

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100121\
 Data File : BF125758.D
 Acq On : 1 Oct 2021 18:15
 Operator : JU/CG
 Sample : M3999-06
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 26498

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 1 % 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-BF092421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125758.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.905	134	139	147	rVB	417341	574136	8.98%	1.476%
2	3.781	283	288	295	rVB	53465	68781	1.08%	0.177%
3	4.710	441	446	452	rBV	643864	667608	10.44%	1.716%
4	4.775	453	457	462	rBV	77575	77573	1.21%	0.199%
5	5.122	505	516	518	rBV	387895	494864	7.74%	1.272%
6	5.146	518	520	524	rVB	429199	366354	5.73%	0.942%
7	5.516	578	583	586	rBV	4665803	4794068	74.97%	12.321%
8	6.510	747	752	755	rBV	4104196	4275291	66.86%	10.988%
9	6.887	813	816	819	rBV	1522658	1144157	17.89%	2.941%
10	7.445	906	911	914	rBV	3412799	3459076	54.09%	8.890%
11	8.169	1030	1034	1037	rBV	1844038	1598188	24.99%	4.107%
12	9.245	1212	1217	1220	rBV	6870075	6394777	100.00%	16.435%
13	9.922	1328	1332	1335	rBV	2233613	1793497	28.05%	4.609%
14	10.710	1461	1466	1469	rBV	4203099	3849287	60.19%	9.893%
15	11.404	1580	1584	1588	rBV	2020972	1675602	26.20%	4.306%
16	12.992	1849	1854	1857	rBV	5752054	5222431	81.67%	13.422%
17	14.039	2028	2032	2041	rBV	1230683	1120166	17.52%	2.879%
18	15.515	2278	2283	2294	rBV	980634	1333511	20.85%	3.427%

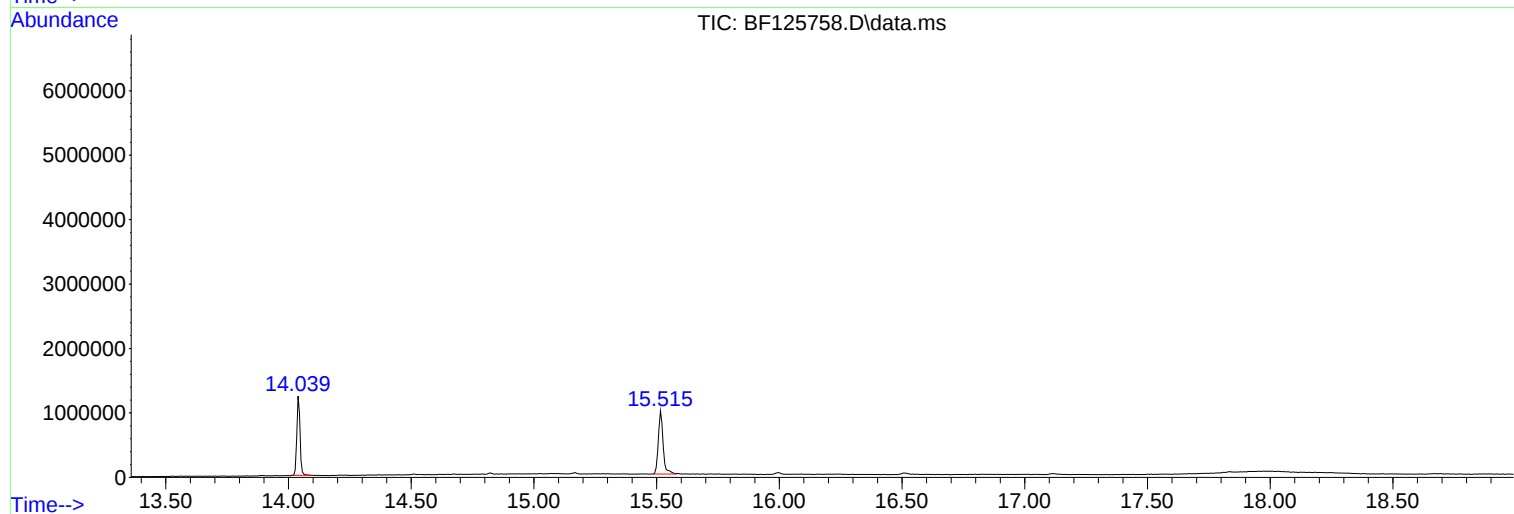
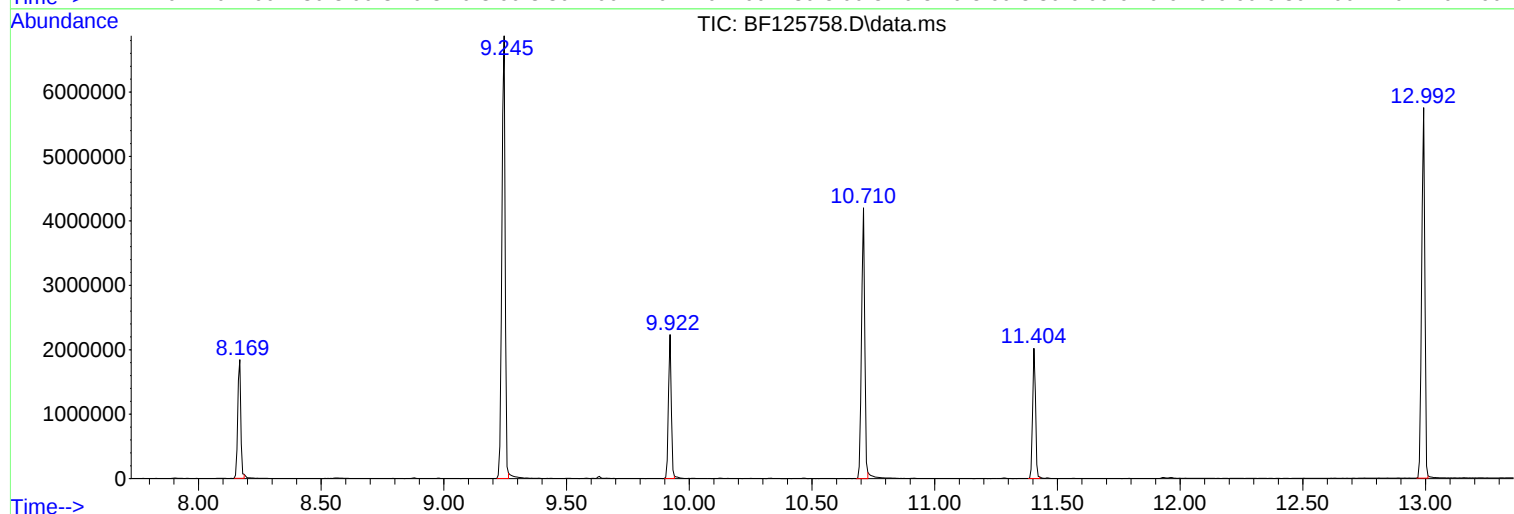
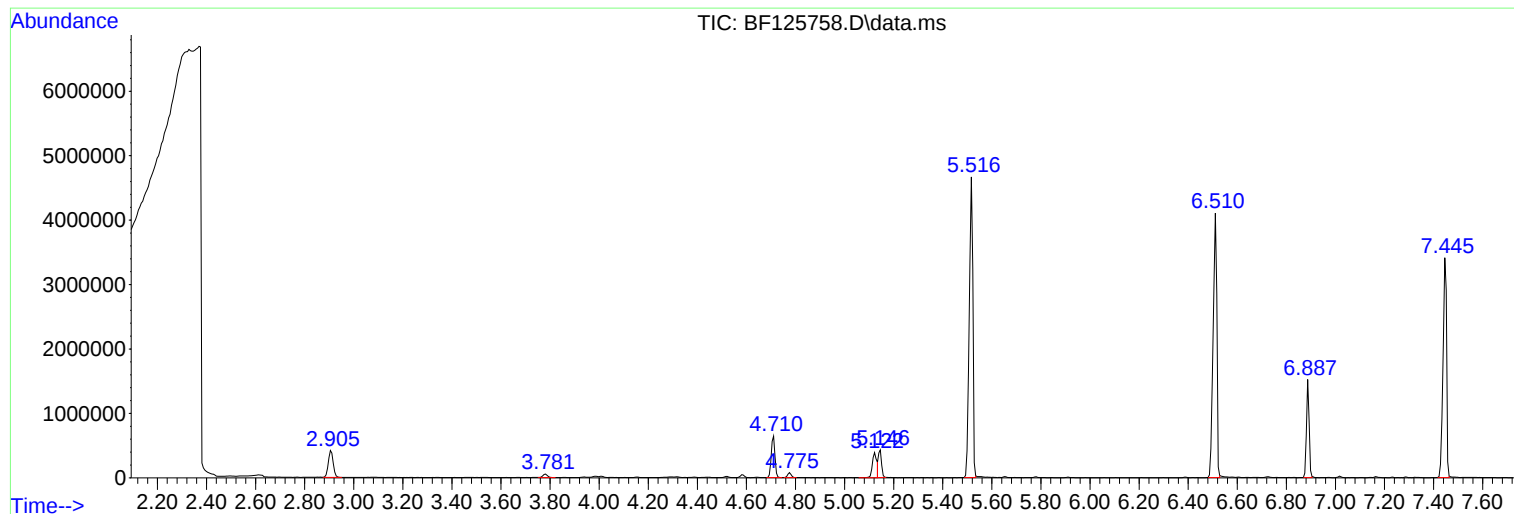
