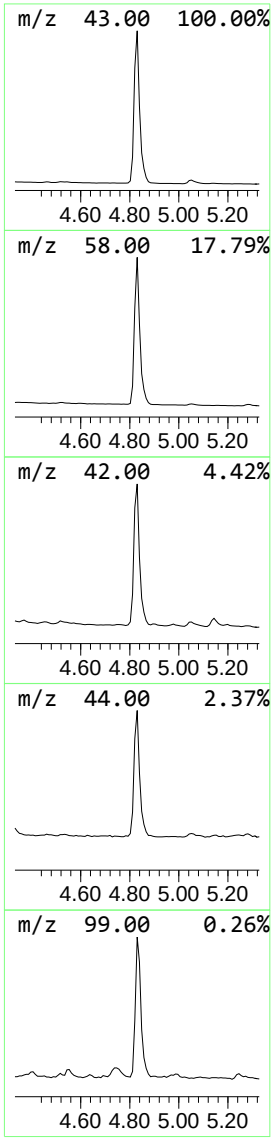
****

Peak Number 3 Acetone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.830	1.23 ng	320815	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetone	58	C3H6O	000067-64-1	4
2	Butane	58	C4H10	000106-97-8	4
3	Ethene, methoxy-	58	C3H6O	000107-25-5	3
4	Diazene, dimethyl-	58	C2H6N2	000503-28-6	3
5	Hydrogen isocyanate	43	CHNO	000075-13-8	2





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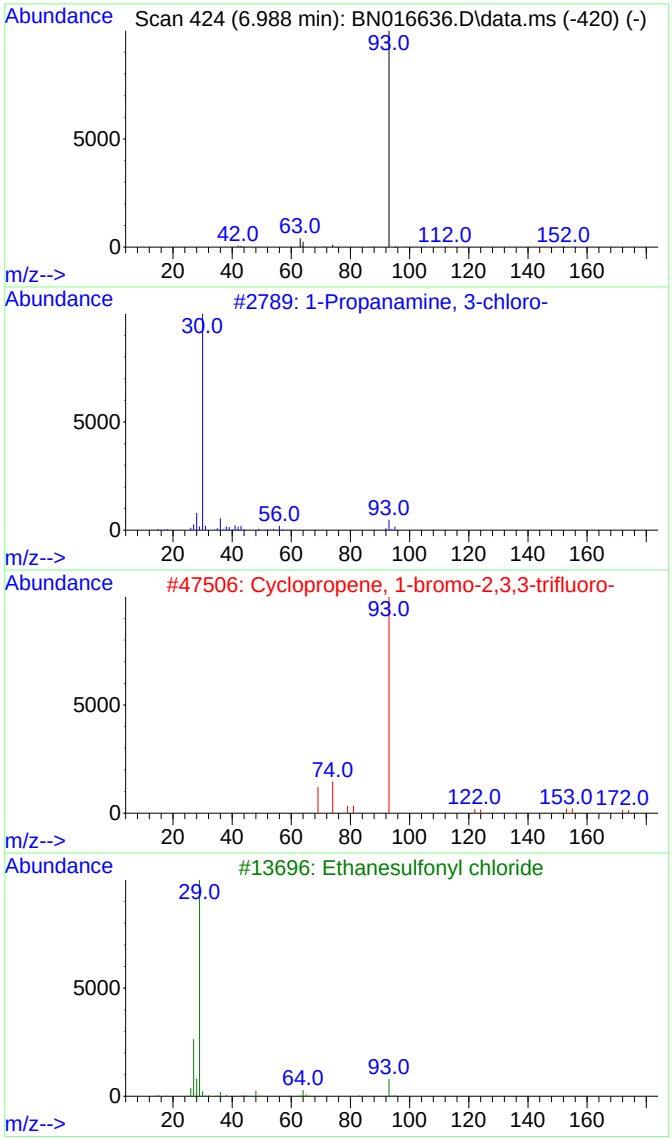
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

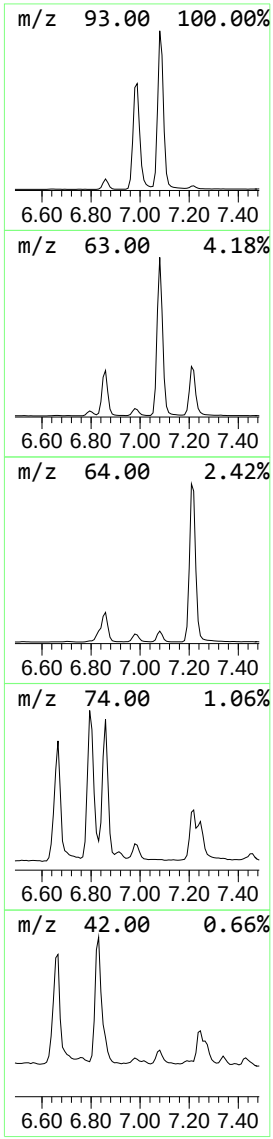
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Propanamine, 3-chloro- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.988	0.10 ng	25872	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 : BN016636.D
Acq On : 01 Oct 2021 15:19
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Sample : M3990-07MSD
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S-836-K1-SO-1-1.5-092921MSD

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

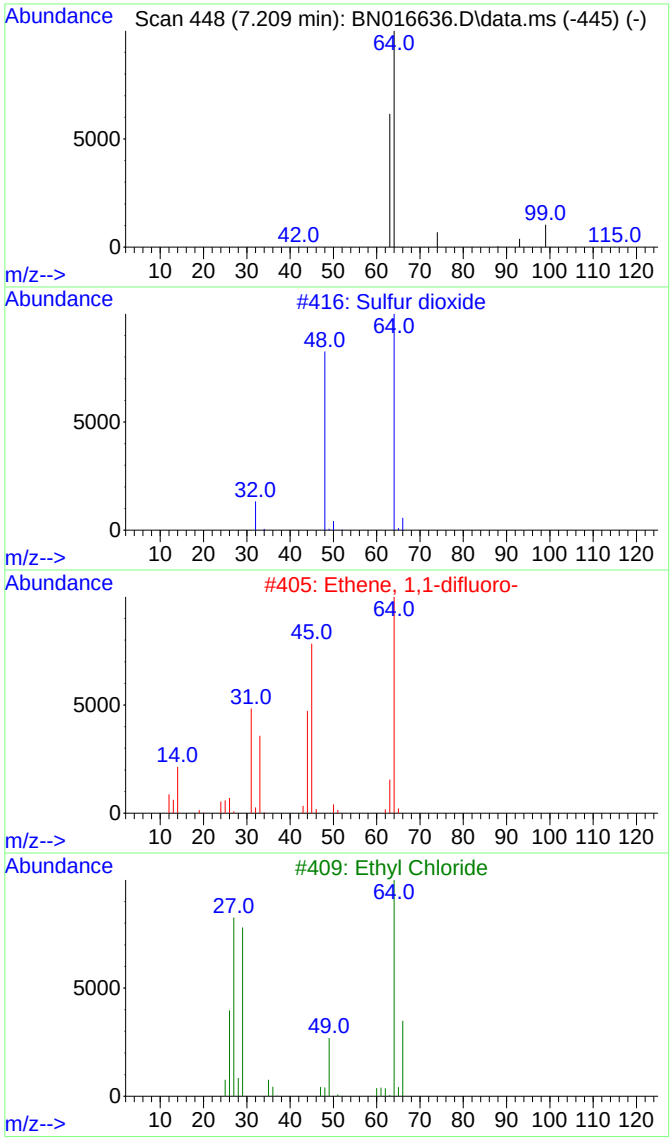
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

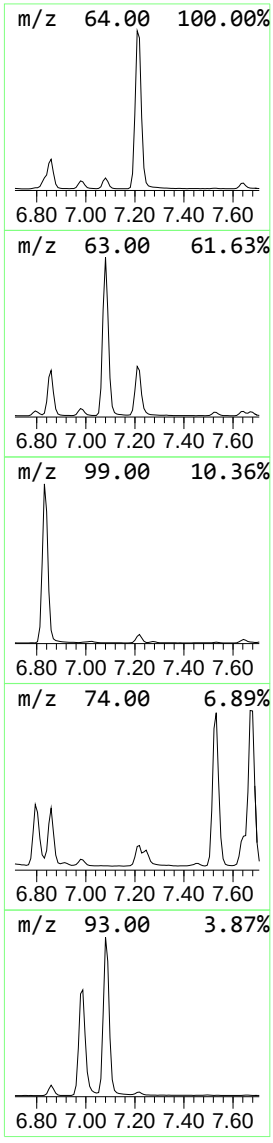
****

Peak Number 5 Sulfur dioxide Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.209	0.08 ng	21808	1,4-Dichlorobenzene-d4	7.642

