Electronic Supplementary Material (ESI) for Chemical Society Reviews.

Supplementary Information

for

Autoxidation vs. antioxidants – the fight for forever

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Table S1: References for the k_p values / BDEs plotted in Figure 1 (ordered by k_p):

Compound	k_p / M^{-1} s^{-1}	Source	BDE kcal / mol	Source
retinal	5656	(Do, Lee et al. 2021)	--	--
7-dehydrocholesterol	2737	(Do, Lee et al. 2021)	--	--
1,4-cyclohexadiene	1400	(Valgimigli and Pratt 2012)	76.0	(Luo 2007)
conjugated linolenic acid 18:3	1235	(Do, Lee et al. 2021)	--	--
vitamin d3	1031	(Do, Lee et al. 2021)	--	--
docosahexaenoic acid 22:6	334	(Xu, Davis et al. 2009)	--	--
arachidonic acid 20:4	197	(Xu, Davis et al. 2009)	--	--
2,4-hexadiene	165	(Do, Lee et al. 2021)	--	--
linolenic acid 18:3	144	(Do, Lee et al. 2021)	--	--
conjugated linoleic acid 18:2	118	(Do, Lee et al. 2021)	--	--
2,4-dimethyl-1,3-pentadiene	97	(Do, Lee et al. 2021)	--	--
indene	80	(Do, Lee et al. 2021)	83.0	(Luo 2007)
1,3-hexadiene	65	(Do, Lee et al. 2021)	--	--
linoleic acid 18:2	62	(Xu, Davis et al. 2009)	--	--
1,3-pentadiene	34	(Do, Lee et al. 2021)	83.3	(Luo 2007)
styrene	17	(Do, Lee et al. 2021)	--	--
1,4-pentadiene	14	(Howard and Ingold 1967)	76.6	(Luo 2007)
cholesterol	11	(Xu, Davis et al. 2009)	83.2	(Porter, Xu et al. 2020)
tetrahydrofuran	4.4	(Valgimigli and Pratt 2012)	92.1	(Luo 2007)
methyl oleate	0.9	(Howard and Ingold 1967)	83.4	(Porter, Xu et al. 2020)
cumene	0.34	(Valgimigli and Pratt 2012)	83.2	(Luo 2007)
hexadecane[a)]	~ 0.01	(Valgimigli and Pratt 2012)	--	--

a) Not shown in Figure 1 for reasons of spacing but mentioned in the text as a reference compound.

Table S2: References for the k_{inh} values / BDEs plotted in Figure 2B (ordered by k_{inh}):

Compound	k_{inh} / M^{-1} s^{-1}	Source	BDE kcal / mol	Source
12	6.60E+08	(Farmer, Haidasz et al. 2017)	70.7	(Farmer, Haidasz et al. 2017)
6	2.80E+08	(Ingold and Pratt 2014)	75.4	(Ingold and Pratt 2014)
5	8.80E+07	(Ingold and Pratt 2014)	76.3	(Ingold and Pratt 2014)
8	3.70E+07	(Hanthorn, Valgimigli et al. 2012)	79.0	(Ingold and Pratt 2014)
2	2.90E+07	(Barclay, Vinqvist et al. 1993)	--	--
10	2.90E+07	(Farmer, Haidasz et al. 2017)	76.1 [b)]	(Lucarini, Pedrielli et al. 1999)
9	8.80E+06	(Foti and Amorati 2009)	78.2 [b)]	(Lucarini, Pedrielli et al. 1999)
4	8.60E+06	(Ingold and Pratt 2014)	78.2	(Ingold and Pratt 2014)
1	5.70E+06	(Ingold and Pratt 2014)	--	--
11	4.50E+06	(Farmer, Haidasz et al. 2017)	77.5	(Farmer, Haidasz et al. 2017)
a-Toc	3.20E+06	(Ingold and Pratt 2014)	77.2	(Poon and Pratt 2018)
3	1.49E+06	(Xi and Barclay 1998)	79.4	(Ingold and Pratt 2014)
Fer-1	3.50E+05	(Poon and Pratt 2018)	--	--
7	1.80E+05	(Hanthorn, Valgimigli et al. 2012)	82.2	(Ingold and Pratt 2014)
Ph_2NH	2.00E+04	(Ingold and Pratt 2014)	84.7	(Ingold and Pratt 2014)
BHT	1.40E+04	(Ingold and Pratt 2014)	79.9	(Poon and Pratt 2018)
PhOH	1.00E+03	(Foti 2007)	87.1	(Ingold and Pratt 2014)

b) This value is 1.1 kcal / mol lower than reported in the referenced publication due to later re-evaluation of the BDE of the reference compound used in the original study (Mulder, Korth et al. 2005).

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