Supplemental Information:

Sequencing Biodegradable and Potentially Biobased Polyesteramide of Sebacic Acid and 3-Amino-1-Propanol by MALDI TOF-TOF Tandem Mass Spectrometry

Paola Rizzarelli [1,*], Stefania La Carta [2], Emanuele Francesco Mirabella [1], Marco Rapisarda [1] and Giuseppe Impallomeni [1]

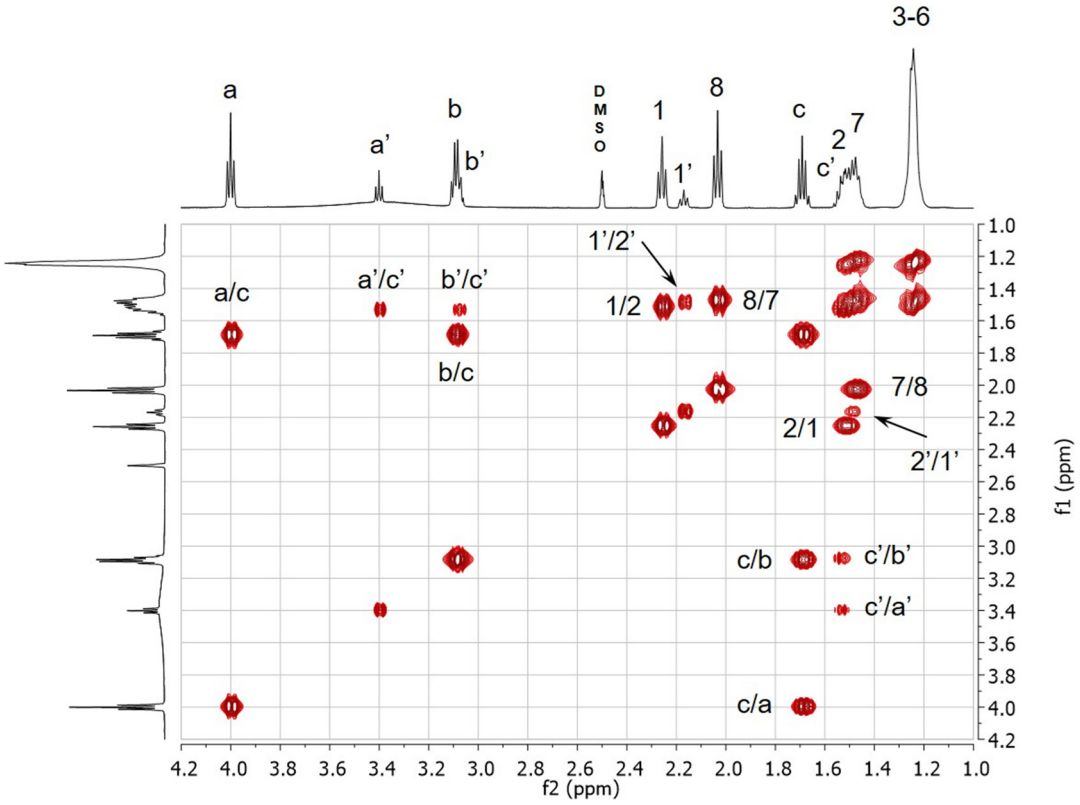


Figure S1. Partial g-COSY spectrum of PEA-Pro in 6d-DMSO at 50 °C showing the 4.2 – 1.0 ppm range.

