LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016702.D
Acq On : 03 Oct 2021 11:12
Operator : CG/JU
Sample : M3892-14
Misc :
ALS Vial : 70 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : S-826-N-SO-1-1.5-092221

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: BN016702.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.511	44	47	59	rVB	21013	51297	5.94%	0.524%
2	3.834	79	82	99	rVB	10553	31245	3.62%	0.319%
3	4.277	128	130	145	rVB	10237	32266	3.74%	0.330%
4	4.821	185	189	196	rVB	70455	125499	14.53%	1.282%
5	5.042	209	213	221	rBV	18770	43436	5.03%	0.444%
6	5.272	235	238	248	rVB	22540	48206	5.58%	0.492%
7	6.333	349	353	361	rVB	13588	30351	3.51%	0.310%
8	6.665	382	389	395	rBV2	11445	34248	3.96%	0.350%
9	6.831	403	407	415	rVB	23658	44586	5.16%	0.455%
10	7.080	430	434	444	rVB	15138	35564	4.12%	0.363%
11	7.246	448	452	459	rVB2	11373	27402	3.17%	0.280%
12	7.642	490	495	500	rVB	47825	93847	10.86%	0.959%
13	7.937	522	527	532	rVB	503743	863843	100.00%	8.825%
14	8.493	580	582	585	rVB	12649	20111	2.33%	0.205%
15	8.734	597	601	603	rBV2	10112	26214	3.03%	0.268%
16	8.784	603	605	610	rVV2	34690	72088	8.35%	0.736%
17	8.949	614	618	621	rVB2	13968	29116	3.37%	0.297%
18	9.697	672	677	680	rBV	39772	101078	11.70%	1.033%
19	9.823	684	687	692	rVB2	14799	26986	3.12%	0.276%
20	10.064	703	706	712	rVB2	34947	87566	10.14%	0.895%
21	10.204	713	717	720	rBV2	255624	479214	55.47%	4.896%
22	10.406	729	733	735	rBV	94195	166366	19.26%	1.700%
23	10.457	735	737	740	rVV2	51952	90012	10.42%	0.920%
24	10.508	740	741	749	rVB4	8586	20353	2.36%	0.208%
25	11.167	789	793	795	rBV	15992	30397	3.52%	0.311%
26	12.003	922	931	940	rBV2	48413	77145	8.93%	0.788%
27	12.074	940	947	962	rVB	15242	25141	2.91%	0.257%
28	12.296	989	997	1011	rVB	16712	26145	3.03%	0.267%
29	12.632	1051	1054	1059	rVB	23610	40645	4.71%	0.415%
30	12.886	1071	1074	1077	rBV2	89667	152887	17.70%	1.562%
31	13.025	1081	1085	1089	rBV	10175	22464	2.60%	0.229%
32	13.190	1092	1098	1101	rVB	107751	228947	26.50%	2.339%
33	13.583	1127	1129	1132	rVB	41004	67450	7.81%	0.689%
34	13.748	1138	1142	1145	rBV	46545	77787	9.00%	0.795%
35	13.824	1145	1148	1151	rVV2	11321	20526	2.38%	0.210%
36	13.989	1158	1161	1163	rBV	18364	29879	3.46%	0.305%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Acq On : 03 Oct 2021 11:12
Operator : CG/JU
Sample : M3892-14
Misc :
ALS Vial : 70 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : S-826-N-SO-1-1.5-092221

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

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Peak separation: 5

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

37	14.129	1168	1172	1180	rBV2	38460	100725	11.66%	1.029%
38	14.269	1180	1183	1186	rBV	132388	193065	22.35%	1.972%
39	14.345	1186	1189	1192	rVV2	53559	90905	10.52%	0.929%
40	14.433	1193	1196	1198	rVB	13749	19924	2.31%	0.204%
41	14.522	1200	1203	1206	rBV2	59310	114209	13.22%	1.167%
42	14.598	1206	1209	1212	rVB	38882	61864	7.16%	0.632%
43	14.713	1212	1218	1219	rBV3	9614	29579	3.42%	0.302%
44	14.751	1219	1221	1223	rVB2	30930	50692	5.87%	0.518%
45	14.814	1223	1226	1230	rVB2	11372	21595	2.50%	0.221%
46	15.093	1243	1248	1251	rBV2	22058	42552	4.93%	0.435%
47	15.169	1251	1254	1256	rBV	68924	95123	11.01%	0.972%
48	15.322	1263	1266	1268	rVB2	13773	24260	2.81%	0.248%
49	15.398	1268	1272	1276	rBV3	14867	33793	3.91%	0.345%
50	15.626	1287	1290	1292	rBV2	19633	42875	4.96%	0.438%
51	15.728	1295	1298	1300	rBV2	55606	123289	14.27%	1.259%
52	15.854	1306	1308	1312	rVB2	27663	48176	5.58%	0.492%
53	16.007	1317	1320	1322	rVB	293805	339696	39.32%	3.470%
54	16.591	1365	1368	1373	rBV	33357	54161	6.27%	0.553%
55	16.677	1373	1375	1379	rVV2	22399	30864	3.57%	0.315%
56	17.017	1397	1403	1405	rVV	97416	198694	23.00%	2.030%
57	17.066	1405	1407	1411	rVV	102519	152629	17.67%	1.559%
58	17.151	1411	1414	1417	rVV2	29111	57620	6.67%	0.589%
59	17.236	1417	1421	1425	rVV	48249	97313	11.27%	0.994%
60	17.309	1425	1427	1432	rVV3	11811	30702	3.55%	0.314%
61	17.431	1435	1437	1443	rVV	13474	25146	2.91%	0.257%
62	17.723	1457	1461	1462	rVV4	9945	24081	2.79%	0.246%
63	17.796	1462	1467	1472	rVV	101819	242754	28.10%	2.480%
64	17.930	1475	1478	1479	rVV	32154	71354	8.26%	0.729%
65	17.967	1479	1481	1483	rVV2	42103	72434	8.39%	0.740%
66	19.068	1689	1697	1699	rBV	101636	133056	15.40%	1.359%
67	19.097	1699	1703	1715	rVV	279153	372861	43.16%	3.809%
68	19.251	1729	1734	1746	rBV	33620	46045	5.33%	0.470%
69	19.460	1767	1776	1788	rVB	255896	360762	41.76%	3.685%
70	19.648	1809	1814	1817	rVV	49508	65160	7.54%	0.666%
71	19.678	1817	1820	1835	rVB	83679	109358	12.66%	1.117%
72	20.006	1884	1886	1888	rBV	24868	29148	3.37%	0.298%
73	20.059	1889	1891	1894	rVV	17546	43960	5.09%	0.449%
74	20.123	1894	1897	1902	rVB3	39160	93739	10.85%	0.958%
75	20.335	1914	1917	1919	rBV	21433	26413	3.06%	0.270%
76	20.856	1964	1966	1970	rBV4	14538	31388	3.63%	0.321%

LSC Area Percent Report

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Operator : CG/JU
Sample : M3892-14
Misc :
ALS Vial : 70 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : S-826-N-SO-1-1.5-092221

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
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Peak separation: 5

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

77	20.919	1970	1972	1974	rVV	20531	35403	4.10%	0.362%
78	20.972	1974	1977	1987	rVB2	114914	206343	23.89%	2.108%
79	21.174	1993	1996	1998	rBV	37082	43657	5.05%	0.446%
80	21.227	1998	2001	2004	rVV2	194694	456255	52.82%	4.661%
81	21.270	2004	2005	2010	rVB	153352	177081	20.50%	1.809%
82	21.610	2034	2037	2040	rBV2	26195	42593	4.93%	0.435%
83	21.748	2048	2050	2053	rBV	28273	49335	5.71%	0.504%
84	21.875	2056	2062	2065	rBV	110614	234892	27.19%	2.400%
85	22.024	2073	2076	2080	rVB2	30310	54636	6.32%	0.558%
86	22.109	2082	2084	2089	rVB3	14717	25862	2.99%	0.264%
87	22.564	2152	2158	2171	rVB2	19923	29217	3.38%	0.298%
88	22.817	2221	2232	2238	rBV	94037	196844	22.79%	2.011%
89	22.896	2249	2255	2271	rVB	109756	179169	20.74%	1.830%
90	22.985	2274	2281	2302	rVB2	27368	51871	6.00%	0.530%
91	23.296	2364	2372	2387	rVB	48465	85907	9.94%	0.878%
92	23.392	2390	2400	2419	rBV2	63326	136867	15.84%	1.398%
93	23.495	2420	2430	2439	rBV2	74349	142798	16.53%	1.459%
94	23.748	2497	2504	2516	rVB	18068	31229	3.62%	0.319%
95	24.097	2597	2606	2618	rVB	29327	58125	6.73%	0.594%
96	24.186	2621	2632	2653	rVV	71251	156284	18.09%	1.597%
97	25.326	2955	2965	2993	rVB	14574	36965	4.28%	0.378%
98	25.778	3082	3097	3120	rVB3	28293	92857	10.75%	0.949%
99	25.921	3126	3139	3161	rBV2	11339	35778	4.14%	0.366%
100	26.476	3287	3301	3330	rVB	14799	46522	5.39%	0.475%

Sum of corrected areas: 9788761

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Data File : BN016702.D
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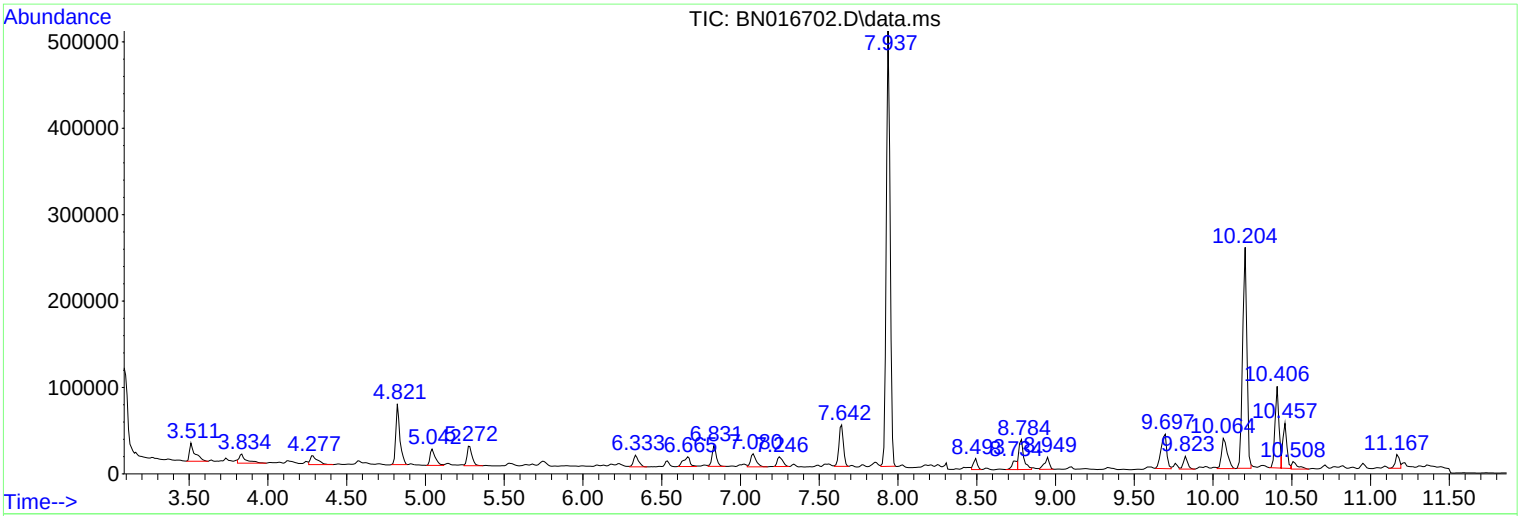
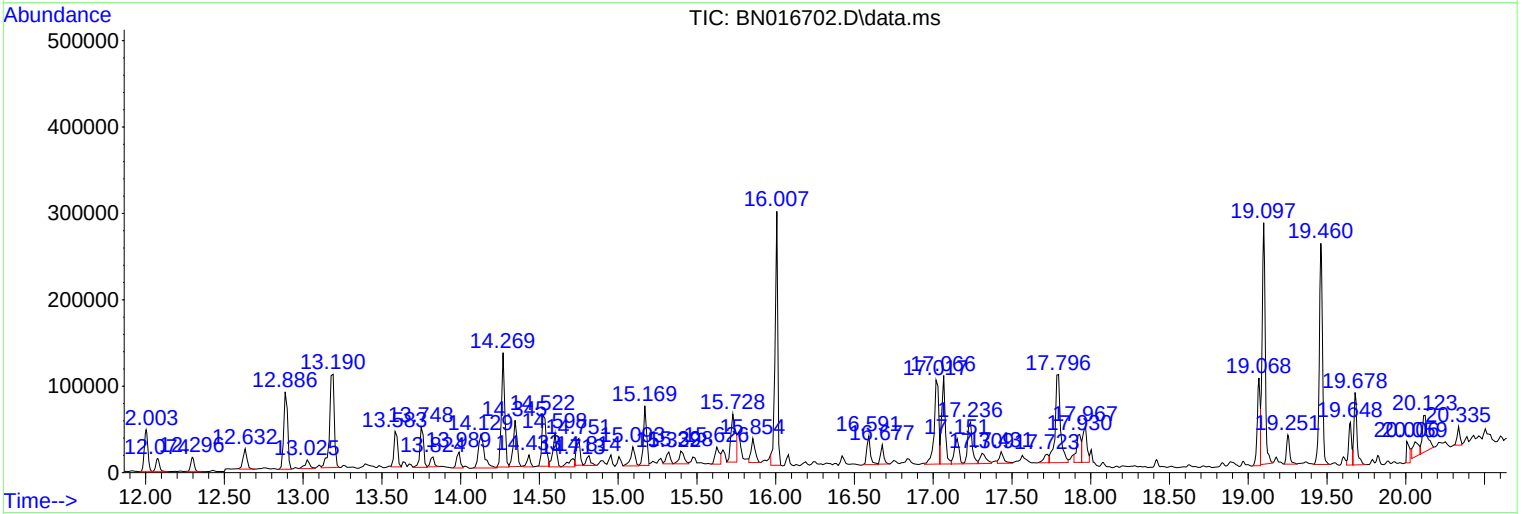
Sample : M3892-14
Misc :
ALS Vial : 70 Sample Multiplier: 1

