LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016665.D
Acq On : 02 Oct 2021 10:32
Operator : CG/JU
Sample : M3829-16
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : EB01-20210917

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: BN016665.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.272	18	21	22	rBV	6596	9851	3.59%	0.234%
2	3.816	76	80	97	rVB	13827	57089	20.81%	1.358%
3	4.092	102	110	122	rVB	12956	47738	17.40%	1.135%
4	4.277	127	130	140	rVB	9923	33261	12.13%	0.791%
5	4.738	177	180	185	rBV	4347	12539	4.57%	0.298%
6	4.821	185	189	204	rVB	69751	160449	58.49%	3.816%
7	5.227	229	233	235	rBV	13267	26205	9.55%	0.623%
8	5.503	259	263	274	rBV2	15506	53118	19.36%	1.263%
9	5.752	284	290	300	rVB2	21851	63546	23.17%	1.511%
10	6.647	383	387	395	rVB	7470	16713	6.09%	0.398%
11	6.822	400	406	417	rVB2	7186	24888	9.07%	0.592%
12	7.015	425	427	434	rVB	4067	8379	3.05%	0.199%
13	7.181	441	445	450	rVB	2840	7548	2.75%	0.180%
14	7.264	450	454	459	rVV2	7215	15915	5.80%	0.379%
15	7.338	459	462	466	rVB	3335	5356	1.95%	0.127%
16	7.633	490	494	499	rBV	54204	111995	40.83%	2.664%
17	7.707	499	502	513	rVB	25022	55376	20.19%	1.317%
18	7.864	515	519	525	rBV	16212	33732	12.30%	0.802%
19	8.113	543	546	549	rBV	2891	6488	2.37%	0.154%
20	8.168	549	552	558	rVV	10682	29415	10.72%	0.700%
21	8.251	558	561	564	rVV	7314	16804	6.13%	0.400%
22	8.306	564	567	569	rVB	13876	17292	6.30%	0.411%
23	8.442	575	578	581	rVV	18355	33122	12.07%	0.788%
24	8.506	581	583	592	rVB2	3059	8138	2.97%	0.194%
25	8.784	601	605	610	rVB	28092	57934	21.12%	1.378%
26	8.886	610	613	616	rVV3	7306	14572	5.31%	0.347%
27	8.949	616	618	622	rVB	9383	14120	5.15%	0.336%
28	9.355	646	650	655	rVB2	4117	8313	3.03%	0.198%
29	9.456	655	658	661	rBV	5812	11020	4.02%	0.262%
30	9.634	669	672	675	rBV	2801	6386	2.33%	0.152%
31	9.735	675	680	685	rVB2	4175	11301	4.12%	0.269%
32	10.204	714	717	720	rBV	4460	9389	3.42%	0.223%
33	10.407	729	733	735	rBV	110942	192901	70.32%	4.588%
34	10.457	735	737	740	rVB2	12920	23407	8.53%	0.557%
35	10.787	759	763	766	rBV3	3298	10534	3.84%	0.251%
36	10.964	774	777	779	rBV3	5596	10367	3.78%	0.247%

LSC Area Percent Report

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Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : EB01-20210917

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	11.053	780	784	789	rVV	32306	67101	24.46%	1.596%
38	11.167	789	793	794	rVV2	3649	9605	3.50%	0.228%
39	11.205	794	796	801	rVB	8702	16096	5.87%	0.383%
40	11.383	806	810	816	rVV2	5229	16578	6.04%	0.394%
41	11.683	848	859	865	rBV	7095	10795	3.94%	0.257%
42	11.741	865	872	882	rVB	5219	8187	2.98%	0.195%
43	12.003	921	931	941	rBV	51992	84440	30.78%	2.008%
44	12.074	941	947	958	rVB	2270	3825	1.39%	0.091%
45	12.274	985	992	996	rBV	2431	4082	1.49%	0.097%
46	12.569	1046	1049	1052	rVB	6512	10931	3.98%	0.260%
47	12.657	1052	1056	1061	rBV2	7074	20814	7.59%	0.495%
48	12.810	1064	1068	1071	rVV2	3697	8218	3.00%	0.195%
49	12.886	1071	1074	1080	rVB	111589	176782	64.44%	4.205%
50	13.178	1094	1097	1101	rBV	30483	61574	22.45%	1.464%
51	13.419	1112	1116	1118	rBV	20531	53996	19.68%	1.284%
52	13.469	1118	1120	1122	rVV	18433	33818	12.33%	0.804%
53	13.520	1122	1124	1127	rVV2	11552	26707	9.74%	0.635%
54	13.634	1131	1133	1135	rVV	12715	29594	10.79%	0.704%
55	13.711	1135	1139	1142	rVV3	25179	83418	30.41%	1.984%
56	13.837	1146	1149	1152	rVB	117995	187928	68.51%	4.470%
57	14.269	1178	1183	1187	rBV2	154446	274316	100.00%	6.524%
58	14.738	1218	1220	1223	rVB	4234	7220	2.63%	0.172%
59	14.814	1223	1226	1228	rVV	8483	15558	5.67%	0.370%
60	14.878	1228	1231	1234	rVB	12404	24067	8.77%	0.572%
61	14.954	1234	1237	1239	rBV3	5229	12781	4.66%	0.304%
62	15.005	1239	1241	1246	rVB	8838	14910	5.44%	0.355%
63	15.106	1246	1249	1252	rBV	119265	152159	55.47%	3.619%
64	15.423	1270	1274	1277	rBV2	6130	10648	3.88%	0.253%
65	15.639	1288	1291	1297	rBV	97416	160126	58.37%	3.808%
66	15.766	1297	1301	1303	rVV3	17595	41750	15.22%	0.993%
67	15.817	1303	1305	1306	rVV	11450	16634	6.06%	0.396%
68	15.855	1306	1308	1312	rVV	24053	39186	14.28%	0.932%
69	15.969	1315	1317	1321	rVB	9967	16737	6.10%	0.398%
70	16.628	1368	1371	1374	rBV2	10781	15709	5.73%	0.374%
71	16.932	1393	1396	1399	rBV2	3534	10263	3.74%	0.244%
72	17.018	1399	1403	1406	rBV	115603	196270	71.55%	4.668%
73	17.602	1448	1451	1455	rBV	7338	11738	4.28%	0.279%
74	17.711	1457	1460	1462	rVV	9891	17528	6.39%	0.417%
75	17.760	1462	1464	1467	rVV	17625	29147	10.63%	0.693%
76	17.833	1467	1470	1472	rVV	7428	11934	4.35%	0.284%

LSC Area Percent Report

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Instrument : BNA_N
ClientSampleId : EB01-20210917

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

77	17.894	1472	1475	1478	rVV	36528	52998	19.32%	1.261%
78	18.016	1482	1485	1504	rVB7	3279	5729	2.09%	0.136%
79	18.234	1524	1529	1539	rVB	3615	5114	1.86%	0.122%
80	18.457	1568	1574	1579	rBV	4045	5351	1.95%	0.127%
81	18.805	1638	1644	1650	rBV	9255	10961	4.00%	0.261%
82	19.063	1688	1696	1713	rBV	154378	207659	75.70%	4.939%
83	19.679	1812	1820	1835	rBV	136647	176914	64.49%	4.208%
84	20.378	1918	1921	1924	rBV	4252	5607	2.04%	0.133%
85	21.026	1979	1982	1993	rBV	33621	42026	15.32%	1.000%
86	21.164	1993	1995	1998	rBV	22473	31398	11.45%	0.747%
87	21.238	1998	2002	2012	rVB2	125040	200780	73.19%	4.775%
88	22.841	2233	2239	2254	rVB	2695	4063	1.48%	0.097%
89	23.423	2401	2409	2415	rBV	3986	6449	2.35%	0.153%
90	23.485	2415	2427	2474	rVB	105122	207440	75.62%	4.934%
91	24.087	2594	2603	2619	rVB	4121	7954	2.90%	0.189%
92	24.857	2818	2828	2849	rVB	3967	9083	3.31%	0.216%
93	25.757	3074	3091	3115	rBV	1250	3722	1.36%	0.089%
94	26.822	3387	3402	3419	rBV2	908	2867	1.05%	0.068%

Sum of corrected areas: 4204486

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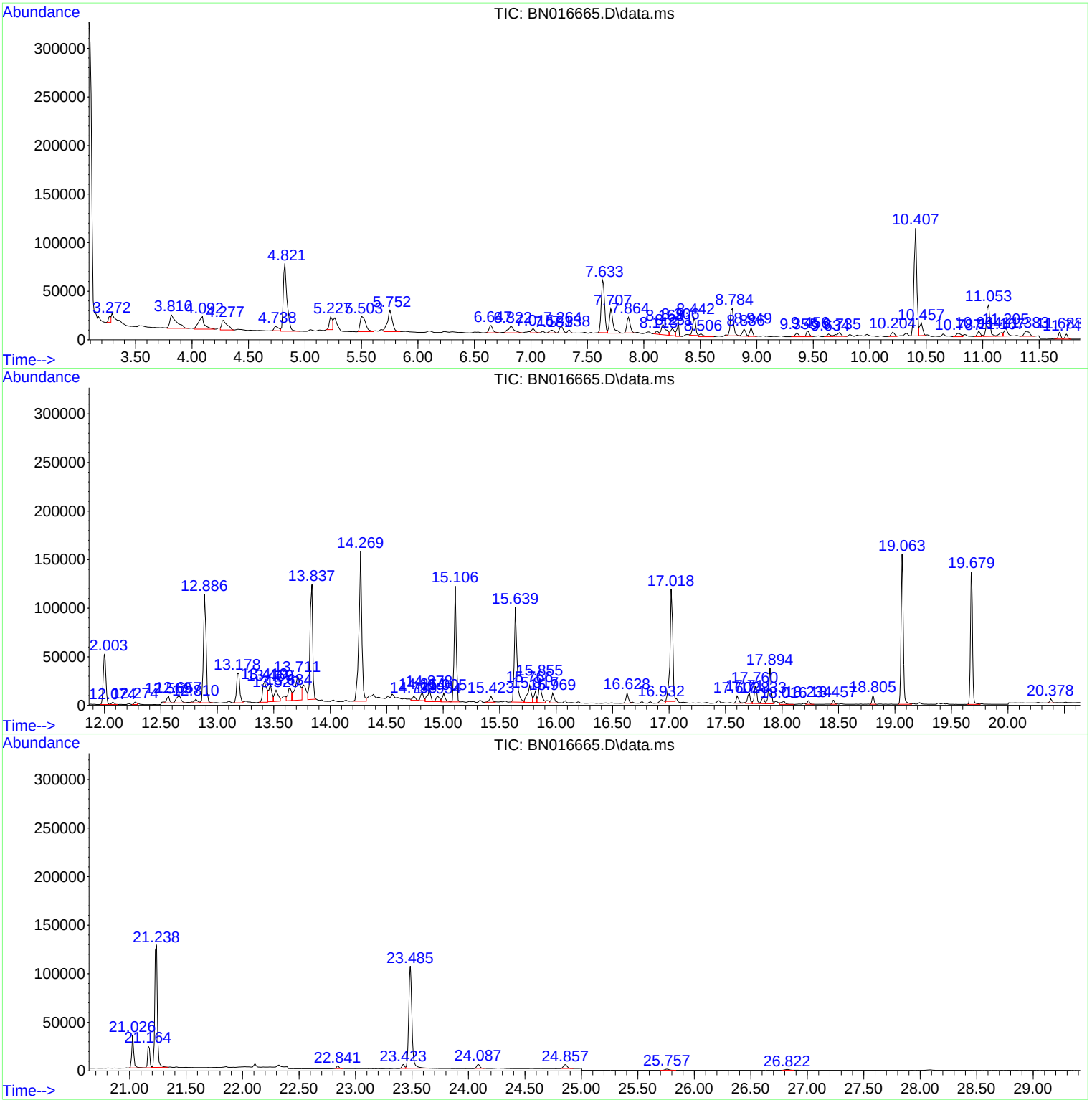
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
EB01-20210917

