LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016623.D
Acq On : 01 Oct 2021 06:35
Operator : CG/JU
Sample : M3986-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : P287-DITCH

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: BN016623.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.502	44	46	48	rBV	2887	5064	2.40%	0.144%
2	3.733	68	71	75	rBV	3308	7148	3.39%	0.203%
3	3.816	78	80	89	rVB2	7291	17057	8.10%	0.483%
4	4.139	112	115	120	rVB	10614	14443	6.86%	0.409%
5	4.498	151	154	156	rBV	19859	36610	17.38%	1.038%
6	4.821	185	189	196	rBV	56125	122627	58.21%	3.476%
7	4.904	196	198	210	rVB	4541	12018	5.71%	0.341%
8	5.181	224	228	234	rBV	5154	17961	8.53%	0.509%
9	5.264	235	237	243	rVB	5621	12851	6.10%	0.364%
10	5.752	288	290	300	rVB3	6683	18072	8.58%	0.512%
11	6.084	323	326	332	rVB2	10029	19665	9.34%	0.557%
12	6.232	339	342	349	rVB	2746	6048	2.87%	0.171%
13	6.647	383	387	395	rBV2	4675	13445	6.38%	0.381%
14	6.757	396	399	403	rBV	3172	5465	2.59%	0.155%
15	6.849	403	409	419	rVB3	7641	26691	12.67%	0.757%
16	6.988	420	424	426	rBV2	3499	8812	4.18%	0.250%
17	7.264	451	454	460	rVB2	6619	15278	7.25%	0.433%
18	7.642	490	495	499	rBV	50259	106916	50.75%	3.031%
19	7.707	499	502	506	rVB	5347	9677	4.59%	0.274%
20	7.864	515	519	527	rBV	15439	33127	15.73%	0.939%
21	8.030	535	537	543	rVB2	3194	6065	2.88%	0.172%
22	8.168	549	552	559	rBV	8889	19868	9.43%	0.563%
23	8.306	565	567	569	rVB2	12350	11223	5.33%	0.318%
24	8.442	574	578	581	rBV	21516	45087	21.40%	1.278%
25	8.784	602	605	606	rBV	24371	45150	21.43%	1.280%
26	8.822	606	608	616	rVB	19869	37620	17.86%	1.066%
27	9.177	633	636	643	rVB3	3059	9241	4.39%	0.262%
28	9.342	646	649	653	rBV	16210	28616	13.58%	0.811%
29	9.659	669	674	677	rBV	17584	36120	17.15%	1.024%
30	9.836	685	688	691	rBV2	2408	6851	3.25%	0.194%
31	9.912	691	694	697	rVV2	2676	8463	4.02%	0.240%
32	10.027	701	703	707	rVB	4205	8844	4.20%	0.251%
33	10.191	713	716	721	rBV2	12435	27168	12.90%	0.770%
34	10.407	729	733	735	rBV	105095	180013	85.45%	5.103%
35	10.457	735	737	739	rVV	12369	21712	10.31%	0.615%
36	10.521	739	742	744	rVB2	3360	7317	3.47%	0.207%

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Instrument : BNA_N
ClientSampleId : P287-DITCH

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	rVB2	9976	25067	11.90%	0.711%
38	11.180	791	794	796	rVV	6927	15274	7.25%	0.433%
39	11.231	796	798	803	rVV	17882	36533	17.34%	1.036%
40	11.345	803	807	810	rVB	45399	83795	39.78%	2.375%
41	12.003	921	931	937	rBV	45932	77933	37.00%	2.209%
42	12.234	967	983	991	rBV3	1425	4964	2.36%	0.141%
43	12.518	1043	1045	1047	rBV2	3965	8755	4.16%	0.248%
44	12.581	1047	1050	1054	rVV	15825	32742	15.54%	0.928%
45	12.657	1054	1056	1061	rVB	6102	14408	6.84%	0.408%
46	12.835	1068	1070	1072	rBV	3968	7391	3.51%	0.210%
47	12.886	1072	1074	1077	rVB	90933	147270	69.91%	4.174%
48	13.190	1094	1098	1102	rBV2	12860	25259	11.99%	0.716%
49	13.558	1124	1127	1132	rVB	11748	21384	10.15%	0.606%
50	13.850	1147	1150	1153	rVB	20362	30225	14.35%	0.857%
51	13.952	1155	1158	1160	rBV	4777	7062	3.35%	0.200%
52	14.269	1180	1183	1186	rVB	145100	210656	100.00%	5.971%
53	14.434	1193	1196	1200	rBV2	6902	11607	5.51%	0.329%
54	14.510	1200	1202	1204	rVV	14460	23074	10.95%	0.654%
55	14.561	1204	1206	1210	rVB	28341	43455	20.63%	1.232%
56	14.814	1222	1226	1228	rVB	13975	21664	10.28%	0.614%
57	14.878	1228	1231	1234	rVB3	4311	10516	4.99%	0.298%
58	14.992	1238	1240	1244	rBV2	10930	21880	10.39%	0.620%
59	15.093	1246	1248	1252	rVB	8746	14307	6.79%	0.406%
60	15.220	1255	1258	1260	rBV2	11579	18813	8.93%	0.533%
61	15.322	1264	1266	1270	rVB	10974	19743	9.37%	0.560%
62	15.487	1276	1279	1284	rBV4	12881	26970	12.80%	0.764%
63	15.639	1288	1291	1295	rVV3	7465	18163	8.62%	0.515%
64	15.766	1299	1301	1305	rVB2	15986	26877	12.76%	0.762%
65	15.956	1313	1316	1324	rVB	32277	75705	35.94%	2.146%
66	16.373	1346	1350	1353	rBV	105815	156570	74.32%	4.438%
67	16.835	1383	1388	1395	rBV	10364	22859	10.85%	0.648%
68	17.018	1400	1403	1406	rBV	113932	171539	81.43%	4.862%
69	17.164	1412	1415	1419	rVB3	7008	13835	6.57%	0.392%
70	17.310	1425	1427	1432	rVB2	4690	8773	4.16%	0.249%
71	17.407	1433	1435	1439	rVB3	4265	8374	3.98%	0.237%
72	17.955	1477	1480	1483	rBV	16353	30494	14.48%	0.864%
73	18.130	1502	1508	1517	rVB	17890	24964	11.85%	0.708%
74	18.462	1570	1575	1580	rBV	3687	5820	2.76%	0.165%
75	18.616	1602	1606	1611	rBV	6425	7859	3.73%	0.223%
76	19.063	1689	1696	1714	rBV	133789	189704	90.05%	5.377%

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Sample : M3986-01
Misc :
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Instrument : BNA_N
ClientSampleId : P287-DITCH

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	19.242	1727	1732	1750	rBV	17021	27498	13.05%	0.779%
78	19.460	1772	1776	1780	rVB	5872	7469	3.55%	0.212%
79	19.679	1813	1820	1831	rBV	125006	156467	74.28%	4.435%
80	19.927	1867	1870	1878	rVB	3142	4052	1.92%	0.115%
81	20.006	1885	1886	1888	rBV	11137	17188	8.16%	0.487%
82	20.059	1889	1891	1895	rVV2	6523	18745	8.90%	0.531%
83	20.973	1974	1977	1981	rBV	22851	41213	19.56%	1.168%
84	21.164	1993	1995	1998	rBV	36268	46816	22.22%	1.327%
85	21.227	1998	2001	2008	rVV	144547	207395	98.45%	5.879%
86	22.109	2081	2084	2087	rBV	8553	12852	6.10%	0.364%
87	23.481	2414	2426	2450	rVB	109602	210441	99.90%	5.965%
88	24.173	2620	2628	2646	rVB	5987	13377	6.35%	0.379%
89	25.761	3078	3092	3117	rVB4	2838	10651	5.06%	0.302%
90	25.983	3146	3157	3189	rVB	4539	14653	6.96%	0.415%
91	26.452	3282	3294	3312	rVB2	1839	5478	2.60%	0.155%
92	26.613	3328	3341	3361	rVB	942	2996	1.42%	0.085%

Sum of corrected areas: 3527907

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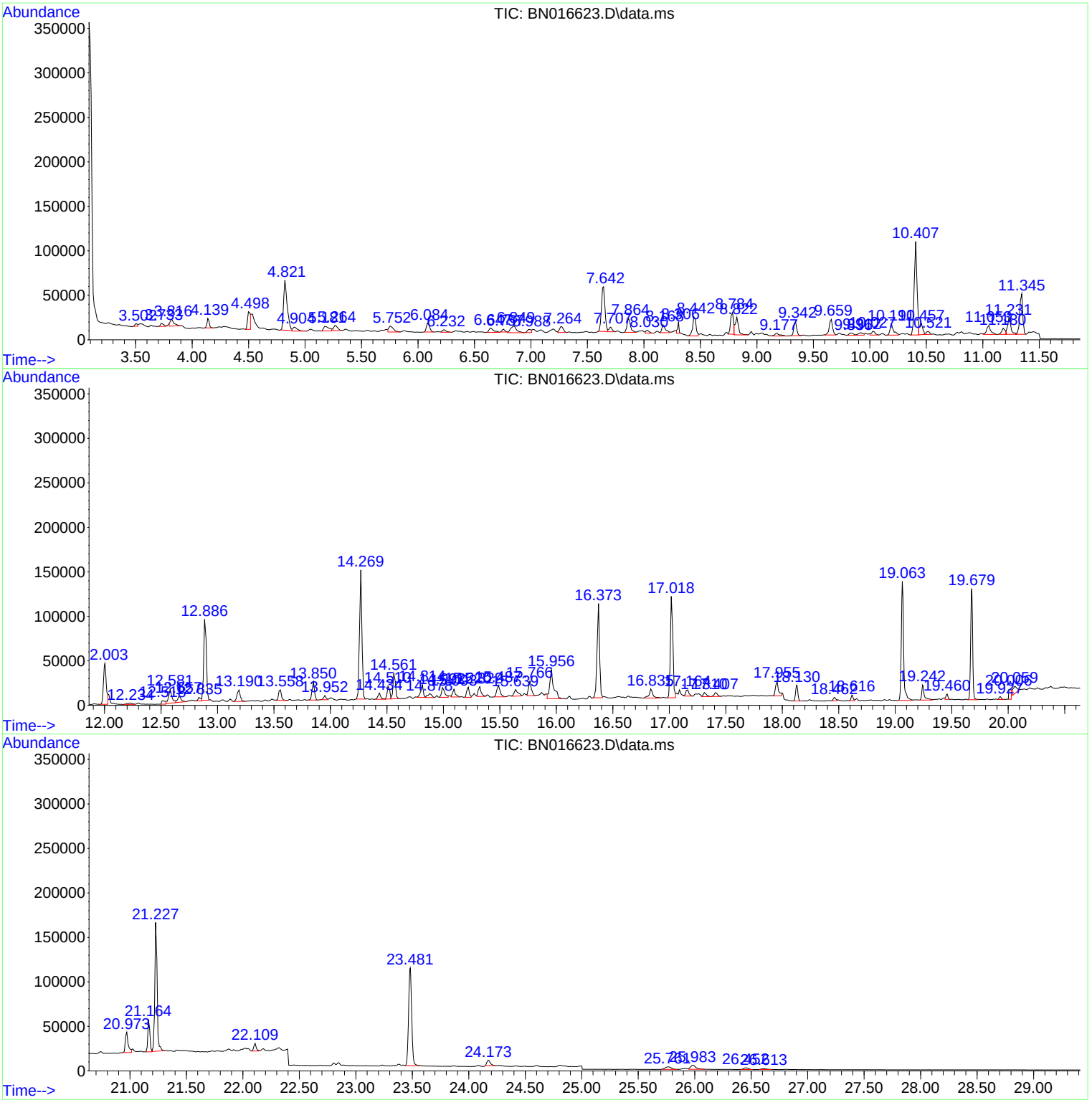
Instrument :
BNA_N
ClientSampleId :
P287-DITCH