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





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Acq On : 01 Oct 2021 15:19
Operator : CG/JU
Sample : M3990-07MSD
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S-836-K1-SO-1-1.5-092921MSD

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

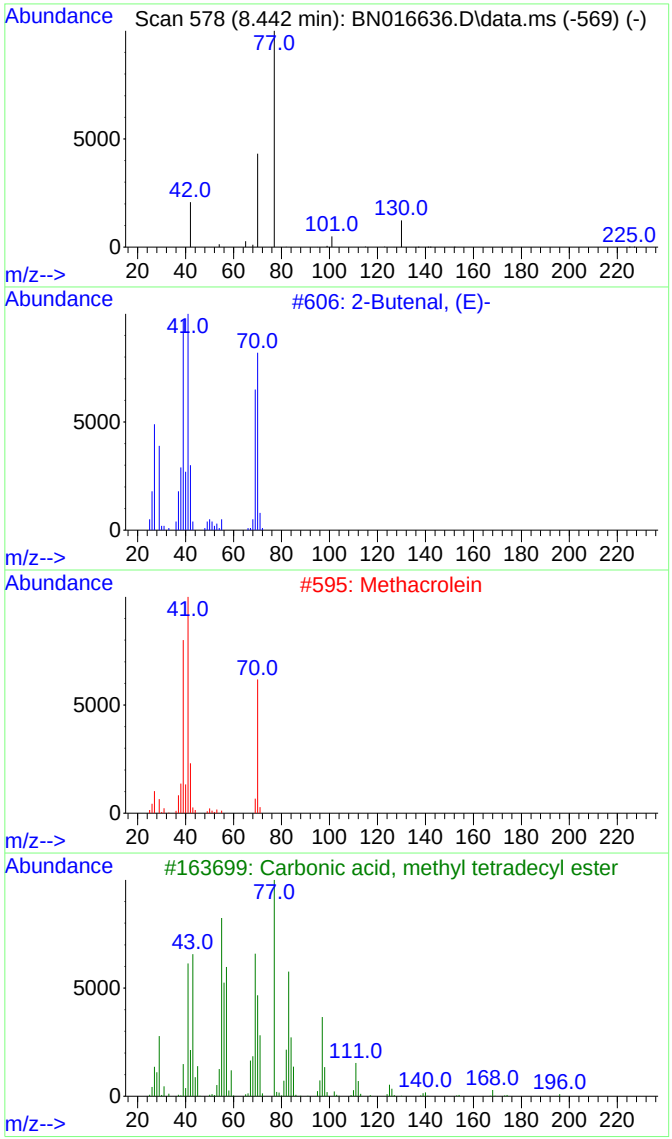
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

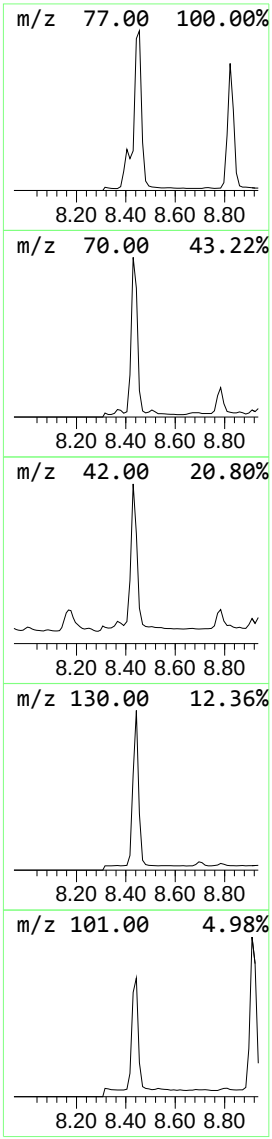
****

Peak Number 6 2-Butenal, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.442	0.38 ng	98093	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenal, (E)-	70	C4H6O	000123-73-9	4
2	Methacrolein	70	C4H6O	000078-85-3	4
3	Carbonic acid, methyl tetradecyl...	272	C16H32O3	1000314-62-5	4
4	(E)-1,3-Butadien-1-ol	70	C4H6O	070411-98-2	4
5	Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	3





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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S-836-K1-SO-1-1.5-092921MSD

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

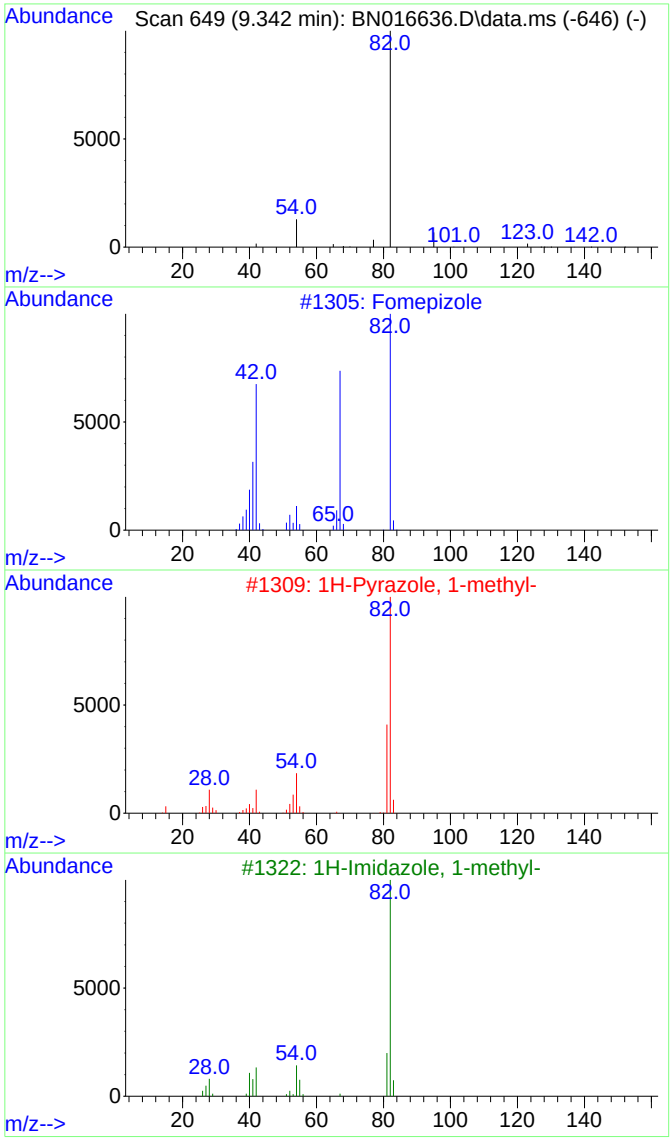
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

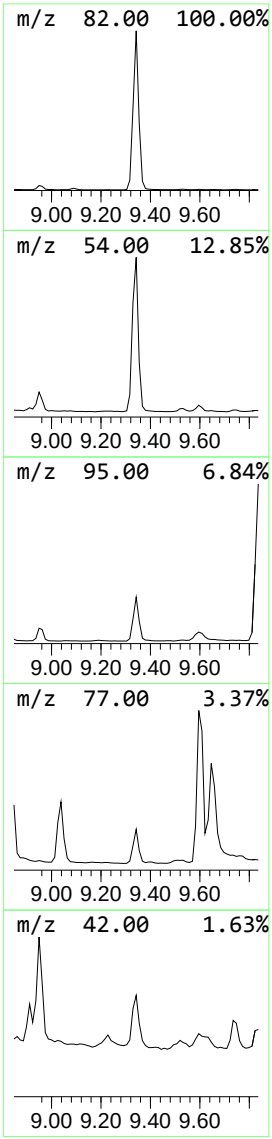
****

Peak Number 7 Fomepizole Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.342	0.19 ng	80177	Naphthalene-d8	10.407

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





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Misc :
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ClientSampleId :
S-836-K1-SO-1-1.5-092921MSD

