

Electronic Supporting Information

Antioxidant Potential of Four Flavonoids from *Scutellaria Baicalensis*: A Computational Investigation on Radical Scavenging Activity and Enzyme Inhibition

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Fig. S1 Optimized structures of the baicalein, wogonin, baicalin, and wogonoside at the M06-2X/6-311+G(d,p) level in the gas phase.

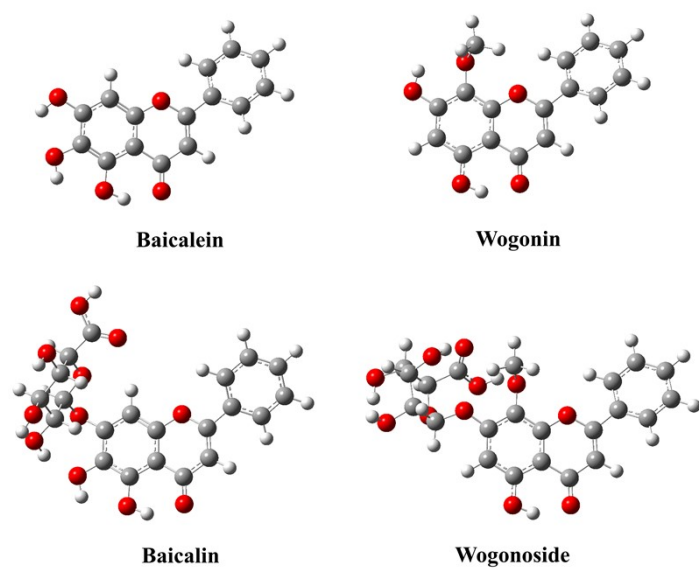
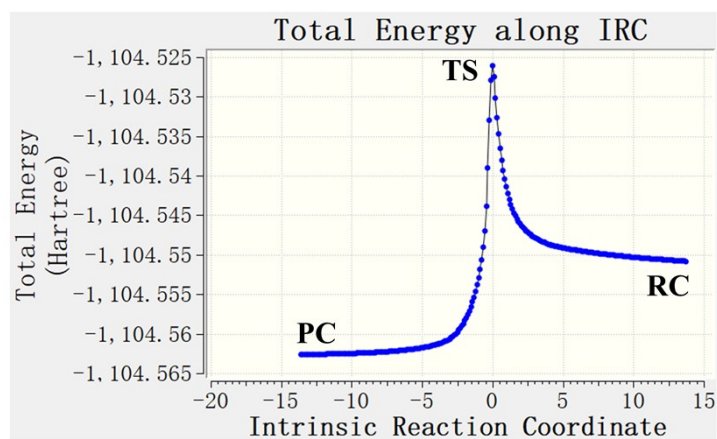
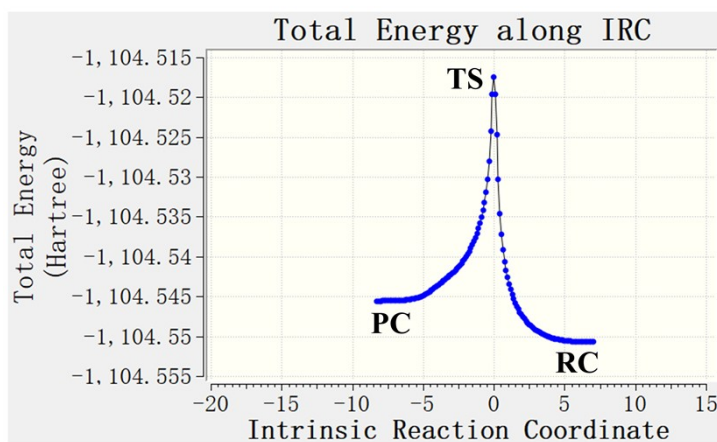


Fig. S2 IRC plots for all transition states related to reactions of baicalein, wogonin, and baicalin and $\cdot\text{OOH}$ radical at the M06-2X/6-311+G(d,p) level in the gas phase.

