Electronic Supplementary Material (ESI) for Analyst.

Electronic Supplementary Information

Assessing the efficiency of supercritical fluid extraction for the decontamination of archaeological bones prior to radiocarbon dating

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1. EGA and Py-GC/MS of reference materials

1.1 EGA-MS analysis of Butvar B98 ™ (Polyvinyl Butyral)

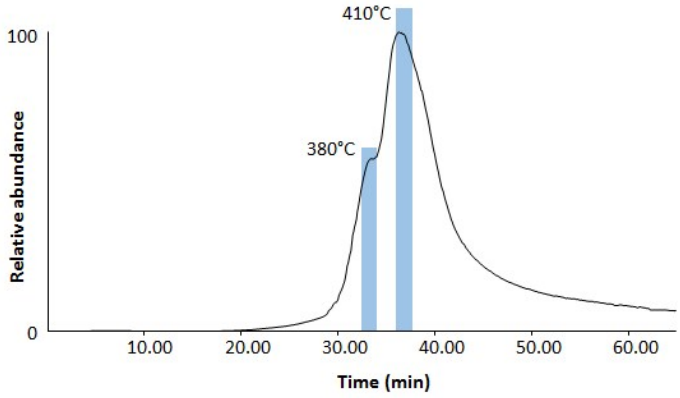

Figure S1: Total Ion Thermogram (TIT) of Butvar B98 ™.

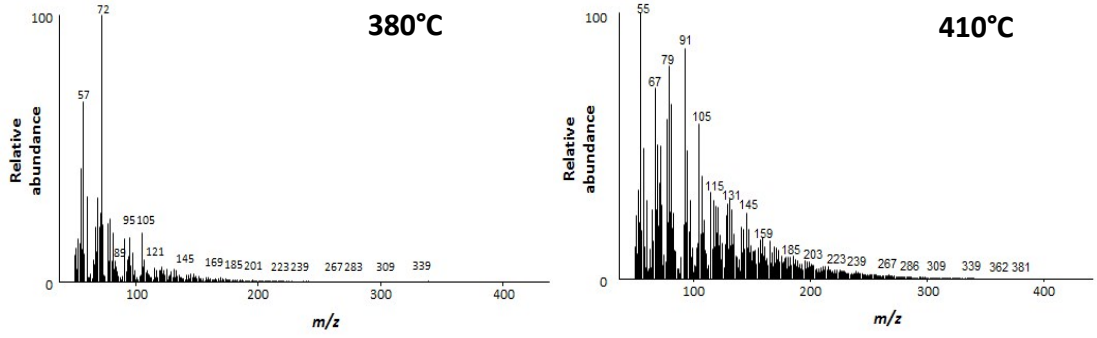

Figure S2: Mass spectra of Butvar B98 ™ at at the temperatures indicated and highlighted in Fig. S1.

1.2 EGA-MS analysis of Paraloid B72 ™

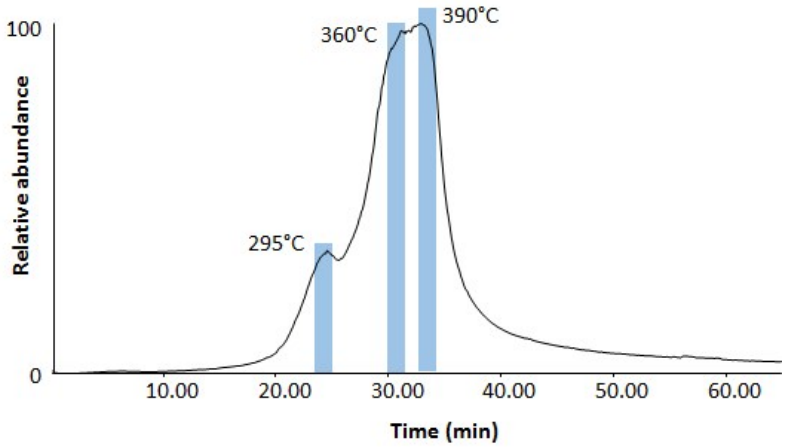

Figure S3: Total Ion Thermogram (TIT) of Paraloid B72 ™.

