LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016704.D
Acq On : 03 Oct 2021 12:24
Operator : CG/JU
Sample : M3892-03
Misc :
ALS Vial : 72 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : S-829-J-SO-2-2.5-092221

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: BN016704.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	42	47	58	rBV	15131	60003	6.05%	0.594%
2	3.834	77	82	97	rVB	17323	67376	6.80%	0.666%
3	4.581	158	163	172	rVV	12266	34211	3.45%	0.338%
4	4.710	173	177	184	rVB	14337	31703	3.20%	0.314%
5	4.821	185	189	196	rVB	28149	66872	6.75%	0.661%
6	5.042	209	213	219	rBV	9785	24992	2.52%	0.247%
7	5.273	234	238	248	rVB	13635	37405	3.77%	0.370%
8	5.531	263	266	274	rVB	4376	12162	1.23%	0.120%
9	5.752	287	290	299	rVB	4004	10426	1.05%	0.103%
10	6.315	347	351	361	rVB2	5572	18204	1.84%	0.180%
11	6.656	383	388	396	rVB2	8500	18601	1.88%	0.184%
12	6.831	403	407	415	rVB2	18699	44218	4.46%	0.437%
13	7.643	490	495	500	rBV	40430	81631	8.24%	0.807%
14	7.938	522	527	533	rVB	150009	266452	26.88%	2.636%
15	8.785	602	605	610	rVB	26166	50503	5.09%	0.500%
16	9.646	668	673	678	rBV	8199	20088	2.03%	0.199%
17	10.065	703	706	712	rVB2	9537	24342	2.46%	0.241%
18	10.191	713	716	723	rBV	49581	90657	9.15%	0.897%
19	10.407	729	733	736	rBV	88594	149599	15.09%	1.480%
20	10.952	773	776	781	rBV2	8380	17344	1.75%	0.172%
21	12.003	922	931	941	rBV	40103	64729	6.53%	0.640%
22	12.632	1050	1054	1057	rBV	27784	47692	4.81%	0.472%
23	12.886	1071	1074	1077	rBV2	74562	127932	12.91%	1.265%
24	13.025	1081	1085	1088	rVV	44103	91567	9.24%	0.906%
25	13.152	1092	1095	1096	rVV	21813	40553	4.09%	0.401%
26	13.190	1096	1098	1102	rVB	20470	35216	3.55%	0.348%
27	13.685	1135	1137	1139	rVB	12038	19427	1.96%	0.192%
28	13.749	1139	1142	1145	rVB	7877	14173	1.43%	0.140%
29	14.117	1168	1171	1173	rBV2	72341	114268	11.53%	1.130%
30	14.167	1173	1175	1180	rVV	31599	48674	4.91%	0.481%
31	14.269	1180	1183	1185	rVV	123156	180670	18.23%	1.787%
32	14.345	1185	1189	1192	rVV3	135048	241783	24.39%	2.392%
33	14.434	1192	1196	1199	rVB2	8002	15000	1.51%	0.148%
34	14.535	1200	1204	1206	rBV2	60656	117688	11.87%	1.164%
35	14.599	1206	1209	1212	rVV	75297	111953	11.29%	1.107%
36	14.713	1212	1218	1219	rVV2	25563	50506	5.10%	0.500%

LSC Area Percent Report

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Operator : CG/JU
Sample : M3892-03
Misc :
ALS Vial : 72 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : S-829-J-SO-2-2.5-092221

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	14.738	1219	1220	1223	rVB2	15427	24567	2.48%	0.243%
38	14.814	1223	1226	1230	rBV	29282	49446	4.99%	0.489%
39	14.954	1234	1237	1239	rVB3	8418	16529	1.67%	0.164%
40	15.005	1239	1241	1244	rBV	13578	19457	1.96%	0.192%
41	15.322	1263	1266	1269	rBV	26239	44099	4.45%	0.436%
42	15.487	1277	1279	1280	rBV	9759	14149	1.43%	0.140%
43	15.626	1287	1290	1295	rBV2	37922	88600	8.94%	0.876%
44	15.753	1295	1300	1304	rVV	150761	382159	38.55%	3.780%
45	15.855	1306	1308	1311	rVB	101064	145408	14.67%	1.438%
46	16.007	1317	1320	1322	rVB	245417	275638	27.81%	2.727%
47	16.251	1337	1340	1345	rVB	13000	21376	2.16%	0.211%
48	16.677	1372	1375	1378	rVB	13585	21027	2.12%	0.208%
49	16.847	1385	1389	1394	rVB3	7651	18285	1.84%	0.181%
50	17.018	1397	1403	1405	rBV	90903	185282	18.69%	1.833%
51	17.066	1405	1407	1410	rVV	301259	413361	41.70%	4.089%
52	17.152	1410	1414	1417	rVV	65524	109901	11.09%	1.087%
53	17.225	1417	1420	1425	rVB	17542	40853	4.12%	0.404%
54	17.431	1432	1437	1440	rBV2	34613	53174	5.36%	0.526%
55	17.797	1462	1467	1472	rVB	38147	80364	8.11%	0.795%
56	17.955	1472	1480	1483	rBV2	14248	48760	4.92%	0.482%
57	18.418	1560	1566	1572	rBV	12799	16924	1.71%	0.167%
58	19.068	1688	1697	1698	rBV	102464	117005	11.80%	1.157%
59	19.098	1698	1703	1713	rVB	728551	991261	100.00%	9.806%
60	19.460	1766	1776	1787	rBV	614767	879308	88.71%	8.698%
61	19.644	1809	1813	1816	rBV	8364	10021	1.01%	0.099%
62	19.679	1816	1820	1824	rBV	81257	98456	9.93%	0.974%
63	20.006	1884	1886	1889	rBV	10631	17087	1.72%	0.169%
64	20.112	1893	1896	1899	rVV2	15371	26479	2.67%	0.262%
65	20.601	1939	1942	1944	rVB2	8374	13864	1.40%	0.137%
66	20.643	1944	1946	1948	rBV	18024	21202	2.14%	0.210%
67	20.718	1951	1953	1957	rVB3	6881	12158	1.23%	0.120%
68	20.803	1958	1961	1963	rVB	15487	21237	2.14%	0.210%
69	20.877	1964	1968	1970	rBV3	10123	25713	2.59%	0.254%
70	20.920	1970	1972	1974	rVV	38856	54621	5.51%	0.540%
71	20.973	1974	1977	1987	rVB2	91855	172929	17.45%	1.711%
72	21.174	1993	1996	1998	rBV2	32946	60593	6.11%	0.599%
73	21.217	1998	2000	2003	rVV2	373327	712455	71.87%	7.048%
74	21.270	2003	2005	2010	rVB	326294	431774	43.56%	4.271%
75	21.387	2012	2016	2023	rBV	50063	83331	8.41%	0.824%
76	21.610	2034	2037	2039	rBV2	7075	11966	1.21%	0.118%

LSC Area Percent Report

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Acq On : 03 Oct 2021 12:24
Operator : CG/JU
Sample : M3892-03
Misc :
ALS Vial : 72 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : S-829-J-SO-2-2.5-092221

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

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

77	21.748	2047	2050	2052	rBV2	7089	15617	1.58%	0.154%
78	21.875	2056	2062	2065	rBV	64606	123724	12.48%	1.224%
79	22.013	2070	2075	2079	rVV2	88949	162872	16.43%	1.611%
80	22.109	2081	2084	2088	rVB2	12847	24770	2.50%	0.245%
81	22.183	2088	2091	2096	rVB	8733	13016	1.31%	0.129%
82	22.290	2096	2101	2102	rBV2	4839	15457	1.56%	0.153%
83	22.564	2151	2158	2174	rVB2	13700	21988	2.22%	0.218%
84	22.728	2201	2206	2217	rVB	7643	11406	1.15%	0.113%
85	22.814	2220	2231	2239	rBV	187280	395363	39.88%	3.911%
86	22.896	2252	2255	2269	rVB	20719	30077	3.03%	0.298%
87	22.985	2273	2281	2304	rVB2	31557	58896	5.94%	0.583%
88	23.242	2351	2356	2362	rBV	7266	9928	1.00%	0.098%
89	23.296	2362	2372	2387	rVB	83797	159408	16.08%	1.577%
90	23.389	2388	2399	2417	rBV	124795	236028	23.81%	2.335%
91	23.488	2418	2428	2436	rBV	68462	131298	13.25%	1.299%
92	23.539	2437	2443	2458	rVB	45223	83282	8.40%	0.824%
93	24.183	2623	2631	2653	rVB	14935	33540	3.38%	0.332%
94	24.607	2747	2755	2779	rVB	14655	34306	3.46%	0.339%
95	25.477	2997	3009	3018	rBV4	8014	21408	2.16%	0.212%
96	25.771	3080	3095	3120	rVB2	43975	135081	13.63%	1.336%
97	26.052	3166	3177	3190	rVB3	6536	16460	1.66%	0.163%
98	26.141	3195	3203	3219	rVB2	4697	11522	1.16%	0.114%
99	26.469	3283	3299	3327	rBV2	26240	84336	8.51%	0.834%

Sum of corrected areas: 10109222

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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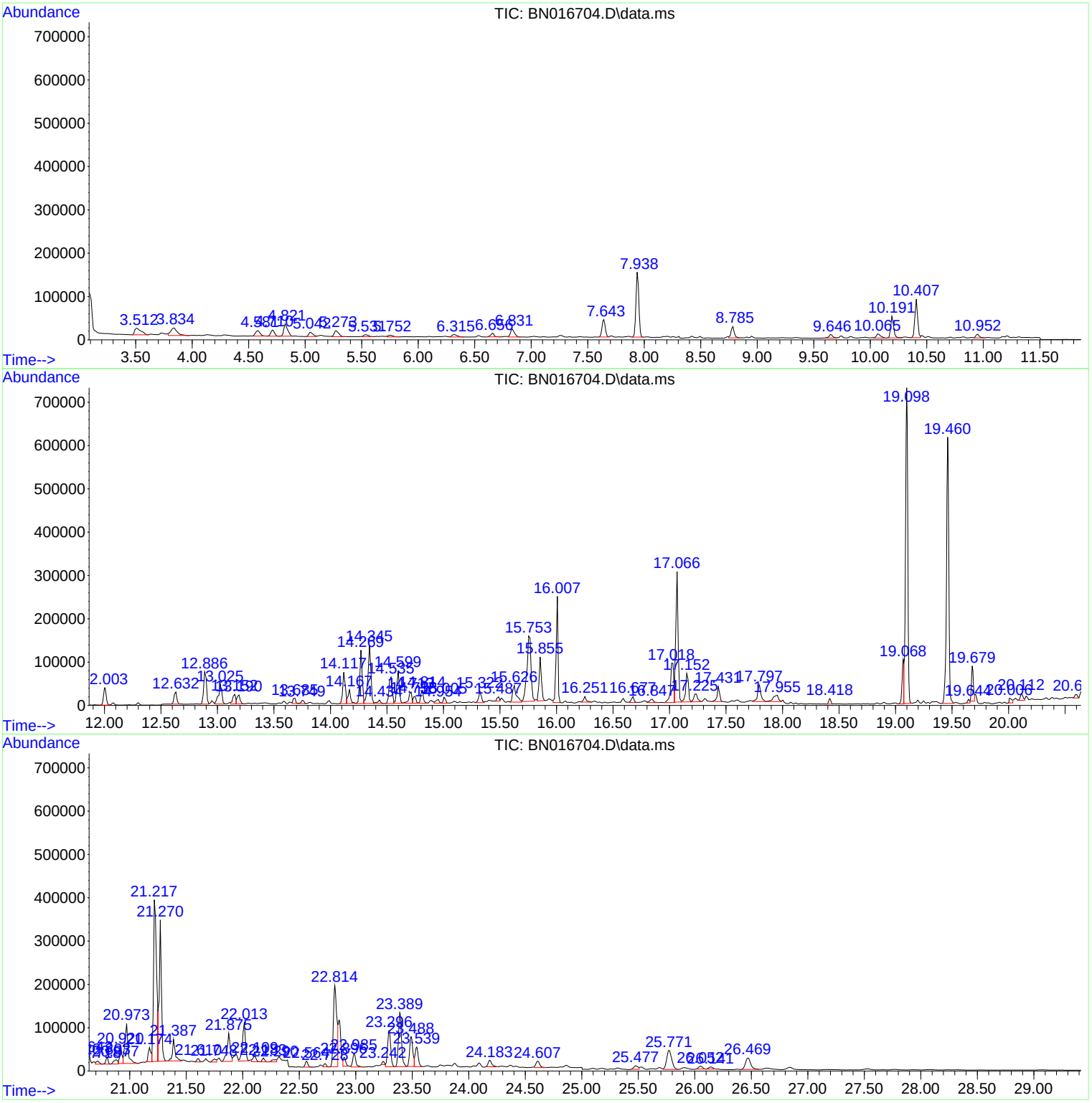
Sample : M3892-03
Misc :
ALS Vial : 72 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-829-J-SO-2-2.5-092221

