Supplementary material to:

N. Benhadria, T. Attar and B. Messaoudi,

Understanding the Link Between the Detection Limit and the Energy Stability of Two Quercetin–Antimony Complexes by Means of Conceptual DFT,

S. Afr. J. Chem., 2020, **73**, 120–124.

Quercetin (Q) **Quercetin-5-sulfonic acid (QSA)**

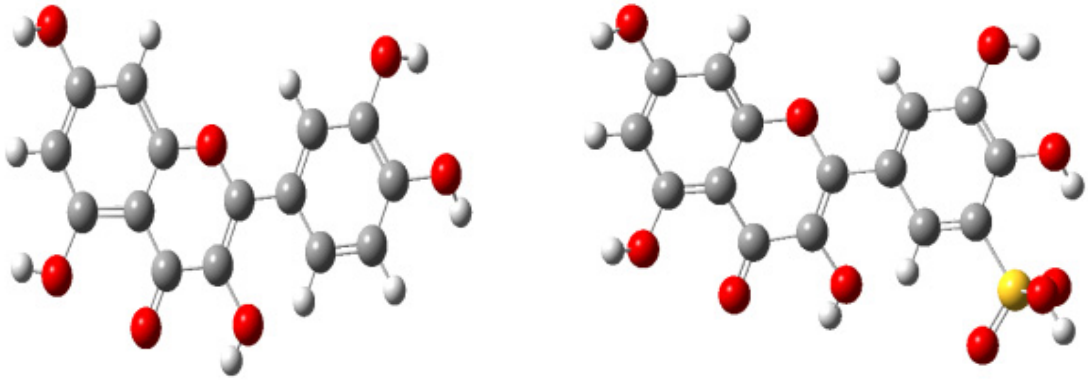


Figure 1S Molecular structures of the quercetin and its derivative.

