Bulgarian Chemical Communications, Volume 50, Special Issue C, (pp. 247 –253) 2018

Antioxidant activity of 3-hydroxyphenol, 2,2'-biphenol, 4,4'-biphenol and 2,2',6,6'-biphenyltetrol**:** theoretical and experimental studies

L. Koleva[1], S. Angelova[1*], M. A. Dettori[2], D. Fabbri[2], G. Delogu[2], V. D. Kancheva[1*]

[1]*Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences, Sofia 1113, Bulgaria*
[2]*CNR-Institute of Biomolecular Chemistry, Traversa La Crucca, I-07100, Sassari, Italy*

Received October 15, 2017; Revised November 3, 2017

A set of selected phenolic compounds (phenol, 3-hydroxyphenol (resorcinol), 2,2'-biphenol, 4,4'-biphenol and 2,2',6,6'-biphenyltetrol) is designed in order to study the structure – antioxidant activity relationship for the compounds with one benzene ring and two C-C bridged benzene rings. The corresponding "dimeric" structures (biphenols and biphenyltetrol) of phenol and resorcinol are handpicked in order to study the influence of the number and mutual position of the substituents (OH group(s) in the aromatic ring) on the antioxidant activity. A combination of theoretical and experimental approaches is applied. Chain-breaking antioxidant activities of compounds under study are determined from the main kinetic parameters of bulk lipid autoxidation. Full geometry optimization of neutral molecules and their corresponding phenoxyl radicals for all compounds under study are obtained by using DFT (B3LYP/6-31+G**) calculations. Good correlation between experimental and predicted activity is achieved.

Keywords: Antioxidants, Protective effect, Bulk lipid autoxidation, Natural phenols, Hydroxylated biphenyls, DFT calculations

INTRODUCTION

Phenols, (ArOH), a major group of antioxidant phytochemicals, are of great importance due to their biological and free radical scavenging activities. They are found in all plants as secondary metabolites produced during the normal cycle of the plant and overproduced under biotic and abiotic stress conditions [1,2]. Generally, phenols are able to control the oxidation of organic compounds by transferring H atom from the phenol OH group(s) to the chain-carrying radicals (ROO•).

In this paper, our study focused on the relationship between antioxidant structure and activity of: phenol (**PhOH**), 3-hydroxyphenol (resorcinol, **Res**), 2,2'-biphenol (***o*-DHB**), 4,4'-biphenol (***p*-DHB**) and 2,2',6,6'-biphenyltetrol (**DRes**) (Figure 1). Biphenols and biphenyltetrol are C_2-symmetrical C-C bridged dimers of phenol and resorcinol, respectively. A combination of theoretical (Density Functional Theory, DFT, calculations) and experimental approaches (bulk lipid autoxidation) is applied.

EXPERIMENTAL AND COMPUTATIONAL DETAILS

Experimental details

All ^{1}H NMR and ^{13}C NMR spectra were recorded on spectrometer Varian Mercury Plus operating at 399.93 MHz and 100.57 MHz, respectively.

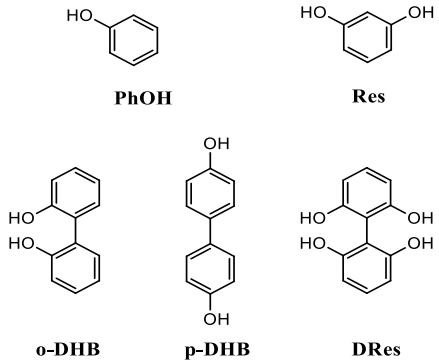


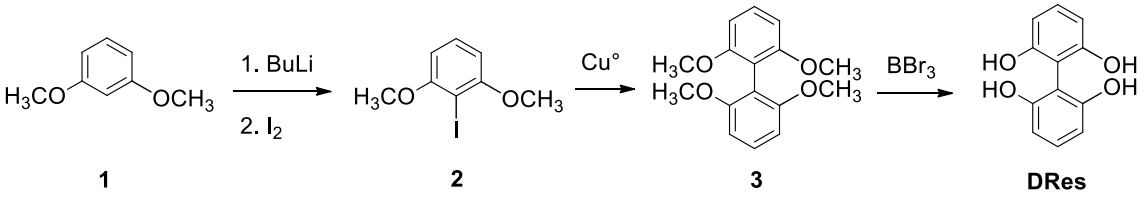
Figure 1. Structures of the studied phenolic compounds.

