Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry This journal is © The Royal Society of Chemistry 2012 S1 Supplementary information contents page

Design and synthesis of screening libraries based on the muurolane natural product scaffold

Emma C. Barnes,^a Vanida Choomuenwai,^{a,b} Katherine T. Andrews,^{a,b} Ronald J. Quinn,^a and Rohan A. Davis^a

^aEskitis Institute, Griffith University, Brisbane, QLD 4111, Australia. ^bQueensland Institute for Medical Research, Herston, QLD 4006, Australia

Contents:

S3	¹ H NMR spectrum for 14-hydroxy-6, 12-muuroloadien-15-oic acid (1) in DMSO- d_6
S4	¹³ C NMR spectrum for 14-hydroxy-6, 12-muuroloadien-15-oic acid (1) in DMSO- d_6
S5	¹ H NMR spectrum for compound 2 in DMSO- d_6
S6	¹³ C NMR spectrum for compound 2 in DMSO- d_6
S7	¹ H NMR spectrum for compound 3 in DMSO- d_6
S8	¹³ C NMR spectrum for compound 3 in DMSO- d_6
S9	¹ H NMR spectrum for compound 4 in DMSO- d_6
S10	¹³ C NMR spectrum for compound 4 in DMSO- d_6
S11	¹ H NMR spectrum for compound 5 in DMSO- d_6
S12	¹³ C NMR spectrum for compound 5 in DMSO- d_6
S13	¹ H NMR spectrum for compound 6 in DMSO- d_6
S14	¹³ C NMR spectrum for compound 6 in DMSO- d_6
S15	¹ H NMR spectrum for compound 7 in DMSO- d_6
S16	¹³ C NMR spectrum for compound 7 in DMSO- d_6
S17	¹ H NMR spectrum for compound 8 in DMSO- d_6
S18	¹³ C NMR spectrum for compound 8 in DMSO- d_6
S19	¹ H NMR spectrum for compound 9 in DMSO- d_6
S20	¹³ C NMR spectrum for compound 9 in DMSO- d_6

Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry This journal is © The Royal Society of Chemistry 20 32 Supplementary information contents page

Contents continued:

- **S21** ¹H NMR spectrum for compound **10** in DMSO- d_6
- **S22** 13 C NMR spectrum for compound **10** in DMSO- d_6
- **S23** ¹H NMR spectrum for compound **11** in DMSO- d_6
- S24 ${}^{13}C$ NMR spectrum for compound 11 in DMSO- d_6
- **S25** ¹H NMR spectrum for compound **12** in DMSO- d_6
- **S26** ¹³C NMR spectrum for compound **12** in DMSO- d_6
- **S27** ¹H NMR spectrum for compound **13** in DMSO- d_6
- **S28** ¹³C NMR spectrum for compound **13** in DMSO- d_6
- **S29** ¹H NMR spectrum for compound **14** in DMSO- d_6
- **S30** ¹³C NMR spectrum for compound **14** in DMSO- d_6

Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry This journal is C The Royal Society of Chemistry 2012

S3 ¹H NMR spectrum for 14-hydroxy-6, 12-muuroloadien-15-oic acid (1) in DMSO- d_6



Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry This journal is C The Royal Society of Chemistry 2012

S4 ¹³C NMR spectrum for 14-hydroxy-6, 12-muuroloadien-15-oic acid (1) in DMSO- d_6





4.5 f1 (ppm)

Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry This journal is © The Royal Society of Chemistry 2012 **S6** ¹³C NMR spectrum for compound 2 in DMSO-*d*₆





Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry This journal is © The Royal Society of Chemistry 2012 **S7** ¹H NMR spectrum for compound 3 in DMSO-*d*₆



Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry This journal is © The Royal Society of Chemistry 2012 **S8** ¹³C NMR spectrum for compound 3 in DMSO-*d*₆



ntrafortantelaki	kainamaji.wikitikajina, sake	and the state of the	arranda magazant	and the second production	itajini)krytajaj	aliter die het stelling die stelling voor stelling die stelling voor stelling die stelling voor stelling voor s	alquariydariyatiya	(tá: várasznák)/já vegt körtyekete	line of the first of the	n na managang kang kang kang kang kang kang ka	and the second second second	h itadi yani k ulan		والرمزيني الرامية	after og sta sta for	ſġĸĨĿŗIJŧĊĸŢĔĸŎĴĴŎĿŊ	for a for the second
	' '			· ·		· · ·						· ·			· · ·		
170	160	150	140	130	120	110	100	90 f1 (ppm)	80	70	60	50	40	30	20	10	0

Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry This journal is © The Royal Society of Chemistry 2012 S9 ¹H NMR spectrum for compound 4 in DMSO-d₆



Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry This journal is © The Royal Society of Chemistry 2012 **S10** ¹³C NMR spectrum for compound 4 in DMSO-*d*₆



Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry This journal is © The Royal Society of Chemistry 2012 S11 ¹H NMR spectrum for compound 5 in DMSO-*d*₆

Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry This journal is C The Royal Society of Chemistry 2012 **S13** ¹H NMR spectrum for compound **6** in DMSO- d_6 Ĥ H Ē 111 Ο OH H₃CO

Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry This journal is © The Royal Society of Chemistry 2012 S14 ¹³C NMR spectrum for compound 6 in DMSO-d₆

Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry This journal is © The Royal Society of Chemistry 2012 **S16** ¹³C NMR spectrum for compound 7 in DMSO-*d*₆

Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry This journal is © The Royal Society of Chemistry 2012 S20 ¹³C NMR spectrum for compound 9 in DMSO-d₆

Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry This journal is © The Royal Society of Chemistry 2012 S22 ¹³C NMR spectrum for compound 10 in DMSO-*d*₆

20

Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry This journal is © The Royal Society of Chemistry 2012 S24 ¹³C NMR spectrum for compound 11 in DMSO-*d*₆

Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry This journal is © The Royal Society of Chemistry 2012 S28 ¹³C NMR spectrum for compound 13 in DMSO-*d*₆

Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry This journal is © The Royal Society of Chemistry 2012 **S30** ¹³C NMR spectrum for compound **14** in DMSO-*d*₆

