LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016684.D
Acq On : 02 Oct 2021 23:09
Operator : CG/JU
Sample : M3892-10
Misc :
ALS Vial : 52 Sample Multiplier: 2

Instrument : BNA_N
ClientSampleId : S-824-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: BN016684.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.373	29	32	44	rVV	8965	24529	5.00%	0.405%
2	3.512	44	47	62	rVB	9446	35326	7.20%	0.583%
3	3.825	78	81	98	rVB	6897	26343	5.37%	0.435%
4	4.277	128	130	140	rVB	6187	18500	3.77%	0.305%
5	4.821	185	189	209	rVB	44650	100143	20.42%	1.654%
6	5.042	210	213	220	rBV	6087	14217	2.90%	0.235%
7	5.273	234	238	255	rVB	18887	44237	9.02%	0.730%
8	6.223	339	341	348	rVB	3094	6429	1.31%	0.106%
9	6.647	384	387	391	rBV	5740	10059	2.05%	0.166%
10	6.831	403	407	417	rVB	19187	38799	7.91%	0.641%
11	7.246	449	452	459	rVB2	6035	17457	3.56%	0.288%
12	7.642	490	495	500	rVB	101023	200308	40.85%	3.307%
13	8.306	565	567	569	rVB	5814	5761	1.17%	0.095%
14	8.785	601	605	612	rBV	27332	55341	11.29%	0.914%
15	8.949	616	618	621	rVB	5806	8757	1.79%	0.145%
16	9.076	625	628	636	rBV2	3652	8337	1.70%	0.138%
17	9.646	669	673	677	rBV	13120	33789	6.89%	0.558%
18	9.912	691	694	696	rBV	3962	6959	1.42%	0.115%
19	10.191	713	716	722	rBV	133625	233804	47.68%	3.860%
20	10.407	729	733	736	rBV	217309	378443	77.18%	6.249%
21	10.457	736	737	739	rVB	7523	7916	1.61%	0.131%
22	10.508	739	741	743	rBV	5578	7946	1.62%	0.131%
23	11.269	798	801	803	rBV	14558	25038	5.11%	0.413%
24	11.307	803	804	809	rVB	4216	8939	1.82%	0.148%
25	11.484	816	818	821	rVB	12047	18500	3.77%	0.305%
26	12.003	922	931	943	rBV	45337	73004	14.89%	1.205%
27	12.632	1050	1054	1059	rBV	20452	37371	7.62%	0.617%
28	12.886	1071	1074	1077	rBV2	87974	146244	29.82%	2.415%
29	13.025	1081	1085	1089	rVV	21118	43544	8.88%	0.719%
30	13.140	1089	1094	1096	rVV3	11575	32039	6.53%	0.529%
31	13.178	1096	1097	1102	rVB	17618	28980	5.91%	0.479%
32	13.393	1111	1114	1119	rVB	7714	12465	2.54%	0.206%
33	13.584	1126	1129	1132	rVB	66130	109571	22.35%	1.809%
34	13.673	1132	1136	1139	rBV	5935	9702	1.98%	0.160%
35	13.749	1139	1142	1145	rVB	10638	16498	3.36%	0.272%
36	14.117	1168	1171	1173	rBV2	27821	48515	9.89%	0.801%

LSC Area Percent Report

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Sample : M3892-10
Misc :
ALS Vial : 52 Sample Multiplier: 2

Instrument : BNA_N
ClientSampleId : S-824-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	14.167	1173	1175	1180	rVB	21187	31634	6.45%	0.522%
38	14.269	1180	1183	1186	rBV	293006	431298	87.96%	7.121%
39	14.345	1186	1189	1192	rVB2	76593	112395	22.92%	1.856%
40	14.434	1193	1196	1197	rBV	9244	13725	2.80%	0.227%
41	14.472	1197	1199	1201	rVV	7128	9225	1.88%	0.152%
42	14.535	1201	1204	1207	rVV2	58687	97199	19.82%	1.605%
43	14.599	1207	1209	1213	rVB2	36892	64469	13.15%	1.064%
44	14.700	1213	1217	1219	rBV2	11218	20653	4.21%	0.341%
45	14.738	1219	1220	1222	rVB	5949	7458	1.52%	0.123%
46	14.802	1222	1225	1228	rBV2	12400	22257	4.54%	0.367%
47	15.005	1238	1241	1245	rVB	7219	11059	2.26%	0.183%
48	15.170	1251	1254	1256	rBV	55231	73750	15.04%	1.218%
49	15.411	1270	1273	1276	rBV	4708	11160	2.28%	0.184%
50	15.474	1276	1278	1280	rVB	4397	7246	1.48%	0.120%
51	15.652	1287	1292	1295	rBV2	42384	94041	19.18%	1.553%
52	15.753	1295	1300	1304	rVV2	67449	178413	36.39%	2.946%
53	15.855	1305	1308	1316	rVV	30225	72704	14.83%	1.200%
54	16.007	1317	1320	1322	rVV	93637	120864	24.65%	1.996%
55	16.081	1322	1326	1332	rVB	23612	41348	8.43%	0.683%
56	16.251	1334	1340	1346	rBV3	5824	19721	4.02%	0.326%
57	16.421	1352	1354	1359	rBV2	1929	6329	1.29%	0.105%
58	16.580	1365	1367	1370	rBV	15285	25458	5.19%	0.420%
59	16.835	1378	1388	1393	rBV5	7798	46976	9.58%	0.776%
60	17.018	1400	1403	1406	rBV	243251	354813	72.36%	5.858%
61	17.249	1418	1422	1425	rBV2	8742	28283	5.77%	0.467%
62	17.444	1425	1438	1444	rBV5	21185	194902	39.75%	3.218%
63	17.955	1477	1480	1483	rVB	15731	26044	5.31%	0.430%
64	19.063	1689	1696	1701	rBV	104912	144349	29.44%	2.383%
65	19.242	1728	1732	1746	rVB	11004	21429	4.37%	0.354%
66	19.460	1771	1776	1782	rBV	10221	13205	2.69%	0.218%
67	19.609	1799	1806	1814	rVV	5320	15042	3.07%	0.248%
68	19.679	1814	1820	1842	rVB	90604	122454	24.97%	2.022%
69	20.006	1884	1886	1899	rBV2	12694	56803	11.58%	0.938%
70	20.335	1914	1917	1918	rBV	6659	8464	1.73%	0.140%
71	20.378	1920	1921	1925	rVB	9348	11362	2.32%	0.188%
72	20.505	1930	1933	1935	rBV2	8191	13189	2.69%	0.218%
73	20.643	1943	1946	1948	rBV	5932	8552	1.74%	0.141%
74	20.792	1958	1960	1974	rVB	11292	18618	3.80%	0.307%
75	20.973	1974	1977	1985	rBV	50769	94792	19.33%	1.565%
76	21.164	1993	1995	1998	rBV	33742	47920	9.77%	0.791%

LSC Area Percent Report

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Acq On : 02 Oct 2021 23:09
Operator : CG/JU
Sample : M3892-10
Misc :
ALS Vial : 52 Sample Multiplier: 2

Instrument : BNA_N
ClientSampleId : S-824-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

77	21.228	1998	2001	2004	rVV	324501	490341	100.00%	8.096%
78	21.270	2004	2005	2010	rVB	25720	25394	5.18%	0.419%
79	21.408	2016	2018	2020	rBV	7236	9885	2.02%	0.163%
80	21.589	2033	2035	2038	rBV	8545	10372	2.12%	0.171%
81	21.875	2057	2062	2067	rBV	22368	55392	11.30%	0.915%
82	22.109	2081	2084	2090	rBV2	6915	13565	2.77%	0.224%
83	22.321	2101	2104	2107	rVB	8974	14244	2.90%	0.235%
84	22.557	2148	2156	2168	rVB	17014	23035	4.70%	0.380%
85	22.803	2220	2228	2235	rBV	15150	27207	5.55%	0.449%
86	22.848	2235	2241	2250	rVV2	19718	35153	7.17%	0.580%
87	22.903	2250	2257	2273	rVB	13154	27443	5.60%	0.453%
88	23.382	2389	2397	2403	rBV	11088	19416	3.96%	0.321%
89	23.485	2415	2427	2465	rVB	247512	488572	99.64%	8.067%
90	24.087	2595	2603	2619	rVB	9162	18331	3.74%	0.303%
91	24.190	2622	2633	2668	rBV	20318	66902	13.64%	1.105%
92	24.549	2730	2738	2765	rVB	6093	14925	3.04%	0.246%
93	24.857	2820	2828	2853	rVB	7678	18437	3.76%	0.304%
94	25.774	3077	3096	3126	rBV4	14790	54182	11.05%	0.895%
95	25.928	3133	3141	3154	rBV	1959	5467	1.11%	0.090%
96	26.459	3281	3296	3328	rVB2	6461	20968	4.28%	0.346%
97	26.637	3331	3348	3376	rBV	6378	23781	4.85%	0.393%

