LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016703.D
Acq On : 03 Oct 2021 11:48
Operator : CG/JU
Sample : M3892-06
Misc :
ALS Vial : 71 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : S-822-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: BN016703.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	57	rVB	5273	19210	1.53%	0.190%
2	4.821	185	189	196	rBV	54143	120460	9.59%	1.192%
3	5.042	210	213	220	rBV	7048	17401	1.39%	0.172%
4	5.273	234	238	254	rVB	14925	38420	3.06%	0.380%
5	6.831	403	407	416	rVB2	19116	47993	3.82%	0.475%
6	7.642	490	495	499	rBV	41559	82157	6.54%	0.813%
7	7.938	523	527	532	rVB	69940	123135	9.81%	1.219%
8	8.784	598	605	609	rBV	26080	56073	4.47%	0.555%
9	10.065	703	706	713	rBV2	5376	13206	1.05%	0.131%
10	10.191	713	716	724	rBV	50216	87765	6.99%	0.869%
11	10.407	729	733	736	rBV	90549	156803	12.49%	1.552%
12	12.003	922	931	940	rBV2	38070	61223	4.88%	0.606%
13	12.078	940	948	960	rVB	14396	22825	1.82%	0.226%
14	12.296	987	997	1012	rVB	10286	16825	1.34%	0.167%
15	12.886	1071	1074	1078	rBV2	69051	120579	9.60%	1.194%
16	13.190	1094	1098	1102	rBV	13206	26451	2.11%	0.262%
17	14.269	1180	1183	1186	rBV	123706	183217	14.59%	1.814%
18	14.332	1186	1188	1192	rVB2	13192	24119	1.92%	0.239%
19	14.523	1198	1203	1206	rBV2	7255	14187	1.13%	0.140%
20	15.322	1263	1266	1269	rBV	14231	22369	1.78%	0.221%
21	15.639	1287	1291	1295	rVB3	4710	13529	1.08%	0.134%
22	15.728	1295	1298	1299	rBV2	8438	15574	1.24%	0.154%
23	15.766	1299	1301	1305	rVB2	14940	26329	2.10%	0.261%
24	16.007	1317	1320	1322	rVB2	29543	35544	2.83%	0.352%
25	17.018	1400	1403	1405	rBV	94324	161389	12.85%	1.597%
26	17.066	1405	1407	1410	rVV	149466	204142	16.26%	2.021%
27	17.151	1410	1414	1417	rVB	29637	48901	3.89%	0.484%
28	17.224	1417	1420	1425	rBV	8502	19164	1.53%	0.190%
29	17.431	1432	1437	1445	rBV2	16966	30550	2.43%	0.302%
30	17.796	1464	1467	1472	rVB	14324	29912	2.38%	0.296%
31	17.955	1473	1480	1483	rBV2	7226	23346	1.86%	0.231%
32	19.068	1689	1697	1699	rBV	92812	124282	9.90%	1.230%
33	19.098	1699	1703	1712	rVV	374039	476367	37.94%	4.715%
34	19.197	1714	1723	1728	rVV3	5754	15143	1.21%	0.150%
35	19.247	1730	1733	1745	rVB3	6849	14966	1.19%	0.148%
36	19.460	1767	1776	1788	rVB	299145	428513	34.12%	4.241%

LSC Area Percent Report

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Instrument : BNA_N
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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % of largest Peak
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Peak separation: 5

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.679	1815	1820	1836	rVB	74976	109142	8.69%	1.080%
38	20.017	1884	1887	1888	rBV	11865	16038	1.28%	0.159%
39	20.463	1927	1929	1931	rVV	12951	21456	1.71%	0.212%
40	20.495	1931	1932	1938	rVV2	36005	66304	5.28%	0.656%
41	20.643	1941	1946	1947	rVV2	11315	28841	2.30%	0.285%
42	20.675	1947	1949	1951	rVV	22576	36413	2.90%	0.360%
43	20.739	1951	1955	1957	rVV	38805	58011	4.62%	0.574%
44	20.781	1957	1959	1960	rVV	59372	83349	6.64%	0.825%
45	20.835	1960	1964	1966	rVV	71017	143826	11.45%	1.424%
46	20.877	1966	1968	1971	rVV	90091	124888	9.95%	1.236%
47	20.930	1971	1973	1975	rVV2	46594	79196	6.31%	0.784%
48	20.973	1975	1977	1979	rVV2	74398	122037	9.72%	1.208%
49	21.004	1979	1980	1983	rVV	52703	65335	5.20%	0.647%
50	21.058	1983	1985	1988	rVB	37820	50508	4.02%	0.500%
51	21.174	1993	1996	1998	rBV	53288	83545	6.65%	0.827%
52	21.227	1998	2001	2004	rVV2	221550	487652	38.83%	4.827%
53	21.270	2004	2005	2012	rVB	181493	212714	16.94%	2.105%
54	21.387	2012	2016	2020	rBV3	24607	72718	5.79%	0.720%
55	21.589	2033	2035	2036	rBV	21984	31895	2.54%	0.316%
56	21.695	2043	2045	2046	rBV	21962	30075	2.40%	0.298%
57	21.727	2046	2048	2050	rBV	20051	19644	1.56%	0.194%
58	21.812	2053	2056	2057	rBV	52590	86132	6.86%	0.853%
59	21.843	2057	2059	2061	rBV	62776	81985	6.53%	0.811%
60	21.886	2061	2063	2065	rBV	108620	201448	16.04%	1.994%
61	21.918	2065	2066	2068	rVB	136568	144554	11.51%	1.431%
62	22.024	2071	2076	2078	rBV	490022	1255719	100.00%	12.429%
63	22.151	2082	2088	2089	rBV	183768	612883	48.81%	6.066%
64	22.183	2089	2091	2093	rBV	166751	253735	20.21%	2.512%
65	22.321	2101	2104	2109	rVV	276666	1184717	94.35%	11.726%
66	22.396	2109	2111	2113	rVB	424123	413492	32.93%	4.093%
67	22.814	2221	2231	2239	rBV	113319	240762	19.17%	2.383%
68	22.896	2252	2255	2272	rVB	16457	24828	1.98%	0.246%
69	22.985	2274	2281	2310	rVB2	17822	34787	2.77%	0.344%
70	23.296	2362	2372	2388	rVB	56802	103115	8.21%	1.021%
71	23.392	2390	2400	2418	rVV2	76042	152675	12.16%	1.511%
72	23.491	2419	2429	2437	rVV	74663	143564	11.43%	1.421%
73	23.539	2437	2443	2471	rVB	42537	83036	6.61%	0.822%
74	24.090	2596	2604	2617	rVB	13362	25612	2.04%	0.254%
75	24.183	2623	2631	2653	rVB	12071	26882	2.14%	0.266%
76	24.861	2823	2829	2848	rVB	8449	17633	1.40%	0.175%

LSC Area Percent Report

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Operator : CG/JU
Sample : M3892-06
Misc :
ALS Vial : 71 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-822-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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Peak separation: 5

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

77	25.771	3080	3095	3119	rVB2	30376	93705	7.46%	0.928%
78	26.473	3283	3300	3333	rVB	17081	55995	4.46%	0.554%

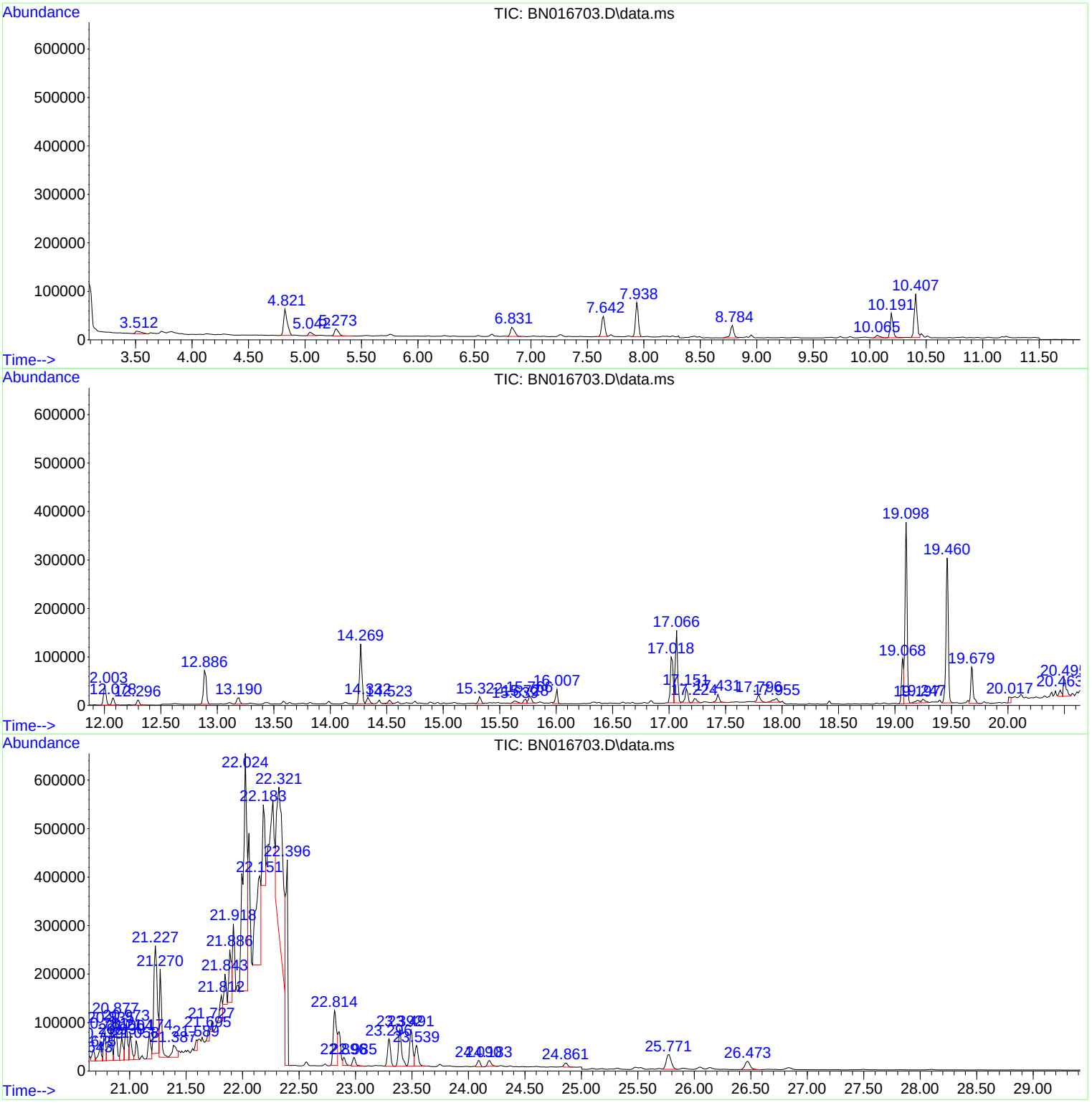
Sum of corrected areas: 10102915

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016703.D
Acq On : 03 Oct 2021 11:48
Operator : CG/JU
Sample : M3892-06
Misc :
ALS Vial : 71 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-822-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\
Data File : BN016703.D
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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