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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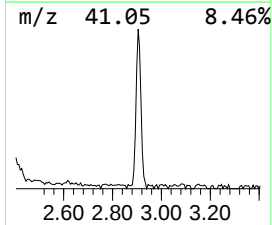
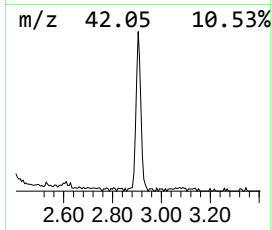
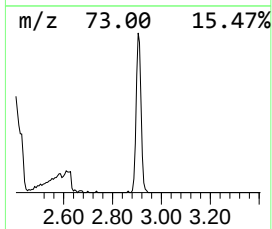
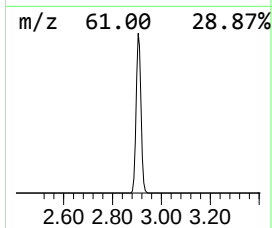
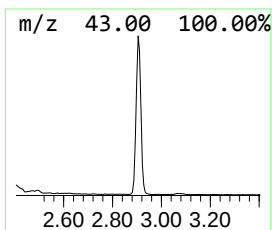
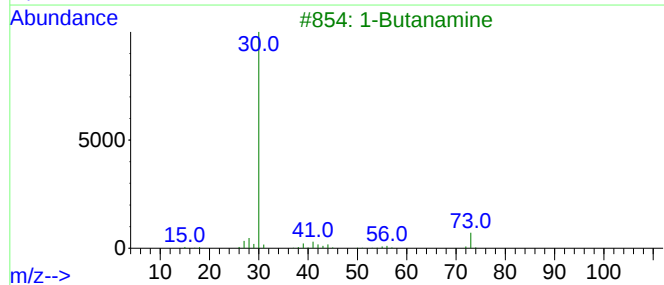
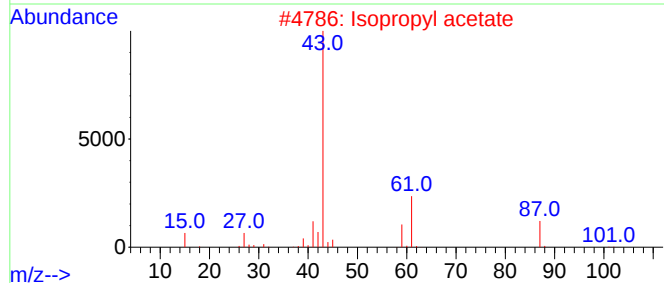
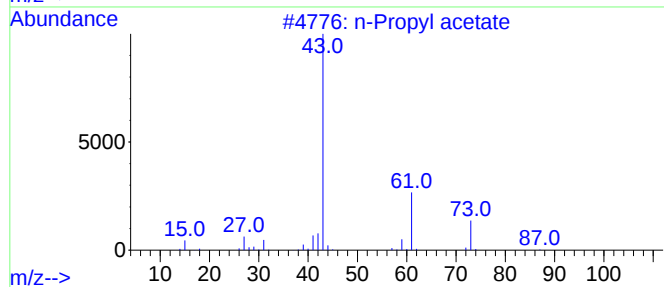
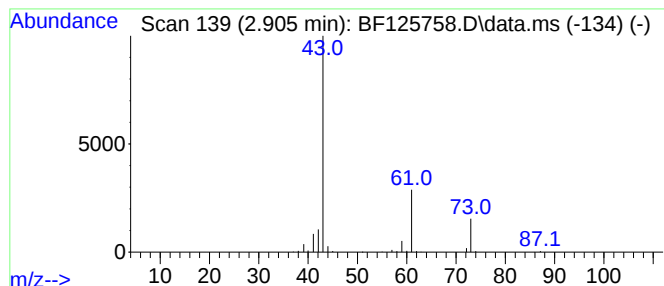
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.905	10.04 ng	574136	1,4-Dichlorobenzene-d4	6.887

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Propyl acetate	102	C5H10O2	000109-60-4	83
2		Isopropyl acetate	102	C5H10O2	000108-21-4	36
3		1-Butanamine	73	C4H11N	000109-73-9	7
4		Pentane	72	C5H12	000109-66-0	5
5		Isobutylamine	73	C4H11N	000078-81-9	5