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 : BN016665.D
Acq On : 02 Oct 2021 10:32
Operator : CG/JU
Sample : M3829-16
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : EB01-20210917

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

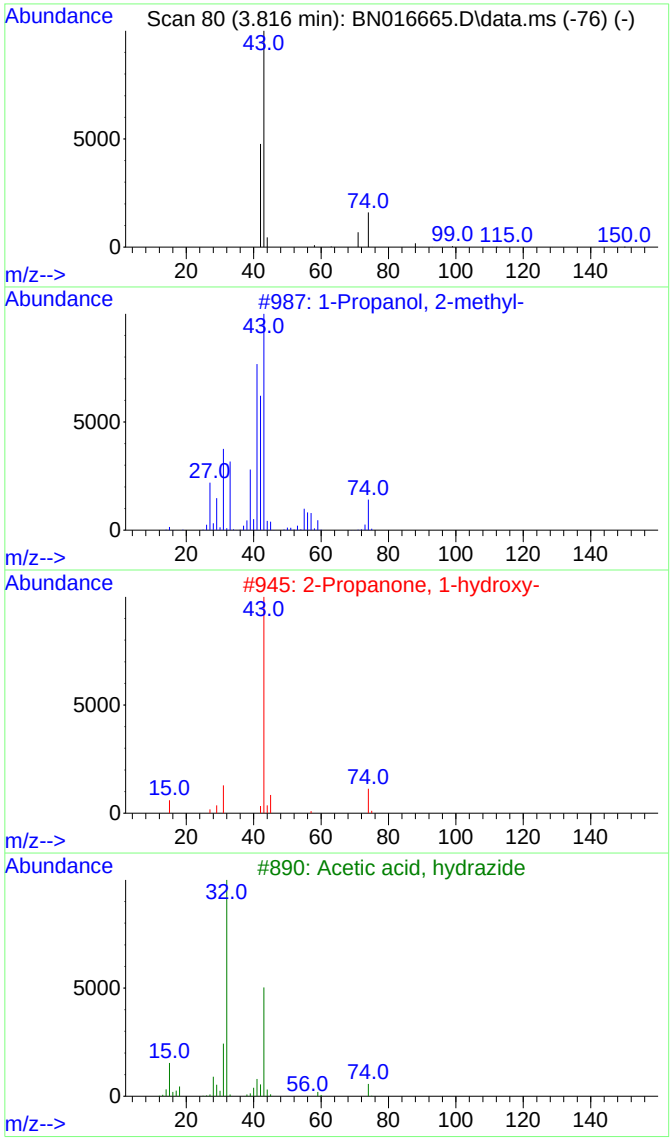
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

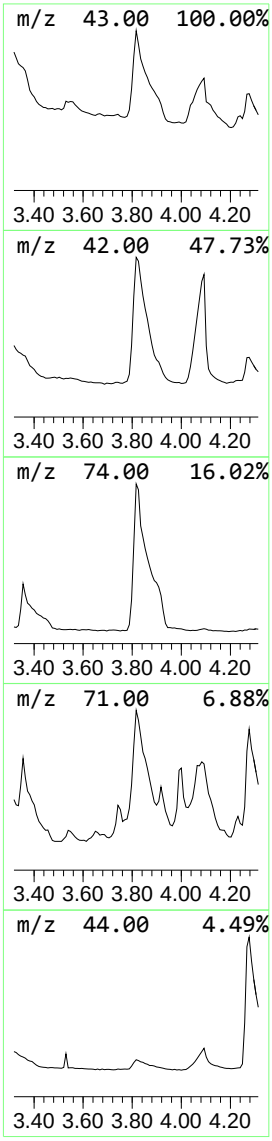
****

Peak Number 1 1-Propanol, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.20 ng	57089	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, hydrazide	74	C2H6N2O	001068-57-1	4
4	Acetic acid, methyl ester	74	C3H6O2	000079-20-9	4
5	1,4-Butanediamine	88	C4H12N2	000110-60-1	3





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016665.D
Acq On : 02 Oct 2021 10:32
Operator : CG/JU
Sample : M3829-16
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
EB01-20210917

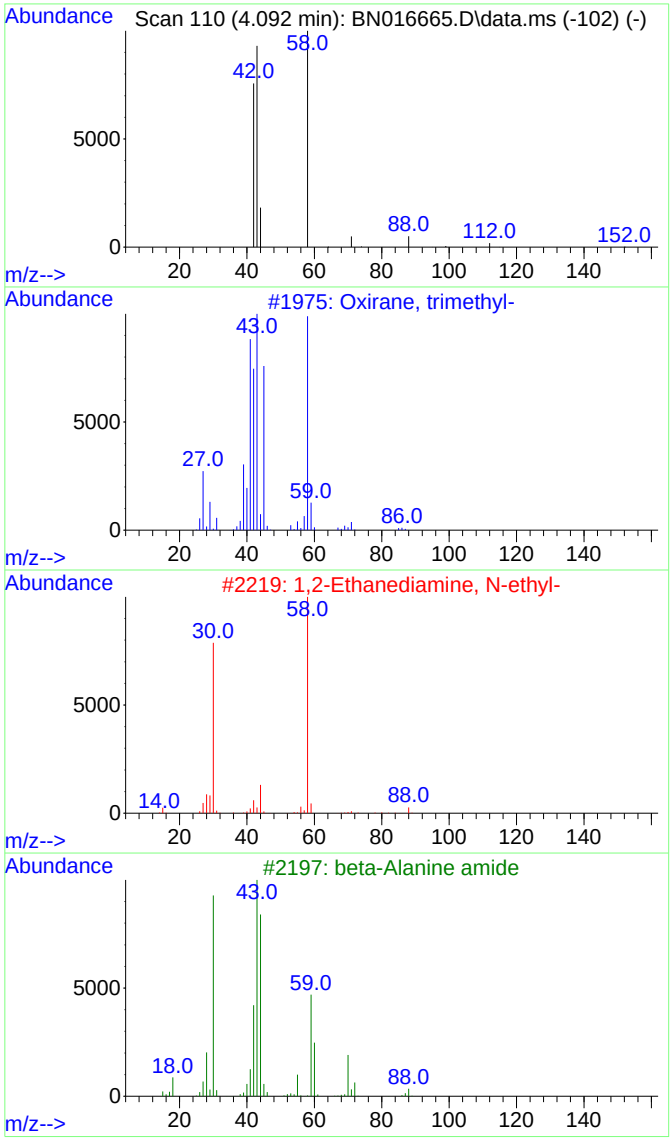
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

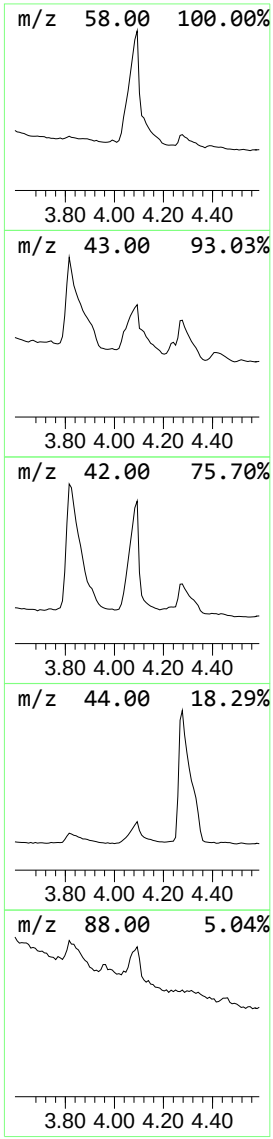
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Oxirane, trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.092	0.17 ng	47738	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, trimethyl-	86	C5H10O	005076-19-7	9
2	1,2-Ethanediamine, N-ethyl-	88	C4H12N2	000110-72-5	5
3	beta-Alanine amide	88	C3H8N2O	004726-85-6	4
4	Butane	58	C4H10	000106-97-8	4
5	2-Aminopropanenitrile, N-acetyl-	112	C5H8N2O	019861-71-3	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
EB01-20210917

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

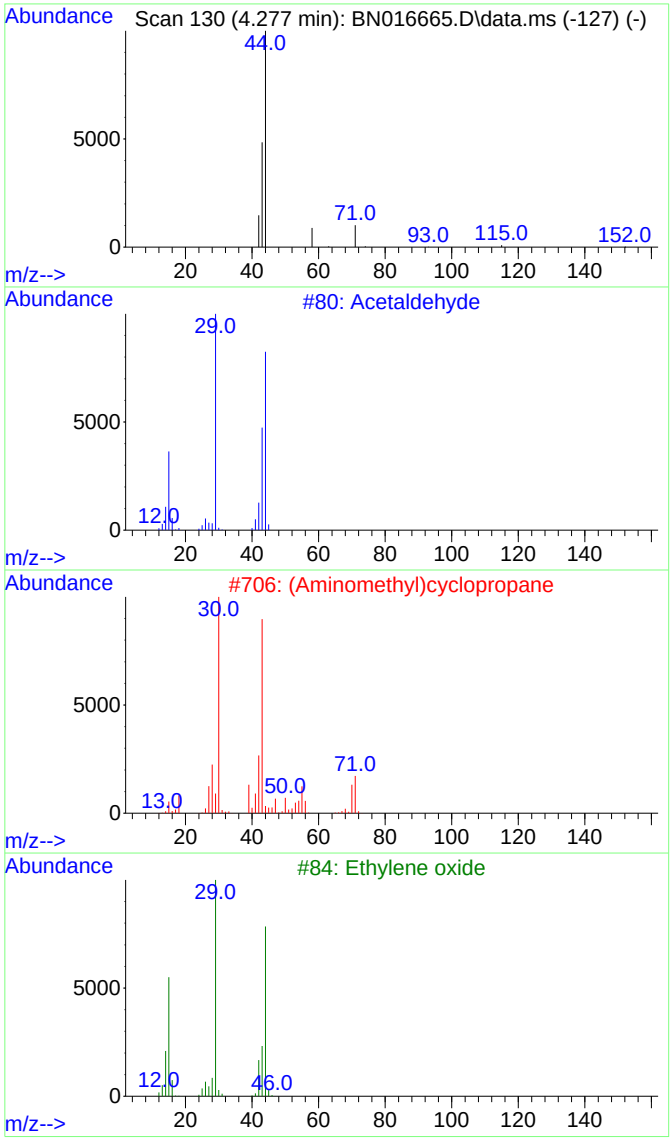
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

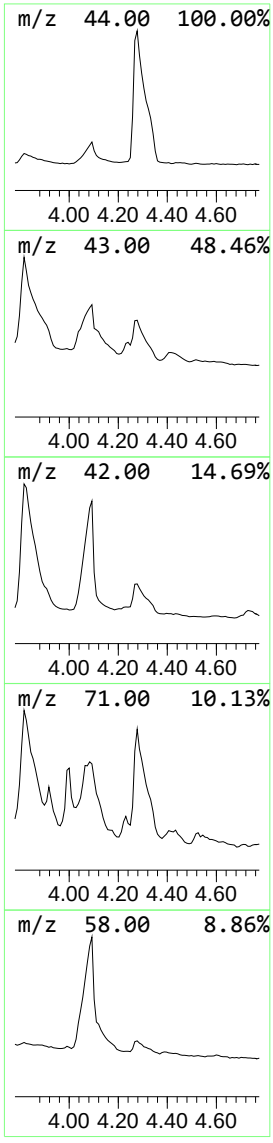
****

Peak Number 3 Acetaldehyde Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.277	0.12 ng	33261	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	7
2	(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	5
3	Ethylene oxide	44	C2H4O	000075-21-8	4
4	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	3
5	Methoxyacetonitrile	71	C3H5NO	001738-36-9	3