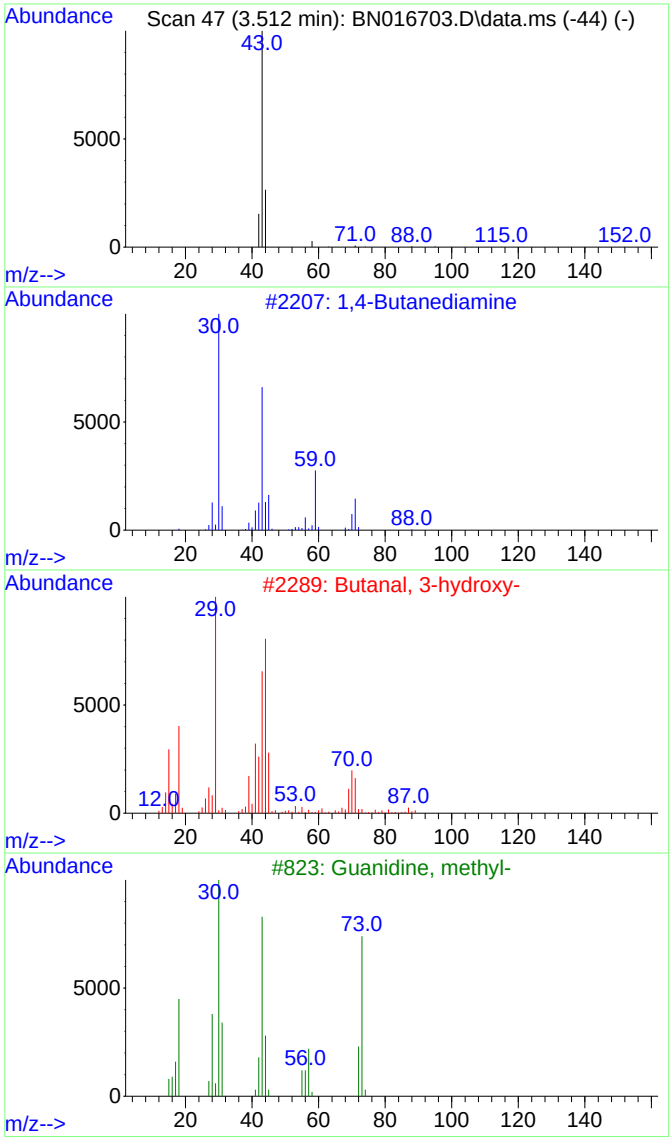
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

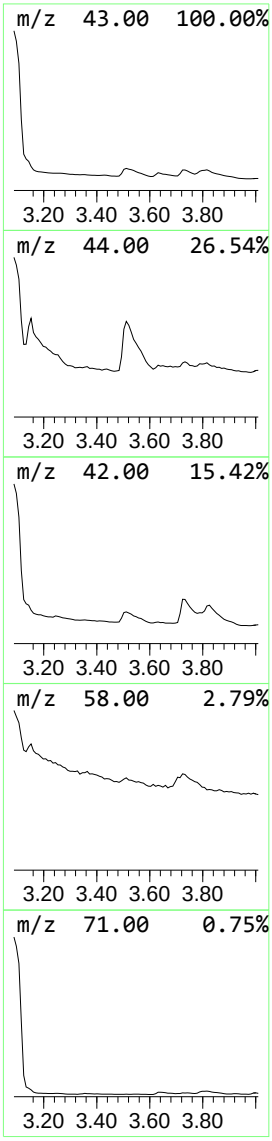
****

Peak Number 1 1,4-Butanediamine Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.512	0.09 ng	19210	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Butanediamine	88	C4H12N2	000110-60-1	5
2	Butanal, 3-hydroxy-	88	C4H8O2	000107-89-1	4
3	Guanidine, methyl-	73	C2H7N3	000471-29-4	4
4	Hydrogen isocyanate	43	CHNO	000075-13-8	3
5	Isobutane	58	C4H10	000075-28-5	3





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016703.D
Acq On : 03 Oct 2021 11:48
Operator : CG/JU
Sample : M3892-06
Misc :
ALS Vial : 71 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-822-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

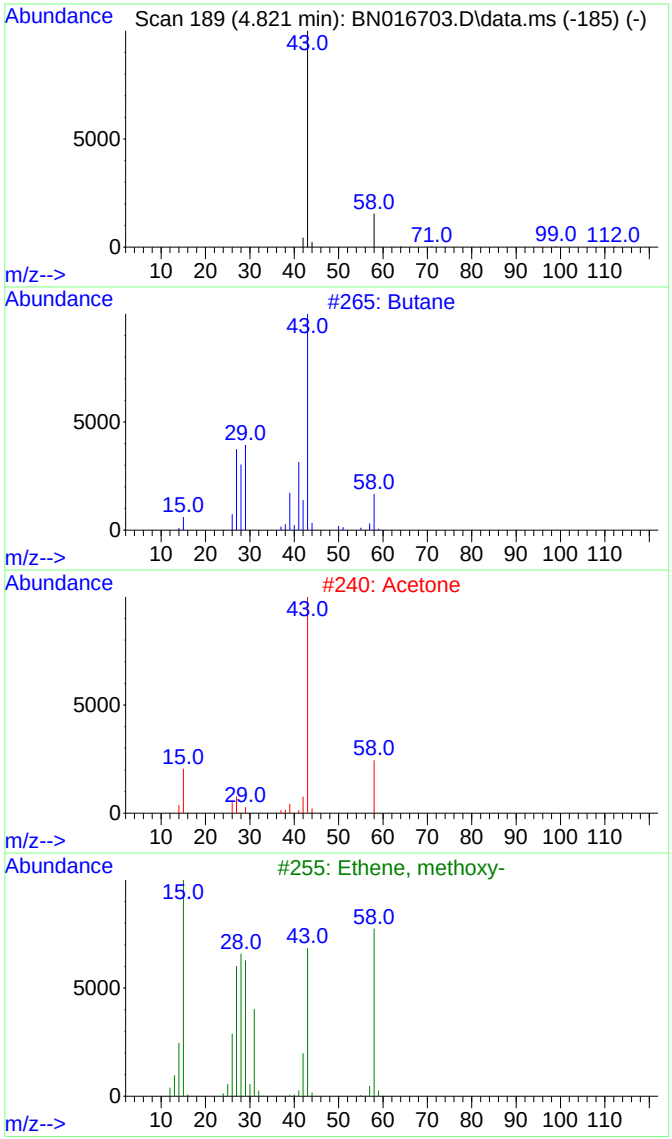
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

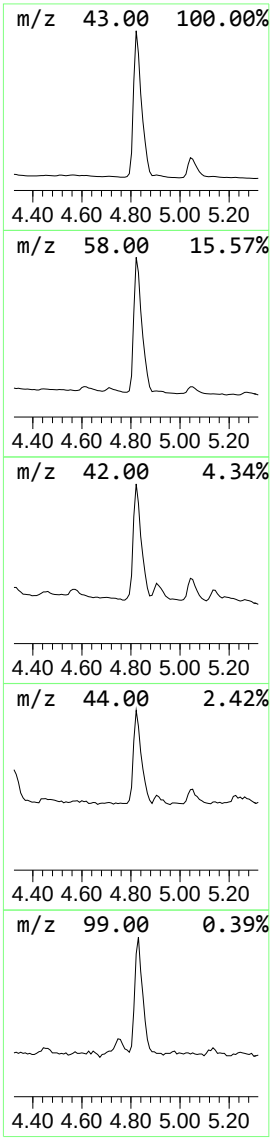
****

Peak Number 2 Butane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.59 ng	120460	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 : BN016703.D
Acq On : 03 Oct 2021 11:48
Operator : CG/JU
Sample : M3892-06
Misc :
ALS Vial : 71 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-822-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

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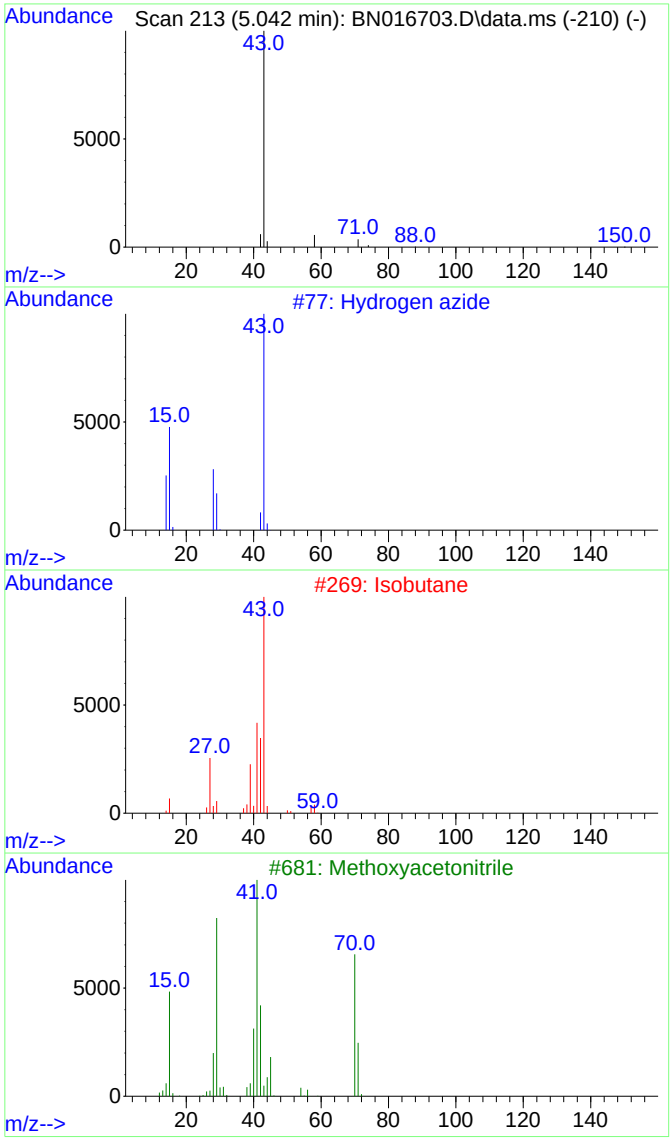
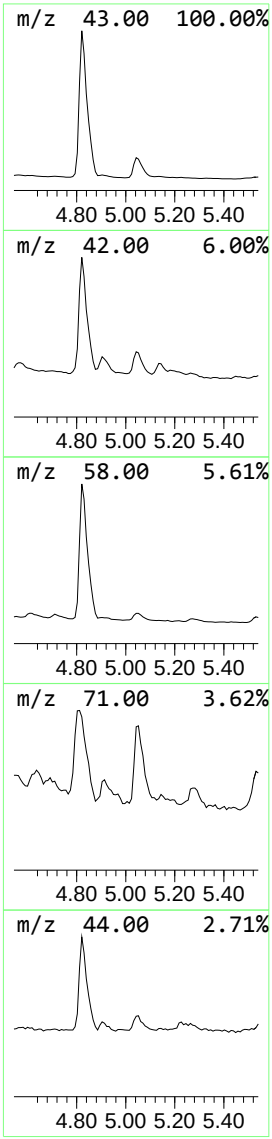
Peak Number 3 Hydrogen azide Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.042	0.08 ng	17401	1,4-Dichlorobenzene-d4	7.642

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	Methoxyacetonitrile	71	C3H5NO	001738-36-9	3
4	Butane	58	C4H10	000106-97-8	3
5	Butanal, 3-hydroxy-	88	C4H8O2	000107-89-1	2





