

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102823\
 Data File : BF136002.D
 Acq On : 28 Oct 2023 13:27
 Operator : CG\JU
 Sample : PB156435BL
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB156435BL

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: BF136002.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	3	13	19	rVB	81442	120691	1.73%	0.262%
2	3.610	253	259	265	rBV	50664	77257	1.11%	0.167%
3	4.463	397	404	407	rBV	2342774	2676150	38.34%	5.800%
4	5.081	500	509	525	rBV	2173674	3565550	51.08%	7.728%
5	5.469	569	575	578	rBV	4667232	5616378	80.47%	12.173%
6	5.851	636	640	645	rVB	184941	143458	2.06%	0.311%
7	6.463	737	744	747	rBV	4354957	5515692	79.03%	11.955%
8	6.828	802	806	809	rVB	1207030	957457	13.72%	2.075%
9	7.392	895	902	905	rBV	3603876	3535715	50.66%	7.663%
10	8.104	1019	1023	1026	rBV	1643662	1296592	18.58%	2.810%
11	9.192	1203	1208	1211	rVB	6259618	6108621	87.52%	13.240%
12	9.863	1318	1322	1325	rBV	1882760	1486908	21.30%	3.223%
13	10.657	1452	1457	1460	rBV	4045793	4143544	59.37%	8.981%
14	11.357	1572	1576	1579	rBV	1831432	1547227	22.17%	3.354%
15	12.963	1843	1849	1852	rBV	6498000	6979650	100.00%	15.128%
16	14.010	2023	2027	2031	rBV	1558605	1333280	19.10%	2.890%
17	15.498	2275	2280	2286	rBV	796959	1033106	14.80%	2.239%

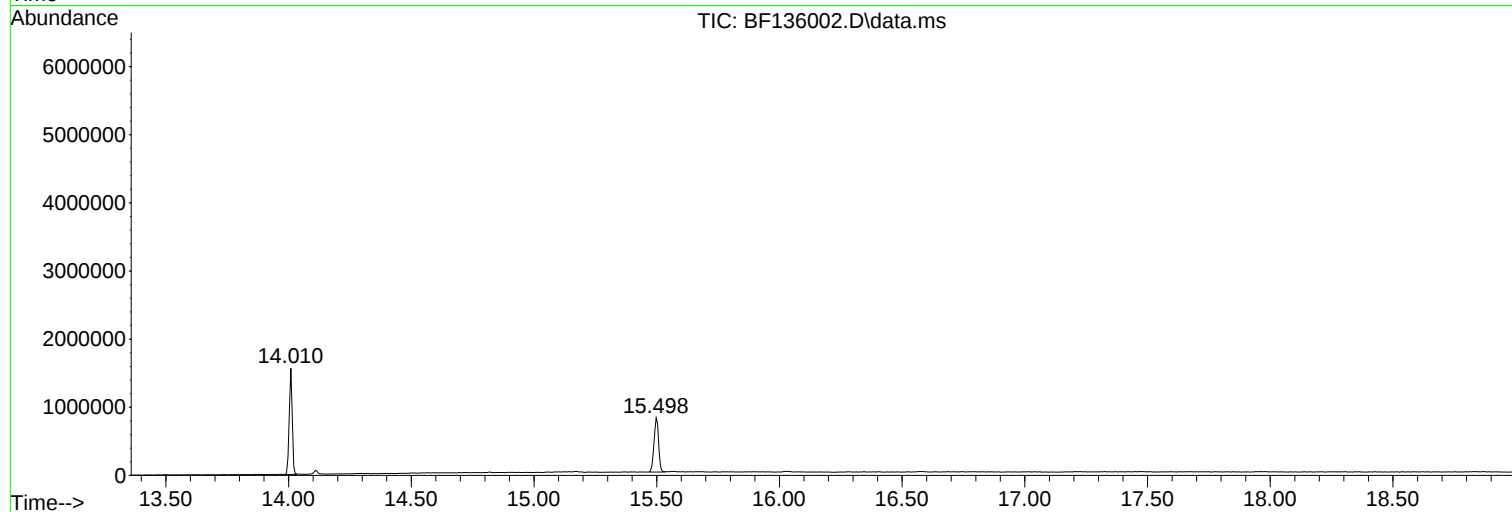
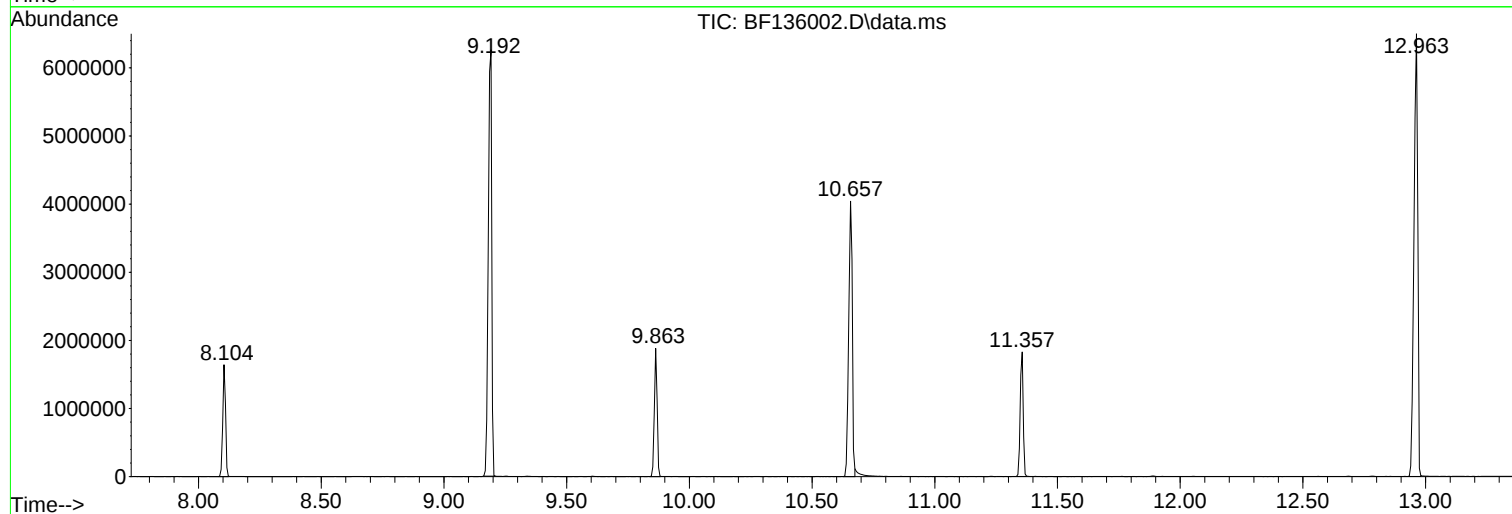
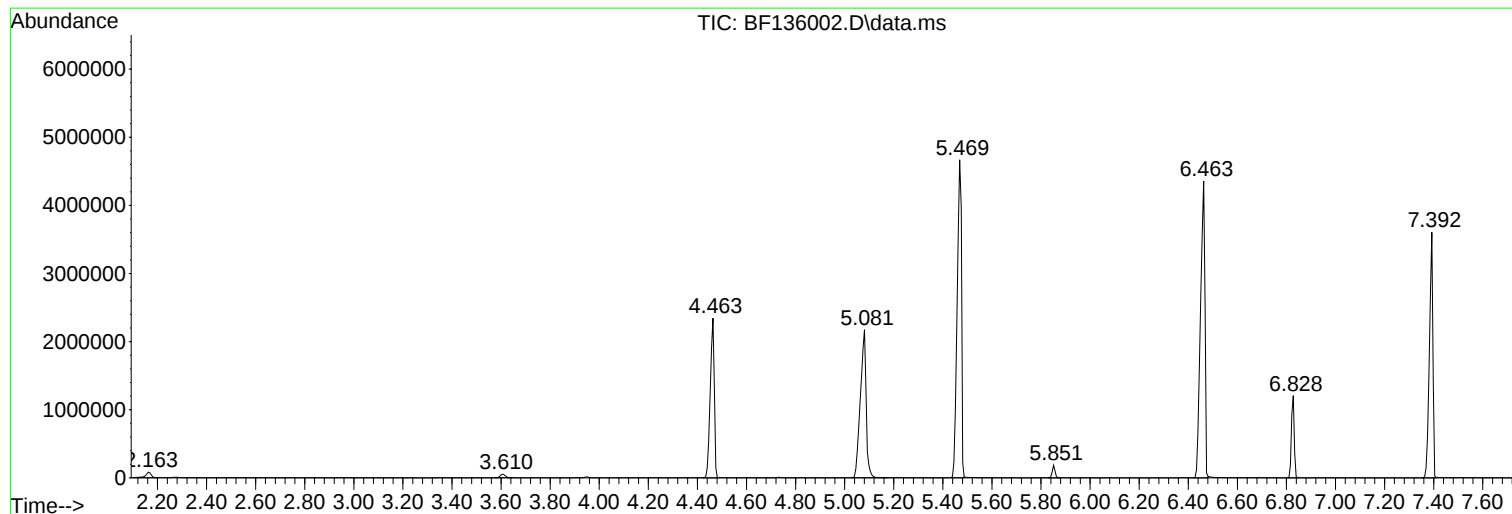
