

ANNEX 7

PARTITION COEFFICIENT: **COMPARISON OF TEST RESULTS AND PREDICTIONS**

Chem. No.	MPD log P _{ow}	SAR -log P _{ow}	Difference [± log units]	Result
4	nd	nd	-	-
6	nd	nd	-	-
16	0.014	<-2.5	-2.5	disagree
17	nd	nd	-	-
21	>4.15	>6	+1.85	disagree
23	-4.68	nd	-	-
24	4.28	6.9	[+1.72]	disagree
26	4.74	>6 (10.8)	[+1.26]	disagree
37	∞	2.5	-	-
44	3.0	nd	-	-
47	3.93	5.3	+1.37	disagree
49	1.65	≥6	+4.35	disagree
50	1.3	nd	-	-

Chem. No.	MPD log P _{ow}	SAR log P _{ow}	Difference [± log units]	Result
53	nd	>6	-	-
54	3.09	2.71	-0.38	agree
61	4.38	>6 (9.2)	[+1.62]	disagree
68	nd	<-2.5	-	-
69	nd	<-2.5	-	-
70	4.4	>6	+1.6	disagree
76	nd	nd	-	-
78	nd	5.9	-	-
79	nd	nd	-	-
87	2.02	2.1	+0.08	agree
96	nd	<-2.5	-	-
99	nd	nd	-	-
101	nd	nd	-	-

Chem. No.	MPD log P _{ow}	SAR log P _{ow}	Difference [± log units]	Result
102	nd	>6 (14.4)	-	-
106	nd	>6 (6.94)	-	-
107	nd	nd	-	-
108	>5	-5	0	agree
110	nd	>6	-	-
113	4.01	>6 (10.8)	[+1.99]	disagree
118	nd	6.8	-	-
124	2.46	1 - 2	-0.96	agree
128	nd	3.4	-	-
133	3.6	3.6	0	agree
144	5.8	>6 (11.8)	[+0.2]	agree
148	nd	>6	-	-
151	4.87	5.3	+0.43	agree

Chem. No.	MPD log P _{ow}	SAR log P _{ow}	Difference [± log units]	Result
155	nd	>6	-	-
156	4.65	3.7	-0.95	agree
164	3.0	>6	+3	disagree
170	-0.823 to -1.148	0	+0.98	agree
173	1.9/2.0	3.8	+1.85	disagree
176	4.5	≥6	+1.5	disagree
182	5.42	>6 (11.2)	[+0.58]	agree
186	5.6	4	-1.6	disagree
192	0.74	<3.8	+3.06	disagree
194	nd	3.6	-	-
196	nd	-1.8	-	-
197	3.6	1.8	-1.8	disagree
200	6.25	>6 (6.7)	[0]	agree

Chem. No.	MPD log P _{ow}	SAR log P _{ow}	Difference [± log units]	Result
204	3.89	>6	+2.11	disagree
214	nd	>6	-	-
216	nd	nd	-	-
217	nd	2.5	-	-
218	3.84	4.1	+0.26	agree
219	1.65	2.3	+0.65	agree
222	nd	reacts	-	-
224	nd	nd	-	-
235	nd	>6	-	-
237	5.1	nd	-	-
239	>3.29	>6 (12.9)	[2.71]	disagree
240	nd	nd	-	-
241	-2.76	[0]	0	agree

Chem. No.	MPD log P _{ow}	SAR log P _{ow}	Difference [± log units]	Result
242	-2.4	<0	[0]	agree
253	nd	>6 (10.5)	-	
256	-1.3	<-2.5	[0]	agree
263	-2.36	<0	[0]	agree
265	<-2.5	≤-1.075	[0]	agree
267	nd	nd	-	
268	4.6	≥5.4	+0.8	agree
269	4.53	5.0	+0.47	agree
270	-1.1 (pH 7.65) +0.55 (pH 8.72)	3	>1	disagree
271	nd	5	-	
275	nd	4.3	-	
278	3.95	5.2	+1.25	disagree
281	4.41	5.2	+0.79	agree

Chem. No.	MPD log P _{ow}	SAR log P _{ow}	Difference [± log units]	Result
283/ 429	nd	nd	-	-
286	≥6	>6	0	agree
287	≥5	>6	1	agree
289	nd	5.5	-	-
291	nd	>6	-	-
292	2.88	3.4	+0.52	agree
300	3.67	4.2	+0.53	agree
307	3.07	3.1	-0.03	agree
309	3.9	>6	+2.1	disagree
312	1.09	<0	-1.09	disagree
318	nd	3 - 4	-	-
320	nd	nd	-	-
321	1.11 (pH 2)	-0.25 (missing fragment)	-1.36	disagree

Chem. No.	MPD log P _{ow}	SAR log P _{ow}	Difference [± log units]	Result
330	<-3	-0.85	[0]	agree
335	-3	nd	-	-
336	<-1	nd	-	-
337	3.05	1.7 - 1.9	-1.15	disagree
340	0.492	-0	-0.49	agree
341	nd	<-2.5	-	-
342	-0.0053	0.55	0.55	agree
344	nd	<-2.5	-	-
348	5.9	>6 (11.5)	[+0.1]	agree
349	>7.24	>6	[0]	agree
354	2.89	3.3	+0.41	agree
355	1.92	>6 (8.0)	+4.08	disagree
360	1.04	3.2	+2.16	disagree

Chem. No.	MPD log P _{ow}	SAR log P _{ow}	Difference [± log units]	Result
361	4.85	>6 (>8)	[+1.15]	disagree
362	2.3	3.0	+0.7	agree
364	nd	<-2.5	-	-
366	3.7	nd	-	-
368	4.3	3.1	-1.2	disagree
369	<-2.5	nd	-	-
370	nd	4.9	-	-
373	4.18	4.4	+0.22	agree
376	>5.7	>6 (11.6)	[+0.3]	agree
379	4.74	4.2	-0.54	agree
381	nd	nd	-	-
383	nd	>6	-	-
386	2.62 / 2.73	3	0.38	agree

Chem. No.	MPD log P _{ow}	SAR log P _{ow}	Difference [± log units]	Result
393	nd	3.6	-	-
394	-2.46	<-2.5	[0]	agree
396	-1.47	-2.4	[0]	agree
398	>2.7	3.3	+0.6	agree
401	-3.27 / 0.758	nd	-	-
406	4.65	5.3	+0.65	agree
411	nd	>6	-	-
413	nd	>6	-	-
414	0.258	2 - 3.5	+2.5	disagree
415	7	>6	[0]	agree
416	nd	>6	-	-
417	5.1	5.4	+0.3	agree
420	3.38	3.8	+0.42	agree

Chem. No.	MPD log P _{ow}	SAR log P _{ow}	Difference [± log units]	Result
421	≥5	5.6	+0.6	agree
425	nd	0.31	-	-
431	4.7	>6 (12.0)	> +1.3	disagree
436	nd	3.5 - 4.6	-	-
437	6.4	>6 (9)	[0]	agree
439	-1.98	2	+3.98	disagree
441	1.37	2.18	+0.81	agree
442	-1.88	≤-2.5	[0]	agree
443	1.96	1.16	-0.8	agree
444	3.39	3.68	+0.29	agree
445	nd	nd	-	-
446	nd	>6	-	-
451	2.63	0.99	1.64	disagree
472	>4.6	>6 (6.78)	+1.4	disagree