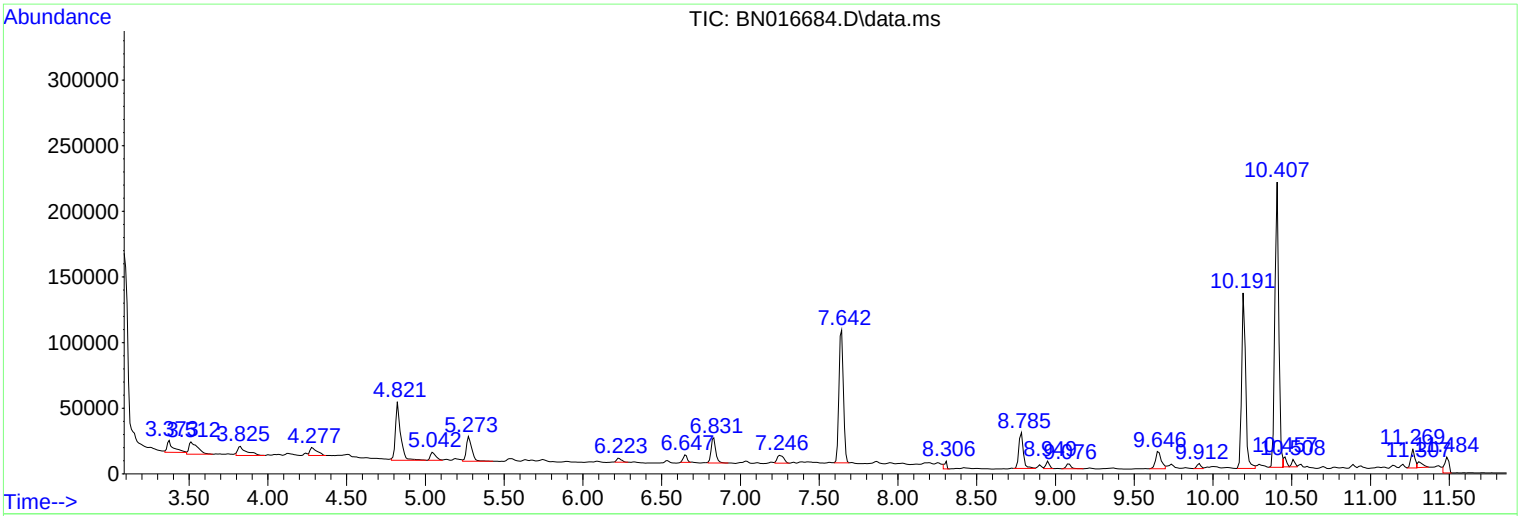
Sum of corrected areas: 6056425

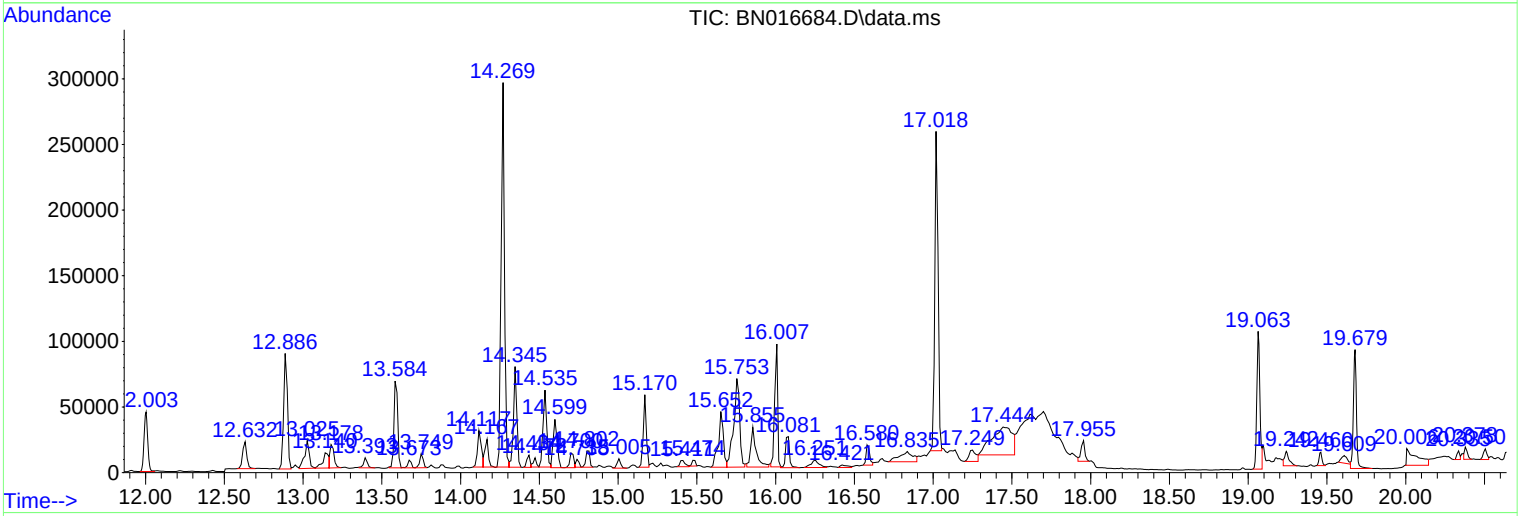
Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016684.D
Acq On : 02 Oct 2021 23:09
Operator : CG/JU
Sample : M3892-10
Misc :
ALS Vial : 52 Sample Multiplier: 2

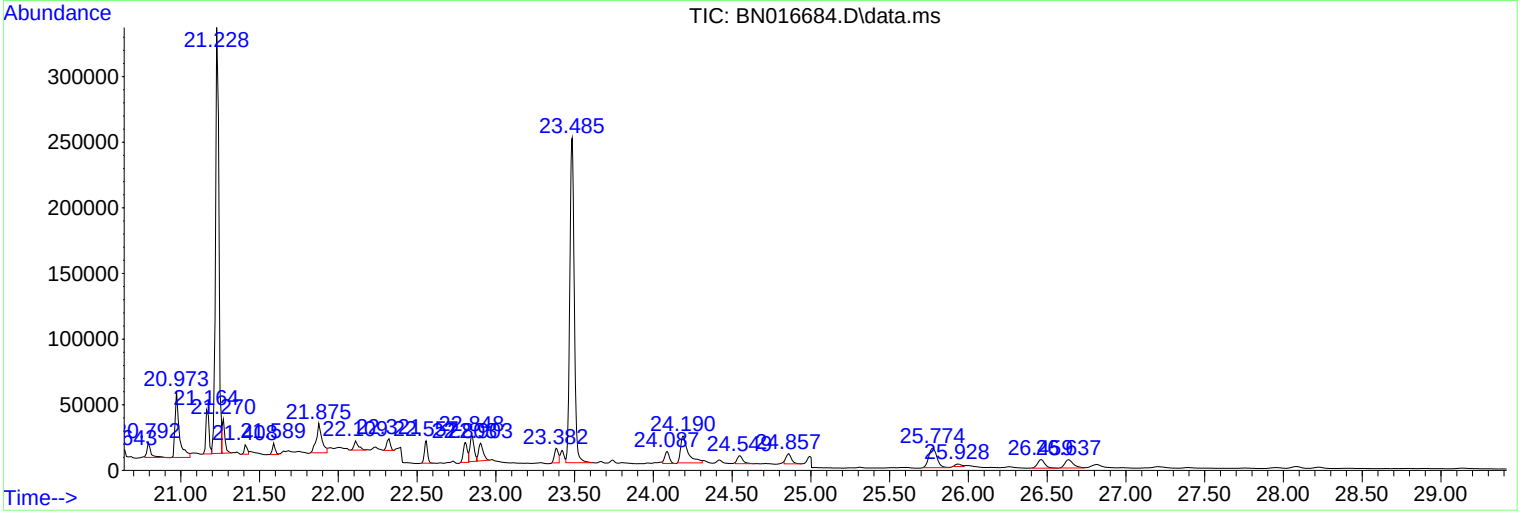
Instrument :
BNA_N
ClientSampleId :
S-824-N-SO-1-1.5-092221

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

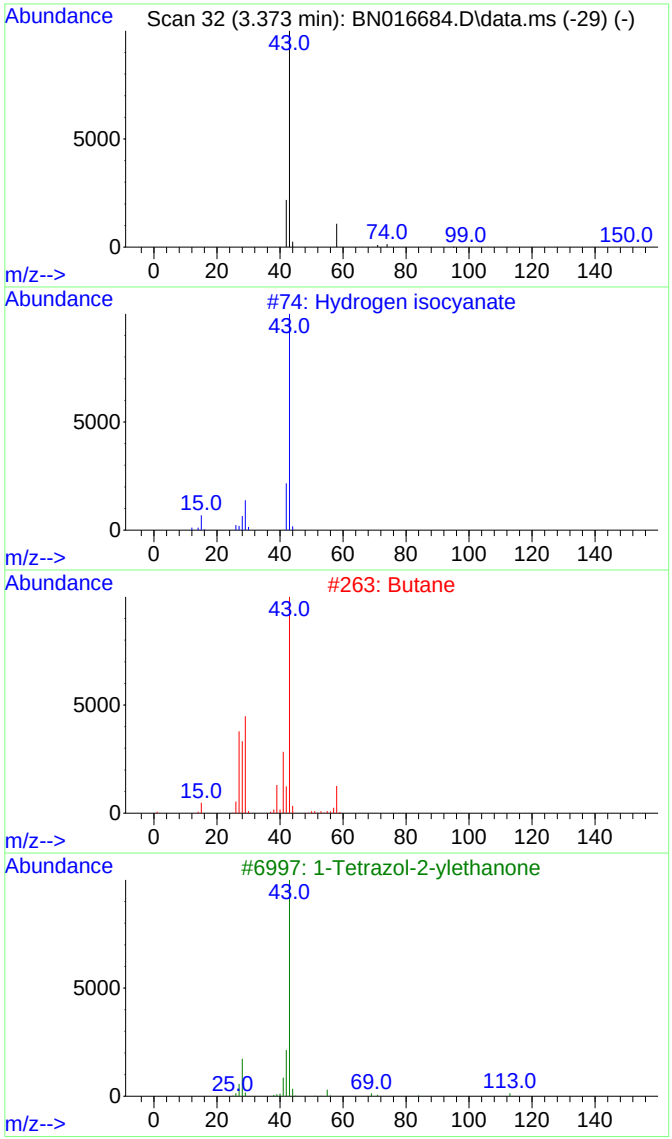
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

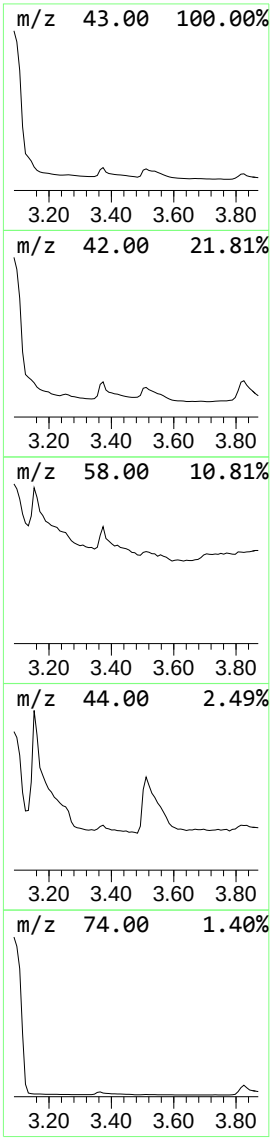
****

Peak Number 1 Hydrogen isocyanate Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.373	0.10 ng	24529	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrogen isocyanate	43	CHNO	000075-13-8	4
2	Butane	58	C4H10	000106-97-8	4
3	1-Tetrazol-2-ylethanone	112	C3H4N4O	051410-11-8	2
4	N-Acetylethylenediamine	102	C4H10N2O	001001-53-2	2
5	Hydrogen azide	43	HN3	007782-79-8	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Acq On : 02 Oct 2021 23:09
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S-824-N-SO-1-1.5-092221

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

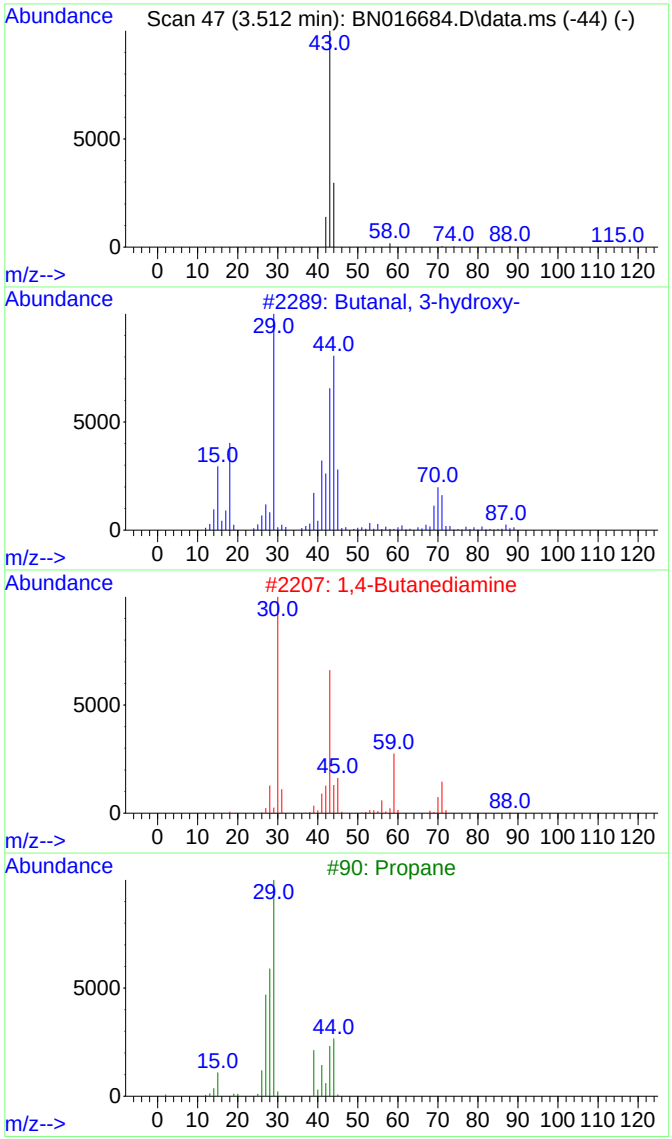
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

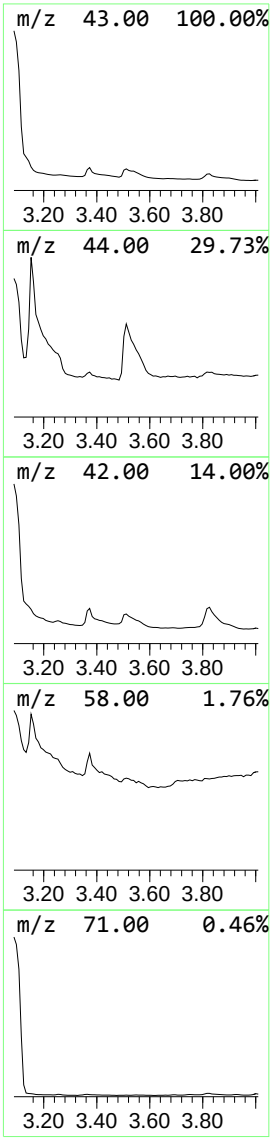
****

Peak Number 2 Butanal, 3-hydroxy- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.512	0.14 ng	35326	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal, 3-hydroxy-	88	C4H8O2	000107-89-1	4
2	1,4-Butanediamine	88	C4H12N2	000110-60-1	4
3	Propane	44	C3H8	000074-98-6	3
4	Hydrogen azide	43	HN3	007782-79-8	3
5	Isobutane	58	C4H10	000075-28-5	2