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

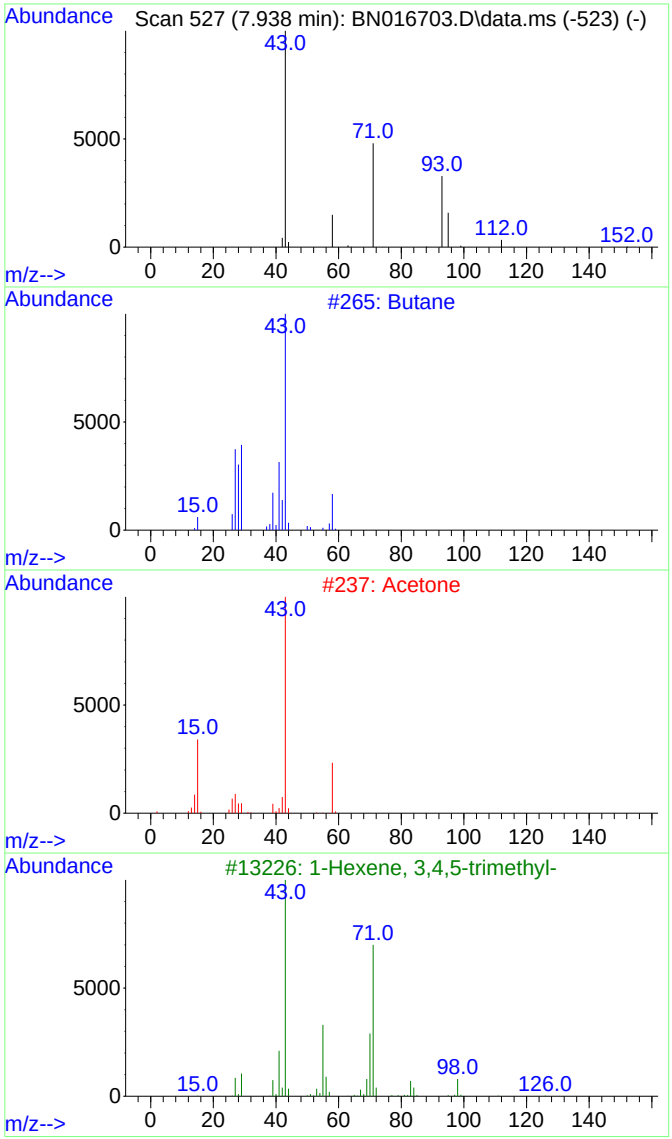
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

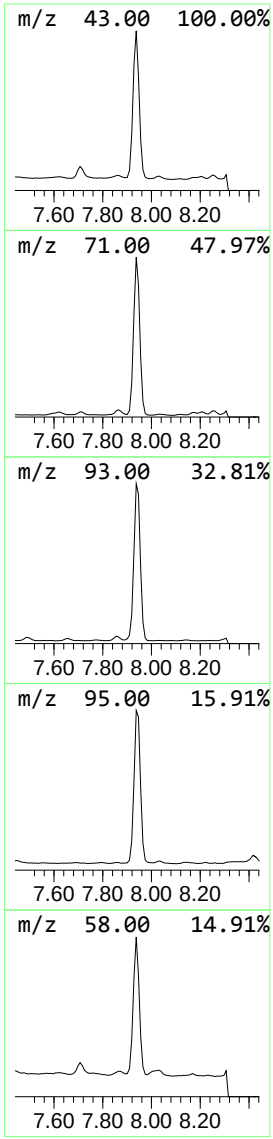
****

Peak Number 4 Butane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.938	0.60 ng	123135	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-Propenamide	71	C3H5NO	000079-06-1	3
5	Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	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

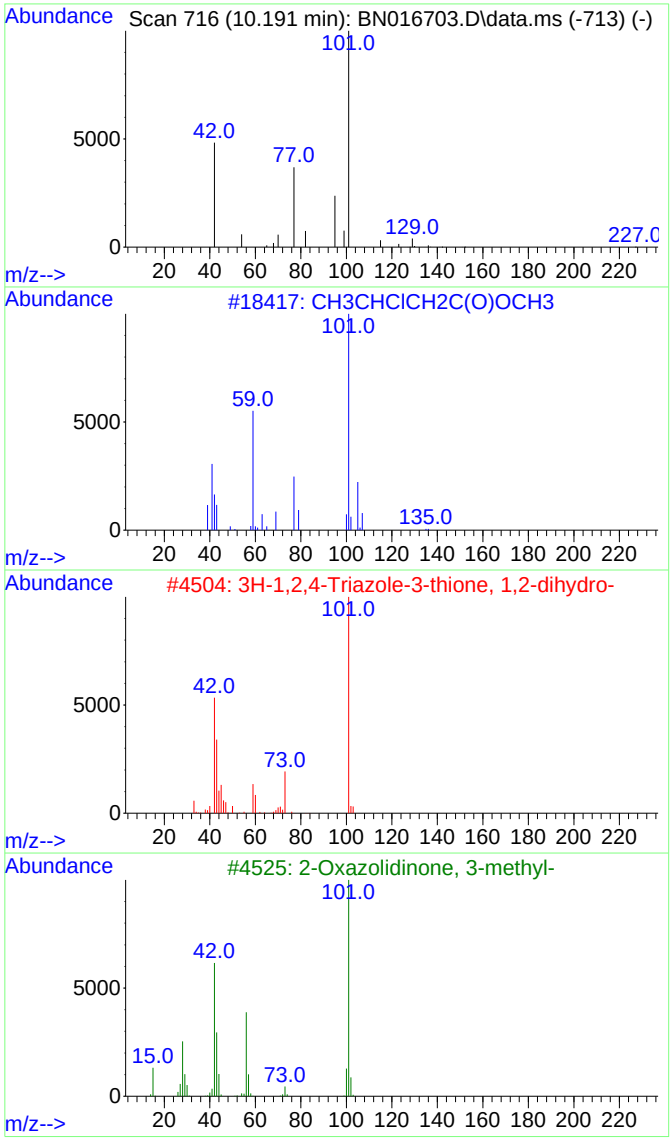
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

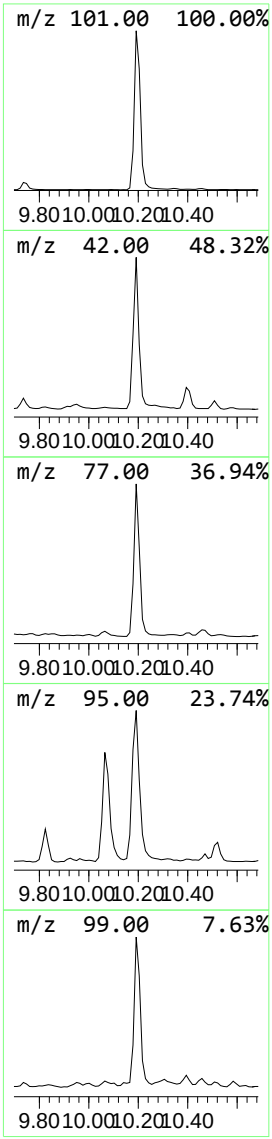
****

Peak Number 5 CH3CHClCH2C(O)OCH3 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.22 ng	87765	Naphthalene-d8	10.407

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	CH3CHClCH2C(O)OCH3	136	C5H9ClO2	000817-76-5	7
2	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
3	2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	5
4	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	5
5	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5





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Data File : BN016703.D
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Sample : M3892-06
Misc :
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Instrument : BNA_N
ClientSampleId : S-822-N-SO-1-1.5-092221

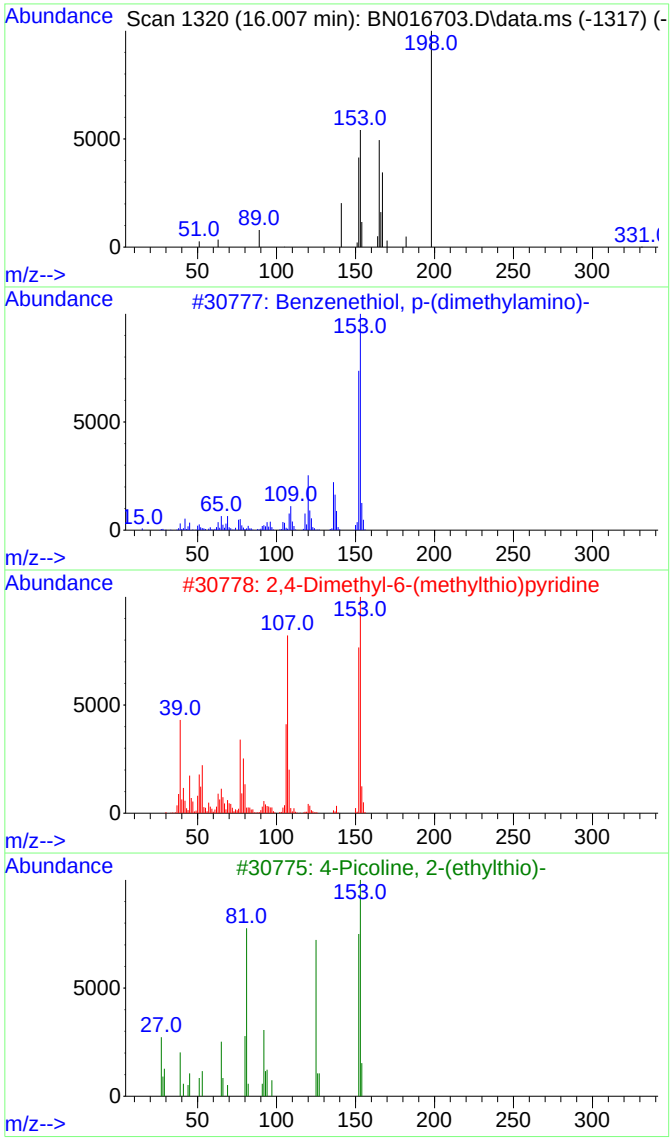
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

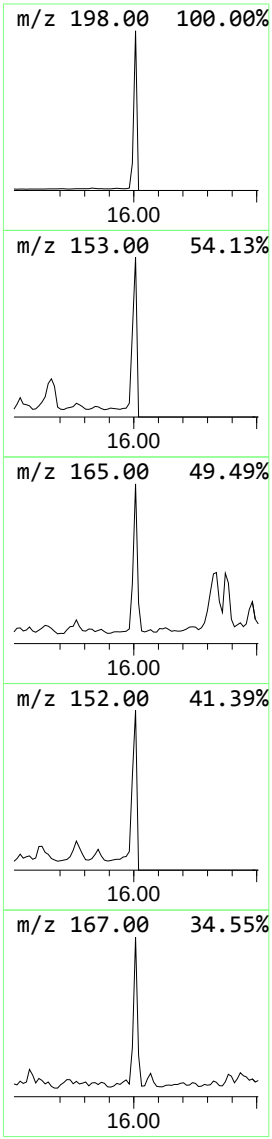
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzenethiol, p-(dimethylam... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.007	0.09 ng	35544	Phenanthrene-d10	17.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenethiol, p-(dimethylamino)-	153	C8H11NS	004946-22-9	10
2	2,4-Dimethyl-6-(methylthio)pyridine	153	C8H11NS	1000305-54-7	9
3	4-Picoline, 2-(ethylthio)-	153	C8H11NS	019006-78-1	9
4	2H-Pyrimido[1,2-a]pyrimidine, 1,...	153	C8H15N3	084030-20-6	9
5	2(1H)-Pyridinethione, 1-ethyl-6-...	153	C8H11NS	019006-73-6	9





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Acq On : 03 Oct 2021 11:48
Operator : CG/JU
Sample : M3892-06
Misc :
ALS Vial : 71 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S-822-N-SO-1-1.5-092221

