LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016626.D
Acq On : 01 Oct 2021 08:23
Operator : CG/JU
Sample : M3833-16
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : RE126D1-20210920

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: BN016626.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.152	6	8	11	rVB	61503	67247	11.82%	2.198%
2	3.253	16	19	44	rVB	73852	304098	53.46%	9.940%
3	3.816	77	80	97	rVB	7503	32911	5.79%	1.076%
4	4.821	185	189	205	rVB	41514	102520	18.02%	3.351%
5	5.264	234	237	245	rVB	5090	14220	2.50%	0.465%
6	6.831	403	407	420	rVB2	3913	13832	2.43%	0.452%
7	7.264	450	454	460	rBV	6285	13807	2.43%	0.451%
8	7.643	490	495	500	rBV	41030	87188	15.33%	2.850%
9	7.864	515	519	526	rBV	3655	7818	1.37%	0.256%
10	8.306	565	567	569	rVB	5995	6001	1.05%	0.196%
11	8.785	601	605	610	rBV	19489	38197	6.72%	1.249%
12	10.191	713	716	725	rBV	66627	105692	18.58%	3.455%
13	10.407	729	733	736	rBV	90193	155010	27.25%	5.067%
14	12.003	920	931	942	rBV2	37540	61668	10.84%	2.016%
15	12.886	1071	1074	1078	rBV	70007	121526	21.36%	3.972%
16	13.178	1094	1097	1100	rBV	136456	203989	35.86%	6.668%
17	14.269	1180	1183	1186	rBV	114939	167411	29.43%	5.472%
18	15.715	1295	1297	1299	rBV	5873	9867	1.73%	0.323%
19	15.766	1299	1301	1305	rVB2	10410	16417	2.89%	0.537%
20	17.018	1400	1403	1406	rBV	90272	135268	23.78%	4.421%
21	18.016	1483	1485	1497	rVB4	4665	6107	1.07%	0.200%
22	18.909	1661	1665	1670	rVB	16872	17997	3.16%	0.588%
23	19.063	1687	1696	1709	rBV	114667	165366	29.07%	5.405%
24	19.177	1715	1719	1728	rVB	6029	6907	1.21%	0.226%
25	19.679	1813	1820	1824	rBV	96347	121961	21.44%	3.986%
26	19.703	1824	1825	1842	rVB	17674	21882	3.85%	0.715%
27	20.006	1885	1886	1888	rBV	4922	6317	1.11%	0.206%
28	20.070	1890	1892	1895	rVV	7857	14296	2.51%	0.467%
29	20.155	1897	1900	1906	rVB	5757	11796	2.07%	0.386%
30	20.335	1912	1917	1919	rBV2	23011	36429	6.40%	1.191%
31	20.378	1919	1921	1925	rBV	8689	15195	2.67%	0.497%
32	20.622	1941	1944	1951	rBV	3877	7879	1.39%	0.258%
33	20.973	1975	1977	1980	rVB	5558	7548	1.33%	0.247%
34	21.026	1980	1982	1986	rVB	21178	24402	4.29%	0.798%
35	21.174	1993	1996	1999	rBV	389947	568817	100.00%	18.592%
36	21.228	1999	2001	2009	rVV	102592	166765	29.32%	5.451%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016626.D
Acq On : 01 Oct 2021 08:23
Operator : CG/JU
Sample : M3833-16
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : RE126D1-20210920

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	21.334	2009	2011	2017	rVB	15912	24456	4.30%	0.799%
38	22.109	2081	2084	2089	rBV2	7906	10725	1.89%	0.351%
39	23.485	2414	2427	2466	rBV	81968	159874	28.11%	5.226%

