

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032823\
 Data File : BM039181.D
 Acq On : 28 Mar 2023 16:02
 Operator : CG/JU
 Sample : PB151601BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PB151601BL

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-BM030823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039181.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.416	187	192	200	rVB	281036	376449	1.84%	0.407%
2	5.028	290	296	305	rBV	2625120	3557734	17.39%	3.842%
3	5.498	369	376	391	rBV	6334375	8963958	43.81%	9.681%
4	7.110	642	650	667	rBV	5859775	9275863	45.33%	10.018%
5	7.934	783	790	800	rBV	999648	1611373	7.87%	1.740%
6	9.110	981	990	1003	rBV	3447833	5745738	28.08%	6.205%
7	10.751	1260	1269	1277	rBV	1321299	2284063	11.16%	2.467%
8	13.210	1679	1687	1703	rBV	9027656	13077084	63.91%	14.123%
9	14.580	1913	1920	1930	rBV	2199210	3161885	15.45%	3.415%
10	16.074	2166	2174	2193	rBV	7074187	10633729	51.97%	11.484%
11	17.327	2380	2387	2396	rBV	2787770	3899430	19.06%	4.211%
12	19.639	2777	2780	2785	rBV	218273	241897	1.18%	0.261%
13	19.950	2827	2833	2838	rBV	16339775	20462662	100.00%	22.099%
14	20.686	2954	2958	2964	rBV	367384	416189	2.03%	0.449%
15	21.509	3093	3098	3103	rBV	3401040	4470402	21.85%	4.828%
16	23.927	3503	3509	3519	rVB2	2216842	4416049	21.58%	4.769%

