Supplementary Information

Medicinal Electrochemistry of Halogenated and Nitrated Pterocarpanquinones

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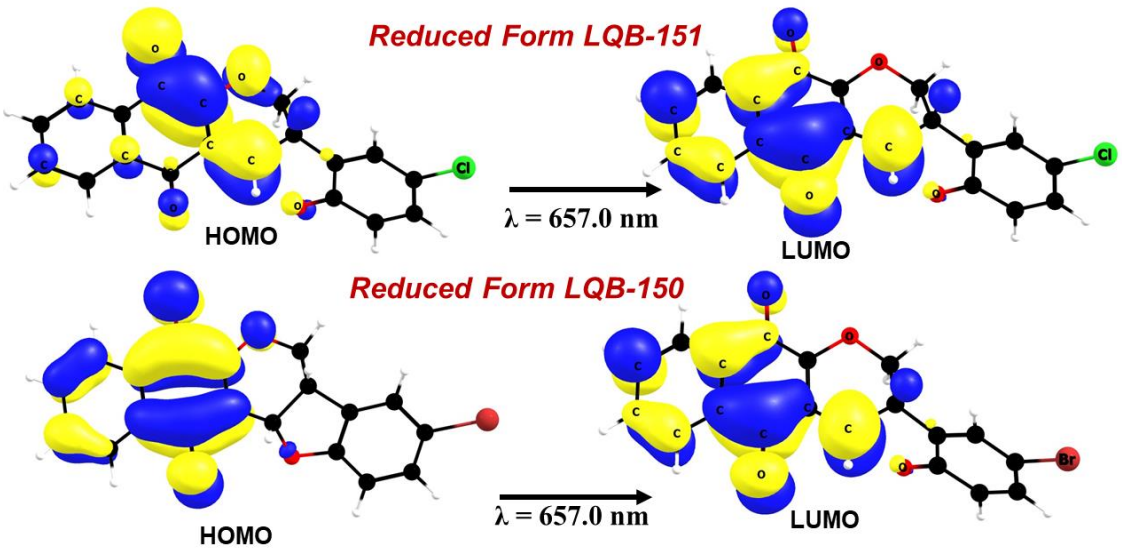

Figure S1. The Kohn-Sham molecular orbitals involved electronic transitions related with the absorption bands at 657 nm in reduced form of **LQB-150** and **LQB-151** molecules.

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Cartesian coordinates of optimized structures of molecules studied

LQB-118

C	−18.004100	3.762694	−0.019674
C	−19.239145	3.129908	0.057831
C	−19.310510	1.778786	0.392978
C	−18.148207	1.059282	0.653622
C	−16.905727	1.684252	0.575945
C	−16.834605	3.045461	0.237260
C	−15.524514	3.724748	0.137982
C	−15.666636	0.910223	0.880643
C	−14.366021	1.571564	0.711142
C	−14.297252	2.879963	0.355953
O	−15.408138	4.910431	−0.118309
O	−15.730195	−0.249655	1.278032
C	−13.131952	0.819229	1.098687
C	−11.862017	1.689864	1.124835
C	−11.954013	2.785004	0.063441
C	−10.811578	0.676593	0.734656
C	−11.468180	−0.406362	0.150608
O	−12.834089	−0.276483	0.163050
C	−10.783512	−1.483770	−0.387891
C	−9.387368	−1.450240	−0.324871
C	−8.713292	−0.378405	0.259848
C	−9.427394	0.701824	0.789993
H	−17.936522	4.811250	−0.278730
H	−20.145086	3.687810	−0.143887
H	−20.273077	1.285888	0.452273
H	−18.196238	0.011440	0.919226

H −7.631141 −0.381183 0.302718

H −8.904153 1.538460 1.238386

H −8.822023 −2.280429 −0.731555

H −11.310605 −2.317749 −0.833856

O −13.167966 3.566984 0.191835

H −11.141820 3.502401 0.143533

H −11.956360 2.349020 −0.938705

H −11.710572 2.128356 2.111117

H −13.289043 0.355063 2.075247

LQB-149

C −18.01016079400689 3.76952216749154 0.07121878153640

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C −19.29890789167244 1.75951267034608 0.38652281534417