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 : BN016623.D
Acq On : 01 Oct 2021 06:35
Operator : CG/JU
Sample : M3986-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_N
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P287-DITCH

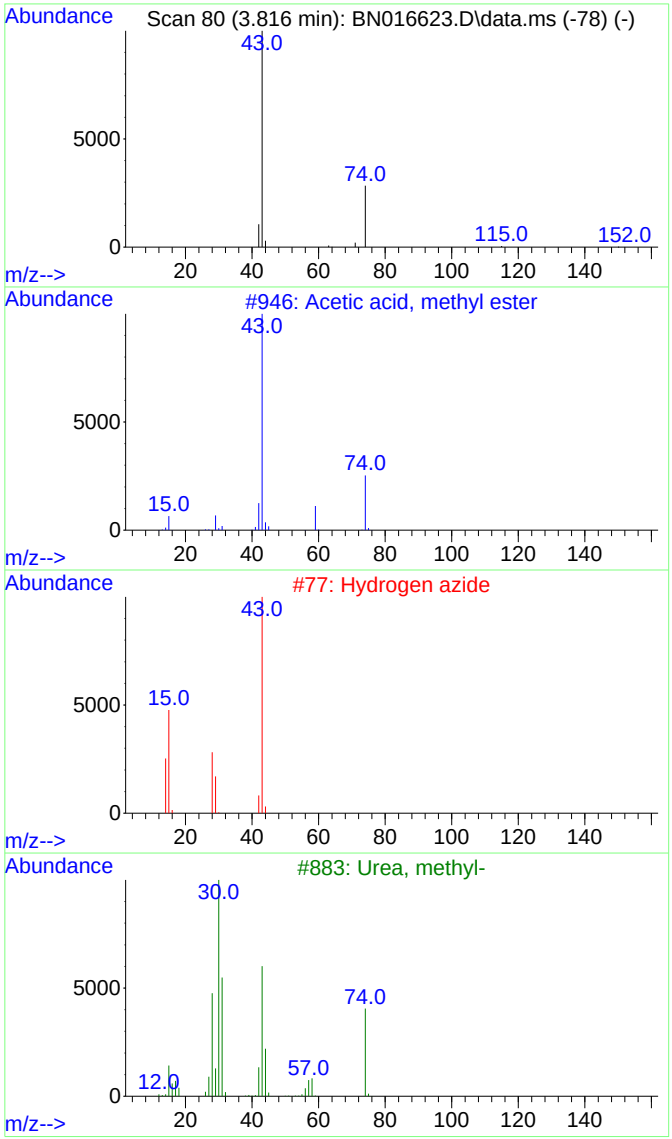
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

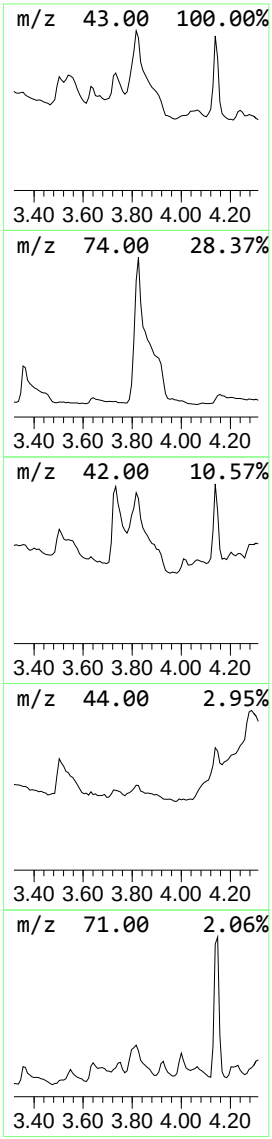
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Acetic acid, methyl ester Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.06 ng	17057	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, methyl ester	74	C3H6O2	000079-20-9	9
2	Hydrogen azide	43	HN3	007782-79-8	4
3	Urea, methyl-	74	C2H6N2O	000598-50-5	4
4	O-Methylisourea	74	C2H6N2O	002440-60-0	3
5	2-(3,3-Dimethyldiaziridin-1-yl)e...	115	C5H13N3	139223-40-8	3





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016623.D
Acq On : 01 Oct 2021 06:35
Operator : CG/JU
Sample : M3986-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : P287-DITCH

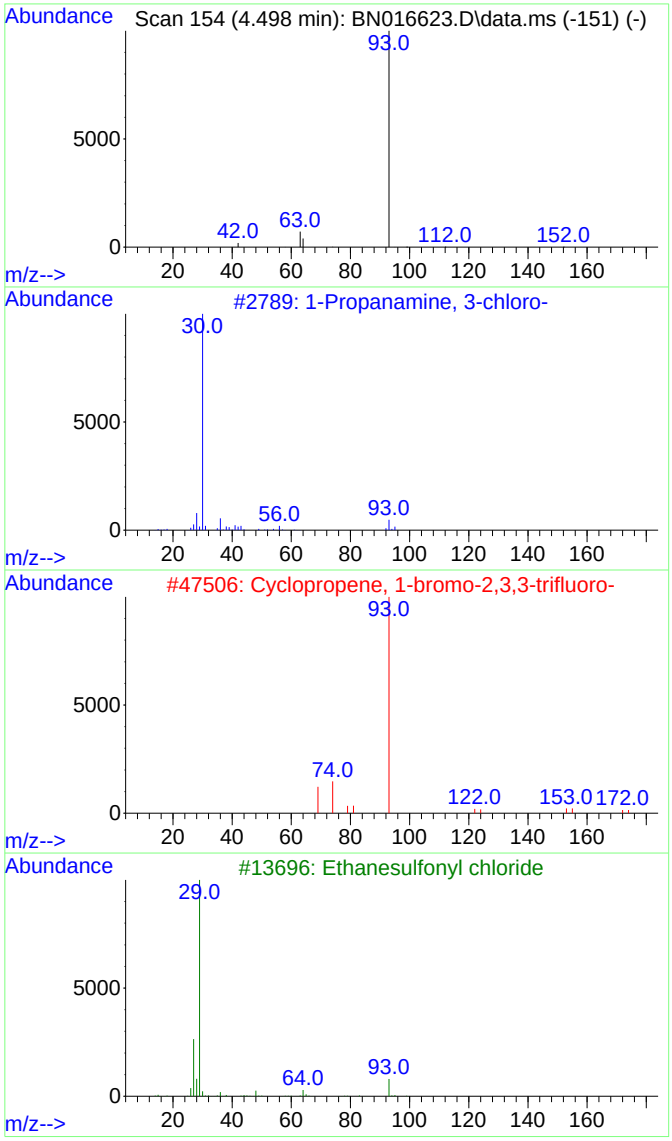
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

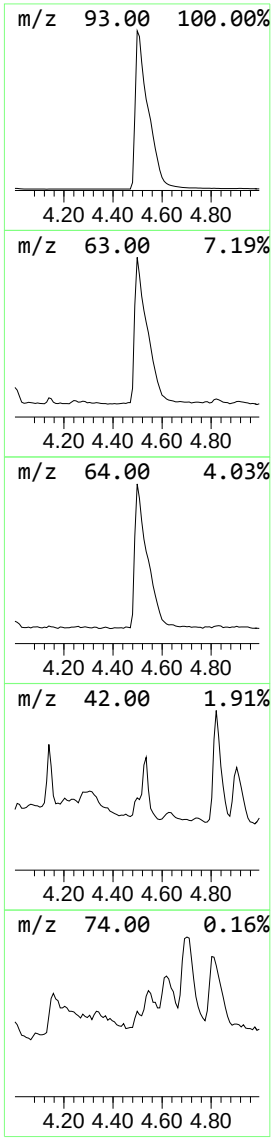
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-Propanamine, 3-chloro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.498	0.14 ng	36610	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





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Sample : M3986-01
Misc :
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Instrument :
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ClientSampleId :
P287-DITCH

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

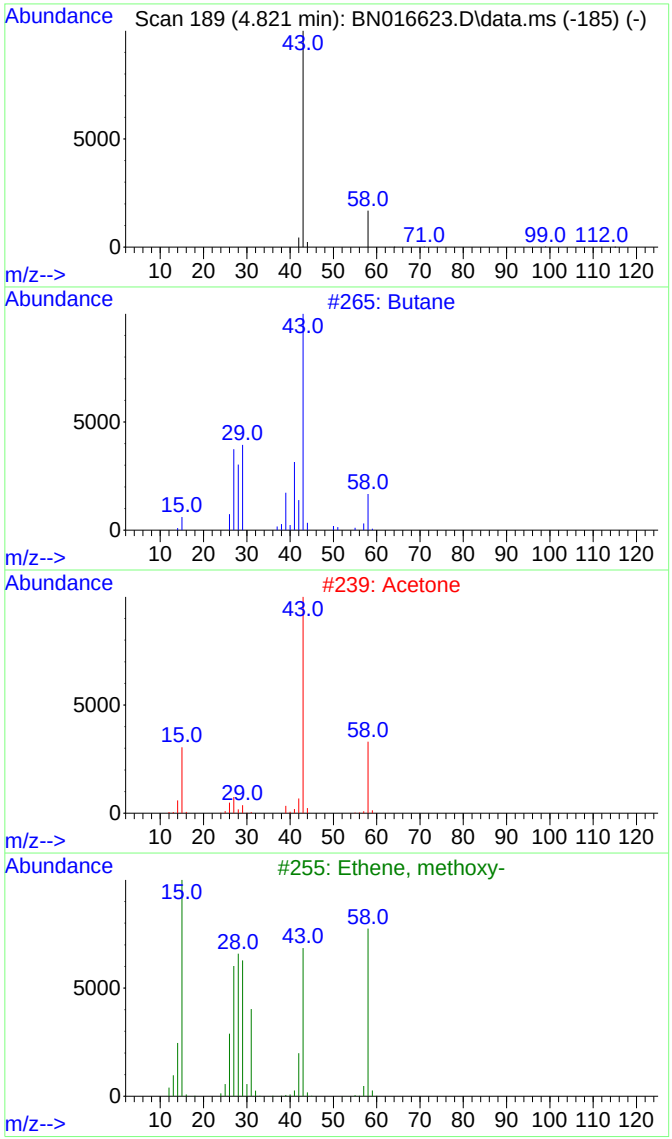
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

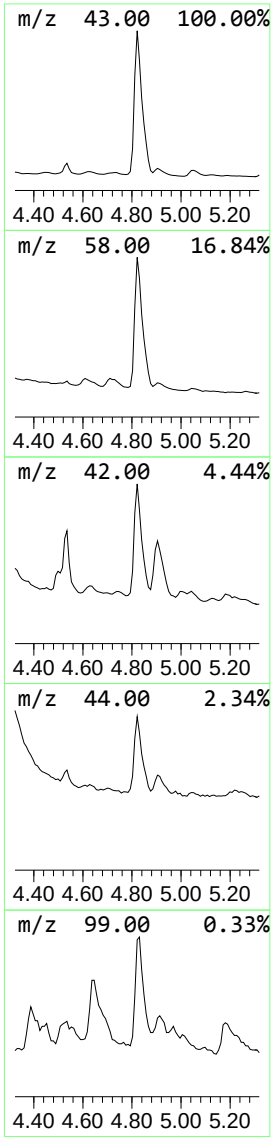
****

Peak Number 3 Butane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.46 ng	122627	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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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