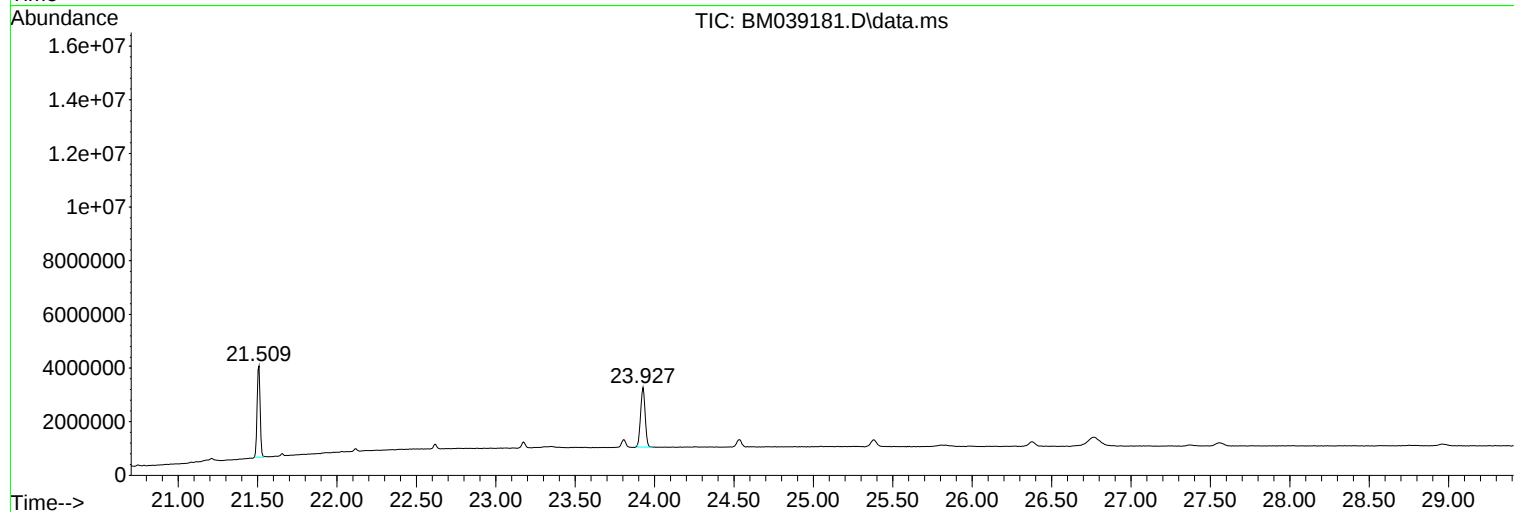
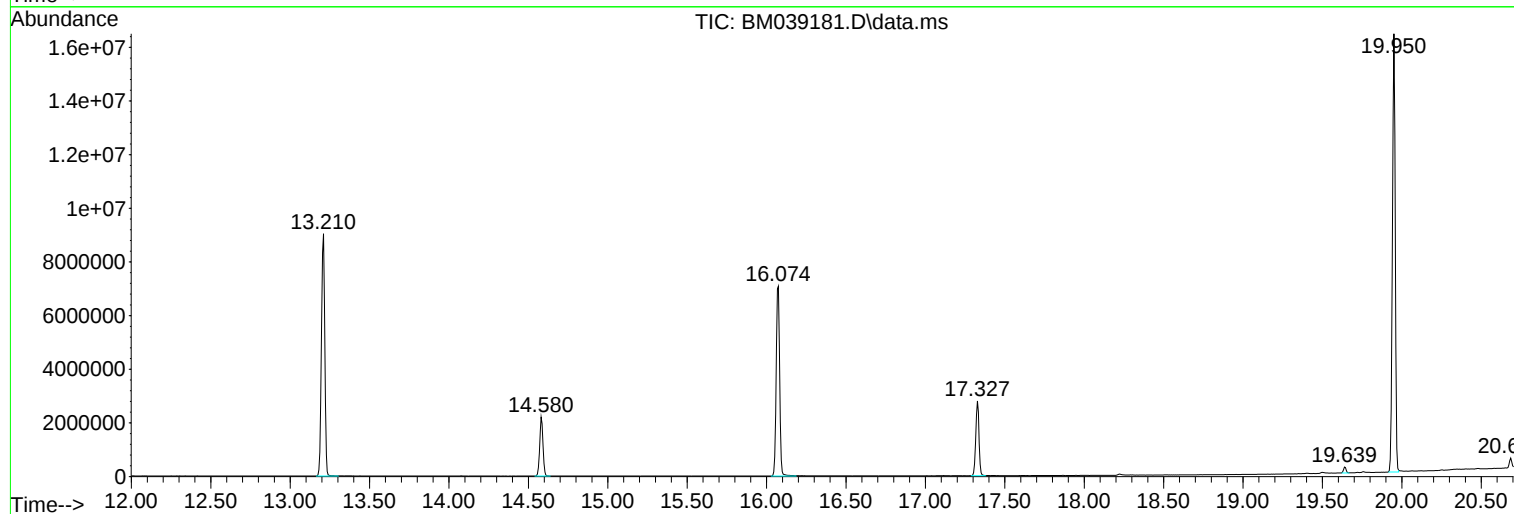
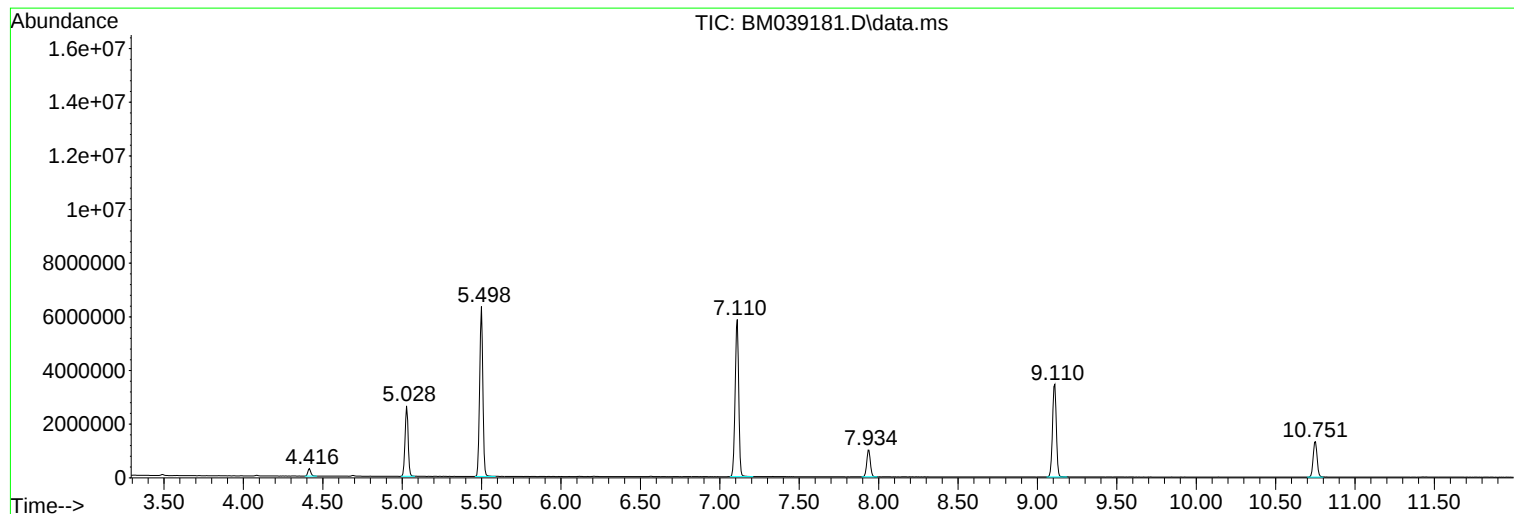
Sum of corrected areas: 92594505