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

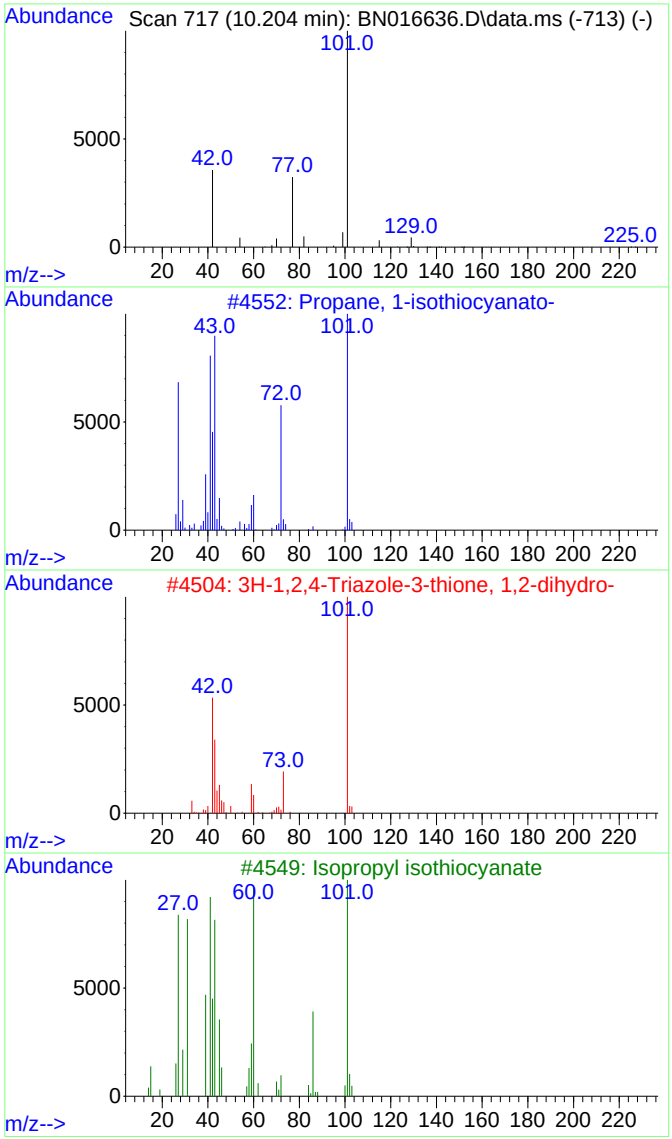
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

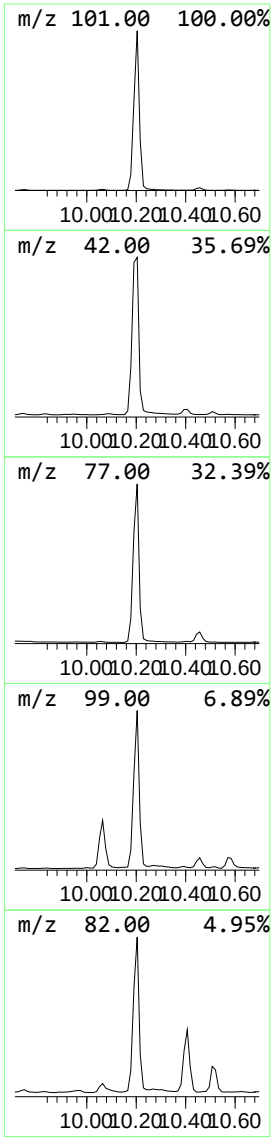
****

Peak Number 8 Propane, 1-isothiocyanato- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.204	0.90 ng	388009	Naphthalene-d8	10.407

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5
2	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
3	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	5
4	2-Pyrrolidinethione	101	C4H7NS	002295-35-4	4
5	3-Aminopropionitrile	70	C3H6N2	000151-18-8	4





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Sample : M3990-07MSD
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-836-K1-SO-1-1.5-092921MSD

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

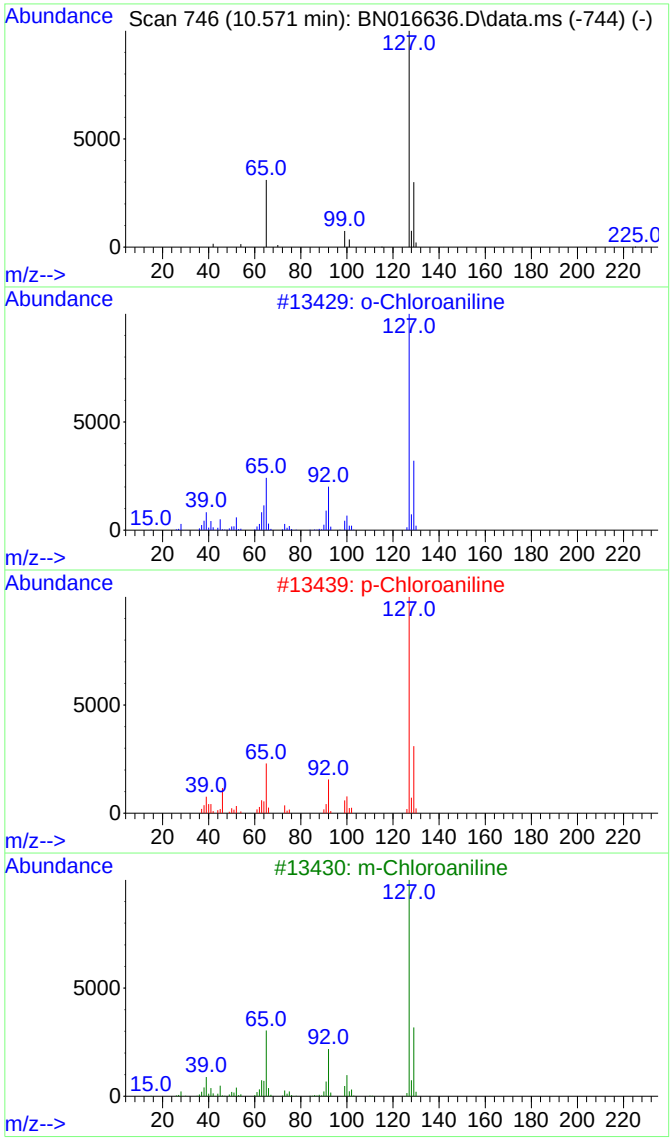
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

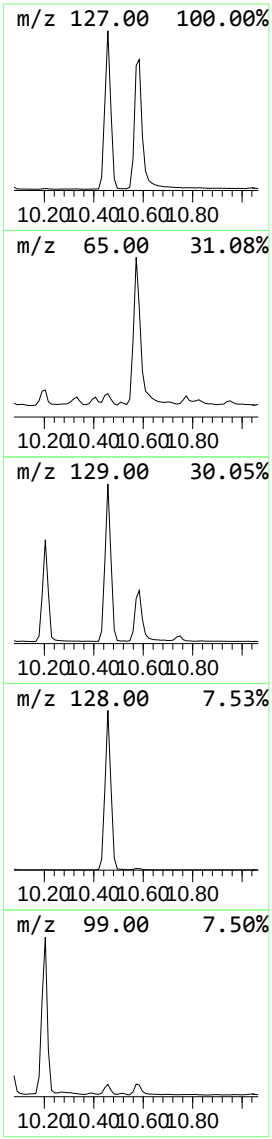
****

Peak Number 9 o-Chloroaniline Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.571	0.07 ng	30628	Naphthalene-d8	10.407

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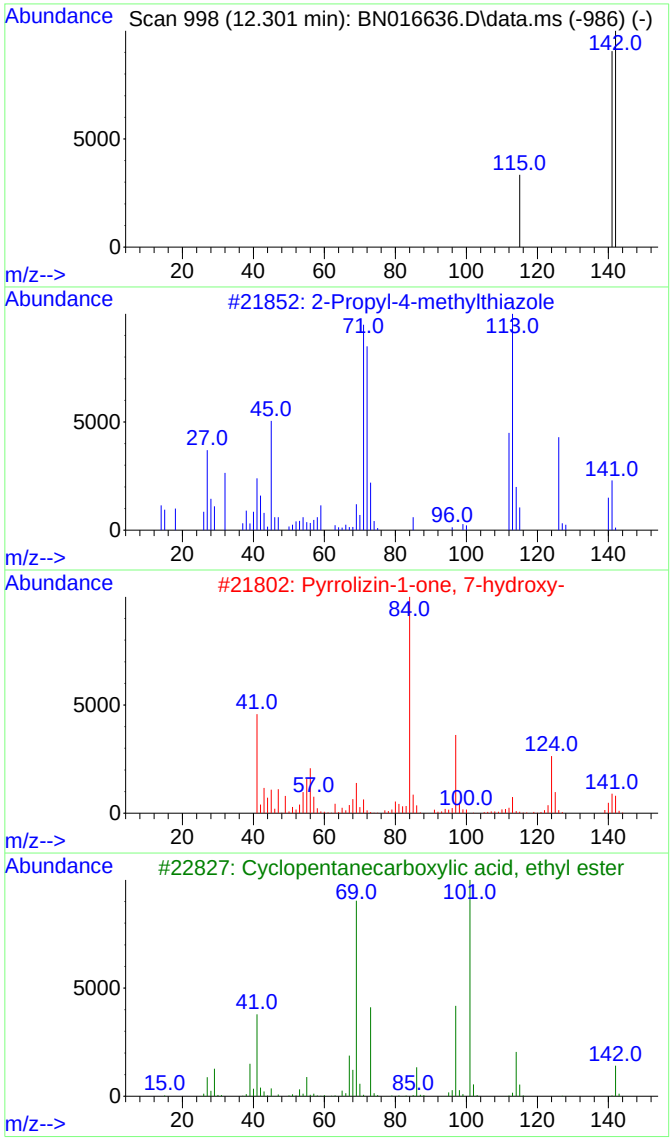
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