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

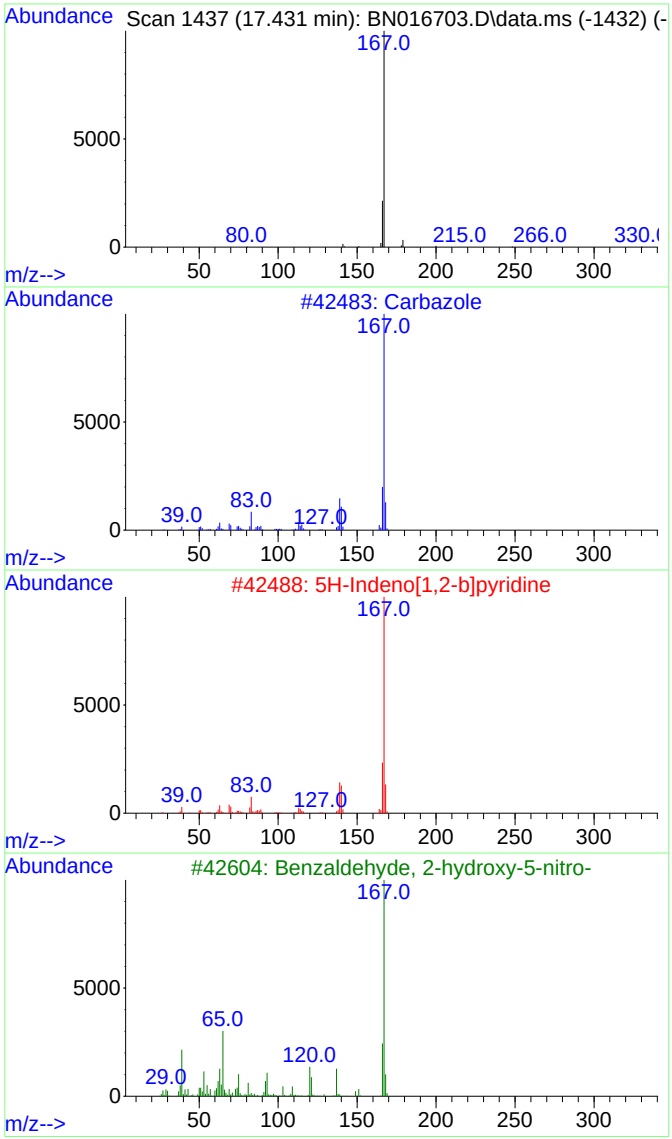
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

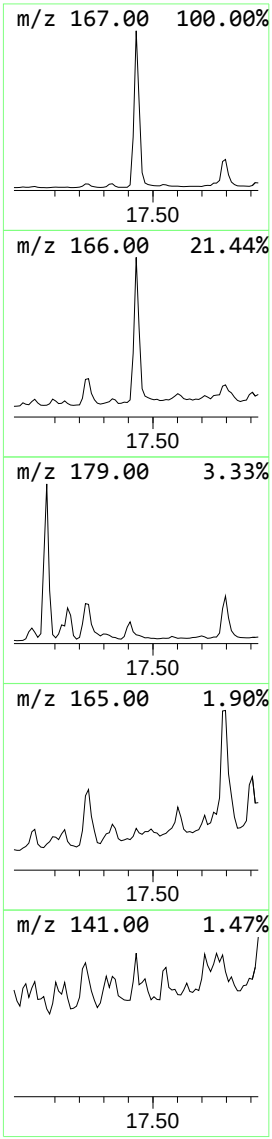
****

Peak Number 7 Carbazole Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.431	0.08 ng	30550	Phenanthrene-d10	17.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbazole	167	C12H9N	000086-74-8	9
2	5H-Indeno[1,2-b]pyridine	167	C12H9N	000244-99-5	9
3	Benzaldehyde, 2-hydroxy-5-nitro-	167	C7H5NO4	000097-51-8	5
4	2-Azaspiro[4.5]decan-3-one, 8-me...	167	C10H17NO	196608-77-2	5
5	benzaldehyde, 2-hydroxy-4-nitro-	167	C7H5NO4	1000404-52-2	5





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ClientSampleId :
S-822-N-SO-1-1.5-092221

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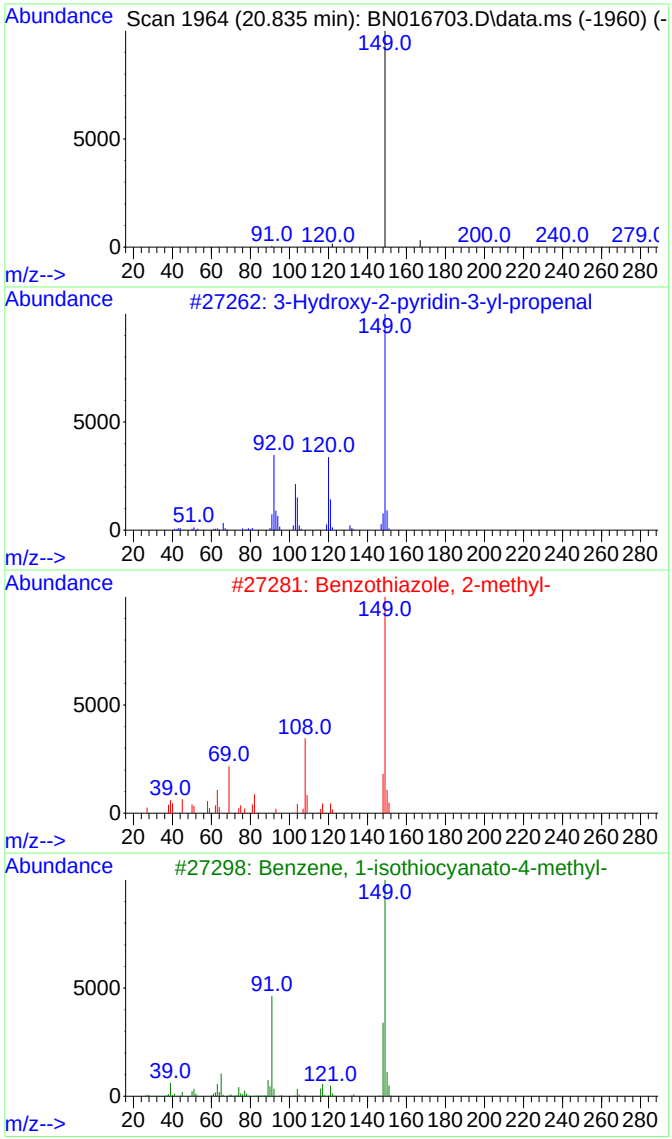
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

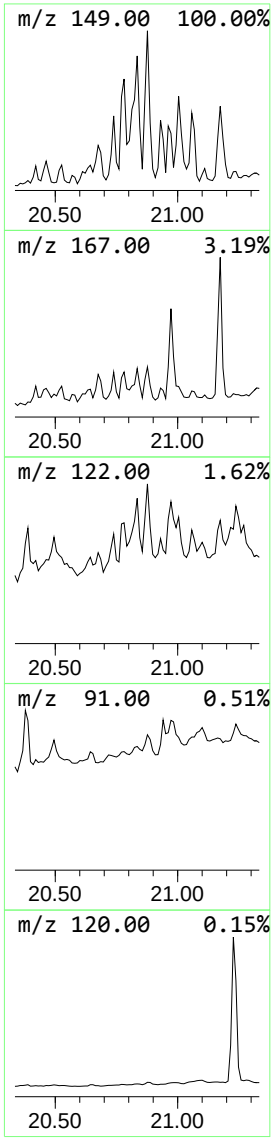
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 3-Hydroxy-2-pyridin-3-yl-pr... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.834	0.12 ng	143826	Chrysene-d12	21.238

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hydroxy-2-pyridin-3-yl-propenal	149	C8H7NO2	1000311-61-6	4
2	Benzothiazole, 2-methyl-	149	C8H7NS	000120-75-2	4
3	Benzene, 1-isothiocyanato-4-methyl-	149	C8H7NS	000622-59-3	4
4	Pyridine, pentamethyl-	149	C10H15N	003748-83-2	4
5	m-Tolyl isothiocyanate	149	C8H7NS	000621-30-7	4





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Misc :
ALS Vial : 71 Sample Multiplier: 1

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

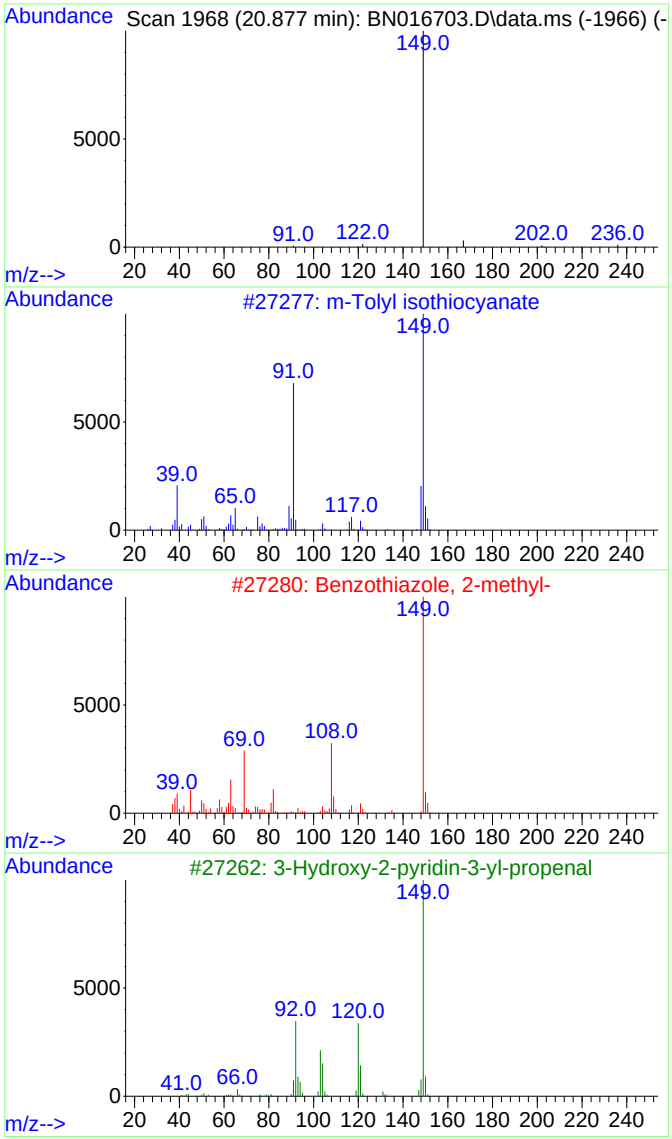
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

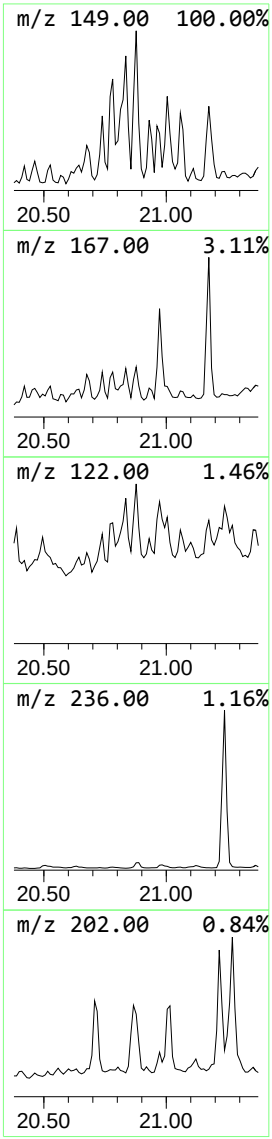
****

Peak Number 9 m-Tolyl isothiocyanate Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.877	0.10 ng	124888	Chrysene-d12	21.238