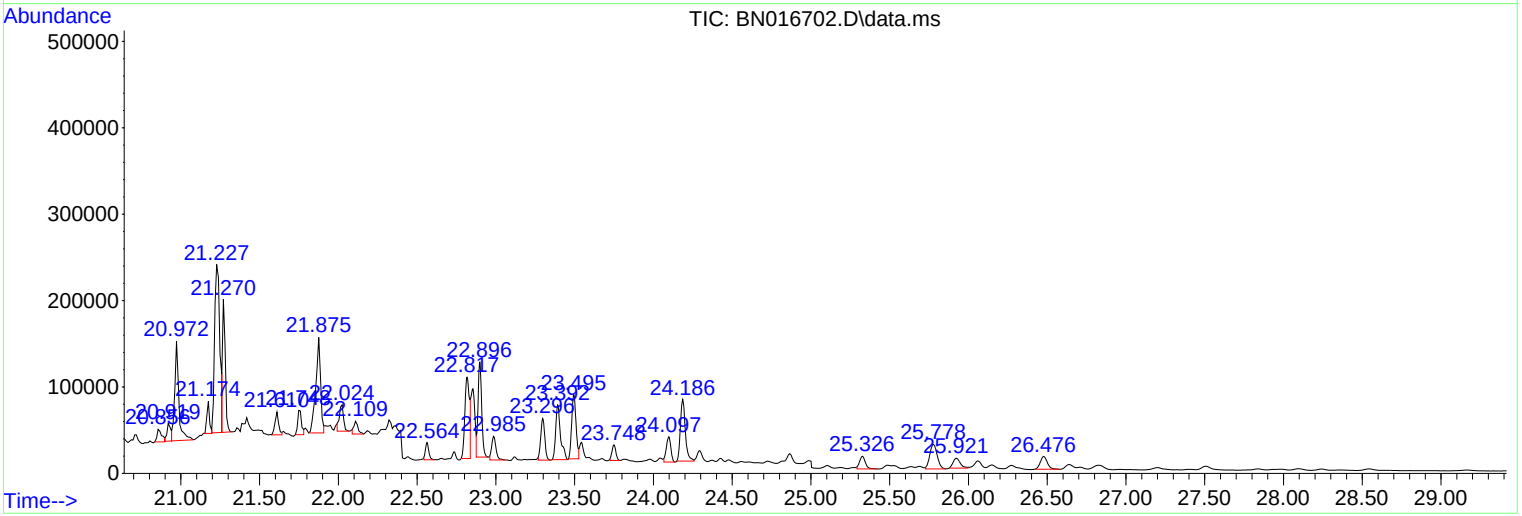
Instrument :
BNA_N
ClientSampleId :
S-826-N-SO-1-1.5-092221

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 : BN016702.D
Acq On : 03 Oct 2021 11:12
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Instrument :
BNA_N
ClientSampleId :
S-826-N-SO-1-1.5-092221

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

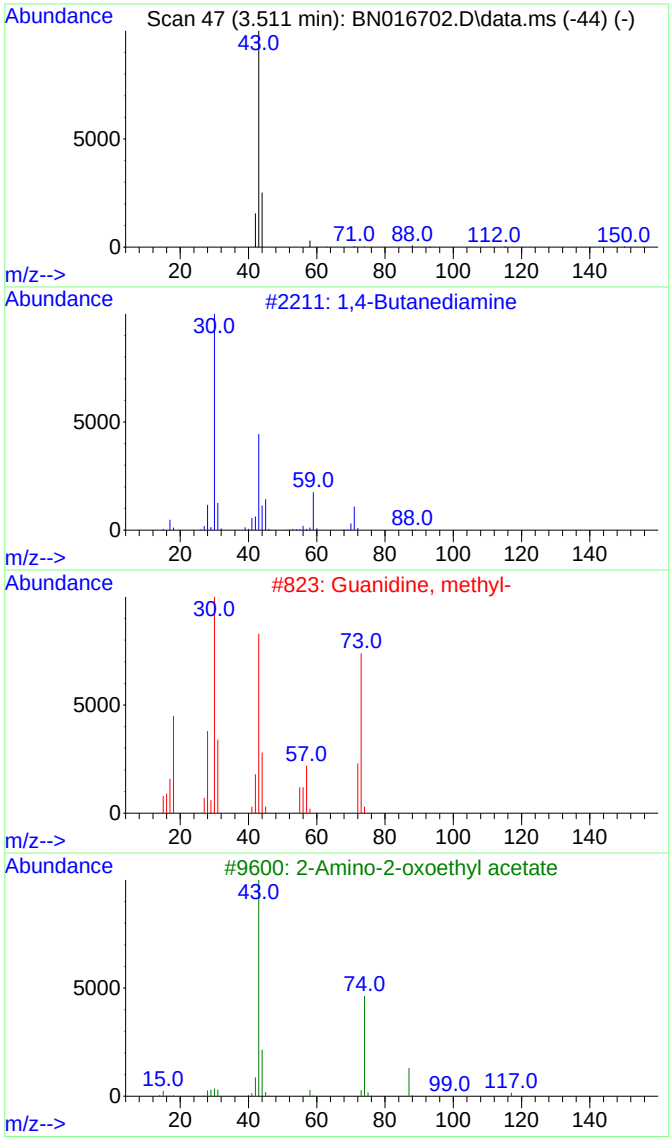
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

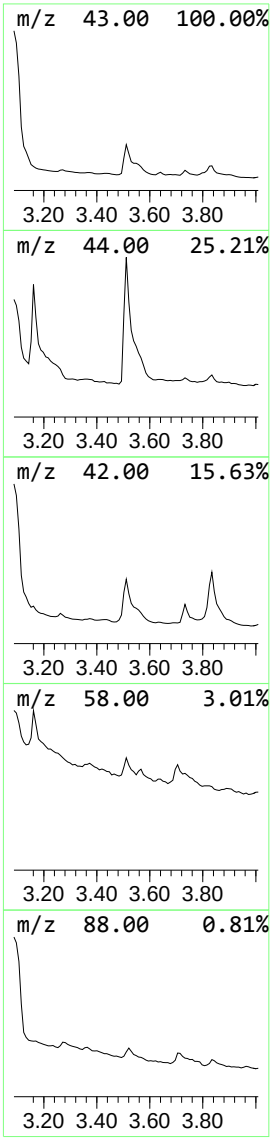
****

Peak Number 1 1,4-Butanediamine Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.511	0.22 ng	51297	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	Guanidine, methyl-	73	C2H7N3	000471-29-4	4
3	2-Amino-2-oxoethyl acetate	117	C4H7NO3	1000500-76-5	4
4	Hydrogen isocyanate	43	CHNO	000075-13-8	3
5	Hydrogen azide	43	HN3	007782-79-8	3





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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ClientSampleId :
S-826-N-SO-1-1.5-092221

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

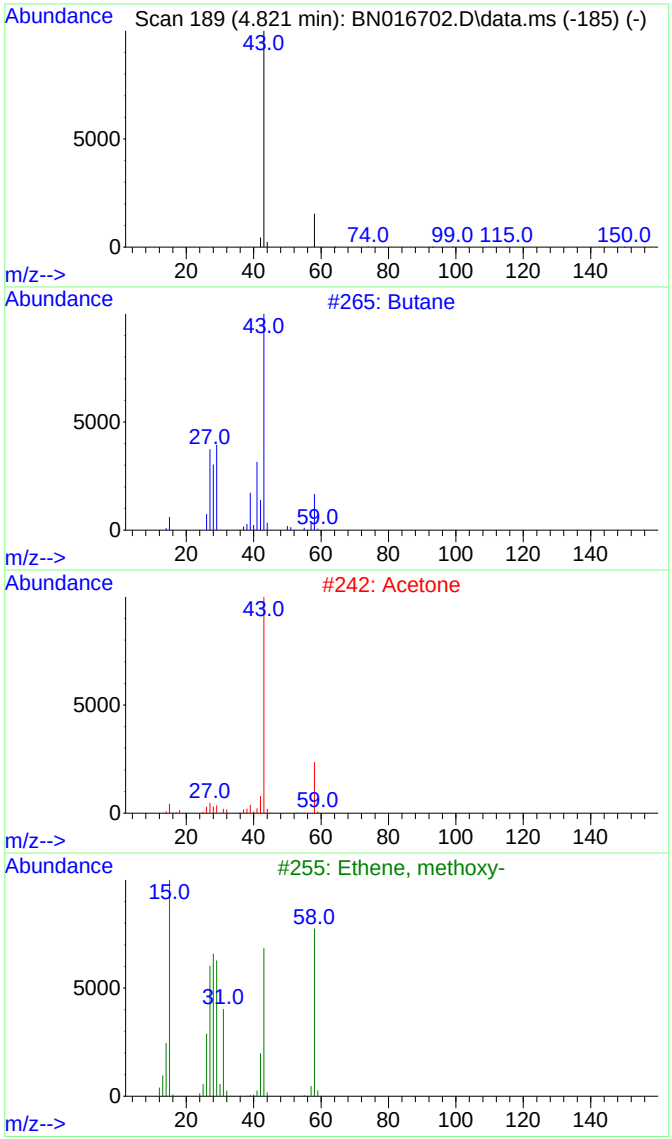
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

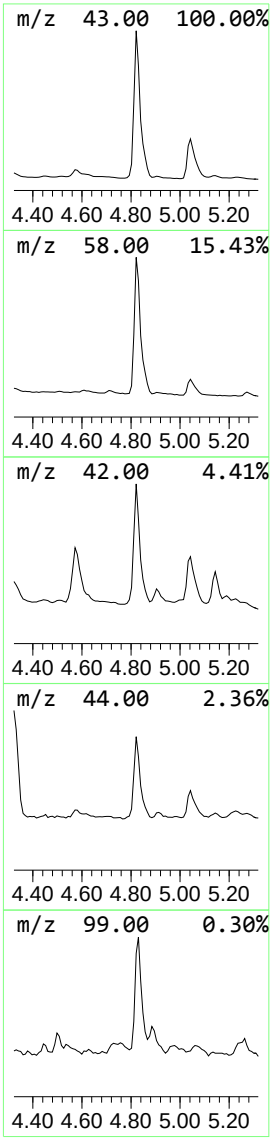
****

Peak Number 2 Butane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.53 ng	125499	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	4
2	Acetone	58	C3H6O	000067-64-1	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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ALS Vial : 70 Sample Multiplier: 1

