Dibenzyl-(1*S**,2*S**)-2,3-dihydro-1*H*-indene-1,2-dicarboxylate

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

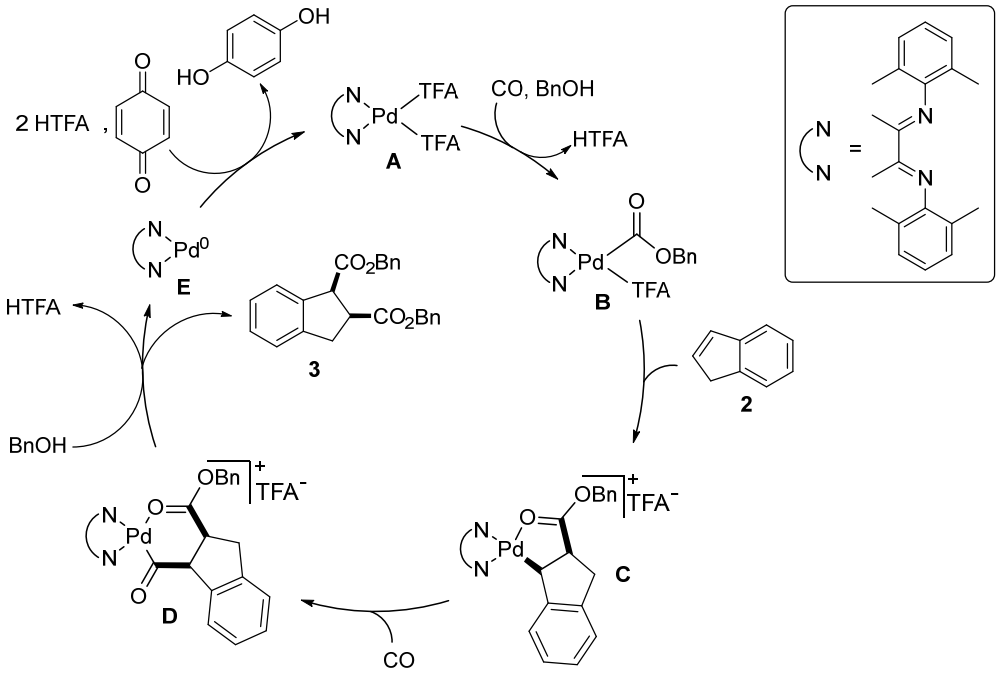
[1] Department of Biomolecular Sciences, University of Urbino "Carlo Bo",Piazza Rinascimento 6, 61029 Urbino (PU), Italy.
[2] Department of Industrial Chemistry "T. Montanari", University of Bologna, Viale Risorgimento 4, 40136 Bologna (BO), Italy
[*]Corresponding Author. diego.olivieri@uniurb.it

Supporting Information

Contents:

1. Proposed Catalytic Cycle S2
2. Computed Equilibrium Geometries and Energies for the Studied Compounds S3
   2.1 Reagents S3
   2.2 Products S4
3. Copies of NMR and ESI-MS spectra S7

1. Proposed catalytic cycle

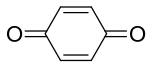


Scheme S1 – Proposed catalytic cycle. Only one enantiomer is shown.

2. Computed Equilibrium Geometries and Energies for the Studied Compounds

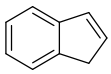
The equilibrium geometries listed below have been obtained at the BP/def2-TZVP level of computation. At such geometries, the difference G-E(el) between the Gibbs free energy and the electronic energy was computed, using the same functional/basis. At the same geometries, a single point energy computation 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

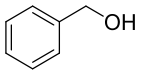
 1*H*-indene **2**

17
G-E(el)= 0.10542102 Eh, E(el)=-347.649774598456 Eh, G=-347.649774598456 Eh

C	-1.42487398529606	1.18491707129125	-0.00202595814128
C	-0.11045216135617	0.70468776351535	-0.00321441855050
C	0.14354576310723	-0.68888627852946	-0.00197595751868
C	-0.90745196777890	-1.59938586378919	0.00037560842325
C	-2.22393934249730	-1.11443024669776	0.00152622908709
C	-2.47723254039692	0.26303814950814	0.00034922490444
C	1.17625770341906	1.40180651828066	-0.00572714581781
C	2.18440809768338	0.49982119768887	-0.00607739064078
C	1.63794506297024	-0.90623816657509	-0.00356667837867
H	-1.62874863970923	2.25754158169293	-0.00294790977900
H	-0.71931379984856	-2.67544561408088	0.00130898147754
H	-3.05884958252628	-1.81699332319751	0.00335328427066
H	-3.50849971117925	0.62029761349453	0.00128425091070
H	1.29054323255727	2.48568004919744	-0.00707511649452
H	3.24880950690866	0.72959215568526	-0.00782057707860
H	1.97732796457824	-1.47823180698758	0.87832491736503
H	1.97548879036458	-1.48125921049697	-0.88415053903889