Chemical shifts are given in ppm (δ) and coupling constants in Hertz; multiplicities are indicated by s (singlet), d (doublet), t (triplet). $CDCl_3$ and acetone-d_6, were used as solvents as indicated below. Shifts are given in ppm relative to the remaining protons of the deuterated solvents used as internal standard (^{1}H, ^{13}C). All reagents were of commercial quality and used as purchased from various producers (Sigma-Aldrich, Merck). Flash chromatography was carried out with silica gel 60 (230-400 mesh, Kiesgel, EM Reagents) eluting with appropriate solution in the stated v:v proportions. Analytical thin-layer chromatography (TLC) was performed with 0.25 mm thick silica gel plates (Polygram® Sil G/UV_{254}, Macherey-Nagel). The purity of all new compounds was judged to be >98% by ^{1}H-NMR spectral determination. **Res** and biphenyls ***o*-DHB** and ***p*-DHB** were purchased from Sigma-Aldrich. **DRes** was prepared as previously described by us [3]. The solvents were used without

* To whom all correspondence should be sent: E-mail: sea@orgchm.bas.bg
vessy.kancheva@abv.bg

additional purification or drying, unless otherwise noted. The melting points of the newly synthesized compounds are uncorrected.

DRes was obtained in three steps starting from resorcinol dimethyl protected compound **1**, quenching of radical with iodine, followed by coupling reaction in presence of Cu(0) and demethylation by BBr_3 in anhydrous dichloromethane (Scheme 1) [3].



Scheme 1. Synthesis of **DRes**.

2-Iodo-1,3-dimethoxybenzene **(2).** To a solution of 1,3-dimethoxybenzene **1** (25 g, 180 mmol) in dry diethyl ether (150 mL) was slowly added butyllithium (112.5 mL of 1.6 M solution in hexanes, 180 mmol) under nitrogen at r.t. The reaction was stirred at r.t for 30 h and then cooled to -35°C. Iodine (45.7 g, 180 mmol) was added and the reaction was stirred for 24 h at 20°C and then poured into 10% chloridric acid (60 mL). The aqueous phase was separated and extracted with ethyl acetate (2 × 60 mL) and the combined organic extracts washed with saturated aqueous sodium thiosulfate (60 mL), brine (60 mL), dried over sodium sulfate, filtered and concentrated in *vacuo*. The product was purified by crystallization (diethyl ether) to give **2** (34 g, 71%) as a white solid; mp 105 -106 °C (Lit.104 °C) [4]; ^{1}H NMR ($CDCl_3$): δ 3.80 (s, 6H), 6.43 (d, J = 8.4, 2H), 7.17 (t, J = 8.4, 1H); ^{13}C NMR ($CDCl_3$): δ 56.6, 76.3, 103.9, 129.8, 159.5; Anal. Calcd for $C_8H_9IO_2$: C, 36.39; H, 3.44; Found: C, 36.40; H, 3.46.

2,2',6,6'-Tetramethoxybiphenyl **(3)**. In a crucible was placed a mixture of 16 g of 2-iodo-1,3-dimethoxybenzene **2** and 30 g of copper bronze. The mixture was covered with a layer (15 g) of copper bronze. The crucible was heated in an oven at 200°C for 2 h. After cooling, the reaction mixture was extracted in a Soxhlet apparatus with acetone. The product was purified by recrystallization from acetone to give **3** as white solid (6.6 g, 85%); mp 175-176 °C (Lit.175-176 °C) [5]; ^{1}H NMR ($CDCl_3$): δ 3.75 (s, 12H), 6.68 (d, J = 8 Hz, 4H), 7.32 (t, J = 8 Hz, 2H); ^{13}C NMR ($CDCl_3$): δ 56.1, 104.4, 112.5, 128.7, 158.4; Anal. Calcd for $C_{16}H_{18}O_4$: C, 70.06; H, 6.61. Found: C, 70.09; H, 6.62.