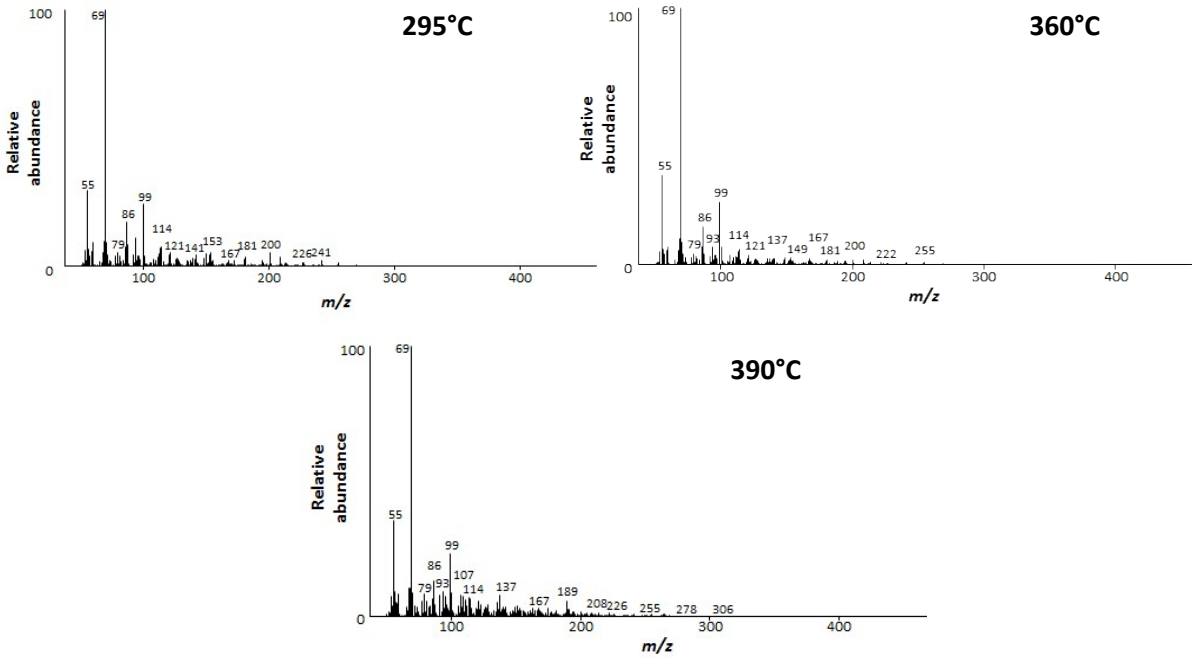

Figure S4: Mass spectra of Paraloid B72 ™ at the temperatures indicated and highlighted in Fig. S3.

1.3 EGA-MS analysis of Polyvinyl acetate

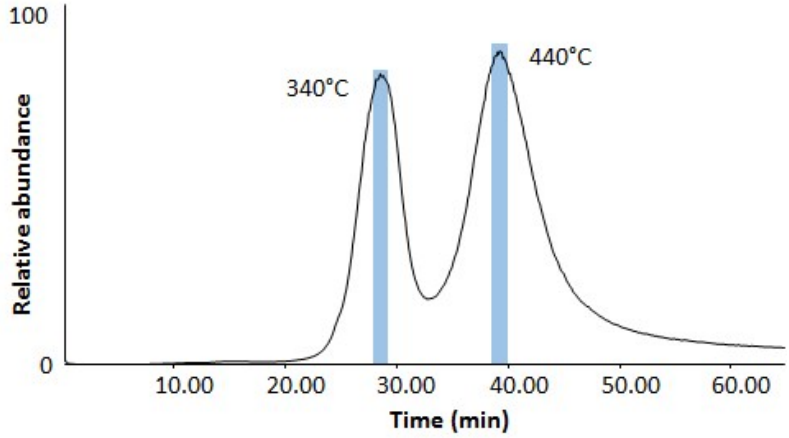

Figure S5: Total Ion Thermogram (TIT) of Polyvinyl acetate.

