LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030122\
Data File : BG052521.D
Acq On : 1 Mar 2022 16:22
Operator : CG/JU
Sample : N1688-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-35

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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_G\Methods\8270-BG020722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG052521.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.837	54	59	66	rBV	23760	35518	1.37%	0.369%
2	5.752	379	385	395	rVB	277771	441760	17.02%	4.586%
3	7.368	654	660	673	rVB	171741	316298	12.19%	3.284%
4	8.220	799	805	812	rBV	107631	180223	6.94%	1.871%
5	8.502	848	853	862	rBV6	9593	26757	1.03%	0.278%
6	8.601	865	870	876	rVB2	28353	50489	1.95%	0.524%
7	9.230	972	977	984	rBV6	12979	31914	1.23%	0.331%
8	9.295	984	988	994	rVV3	20594	50404	1.94%	0.523%
9	9.394	998	1005	1013	rVB	384251	700806	27.00%	7.276%
10	10.029	1102	1113	1120	rVB4	17418	39599	1.53%	0.411%
11	11.057	1280	1288	1294	rBV	143406	252053	9.71%	2.617%
12	13.489	1691	1702	1711	rBV	1051178	1599790	61.65%	16.609%
13	14.863	1928	1936	1946	rVB	232056	367213	14.15%	3.812%
14	16.356	2182	2190	2198	rBV	808775	1311321	50.53%	13.614%
15	17.613	2398	2404	2413	rBV	310791	475108	18.31%	4.933%
16	18.488	2548	2553	2559	rBV7	14528	27781	1.07%	0.288%
17	18.553	2561	2564	2571	rVB	24145	33989	1.31%	0.353%
18	20.209	2840	2846	2859	rVB	1999406	2595114	100.00%	26.943%
19	21.537	3069	3072	3079	rBV8	11553	30140	1.16%	0.313%
20	21.930	3132	3139	3148	rBV	299014	531569	20.48%	5.519%
21	25.396	3719	3729	3740	rVB2	174346	534197	20.58%	5.546%

