LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016683.D
Acq On : 02 Oct 2021 22:33
Operator : CG/JU
Sample : M3892-12
Misc :
ALS Vial : 51 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : S-825-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: BN016683.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.512	44	47	49	rBV	6221	13610	4.94%	0.236%
2	3.816	77	80	97	rVB	6526	26267	9.54%	0.456%
3	4.277	128	130	146	rVB	6028	22232	8.07%	0.386%
4	4.821	185	189	200	rVB	36546	79602	28.91%	1.381%
5	5.042	210	213	220	rBV	4326	11510	4.18%	0.200%
6	5.273	234	238	247	rVB	17029	40087	14.56%	0.695%
7	6.333	349	353	361	rVB	6460	17087	6.21%	0.296%
8	6.536	371	375	381	rVB	4676	8695	3.16%	0.151%
9	6.831	403	407	418	rVB	18209	44119	16.02%	0.765%
10	7.080	430	434	441	rVB	5056	13380	4.86%	0.232%
11	7.264	450	454	459	rVB3	4044	9748	3.54%	0.169%
12	7.642	490	495	500	rBV	49665	102321	37.16%	1.775%
13	7.938	523	527	533	rVB	21314	39321	14.28%	0.682%
14	8.784	601	605	610	rVV	22738	46319	16.82%	0.803%
15	9.684	668	676	679	rBV	62604	163942	59.54%	2.843%
16	9.735	679	680	685	rVV	4143	10674	3.88%	0.185%
17	10.191	713	716	723	rBV	51705	99678	36.20%	1.729%
18	10.407	729	733	736	rBV	105707	184224	66.91%	3.195%
19	10.508	739	741	748	rVB3	4982	8941	3.25%	0.155%
20	11.091	784	787	790	rVB2	6525	12065	4.38%	0.209%
21	12.003	922	931	941	rBV	40687	66080	24.00%	1.146%
22	12.632	1050	1054	1057	rBV	112830	196704	71.44%	3.412%
23	12.886	1071	1074	1077	rBV	78035	126029	45.77%	2.186%
24	13.000	1080	1083	1089	rVB	32281	85687	31.12%	1.486%
25	13.152	1089	1095	1096	rBV	82530	147990	53.75%	2.567%
26	13.190	1096	1098	1102	rVB	32907	58653	21.30%	1.017%
27	13.584	1127	1129	1132	rVV	106124	173791	63.12%	3.014%
28	13.672	1134	1136	1139	rVV	67126	115948	42.11%	2.011%
29	13.749	1139	1142	1145	rVV	13300	22496	8.17%	0.390%
30	13.888	1150	1153	1158	rVB	6259	11566	4.20%	0.201%
31	13.990	1158	1161	1163	rBV	6193	11439	4.15%	0.198%
32	14.117	1167	1171	1174	rBV2	64058	130276	47.31%	2.259%
33	14.167	1174	1175	1179	rVV	17443	20740	7.53%	0.360%
34	14.269	1180	1183	1186	rVV	140998	211908	76.96%	3.675%
35	14.345	1186	1189	1194	rVV2	123758	197741	71.82%	3.430%
36	14.434	1194	1196	1200	rVB	8009	12181	4.42%	0.211%

LSC Area Percent Report

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Operator : CG/JU
Sample : M3892-12
Misc :
ALS Vial : 51 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : S-825-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

37	14.535	1200	1204	1207	rBV2	88350	154017	55.94%	2.671%
38	14.599	1207	1209	1213	rVV2	55139	90129	32.73%	1.563%
39	14.700	1213	1217	1219	rVV2	30887	59153	21.48%	1.026%
40	14.738	1219	1220	1223	rVV	14569	19630	7.13%	0.340%
41	14.814	1223	1226	1229	rVV	34688	62367	22.65%	1.082%
42	14.878	1229	1231	1234	rVV	3925	8616	3.13%	0.149%
43	14.954	1234	1237	1239	rVV	3836	8555	3.11%	0.148%
44	15.005	1239	1241	1244	rVV	26606	38077	13.83%	0.660%
45	15.144	1250	1252	1256	rVV2	3956	9566	3.47%	0.166%
46	15.220	1256	1258	1260	rVV	5914	12055	4.38%	0.209%
47	15.271	1260	1262	1264	rVV	70315	97172	35.29%	1.685%
48	15.309	1264	1265	1271	rVV2	4574	13762	5.00%	0.239%
49	15.411	1271	1273	1276	rVV	5255	14147	5.14%	0.245%
50	15.474	1276	1278	1280	rVV	10157	19424	7.05%	0.337%
51	15.512	1280	1281	1287	rVV	5305	13946	5.06%	0.242%
52	15.626	1287	1290	1295	rVV3	13123	45629	16.57%	0.791%
53	15.753	1295	1300	1304	rVV2	50189	136814	49.69%	2.373%
54	15.855	1305	1308	1312	rVV2	18853	69648	25.29%	1.208%
55	15.931	1312	1314	1317	rVV3	13184	32738	11.89%	0.568%
56	16.007	1317	1320	1322	rVV	145193	192249	69.82%	3.334%
57	16.239	1337	1339	1345	rVB4	5798	17219	6.25%	0.299%
58	16.835	1384	1388	1392	rBV2	5119	10561	3.84%	0.183%
59	16.969	1394	1399	1400	rBV2	3063	8612	3.13%	0.149%
60	17.018	1400	1403	1405	rVV	122099	181328	65.86%	3.145%
61	17.066	1405	1407	1410	rVV	15660	27795	10.09%	0.482%
62	17.139	1410	1413	1418	rVV2	13098	29123	10.58%	0.505%
63	17.249	1418	1422	1425	rVV	9726	25682	9.33%	0.445%
64	17.310	1425	1427	1432	rVV2	4924	12127	4.40%	0.210%
65	17.821	1465	1469	1476	rVV	6962	35621	12.94%	0.618%
66	17.943	1476	1479	1491	rVB2	14767	38171	13.86%	0.662%
67	18.964	1671	1676	1681	rBV	8942	10112	3.67%	0.175%
68	19.063	1689	1696	1699	rBV	84289	113072	41.07%	1.961%
69	19.093	1699	1702	1714	rVV	60867	90293	32.79%	1.566%
70	19.177	1714	1719	1727	rVV	14065	18254	6.63%	0.317%
71	19.242	1727	1732	1744	rVV2	9228	13154	4.78%	0.228%
72	19.455	1767	1775	1796	rVB	48169	69470	25.23%	1.205%
73	19.679	1814	1820	1833	rVB	65887	84922	30.84%	1.473%
74	20.006	1885	1886	1889	rBV	7333	11789	4.28%	0.204%
75	20.335	1914	1917	1919	rBV	11236	15035	5.46%	0.261%
76	20.378	1919	1921	1925	rVB	7622	10919	3.97%	0.189%

LSC Area Percent Report

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Acq On : 02 Oct 2021 22:33
Operator : CG/JU
Sample : M3892-12
Misc :
ALS Vial : 51 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : S-825-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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Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
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77	20.633	1943	1945	1948	rBV	12749	17130	6.22%	0.297%
78	20.792	1958	1960	1963	rBV	16821	20019	7.27%	0.347%
79	20.973	1974	1977	1989	rVB	37465	76973	27.96%	1.335%
80	21.164	1993	1995	1998	rVV	28330	39939	14.51%	0.693%
81	21.227	1998	2001	2003	rVV2	171817	275344	100.00%	4.776%
82	21.270	2003	2005	2009	rVV	42144	59866	21.74%	1.038%
83	21.589	2033	2035	2039	rBV3	6071	10188	3.70%	0.177%
84	21.875	2057	2062	2071	rVV	38310	93100	33.81%	1.615%
85	22.024	2074	2076	2081	rVV5	4688	14011	5.09%	0.243%
86	22.109	2081	2084	2089	rVB2	9837	16113	5.85%	0.279%
87	22.321	2100	2104	2107	rBV2	7330	13820	5.02%	0.240%
88	22.557	2149	2156	2176	rVB2	10068	14499	5.27%	0.251%
89	22.807	2219	2229	2235	rBV	34308	66380	24.11%	1.151%
90	22.903	2250	2257	2272	rBV	19941	41918	15.22%	0.727%
91	23.289	2361	2370	2384	rVB	13207	23598	8.57%	0.409%
92	23.385	2388	2398	2404	rBV	19184	35914	13.04%	0.623%
93	23.485	2416	2427	2467	rVB	118812	244801	88.91%	4.246%
94	24.090	2595	2604	2621	rVB	12224	25520	9.27%	0.443%
95	24.196	2625	2635	2653	rBV	11503	34865	12.66%	0.605%
96	24.857	2822	2828	2853	rVB2	10862	25054	9.10%	0.435%
97	25.768	3077	3094	3120	rBV3	19739	67028	24.34%	1.163%
98	26.459	3281	3296	3329	rVB	10017	32295	11.73%	0.560%
99	26.640	3333	3349	3379	rVV2	8902	32693	11.87%	0.567%
100	26.815	3386	3400	3433	rVB3	4868	20629	7.49%	0.358%

Sum of corrected areas: 5765701

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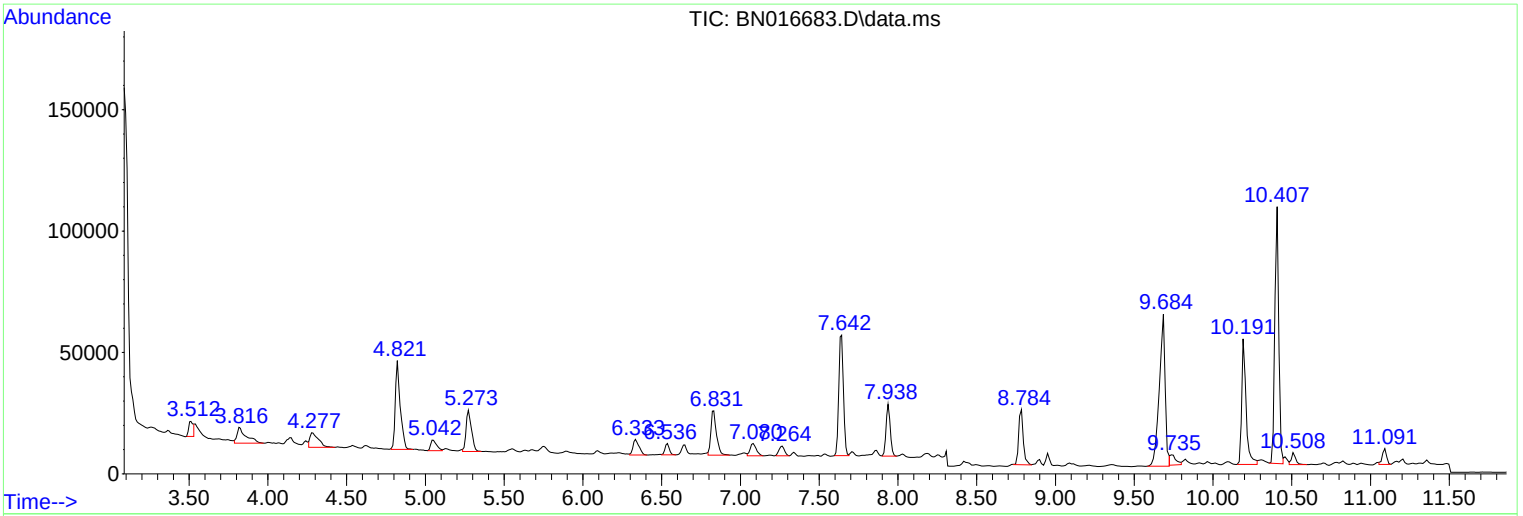
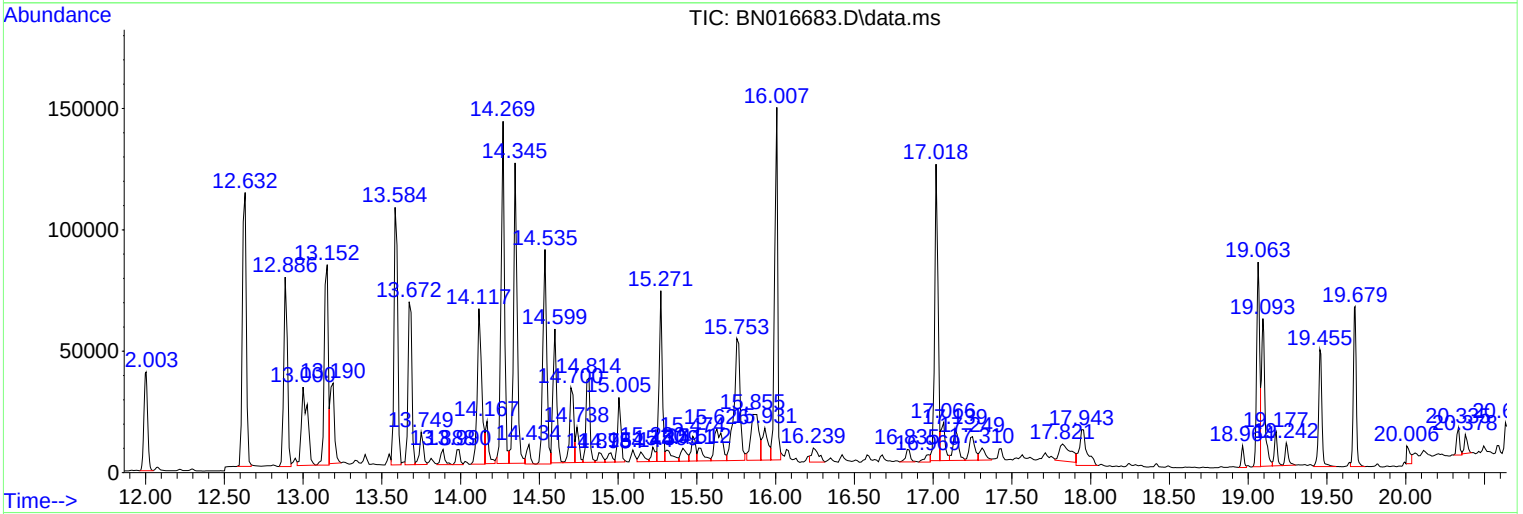
Misc :
ALS Vial : 51 Sample Multiplier: 1