Sum of corrected areas: 46137276

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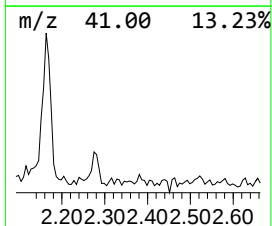
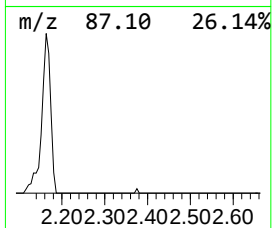
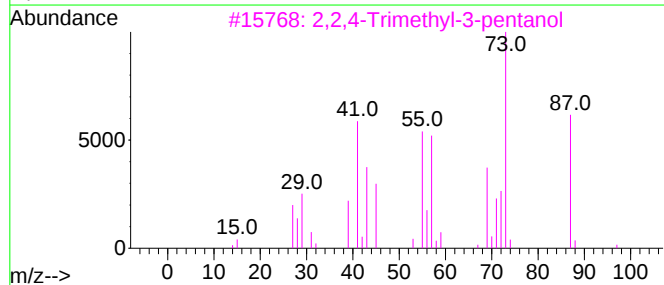
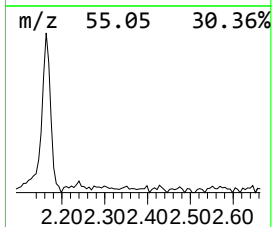
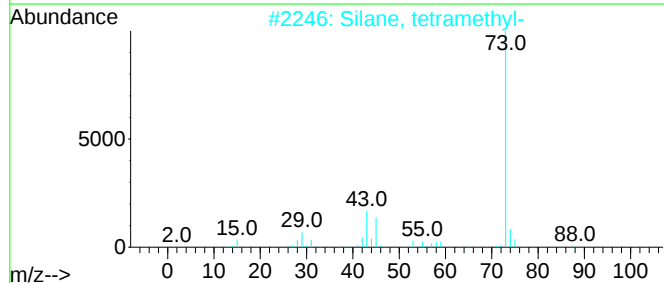
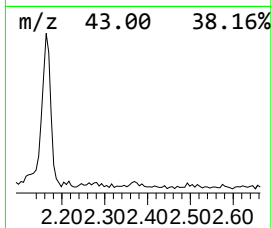
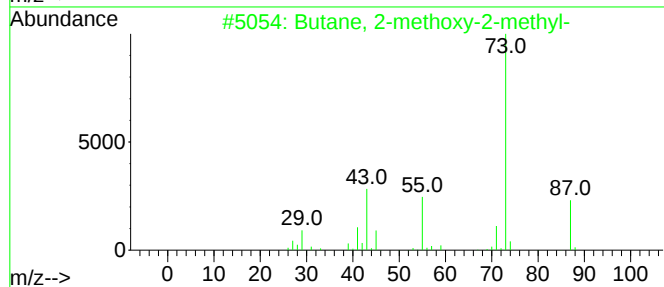
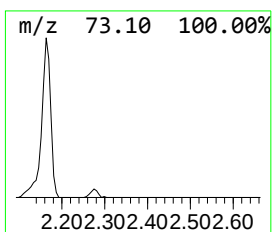
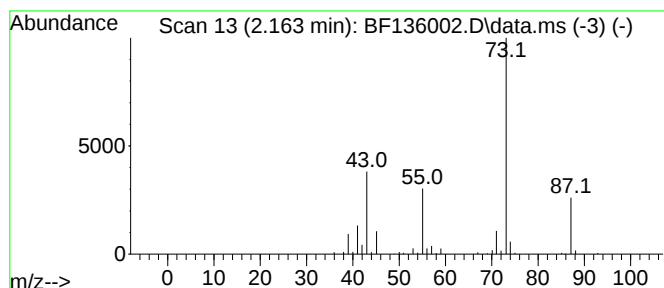
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.163	2.52 ng	120691	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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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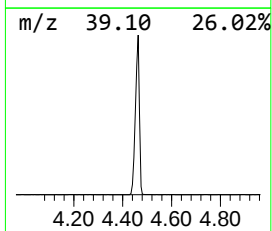
