Supporting Information

Table S1. Experimental antiradical and antioxidant activities in scaled and logarithmic units [log(I%+100)] of the selected anthocyanidins and anthocyanins (Kähkönen and Heinonen, 2003).

Table S2. Numerical values of the descriptors of the anthocyanins analyzed.

Figure S1. Dispersion plot of residuals for the proposed QSAR models of Eqs. (**1**)-(**7**).

Table S1. Experimental antiradical and antioxidant activities in scaled and logarithmic units [log(I%+100)] of the selected anthocyanidins and anthocyanins (Kähkönen and Heinonen, 2003).

ID	DPPH[a]	MeLo emulsion[b]		LDL[c]			MeLo bulk[b]
	17 µM	50 µM	250 µM	2.5 µM	10 µM	25 µM	50 µM
1	4.87520	4.97673	5.00395	4.68213	4.87520	5.25750	4.57471^
2	4.89035	5.04986^	5.21494^	4.57471	5.26786	5.28827^	4.40672
3	4.95583	5.11799	5.20949	4.57471	5.26786	5.28827	4.73620
4	4.89035	5.00395	5.21494	4.66344^	5.06890	5.27300	4.79579
5	4.70048	4.92725	5.15906	4.58497	4.53260	4.57471	4.35671
6	4.82028	5.09375	5.23644	4.82028	5.21494	5.28320	4.36945
7	4.78749	4.96981	5.12396	4.41884	4.34381	4.58497	4.89035
8	4.88280^[d]	5.02388	5.20949	4.51086^	5.25750	5.25750	4.78749^
9	4.95583	5.01728	5.13580	4.55388	5.24702	5.26269^	4.77068
10	4.83628	4.96284	4.99043	4.55388	4.67283	5.28320	
11	4.81218^	5.07517	5.23111	4.38203	5.06890	5.20949	4.89035
12	4.83628	5.20401	5.24702	4.41884	4.46591	4.73620	4.46591
13	4.82831^	4.99043	5.22036		5.22575^	5.24175	
14	4.78749	4.54329	5.23644		4.52179^	5.28320	
15	4.80402	4.82831	5.17615		5.25227	5.28827	
16	4.83628	5.01064^	5.17048		5.28827^	5.29330	
17	4.66344	4.78749^	5.14749^		4.39445	5.26786	
18	4.82831	4.79579	5.18178		4.70953	5.17615^	
19	4.88280	3.76120	4.99043		5.28827	5.28827	
20	4.79579	4.94164^	5.17615		4.70953^	5.03044^	
21	4.73620^	5.00395	5.15329^		4.70048	4.82831	
22	4.80402	4.91998	5.26786		4.56435	5.28827	
23	4.83628	4.92725	5.15906		5.28827	5.28320	

[a]scavenged radicals (%) after 4 min reaction time, *n* = 3;
[b]inhibition (%) of the formation of methyl linoleate (MeLo) hydroperoxide after 72 h of oxidation, *n* = 2;
[c]inhibition (%) of hexanal formation after 2 h of oxidation, *n* = 3.

[d]test set compound.

Table S2. Numerical values of the descriptors of the anthocyanins analyzed.

ID	*GATS6p*	*qub1*	*D714*	*VR1.Dzm*	*VR2.Dzs*	*qub2*	*qub3*
1	0.9595382	24.2077080	0	439.3058750	10.5443196	14.1850729	0.0000000
2	0.9444419	25.0929249	0	230.6142279	9.0916054	9.9671933	0.0000000
3	0.9173768	25.2191699	0	212.6895961	9.1364230	10.2901955	0.0000000
4	0.9827300	24.5967535	0	213.2189258	9.2265283	9.4181651	0.0051214
5	0.9898621	25.1023070	0	227.0914828	10.8282287	9.8147907	0.0039714
6	0.9948505	24.2769590	0	302.5558701	13.7133916	9.2200064	0.0065081
7	0.9665389	25.6188102	0	301.1697163	9.5727536	11.3646377	0.0000000
8	0.9647003	24.8094932	0	380.0264673	11.1003310	11.0978371	0.0000000
9	0.9560476	24.4800395	0	854.7615926	18.8573963	10.9948782	0.0000000
10	0.9879946	25.1034341	0	498.0462474	22.7324794	11.0961241	0.0034002
11	0.9965436	24.7921402	0	462.2880102	16.0950726	10.9505134	0.0026732
12	1.0022293	24.7705620	0	1433.4373248	23.4450686	10.8797640	0.0044255
13	0.9647003	24.8094932	0	380.0264673	11.1003310	11.0978371	0.0000000
14	0.9879946	25.1034341	0	498.0462474	22.7324794	11.0961241	0.0034002
15	1.0022293	24.7705620	0	1433.4373248	23.4450686	10.8797640	0.0044255
16	1.0138353	24.2291058	0	319.6902060	12.6497137	10.6447366	0.0000000
17	1.0343070	24.2649297	0	457.3088966	18.4478937	10.5403630	0.0036237
18	1.0128248	23.3713220	1	4614.0097769	16.4750633	10.8539321	0.0264858
19	1.0077228	23.2621313	1	1213.4819420	15.7698658	10.7620869	0.0258698
20	1.0160480	24.2586855	0	517.0118902	12.3940145	11.3924700	0.0000000
21	1.0404010	24.5118564	0	727.9515823	14.8011700	11.3488489	0.0033721
22	1.0379875	23.4955287	0	1845.3619433	32.8435839	11.2770147	0.0000000
23	1.0274062	24.2451552	0	979.1123393	14.9875807	11.3965758	0.0000000
24	0.8454556	24.6694822	0	223.3251380	9.9057353	9.4258817	0.0069429
25	0.7972004	25.0915104	0	259.0299798	21.5834563	9.7570943	0.0203226
26	0.8930368	25.1650840	0	267.8713982	10.4915801	9.8425247	0.0000000
27	1.0141277	24.3109337	0	360.9663106	9.6772319	9.1971440	0.0046734
28	0.9200598	25.5184453	0	417.4618615	10.6489782	9.7400306	0.0000000
29	0.9135260	25.1830088	0	436.2273250	19.1067218	11.0999639	0.0045924