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

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016704.D
Acq On : 03 Oct 2021 12:24
Operator : CG/JU
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Instrument :
BNA_N
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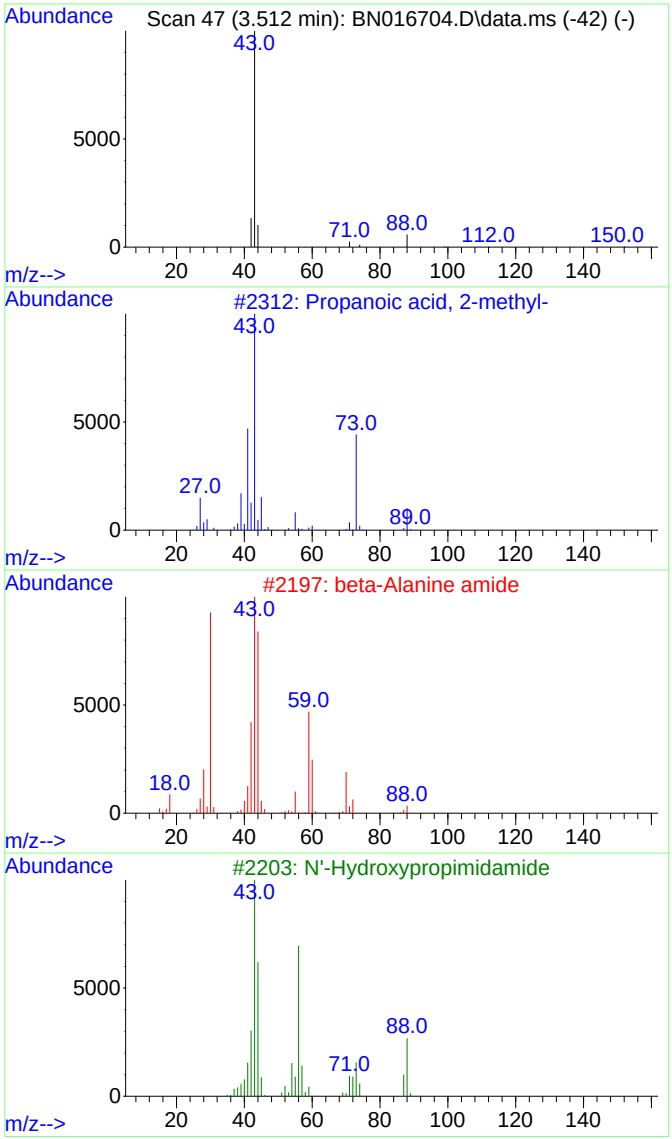
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

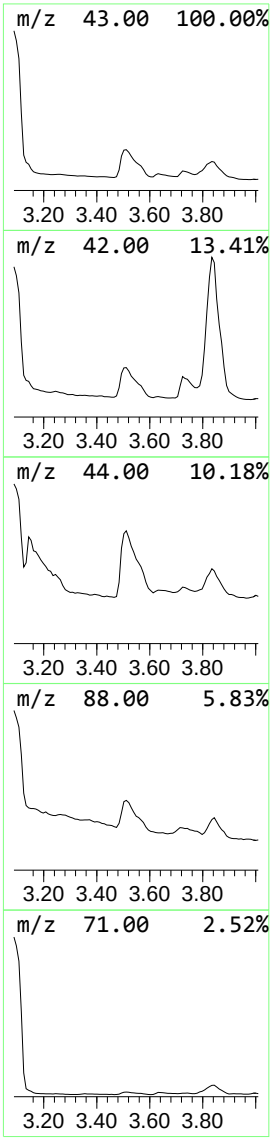
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Propanoic acid, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.512	0.29 ng	60003	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	4
2	beta-Alanine amide	88	C3H8N2O	004726-85-6	4
3	N'-Hydroxypropimidamide	88	C3H8N2O	029335-36-2	4
4	1,4-Butanediamine	88	C4H12N2	000110-60-1	4
5	1-Butanol	74	C4H10O	000071-36-3	3





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016704.D
Acq On : 03 Oct 2021 12:24
Operator : CG/JU
Sample : M3892-03
Misc :
ALS Vial : 72 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-829-J-SO-2-2.5-092221

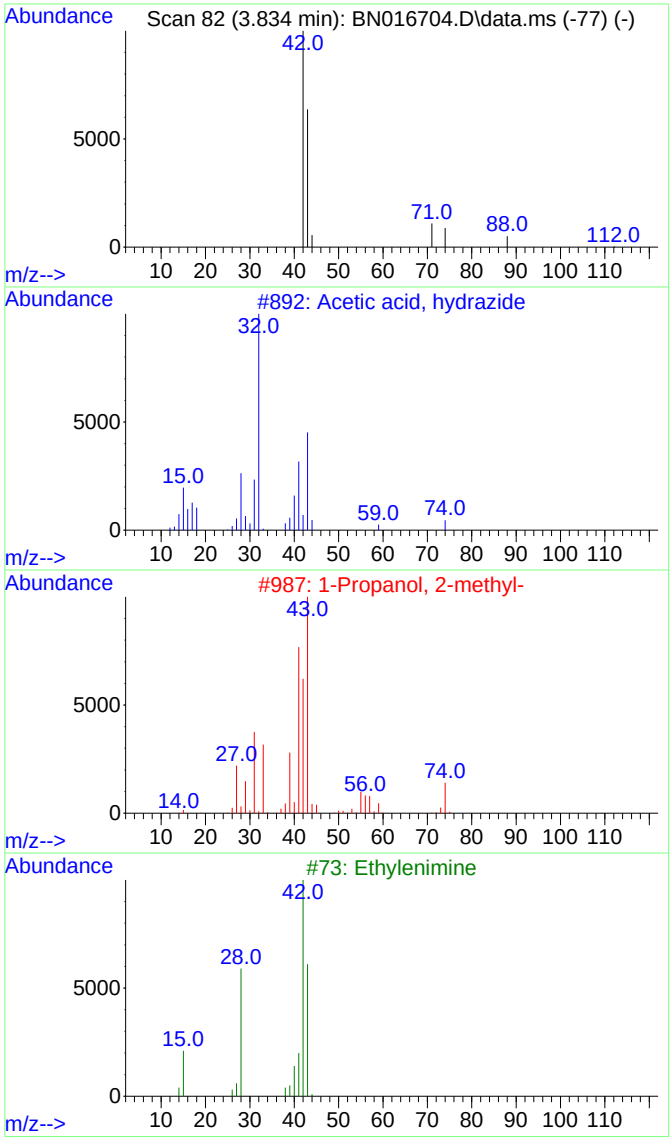
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

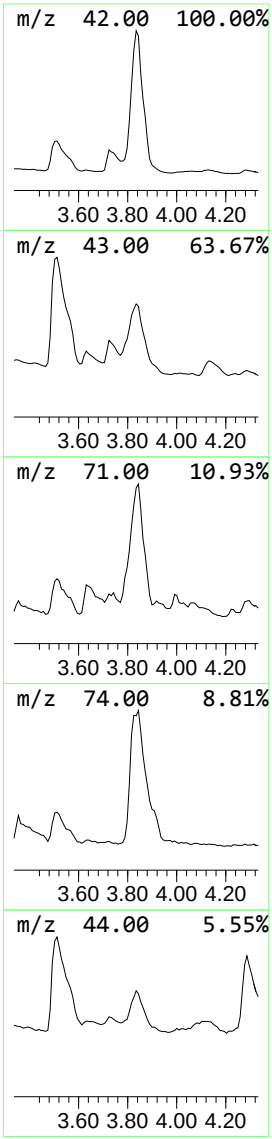
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Acetic acid, hydrazide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.834	0.33 ng	67376	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, hydrazide	74	C2H6N2O	001068-57-1	4
2	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	4
3	Ethylenimine	43	C2H5N	000151-56-4	4
4	1,4-Butanediamine	88	C4H12N2	000110-60-1	4
5	Cyanamide	42	CH2N2	000420-04-2	3





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Acq On : 03 Oct 2021 12:24
Operator : CG/JU
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ALS Vial : 72 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-829-J-SO-2-2.5-092221

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

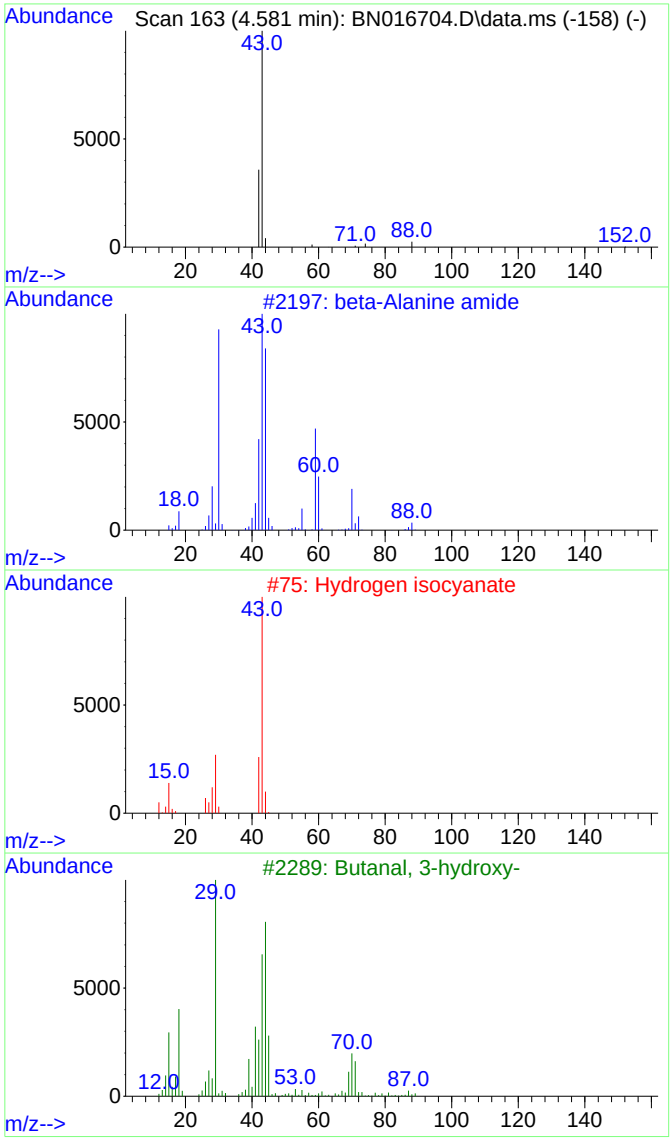
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