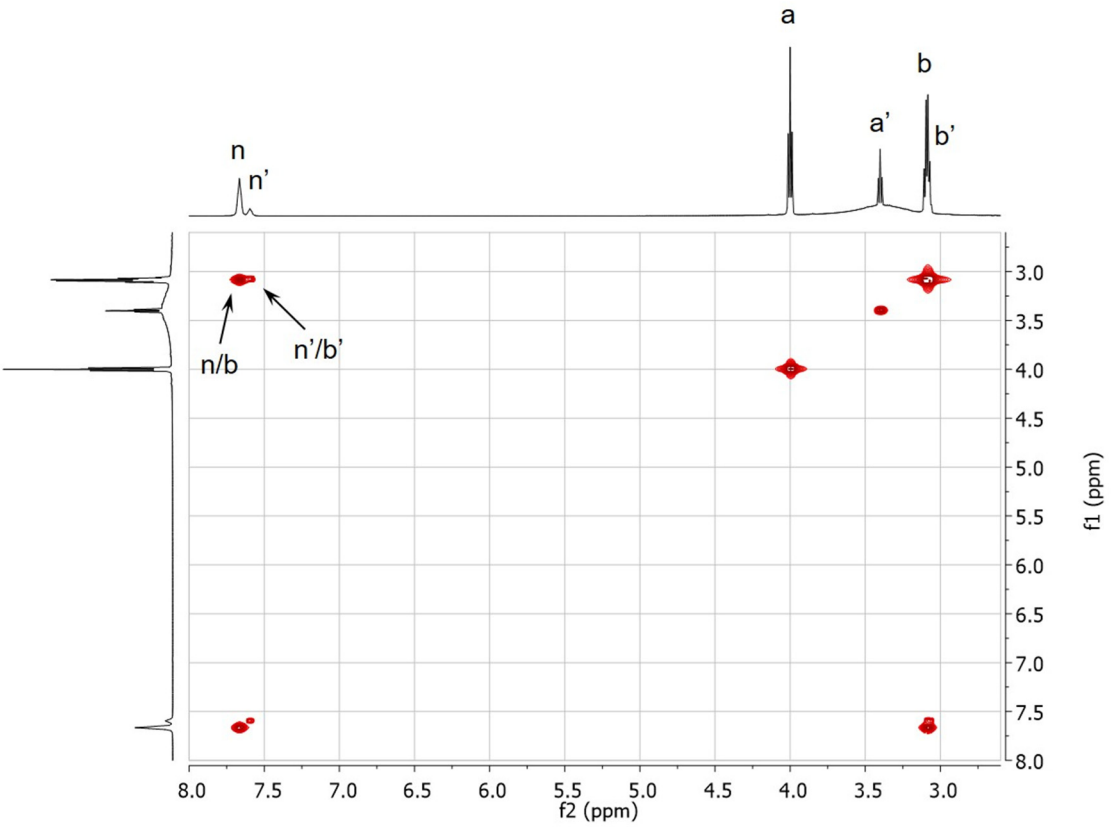


Figure S2. Partial g-COSY spectrum of PEA-Pro in 6d-DMSO at 50°C showing the 8.0 – 2.6 ppm range.

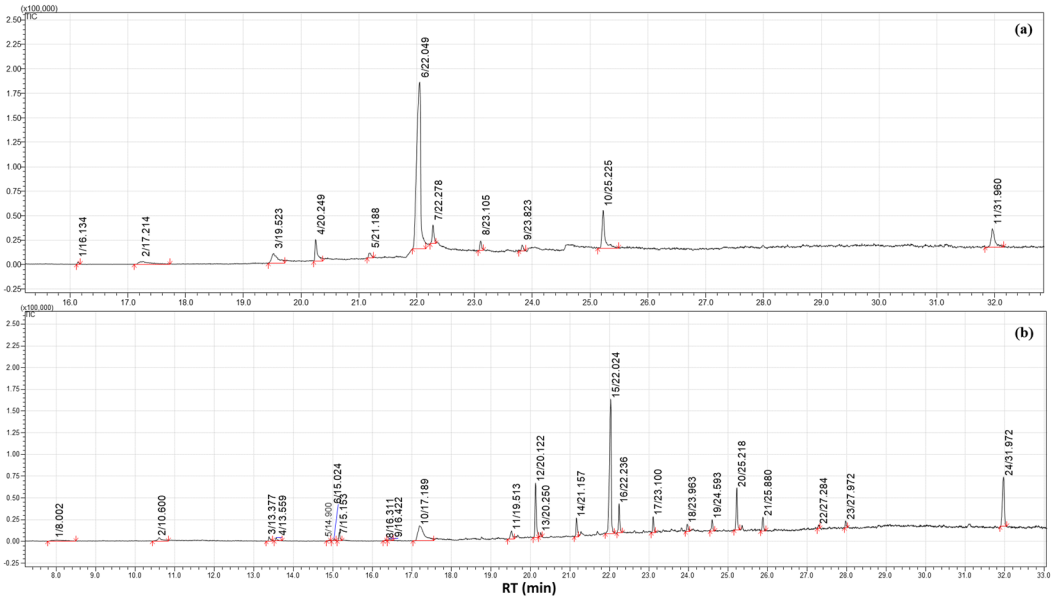
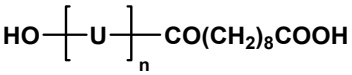
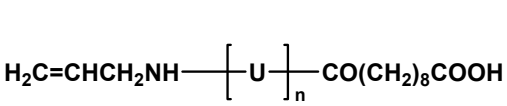
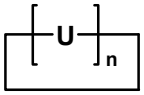
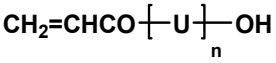
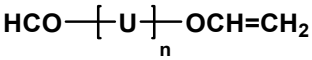
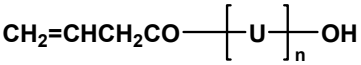