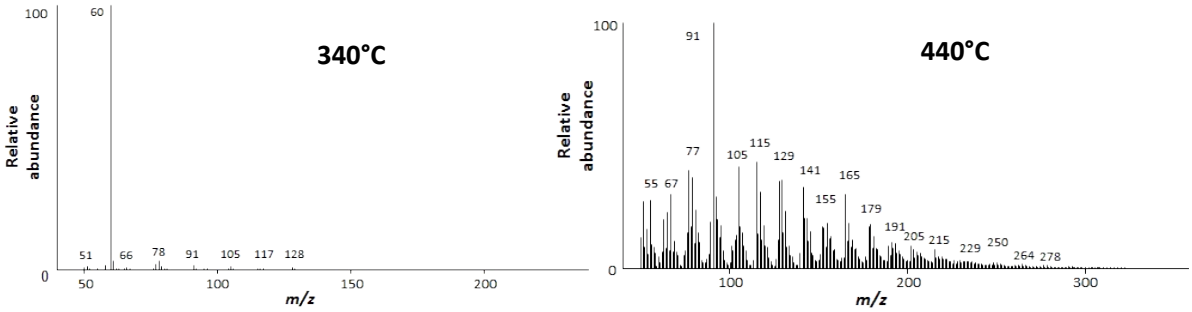

Figure S6: Mass spectra of Polyvinyl acetate at the temperatures indicated and highlighted in Fig. S5.

1.4 EGA-MS analysis of Animal glue

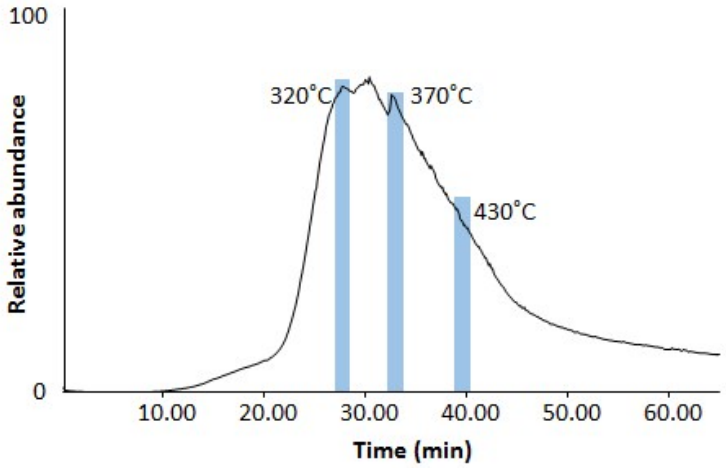

Figure S7: Total Ion Thermogram (TIT) of animal glue.

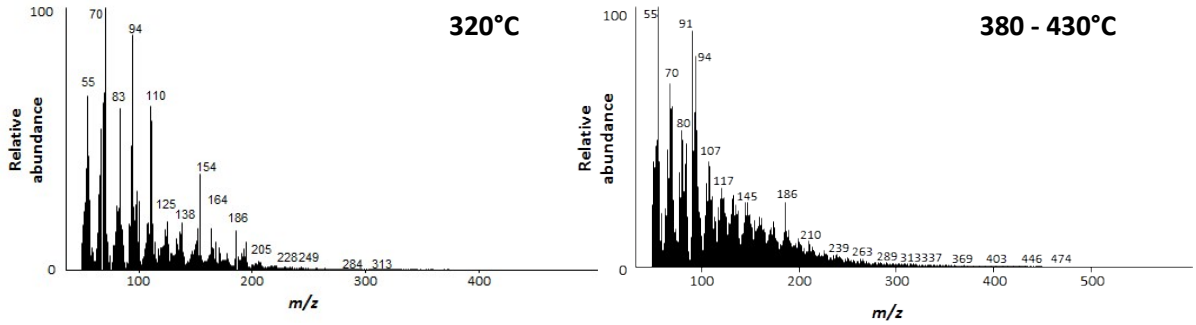

Figure S8: Mass spectra of animal glue at the temperatures indicated and highlighted in Fig. S7.