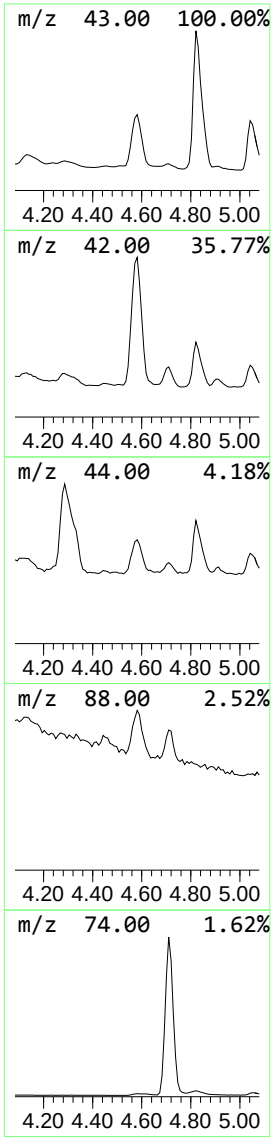
****

Peak Number 3 beta-Alanine amide Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.581	0.17 ng	34211	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	beta-Alanine amide	88	C3H8N2O	004726-85-6	5
2	Hydrogen isocyanate	43	CHNO	000075-13-8	3
3	Butanal, 3-hydroxy-	88	C4H8O2	000107-89-1	3
4	CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	2
5	Hydrogen azide	43	HN3	007782-79-8	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Sample : M3892-03
Misc :
ALS Vial : 72 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-829-J-SO-2-2.5-092221

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

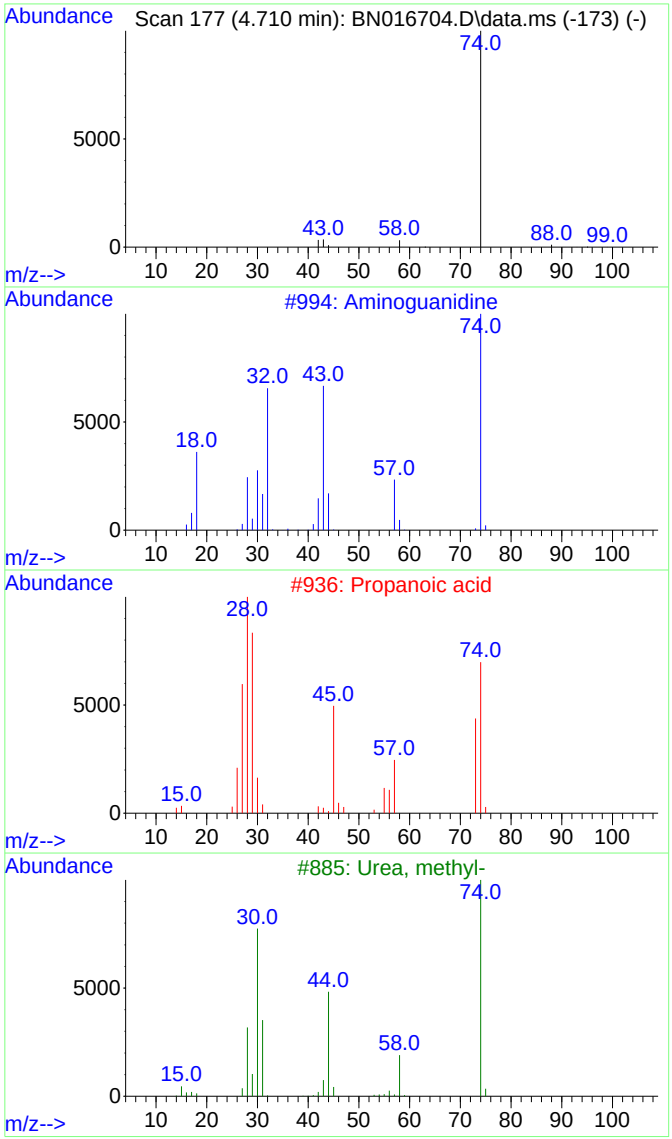
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

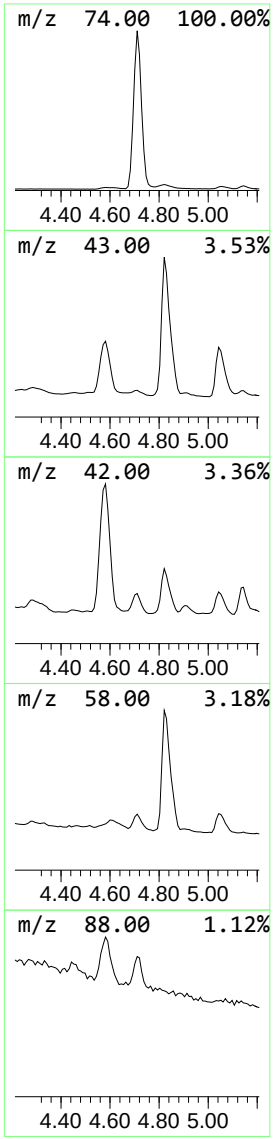
****

Peak Number 4 Aminoguanidine Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.710	0.16 ng	31703	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aminoguanidine	74	CH6N4	000079-17-4	3
2	Propanoic acid	74	C3H6O2	000079-09-4	3
3	Urea, methyl-	74	C2H6N2O	000598-50-5	3
4	Ethyl ether	74	C4H10O	000060-29-7	3
5	Thiirane, methyl-	74	C3H6S	001072-43-1	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016704.D
Acq On : 03 Oct 2021 12:24
Operator : CG/JU
Sample : M3892-03
Misc :
ALS Vial : 72 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : S-829-J-SO-2-2.5-092221

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

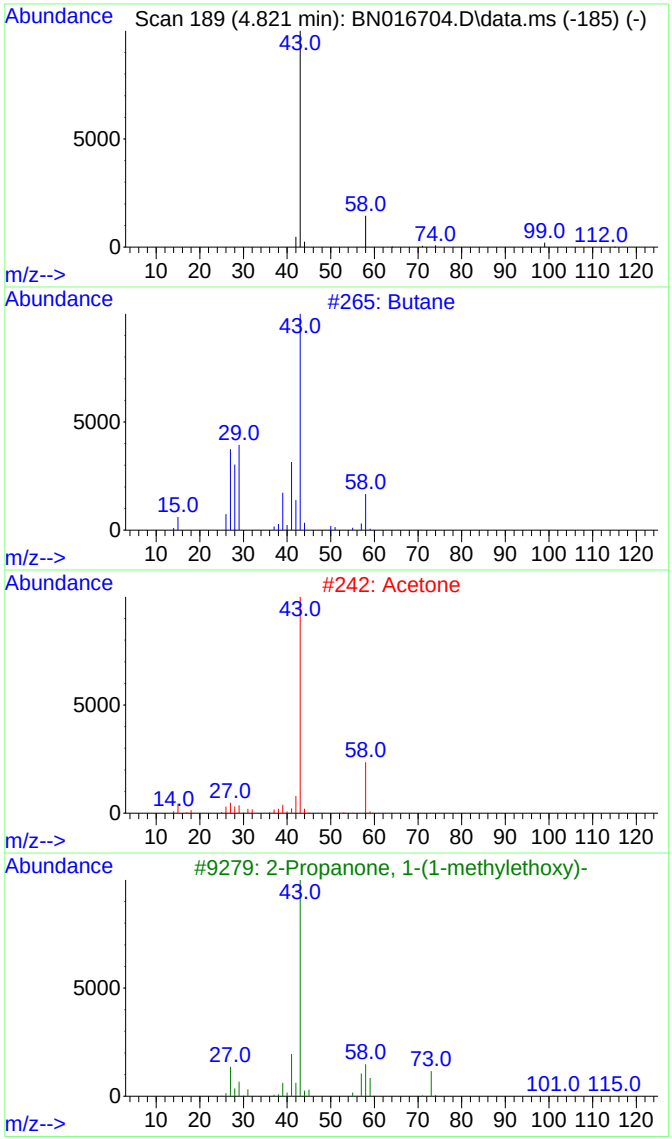
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

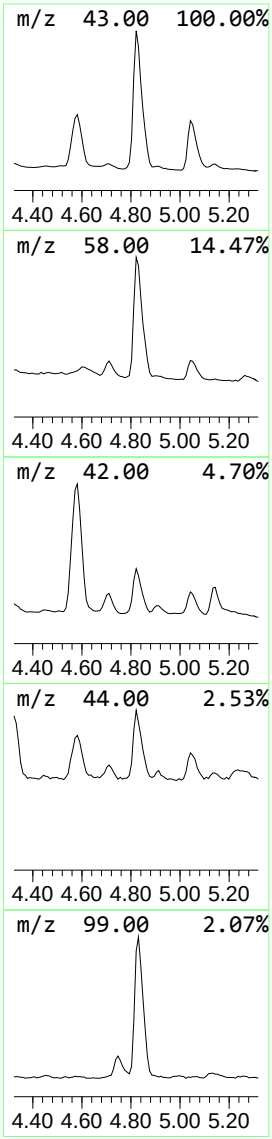
****

Peak Number 5 Butane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.33 ng	66872	1,4-Dichlorobenzene-d4	7.643

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	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	4
4	Ethene, methoxy-	58	C3H6O	000107-25-5	3
5	Diazene, dimethyl-	58	C2H6N2	000503-28-6	3





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Acq On : 03 Oct 2021 12:24
Operator : CG/JU
Sample : M3892-03
Misc :
ALS Vial : 72 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-829-J-SO-2-2.5-092221

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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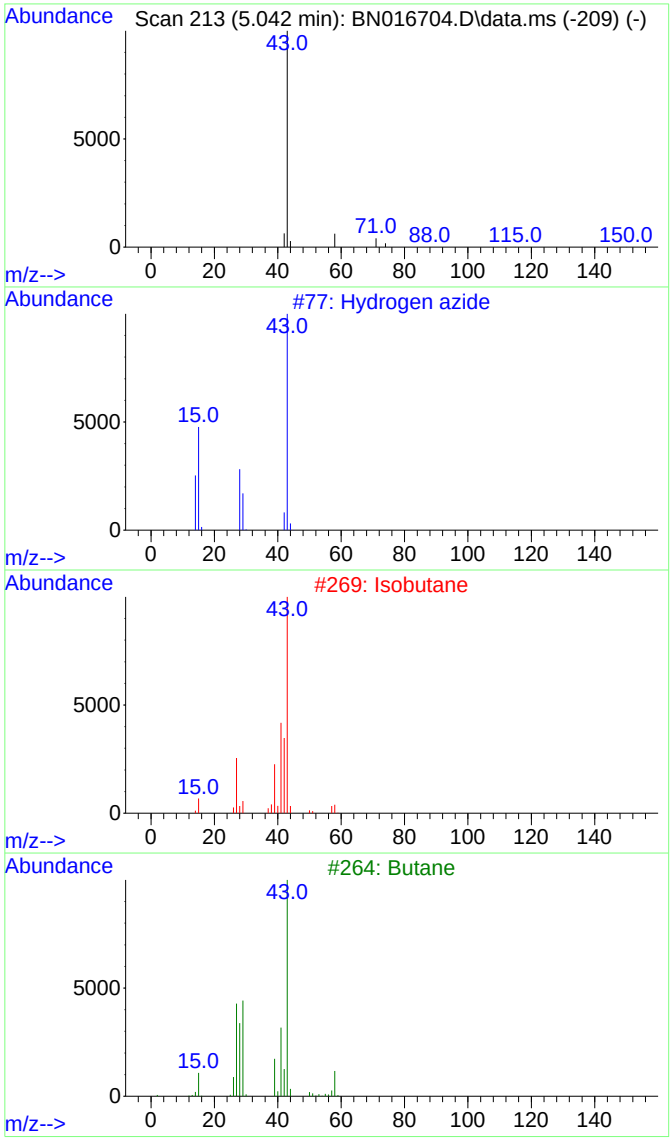
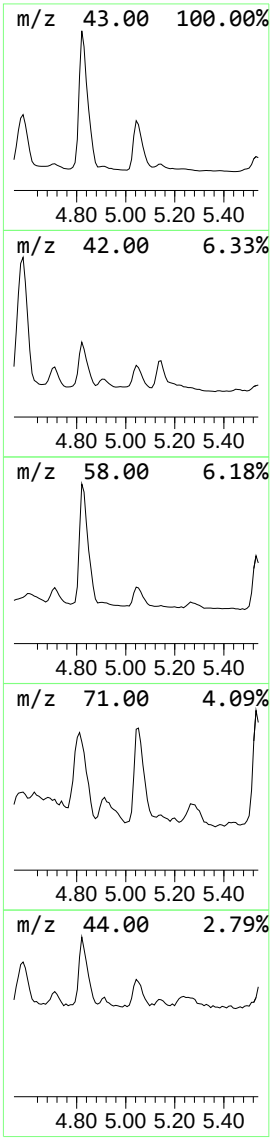
Peak Number 6 Hydrogen azide Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.042	0.12 ng	24992	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrogen azide	43	HN3	007782-79-8	4
2	Isobutane	58	C4H10	000075-28-5	4
3	Butane	58	C4H10	000106-97-8	4
4	Methoxyacetonitrile	71	C3H5NO	001738-36-9	3
5	Hydrogen isocyanate	43	CHNO	000075-13-8	2





