Verma protocol

Bronwen Dekker

Method Article

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Abstract

Introduction

This protocol is here to upload the Verma figures.

Procedure

See the figures.

Figures

<u>Code</u>	<u>System</u>	<u>Hits*</u>
<u>1</u>	<u>Guppy</u>	<u>35</u>
<u>1</u>	<u>Mouse</u>	<u>461</u>
<u>1</u>	<u>Chloroplast</u>	<u>76</u>
<u>1</u>	<u>Liver</u>	<u>424</u>
<u>1</u>	<u>Human</u>	<u>1989</u> etc.

Figure 1

1

<u>Code</u>	<u>Class</u>	<u>Hits</u>
<u>2</u>	<u>B4V</u>	<u>424</u>
<u>2</u>	<u>B6F</u>	<u>208</u>
<u>2</u>	<u>B2A</u>	<u>1028</u> etc.

Figure 2

2

<u>Code</u>	<u>Action</u>	<u>Hits</u>
<u>4</u>	<u>Pen Perm</u> (cell penetration)	<u>272</u>
<u>4</u>	<u>Hemolysis</u>	<u>52</u>
<u>4</u>	<u>Narcosis</u>	<u>86</u>
<u>4</u>	<u>I50</u>	<u>938</u>
<u>4</u>	<u>IC50</u>	<u>3790</u>
<u>4</u>	<u>Kill</u>	<u>199</u> etc.

Figure 3

3

Set No. 12865

System L1210 CELLS
Class B4C ; Cells in culture
Compound X-PHENOLS
Action IC50: CASPASE-MEDIATED APOPTOSIS OF X-PHENOLS
Equation $\log 1/C = 1.06(\pm 0.12)B5_2 + 0.33(\pm 0.20)B5_3 - 0.18(\pm 0.09)n_{2,4} - 0.92(0.46)$
(1)
Stats $n = 51$ $DF = 47$ $s = 0.349$ $r = 0.941$ $q^2 = 0.866$
omit = 1

Figure 4

4

No.	Command (press ENTER followed by <u>sea</u> command)	Hits
1	qsar:bio> <u>15</u> " <u>log1/C</u> "	<u>8607</u>
2	qsar:bio> <u>15</u> not <u>**2 bilin</u>	<u>6549</u>
3	qsar:bio> <u>15</u> " <u>logP</u> " " <u>ClogP</u> "	<u>3104</u>
4	qsar:bio> <u>15</u> not "S	<u>2638</u>
5	qsar:bio> <u>15</u> not <u>ES B1 B5 MR Pi PKA</u>	<u>2092</u>
6	qsar:bio> <u>16</u> <u>0.6<LOGP<1< B></u>	<u>639</u>
7	qsar:bio> <u>16</u> <u>0<CONST<0.5< B></u>	<u>55</u>

Figure 5

5

No.	Command (press ENTER followed by <u>sea</u> command)	Hits
1	qsar:bio> <u>15</u> <u>logP</u>	<u>6953</u>
2	qsar:bio> <u>15</u> <u>logP**2 bilin(logP) bilin(ClogP)</u>	<u>1786</u>
3	qsar:bio> <u>17</u> <u>1.5<logP<2.5</u>	<u>170</u>

Figure 6

6

No.	Command (press ENTER followed by <u>sea</u> command)	Hits
1	qsar:bio> <u>16</u> <u>ClogP>0</u>	<u>4377</u>
2	qsar:bio> <u>16</u> <u>ClogP**2<0</u>	<u>696</u>

Figure 7

7

No.	Command (press ENTER followed by <u>sea</u> command)	Hits
1	qsar:bio> <u>16 ClogP<0</u>	<u>2795</u>
2	qsar:bio> <u>16 ClogP**2>0</u>	<u>158</u>

Figure 8

8

No.	Command (press ENTER followed by <u>sea</u> command)	Hits
1	qsar:bio> <u>16 ClogP>0</u>	<u>4377</u>
2	qsar:bio> <u>16 bilin(ClogP)<0</u>	<u>602</u>

Figure 9

9

No.	Command (press ENTER followed by <u>sea</u> command)	Hits
1	qsar:bio> <u>16 ClogP<0</u>	<u>2795</u>
2	qsar:bio> <u>16 bilin(ClogP)>0</u>	<u>57</u>

Figure 10

10

QSAR DB name: BIO
 THOR DB name: QSAR_MC\$BIGDATA:MASTER
 Dataset name: BIO_12675
 Substituents: 15 Parameters: 7 SMILES: 15
 Equations: 1
 Active: 14 Starred: 1 Inactive: 0
 System: DNA
 Class: B1 ; Nonenzymatic Macromolecules:
 Compound: THIOACRIDONE DERIVATIVES
 Action: K: BINDING CONSTANT
 Reference: DHEYONGERA, J.P., GELDENHUYS, W.J., DEKKER,
 T.G., VAN DER SCHYF, C.J., BIOORG. MED. CHEM.,
 13, 689-698(2005) R7466
 Source: RAJESHWAR PRASAD VERMA
 Analysis: UNKNOWN
 Date: 2006 October 26
 Parameters: YPRED DEV LOGK CLOGP CMR NVE MGVOL