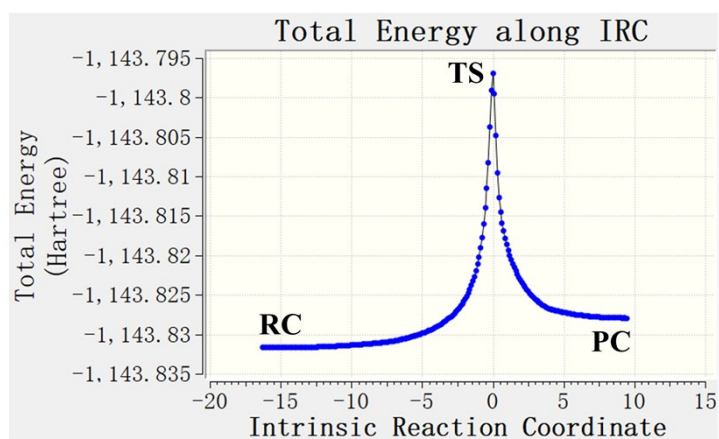
Baicalein-6-OH + $\cdot\text{OOH}$



Baicalein-7-OH + $\cdot\text{OOH}$



Wogonin-7-OH + $\cdot$ OOH



Baicalin-6-OH + $\cdot$ OOH

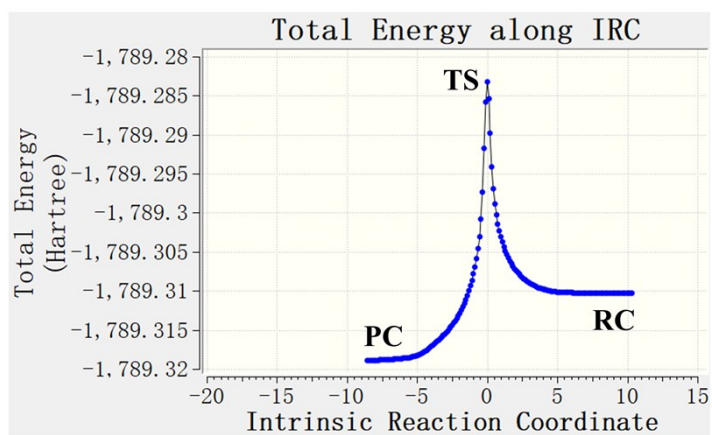


Table S1 Optimized coordinates (x, y, z) of baicalein, wogonin, baicalin, and wogonoside at the M06-2X level.

Baicalein

O	-0.61586400	-0.73280300	0.06668400
O	3.37957400	1.94573200	-0.11461300
O	4.85927900	-0.34358900	0.02003500
O	3.64508600	-2.73851500	0.17069000
O	0.97599800	3.00280900	-0.17651800
C	1.32346000	0.67764100	-0.02874400
C	0.74240300	-0.59129300	0.04942300
C	-1.41623700	0.35110100	-0.00435800
C	2.72874900	0.77158600	-0.03987000
C	0.49091300	1.86908300	-0.10346900
C	-0.93413100	1.61119400	-0.09774000
C	-2.84641200	-0.01182800	0.00873400
C	1.49771000	-1.75087100	0.11842700
C	3.49572700	-0.37568700	0.02698600
C	2.88184500	-1.63058400	0.10563300
C	-3.80853500	0.90988200	0.43045300
C	-3.24957300	-1.28331000	-0.40746600
C	-5.15400200	0.56975100	0.41859400
C	-4.59759200	-1.61767900	-0.42082900
C	-5.55224200	-0.69316200	-0.01021800
H	-1.60615000	2.45125900	-0.19519600
H	1.03096400	-2.72360100	0.18314300
H	-3.50394100	1.88475300	0.79116100
H	-2.50488700	-2.00112400	-0.72620600
H	-5.89204600	1.28811200	0.75391400
H	-4.90260800	-2.60264500	-0.75268400
H	-6.60292100	-0.95708600	-0.01800600
H	2.69751200	2.65496500	-0.15754900
H	5.14489200	0.57668000	-0.03594900
H	4.57409900	-2.47532200	0.15380700