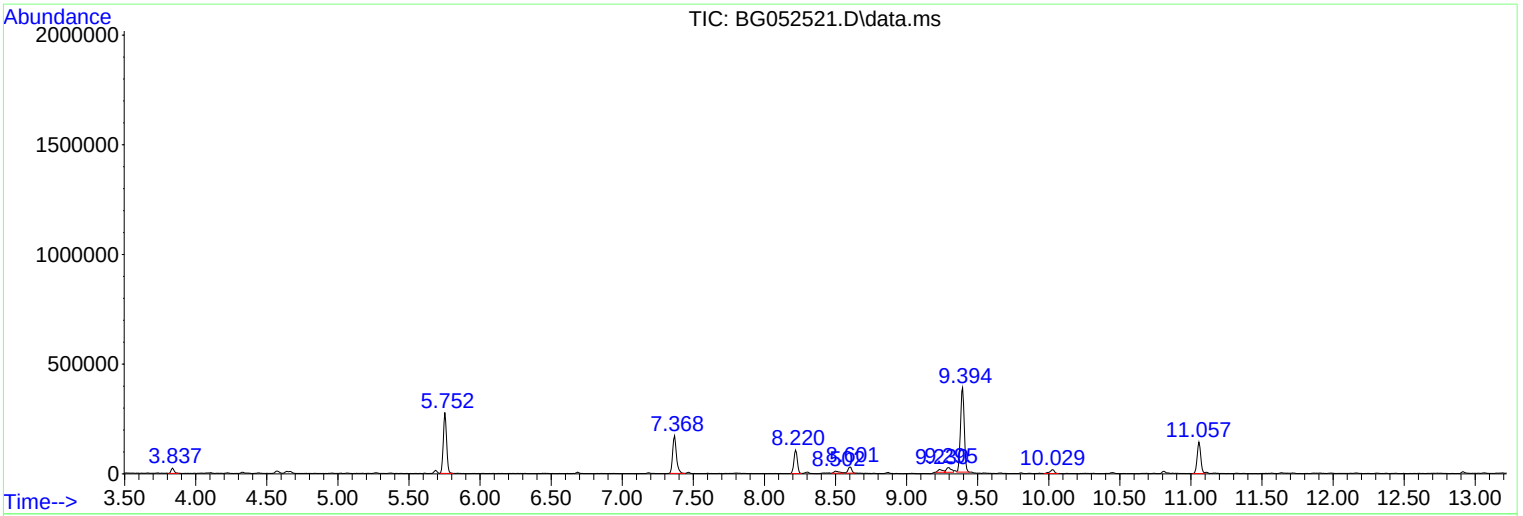
Sum of corrected areas: 9632043

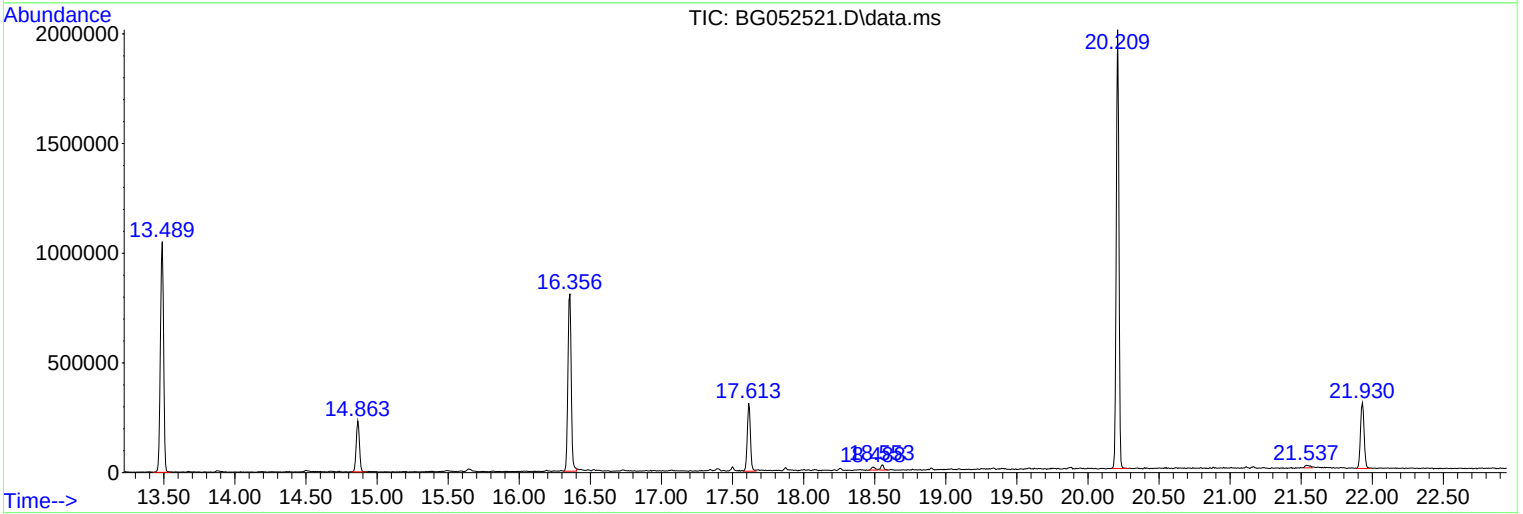
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030122\
Data File : BG052521.D
Acq On : 1 Mar 2022 16:22
Operator : CG/JU
Sample : N1688-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

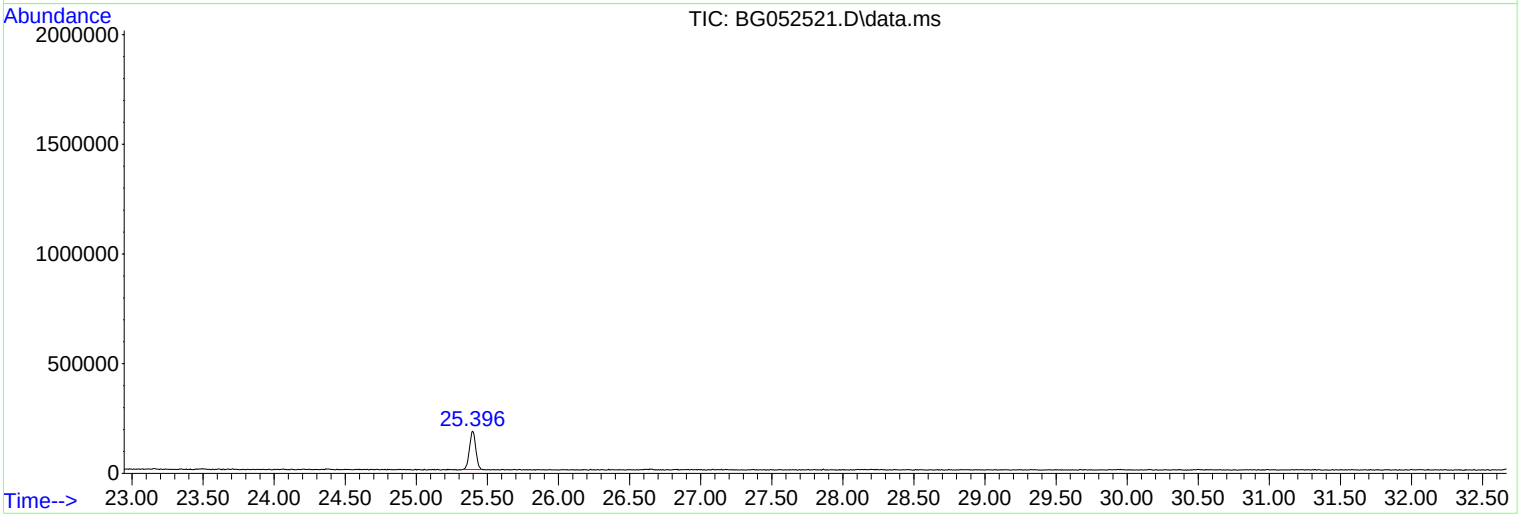
Instrument :
BNA_G
ClientSampleId :
MW-35

