

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042624\
 Data File : BF137731.D
 Acq On : 26 Apr 2024 12:18
 Operator : CG\JU
 Sample : PB160534BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB160534BL

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BF042324.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137731.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	5	10	16	rVB	763940	917336	8.74%	1.480%
2	4.734	446	450	454	rBV	762425	716103	6.82%	1.156%
3	5.328	543	551	554	rBV	4257847	6537180	62.25%	10.548%
4	5.693	608	613	616	rBV	5561990	5515328	52.52%	8.900%
5	6.081	676	679	683	rBV	392365	322654	3.07%	0.521%
6	6.669	773	779	782	rBV	5252078	5417290	51.58%	8.741%
7	7.063	842	846	849	rVB	1839542	1688589	16.08%	2.725%
8	7.622	935	941	944	rBV	4955574	5069802	48.28%	8.181%
9	8.345	1059	1064	1067	rBV	2431058	2282457	21.73%	3.683%
10	9.422	1241	1247	1250	rBV	9671980	9672173	92.10%	15.607%
11	10.104	1358	1363	1367	rBV	3054521	2640695	25.15%	4.261%
12	10.898	1493	1498	1501	rBV	4251056	4184493	39.85%	6.752%
13	11.598	1613	1617	1621	rBV	3095141	2743506	26.12%	4.427%
14	13.192	1883	1888	1891	rBV	10498703	10501706	100.00%	16.946%
15	14.251	2064	2068	2078	rVB	2419851	2176934	20.73%	3.513%
16	15.821	2329	2335	2350	rBV	1215519	1586701	15.11%	2.560%

Sum of corrected areas: 61972947

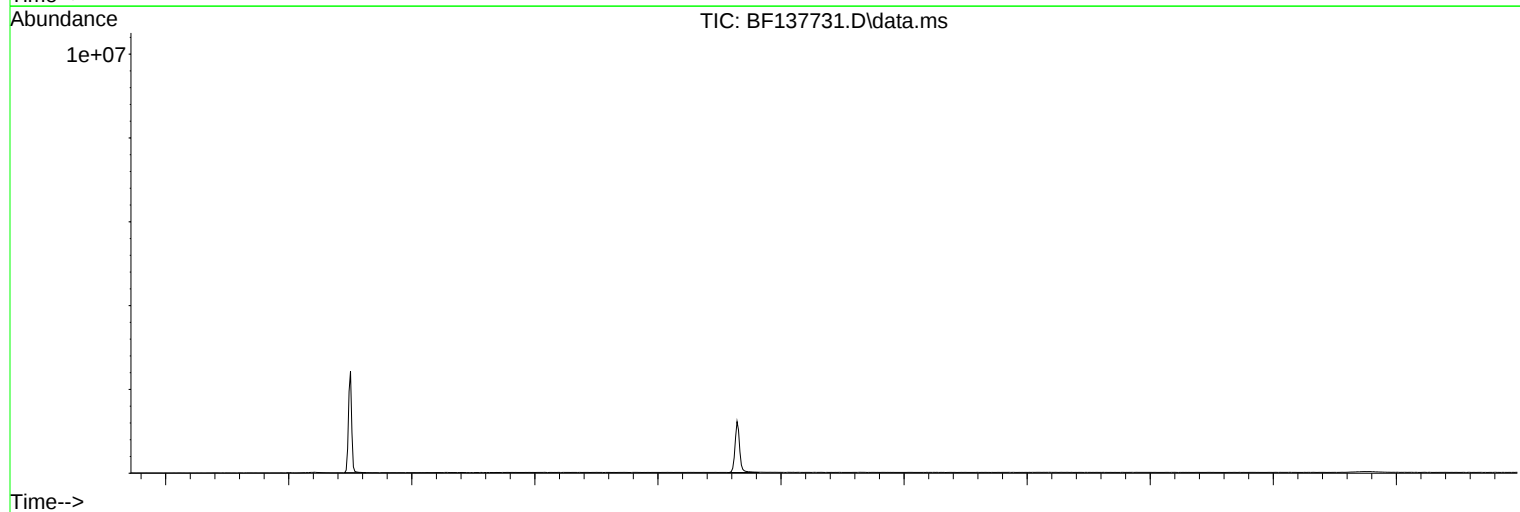
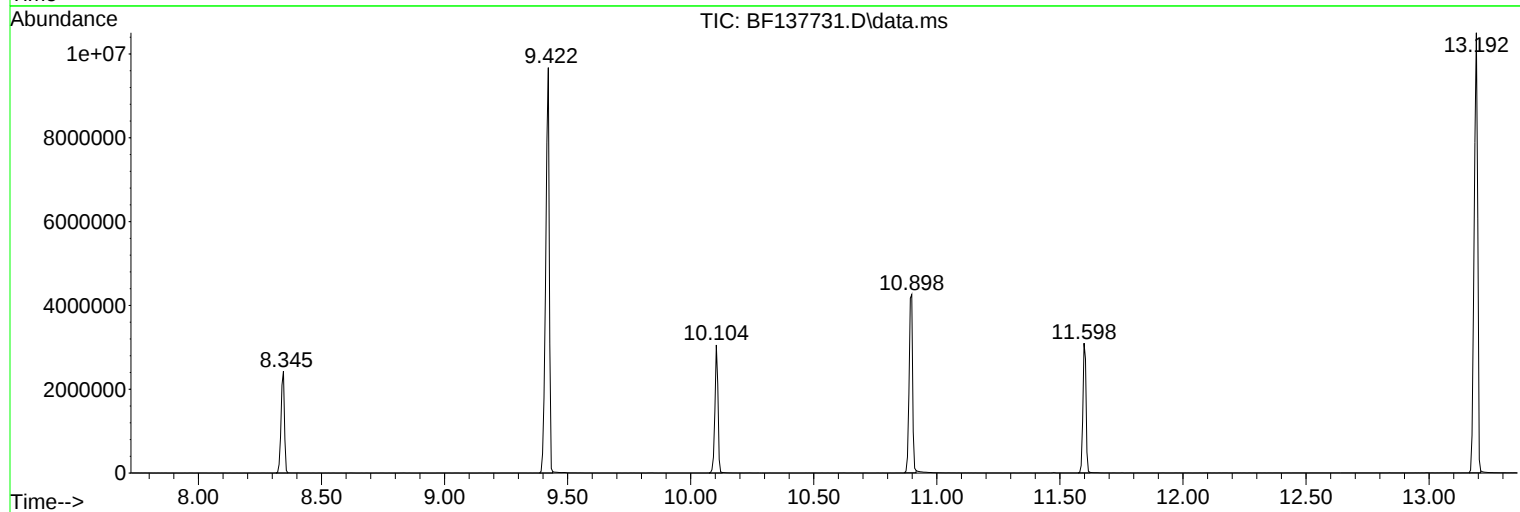
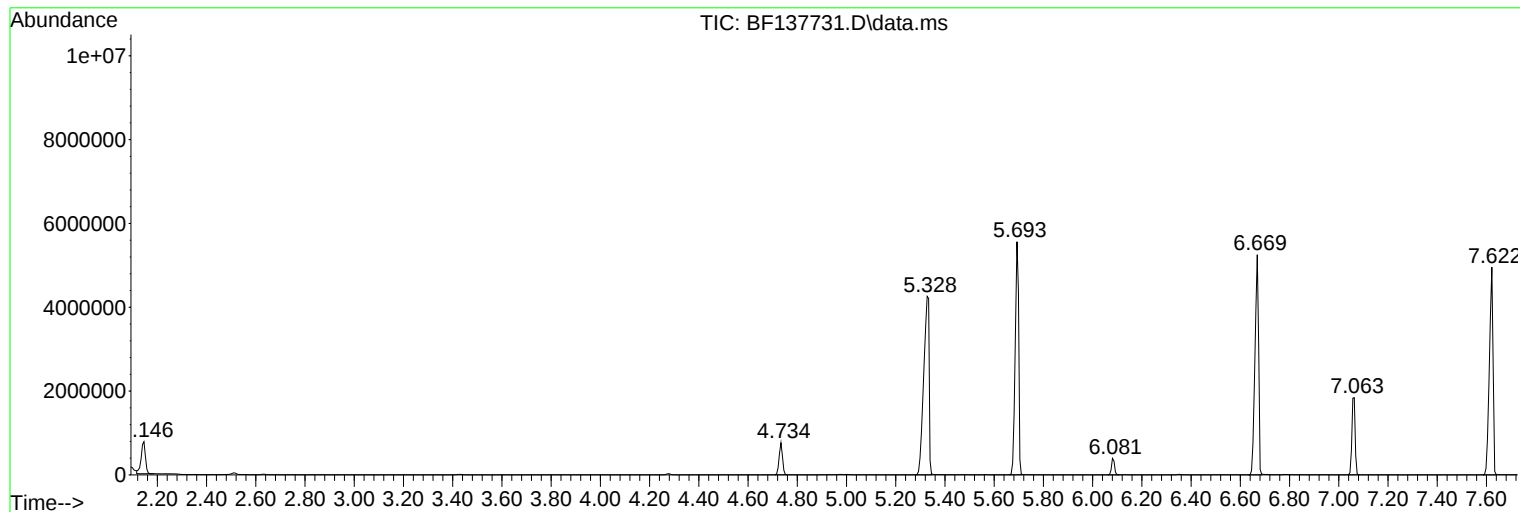
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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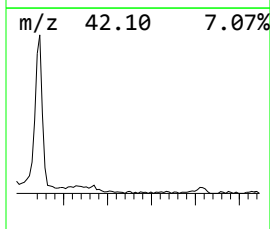