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Misc :
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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

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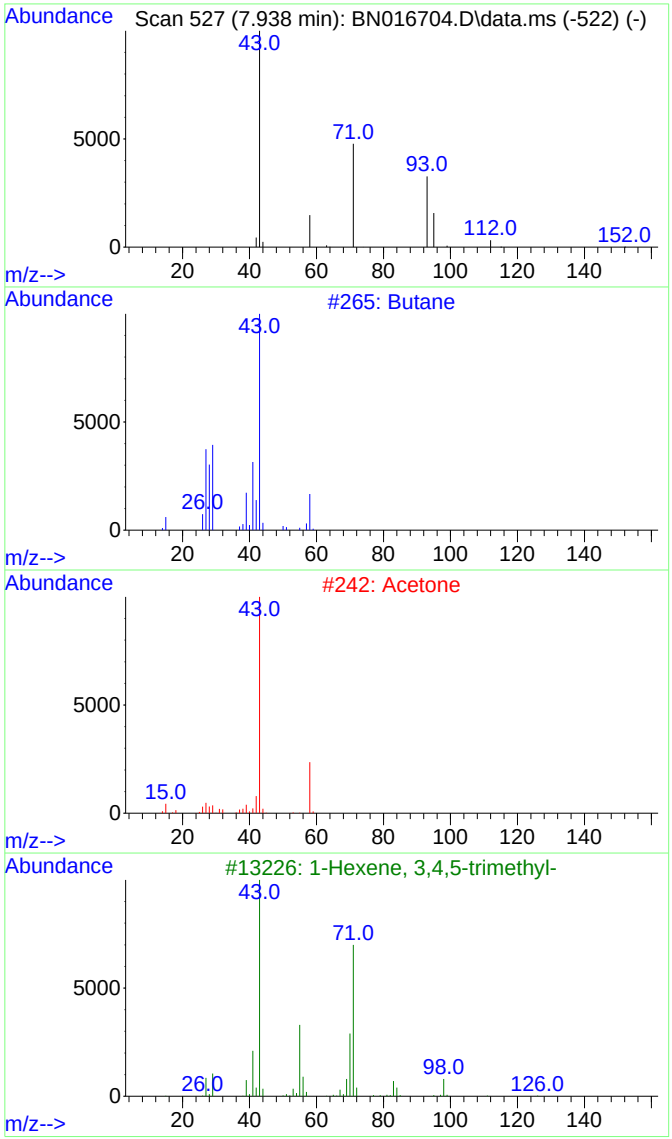
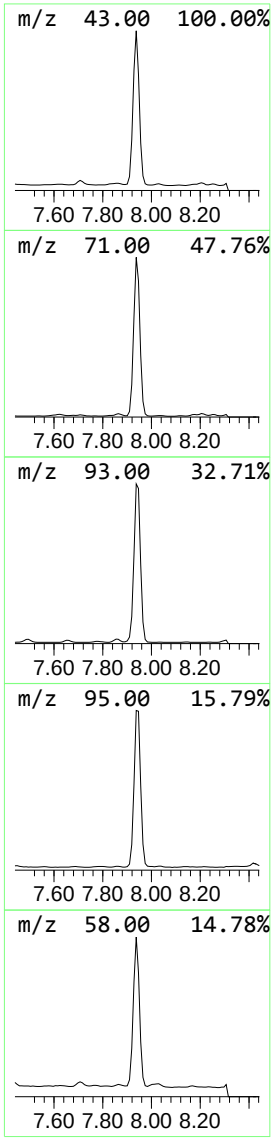
Peak Number 7 Butane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.938	1.31 ng	266452	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	4
2	Acetone	58	C3H6O	000067-64-1	4
3	1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	4
4	2-Propenamide	71	C3H5NO	000079-06-1	3
5	Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	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

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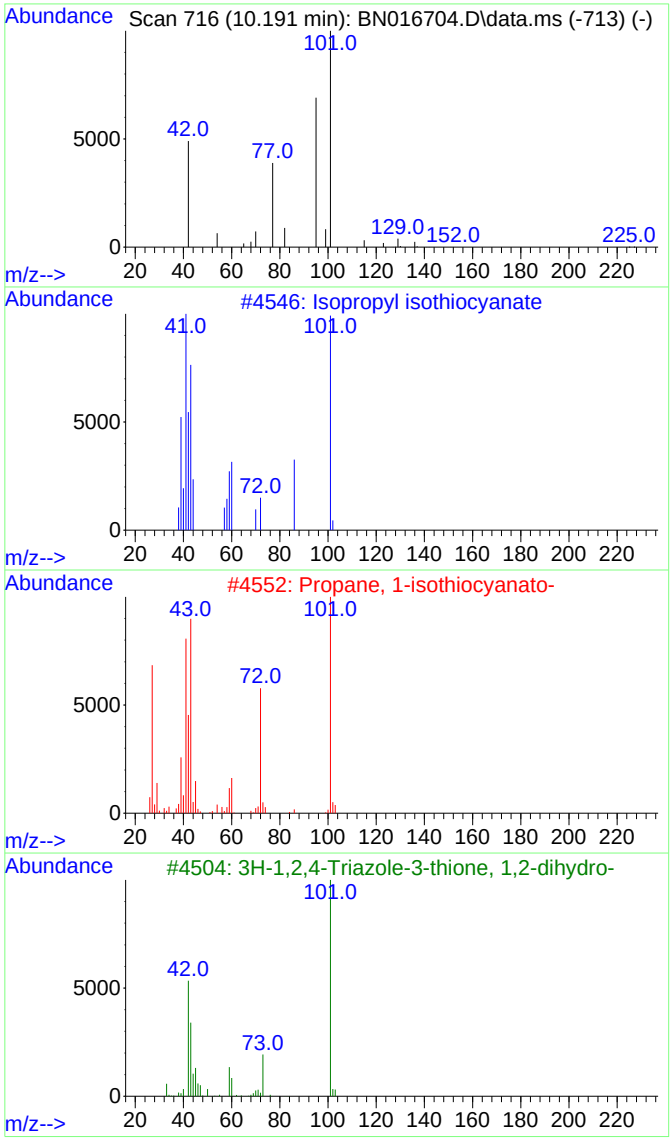
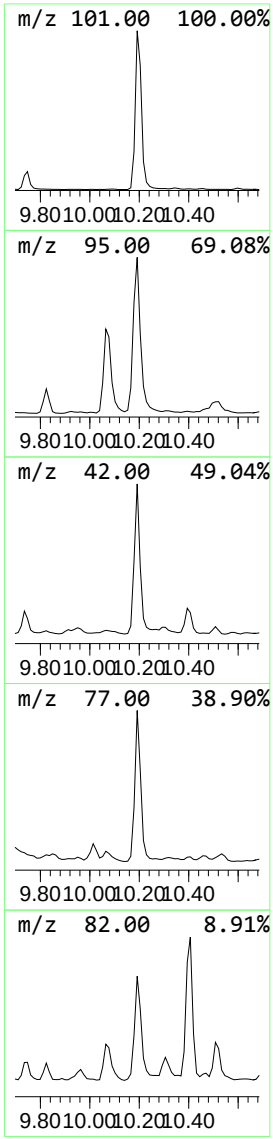
Peak Number 8 Isopropyl isothiocyanate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.24 ng	90657	Naphthalene-d8	10.407

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	9
2	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5
3	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
4	2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	5
5	2-Pyrimidinamine	95	C4H5N3	000109-12-6	5





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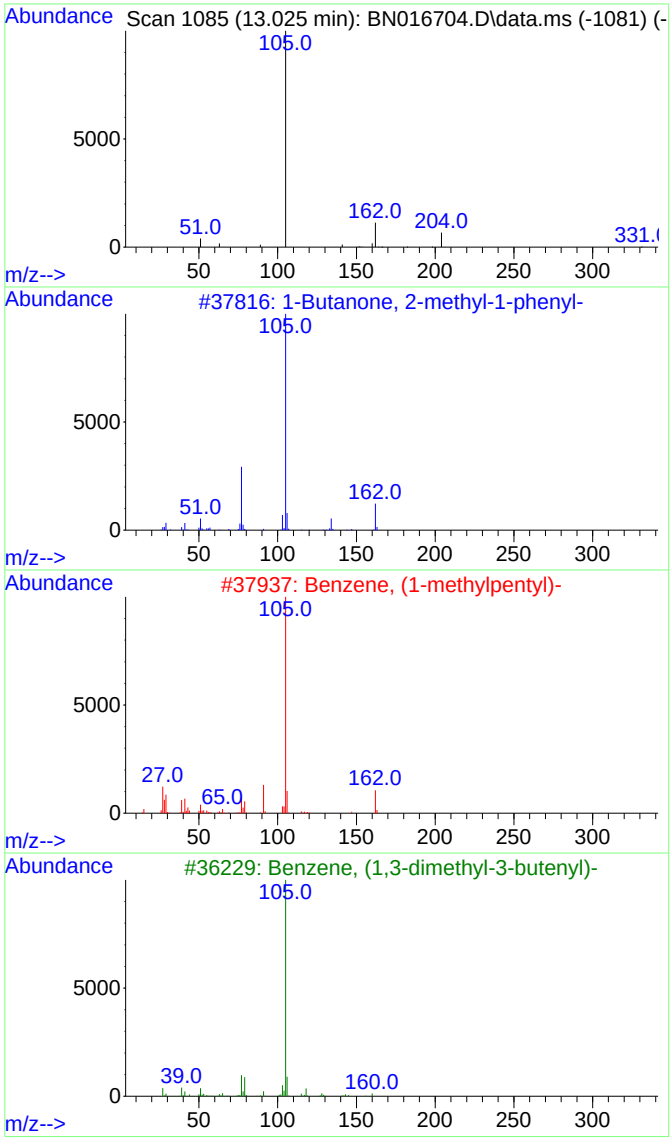
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

