Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122022\
Data File : BG056039.D
Acq On : 20 Dec 2022 21:12
Operator : CG/JU
Sample : N6051-01 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-591

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-BG121322.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056039.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.399	15	19	25	rBB2	4942	7735	2.66%	0.396%
2	5.415	357	362	366	rBB	3284	4529	1.56%	0.232%
3	5.885	436	442	449	rBB	27546	42237	14.53%	2.165%
4	7.494	710	716	721	rBV2	28663	47462	16.33%	2.432%
5	8.370	859	865	871	rBB	40170	67181	23.11%	3.443%
6	9.539	1058	1064	1070	rBB2	18073	30652	10.55%	1.571%
7	11.202	1340	1347	1354	rBB2	54970	94584	32.54%	4.847%
8	13.599	1749	1755	1761	rVB	63359	94948	32.66%	4.866%
9	14.974	1983	1989	1995	rBV2	100929	150034	51.62%	7.689%
10	16.449	2235	2240	2247	rVB	63927	96105	33.06%	4.925%
11	17.712	2446	2455	2459	rBV	133411	200774	69.07%	10.289%
12	17.753	2459	2462	2467	rVB	17593	22865	7.87%	1.172%
13	17.841	2474	2477	2485	rVB3	3183	4837	1.66%	0.248%
14	18.552	2594	2598	2600	rBV	3072	3447	1.19%	0.177%
15	18.576	2600	2602	2607	rVB	3191	3812	1.31%	0.195%
16	18.623	2607	2610	2616	rBV2	3763	5283	1.82%	0.271%
17	18.775	2630	2636	2639	rBV2	3977	7157	2.46%	0.367%
18	19.063	2679	2685	2689	rBV	2564	3899	1.34%	0.200%
19	19.104	2689	2692	2696	rVB2	3240	4087	1.41%	0.209%
20	19.463	2749	2753	2762	rBV7	5613	11401	3.92%	0.584%
21	19.621	2774	2780	2782	rBV4	2663	3684	1.27%	0.189%
22	19.739	2794	2800	2807	rBV	55287	74460	25.62%	3.816%
23	20.062	2851	2855	2857	rVV2	9667	13599	4.68%	0.697%
24	20.097	2857	2861	2866	rVV	41248	61158	21.04%	3.134%
25	20.162	2869	2872	2876	rVV3	2739	3178	1.09%	0.163%
26	20.279	2887	2892	2898	rVB	137397	177361	61.02%	9.089%
27	20.403	2909	2913	2914	rBV3	4536	4299	1.48%	0.220%
28	20.579	2932	2943	2948	rBV5	7561	19180	6.60%	0.983%
29	20.673	2955	2959	2962	rBV6	4712	8252	2.84%	0.423%
30	20.738	2968	2970	2973	rVB4	5261	5773	1.99%	0.296%
31	20.885	2992	2995	2996	rBV3	5432	5171	1.78%	0.265%
32	20.926	2999	3002	3009	rVV7	5067	9458	3.25%	0.485%
33	21.314	3065	3068	3072	rBV6	2479	3438	1.18%	0.176%
34	21.560	3107	3110	3111	rBV3	4041	5430	1.87%	0.278%
35	21.601	3115	3117	3125	rVB8	5690	9577	3.29%	0.491%
36	21.666	3125	3128	3129	rBV3	4384	4408	1.52%	0.226%

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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-BG121322.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	22.019	3178	3188	3193	rVV3	142800	290678	100.00%	14.897%
38	22.060	3193	3195	3202	rVB	15985	26855	9.24%	1.376%
39	22.289	3232	3234	3240	rBV6	2879	4120	1.42%	0.211%
40	22.436	3258	3259	3262	rBV3	3103	3264	1.12%	0.167%
41	22.800	3319	3321	3325	rVB4	4007	3808	1.31%	0.195%
42	23.223	3389	3393	3395	rBV5	4452	7219	2.48%	0.370%
43	23.299	3404	3406	3409	rBV4	3133	3983	1.37%	0.204%
44	24.169	3552	3554	3558	rVB5	3332	3772	1.30%	0.193%
45	24.392	3587	3592	3597	rBV2	8646	20615	7.09%	1.056%
46	25.344	3747	3754	3760	rBV2	7287	19512	6.71%	1.000%
47	25.503	3772	3781	3794	rBV2	68314	242199	83.32%	12.412%
48	26.607	3967	3969	3971	rVB2	3732	3121	1.07%	0.160%
49	26.625	3971	3972	3975	rBV3	2551	3260	1.12%	0.167%
50	28.370	4267	4269	4272	rBV3	2332	3170	1.09%	0.162%
51	29.715	4494	4498	4501	rVB6	2654	4253	1.46%	0.218%