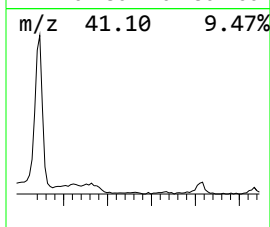
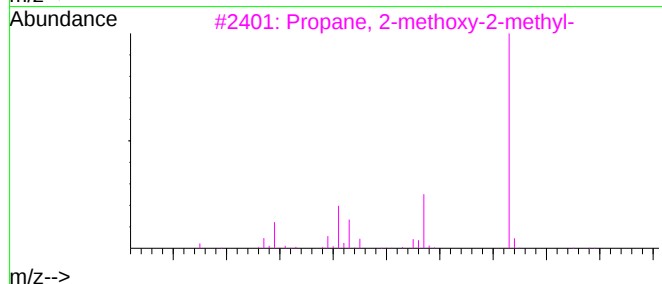
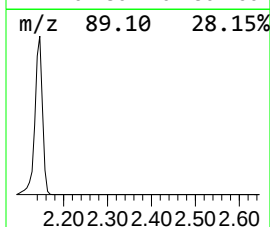
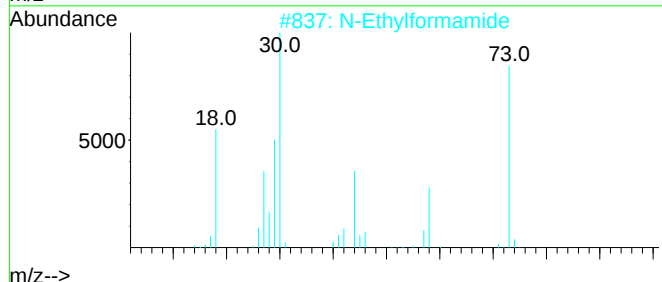
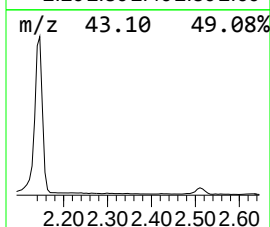
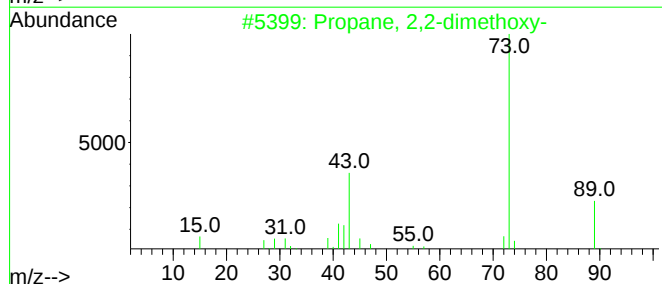
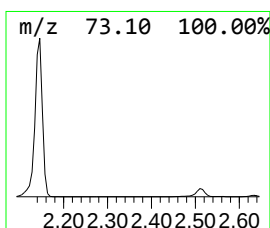
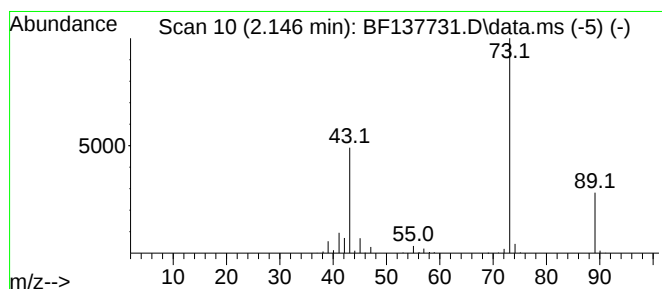
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown2.146 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	10.87 ng	917336	1,4-Dichlorobenzene-d4	7.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	45
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4	2-Acetamido-N-methylacetamide	130	C5H10N2O2	007606-79-3	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9