Instrument :
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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

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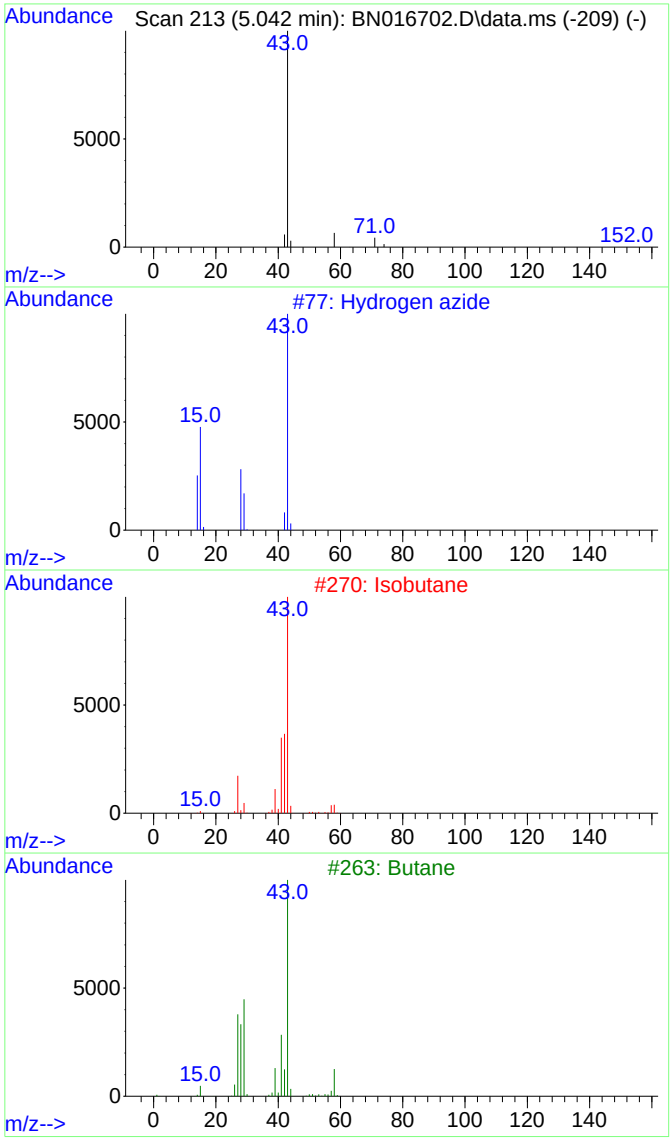
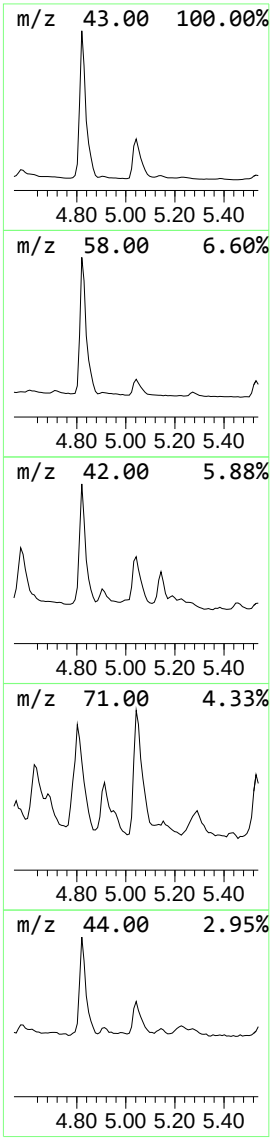
Peak Number 3 Hydrogen azide Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.042	0.19 ng	43436	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrogen azide	43	HN3	007782-79-8	4
2	Isobutane	58	C4H10	000075-28-5	4
3	Butane	58	C4H10	000106-97-8	3
4	Methoxyacetonitrile	71	C3H5NO	001738-36-9	2
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

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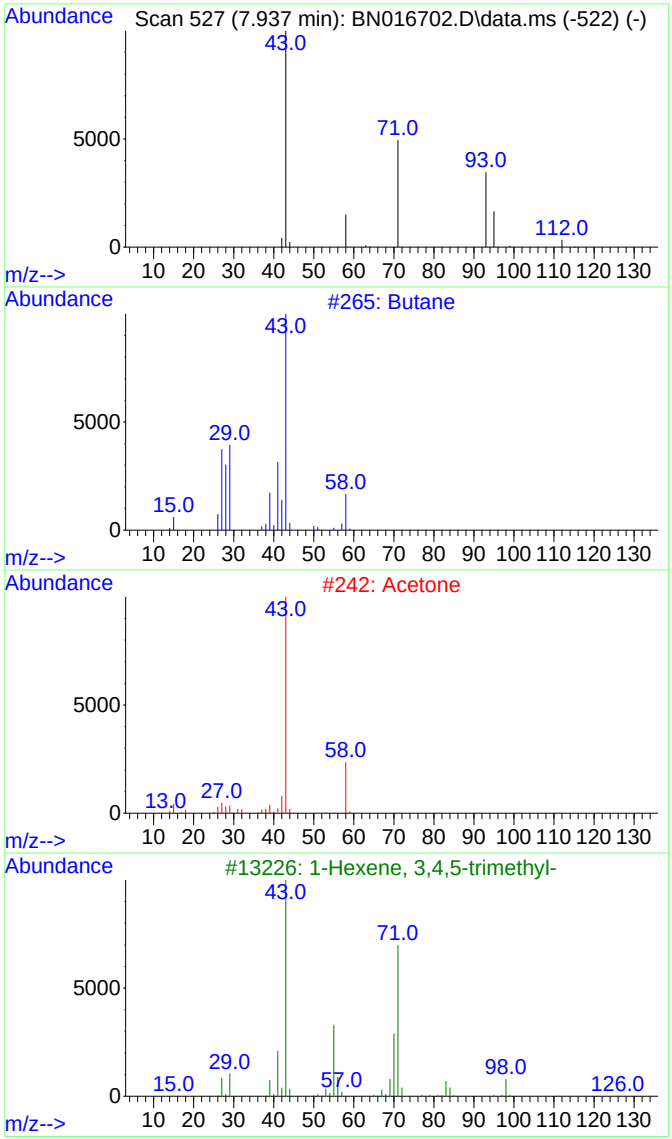
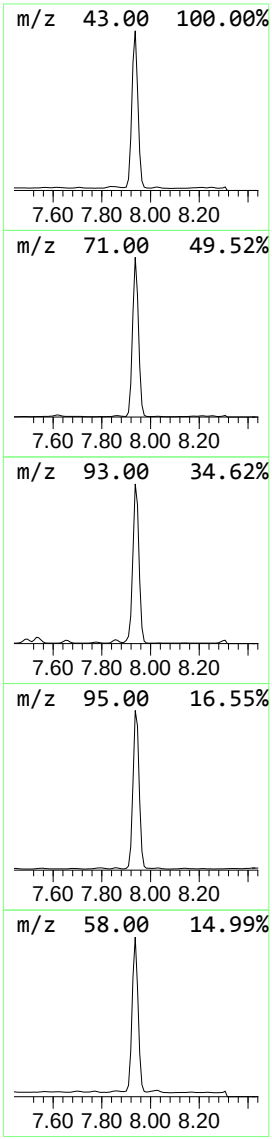
Peak Number 4 Butane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.937	3.68 ng	863843	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	4
2	Acetone	58	C3H6O	000067-64-1	4
3	1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	4
4	2-Propenamide	71	C3H5NO	000079-06-1	3
5	4-Hepten-2-one, (E)-	112	C7H12O	036678-43-0	3





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016702.D
Acq On : 03 Oct 2021 11:12
Operator : CG/JU
Sample : M3892-14
Misc :
ALS Vial : 70 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-826-N-SO-1-1.5-092221

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

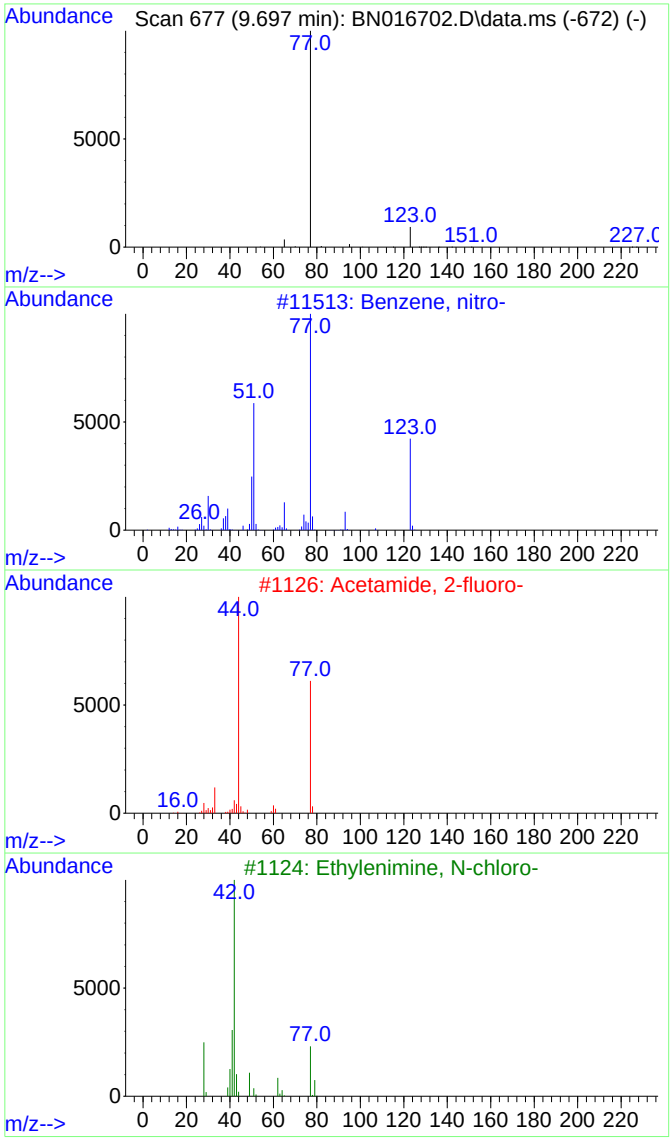
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

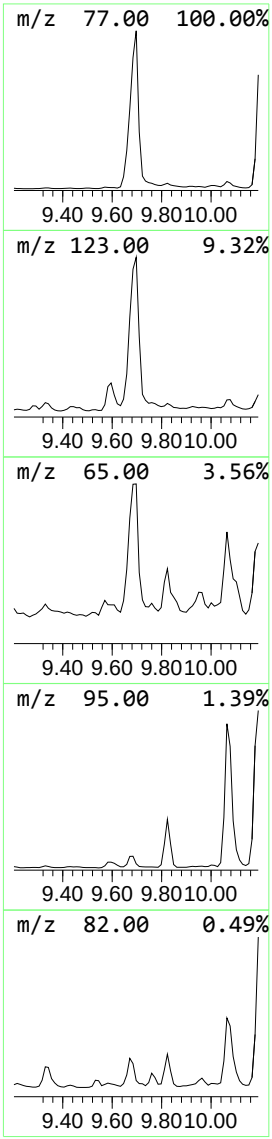
****

Peak Number 5 Benzene, nitro- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.697	0.24 ng	101078	Naphthalene-d8	10.406

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, nitro-	123	C6H5NO2	000098-95-3	3
2	Acetamide, 2-fluoro-	77	C2H4FNO	000640-19-7	2
3	Ethylenimine, N-chloro-	77	C2H4ClN	010165-13-6	1
4	ClCH2C(O)OCH(CH3)2	136	C5H9ClO2	000105-48-6	1
5	Acetic acid, chloro-, 1-methylbu...	164	C7H13ClO2	090380-52-2	1





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Operator : CG/JU
Sample : M3892-14
Misc :
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Instrument :
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ClientSampleId :
S-826-N-SO-1-1.5-092221

