

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032923\
 Data File : BM039213.D
 Acq On : 29 Mar 2023 20:18
 Operator : CG/JU
 Sample : PB151658BL
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PB151658BL

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_M\Methods\8270-BM032923.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039213.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.404	185	190	199	rVB	235965	307783	2.14%	0.445%
2	5.016	288	294	309	rVB	2219403	2988649	20.81%	4.324%
3	5.487	367	374	388	rBV	5237377	7350942	51.20%	10.636%
4	7.098	640	648	664	rBV	4630014	7380586	51.40%	10.678%
5	7.928	782	789	801	rVB	855390	1363529	9.50%	1.973%
6	9.098	979	988	1000	rBV	2785753	4699149	32.73%	6.799%
7	10.739	1258	1267	1278	rBV	1067829	1856427	12.93%	2.686%
8	13.198	1676	1685	1701	rBV	6949050	10029224	69.85%	14.511%
9	14.568	1911	1918	1935	rBV	1540905	2332816	16.25%	3.375%
10	16.062	2165	2172	2194	rBV	5246131	7578417	52.78%	10.965%
11	17.315	2379	2385	2399	rBV	1832735	2736008	19.05%	3.959%
12	19.639	2776	2780	2786	rBV	116898	145440	1.01%	0.210%
13	19.944	2826	2832	2845	rBV	11781536	14358696	100.00%	20.775%
14	20.680	2954	2957	2963	rBV	184682	213330	1.49%	0.309%
15	21.503	3092	3097	3106	rBV	2226616	2889082	20.12%	4.180%
16	23.921	3502	3508	3516	rVB2	1444453	2886504	20.10%	4.176%

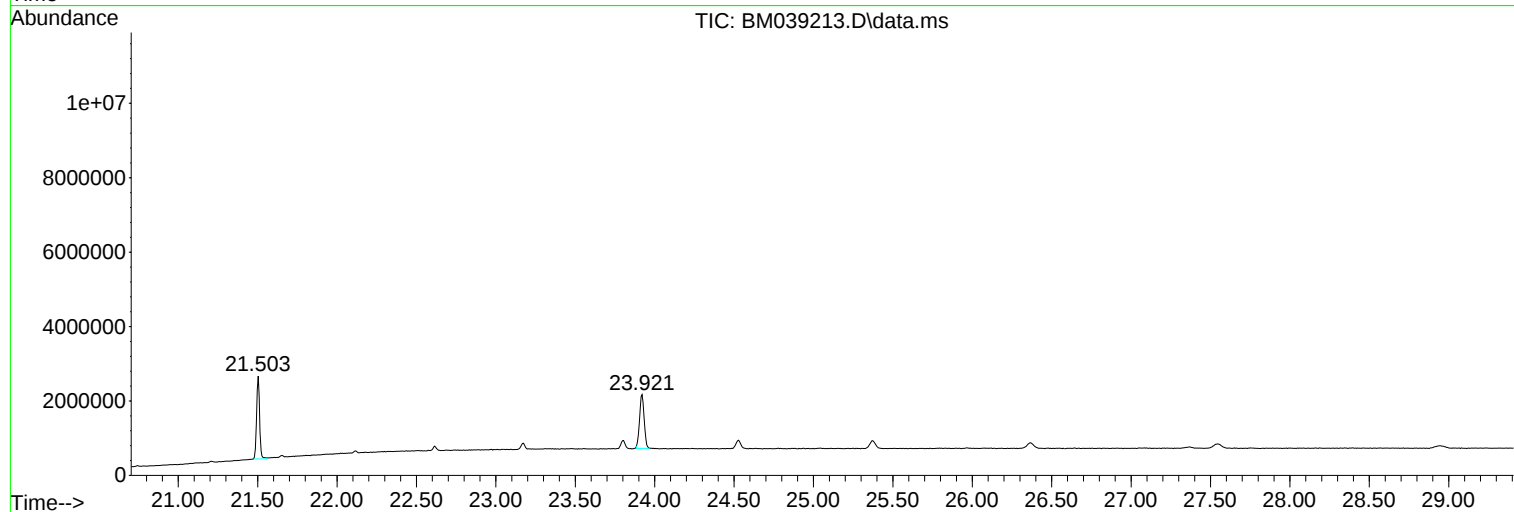
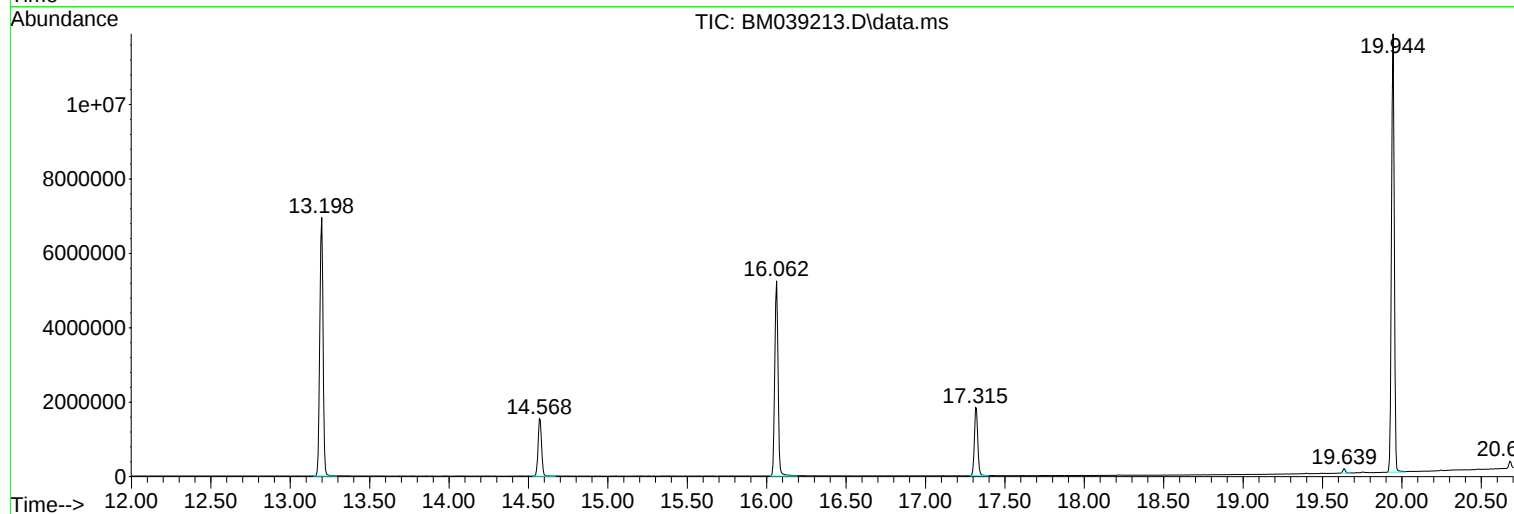
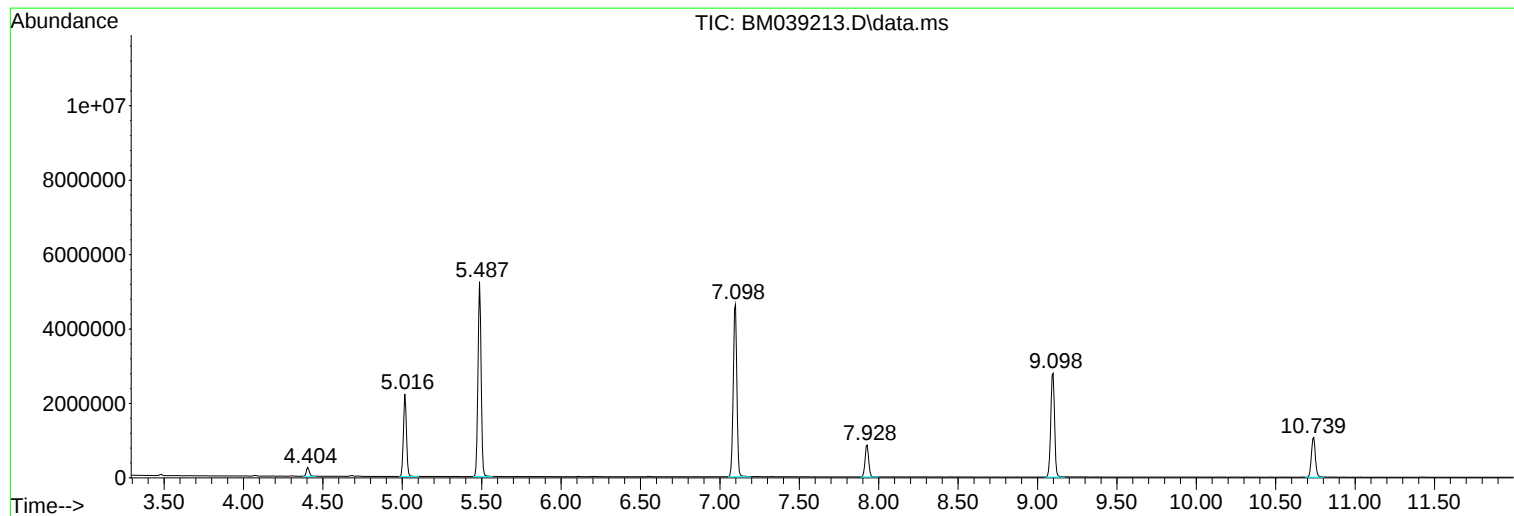
Sum of corrected areas: 69116582