2,2',6,6'-Tetrahydroxybiphenyl (**DRes**). 2,2',6,6'-Tetramethoxybiphenyl **3** (4.7 g, 16.7 mmol) was dissolved in dry dichloromethane (110 mL) and cooled to -78 °C. A solution of boron tribromide (6.3 mL, 66.9 mmol) in dichlorom ethane (23 mL) was added dropwise under nitrogen. The solution was allowed to reach room temperature during 5 h. Water was carefully added to the reaction mixture. The solution was extracted several times with diethyl ether. The combined organic solutions were dried and evaporated. The residue was crystallized from ethanol to obtain *2,2',6,6'*-tetrahydroxybiphenyl **DRes** (2.84 g, 78%; mp 193-194 °C (Lit. 191-192 °C) [6]; ^{1}H NMR (acetone-d_6): δ 6.47 (d, J = 8 Hz, 4H), 7.02 (t, J = 8 Hz, 2H); ^{13}C NMR (acetone-d_6): δ 107.28, 129.04, 156.52, 205.51; Anal. Calcd for $C_{12}H_{10}O_4$: C, 66.05; H, 4.62. Found: C, 66.08; H, 4.65.

Chain-breaking antioxidant activity

Triacylglycerols of commercially available sunflower oil (TGSO) were cleaned from pro- and antioxidants by adsorption chromatography and stored under nitrogen at temperature 20 °C. Fatty acid composition of the lipid substrate was determined by GC analysis of the methyl esters: 16:0 (6.7%); 18:0 (3.6%); 18:1 (25.1%); 18:2 (63.7%); 20:0 (0.2%); 22:0 (0.7%); the numbers x:y indicate, respectively, the number of carbon atoms and double bonds in the fatty acid. Lipid samples containing various inhibitors were prepared directly before use. Aliquots of the antioxidant solutions in purified acetone were added to the lipid sample. Solvents were removed under a nitrogen flow. Lipid autoxidation was carried out in a thermostatic bath at (80±0.2) °C by blowing air through the samples in special vessels. The oxidation process was monitored by withdrawing samples at measured time intervals and subjecting them to iodometric determination of the primary products (lipid hydroxyperoxides, LOOH) concentration, i.e. the peroxide value (PV). All compounds were subjected to lipid autoxidation at 80 °C at two concentrations, 0.1 and 1.0 mM, respectively. All kinetic data are expressed as the average of two independent measurements which were processed using the computer program Origin 6.1 and Microsoft Excel 2010. The basic kinetic scheme of lipid autoxidation is published elsewhere [7].

Determination of the main kinetic parameters of the studied compounds [8-10]

Protection factor (PF) is a measure for the antioxidant efficiency i.e. $PF = IP_A/IP_C$ and means how many times the oxidation stability of lipid substrate increased in presence of an antioxidant. IP_C and IP_A are the induction periods of control sample and in presence of an inhibitor.

Inhibition degree (ID) is a measure of the antioxidant reactivity, e.g. how many times the antioxidant shortens the oxidation chain length, i.e. $ID = R_C/R_A$. The initial oxidation rates R_C in the absence and R_A in the presence of antioxidant were found from the tangents at the initial phase of the kinetic curves of hydroperoxides accumulation.

Antioxidant capacity (Rm) is a measure of the consumption of the antioxidant during the induction period.

Radical scavenging activity: the capacity of studied compounds to scavenge free radicals was estimated by DPPH radical test in acetone solution. Experimental details are previously presented [11]. The main kinetic parameters of the process are radical scavenging activity (%RSA) and stoichiometric coefficient (n) that shows how many radicals are trapped by one molecule of antioxidants. All these kinetic parameters are determined and compared.

Computational details

Unrestricted open-shell approach (Becke three-parameter hybrid functional B3LYP [12] and 6-31+G(d,p) [13,14] basis set) was used to optimize the geometry of compounds studied and their radicals without symmetry constraints with the default convergence criteria using the Gaussian 09 program [15]. Frequency calculations for each optimized structure are performed at the same level of theory. No imaginary frequency is found for the lowest energy configurations of any of the optimized structures. Unscaled thermal corrections to enthalpy are added to the total energy values. The BDEs for the generation of the respective radicals from the parent compounds are calculated by the formula

$$BDE = H_{298}(AO^{\bullet}) + E_T(H^{\bullet}) - H_{298}(AOH) \quad (1)$$

where $H_{298}(AO^{\bullet})$ and $H_{298}(AOH)$ are enthalpies calculated at 298 K for radical species, $AO^{\bullet}$ and neutral molecule AOH, respectively, and $E_T(H^{\bullet})$ (calculated total energy of $H^{\bullet}$) is -313.93 kcal mol^{-1}.

Solvation effects are accounted for by employing the polarizable continuum model [16] (PCM) as implemented in the Gaussian 09 suite of programs: all structures are optimized in acetone surrounding environment. PyMOL molecular graphics system was used for generation of the molecular graphics images [17].