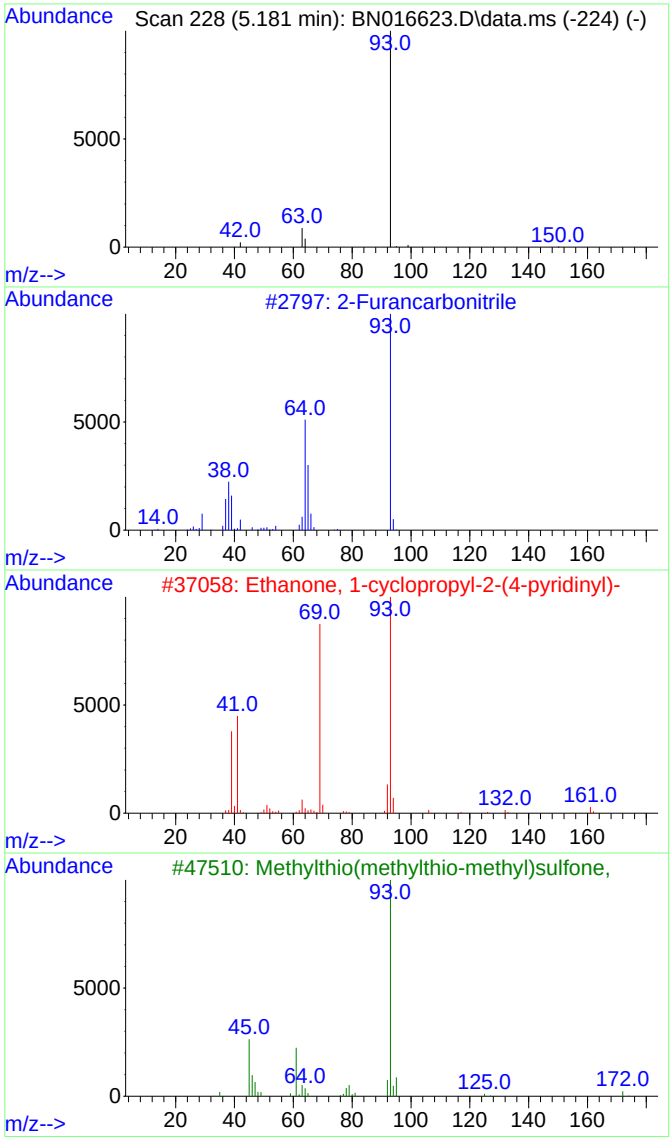
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

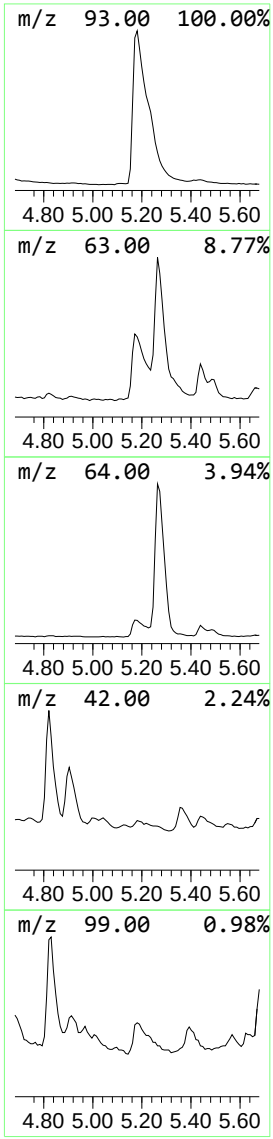
****

Peak Number 4 2-Furancarbonitrile Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.181	0.07 ng	17961	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Furancarbonitrile	93	C5H3NO	000617-90-3	3
2	Ethanone, 1-cyclopropyl-2-(4-pyr...	161	C10H11NO	006580-95-6	2
3	Methylthio(methylthio-methyl)sul...	172	C3H8O2S3	058000-45-6	1
4	2,3,5-trithiahexane 5-oxide	156	C3H8OS3	042474-27-1	1
5	Nortricyclyl bromide	172	C7H9Br	1000342-32-2	1





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BNA_N
ClientSampleId :
P287-DITCH

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

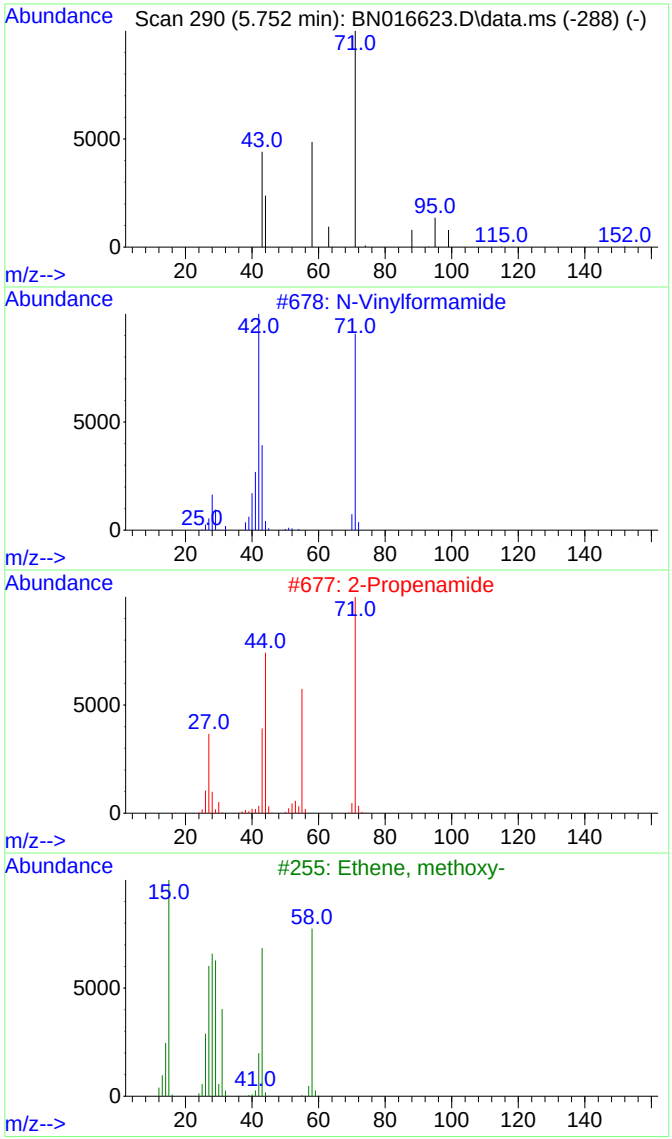
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

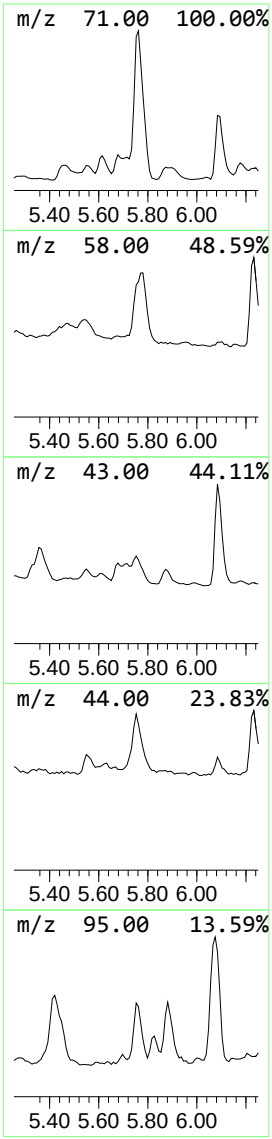
****

Peak Number 5 N-Vinylformamide Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.752	0.07 ng	18072	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-Vinylformamide	71	C3H5NO	013162-05-5	4
2	2-Propenamide	71	C3H5NO	000079-06-1	4
3	Ethene, methoxy-	58	C3H6O	000107-25-5	4
4	Propylene oxide	58	C3H6O	000075-56-9	3
5	Methoxyacetonitrile	71	C3H5NO	001738-36-9	3





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016623.D
Acq On : 01 Oct 2021 06:35
Operator : CG/JU
Sample : M3986-01
Misc :
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Instrument :
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P287-DITCH

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

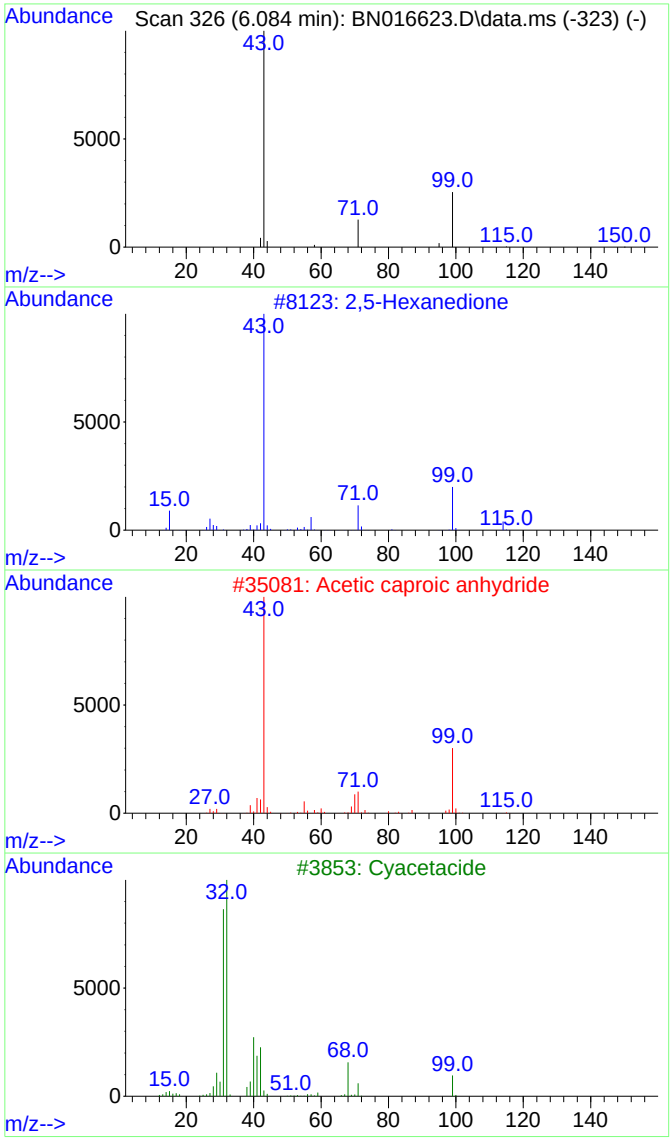
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

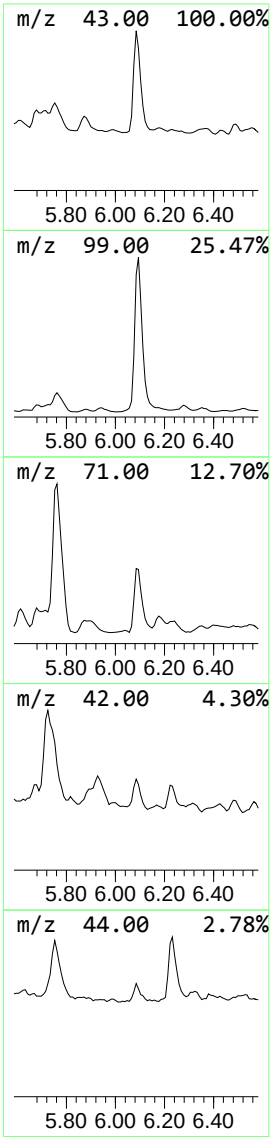
****

Peak Number 6 2,5-Hexanedione Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.084	0.07 ng	19665	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Hexanedione	114	C6H10O2	000110-13-4	9
2	Acetic caproic anhydride	158	C8H14O3	092351-84-3	9
3	Cyacetacide	99	C3H5N3O	000140-87-4	4
4	Pentanoic acid, 4-oxo-, methyl e...	130	C6H10O3	000624-45-3	4
5	2-Hexanone, 6-bromo-	178	C6H11BrO	010226-29-6	4