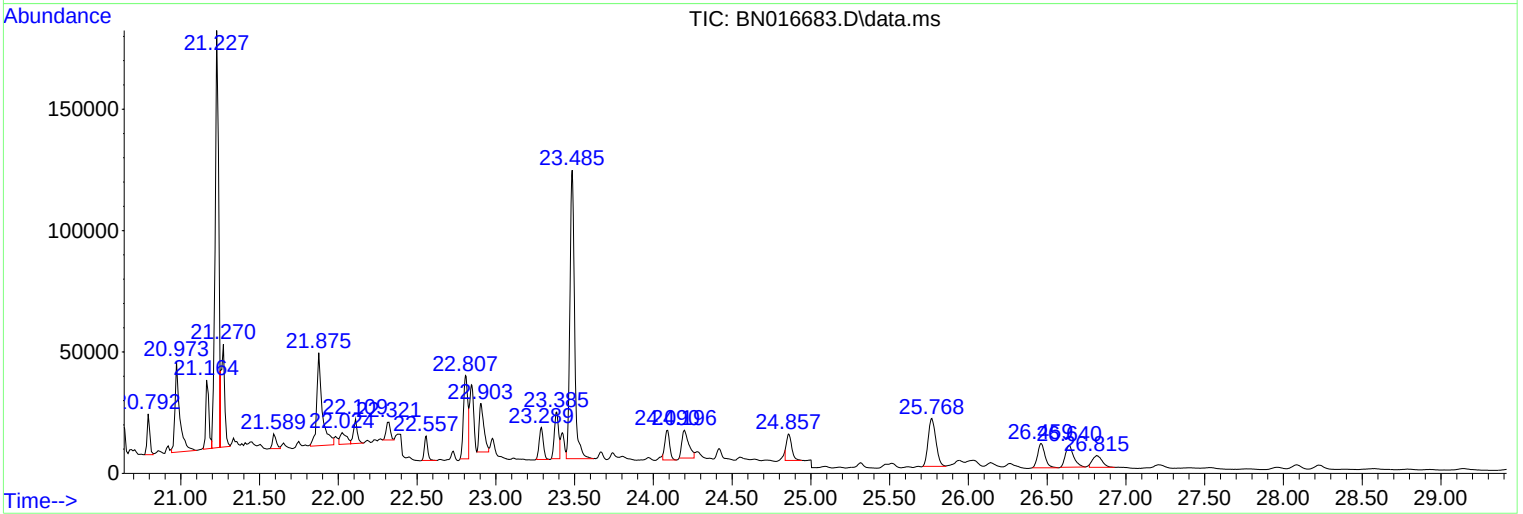
Instrument :
BNA_N
ClientSampleId :
S-825-N-SO-1-1.5-092221

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\
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Instrument :
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S-825-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

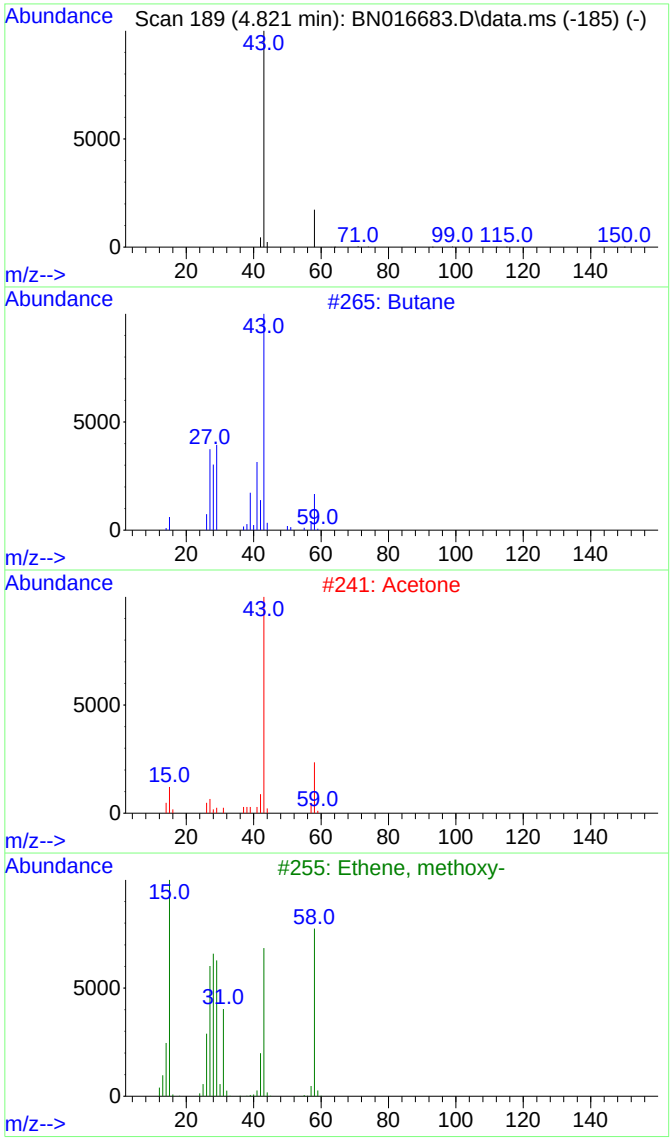
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

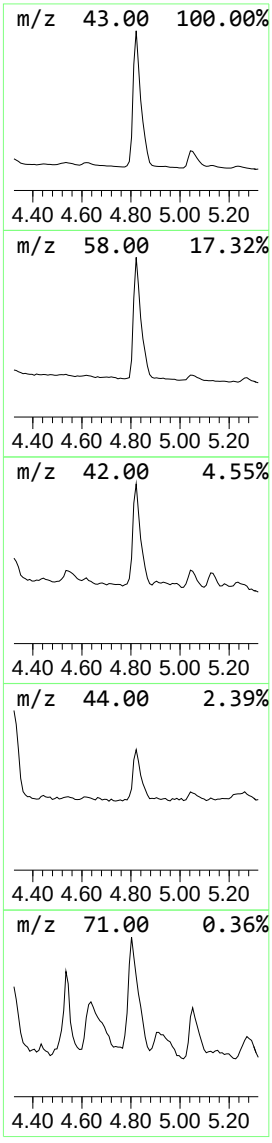
****

Peak Number 1 Butane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.31 ng	79602	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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BNA_N
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

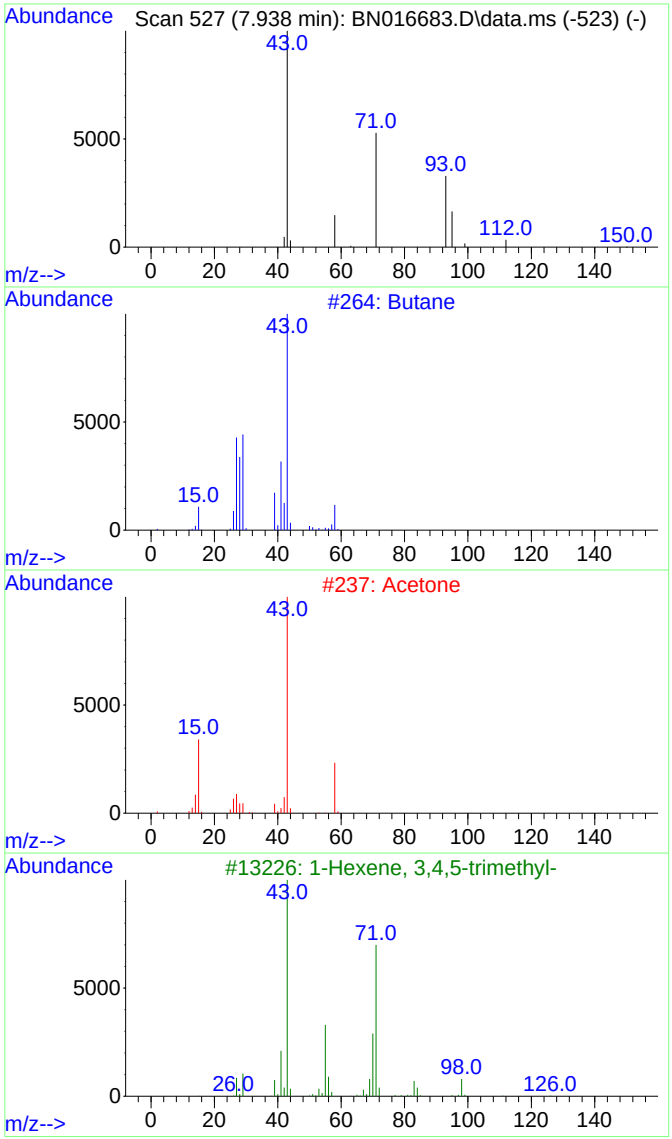
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

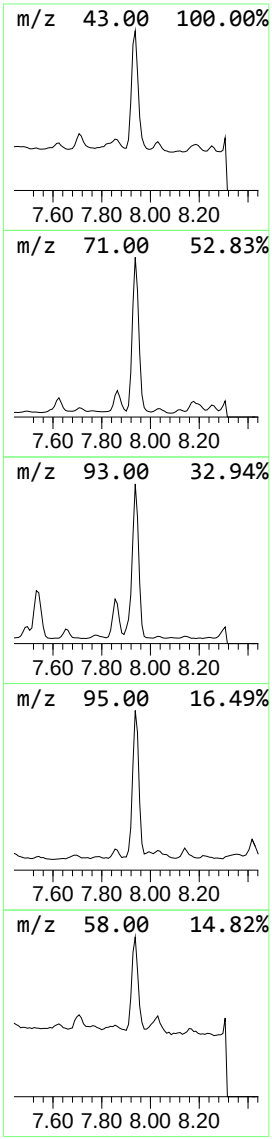
****

Peak Number 2 Butane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.938	0.15 ng	39321	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-Furanmethanamine, tetrahydro-	101	C5H11NO	004795-29-3	4
5	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	4