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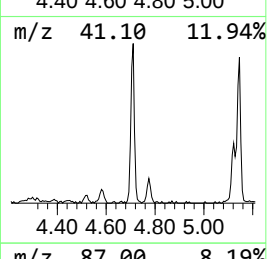
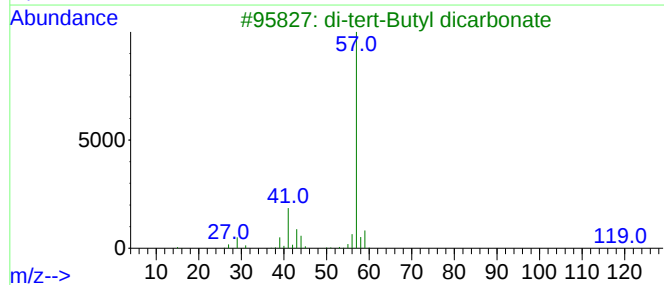
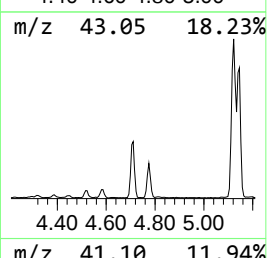
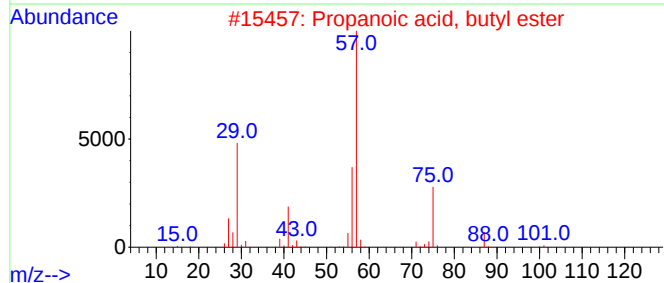
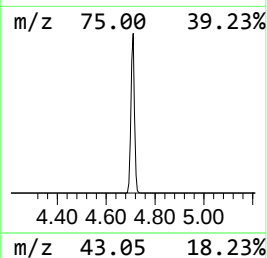
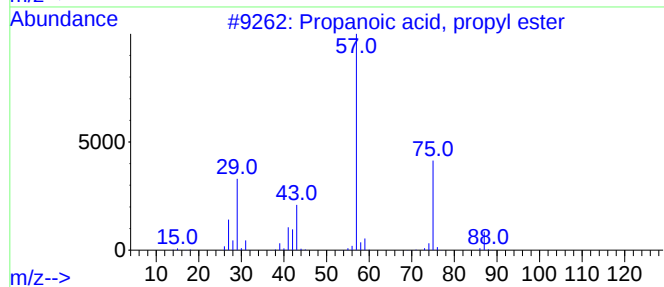
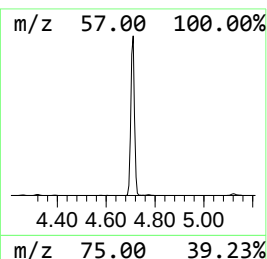
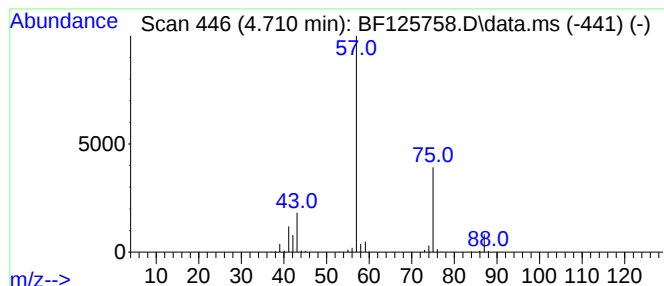
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.710	11.67 ng	667608	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	39
3			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
4			2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
5			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	5



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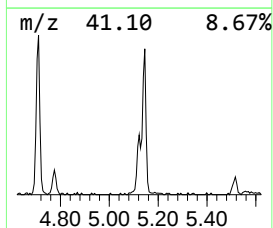
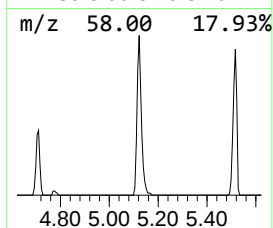