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ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_N
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

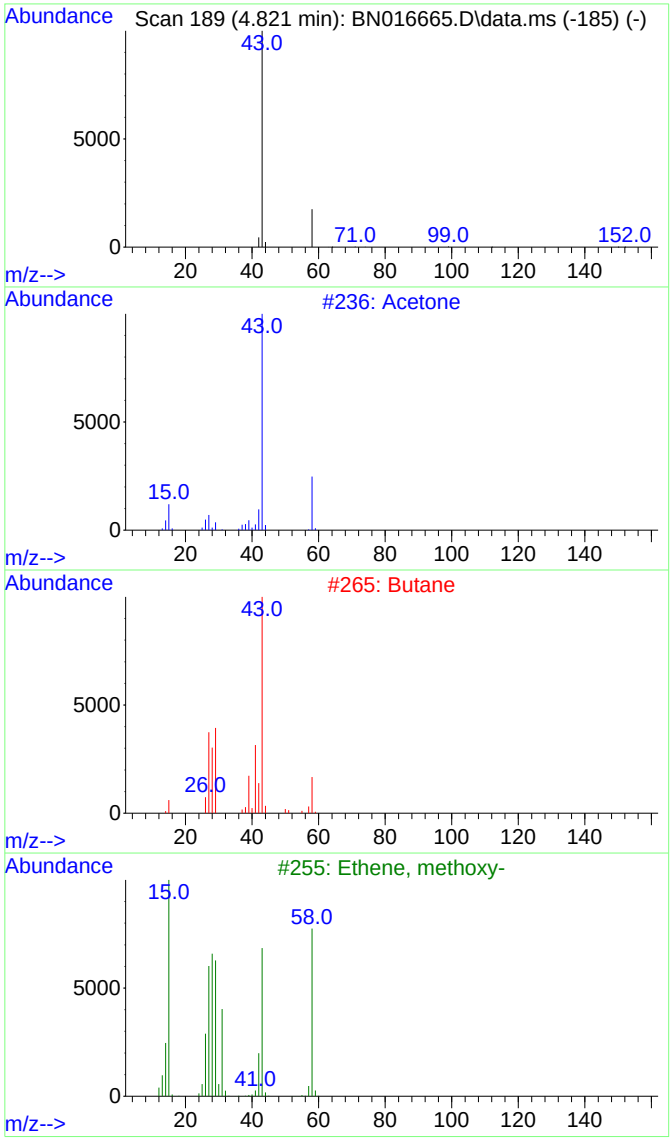
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

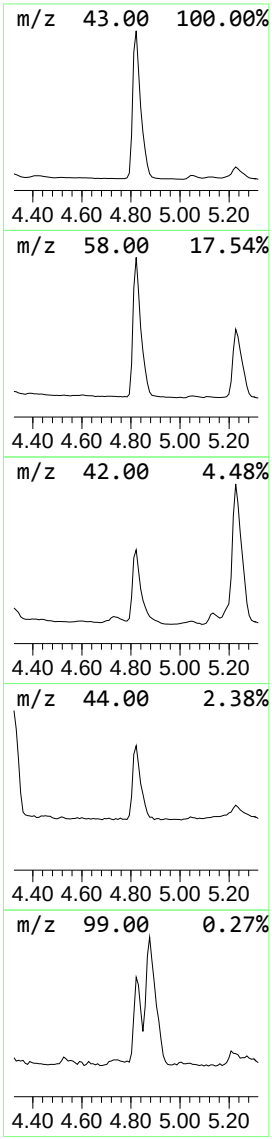
****

Peak Number 4 Acetone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.57 ng	160449	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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Misc :
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Instrument : BNA_N
ClientSampleId : EB01-20210917

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

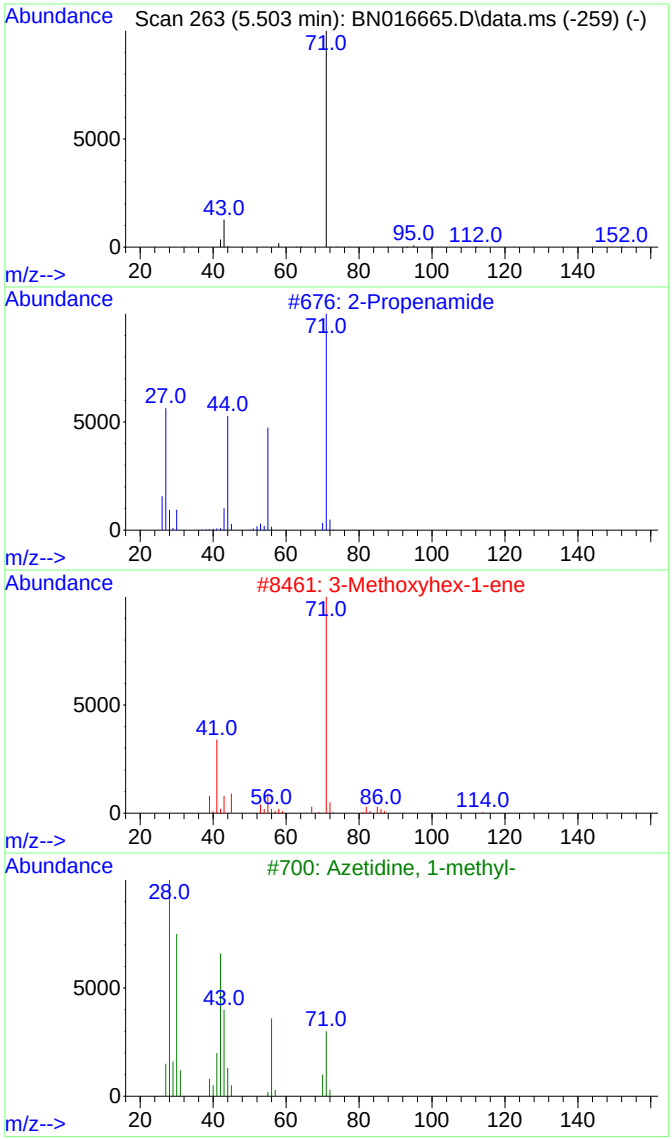
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

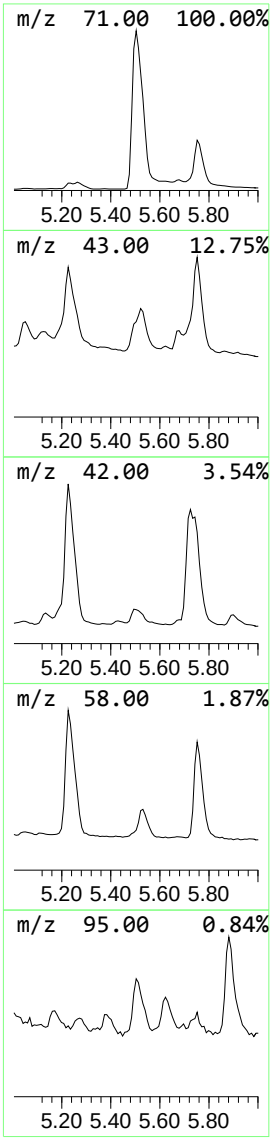
****

Peak Number 5 2-Propenamide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.503	0.19 ng	53118	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenamide	71	C3H5NO	000079-06-1	3
2	3-Methoxyhex-1-ene	114	C7H14O	108811-41-2	2
3	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	2
4	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	2
5	Aziridine, 2,2-dimethyl-	71	C4H9N	002658-24-4	1





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Data File : BN016665.D
Acq On : 02 Oct 2021 10:32
Operator : CG/JU
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ALS Vial : 33 Sample Multiplier: 1

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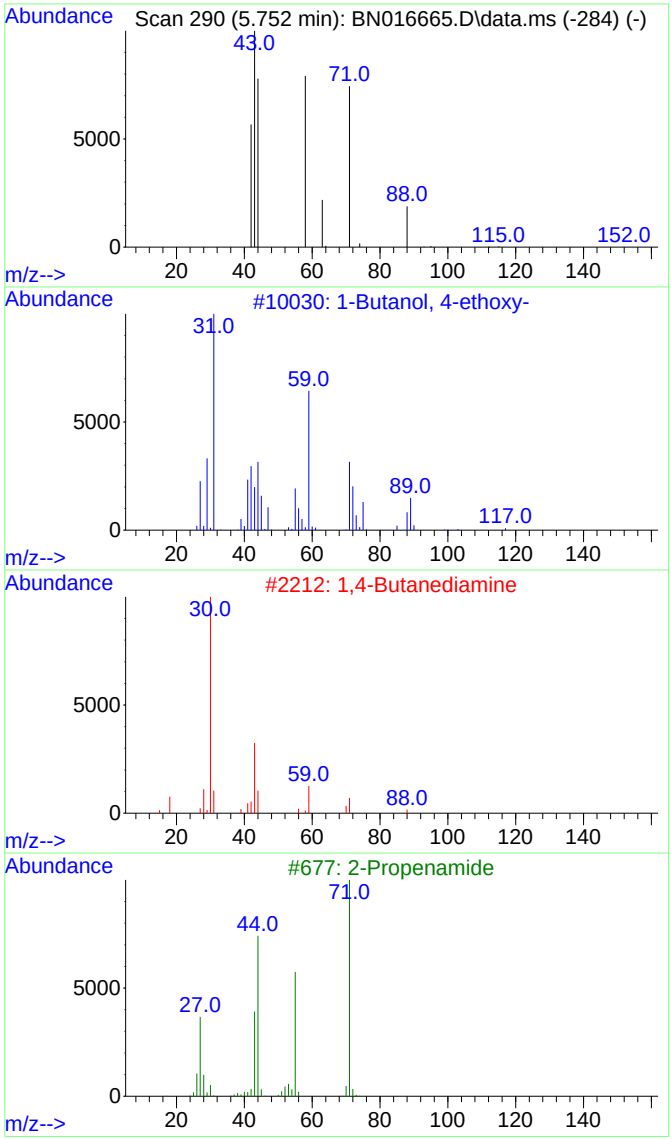
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

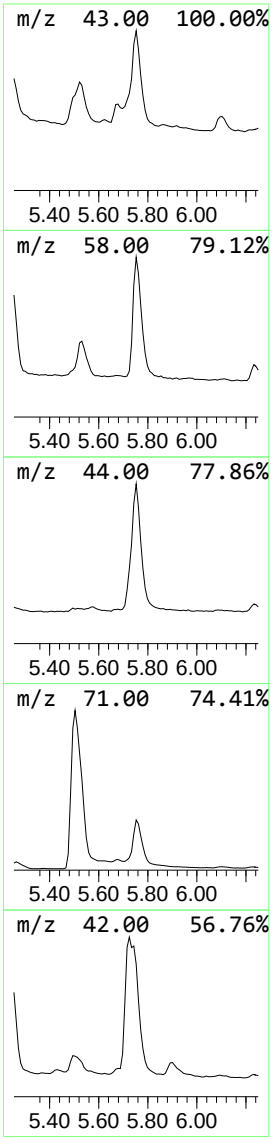
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Butanol, 4-ethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.752	0.23 ng	63546	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol, 4-ethoxy-	118	C6H14O2	000111-73-9	9
2	1,4-Butanediamine	88	C4H12N2	000110-60-1	7
3	2-Propenamide	71	C3H5NO	000079-06-1	5
4	N-Vinylformamide	71	C3H5NO	013162-05-5	5
5	Ethanediamide	88	C2H4N2O2	000471-46-5	4