C −18.13022656054967 1.03505015535961 0.58572612746701

C −16.89346273003031 1.67171670895352 0.53254491832320

C −16.83189711620744 3.04459045217022 0.25135756836913

C −15.52435630964335 3.72701451406922 0.11550055619068

C −15.65062613666566 0.89860987447555 0.81869039162486

C −14.35719466484633 1.57820975966514 0.67323725494556

C −14.29198973752636 2.88781364561488 0.32522425593992

O −15.41820117955130 4.90405935326480 −0.16787938624719

O −15.70298007450067 −0.26559680604049 1.19382321286485

C −13.12561576446068 0.84108826927738 1.07840669906042

C −11.85714903072352 1.70999239037794 1.11063291750856

C −11.94665828086470 2.80734945087943 0.05281453804177

C −10.80822535358011 0.69677013397579 0.72509903702930

C −11.46996337717720 −0.39350857284192 0.14587244792354

O −12.81054728024167 −0.26409595040015 0.15223926709419

C −10.78856974740723 −1.48804357499277 −0.37307841344083

C −9.40429938746019 −1.47746913762358 −0.28974164555625

C −8.74659297370848 −0.38850402294717 0.28066080917105

C −9.43472905565623 0.72057626461444 0.78725046763524

H −17.95358050427234 4.83097217708984 −0.13145280236299

H −20.15133441562950 3.69765472351532 0.00431912824830

H −20.25705801391841 1.25551341399554 0.42720351064843

H −18.16858414114605 −0.02669221213474 0.79100605295057

H −8.89374422796588 1.55092511384129 1.21794593343121

H −8.82989841383987 −2.31170607119524 −0.66584457601577

H −11.31704542192686 −2.32275608768042 −0.81418027922809

O −13.16483917488746 3.57574608449876 0.16839906989348

H −11.13946364132187 3.52962362013777 0.15057713662039

H −11.92380326369737 2.37806736052210 −0.95312734106660

H −11.70648417900743 2.14722231248589 2.09754121144405

H −13.29160034874908 0.37351915681805 2.05142590617233

N −7.29398261527150 −0.40071115623859 0.34287967819895

O −6.71516587680953 0.64745313185954 0.62091169986568

O −6.70696225991215 −1.45537778542401 0.11147021191704

LQB-150

C −17.998067 3.752595 −0.047853

C −19.231858 3.118384 0.021527

C −19.305161 1.773474 0.378290

C −18.145686 1.062097 0.665725

C −16.903240 1.687628 0.592617

C −16.830402 3.042721 0.235200

C −15.519828 3.727405 0.150529

C −15.666430 0.917756 0.920609

C	−14.364377	1.573658	0.730880
C	−14.293451	2.881065	0.372232
O	−15.407676	4.913454	−0.096735
O	−15.735472	−0.228321	1.349314
C	−13.130181	0.819835	1.110833
C	−11.858238	1.687071	1.135806
C	−11.951236	2.784029	0.077181
C	−10.814989	0.671546	0.738110
C	−11.478983	−0.404768	0.149309
O	−12.835390	−0.274778	0.167207
C	−10.792495	−1.475501	−0.399630
C	−9.397346	−1.449149	−0.348752
C	−8.740508	−0.375824	0.240822
C	−9.432441	0.705579	0.786088
H	−17.930427	4.797108	−0.322434
H	−20.136009	3.670714	−0.202449
H	−20.267391	1.279229	0.433266
H	−18.194900	0.018981	0.948644
H	−8.910710	1.541464	1.233224
H	−8.836594	−2.275620	−0.764285
H	−11.313194	−2.309177	−0.852821
O	−13.162867	3.565641	0.207510
H	−11.135661	3.497710	0.160021
H	−11.949365	2.352669	−0.927172
H	−11.701154	2.120654	2.122935
H	−13.282908	0.349107	2.084269
Br	−6.812070	−0.378337	0.306085

LQB-151

C	−17.997853	3.753269	−0.047663
C	−19.232055	3.120025	0.022660
C	−19.306048	1.775230	0.379788
C	−18.146905	1.063135	0.666967
C	−16.904094	1.687945	0.593429
C	−16.830536	3.042735	0.235020
C	−15.519640	3.726544	0.148881
C	−15.667562	0.917656	0.921501
C	−14.365160	1.572181	0.729408
C	−14.293672	2.879460	0.370264
O	−15.406984	4.912361	−0.099258
O	−15.737217	−0.227600	1.352377
C	−13.131037	0.817933	1.109097
C	−11.859469	1.685488	1.135694
C	−11.951197	2.782053	0.076474
C	−10.815469	0.670638	0.739387
C	−11.478141	−0.405534	0.148776
O	−12.835247	−0.275626	0.164881
C	−10.790556	−1.475450	−0.400618
C	−9.395688	−1.448048	−0.349149
C	−8.742019	−0.374409	0.241712
C	−9.433206	0.705897	0.788189
H	−17.929604	4.797646	−0.322613
H	−20.135922	3.672973	−0.200938
H	−20.268626	1.281716	0.435170
H	−18.196719	0.020136	0.950267
H	−8.906006	1.538518	1.235386
H	−8.827752	−2.270510	−0.763368