Sum of corrected areas: 1951284

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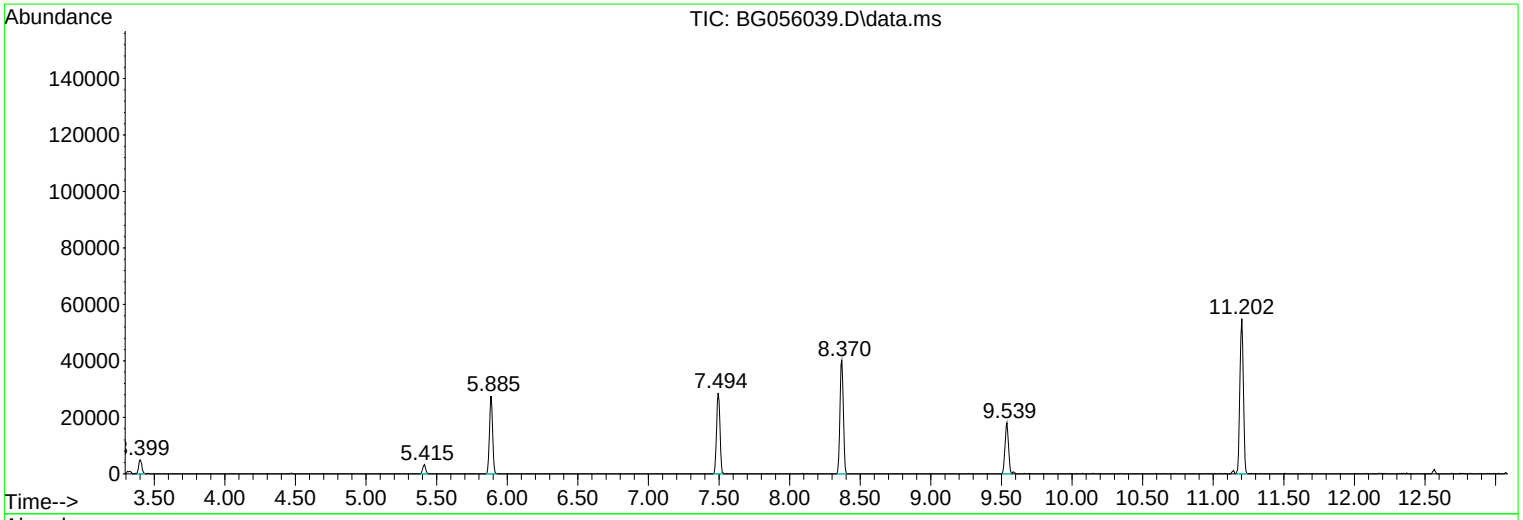
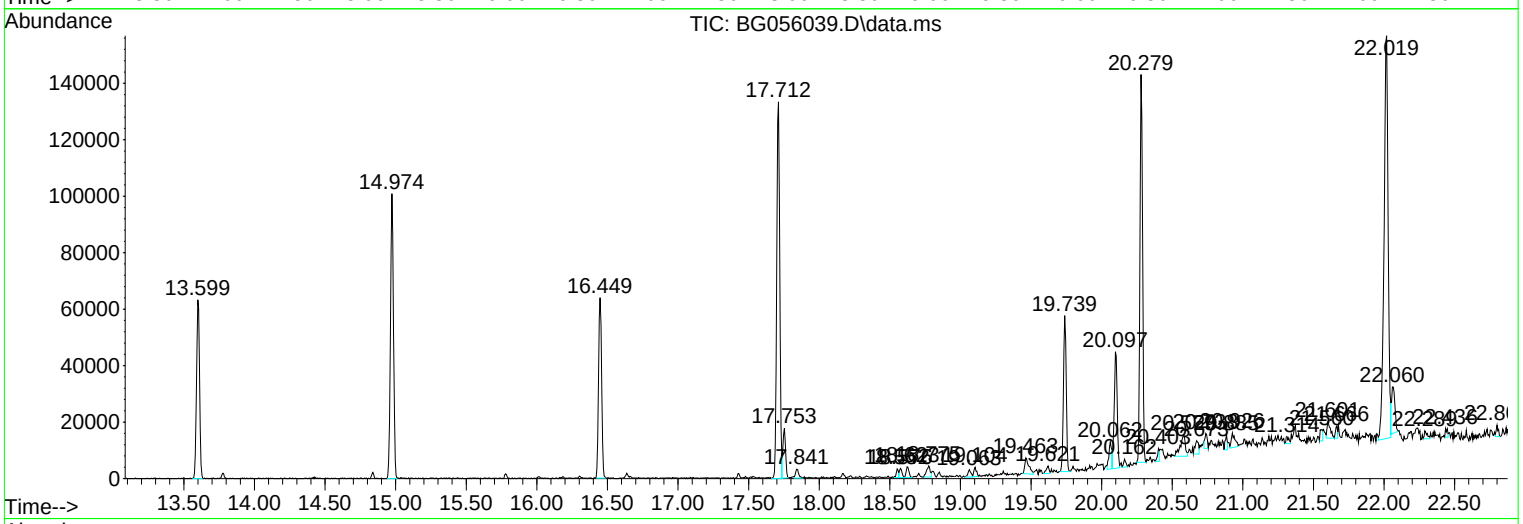
Misc :
ALS Vial : 16 Sample Multiplier: 1