1.5 Py-GC/MS of Butvar B98 ™

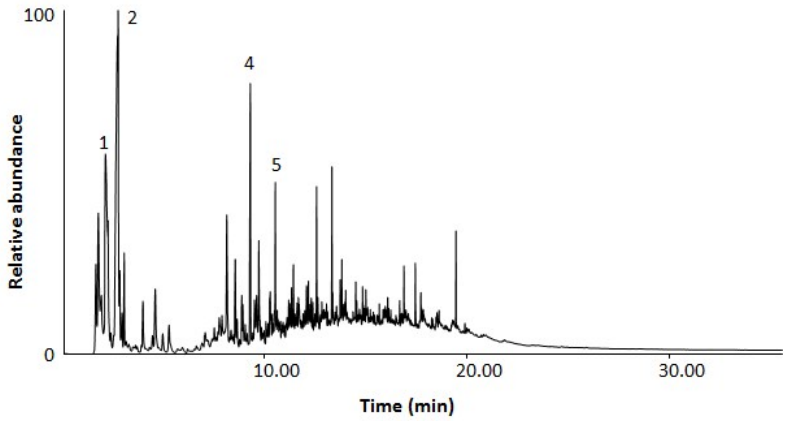

Figure S9: Total Ion Chromatogram (TIC) of Butvar B98 ™ obtained by Py-GC/MS. Peaks are numbered according to Table S1

Table S1: Principal pyrolysis products of Butvar B98 ™ obtained by Py-GC/MS.

	Compound	R_t (min)	m/z
1	Butanal	2,1	**72**, 57
2	Crotonaldehyde	2,7	**70**, 55
4	Benzaldehyde	9,3	106, 95, **77**, 74, 51
5	Acetophenone	10,5	120, **105**, 91, 77, 74, 51

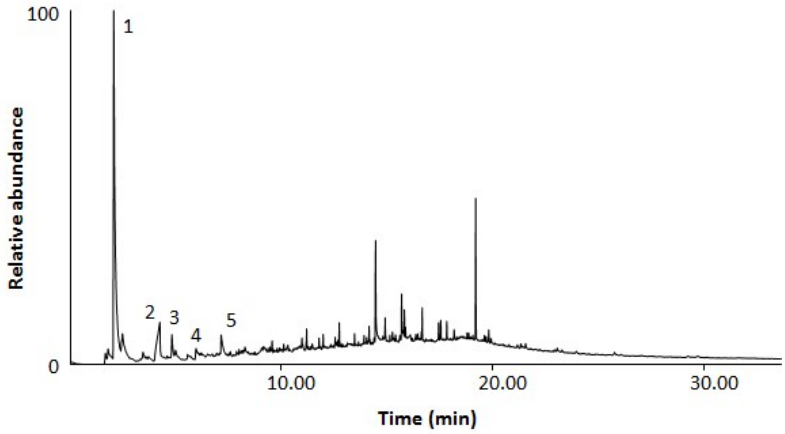

Figure S10: Total Ion Chromatogram (TIC) of Butvar B98 ™ obtained by Py-GC/MS using the micro reaction sampler. Peaks are numbered according to Table S2.

Table S2: Principal pyrolysis products of Butvar B89 obtained by Py-GC/MS using the micro reaction sampler.

