Molbank **2016**, 2016, M916: S1 of S20

Supplementary Materials: 2-C-Alkynyl and 2-C-cis-Alkenyl β -Mannosides with Acetal Protected γ -Aldehyde Functionality via 2-Uloside Alkynylation and Lindlar Hydrogenation

Daniel Borowski, Melchior Menzel and Thomas Ziegler

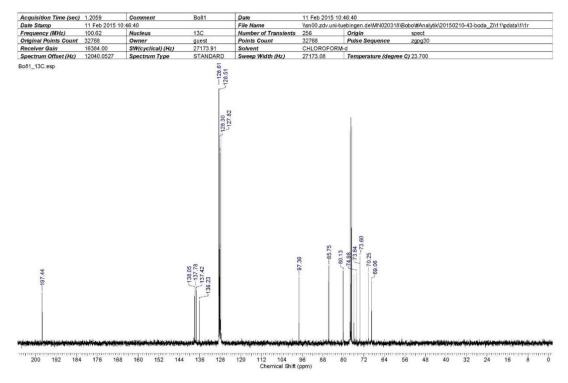


Figure S1. Compound 2 ¹³C-NMR.

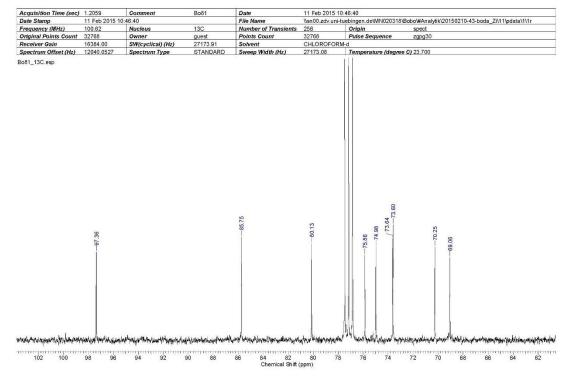


Figure S2. Compound 2 ¹³C-NMR Zoom.

Acquisition Time (sec)	4.0894	Comment	Bo81.7	Date	29 Aug 2016	16:21:52
Date Stamp	29 Aug 2016 1	16:21:52		File Name	\\sn00.zdv.ur	ni-tuebingen.de\MN020318\Bobo\#Analytik\20160829-14-boda_Zi\10\PDATA\1\1r
Frequency (MHz)	400.16	Nucleus	1H	Number of Transients	16	Origin spect
Original Points Count	32768	Owner	nmrsu	Points Count	65536	Pulse Sequence zg30
Receiver Gain	200.95	SW(cyclical) (Hz)	8012.82	Solvent	CHLOROFO	RM-d
Spectrum Offset (Hz)	2461.2754	Spectrum Type	STANDARD	Sweep Width (Hz)	8012.70	Temperature (degree C) 25.124

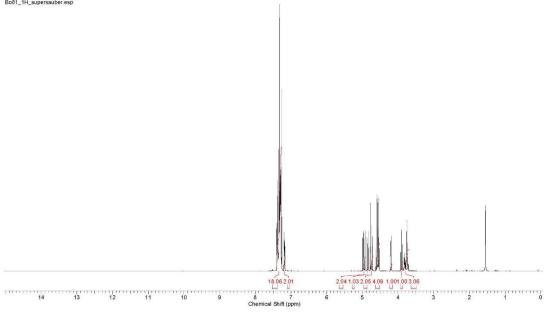


Figure S3. Compound **2** ¹H-NMR.

Acquisition Time (sec)	4.0894	Comment	Bo81.7	Date	29 Aug 2016	16:21:52
Date Stamp	29 Aug 2016 16	:21:52		File Name	\\sn00.zdv.uni	i-tuebingen.de\MN020318\Bobo\#Analytik\20160829-14-boda_Zi\10\PDATA\1\1r
Frequency (MHz)	400.16	Nucleus	1H	Number of Transients	16	Origin spect
Original Points Count	32768	Owner	nmrsu	Points Count	65536	Pulse Sequence zg30
Receiver Gain	200.95	SW(cyclical) (Hz)	8012.82	Solvent	CHLOROFOR	RM-d
Spectrum Offset (Hz)	2461.2754	Spectrum Type	STANDARD	Sweep Width (Hz)	8012.70	Temperature (degree C) 25.124

Bo81_1H_supersauber.esp

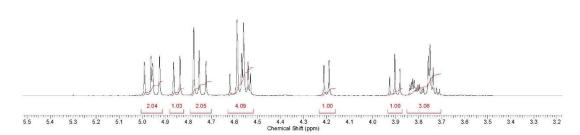


Figure S4. Compound 2 ¹H-NMR Zoom.

