Bis(2-hydroxyethyl) 2-phenylsuccinate

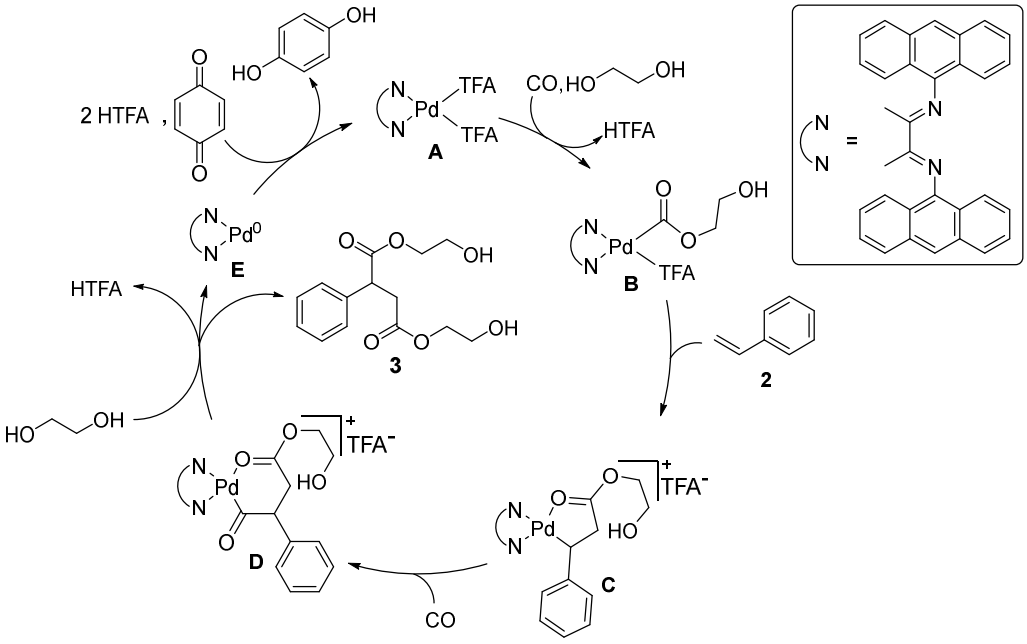
Diego Olivieri,[1,*] Riccardo Tarroni,[2] Carla Carfagna[2]

[1] Department of Biomolecular Sciences, University of Urbino "Carlo Bo",Piazza Rinascimento 6, 61029 Urbino (PU), Italy
[2] Department of Industrial Chemistry "T. Montanari", University of Bologna, Viale Risorgimento 4, 40136 Bologna (BO), Italy
[*]Corresponding Author. diego.olivieri@uniurb.it

Supporting Information

Contents:

1. Proposed Catalytic Cycle

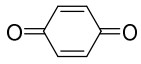


Scheme S1. Proposed catalytic cycle.

2. Computed Equilibrium Geometries and Energies for the Studied Compounds

The equilibrium geometries listed below have been obtained at the BP/def2-TZVP level of computation. At such geometries, the difference G-E(el) between the Gibbs free energy and the electronic energy was computed, using the same functional/basis. At the same geometries, a single point energy computation at the SMD(THF) M06-D0/def2-QZVPP level was performed, and the final free energy G was obtained by summing the electronic energy E(el) with the previously obtained G-E(el) value.

2.1. Reagents

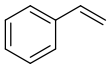


p-benzoquinone

12

G-E(el) = 0.0515645400 Eh, E(el)= -381.397747184337 Eh, G=-381.3461826443 Eh

C	-0.69772192294653	1.26861790785852	-0.00000140006457
C	0.05351696306028	-0.01132172284729	-0.00000013002152
C	-0.73813544694518	-1.26666777229364	-0.00000018062878
C	-2.04488339635816	1.29008857242105	-0.00000265060198
C	-2.83653505276387	0.03474276756148	-0.00000291090888
C	-2.08529690976939	-1.24519659166116	-0.00000138504936
O	-4.06803205352178	0.05437412046137	-0.00000352264059
O	1.28501381144993	-0.03095302833435	0.00000089598761
H	-0.09346365790323	2.17818741505972	-0.00000125745533
H	-0.16317461792976	-2.19503496940567	0.00000088652390
H	-2.61984420918914	2.21845517037904	-0.00000354679325
H	-2.68955514118318	-2.15476548819908	-0.00000138734725