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

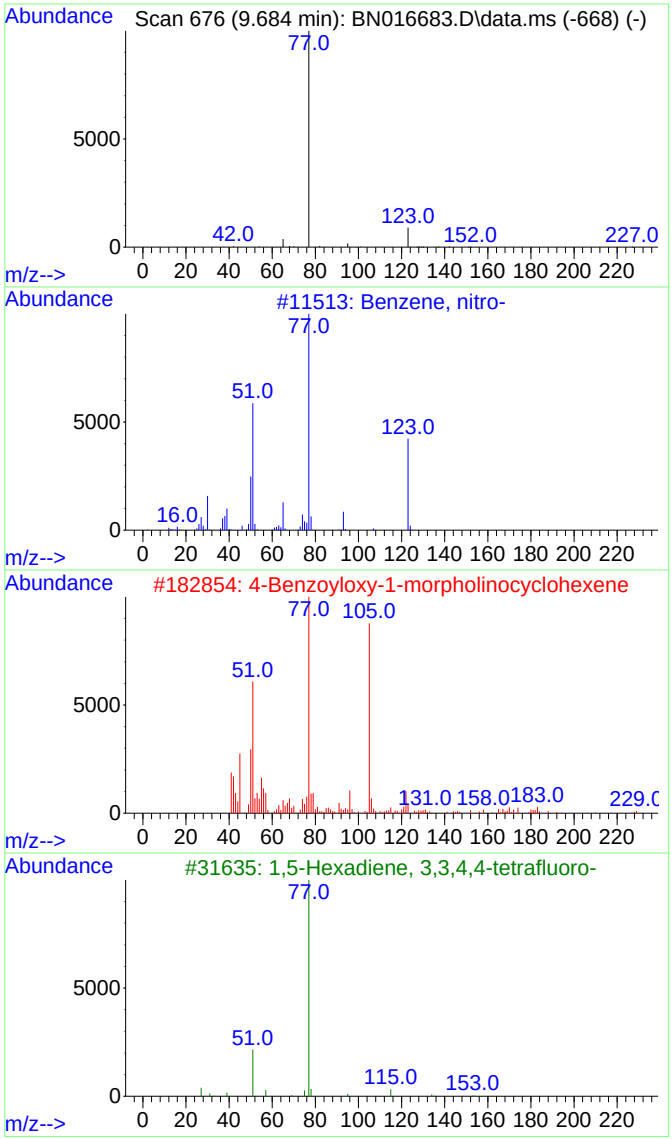
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

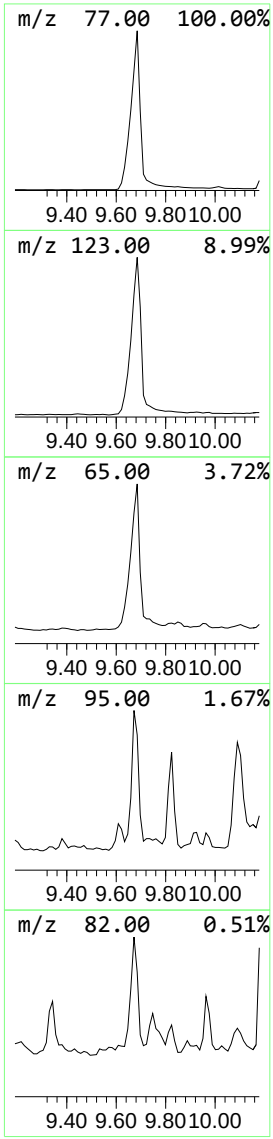
****

Peak Number 3 Benzene, nitro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.684	0.36 ng	163942	Naphthalene-d8	10.407

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, nitro-	123	C6H5NO2	000098-95-3	2
2	4-Benzoyloxy-1-morpholinocyclohe...	287	C17H21NO3	037138-56-0	1
3	1,5-Hexadiene, 3,3,4,4-tetrafluoro-	154	C6H6F4	001763-21-9	1
4	Silanamine, N-silyl-	77	H7NSi2	005702-11-4	1
5	Mercaptamine	77	C2H7NS	000060-23-1	1





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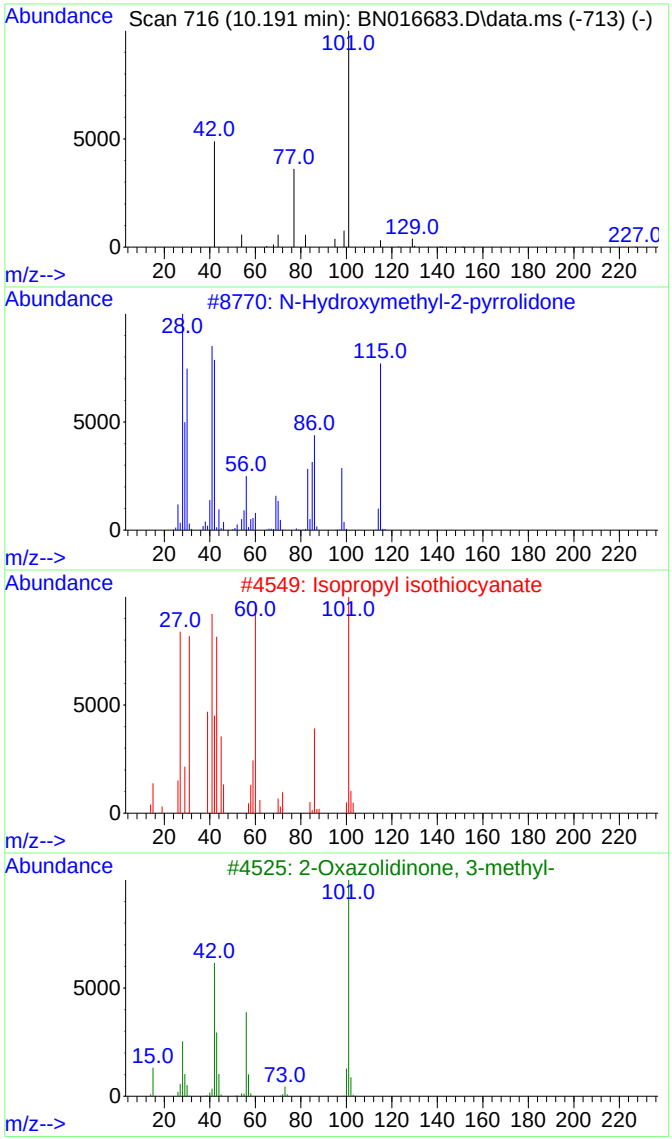
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

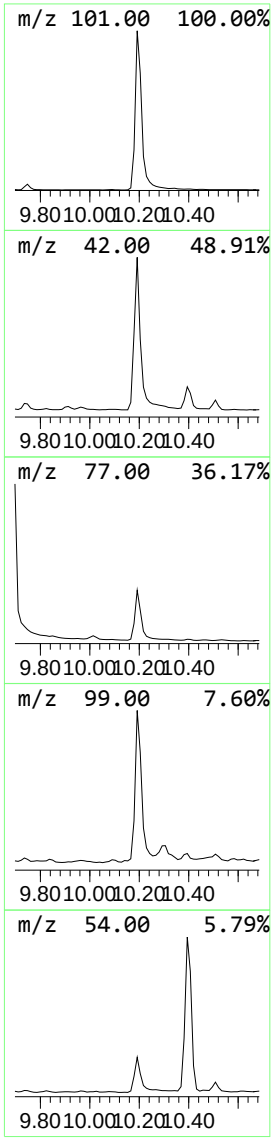
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 N-Hydroxymethyl-2-pyrrolidone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.22 ng	99678	Naphthalene-d8	10.407

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-Hydroxymethyl-2-pyrrolidone	115	C5H9NO2	1000426-51-3	7
2	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	5
3	2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	5
4	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
5	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016683.D
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Operator : CG/JU
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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
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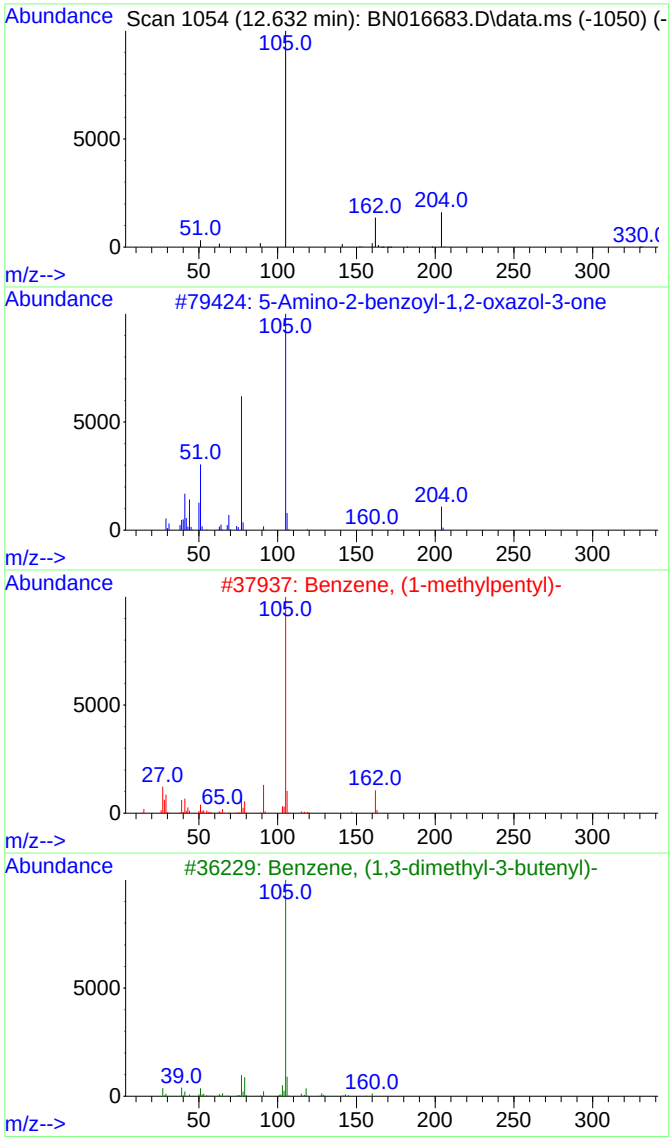
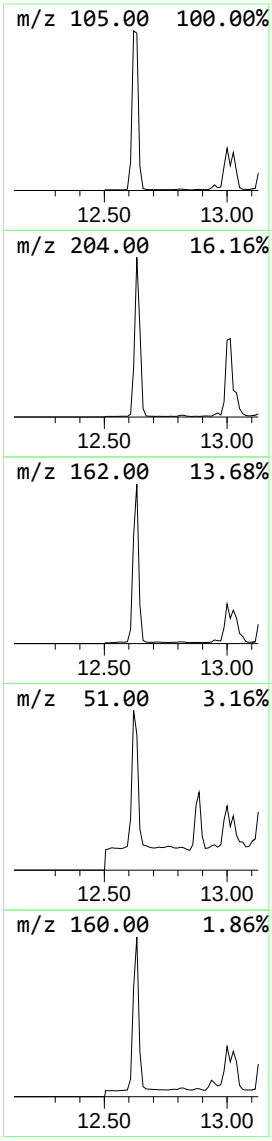
****
Peak Number 5 5-Amino-2-benzoyl-1,2-oxazo... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.632	0.37 ng	196704	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Amino-2-benzoyl-1,2-oxazol-3-one	204	C10H8N2O3	090771-25-8	5
2	Benzene, (1-methylpentyl)-	162	C12H18	006031-02-3	5
3	Benzene, (1,3-dimethyl-3-butenyl)-	160	C12H16	056851-51-5	4
4	1-Butanone, 3-methyl-1-phenyl-	162	C11H14O	000582-62-7	4
5	Phenyl tert-butyl ketone	162	C11H14O	000938-16-9	4





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Acq On : 02 Oct 2021 22:33
Operator : CG/JU
Sample : M3892-12
Misc :
ALS Vial : 51 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S-825-N-SO-1-1.5-092221