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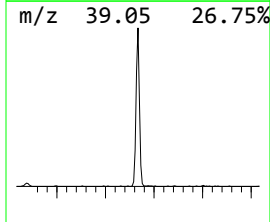
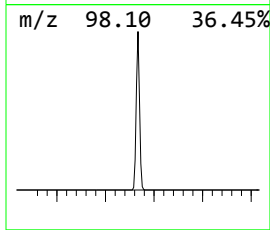
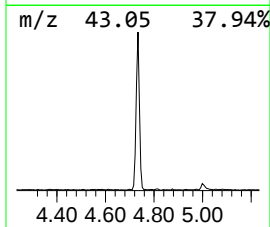
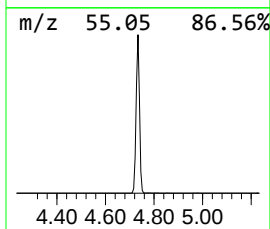
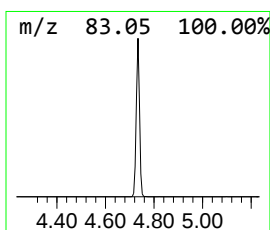
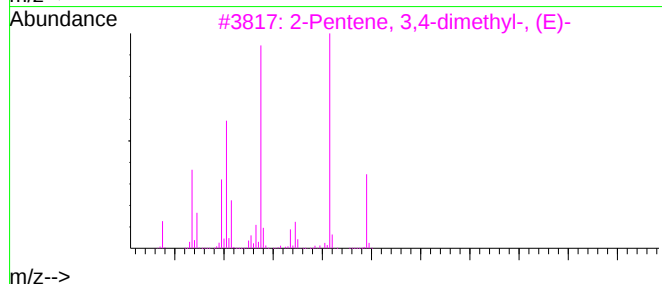
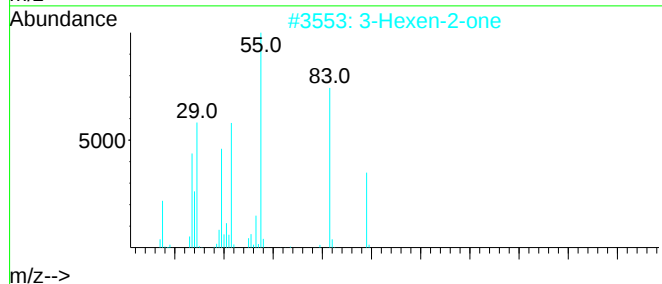
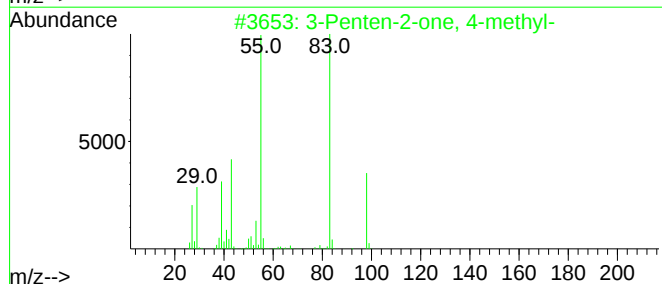
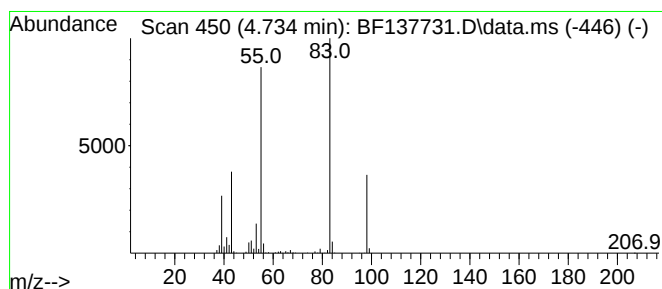
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.734	8.48 ng	716103	1,4-Dichlorobenzene-d4	7.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2	3-Hexen-2-one	98	C6H10O	000763-93-9	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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

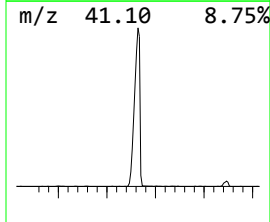
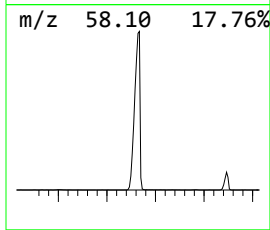
