

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102823\
 Data File : BF136000.D
 Acq On : 28 Oct 2023 12:26
 Operator : CG\JU
 Sample : PB156392BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB156392BL

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_F\Methods\8270-BF102523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136000.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.151	3	11	18	rVB	73052	102519	1.83%	0.268%
2	4.457	397	403	407	rBV	2010322	2282383	40.74%	5.969%
3	5.075	500	508	519	rBV	2031206	3041274	54.28%	7.953%
4	5.469	569	575	578	rBV	4064634	4398114	78.50%	11.501%
5	5.851	636	640	644	rVB	162445	127512	2.28%	0.333%
6	6.463	737	744	746	rBV	3607022	4315476	77.03%	11.285%
7	6.828	802	806	809	rVB	1165127	908213	16.21%	2.375%
8	7.392	896	902	904	rBV	2839939	2752503	49.13%	7.198%
9	8.104	1020	1023	1026	rVB	1543151	1209424	21.59%	3.163%
10	9.186	1203	1207	1210	rBV	5481756	4985377	88.99%	13.037%
11	9.863	1318	1322	1325	rBV	1789713	1385448	24.73%	3.623%
12	10.657	1452	1457	1460	rBV	3542863	3301190	58.92%	8.633%
13	11.357	1572	1576	1579	rBV	1793710	1442821	25.75%	3.773%
14	12.963	1844	1849	1852	rBV	5749814	5602485	100.00%	14.651%
15	14.009	2023	2027	2031	rBV	1496719	1282459	22.89%	3.354%
16	14.109	2039	2044	2048	rBV	62362	72698	1.30%	0.190%
17	15.498	2275	2280	2287	rVB	791859	1029700	18.38%	2.693%

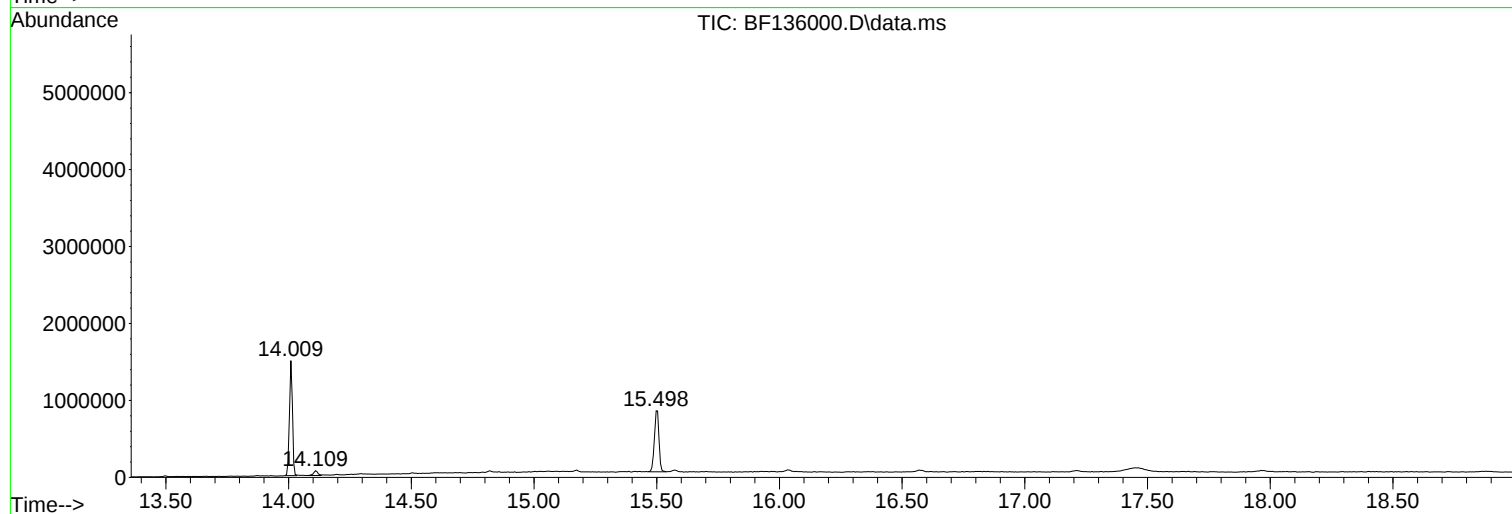
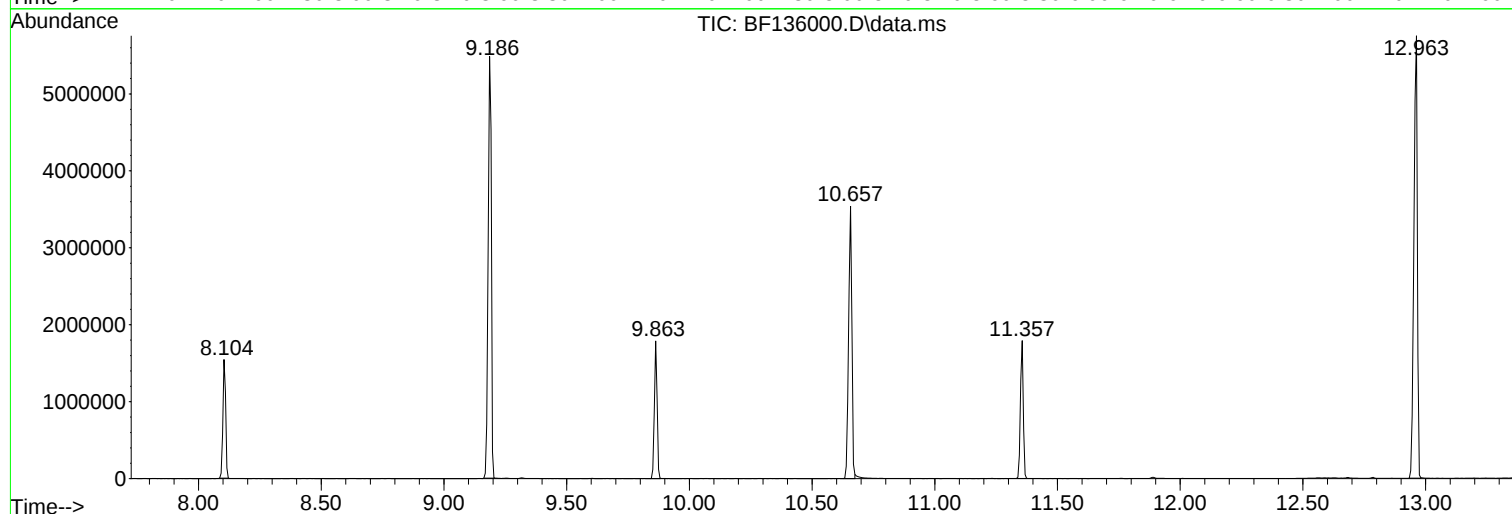
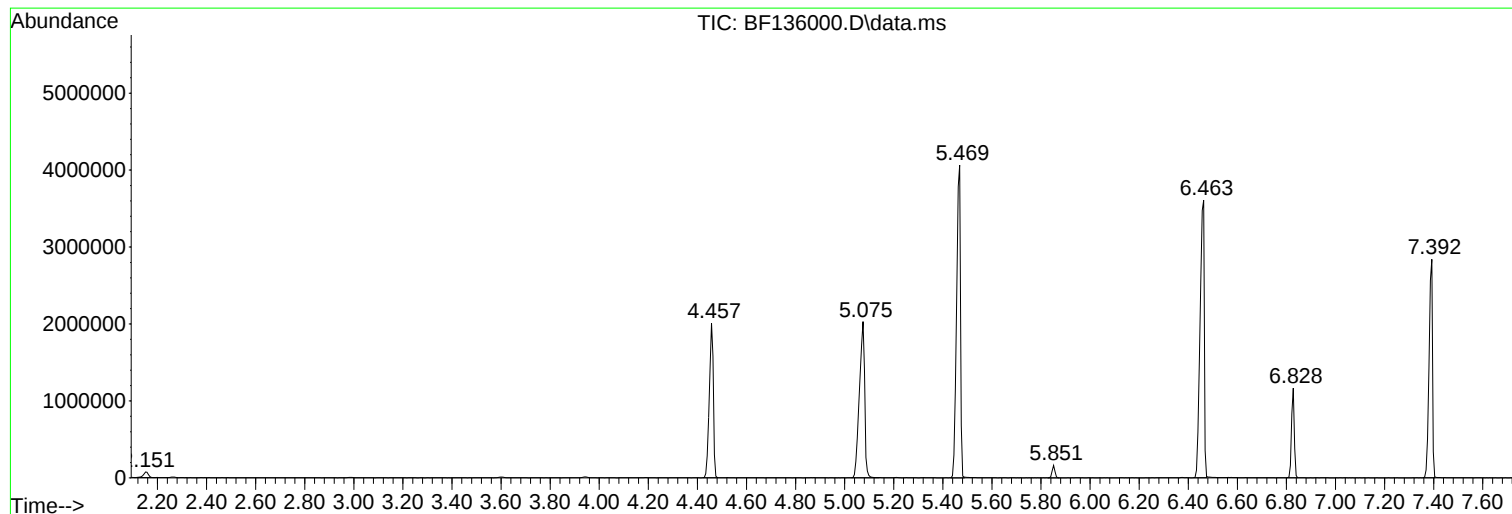
