

SUPPORTING INFORMATION

Development of an antimicrobial and antioxidant hydrogel/nano-electrospun composite for multifunctional wound dressing

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Supplementary data file 1. FT-IR spectra for PCL (a), PGAL (b) and PCL-g-PGAL (c)

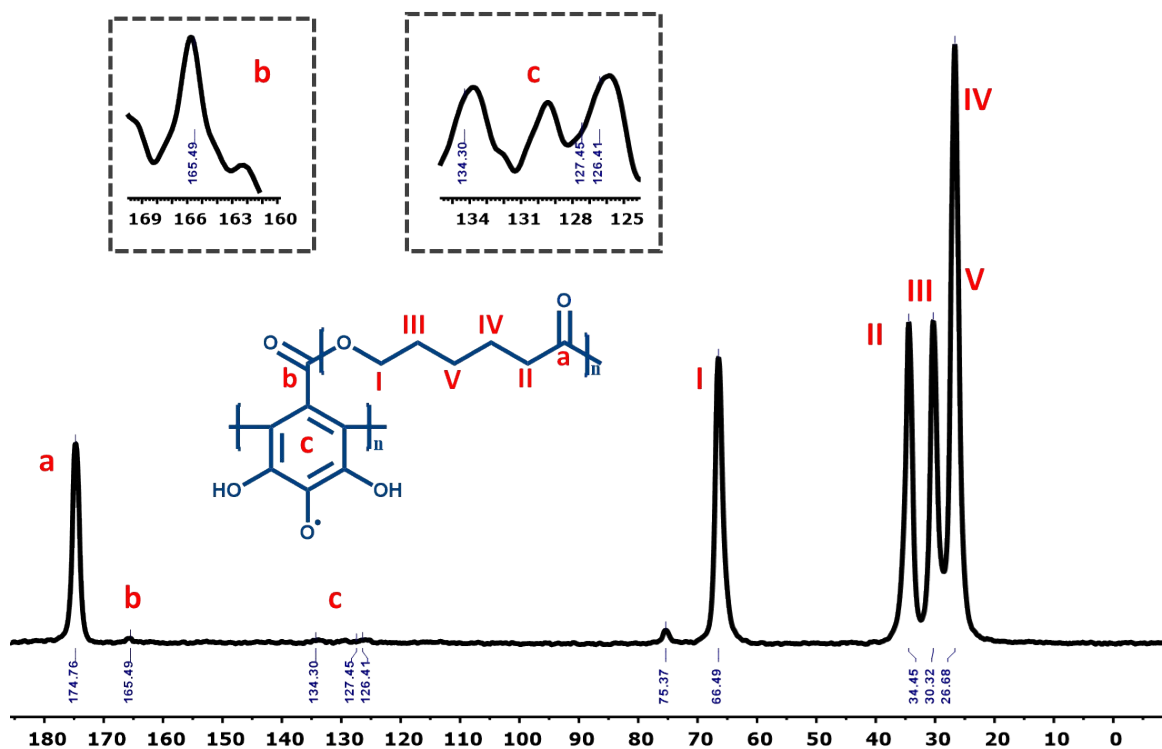


Figure S1. Representative CP/MAS ^{13}C -NMR spectrum of the PCL-g-PGAL, taken at 400 MHz with spinning frequency of 10 kHz.

Supplementary data file 2. FT-IR spectra for PCL (a), PGAL (b) and PCL-g-PGAL (c)