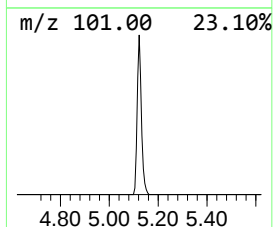
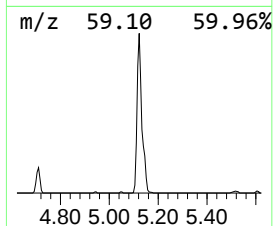
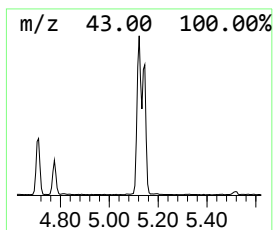
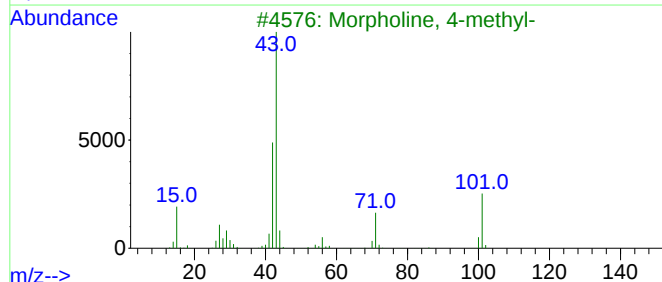
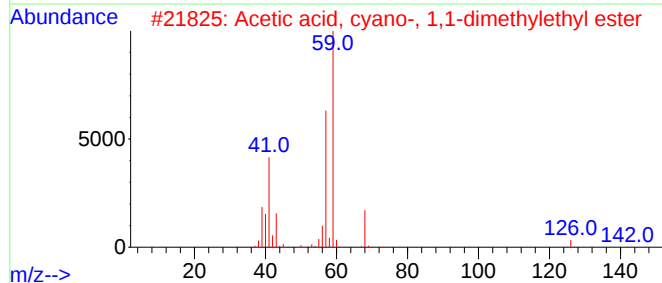
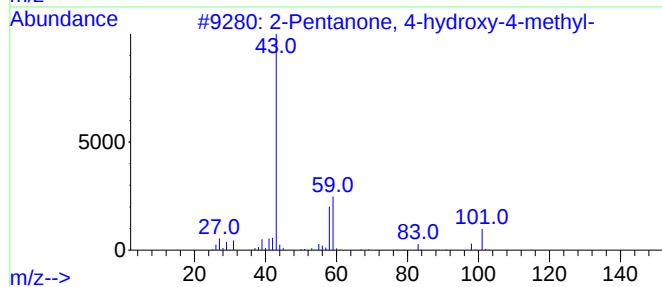
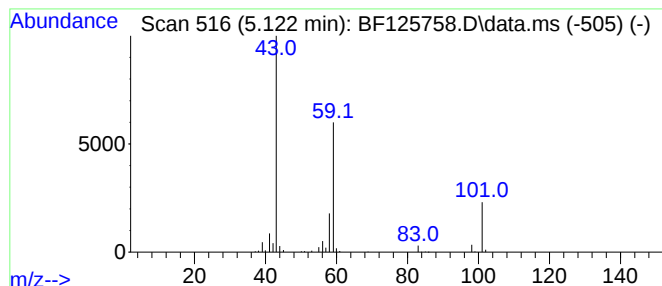
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.122	8.65 ng	494864	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Acetone	58	C3H6O	000067-64-1	9



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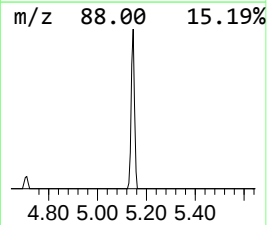
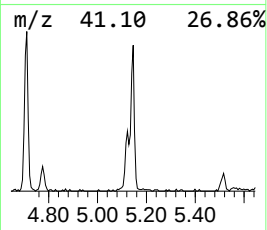
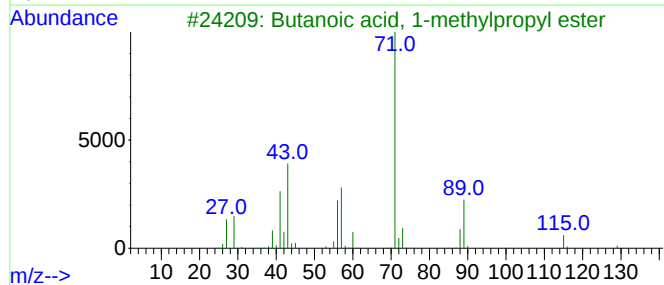
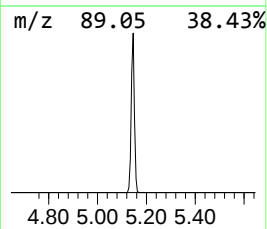
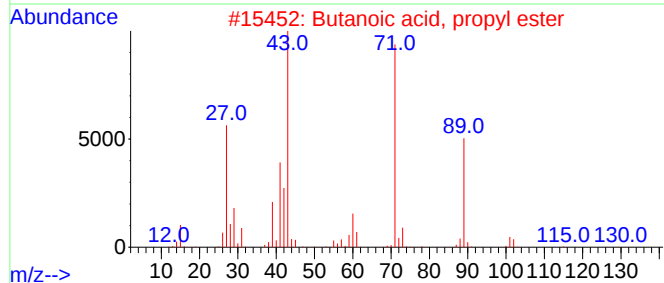
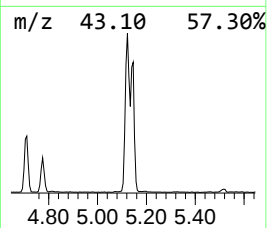
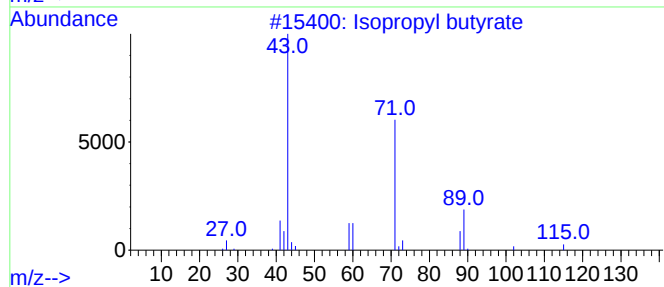