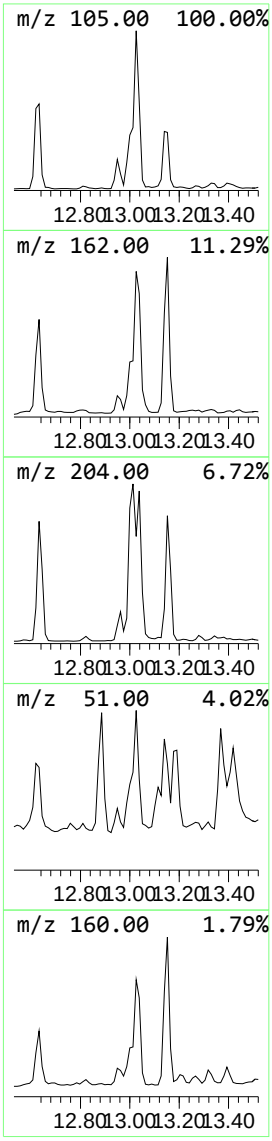
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1-Butanone, 2-methyl-1-phenyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.025	0.20 ng	91567	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	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	1,1,1-Trifluoro-2-(4-methylpheny...	204	C10H11F3O	076953-97-4	4
5	1-Butanone, 3-methyl-1-phenyl-	162	C11H14O	000582-62-7	4





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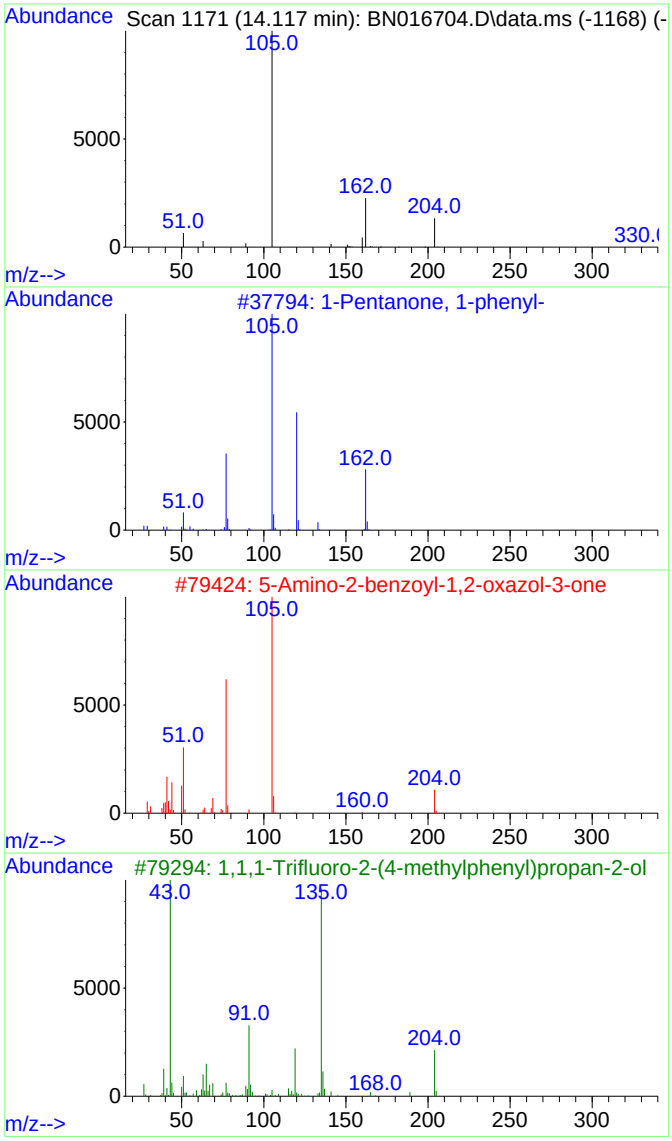
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

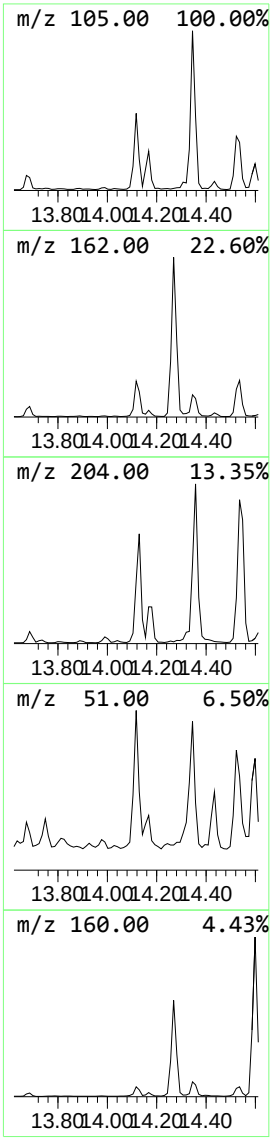
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.117	0.25 ng	114268	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	5-Amino-2-benzoyl-1,2-oxazol-3-one	204	C10H8N2O3	090771-25-8	5
3	1,1,1-Trifluoro-2-(4-methylpheny...	204	C10H11F3O	076953-97-4	5
4	Benzene, 1-methyl-2-(1-ethylprop...	162	C12H18	054410-74-1	4
5	Benzaldehyde, 4-(2-propenyloxy)-	162	C10H10O2	040663-68-1	4





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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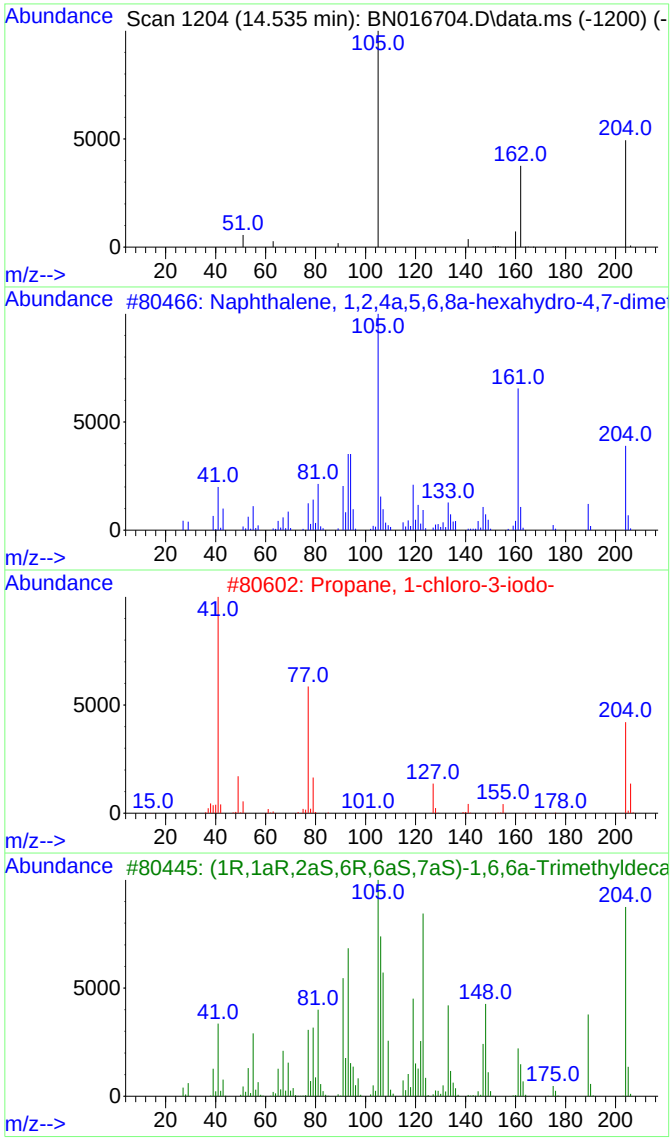
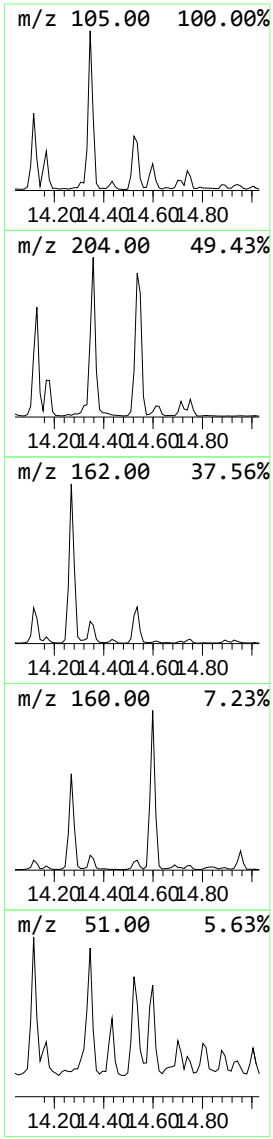
****
Peak Number 11 Naphthalene, 1,2,4a,5,6,8a-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.535	0.26 ng	117688	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	031983-22-9	7
2	Propane, 1-chloro-3-iodo-	204	C3H6ClI	006940-76-7	5
3	(1R,1aR,2aS,6R,6aS,7aS)-1,6,6a-T...	204	C15H24	026620-70-2	4
4	[1,2,4]Oxadiazole-3-carboxylic a...	204	C10H8N2O3	1000310-82-1	4
5	3H-3a,7-Methanoazulene, 2,4,5,6,...	204	C15H24	002387-78-2	4





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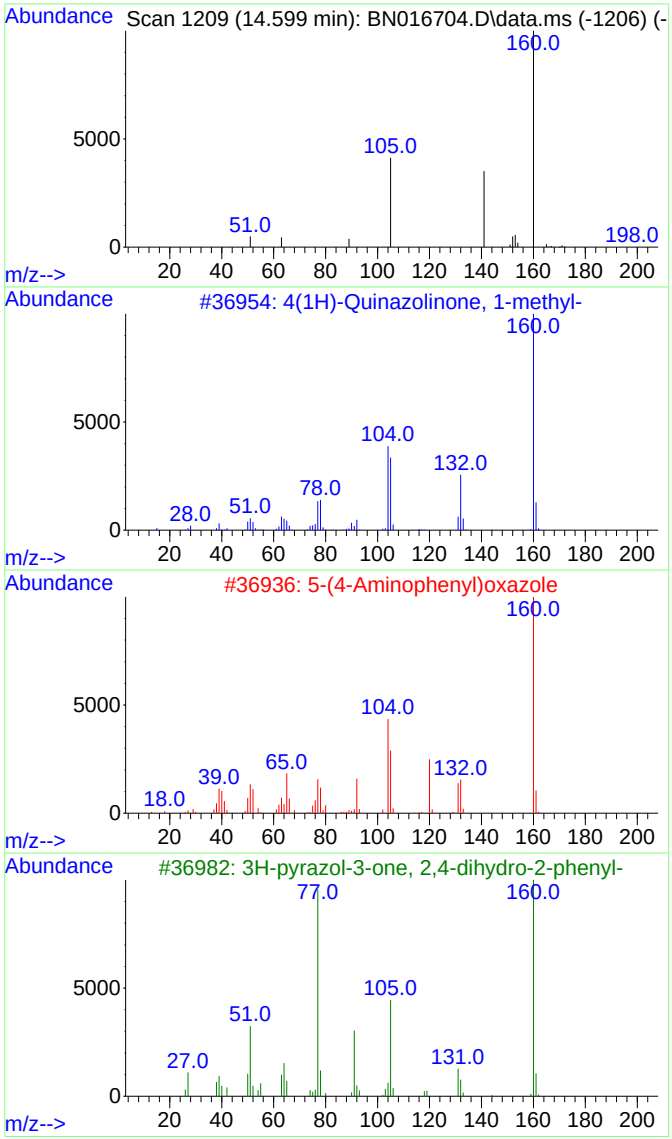
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