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Acq On : 02 Oct 2021 10:32
Operator : CG/JU
Sample : M3829-16
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
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ClientSampleId :
EB01-20210917

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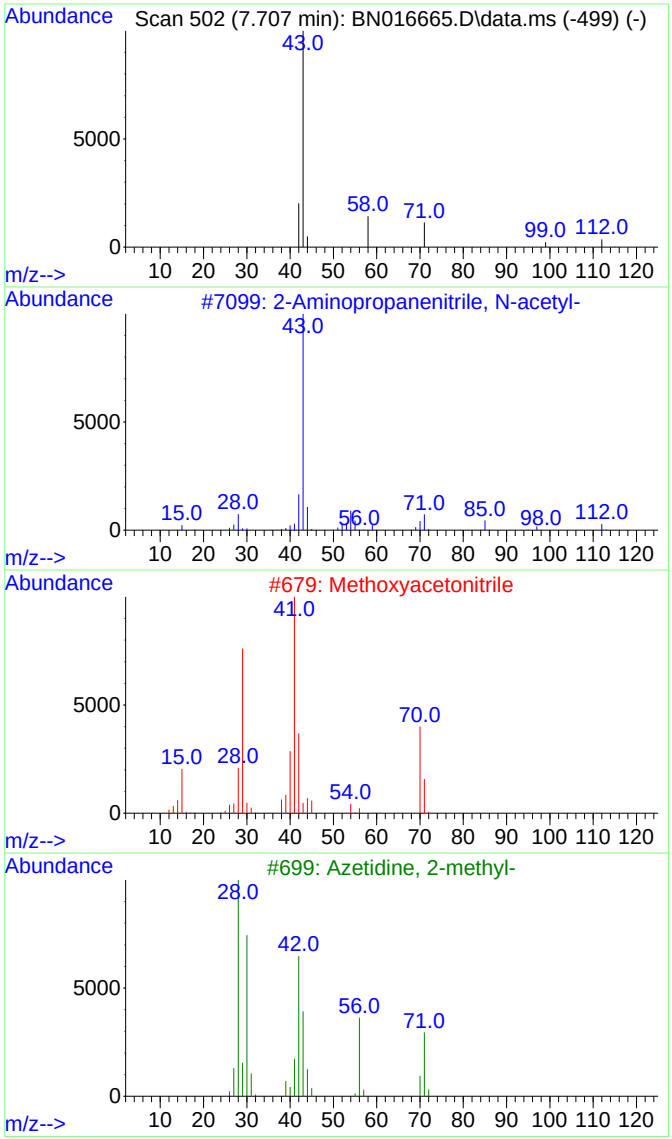
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

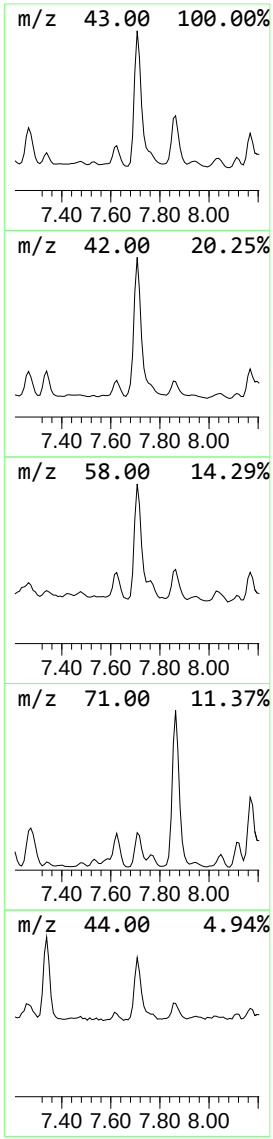
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2-Aminopropanenitrile, N-ac... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.707	0.20 ng	55376	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Aminopropanenitrile, N-acetyl-	112	C5H8N2O	019861-71-3	7
2	Methoxyacetonitrile	71	C3H5NO	001738-36-9	4
3	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	4
4	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	4
5	Butane	58	C4H10	000106-97-8	4





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Sample : M3829-16
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ClientSampleId : EB01-20210917

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

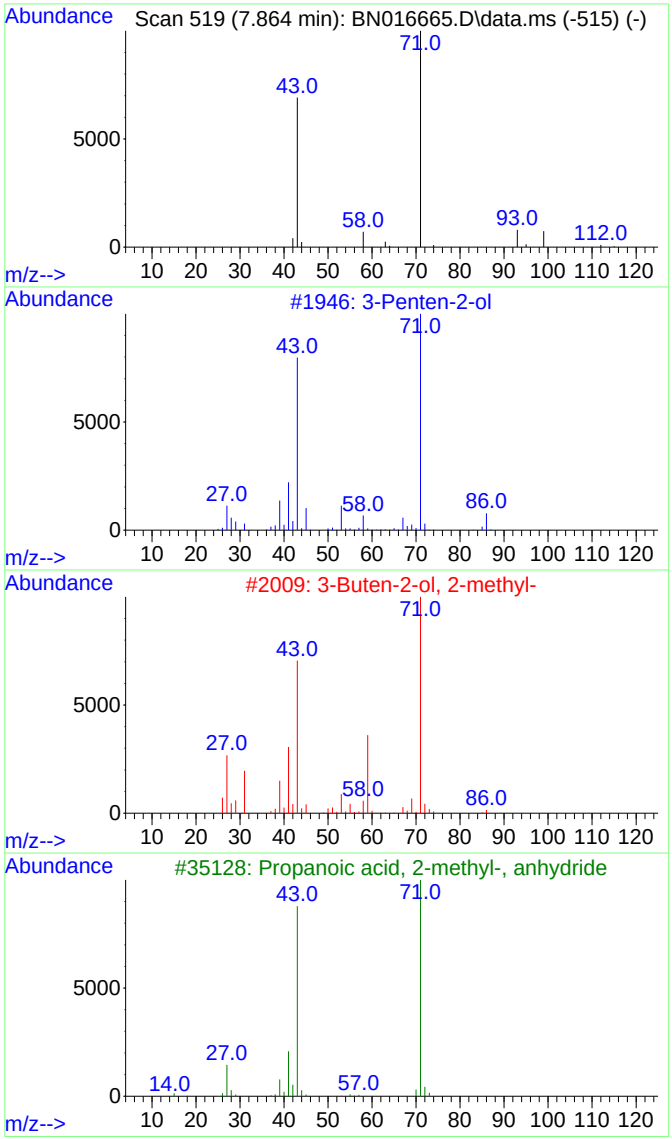
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

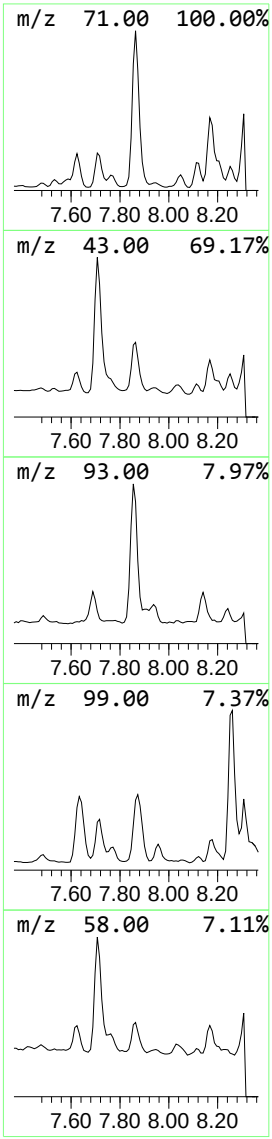
****

Peak Number 8 3-Penten-2-ol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.864	0.12 ng	33732	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-ol	86	C5H10O	001569-50-2	4
2	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	4
3	Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	4
4	Butane, 2-iodo-3-methyl-	198	C5H11I	018295-27-7	4
5	2-Propenamide	71	C3H5NO	000079-06-1	3





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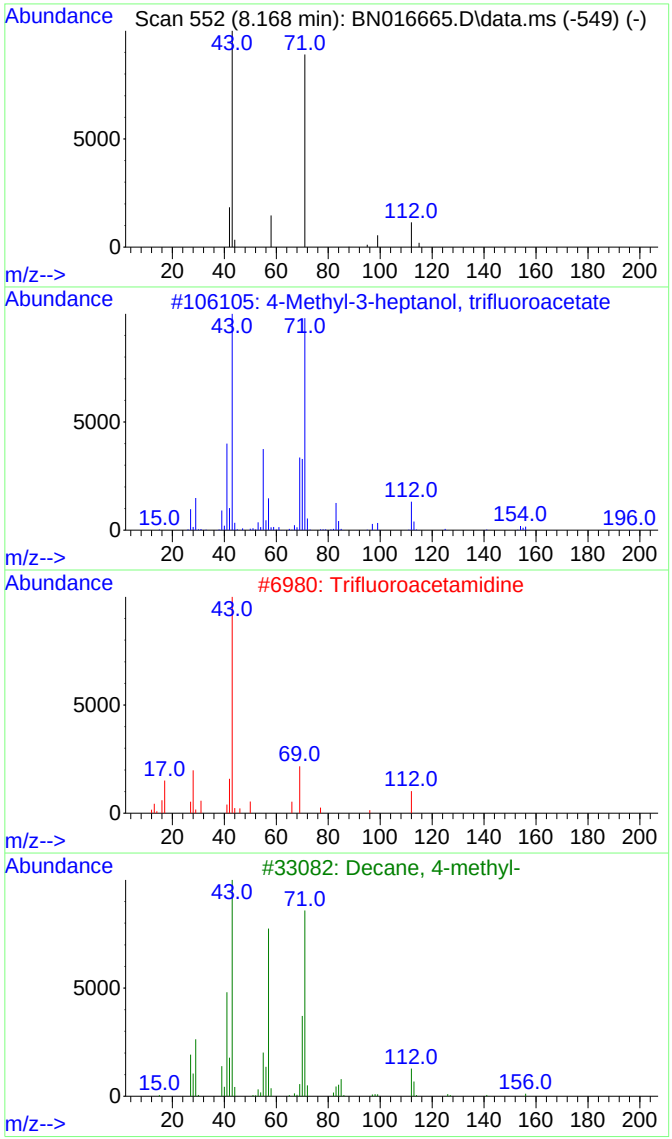
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

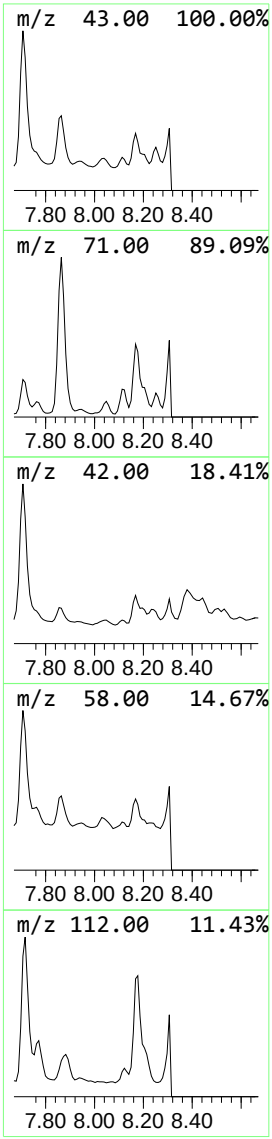
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 4-Methyl-3-heptanol, triflu... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.168	0.11 ng	29415	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methyl-3-heptanol, trifluoroac...	226	C10H17F3O2	1000365-51-8	43
2	Trifluoroacetamidine	112	C2H3F3N2	000354-37-0	9
3	Decane, 4-methyl-	156	C11H24	002847-72-5	9
4	n-Butyric acid 2-ethylhexyl ester	200	C12H24O2	025415-84-3	9
5	Butane	58	C4H10	000106-97-8	7