Figure S3. Total ion current (TIC) trace of pyrolysis products of PEA-Pro at **(a)** 350 °C and **(b)** 400 °C.

Table S1. Structure assignments of product ions appearing in the MALDI-TOF/TOF-MS/MS spectra of the PEA-Pro sample (precursor ions at *m*/*z* 1189.8, 1228.8, 1246.8 and 1303.9).

Structure	n	[M+Na$^+$]	[M+H$^+$]
	4	1189.78	
	3	948.61	
	2	707.44	/
	1	466.27	
	0	225.10	
	4	1228.83	
	3	987.66	
	2	746.48	/
	1	505.32	
	0	264.18	
	5	1228.83	
	4	987.66	
	3	746.48	
	2	505.32	
	1	264.18	242.18
	4	1059.83	
	3	818.50	
	2	577.37	/
	1	336.21	
	0	95.04	
			
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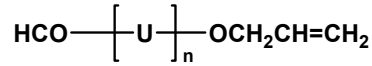
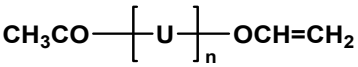
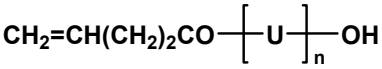
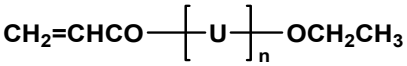
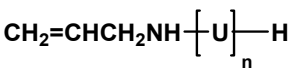
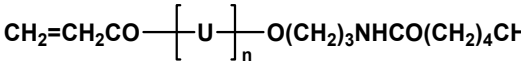
	2	591.35	/
	1	350.18	
	0	109.01	
			
	3	846.82	
	2	605.63	
	1	364.34	/
	0	123.09	
	4	1044.63	1022.62
	3	803.52	781.48
	2	562.38	540.40
	1	321.22	299.23
	0	80.59	58.04
	2	744.47	
	1	503.30	/
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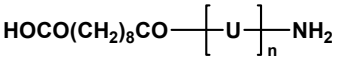
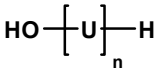
	1	465.30	
	0	224.15	/
	3	1005.68	
	2	764.50	/
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	4	1172.80	
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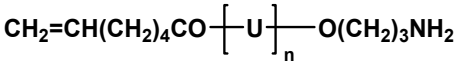
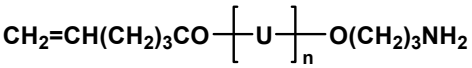
	2	690.53	/
	1	449.33	
	0	208.10	
			