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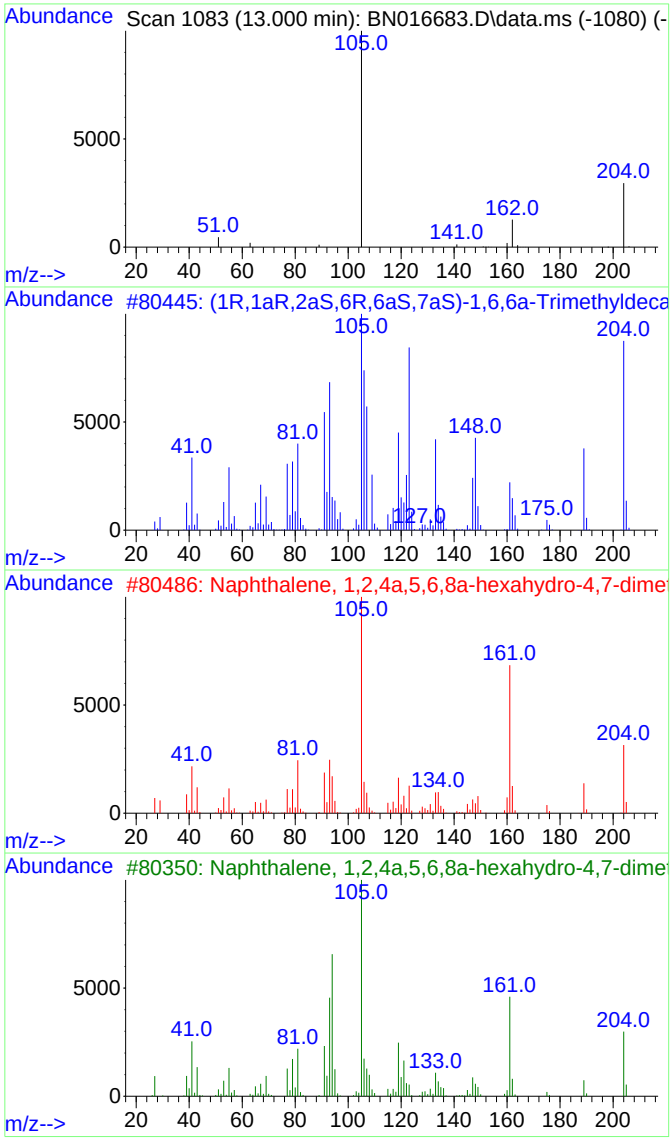
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

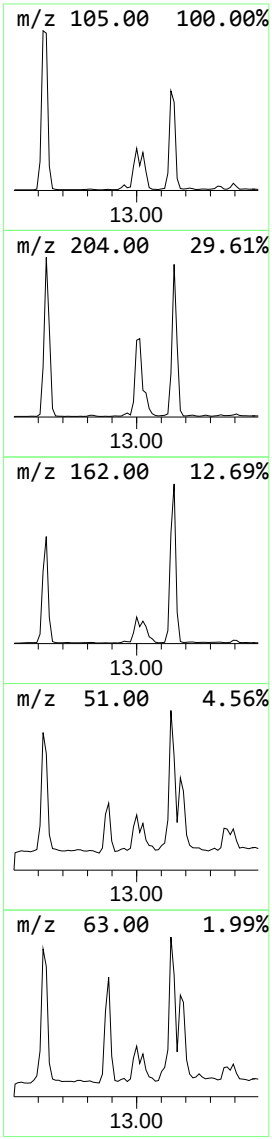
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (1R,1aR,2aS,6R,6aS,7aS)-1,6... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.000	0.16 ng	85687	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1R,1aR,2aS,6R,6aS,7aS)-1,6,6a-T...	204	C15H24	026620-70-2	9
2	Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	024406-05-1	7
3	Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	000483-75-0	7
4	.alpha.-Muurolene	204	C15H24	010208-80-7	7
5	(1R,3aS,8aS)-7-Isopropyl-1,4-dim...	204	C15H24	036577-33-0	7





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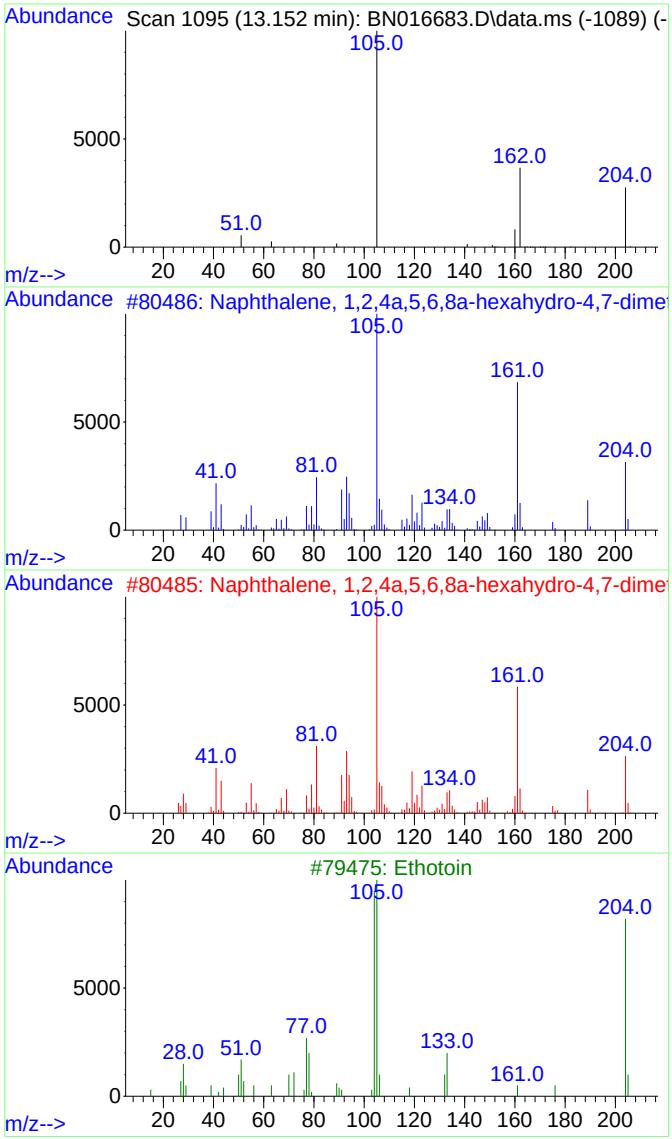
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

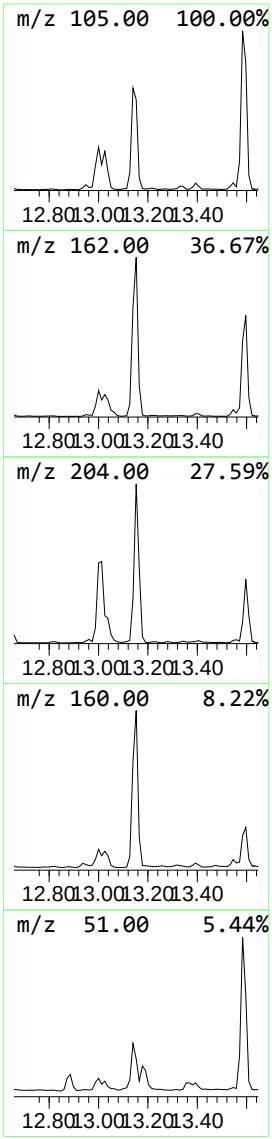
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Naphthalene, 1,2,4a,5,6,8a-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.152	0.28 ng	147990	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	024406-05-1	7
2	Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	017627-24-6	7
3	Ethotoin	204	C11H12N2O2	000086-35-1	5
4	(1R,1aR,2aS,6R,6aS,7aS)-1,6,6a-T...	204	C15H24	026620-70-2	4
5	Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	031983-22-9	4





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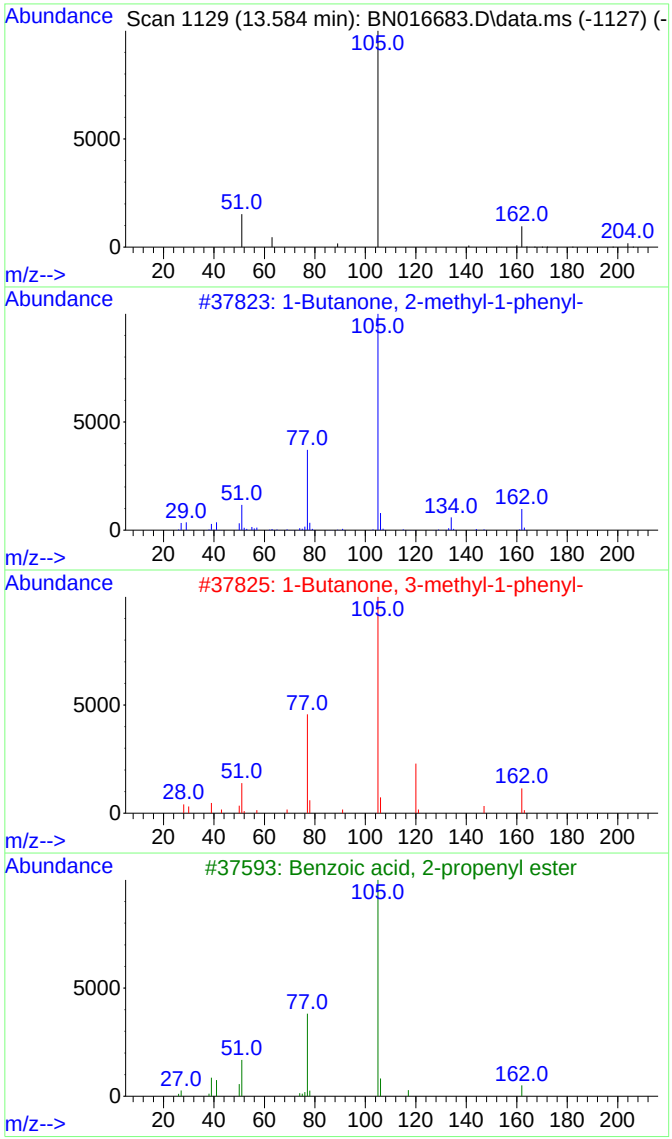
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

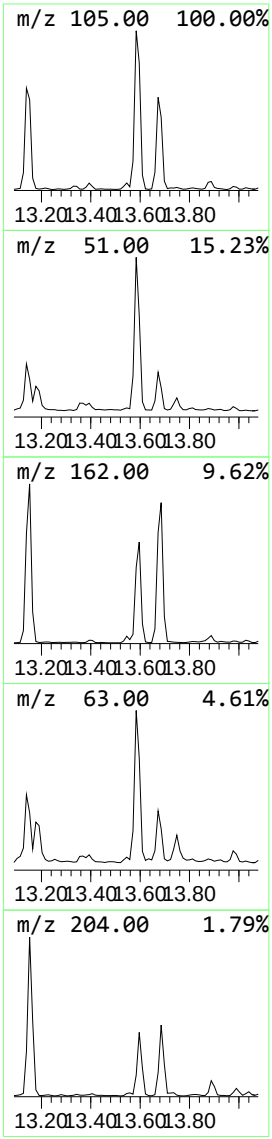
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1-Butanone, 2-methyl-1-phenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.584	0.33 ng	173791	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanone, 2-methyl-1-phenyl-	162	C11H14O	000938-87-4	7
2	1-Butanone, 3-methyl-1-phenyl-	162	C11H14O	000582-62-7	7
3	Benzoic acid, 2-propenyl ester	162	C10H10O2	000583-04-0	5
4	Cyclobutyl phenyl ketone	160	C11H12O	005407-98-7	4
5	1,3-Butanedione, 1-phenyl-	162	C10H10O2	000093-91-4	4





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Misc :
ALS Vial : 51 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S-825-N-SO-1-1.5-092221