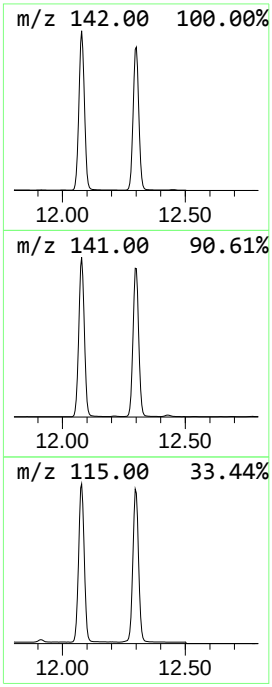
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2-Propyl-4-methylthiazole Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.301	0.41 ng	175595	Naphthalene-d8	10.407

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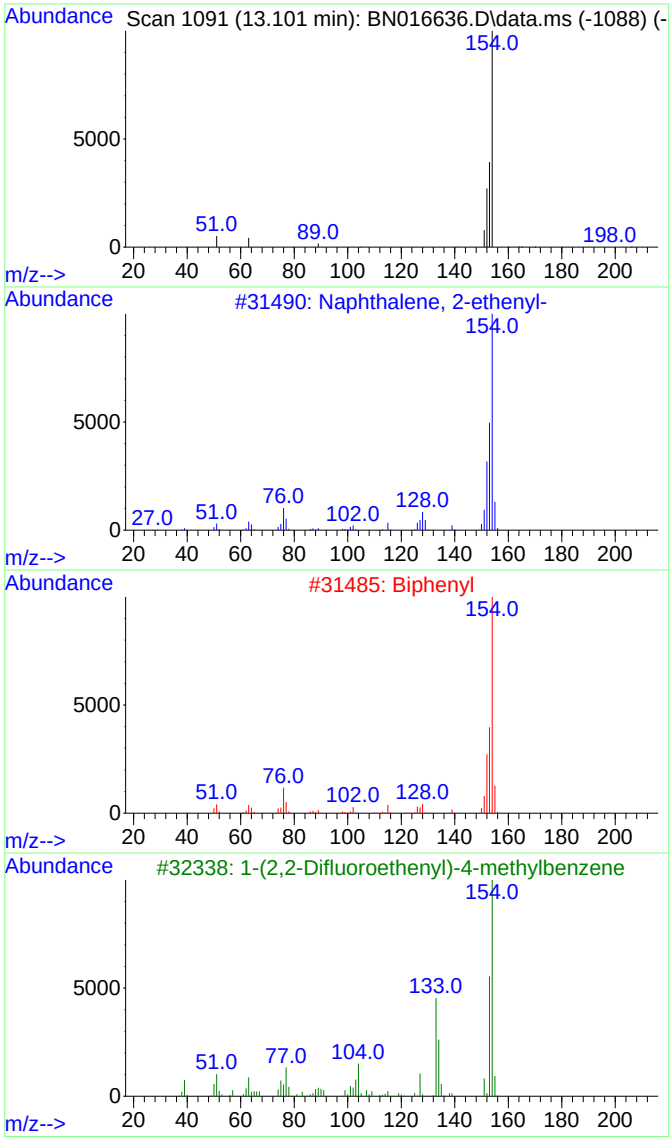
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

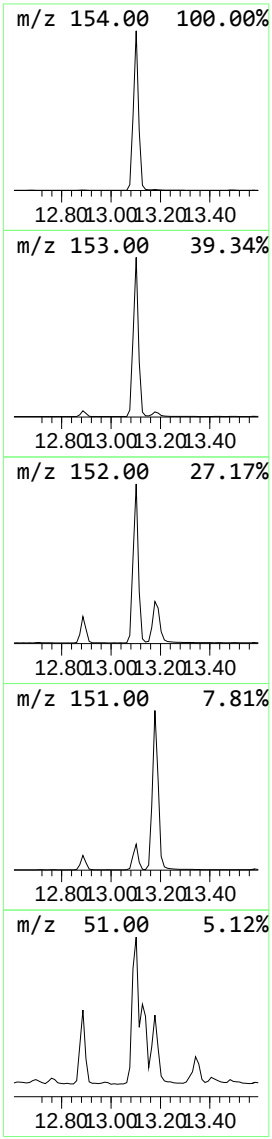
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Naphthalene, 2-ethenyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.101	0.39 ng	182474	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	50
2	Biphenyl	154	C12H10	000092-52-4	45
3	1-(2,2-Difluoroethenyl)-4-methyl...	154	C9H8F2	1000305-64-2	9
4	Octahydro-1H-pyrido(1,2-c)pyrimi...	154	C8H14N2O	015932-63-5	5
5	Furane-2-carboxaldehyde, iminose...	152	C6H8N4O	004353-50-8	5





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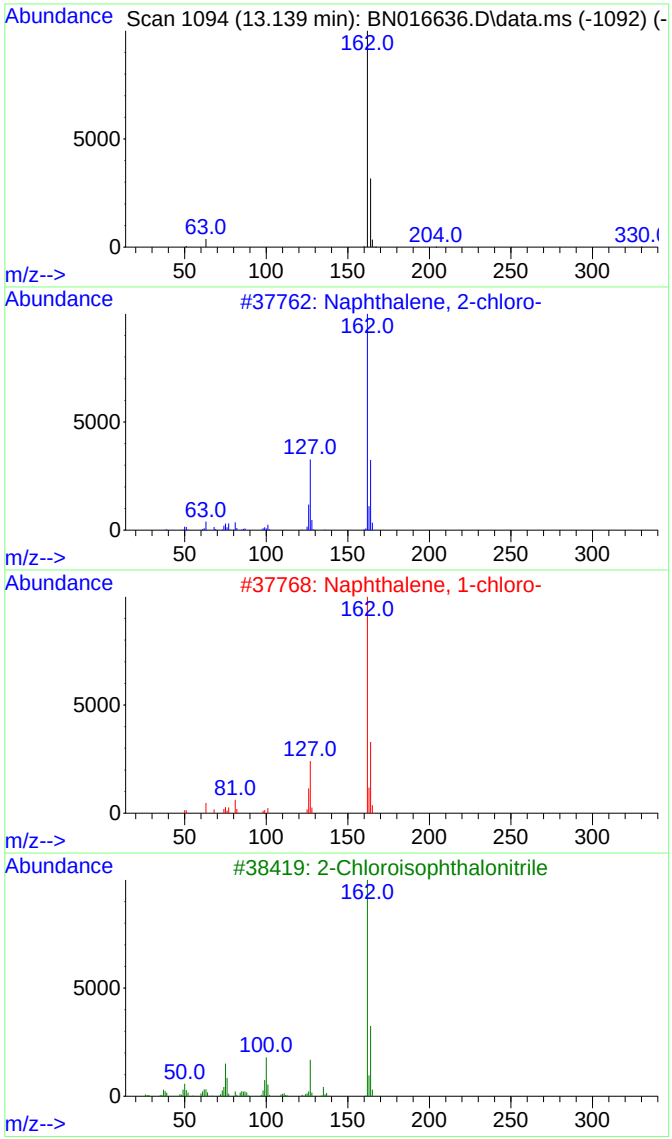
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

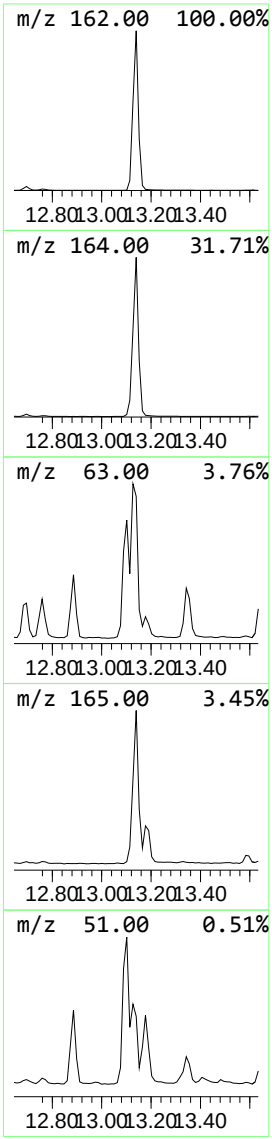
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Naphthalene, 2-chloro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.140	0.29 ng	133129	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	2-Chloroisophthalonitrile	162	C8H3ClN2	028442-78-6	7
4	3-Chlorophthalonitrile	162	C8H3ClN2	076241-79-7	7
5	3-Chloro-4-fluorothiophenol	162	C6H4ClFS	060811-23-6	5