styrene **2**

16

G-E(el)=-381.397747184337 Eh, E(el)=-309.5450190993 Eh, G=-309.4468602193 Eh

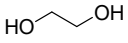
C	-0.68875943122844	1.18003600038322	-0.00000209832308
C	-0.00333610583797	-0.04987345747510	0.00000088720413
C	-0.77150267138694	-1.23153402765603	0.00000054495520
C	-2.08339282947397	1.23354602275942	-0.00000372593839
C	-2.82778042525976	0.05200881237894	-0.00000312098468
C	-2.16305927104588	-1.18060747830200	-0.00000120099964
C	1.46567838780783	-0.04470017217921	0.00000406662129
C	2.28903727923755	-1.10500677471459	0.00002463429669
H	-0.11022339301283	2.10699294508833	-0.00000263643853
H	-0.27287774388765	-2.20212239759723	0.00000043782575
H	-2.58952836474248	2.20041078314422	-0.00000573419912
H	-3.91823665577215	0.08778192473060	-0.00000469512648
H	-2.73746108141220	-2.10872096836557	-0.00000173836811
H	1.91461657975477	0.95458323489824	-0.00001106793748
H	1.92505688574251	-2.13389980496783	0.00004258144602
H	3.37080898251761	-0.97279200612540	0.00002486996644

CO, carbon monoxide

2

G-E(el)=-0.0142967500 Eh, E(el)=-113.304174256452 Eh G=-113.3184710065 Eh

C	-0.00113237570858	0.00000000000000	0.00000000000000
O	1.13542382470858	0.00000000000000	0.00000000000000



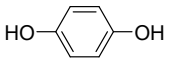
Ethylene glycol

10

G-E(el)=0.0544989600 Eh, E(el)=-230.2440952537 Eh, G=-230.1895962937 Eh

C	0.01048292093598	0.00178031045372	-0.00000063839532
C	1.53043159106164	-0.00177974263275	-0.00000098557542
O	-0.40577245051564	1.37292749921339	-0.00000233458471
O	1.94668695292545	-1.37292693077150	0.00000084131983
H	-0.35384954751836	-0.53470744759104	0.89508426162267
H	-0.35384986280219	-0.53470986827043	-0.89508396067919
H	1.89476451345150	0.53471042232774	0.89508231007099
H	1.89476396076518	0.53470801319674	-0.89508592856948
H	-1.37656246366617	1.38977255923497	-0.00000324498636
H	2.91747696836259	-1.38977208316084	-0.00000144522300

2.2. Products

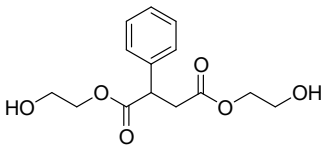


1,4-hydroquinone

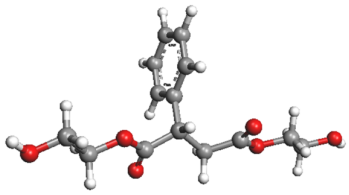
14

G-E(el)=0.0743608600 Eh, E(el)=-382.6383156546 Eh, G=-382.5639547946 Eh

C	-0.68215027586900	1.21002493726280	-0.00000069097962
C	0.01196476359252	-0.00649125663146	0.00000077090025
C	-0.70533843053886	-1.20691071892116	0.00000003364292
C	-2.07768003273654	1.23033178032757	-0.00000283105606
C	-2.79498322820987	0.02991235360700	-0.00000360181054
C	-2.10086820193299	-1.18660387499305	-0.00000215472879
O	-4.17106162232196	0.10646986581309	-0.00000562669810
O	1.38804317636934	-0.08304873323690	0.00000270224669
H	-0.13014956481664	2.15394413520904	-0.00000022843305
H	-0.16219112997426	-2.15228197520693	0.00000117225381
H	-2.62082733214218	2.17570297630405	-0.00000400951393
H	-2.65286892434320	-2.13052310507567	-0.00000267155780
H	-4.53088636716271	-0.79752138498920	-0.00000700596586
H	1.74786784108635	0.82094258053082	0.00000442470008