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



Benzyl alcohol

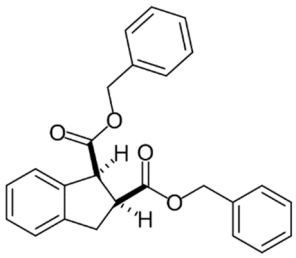
16
G-E(el)= 0.0980852100 Eh, E(el)= -346.6959640240 Eh, G= -346.5978788140 Eh
O	4.73308170205998	0.33407718531542	1.40732720757753
C	4.31490541968001	0.04629080216071	0.05811935651958
C	0.68654265495359	1.20859381893345	0.01083670347111
C	-0.00139806609842	-0.00901289401698	-0.01729162553214
C	0.71298460026377	-1.20936101560997	-0.02671730072590
C	2.08199492675303	1.22247290376531	0.02646359225388
C	2.80950855674407	0.02325784661546	0.01813480204830
C	2.11039369633157	-1.19010562585552	-0.00688659573022
H	4.69542683429739	0.82074821211799	-0.63412893504676
H	4.71081222615601	-0.93136850247208	-0.27326176062782
H	0.13259565611685	2.14892146753398	0.01639801156880
H	-1.09251115202587	-0.02086766445287	-0.03350132686119
H	0.18181667082059	-2.16245176377148	-0.04830328695563
H	2.61839009320008	2.17355718524495	0.05067164713610
H	2.66855966801457	-2.12924964986431	-0.00995078420595
H	5.70228825173277	0.42090532235595	1.40014727511031

2.2 Products

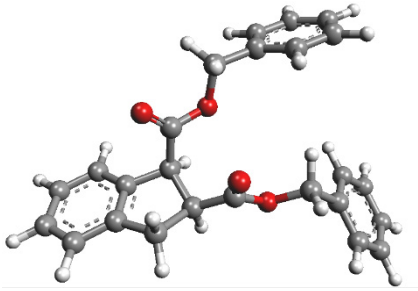


1,4-hydroquinone

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



Dibenzyl-(1*S**,2*S**)-2,3-dihydro-1*H*-indene-1,2-dicarboxylate **3**



51

G-E(el)=0.3451148500 Eh, E(el)=-1266.5667099412 Eh, G=-1266.2215950912 Eh

C	0.95384077929463	1.69055132366381	-1.09582748869915
C	0.19681414235255	1.22253847571901	-0.02299167010006
C	-0.31400096886663	-0.08335347509813	-0.01803990440948
C	-0.06642895081126	-0.93801853684386	-1.09241813539024
C	0.69943511967066	-0.47357201502810	-2.16832314562170
C	1.20745735576684	0.83030851957546	-2.17031520076359
C	-0.21978466230403	1.96682590462098	1.22899415973038
C	-0.59885679729019	0.77359937379260	2.19104790781785
C	-1.10535800941619	-0.33788298388548	1.24318107445451
C	-1.40397618013417	2.90471178376160	0.96136659354038
O	-2.18104886630094	2.82274833484407	0.03404763200467
O	-1.47278466650600	3.85921402780824	1.93062826819589
C	-1.56870412261108	1.14023269699698	3.30052019890230
O	-2.77841903012639	1.20753639205808	3.18663226128915
O	-0.89942588584602	1.38708022705689	4.45622805774592
C	-2.62756812009307	4.75523628962251	1.82097425102232
C	-3.44588211443995	6.36662814215542	5.17347424187152
C	-2.57134668215197	7.45617757041534	5.18305442558823
C	-1.71557290266001	7.67012312755047	4.09746485471889
C	-3.46096730971790	5.49198252829235	4.08332068879561
C	-2.60665310157718	5.69678359273441	2.99083146607160
C	-1.73661573884622	6.79752910876092	3.00837039948219
C	-1.73440539947298	1.79997036381687	5.58806873306587
C	0.64930799044956	3.21356022765868	8.19838273282715
C	0.81279920249785	2.11832231423247	9.05176171541089
C	0.14245170039567	0.92161818438572	8.78315770131236
C	-0.18063500388679	3.11104266773214	7.08019380297689
C	-0.85480973495138	1.91364537892446	6.79973542585327
C	-0.68630286704533	0.82210533529084	7.66349406394135
H	1.34761145014506	2.70904895124085	-1.10181850518566
H	-0.45838489941740	-1.95724460998988	-1.09613587514104
H	0.90618350633236	-1.13556124496239	-3.01092925094958
H	1.80677495936633	1.17762567727870	-3.01333667205705
H	-2.18632992012201	-0.21761298514929	1.06414167500356
H	-0.94698359403706	-1.34047039833672	1.66590884348080