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.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_G\Data\BG030122\
Data File : BG052521.D
Acq On : 1 Mar 2022 16:22
Operator : CG/JU
Sample : N1688-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-35

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

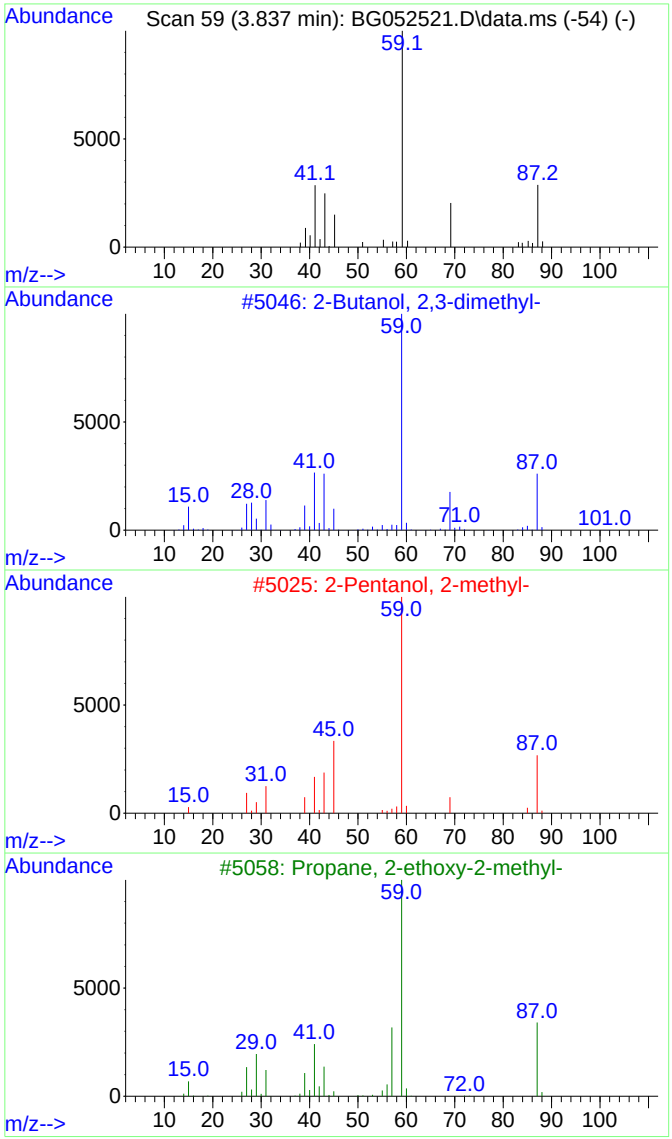
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