	Compound	R_t (min)	m/z
1	Butanal	2,1	**72**, 57
2	Crotonaldehyde	2,7	**70**, 55
3	Butanoic Acid	4,3	94, 88, 73, **60**
4	Benzaldehyde	6,1	106, 95, **77**, 74, 51
5	Acetophenone	7,2	120, **105**, 91, 77, 74, 51

1.6 Py-GC/MS of Paraloid B72 ™

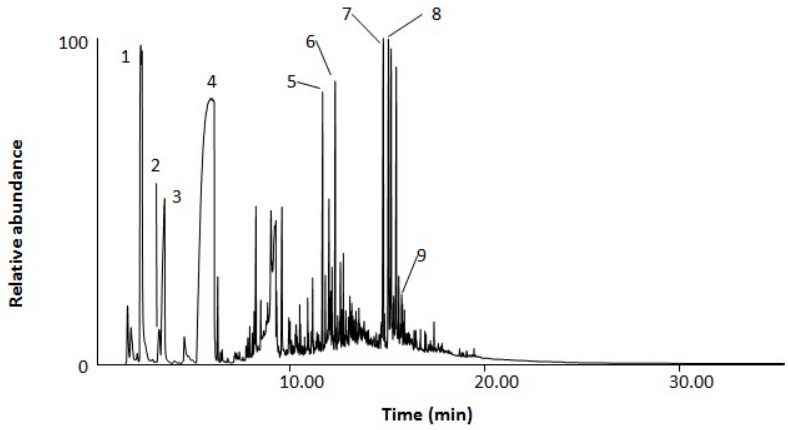

Figure S11: Total Ion Chromatogram (TIC) of Paraloid B72 ™ obtained by Py-GC/MS. Peaks are numbered according to Table S3.

Table S3: Principal pyrolysis products of Paraloid B72 ™ obtained by Py-GC/MS.

	Compound	Rt (min)	m/z	
1	MA	2,3	**55**	**Monomers**
2	EA	2,9	85, 73, **55**	
3	MMA	3,0	85, **69**, 59	
4	EMA	5,8	99, 86, **69**	
5	MA-MA	11,6	141, **110**, 81	**Dimers**
6	MA-EMA	12,3	169, 155, 126, **67**	
7	3MA	14,8	227, 196, 165, **134**, 106, 79	**Trimers**
8	2MA-EMA	15,0	255, 241, 224, 20,8, 152, **93**	
9	MA-2EMA	15,7	283, 269, 224, 200, **107**	

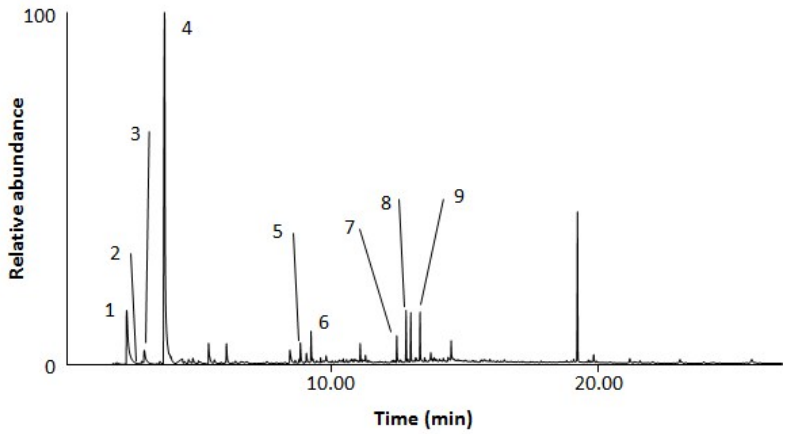

Figure S12 Total Ion Chromatogram (TIC) of Paraloid B72 ™ obtained by Py-GC/MS using the micro reaction sampler. Peaks are numbered according to Table S4.

Table S4: Principal pyrolysis products of Paraloid B72 ™ obtained by Py-GC/MS using the micro reaction sampler.

