Supplementary Materials

Investigation of Physicochemical Properties of *N*-Alkoxyphenylhydroxynaphthalene-carboxamides †

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† Preliminary results were presented at The 21th Electronic Conference on Synthetic Organic Chemistry (ECSOC-21, http://sciforum.net/conference/ecsoc-21/paper/4719), 1–30 November 2017 (paper 4719).

Table S1. Matrix of correlation coefficients (n=19, α=0.05) of linear relationships between particular partition coefficients and experimental lipophilicity data (log*k*) for *N*-substituted 3-hydroxynaphthalene-2-carboxanilides **1a–19a** (series A).

	log*k*	**logP**[a]	**miLogP**[b]	**ClogP**[c]	**ClogP**[d]	**ClogP**[e]	**ClogP**[f]	**ClogP**[g]	**MlogP**[h]	**AlogP**[i]	**ClogP**[j]	**ClogP**[k]
log*k*	1											
logP[a]	0.93	1										
miLogP[b]	0.98	0.97	1									
ClogP[c]	0.98	0.97	0.99	1								
ClogP[d]	0.96	0.96	0.98	0.99	1							
ClogP[e]	0.88	0.88	0.90	0.89	0.88	1						
ClogP[f]	0.96	0.96	0.98	0.99	1.00	0.88	1					
ClogP[g]	0.99	0.95	0.98	0.98	0.96	0.93	0.96	1				
MlogP[h]	0.94	0.93	0.95	0.97	0.99	0.86	0.99	0.94	1			
AlogP[i]	0.98	0.97	0.99	0.99	0.99	0.90	0.99	0.98	0.96	1		
ClogP[j]	0.87	0.91	0.90	0.90	0.89	0.99	0.89	0.93	0.87	0.89	1	
ClogP[k]	0.93	0.95	0.97	0.98	0.99	0.88	0.99	0.95	0.98	0.98	0.90	1

[a] clogPS, [b] Molinspirations, [c] OSIRIS property explorer, [d] HyperChem 7.0, [e] Sybyl X, [f] Marvin Sketch (ChemAxon) 15, [g] ChemSketch 2015, [h] Dragon 6.0, [i] Dragon 6.0, [j] Kowwin, [k] XlogP3.

Table S2. Matrix of correlation coefficients (n=19, α=0.05) of linear relationships between particular partition coefficients and experimental lipophilicity data for *N*-substituted 1-hydroxynaphthalene-2-carboxanilides **1b–19b** (series B).

	log*k*	**logP**[a]	**miLogP**[b]	**ClogP**[c]	**ClogP**[d]	**ClogP**[e]	**ClogP**[f]	**ClogP**[g]	**MlogP**[h]	**AlogP**[i]	**ClogP**[j]	**ClogP**[k]
log*k*	1											
logP[a]	0.75	1										
miLogP[b]	0.79	0.98	1									
ClogP[c]	0.80	0.98	0.99	1								
ClogP[d]	0.78	0.96	0.98	0.99	1							
ClogP[e]	0.47	0.90	0.90	0.89	0.88	1						
ClogP[f]	0.80	0.97	0.99	0.99	0.99	0.88	1					
ClogP[g]	0.74	0.96	0.90	0.98	0.96	0.93	0.97	1				
MlogP[h]	0.76	0.92	0.95	0.97	0.99	0.86	0.98	0.94	1			
AlogP[i]	0.80	0.98	0.99	0.99	0.99	0.89	0.99	0.98	0.96	1		
ClogP[j]	0.47	0.91	0.90	0.90	0.89	0.99	0.89	0.93	0.87	0.89	1	
ClogP[k]	0.79	0.97	0.99	0.99	0.99	0.88	0.99	0.97	0.97	0.99	0.89	1

[a] clogPS, [b] Molinspirations, [c] OSIRIS property explorer, [d] HyperChem 7.0, [e] Sybyl X, [f] Marvin Sketch (ChemAxon) 15, [g] ChemSketch 2015, [h] Dragon 6.0, [i] Dragon 6.0, [j] Kowwin, [k] XlogP3.

Table S3. Matrix of correlation coefficients (n=19, α=0.05) of linear relationships between particular partition coefficients and experimental lipophilicity data for *N*-substituted 2-hydroxynaphthalene-1-carboxanilides **1c–19c** (series C).