H	−11.310559	−2.308774	−0.855076
O	−13.162961	3.563651	0.205101
H	−11.135685	3.495744	0.159903
H	−11.948233	2.350262	−0.927675
H	−11.704063	2.119541	2.122887
H	−13.284105	0.346755	2.082287
Cl	−6.966598	−0.373058	0.301015

Reduced form **LQB-118**

C	2.190708	1.234543	0.433874
C	1.159336	0.164120	0.397278
C	1.553393	−1.199158	0.155092
C	2.850903	−1.620869	−0.121408
O	3.220131	−2.817369	−0.358602
O	1.918200	2.408952	0.686764
O	0.552407	−2.166580	0.224649
C	−0.727426	−1.730745	−0.251273
H	−0.666141	−1.467128	−1.310551
H	−1.394800	−2.584972	−0.130580
C	−2.577875	−0.004159	0.029765
C	−3.703444	−0.100130	0.843538
C	−2.681921	0.575798	−1.297440
C	−4.970477	0.340913	0.445407
H	−3.587750	−0.536900	1.832993
C	−4.001751	1.012472	−1.668699
C	−5.099365	0.900393	−0.828415
H	−4.114104	1.448749	−2.657413
H	−6.069788	1.251625	−1.169003
O	−1.686301	0.691446	−2.084182

C	3.888097	−0.538403	−0.098539
C	3.588206	0.818076	0.152895
C	5.224308	−0.882815	−0.347519
C	4.606802	1.776241	0.156640
C	6.227853	0.076650	−0.345952
H	5.446574	−1.924201	−0.541108
C	5.923959	1.416212	−0.092980
H	4.345437	2.807741	0.357904
H	7.253564	−0.216384	−0.541673
H	6.706497	2.165656	−0.090915
C	−0.147036	0.506455	0.588284
H	−0.400215	1.542981	0.772057
C	−1.242834	−0.518501	0.541128
H	−1.420130	−0.870698	1.567745
H	−5.822872	0.250759	1.108364

Reduced form **LQB-149**

C	2.271099	1.167910	0.601339
C	1.317243	0.125466	0.395219
C	1.692440	−1.168030	−0.068525
C	3.010253	−1.545000	−0.424823
O	3.345842	−2.724780	−0.833855
O	1.957195	2.315523	1.082829
O	0.753827	−2.195313	−0.113614
C	−0.597126	−1.798914	−0.257060
H	−0.752725	−1.352932	−1.249147
H	−1.195352	−2.709049	−0.196158
C	−2.350283	−0.185976	0.458259
C	−3.637837	−0.656780	0.548522

C	−2.077222	1.030136	−0.195013
C	−4.664348	0.116186	−0.021003
H	−3.868146	−1.595635	1.031954
C	−3.093761	1.783302	−0.786982
C	−4.393953	1.314873	−0.688830
H	−2.874962	2.713903	−1.294151
H	−5.209295	1.879174	−1.117919
O	−0.784976	1.359535	−0.197454
C	3.980551	−0.475302	−0.269086
C	3.638175	0.832049	0.230247
C	5.338196	−0.718348	−0.604909
C	4.661835	1.796060	0.363517
C	6.312060	0.245859	−0.467906
H	5.582723	−1.706559	−0.977297
C	5.972220	1.527890	0.025912
H	4.376081	2.770338	0.744284
H	7.340012	0.025039	−0.737162
H	6.736249	2.290186	0.134980
N	−6.029288	−0.342533	0.078914
O	−6.261429	−1.378810	0.719624
O	−6.923767	0.310630	−0.479141
C	−0.081484	0.409147	0.786954
H	−0.114621	0.977751	1.717939
C	−1.025181	−0.799092	0.823138
H	−1.014403	−1.276107	1.803816