	Compound	Rt (min)	m/z	
1	Methyl acrylate (MA)	2,3	**55**	**Monomers**
2	Ethyl acrylate (EA)	2,9	85, 73, **55**	
3	Methyl methacrylate (MMA)	3,0	100, 85, **69**, 59	
4	Ethyl methacrylate (EMA)	3,7	99, 86, **69**	
5	MA-MA	8,8	141, **110**, 81	**Dimers**
6	MA-EMA	9,2	169, 155, **126**, 67	
7	3MA	12,4	227, 196, 165, **134**	**Trimers**
8	2MA-EMA	12,8	255, 241, 224, 208, 152, **93**	
9	MA-2EMA	13,3	283, 269, 224, **200**, 107	

1.7 Py-GC/MS of Polyvinyl Acetate

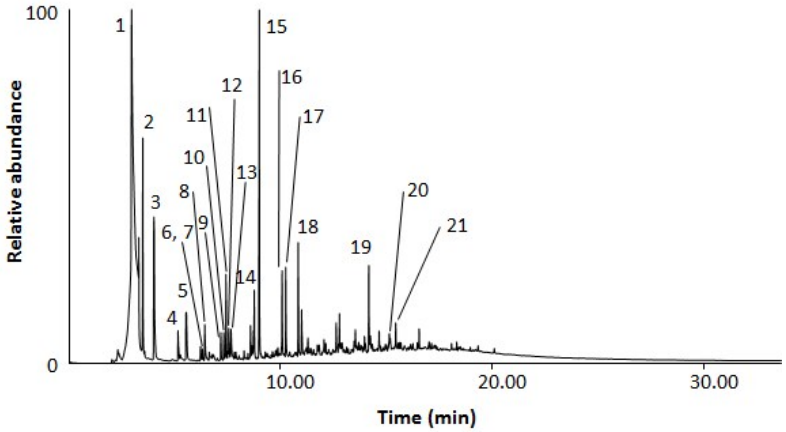

Figure S13: Total Ion Chromatogram (TIC) of polyvinyl acetate obtained by Py-GC/MS using the micro reaction sampler. Peaks are numbered according to Table S5.

Table S5: Principal pyrolysis products of polyvinyl acetate obtained by Py-GC/MS using the micro reaction sampler.

	Compound	R_t (min)	m/z
1	Acetic Acid	3,4	60
2	Acetic Acid, (trimethylsilyl)-	3,6	117, **75**, 60
3	Toluene	4,1	**91**, 65, 51
4	Ethylbenzene	5,2	106, **91**, 77, 65
5	Styrene	5,6	**104**, 78, 63, 51
6	Propylbenzene	6,4	120, 105, **91**, 78, 65, 51
7	Benzaldehyde	6,5	**106**, 91, 77, 63, 51
8	Isopropylbenzene	6,7	120, **105**, 91, 77, 63, 51
9	1-propenylbenzene	7,2	**117**, 103, 91, 77, 65, 51
10	2-propenylbenzene	7,4	**117**, 103, 91, 77, 58, 51
11	1H-indene	7,5	**116**, 89, 74, 63
12	Acetic Acid, Phenyl Esther	7,6	116, **94**, 77, 66, 51
13	Acetophenone	7,7	120, **105**, 91, 77, 51
14	1-methyl-1H-indene	8,6	**130**, 115, 102, 89, 77, 64, 51
15	Naphtalene	9	**128**, 102, 87, 75, 64, 51
16	1-methylnaphtalene	10,1	**142**, 115, 102, 89, 71, 63, 51
17	2-methylnaphtalene	10,3	**142**, 115, 102, 89, 71, 57, 51
18	Biphenyl	10,9	**154**, 139, 128, 115, 102,76, 63, 51
19	Anthracene	14,2	**178**, 152, 89, 76, 63, 51
20	1-phenylnaphtalene	14,7	**204**, 101, 89, 76, 63, 51
21	2-methylanthracene	15,2	**192**, 165, 152, 115, 94, 82, 69, 51