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ALS Vial : 52 Sample Multiplier: 2

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

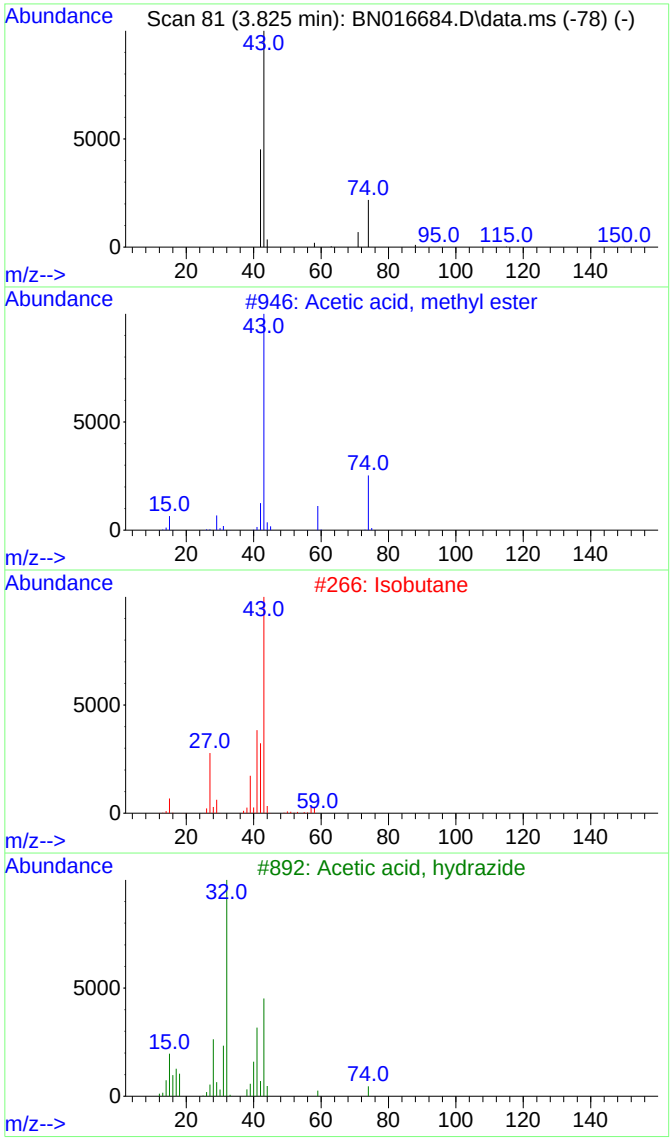
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

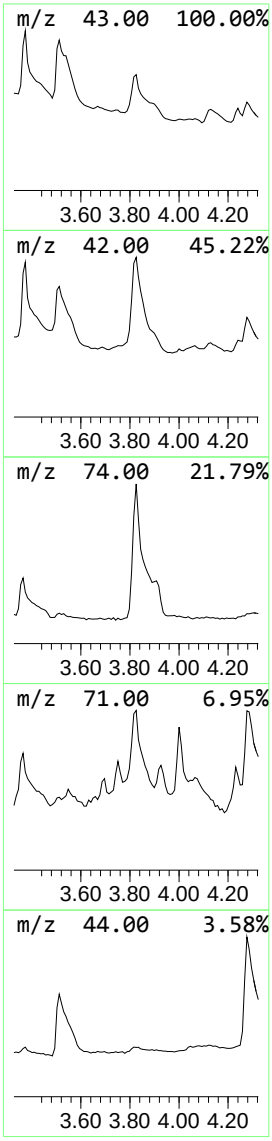
****

Peak Number 3 Acetic acid, methyl ester Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.825	0.11 ng	26343	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	5
2	Isobutane	58	C4H10	000075-28-5	3
3	Acetic acid, hydrazide	74	C2H6N2O	001068-57-1	3
4	1,4-Butanediamine	88	C4H12N2	000110-60-1	3
5	Ethyl ether	74	C4H10O	000060-29-7	3





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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

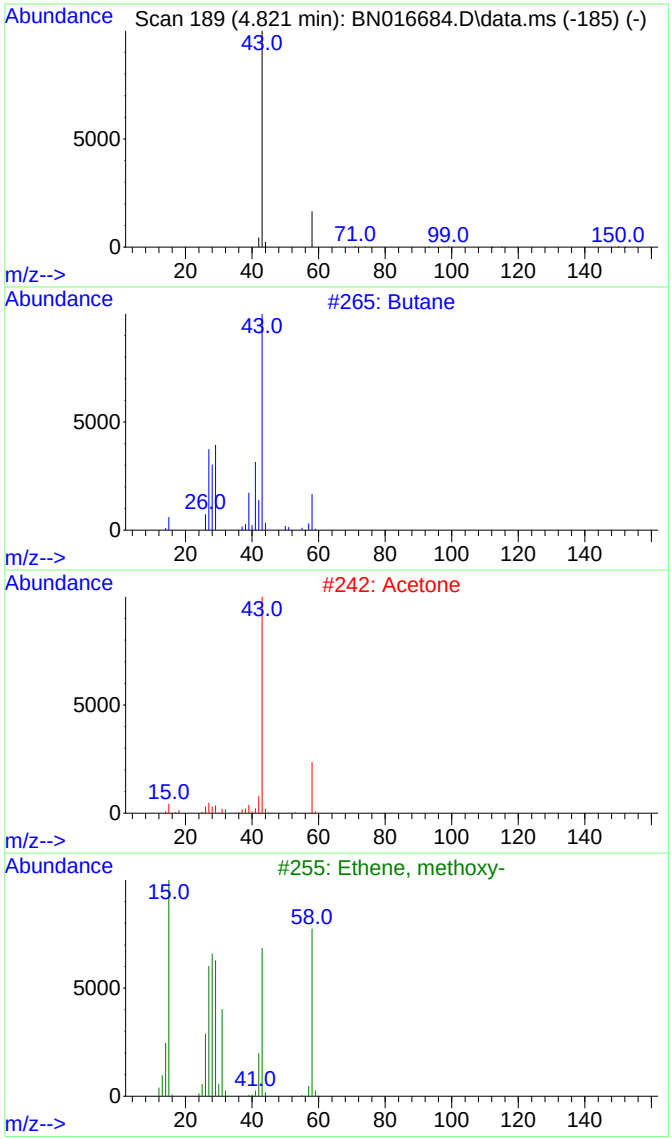
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

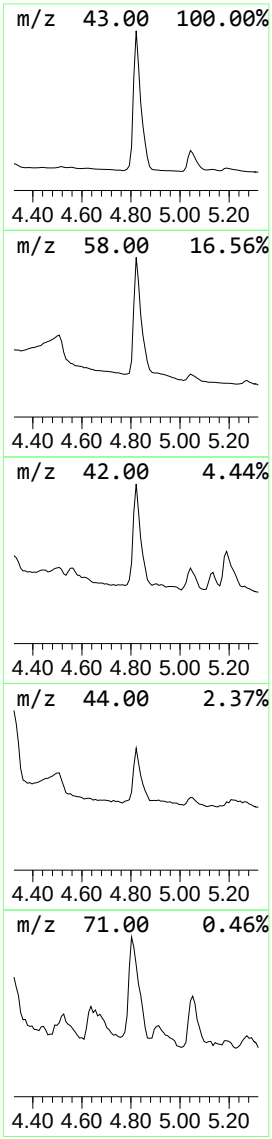
****

Peak Number 4 Butane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.40 ng	100143	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





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016684.D
Acq On : 02 Oct 2021 23:09
Operator : CG/JU
Sample : M3892-10
Misc :
ALS Vial : 52 Sample Multiplier: 2

Instrument :
BNA_N
ClientSampleId :
S-824-N-SO-1-1.5-092221

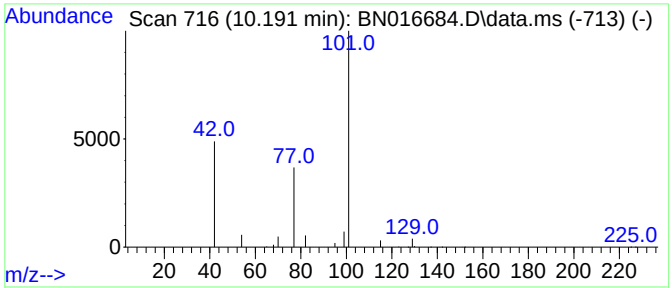
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

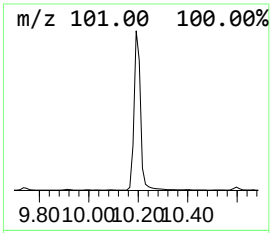
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

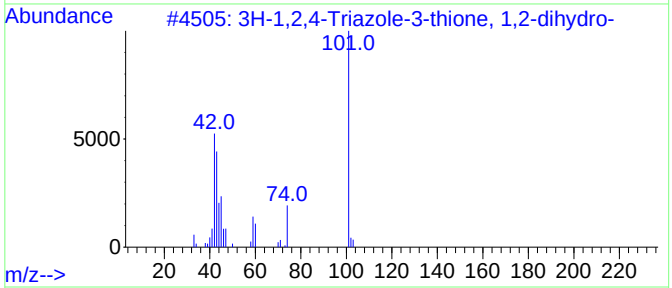
****
Peak Number 5 3H-1,2,4-Triazole-3-thione,... Concentration Rank 1

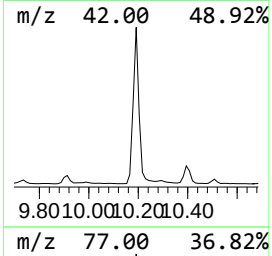
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.49 ng	233804	Naphthalene-d8	10.407

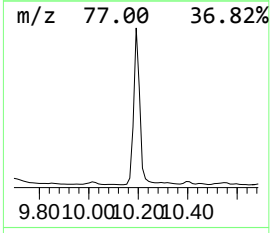
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
2	2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	5
3	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	5
4	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5
5	3-Aminopropionitrile	70	C3H6N2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

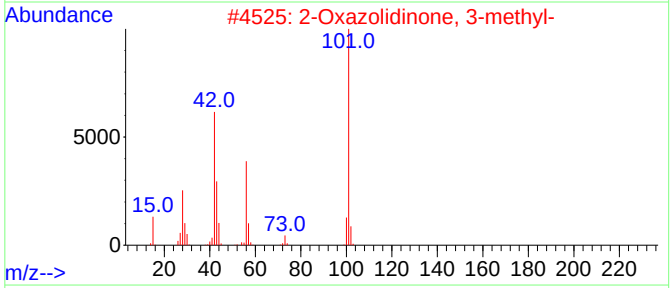


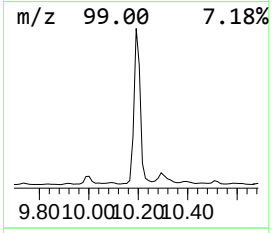


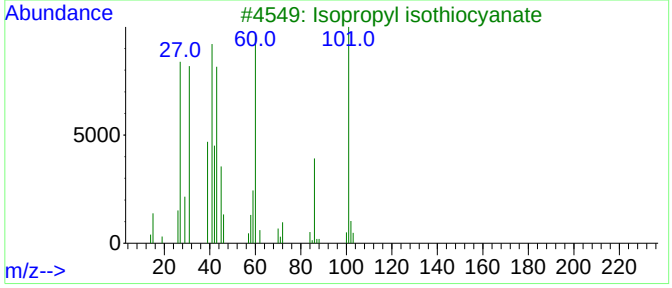


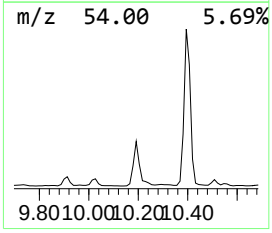












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Acq On : 02 Oct 2021 23:09
Operator : CG/JU
Sample : M3892-10
Misc :
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Instrument :
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ClientSampleId :
S-824-N-SO-1-1.5-092221

