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Supplemental Material for

# A Widespread Bacterial Phenazine

### Forms Conjugates with Biogenic Thiols and Crosslinks Proteins

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## Analytical data of compounds 3 and 4



**Figure S1**: Selected <sup>1</sup>H,<sup>13</sup>C HMBC and <sup>1</sup>H,<sup>1</sup>H COSY correlations of panphenazines **3** and **4**.

	3		4	
Position	$\delta_{H^a}$ (J in Hz)	δ <sub>C</sub> <sup>b</sup>	$\delta_{\rm H^a}$ ( <i>J</i> in Hz)	δc <sup>b</sup>
1	-	_c	-	_c
2	8.62, d (7.0)	135.5	8.32, m	134.7
3	8.03, dd (8.7, 7.0)	131.7	-	143.3
4	8.40, dd (8.7, 1.3)	134.8	8.17, d (2.2)	126.6
4a	-	144.6	-	144.8
5a	-	145.3	-	145.1
6	8.05, d (2.1)	123.2	8.22, dd (7.6, 2.2)	130.2
7	-	145.2	7.96, m	133.0
8	7.87, dd (9.1, 2.1)	134.3	7.96, m	132.8
9	8.18, d (9.1)	129.4	8.28, dd (7.6, 2.2)	129.9
9a	-	141.0	-	142.0
10a	-	140.8	-	140.4
1`	3.38, m	32.0	3.39, m	32.3
2`	3.59,td (6.90, 1.5)	39.3	3.59, t (6.8)	39.2
3`	-	174.1	-	174.1
4`	2.43, t (6.7)	36.5	2.42, t (6.6)	36.5
5`	3.48, m	36.4	3.49, m	36.3
6`	-	176.1	-	176.1
7`	3.87, s	77.3	3.87, s	77.3
8`	-	40.4	-	40.4
9`/10`	0.89, s	21.3/20.9	0.89, s	21.3/20.9
11`	3.39, m	70.4	3.40, m	70.4
соон	-	169.7	-	170.2

**Table S1**: NMR spectroscopic data for Compounds **3** and **4** in methanol-*d*4.

<sup>a</sup> recorded at 600.3 MHz, <sup>b</sup> recorded at 150.9 MHz; <sup>c</sup> signals not detectable.

### Binding of phenazine to biogenic thiols



#### Conjugate formation of PCA with pantetheine following irradiation at 370 nm

**Figure S2.** SIM-HRMS (m/z = 501.1788-501.1828) analysis of the obtained product after incubation of PCA and pantetheine with irradiation at 370 nm; comparison with the isolated reference compounds **3** and **4**. SIM: selected ion monitoring.



#### Coupling of PCA to cysteine and glutathione

**Figure S3**. HRMS(/MS) spectrum of PCA-cysteine adduct ([M+H]<sup>+</sup>) after incubation of PCA with cysteine under sunlight.



**Figure S4**. HRMS(/MS) spectrum of PCA-glutathione-adduct ([M+H]<sup>+</sup>) after incubation of PCA with glutathione under sunlight.

#### Conjugate formation of PCA with pantetheine in presence of AIBN



**Figure S5**. SIM-MS spectrum of the product after incubation of PCA with pantetheine in presence of AIBN in the dark (top). MS spectrum of PCA-pantetheine-adduct ([M+Na]<sup>+</sup>) (bottom).



Synthesis of phenazine probes 9 (with biotin) and 10 (with rhodamine).

Figure S6: Synthesis of biotin- and rhodamine-B-tagged phenazine probes.

### Phenazine-protein binding assays with KS-B



**Figure S7.** SDS-PAGE (12% gel) after incubation of KS-B with rhodamine-B-labelled phenazine probe **10** under the following conditions: A)  $\lambda$  = 370 nm, 20 h, in H<sub>2</sub>O, B)  $\lambda$  = 370 nm, 20 h, DMSO, C) sunlight, 8 h, H<sub>2</sub>O, D) D: sunlight, 8 h, DMSO, E) E: AIBN, 20 h, DMSO, F) F: AIBN, 20 h, H<sub>2</sub>O.