bis(2-hydroxyethyl) 2-phenylsuccinate **3**



38

G-E(el)=0.2486548100 Eh, E(el)=-995.5636333227 Eh, G=-995.3149785127 Eh

C	1.59522761807069	0.08873567798804	0.04970703172850
C	0.06203490119733	-0.03831259878273	0.04724839173074
C	2.12415106618459	0.54089776469193	1.39722077740121
O	3.29504464233361	1.21661492598407	1.25471317072530
O	1.60820957119306	0.30706615652829	2.47273897809469
C	-0.39700951322592	-0.87328066633966	-1.14575517340623
O	-1.62724576591583	-1.39894309997964	-0.91510167418211
O	0.22858412672244	-1.04225647569471	-2.17454134357136
C	3.92771841497021	1.63567205034601	2.49021924071786
C	5.19659480500137	2.37254482809965	2.09698848361045
O	5.81951023099111	2.77634828852597	3.31999052652607
C	-2.19838754322094	-2.15938913645426	-2.00905249303705
C	-3.56630896894097	-2.62657294515764	-1.54191192013898
O	-4.11850657442222	-3.38597440598154	-2.62144944945492
C	-1.88998967284518	3.83794797478447	0.02032087374976
C	-1.19762380896300	3.39329948406353	-1.10991586912139
C	-0.57331077536632	2.14429602759528	-1.10424690238910
C	-1.95509253176877	3.02452800385576	1.15413541710815
C	-1.33353046702454	1.77284503371277	1.15781831521615
C	-0.63517162779025	1.31999667699837	0.03049979055247
H	2.05036644839095	-0.89344144967491	-0.16085482505839
H	-0.24643415996826	-0.56326132472830	0.96288049839421
H	4.15417223132457	0.75638651519490	3.11016572260429
H	3.24621411196657	2.28783306941727	3.05424898835468
H	4.93907842525622	3.24130849295814	1.46398157585369
H	5.84885996805204	1.70038126639697	1.50980661279881
H	6.63237200585192	3.25916604643243	3.09789350251629
H	-1.54772262187384	-3.01207117707978	-2.25014935844706
H	-2.27782703382880	-1.52359892509068	-2.90228978771564
H	-4.19305227573030	-1.75006740363390	-1.29654249705380
H	-3.45642372087508	-3.23813304172844	-0.62759822458203
H	-5.00389936835230	-3.68440843779880	-2.35651500502833
H	1.94644691307560	0.76268950602640	-0.74118992304765
H	-2.37695687462634	4.81441170652873	0.01634546002111
H	-1.14459575105178	4.02057132334004	-2.00142230849443
H	-0.04043469913185	1.80153803756851	-1.99430316072467
H	-2.49093423107390	3.36441050882042	2.04204438705750
H	-1.37796765458590	1.14259169426702	2.04771199469121

3. Copies of NMR Spectra

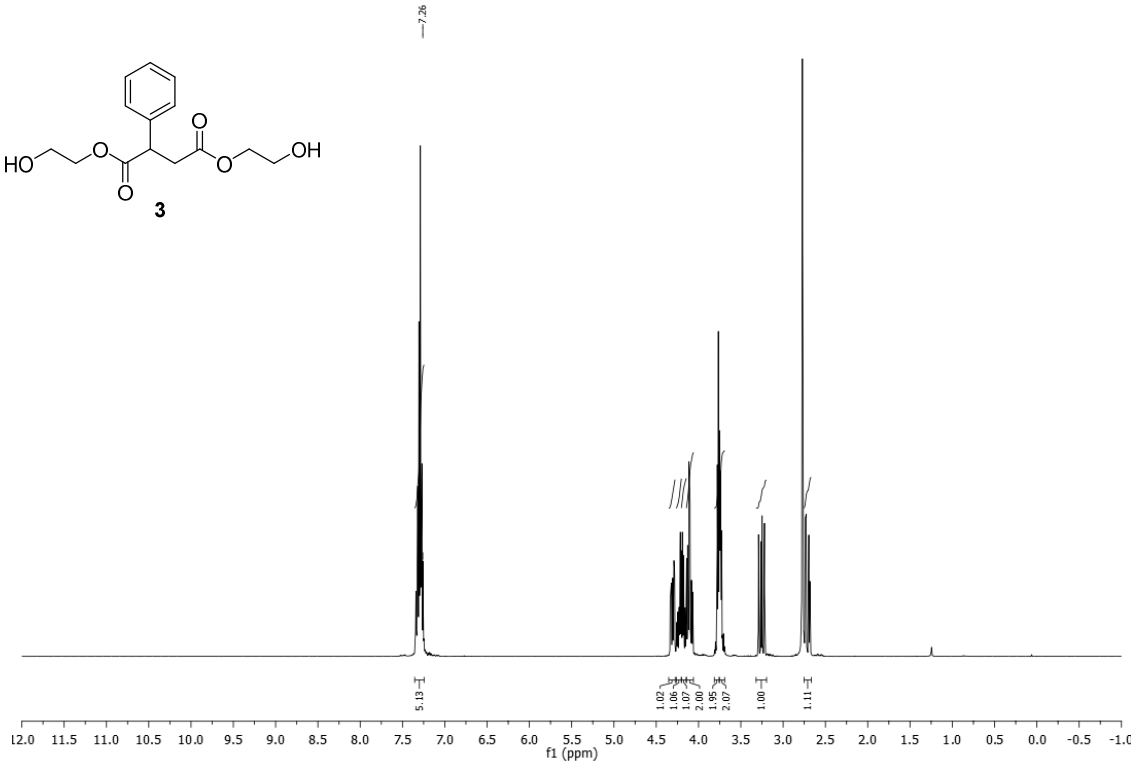


Figure S1. –^{1}H-NMR spectrum.