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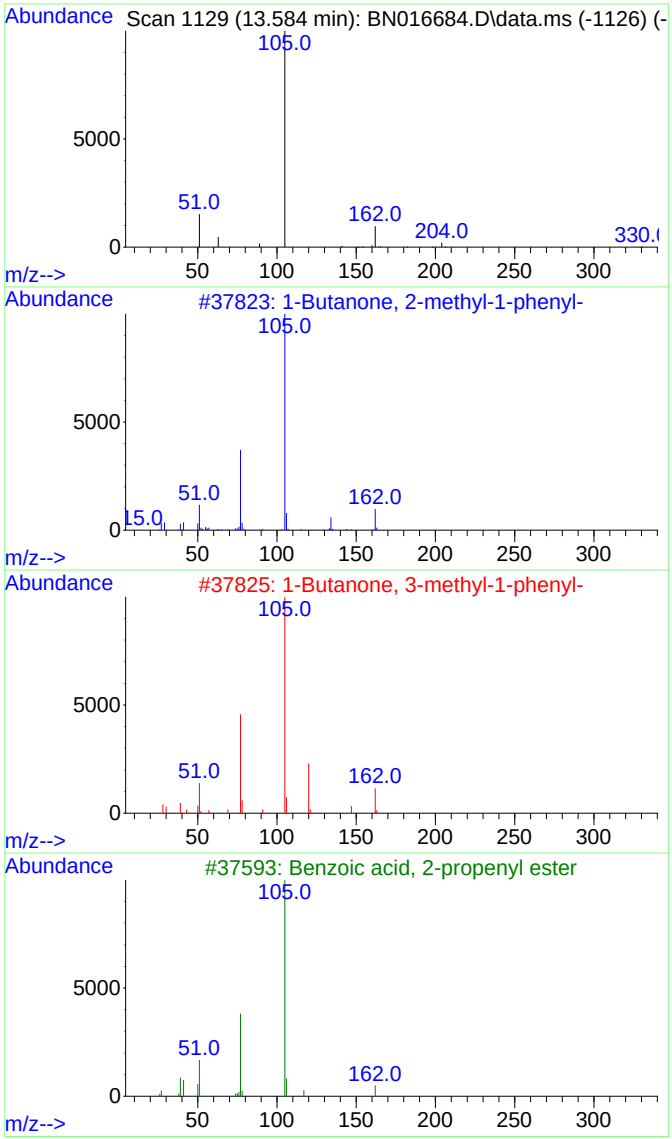
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

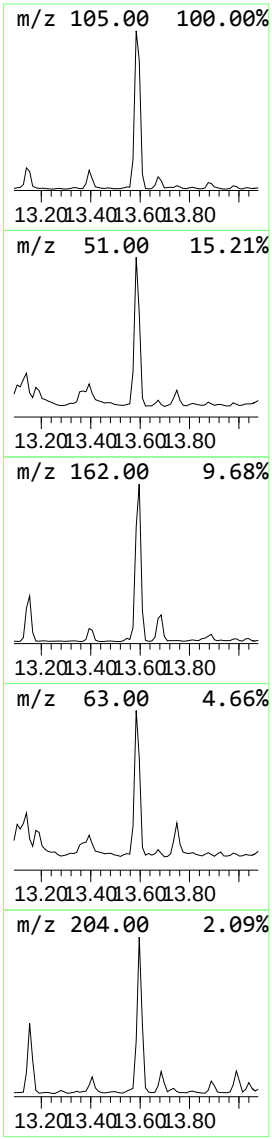
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Butanone, 2-methyl-1-phenyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.584	0.20 ng	109571	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	Benzene, (1,3-dimethyl-3-butenyl)-	160	C12H16	056851-51-5	4





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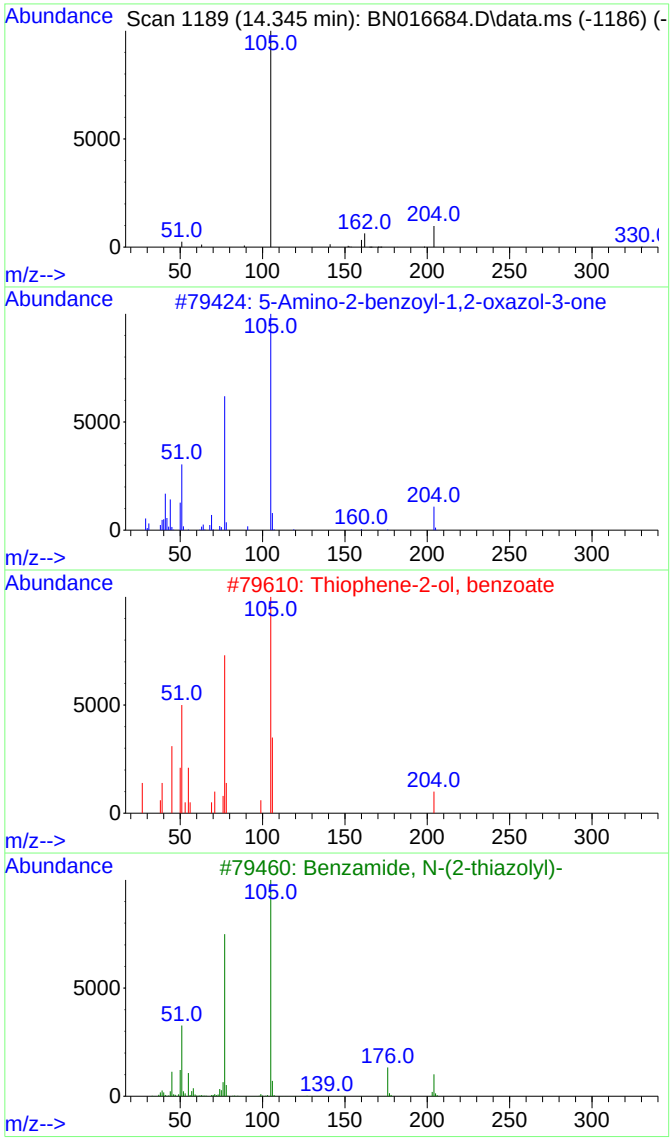
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

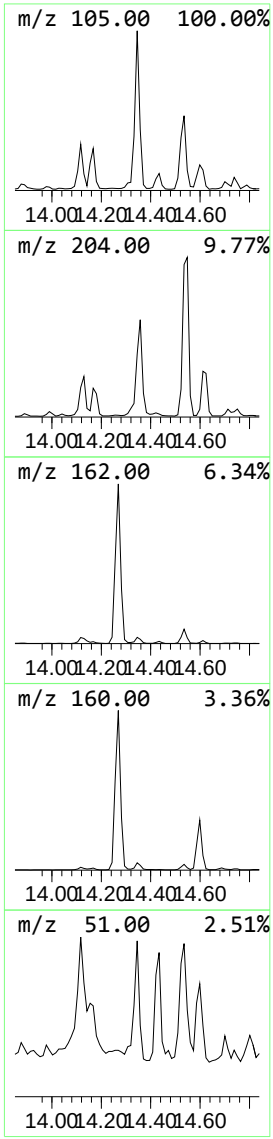
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 5-Amino-2-benzoyl-1,2-oxazo... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.345	0.21 ng	112395	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	Thiophene-2-ol, benzoate	204	C11H8O2S	016693-98-4	4
3	Benzamide, N-(2-thiazolyl)-	204	C10H8N2OS	013053-82-2	4
4	1,3,5-Hexanetrione, 1-phenyl-	204	C12H12O3	001469-95-0	3
5	Benzoic acid, 2-propenyl ester	162	C10H10O2	000583-04-0	3





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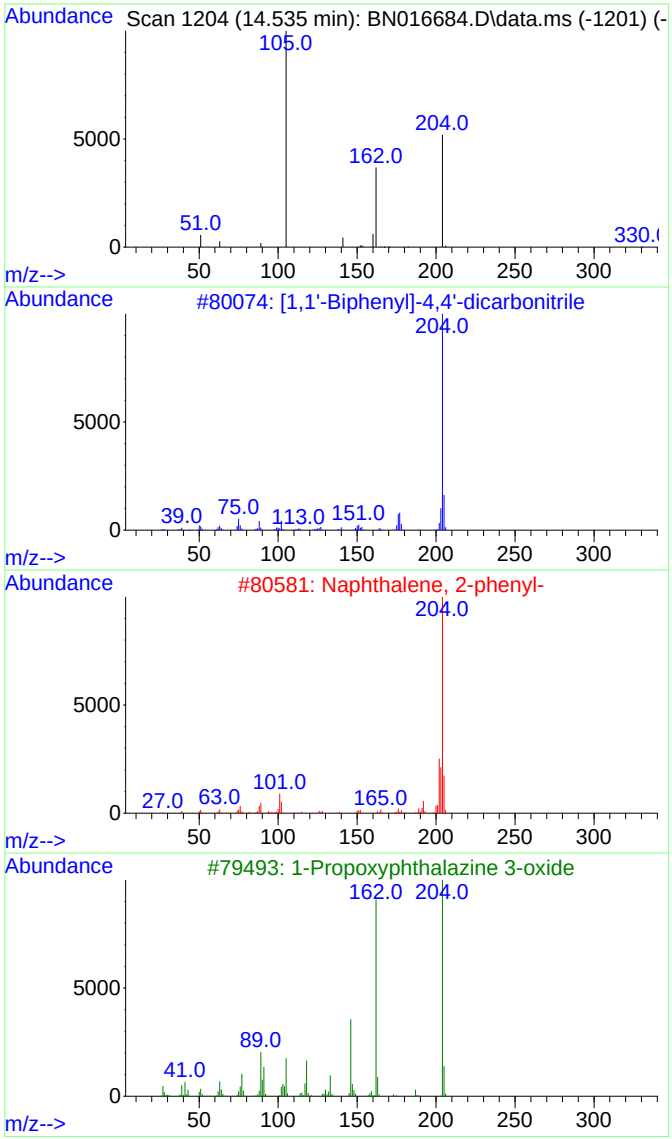
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

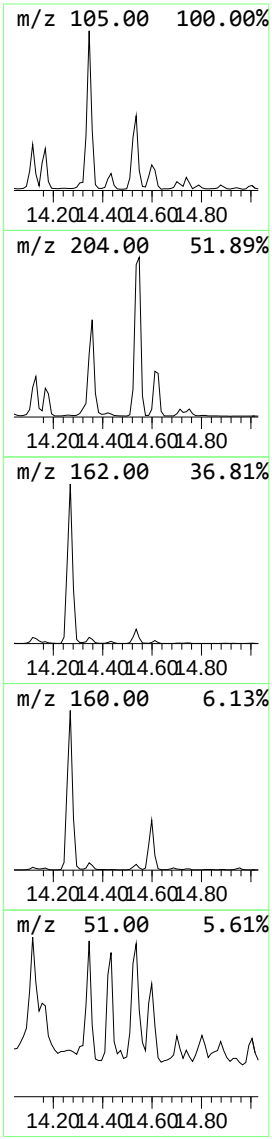
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 [1,1'-Biphenyl]-4,4'-dicarb... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.535	0.18 ng	97199	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	[1,1'-Biphenyl]-4,4'-dicarbonitrile	204	C14H8N2	001591-30-6	9
2	Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	7
3	1-Propoxyphthalazine 3-oxide	204	C11H12N2O2	091350-93-5	7
4	Coumarin, 3,4-dihydro-4,4,6,8-te...	204	C13H16O2	249629-60-5	7
5	Naphthalene, 1-phenyl-	204	C16H12	000605-02-7	7