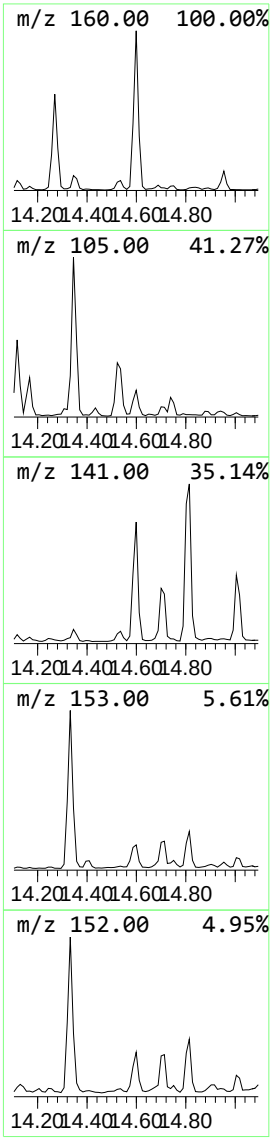
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 4(1H)-Quinazolinone, 1-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.599	0.25 ng	111953	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4(1H)-Quinazolinone, 1-methyl-	160	C9H8N2O	003476-68-4	4
2	5-(4-Aminophenyl)oxazole	160	C9H8N2O	001008-95-3	4
3	3H-pyrazol-3-one, 2,4-dihydro-2-...	160	C9H8N2O	1000404-39-1	4
4	2-Indolinone, 3-(methylimino)-	160	C9H8N2O	002058-70-0	4
5	2-(2-Thienylmethylene)malononitrile	160	C8H4N2S	028162-32-5	4





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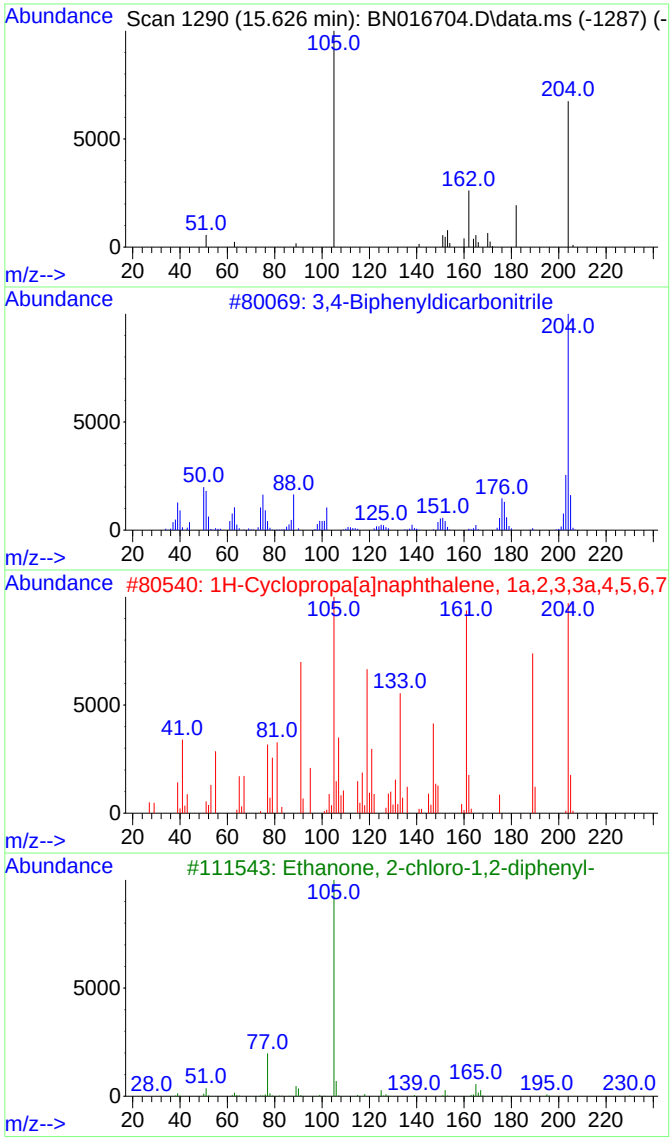
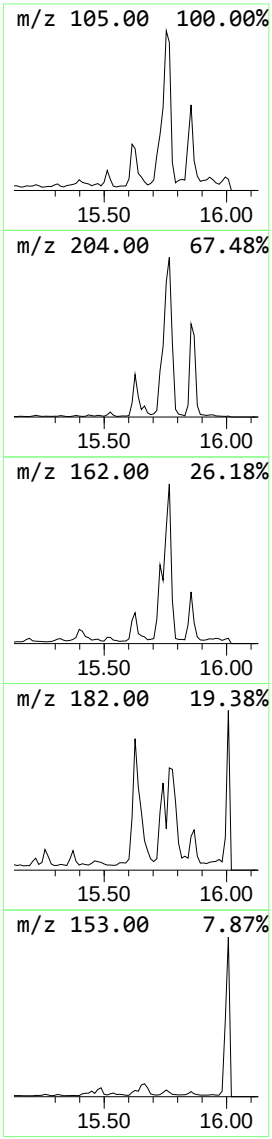
****
Peak Number 13 3,4-Biphenyldicarbonitrile Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.626	0.20 ng	88600	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Biphenyldicarbonitrile	204	C14H8N2	004128-63-6	9
2	1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	000489-29-2	9
3	Ethanone, 2-chloro-1,2-diphenyl-	230	C14H11ClO	000447-31-4	9
4	Tetracyano-p-quinodimethane	204	C12H4N4	001518-16-7	7
5	9,10-ethenoanthracene, 9,10-dihy...	204	C16H12	1000400-47-8	7





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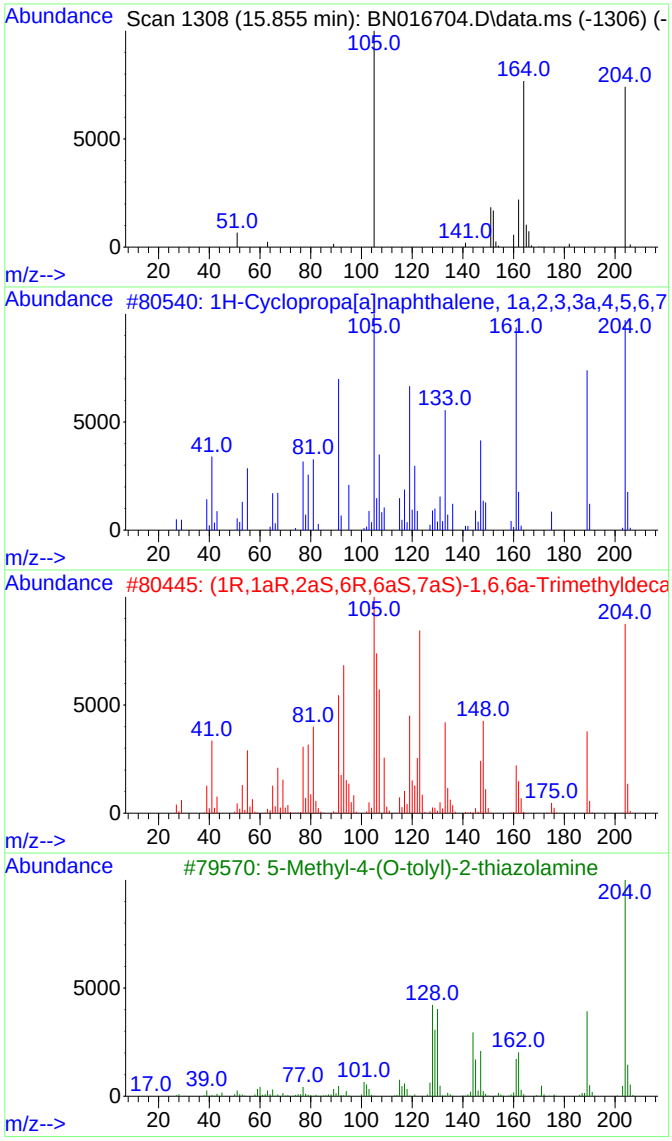
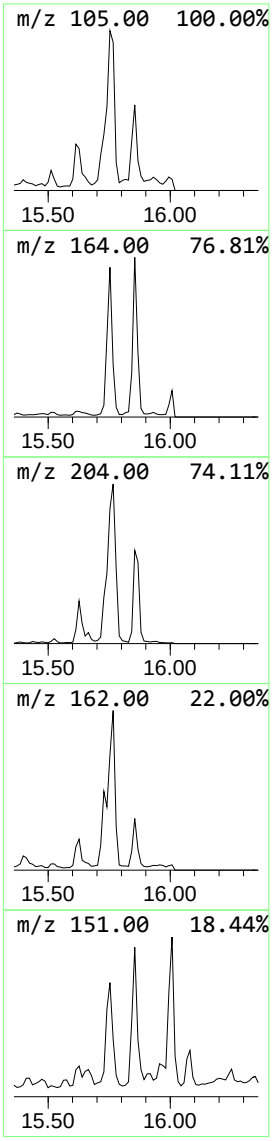
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 1H-Cyclopropa[a]naphthalene... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.855	0.31 ng	145408	Phenanthrene-d10	17.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	000489-29-2	9
2	(1R,1aR,2aS,6R,6aS,7aS)-1,6,6a-T...	204	C15H24	026620-70-2	9
3	5-Methyl-4-(O-tolyl)-2-thiazolamine	204	C11H12N2S	016942-68-0	9
4	3,4-Dimethoxyphenethanamine, N-p...	299	C18H21NO3	004876-02-2	9
5	2-Benzothiazolamine, N-methyl-	164	C8H8N2S	016954-69-1	7





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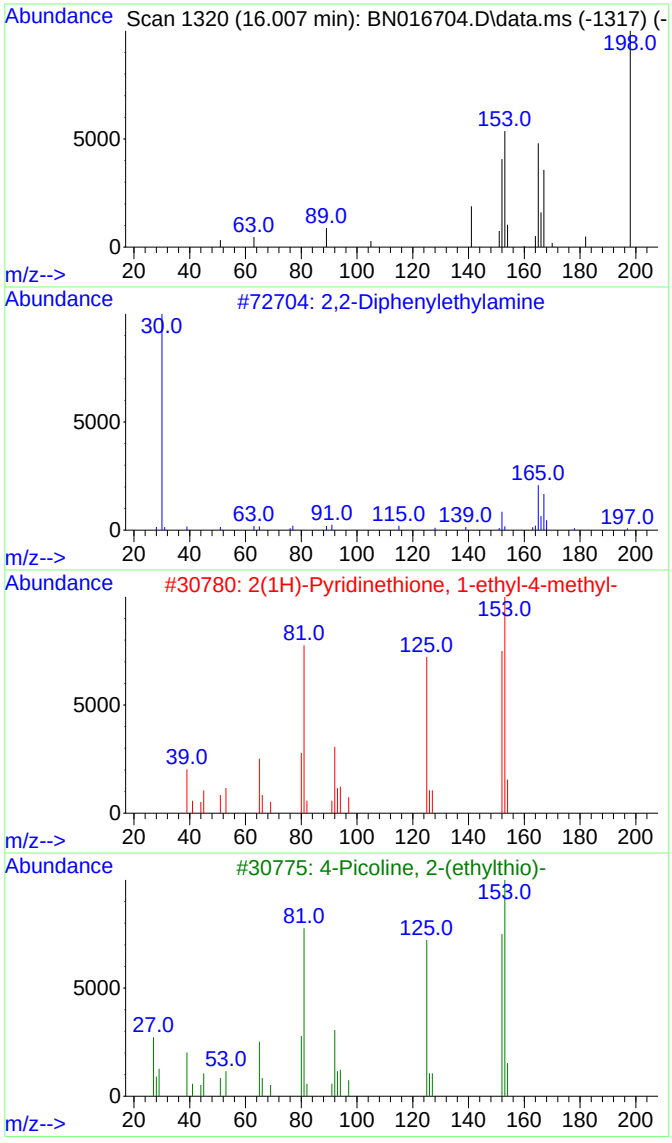
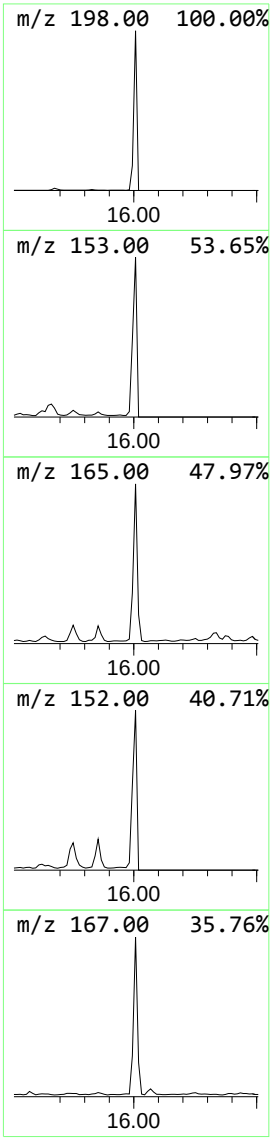
****
Peak Number 15 2,2-Diphenylethylamine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.007	0.60 ng	275638	Phenanthrene-d10	17.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2-Diphenylethylamine	197	C14H15N	003963-62-0	12
2	2(1H)-Pyridinethione, 1-ethyl-4-...	153	C8H11NS	019006-72-5	9
3	4-Picoline, 2-(ethylthio)-	153	C8H11NS	019006-78-1	9
4	2(1H)-Pyridinethione, 1-ethyl-6-...	153	C8H11NS	019006-73-6	9
5	2,4-Dimethyl-6-(methylthio)pyridine	153	C8H11NS	1000305-54-7	9