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

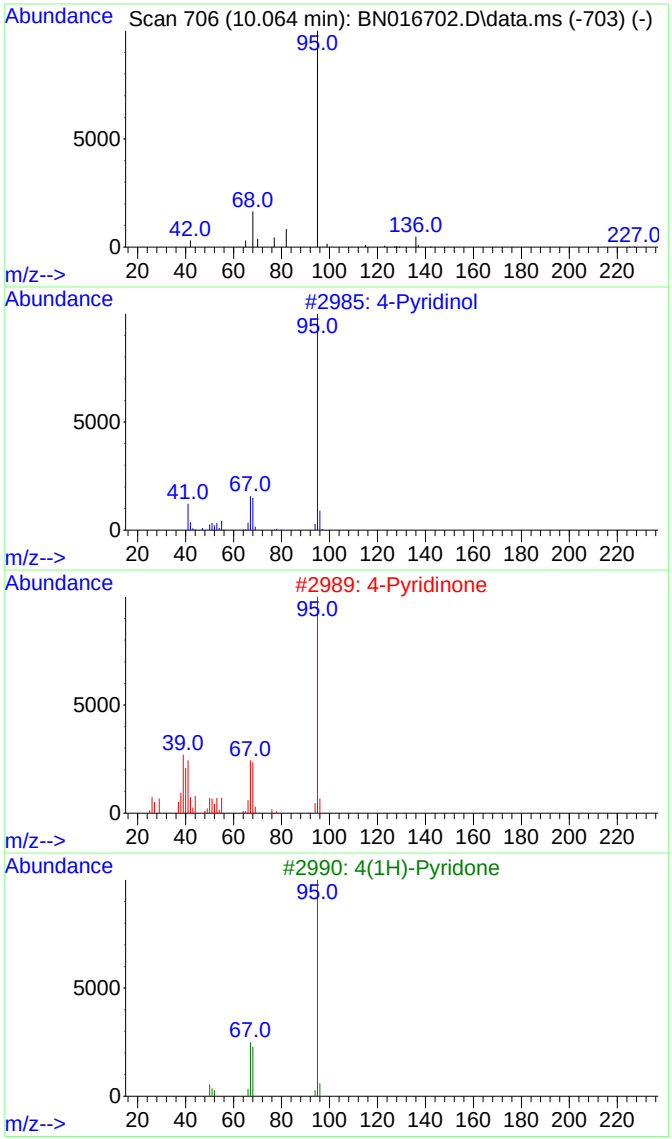
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

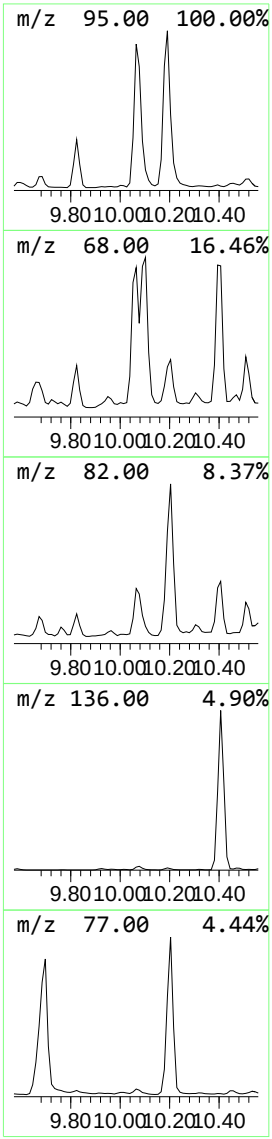
****

Peak Number 6 4-Pyridinol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.064	0.21 ng	87566	Naphthalene-d8	10.406

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Pyridinol	95	C5H5NO	000626-64-2	7
2	4-Pyridinone	95	C5H5NO	1000433-50-4	4
3	4(1H)-Pyridone	95	C5H5NO	000108-96-3	4
4	Pyridine, 1-oxide	95	C5H5NO	000694-59-7	4
5	3-Pyridinol	95	C5H5NO	000109-00-2	4





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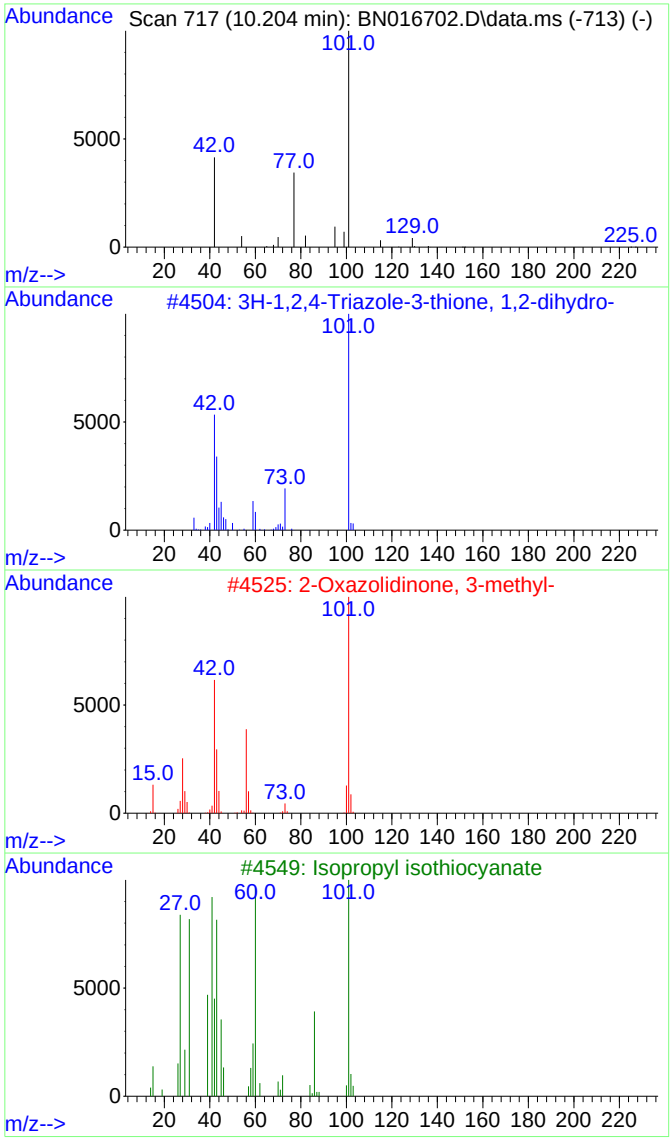
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

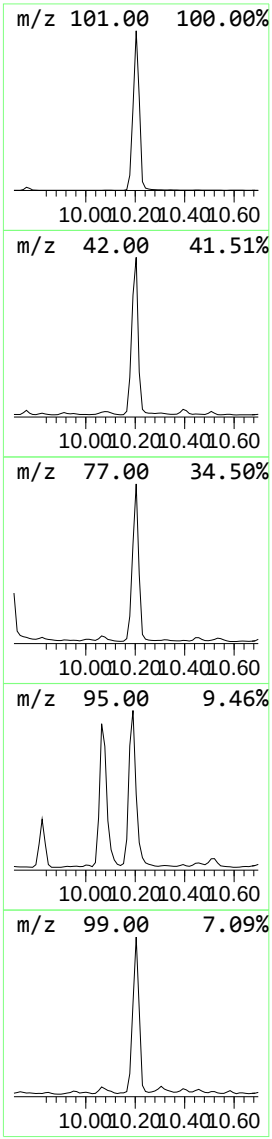
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 3H-1,2,4-Triazole-3-thione,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.204	1.15 ng	479214	Naphthalene-d8	10.406

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
2	2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	5
3	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	5
4	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5
5	3-Aminopropionitrile	70	C3H6N2	000151-18-8	4





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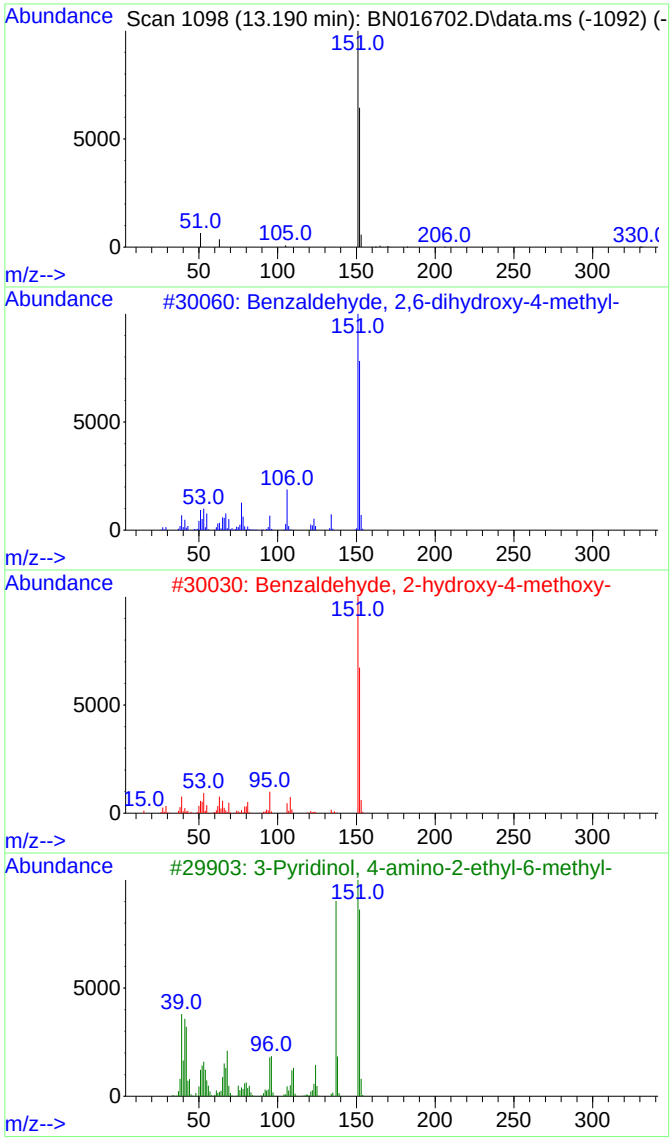
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

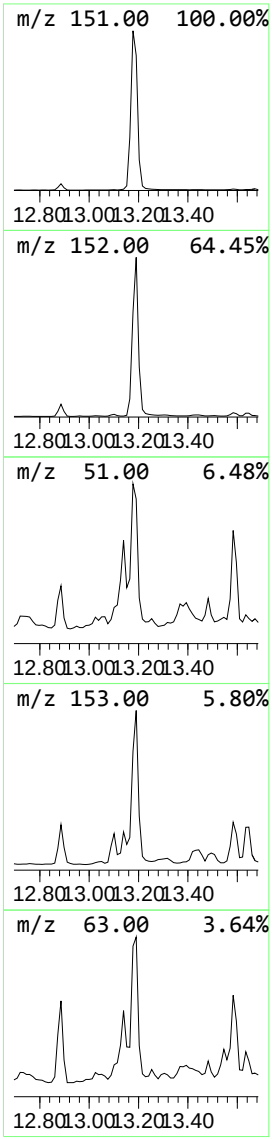
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzaldehyde, 2,6-dihydroxy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.190	0.47 ng	228947	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 2,6-dihydroxy-4-me...	152	C8H8O3	000526-37-4	56
2	Benzaldehyde, 2-hydroxy-4-methoxy-	152	C8H8O3	000673-22-3	9
3	3-Pyridinol, 4-amino-2-ethyl-6-m...	152	C8H12N2O	1010351-35-8	9
4	2,4-Dihydroxy-3-methylbenzaldehyde	152	C8H8O3	006248-20-0	9
5	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	9