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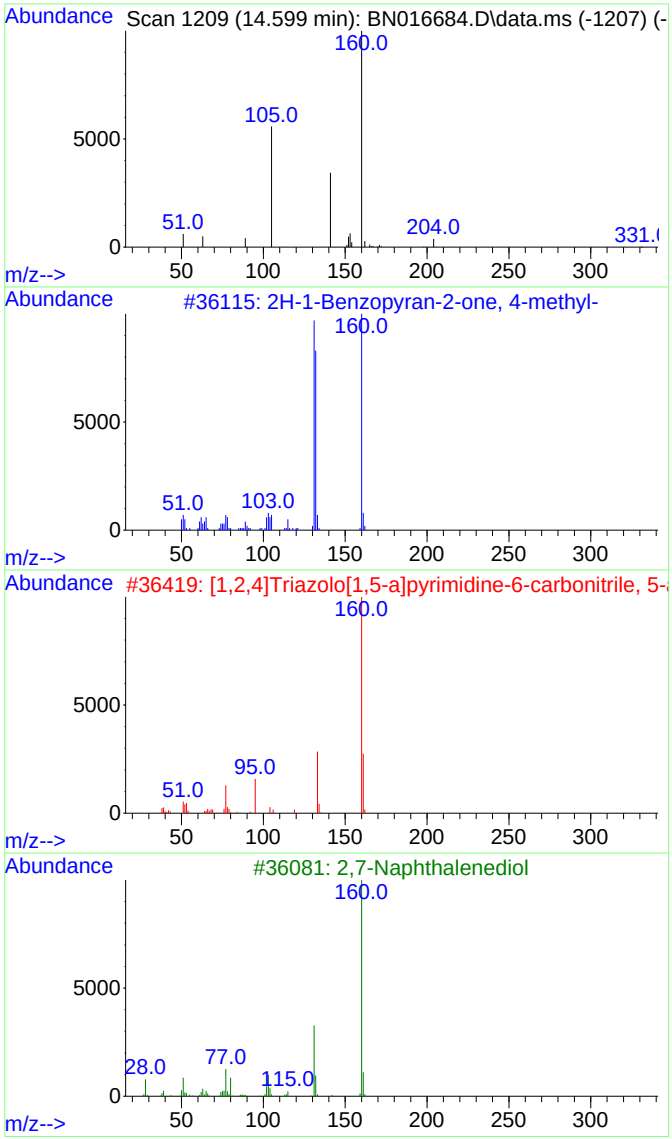
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

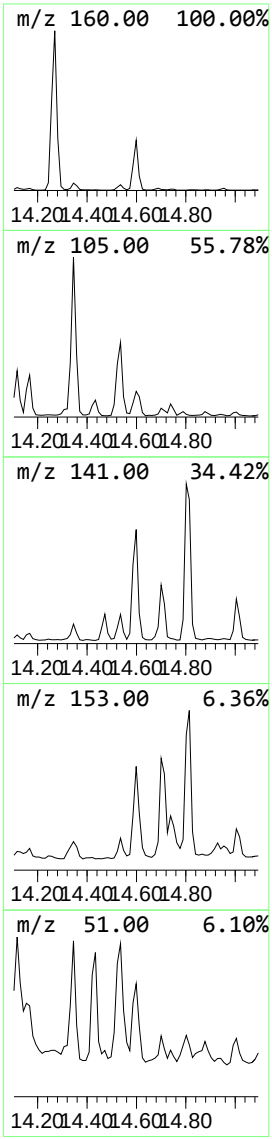
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 2H-1-Benzopyran-2-one, 4-me... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.599	0.12 ng	64469	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	2,7-Naphthalenediol	160	C10H8O2	000582-17-2	5
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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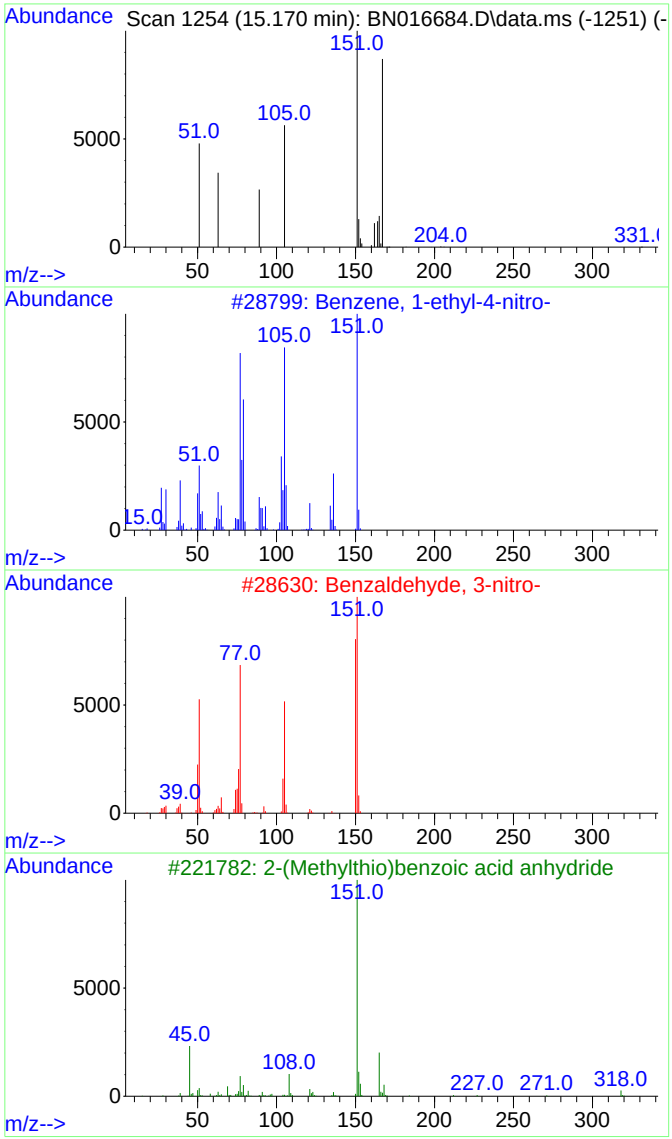
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

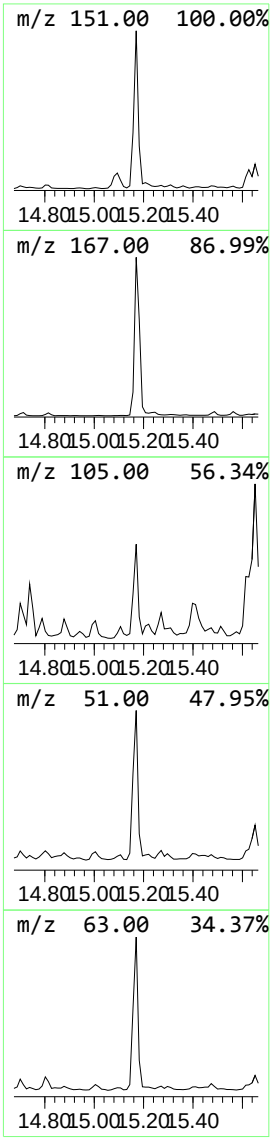
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 1-ethyl-4-nitro- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.170	0.14 ng	73750	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-4-nitro-	151	C8H9NO2	000100-12-9	38
2	Benzaldehyde, 3-nitro-	151	C7H5NO3	000099-61-6	25
3	2-(Methylthio)benzoic acid anhyd...	318	C16H14O3S2	1000374-99-4	10
4	D-4,4'-Biphenylalanine	241	C15H15NO2	170080-13-4	10
5	1H-Indole, 4-chloro-	151	C8H6ClN	025235-85-2	9





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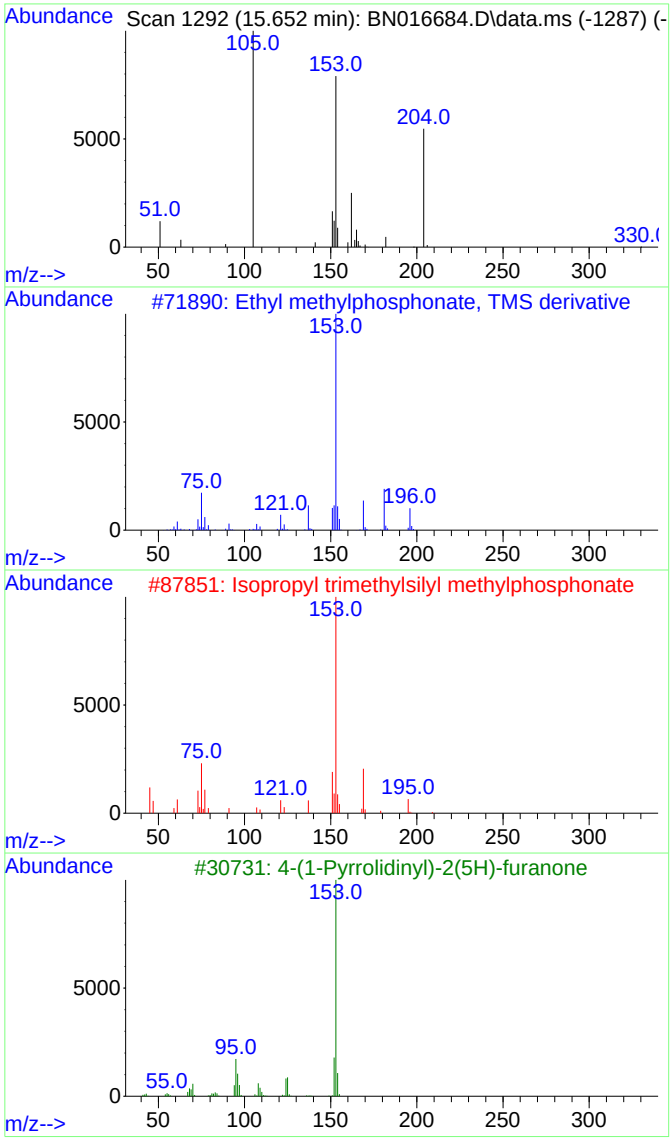
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

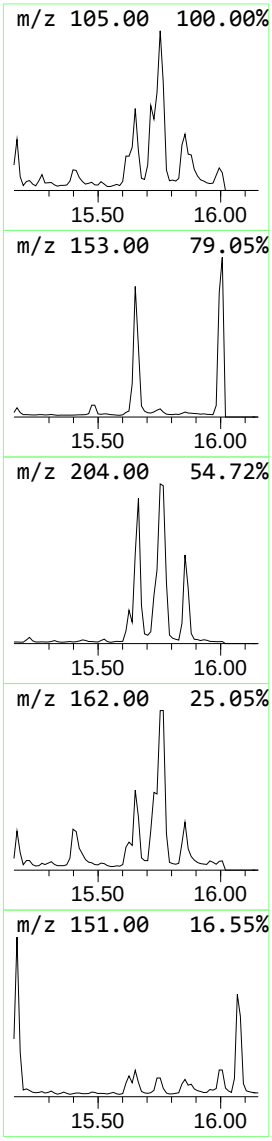
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Ethyl methylphosphonate, TM... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.652	0.21 ng	94041	Phenanthrene-d10	17.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl methylphosphonate, TMS der...	196	C6H17O3PSi	057451-30-6	37
2	Isopropyl trimethylsilyl methylp...	210	C7H19O3PSi	199116-08-0	25
3	4-(1-Pyrrolidinyl)-2(5H)-furanone	153	C8H11NO2	1000427-46-1	9
4	Benzenamine, 3,5-dimethoxy-	153	C8H11NO2	010272-07-8	9
5	Pyridine-2,4-diol, 3,5,6-trimethyl-	153	C8H11NO2	109371-16-6	9





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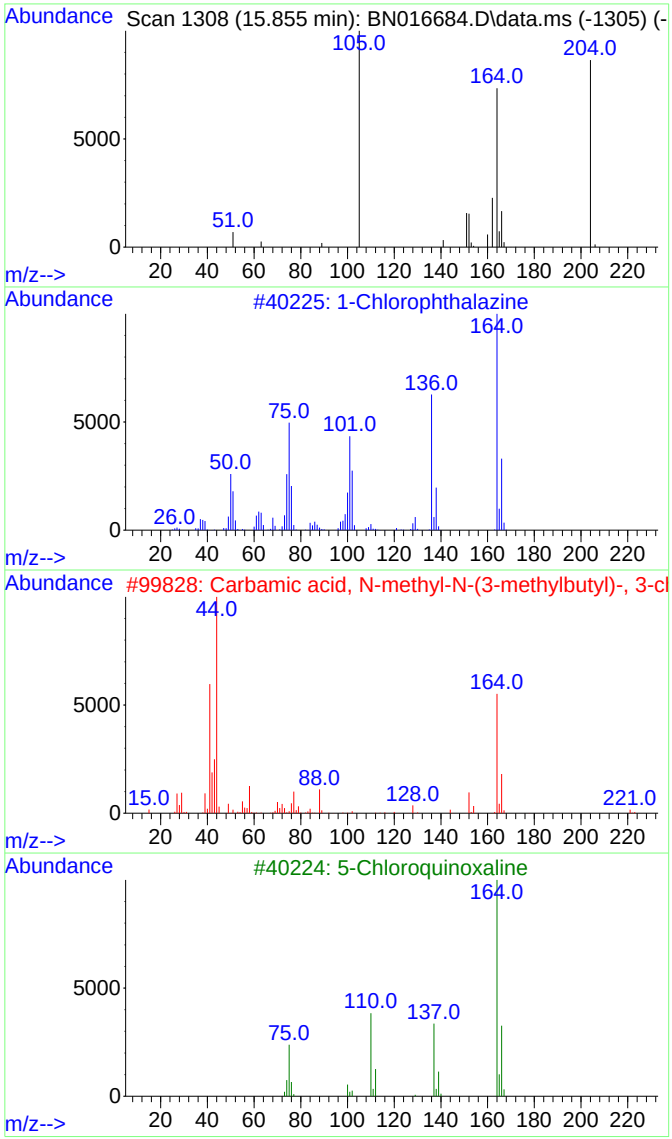
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