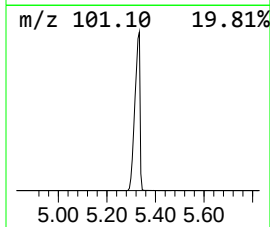
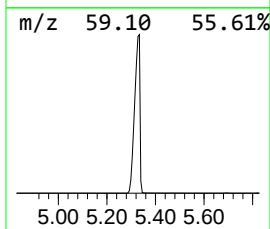
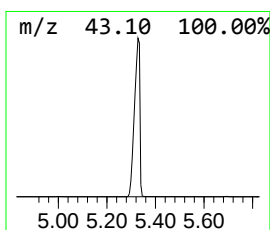
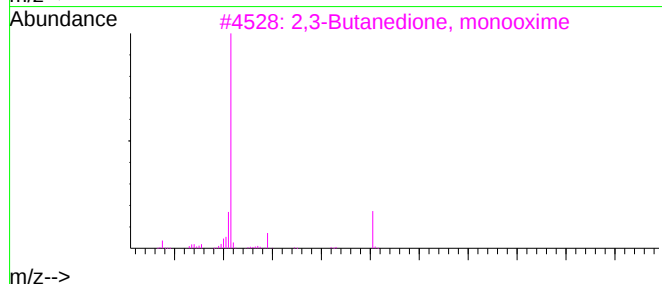
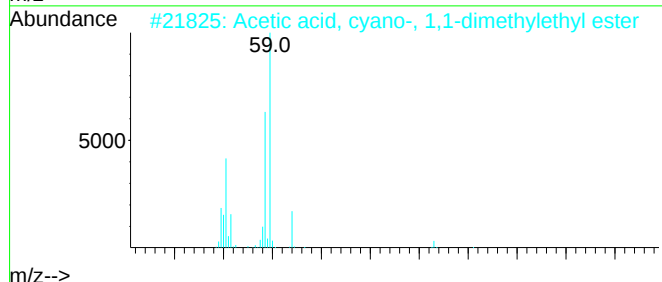
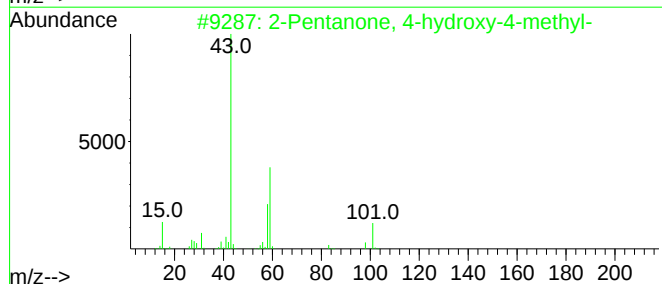
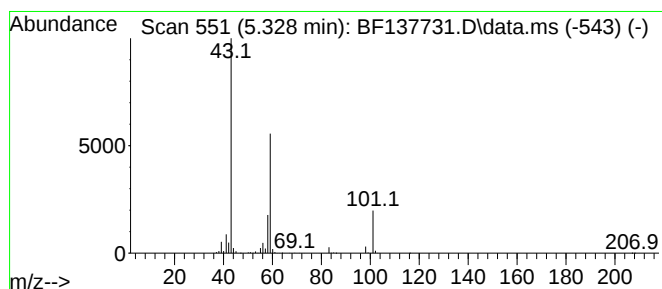
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.328	77.43 ng	6537180	1,4-Dichlorobenzene-d4	7.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
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	10
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9



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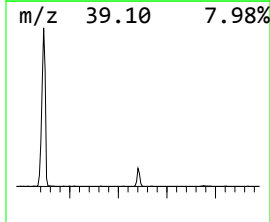
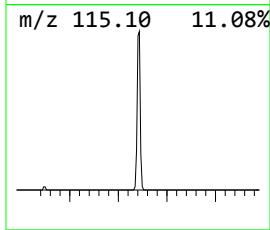
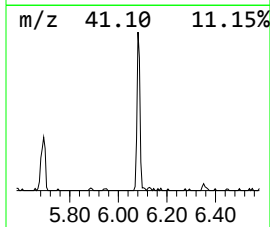