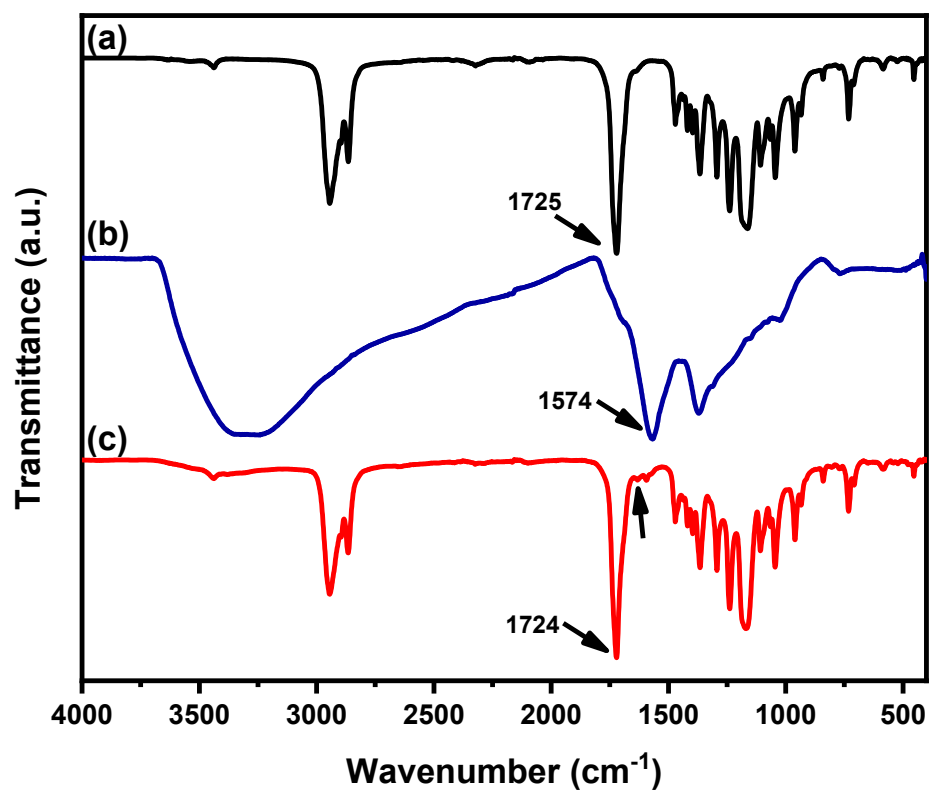


Figure S2. FT-IR spectra for PCL (a), PGAL (b) and PCL-g-PGAL (c)