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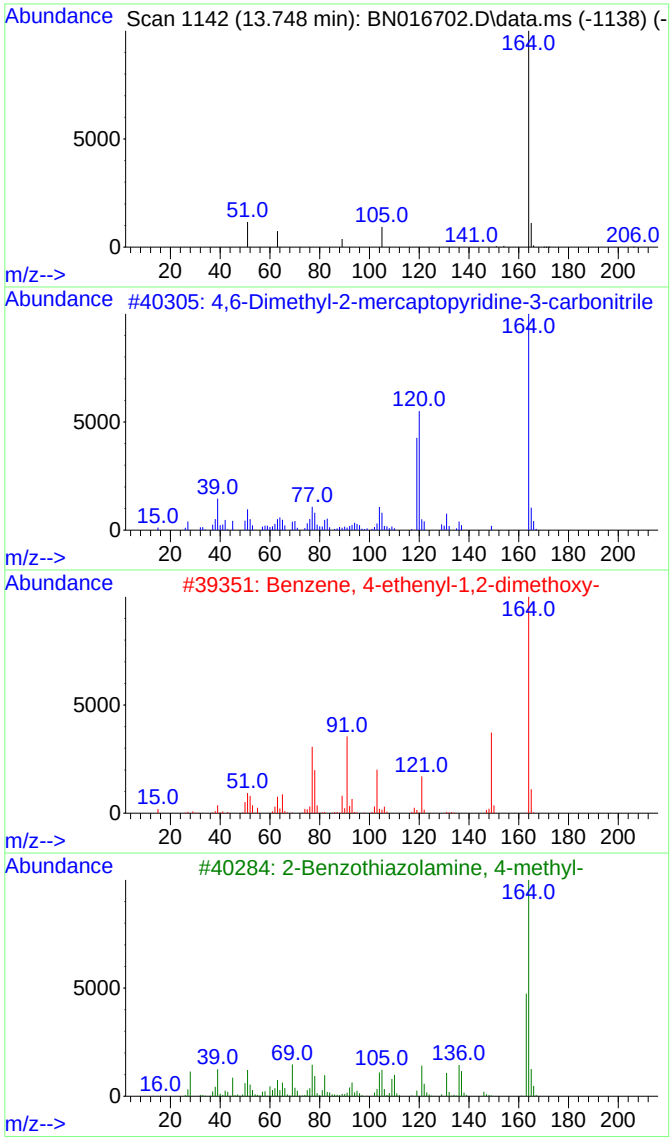
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

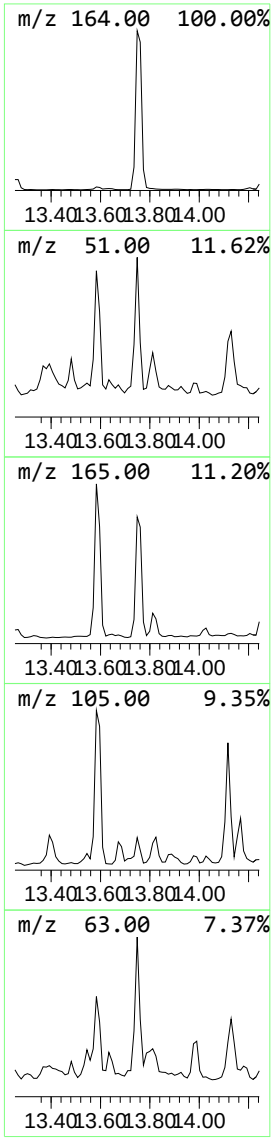
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 4,6-Dimethyl-2-mercaptopyri... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.748	0.16 ng	77787	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,6-Dimethyl-2-mercaptopyridine-...	164	C8H8N2S	054585-47-6	9
2	Benzene, 4-ethenyl-1,2-dimethoxy-	164	C10H12O2	006380-23-0	9
3	2-Benzothiazolamine, 4-methyl-	164	C8H8N2S	001477-42-5	9
4	4-Methoxy-2-allylphenol	164	C10H12O2	1000306-52-7	9
5	p-Coumaric acid	164	C9H8O3	007400-08-0	7





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

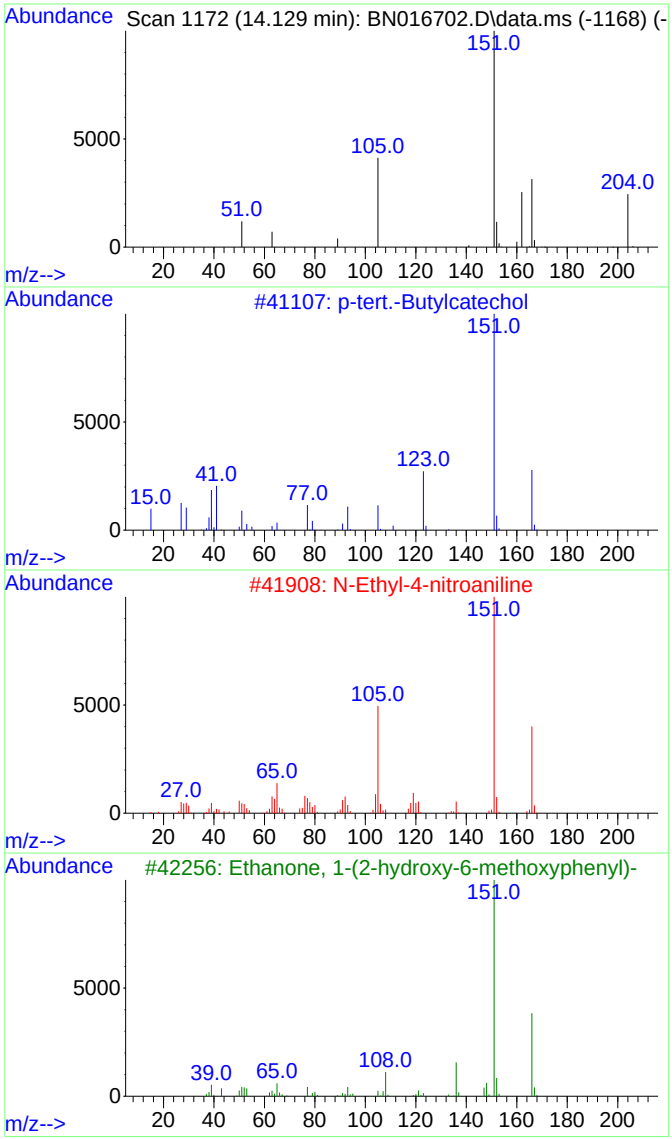
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

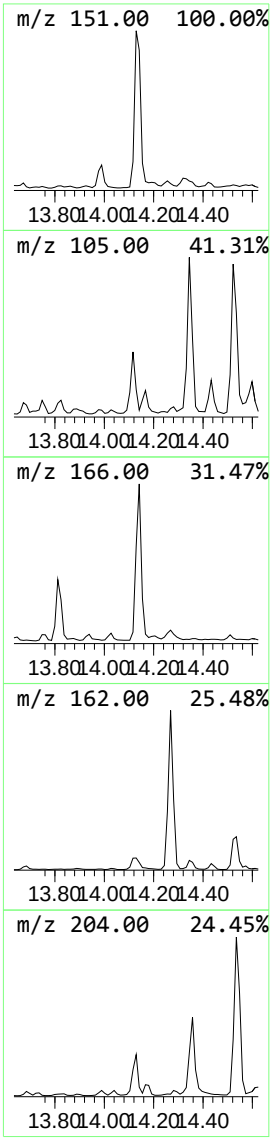
****

Peak Number 10 p-tert.-Butylcatechol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.129	0.21 ng	100725	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-tert.-Butylcatechol	166	C10H14O2	000098-29-3	53
2	N-Ethyl-4-nitroaniline	166	C8H10N2O2	003665-80-3	50
3	Ethanone, 1-(2-hydroxy-6-methoxy...	166	C9H10O3	000703-23-1	49
4	Ethanone, 1-(2-hydroxy-4-methoxy...	166	C9H10O3	000552-41-0	38
5	Benzenethiol, 4-(1,1-dimethyleth...	166	C10H14S	002396-68-1	38





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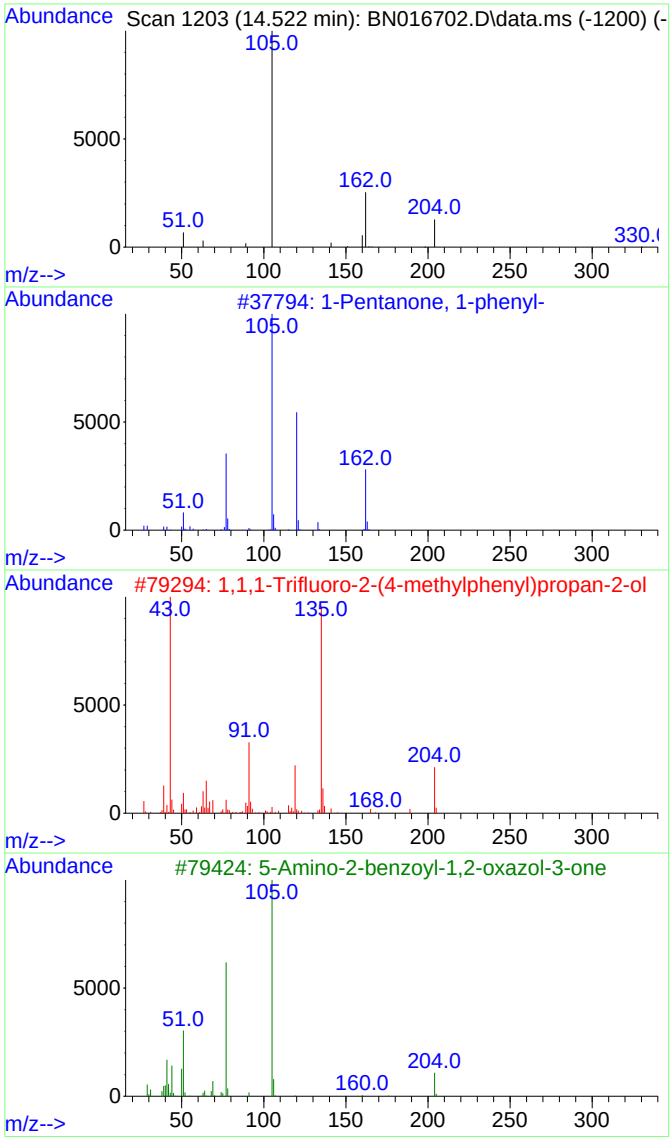
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

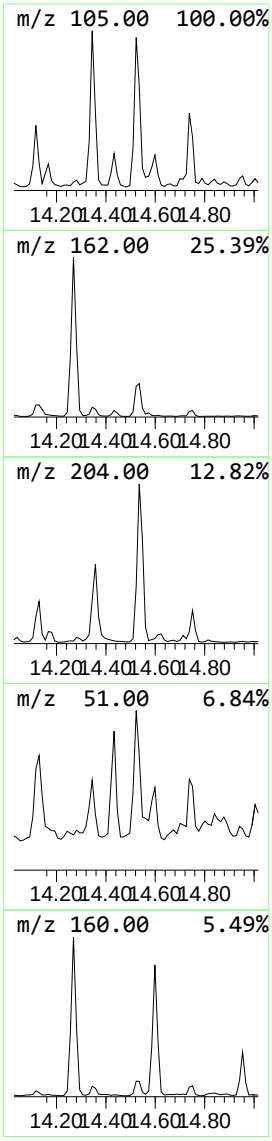
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 1-Pentanone, 1-phenyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.522	0.24 ng	114209	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanone, 1-phenyl-	162	C11H14O	001009-14-9	5
2	1,1,1-Trifluoro-2-(4-methylpheny...	204	C10H11F3O	076953-97-4	5
3	5-Amino-2-benzoyl-1,2-oxazol-3-one	204	C10H8N2O3	090771-25-8	5
4	Spiro[bicyclo[4.2.0]octa-1,3,5-t...	162	C10H10O2	014458-33-4	4
5	Benzene, 1-methyl-2-(1-ethylprop...	162	C12H18	054410-74-1	4