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.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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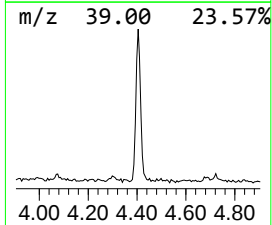
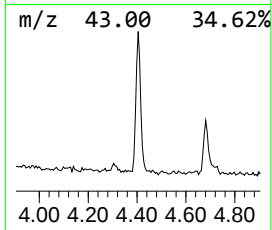
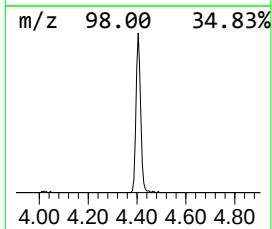
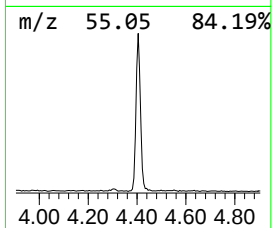
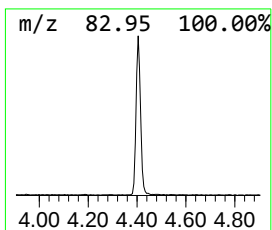
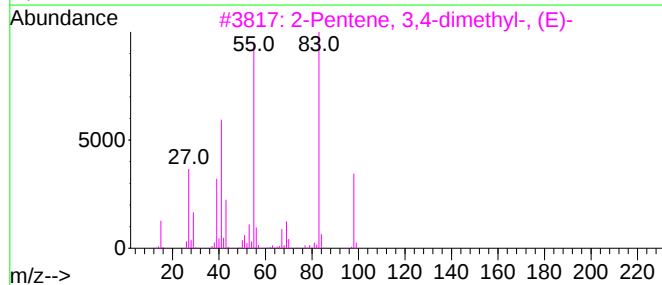
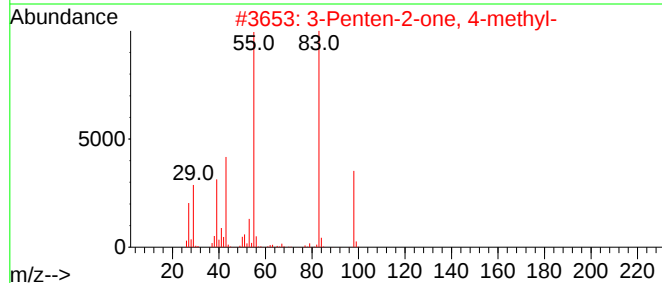
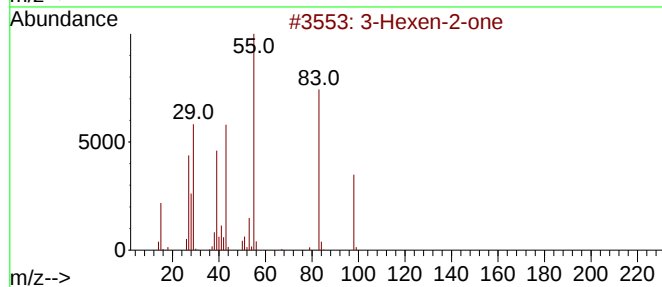
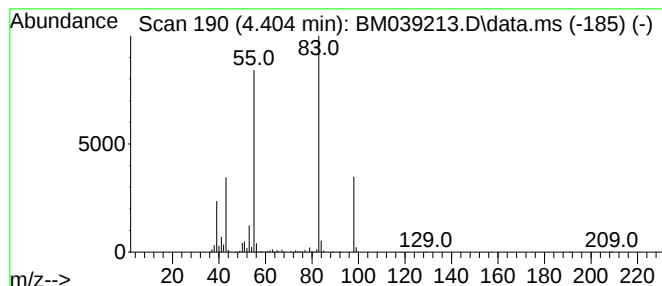
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Hexen-2-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.404	4.51 ng	307783	1,4-Dichlorobenzene-d4	7.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	91