H	0.34328017720211	0.45197127300568	2.65658869785033
H	0.58545341472016	2.56604673437745	1.67620140377028
H	-2.55399376800192	5.28688675790113	0.86098833901538
H	-3.53820383969552	4.14150218931835	1.80397030136358
H	-4.12032963462145	6.19851517308789	6.01468512182785
H	-2.56026407719647	8.14187988321780	6.03183743830383
H	-1.03576364980039	8.52378560313788	4.09746520002346
H	-4.14663239949440	4.64182056766480	4.07356873568645
H	-1.07186046344223	6.97004538595496	2.15902193009120
H	-2.20299110552206	2.76024188418985	5.32916794811529
H	-2.52862440667605	1.05234796441549	5.72167376643854
H	1.16671439078455	4.15139004157423	8.40702509353324
H	1.45836209937003	2.19888961972649	9.92784078505659
H	0.26270779166484	0.06551730238155	9.44900469517720
H	-0.31084549573218	3.96791370393124	6.41580883030251
H	-1.21165207719833	-0.11290654058099	7.45574720065807

3. Copies of NMR and ESI-MS spectra

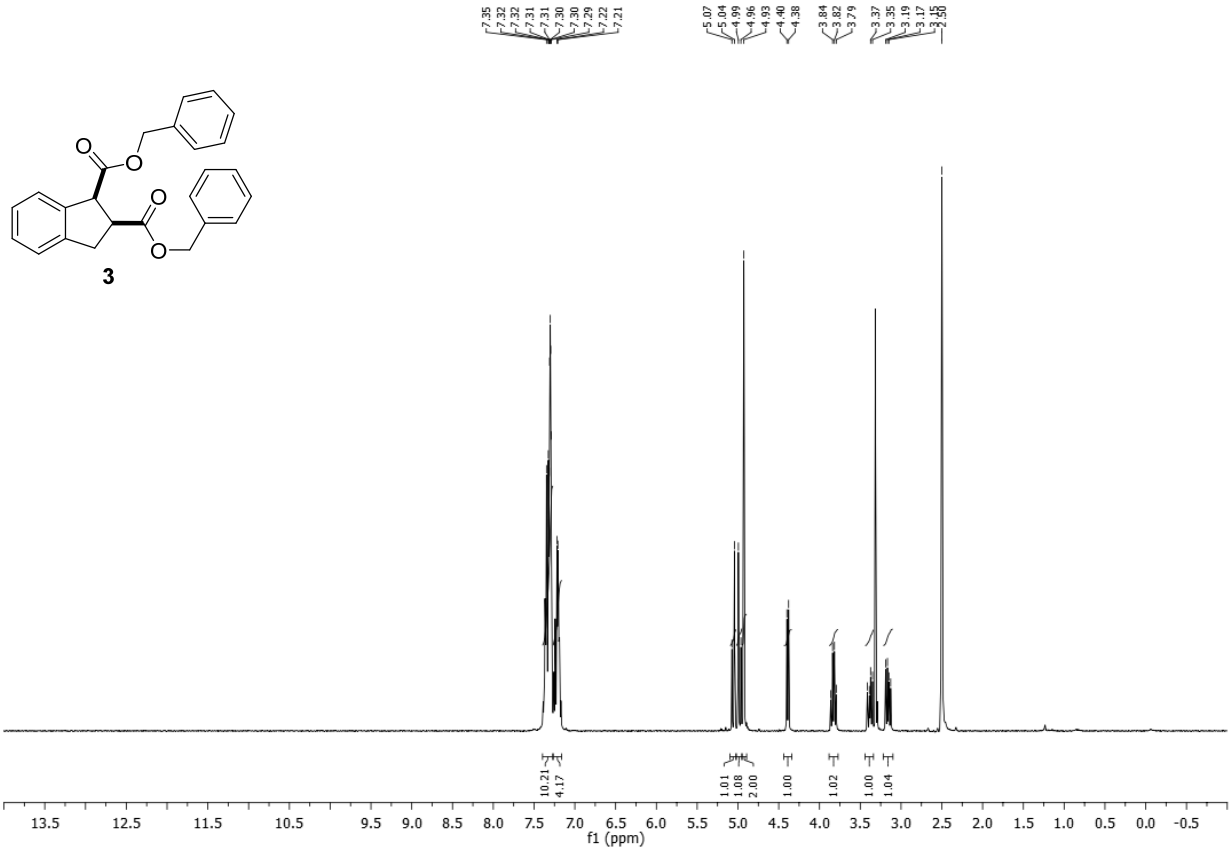


Figure S1 –^{1}H-NMR spectrum

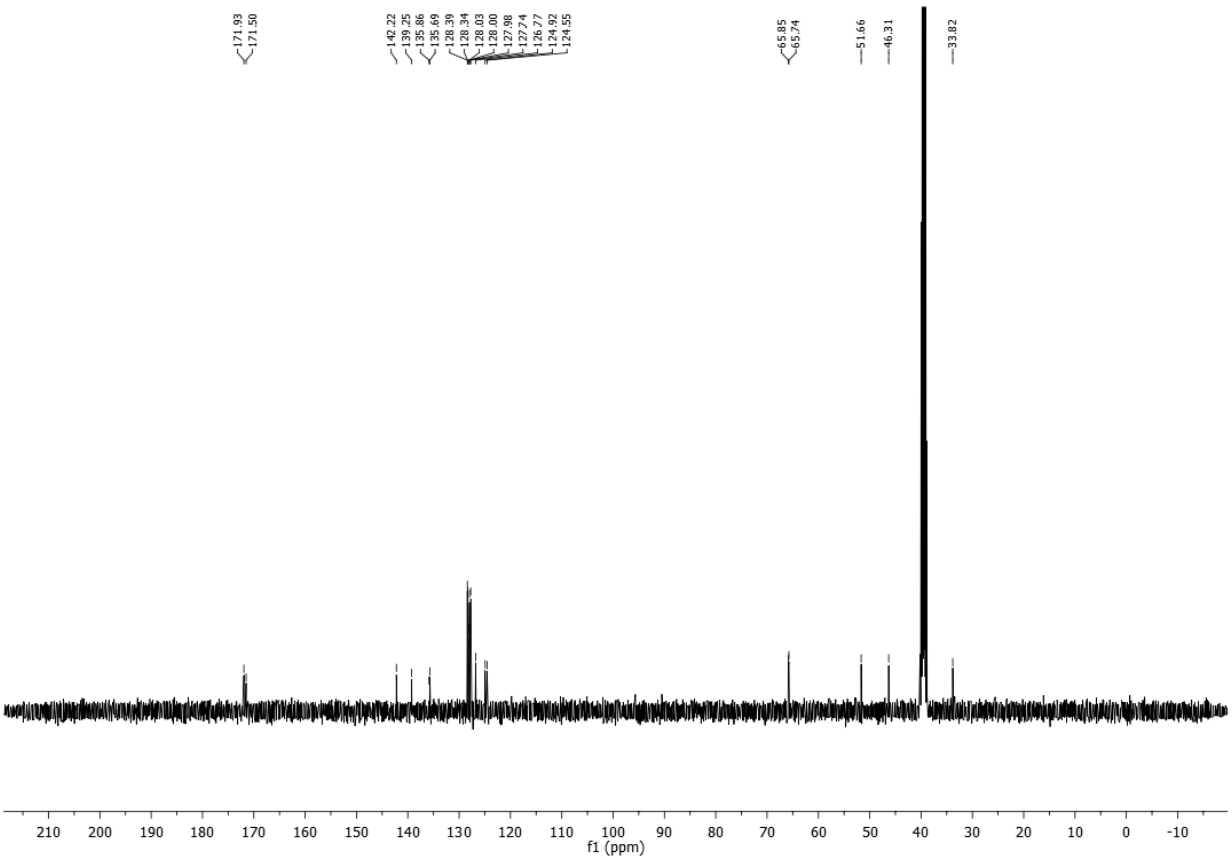


Figure S2 – ^{13}C-NMR spectrum

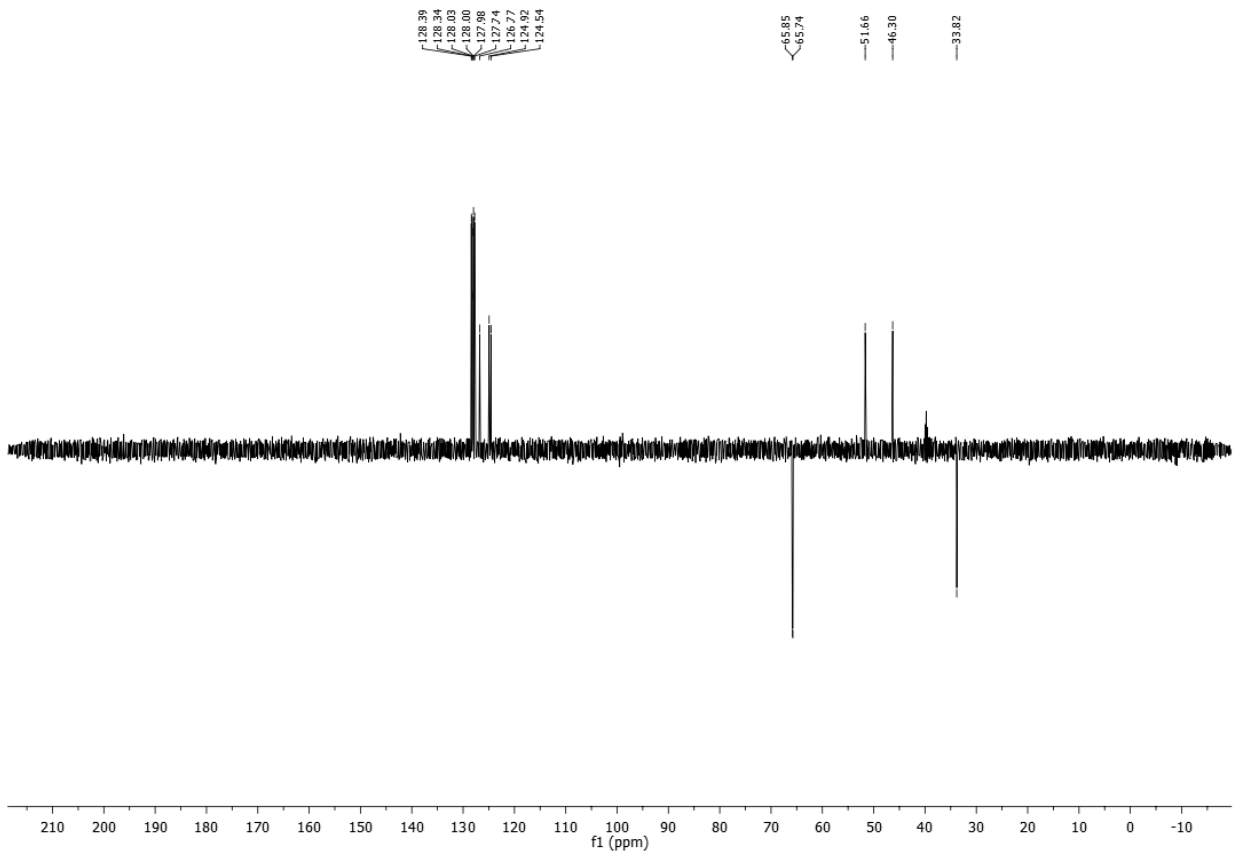


Figure S3 – DEPT 135 (CH and CH_3 positive, CH_2 negative)