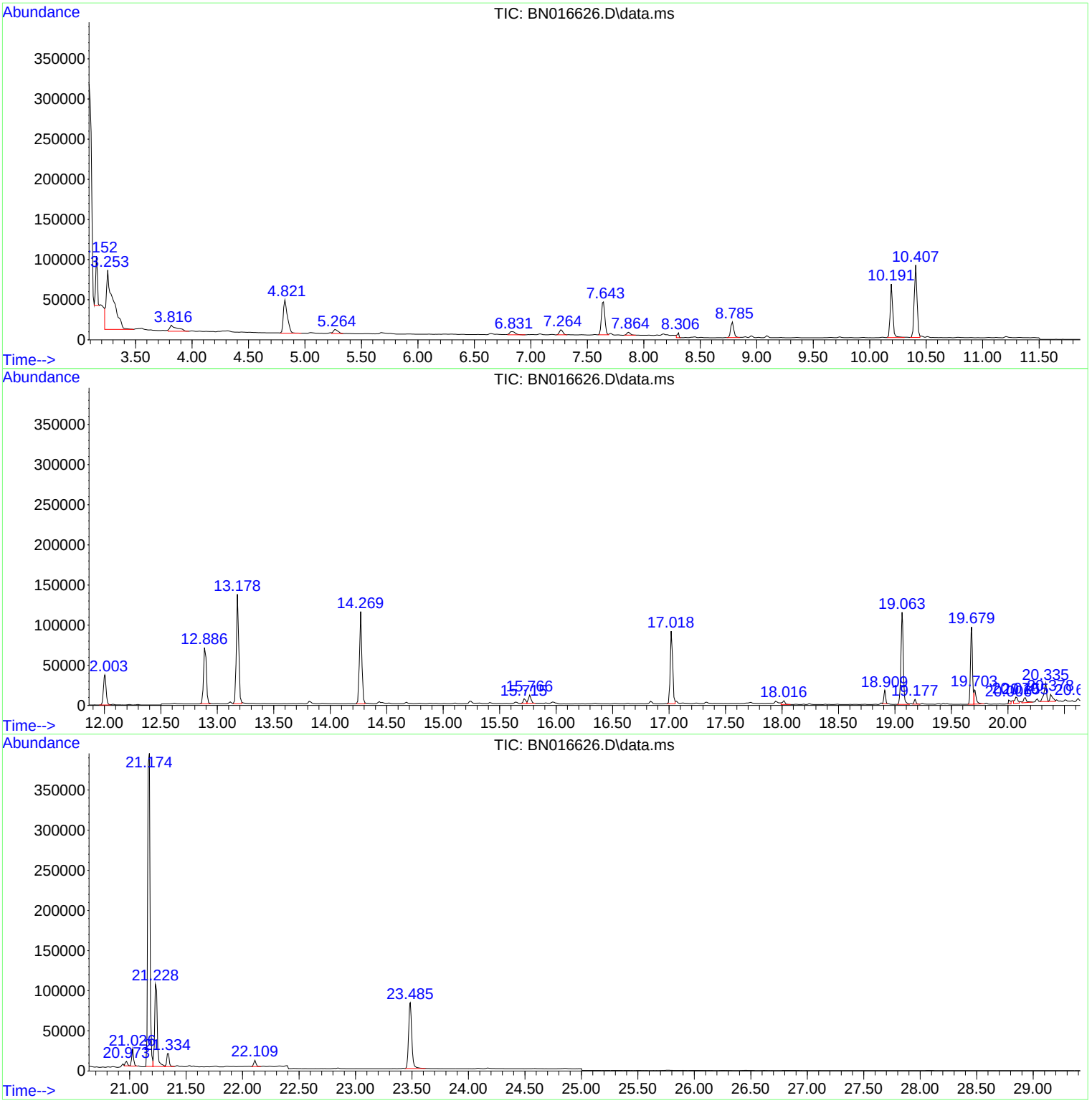
Sum of corrected areas: 3059406

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016626.D
Acq On : 01 Oct 2021 08:23
Operator : CG/JU
Sample : M3833-16
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE126D1-20210920

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 : BN016626.D
Acq On : 01 Oct 2021 08:23
Operator : CG/JU
Sample : M3833-16
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE126D1-20210920

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

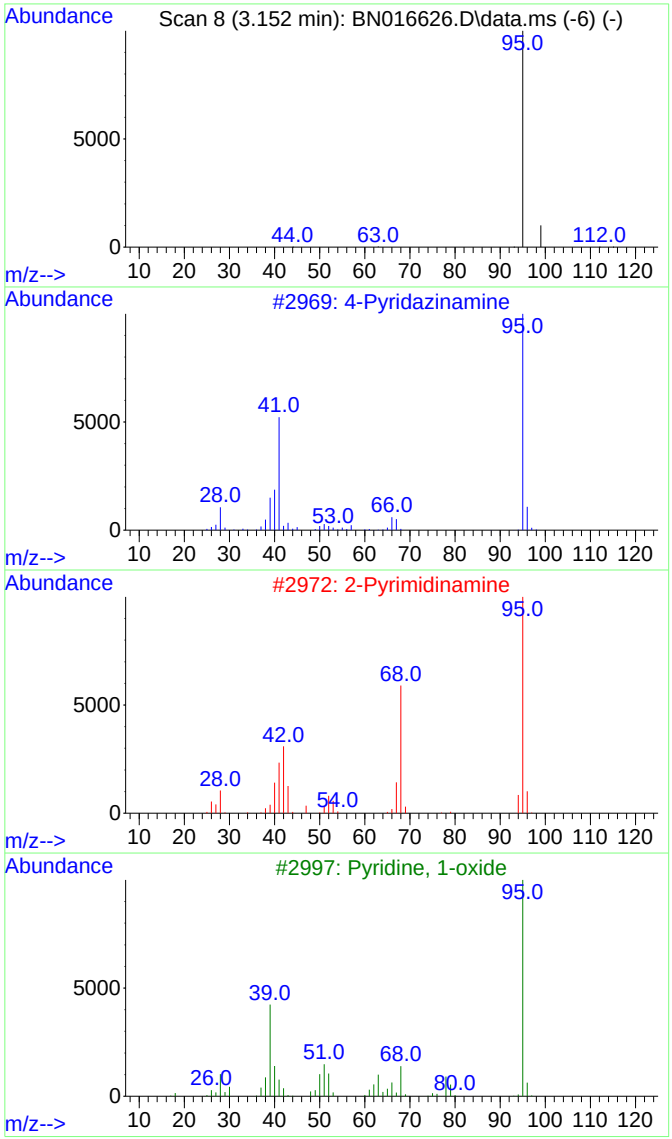
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

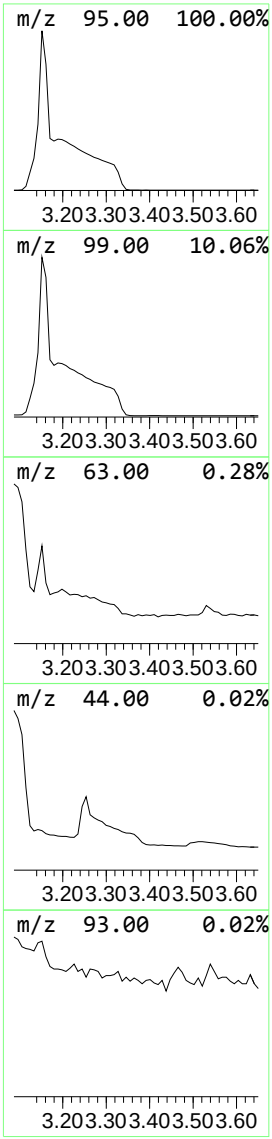
****

Peak Number 1 4-Pyridazinamine Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.152	0.31 ng	67247	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Pyridazinamine	95	C4H5N3	020744-39-2	2
2	2-Pyrimidinamine	95	C4H5N3	000109-12-6	2
3	Pyridine, 1-oxide	95	C5H5NO	000694-59-7	2
4	3-Pyridinol	95	C5H5NO	000109-00-2	2
5	4-Pyridinol	95	C5H5NO	000626-64-2	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016626.D
Acq On : 01 Oct 2021 08:23
Operator : CG/JU
Sample : M3833-16
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE126D1-20210920