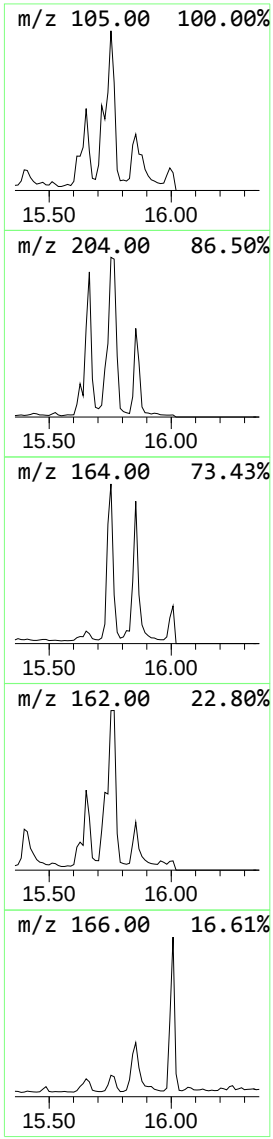
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 1-Chlorophthalazine Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.855	0.16 ng	72704	Phenanthrene-d10	17.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Chlorophthalazine	164	C8H5ClN2	005784-45-2	16
2	Carbamic acid, N-methyl-N-(3-met...	221	C10H20ClNO2	1010437-32-0	16
3	5-Chloroquinoxaline	164	C8H5ClN2	062163-09-1	16
4	Tetracyano-p-quinodimethane	204	C12H4N4	001518-16-7	9
5	4-Chloro-1,5-naphthyridine	164	C8H5ClN2	007689-63-6	9





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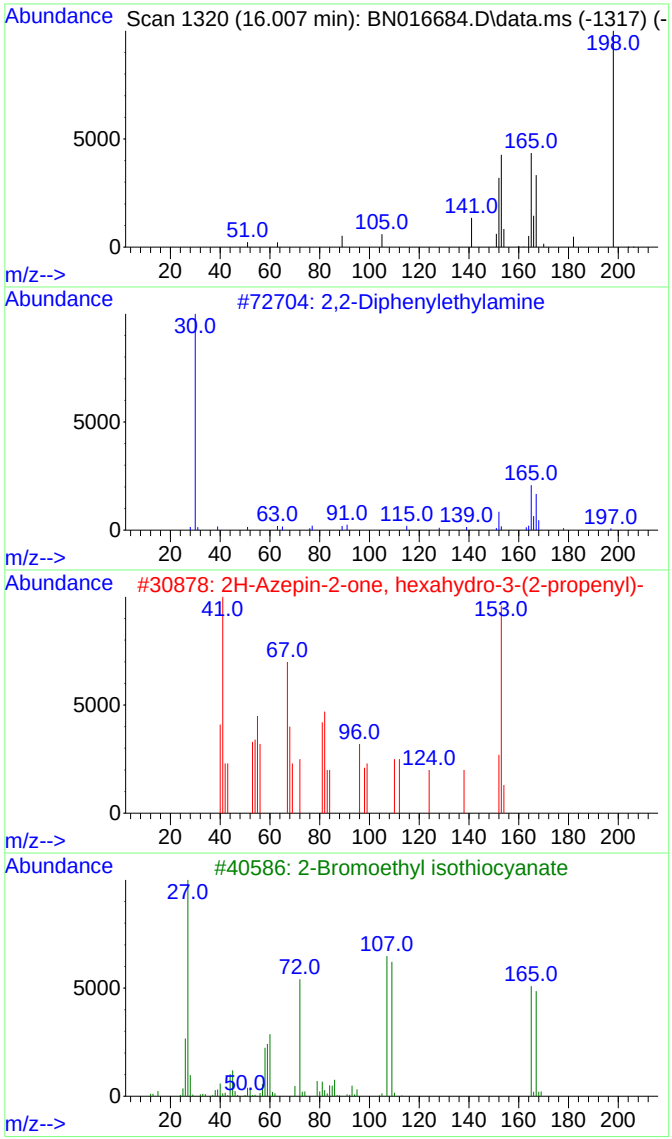
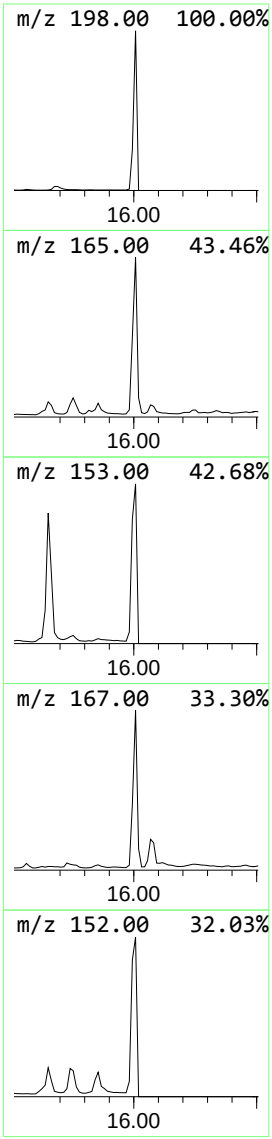
Peak Number 13 2,2-Diphenylethylamine Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.007	0.27 ng	120864	Phenanthrene-d10	17.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2-Diphenylethylamine	197	C14H15N	003963-62-0	9
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	Z-2-Propenoic acid, 3-iodo-	198	C3H3IO2	1000308-86-8	4





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Misc :
ALS Vial : 52 Sample Multiplier: 2

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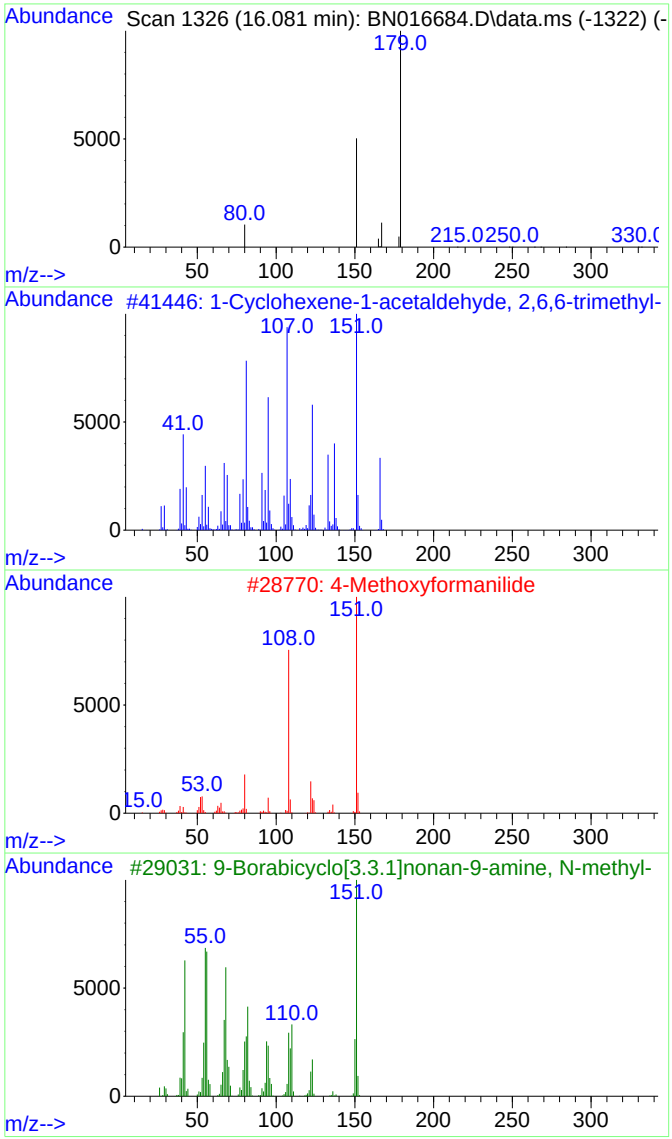
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

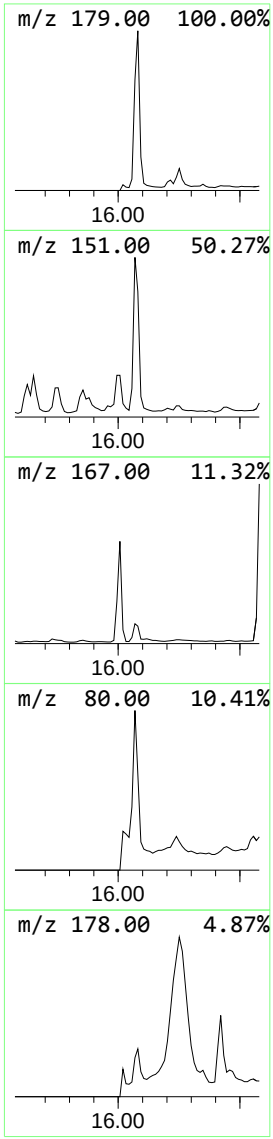
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 1-Cyclohexene-1-acetaldehyd... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.081	0.09 ng	41348	Phenanthrene-d10	17.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Cyclohexene-1-acetaldehyde, 2,...	166	C11H18O	000472-66-2	5
2	4-Methoxyformanilide	151	C8H9NO2	005470-34-8	4
3	9-Borabicyclo[3.3.1]nonan-9-amin...	151	C9H18BN	063366-66-5	4
4	Thiazolo[5,4-d]pyrimidine, 5-met...	151	C6H5N3S	013554-89-7	4
5	Benzofuran-4(5H)-one, 6,7-dihydr...	151	C8H9NO2	061190-46-3	4





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TIC Integration Parameters: LSCINT.P

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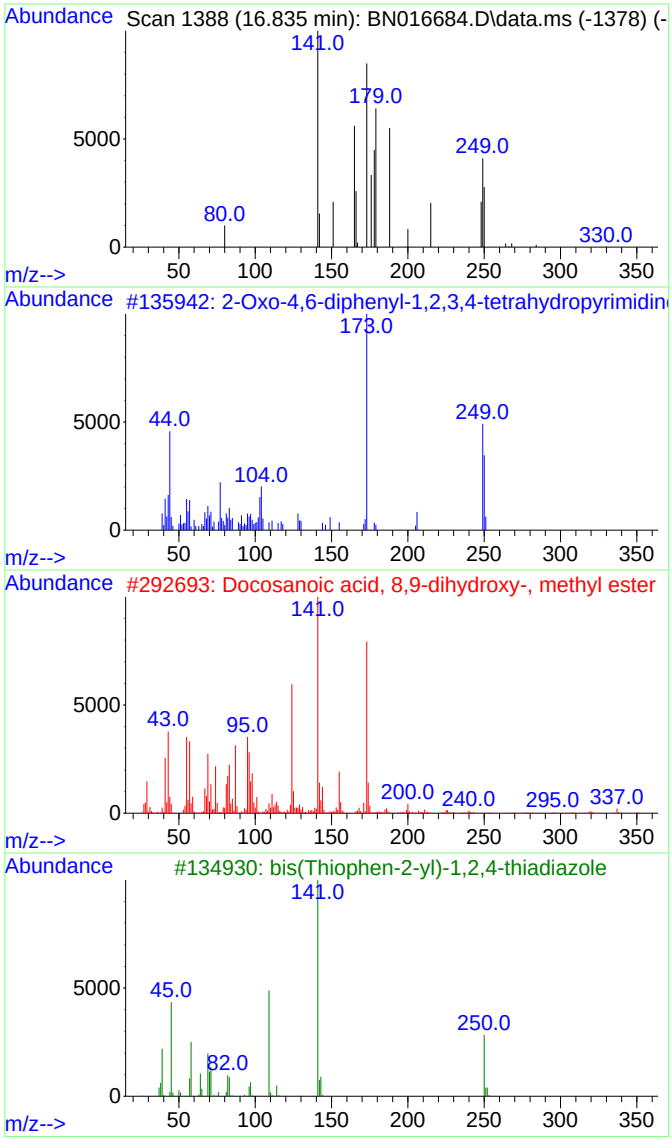
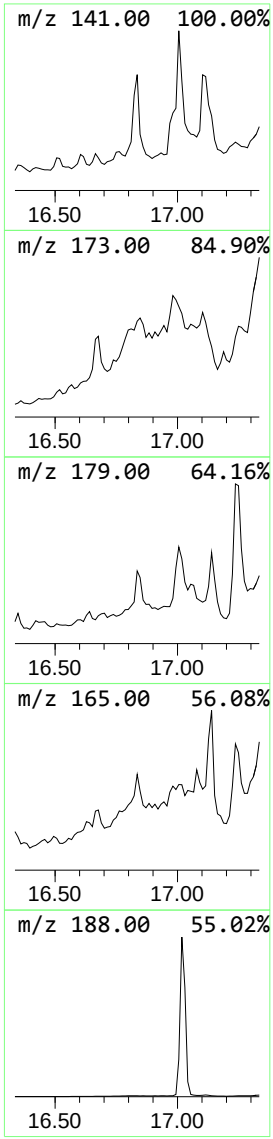
Peak Number 15 2-Oxo-4,6-diphenyl-1,2,3,4-... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.835	0.11 ng	46976	Phenanthrene-d10	17.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Oxo-4,6-diphenyl-1,2,3,4-tetra...	250	C16H14N2O	004113-79-5	10
2	Docosanoic acid, 8,9-dihydroxy-,...	386	C23H46O4	056555-06-7	10
3	bis(Thiophen-2-yl)-1,2,4-thiadia...	250	C10H6N2S3	089767-78-2	9
4	Oxazole, 2-ethyl-4,5-diphenyl-	249	C17H15NO	020662-94-6	9
5	Naphthalene, 1-(chloromethyl)-	176	C11H9Cl	000086-52-2	9