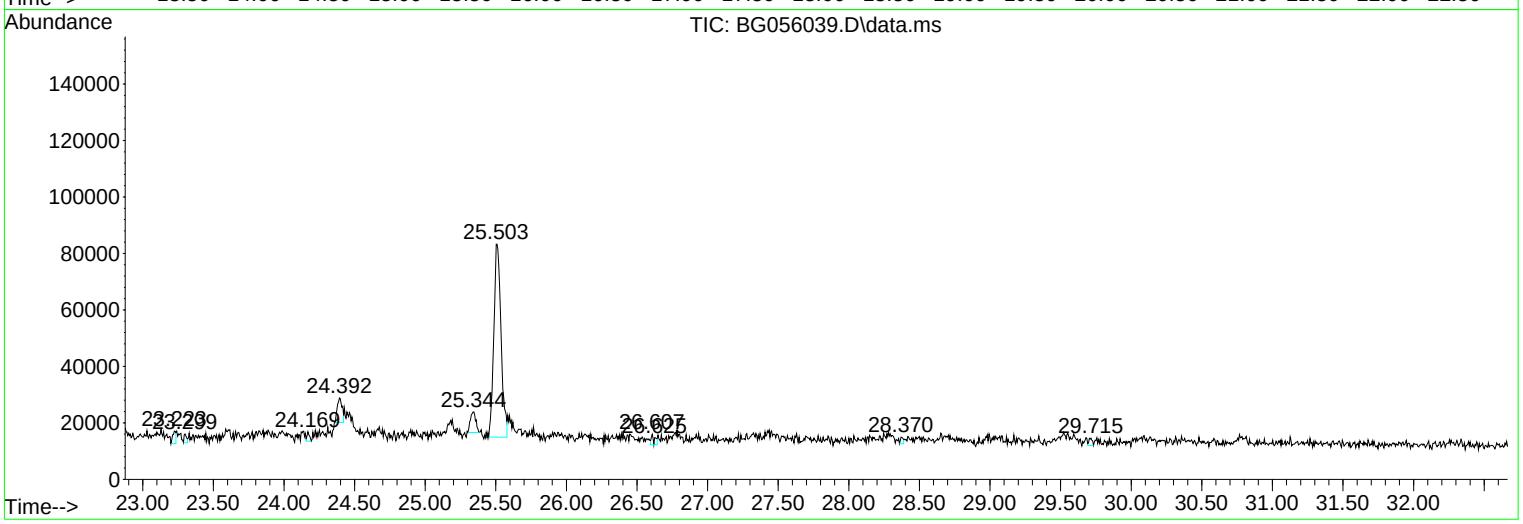
Instrument :
BNA_G
ClientSampleId :
SP-591

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.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\BG122022\
Data File : BG056039.D
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Operator : CG/JU
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Instrument :
BNA_G
ClientSampleId :
SP-591