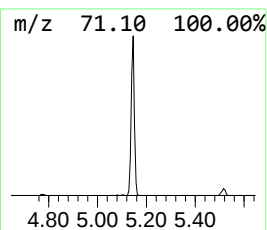
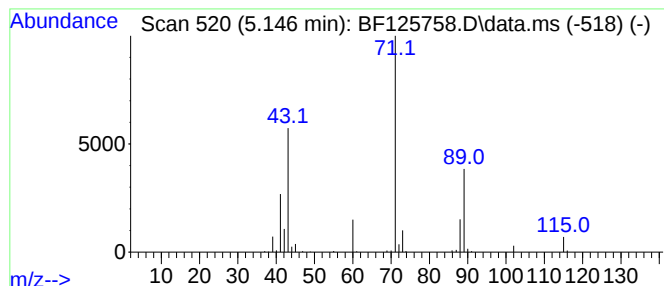
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Peak Number 4 Isopropyl butyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.146	6.40 ng	366354	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	83
2			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	53
3			Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	50
4			Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	43
5			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	40



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	2.905	10.0	ng	574136	1	6.887	1144160	20.0
Propanoic acid,...	4.710	11.7	ng	667608	1	6.887	1144160	20.0
2-Pentanone, 4-...	5.122	8.7	ng	494864	1	6.887	1144160	20.0
Isopropyl butyrate	5.146	6.4	ng	366354	1	6.887	1144160	20.0