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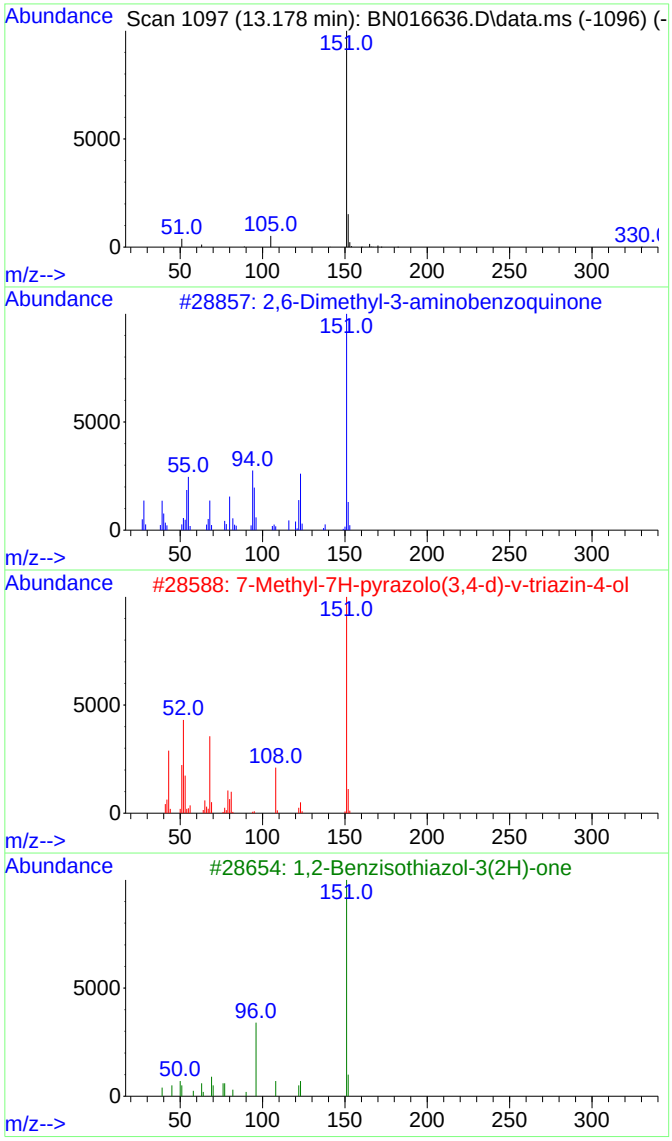
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

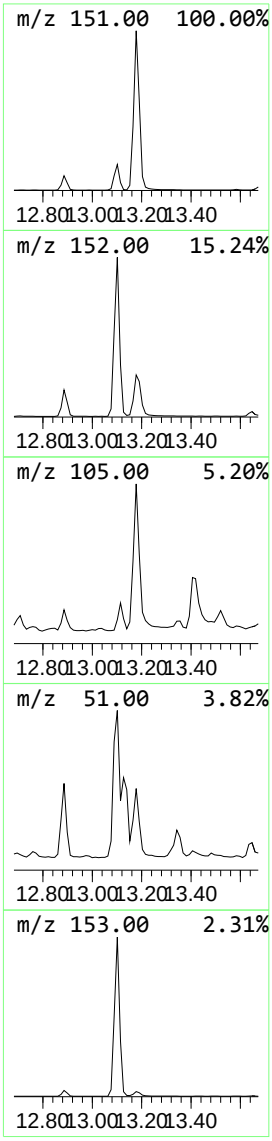
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 2,6-Dimethyl-3-aminobenzoqu... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.178	0.13 ng	58936	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Dimethyl-3-aminobenzoquinone	151	C8H9NO2	090005-56-4	7
2	7-Methyl-7H-pyrazolo(3,4-d)-v-tr...	151	C5H5N5O	018213-76-8	7
3	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	7
4	Butane-1,3-dione, 1-(pyrrol-2-yl)-	151	C8H9NO2	022441-25-4	5
5	1H-Indole, 4-chloro-	151	C8H6ClN	025235-85-2	4





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Misc :
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Instrument :
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ClientSampleId :
S-836-K1-SO-1-1.5-092921MSD

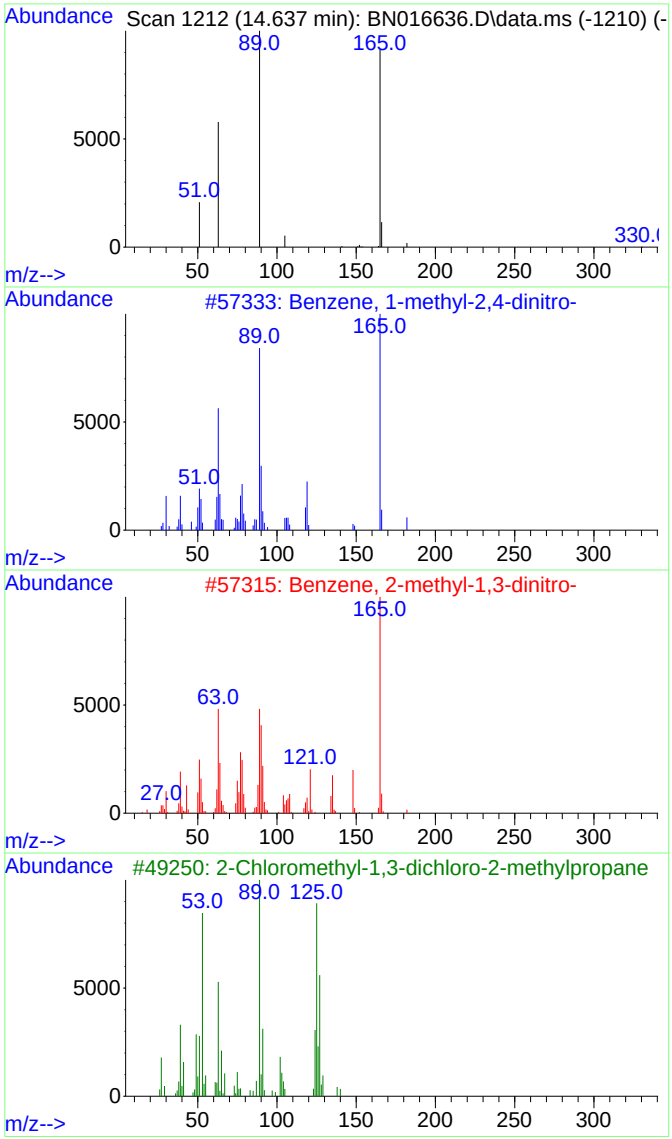
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

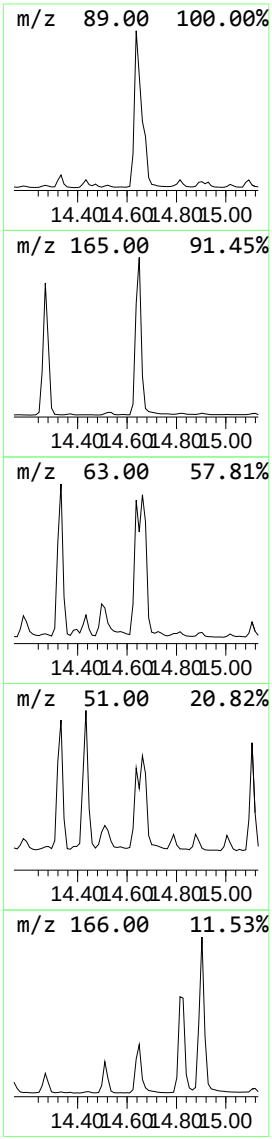
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.637	0.10 ng	44643	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-2,4-dinitro-	182	C7H6N2O4	000121-14-2	74
2	Benzene, 2-methyl-1,3-dinitro-	182	C7H6N2O4	000606-20-2	38
3	2-Chloromethyl-1,3-dichloro-2-me...	174	C5H9Cl3	001067-09-0	9
4	Ethanol, 1-(4-nitrophenyl)-2-[1-...	304	C17H24N2O3	1000264-75-7	9
5	5-[2-Chlorophenyl]tetraazole	180	C7H5ClN4	050907-46-5	9