RESULTS AND DISCUSSION

Chain-breaking antioxidant activity

Figure 2 (a-d) presents the kinetics of TGSO autoxidation at 80ºC in absence and in presence of **Res** and **DRes** at concentrations 0.1 mM and 1.0 mM. The main kinetic parameters determined are shown in Table 1.

Res manifested no antioxidant effect (PF) at lower concentration (0.1 mM) where a small pro-oxidant effect appears. At higher concentration (1.0 mM) **Res** showed the same activity as the control lipid (TGSO) sample, however ID increased 2-fold and Rm 10-fold growing the concentration. These data suggest a significant role of the side reactions with participation of **Res**. The lack of antioxidant activity was expected because of the *meta* positions of phenol OH groups and more difficult H-atom abstraction from **Res** to the lipid peroxide radicals.

DRes also demonstrated pro-oxidant effect at lower concentration and no effect at higher concentration. Its antioxidant reactivity (ID) shows low values at both concentrations, however the antioxidant capacity (Rm) grows significantly (10-fold) at higher concentration.

Protection factor of ***o*-DHB** increased 2.4-fold at higher concentration, however inhibition degree does not change, and the main rate of antioxidant consumption (Rm) increased 4.6-fold (Figure 3 and Table 1). These data confirm the participation of ***o*-DHB** in side reactions, leading to a decrease in its antioxidant capacity. Effect of the positions of phenolic OH groups was studied for ***o*-DHB** and ***p*-DHB**. A comparison of ***o*-DHB** and ***p*-DHB** demonstrates 2-fold higher antioxidant efficiency (PF) and reactivity (ID) for ***o*-DHB** at lower concentration (0.1 mM). Rm does not demonstrate significant differences between ***o*-DHB** and ***p*-DHB**.

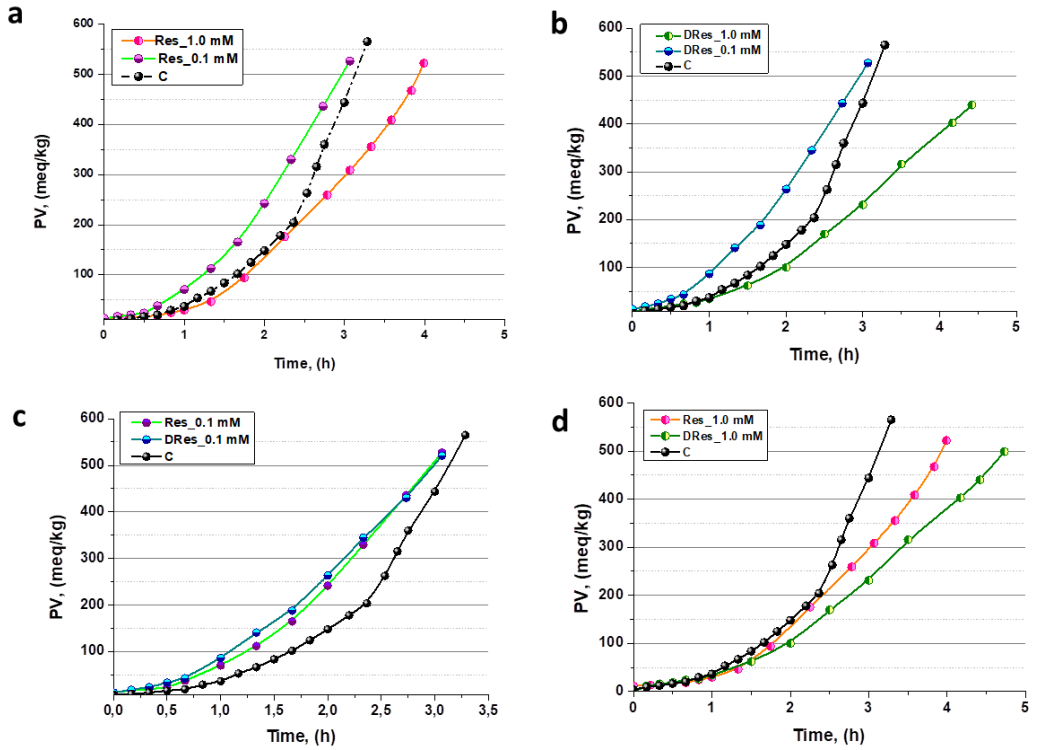


Figure 2. Kinetics of TGSO autoxidation at 80° C in absence (C) and in presence of 0.1 mM and 1.0 mM of **Res** and **DRes.**

Table 1. The main kinetic parameters, characterizing TGSO autoxidation at 80°C in presence of 0.1 mM and 1.0 mM of the tested compounds.