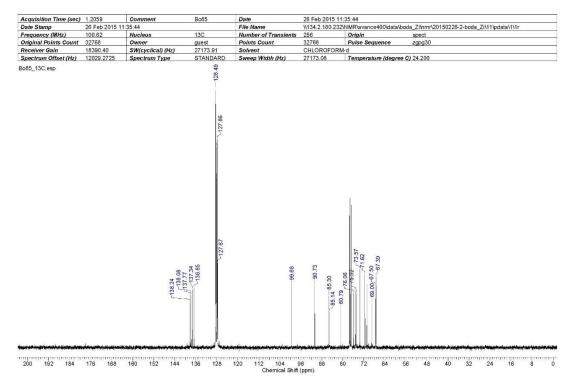


Figure S5. Compound 3a ¹³C-NMR.

Acquisition Time (sec)	1.2059	Comment	Bo85	Date	26 Feb 2015	11:35:44
Date Stamp	26 Feb 2015 11	1:35:44		File Name	\\134.2.180.2	232\NMR\avance400\data\boda_Zi\nmr\20150226-2-boda_Zi\11\pdata\1\1r
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	256	Origin spect
Original Points Count	32768	Owner	guest	Points Count	32768	Pulse Sequence zgpg30
Receiver Gain	18390.40	SW(cyclical) (Hz)	27173.91	Solvent	CHLOROFO	RM-d
Spectrum Offset (Hz)	12029.2725	Spectrum Type	STANDARD	Sweep Width (Hz)	27173.08	Temperature (degree C) 24.200

Bo85_13C.esp

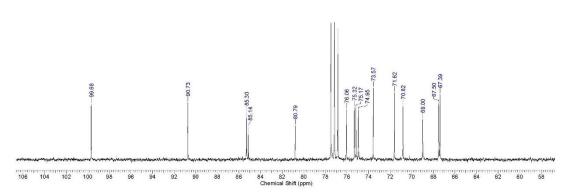


Figure S6. Compound 3a ¹³C-NMR Zoom.

Acquisition Time (sec)	3.9584	Comment	Bo85	Date	26 Feb 2015	11:25:04			
Date Stamp	26 Feb 2015 11	1:25:04		File Name	\\134.2.180.2	32\NMR\avance400\data	\boda_Zi\nmr\20150	0226-2-boda_Zi\10\pdata\1\	1r
Frequency (MHz)	400.16	Nucleus	1H	Number of Transients	32	Origin	spect	Original Points Count	32768
Owner	guest	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	35.90	SW(cyclical) (Hz)	8278.15
Solvent	CHLOROFOR	M-d		Spectrum Offset (Hz)	2463.1875	Spectrum Type	STANDARD	Sweep Width (Hz)	8277.89

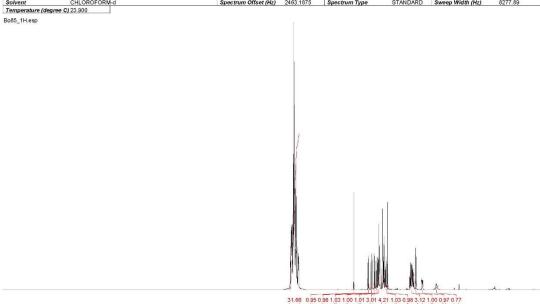


Figure S7. Compound 3a ¹H-NMR.