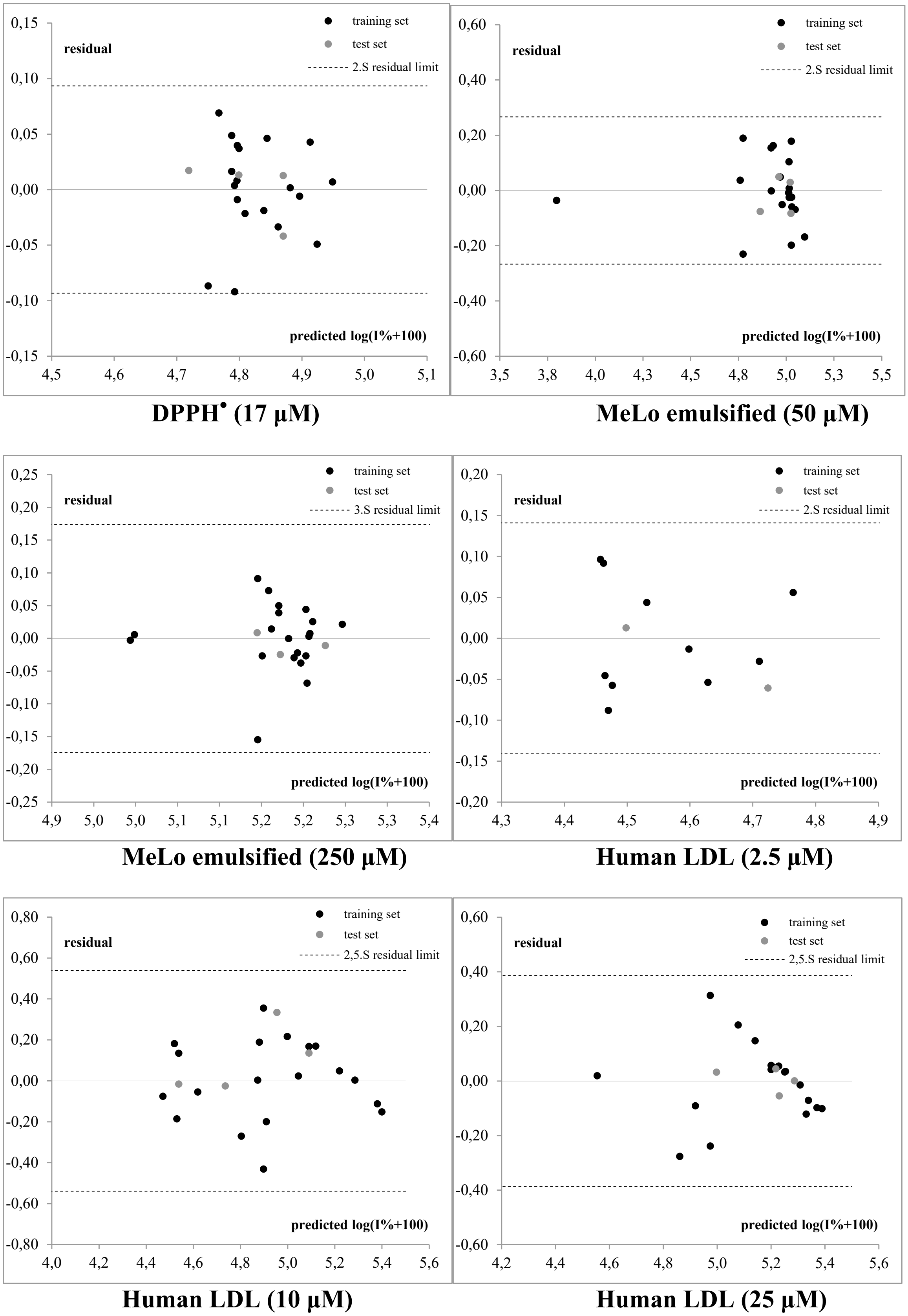
30	0.9965436	24.7921402	0	462.2880102	16.0950726	10.9505134	0.0026732
31	0.9393208	24.9074098	0	333.2710901	10.2759109	11.0287731	0.0000000
32	1.0146264	24.8237808	0	715.4493494	37.9318844	10.8667426	0.0031410
33	0.9478676	25.8248541	0	292.2999849	9.4851529	11.3815195	0.0000000
34	1.0017479	24.1654211	0	397.2840097	17.4900129	10.6430082	0.0000000
35	1.0179297	24.7637541	0	332.6453799	15.3298220	10.8086932	0.0000000
36	0.9837704	24.3440972	0	327.0866460	14.7955051	10.5664336	0.0000000
37	1.0017479	24.1654211	0	397.2840097	17.4900129	10.6430082	0.0000000
38	0.9209631	24.2775951	0	851.0157352	16.9566438	10.4629355	0.0145854
39	1.0561779	24.0319956	0	731.3183920	13.0466126	10.3153987	0.0033502
40	0.9957533	25.0001484	0	363.6324078	13.5925907	10.8278697	0.0000000
41	1.0114191	23.8108166	0	538.9341489	12.7987865	11.2202188	0.0000000
42	1.0304516	24.7829292	0	543.5689477	12.7976608	11.5145479	0.0025523
43	1.0158060	25.1713359	0	541.7817267	13.4797879	11.7121372	0.0000000
44	0.9984894	24.3148520	0	514.8615749	12.3825237	11.3416090	0.0000000