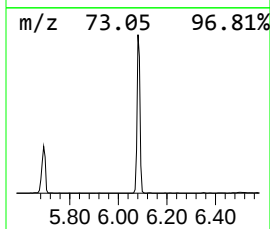
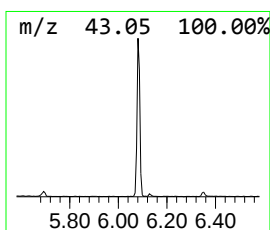
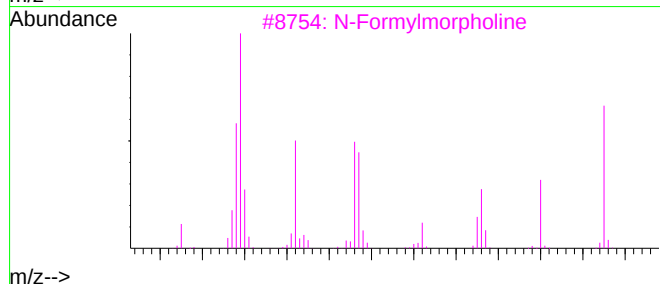
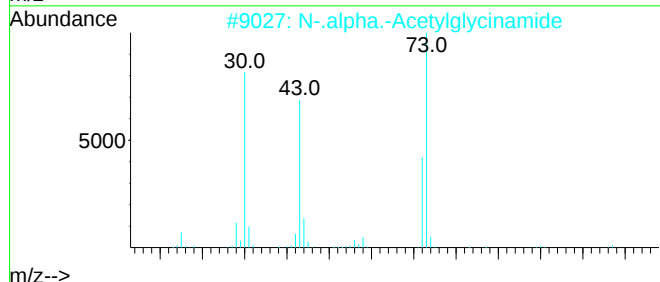
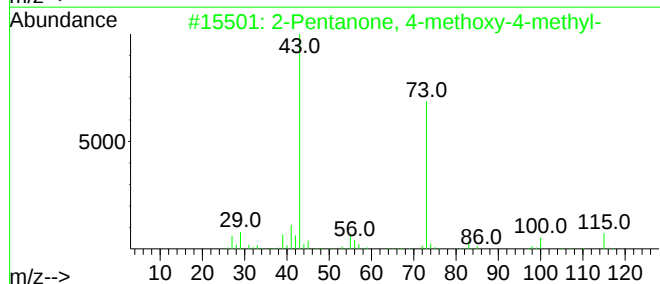
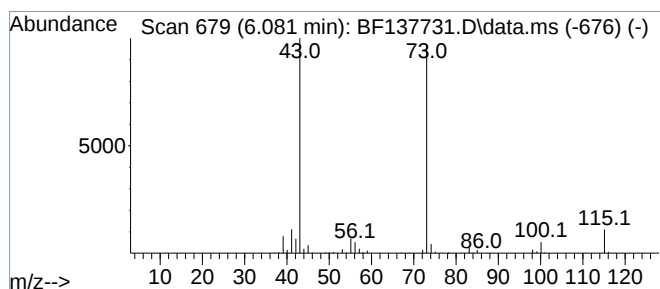
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.081	3.82 ng	322654	1,4-Dichlorobenzene-d4	7.063

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	N-Formylmorpholine	115	C5H9NO2	004394-85-8	10
4	Morpholine, 2,6-dimethyl-	115	C6H13NO	000141-91-3	9
5	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown2.146	2.146	10.9	ng	917336	1	7.063	1688590	20.0
3-Penten-2-one,...	4.734	8.5	ng	716103	1	7.063	1688590	20.0
2-Pentanone, 4-...	5.328	77.4	ng	6537180	1	7.063	1688590	20.0
2-Pentanone, 4-...	6.081	3.8	ng	322654	1	7.063	1688590	20.0