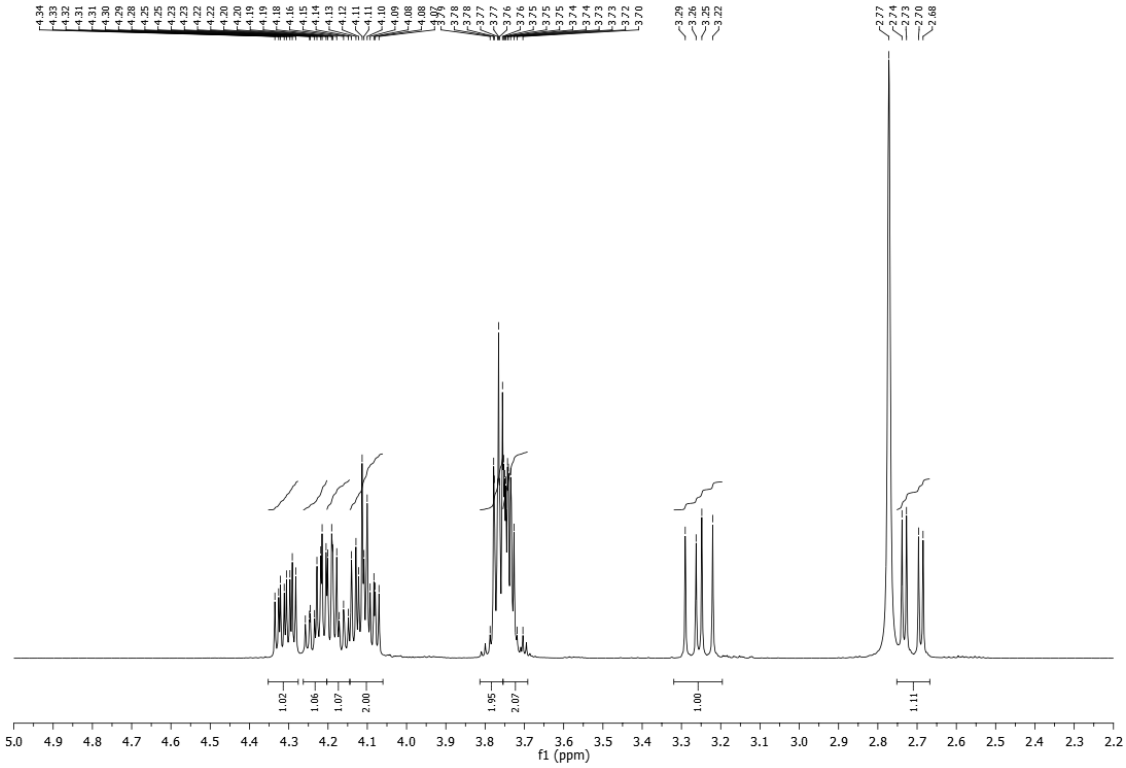


Figure S2. –Zoom of the ^{1}H-NMR spectrum (from 5.0 ppm to 2.2 ppm).