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

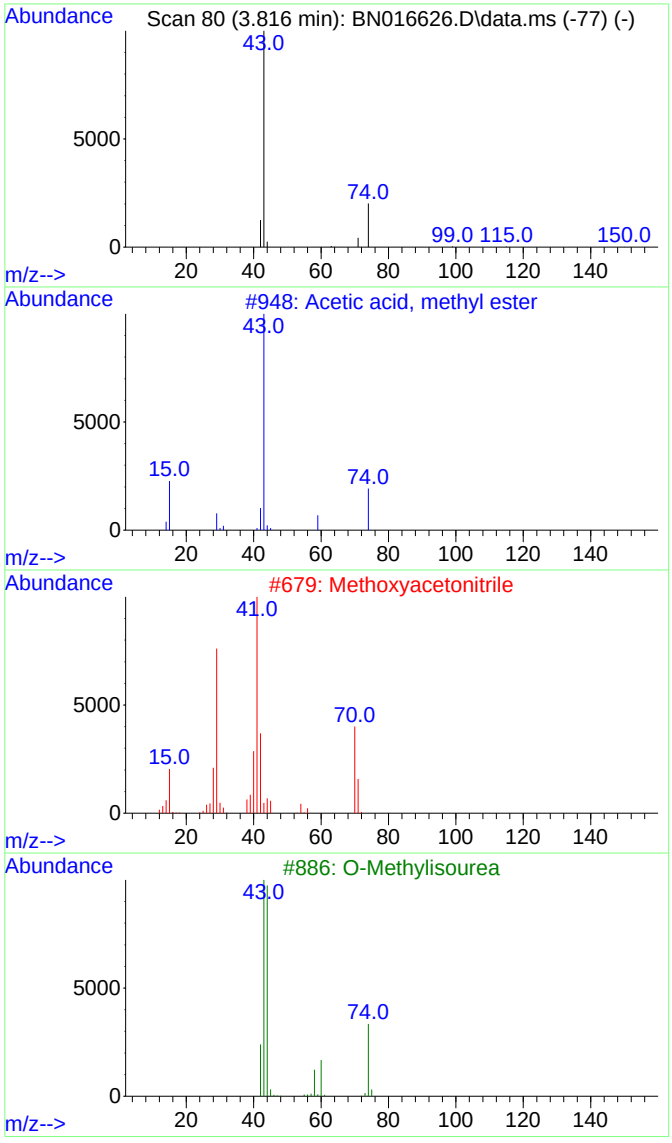
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

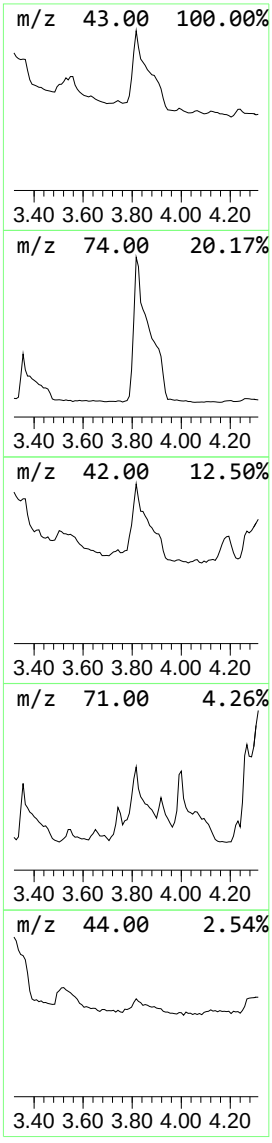
****

Peak Number 2 Acetic acid, methyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.15 ng	32911	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, methyl ester	74	C3H6O2	000079-20-9	9
2	Methoxyacetonitrile	71	C3H5NO	001738-36-9	4
3	O-Methylisourea	74	C2H6N2O	002440-60-0	4
4	Hydrogen azide	43	HN3	007782-79-8	4
5	1-Ethyl-1-methylhydrazine	74	C3H10N2	004986-48-5	3





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016626.D
Acq On : 01 Oct 2021 08:23
Operator : CG/JU
Sample : M3833-16
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE126D1-20210920

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

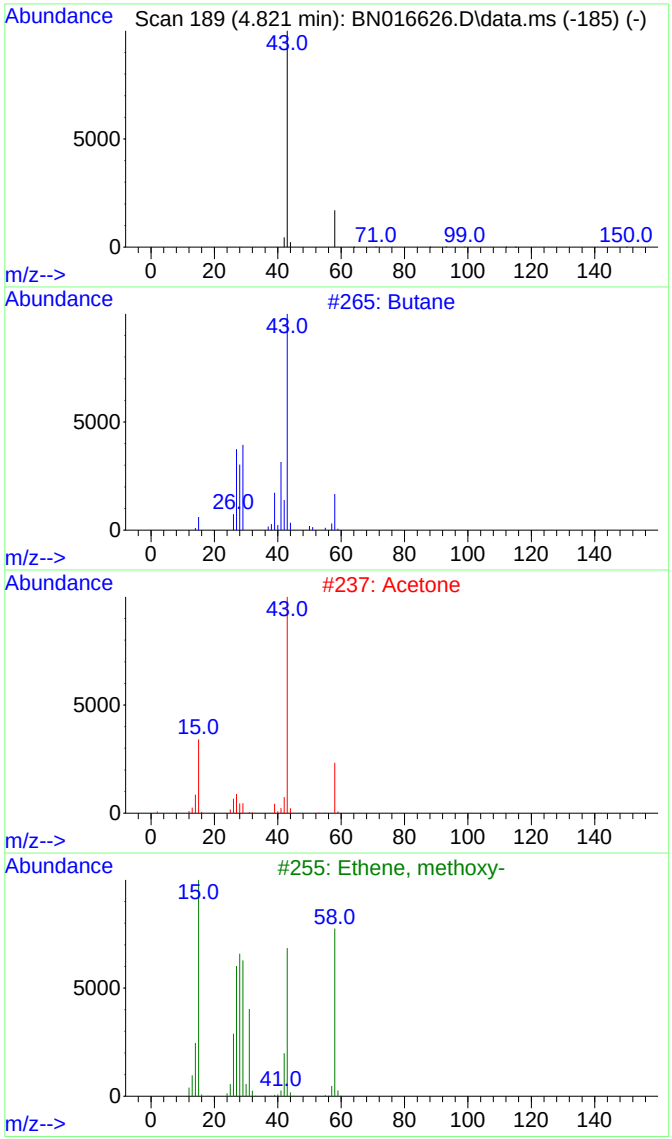
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