Compd.	Conc.	IP_A, h	PF -	R_A 10^{-6}, M/s	ID -	Rm 10^{-8}, M/s	RRm 10^3 -	Activity
Res[a]	0.1 1.0	1.3±0.2 2.3±0.3	0.6 1.1	2.9±0.4 1.5±0.2	1.2 2.3	2.1±0.2 12.1±1.2	7.24 80.7	prooxidant no activity
DRes[a]	0.1 1.0	1.3±0.2 1.7±0.2	0.7 0.8	4.7±0.5 3.3±0.5	0.7 1.0	2.1±0.2 16.3±1.5	4.5 49.4	prooxidant no activity
o-DHB[b]	0.1 1.0	2.5±0.2 6.0±0.5	2.5 6.0	4.6±0.6 4.2±0.3	1.8 2.0	1.1±0.2 4.6±0.3	2.4 10.9	weak moderate
p-DHB[b]	0.1	1.1±0.1	1.1	7.5±2.0	1.1	2.5±0.2	3.3	no activity

Control sample: [a]IP_C=(2.0±0.3) h, R_C =3.4×10^{-6} M/s.; [b]IP_C=(1.0±0.2) h, R_C=8.3×10^{-6} M/s

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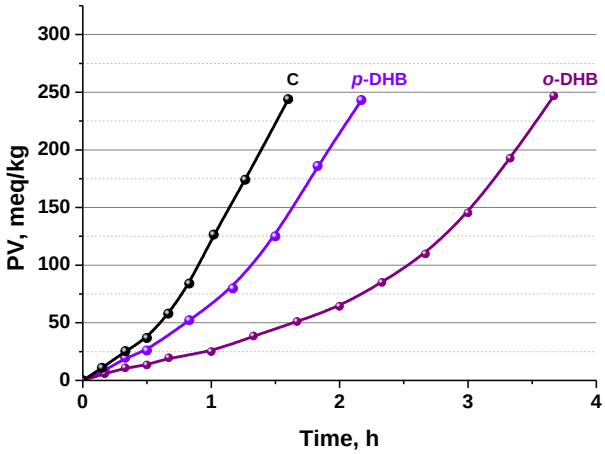

Figure 3. Kinetics of TGSO autoxidation at 80° C in absence (C) and in presence of 0.1 mM of ***o*-DHB** and ***p*-DHB**.

Figure 2 and Table 1 present the kinetic data of TGSO in presence of **Res** and **DRes**. **Res** and **DRes** at low concentration (0.1 mM) demonstrate similar pro-oxidant activity (PF), however ID and Rm values for **DRes** are lower in comparison to the values for **Res** (almost 2-fold).

At higher concentration (1.0 mM) **DRes** is less active than **Res** (PF), 2-fold lower for **DRes** for Rm. Interestingly, the increase of the number of phenol OH-groups in *ortho* positions to the C-C single bond (**DRes**) does not lead to a proportional increase in the antioxidant activity in comparison to the dimer with two phenol OH groups (***o*-DHB**). This result may be is due to the orthogonal position of the two aromatic rings in **DRes** that excludes a hypothetical conjugation between the two aromatic

rings. In fact the kinetic parameters for **DRes** are comparable with these for **Res** (having two phenol-OH groups in *meta*-position).

Radical scavenging activity

The results presented in Table 2 show a weak radical scavenging activity of studied compounds towards DPPH radical. A possible explanation is formation of inactive (to scavenge free radicals) complexes between the solute and acetone molecules.

Table 2. Radical scavenging activity towards DPPH radical in acetone solution.

Compound	Reaction time, min	Concentration, μM			
		25		39	
		RSA, %	n	RSA, %	n
DRes	2 min (fast kinetics)	3.21	0.13	4.42	0.11
	20 min (total kinetics)	17.49	0.70	23.03	0.57
o-DHB	2 min (fast kinetics)	0.21	0.01	0.9	0.02
	20 min (total kinetics)	2.33	0.10	4.28	0.10
p-DHB	2 min (fast kinetics)	0.70	0.03	0.63	0.02
	20 min (total kinetics)	1.48	0.06	1.50	0.04

DFT calculations

The geometries of the parent compounds and possible phenoxyl radical species are optimized at UB3LYP/6-31+G(d,p) level. The optimized geometries only of the thermodynamically preferred rotamers of the parent compounds are presented in Figure 4. The calculated enthalpies, H_{298}, for the parent compounds and radical species (radicals and biradicals) are given in Table 3. The BDEs derived from the respective enthalpy values are also listed in Table 3 and presented in Figure 4. The values in gas phase and in acetone are compared.