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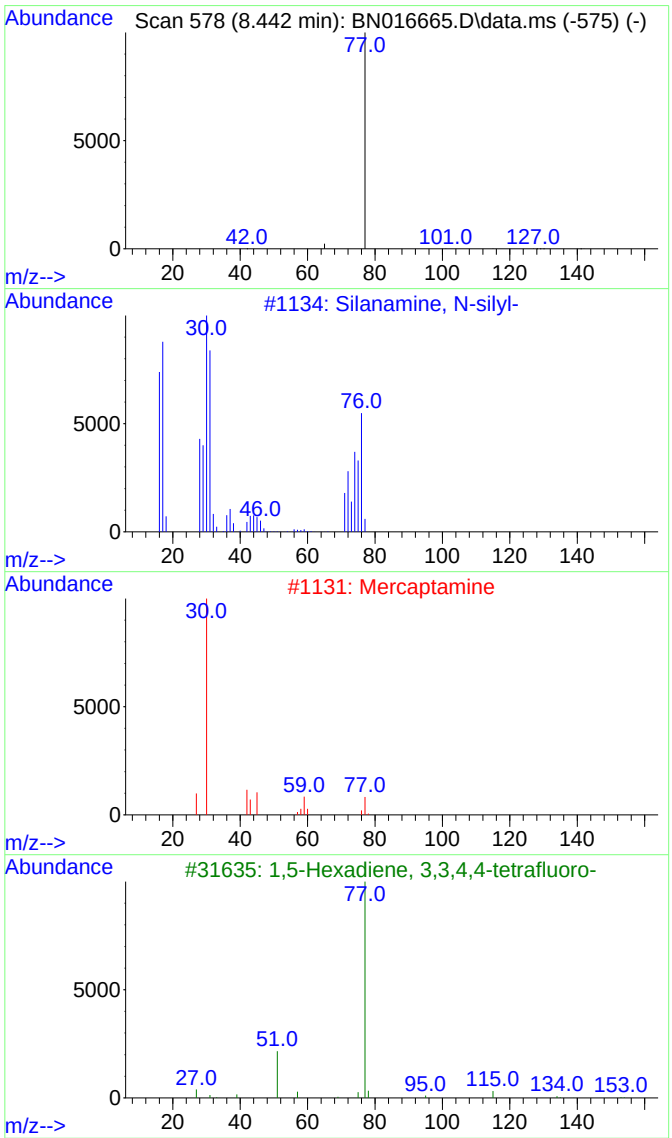
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

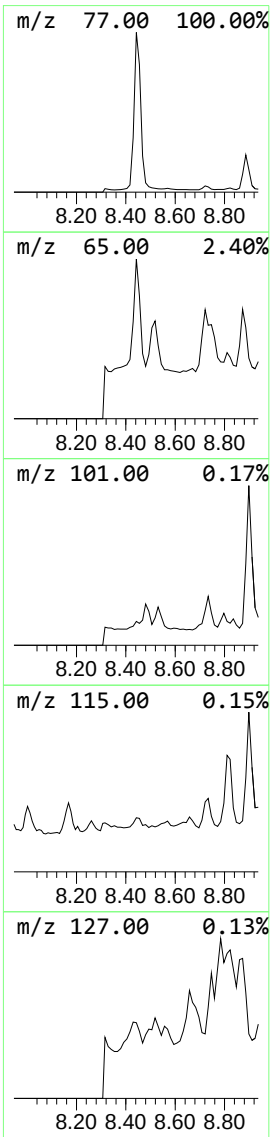
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Silanamine, N-silyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.442	0.12 ng	33122	1,4-Dichlorobenzene-d4	7.642

Hit# of 4	Tentative ID	MW	MolForm	CAS#	Qual
1	Silanamine, N-silyl-	77	H7NSi2	005702-11-4	1
2	Mercaptamine	77	C2H7NS	000060-23-1	1
3	1,5-Hexadiene, 3,3,4,4-tetrafluoro-	154	C6H6F4	001763-21-9	1
4	1-Propyne, 3-chloro-	74	C3H3Cl	000624-65-7	1





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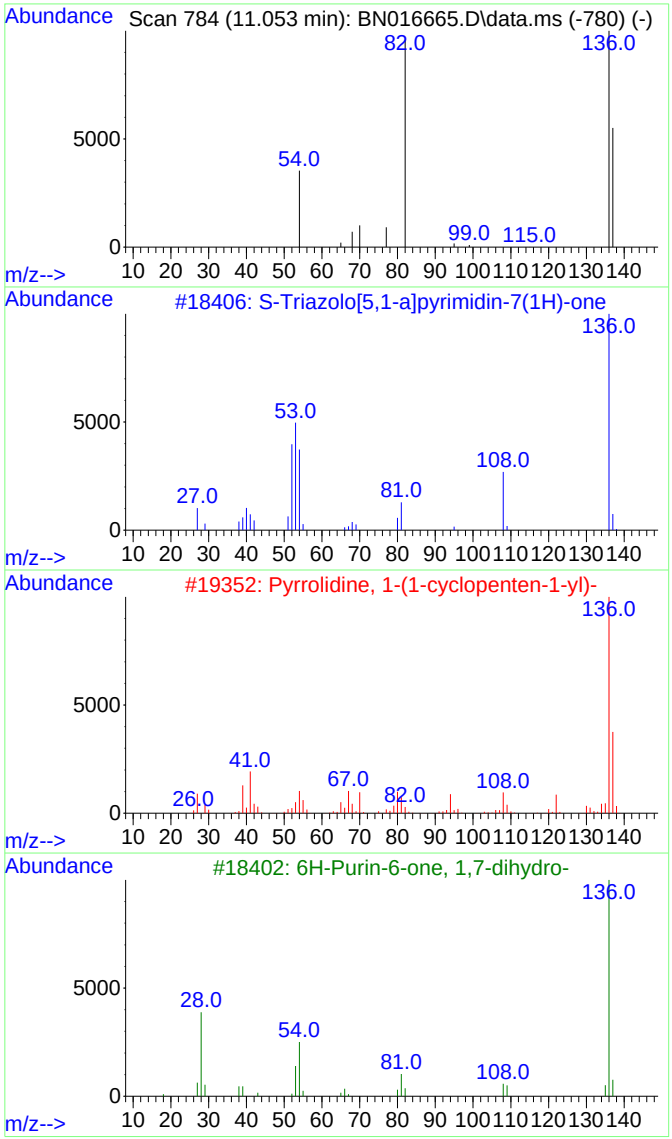
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

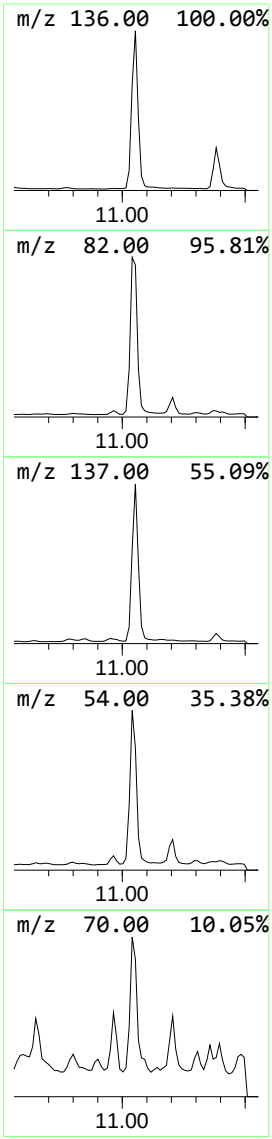
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 S-Triazolo[5,1-a]pyrimidin-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.053	0.14 ng	67101	Naphthalene-d8	10.407

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	S-Triazolo[5,1-a]pyrimidin-7(1H)...	136	C5H4N4O	004866-61-9	9
2	Pyrrolidine, 1-(1-cyclopenten-1-...	137	C9H15N	007148-07-4	9
3	6H-Purin-6-one, 1,7-dihydro-	136	C5H4N4O	000068-94-0	7
4	Benzenemethanamine, 4-methoxy-	137	C8H11NO	002393-23-9	5
5	2-Cyclopenten-1-one	82	C5H6O	000930-30-3	4





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

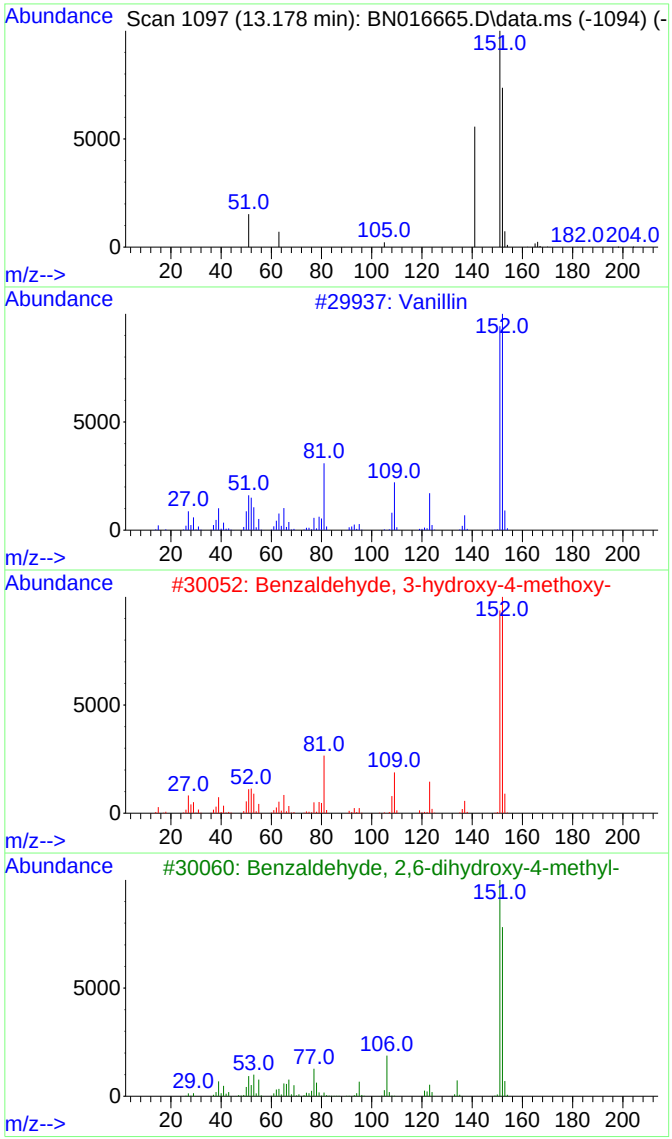
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

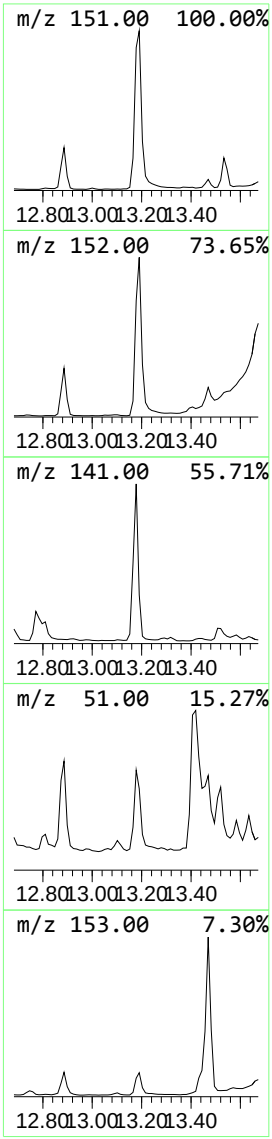
****

Peak Number 12 Vanillin Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.178	0.09 ng	61574	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Vanillin	152	C8H8O3	000121-33-5	59
2	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	45
3	Benzaldehyde, 2,6-dihydroxy-4-me...	152	C8H8O3	000526-37-4	45
4	Benzaldehyde, 2-hydroxy-4-methoxy-	152	C8H8O3	000673-22-3	9
5	1H-Indene, 4,7-difluoro-	152	C9H6F2	130408-18-3	9