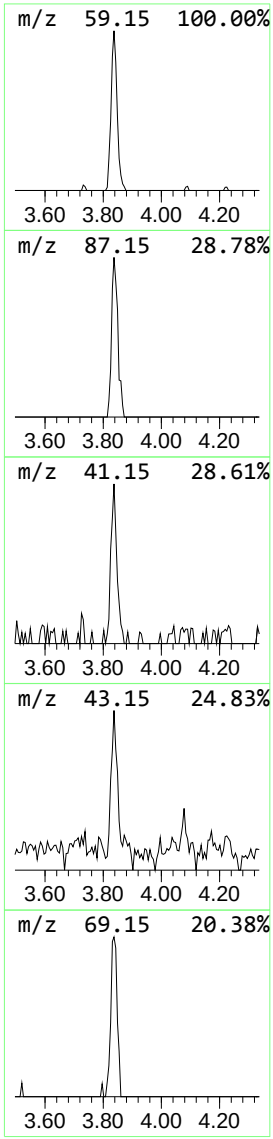
****

Peak Number 1 2-Butanol, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.837	3.94 ng	35518	1,4-Dichlorobenzene-d4	8.220

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	83
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	83
3	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	72
4	3-Heptanol	116	C7H16O	000589-82-2	40
5	DL-Lactamide, N,O-dimethyl-	117	C5H11NO2	1000452-56-3	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030122\
Data File : BG052521.D
Acq On : 1 Mar 2022 16:22
Operator : CG/JU
Sample : N1688-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-35

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

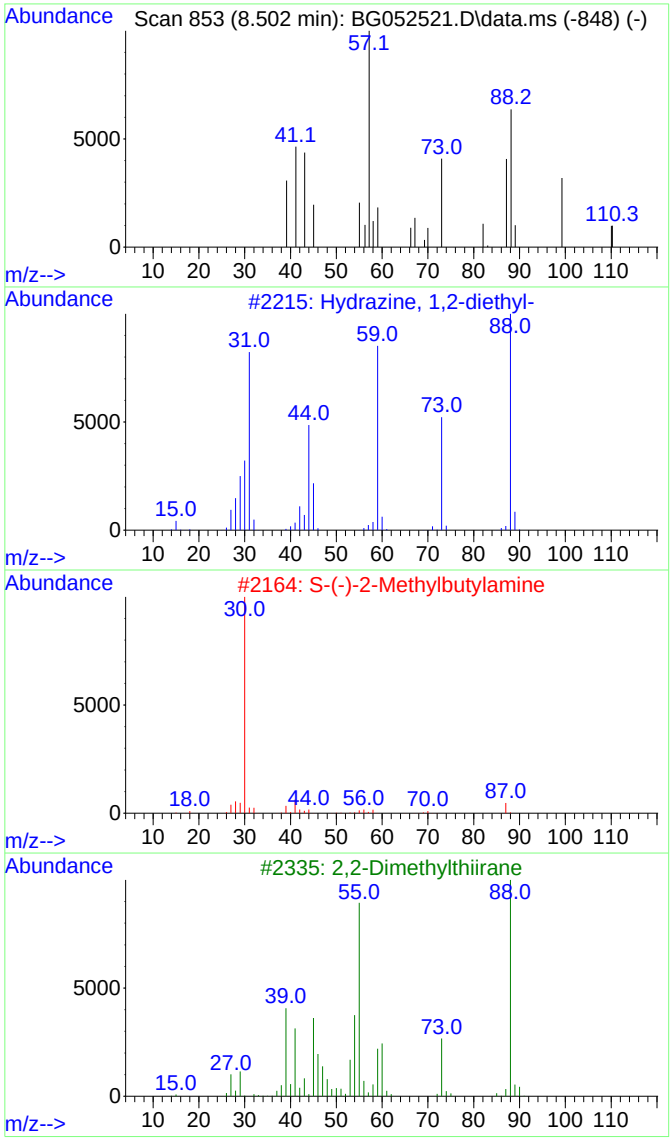
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

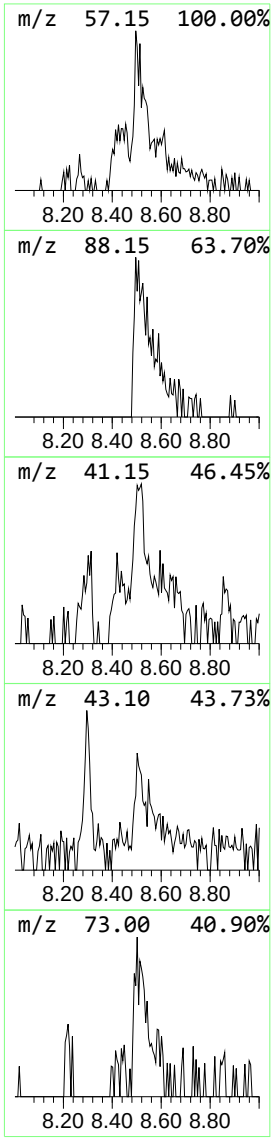
****

Peak Number 2 unknown8.502 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.502	2.97 ng	26757	1,4-Dichlorobenzene-d4	8.220