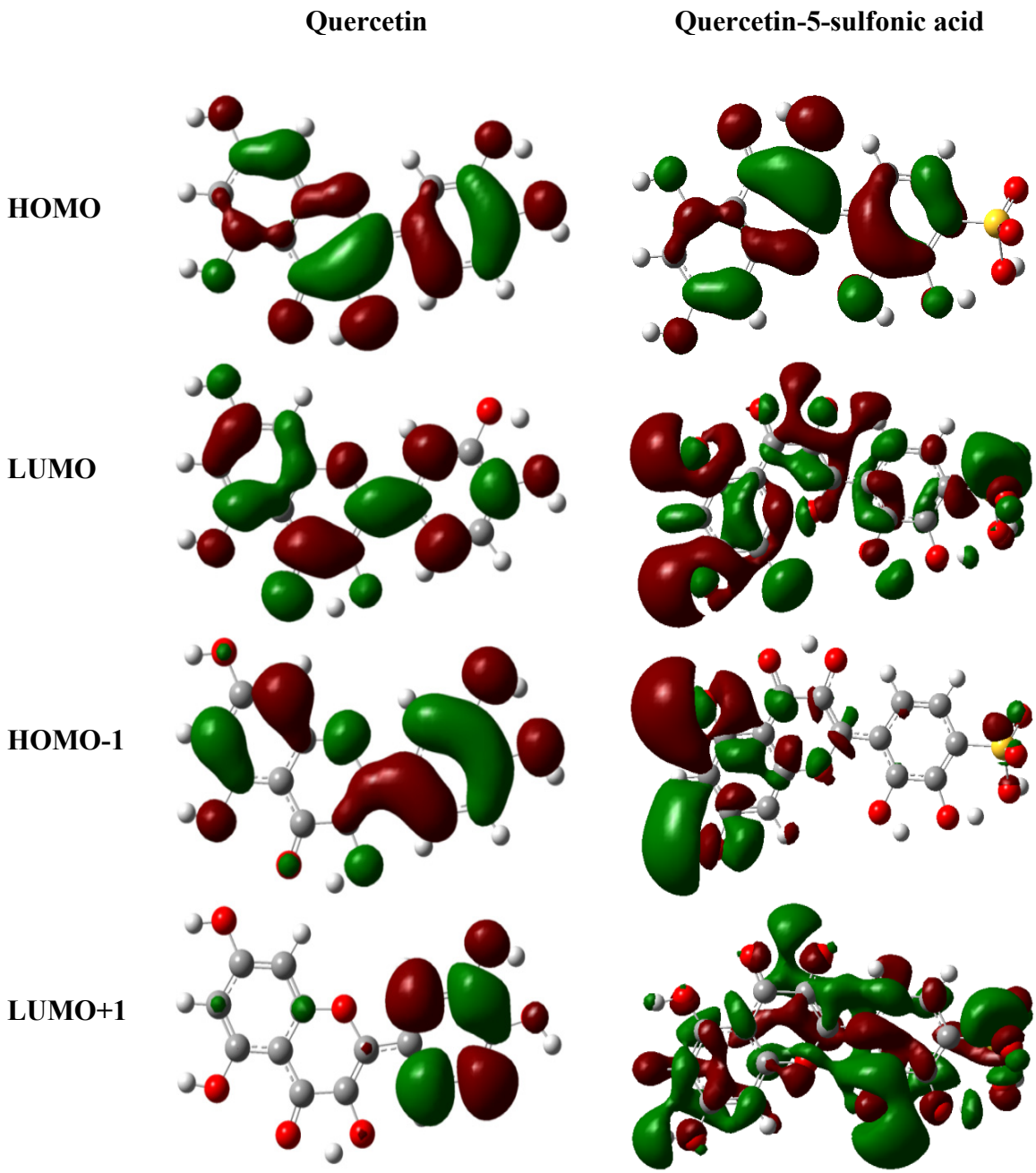


Figure 2S Calculated HOMO, LUMO, HOMO-1 and LUMO+1 molecular orbitals of the studied molecules at the HF/3-21G level of theory.

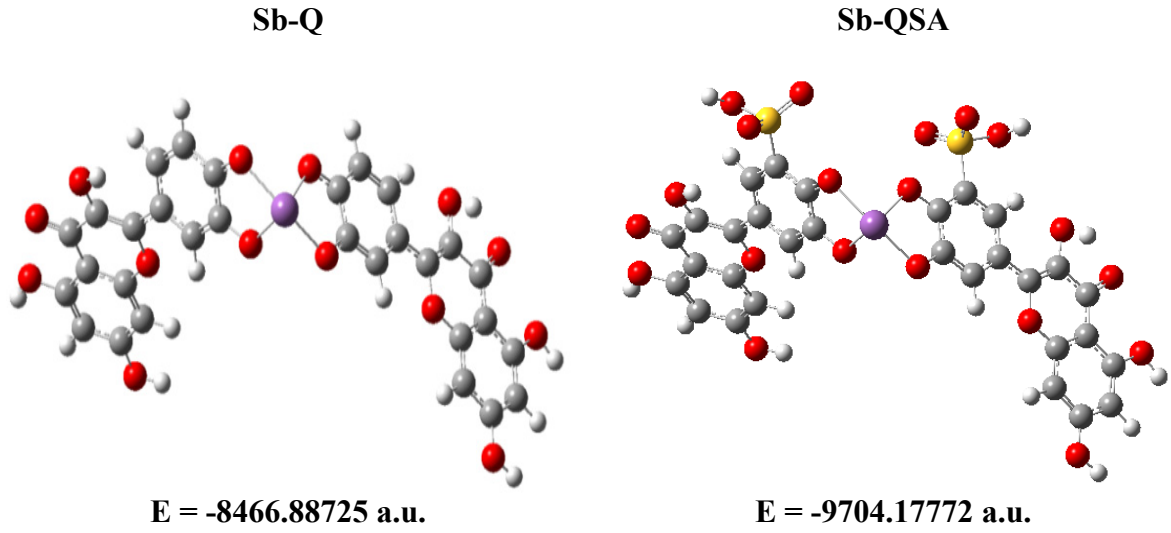


Figure 3S Molecular structures of Sb-Q and Sb-QSA complexes at the LSDA/3-21G(d) level of theory

LSDA/3-21G(d) Cartesian coordinates of the optimized stationary points (Ligands and complexes) calculated.

Quercetin

C	-4.38829000	0.83764700	0.00000000
C	-3.77058400	-0.40025300	-0.00001500
C	-2.36298700	-0.48069300	0.00002400
C	-1.63206600	0.72388500	0.00002000
C	-2.25369500	1.96096400	-0.00021600
C	-3.63785000	2.01961600	-0.00021600
H	-5.48378800	0.89294900	0.00054500
H	-1.66112500	2.87455800	-0.00068500
C	0.46427000	-0.45632600	-0.00007200
C	-0.20604800	-1.63864300	0.00003400
C	1.88553100	-0.26772300	-0.00016300
C	2.73953200	-1.38082200	-0.00042400
C	2.41157100	1.03350500	0.00013200
C	4.11611800	-1.18627500	-0.00044700

H	2.28172800	-2.37523800	-0.00062400
C	3.77594400	1.21915200	0.00009400
H	1.74275900	1.89518700	0.00049700
C	4.62399200	0.09653500	-0.00017600
H	4.78852500	-2.05116200	-0.00077500
O	-4.44777600	-1.57333400	0.00011500
H	-5.43575900	-1.40237700	0.00015900
O	-4.21135700	3.25367200	0.00002500
H	-5.20943400	3.17334500	-0.00054800
O	-0.26781800	0.72206500	-0.00005200
O	0.32915900	-2.87463300	0.00007000
H	-0.60729600	-3.43139400	-0.00017000
O	4.37717800	2.44069200	0.00044800
H	5.37180600	2.22543000	0.00030900
O	5.95183000	0.47598600	-0.00023600
H	6.56725000	-0.30851200	0.00348300
O	-2.10598500	-2.90697800	0.00033600
C	-1.65818700	-1.71265900	0.00011900