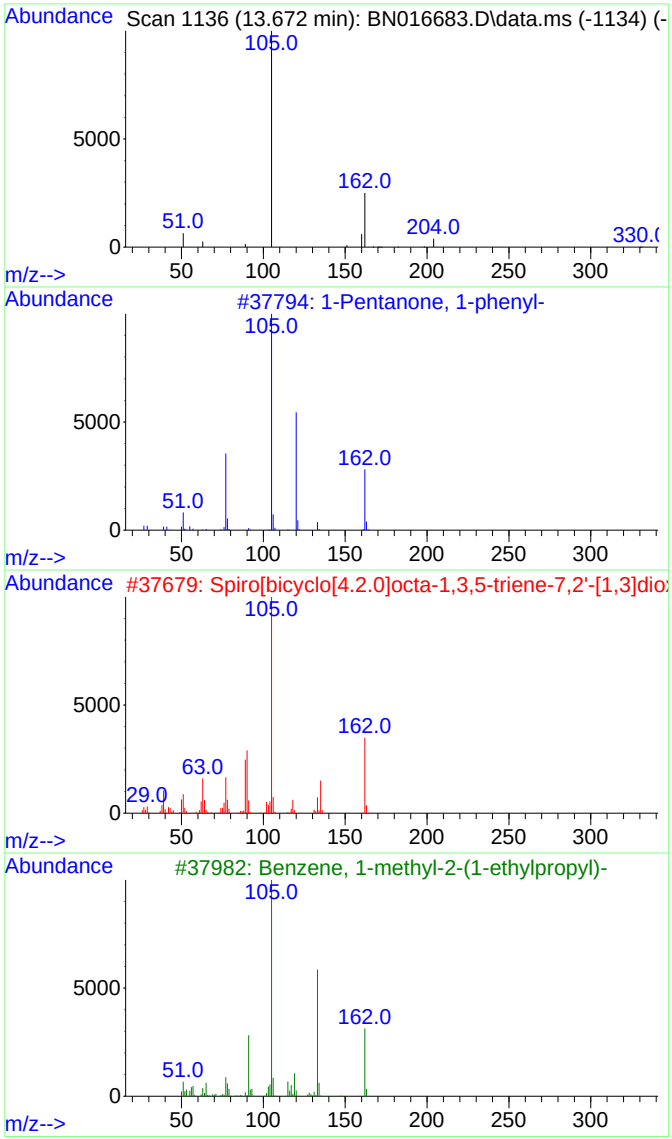
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

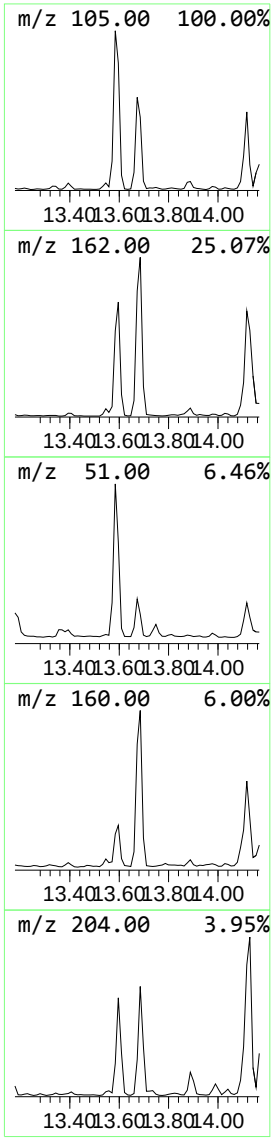
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1-Pentanone, 1-phenyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.672	0.22 ng	115948	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	Spiro[bicyclo[4.2.0]octa-1,3,5-t...	162	C10H10O2	014458-33-4	4
3	Benzene, 1-methyl-2-(1-ethylprop...	162	C12H18	054410-74-1	4
4	Benzaldehyde, 4-(2-propenyloxy)-	162	C10H10O2	040663-68-1	4
5	1-Butanone, 3-methyl-1-phenyl-	162	C11H14O	000582-62-7	4





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Operator : CG/JU
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Misc :
ALS Vial : 51 Sample Multiplier: 1

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

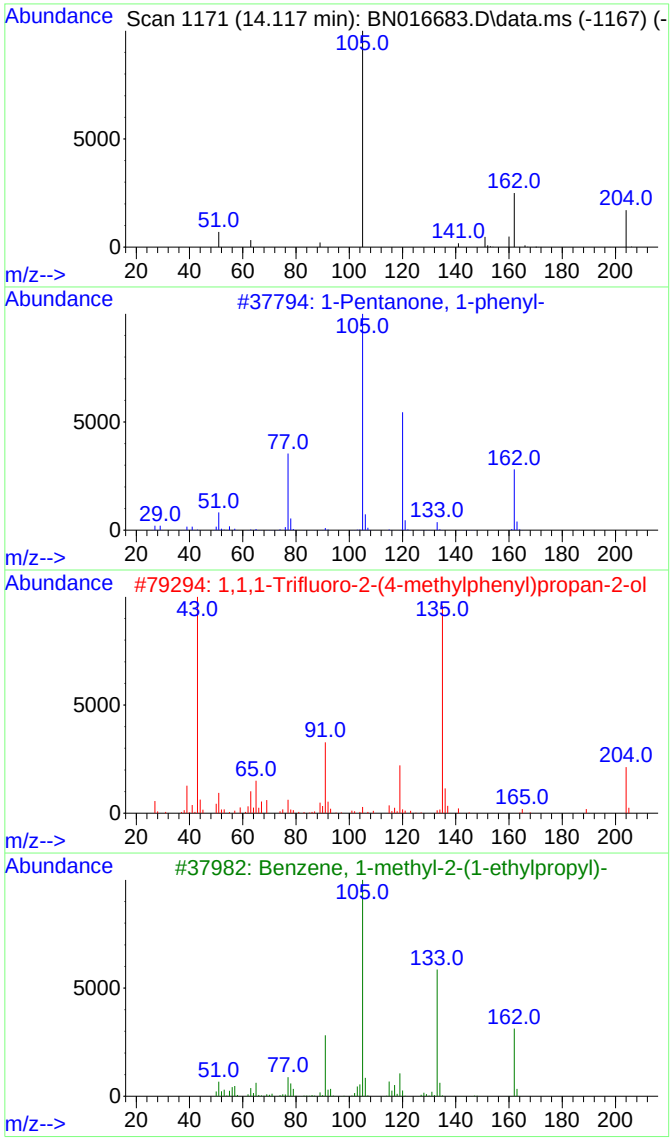
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

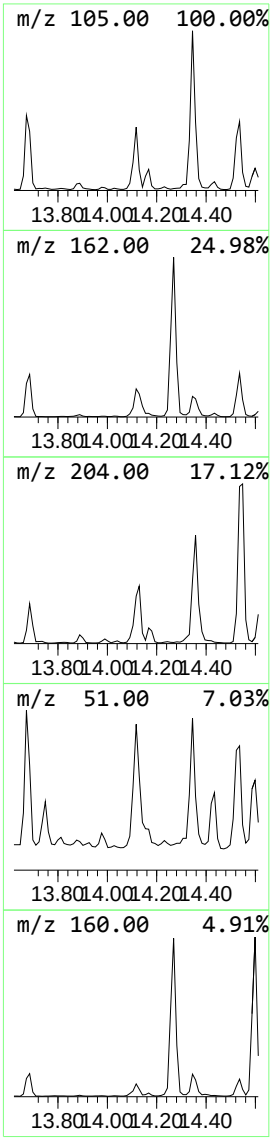
****

Peak Number 10 1-Pentanone, 1-phenyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.117	0.25 ng	130276	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	Benzene, 1-methyl-2-(1-ethylprop...	162	C12H18	054410-74-1	4
4	Spiro[bicyclo[4.2.0]octa-1,3,5-t...	162	C10H10O2	014458-33-4	4
5	Phenylglyoxylic acid, butyl ester	206	C12H14O3	1000453-46-6	4





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Sample : M3892-12
Misc :
ALS Vial : 51 Sample Multiplier: 1

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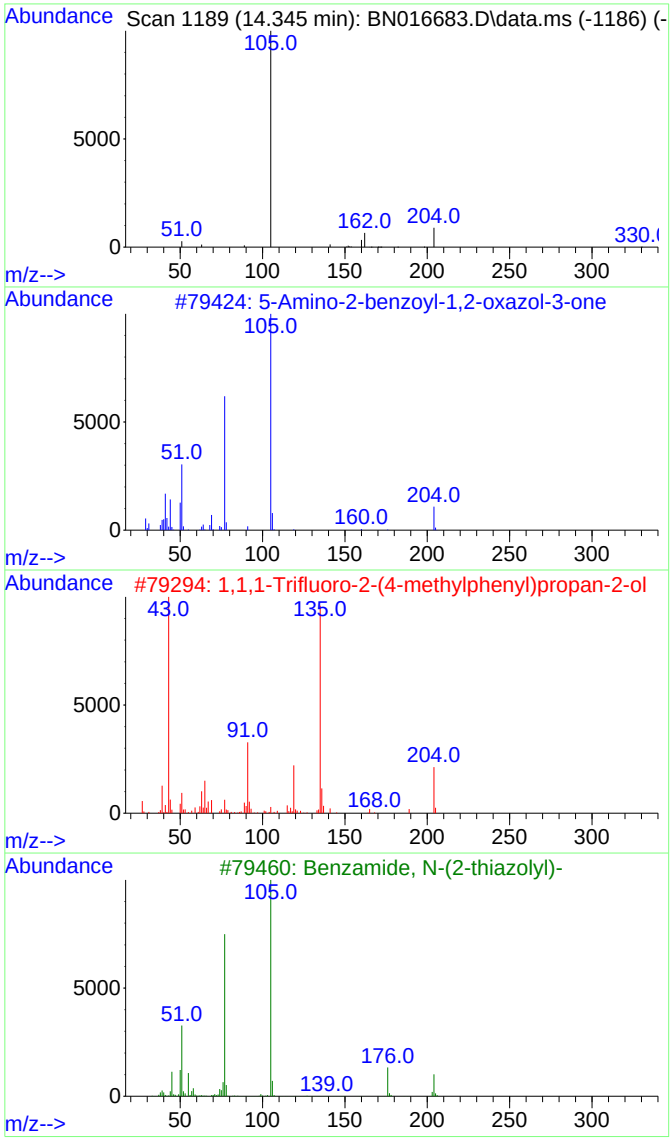
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

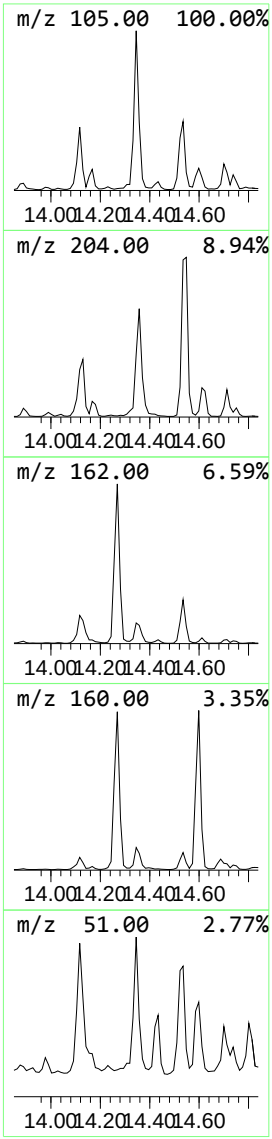
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 5-Amino-2-benzoyl-1,2-oxazo... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.345	0.37 ng	197741	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Amino-2-benzoyl-1,2-oxazol-3-one	204	C10H8N2O3	090771-25-8	4
2	1,1,1-Trifluoro-2-(4-methylpheny...	204	C10H11F3O	076953-97-4	4
3	Benzamide, N-(2-thiazolyl)-	204	C10H8N2OS	013053-82-2	3
4	1-Butanone, 2-methyl-1-phenyl-	162	C11H14O	000938-87-4	3
5	Thiophene-2-ol, benzoate	204	C11H8O2S	016693-98-4	3





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Sample : M3892-12
Misc :
ALS Vial : 51 Sample Multiplier: 1

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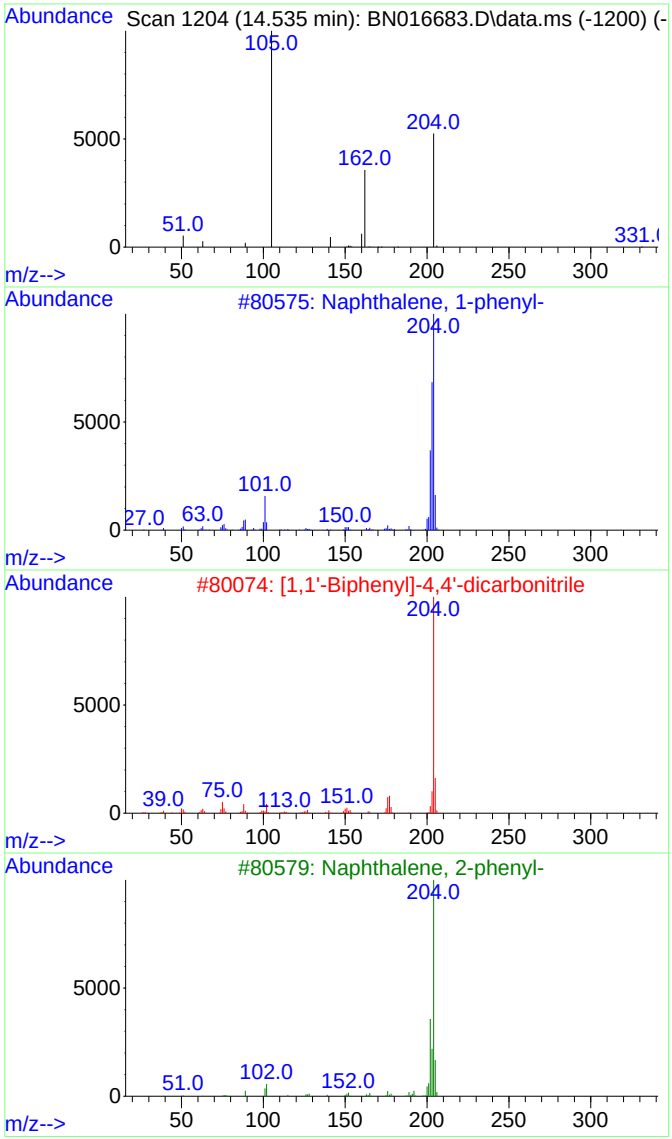
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