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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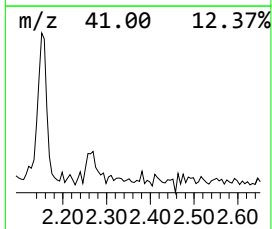
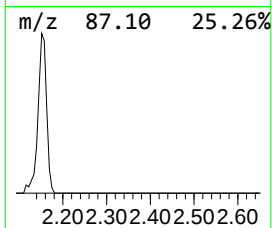
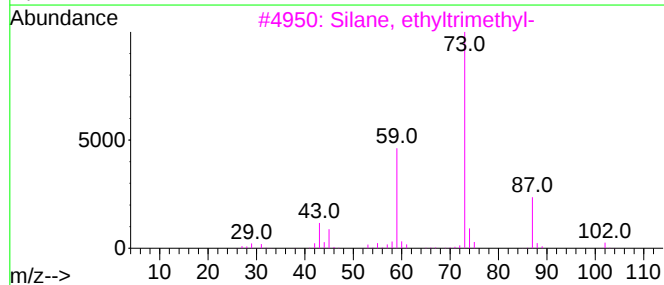
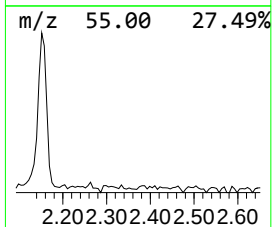
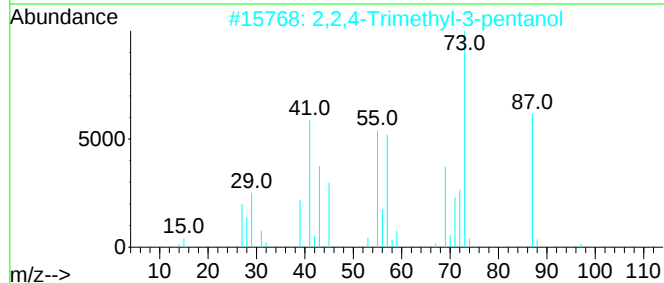
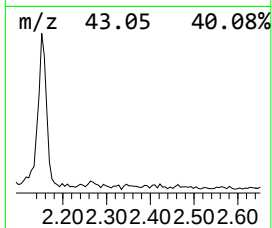
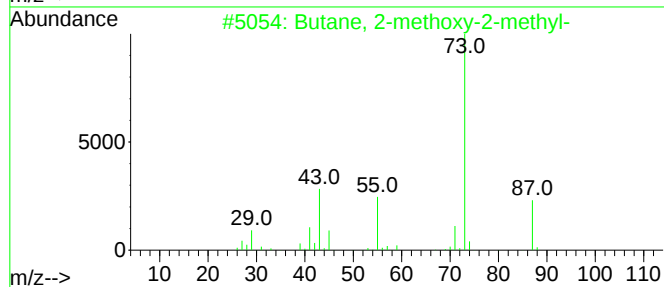
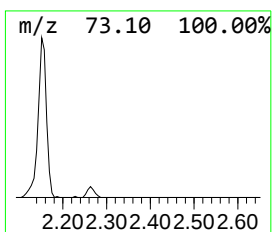
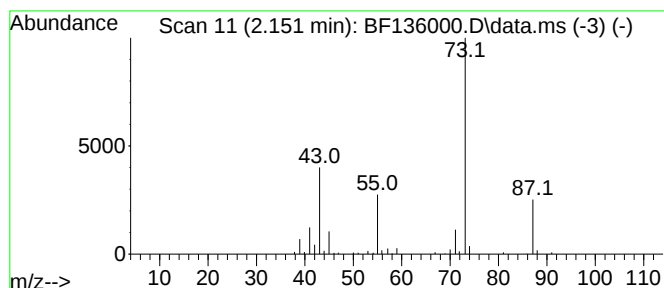
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.151	2.26 ng	102519	1,4-Dichlorobenzene-d4	6.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3			Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	17
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	16