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Acq On : 01 Oct 2021 06:35
Operator : CG/JU
Sample : M3986-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : P287-DITCH

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

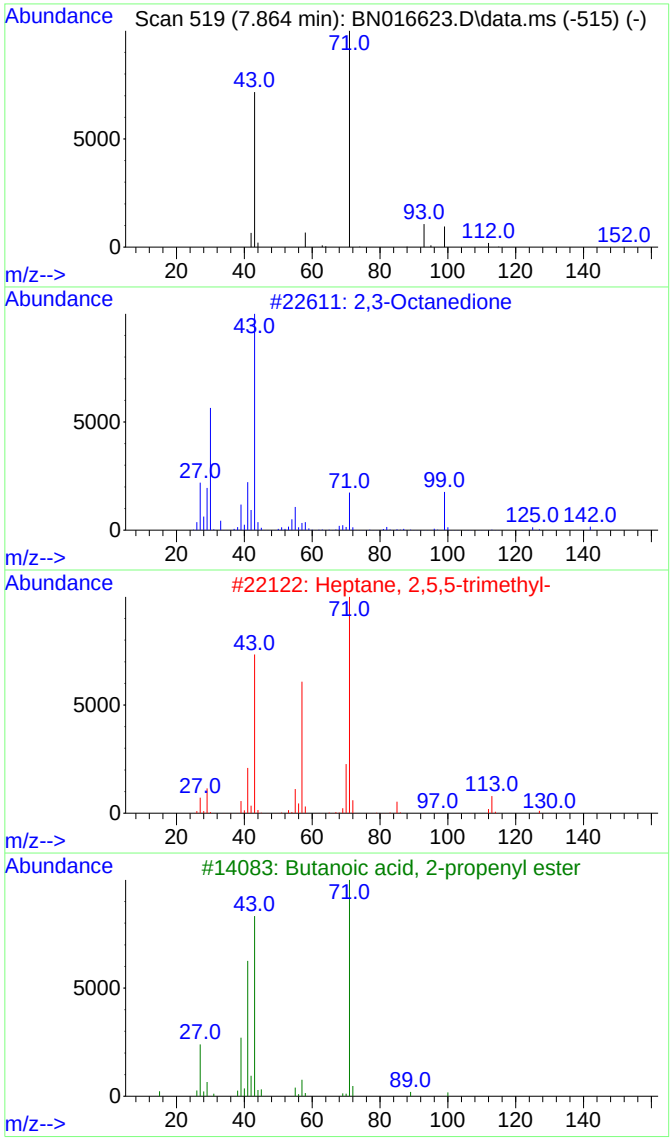
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

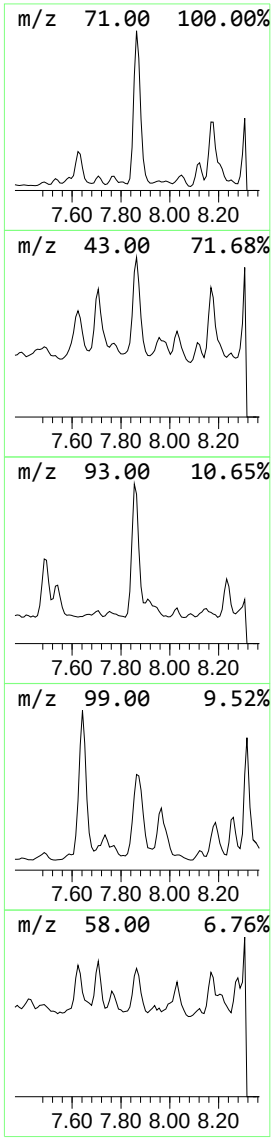
****

Peak Number 7 2,3-Octanedione Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.864	0.12 ng	33127	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Octanedione	142	C8H14O2	000585-25-1	4
2	Heptane, 2,5,5-trimethyl-	142	C10H22	001189-99-7	4
3	Butanoic acid, 2-propenyl ester	128	C7H12O2	002051-78-7	4
4	3-Penten-2-ol	86	C5H10O	001569-50-2	4
5	Pentane, 3-bromo-	150	C5H11Br	001809-10-5	4





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Sample : M3986-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
P287-DITCH

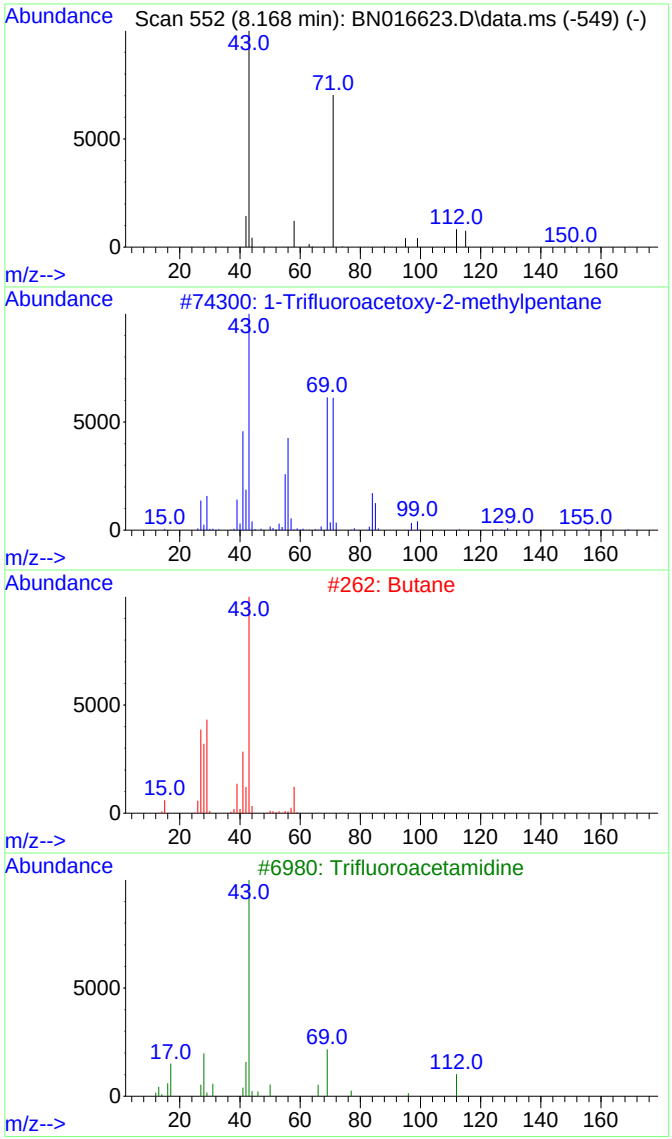
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

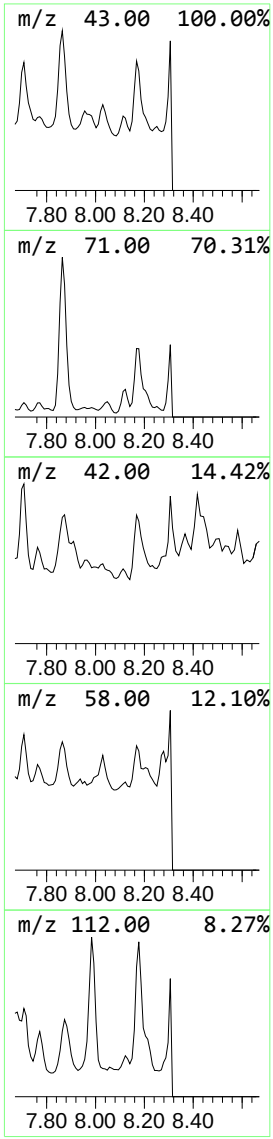
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1-Trifluoroacetoxy-2-methyl... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.168	0.07 ng	19868	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Trifluoroacetoxy-2-methylpentane	198	C8H13F3O2	155089-96-6	9
2	Butane	58	C4H10	000106-97-8	7
3	Trifluoroacetamidine	112	C2H3F3N2	000354-37-0	5
4	5-Amino-3,4-dimethyl-isoxazole	112	C5H8N2O	019947-75-2	5
5	Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	4





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ClientSampleId :
P287-DITCH

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

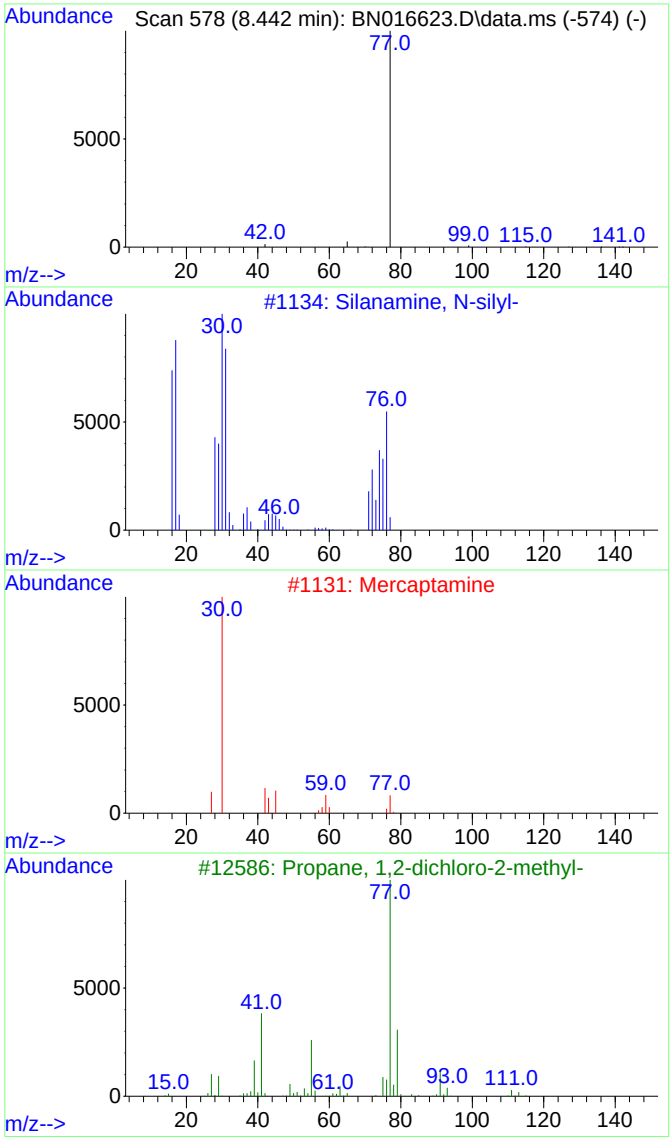
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

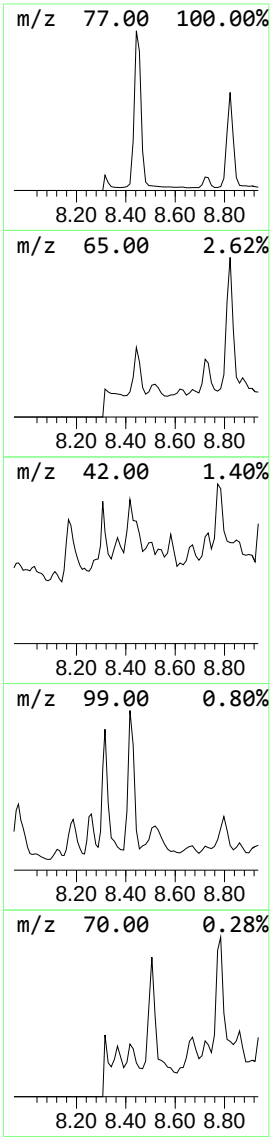
****

Peak Number 9 Silanamine, N-silyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.442	0.17 ng	45087	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	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	Propane, 1,2-dichloro-2-methyl-	126	C4H8Cl2	000594-37-6	1
4	Propane, 2,2-dichloro-	112	C3H6Cl2	000594-20-7	1
5	Silanamine, N-phenyl-	123	C6H9NSi	005578-85-8	1