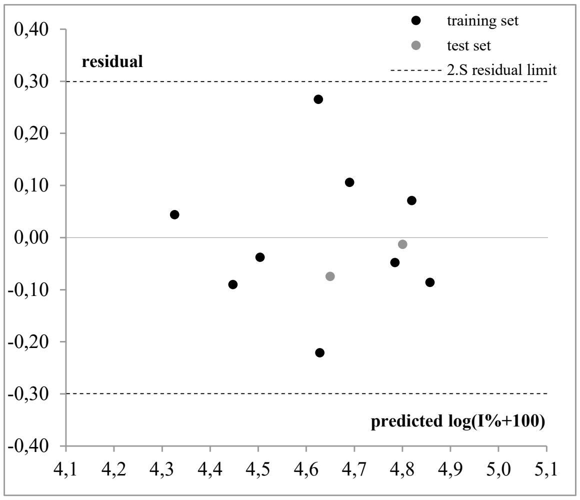
Table S2. (continued)

ID	***qub4***	***ATSC8e***	***qub5***	***qub6***	***D284***	***minHBint4***	***qub7***	***D458***
1	40.0439403	-1.6826154	22.6026283	17.1197224	4.067	5.2117991	39.2979036	0.464
2	40.7610891	-2.0441039	18.1846904	14.9989257	4.325	5.2140609	27.5377080	0.456
3	41.6180733	-2.4216115	20.7636603	15.4164667	4.271	5.2163227	35.7562228	0.514
4	39.9225180	-2.3800805	15.4347052	14.5849390	4.536	5.1670872	19.6361929	0.479
5	41.0288559	-2.7329646	18.0298453	15.1592456	4.604	2.7567706	26.6210201	0.389
6	39.5689340	-2.5058470	15.5328725	14.5496979	4.324	5.1213477	19.4008223	0.344
7	42.0986691	-1.6889734	17.9255733	16.6426438	4.936	2.1859590	33.1390689	0.527
8	41.9071487	-1.5991055	19.7346686	16.2470200	5.133	2.1755798	37.7435736	0.520
9	42.2634279	-1.5813855	21.3994286	16.1388959	5.067	2.1652006	42.8685723	0.541
10	42.2219707	-1.9315046	17.8616420	16.3662178	5.253	2.1564707	32.1761237	0.508
11	42.1535056	-1.8842032	19.5378111	16.2399669	5.267	2.1462696	36.4902906	0.455
12	42.2017822	-1.5470488	17.7884416	16.1841496	5.077	2.1267016	31.2655373	0.410
13	41.9071487	-1.5991055	19.7346686	16.2470200	5.133	2.1755798	37.7435736	0.520