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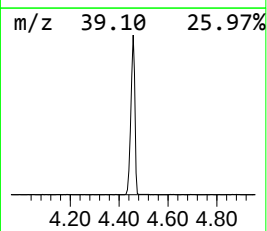
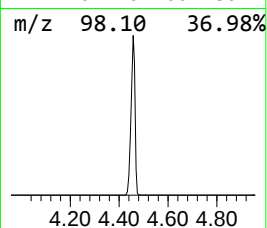
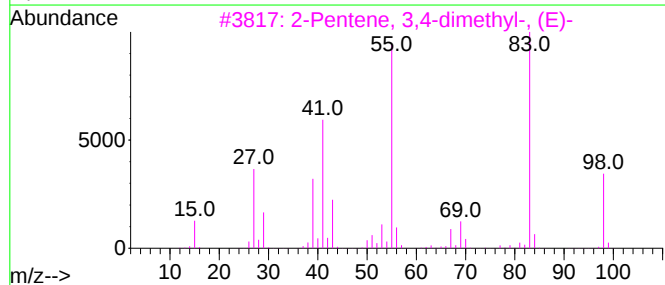
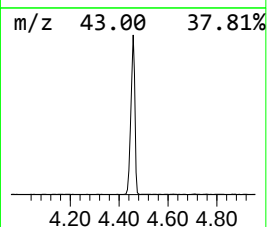
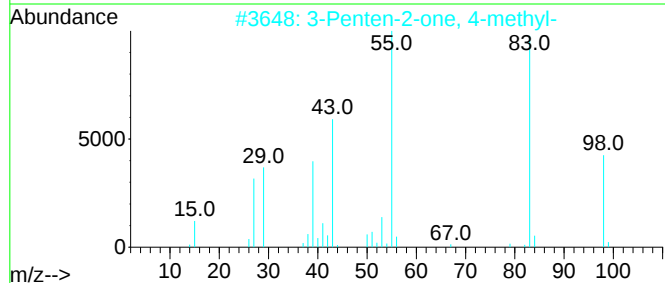
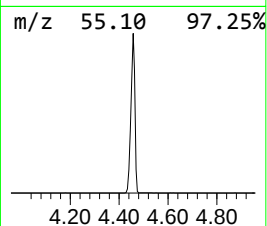
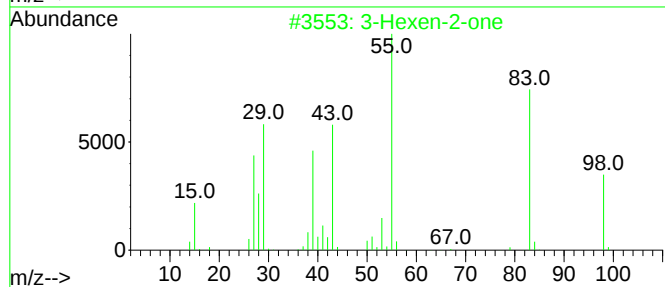
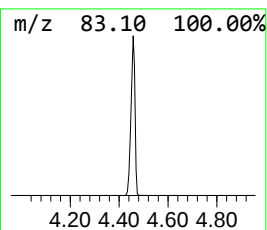
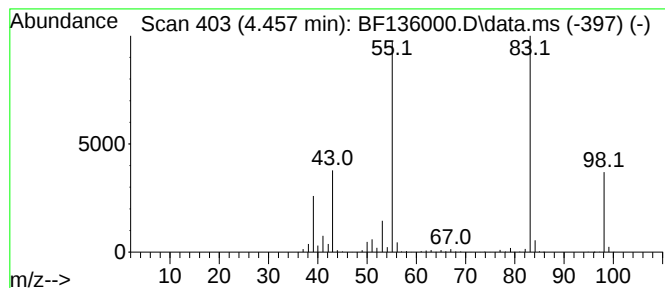
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.457	50.26 ng	2282380	1,4-Dichlorobenzene-d4	6.828

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-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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ALS Vial : 3 Sample Multiplier: 1

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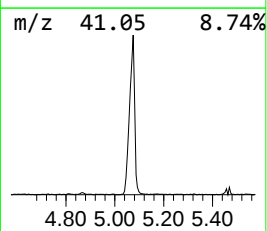