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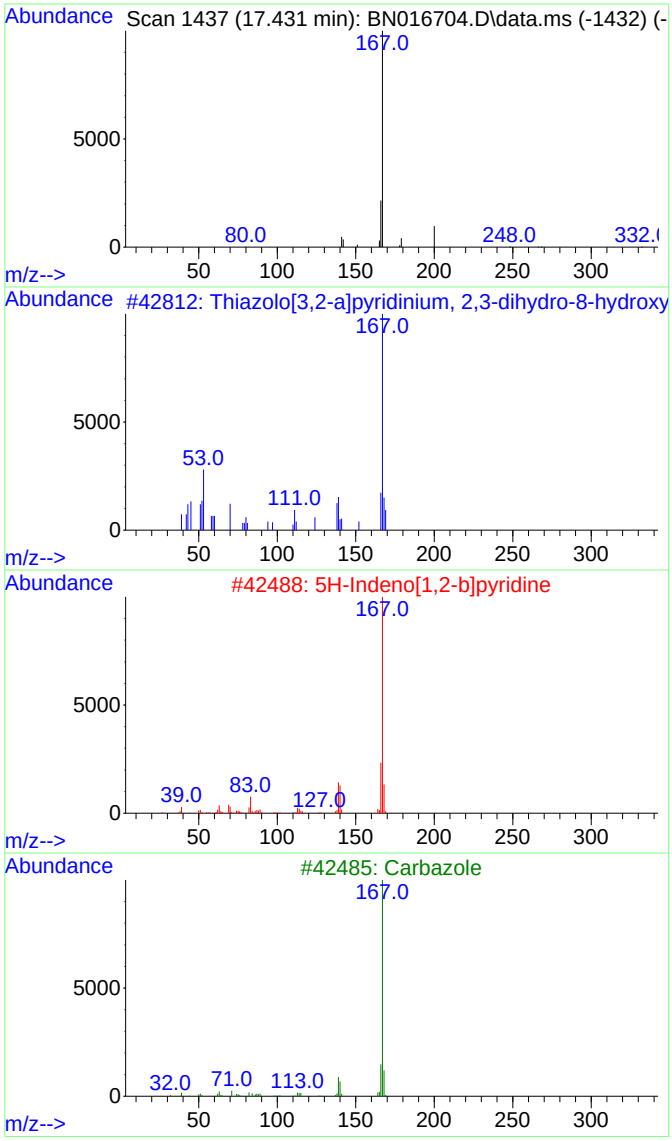
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

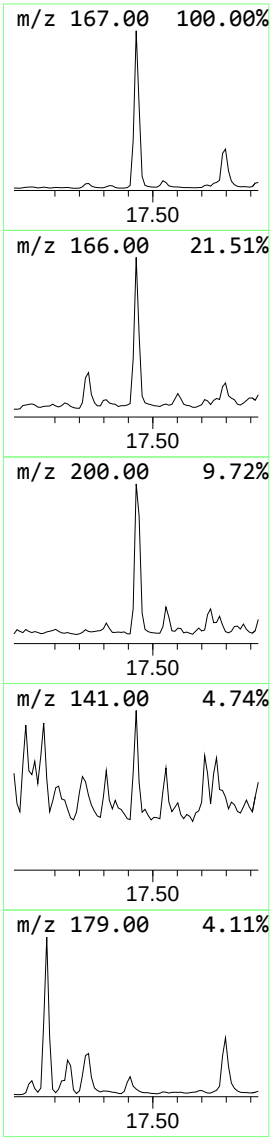
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 Thiazolo[3,2-a]pyridinium, ... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.432	0.11 ng	53174	Phenanthrene-d10	17.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiazolo[3,2-a]pyridinium, 2,3-d...	167	C8H9NOS	023003-43-2	7
2	5H-Indeno[1,2-b]pyridine	167	C12H9N	000244-99-5	7
3	Carbazole	167	C12H9N	000086-74-8	7
4	5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	5
5	Benzaldehyde, 2-hydroxy-5-nitro-	167	C7H5NO4	000097-51-8	5





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Data File : BN016704.D
Acq On : 03 Oct 2021 12:24
Operator : CG/JU
Sample : M3892-03
Misc :
ALS Vial : 72 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-829-J-SO-2-2.5-092221

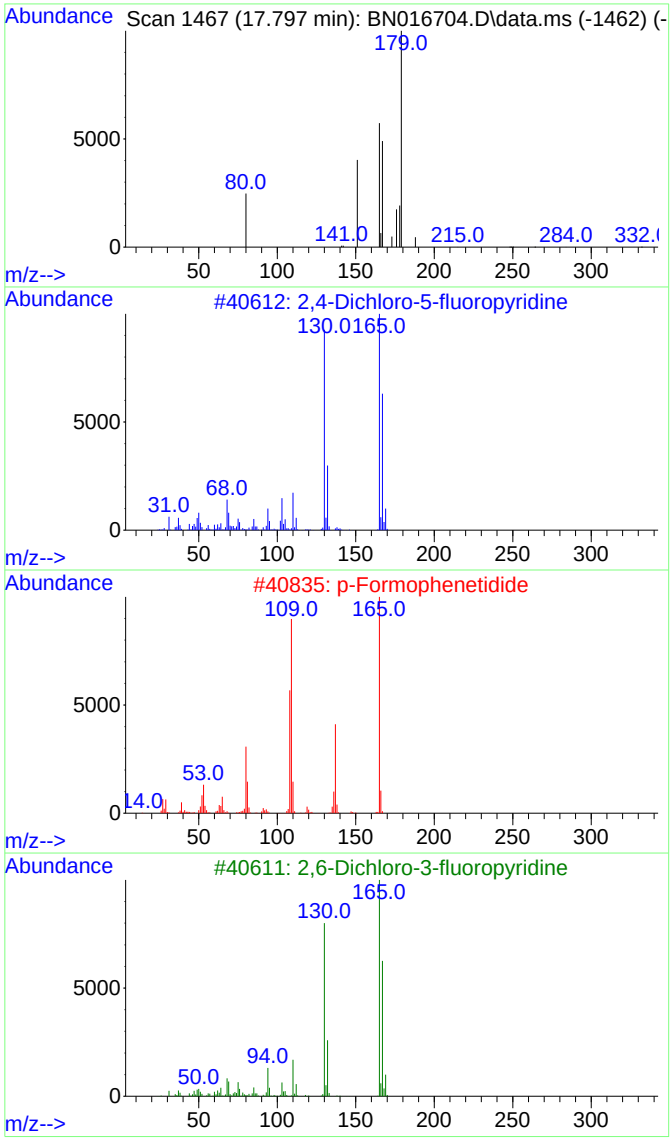
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

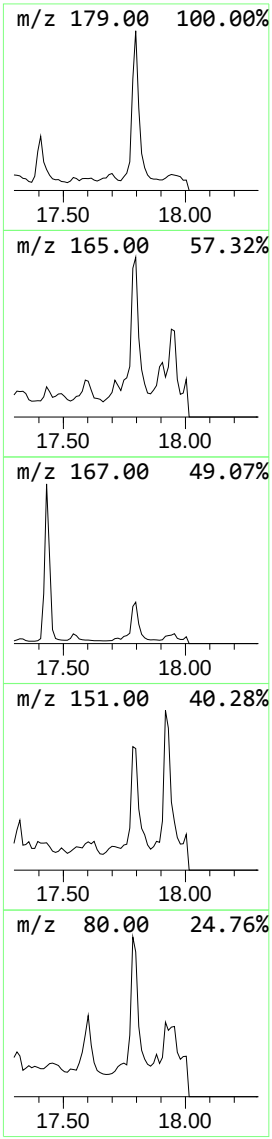
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 2,4-Dichloro-5-fluoropyridine Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.797	0.17 ng	80364	Phenanthrene-d10	17.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Dichloro-5-fluoropyridine	165	C5H2Cl2FN	189281-48-9	9
2	p-Formophenetidide	165	C9H11NO2	061587-14-2	9
3	2,6-Dichloro-3-fluoropyridine	165	C5H2Cl2FN	052208-50-1	9
4	s-Triazolo[4,3-a]pyridine-3-thio...	165	C7H7N3S	005528-58-5	9
5	s-Triazolo[4,3-a]pyridine-3-thio...	165	C7H7N3S	004926-22-1	7





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016704.D
Acq On : 03 Oct 2021 12:24
Operator : CG/JU
Sample : M3892-03
Misc :
ALS Vial : 72 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-829-J-SO-2-2.5-092221

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

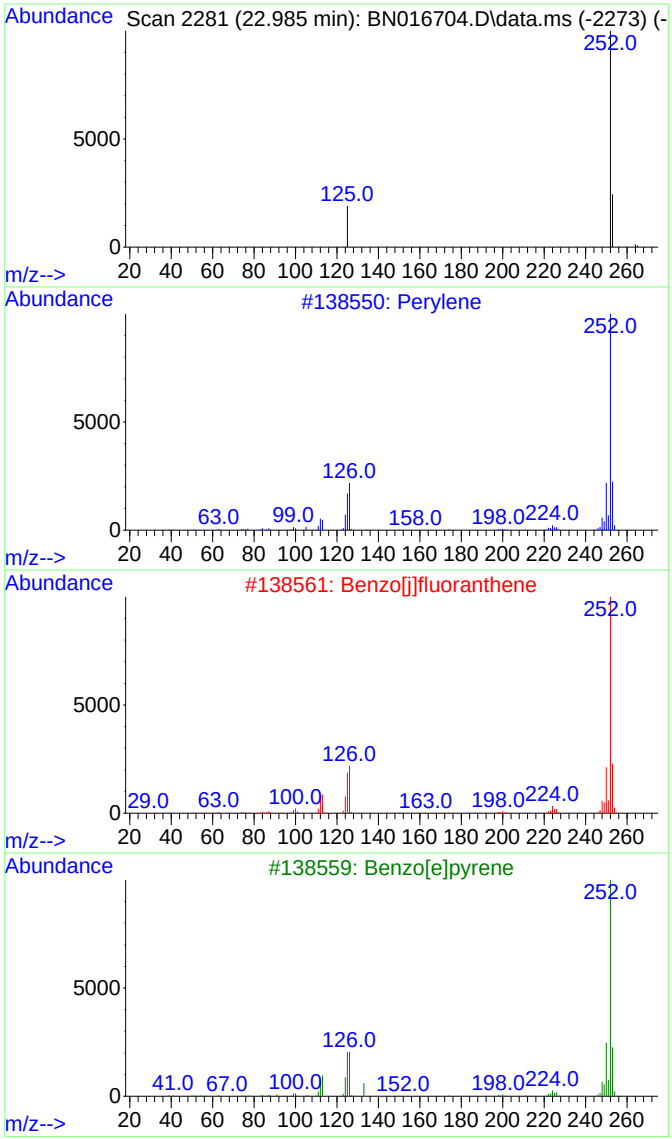
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