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Sample : M3990-07MSD
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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S-836-K1-SO-1-1.5-092921MSD

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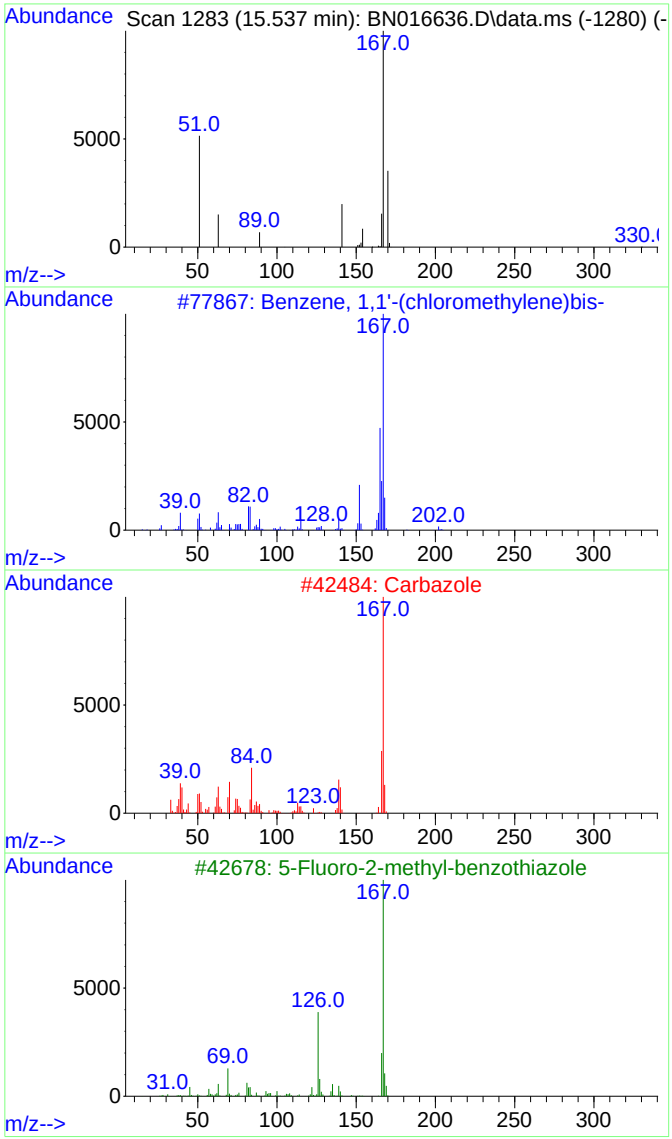
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

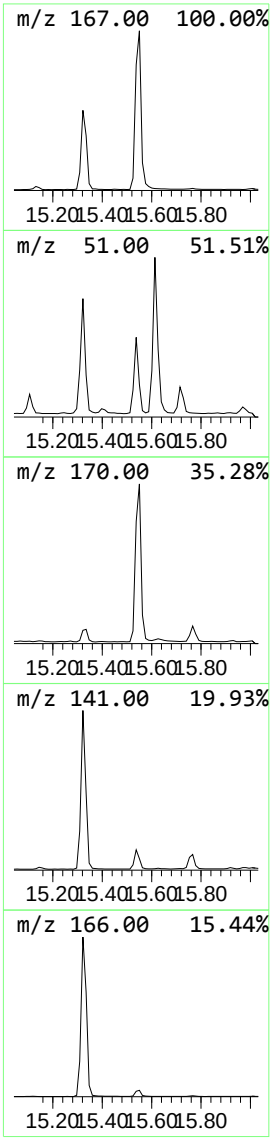
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 Benzene, 1,1'-(chloromethyl... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.537	0.12 ng	56993	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-(chloromethylene)bis-	202	C13H11Cl	000090-99-3	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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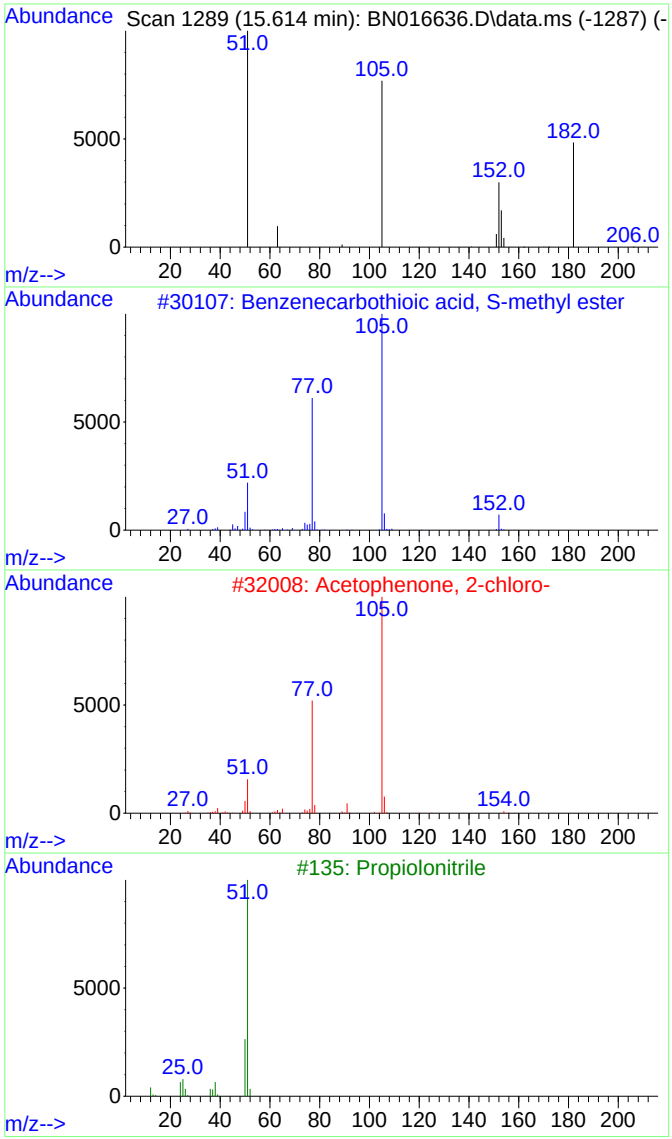
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

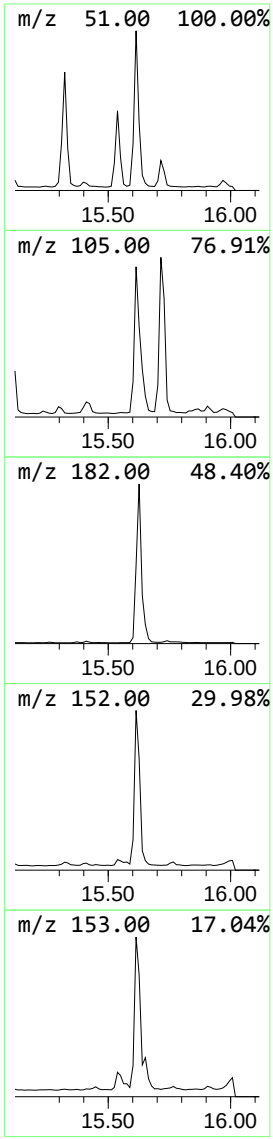
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 Benzenecarbothioic acid, S-... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.614	0.15 ng	69322	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 : BN016636.D
Acq On : 01 Oct 2021 15:19
Operator : CG/JU
Sample : M3990-07MSD
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-836-K1-SO-1-1.5-092921MSD