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	m-Tolyl isothiocyanate	149	C8H7NS	000621-30-7	4
2	Benzothiazole, 2-methyl-	149	C8H7NS	000120-75-2	4
3	3-Hydroxy-2-pyridin-3-yl-propenal	149	C8H7NO2	1000311-61-6	4
4	Pyridine, pentamethyl-	149	C10H15N	003748-83-2	4
5	Benzene, 1-isothiocyanato-4-methyl-	149	C8H7NS	000622-59-3	4





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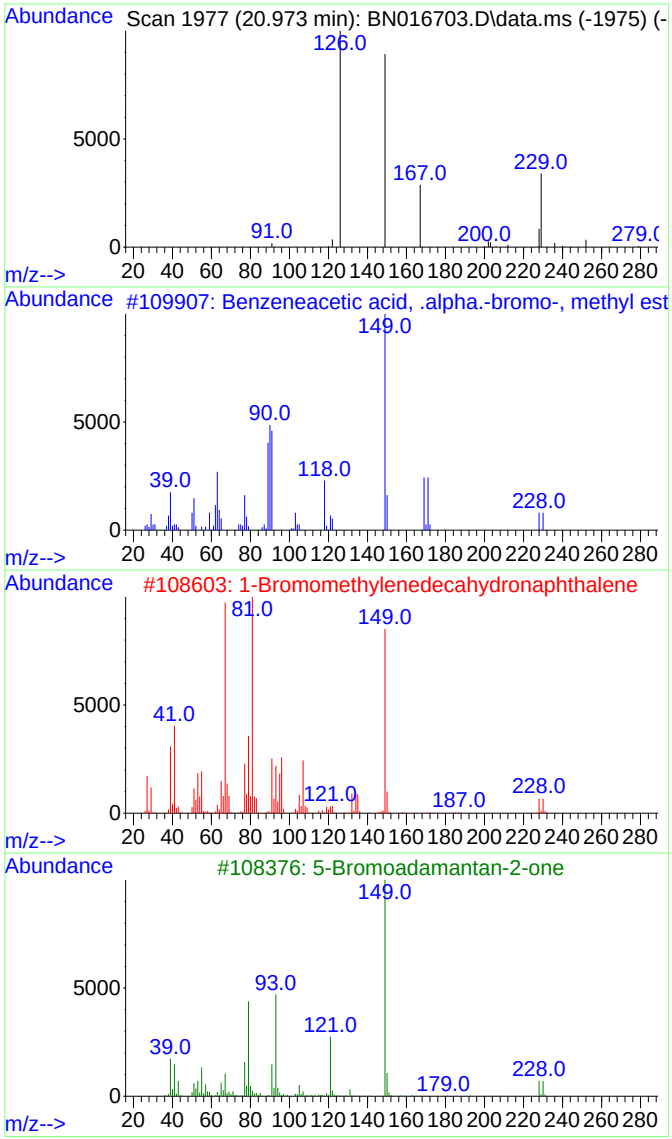
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

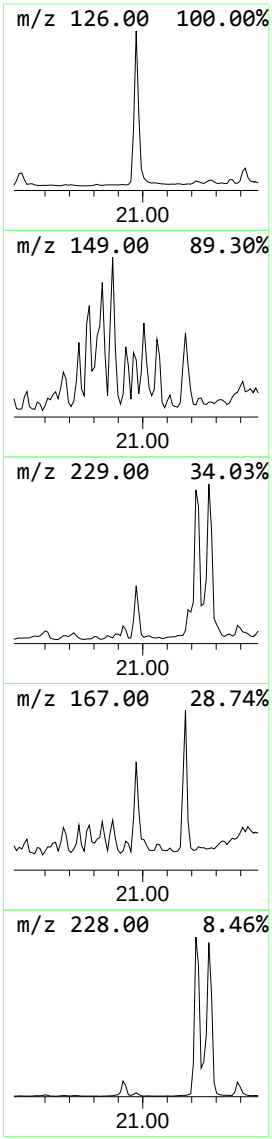
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzeneacetic acid, .alpha.... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.973	0.10 ng	122037	Chrysene-d12	21.238

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneacetic acid, .alpha.-brom...	228	C9H9BrO2	003042-81-7	7
2	1-Bromomethylenedecahydronaphtha...	228	C11H17Br	1000191-97-5	7
3	5-Bromoadamantan-2-one	228	C10H13BrO	020098-20-8	5
4	Nicotinic acid, 1,2-dihydro-4,6-...	167	C8H9NO3	024667-09-2	5
5	Tricyclo[3.3.1.1(3,7)]decanone, ...	228	C10H13BrO	032456-49-8	4





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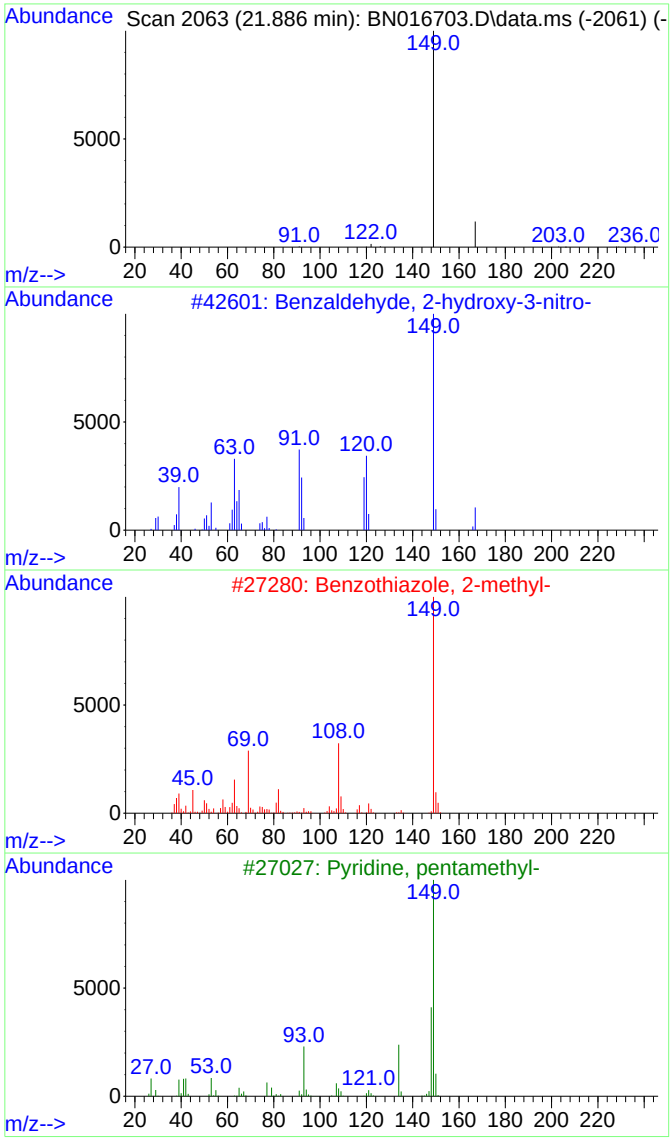
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

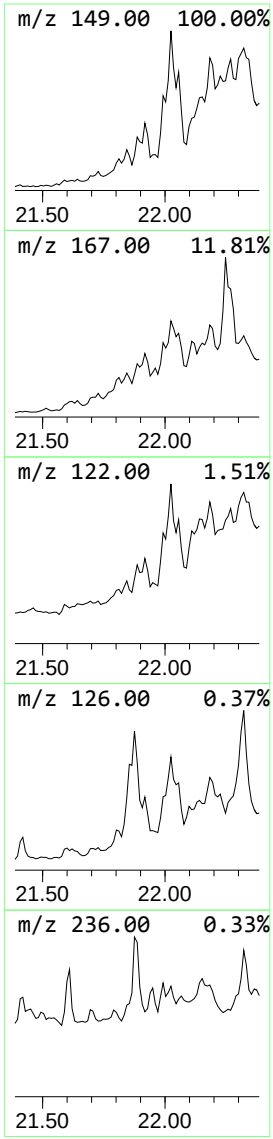
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Benzaldehyde, 2-hydroxy-3-n... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.886	0.17 ng	201448	Chrysene-d12	21.238

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 2-hydroxy-3-nitro-	167	C7H5NO4	005274-70-4	4
2	Benzothiazole, 2-methyl-	149	C8H7NS	000120-75-2	4
3	Pyridine, pentamethyl-	149	C10H15N	003748-83-2	4
4	m-Tolyl isothiocyanate	149	C8H7NS	000621-30-7	4
5	Benzene, 1-isothiocyanato-4-methyl-	149	C8H7NS	000622-59-3	4





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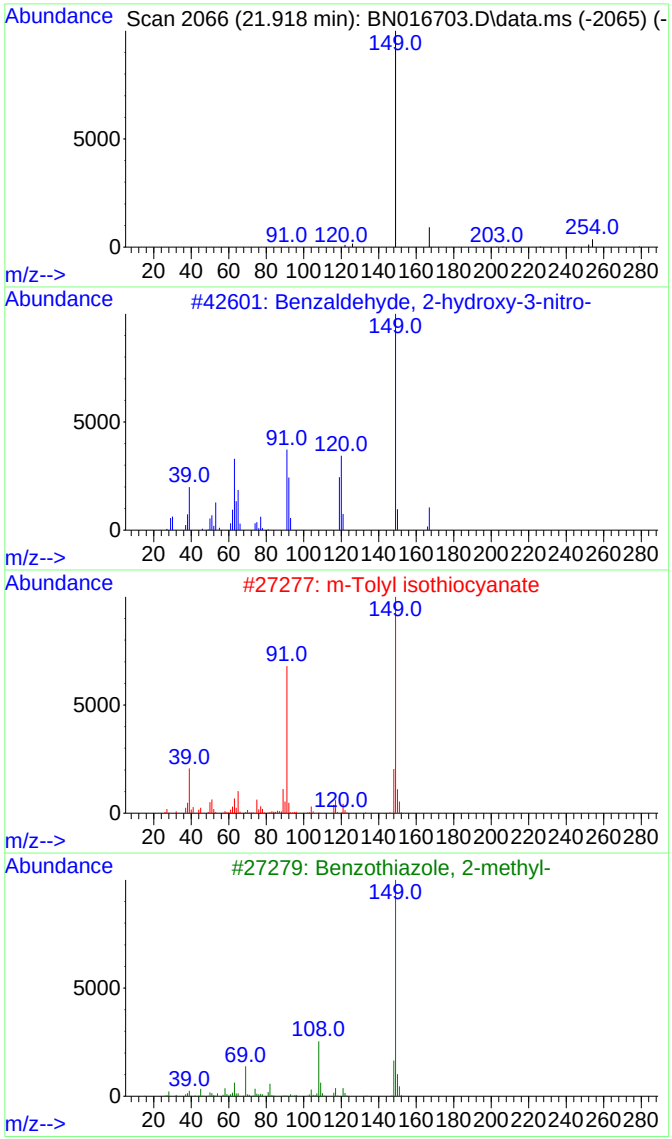
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

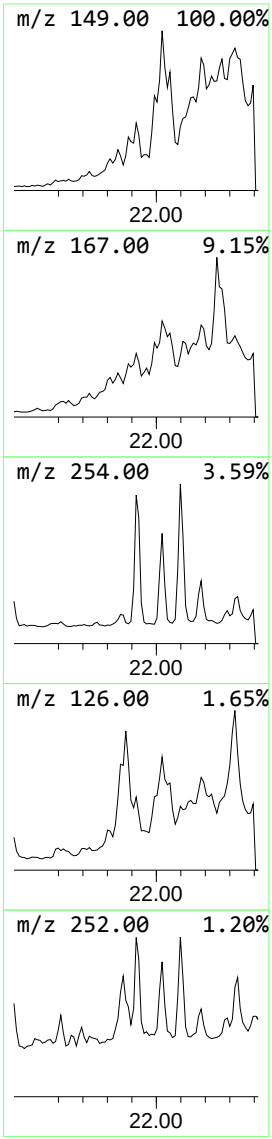
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Benzaldehyde, 2-hydroxy-3-n... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.918	0.12 ng	144554	Chrysene-d12	21.238