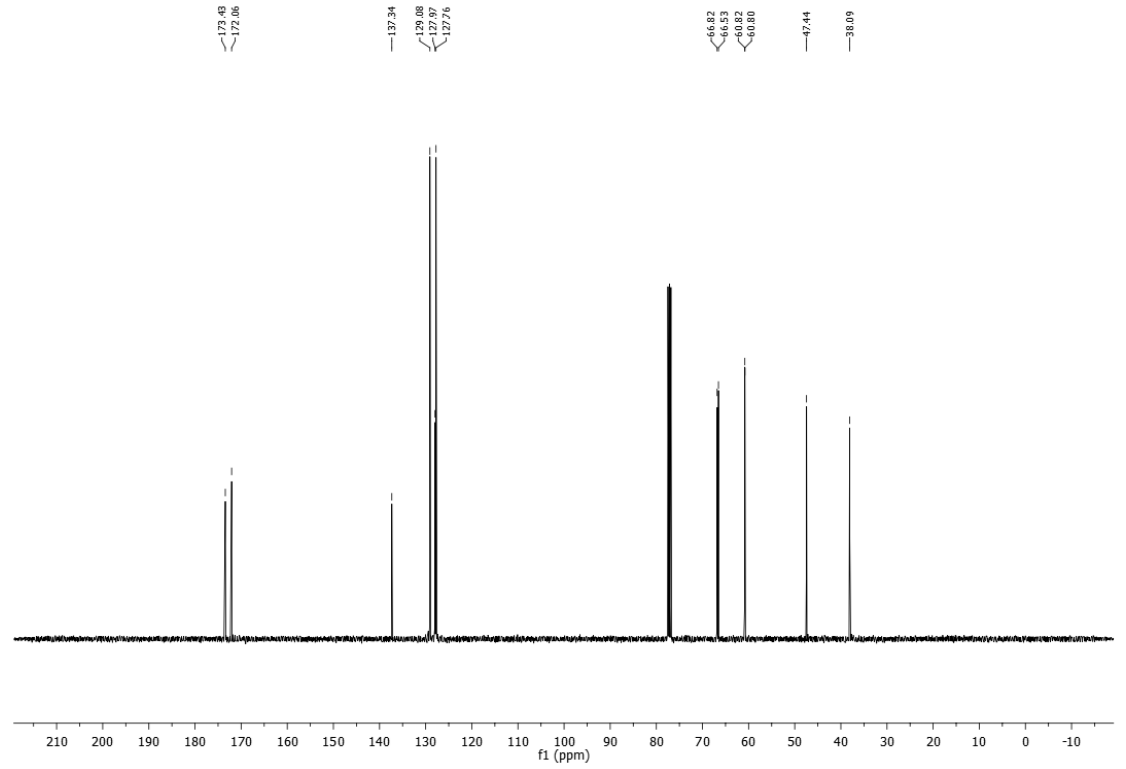


Figure S3. –^{13}C-NMR spectrum.

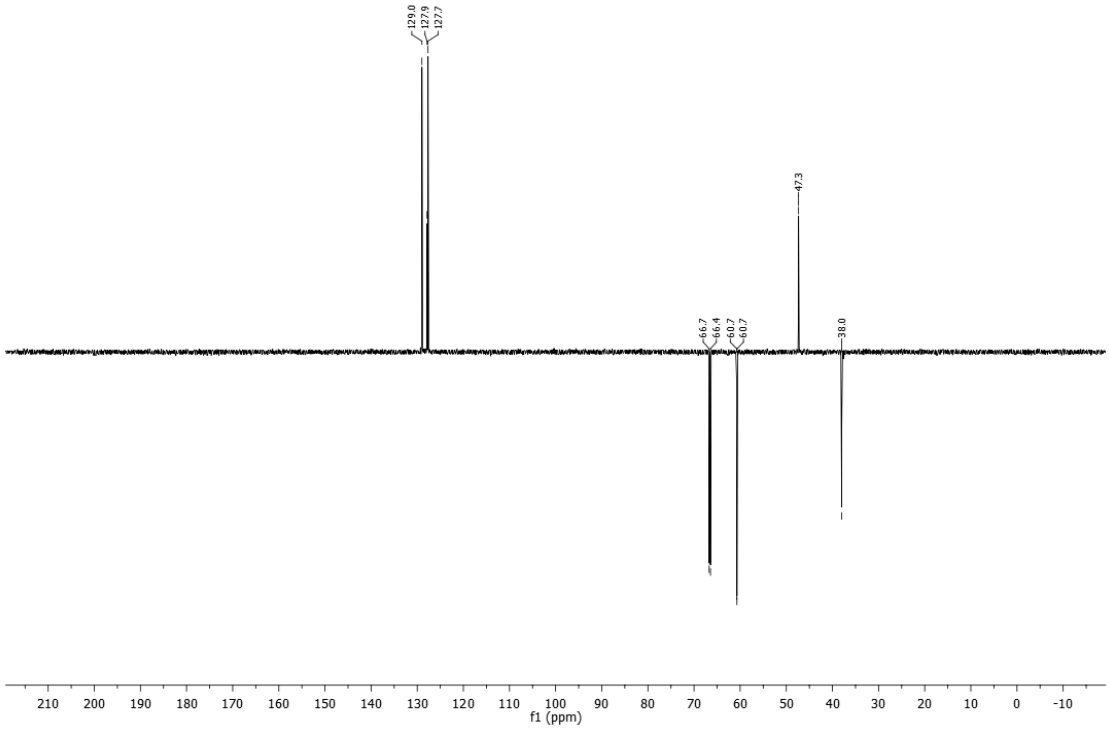


Figure S4. –DEPT 135 (CH and CH_3 positive, CH_2 negative).