# Tryptic mass fingerprinting of labelled KS-B

-	-

Protein:	RhiE KsBb						
Intensity covera	ge: 54.2 % (250	1997 cnts) Seque	nce coverage MS:	42.5 % Sequ	ence coverage MS/	MS: 5.5 %	pl: 5.9
10	20	30	40	50	60	70	80
мкннннннн	GGLVPRGSHG	GSSGERVEDN	ELANYIAVIG	LGGYYPGADS	IDELWQNLAN	GVDCMSDFPA	DRWDHSKIYY
90	100	110	120	130	140	150	160
KNRKVLGKTT	CI <mark>NGS</mark> FIKDV	DKFDYSYFKM	PKVYADHMSP	EVRLFLQVAV	HTFEDAGYSK	ETLLSRYNGD	VGVLLGTMSN
170	180	190	200	210	220	230	240
DYHYYGFESN	VFRGSMASGS	GMATIPMTVS	YFYGLTGPSL	FIDTMCSSSS	TCIHTACQML	KHDETKMVLA	GGLNLMYHPY
250	260	270	280	290	300	310	320
TTVNTSQGNF	TSITSESVNS	YGVGADGTVI	GEGIGAVLLK	RLDRAIADRD	QIYGVIKGSA	MTNAGERNGF	NVPNPDLQTI
330	340	350	360	370	380	390	400
AIRQAMDQAK	VHPSSISYIE	GHGSGTKLGD	PIEVLGLNNA	FRWATDDKQF	CYLGSIKSNI	GHLLAASGIA	GLTKTLLQF
410	420	430	440	450	460	470	480
HKQIAPSIHS	SQLNQDIDFA	DTPFVVPQQL	IEWRQPERII	NGRKQVFPRR	AGLTSIAAGG	MNAHMIVEEY	PEPADSAGQI
490	500	510	520	530	540	550	560
SEDQLVFVFS	VHKLALLAQ <mark>N</mark>	LTSFRDWLAS	SEAPLAQIAY	TLQVGKNNLR	NRLAIRCRTR	QALSRALNAC	IDGHYQSSAI
570	580	590	600	610	620	630	640
SKIFYRFQES	DAVQPLESDL	NDPLAPLLTQ	WLNGDSQVDW	ASLYAQPPVR	ISLPAYRFEK	TRCWYTEEGY	ESSIVNPLME
650	660	670	680	690	700	710	720
KNKLHPLVAK	NCSTPQPGAI	FRTDFVEDEL	LDYVYSGRGG	RRLSAFNFAD	VALAMPALAS	RFDGRTLSVS	CAFEHYIADU
730	740	750	760	770	780	790	800
TTVTGLEYRL	FEIDSEQLEL	EFDFRRSGEQ	PTHLGFAVIN	PLTSDEPPLP	QQWLDDAREL	LNRQALQAGR	QLSAAEVSQR
810	820	830	840	850	860	870	880
LAQAGYDFAP	YLDHDGELTI	GRSGLVLKGR	PPVNRHNHYA	DNVQLSPYLA	TTIDKALYLL	LDELGLPQGR	VIVRNIERLO
890	900	910	920	930	940	950	
CYHTPAGGFS	VVLSGIGLND	NELSLSLLVL	DEREQICVKL	DKVSLYLGKQ	EVASVDRKHS	LLTGT	

**Figure S8.1.** Tryptic mass fingerprinting of KS-B after incubation with **9** and AIBN followed by affinity chromatography.