Wogonin

O	0.38504700	0.38942700	-0.06063600
O	-1.24909700	2.60498400	-0.17512400
O	-3.50408700	-2.42504000	-0.00626400
O	-3.92774400	2.26008800	-0.20270600
O	-1.06371700	-3.40523400	0.05141200
C	-1.51702700	-1.09032700	-0.02377400
C	-0.96127400	0.19365000	-0.06525500
C	1.22842400	-0.67028100	-0.03219000
C	-1.75378600	1.33085600	-0.10464900
C	-0.63627500	-2.24926500	0.01482700
C	-2.92800100	-1.22043300	-0.04111000
C	0.78514300	-1.94344400	-0.00602000
C	2.64076300	-0.24617200	-0.05272100
C	-3.14271600	1.16842200	-0.13589900
C	-3.73197000	-0.09201000	-0.10214100
C	3.64408100	-1.09179700	0.42814100
C	2.98450600	1.01091900	-0.55810700
C	4.97237500	-0.69203400	0.38758300
C	4.31604600	1.40480400	-0.59858000
C	5.31205400	0.55543600	-0.12845600
C	-0.62820600	3.05986900	1.03058200
H	1.48027200	-2.77022700	-0.02363100
H	-4.80867300	-0.18998600	-0.12796400
H	3.38481300	-2.05288800	0.85525400
H	2.20737700	1.66825100	-0.92777800
H	5.74301800	-1.35125500	0.76798100
H	4.57579300	2.37662500	-1.00042000
H	6.34964500	0.86542800	-0.15884500
H	-2.79201600	-3.09973800	0.02514500
H	-3.35174400	3.02875900	-0.31142400
H	-0.34974100	4.09802600	0.85980400
H	-1.33026900	2.99445400	1.86650000
H	0.26349400	2.46960800	1.24853300

Baicalin

O	2.33967900	-1.03540700	-1.04448800
O	2.09107100	1.08224100	-1.83811100
O	4.58612100	0.12404100	2.20809100
O	4.12079800	1.94699700	0.09305800
O	4.36056500	-2.59891000	1.52166200
O	3.01051900	-4.37290000	-0.69575600
O	1.15081400	-3.30854400	-0.04122300
O	-2.32440700	-0.04098400	-0.48151500
O	1.84112100	3.53534800	-0.71159500
O	-0.47480200	4.31003900	0.40751800
O	-2.91815200	3.65732400	1.10242300
C	4.26224900	-0.26364900	0.89132700
C	3.37765500	0.75847200	0.20333600
C	3.54137600	-1.59596800	0.97594800
C	2.97026500	0.21959400	-1.16834100
C	3.14496100	-2.02370500	-0.44040800
C	2.30160000	-3.28688100	-0.36944400
C	0.91009300	1.38857000	-1.20842700
C	-0.13491900	0.47574900	-1.14749300
C	0.78336000	2.67441500	-0.67649500
C	-1.31488700	0.87499500	-0.54105600
C	-1.48456700	2.15729700	-0.01352300
C	-0.41326900	3.06077200	-0.08719500
C	-2.74462400	2.53272600	0.62438100
C	-3.49257300	0.26835600	0.11279900
C	-3.73751400	1.48263100	0.66045000
C	-4.43157900	-0.86894500	0.11211600
C	-3.94141700	-2.17521800	0.02845300
C	-5.80924100	-0.65316000	0.20222600
C	-4.82104900	-3.24966500	0.05556100
C	-6.68346800	-1.73085000	0.22426900
C	-6.19121500	-3.03105800	0.15453600
H	5.18131600	-0.39286700	0.29964000
H	2.47290200	0.90580500	0.81000700
H	2.62244100	-1.46894700	1.56472400
H	3.84884300	0.15423400	-1.82069200
H	4.04860500	-2.22032700	-1.03046200

H	4.95003100	1.01542400	2.16955400
H	3.53515800	2.64514700	-0.23389300
H	4.72471800	-2.25552800	2.34505300
H	-0.01637000	-0.52299900	-1.54202700
H	2.44507500	-5.14589200	-0.56052600
H	-4.67245800	1.67849400	1.16478900
H	1.55335400	4.37084100	-0.31851200
H	-1.37374200	4.42862400	0.79281900
H	-2.87446500	-2.34339300	-0.04700200
H	-6.19968300	0.35695300	0.23001600
H	-4.43397200	-4.25973400	-0.00019500
H	-7.75051700	-1.55563200	0.28633000
H	-6.87525600	-3.87102100	0.17174500