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrazine, 1,2-diethyl-	88	C4H12N2	001615-80-1	12
2	S-(-)-2-Methylbutylamine	87	C5H13N	020626-52-2	9
3	2,2-Dimethylthiirane	88	C4H8S	003772-13-2	9
4	1-Pentanamine	87	C5H13N	000110-58-7	9
5	Methyl propionate	88	C4H8O2	000554-12-1	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030122\
Data File : BG052521.D
Acq On : 1 Mar 2022 16:22
Operator : CG/JU
Sample : N1688-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-35

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

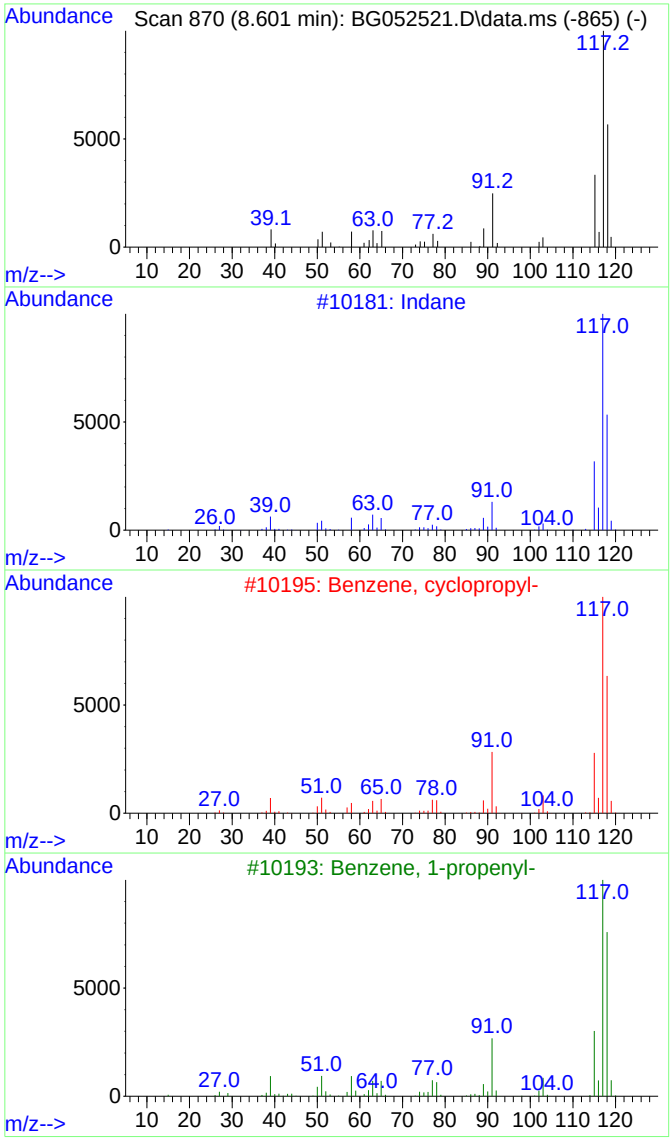
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

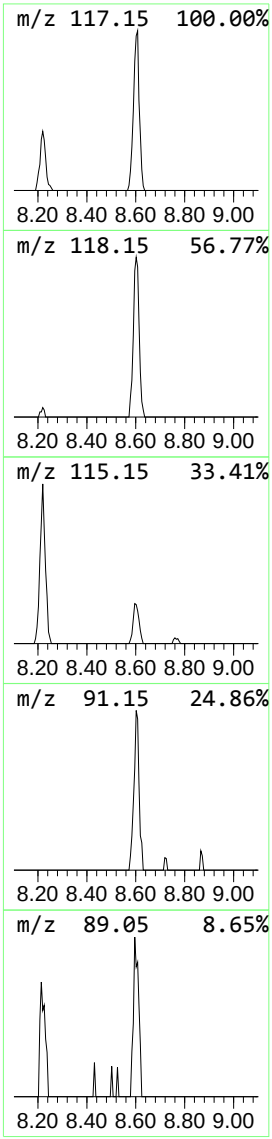
****

Peak Number 3 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.601	5.60 ng	50489	1,4-Dichlorobenzene-d4	8.220