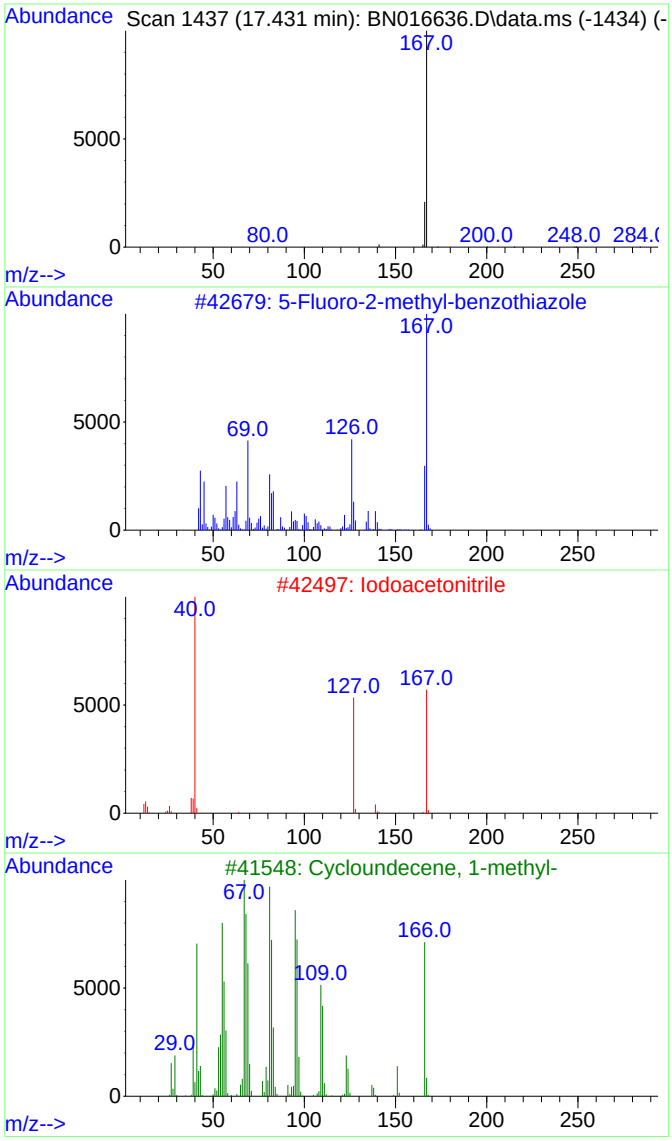
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

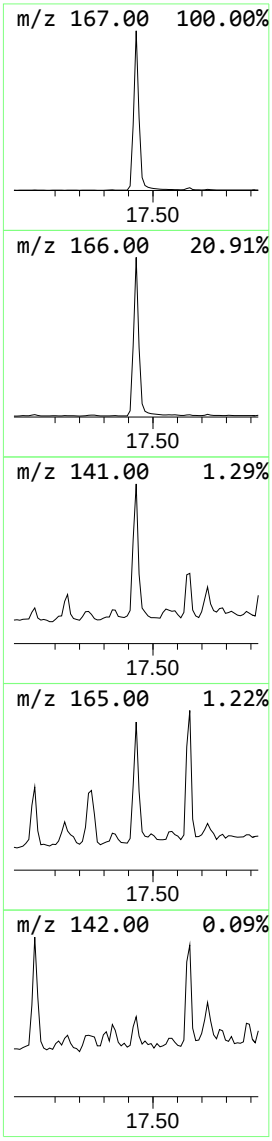
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 5-Fluoro-2-methyl-benzothia... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.431	0.35 ng	135231	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





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Data File : BN016636.D
Acq On : 01 Oct 2021 15:19
Operator : CG/JU
Sample : M3990-07MSD
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-836-K1-SO-1-1.5-092921MSD

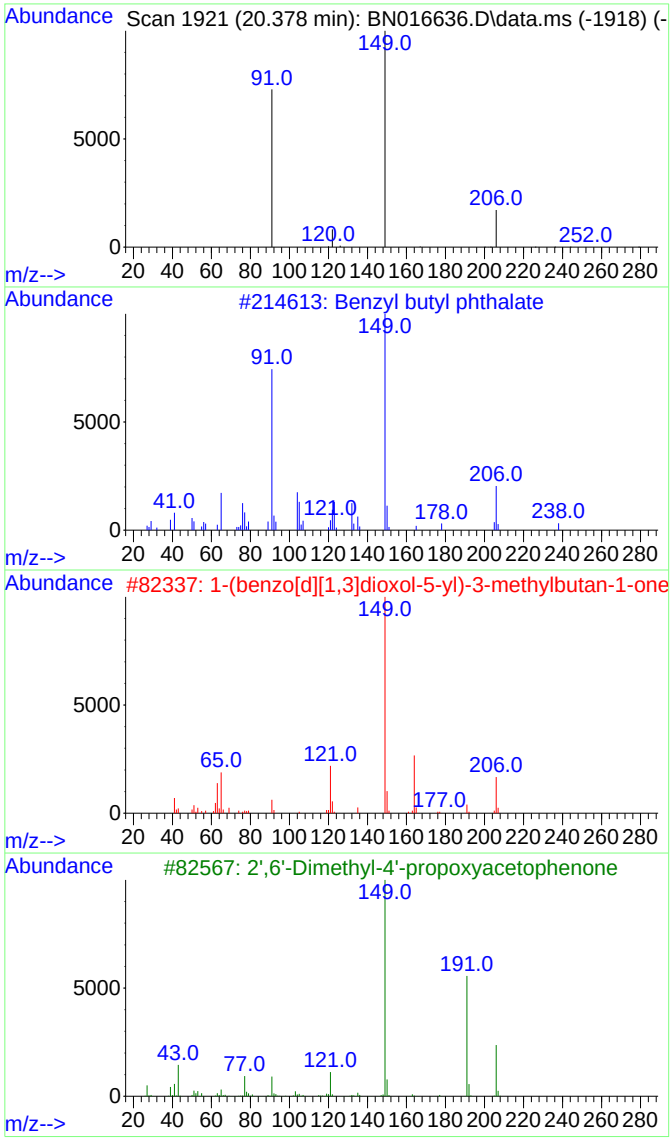
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

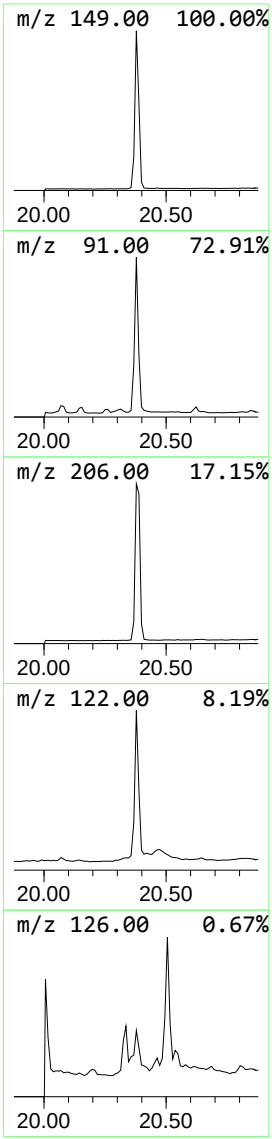
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 Benzyl butyl phthalate Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.378	0.10 ng	108965	Chrysene-d12	21.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzyl butyl phthalate	312	C19H20O4	000085-68-7	40
2	1-(benzo[d][1,3]dioxol-5-yl)-3-m...	206	C12H14O3	1000456-66-2	9
3	2',6'-Dimethyl-4'-propoxyacetoph...	206	C13H18O2	1010195-98-1	5
4	1,3,2-Dioxarsenane, 2-butyl-	206	C7H15AsO2	042541-33-3	5
5	2-tert-Butyl-6-methylphenol, n-p...	206	C14H22O	1000395-19-2	5





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Acq On : 01 Oct 2021 15:19
Operator : CG/JU
Sample : M3990-07MSD
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-836-K1-SO-1-1.5-092921MSD

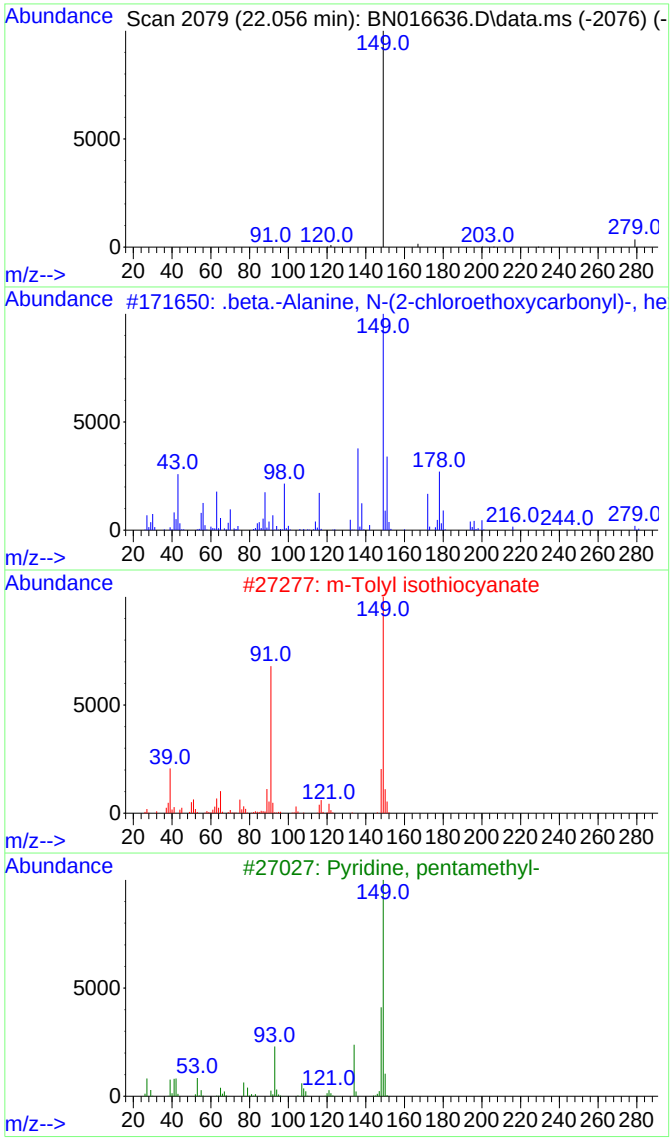
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