Protein:	BhiFKs8h						
Intensity covera	ge: 49.7 % (228)	3686 cnts) Sequer	nce coverage MS:	16.3% Sequ	ence coverage MS/1	¥5: 83%	pl: 5.9
10	20	30	10	50	E.	70	80
мкннннннн	GGLVPRGSHG	GSSGERVEDN	ELANYIAVIG	LGGYYPGADS	IDELCONLAN	GVOCMSOFPA	DRWDHSKIY
90	100	110	120	130	140	_50	160
KNRKVLGKTT	CI <mark>NGS</mark> FIKDV	DKFDYSYFKM	PKVYADHMSP	EVRLFLQVAV	HIFECAGESE	ETLLSRYNGD	VGVLLGTMS
170	180	190	200	210	220	230	240
DYHYYGFESN	VFRGSMASGS	GMATIPMTVS	YFYGLTGPSL	FIDTMCSSSE	TCIETACOBL	ZHOETKMVLA	GGLNLMYHP
250	2.60	270	280	290	300	310	320
TTV <mark>NTS</mark> QG <mark>NF</mark>	TSITSESVNS	YGVGADGTVI	GEGIGAVLLK	RLDRAIADRE	QIYGVIRGEN	STNAGERNGF	NVPNPDLQTI
330	340	350	3.60	370	350	390	400
AIRQAMDQAK	VHPSSISYIE	GHGSGTKLGD	PIEVLGLNNA	FRWATDDKQF	CYLGEDRENI	GHLLAASGIA	GLTKTLLQF
410	420	430	440	450	460	470	480
HKQIAPSIHS	SQLNQDIDFA	DTPFVVPQQL	IEWRQPERII	NGRKQVFPRF	AGLIEINAGG	INABMIVEEY	PEPADSAGQI
490	500	510	520	530	541	550	560
SEDQLVFVFS	VHKLALLAQ <mark>N</mark>	LTSFRDWLAS	SEAPLAQIAY	TLQVGKNNLF	NRLAIRCRIR	CALSRALNAC	IDGHYQSSAD
570	580	590	600	610	620	630	640
SKIFYRFQES	DAVQPLESDL	NDPLAPLLTQ	WLNGDSQVDW	ASLYAQPPVE	IELFATEFER	TROWYTEEGY	ESSIVNPLMF
650	660	670	680	690	700	710	720
KNKLHPLVAK	NCSTPQPGAI	FRTDFVEDEL	LDYVYSGRGG	RRLSAFNFAC	VALAEFALAS	RFOGRTLSVS	CAFEHYIADU
730	740	750	760	770	780	790	800
TTVTGLEYRL	FEIDSEQLEL	EFDFRRSGEQ	PTHLGFAVIN	PLTSDEPPLF	QQUICCAREL	LNRCALQAGR	QLSAAEVSQF
810	820	830	840	850	867	870	880
LAQAGYDFAP	VLDHDGELTT	GREGLVLKGR	PPVNRHNHVA	DNVQLSPVLA	LIP ISTITT	LOKINGL/PQGR	VIVENTERLO
890	900	910	920	930	542	950	
CYNTRAGGES	VVLSCICLND	NELSLSLLVL	DEREOICVKL	DKVSLVLGKO	FVAEVODERES	LATGT	

Figure S8.2. Tryptic mass fingerprinting of KS-B after crosslinking with 10 under UV light (1).

Protein:	RhiE KsBb						
Intensity covera	ige: 54.9 % (117.	3386 cnts) Seque	nce coverage MS:	14.5 % Sequ	ence coverage MS/I	MS: RR%	pl: 5.9
10	20	30	40	50	60	70	80
мкниннини	GGLVPRGSHG	GSSGERVEDN	ELANVIAVIG	LGGYYPGADS	IDELWQNLAN	GVDCMSDFPA	DRWDHSKIY
90	100	110	120	130	140	150	160
KNRKVLGKTT	CI <mark>NGS</mark> FIKDV	DKFDYSYFKN	PKVYADIIMSP	EVRLFLQVAV	HTFEDAGYSK	ETLLSRYNGD	VGVLLGTMS
170	180	190	200	210	220	230	2.40
DYHYYGFESN	VFRGSMASGS	GMATIPMTVS	YFYGLTGPSL	FIDTMC3333	TCIHTACQML	KHDETKHVLA	GGLNL MYHP
2.50	2.60	270	260	290	300	310	320
TTV <mark>NTSQGNF</mark>	TSITSESVNS	YGVGADGTVI	GEGIGAVLLK	RLDRAIADRD	Q1YGV1KG5A	MINAGERNGF	NVPNPDLQTI
330	340	350	360	370	380	390	400
AIRQAMDQAK	VHPSSISYIE	GHGSGTKLGD	PIEVLGLNNA	FRUATDDKQF	CYLGSIKSNI	GHLLAASGIA	GLTKTLLQF
410	420	430	440	450	460	470	480
HKQIAPSIHS	SQLNQDIDFA	DIFFAAROOF	TEWRQPERII	NGRKQVFPRR	AGLTSIAAGG	MNAHMIVEEY	PEPADSAGQI
490	500	510	520	530	540	550	560
SEDQLVFVFS	VHKLALLAQ <mark>N</mark>	LTSFRDWLAS	SEAPLAQIAY	TLQVGKNNLR	NRLAIRCRTR	QALSRALNAC	IDGHYQSSAI
570	580	590	600	610	620	630	640
SKIFYRFQES	DAVQPLESDL	NDPLAPLLTQ	WLNGDSQVDW	ASLYAQPPVR	ISLPAYRFEK	TRCWYTEEGY	ESSIVNPLM
650	660	670	680	690	700	710	720
KNKLHPLVAK	NCSTPQPGAI	FRTDFVEDEL	LDYVYSGRGG	RRLSAFNFAD	VALAMPALAS	RFDGRTLSVS	CAFEHYIAD
730	740	750	760	770	780	790	800
TTVTGLEYRL	FEIDSEOLEL	EFDFRRSGEO	PTHLGFAVIN	PLTSDEPPLP	OOWLDDAREL	LNROALOAGR	OLSAAEVSON
810	820	830	840	850	860	870	880
LAQAGYDFAP	YLDHDGELTI	GREGLVLKGR	PPVNRHNHYA	DNVQLSPYLA	TTIDKALVLL	LDELGLPQGR	VIVENIERL
890	900	910	920	930	940	950	
CYHTPACCFS	VVLSCICLND	NELSLSLLVL	DEREQICVKL	DKVSLYLCKQ	EVASVDRKHS	LLTCT	