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	87
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	74
3	Benzene, 1-propenyl-	118	C9H10	000637-50-3	74
4	Deltacyclene	118	C9H10	007785-10-6	72
5	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030122\
Data File : BG052521.D
Acq On : 1 Mar 2022 16:22
Operator : CG/JU
Sample : N1688-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-35

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

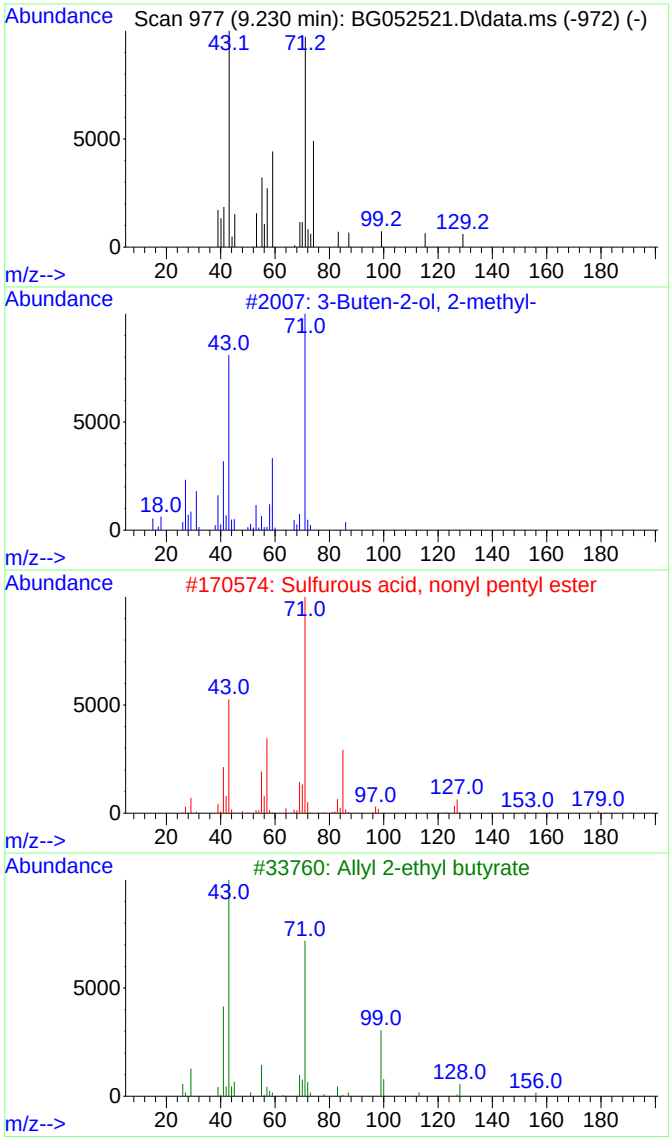
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

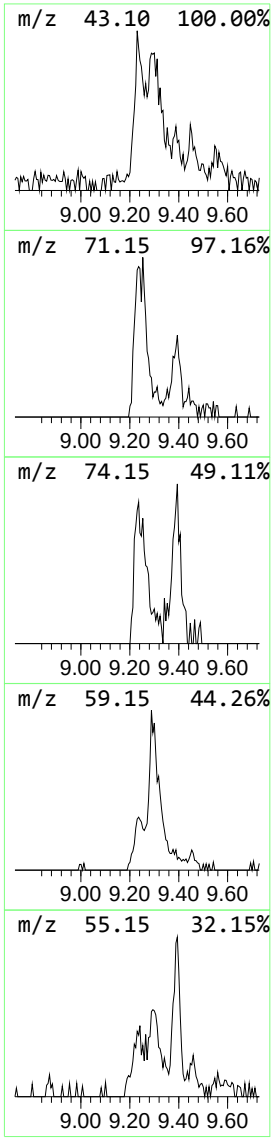
****

Peak Number 4 3-Buten-2-ol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.230	3.54 ng	31914	1,4-Dichlorobenzene-d4	8.220

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	50
2	Sulfurous acid, nonyl pentyl ester	278	C14H30O3S	1000309-14-2	38
3	Allyl 2-ethyl butyrate	156	C9H16O2	007493-69-8	37
4	1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	35
5	Butane, 2,2'-[methylenebis(oxy)]...	188	C11H24O2	054699-28-4	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030122\
Data File : BG052521.D
Acq On : 1 Mar 2022 16:22
Operator : CG/JU
Sample : N1688-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-35