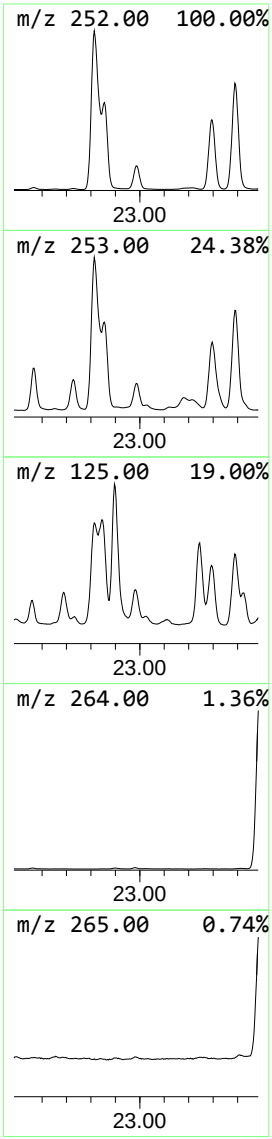
****

Peak Number 18 Perylene Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.985	0.18 ng	58896	Perylene-d12	23.488

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	9
2	Benzo[j]fluoranthene	252	C20H12	000205-82-3	9
3	Benzo[e]pyrene	252	C20H12	000192-97-2	9
4	Benzo[a]pyrene	252	C20H12	000050-32-8	9
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	9





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Data File : BN016704.D
Acq On : 03 Oct 2021 12:24
Operator : CG/JU
Sample : M3892-03
Misc :
ALS Vial : 72 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-829-J-SO-2-2.5-092221

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

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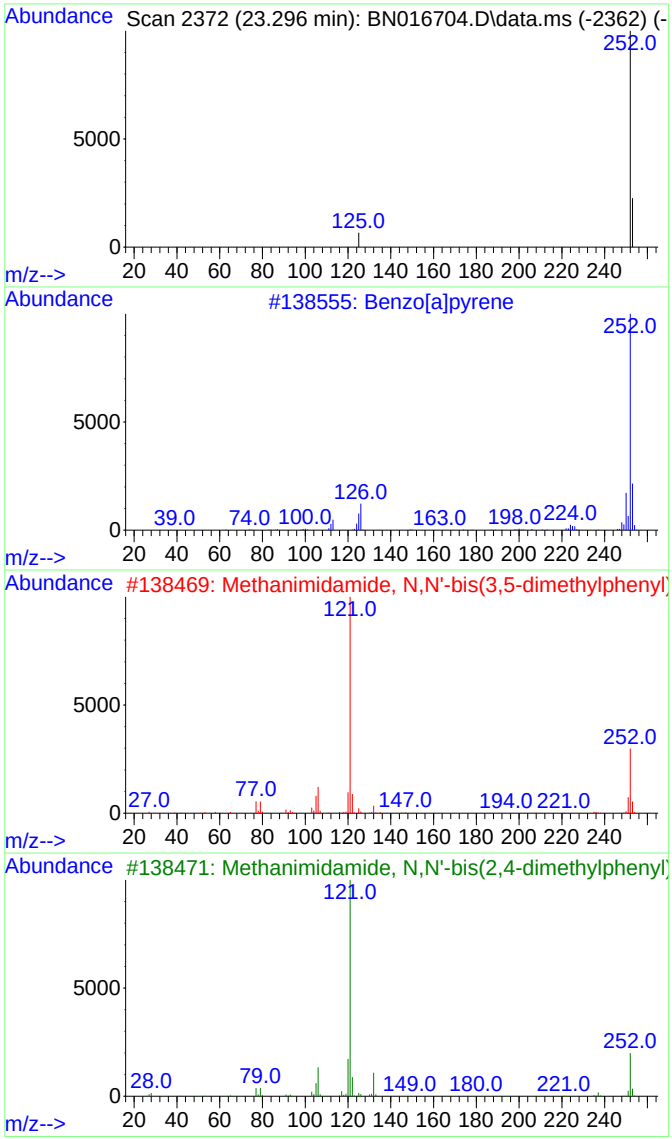
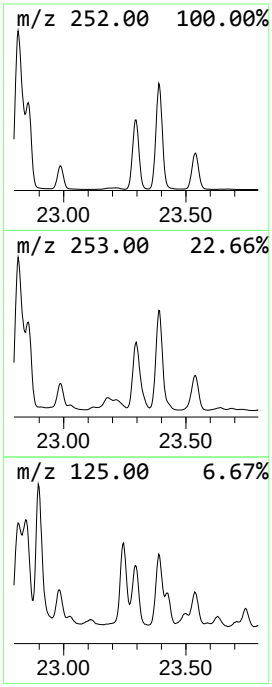
Peak Number 19 Benzo[a]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.296	0.49 ng	159408	Perylene-d12	23.488

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[a]pyrene	252	C20H12	000050-32-8	9
2	Methanimidamide, N,N'-bis(3,5-di...	252	C17H20N2	064107-05-7	5
3	Methanimidamide, N,N'-bis(2,4-di...	252	C17H20N2	016596-04-6	5
4	1-Phenyl-3-(4-methoxyphenyl)-2-p...	252	C16H16N2O	003314-43-0	5
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	5





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Data File : BN016704.D
Acq On : 03 Oct 2021 12:24
Operator : CG/JU
Sample : M3892-03
Misc :
ALS Vial : 72 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-829-J-SO-2-2.5-092221

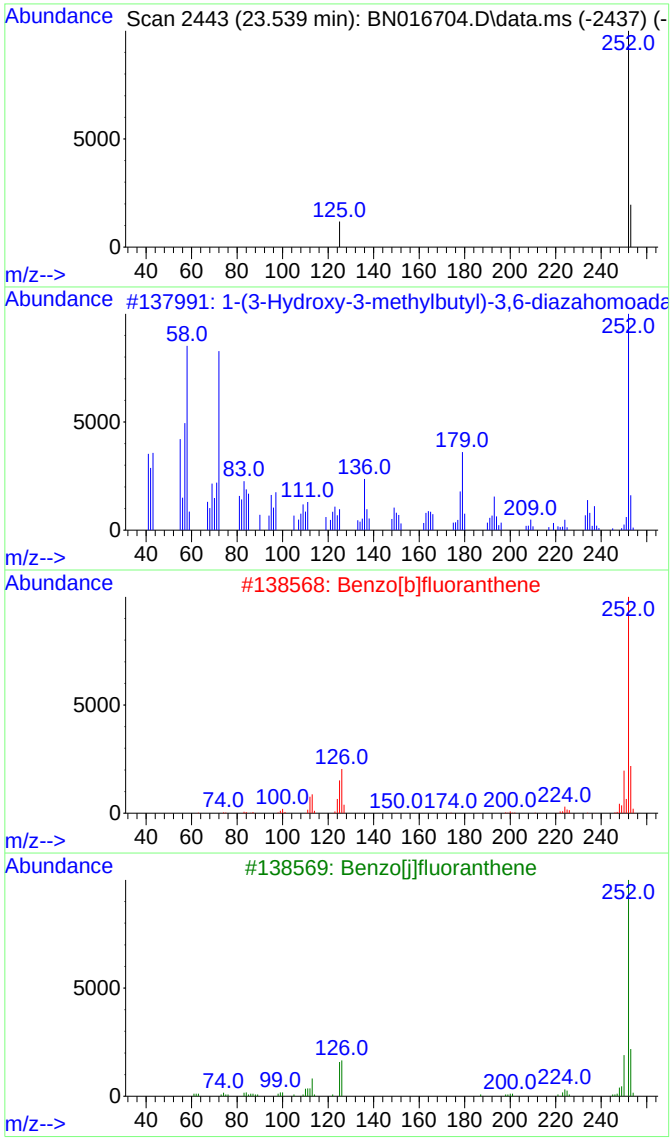
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

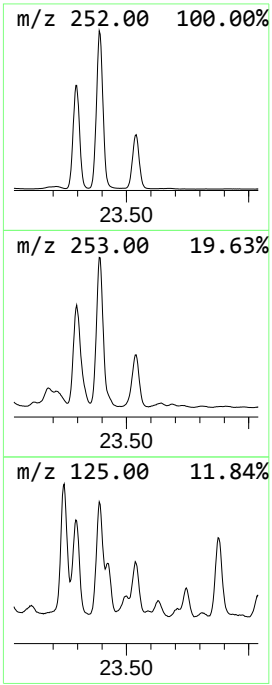
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 1-(3-Hydroxy-3-methylbutyl)... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.539	0.25 ng	83282	Perylene-d12	23.488

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(3-Hydroxy-3-methylbutyl)-3,6-...	252	C14H24N2O2	1000216-02-0	9
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	9
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	9
4	Gama-carbolin-1-one, 5,7-difluor...	252	C12H10F2N2O2	062223-53-4	9
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016704.D
Acq On : 03 Oct 2021 12:24
Operator : CG/JU
Sample : M3892-03
Misc :
ALS Vial : 72 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : S-829-J-SO-2-2.5-092221

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
Propanoic acid,...	3.512	0.3	ng	60003	1	7.643	81631	0.4
Acetic acid, hy...	3.834	0.3	ng	67376	1	7.643	81631	0.4
beta-Alanine amide	4.581	0.2	ng	34211	1	7.643	81631	0.4
Aminoguanidine	4.710	0.2	ng	31703	1	7.643	81631	0.4
Butane	4.821	0.3	ng	66872	1	7.643	81631	0.4
Hydrogen azide	5.042	0.1	ng	24992	1	7.643	81631	0.4
Butane	7.938	1.3	ng	266452	1	7.643	81631	0.4
Isopropyl isoth...	10.191	0.2	ng	90657	2	10.407	149599	0.4
1-Butanone, 2-m...	13.025	0.2	ng	91567	3	14.269	180670	0.4
1-Pentanone, 1-...	14.117	0.3	ng	114268	3	14.269	180670	0.4
Naphthalene, 1,...	14.535	0.3	ng	117688	3	14.269	180670	0.4
4(1H)-Quinazoli...	14.599	0.2	ng	111953	3	14.269	180670	0.4
3,4-Biphenyldic...	15.626	0.2	ng	88600	3	14.269	180670	0.4
1H-Cyclopropa[a...	15.855	0.3	ng	145408	4	17.030	185282	0.4
2,2-Diphenyleth...	16.007	0.6	ng	275638	4	17.030	185282	0.4
Thiazolo[3,2-a]...	17.432	0.1	ng	53174	4	17.030	185282	0.4
2,4-Dichloro-5-...	17.797	0.2	ng	80364	4	17.030	185282	0.4
Perylene	22.985	0.2	ng	58896	6	23.488	131298	0.4
Benzo[a]pyrene	23.296	0.5	ng	159408	6	23.488	131298	0.4
1-(3-Hydroxy-3-...	23.539	0.3	ng	83282	6	23.488	131298	0.4