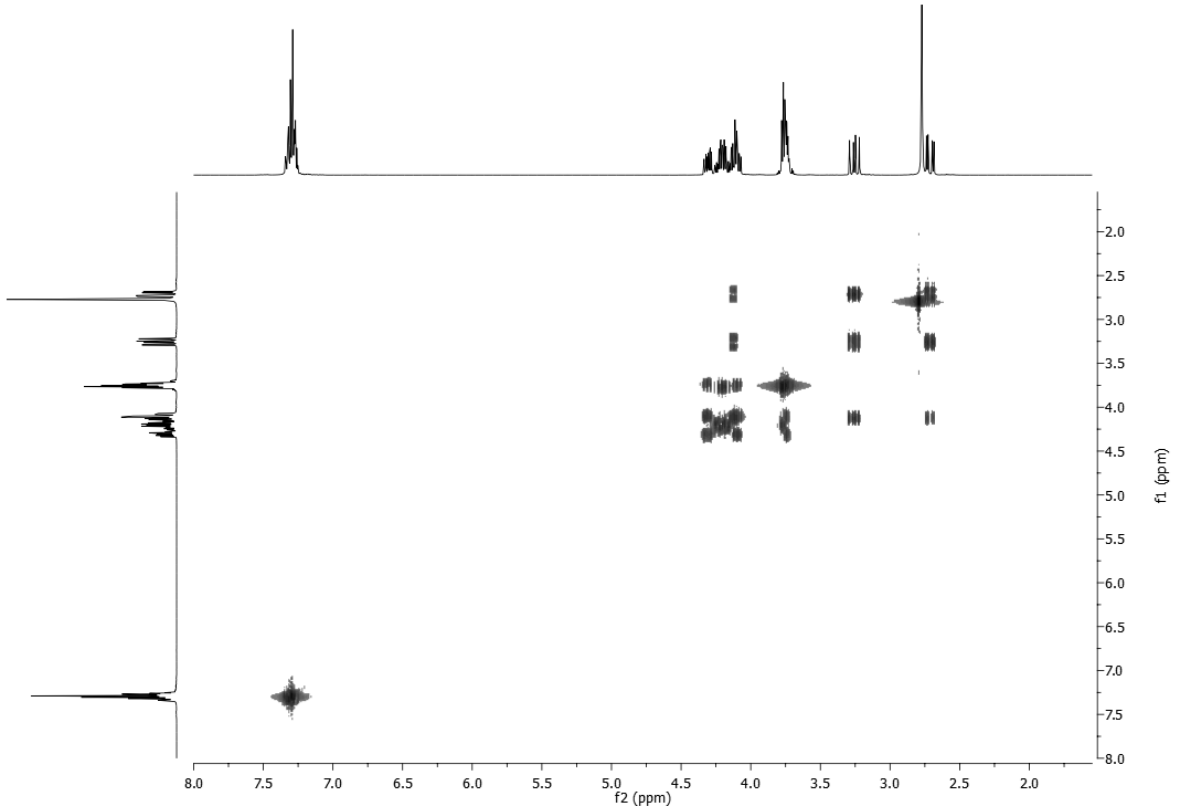


Figure S5. –COSY spectrum.