Figure S8.3. Tryptic mass fingerprinting of KS-B after crosslinking with 10 under UV light (1).

Protein:	RhiE KeBb						
Intensity covera	ge: 47.8 % (976	679 cnts) Seque	nce coverage MS:	14.4 % Sequ	ence coverage MS/I	MS: 6.6 %	pl: 5.9
10	20	30	40	50	60	70	80
икниннинн	GGLVPRGSHG	GSSGERVEDN	ELANYIAVIG	LGGYYPGADS	IDELUQNLAN	GVDCMSDFPA	DRWDHSKIY
90	100	110	120	130	140	150	160
KNRKVLGKTT	CI <mark>NGS</mark> FIKDV	DEEDYSYFEN	PKVYADHMSP	EABTEFTOATA	HTFEDIGYSK	ETLLSRYNGD	VGVLLGTHSI
170	180	190	200	210	220	230	240
DYHYYGFESN	VERGSMASGS	GMATIPMTVS	YFYGI.TGPSI.	FIDTMCSSSS	TOTHTACOMI.	KHDETKMVLA	GGLNLMYHPY
250	260	270	280	290	300	310	320
TTVNTSOGNF	TSITSESVNS	YGVGADGTVI	GEGIGAVLLK	RLDRAIADRD	OIYGVIKGSA	MTNAGERNGF	NVPNPDLOTI
330	340	350	3 60	370	360	390	400
AIRQAMDQAK	VHPSSISYIE	GHGSGTKLGD	PIEVLGLNNA	FRUATDDKQF	CYLGSIKSNI	GHLLAASGIA	GLTKTLLQFI
410	420	430	440	450	460	470	480
HKQIAPSIHS	SQLNQDIDFA	DTPFVVPQQL	IEWRQPERII	NGRKQVFPRR	AGLTSIAAGG	MNAHMIVEEY	PEPADSAGQI
490	500	510	520	530	.540	550	560
SEDQLVFVFS	VHKLALLAQ <mark>N</mark>	LT3FRDWLAS	SEAPLAQIAY	TLQVGKNNLR	NRLAIRCRTR	QALSRALNAC	IDGHYQSSAI
570	580	590	600	610	620	630	640
SKIFYRFQES	DAVQPLESDL	NDPLAPLLTQ	WLNGDSQVDW	ASLYAQPPVR	IGLPAYRFEK	TRCUYTEEGY	ESSIVNPLM
650	660	670	680	690	700	710	720
KNKLHPLVAK	NCSTPQPGAI	FRTDFVEDEL	LDYVYSCRCC	RRLSAFNFAD	VALAMPALAS	RFDGRTLSVS	CAFEHVIADU
730	740	750	760	770	780	790	800
TTVTGLEYRL	FEIDSEQLEL	EFDFRRSGEQ	PTHLGFAVIN	PLTSDEPPLP	QQWLDDAREL	LNRQALQAGR	QLSAAEVSQR
810	820	830	840	850	860	870	880
LAQAGYDFAP	YLDHDGELTI	GREGLVLKGR	PPVNRHNHYA	DNVQLSPYLA	TTIDKALVLL	LDELGLPQGR	VIVRNIERLO
890	900	910	920	930	940	950	
CYHTPAGGES	VVLSGIGLND	NELSLSLLVL	DEREQICVKL	DKVSLYLGKQ	EVASVDRKHS	LLTGT	

Figure S8.4. Tryptic mass fingerprinting of KS-B after crosslinking with 10 under UV light (1).