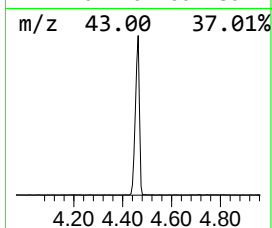
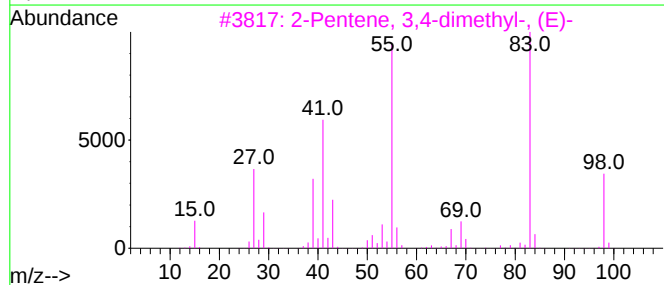
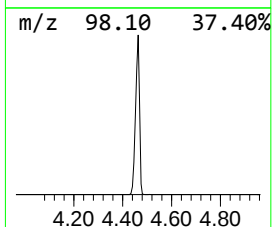
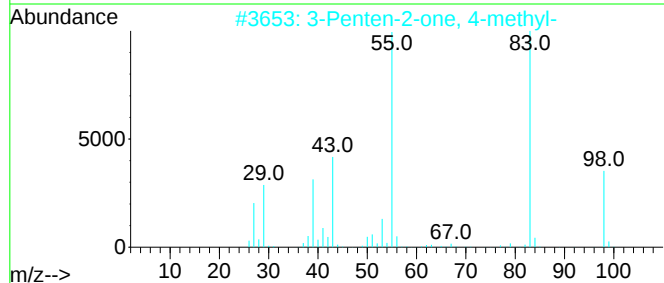
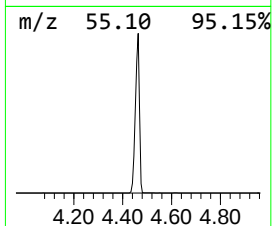
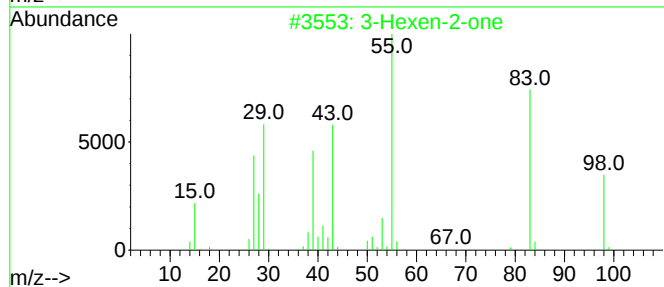
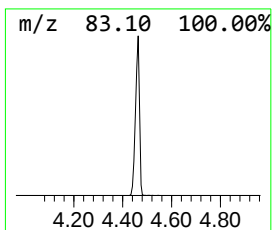
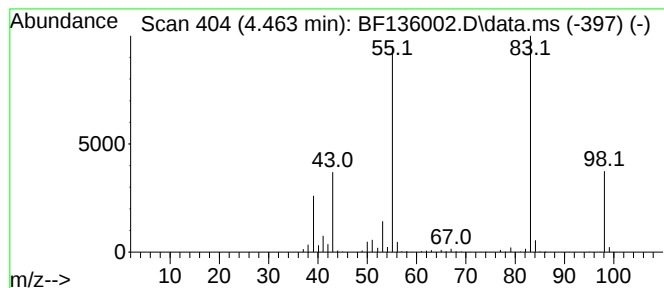
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.463	55.90 ng	2676150	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 : 5 Sample Multiplier: 1

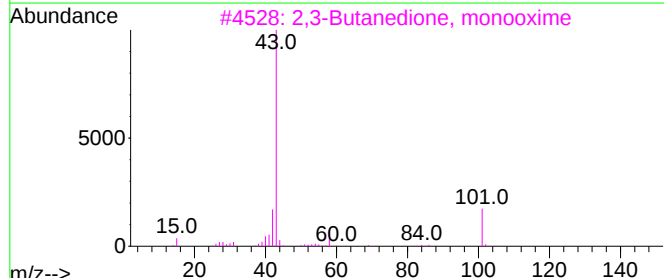
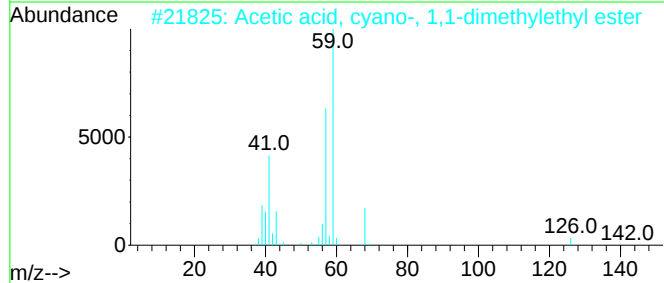
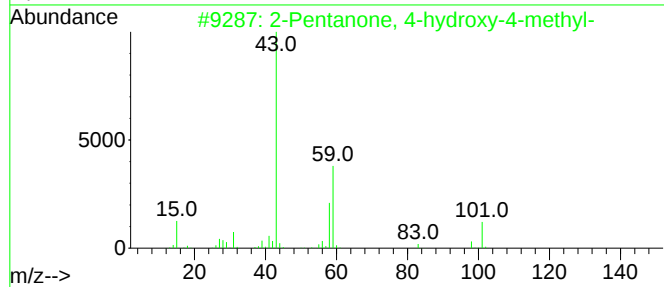
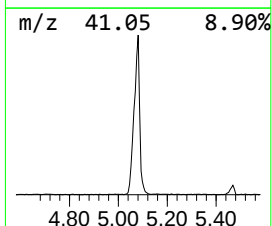
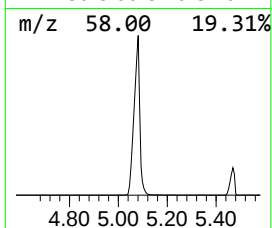