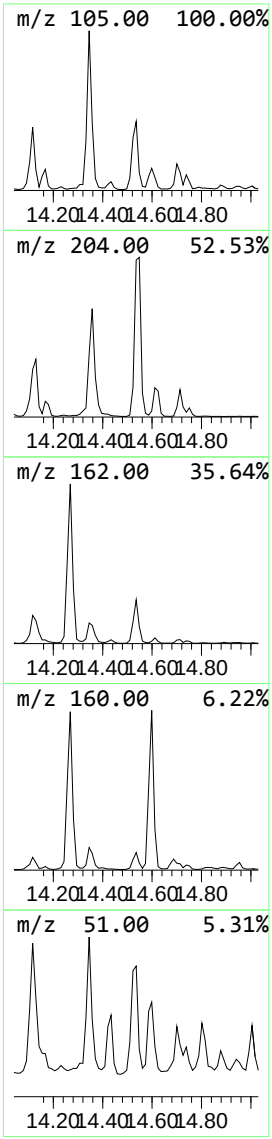
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Naphthalene, 1-phenyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.535	0.29 ng	154017	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-phenyl-	204	C16H12	000605-02-7	7
2	[1,1'-Biphenyl]-4,4'-dicarbonitrile	204	C14H8N2	001591-30-6	7
3	Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	7
4	1-Propoxyphthalazine 3-oxide	204	C11H12N2O2	091350-93-5	7
5	Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	031983-22-9	7





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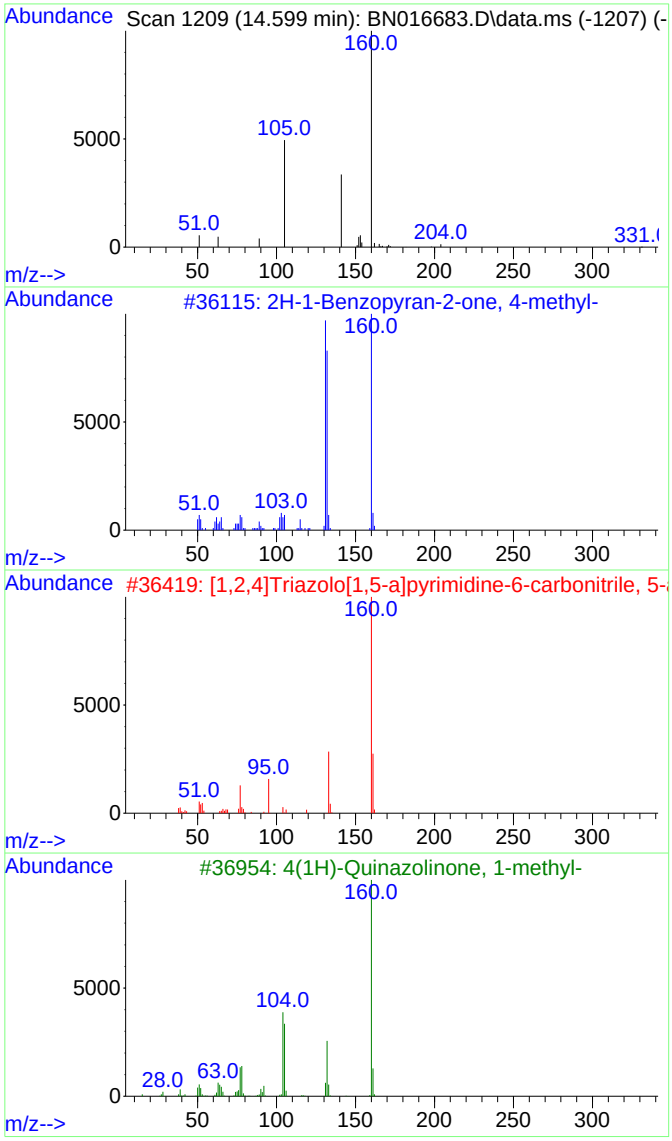
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

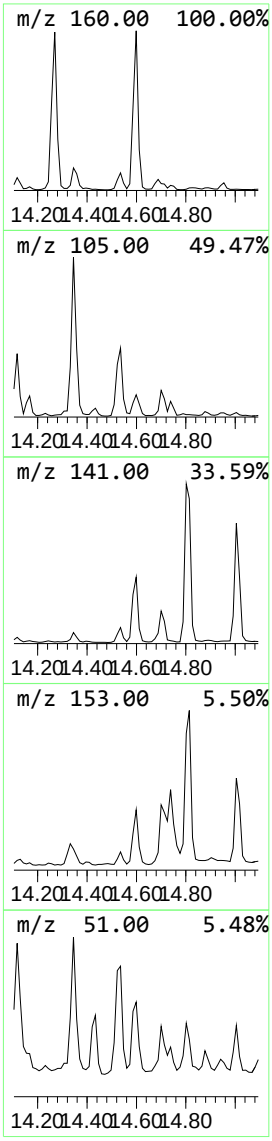
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 2H-1-Benzopyran-2-one, 4-me... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.599	0.17 ng	90129	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-1-Benzopyran-2-one, 4-methyl-	160	C10H8O2	000607-71-6	5
2	[1,2,4]Triazolo[1,5-a]pyrimidine...	160	C6H4N6	1000337-63-1	5
3	4(1H)-Quinazolinone, 1-methyl-	160	C9H8N2O	003476-68-4	4
4	3H-pyrazol-3-one, 2,4-dihydro-2-...	160	C9H8N2O	1000404-39-1	4
5	5-(3-Aminophenyl)oxazole	160	C9H8N2O	1000342-39-6	4





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ALS Vial : 51 Sample Multiplier: 1

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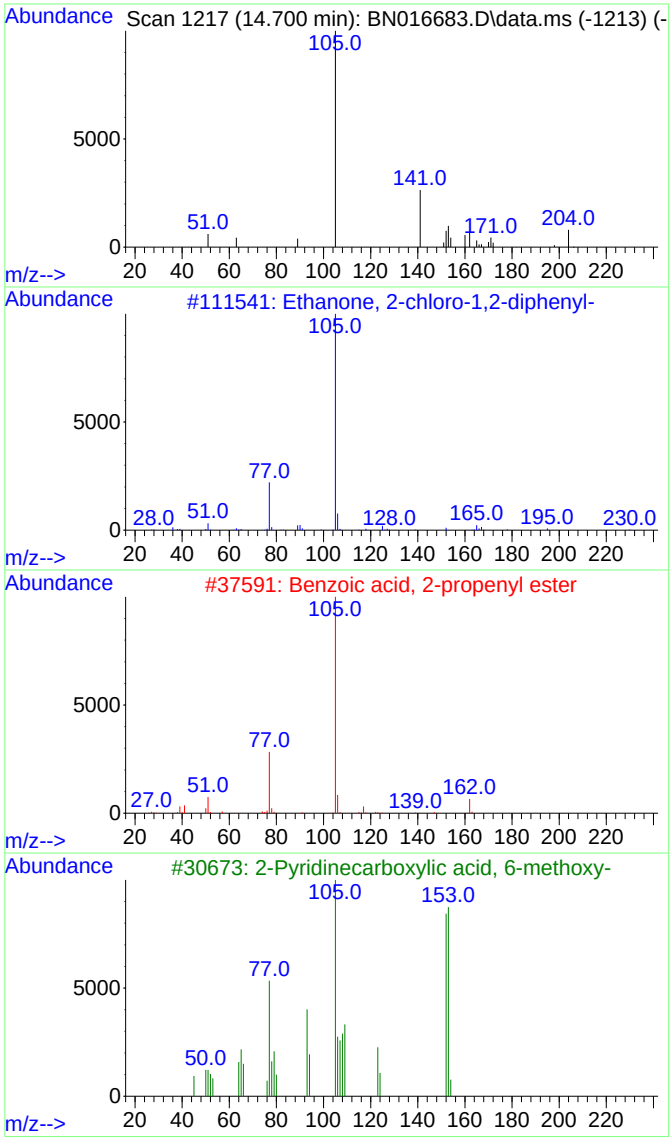
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

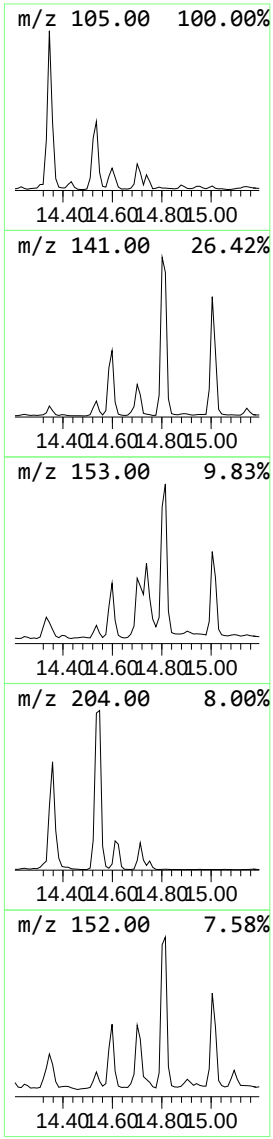
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 Ethanone, 2-chloro-1,2-diph... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.700	0.11 ng	59153	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 2-chloro-1,2-diphenyl-	230	C14H11ClO	000447-31-4	9
2	Benzoic acid, 2-propenyl ester	162	C10H10O2	000583-04-0	4
3	2-Pyridinecarboxylic acid, 6-met...	153	C7H7NO3	026893-73-2	4
4	2-(2-Nitrophenyl)-1-phenylethan-...	241	C14H11NO3	1000482-55-3	4
5	N-(2-Bromophenyl)-N'-(4-methylbe...	374	C18H19BrN2O2	328019-20-1	4





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Sample : M3892-12
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Instrument :
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ClientSampleId :
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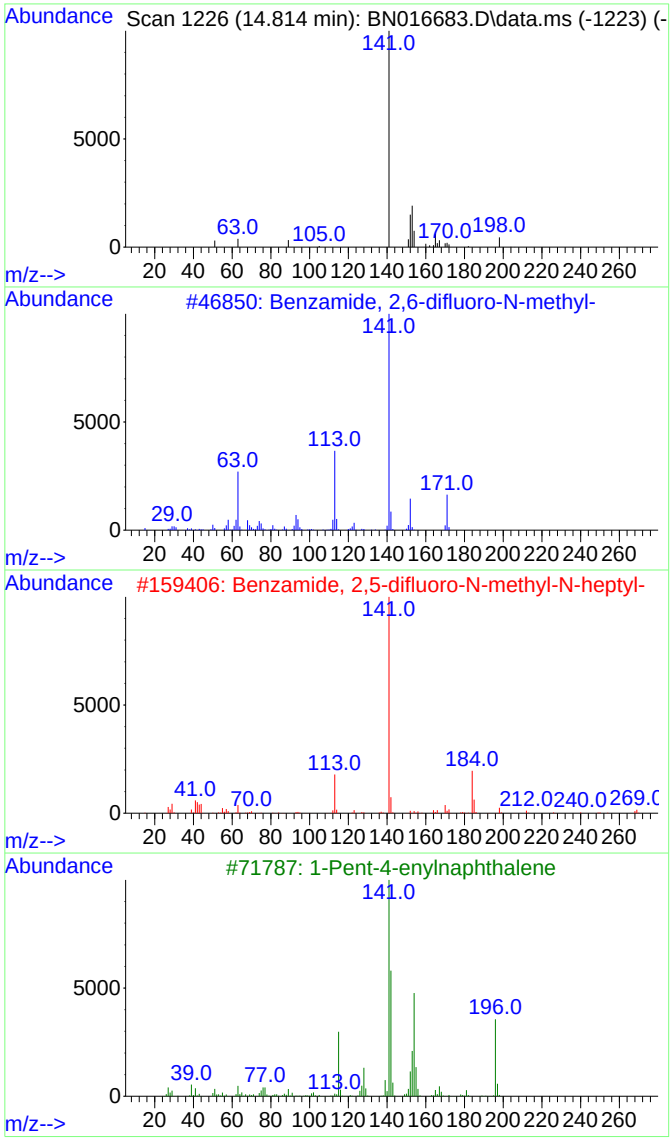
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