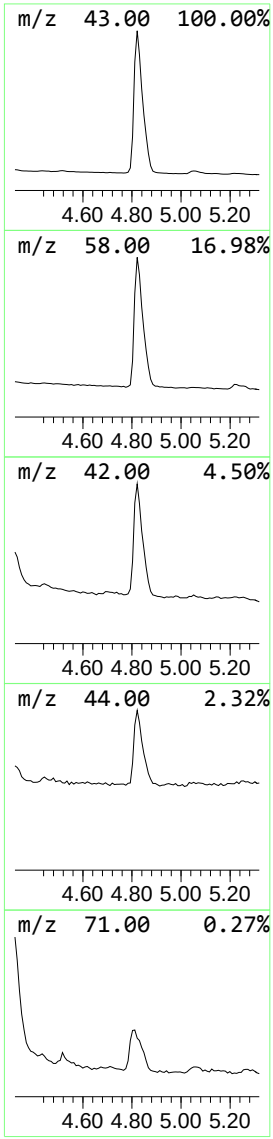
****

Peak Number 3 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.47 ng	102520	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	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 : BN016626.D
Acq On : 01 Oct 2021 08:23
Operator : CG/JU
Sample : M3833-16
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE126D1-20210920

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

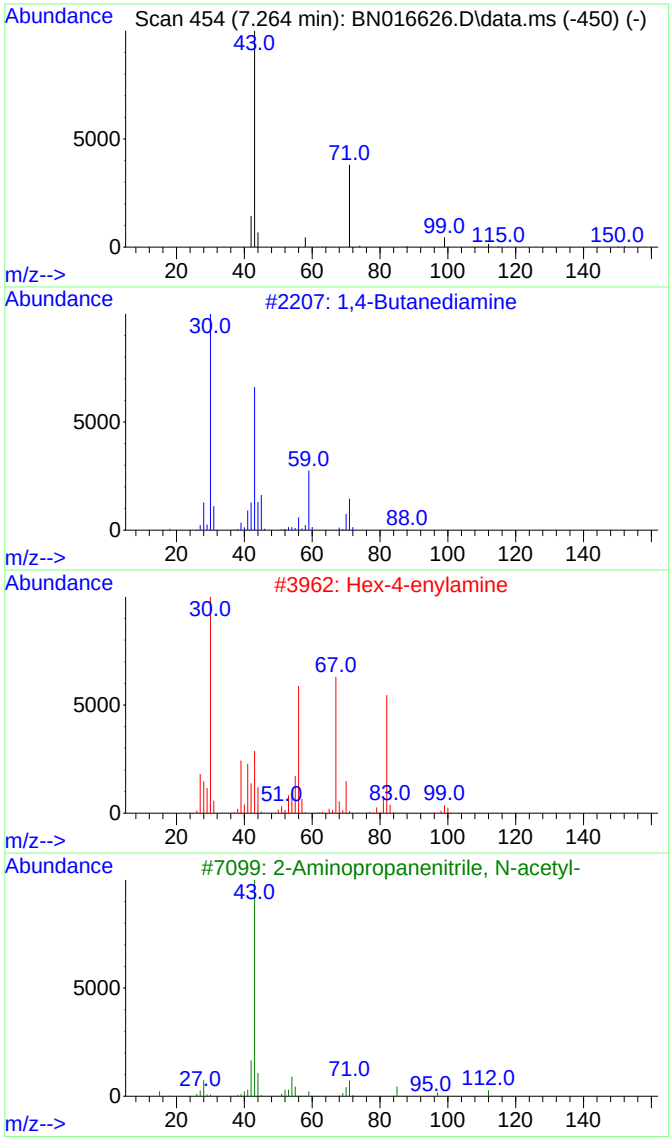
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

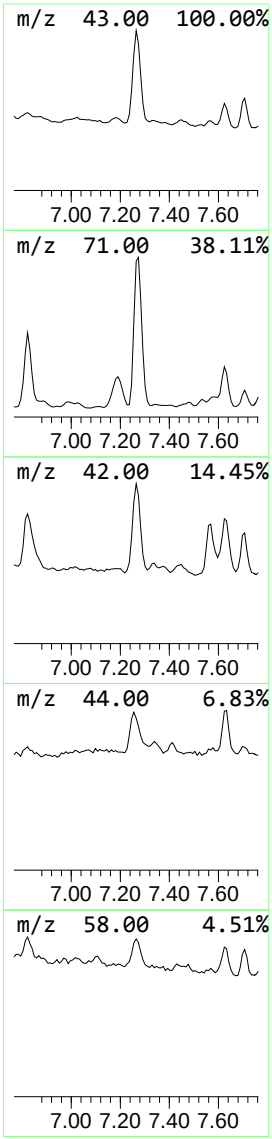
****

Peak Number 4 1,4-Butanediamine Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.264	0.06 ng	13807	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Butanediamine	88	C4H12N2	000110-60-1	5
2	Hex-4-enylamine	99	C6H13N	055108-01-5	4
3	2-Aminopropanenitrile, N-acetyl-	112	C5H8N2O	019861-71-3	4
4	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	4
5	Isobutane	58	C4H10	000075-28-5	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016626.D
Acq On : 01 Oct 2021 08:23
Operator : CG/JU
Sample : M3833-16
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE126D1-20210920

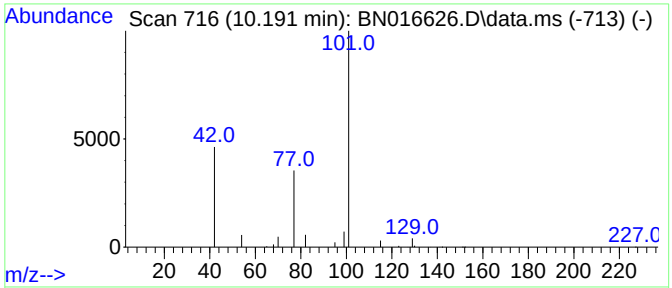
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

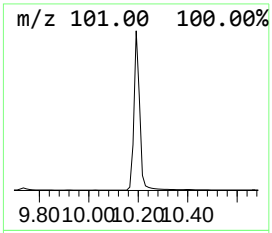
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

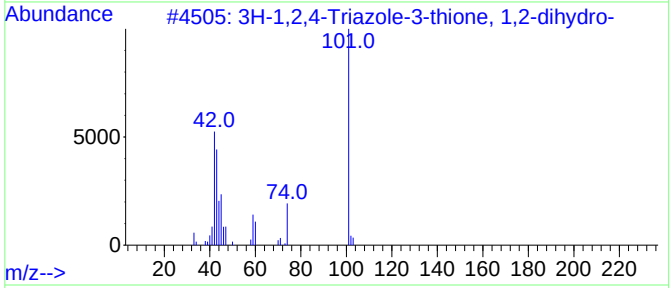
****
Peak Number 5 3H-1,2,4-Triazole-3-thione,... Concentration Rank 4