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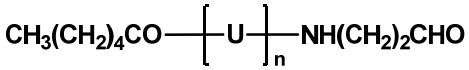
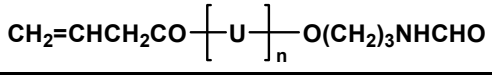
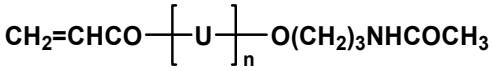
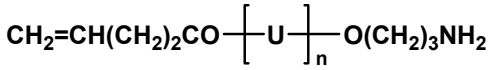
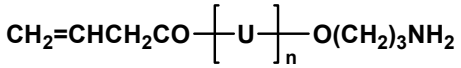
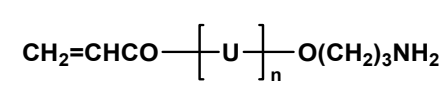
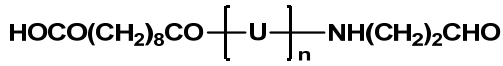
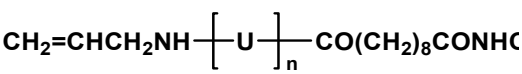
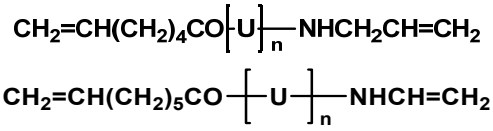
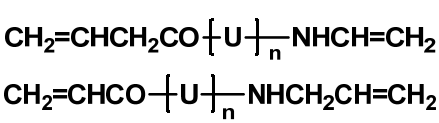
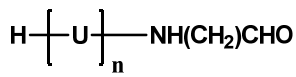
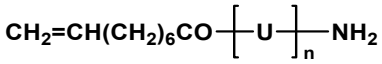
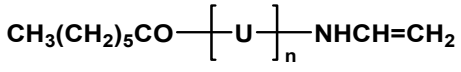
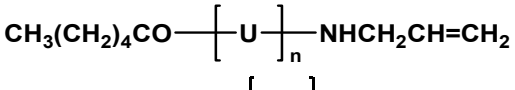
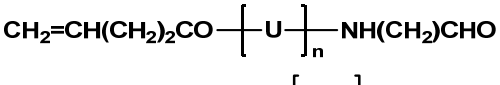
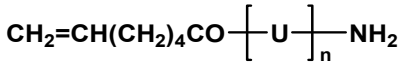
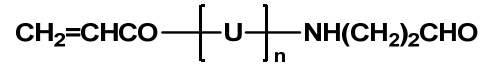
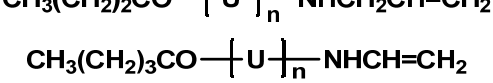
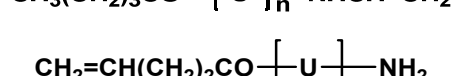
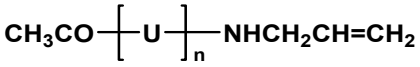
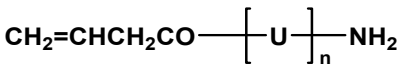
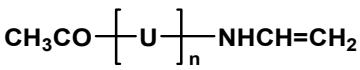
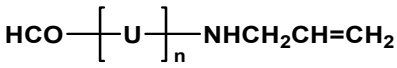
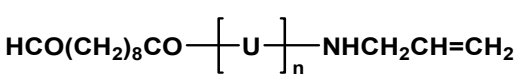
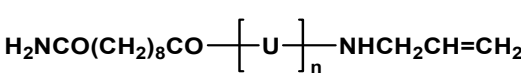
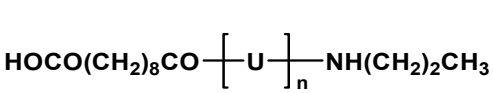
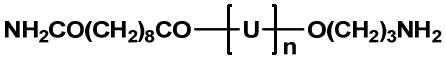
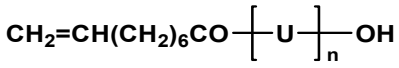
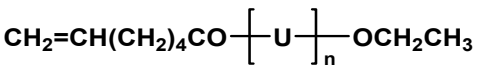
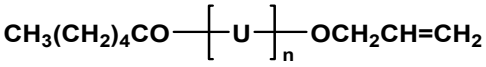
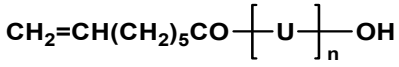
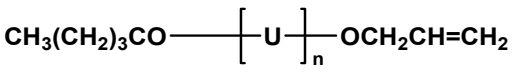
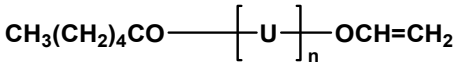
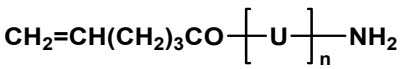
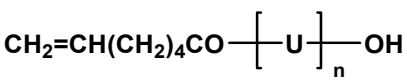
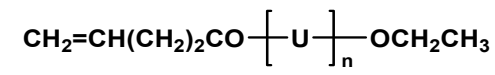
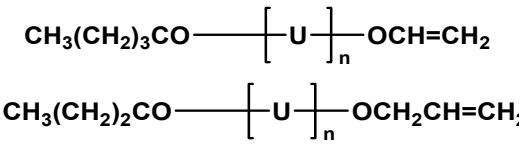
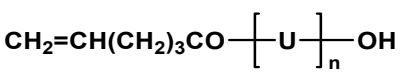
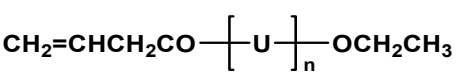
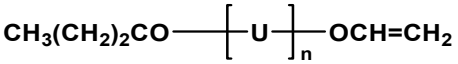
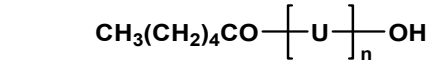
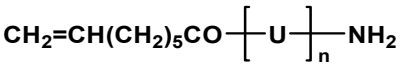
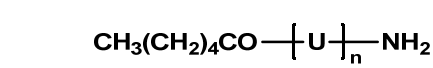
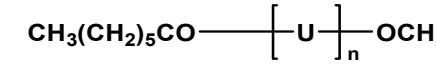
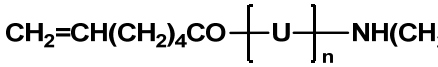
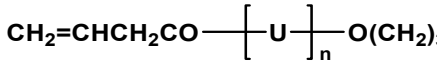
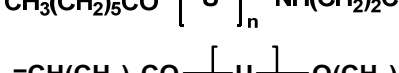
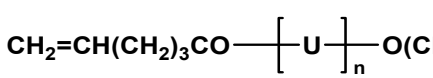
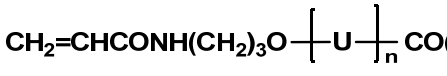
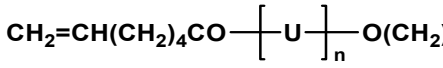
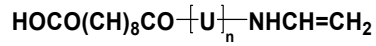
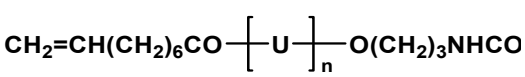
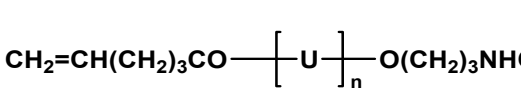
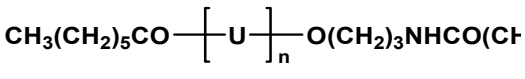
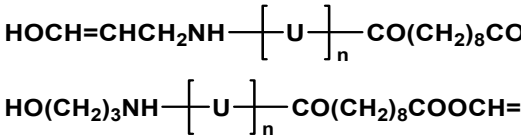
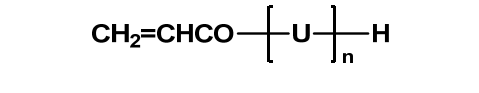
	2	676.49	/
	1	435.32	
	0	194.09	
			