9 8 Chemical Shift (ppm)

Acquisition Time (sec)	3.9584	Comment	Bo85	Date	26 Feb 2015	11:25:04			
Date Stamp	26 Feb 2015	11:25:04		File Name	\\134.2.180.2	32\NMR\avance400\data	Nboda_Zi\nmr\20150	0226-2-boda_Zi\10\pdata\1\	1r
Frequency (MHz)	400.16	Nucleus	1H	Number of Transients	32	Origin	spect	Original Points Count	32768
Owner	guest	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	35.90	SW(cyclical) (Hz)	8278.15
Solvent	CHLOROFOR	RM-d		Spectrum Offset (Hz)	2463.1875	Spectrum Type	STANDARD	Sweep Width (Hz)	8277.89
Tomporatum (doarno C		10.54		opectium onoci (riz)	2400.1070	орессии турс	01/440/410	Officep friday (1/2)	0277.

Temperature Bo85_1H.esp

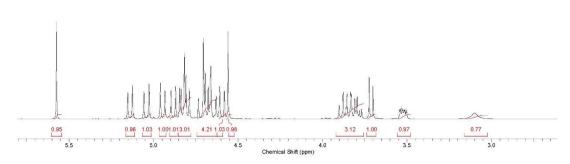


Figure S8. Compound 3a ¹H-NMR Zoom.

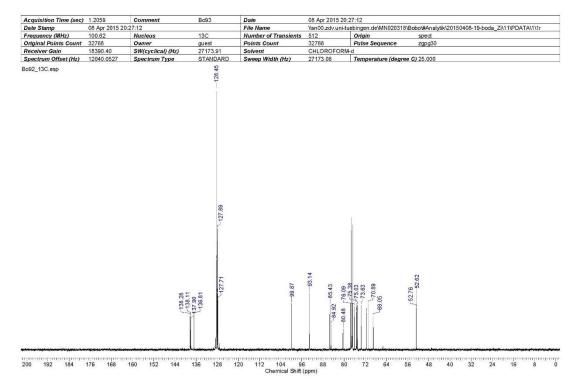


Figure S9. Compound 3b ¹³C-NMR.

Acquisition Time (sec)	1.2059	Comment	Bo93	Date	08 Apr 2015 2	20:27:12
Date Stamp	08 Apr 2015 20):27:12		File Name	\\sn00.zdv.un	i-tuebingen.de\MN020318\Bobo\#Analytik\20150408-19-boda_Zi\11\PDATA\1\1r
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	512	Origin spect
Original Points Count	32768	Owner	guest	Points Count	32768	Pulse Sequence zgpg30
Receiver Gain	18390.40	SW(cyclical) (Hz)	27173.91	Solvent	CHLOROFOR	RM-d
Spectrum Offset (Hz)	12040.0527	Spectrum Type	STANDARD	Sweep Width (Hz)	27173.08	Temperature (degree C) 25.000

Bo92_13C.esp

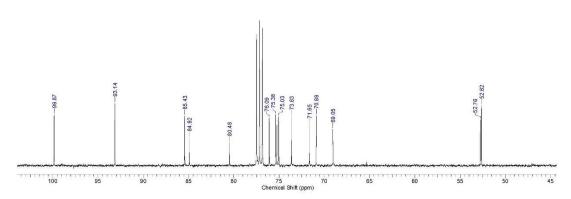


Figure S10. Compound 3b ¹³C-NMR Zoom.

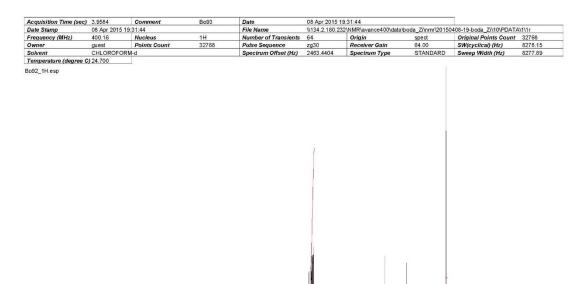


Figure S11. Compound 3b ¹H-NMR.