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Acq On : 02 Oct 2021 23:09
Operator : CG/JU
Sample : M3892-10
Misc :
ALS Vial : 52 Sample Multiplier: 2

Instrument :
BNA_N
ClientSampleId :
S-824-N-SO-1-1.5-092221

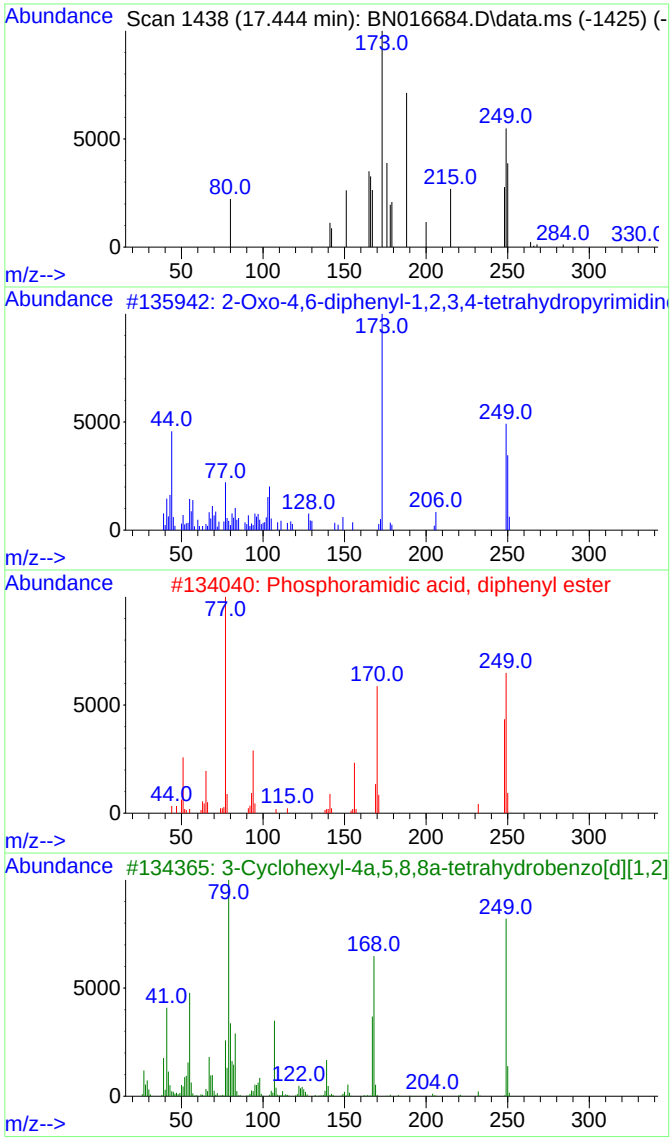
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

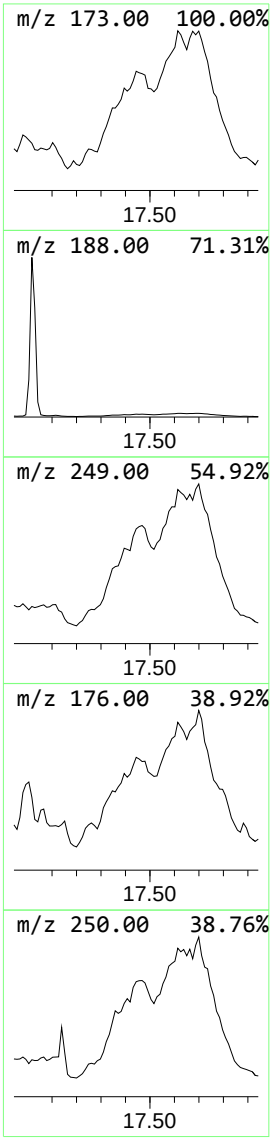
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 2-Oxo-4,6-diphenyl-1,2,3,4-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.444	0.44 ng	194902	Phenanthrene-d10	17.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Oxo-4,6-diphenyl-1,2,3,4-tetra...	250	C16H14N2O	004113-79-5	25
2	Phosphoramidic acid, diphenyl ester	249	C12H12NO3P	002015-56-7	9
3	3-Cyclohexyl-4a,5,8,8a-tetrahydr...	249	C14H19NO3	063013-26-3	9
4	Naphthalene, 1,2,3,4-tetrahydro-...	188	C14H20	081603-43-2	9
5	(1,5-Cyclooctanediylboryl)-.eta....	249	C14H24BNS	1000161-66-4	9





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Operator : CG/JU
Sample : M3892-10
Misc :
ALS Vial : 52 Sample Multiplier: 2

Instrument :
BNA_N
ClientSampleId :
S-824-N-SO-1-1.5-092221

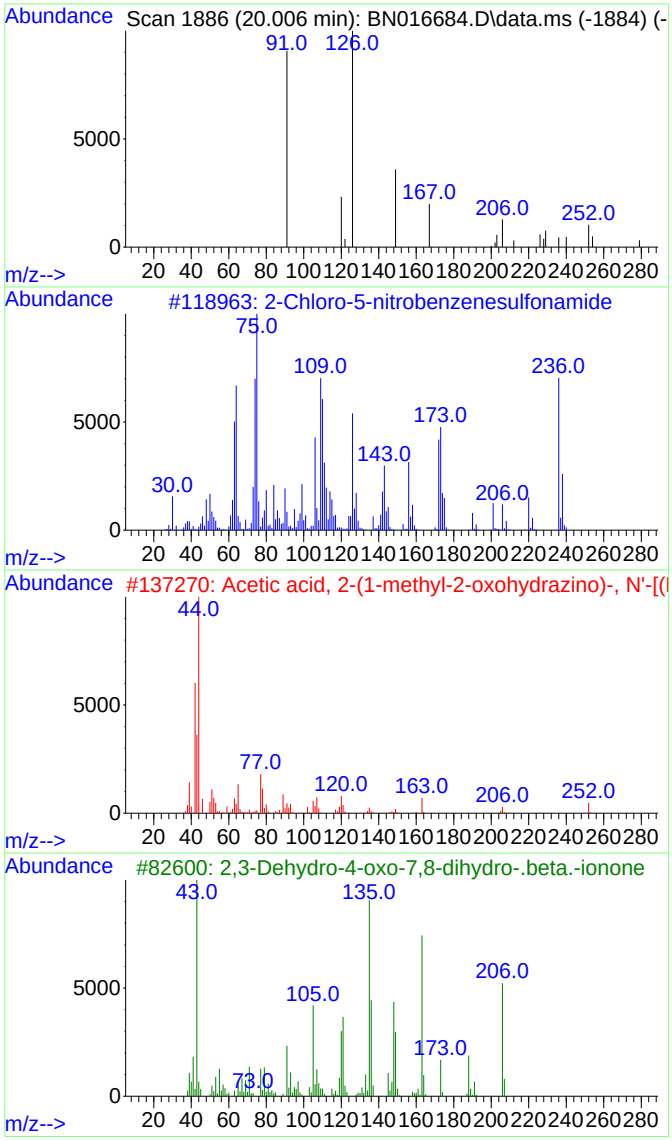
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

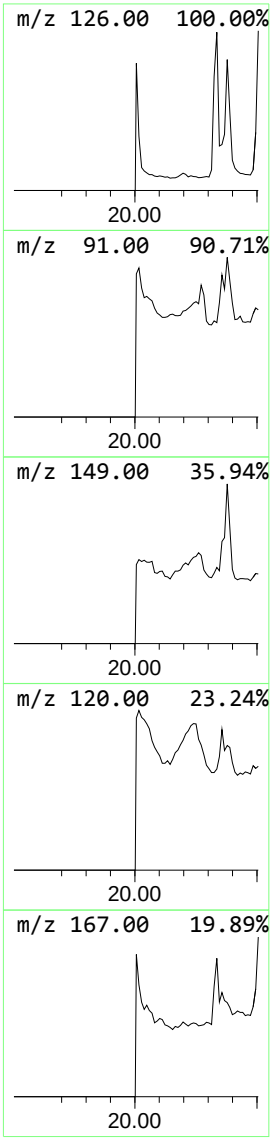
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 2-Chloro-5-nitrobenzenesulf... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.006	0.09 ng	56803	Chrysene-d12	21.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chloro-5-nitrobenzenesulfonamide	236	C6H5ClN2O4S	000096-72-0	5
2	Acetic acid, 2-(1-methyl-2-oxohy...	252	C10H12N4O4	1000327-59-6	5
3	2,3-Dehydro-4-oxo-7,8-dihydro-.b...	206	C13H18O2	083646-60-0	5
4	Octanehydrazide, N2-(2-thenylide...	252	C13H20N2OS	339302-09-9	5
5	1-Methoxy-4-methyl-2-nitrobenzene	167	C8H9NO3	000119-10-8	4





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Acq On : 02 Oct 2021 23:09
Operator : CG/JU
Sample : M3892-10
Misc :
ALS Vial : 52 Sample Multiplier: 2

Instrument : BNA_N
ClientSampleId : S-824-N-SO-1-1.5-092221

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

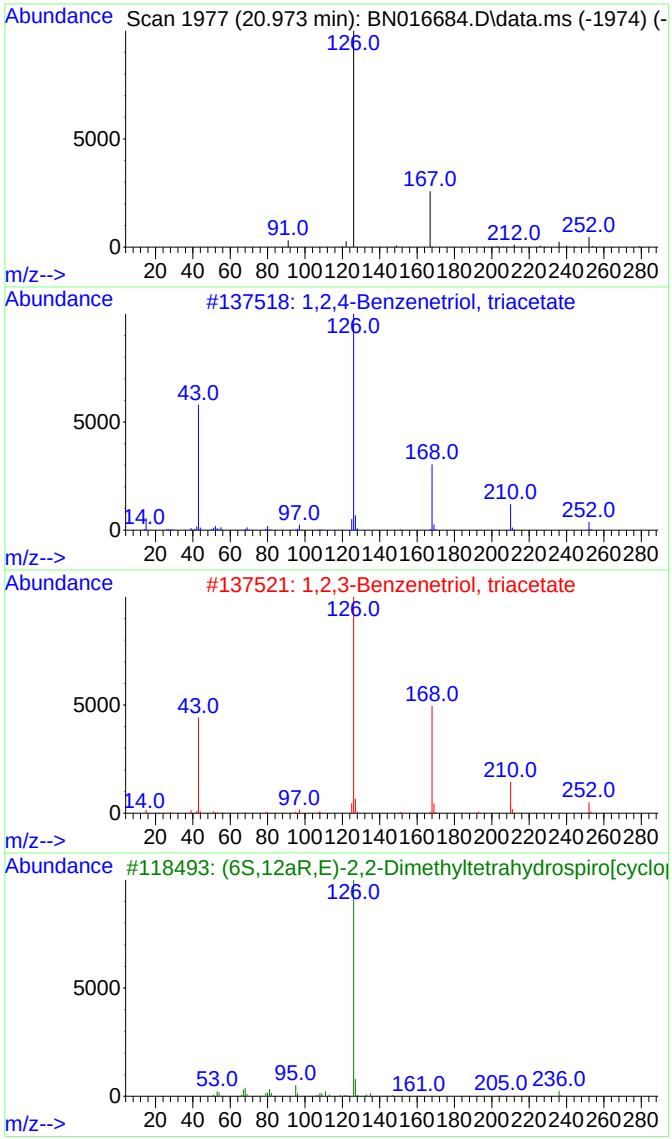
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