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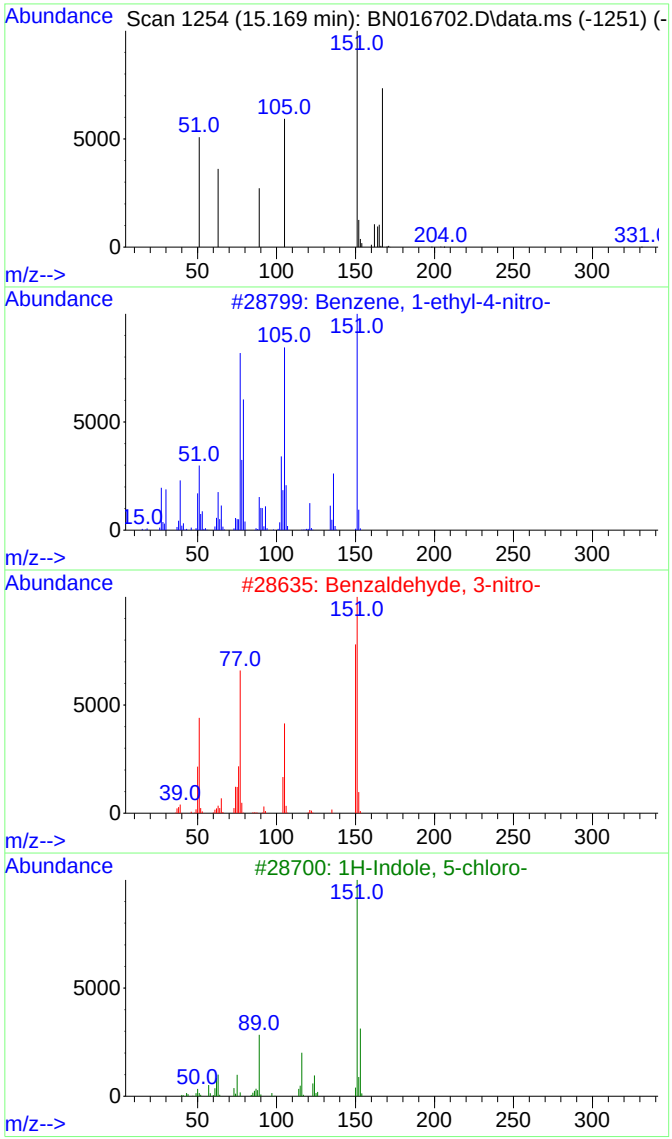
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

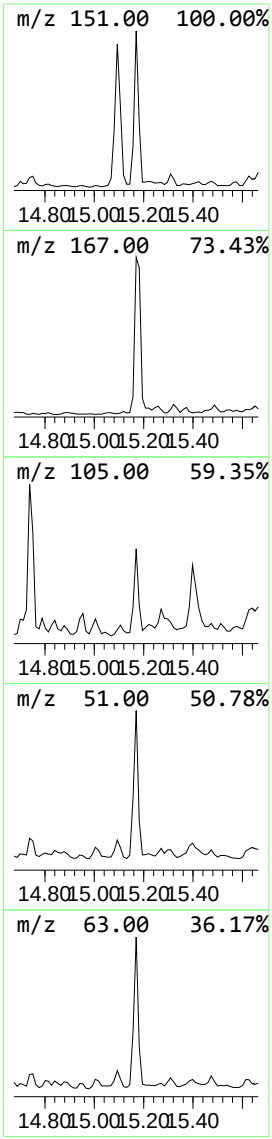
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Benzene, 1-ethyl-4-nitro- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.169	0.20 ng	95123	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-4-nitro-	151	C8H9NO2	000100-12-9	38
2	Benzaldehyde, 3-nitro-	151	C7H5NO3	000099-61-6	25
3	1H-Indole, 5-chloro-	151	C8H6ClN	017422-32-1	9
4	1H-Indole, 4-chloro-	151	C8H6ClN	025235-85-2	9
5	Benzaldehyde, 4-methoxy-, oxime	151	C8H9NO2	003235-04-9	9





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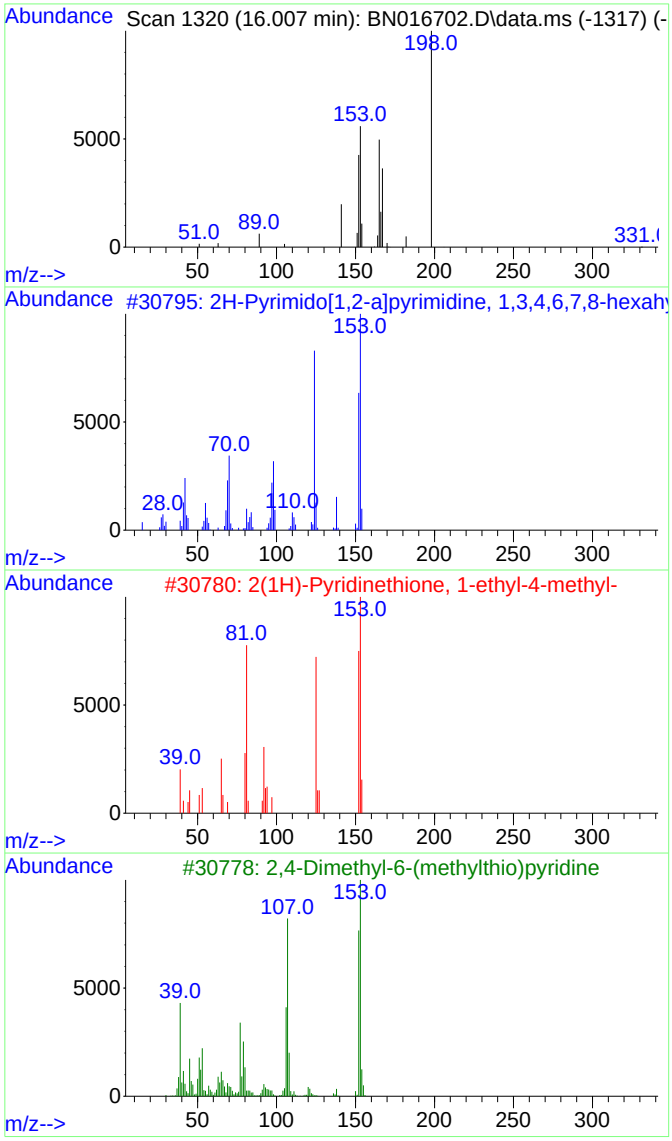
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

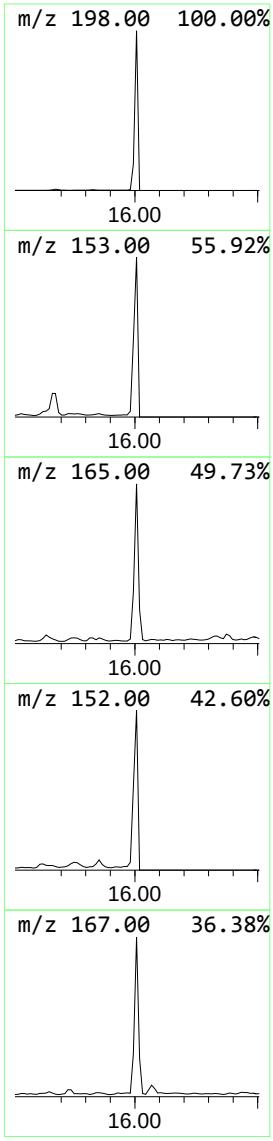
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 2H-Pyrimido[1,2-a]pyrimidin... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.007	0.68 ng	339696	Phenanthrene-d10	17.029

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Pyrimido[1,2-a]pyrimidine, 1,...	153	C8H15N3	084030-20-6	9
2	2(1H)-Pyridinethione, 1-ethyl-4-...	153	C8H11NS	019006-72-5	9
3	2,4-Dimethyl-6-(methylthio)pyridine	153	C8H11NS	1000305-54-7	9
4	Benzenethiol, p-(dimethylamino)-	153	C8H11NS	004946-22-9	9
5	4-Picoline, 2-(ethylthio)-	153	C8H11NS	019006-78-1	9





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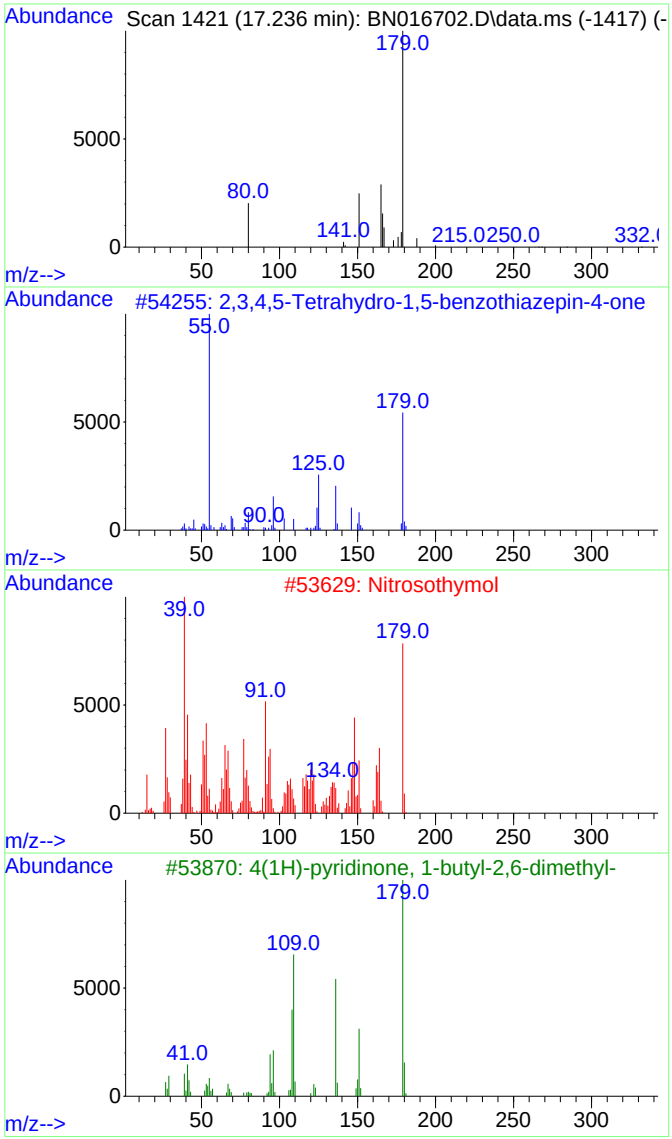
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

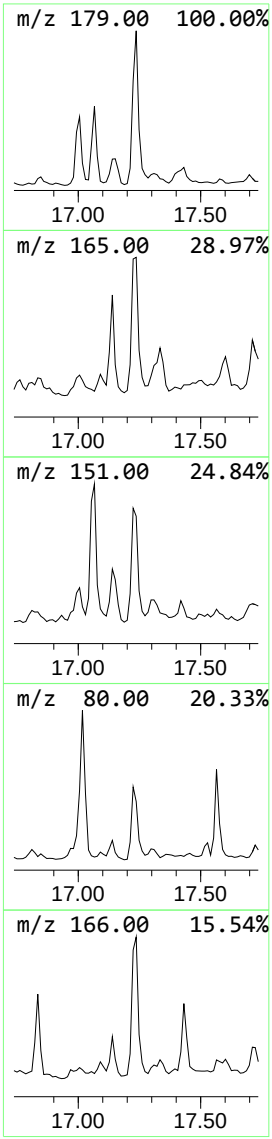
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 2,3,4,5-Tetrahydro-1,5-benz... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.236	0.20 ng	97313	Phenanthrene-d10	17.029

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3,4,5-Tetrahydro-1,5-benzothia...	179	C9H9NOS	053454-43-6	5
2	Nitrosothymol	179	C10H13NO2	002364-54-7	5
3	4(1H)-pyridinone, 1-butyl-2,6-di...	179	C11H17NO	1000404-82-3	5
4	2-Amino-4-hydroxy-6-(trifluorome...	179	C5H4F3N3O	001513-69-5	5
5	Benzo[f]quinoline	179	C13H9N	000085-02-9	5