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5			2,4-Azetidinedione, 3,3-diethyl-	141	C7H11NO2	042282-85-9	78



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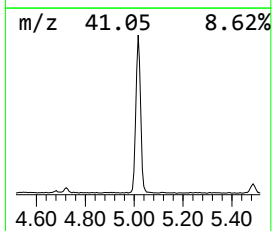
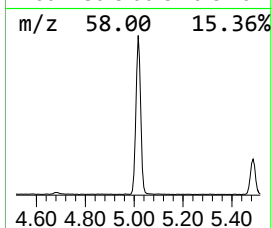
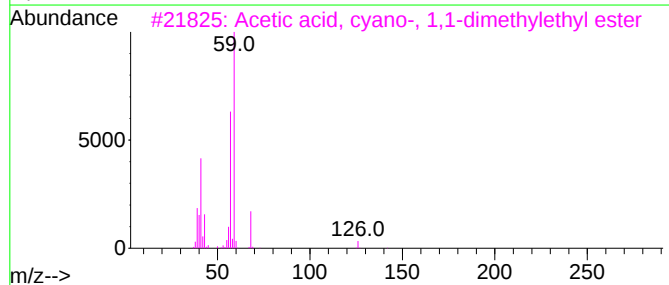
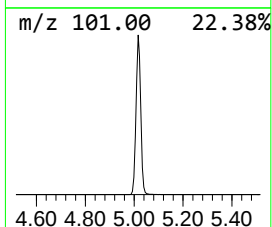
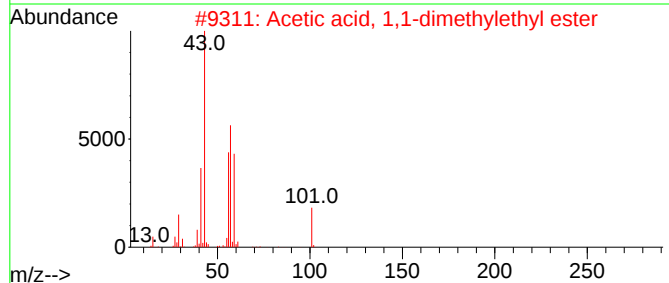
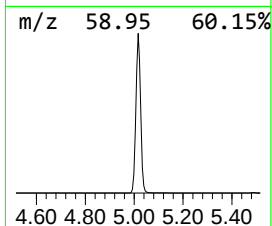
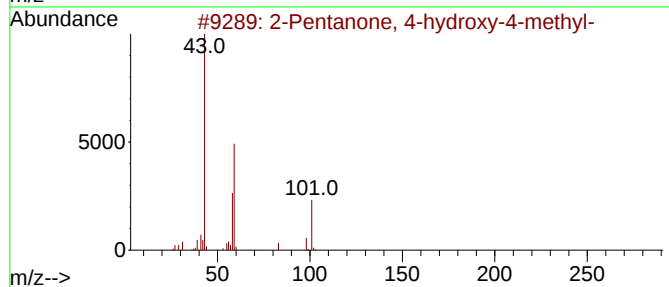
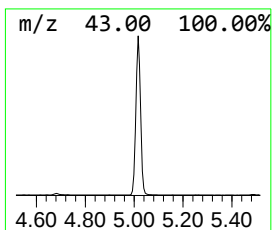
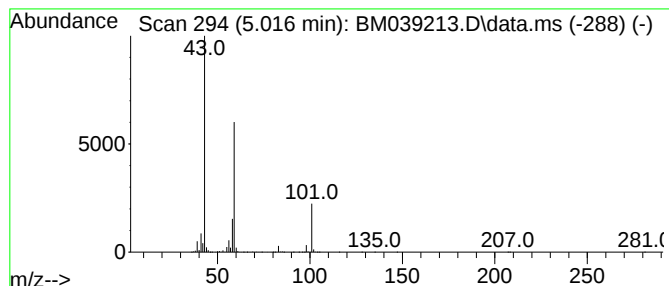
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	43.84 ng	2988650	1,4-Dichlorobenzene-d4	7.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Hexen-2-one	4.404	4.5	ng	307783	1	7.928	1363530	20.0
2-Pentanone, 4-...	5.016	43.8	ng	2988650	1	7.928	1363530	20.0