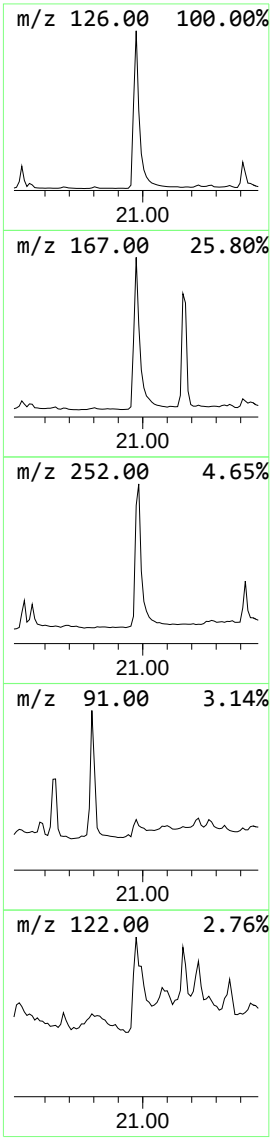
****

Peak Number 18 1,2,4-Benzenetriol, triacetate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.973	0.15 ng	94792	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	(6S,12aR,E)-2,2-Dimethyltetrahyd...	236	C14H24N2O	155975-43-2	4
4	Phloroglucinol triacetate	252	C12H12O6	002999-40-8	4
5	cis-6-Octadecenoic acid, 4,4-dim...	335	C22H41NO	1000333-21-8	4





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ALS Vial : 52 Sample Multiplier: 2

Instrument :
BNA_N
ClientSampleId :
S-824-N-SO-1-1.5-092221

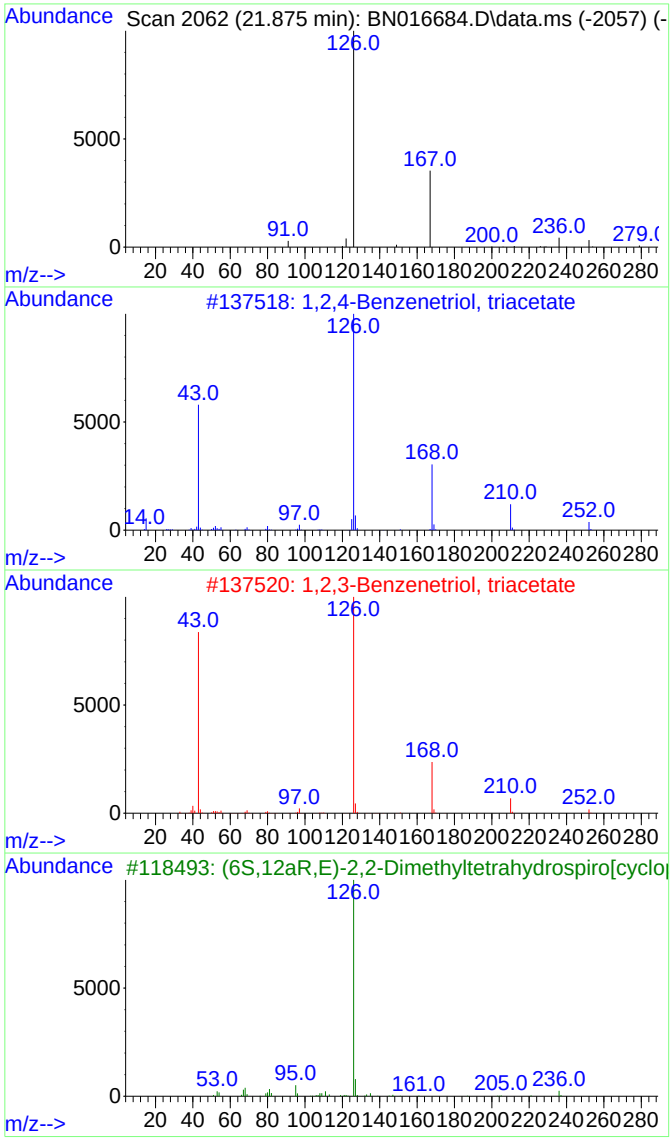
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

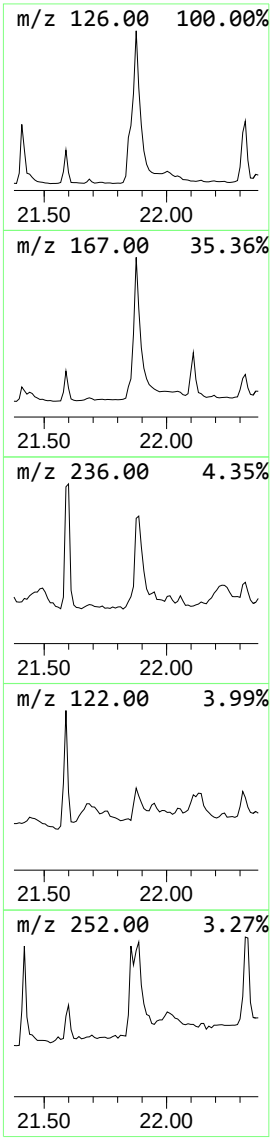
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 1,2,4-Benzenetriol, triacetate Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.875	0.09 ng	55392	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	(6S,12aR,E)-2,2-Dimethyltetrahyd...	236	C14H24N2O	155975-43-2	4
4	Phloroglucinol triacetate	252	C12H12O6	002999-40-8	4
5	4(1H)-Oxopyridine-1-carboxylic a...	167	C8H9NO3	057330-83-3	4





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Acq On : 02 Oct 2021 23:09
Operator : CG/JU
Sample : M3892-10
Misc :
ALS Vial : 52 Sample Multiplier: 2

Instrument :
BNA_N
ClientSampleId :
S-824-N-SO-1-1.5-092221

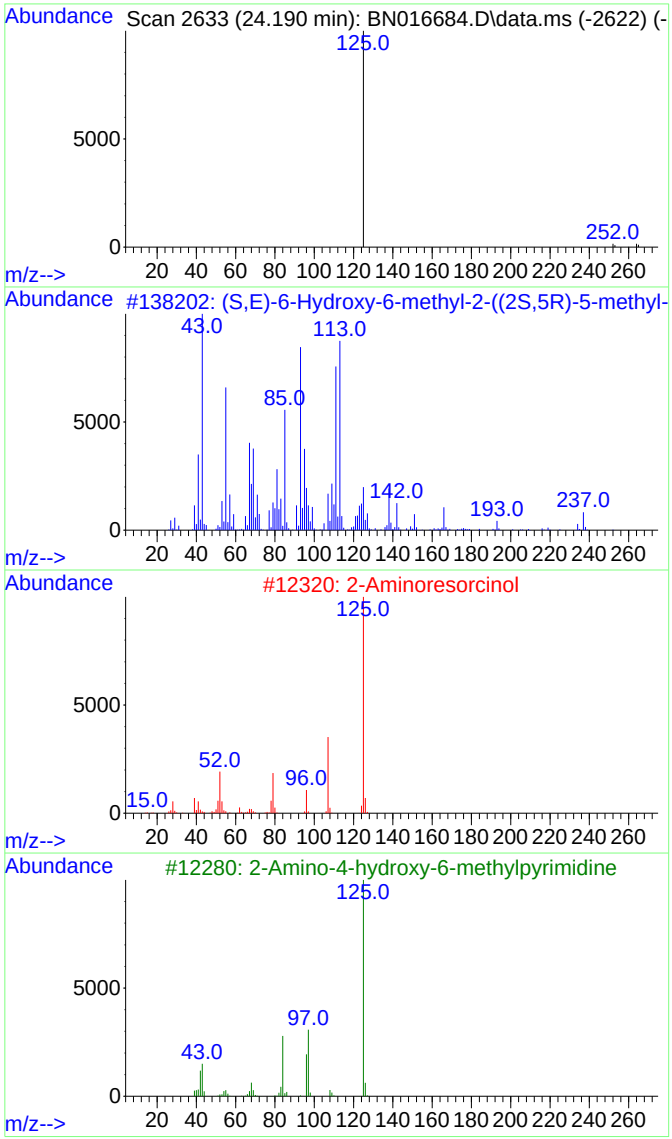
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

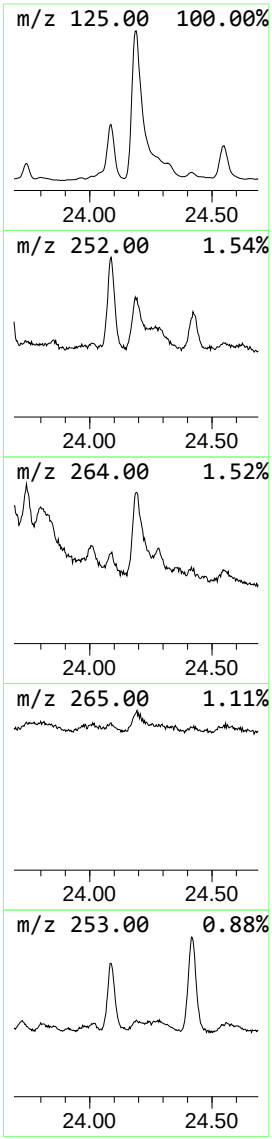
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 (S,E)-6-Hydroxy-6-methyl-2-... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.190	0.11 ng	66902	Perylene-d12	23.485

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





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016684.D
Acq On : 02 Oct 2021 23:09
Operator : CG/JU
Sample : M3892-10
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ALS Vial : 52 Sample Multiplier: 2

Instrument :
BNA_N
ClientSampleId :
S-824-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
Hydrogen isocya...	3.373	0.1	ng	24529	1	7.642	200308	0.4
Butanal, 3-hydr...	3.512	0.1	ng	35326	1	7.642	200308	0.4
Acetic acid, me...	3.825	0.1	ng	26343	1	7.642	200308	0.4
Butane	4.821	0.4	ng	100143	1	7.642	200308	0.4
3H-1,2,4-Triazo...	10.191	0.5	ng	233804	2	10.407	378443	0.4
1-Butanone, 2-m...	13.584	0.2	ng	109571	3	14.269	431298	0.4
5-Amino-2-benzo...	14.345	0.2	ng	112395	3	14.269	431298	0.4
[1,1'-Biphenyl]...	14.535	0.2	ng	97199	3	14.269	431298	0.4
2H-1-Benzopyran...	14.599	0.1	ng	64469	3	14.269	431298	0.4
Benzene, 1-ethy...	15.170	0.1	ng	73750	3	14.269	431298	0.4
Ethyl methylpho...	15.652	0.2	ng	94041	4	17.018	354813	0.4
1-Chlorophthala...	15.855	0.2	ng	72704	4	17.018	354813	0.4
2,2-Diphenyleth...	16.007	0.3	ng	120864	4	17.018	354813	0.4
1-Cyclohexene-1...	16.081	0.1	ng	41348	4	17.018	354813	0.4
2-Oxo-4,6-diphe...	16.835	0.1	ng	46976	4	17.018	354813	0.4
2-Oxo-4,6-diphe...	17.444	0.4	ng	194902	4	17.018	354813	0.4
2-Chloro-5-nitr...	20.006	0.1	ng	56803	5	21.227	490341	0.4
1,2,4-Benzenetr...	20.973	0.2	ng	94792	5	21.227	490341	0.4
1,2,4-Benzenetr...	21.875	0.1	ng	55392	5	21.227	490341	0.4
(S,E)-6-Hydroxy...	24.190	0.1	ng	66902	6	23.485	488572	0.4