Wogonoside

O	3.51621200	0.39831800	-1.29930500
O	2.04050700	0.39292700	0.48126800
O	3.83998400	-1.56213100	1.83853900
O	5.44263500	1.43731700	0.53648900
O	6.11081100	-0.93109800	-0.96575300
O	1.47215500	-1.39986200	-1.85225200
O	2.35560100	-2.67580000	-0.24815700
O	-2.58557800	-0.10631300	0.12842800
O	-0.14938400	-1.19334900	0.31851200
O	-0.66346700	4.27496600	-0.14838100
O	-3.25423400	3.87410700	-0.32735200
C	4.73838200	-0.84156000	1.03269100
C	4.34687400	0.64548800	0.97902700
C	4.90645400	-1.39479100	-0.39644300
C	3.24313200	0.93348800	-0.03727800
C	3.74415300	-1.00437600	-1.31666700
C	2.45702900	-1.78348000	-1.05773100
C	0.84575000	1.01394400	0.26474300
C	-0.27005300	0.16743500	0.25614700
C	0.70506300	2.39440500	0.13656300
C	-1.52728700	0.74454700	0.11687200
C	-1.70173900	2.12295800	-0.03314300
C	-0.55832600	2.95023600	-0.02230200
C	-3.04597300	2.66636900	-0.19573900
C	-3.84383100	0.36476900	-0.03157500
C	-4.10795000	1.67798300	-0.20197100
C	-4.84177400	-0.72115000	-0.01363300
C	0.12538200	-1.70776500	1.62820600
C	-4.44213900	-2.03918000	-0.25240100
C	-6.18881500	-0.44669100	0.23952500
C	-5.38242500	-3.06160900	-0.25910600
C	-7.12321900	-1.47227800	0.23386900
C	-6.72330500	-2.78153500	-0.01902600
H	5.72762600	-0.90239000	1.50089900
H	3.99280500	0.95807500	1.96584300
H	4.97461600	-2.48329100	-0.34878100
H	3.17554700	2.00701800	-0.19691700

H	4.04528600	-1.22351300	-2.34398900
H	3.26752600	-2.10965600	1.28393900
H	6.13793400	1.40500100	1.19975900
H	6.08822900	0.03478800	-0.95845300
H	1.54698800	3.07039500	0.17191400
H	0.65143900	-1.76307600	-1.47614000
H	-5.11832100	2.02267700	-0.36575900
H	-1.61635900	4.49324600	-0.24534600
H	0.23140700	-2.78418100	1.51505600
H	1.05625300	-1.28470700	2.01243100
H	-0.70753000	-1.47499900	2.29638300
H	-3.39724000	-2.25453100	-0.43606500
H	-6.50600900	0.56445900	0.46286700
H	-5.06602100	-4.07943100	-0.45201100
H	-8.16390100	-1.25088300	0.43651200
H	-7.45448700	-3.58090400	-0.02220900

Table S2. The transition states coordinates (x, y, z) and imaginary frequencies for the reactions between the baicalein, wogonin, and baicalin and $\cdot\text{OOH}$ radical at the M06-2X level.

The TS coordinate of Baicalein-6-OH + $\cdot\text{OOH}$ (Imaginary frequency: $2768i\text{ cm}^{-1}$)