Supplementary data file 3. DPPH analysis for PCL-g-PGAL

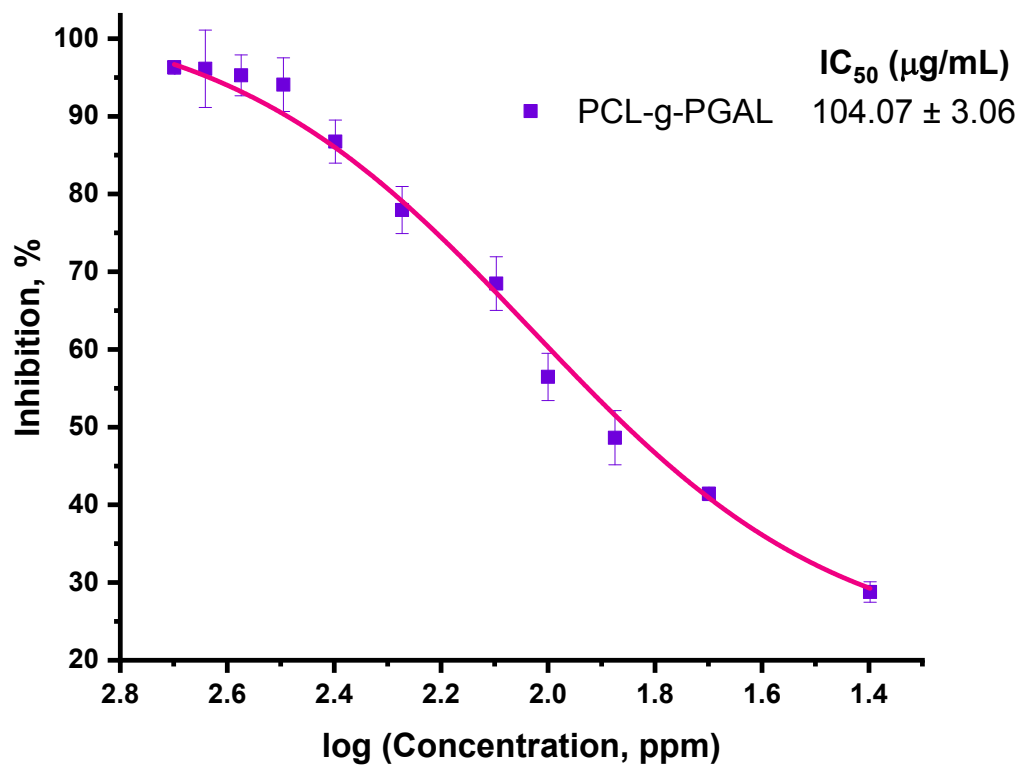


Figure S3. Reduction of the DPPH radical in the presence of PCL-g-PGAL. Values expressed as mean percent inhibition of DPPH in 3 experiments.

Supplementary data file for the optimized coordinates for S1 at the M06-2X/6-311++G(d,p) level of theory.

C	-7.11550	-0.00530	-0.20840
C	-5.76910	0.44590	0.32180
C	-4.61020	-0.27520	-0.36130
C	-3.25510	0.17050	0.18170
H	-7.24200	-1.08170	-0.04250
H	-7.17440	0.18150	-1.28720
H	-5.73520	0.26490	1.40130
H	-5.67440	1.52650	0.17100
H	-4.64870	-0.09030	-1.44090
H	-4.71820	-1.35730	-0.22380
H	-3.20480	-0.02740	1.25640
H	-3.14400	1.25170	0.05500
C	-2.10500	-0.54060	-0.51760
H	-2.17950	-1.62740	-0.40680
H	-2.10700	-0.34560	-1.59470
O	-8.13110	0.72350	0.47570
H	-8.98770	0.44540	0.14020
C	-0.76180	-0.13240	0.01010
O	-0.53760	0.62930	0.90370
C	2.11910	0.67740	-0.34490
C	1.54470	-0.55570	-0.35900
C	2.31790	-1.75250	-0.08010
C	3.74190	-1.55300	0.20700
C	4.30980	-0.29050	0.22530
C	3.50340	0.80480	-0.04770
O	1.85790	-2.90130	-0.06940
O	0.23340	-0.77890	-0.68150

O	4.45560	-2.63840	0.45170
C	4.14810	2.15060	-0.02510
O	3.29260	3.13790	-0.30100
O	5.31470	2.33080	0.21510
H	1.53150	1.55940	-0.55780
H	3.85980	-3.40650	0.39070
H	5.36140	-0.16130	0.44560
H	3.76970	3.98010	-0.27160

Optimized coordinates for S2 at the M06-2X/6-311++G(d,p) level of theory

C	-2.62890	0.87450	0.07750
C	-3.81670	1.56770	0.06770
C	-5.08990	0.86800	-0.01330
C	-5.05550	-0.58510	-0.08240
C	-3.85950	-1.26000	-0.06710
C	-2.66470	-0.52680	0.01100
O	-6.16730	1.49020	-0.02390
O	-3.86070	2.89710	0.13270
O	-6.22710	-1.21500	-0.15910
C	-1.39280	-1.31680	0.03080
O	-1.36010	-2.52350	0.04730
H	-1.68850	1.40400	0.13860
H	-4.79290	3.16960	0.11090
H	-6.93000	-0.54470	-0.15380
H	-3.83260	-2.34040	-0.11470
C	0.96190	-1.22060	0.06590
C	2.04260	-0.16510	-0.00980
C	3.43300	-0.79010	0.07890
C	4.53930	0.25420	-0.04530

H	1.02010	-1.79650	0.99300
H	1.01320	-1.91410	-0.77640
H	1.90370	0.55120	0.80570
H	1.93960	0.38500	-0.95020
H	3.55090	-1.54080	-0.71090
H	3.53550	-1.31880	1.03330
H	4.41600	1.01660	0.72950
H	4.45460	0.76750	-1.00760
C	5.92130	-0.37140	0.07550
H	6.04700	-0.87560	1.03890
H	6.07870	-1.13880	-0.68930
O	-0.31150	-0.54510	0.02890
C	7.03750	0.62760	-0.05640
O	6.90820	1.80860	-0.25780
O	8.24290	0.05080	0.07790
H	8.92250	0.73460	-0.01370