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.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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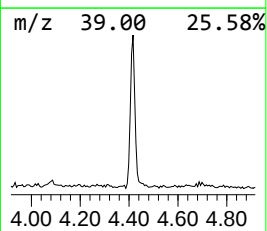
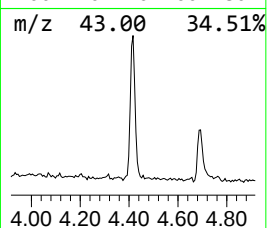
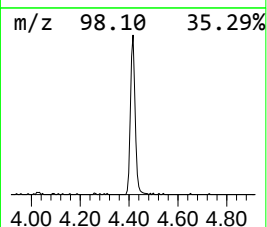
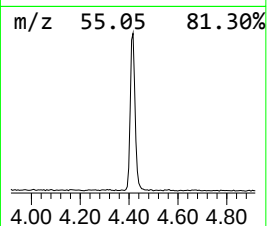
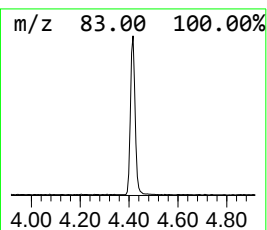
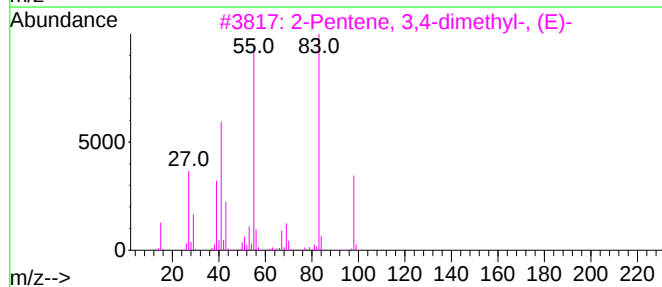
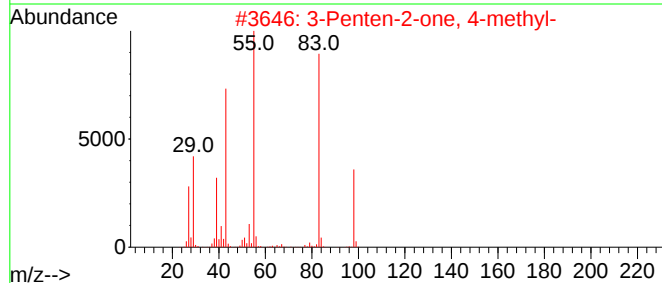
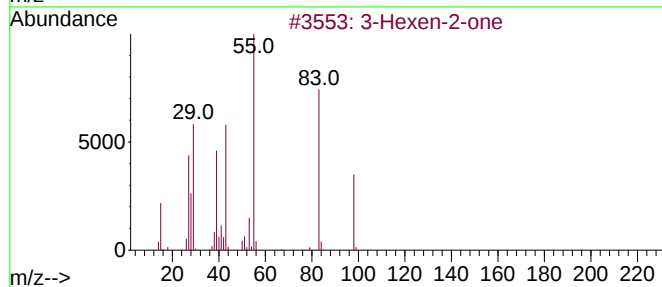
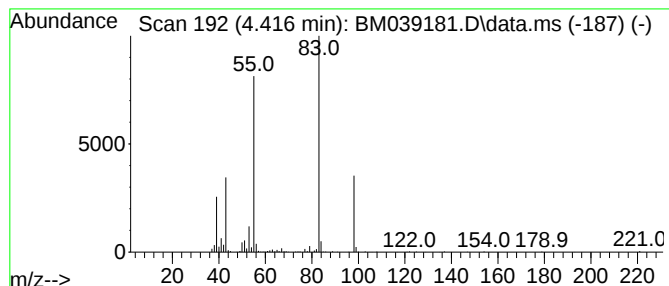
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.416	4.67 ng	376449	1,4-Dichlorobenzene-d4	7.939