Phenol and resorcinol: in the gas phase they are characterized by consistently high BDE values for **PhOH (r)** and **Res (r)** radical species generation (81.76 kcal/mol and 82.77 kcal/mol, respectively); the biradical generation from **Res (r)** is characterized with lower BDE value – 81.54 kcal/mol. In acetone medium the BDEs for **PhOH (r)** and **Res (r)** decrease, while that for the **Res (br)** generation increases.

Biphenols: the Ar-Ar dihedral angles in the parent biphenols ***o*-DHB** (with H bond between the OH groups) and ***p*-DHB** are 50° and 40°, respectively. In the radical species the Ar-Ar dihedral angles angles decrease (31° and 29°, respectively), but for the biradicals species an increase (to 64° and 48°, respectively) is observed. In the gas phase ***o***- and ***p*-DHB** are characterized by lower BDE values (in comparison to phenol) for radical species generation (75.31 and 78.61 kcal/mol, respectively), while the BDEs for the biradical species (**br**) generation are higher than those for the first H-atom abstraction (generation of **PhOH (r)**, ***o*-DHB (r)** and ***p*-DHB (r)**). In acetone medium the BDE for ***o*-DHB (r)** increases (ΔBDE= 1.48 kcal/mol), for ***o*-DHB (br)** decreases noticeably (ΔBDE= 4.09 kcal/mol). In acetone medium the BDE for ***p*-DHB (r)** decreases (ΔBDE= 1.79 kcal/mol), while for ***p*-DHB (br)** the BDE changes slightly (ΔBDE= 0.58 kcal/mol).

Biphenyltetrol (**DRes**): the benzene rings of **DRes** lie in perpendicular planes and the BDE for the first H-atom abstraction from **DRes** has almost the same value (82.72 kcal/mol) as from "monomeric" **Res** (82.77 kcal/mol), while for **DRes (r)** the angle between the distinct planes of the benzene rings is ~53°. Two possible biradicals can be generated from **DRes (r)**: **DRes (br1)** (formed after H-atom abstraction from the same ring, with 36° angle between the planes) and **DRes (br2)** (formed after H-atom abstraction from the second ring, 40° angle). The BDEs for the second H-atom abstraction are lower than for the first one both in the gas phase and in acetone medium. The second H-atom abstraction from the second ring is characterized by lower BDEs in the gas phase and in acetone medium.

CONCLUSIONS

Although ***o*-DHB** manifests a weak/moderate antioxidant activity it shows higher antioxidant efficiency than ***p*-DHB.** The latest is a result of the lower BDE (75.31 kcal/mol) than that of ***p*-DHB** (78.61 kcal/mol). There is agreement between the theoretically predicted and experimentally observed antioxidant properties for these compounds. Bond dissociation enthalpies calculated for **Res** and **DRes** are of the same order, i.e. their antioxidant activity is expected to be similar. There is an excellent agreement between the theoretically calculated BDEs and experimental data (**Res** and **DRes** show the same antioxidant efficiency at low concentration). The discrepancy between the

theoretical BDE values and experimental results at higher concentrations can be explained by the side reactions that take place to a greater extend and that are not accounted for in the calculations.

Table 3. UB3LYP/6-31+G(d,p) calculated enthalpies (H_{298}) at 298 K (Hartree) in the gas phase and BDEs (kcal/mol).