8 Chemical Shift (ppm)

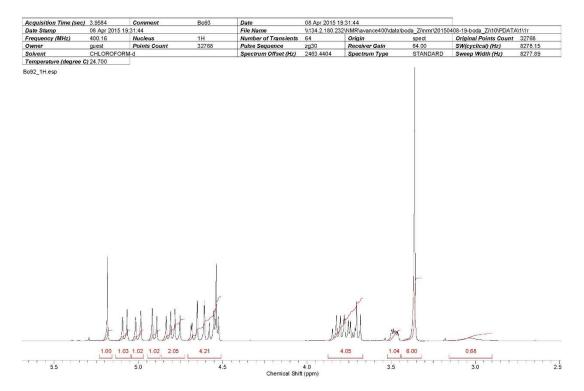


Figure S12. Compound 3b ¹H-NMR Zoom.

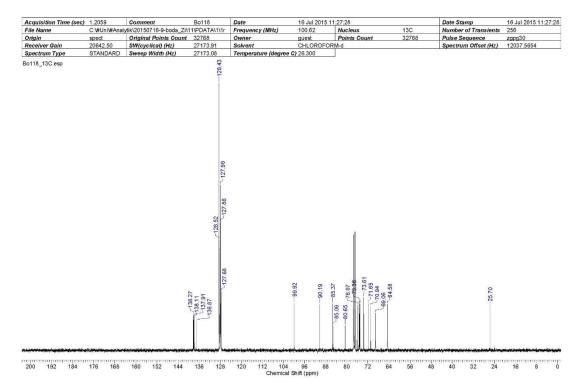


Figure S13. Compound **3c** ¹³C-NMR.

Acquisition Time (sec)	1.2059	Comment	Bo118	Date	16 Jul 2015 11	1:27:28		Date Stamp	16 Jul 2015 11:27:28
File Name	C:\#Uni\#Analy	ytik\20150716-9-boda_Zi\1	1\PDATA\1\1r	Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	256
Origin	spect	Original Points Count	32768	Owner	guest	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	20642.50	SW(cyclical) (Hz)	27173.91	Solvent	CHLOROFOR	M-d		Spectrum Offset (Hz)	12037.5654
Spectrum Type	STANDARD	Sweep Width (Hz)	27173.08	Temperature (degree C	2) 26.300				

Bo118_13C.esp

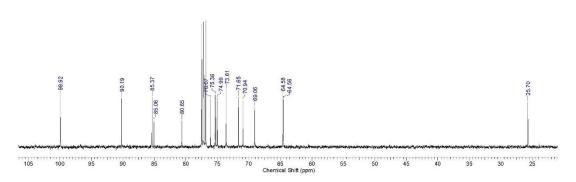


Figure S14. Compound 3c 13 C-NMR Zoom.

Acquisition Time (sec)	3.9584	Comment	Bo118	Date	17 Jul 2015	23:05:04		Date Stamp	17 Jul 2015 23:05:04
File Name	C:\#Uni\#Ana	lytik\20150717-24-box	ta_Zi\10\PDATA\1\1	г		Frequency (MHz)	400.16	Nucleus	1H
Number of Transients	32	Origin	spect	Original Points Count	32768	Owner	guest	Points Count	32768
Pulse Sequence	zg30	Receiver Gain	45.30	SW(cyclical) (Hz)	8278.15	Solvent	CHLOROF	ORM-d	1222
Spectrum Offset (Hz)	2462 9351	Spectrum Type	STANDARD	Sween Width (Hz)	8277.89	Temperature (degree	C) 26 200		

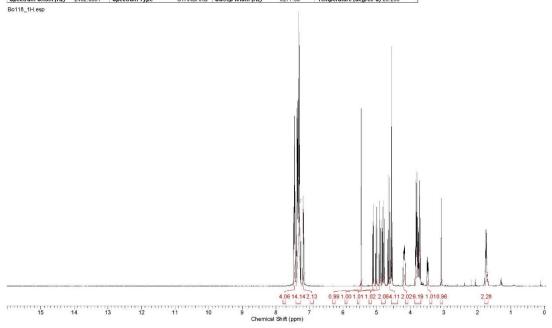


Figure S15. Compound 3c 1H-NMR.