Quercetin-5-sulfonic acid

C	-5.56690700	-0.83002600	0.02177200
C	-4.97799400	0.42090400	0.00644000
C	-3.57175900	0.53094800	0.00058200
C	-2.81471100	-0.65765700	0.01084300
C	-3.40774200	-1.90836300	0.02590300
C	-4.78974000	-1.99640700	0.03163800
H	-6.66078700	-0.91042400	0.02640500
H	-2.78601500	-2.80221100	0.03427800
C	-0.74011200	0.55303800	-0.00700000
C	-1.43219800	1.72679800	-0.01678900
C	0.68350800	0.40550900	-0.00728300

C	1.49506200	1.56650300	-0.01550500
C	1.30060600	-0.84911100	-0.02233800
C	2.86716200	1.47997500	-0.01924400
H	0.97034900	2.52833700	-0.02664700
C	2.70507200	-0.93054100	-0.01962600
C	3.47881700	0.21759700	-0.00673500
H	3.49833800	2.37219100	-0.04890800
O	-5.33829300	-3.24095800	0.04685600
H	-6.33784100	-3.18175000	0.05204700
O	-5.67773800	1.57995000	-0.00359400
H	-6.66245900	1.39183000	0.00386200
O	-0.93291300	2.97442900	-0.03039500
H	-1.89173300	3.50762600	-0.03344500
O	3.15753900	-2.21577200	-0.07096200
H	4.16772000	-2.18052700	-0.35146700
O	-1.45367600	-0.63108800	0.00638800
C	-2.89046100	1.77175400	-0.01399500
O	-3.35485300	2.96000600	-0.02542600
O	0.66919600	-2.04618700	-0.05897600
H	1.45330100	-2.71214600	-0.08991400
O	5.39762800	-1.34417400	-0.66614000
H	5.80886700	-1.19932100	-1.57291200
O	5.81484800	1.14236600	-0.68956000
O	5.64246700	-0.14931400	1.48866000
S	5.18843700	0.12167600	0.13874400

Complex Sb-Quercetin

C	-2.38770100	-1.96521800	-0.50926300
C	-3.25722400	-0.89656200	-0.49815300
C	-4.47670200	-0.99071000	0.18454300
C	-4.79598000	-2.17689300	0.89051000

C	-3.93142900	-3.25481800	0.86767000
C	-2.73004100	-3.17928800	0.16102900
H	-2.99842700	0.02787300	-1.01692500
H	-5.66654400	-2.19232100	1.55580400
H	-4.15058900	-4.17062100	1.42075600
C	3.82884500	-0.74265800	0.83247800
C	3.22641900	-1.13423100	-0.36749100
C	2.12259700	-1.96603600	-0.34251100
C	1.60841500	-2.41719200	0.91694800
C	2.23208900	-2.04030100	2.10708700
C	3.32485300	-1.20356900	2.07579100
H	3.62536200	-0.78331200	-1.32015100
H	1.82313300	-2.41068300	3.04939900
H	3.83490800	-0.86768200	2.98461200
O	-1.20089500	-1.94173900	-1.16116400
O	-1.86704500	-4.19214500	0.05042700
O	0.53234000	-3.21632800	0.88647000
O	1.50018100	-2.42905500	-1.43572700
Sb	-0.13245500	-3.66331700	-1.00684500
O	5.35767700	0.51386900	-0.45818500
O	5.44351800	0.34036000	3.17676400
H	6.27173100	0.94693600	3.58045100
C	6.42462300	1.34252800	-0.66514000
C	6.72180100	1.65839100	-1.97711000
H	6.12149000	1.25559600	-2.79154500
C	7.79684200	2.49508300	-2.24297300
C	8.56400500	3.00641100	-1.19000200
H	9.41201300	3.66598800	-1.40946800
C	8.26874900	2.69303500	0.12461400
C	7.17893300	1.84511100	0.41395500