Structure	n	[M+Na$^+$]	[M+H$^+$]
			
	3 2 1 0	903.59 662.42 421.30 180.10	/
	3 2 1 0	889.74 648.40 407.29 166.09	/
	4 3 2 1 0	1116.73 875.61 634.49 393.28 152.06	/
	3 2 1 0	1003.76 762.51 521.36 280.17	/
	3 2 1 0	1026.91 785.69 544.36 303.19	/
	3 2 1 0	913.62 672.45 431.28 190.11	/
	4 3 2 1 0	1089.80 857.68 616.40 375.27 134.08	/
	4 3 2 1 0	1060.79 819.59 578.44 337.25 96.47	/
			
	2 1 0	660.54 419.30 178.11	/
			
			
			
	2 1 0	632.42 391.25 150.08	/
			
	2 1 0	604.39 363.22 122.05	/

Structure	n	[M+Na$^+$]	[M+H$^+$]
			
			
	2 1 0	590.37 349.20 108.03	/
			
	2 1 0	730.54 489.38 248.16	/
	2 1 0	745.63 504.33 263.19	/
	3 2 1 0	989.68 748.51 507.29 266.16	/
	3 2 1 0	1004.78 763.58 522.39 281.25	/
			
	3 2 1 0	902.57 661.49 420.45 179.19	/
			
			
	2 1 0	647.42 406.25 165.11	/
			
	2 1 0	618.49 377.23 136.06	/
			
	4 3 2 1 0	1115.74 874.57 633.40 392.23 151.06	/
			
			
	2 1 0	619.49 378.26 137.07	/
			

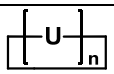
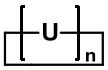
Structure	n	[M+Na$^+$]	[M+H$^+$]
	1 0	380.23 139.06	/
	3 2 1 0	887.65 646.48 405.27 164.10	/
	2 1 0	620.40 379.25 138.08	/
	2 1 0	663.44 422.33 181.07	/
	2 1 0	688.52 447.31 206.12	/
	2 1 0	702.45 461.41 220.13	/
	3 2 1 0	945.73 704.53 463.35 222.06	/
	3 2 1 0	959.69 718.52 477.33 236.14	/
	2 1 0	733.54 492.29 251.12	/
	3 2 1 0	973.17 732.57 491.34 250.14	/