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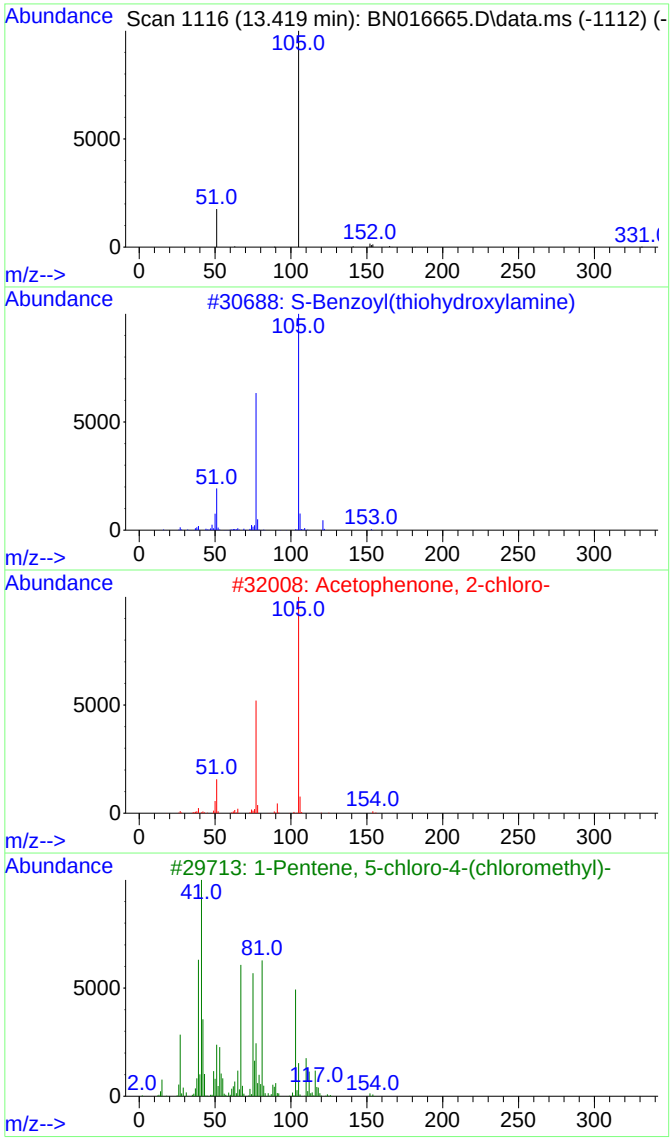
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

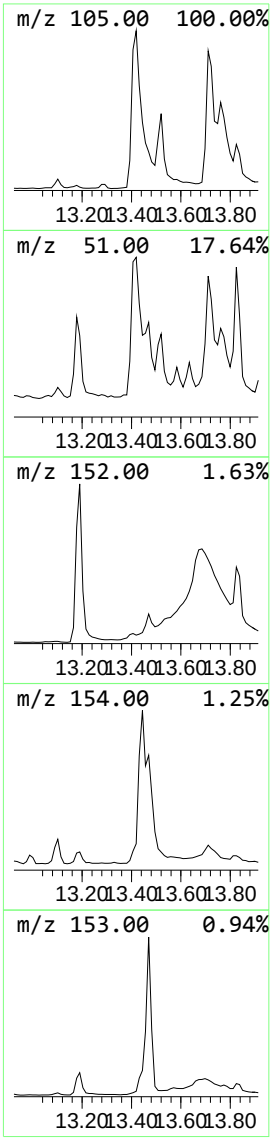
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 S-Benzoyl(thiohydroxylamine) Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.419	0.08 ng	53996	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	S-Benzoyl(thiohydroxylamine)	153	C7H7NOS	025740-80-1	5
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	4
3	1-Pentene, 5-chloro-4-(chloromet...	152	C6H10Cl2	027990-74-5	3
4	2,2-Bis[4-(benzoyloxy)phenyl]pro...	436	C29H24O4	002297-14-5	2
5	Oxazol-5(4H)-one, 4-[5-(2,5-dich...	383	C20H11Cl2NO3	329795-32-6	2





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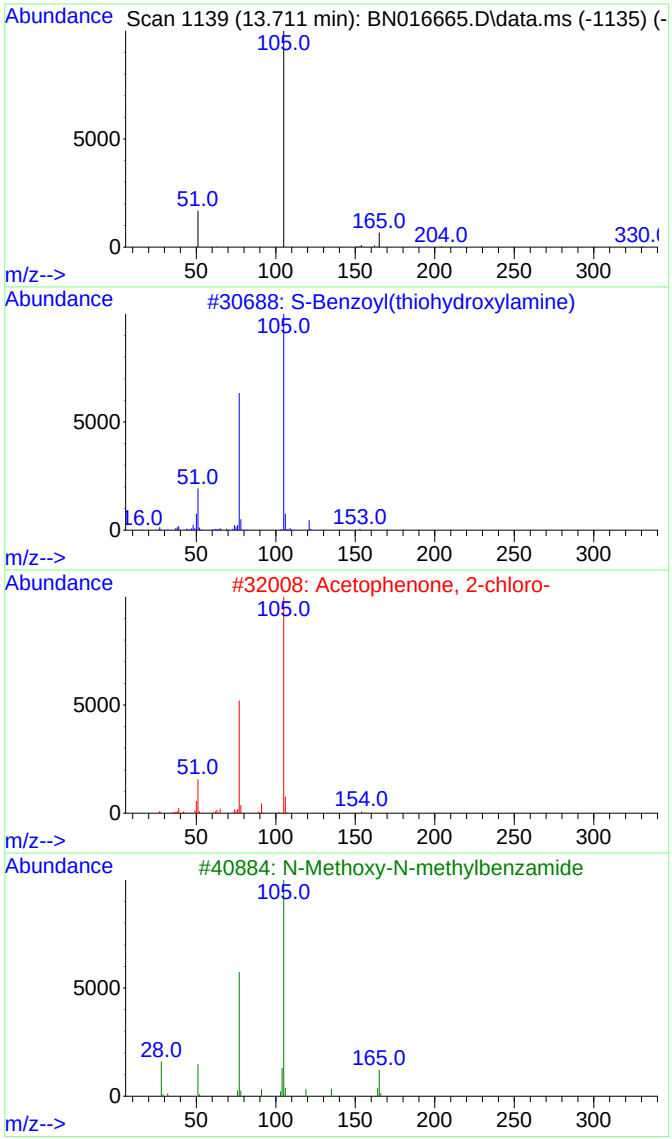
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

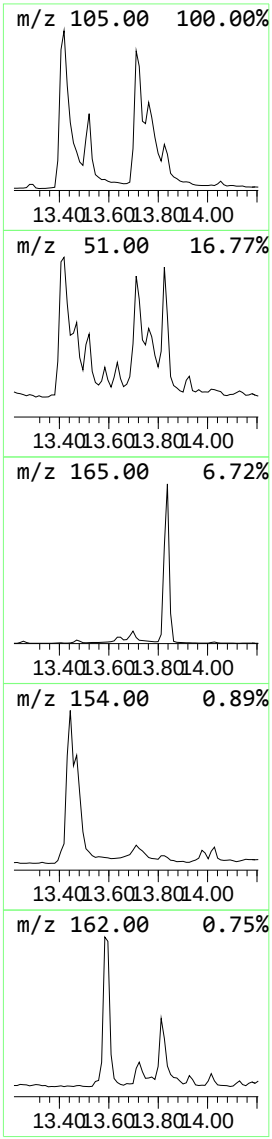
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 S-Benzoyl(thiohydroxylamine) Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.711	0.12 ng	83418	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	S-Benzoyl(thiohydroxylamine)	153	C7H7NOS	025740-80-1	5
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	4
3	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	3
4	2-Amino-1-(o-methoxyphenyl)propane	165	C10H15NO	015402-84-3	2
5	1-(4-Nitrophenyl)-2-phenylethane...	255	C14H9NO4	022711-24-6	2





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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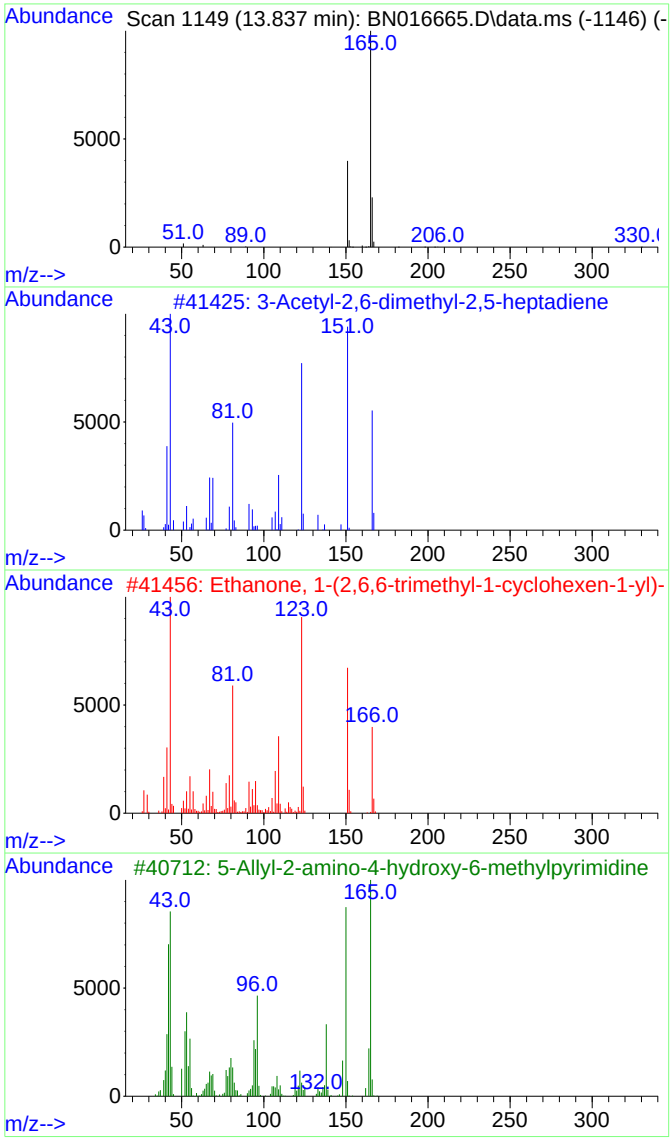
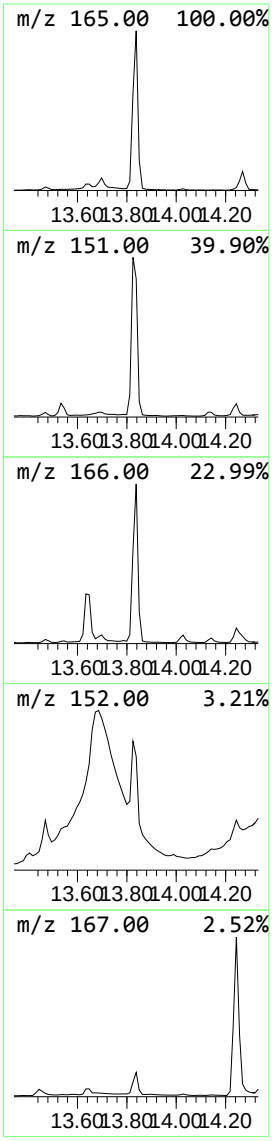
****
Peak Number 15 3-Acetyl-2,6-dimethyl-2,5-h... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.837	0.27 ng	187928	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Acetyl-2,6-dimethyl-2,5-heptad...	166	C11H18O	1000432-11-5	7
2	Ethanone, 1-(2,6,6-trimethyl-1-c...	166	C11H18O	001197-92-8	5
3	5-Allyl-2-amino-4-hydroxy-6-meth...	165	C8H11N3O	006957-86-4	5
4	7-Methyl-6-oxo-1,2,3,4-tetrahydr...	165	C8H11N3O	026955-14-6	4
5	N,N-Dimethyl-2H-1,3-benzodioxol-...	165	C9H11NO2	1000388-48-7	4