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Operator : CG/JU
Sample : M3986-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : P287-DITCH

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

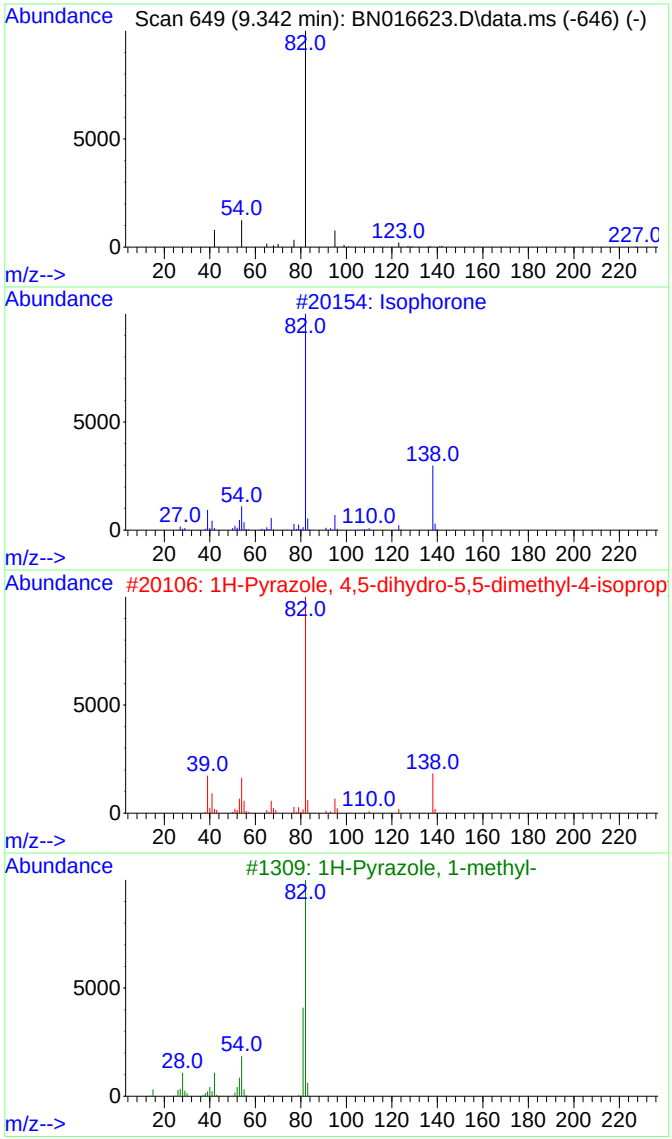
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

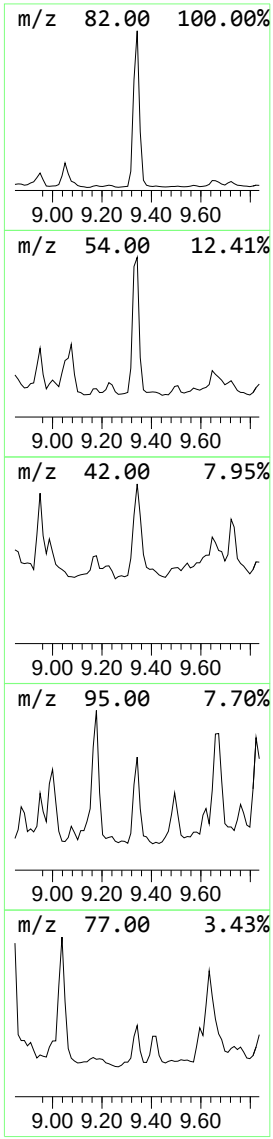
****

Peak Number 10 Isophorone Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.342	0.06 ng	28616	Naphthalene-d8	10.407

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isophorone	138	C9H14O	000078-59-1	40
2	1H-Pyrazole, 4,5-dihydro-5,5-dim...	138	C8H14N2	106251-09-6	9
3	1H-Pyrazole, 1-methyl-	82	C4H6N2	000930-36-9	7
4	3-Hepten-2-one, O-methyloxime	141	C8H15NO	056336-01-7	5
5	Fomepizole	82	C4H6N2	007554-65-6	5





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ALS Vial : 26 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P287-DITCH

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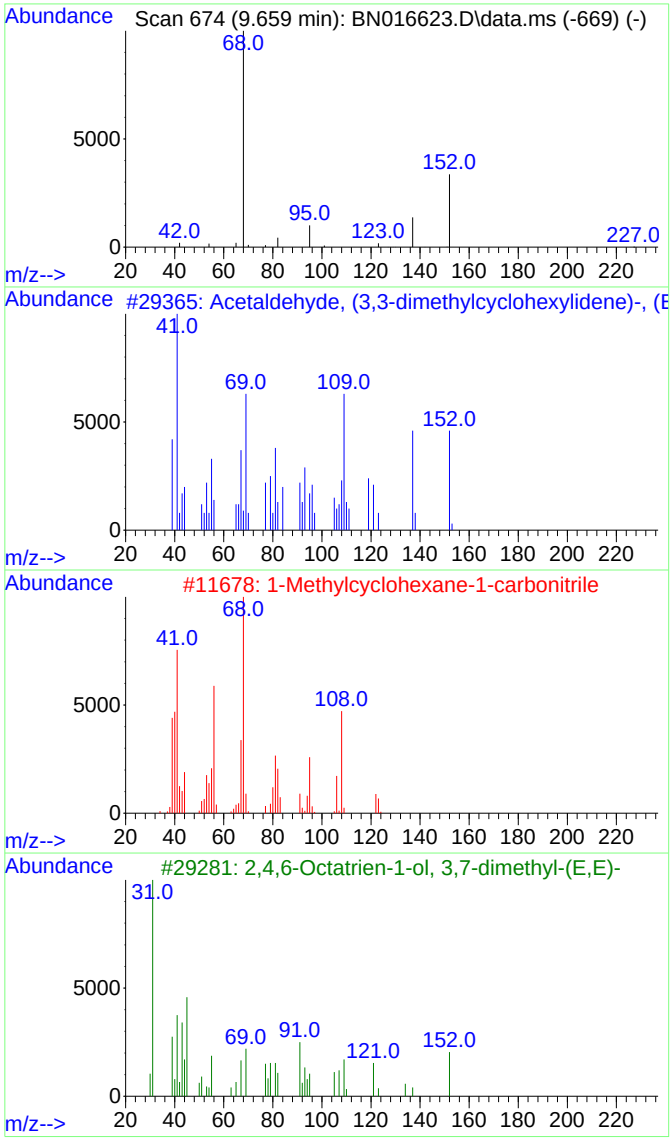
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

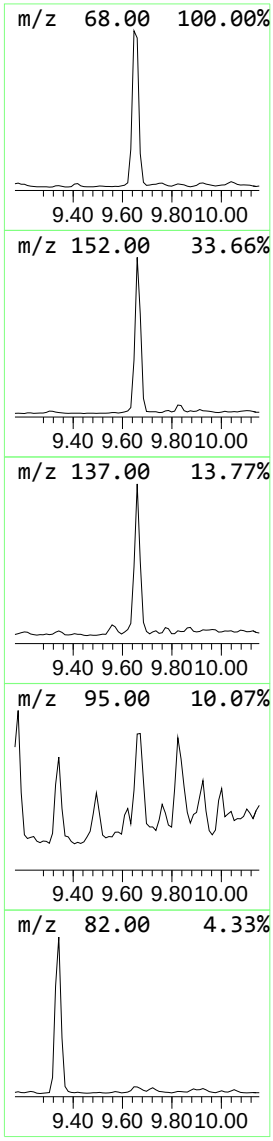
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Acetaldehyde, (3,3-dimethyl... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.659	0.08 ng	36120	Naphthalene-d8	10.407

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde, (3,3-dimethylcyclo...	152	C10H16O	026532-25-2	4
2	1-Methylcyclohexane-1-carbonitrile	123	C8H13N	062718-34-7	3
3	2,4,6-Octatrien-1-ol, 3,7-dimeth...	152	C10H16O	089155-85-1	3
4	1H-Imidazole	68	C3H4N2	000288-32-4	3
5	1,2-Propadiene-1,3-dione	68	C3O2	000504-64-3	3





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Misc :
ALS Vial : 26 Sample Multiplier: 1

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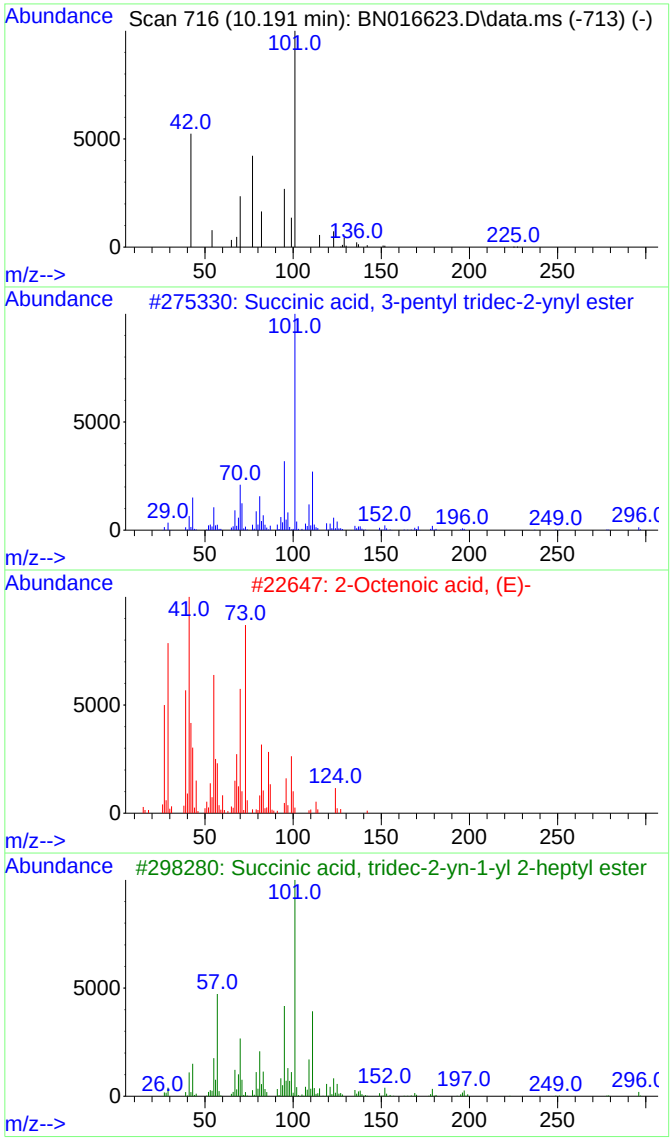
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

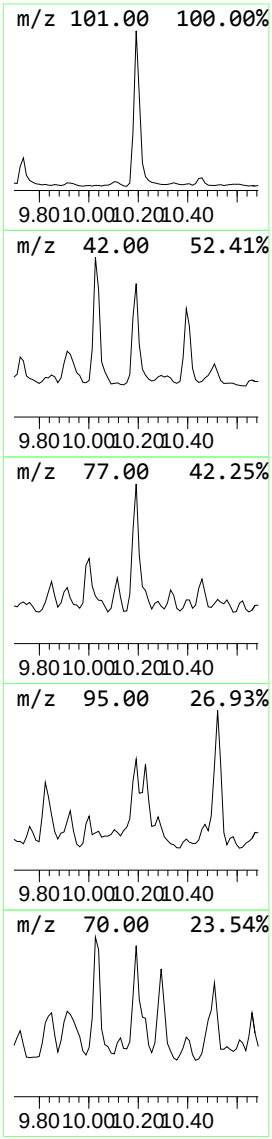
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Succinic acid, 3-pentyl tri... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.06 ng	27168	Naphthalene-d8	10.407