O	1.34291600	0.74598000	0.01066800
O	-2.68488200	-1.77053900	-0.59579500
O	-4.07338500	0.60557500	-0.55531400
O	-2.82367500	2.90877100	-0.13509700
O	-0.33889900	-2.91690700	-0.48140000
C	-0.62336800	-0.58584100	-0.29915300
C	-0.00582500	0.65746300	-0.12405500
C	2.11758000	-0.36418300	-0.02899100
C	-2.02614100	-0.63279100	-0.44254400
C	0.17387700	-1.80377000	-0.33668600
C	1.60295000	-1.60025500	-0.20363100
C	3.54982100	-0.04630000	0.11713700
C	-0.71440200	1.85383900	-0.06789000
C	-2.77082900	0.56022700	-0.39754800
C	-2.08955900	1.79240900	-0.19131700
C	4.44499400	-1.01191700	0.58570000
C	4.02351500	1.22445200	-0.21960200
C	5.79587900	-0.71494400	0.69822800
C	5.37703500	1.51531100	-0.10850600
C	6.26565800	0.54772200	0.34823900
H	2.25007800	-2.46257900	-0.27064300
H	-0.20691600	2.79730500	0.07488100
H	4.08259000	-1.98762100	0.88569200
H	3.33081200	1.97615000	-0.57526000
H	6.48148400	-1.46695500	1.06903400
H	5.73789300	2.49995400	-0.37958300
H	7.32050000	0.77782500	0.43735800
H	-2.02208900	-2.50153100	-0.58935800
H	-4.68042300	-0.15831200	0.01226400
H	-3.75061000	2.65097400	-0.25618200
O	-5.31623300	-0.79343300	0.85712300
O	-6.45572000	-0.08907500	1.09459500
H	-6.47140600	0.00327600	2.05726500

The TS coordinate of Baicalein-7-OH + $\cdot$ OOH (Imaginary frequency: 3220i cm⁻¹)

O	-1.19287500	-0.61730200	0.03940100
O	2.19408100	2.79776500	-0.11048400
O	4.07326400	0.86671600	-0.04085900
O	3.36500400	-1.73371600	0.06202300
O	-0.35851900	3.36262200	-0.12834600
C	0.43636800	1.14982400	-0.03916600
C	0.11653000	-0.22748000	0.01460300
C	-2.18858600	0.29425900	0.00049500
C	1.78231500	1.52136000	-0.05873700
C	-0.61621900	2.15498000	-0.07867800
C	-1.96307900	1.62598000	-0.06759800
C	-3.51975800	-0.34055800	0.01799900
C	1.07026300	-1.21090700	0.05030600
C	2.77542400	0.54308000	-0.02478700
C	2.43948900	-0.84761700	0.03087600
C	-4.64076600	0.37195000	0.45332300
C	-3.66918300	-1.66352200	-0.40698900
C	-5.89340500	-0.22506200	0.44624200
C	-4.92579000	-2.25495400	-0.41598100
C	-6.03974100	-1.53826300	0.00821100
H	-2.78642900	2.32117800	-0.13955100
H	0.80161200	-2.25679800	0.09641800
H	-4.53106500	1.38472100	0.82131800
H	-2.80091200	-2.21958300	-0.73576400
H	-6.75528200	0.33208200	0.79247900
H	-5.03434000	-3.27810000	-0.75454900
H	-7.01851500	-2.00261800	0.00419700
H	1.38615900	3.36338600	-0.13058100
H	4.15643800	1.83035600	-0.07562100
H	4.53775200	-1.41002600	0.06201300
O	5.67639000	-1.20800800	0.07391200
O	6.22832700	-2.45704100	0.14236700
H	7.17603900	-2.27130300	0.17483000

The TS coordinate of Wogonin-7-OH + [•]OOH (Imaginary frequency: 3365i cm⁻¹)