	log*k*	**logP**[a]	**miLogP**[b]	**ClogP**[c]	**ClogP**[d]	**ClogP**[e]	**ClogP**[f]	**ClogP**[g]	**MlogP**[h]	**AlogP**[i]	**ClogP**[j]	**ClogP**[k]
log*k*	1											
logP[a]	0.75	1										
miLogP[b]	0.79	0.98	1									
ClogP[c]	0.80	0.98	0.99	1								
ClogP[d]	0.78	0.96	0.98	0.99	1							
ClogP[e]	0.47	0.90	0.90	0.89	0.88	1						
ClogP[f]	0.80	0.97	0.99	0.99	0.99	0.88	1					
ClogP[g]	0.74	0.96	0.98	0.98	0.96	0.93	0.97	1				
MlogP[h]	0.76	0.92	0.95	0.97	0.99	0.86	0.98	0.94	1			
AlogP[i]	0.80	0.98	0.99	0.99	0.99	0.89	0.99	0.98	0.96	1		
ClogP[j]	0.47	0.91	0.90	0.90	0.89	0.99	0.89	0.93	0.87	0.89	1	
ClogP[k]	0.79	0.97	0.99	0.99	0.99	0.88	0.99	0.97	0.97	0.99	0.89	1

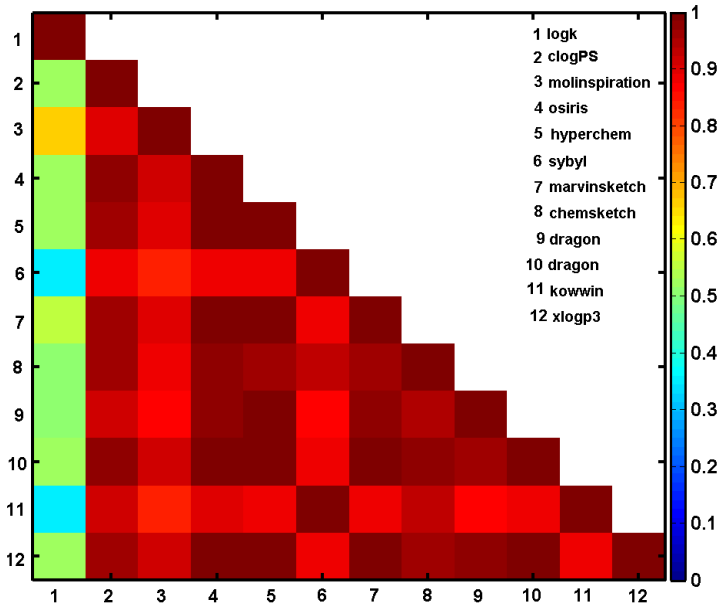
[a] clogPS, [b] Molinspirations, [c] OSIRIS property explorer, [d] HyperChem 7.0, [e] Sybyl X, [f] Marvin Sketch (ChemAxon) 15, [g] ChemSketch 2015, [h] Dragon 6.0, [i] Dragon 6.0, [j] Kowwin, [k] XlogP3.

Table S4. Matrix of correlation coefficients (n=57, α=0.05) of linear relationships between particular partition coefficients and experimental lipophilicity data for entire ensemble of compounds (series A, B, C).

	log*k*	**logP**[a]	**miLogP**[b]	**ClogP**[c]	**ClogP**[d]	**ClogP**[e]	**ClogP**[f]	**ClogP**[g]	**MlogP**[h]	**AlogP**[i]	**ClogP**[j]	**ClogP**[k]
log*k*	1											
logP[a]	0.52	1										
miLogP[b]	0.66	0.90	1									
ClogP[c]	0.53	0.97	0.91	1								
ClogP[d]	0.52	0.96	0.90	0.99	1							
ClogP[e]	0.35	0.89	0.83	0.89	0.88	1						
ClogP[f]	0.56	0.96	0.90	0.99	0.99	0.88	1					
ClogP[g]	0.50	0.96	0.89	0.98	0.96	0.93	0.96	1				
MlogP[h]	0.50	0.92	0.87	0.97	0.99	0.86	0.98	0.94	1			
AlogP[i]	0.53	0.97	0.91	0.99	0.99	0.89	0.99	0.98	0.96	1		
ClogP[j]	0.35	0.91	0.83	0.90	0.89	0.99	0.89	0.93	0.87	0.89	1	
ClogP[k]	0.52	0.96	0.91	0.99	0.99	0.88	0.99	0.96	0.97	0.99	0.89	1

[a] clogPS, [b] Molinspirations, [c] OSIRIS property explorer, [d] HyperChem 7.0, [e] Sybyl X, [f] Marvin Sketch (ChemAxon) 15, [g] ChemSketch 2015, [h] Dragon 6.0, [i] Dragon 6.0, [j] Kowwin, [k] XlogP3.

Figure S1. Matrix of correlation coefficients of linear relationships between experimental lipophilicity (log*k*[1]) and calculated lipophilicity with clogPS[2], Molinspirations[3], OSIRIS property explorer[4], HyperChem 7.0[5], Sybyl X[6], Marvin Sketch (ChemAxon) 15[7], ChemSketch 2015[8], Dragon 6.0[9], Dragon 6.0[10], Kowwin[11], XlogP3[12] methods for the entire ensemble of compounds (series A, B, C).



Scheme S1. Basic methods for in silico lipophilicity specification.