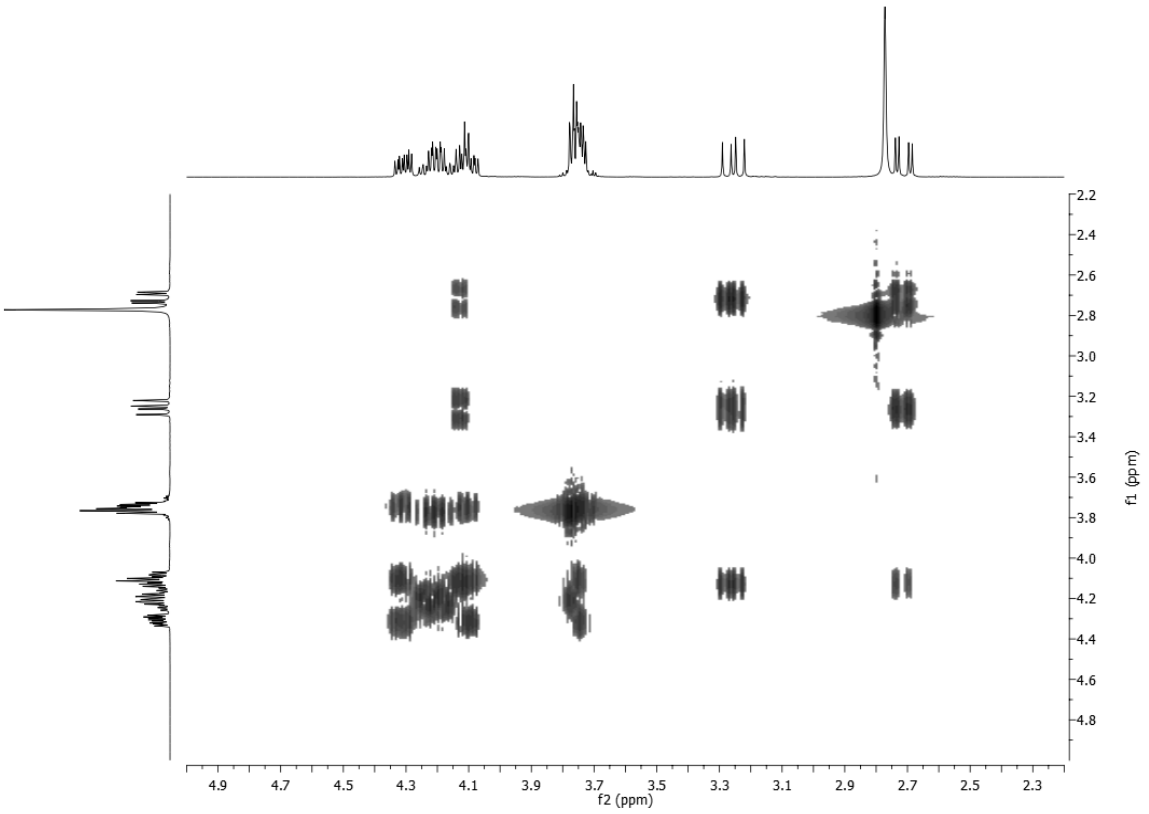


Figure S6. –Zoom of the COSY spectrum (from 5.0 ppm to 2.2 ppm).

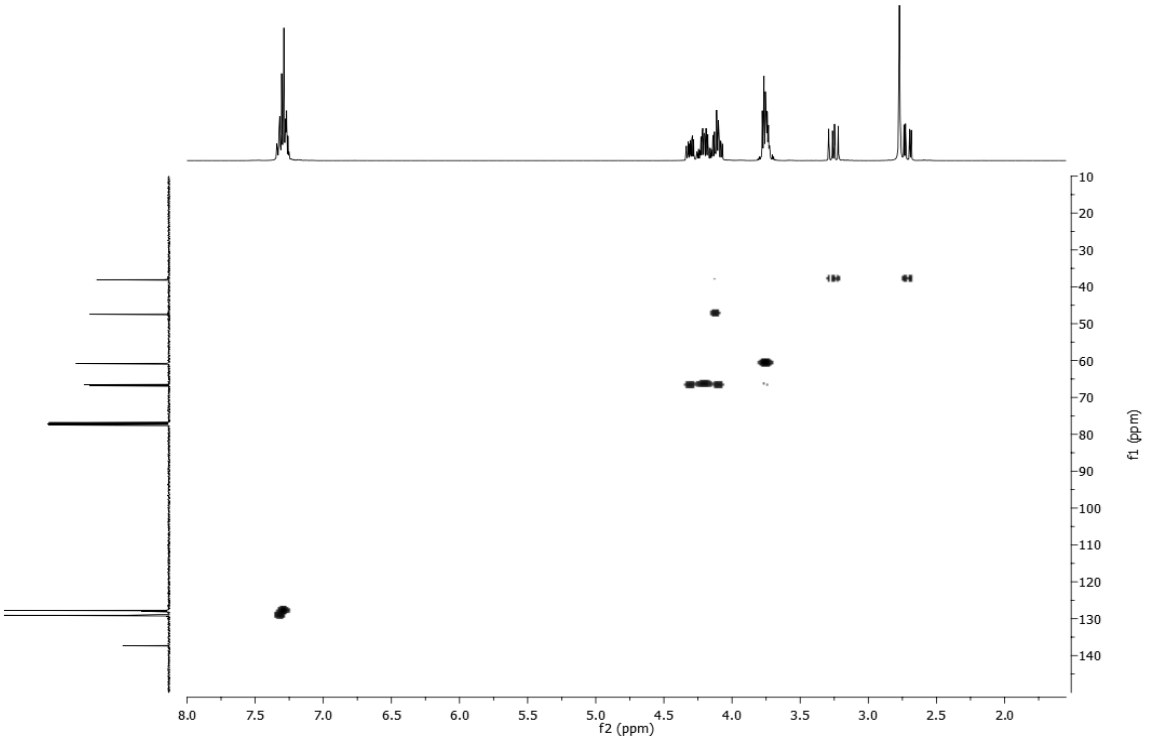


Figure S7. –HSQC spectrum.