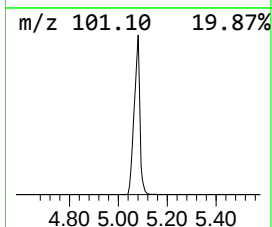
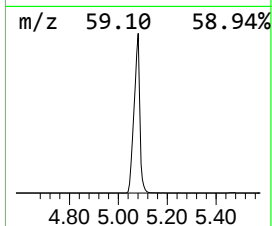
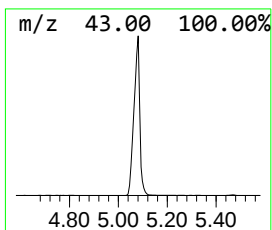
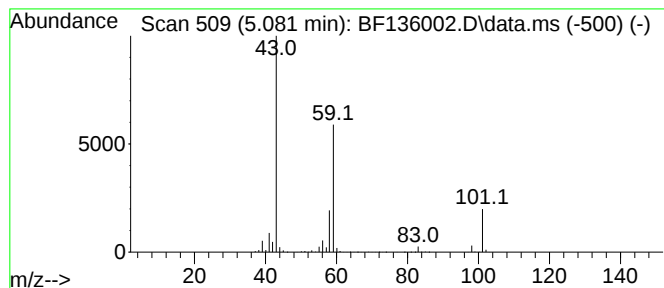
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.081	74.48 ng	3565550	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	17
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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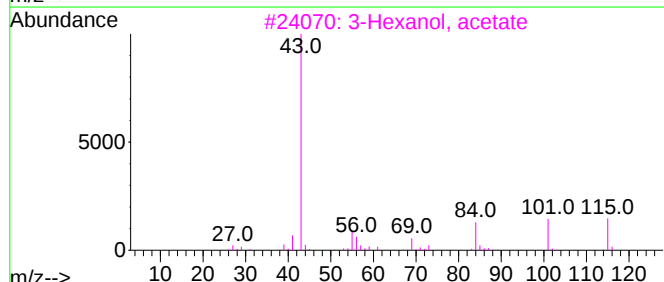
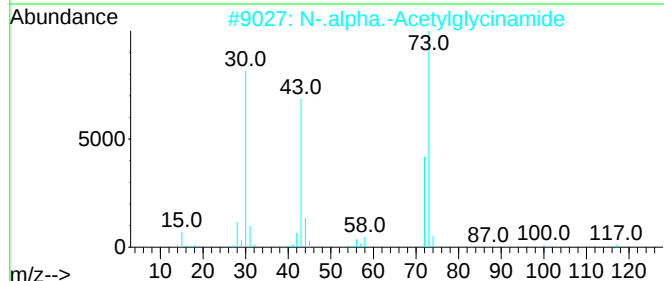
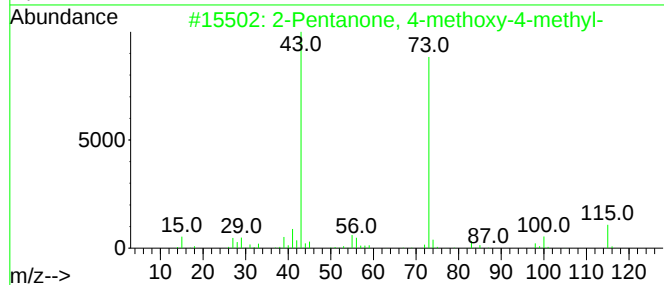
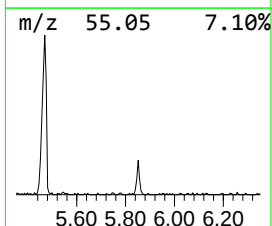
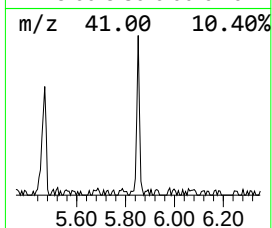
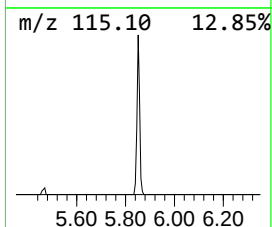
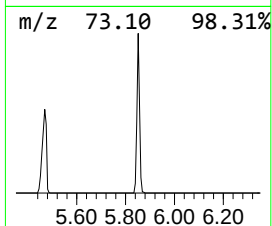