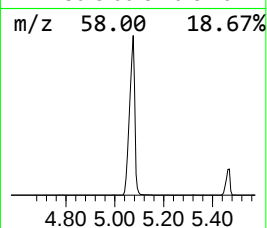
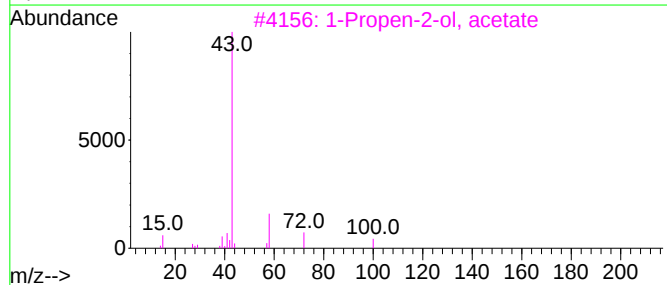
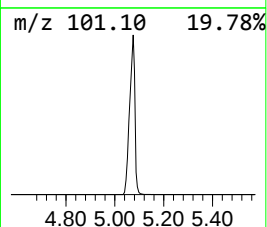
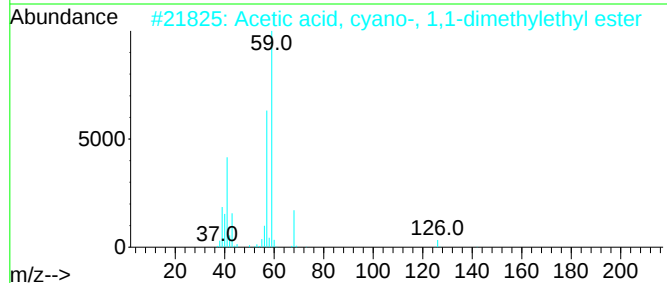
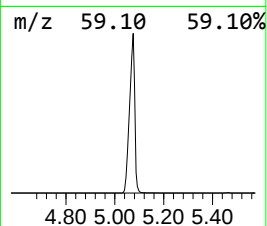
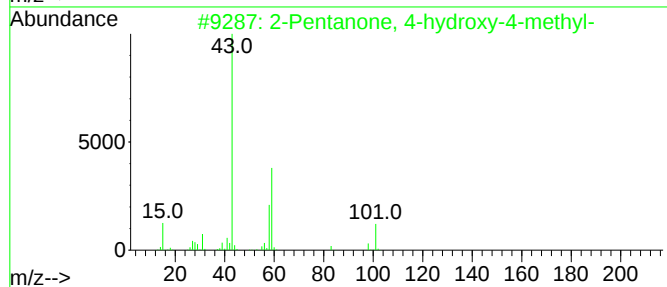
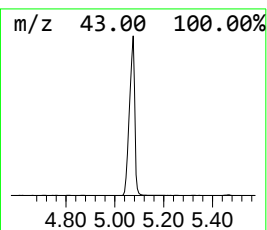
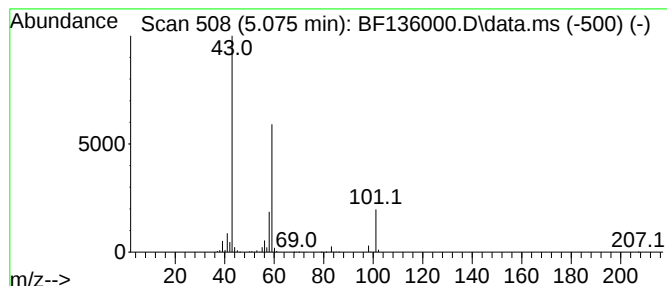
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	66.97 ng	3041270	1,4-Dichlorobenzene-d4	6.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	Acetone	58	C3H6O	000067-64-1	9		



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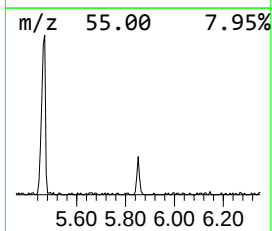
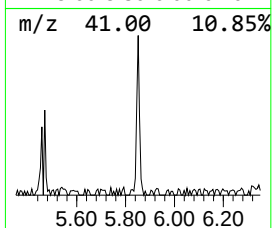
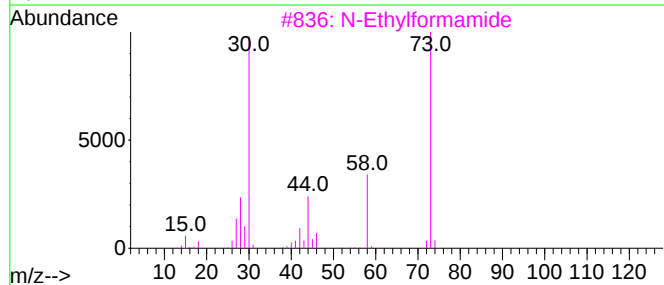
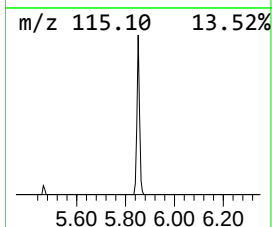