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 2-hydroxy-3-nitro-	167	C7H5NO4	005274-70-4	4
2	m-Tolyl isothiocyanate	149	C8H7NS	000621-30-7	4
3	Benzothiazole, 2-methyl-	149	C8H7NS	000120-75-2	4
4	Benzene, 1-isothiocyanato-4-methyl-	149	C8H7NS	000622-59-3	4
5	Disulfide, 1-(1-propenyldithio)p...	254	C9H18S4	126876-37-7	4





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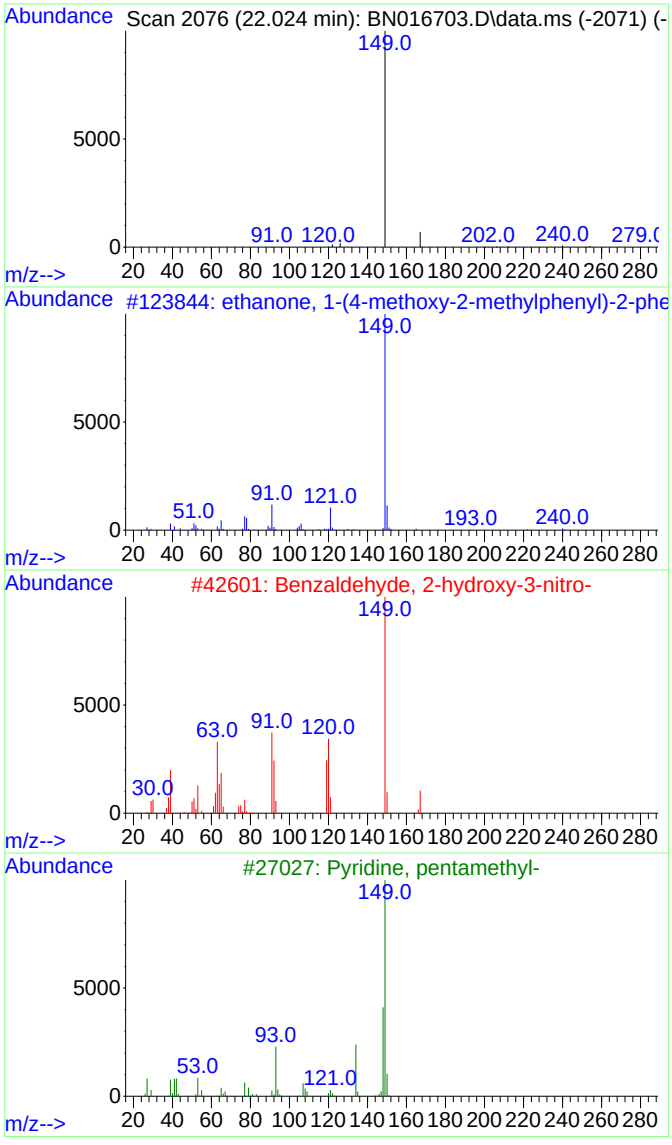
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

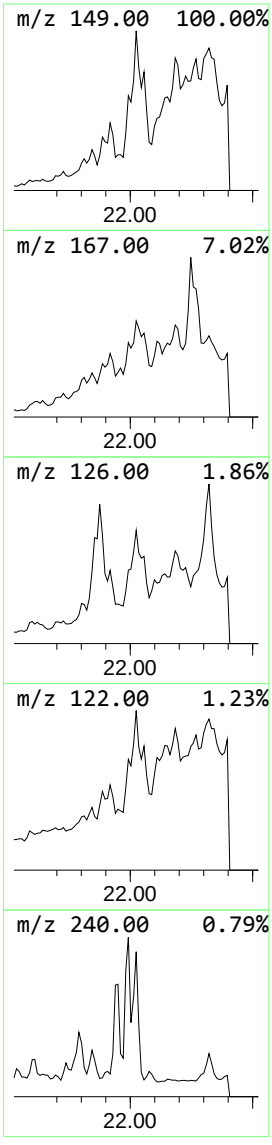
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 ethanone, 1-(4-methoxy-2-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.024	1.03 ng	1255720	Chrysene-d12	21.238

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	ethanone, 1-(4-methoxy-2-methylp...	240	C16H16O2	1000401-19-7	5
2	Benzaldehyde, 2-hydroxy-3-nitro-	167	C7H5NO4	005274-70-4	4
3	Pyridine, pentamethyl-	149	C10H15N	003748-83-2	4
4	3-Hydroxy-2-pyridin-3-yl-propenal	149	C8H7NO2	1000311-61-6	4
5	Benzothiazole, 2-methyl-	149	C8H7NS	000120-75-2	4





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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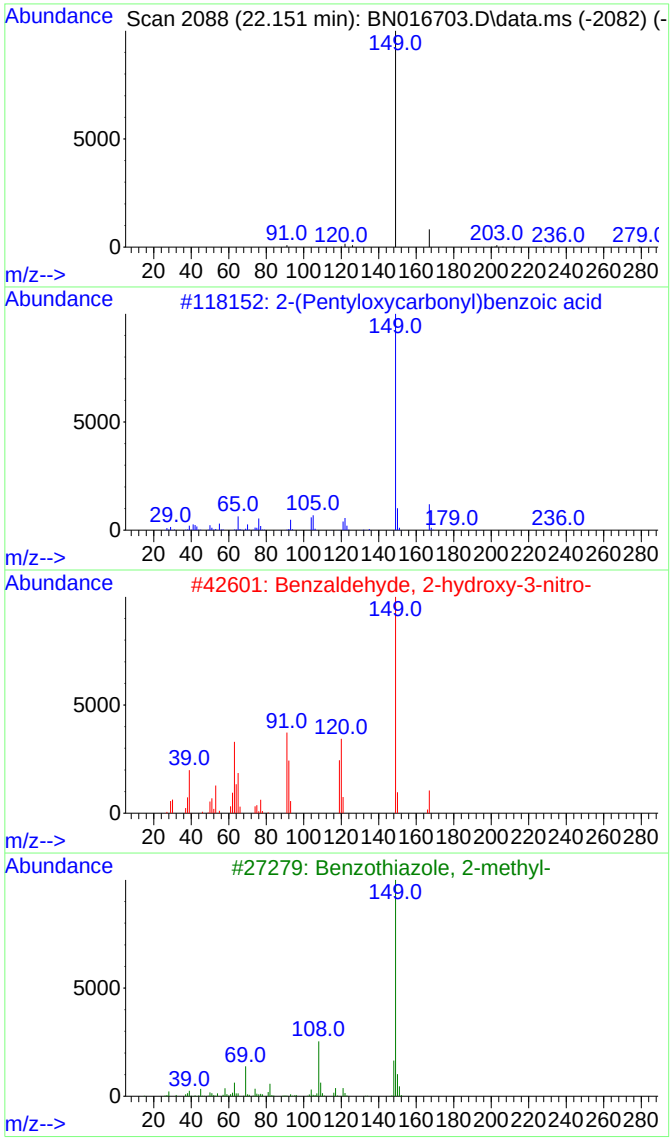
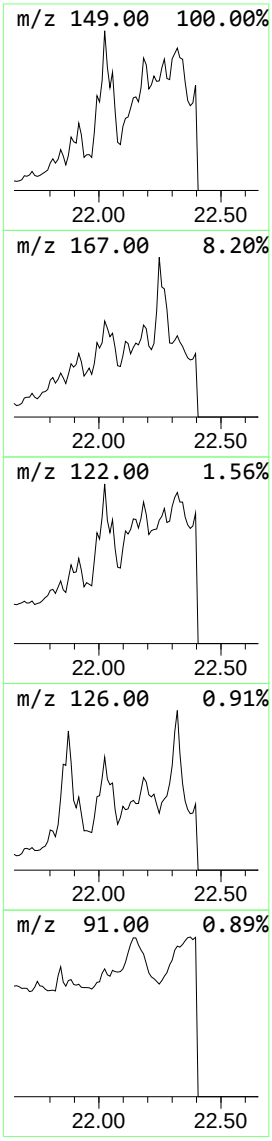
****
Peak Number 14 2-(Pentyloxycarbonyl)benzoi... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.151	0.50 ng	612883	Chrysene-d12	21.238

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(Pentyloxycarbonyl)benzoic acid	236	C13H16O4	024539-56-8	5
2	Benzaldehyde, 2-hydroxy-3-nitro-	167	C7H5NO4	005274-70-4	4
3	Benzothiazole, 2-methyl-	149	C8H7NS	000120-75-2	4
4	m-Tolyl isothiocyanate	149	C8H7NS	000621-30-7	4
5	3-Hydroxy-2-pyridin-3-yl-propenal	149	C8H7NO2	1000311-61-6	4





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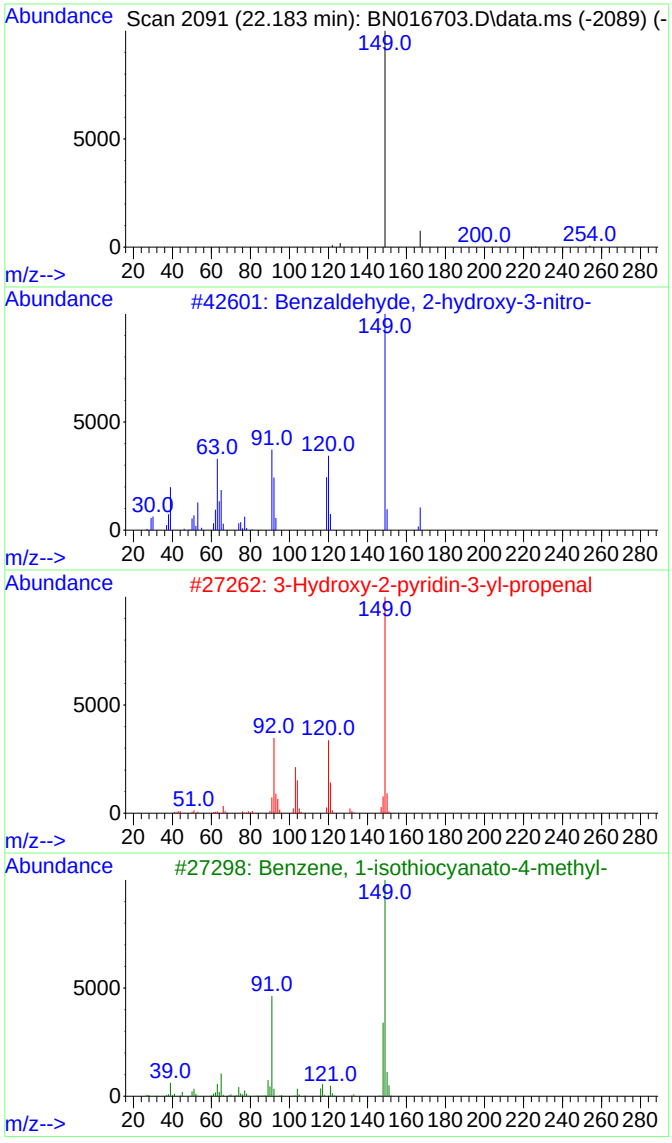
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