Reduced form **LQB-150**

C	2.195009	1.246726	0.402076
C	1.157383	0.180985	0.384540
C	1.544758	−1.186263	0.156676
C	2.841895	−1.620126	−0.102264
O	3.202837	−2.821104	−0.326623
O	1.927576	2.428150	0.624894
O	0.537516	−2.148003	0.220436
C	−0.735862	−1.703391	−0.260235
H	−0.668050	−1.436803	−1.318906
H	−1.410210	−2.552880	−0.145679
C	−2.581401	0.019965	0.022740
C	−3.708954	−0.131916	0.825175
C	−2.685543	0.626289	−1.292660
C	−4.965248	0.293026	0.400942
H	−3.599560	−0.590564	1.802181
C	−4.010547	1.043724	−1.664569
C	−5.120054	0.883191	−0.847756
H	−4.130858	1.503785	−2.640604
H	−6.094566	1.217080	−1.185253
O	−1.686789	0.780216	−2.065626
C	3.887168	−0.546116	−0.079622
C	3.592648	0.816659	0.140862
C	5.224061	−0.904724	−0.303156
C	4.616993	1.768630	0.134208
C	6.233328	0.048519	−0.311803
H	5.441493	−1.951726	−0.470600
C	5.934449	1.395291	−0.093712
H	4.360212	2.806008	0.309289

H	7.259496	−0.254814	−0.488435
H	6.721246	2.140214	−0.101716
C	−0.147305	0.533691	0.570272
H	−0.395063	1.574033	0.737462
C	−1.245068	−0.489145	0.534252
H	−1.418537	−0.840443	1.561430
Br	−6.504902	0.054017	1.558356

Reduced form **LQB-151**

C	2.192290	1.242095	0.419240
C	1.156152	0.174966	0.394243
C	1.545823	−1.191324	0.164082
C	2.845675	−1.623610	−0.083191
O	3.212097	−2.825531	−0.293081
O	1.924133	2.421028	0.654387
O	0.539679	−2.155350	0.222800
C	−0.734948	−1.712600	−0.255877
H	−0.669434	−1.447159	−1.314993
H	−1.407831	−2.562990	−0.139230
C	−2.579899	0.012934	0.024236
C	−3.710658	−0.138611	0.821613
C	−2.677498	0.626047	−1.288589
C	−4.962008	0.295255	0.393992
H	−3.611354	−0.601161	1.798162
C	−3.999300	1.050746	−1.663870
C	−5.112099	0.892108	−0.851256
H	−4.112933	1.515970	−2.638132
H	−6.086041	1.231588	−1.185691
O	−1.675242	0.779681	−2.056971

C	3.886722	−0.545444	−0.072420
C	3.589202	0.816770	0.147379
C	5.222265	−0.899331	−0.310639
C	4.610013	1.772411	0.129210
C	6.227640	0.057842	−0.333330
H	5.441779	−1.945695	−0.479246
C	5.926191	1.403729	−0.113266
H	4.351372	2.809263	0.304718
H	7.252606	−0.241809	−0.522779
H	6.709967	2.151640	−0.131421
Cl	−6.384641	0.084332	1.461583
C	−0.149369	0.524577	0.579011
H	−0.399532	1.563785	0.749550
C	−1.245860	−0.498769	0.538715
H	−1.422036	−0.850637	1.565183