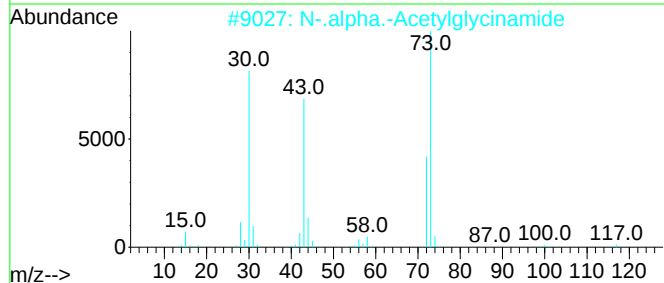
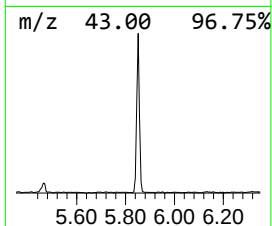
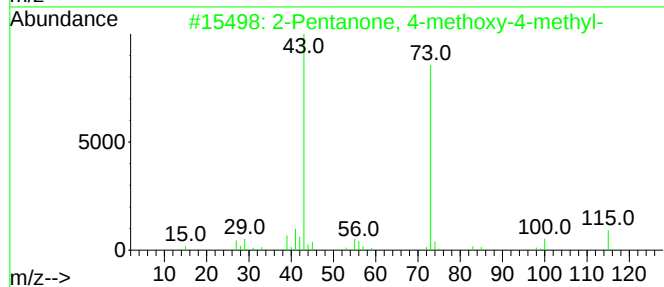
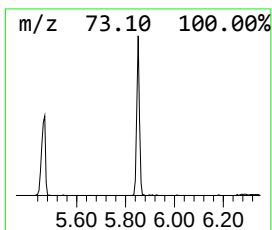
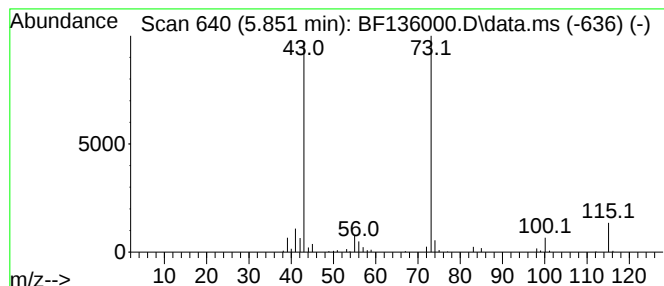
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Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.851	2.81 ng	127512	1,4-Dichlorobenzene-d4	6.828

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	40
3		N-Ethylformamide	73	C3H7NO	000627-45-2	16
4		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.151	2.3	ng	102519	1	6.828	908213	20.0
3-Hexen-2-one	4.457	50.3	ng	2282380	1	6.828	908213	20.0
2-Pentanone, 4-...	5.075	67.0	ng	3041270	1	6.828	908213	20.0
2-Pentanone, 4-...	5.851	2.8	ng	127512	1	6.828	908213	20.0