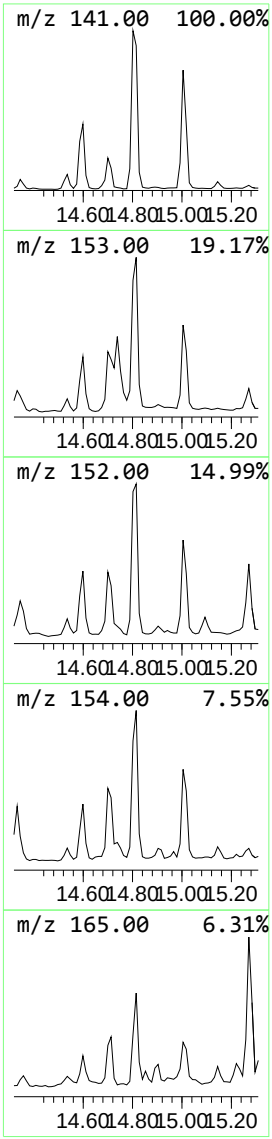
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 Benzamide, 2,6-difluoro-N-m... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.814	0.12 ng	62367	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, 2,6-difluoro-N-methyl-	171	C8H7F2NO	1010419-67-9	38
2	Benzamide, 2,5-difluoro-N-methyl...	269	C15H21F2NO	1000437-04-9	9
3	1-Pent-4-enylnaphthalene	196	C15H16	093359-74-1	9
4	1,6-Dioxaspiro[4.5]decane, 2-eth...	170	C10H18O2	076495-09-5	5
5	1-Chloro-4-methoxy-2-phenylbutane	198	C11H15ClO	1010216-63-6	5





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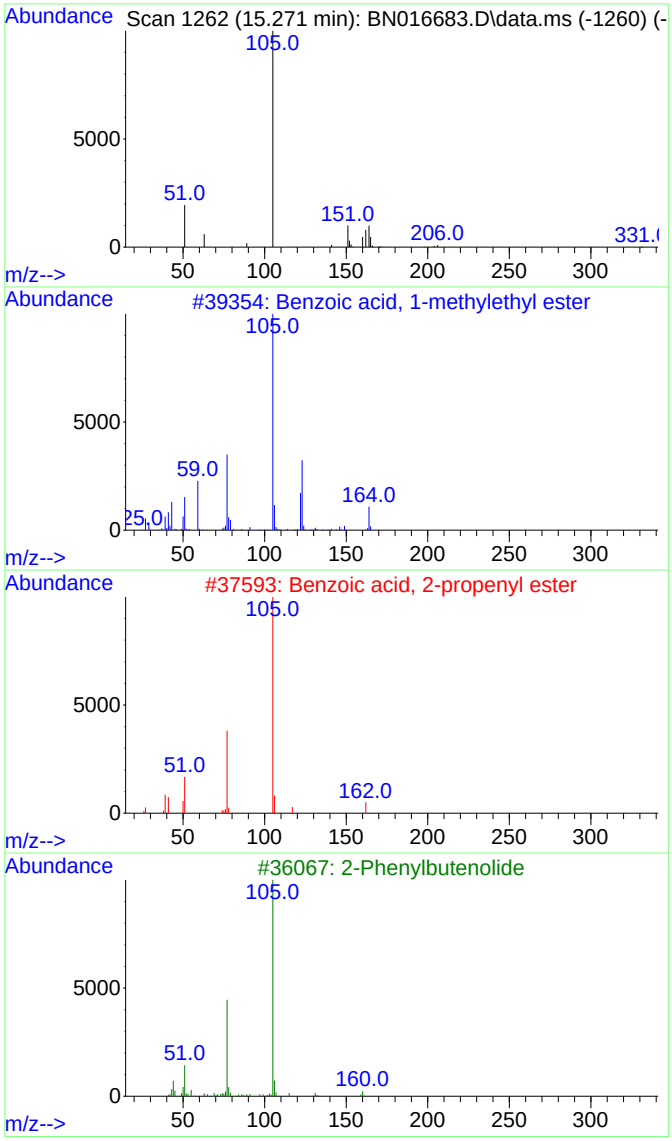
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

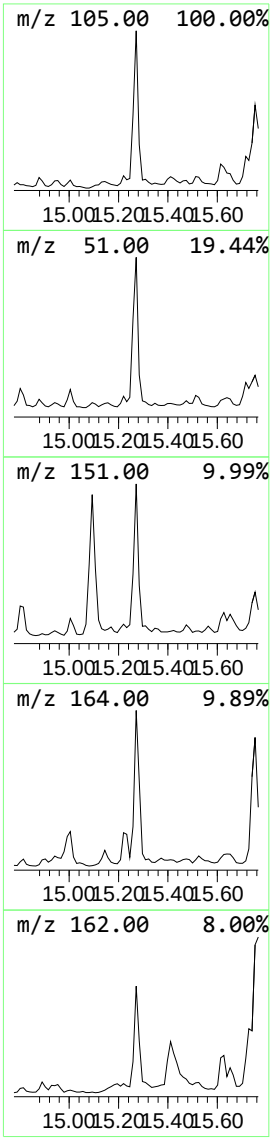
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 Benzoic acid, 1-methylethyl... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.271	0.18 ng	97172	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 1-methylethyl ester	164	C10H12O2	000939-48-0	7
2	Benzoic acid, 2-propenyl ester	162	C10H10O2	000583-04-0	5
3	2-Phenylbutenolide	160	C10H8O2	001955-39-1	5
4	E-2-Hexenyl benzoate	204	C13H16O2	076841-70-8	5
5	1-Benzoyl-1,4-diazepane	204	C12H16N2O	059939-75-2	4





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Data File : BN016683.D
Acq On : 02 Oct 2021 22:33
Operator : CG/JU
Sample : M3892-12
Misc :
ALS Vial : 51 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-825-N-SO-1-1.5-092221

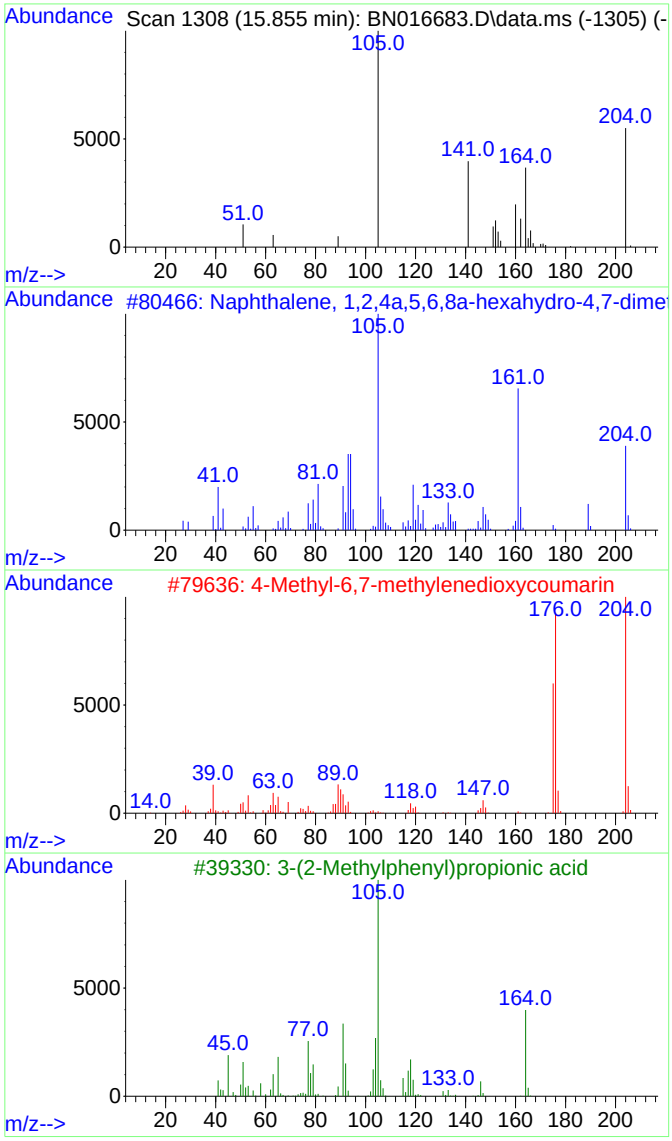
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

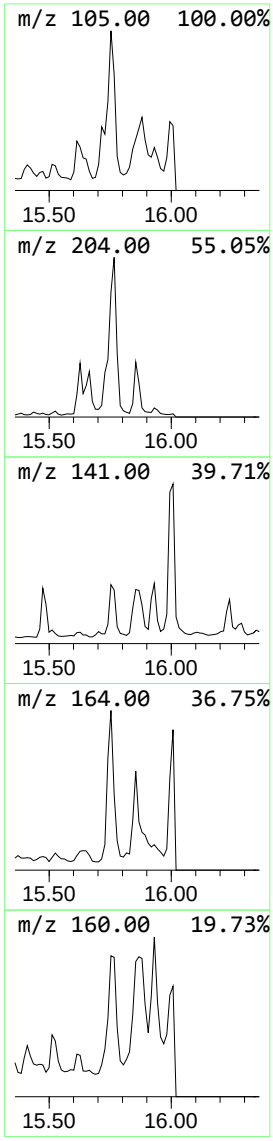
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 Naphthalene, 1,2,4a,5,6,8a-... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.855	0.15 ng	69648	Phenanthrene-d10	17.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	031983-22-9	9
2	4-Methyl-6,7-methylenedioxycoumarin	204	C11H8O4	015071-04-2	9
3	3-(2-Methylphenyl)propionic acid	164	C10H12O2	022084-89-5	9
4	Hydantoin, 5-benzylidene-2-thio-	204	C10H8N2OS	000583-46-0	9
5	3'-Carboxybenzo[1',2',-b]-1,4-di...	204	C11H12N2O2	138023-41-3	9





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
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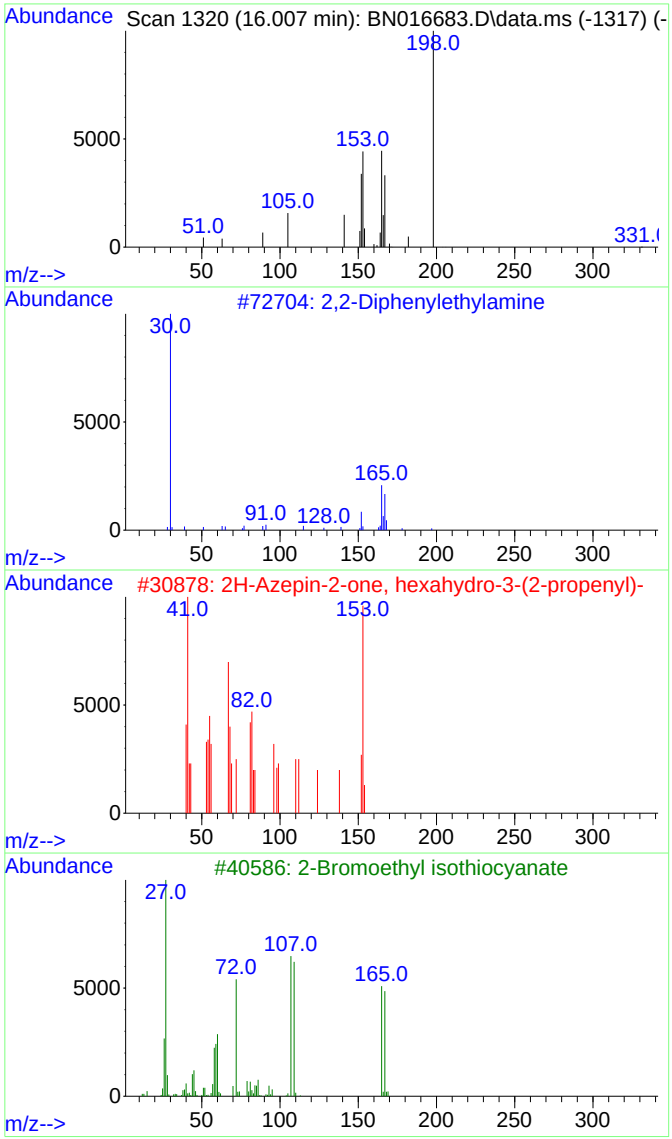
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