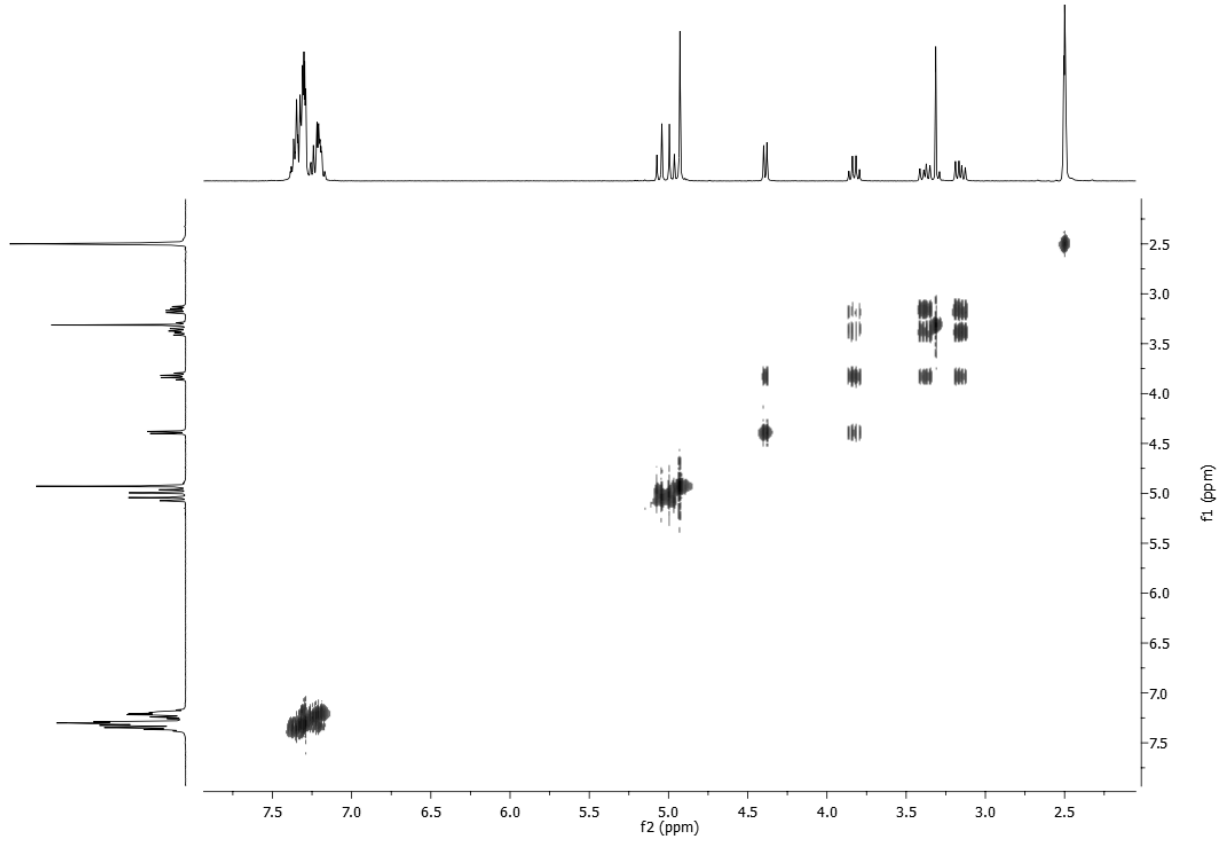


Figure S4 – COSY spectrum

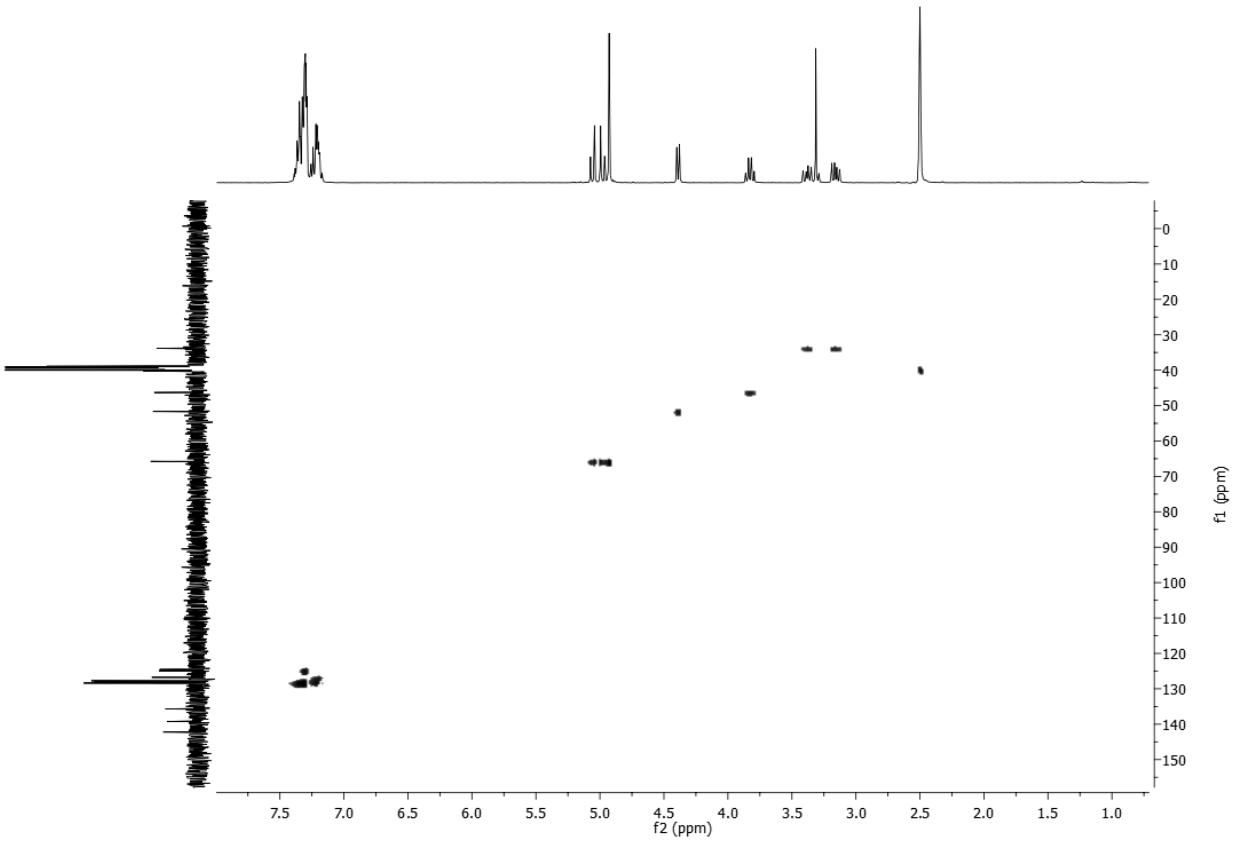