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Succinic acid, 3-pentyl tridec-2...	366	C22H38O4	1000370-92-5	25
2	2-Octenoic acid, (E)-	142	C8H14O2	001871-67-6	9
3	Succinic acid, tridec-2-yn-1-yl ...	394	C24H42O4	1000390-57-6	9
4	Succinic acid, tridec-2-yn-1-yl ...	380	C23H40O4	1000390-69-6	9
5	3-Methyl-1-pyrrolidino-1-aza-1,3...	138	C8H14N2	1000090-58-0	9





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Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : P287-DITCH

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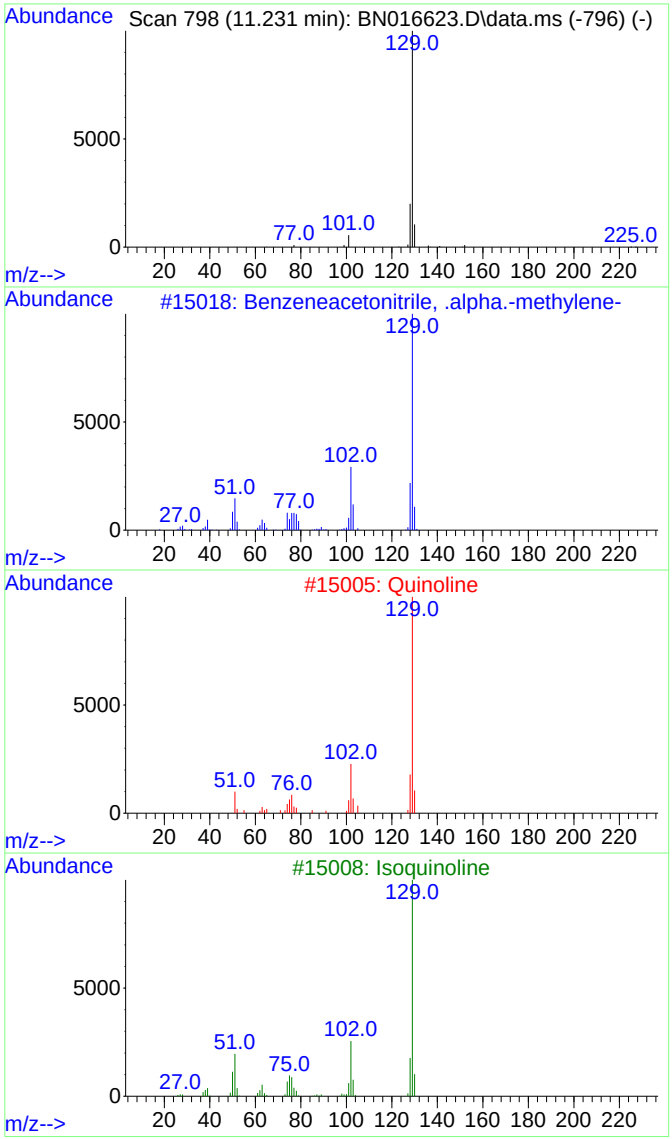
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

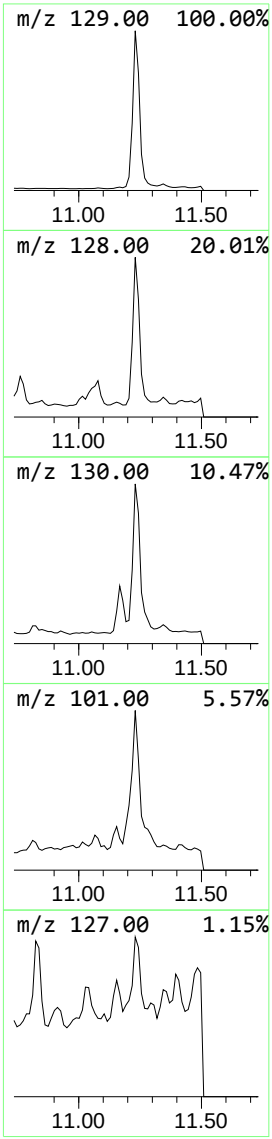
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Benzeneacetonitrile, .alpha... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.230	0.08 ng	36533	Naphthalene-d8	10.407

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneacetonitrile, .alpha.-met...	129	C9H7N	000495-10-3	78
2	Quinoline	129	C9H7N	000091-22-5	78
3	Isoquinoline	129	C9H7N	000119-65-3	78
4	2-Propenenitrile, 3-phenyl-, (E)-	129	C9H7N	001885-38-7	56
5	2H-Azepine-2-thione, hexahydro-	129	C6H11NS	007203-96-5	9





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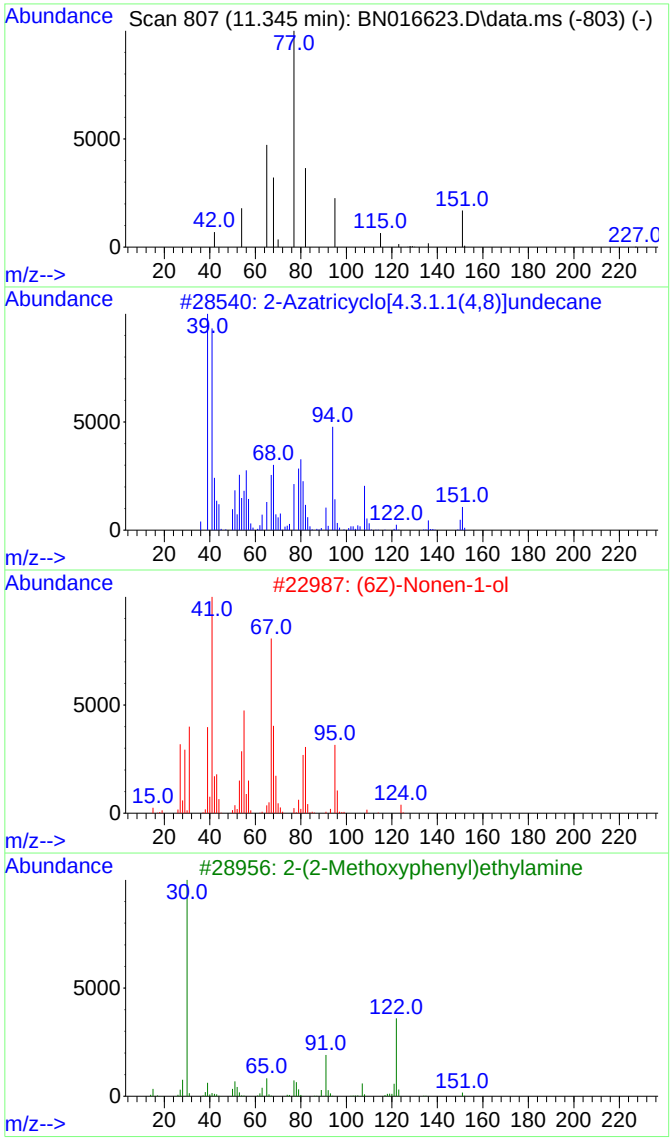
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

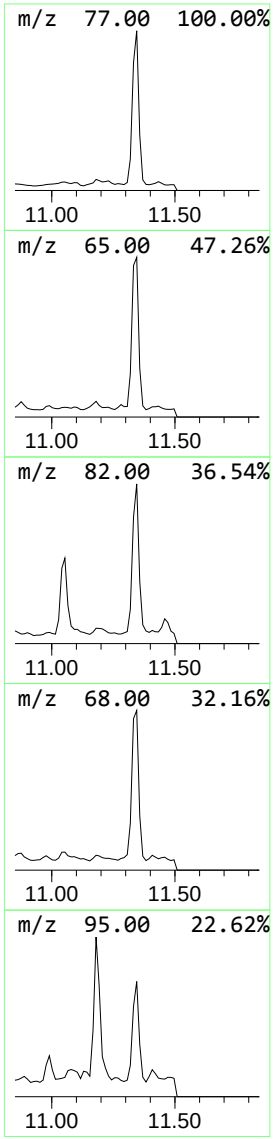
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 2-Azatricyclo[4.3.1.1(4,8)]... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.345	0.19 ng	83795	Naphthalene-d8	10.407

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Azatricyclo[4.3.1.1(4,8)]undecane	151	C10H17N	1010362-59-3	7
2	(6Z)-Nonen-1-ol	142	C9H18O	035854-86-5	4
3	2-(2-Methoxyphenyl)ethylamine	151	C9H13NO	002045-79-6	3
4	5-Hydroxy-1-phenyl-1H-1,2,3-tria...	280	C15H12N4O2	133346-51-7	2
5	N-(2-Benzyloxy-ethyl)-benzenesul...	291	C15H17NO3S	1000296-69-8	2