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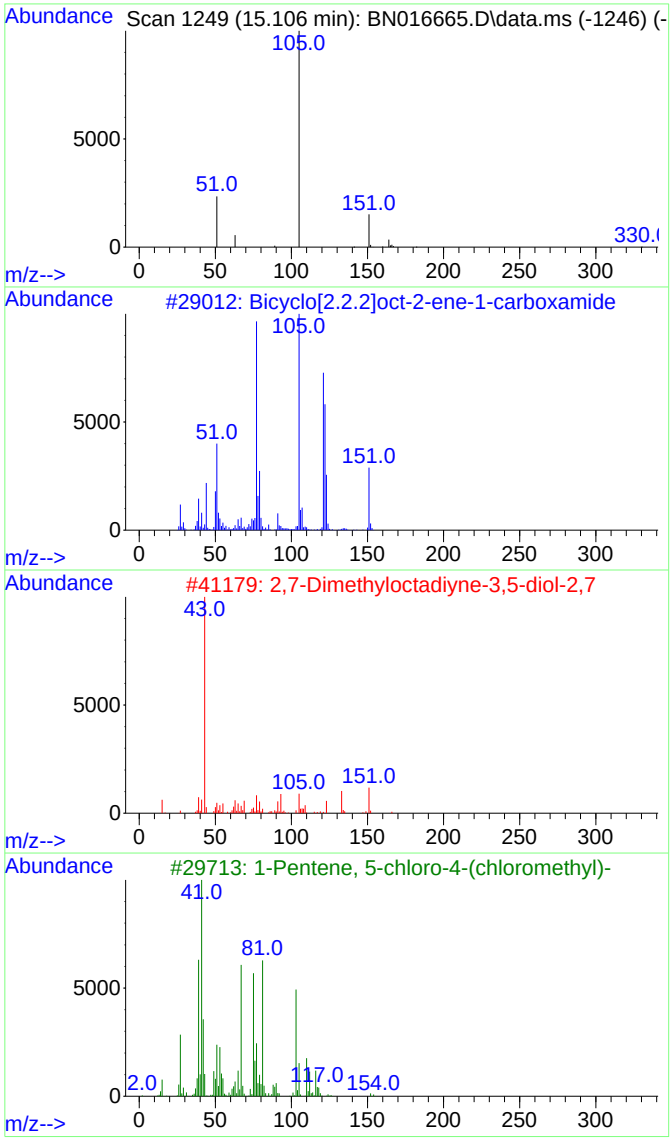
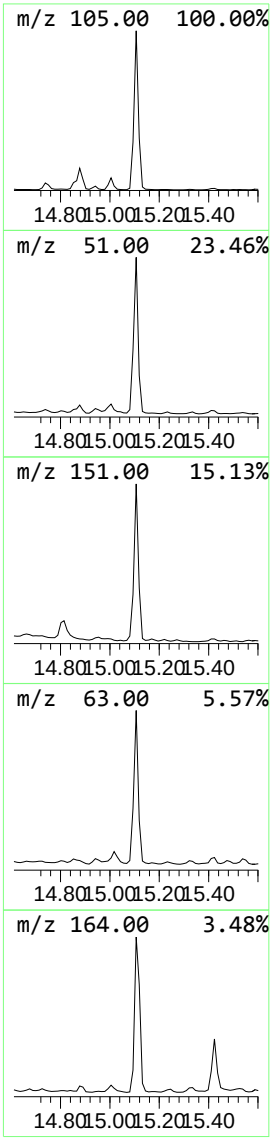
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 Bicyclo[2.2.2]oct-2-ene-1-c... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.106	0.22 ng	152159	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.2]oct-2-ene-1-carbox...	151	C9H13NO	1000211-27-6	4
2	2,7-Dimethyloctadiyne-3,5-diol-2,7	166	C10H14O2	005929-72-6	4
3	1-Pentene, 5-chloro-4-(chloromet...	152	C6H10Cl2	027990-74-5	3
4	Ethanone, 2-(formyloxy)-1-phenyl-	164	C9H8O3	055153-12-3	3
5	5-Nitro-m-xylene	151	C8H9NO2	000099-12-7	3





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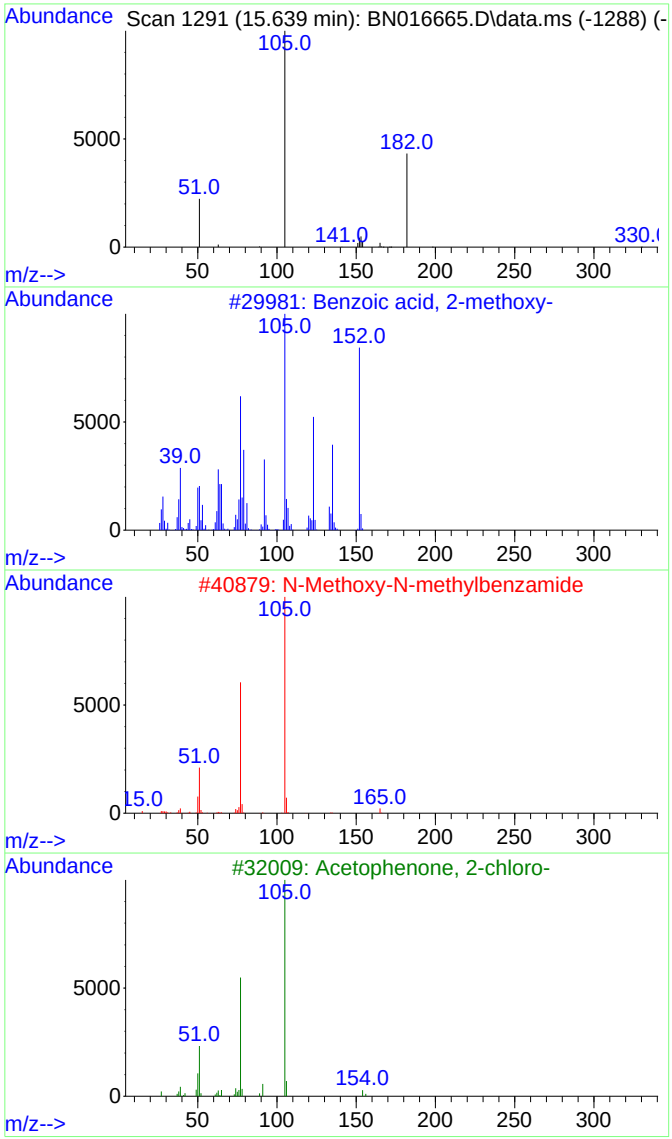
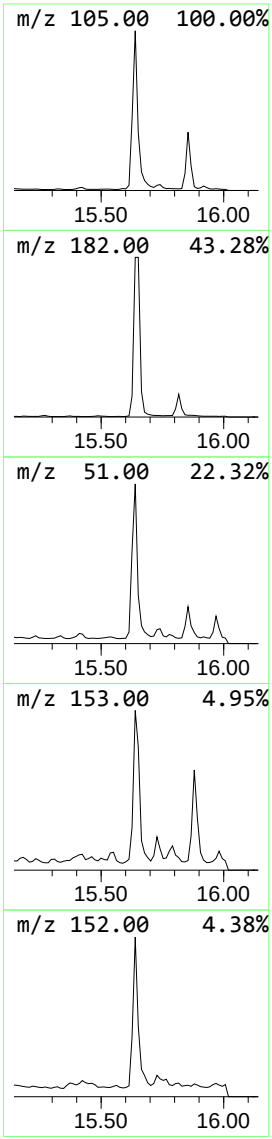
****

Peak Number 17 Benzoic acid, 2-methoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.639	0.23 ng	160126	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2-methoxy-	152	C8H8O3	000579-75-9	9
2	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	5
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	5
4	3-(4-Methoxy-1,2,5-oxadiazol-3-y...	182	C6H6N4O3	1000459-91-2	3
5	Benzeneethanamine, 4-methoxy-	151	C9H13NO	000055-81-2	3





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Acq On : 02 Oct 2021 10:32
Operator : CG/JU
Sample : M3829-16
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
EB01-20210917

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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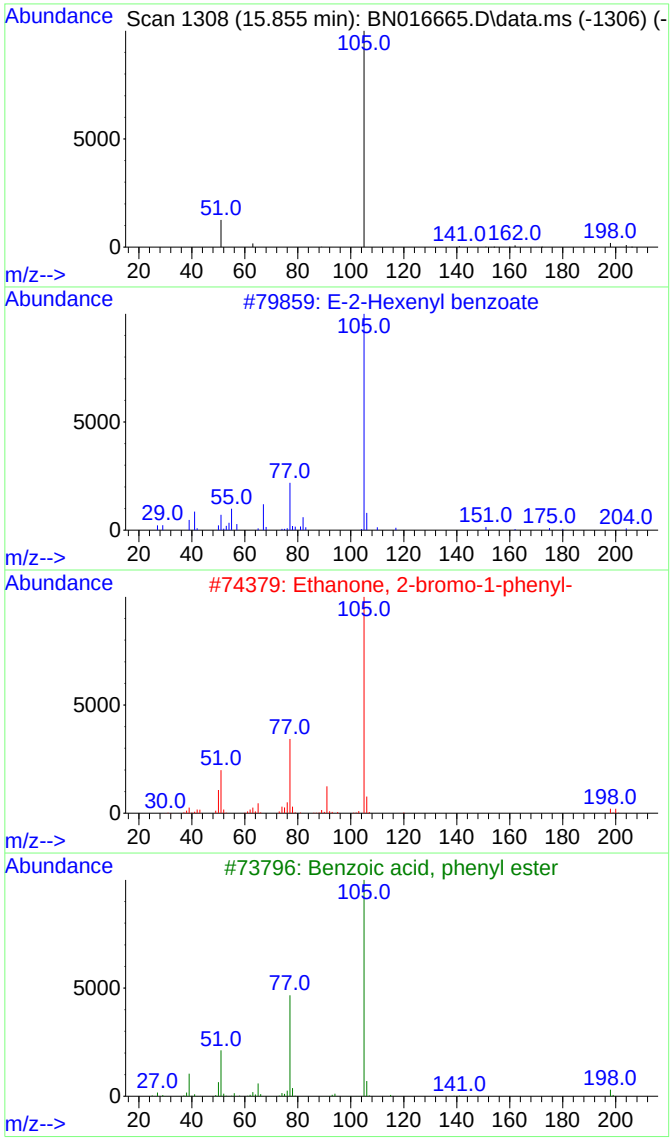
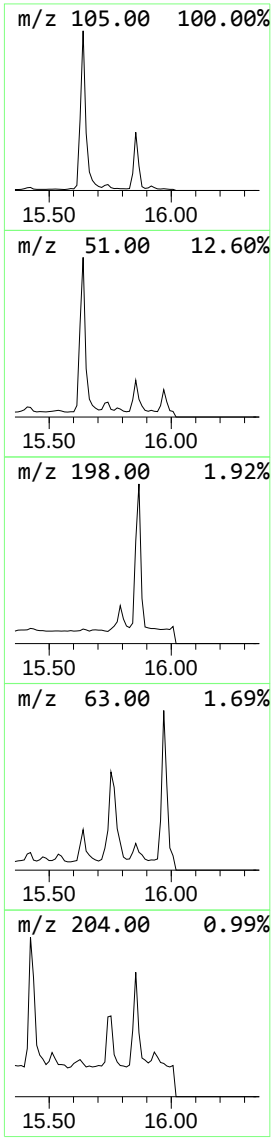
Peak Number 18 E-2-Hexenyl benzoate Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.855	0.08 ng	39186	Phenanthrene-d10	17.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-2-Hexenyl benzoate	204	C13H16O2	076841-70-8	5
2	Ethanone, 2-bromo-1-phenyl-	198	C8H7BrO	000070-11-1	4
3	Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	4
4	1-Chloro-4-methoxy-2-phenylbutane	198	C11H15ClO	1010216-63-6	3
5	2-Benzoylamino-2-methyl-propioni...	403	C19H18BrNO4	1000295-31-8	2