Figure S5 – HSQC spectrum

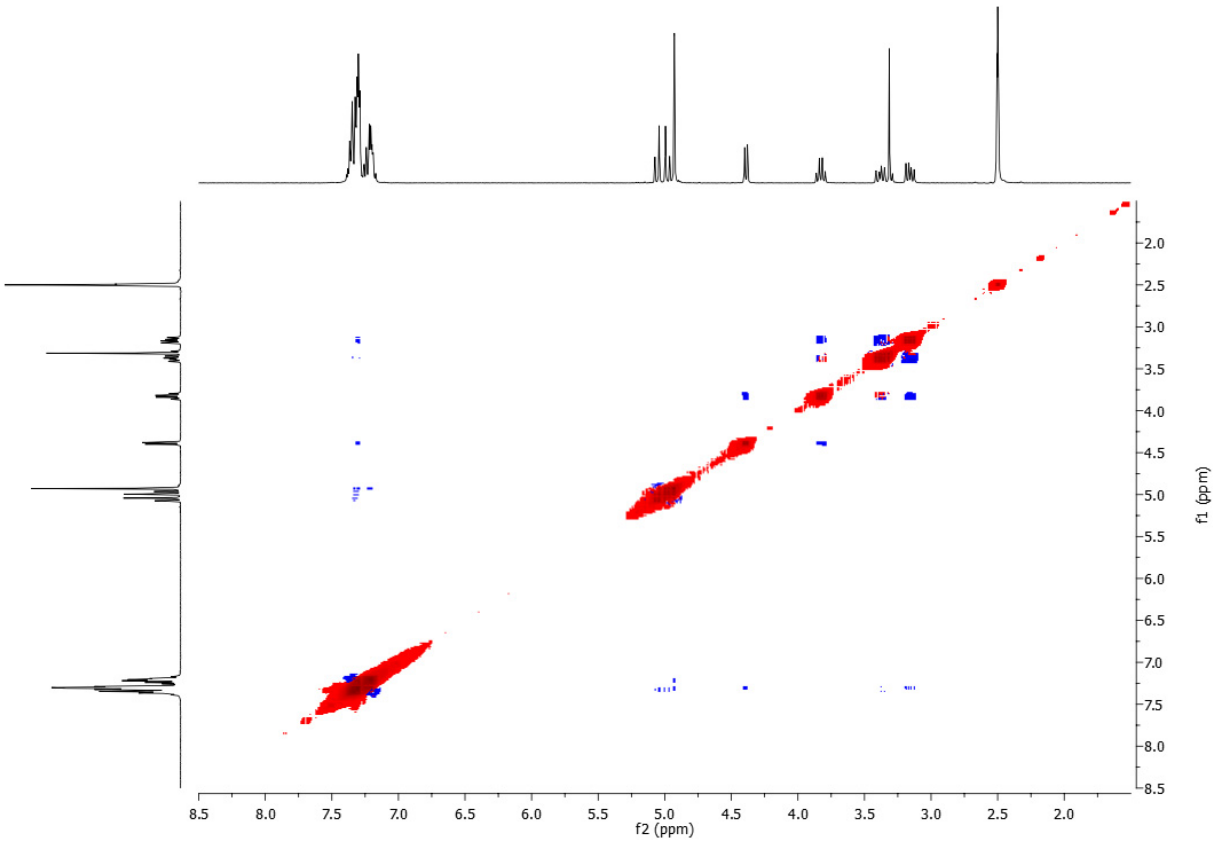