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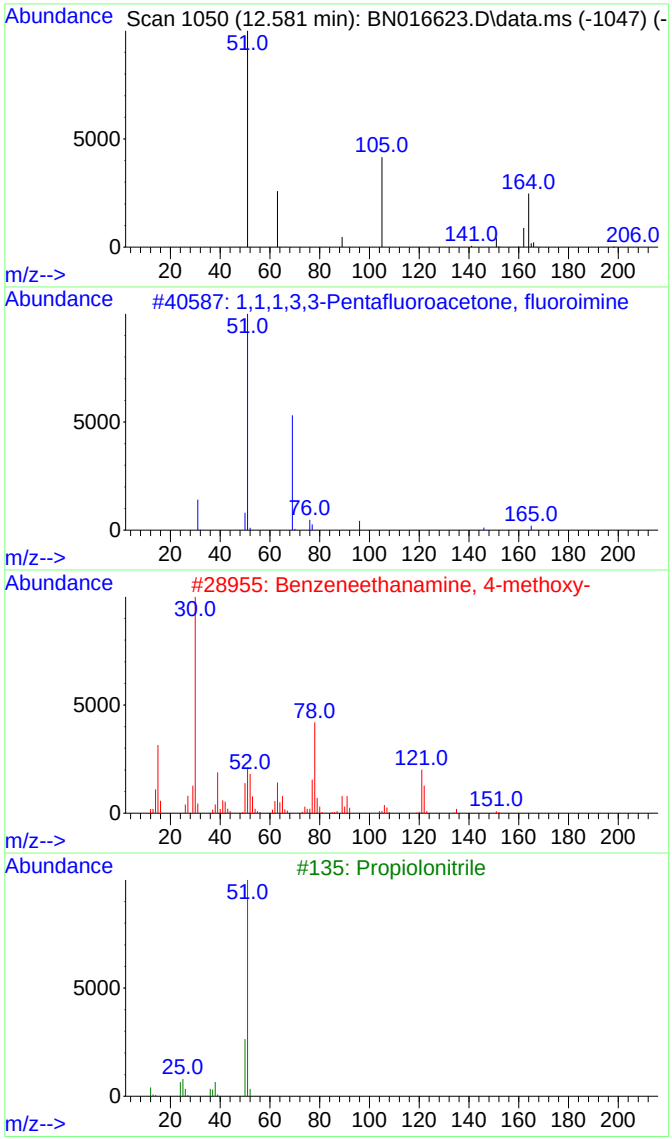
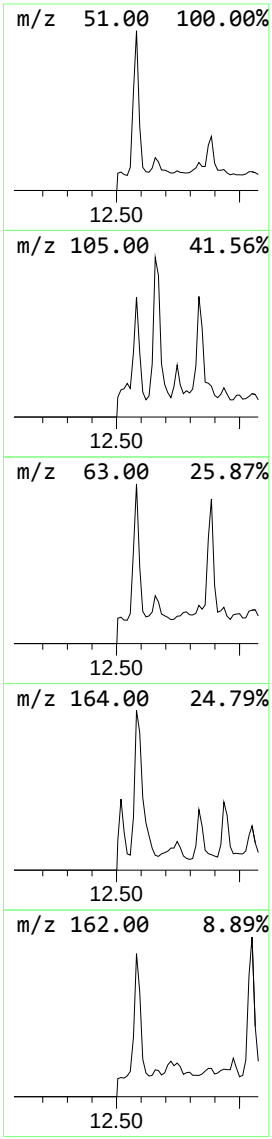
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 1,1,1,3,3-Pentafluoroaceton... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.581	0.06 ng	32742	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,1,3,3-Pentafluoroacetone, fl...	165	C3HF6N	1000284-28-6	4
2	Benzeneethanamine, 4-methoxy-	151	C9H13NO	000055-81-2	3
3	Propiolonitrile	51	C3HN	001070-71-9	3
4	Benzene, 1-azido-2-nitro-	164	C6H4N4O2	001516-58-1	2
5	2H-Pyran, 2-(2,5-hexadiynyloxy)t...	178	C11H14O2	040924-58-1	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
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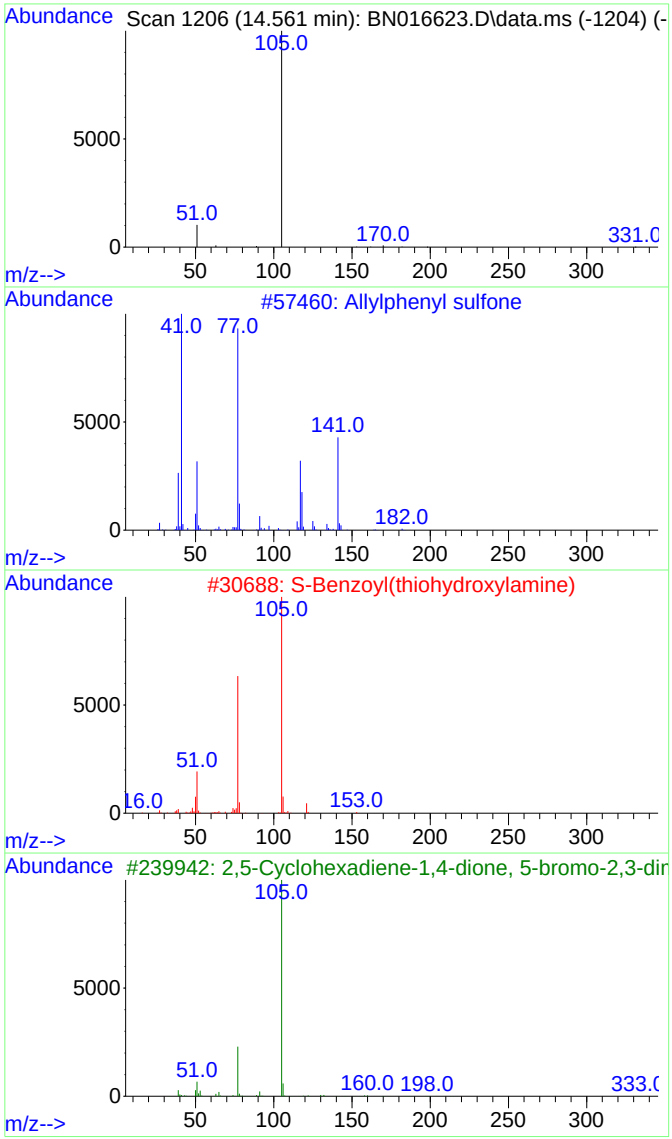
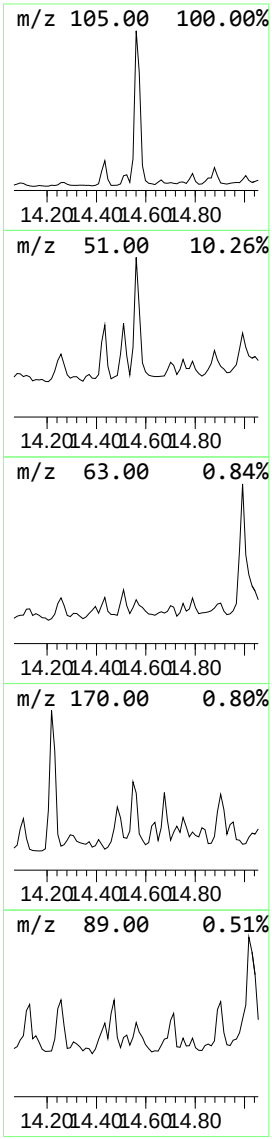
****

Peak Number 16 Allylphenyl sulfone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.561	0.08 ng	43455	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Allylphenyl sulfone	182	C9H10O2S	016212-05-8	2
2	S-Benzoyl(thiohydroxylamine)	153	C7H7NOS	025740-80-1	2
3	2,5-Cyclohexadiene-1,4-dione, 5-...	333	C15H12BrNO3	296243-33-9	2
4	2-Chloro-1-phenyl-1-propanone	168	C9H9ClO	006084-17-9	2
5	2,2-Bis[4-(benzoyloxy)phenyl]pro...	436	C29H24O4	002297-14-5	2





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P287-DITCH

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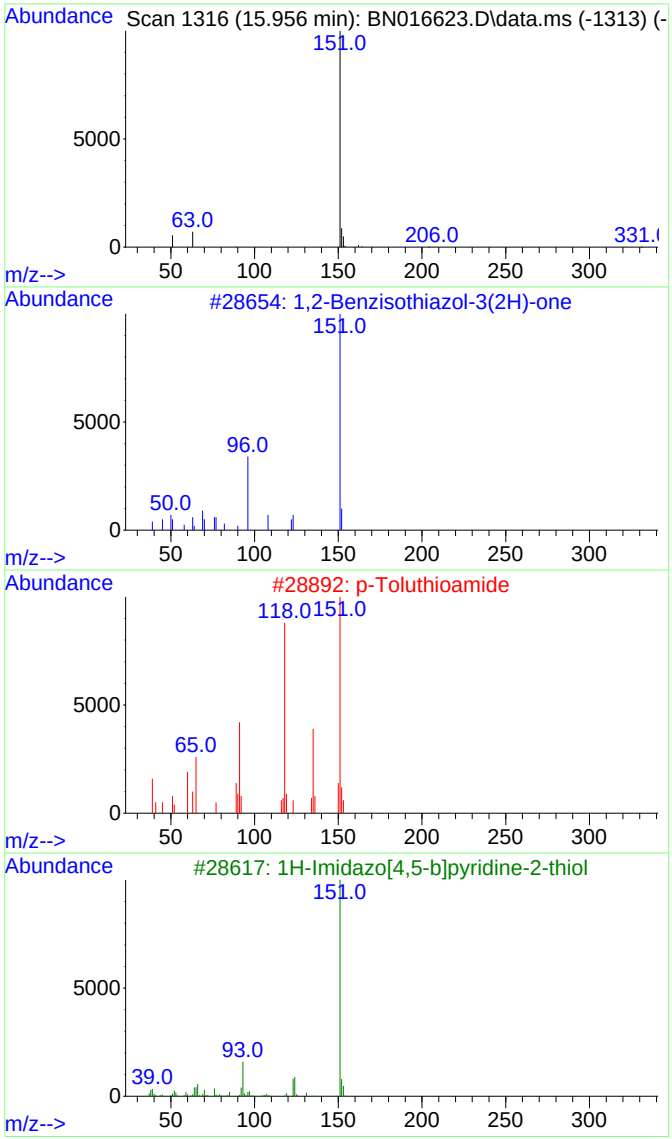
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

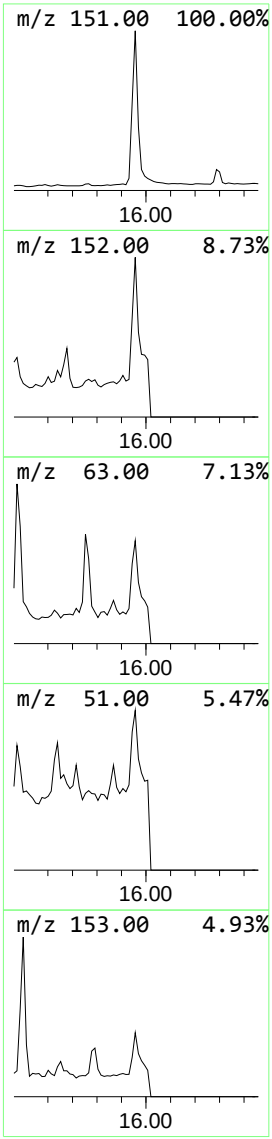
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 1,2-Benzisothiazol-3(2H)-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.956	0.18 ng	75705	Phenanthrene-d10	17.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	9
2	p-Toluthioamide	151	C8H9NS	002362-62-1	7
3	1H-Imidazo[4,5-b]pyridine-2-thiol	151	C6H5N3S	029448-81-5	7
4	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	7
5	2H-1,4-Benzothiazine, 3,4-dihydro-	151	C8H9NS	003080-99-7	7





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016623.D
Acq On : 01 Oct 2021 06:35
Operator : CG/JU
Sample : M3986-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
P287-DITCH

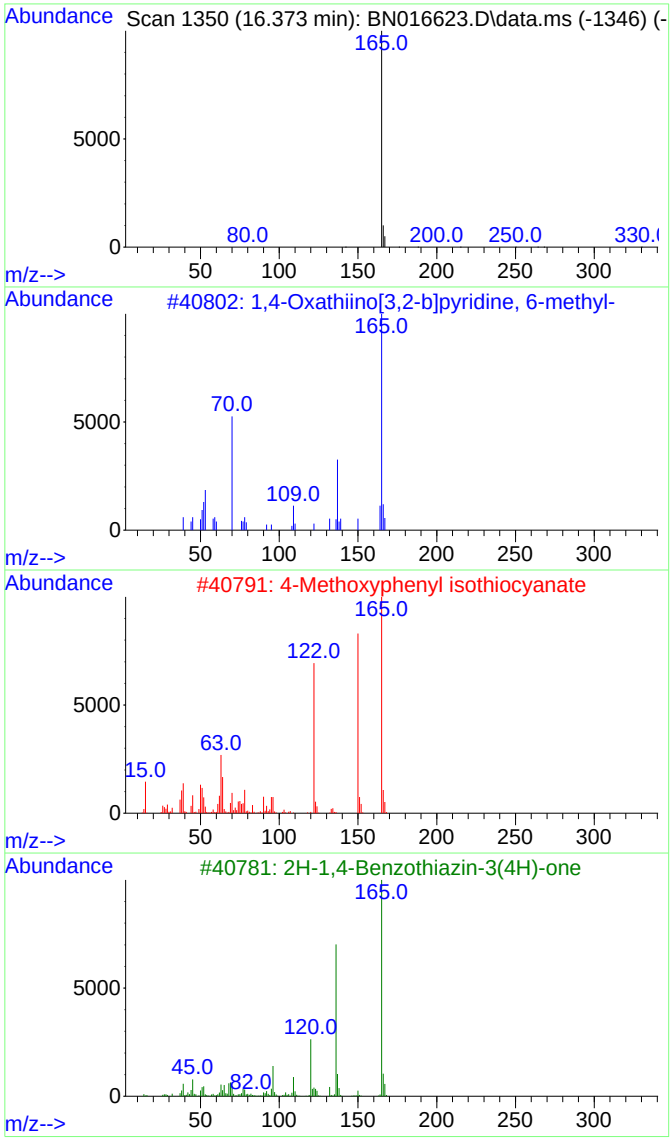
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