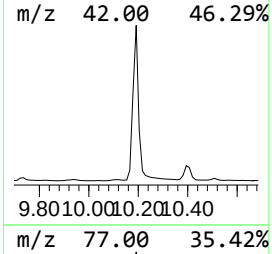
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.27 ng	105692	Naphthalene-d8	10.407

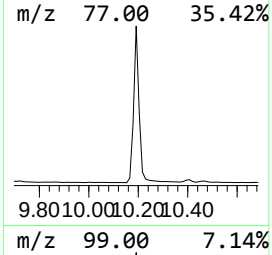
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
2	2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	5
3	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	5
4	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5
5	3-Aminopropionitrile	70	C3H6N2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

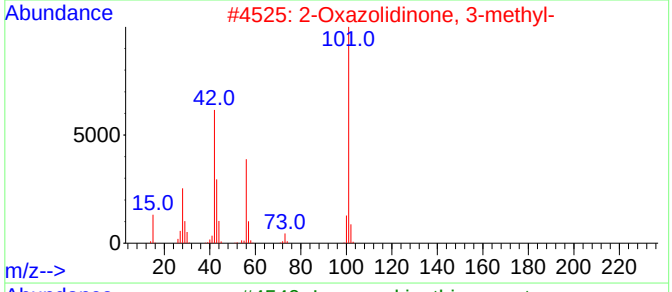


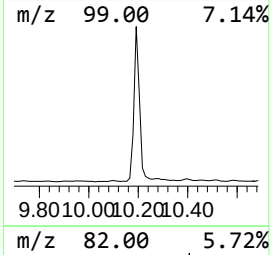


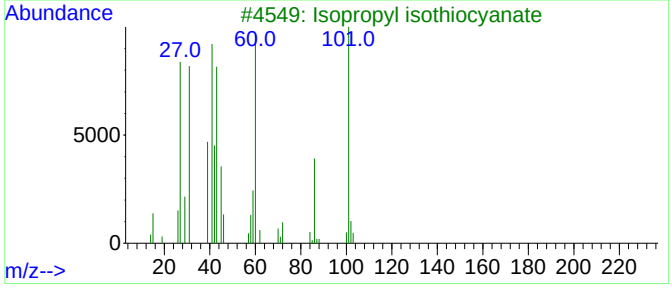


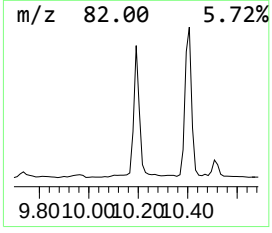












Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016626.D
Acq On : 01 Oct 2021 08:23
Operator : CG/JU
Sample : M3833-16
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE126D1-20210920

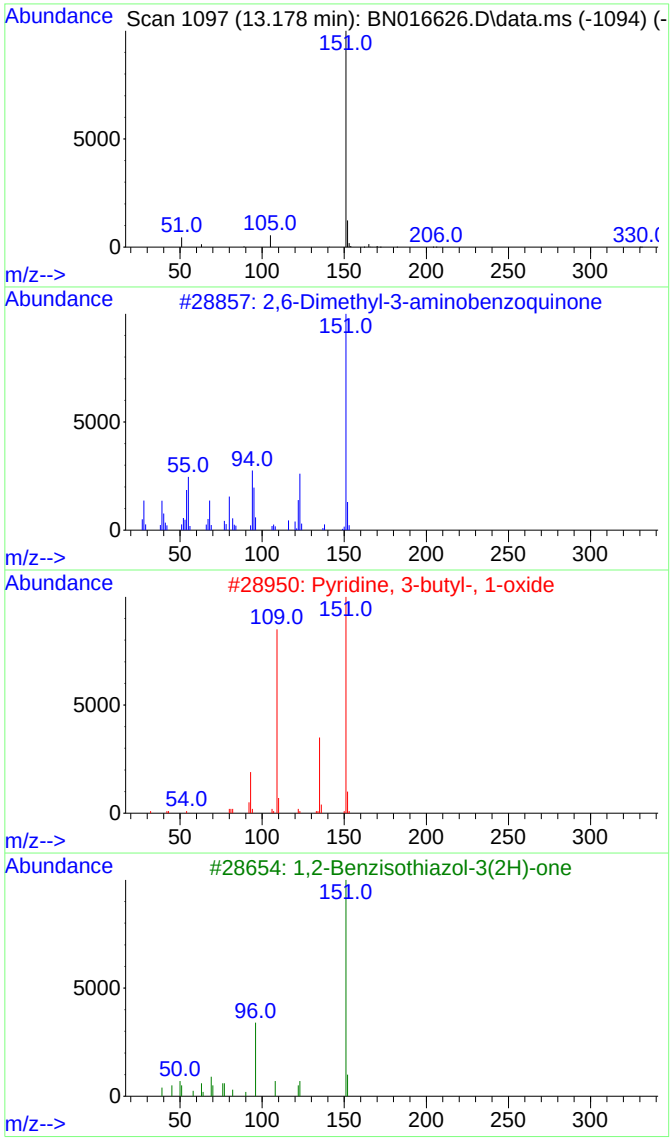
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

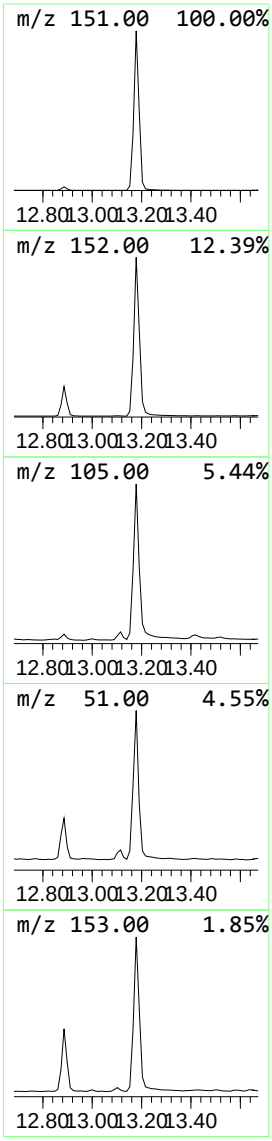
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2,6-Dimethyl-3-aminobenzoqu... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.178	0.49 ng	203989	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Dimethyl-3-aminobenzoquinone	151	C8H9NO2	090005-56-4	7
2	Pyridine, 3-butyl-, 1-oxide	151	C9H13NO	031396-33-5	7
3	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	7
4	7-Methyl-7H-pyrazolo(3,4-d)-v-tr...	151	C5H5N5O	018213-76-8	7
5	Carbamic acid, phenyl-, methyl e...	151	C8H9NO2	002603-10-3	7