O	-0.74162000	-0.16685200	-0.10428500
O	1.56143600	-1.68886100	-0.37368000
O	2.01057500	3.77026200	-0.00366200
O	3.92313400	-0.48212100	-0.51390300
O	-0.60033700	3.87723400	0.23537100
C	0.57823300	1.84625600	-0.02021800
C	0.46607100	0.46163000	-0.12327100
C	-1.88020900	0.55321000	0.02183600
C	1.58770600	-0.35585700	-0.27809600
C	-0.63133100	2.64993000	0.13333800
C	1.87850400	2.44495100	-0.09454100
C	-1.87316600	1.89711300	0.13745200
C	-3.08147300	-0.29985400	-0.00962200
C	2.88142800	0.25736700	-0.36110800
C	2.99509500	1.66131700	-0.25865000
C	-4.24633200	0.09373600	0.65330600
C	-3.06198800	-1.50654600	-0.71406300
C	-5.38023800	-0.70558200	0.60185200
C	-4.20036800	-2.30029700	-0.76570300
C	-5.36038800	-1.90210600	-0.10868400
C	0.77210400	-2.45919000	0.53842500
H	-2.80130200	2.44732000	0.19735500
H	3.97625200	2.11248900	-0.31467400
H	-4.25706700	1.01196100	1.22836700
H	-2.16120100	-1.80700500	-1.23503500
H	-6.27764600	-0.39863000	1.12482400
H	-4.18274300	-3.22907000	-1.32275800
H	-6.24639700	-2.52420100	-0.14721900
H	1.11858600	4.16325800	0.10619500
H	3.84728400	-1.61898000	-0.23461200
H	1.31196600	-3.39615900	0.65947600
H	0.69431500	-1.94372600	1.49758500
H	-0.22321400	-2.63404200	0.13178000
O	3.86088600	-2.71835000	0.24888200
O	5.16699600	-2.93555500	0.60766100
H	5.09072600	-3.44573300	1.42412800

The TS coordinate of Baicalin-6-OH + $\cdot$ OOH (Imaginary frequency: 3372i cm⁻¹)

O	1.78082900	-1.87405400	-1.00498500
O	1.94138400	0.19985300	-1.91831700
O	4.47681400	-1.08790600	2.00891900
O	4.27385600	0.67200400	-0.19575300
O	3.58439900	-3.71784400	1.53820400
O	1.72794000	-5.25746200	-0.44828100
O	0.18570400	-3.76508100	0.19438700
O	-2.57135700	0.09137500	-0.49878600
O	2.26494700	2.60663200	-0.69172000
O	0.18093000	3.88949000	0.44175600
O	-2.32716500	3.79204700	1.15608800
C	3.96965500	-1.46233900	0.74755900
C	3.29163400	-0.30017500	0.04657600
C	2.97484600	-2.58536800	0.97153900
C	2.66385500	-0.80267900	-1.25359300
C	2.38777300	-2.98640000	-0.38577500
C	1.29329800	-4.02118300	-0.18052700
C	0.88541600	0.75974100	-1.25157500
C	-0.33062800	0.11712200	-1.18998400
C	1.09093100	2.04801900	-0.67877500
C	-1.39315400	0.76220000	-0.55224600
C	-1.26817400	2.03515200	-0.00097900
C	-0.02041900	2.68281200	-0.06911800
C	-2.40926400	2.66702800	0.65585500
C	-3.64513500	0.63628500	0.11279300
C	-3.61124800	1.86286200	0.68358400
C	-4.80925700	-0.26720900	0.09718700
C	-4.61891600	-1.64812900	-0.00442600
C	-6.10524900	0.24663700	0.19271900
C	-5.71426400	-2.50189500	0.00988000
C	-7.19577400	-0.61154100	0.20196800
C	-7.00240300	-1.98724100	0.11395200
H	4.78602800	-1.83286900	0.10872500
H	2.49493100	0.08665000	0.69872100
H	2.15506200	-2.21735700	1.60389000
H	3.44955900	-1.09577700	-1.95928600
H	3.17907100	-3.41324400	-1.01438200

H	5.00961400	-0.29452000	1.88283500
H	3.82383800	1.48176900	-0.48405100
H	4.08896700	-3.41851700	2.30269300
H	-0.45196500	-0.87346800	-1.60490700
H	1.01684100	-5.87444900	-0.22675000
H	-4.47634900	2.25152400	1.20086900
H	2.39379400	3.68316600	-0.22284500
H	-0.67193300	4.19129300	0.84012500
H	-3.61535100	-2.04722700	-0.08198400
H	-6.26250400	1.31766900	0.23475100
H	-5.55996200	-3.57169700	-0.05950100
H	-8.19787400	-0.20597200	0.26803500
H	-7.85500400	-2.65559900	0.12116900
O	2.68223700	4.75007300	0.21391800
O	4.02889800	4.81665000	0.01215900
H	4.25675800	5.70020700	0.33150800