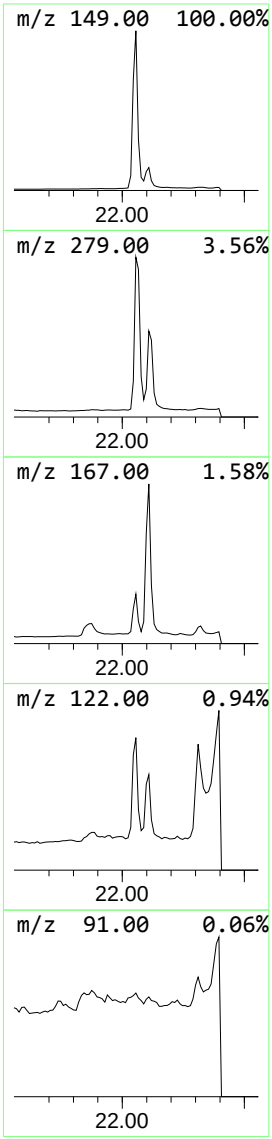
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 .beta.-Alanine, N-(2-chloro... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.056	0.16 ng	167758	Chrysene-d12	21.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Alanine, N-(2-chloroethox...	279	C12H22ClNO4	1010328-58-4	4
2	m-Tolyl isothiocyanate	149	C8H7NS	000621-30-7	4
3	Pyridine, pentamethyl-	149	C10H15N	003748-83-2	4
4	Phthalic acid, 7-bromoheptyl oct...	454	C23H35BrO4	1000415-52-2	4
5	Benzene, 1-isothiocyanato-4-methyl-	149	C8H7NS	000622-59-3	4





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Data File : BN016636.D
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Operator : CG/JU
Sample : M3990-07MSD
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-836-K1-SO-1-1.5-092921MSD

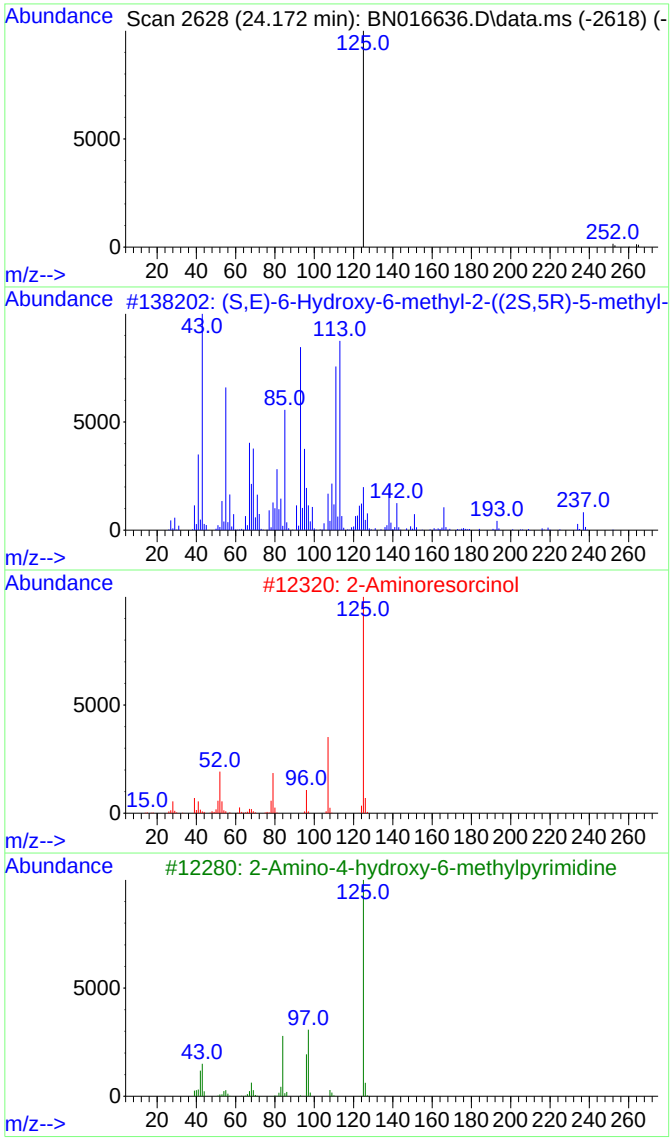
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

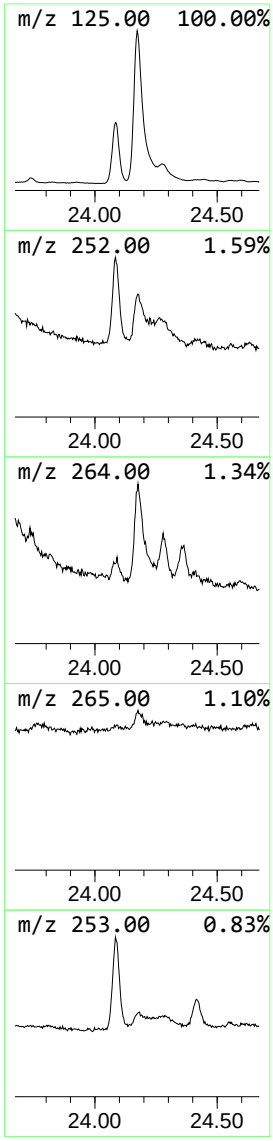
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 (S,E)-6-Hydroxy-6-methyl-2-... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.172	0.07 ng	37901	Perylene-d12	23.481

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S,E)-6-Hydroxy-6-methyl-2-((2S,...	252	C15H24O3	088243-64-5	3
2	2-Aminoresorcinol	125	C6H7NO2	003163-15-3	2
3	2-Amino-4-hydroxy-6-methylpyrimi...	125	C5H7N3O	003977-29-5	2
4	2(1H)-Pyrimidinone, 4-amino-5-me...	125	C5H7N3O	000554-01-8	2
5	2,4-Diamino-6-methyl-1,3,5-triazine	125	C4H7N5	000542-02-9	2





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016636.D
Acq On : 01 Oct 2021 15:19
Operator : CG/JU
Sample : M3990-07MSD
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : S-836-K1-SO-1-1.5-092921MSD

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
1,4-Butanediamine	3.530	0.2	ng	50587	1	7.642	103940	0.4
1-Propanol, 2-m...	3.843	0.2	ng	38991	1	7.642	103940	0.4
Acetone	4.830	1.2	ng	320815	1	7.642	103940	0.4
1-Propanamine, ...	6.988	0.1	ng	25872	1	7.642	103940	0.4
Sulfur dioxide	7.209	0.1	ng	21808	1	7.642	103940	0.4
2-Butenal, (E)-	8.442	0.4	ng	98093	1	7.642	103940	0.4
Fomepizole	9.342	0.2	ng	80177	2	10.407	172256	0.4
Propane, 1-isot...	10.204	0.9	ng	388009	2	10.407	172256	0.4
o-Chloroaniline	10.571	0.1	ng	30628	2	10.407	172256	0.4
2-Propyl-4-meth...	12.301	0.4	ng	175595	2	10.407	172256	0.4
Naphthalene, 2-...	13.101	0.4	ng	182474	3	14.269	186177	0.4
Naphthalene, 2-...	13.140	0.3	ng	133129	3	14.269	186177	0.4
2,6-Dimethyl-3-...	13.178	0.1	ng	58936	3	14.269	186177	0.4
Benzene, 1-meth...	14.637	0.1	ng	44643	3	14.269	186177	0.4
Benzene, 1,1'-(...	15.537	0.1	ng	56993	3	14.269	186177	0.4
Benzenecarbothi...	15.614	0.1	ng	69322	3	14.269	186177	0.4
5-Fluoro-2-meth...	17.431	0.3	ng	135231	4	17.017	154908	0.4
Benzyl butyl ph...	20.378	0.1	ng	108965	5	21.227	424329	0.4
.beta.-Alanine,...	22.056	0.2	ng	167758	5	21.227	424329	0.4
(S,E)-6-Hydroxy...	24.172	0.1	ng	37901	6	23.481	204522	0.4