Acquisition Time (sec)	3.9584	Comment	Bo118	Date	17 Jul 2015	23:05:04		Date Stamp	17 Jul 2015 23:05:04
File Name	C:\#Uni\#Anal	lytik\20150717-24-box	da_Zi\10\PDATA\1\1	r		Frequency (MHz)	400.16	Nucleus	1H
Number of Transients	32	Origin	spect	Original Points Count	32768	Owner	guest	Points Count	32768
Pulse Sequence	zg30	Receiver Gain	45.30	SW(cyclical) (Hz)	8278.15	Solvent	CHLOROF	ORM-d	
Spectrum Offset (Hz)	2462.9351	Spectrum Type	STANDARD	Sweep Width (Hz)	8277.89	Temperature (degree	C) 26.200		

Bo118_1H.esp

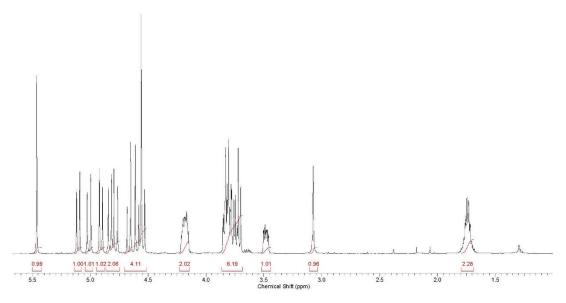


Figure S16. Compound 3c ¹H-NMR Zoom.

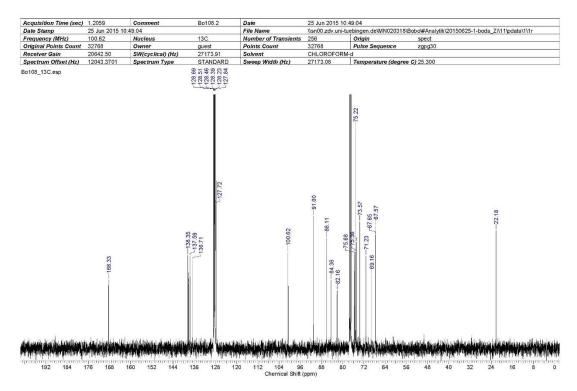


Figure S17. Compound 3d ¹³C-NMR.

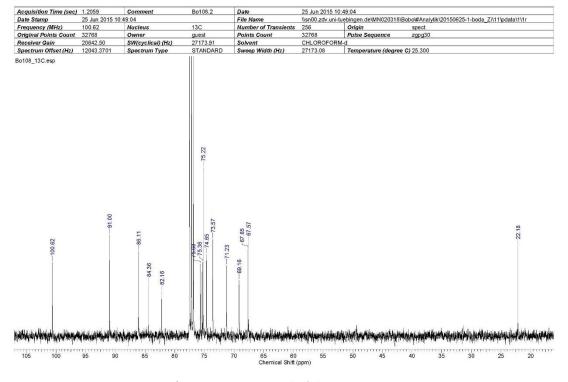


Figure S18. Compound 3d 13 C-NMR Zoom.

Acquisition Time (sec)	3.9584	Comment	Bo108.2	Date	25 Jun 2015	5 10:38:24
Date Stamp	25 Jun 2015 10	0:38:24		File Name	\\sn00.zdv.u	ni-tuebingen.de\MN020318\Bobo\#Analytik\20150625-1-boda_Zi\10\PDATA\1\
Frequency (MHz)	400.16	Nucleus	1H	Number of Transients	32	Origin spect
Original Points Count	32768	Owner	guest	Points Count	32768	Pulse Sequence zg30
Receiver Gain	90.50	SW(cyclical) (Hz)	8278.15	Solvent	CHLOROFO	DRM-d
Spectrum Offset (Hz)	2460 0828	Spectrum Type	STANDARD	Sween Width (Hz)	8277.89	Temperature (degree C) 24 900

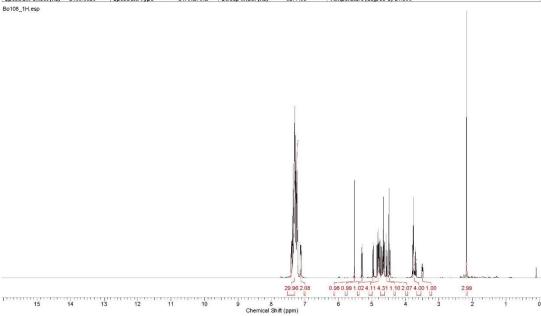


Figure S19. Compound 3d ¹H-NMR.