14	42.2219707	-1.9315046	17.8616420	16.3662178	5.253	2.1564707	32.1761237	0.508
15	42.2017822	-1.5470488	17.7884416	16.1841496	5.077	2.1267016	31.2655373	0.410
16	40.0964877	-1.9731000	19.0857701	15.9336768	5.166	2.5408522	33.2770243	0.432
17	39.6409107	-2.3014397	17.1126483	15.9290960	5.287	2.5337448	27.4903314	0.445
18	41.5028024	-1.5643521	17.8873140	16.1677563	5.260	1.8257517	38.8049173	0.587
19	42.0972865	-1.6023920	19.2084937	16.0854221	5.216	1.8208865	42.7134631	0.597
20	42.6225662	-2.1044280	20.5622107	16.4599391	4.959	2.0063552	42.1516533	0.525
21	43.1278338	-2.0251529	19.0284949	16.5502201	5.000	1.9538408	36.9367103	0.438
22	42.1269541	-1.8084582	19.3808257	16.6935905	5.282	1.4010092	42.0478227	0.558
23	42.3540341	-0.2198885	17.9764524	16.9862785	5.604	1.0665747	34.6664462	0.552
24	40.0404853	-2.4645950	15.4305747	14.6385744	4.593	5.1744667	19.5904863	0.597
25	40.4924805	-2.8752062	18.0251529	15.1479422	4.438	5.1766999	25.1466888	0.712
26	40.1534805	-1.4852988	18.1669212	14.9889019	4.153	5.2144907	25.5575637	0.551
27	39.7509309	-3.1734737	15.5288992	14.5567649	4.477	2.6702900	19.3651639	0.443
28	40.1247192	-1.1768379	15.2597517	14.9755209	4.503	5.2122289	19.7583149	0.493
29	42.2277053	-2.0889259	17.8577901	16.4114458	5.253	2.1586668	32.1510141	0.573
30	42.1535056	-1.8842032	19.5378111	16.2399669	5.267	2.1462696	36.4902906	0.455
31	41.4282041	-0.8071478	19.7192826	16.2621263	4.992	2.1736497	36.4222989	0.558
32	42.2472882	-2.3530741	17.7847666	16.2014706	5.177	2.1289773	31.2466308	0.472
33	42.0699313	-0.8789872	17.9054349	16.7541034	5.195	2.1840289	33.0813155	0.537
34	41.0158569	-1.9594753	20.8785888	15.9638383	5.092	2.5222871	38.8838596	0.463
35	39.6485076	-2.0672907	17.1298325	16.1932245	4.954	2.5594173	28.1934819	0.436
36	39.5591485	-1.1784400	19.0692606	15.9544628	5.012	2.5366283	31.8703634	0.481
37	41.0158569	-1.9594753	20.8785888	15.9638383	5.092	2.5222871	38.8838596	0.463
38	39.7256313	-2.4445867	18.9124111	15.9602572	5.185	2.5139719	31.1758534	0.598
39	39.5682526	-2.7099967	17.0761422	15.7915140	5.195	2.4294507	26.7920681	0.424
40	39.6148932	-1.2530755	17.1081969	16.3232959	5.236	2.5551934	28.1341430	0.450
41	42.8894242	-2.0999518	21.7920533	16.2339703	4.935	1.9969316	45.8968580	0.538
42	43.0552314	-2.4251695	19.1392159	16.7173745	5.065	1.9849501	37.8757935	0.513
43	42.8952217	-2.1539800	19.2467230	16.9412851	4.796	2.0157788	38.8562704	0.530
44	42.2555071	-1.3194960	20.5504602	16.4602344	4.868	2.0046028	41.1687174	0.548

Figure S1. Dispersion plot of residuals for the proposed QSAR models of Eqs. (**1**)-(**7**).





MeLo in bulk (50 µM)

The Replacement Method (RM) procedure

The procedure of the RM technique is as follows: choose *d* descriptors, $\{X_1, X_2,\ldots,X_d\}$ at random and do a linear regression. Choose one of the descriptors of this set, called X_i, and replaced it by each of the *D* descriptors set (except itself) keeping the best resulting set. Since one can start replacing any of the *d* descriptors in the initial model, then a regression equation with *d* variables has *d* possible paths to achieve the final result; one example, the choice above will develop into path *i*. Next choose the variable with greatest relative error in it is coefficient (except the one replaced in the previous step) and replace it with all the D descriptors (except itself) keeping again the best set. Replace the entire remaining variable having greatest relative error in the coefficient and repeat the whole process. The process will repeat as many times as needed until the set of descriptors remains unchanged. At the end, we have the best model for the path *i*. Proceed in exactly the same way for all possible paths i=1, 2,…,*d*, compare the resulting models, and keep the best one. Our numerical experiments show that in this way one obtains a model almost as good as the best one with much less than $D!/(D-d)!d!$ linear regressions when this combinatorial number is large.