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016626.D
Acq On : 01 Oct 2021 08:23
Operator : CG/JU
Sample : M3833-16
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : RE126D1-20210920

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

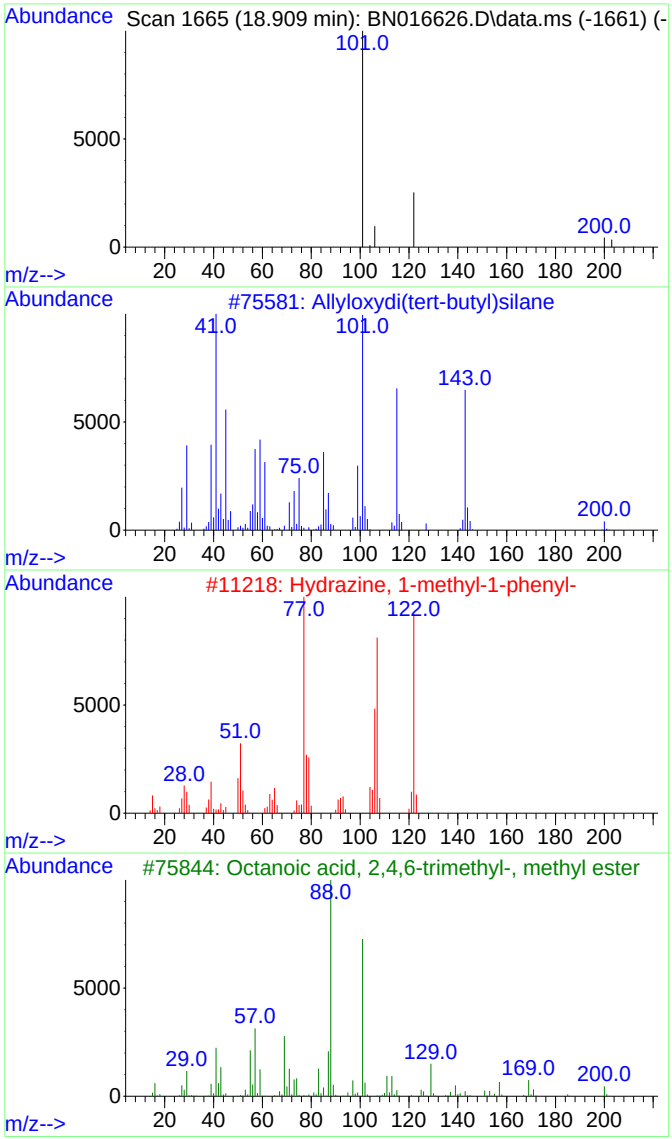
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

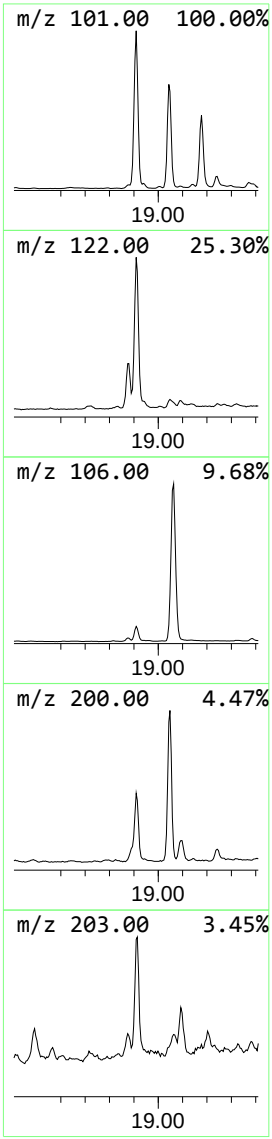
****

Peak Number 7 Allyloxydi(tert-butyl)silane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.909	0.05 ng	17997	Phenanthrene-d10	17.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Allyloxydi(tert-butyl)silane	200	C11H24OSi	1000279-09-4	4
2	Hydrazine, 1-methyl-1-phenyl-	122	C7H10N2	000618-40-6	4
3	Octanoic acid, 2,4,6-trimethyl-,...	200	C12H24O2	054984-07-5	4
4	Decanoic acid, ethyl ester	200	C12H24O2	000110-38-3	3
5	1,2-Propanediol, 3-(methylthio)-	122	C4H10O2S	022551-26-4	3





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016626.D
Acq On : 01 Oct 2021 08:23
Operator : CG/JU
Sample : M3833-16
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE126D1-20210920