Acquisition Time (sec)	3.9584	Comment	Bo108.2	Date	25 Jun 2015	5 10:38:24
Date Stamp	25 Jun 2015 10	:38:24		File Name	\\sn00.zdv.u	uni-tuebingen.de\MN020318\Bobo\#Analytik\20150625-1-boda_Zi\10\PDATA\1\1r
Frequency (MHz)	400.16	Nucleus	1H	Number of Transients	32	Origin spect
Original Points Count	32768	Owner	guest	Points Count	32768	Pulse Sequence zg30
Receiver Gain	90.50	SW(cyclical) (Hz)	8278.15	Solvent	CHLOROFO	ORM-d
Spectrum Offset (Hz)	2460.0828	Spectrum Type	STANDARD	Sweep Width (Hz)	8277.89	Temperature (degree C) 24,900

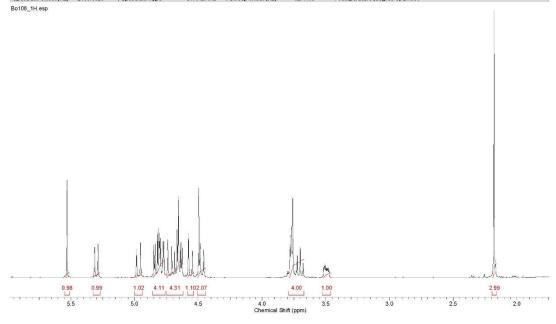


Figure S20. Compound 3d ¹H-NMR Zoom.

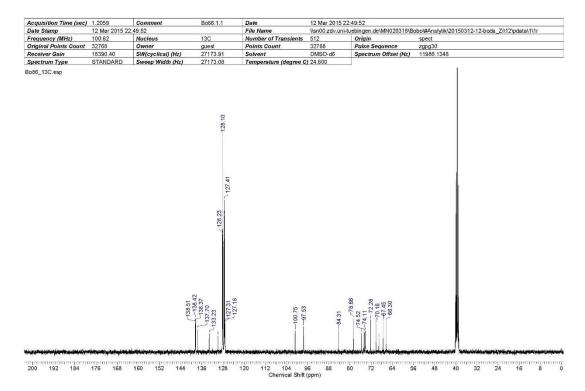


Figure S21. Compound 4a 13C-NMR.

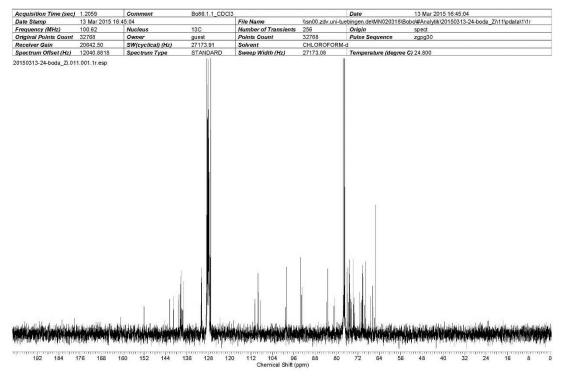


Figure S22. Compound 4a ¹³C-NMR chloroform.

Acquisition Time (sec)	1.2059	Comment	Bo86.1.1	Date	12 Mar 2015 2	22:49:52
Date Stamp	12 Mar 2015 22	2:49:52		File Name	\\sn00.zdv.uni	i-tuebingen.de\MN020318\Bobo\#Analytik\20150312-12-boda_Zi\12\pdata\1\1r
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	512	Origin spect
Original Points Count	32768	Owner	guest	Points Count	32768	Pulse Sequence zgpg30
Receiver Gain	18390.40	SW(cyclical) (Hz)	27173.91	Solvent	DMSO-d6	Spectrum Offset (Hz) 11986.1348
Amount of the court			07170.00		11.04.000	

Bo86_13C.esp

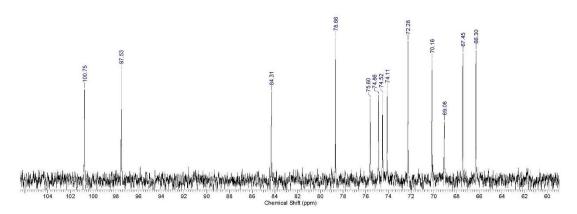


Figure S23. Compound 4a ¹³C-NMR Zoom.