Figure 11

12

$$\log K = -0.77(\pm 0.28)\text{Clog } P + 0.95(\pm 0.14)\text{CMR} - 4.67(\pm 1.76) \quad (2)$$

$$n = 14, \quad r = 0.981, \quad q^2 = 0.933, \quad \text{SS1} = 22.23, \quad \text{DEV+} = 6$$

$$\text{DF} = 11, \quad r^2 = 0.963, \quad s = 0.275, \quad \text{SS2} = 0.831, \quad \text{DEV-} = 8$$

Figure 12

13

#	R ₁	R ₂	R ₃	log K	Ypred.	Dev	Clog P	CMR
1	NH(CH ₂) ₂ N(CH ₃) ₂	H	CH ₃	2.93	2.46	0.48	2.99	9.98
2	NH(CH ₂) ₂ N(CH ₃) ₂	Cl	CH ₃	2.04	2.25	-0.21	3.86	10.47
3	NH(CH ₂) ₂ N(CH ₃) ₂	CH ₃	CH ₃	2.36	2.51	-0.15	3.49	10.44
*4	NH(CH ₂) ₂ N(CH ₃) ₂	H	H	4.41	2.56	1.85	2.28	9.52
5	NH(CH ₂) ₂ N(CH ₃) ₂	Cl	H	2.08	2.21	-0.13	3.35	10.01
6	NH(CH ₂) ₂ N(CH ₃) ₂	CH ₃	H	2.43	2.62	-0.19	2.78	9.98
7	N(CH ₂ CH ₂ Cl) ₂	H	H	2.04	1.88	0.16	3.93	10.13
8	N(CH ₂ CH ₂ Cl) ₂	Cl	H	1.95	1.62	0.33	4.86	10.62
9	N(CH ₂ CH ₂ Cl) ₂	CH ₃	H	1.78	1.93	-0.15	4.42	10.59
10	Cl	H	H	-0.1	-0.33	0.23	3.46	7.41
11	Cl	Cl	H	-0.22	-0.46	0.24	4.23	7.91
12	Cl	CH ₃	H	-0.15	-0.27	0.12	3.96	7.88
13	Cl	H	CH ₃	-0.52	-0.15	-0.37	3.8	7.88
14	Cl	Cl	CH ₃	-0.4	-0.25	-0.15	4.52	8.37
15	Cl	CH ₃	CH ₃	-0.3	-0.1	-0.2	4.3	8.34

Figure 13

13a

<u>C</u> (concentration of the activity)	<u>Enter transformation</u> (log1/C in molar concentration)
Nano molar (nM)	<u>9 - log C</u>
Mili molar (mM)	<u>3 - log C</u>

Figure 14

14

No.	Substituent	log1/C	BDE
1	NH ₂	4.61	-9.25
2	OC ₆ H ₁₃	5.34	-6.30
3	Me	3.82	-2.22
4	CMe ₃	3.86	-1.54
5	H	3.27	0.00
6	OMe	4.41	-6.01
7	C ₃ H ₇	3.72	-2.01
8	C(Me) ₂ C ₆ H ₄ -4-OH	4.18	-1.88
9	C ₂ H ₅	3.79	-1.90
10	C ₈ H ₁₇	4.66	-2.17

Figure 15

15

Figure 16

16

<u>*OCCCCC</u>	4- <i>n</i> -hexyloxyphenol
<u>*C</u>	4-methylphenol
<u>*C(C)(C)C</u>	4- <i>t</i> -butylphenol
<u>*H</u>	phenol
<u>*OC</u>	4-methoxyphenol
<u>*CCC</u>	4- <i>n</i> -propylphenol
<u>*C(C)(C)c2ccc(O)cc2</u>	4-CMe ₂ C ₆ H ₄ (4-OH)-phenol
<u>*CC</u>	4-ethylphenol
<u>*CCCCCCC</u>	4- <i>n</i> -octylphenol

Figure 17

17

Oc1ccc(*)cc1
1

Figure 18

17a

	S.D.	BDE	Clog <i>P</i>	CMR	NVE	MgVol	MW	S+	CONST
1	.437	-.15							3.66
2	.457							-1.09	3.66
3	.525				.02				3.12
4	.531						.01		3.12
5	.538					.76			3.21
6	.550			.21					3.24
7	.594		.14						3.79

Figure 19

18

	S.D.	BDE	Clog <i>P</i>	CMR	NVE	MgVol	MW	S+	CONS
1	.142	-.20	.27						2.74
2	.176		.28					-1.52	2.69
3	.205	-.17				.89			2.50
4	.218	-.16			.02				2.51
5	.234	-.17		.25					2.51
6	.238	-.16					.01		2.51
7	.241					.90		-1.21	2.47
8	.249				.02			-1.16	2.48
9	.268						.01	-1.16	2.49
10	.269			.25				-1.22	2.49

Figure 20