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

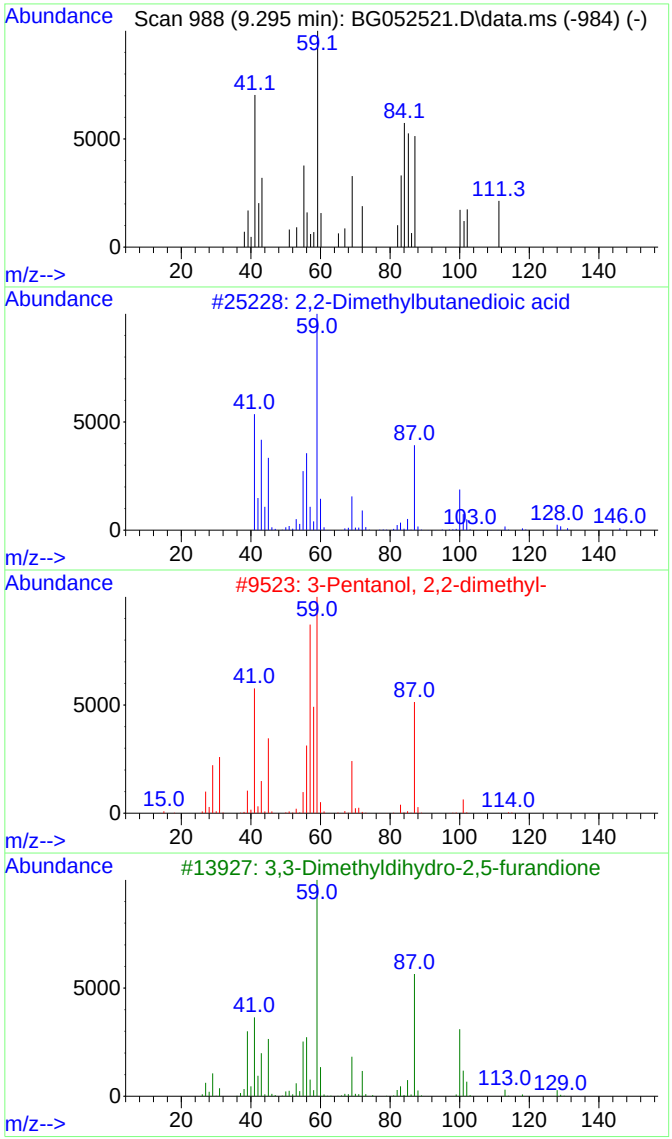
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

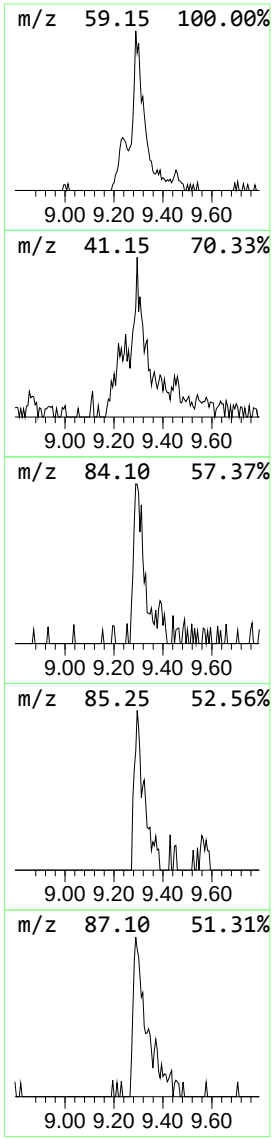
****

Peak Number 5 unknown9.295 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.295	5.59 ng	50404	1,4-Dichlorobenzene-d4	8.220

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2-Dimethylbutanedioic acid	146	C6H10O4	000597-43-3	25
2	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	17
3	3,3-Dimethyldihydro-2,5-furandione	128	C6H8O3	017347-61-4	16
4	Pentane, 3-ethoxy-	116	C7H16O	036749-13-0	12
5	1,3-Propanediol, 2,2-diethyl-	132	C7H16O2	000115-76-4	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030122\
Data File : BG052521.D
Acq On : 1 Mar 2022 16:22
Operator : CG/JU
Sample : N1688-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-35