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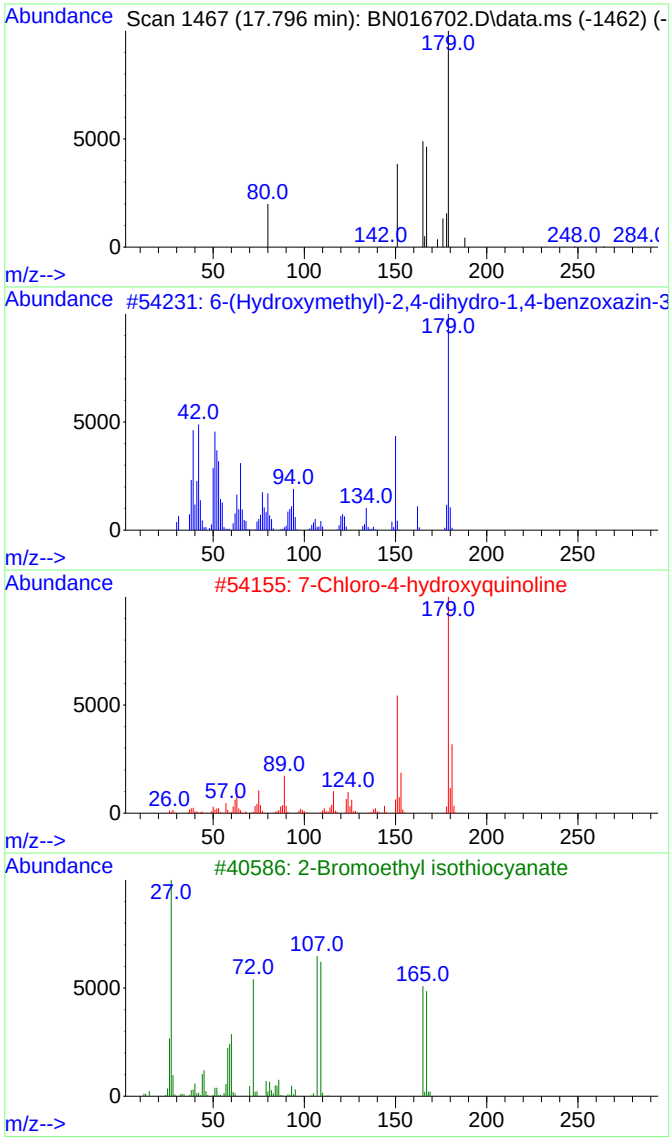
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

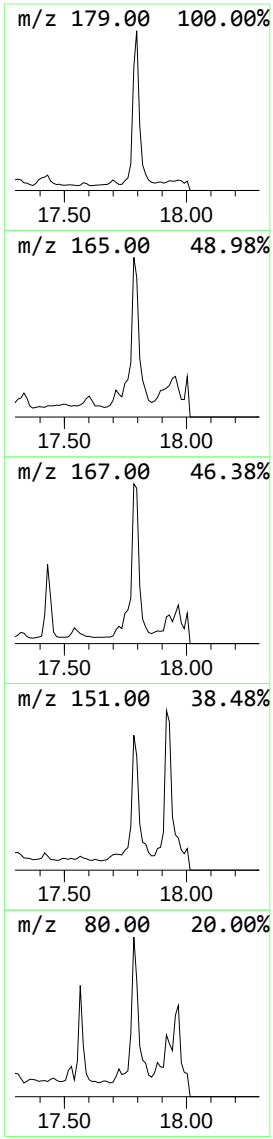
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 6-(Hydroxymethyl)-2,4-dihyd... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.796	0.49 ng	242754	Phenanthrene-d10	17.029

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-(Hydroxymethyl)-2,4-dihydro-1,...	179	C9H9NO3	615568-17-7	9
2	7-Chloro-4-hydroxyquinoline	179	C9H6ClNO	000086-99-7	5
3	2-Bromoethyl isothiocyanate	165	C3H4BrNS	001483-41-6	5
4	1H-Purin-2-amine, 6-methoxy-N-me...	179	C7H9N5O	050704-44-4	5
5	2-Amino-4,6-pteridinediol	179	C6H5N5O2	005979-01-1	5





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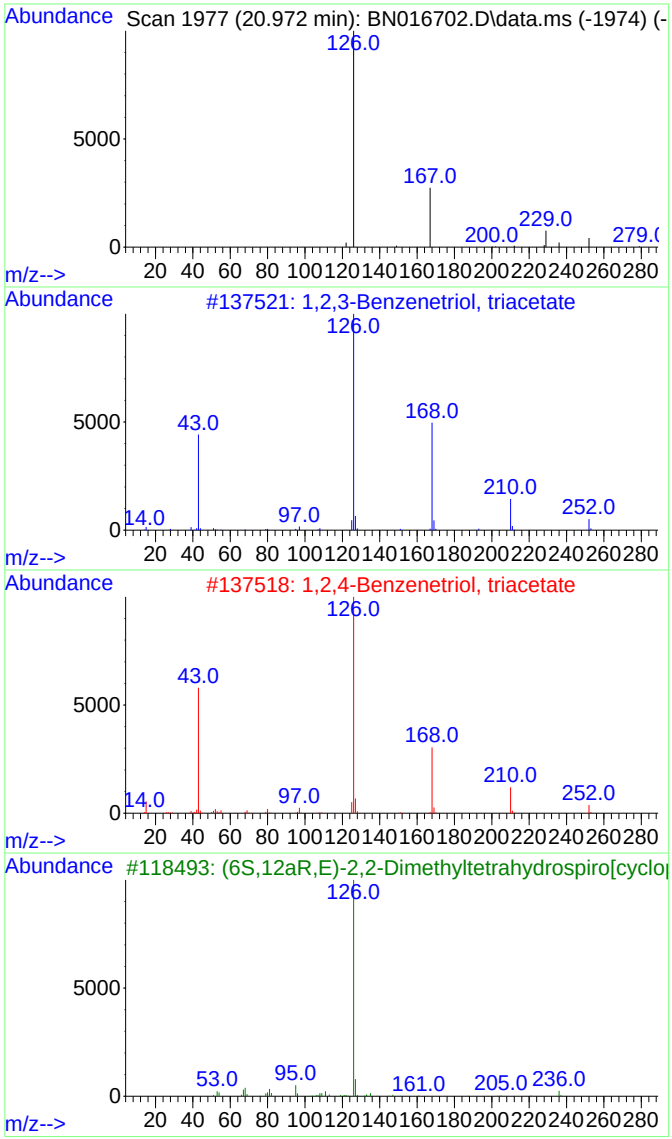
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

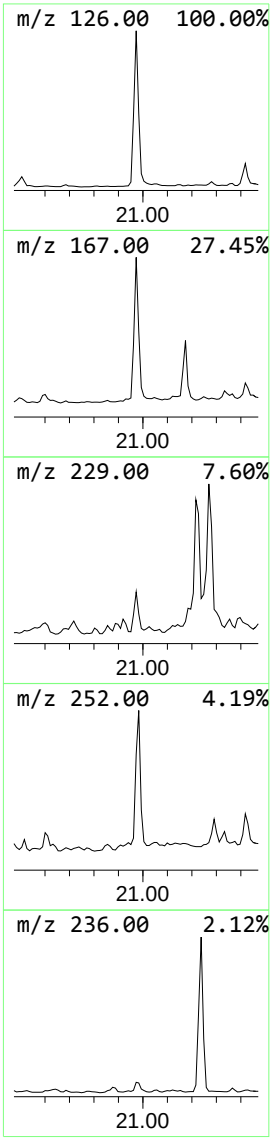
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 1,2,3-Benzenetriol, triacetate Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.972	0.18 ng	206343	Chrysene-d12	21.238

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,3-Benzenetriol, triacetate	252	C12H12O6	000525-52-0	4
2	1,2,4-Benzenetriol, triacetate	252	C12H12O6	000613-03-6	4
3	(6S,12aR,E)-2,2-Dimethyltetrahyd...	236	C14H24N2O	155975-43-2	4
4	Phloroglucinol triacetate	252	C12H12O6	002999-40-8	4
5	N-[[6-Cyclooctylaminohexyl]aziri...	252	C16H32N2	1010256-12-1	4





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Data File : BN016702.D
Acq On : 03 Oct 2021 11:12
Operator : CG/JU
Sample : M3892-14
Misc :
ALS Vial : 70 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-826-N-SO-1-1.5-092221

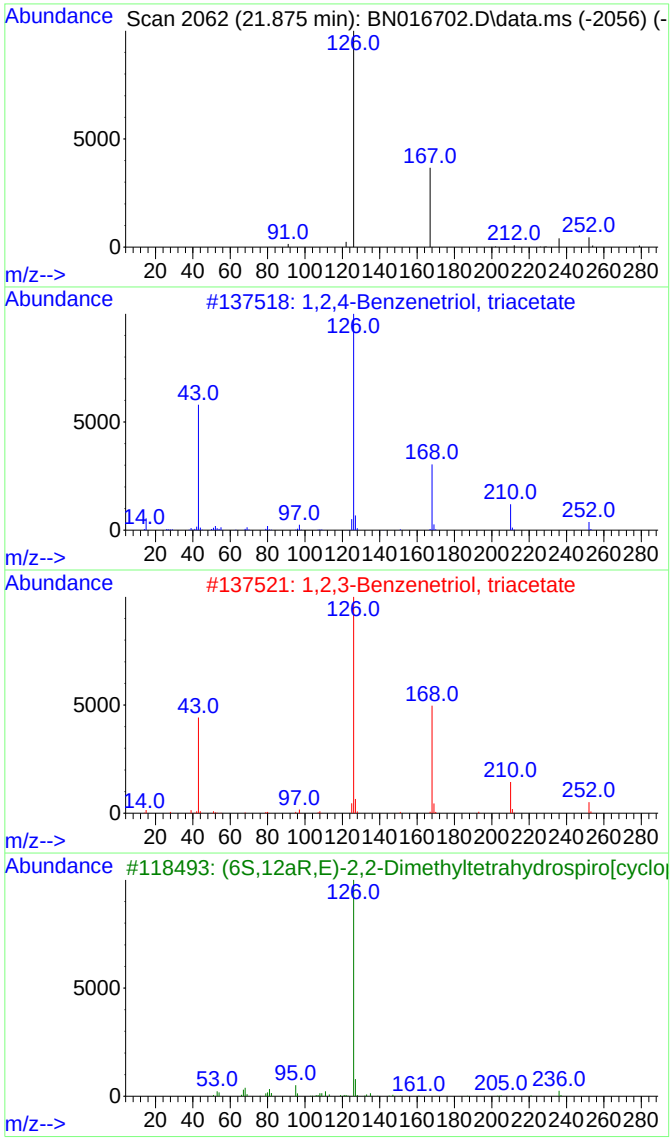
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

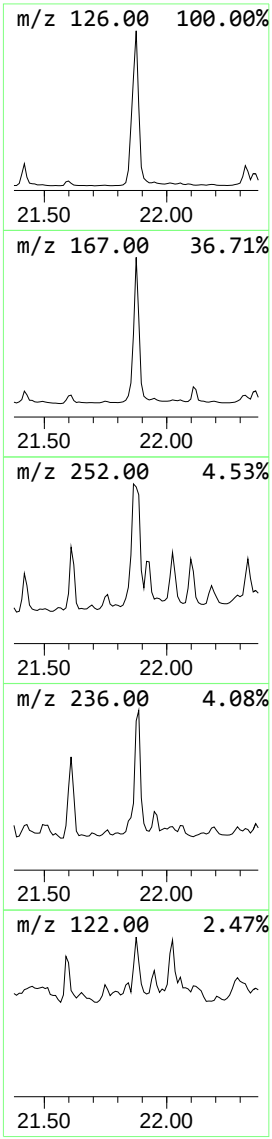
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 1,2,4-Benzenetriol, triacetate Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.875	0.21 ng	234892	Chrysene-d12	21.238

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Benzenetriol, triacetate	252	C12H12O6	000613-03-6	4
2	1,2,3-Benzenetriol, triacetate	252	C12H12O6	000525-52-0	4
3	(6S,12aR,E)-2,2-Dimethyltetrahyd...	236	C14H24N2O	155975-43-2	4
4	Phloroglucinol triacetate	252	C12H12O6	002999-40-8	4
5	N-[[6-Cyclooctylaminohexyl]aziri...	252	C16H32N2	1010256-12-1	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Misc :
ALS Vial : 70 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-826-N-SO-1-1.5-092221