Piutein. Intensity covera	NhĩE Ks0b ge: 47.8 % (154)	3905 cnts) Sequer	nce coverage MS:	35.7 % Seque	ance coverage MS/I	MS: 8.3%	pl: 5.9
10	20	30	10	50	60	70	80
мкннннннн	GGLVPRGSHG	GSSGERVEDN	ELANYIAVIG	LGGYYPGADS	IDELUQNLAN	GVDCMSDFPA	DRUDHSKIY
90	100	110	120	130	110	150	160
<b>KNRKVLGKTT</b>	CI <mark>NGS</mark> FIKDV	DKFDYSYFKM	PKVYADHMSP	EVRLFLQVAV	HTFEDAGYSK	ETLLSRYNGD	VGVLLGTMS
170	100	190	200	210	220	200	240
DYHYYGFESN	VFRGSMASGS	GMATIPMTVS	YFYGLTGPSL	FIDTHCSSSS	TCIHTACQML	KHDETKMVLA	GGLNLMYHP
250	2.60	270	200	290	000	010	020
TTVNTSQCNF	TSITSESVNS	YCVCADCTVI	CECICAVLLK	RLDRAIADRD	QIVCVINCSA	MINAGERNGE	NVPNPDLQTI
22011	5411	2611	2411		100	2000	2010
AIRQAMDQAK	VHPSSISYIE	GHGSGTKLGD	PIEVLGLNNA	FRWATDDKQF	CYLGSIKSNI	GHLLAASGIA	GLTKTLLQFI
						100	
410	420	430	440	450	460	470	480
HKQIAPSIHS	SQUNQDIDFA	DTPFVVPQQL	IEWROPERII	NGRKQVFPRR	AGLTSTAAGG	MNAHMIVEEY	PEPADSAGQ.
490	500	510	520	500	540	550	560
SEDQLVFVFS	VHKLALLAQ <mark>N</mark>	LTSFRDWLAS	SEAPLAQIAY	TLQVGKNNLR	NRLAIRCRTR	QALSRALNAC	IDGHYQSSAI
570	500	590	600	610	620	630	640
SKIFYRFQES	DAVQPLESDL	NDPLAPLLTQ	ULNCDSQVDU	ASLYAQPPVR	ISLPAYRFEK	TRCWYTEEGY	ESSIVNPLM
650	660	670	600	690	700	710	720
KNKLHPLVAK	NCSTPQPGAI	FRTDFVEDEL	LDYVYSCRCC	RRLSAFNFAD	VALAMPALAS	RFDCRTLSVS	CAFEHYIADU
730	740	750	760	770	780	790	800
TTVTGLEYRL	FEIDSEQLEL	EFDFRRGGEQ	PTHLGFAVIN	PLTSDEPPLP	QQULDDAREL	LNRQALQAGR	QUCAREVOQR
810	820	830	840	850	860	870	880
LAQAGYDFAP	YLDHDGELTI	GRSGLVLKGR	PPVNRHNHYA	DNVQLSPYLA	TTIDKALYLL	LDELGLPQGR	VIVRNIERLO
890	900	910	920	930	940	950	
CYNTPAGGES	VVLSGTGLND	NELSLSLLVL	DEREOICVKL	DKVSLYLGKO	EVASVDRKHS	LLTGT	

Figure S8.5. Tryptic mass fingerprinting of KS-B after crosslinking with 10 under UV light (1).