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

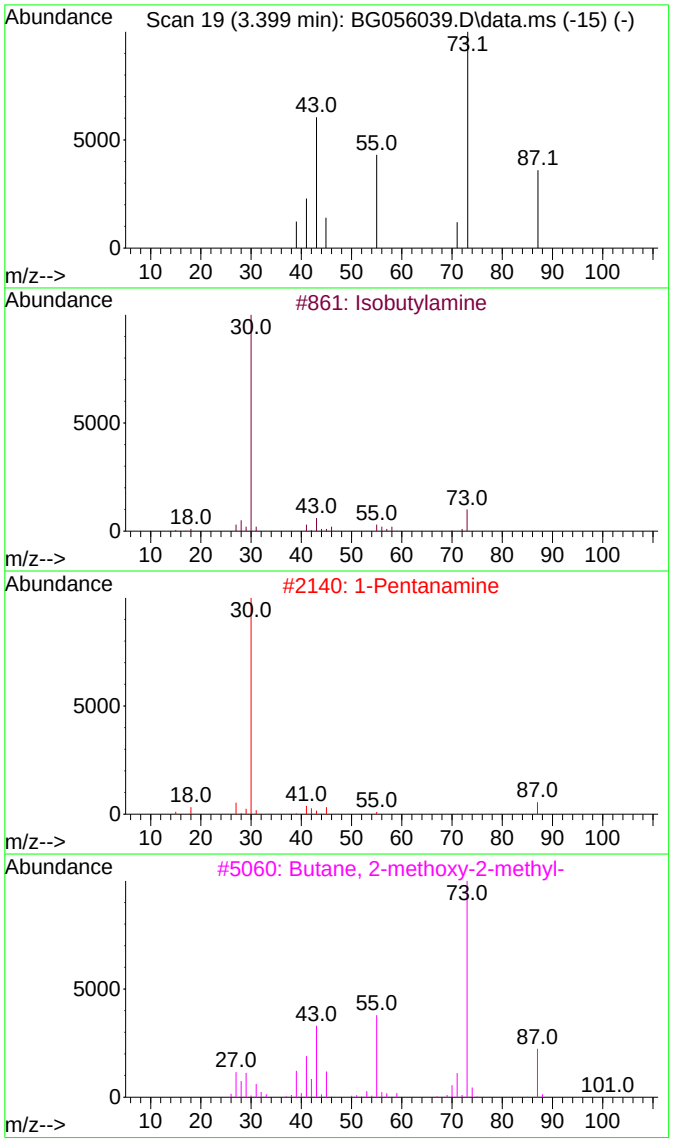
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

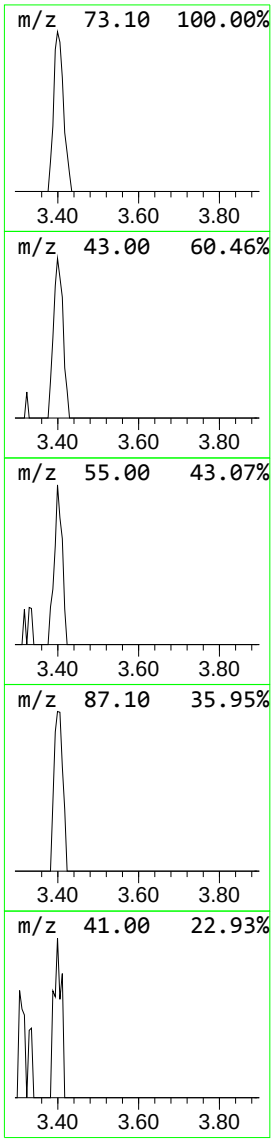
****

Peak Number 1 unknown3.399 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.399	2.30 ng	7735	1,4-Dichlorobenzene-d4	8.370

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutylamine	73	C4H11N	000078-81-9	5
2	1-Pentanamine	87	C5H13N	000110-58-7	4
3	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	4
4	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	4
5	3,4-Hexanediol, 2,5-dimethyl-	146	C8H18O2	022607-11-0	4





Tentatively Identified Compound (LSC) summary

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Data File : BG056039.D
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Sample : N6051-01 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-591

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
unknown3.399	3.399	2.3	ng	7735	1	8.370	67181	20.0