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

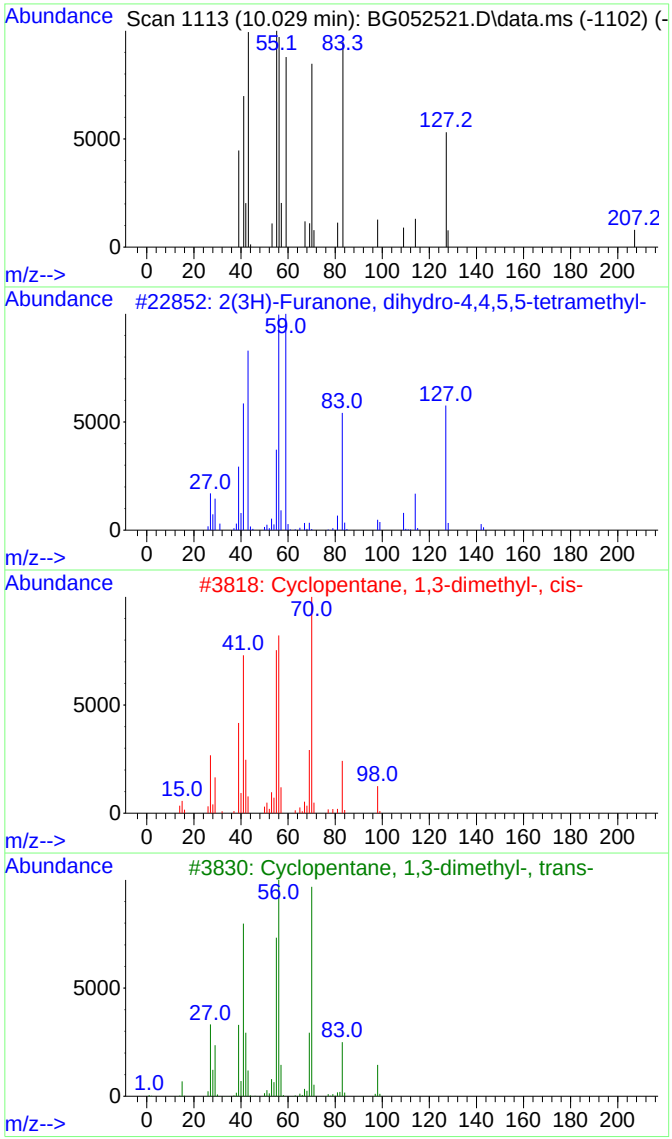
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

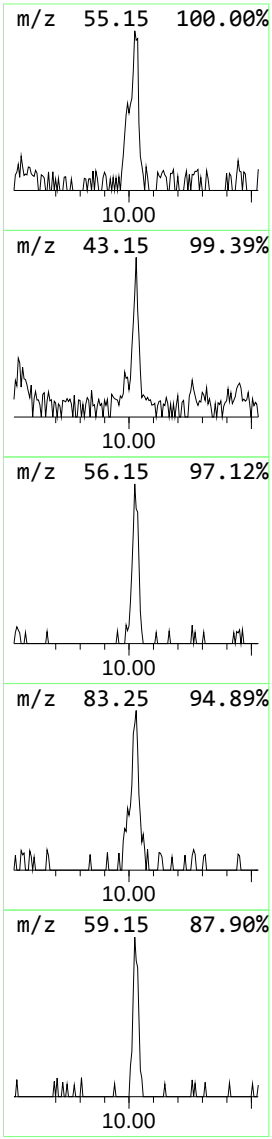
****

Peak Number 6 unknown10.029 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.029	3.14 ng	39599	Naphthalene-d8	11.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Furanone, dihydro-4,4,5,5-...	142	C8H14O2	016466-24-3	47
2	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	43
3	Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	38
4	Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	38
5	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030122\
Data File : BG052521.D
Acq On : 1 Mar 2022 16:22
Operator : CG/JU
Sample : N1688-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-35

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.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
2-Butanol, 2,3-...	3.837	3.9	ng	35518	1	8.220	180223	20.0
unknown8.502	8.502	3.0	ng	26757	1	8.220	180223	20.0
Indane	8.601	5.6	ng	50489	1	8.220	180223	20.0
3-Buten-2-ol, 2...	9.230	3.5	ng	31914	1	8.220	180223	20.0
unknown9.295	9.295	5.6	ng	50404	1	8.220	180223	20.0
unknown10.029	10.029	3.1	ng	39599	2	11.057	252053	20.0