Structure	H_{298}		BDE	
	gas phase	acetone	gas phase	acetone
PhOH	-307.383018	-307.389653		
PhOH (r)	-306.752447	-306.760335	81.76	80.97
o-DHB				
o-DHB (r)	-612.968012	-612.976369	75.31	76.79
o-DHB (br)	-612.323554	-612.338417	90.48	86.39
p-DHB				
p-DHB (r)	-612.962677	-612.977519	78.61	76.82
p-DHB (br)	-612.325169	-612.339322	86.12	86.54
Res				
Res (r)	-381.971644	-381.984213	82.77	81.20
Res (br)	-381.341432	-381.351743	81.54	82.95
DRes				
DRes (r)	-763.404066	-763.417064	82.72	80.28
DRes (br1)	-762.782027	-762.793415	76.41	77.41
DRes (br2)	-762.783847	-762.794883	75.27	76.49

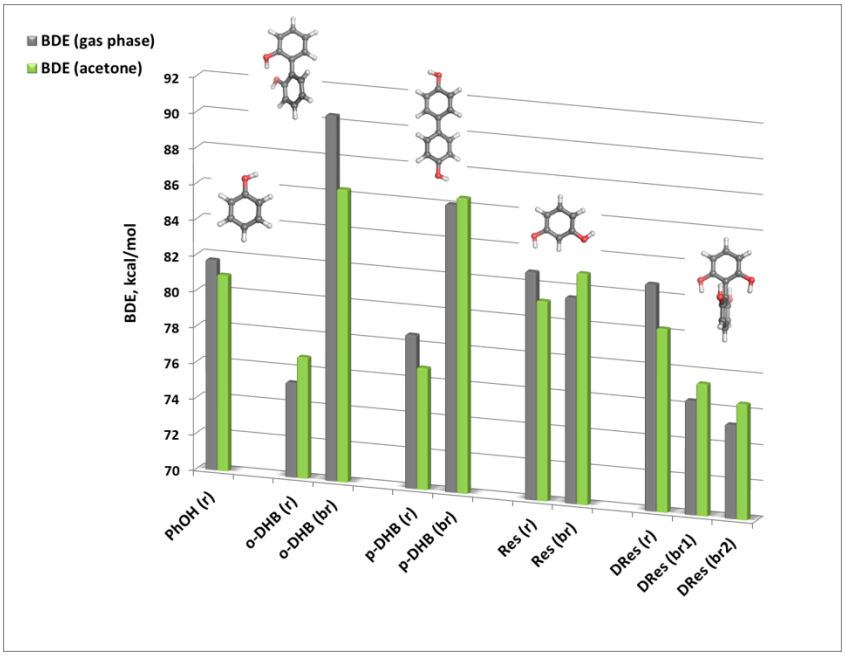

Figure 4. BDEs (in kcal/mol) in gas phase (grey) and in acetone (green).

Acknowledgements: *The financial support by the CNR-BAS bilateral project №0012242 23/02/2016 is gratefully acknowledged. Technical assistance of Dr. Jordan Nechev in radical scavenging activity experiments is gratefully acknowledged.*

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АНТИОКСИДАНТНА АКТИВНОСТ НА 3-ХИДРОКСИФЕНОЛ, 2,2'-БИФЕНОЛ, 4,4'-БИФЕНОЛ И 2,2',6,6'-БИФЕНИЛТЕТРОЛ**:** ТЕОРЕТИЧНО И ЕКСПЕРИМЕНТАЛНО ИЗСЛЕДВАНЕ

Л. Колева[1], С. Ангелова[1*], М. А. Деттори[2], Д. Фаббри[2], Дж. Делогу[2], В. Д. Кънчева[1*]

[1] Институт по органична химия с Център по фитохимия – Българска академия на науките, София 1113, България

[2] Национален съвет за научни изследвания – Институт по биомолекулярна химия, Сассари I-07100, Италия

Постъпила на 15 октомври, 2017 г.; коригирана на 3 ноември, 2017 г.

(Резюме)

Изследвана е зависимостта структура - антиоксидантна активност за избрани фенолни съединения с едно бензеново ядро и две С-С свързани бензенови ядра (фенол, 3-хидроксифенол (резорцинол), 2,2'-бифенол, 4,4'-бифенол и 2,2',6,6'-бифенилтетрол). Съответните "димерни" структури (бифеноли и бифенилтетрол) на фенол и резорцин са така подбрани, че да може да се изследва влиянието на броя и взаимното положение на заместителите (ОН група/и в ароматния пръстен) върху антиоксидантната активност. Използвана е комбинация от теоретични и експериментални подходи. Антиоксидантната активност на изследваните съединения е определена от основните кинетичните параметри на липидното автоокисление в хомогенна среда. Молекулите на всички изследвани съединения и техните съответни феноксилни радикали са оптимизирани на теоретично ниво B3LYP/6-31+G**. Постигната е добра корелация между теоретично предсказаната и експериментално определената антиоксидантна активност.