Figure S6 – NOESY spectrum

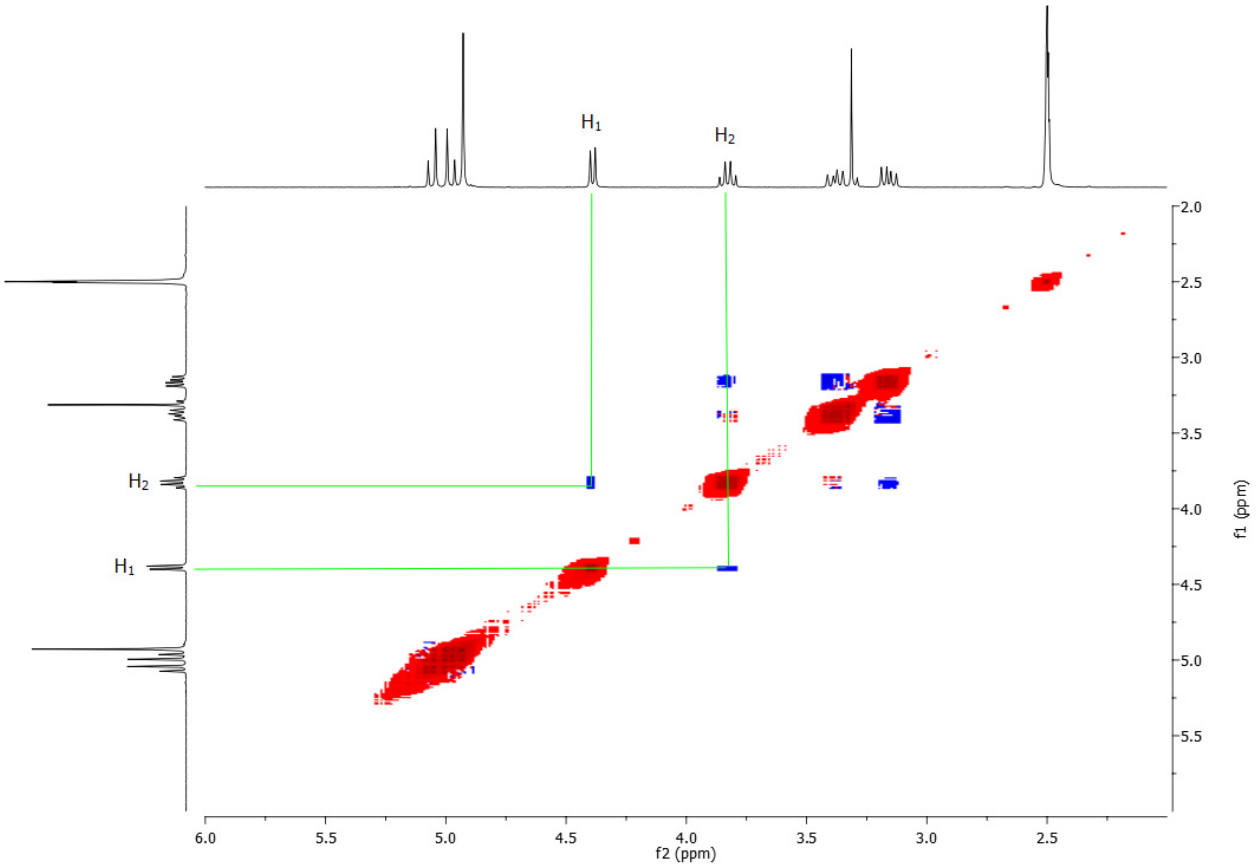
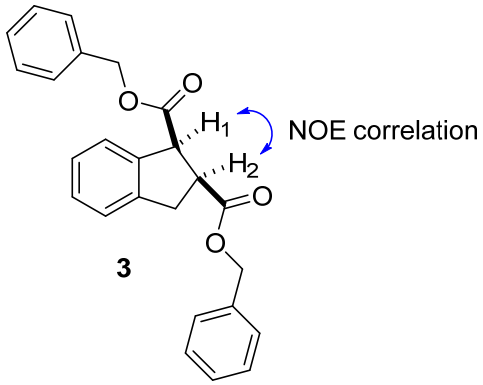