C	5.66494500	0.59445900	1.88130300
C	4.95819600	0.12459700	0.80926700
C	6.81415400	1.48087200	1.73175800
O	7.33864400	1.80846800	2.84778200
O	8.97140000	3.15567400	1.18314600
H	9.72245600	3.74508600	0.87704000
O	8.05223400	2.77932400	-3.54577400
H	8.84521000	3.38548300	-3.62785000
C	-5.37002100	0.13278600	0.17419600
C	-6.72346000	0.07523300	0.35771600
C	-7.57481500	1.27043400	0.38530300
O	-4.75196900	1.33047800	-0.11220200
O	-7.39424000	-1.09427900	0.51543500
H	-6.80676500	-1.85764200	0.19967800
O	-8.79699400	1.17769900	0.59594900
O	-4.80071300	6.05155300	-0.68183800
H	-3.82396400	5.90362700	-0.84662200
C	-4.75288600	3.64801900	-0.40455000
H	-3.68045800	3.55570200	-0.59049100
C	-5.47382600	2.49708900	-0.12784300
C	-5.41647900	4.86595900	-0.42451600
C	-6.84707100	2.50302700	0.13122600
C	-7.50216800	3.75488100	0.10713500
C	-6.78615800	4.90733600	-0.16795800
H	-7.27378500	5.88582100	-0.18957600
O	-8.83281200	3.77294900	0.35853700
H	-9.16823200	4.71799500	0.30691300

Complex Sb-Quercetin-5-sulfonic acid

C	-2.18179700	-0.87545700	-1.22811000
C	-2.91728500	0.26215100	-0.98239400

C	-4.16490300	0.17215900	-0.34661200
C	-4.65018200	-1.08447000	0.07001800
C	-3.91707300	-2.22702100	-0.19124200
C	-2.68634700	-2.15547100	-0.84876700
H	-2.53438900	1.23925800	-1.28014300
H	-5.53913000	-1.19820800	0.69842500
C	4.01113900	-0.50773800	0.24789900
C	3.40705000	-0.63392200	-1.00909000
C	2.24661300	-1.37119300	-1.14504100
C	1.67288300	-1.99960700	0.00285900
C	2.30232800	-1.88318500	1.24468900
C	3.45203300	-1.13614000	1.38164400
H	3.85252200	-0.15005000	-1.87926000
H	3.92774800	-1.02066500	2.36067300
O	-0.98559200	-0.86748900	-1.85661300
O	-1.96351000	-3.22085000	-1.16839500
O	0.54858600	-2.70380300	-0.16430700
O	1.61299100	-1.58747300	-2.30685000
Sb	-0.13937600	-2.69829200	-2.11058000
O	5.65839200	0.83616300	-0.78153200
O	5.63732600	0.00792100	2.75950900
H	6.49045600	0.47230100	3.28192100
C	6.78801700	1.60655100	-0.82278500
C	7.14312000	2.12190000	-2.05379500
H	6.54009700	1.91203300	-2.93599900
C	8.28191800	2.91022300	-2.15215300
C	9.05207800	3.17403600	-1.01382500
H	9.94927200	3.79812100	-1.10088000
C	8.69893600	2.65945300	0.22080700
C	7.54526700	1.85544400	0.33977100

C	5.91097900	0.47612000	1.53748700
C	5.20128100	0.26155900	0.38983600
C	7.12226200	1.29096700	1.56639400
O	7.63605100	1.37445500	2.73028600
O	9.40008800	2.87705100	1.35529300
H	10.19958400	3.45413900	1.17368900
O	8.59276300	3.39438200	-3.38086100
H	9.42901900	3.94446900	-3.34641700
C	-4.91616300	1.37216000	-0.11646600
C	-6.26812100	1.44589400	0.08622400
C	-6.95908000	2.71120700	0.37850900
O	-4.15355200	2.51600900	-0.16702400
O	-7.08759600	0.37108900	0.02306700
H	-6.62361400	-0.39345700	-0.45201500
O	-8.18155900	2.72853000	0.60198600
O	-3.60290600	7.22448200	0.21524200
H	-2.65081900	6.99478500	0.00575000
C	-3.85864700	4.82709700	0.00934300
H	-2.80544100	4.64117300	-0.21259900
C	-4.72063000	3.74434200	0.06698300
C	-4.36358600	6.09837400	0.24565400
C	-6.08239400	3.86878200	0.35257300
C	-6.57510200	5.17204700	0.59074800
C	-5.71805900	6.25782900	0.53369600
H	-6.07799200	7.27420900	0.71519900
O	-7.89303300	5.30313600	0.86791200
H	-8.11027000	6.27217100	1.01632700
O	2.62512900	-2.23614600	3.74246600
H	3.06126800	-3.06534100	4.11469800
O	-5.84894800	-3.32145600	1.02284200

H	-5.83591100	-3.69248500	1.96033800
S	1.56035400	-2.68389600	2.60004200
S	-4.49160800	-3.80407400	0.26152200
O	-4.87555500	-4.53379100	-0.93322900
O	-3.64164200	-4.41325000	1.27603500
O	0.28632500	-2.06161100	2.90404300
O	1.68581900	-4.13067100	2.46084400