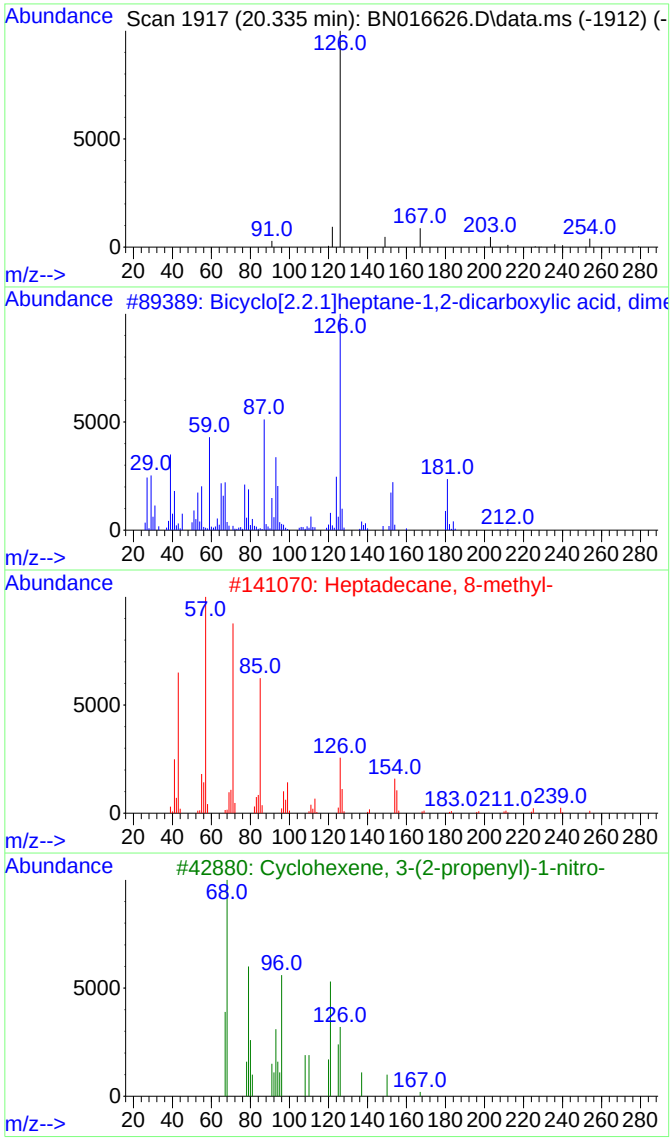
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

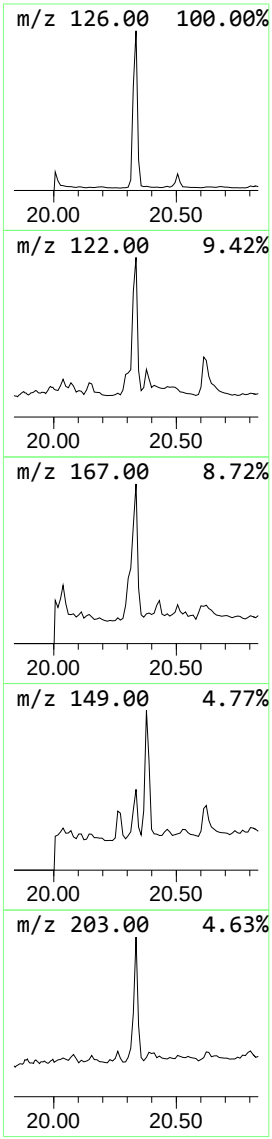
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Bicyclo[2.2.1]heptane-1,2-d... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.336	0.09 ng	36429	Chrysene-d12	21.238

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptane-1,2-dicarb...	212	C11H16O4	1000191-44-2	4
2	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	3
3	Cyclohexene, 3-(2-propenyl)-1-ni...	167	C9H13NO2	112683-38-2	3
4	Propanedioic acid, (3-methylbuty...	200	C10H16O4	053618-21-6	3
5	N-(tert-Butyl)-2-piperidinecarbo...	226	C12H22N2O2	1000505-19-4	3





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016626.D
Acq On : 01 Oct 2021 08:23
Operator : CG/JU
Sample : M3833-16
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE126D1-20210920

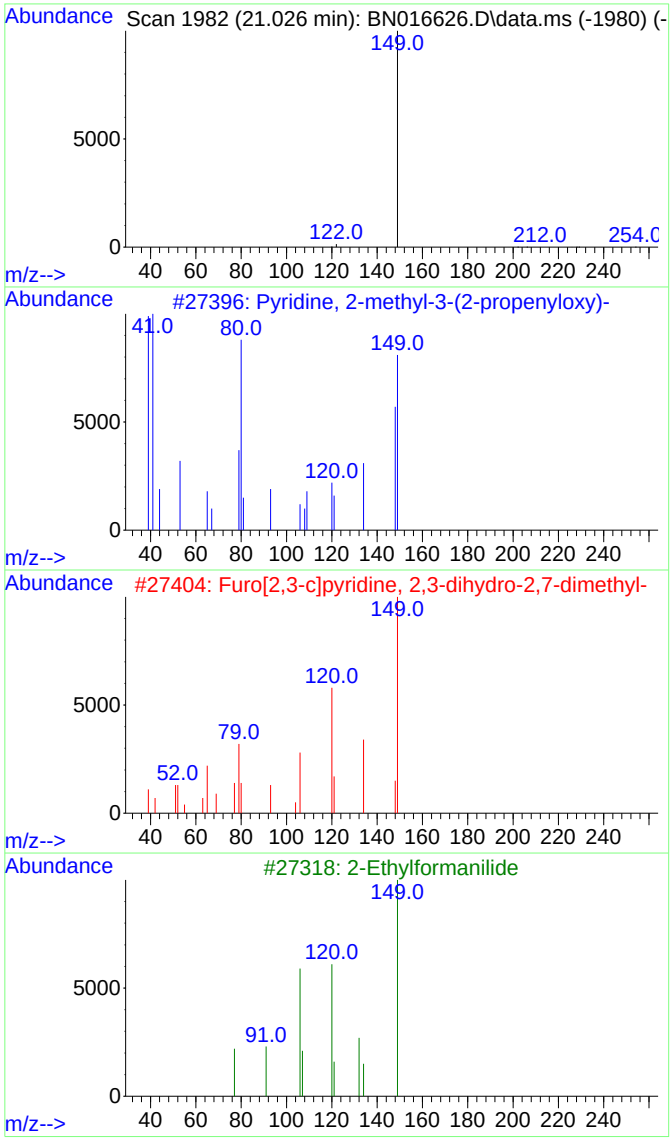
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

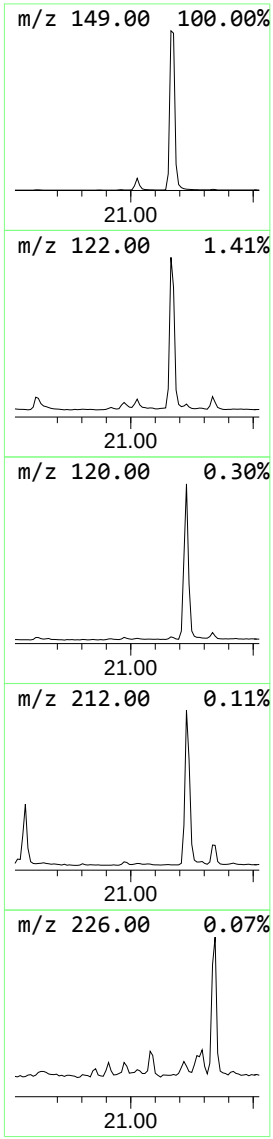
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Pyridine, 2-methyl-3-(2-pro... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.026	0.06 ng	24402	Chrysene-d12	21.238