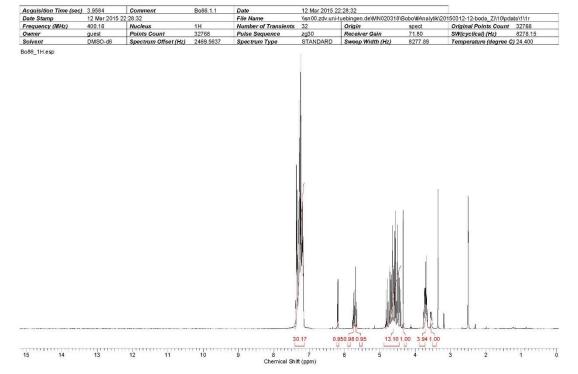


Figure S24. Compound 4a ¹H-NMR.

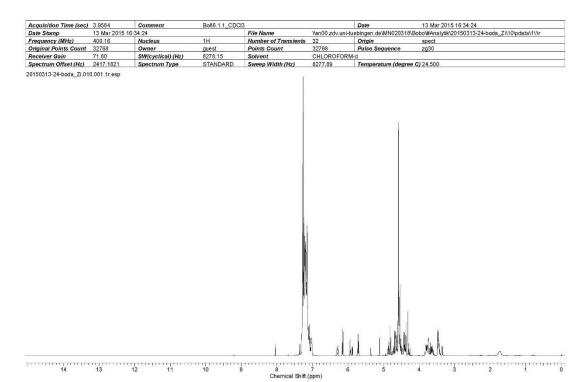


Figure S25. Compound 4a ¹H-NMR chloroform.

Acquisition Time (sec)	3.9584	Comment	Bo86.1.1	Date	12 Mar 2015 2	2:28:32			
Date Stamp	12 Mar 2015 22	:28:32		File Name	\\sn00.zdv.uni-tuebingen.de\MN020318\Bobo\#Analytik\20150312-12-boda_Zi\10\pdata				
Frequency (MHz)	400.16	Nucleus	1H	Number of Transients	32	Origin	spect	Original Points Count 32768	
Owner	guest	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	71.80	SW(cyclical) (Hz) 8278.15	
Solvent	DMSO-d6	Spectrum Offset (Hz)	2469.5637	Spectrum Type	STANDARD	Sweep Width (Hz)	8277.89	Temperature (degree C) 24.400	

Bo86_1H.esp

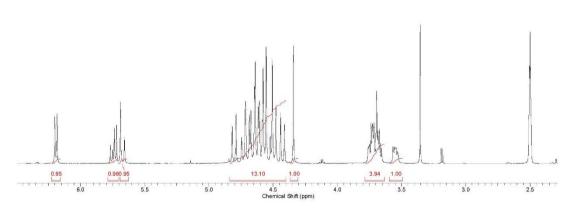


Figure S26. Compound 4a ¹H-NMR Zoom.

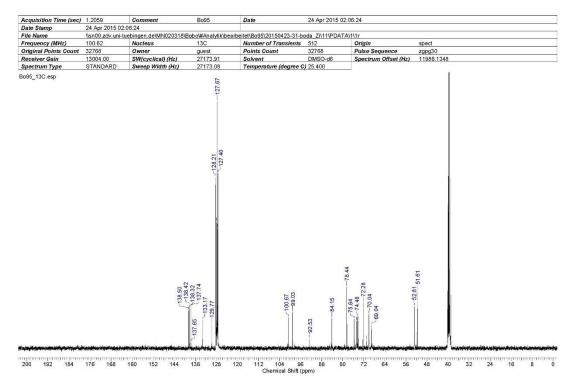


Figure S27. Compound 4b 13C-NMR.