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Data File : BN016665.D
Acq On : 02 Oct 2021 10:32
Operator : CG/JU
Sample : M3829-16
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
EB01-20210917

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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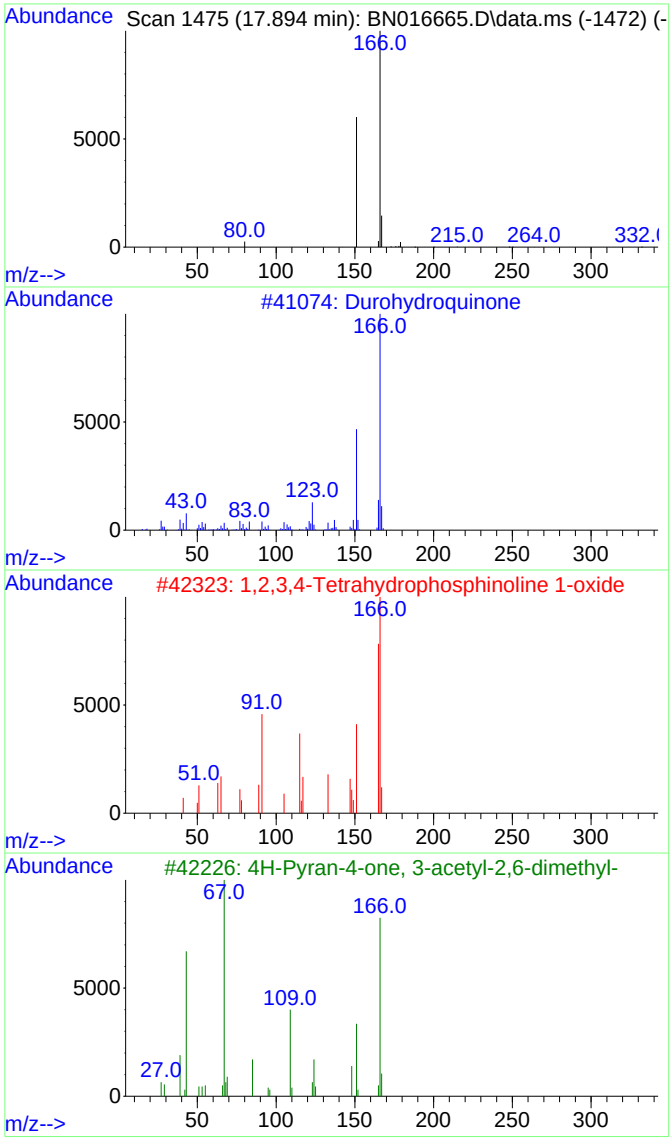
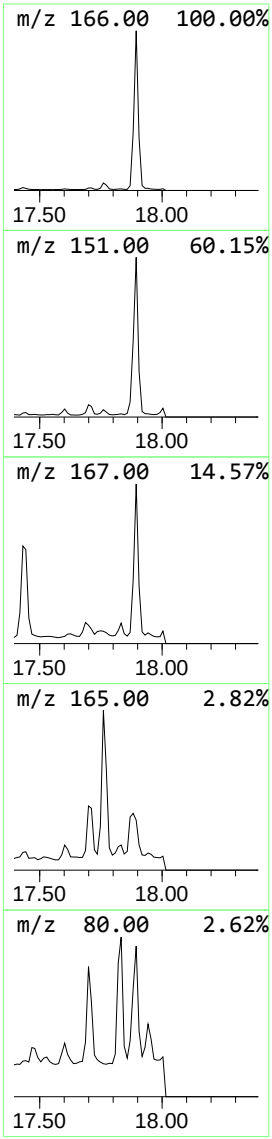
Peak Number 19 Durohydroquinone Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.894	0.11 ng	52998	Phenanthrene-d10	17.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Durohydroquinone	166	C10H14O2	000527-18-4	9
2	1,2,3,4-Tetrahydrophosphinoline ...	166	C9H11OP	052221-85-9	9
3	4H-Pyran-4-one, 3-acetyl-2,6-dim...	166	C9H10O3	007521-38-2	9
4	Phenol, 3-methoxy-2,4,5-trimethyl-	166	C10H14O2	034883-04-0	9
5	Benzaldehyde, 2,5-dimethoxy-	166	C9H10O3	000093-02-7	9





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Data File : BN016665.D
Acq On : 02 Oct 2021 10:32
Operator : CG/JU
Sample : M3829-16
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
EB01-20210917

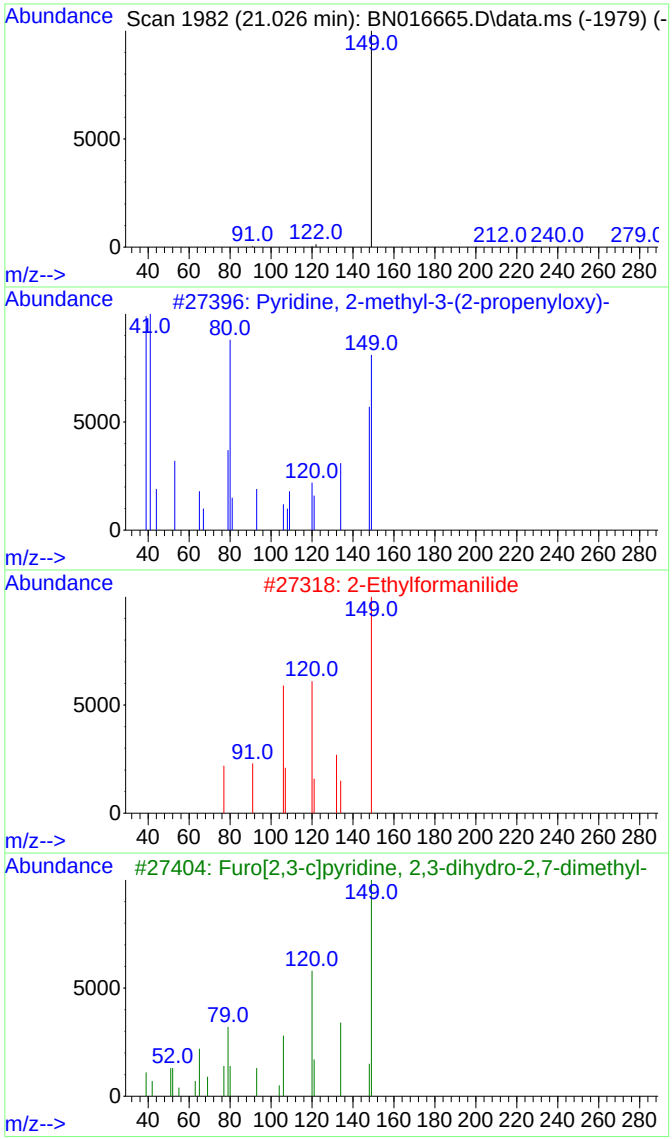
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

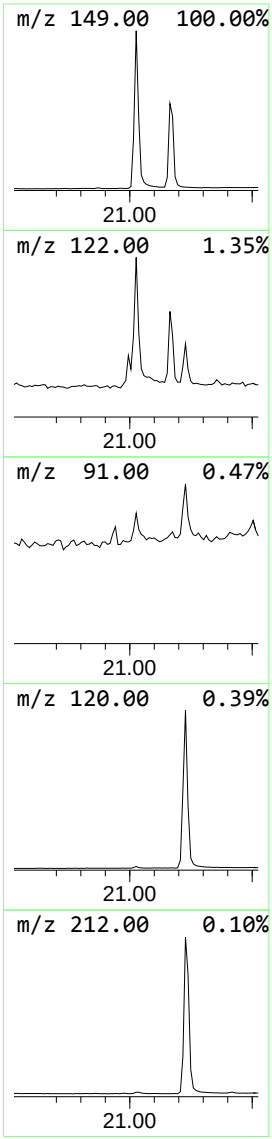
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 Pyridine, 2-methyl-3-(2-pro... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.026	0.08 ng	42026	Chrysene-d12	21.238

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine, 2-methyl-3-(2-propenyl...	149	C9H11NO	069022-75-9	2
2	2-Ethylformanilide	149	C9H11NO	002860-30-2	2
3	Furo[2,3-c]pyridine, 2,3-dihydro...	149	C9H11NO	069022-82-8	2
4	6,7-Dimethyl-triazolo(4,3-b)(1,2...	149	C6H7N5	061139-73-9	2
5	Carbamodithioic acid, dimethyl-,...	149	C5H11NS2	000617-38-9	2





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016665.D
Acq On : 02 Oct 2021 10:32
Operator : CG/JU
Sample : M3829-16
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : EB01-20210917

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-Propanol, 2-m...	3.816	0.2	ng	57089	1	7.642	111995	0.4
Oxirane, trimet...	4.092	0.2	ng	47738	1	7.642	111995	0.4
Acetaldehyde	4.277	0.1	ng	33261	1	7.642	111995	0.4
Acetone	4.821	0.6	ng	160449	1	7.642	111995	0.4
2-Propenamide	5.503	0.2	ng	53118	1	7.642	111995	0.4
1-Butanol, 4-et...	5.752	0.2	ng	63546	1	7.642	111995	0.4
2-Aminopropanen...	7.707	0.2	ng	55376	1	7.642	111995	0.4
3-Penten-2-ol	7.864	0.1	ng	33732	1	7.642	111995	0.4
4-Methyl-3-hept...	8.168	0.1	ng	29415	1	7.642	111995	0.4
Silanamine, N-s...	8.442	0.1	ng	33122	1	7.642	111995	0.4
S-Triazolo[5,1-...	11.053	0.1	ng	67101	2	10.407	192901	0.4
Vanillin	13.178	0.1	ng	61574	3	14.269	274316	0.4
S-Benzoyl(thioh...	13.419	0.1	ng	53996	3	14.269	274316	0.4
S-Benzoyl(thioh...	13.711	0.1	ng	83418	3	14.269	274316	0.4
3-Acetyl-2,6-di...	13.837	0.3	ng	187928	3	14.269	274316	0.4
Bicyclo[2.2.2]o...	15.106	0.2	ng	152159	3	14.269	274316	0.4
Benzoic acid, 2...	15.639	0.2	ng	160126	3	14.269	274316	0.4
E-2-Hexenyl ben...	15.855	0.1	ng	39186	4	17.018	196270	0.4
Durohydroquinone	17.894	0.1	ng	52998	4	17.018	196270	0.4
Pyridine, 2-met...	21.026	0.1	ng	42026	5	21.238	200780	0.4