Structure	n	[M+Na$^+$]	[M+H$^+$]
			
	2 1 0	772.71 531.44 290.22	/
	3 2 1 0	1029.69 788.52 547.35 306.18	/
	3 2 1 0	1031.11 790.67 549.38 308.21	/
	3 2 1 0	802.51 561.34 320.17 79.00	/
	3 2 1 0	930.63 689.46 448.31 207.14	/

* U = -NH(CH$_2$)$_3$OCO(CH$_2$)$_8$CO- or -O(CH$_2$)$_3$NHCO(CH$_2$)$_8$CO-.

Table S2. Structure assignment of the degradation products derived from the pyrolysis of the PEA-pro at 350 and 400 °C.

RT (min)	Possible structure (Mol Wt)	Ion EI[a] (*m*/*z*)	A%[b] 350 °C	A%[b] 400 °C
8.002	**CH$_3$(CH$_2$)$_4$COOH* (116)**	73	/	1.31
10.600	**CH$_3$(CH$_2$)$_7$COOH* (158)**	129	/	1.99
13.377	**CH$_3$(CH$_2$)$_4$CONHCH$_2$CH=CH$_2$* (155)**	140	/	0.96
13.559	**CH$_3$(CH$_2$)$_5$CONHCH$_2$CH=CH$_2$* (169)**	126	/	0.63
14.900	**unidentified**	99	/	0.07
15.024	**CH$_3$(CH$_2$)$_6$CONHCH$_2$CH=CH$_2$ (183)**	112	/	0.43
15.154	**unidentified**	168	/	1.33
16.134	**unidentified**	177	0.28	/
16.311	**unidentified**	112	/	0.15
16.422	**unidentified**	112	/	0.45
17.214/ 17.189	**HOCO(CH$_2$)$_8$COOH (202)**	138	2.96	12.15
19.522/ 19.513	**NC(CH$_2$)$_8$CN (164)**	164	5.92	2.54
20.122	**NC(CH$_2$)$_8$CONHCH$_2$CH=CH$_2$ (222)**	221	/	9.69
20.249	**CH$_3$(CH$_2$)$_6$CONHCH$_2$CH=CH$_2$ (183)**	183	5.30	0.55
21.188/ 21.158	**NC(CH$_2$)$_8$CONHCH=CH$_2$ (208)**	207	1.28	3.43

RT (min)	Possible structure (Mol Wt)	Ion EI[a] (*m*/*z*)	A%[b] 350 °C	A%[b] 400 °C
22.049/ 22.024	 or $HOCO(CH_2)_8CONHCH_2CH=CH_2$ (241)	241	61.83	30.49
22.278/ 22.236	 or $HOCO(CH_2)_8CONHCH_2CH=CH_2$ (241)	241	3.22	4.76
23.100	$CH_2=CHCH_2OCO(CH_2)_8CONHCH_2CH=CH_2$ (281)	281	/	2.43
23.104	unidentified	182	1.52	/
23.822	$CH_3CH_2OCO(CH_2)_8CONHCH_2CH=CH_2$ (269)	269	0.91	/
23.963	unidentified	281	/	1.61
24.593	$CH_2=CHCH_2NHCO(CH_2)_8CONH(CH_2)_3OH$ (298)	281	/	2.03
25.225/ 25.218	$CH_3(CH_2)_2NH(CH_2)_3OCO(CH_2)_8CN$ (282) or $CH_2=CHCH_2OCO(CH_2)_8CONHCH_2CH=CH_2$ or $CH_2=CHCH_2COO(CH_2)_3NHCO(CH_2)_6CH=CH_2$ (281)	265	10.47	6.73
25.880	$CH_3(CH_2)_2O(CH_2)_3NHCO(CH_2)_8CN$ (282)	281	/	2.36
27.284	unidentified	429	/	0.59
27.972	unidentified	429	/	1.05
31.960	unidentified	429	6.31	/
31.972	unidentified	429	/	12.27

a: Molecular ion or major fragment; b: Area %.