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	C7H11N02	042282-85-9	78



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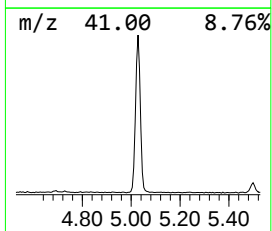
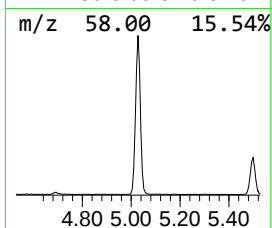
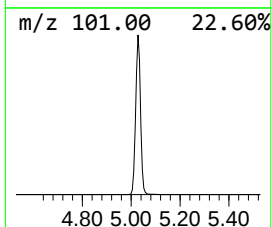
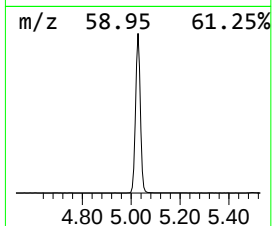
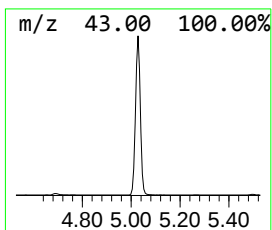
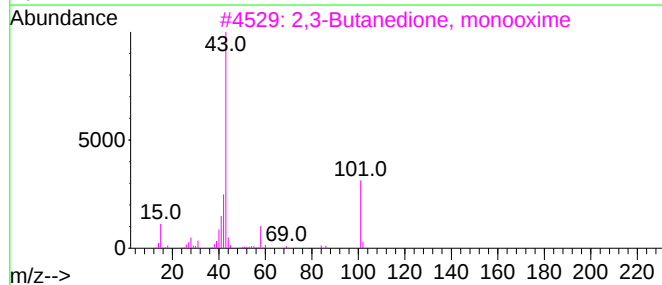
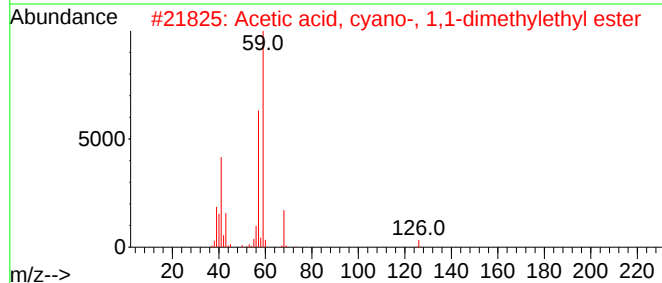
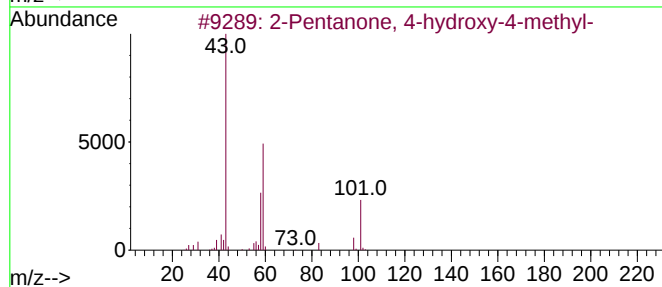
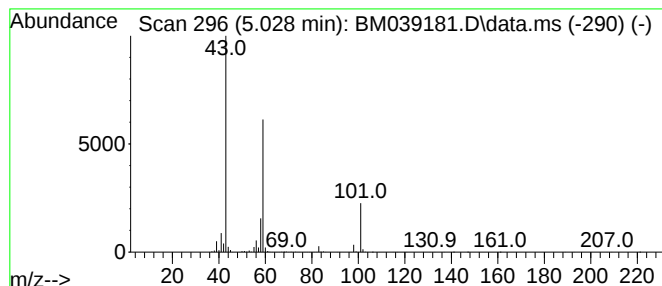
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.028	44.16 ng	3557730	1,4-Dichlorobenzene-d4	7.939

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Hexen-2-one	4.416	4.7	ng	376449	1	7.939	1611370	20.0
2-Pentanone, 4-...	5.028	44.2	ng	3557730	1	7.939	1611370	20.0