Protein:	RhiE K∞Bb						
Intensity covera	ger 40.7 % (173.	2434 cnts) Sieque	nce coverage MS <sup>+</sup>	35.9 % Seque	ence coverage MS/I	MS: 6.6 %	pl: 5.9
10	20	30	40	50	60	70	80
мкниннини	GGLVPRGSHG	GSSGERVEDN	ELANYIAVIG	LGGYYPGADS	IDELWONLAN	GVDCMSDFPA	DRWDHSKIYY
90	100	110	120	130	140	150	160
KNRKVLGKTT	CI <mark>NGS</mark> FIKDV	DKFDYSYFKN	PKVYADHMSP	EVRLFLOVAV	HTFEDAGYSK	ETLLSRYNGD	VGVLLGTMSN
170	180	190	200	210	220	230	240
DYHYYGFESN	VFRGSMASGS	GMATIPMTVS	VFYGLTGPSI.	FIDTMCSSSS	TOTHTACOMI.	KHDETKMVLA	GGLNLMYHPY
250	2.60	270	280	290	300	310	320
TTV <mark>NTS</mark> QG <mark>NF</mark>	TSITSESVNS	YGYGADGTVI	GEGIGAVLLK	RLDRATADED	QTYGVTKGSA	MTNAGERNGE	NVPNPDI.QTI
330	340	350	3 60	370	380	390	400
AIRQAMDQAK	VHPSSISVIE	CHCSCTKLCD	PIEVLCLNNA	FRUATDDKQF	CYLCSIKSNI	CHLLAASCIA	CLTKTLLQFI
110	120	130	110	150	160	170	180
HKOIAPSIHS	SOLNODIDFA	DTPFVVPOOL	IEUROPERII	NGRKOVFPRR	AGLTSIAAGG	MNAHMIVEEY	PEPADSAGO
490	500	510	520	530	540	550	560
SEDQLVEVES	VHKI. AT. I. AQ <mark>N</mark>	I.TSFRDMLAS	SEAPLAQUAY	TI.QVGKNNI.R	NRLATECETE	QALSRALNAC	IDGHYQSSAT
570	580	590	600	610	620	630	640
SKIFYRFORS	DAVQPI.ESDI.	NDPLAPLITQ	MLNGDSQVDW	ASI.VAQPPVR	TSLPAYREEK	TRCHYTEEGY	ESSIVNPLME
650	660	670	680	690	700	710	720
KNKLHÞLVAK	NCS TPOPGAI	FRTDFVEDEL	LDYVYSGRGG	PRLSAFNFAD	VALAMPALAS	REDGRTLSVS	CAFEHVIADU
730	740	750	760	770	780	790	800
TTVTGLEYRL	FEIDSEQLEL	EFDFRRSGEQ	PTHLGFAVIN	PLTSDEPPLP	QQULDDAREL	LNRQALQAGR	QUSINEVSQR
							1
810	820	830	840	850	860	870	880
LAQAGYDF AP	YLDHDGELTI	GRIGLVLKGR	PPVNRIINIIYA	DNVQLOPYLA	TTIDKALYLL	LDELGLPQGR	VIVRNIERLO
890	900	910	920	930	940	950	
CVITTRAGES	VAL COTOLND	NELCICIUM	DEPENTCURI	DEVCI VI GRO	FURCUDDUIC	LITGT	

CYHTPAGGFS VVLSGIGLND NELSLSLLVL DEREQICVKL DKVSLYLGKQ EVASVDRKHS LLTGT

Figure S8.6. Tryptic mass fingerprinting of KS-B after crosslinking with 10 under UV light (1).

#### Phenazine-protein binding assays with carbonic anhydrase III and albumin



**Figure S9.** A) Scheme for the functionalization of carbonic anhydrase III by probe **10** after irradiation with UV-light. B) SDS-PAGE (10%) of carbonic anhydrase III after the incubation with probe **10** or rhodamine B in water; a) rhodamine B, 370 nm, 10 h; b) **10**, 370 nm, 15 min; c) **10**, 370 nm, 30 min; d) **10**, 370 nm, 1 h; e) **10**, 370 nm, 5 h; f) **10**, 370 nm, 10 h, C) carbonic anhydrase III control, L: Ladder. The fluorescent bands would correspond to potential conjugates of carbonic anhydrase III and **9** with n>5.



**Figure S10.** SDS-PAGE (10%) of albumin after the incubation with probe **10** or rhodamine B in water (left picture: under white light; right picture at 370 nm); L, Ladder, a) rhodamine B, 370 nm, 10 h; b) **10**, 370 nm, 15 min; c) **10**, 370 nm, 30 min; d) **10**, 370 nm, 1 h; e) **10**,

370 nm, 5 h; f) **10**, 370 nm, 10 h, C) albumin control. The fluorescent band potentially corresponds to a 70 kDa monoadduct of **10** and albumin.