Optimized coordinates for S1-TS at the M06-2X/6-311++G(d,p) level of theory

O	1.02480	1.87480	-0.73150
O	0.59500	0.75660	1.29750
O	-0.36010	-0.23710	-0.77680
C	0.95880	0.48690	0.20310
H	1.17450	1.66630	-1.66580
H	0.03020	2.19030	-0.63400
C	-4.32190	0.46350	0.25270
C	-3.46860	1.52190	0.16170
C	-2.07690	1.33480	-0.20790
C	-1.58970	-0.02780	-0.44660

C	-2.51430	-1.08700	-0.34960
C	-3.82790	-0.84280	-0.01330
O	-1.35990	2.36520	-0.34070
O	-3.87090	2.78150	0.39120
C	-4.73910	-2.02330	0.07640
O	-5.98470	-1.69180	0.43040
O	-4.39970	-3.15850	-0.14500
H	-5.35760	0.62070	0.51970
H	-3.10910	3.36590	0.25440
H	-2.17170	-2.09620	-0.53700
H	-6.51770	-2.49920	0.47260
C	7.08570	-1.08510	-0.09910
C	5.93530	-0.18320	0.30250
C	4.59000	-0.72570	-0.17270
C	3.42870	0.17670	0.23700
H	7.11580	-1.19000	-1.19000
H	6.94800	-2.08260	0.33440
H	6.10380	0.81350	-0.11880
H	5.93120	-0.07860	1.39250
H	4.43120	-1.72870	0.23930
H	4.60070	-0.83070	-1.26350
H	3.58300	1.18170	-0.16750
H	3.39760	0.26860	1.32670
C	2.09170	-0.37650	-0.26030
H	2.07200	-0.46540	-1.34710
H	1.90400	-1.36840	0.15830
O	8.29600	-0.50240	0.37530
H	9.02980	-1.06790	0.11970

Optimized coordinates for S2-TS at the M06-2X/6-311++G(d,p) level of theory

O	-0.71790	-0.68850	1.98980
O	-0.20740	1.22090	0.54160
O	-0.16140	-1.08560	-0.07930
C	-0.86560	0.21440	0.54100
H	-1.56320	-1.01470	2.32520
H	-0.22300	-1.36340	1.04040
C	1.13890	-0.86380	-0.66360
C	2.24630	-0.93590	0.37090
C	3.61700	-0.75290	-0.27630
C	4.75050	-0.83750	0.74420
H	1.25380	-1.63280	-1.42840
H	1.11110	0.11650	-1.14300
H	2.20250	-1.90740	0.87640
H	2.08250	-0.16180	1.12670
H	3.65310	0.21680	-0.78370
H	3.76500	-1.52110	-1.04400
H	4.72200	-1.81340	1.23670
H	4.60450	-0.08180	1.52120
C	6.12540	-0.65360	0.11420
H	6.92190	-0.87970	0.83080
H	6.27510	-1.33030	-0.73130
C	6.37890	0.75420	-0.35780
O	5.72850	1.72580	-0.06440
O	7.46150	0.82960	-1.14820
H	7.59680	1.75590	-1.39560
C	-2.95720	-1.04660	-0.17040
C	-4.30340	-1.03310	-0.45020

C	-5.07130	0.19910	-0.37970
C	-4.36090	1.40950	-0.00540
C	-3.01330	1.37820	0.27050
C	-2.33040	0.15770	0.18700
O	-6.29110	0.21600	-0.63530
O	-4.96310	-2.13610	-0.80210
O	-5.07020	2.53540	0.05440
H	-2.40140	-1.97160	-0.24040
H	-5.89140	-1.89350	-0.95370
H	-5.98880	2.32370	-0.18070
H	-2.48310	2.28090	0.54370