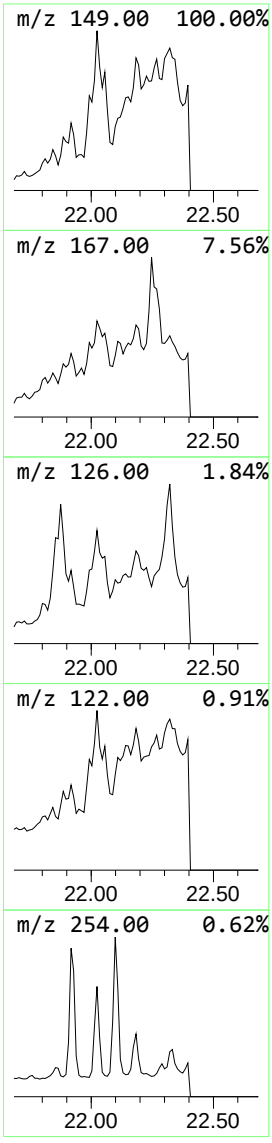
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 Benzaldehyde, 2-hydroxy-3-n... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.183	0.21 ng	253735	Chrysene-d12	21.238

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 2-hydroxy-3-nitro-	167	C7H5NO4	005274-70-4	4
2	3-Hydroxy-2-pyridin-3-yl-propenal	149	C8H7NO2	1000311-61-6	4
3	Benzene, 1-isothiocyanato-4-methyl-	149	C8H7NS	000622-59-3	4
4	Ethanone, 2-(1-methylethoxy)-1,2...	254	C17H18O2	006652-28-4	3
5	3-Carbamoyl-2-pyrazinecarboxylic...	167	C6H5N3O3	067367-37-7	3





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TIC Library : C:\Database\NIST20.L
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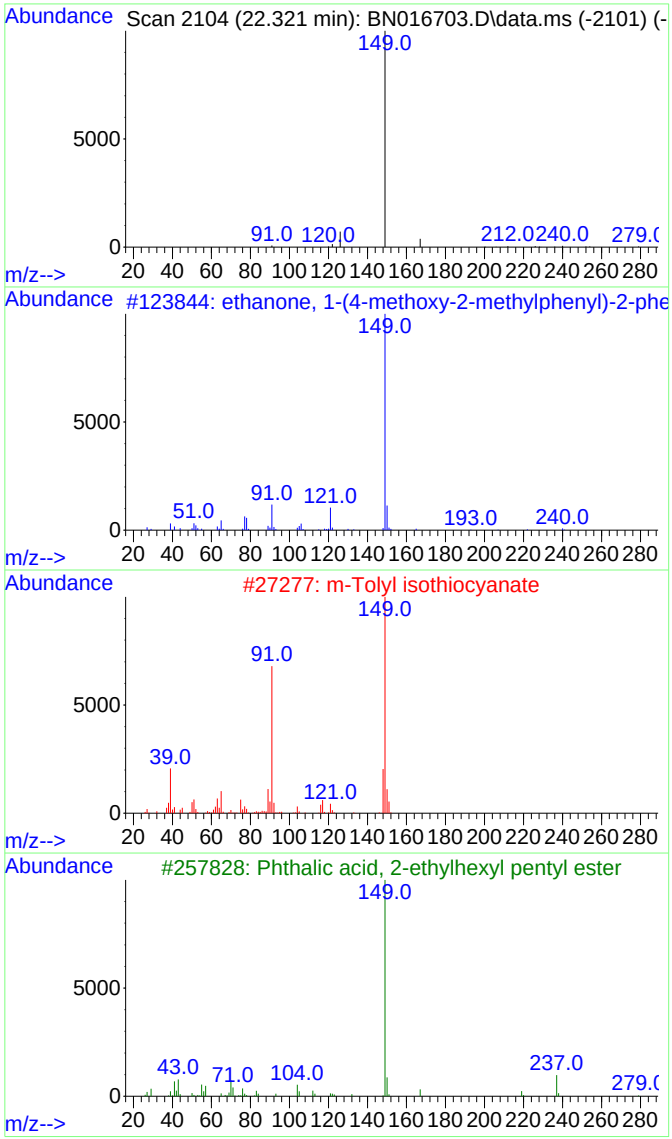
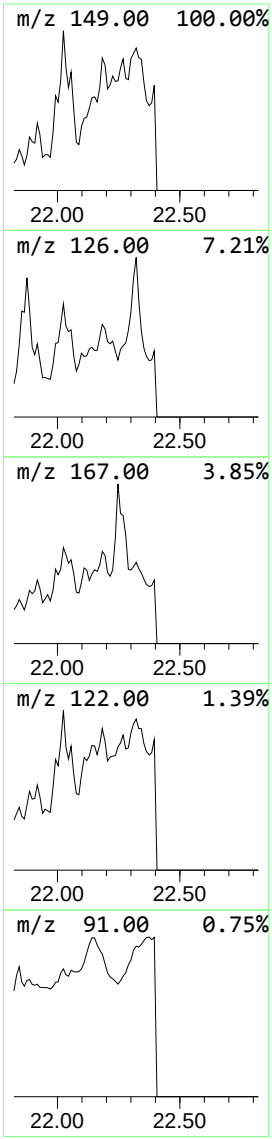
****
Peak Number 16 ethanone, 1-(4-methoxy-2-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.321	0.97 ng	1184720	Chrysene-d12	21.238

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	ethanone, 1-(4-methoxy-2-methylp...	240	C16H16O2	1000401-19-7	5
2	m-Tolyl isothiocyanate	149	C8H7NS	000621-30-7	4
3	Phthalic acid, 2-ethylhexyl pent...	348	C21H32O4	1000309-01-3	4
4	Benzothiazole, 2-methyl-	149	C8H7NS	000120-75-2	4
5	3-Hydroxy-2-pyridin-3-yl-propenal	149	C8H7NO2	1000311-61-6	4





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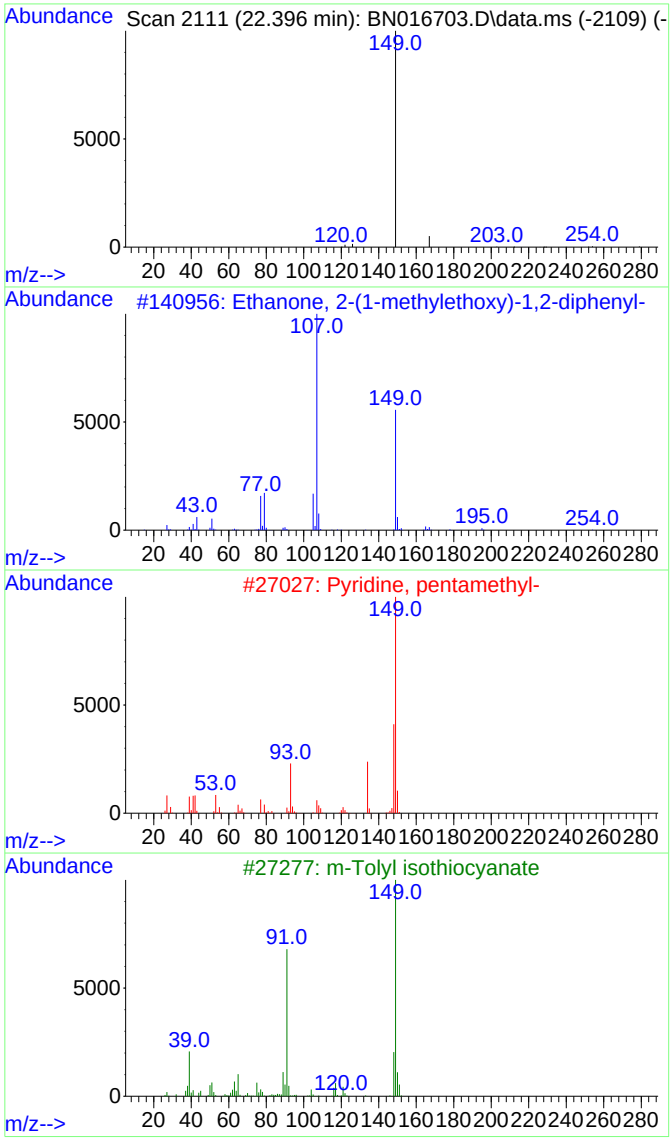
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

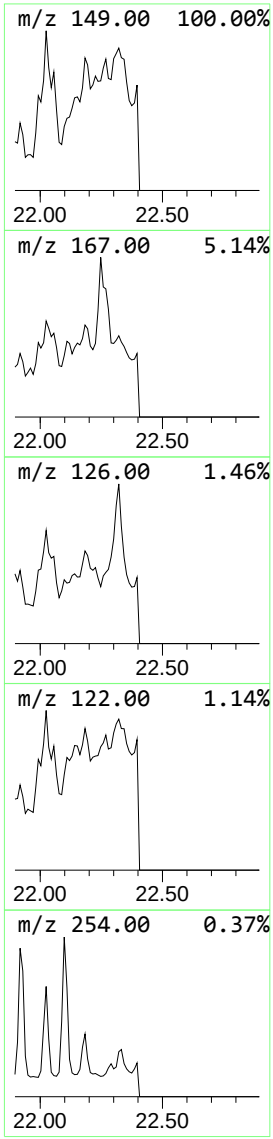
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 Ethanone, 2-(1-methylethoxy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.396	1.15 ng	413492	Perylene-d12	23.491

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 2-(1-methylethoxy)-1,2...	254	C17H18O2	006652-28-4	4
2	Pyridine, pentamethyl-	149	C10H15N	003748-83-2	4
3	m-Tolyl isothiocyanate	149	C8H7NS	000621-30-7	4
4	Benzothiazole, 2-methyl-	149	C8H7NS	000120-75-2	4
5	3-Hydroxy-2-pyridin-3-yl-propenal	149	C8H7NO2	1000311-61-6	4





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Data File : BN016703.D
Acq On : 03 Oct 2021 11:48
Operator : CG/JU
Sample : M3892-06
Misc :
ALS Vial : 71 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : S-822-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

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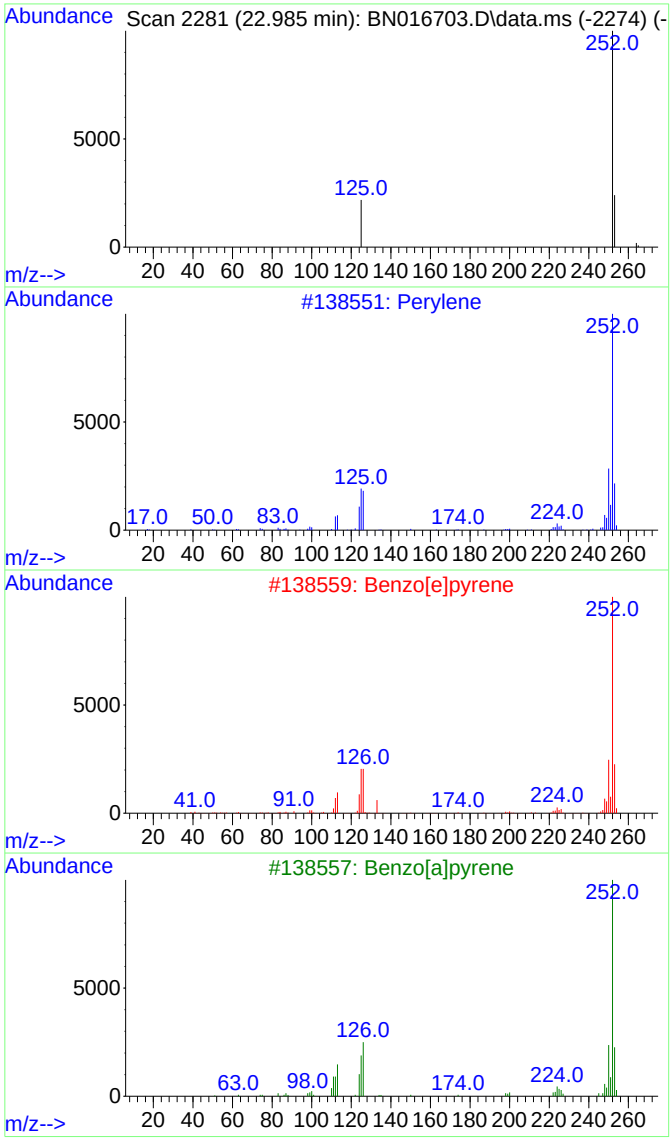
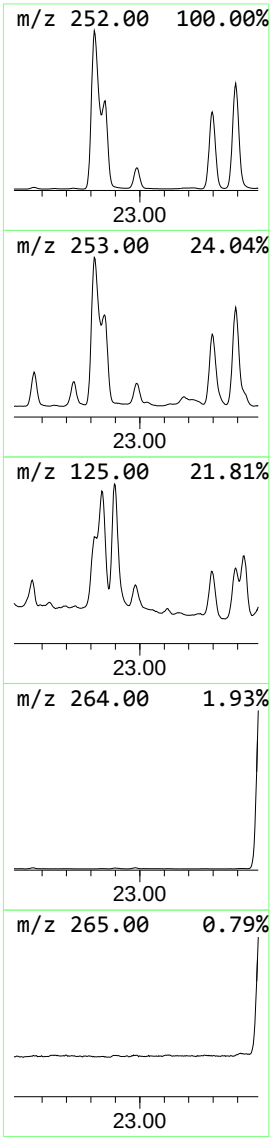
Peak Number 18 Perylene Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.985	0.10 ng	34787	Perylene-d12	23.491