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

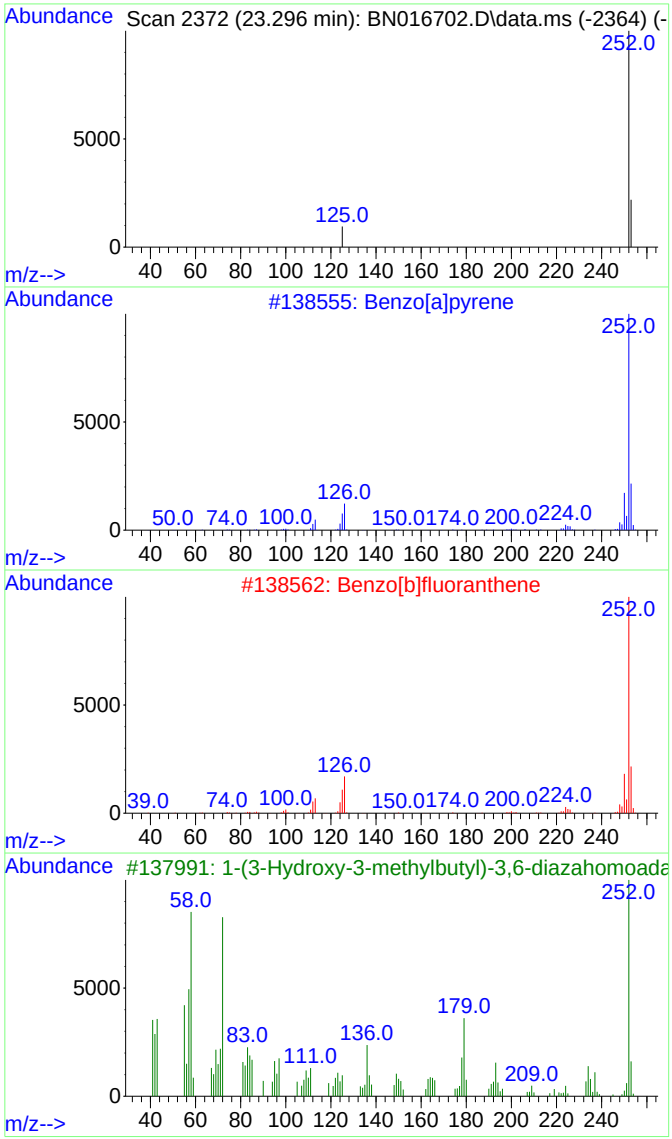
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

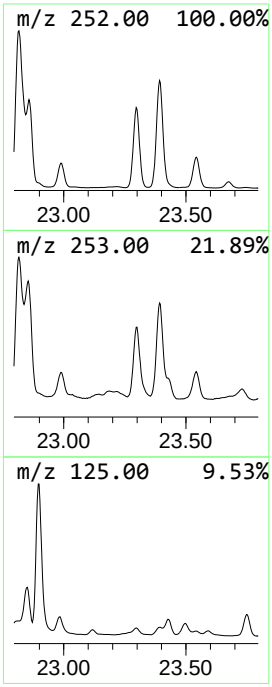
****

Peak Number 18 Benzo[a]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.296	0.24 ng	85907	Perylene-d12	23.494

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[a]pyrene	252	C20H12	000050-32-8	9
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	9
3	1-(3-Hydroxy-3-methylbutyl)-3,6-...	252	C14H24N2O2	1000216-02-0	9
4	Perylene	252	C20H12	000198-55-0	9
5	Benzo[e]pyrene	252	C20H12	000192-97-2	9





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Data File : BN016702.D
Acq On : 03 Oct 2021 11:12
Operator : CG/JU
Sample : M3892-14
Misc :
ALS Vial : 70 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-826-N-SO-1-1.5-092221

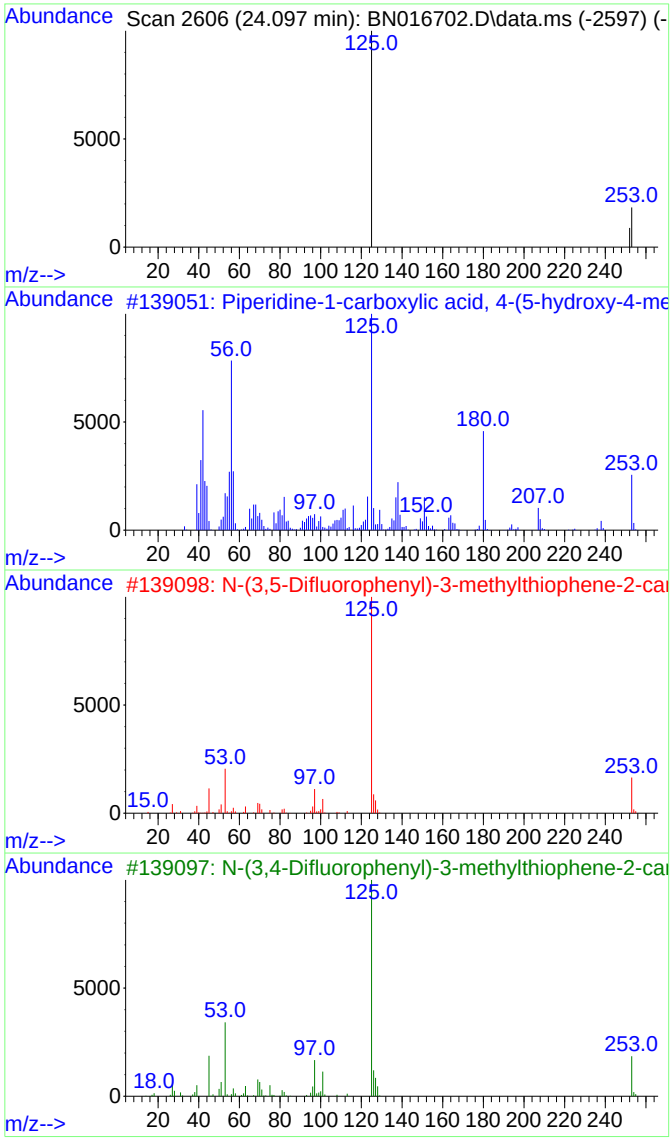
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

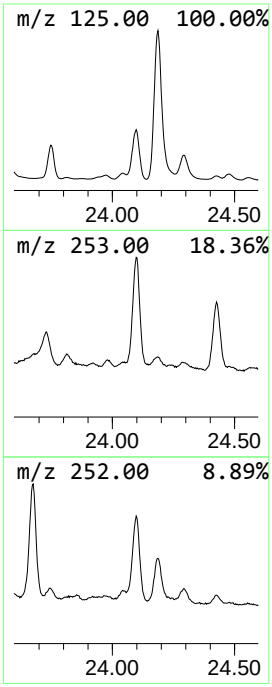
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 Piperidine-1-carboxylic aci... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.097	0.16 ng	58125	Perylene-d12	23.494

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Piperidine-1-carboxylic acid, 4-...	253	C12H19N3O3	1000316-66-8	5
2	N-(3,5-Difluorophenyl)-3-methylt...	253	C12H9F2NOS	1000436-25-2	4
3	N-(3,4-Difluorophenyl)-3-methylt...	253	C12H9F2NOS	1000436-25-1	4
4	Furane-2-carboxylic acid, 5-(4-c...	252	C12H9ClO4	074556-57-3	4
5	3-Cyclopentylpropionic acid, 3-c...	252	C14H17ClO2	1000325-52-2	4





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Data File : BN016702.D
Acq On : 03 Oct 2021 11:12
Operator : CG/JU
Sample : M3892-14
Misc :
ALS Vial : 70 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-826-N-SO-1-1.5-092221

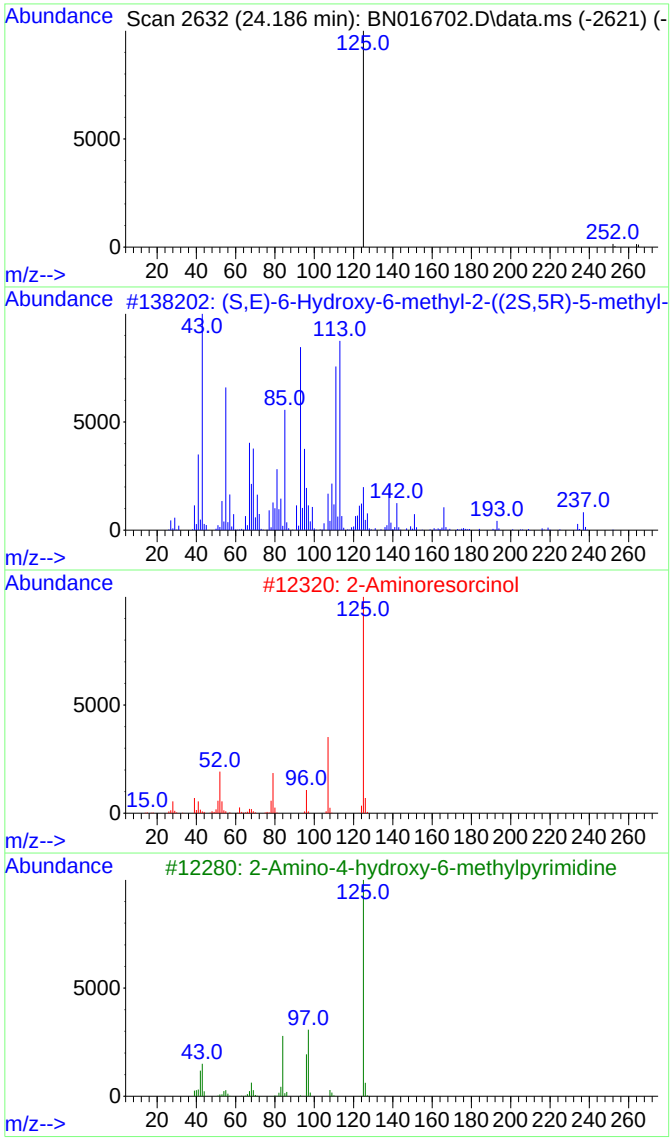
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

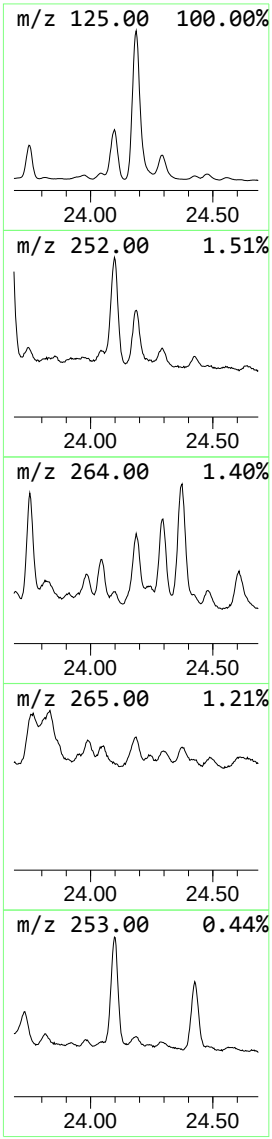
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 (S,E)-6-Hydroxy-6-methyl-2-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.186	0.44 ng	156284	Perylene-d12	23.494

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 : BN016702.D
Acq On : 03 Oct 2021 11:12
Operator : CG/JU
Sample : M3892-14
Misc :
ALS Vial : 70 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-826-N-SO-1-1.5-092221

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	3.511	0.2	ng	51297	1	7.642	93847	0.4
Butane	4.821	0.5	ng	125499	1	7.642	93847	0.4
Hydrogen azide	5.042	0.2	ng	43436	1	7.642	93847	0.4
Butane	7.937	3.7	ng	863843	1	7.642	93847	0.4
Benzene, nitro-	9.697	0.2	ng	101078	2	10.406	166366	0.4
4-Pyridinol	10.064	0.2	ng	87566	2	10.406	166366	0.4
3H-1,2,4-Triazo...	10.204	1.2	ng	479214	2	10.406	166366	0.4
Benzaldehyde, 2...	13.190	0.5	ng	228947	3	14.269	193065	0.4
4,6-Dimethyl-2-...	13.748	0.2	ng	77787	3	14.269	193065	0.4
p-tert.-Butylca...	14.129	0.2	ng	100725	3	14.269	193065	0.4
1-Pentanone, 1-...	14.522	0.2	ng	114209	3	14.269	193065	0.4
Benzene, 1-ethy...	15.169	0.2	ng	95123	3	14.269	193065	0.4
2H-Pyrimido[1,2...	16.007	0.7	ng	339696	4	17.029	198694	0.4
2,3,4,5-Tetrahy...	17.236	0.2	ng	97313	4	17.029	198694	0.4
6-(Hydroxymethy...	17.796	0.5	ng	242754	4	17.029	198694	0.4
1,2,3-Benzenetr...	20.972	0.2	ng	206343	5	21.238	456255	0.4
1,2,4-Benzenetr...	21.875	0.2	ng	234892	5	21.238	456255	0.4
Benzo[a]pyrene	23.296	0.2	ng	85907	6	23.494	142798	0.4
Piperidine-1-ca...	24.097	0.2	ng	58125	6	23.494	142798	0.4
(S,E)-6-Hydroxy...	24.186	0.4	ng	156284	6	23.494	142798	0.4