Spectral data for the product of reductive thioalkylation, compound **1**

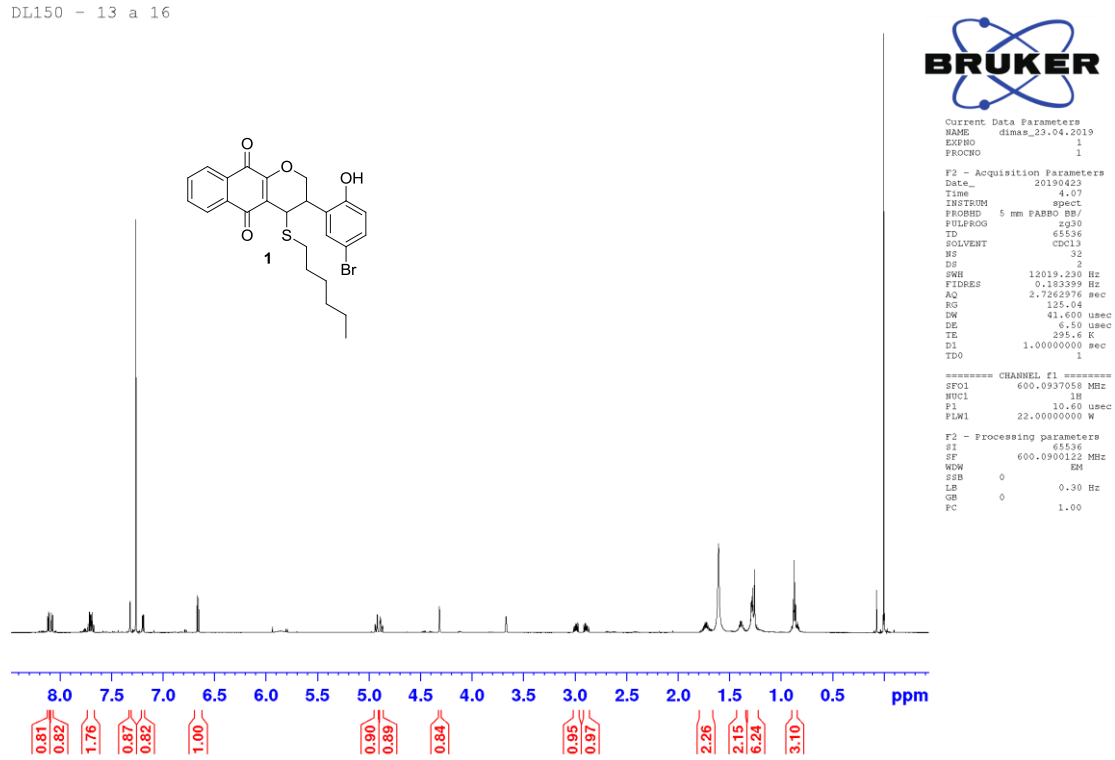

Figure S2. ^{1}H NMR (600 MHz, $CDCl_3$) of compound **1**.

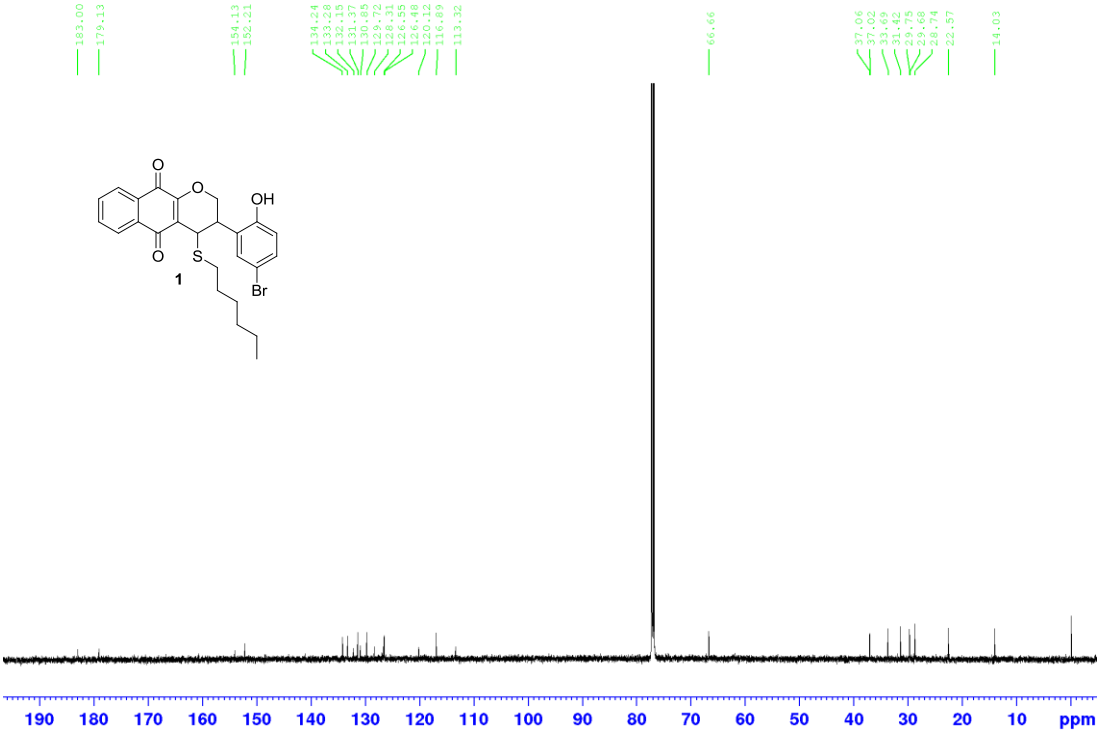

Figure S3. ^{13}C NMR (150 MHz, $CDCl_3$) of compound **1**.

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