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	9
2	Benzo[e]pyrene	252	C20H12	000192-97-2	9
3	Benzo[a]pyrene	252	C20H12	000050-32-8	9
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	9
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	9





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Data File : BN016703.D
Acq On : 03 Oct 2021 11:48
Operator : CG/JU
Sample : M3892-06
Misc :
ALS Vial : 71 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-822-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

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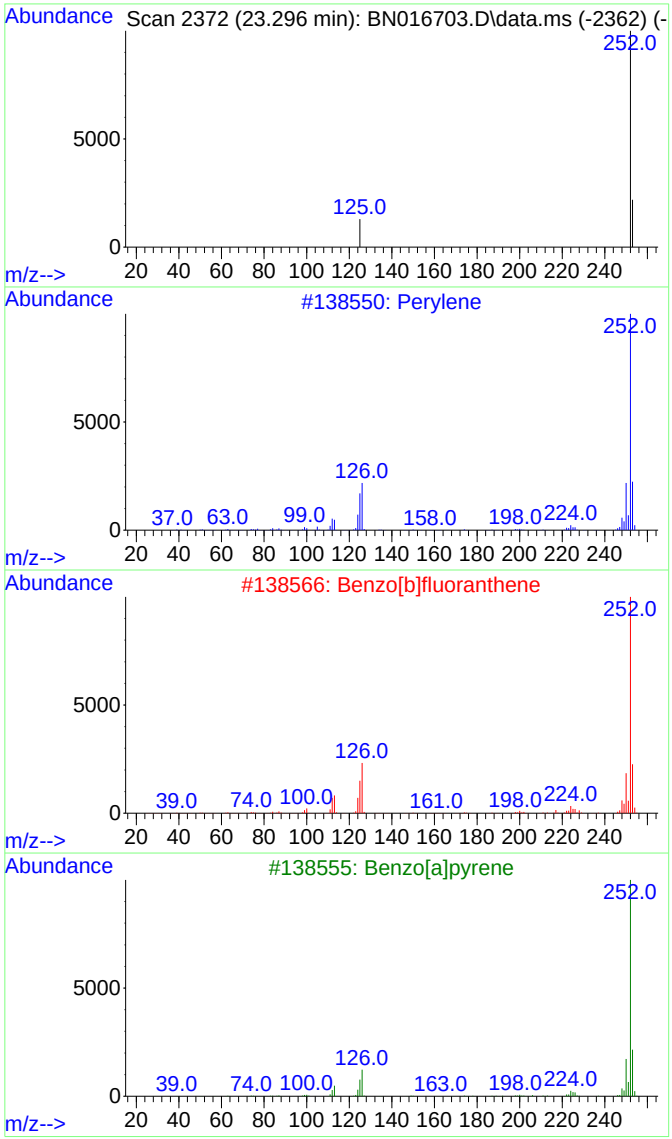
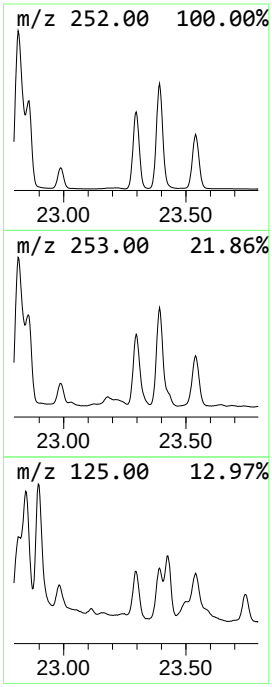
Peak Number 19 Perylene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.296	0.29 ng	103115	Perylene-d12	23.491

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	9
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	9
3	Benzo[a]pyrene	252	C20H12	000050-32-8	9
4	Benzo[e]pyrene	252	C20H12	000192-97-2	9
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016703.D
Acq On : 03 Oct 2021 11:48
Operator : CG/JU
Sample : M3892-06
Misc :
ALS Vial : 71 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-822-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

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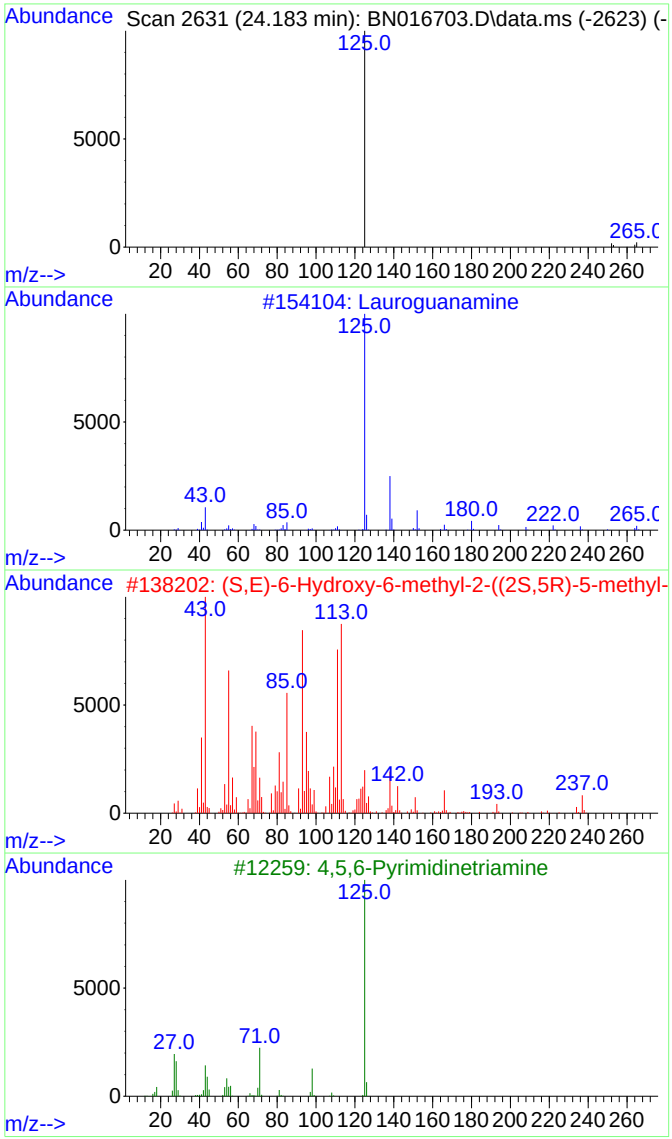
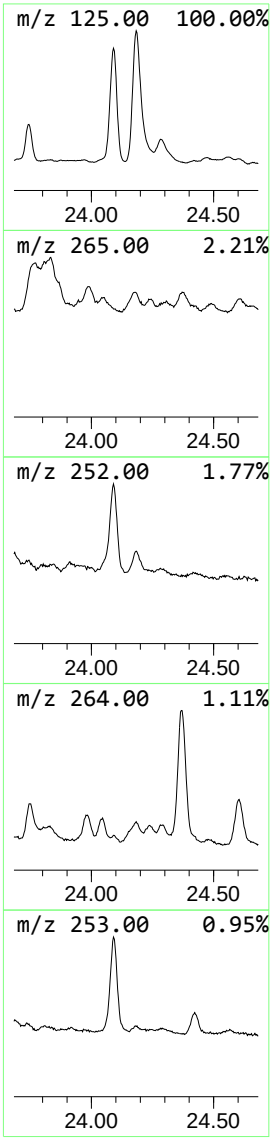
Peak Number 20 Lauroguanamine Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.183	0.07 ng	26882	Perylene-d12	23.491

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lauroguanamine	265	C14H27N5	002533-34-8	5
2	(S,E)-6-Hydroxy-6-methyl-2-((2S,...	252	C15H24O3	088243-64-5	3
3	4,5,6-Pyrimidinetriamine	125	C4H7N5	000118-70-7	2
4	2-Amino-4-hydroxy-6-methylpyrimi...	125	C5H7N3O	003977-29-5	2
5	Pyridine, 4-methoxy-1-oxide-	125	C6H7NO2	001122-96-9	2





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016703.D
Acq On : 03 Oct 2021 11:48
Operator : CG/JU
Sample : M3892-06
Misc :
ALS Vial : 71 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-822-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
1,4-Butanediamine	3.512	0.1	ng	19210	1	7.642	82157	0.4
Butane	4.821	0.6	ng	120460	1	7.642	82157	0.4
Hydrogen azide	5.042	0.1	ng	17401	1	7.642	82157	0.4
Butane	7.938	0.6	ng	123135	1	7.642	82157	0.4
CH3CHClCH2C(O)OCH3	10.191	0.2	ng	87765	2	10.407	156803	0.4
Benzenethiol, p...	16.007	0.1	ng	35544	4	17.018	161389	0.4
Carbazole	17.431	0.1	ng	30550	4	17.018	161389	0.4
3-Hydroxy-2-pyr...	20.834	0.1	ng	143826	5	21.238	487652	0.4
m-Tolyl isothio...	20.877	0.1	ng	124888	5	21.238	487652	0.4
Benzeneacetic a...	20.973	0.1	ng	122037	5	21.238	487652	0.4
Benzaldehyde, 2...	21.886	0.2	ng	201448	5	21.238	487652	0.4
Benzaldehyde, 2...	21.918	0.1	ng	144554	5	21.238	487652	0.4
ethanone, 1-(4-...	22.024	1.0	ng	1255720	5	21.238	487652	0.4
2-(Pentyloxycar...	22.151	0.5	ng	612883	5	21.238	487652	0.4
Benzaldehyde, 2...	22.183	0.2	ng	253735	5	21.238	487652	0.4
ethanone, 1-(4-...	22.321	1.0	ng	1184720	5	21.238	487652	0.4
Ethanone, 2-(1-...	22.396	1.2	ng	413492	6	23.491	143564	0.4
Perylene	22.985	0.1	ng	34787	6	23.491	143564	0.4
Perylene	23.296	0.3	ng	103115	6	23.491	143564	0.4
Lauroguanamine	24.183	0.1	ng	26882	6	23.491	143564	0.4