Figure S7 – Zoom of the NOESY spectrum (from 6.0 ppm to 2.0 ppm for both f1 and f2). Observed NOE correlation for H_1 (4.39 ppm) and H_2 (3.83 ppm).



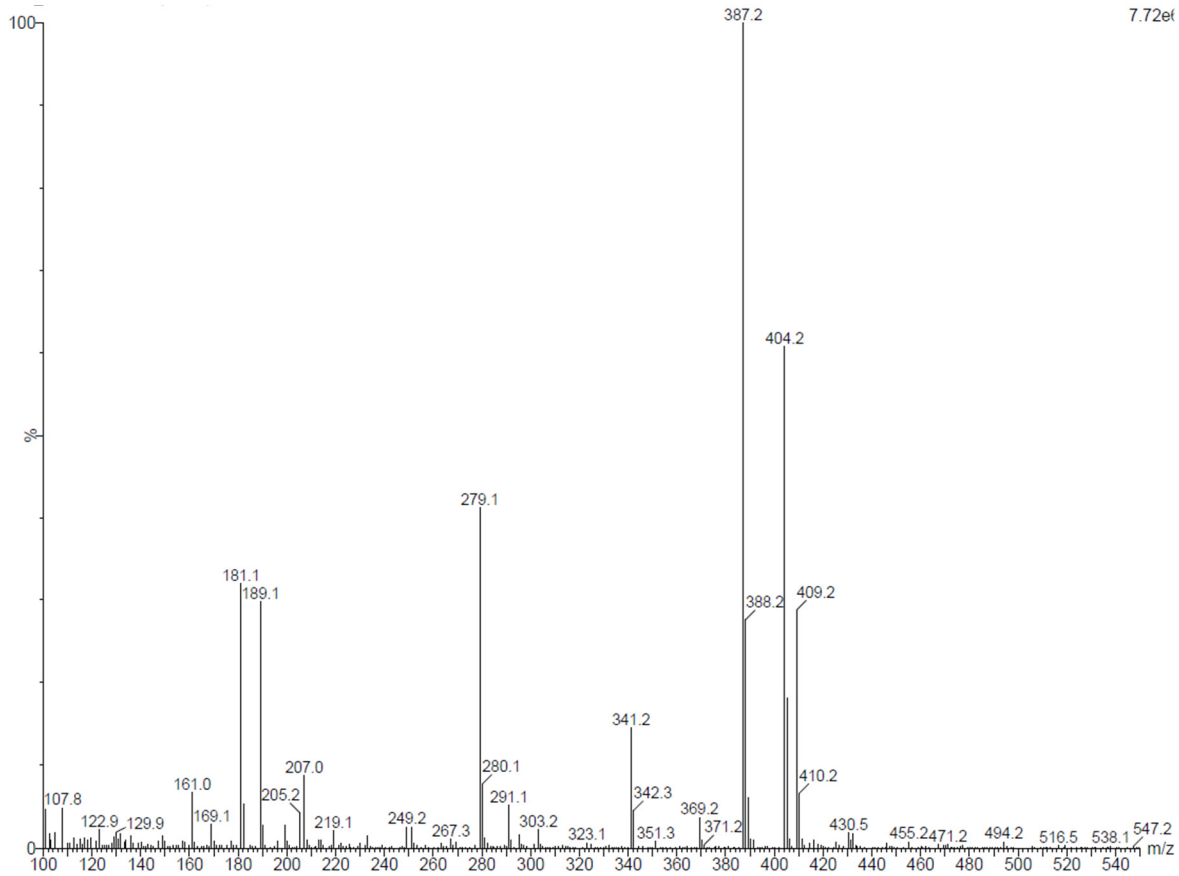


Figure S8 – ESI-MS (ESI+) spectrum of compound **3**