## Tryptic mass fingerprinting of labelled albumin

	-	-	-			
	-	-				-
-				ſ		
	Π	Π	Π			
					1	

Protein: Intensity covera	BSA ge: 51.2 % (1748	6939 cnts) Sequer	nce coverage MS:	52.2 % Sequ	ence coverage MS/I	MS: 5.1 %	pl: 5.8
10	20	30	40	50	60	70	80
MKWVTFISLL	LLFSSAYSRG	VFRRDTHKSE	IAHRFKDLGE	EHFKGLVLIA	FSQYLQQCPF	DEHVKLVNEL	TEFAKTCVAD
90	100	110	120	130	140	150	160
ESHAGCEKSL	HTLFGDELCK	VASLRETYGD	MADCCEKQEP	ERNECFLSHK	DDSPDLPKLK	PDPNTLCDEF	KADEKKFWGK
170	180	190	200	210	220	230	240
YLYEIARRHP	YFYAPELLYY	ANKYNGVFQE	CCQAEDKGAC	LLPKIETMRE	KVLASSARQR	LRCASIQKFG	ERALKAWSVA
250	2.60	270	280	290	300	310	320
RLSQKFPKAE	FVEVTKLVTD	LTKVHKECCH	GDLLECADDR	ADLAKYICDN	QDTISSKLKE	CCDKPLLEKS	HCIAEVEKDA
220	340	350	3.60	370	390	200	400
IPENLPPLTA	DFAEDKDVCK	NYQEAKDAFL	GSFLYEYSRR	HPEYAVSVLL	RLAKEYEATL	EECCAKDDPH	ACYSTVFDKL
410	420	430	440	450	460	470	480
KHLVDEPQNL	IKQNCDQFEK	LGEYGFQNAL	IVRYTRKVPQ	VSTPTLVEVS	RSLGKVGTRC	CTKPESERMP	CTEDYLSLIL
490	500	510	520	530	540	550	560
NRLCVLHEKT	PVSEKVTKCC	TESLVNRRPC	FSALTPDETY	VPKAFDEKLF	TFHADICTLP	DTEKQIKKQT	ALVELLKHKP
		_					
570	580	590	600	610			
KATEEQLKTV	MENFVAFVDK	CCAADDKEAC	FAVEGPKLVV	STQTALA			

**Figure S11.** Tryptic mass fingerprinting of albumin after functionalization with **10** under UV light (1).



**Figure S12.** A) Model of the rhodamine-based probe (**10**) crosslinked to the Cys<sub>557</sub> of albumin under UV light (PDB code 4F5S) B) MALDI-MS/MS spectrum of the rhodamine-based probe (**10**)-linked peptide of albumin.

		Inhibition zone (mm)										
Cpd.	B. sub	S. aur	E. col	P. aer	MRSA	VRE	M. vac	S. sal	C. alb	P. not		
3	0	0	17	0	0	15	13	20	0	0		
4	10	0	0	15	0	0	13	0	0	0		
PCA (2)	31	25	32	0	20	0	27	20	35	16		

### Antimicrobial properties of isolated phenazines 3 and 4

**Table S2**. Antimicrobial properties of the phenazine-pantetheine conjugates **3** and **4** in comparison with PCA (**2**). *B. sub: Bacillus subtilis* ATCC 6633; *S. aur: Staphylococcus aureus* SG 511; *E. col: Escherichia coli* SG 458; *P. aer: Pseudomonas aeruginosa* SG 137; MRSA: Methicillin- and quinolone-resistant *Staphylococcus aureus* 134/93; VRE: Vancomycin-resistant *Enterococcus faecalis* 1528; *M. vac: Mycobacterium vaccae* IMET 10670; *S. sal: Sporobolomyces salmonicolor* SBUG 549; *C. alb: Candida albicans* BSMY 212; *P. not: Penicillium notatum* JP36; cpd, compound; PCA: phenazine-1-carboxylic acid (**2**).



<sup>&</sup>lt;sup>13</sup>C NMR spectrum (150 MHz, MeOD) of **3**.



COSY and HSQC spectra of compound 3.



HMBC spectrum of compound **3**.



<sup>13</sup>C NMR spectrum (150 MHz, MeOD) of **4**.



COSY and HSQC spectra of compound 4.



HMBC spectrum of compound 4.



 $^{\rm 13}{\rm C}$  NMR spectrum (125 MHz, DMSO-D<sub>6</sub>) of **5**.



<sup>1</sup>H NMR spectrum (600 MHz, DMSO-D<sub>6</sub>) of **6**.



<sup>1</sup>H NMR spectrum (500 MHz, DMSO-D<sub>6</sub>) of **7**.







<sup>1</sup>H NMR spectrum (600 MHz,  $CDCl_3$ ) of **10**.



<sup>1</sup>H NMR spectrum (600 MHz, MeOD) of **11**.