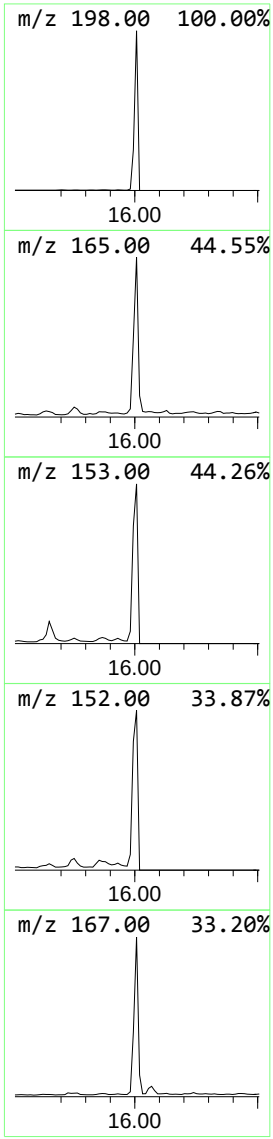
****

Peak Number 18 2,2-Diphenylethylamine Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.007	0.42 ng	192249	Phenanthrene-d10	17.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2-Diphenylethylamine	197	C14H15N	003963-62-0	16
2	2H-Azepin-2-one, hexahydro-3-(2-...	153	C9H15NO	029559-34-0	5
3	2-Bromoethyl isothiocyanate	165	C3H4BrNS	001483-41-6	5
4	Methyl 2-(dimethylhydrazono)-3,3...	198	C6H9F3N2O2	1000489-35-4	4
5	1-Methyl-1,8-diazaundecan-2,9-dione	198	C10H18N2O2	1000298-94-5	4





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Data File : BN016683.D
Acq On : 02 Oct 2021 22:33
Operator : CG/JU
Sample : M3892-12
Misc :
ALS Vial : 51 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-825-N-SO-1-1.5-092221

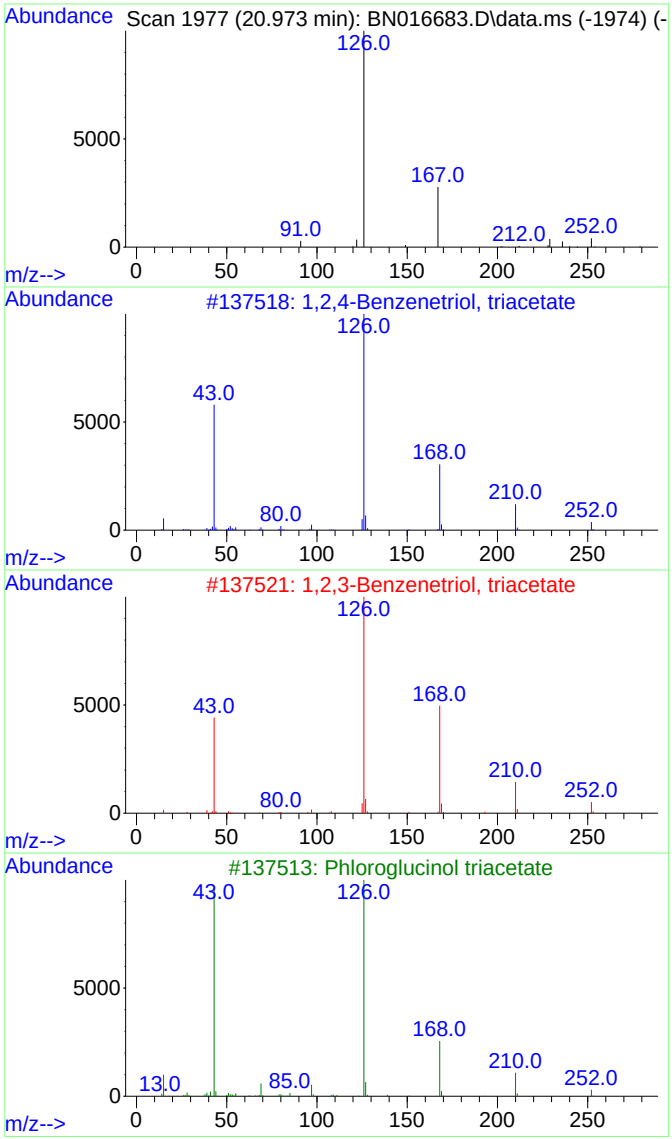
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

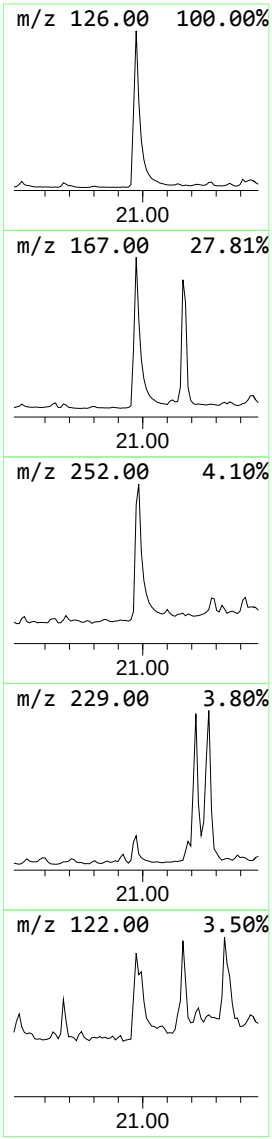
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 1,2,4-Benzenetriol, triacetate Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.973	0.11 ng	76973	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	Bicyclo[2.2.1]heptane-1,2-dicarb...	212	C11H16O4	1000191-44-2	4





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Sample : M3892-12
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ALS Vial : 51 Sample Multiplier: 1

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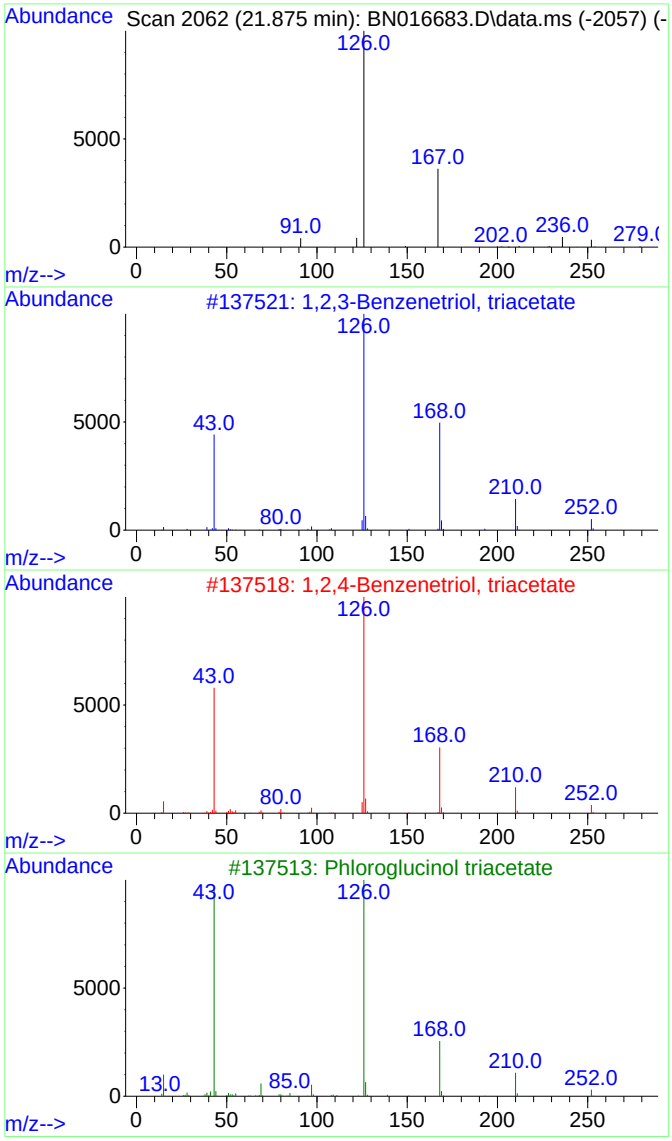
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

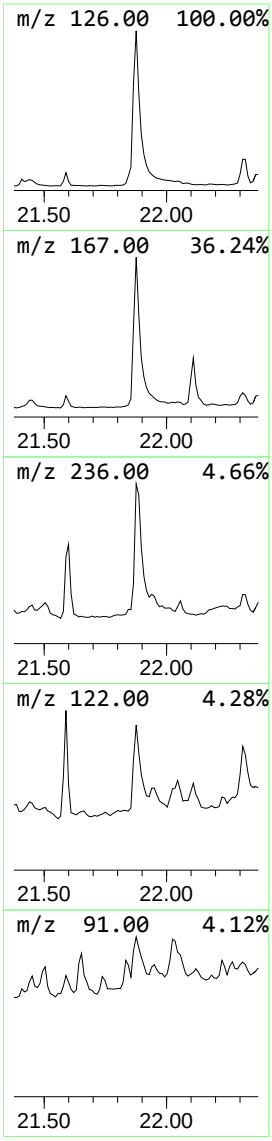
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 1,2,3-Benzenetriol, triacetate Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.875	0.14 ng	93100	Chrysene-d12	21.227

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	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 : BN016683.D
Acq On : 02 Oct 2021 22:33
Operator : CG/JU
Sample : M3892-12
Misc :
ALS Vial : 51 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-825-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
Butane	4.821	0.3	ng	79602	1	7.642	102321	0.4
Butane	7.938	0.2	ng	39321	1	7.642	102321	0.4
Benzene, nitro-	9.684	0.4	ng	163942	2	10.407	184224	0.4
N-Hydroxymethyl...	10.191	0.2	ng	99678	2	10.407	184224	0.4
5-Amino-2-benzo...	12.632	0.4	ng	196704	3	14.269	211908	0.4
(1R,1aR,2aS,6R,...	13.000	0.2	ng	85687	3	14.269	211908	0.4
Naphthalene, 1,...	13.152	0.3	ng	147990	3	14.269	211908	0.4
1-Butanone, 2-m...	13.584	0.3	ng	173791	3	14.269	211908	0.4
1-Pentanone, 1-...	13.672	0.2	ng	115948	3	14.269	211908	0.4
1-Pentanone, 1-...	14.117	0.2	ng	130276	3	14.269	211908	0.4
5-Amino-2-benzo...	14.345	0.4	ng	197741	3	14.269	211908	0.4
Naphthalene, 1-...	14.535	0.3	ng	154017	3	14.269	211908	0.4
2H-1-Benzopyran...	14.599	0.2	ng	90129	3	14.269	211908	0.4
Ethanone, 2-chl...	14.700	0.1	ng	59153	3	14.269	211908	0.4
Benzamide, 2,6-...	14.814	0.1	ng	62367	3	14.269	211908	0.4
Benzoic acid, 1...	15.271	0.2	ng	97172	3	14.269	211908	0.4
Naphthalene, 1,...	15.855	0.2	ng	69648	4	17.018	181328	0.4
2,2-Diphenyleth...	16.007	0.4	ng	192249	4	17.018	181328	0.4
1,2,4-Benzenetr...	20.973	0.1	ng	76973	5	21.227	275344	0.4
1,2,3-Benzenetr...	21.875	0.1	ng	93100	5	21.227	275344	0.4