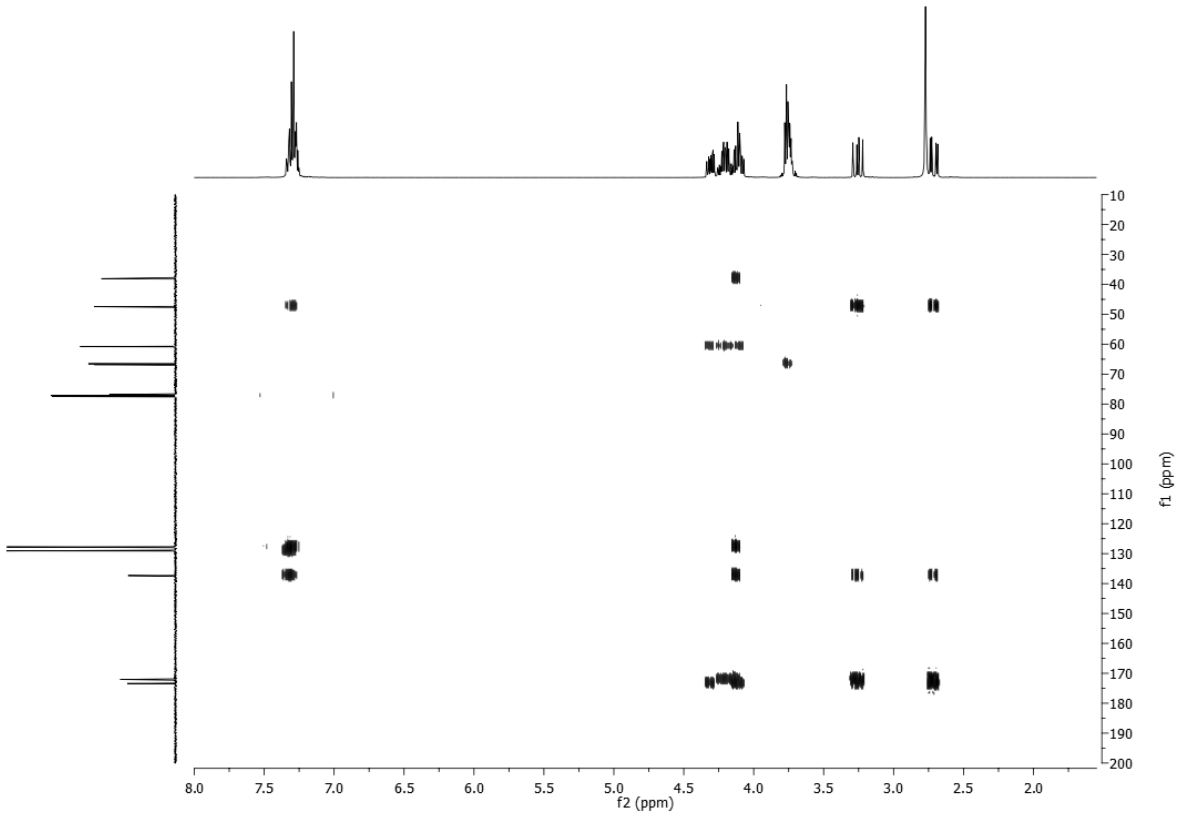


Figure S8. –HMBC spectrum.

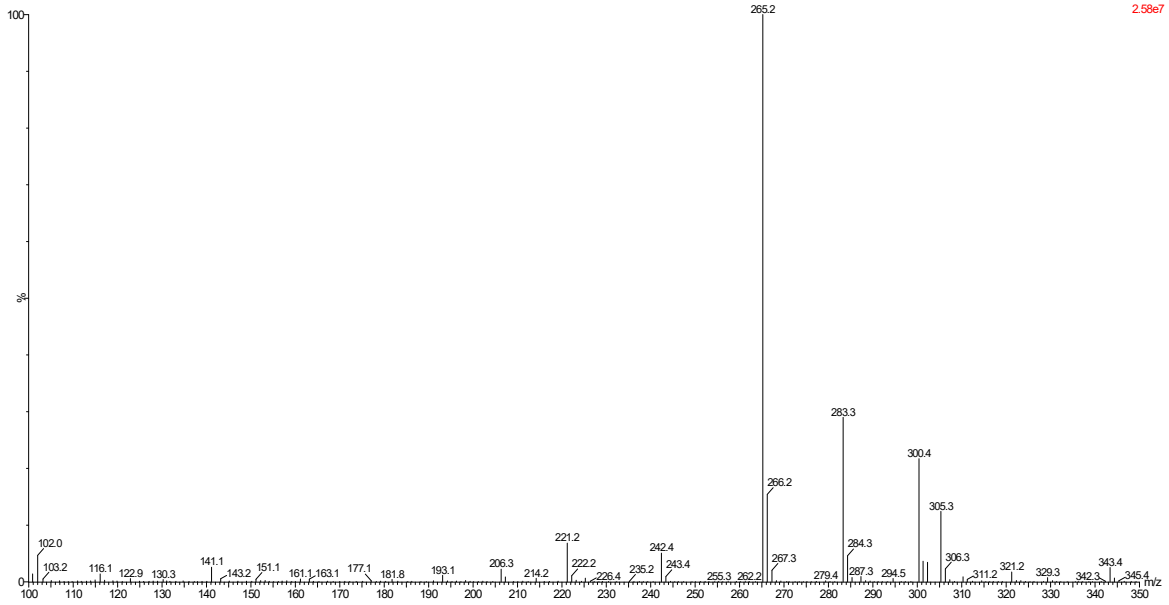


Figure S9. –ESI-MS (ESI+) spectrum of compound **3.**