1.8 Py-GC/MS of Animal Glue

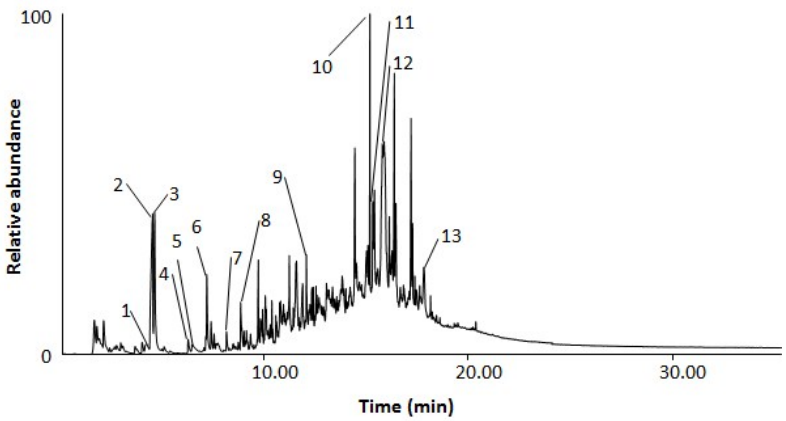

Figure S14: Total Ion Chromatogram (TIC) of animal glue obtained by Py-GC/MS using the micro reaction sampler. Peaks are numbered according to Table S5.. Peaks are numbered according to Table S6.

Table S6: Principal pyrolysis products of animal glue obtained by Py-GC/MS.

	Compound	**Rt (min)**	**m/z**
1	Pyridine	4,2	**79**, 52
2	Pyrrole	4,5	**67**
3	Toluene	4,6	**91,** 65, 51
4	1-ethyl-1H-pyrrole	6,2	95, **80**, 67, 53
5	2-methylpyridine	6,5	**93**, 78, 66, 51
6	2-methyl-1H-pyrrole	7,2	**80**, 53
7	Styrene	8,1	**104**, 71, 51
8	2-ethyl-1H-pyrrole	8,8	95, **80**, 53
9	Benzenepropanenitrile	12	**91**, 131
10	Diketodipyrrole	15,1	**186**, 130, 93, 65
11	Cyclo (Pro-Ala)	15,3	168, 125, 97, **70**
12	Cyclo (Pro-Gly)	15,8	154, 111, **83**, 70
13	Cyclo (Pro-Hyp)	17,8	210, 124, 86, **70**

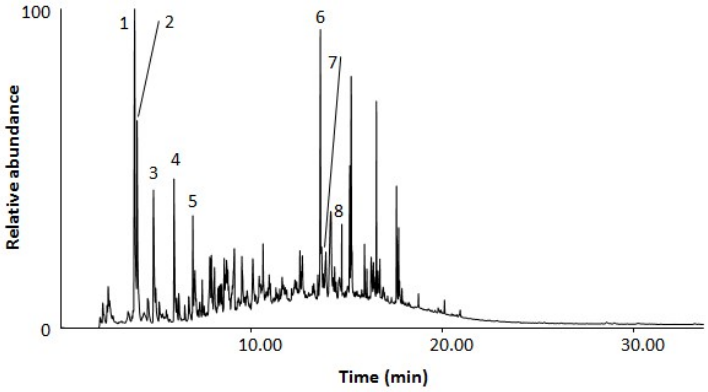

Figure S15: Total Ion Chromatogram (TIC) of animal glue obtained by Py-GC/MS using the micro reaction sampler. Peaks are numbered according to Table S7.

Table S7: Principal products of pyrolysis obtained by Py-GC/MS of animal glue using the micro reaction sampler.

	Compound	Rt (min)	m/z
1	Pyrrole	4,0	**67**
2	Toluene	4,1	**91**, 65, 51
3	3-methyl-1H-pyrrole	4,9	**80**, 53
4	2-ethyl-1H-pyrrole	6,0	**95**, 80, 53
5	5-methyl-2(1H)-pyridinone	7,0	109, **80**, 53
6	Diketodipyrrole	13,6	**186**, 130, 93, 65
7	Cyclo (Pro-Ala)	13,9	168, 125, 97, **70**
8	Cyclo (Pro-Gly)	14,2	154, 111, **83**, 70

2) Py-GC/MS data on archaeological samples

The pyrolysis data and radiocarbon data obtained on all the archaeological samples is archived at the University of Pisa and the University of Oxford, respectively. It can be accessed on request by contacting the authors of the article.