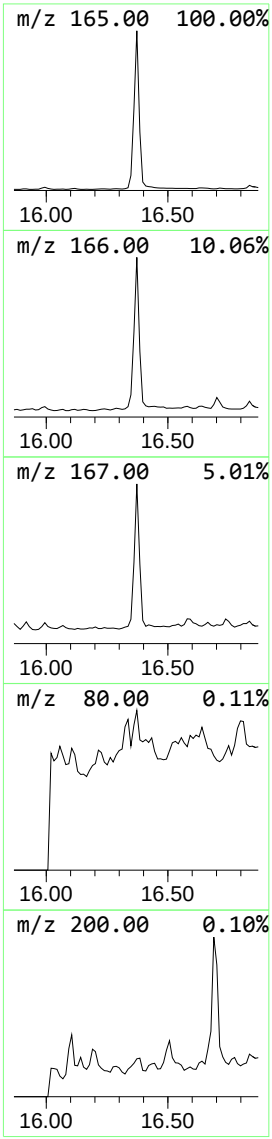
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 1,4-Oxathiino[3,2-b]pyridin... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.373	0.37 ng	156570	Phenanthrene-d10	17.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Oxathiino[3,2-b]pyridine, 6-...	165	C8H7NOS	056114-39-7	7
2	4-Methoxyphenyl isothiocyanate	165	C8H7NOS	002284-20-0	7
3	2H-1,4-Benzothiazin-3(4H)-one	165	C8H7NOS	005325-20-2	7
4	4-(2-Thienyl)-1H-pyrazol-5-amine	165	C7H7N3S	091447-40-4	7
5	s-Triazolo[4,3-a]pyridine-3-thio...	165	C7H7N3S	005528-58-5	7





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016623.D
Acq On : 01 Oct 2021 06:35
Operator : CG/JU
Sample : M3986-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
P287-DITCH

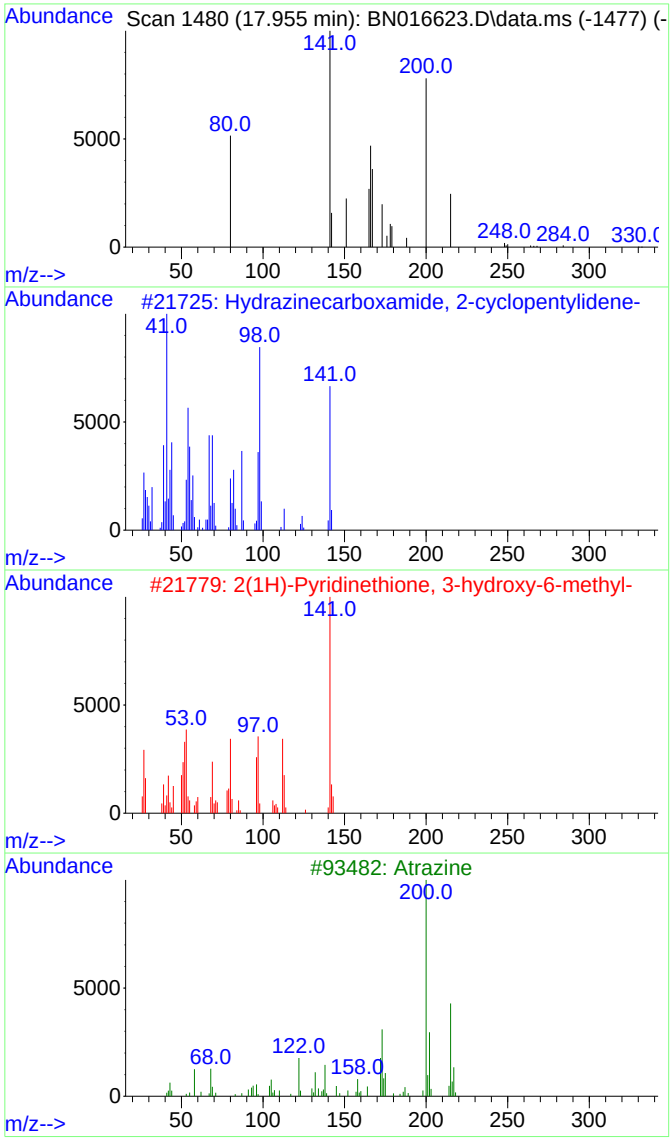
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

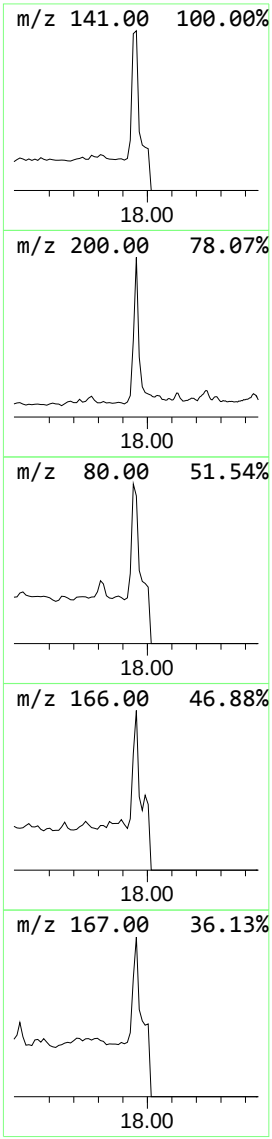
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 Hydrazinecarboxamide, 2-cyc... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.955	0.07 ng	30494	Phenanthrene-d10	17.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrazinecarboxamide, 2-cyclopen...	141	C6H11N3O	005459-00-7	9
2	2(1H)-Pyridinethione, 3-hydroxy-...	141	C6H7NOS	022989-67-9	9
3	Atrazine	215	C8H14ClN5	001912-24-9	9
4	2-Chloro-1-(1H-pyrrol-2-yl)ethan...	215	C9H14ClNOSi	1000485-05-7	9
5	Isothiocyanic acid, hexamethylen...	200	C8H12N2S2	005586-70-9	7





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016623.D
Acq On : 01 Oct 2021 06:35
Operator : CG/JU
Sample : M3986-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
P287-DITCH

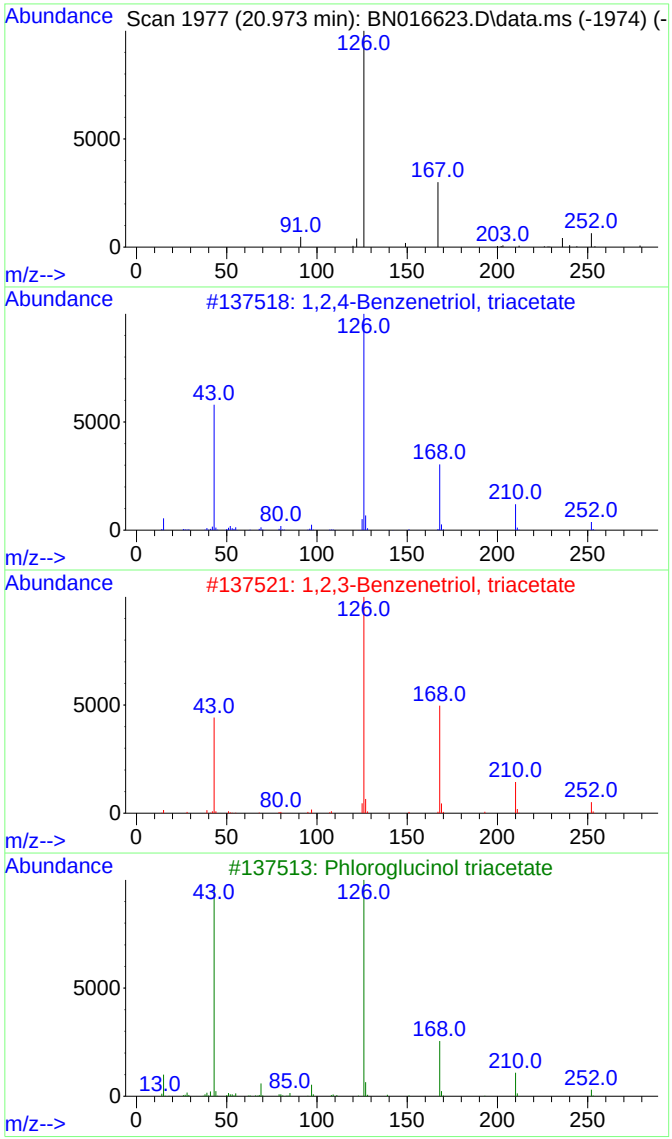
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

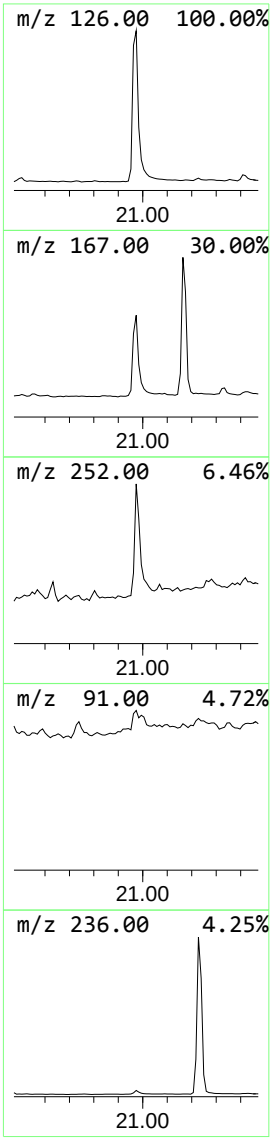
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 1,2,4-Benzenetriol, triacetate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.973	0.08 ng	41213	Chrysene-d12	21.227

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	Phloroglucinol triacetate	252	C12H12O6	002999-40-8	4
4	(6S,12aR,E)-2,2-Dimethyltetrahyd...	236	C14H24N2O	155975-43-2	4
5	N-[[6-Cyclooctylaminohexyl]aziri...	252	C16H32N2	1010256-12-1	4





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016623.D
Acq On : 01 Oct 2021 06:35
Operator : CG/JU
Sample : M3986-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : P287-DITCH

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
Acetic acid, me...	3.816	0.1	ng	17057	1	7.642	106916	0.4
1-Propanamine, ...	4.498	0.1	ng	36610	1	7.642	106916	0.4
Butane	4.821	0.5	ng	122627	1	7.642	106916	0.4
2-Furancarbonit...	5.181	0.1	ng	17961	1	7.642	106916	0.4
N-Vinylformamide	5.752	0.1	ng	18072	1	7.642	106916	0.4
2,5-Hexanedione	6.084	0.1	ng	19665	1	7.642	106916	0.4
2,3-Octanedione	7.864	0.1	ng	33127	1	7.642	106916	0.4
1-Trifluoroacet...	8.168	0.1	ng	19868	1	7.642	106916	0.4
Silanamine, N-s...	8.442	0.2	ng	45087	1	7.642	106916	0.4
Isophorone	9.342	0.1	ng	28616	2	10.407	180013	0.4
Acetaldehyde, (...	9.659	0.1	ng	36120	2	10.407	180013	0.4
Succinic acid, ...	10.191	0.1	ng	27168	2	10.407	180013	0.4
Benzeneacetonit...	11.230	0.1	ng	36533	2	10.407	180013	0.4
2-Azatricyclo[4...	11.345	0.2	ng	83795	2	10.407	180013	0.4
1,1,1,3,3-Penta...	12.581	0.1	ng	32742	3	14.269	210656	0.4
Allylphenyl sul...	14.561	0.1	ng	43455	3	14.269	210656	0.4
1,2-Benzisothia...	15.956	0.2	ng	75705	4	17.018	171539	0.4
1,4-Oxathiino[3...	16.373	0.4	ng	156570	4	17.018	171539	0.4
Hydrazinecarbox...	17.955	0.1	ng	30494	4	17.018	171539	0.4
1,2,4-Benzenetr...	20.973	0.1	ng	41213	5	21.227	207395	0.4