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine, 2-methyl-3-(2-propenyl...	149	C9H11NO	069022-75-9	2
2	Furo[2,3-c]pyridine, 2,3-dihydro...	149	C9H11NO	069022-82-8	2
3	2-Ethylformanilide	149	C9H11NO	002860-30-2	2
4	6,7-Dimethyl-triazolo(4,3-b)(1,2...	149	C6H7N5	061139-73-9	2
5	1H-Pyrazole-1-propanenitrile, 3,...	149	C8H11N3	005589-97-9	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016626.D
Acq On : 01 Oct 2021 08:23
Operator : CG/JU
Sample : M3833-16
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : RE126D1-20210920

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

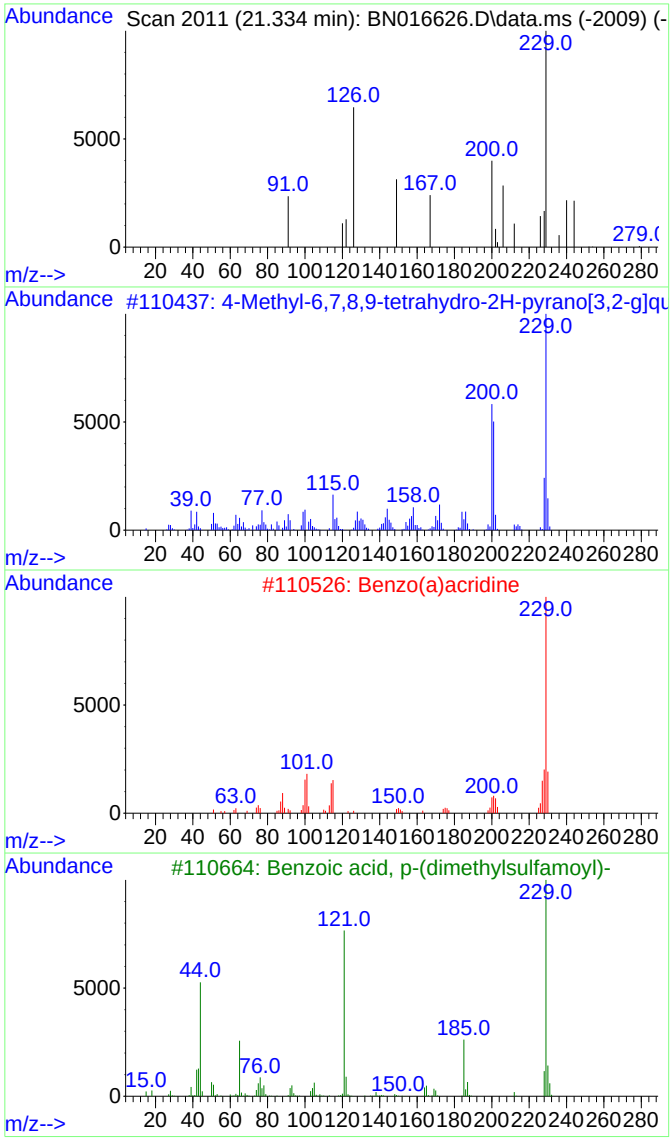
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

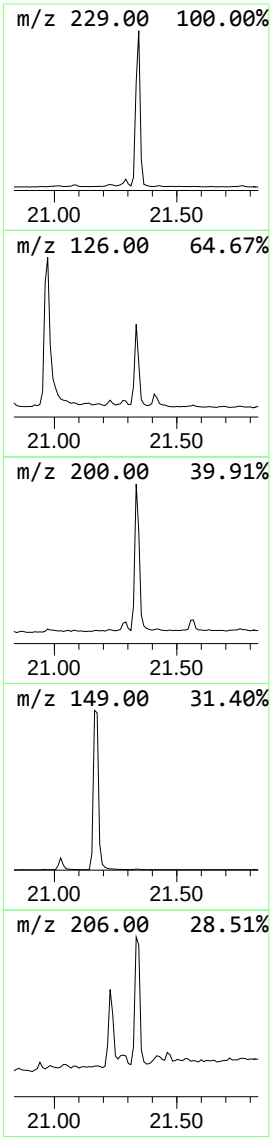
****

Peak Number 10 4-Methyl-6,7,8,9-tetrahydro... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.334	0.06 ng	24456	Chrysene-d12	21.238

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methyl-6,7,8,9-tetrahydro-2H-p...	229	C14H15NO2	065292-83-3	35
2	Benzo(a)acridine	229	C17H11N	000225-11-6	10
3	Benzoic acid, p-(dimethylsulfamo...	229	C9H11NO4S	001206-37-7	9
4	Coumarin, 4-piperidino-	229	C14H15NO2	014290-47-2	9
5	Pyrimidine-4-ol, 2,6-diamino-5-b...	229	C11H11N5O	025477-74-1	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016626.D
Acq On : 01 Oct 2021 08:23
Operator : CG/JU
Sample : M3833-16
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : RE126D1-20210920

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
4-Pyridazinamine	3.152	0.3	ng	67247	1	7.643	87188	0.4
Acetic acid, me...	3.816	0.2	ng	32911	1	7.643	87188	0.4
Butane	4.821	0.5	ng	102520	1	7.643	87188	0.4
1,4-Butanediamine	7.264	0.1	ng	13807	1	7.643	87188	0.4
3H-1,2,4-Triazo...	10.191	0.3	ng	105692	2	10.407	155010	0.4
2,6-Dimethyl-3-...	13.178	0.5	ng	203989	3	14.269	167411	0.4
Allyloxydi(tert...	18.909	0.1	ng	17997	4	17.018	135268	0.4
Bicyclo[2.2.1]h...	20.336	0.1	ng	36429	5	21.238	166765	0.4
Pyridine, 2-met...	21.026	0.1	ng	24402	5	21.238	166765	0.4
4-Methyl-6,7,8,...	21.334	0.1	ng	24456	5	21.238	166765	0.4