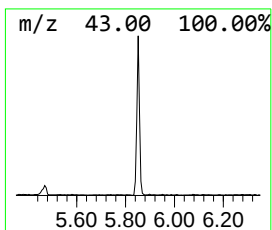
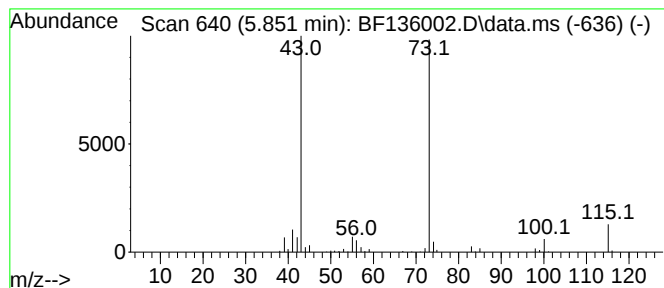
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Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.851	3.00 ng	143458	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	38
3			3-Hexanol, acetate	144	C8H16O2	040780-64-1	25
4			N-Formylmorpholine	115	C5H9NO2	004394-85-8	10
5			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	10



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.163	2.5	ng	120691	1	6.828	957457	20.0
3-Hexen-2-one	4.463	55.9	ng	2676150	1	6.828	957457	20.0
2-Pentanone, 4-...	5.081	74.5	ng	3565550	1	6.828	957457	20.0
2-Pentanone, 4-...	5.851	3.0	ng	143458	1	6.828	957457	20.0