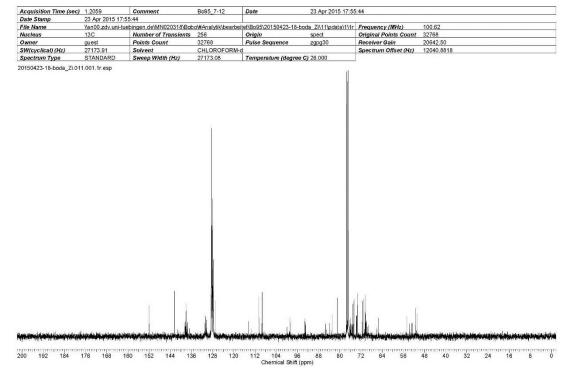


Figure S28. Compound 4b ¹³C-NMR chloroform.

Acquisition Time (sec)	1.2059	Comment	Bo95	Date	24 Apr 2015 02:06:24					
Date Stamp	24 Apr 2015 02	:06:24								
File Name	\\sn00.zdv.uni-t	\\sn00.zdv.uni-tuebingen.de\MN020318\Bobo\#Analytik\bearbeitet\Bo95\20150423-31-boda Zi\11\PDATA\1\1r								
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	512	Origin	spect			
Original Points Count	32768	Owner	guest	Points Count	32768	Pulse Sequence	zgpg30			
Receiver Gain	13004.00	SW(cyclical) (Hz)	27173.91	Solvent	DMSO-d6	Spectrum Offset (Hz)	11986.1348			
Spectrum Tupe	STANDARD	Suroon Wildth (Hz)	27173 08	Tompomtum (dogmo (2) 25 400					

Bo95_13C.esp

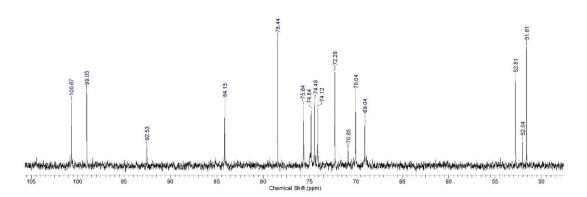


Figure S29. Compound 4b ¹³C-NMR Zoom.

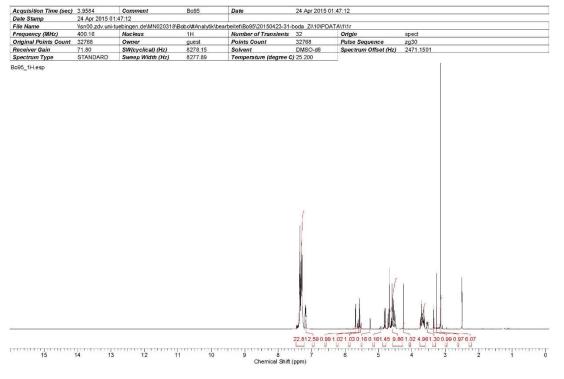


Figure S30. Compound 4b ¹H-NMR.

Acquisition Time (sec)	3.9584	Comment	Bo95_7-12	Date	23 Apr 2015 17:4	5:04	
Date Stamp	23 Apr 2015 17	:45:04				23	
File Name	\\sn00.zdv.uni-t	uebingen.de\MN020318\Bol	bo\#Analytik\bearb	neitet\Bo95\20150423-1	3-boda_Zi\10\pdata\1\	frequency (MHz)	400.16
Nucleus	1H	Number of Transients	32	Origin	spect	Original Points Count	32768
Owner	guest	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	64.00
SW(cyclical) (Hz)	8278.15	Solvent	CHLOROFORM	l-d		Spectrum Offset (Hz)	2463.1877
Spectrum Type	STANDARD	Sweep Width (Hz)	8277.89	Temperature (degre	e C) 25.700		

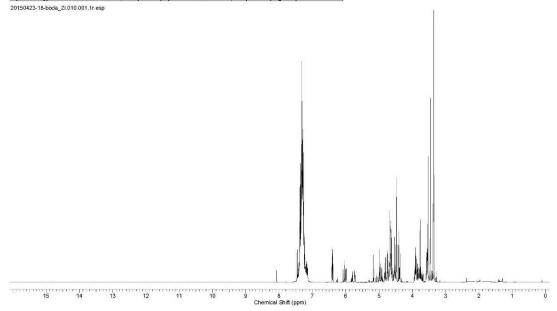


Figure S31. Compound 4b ¹H-NMR chloroform.

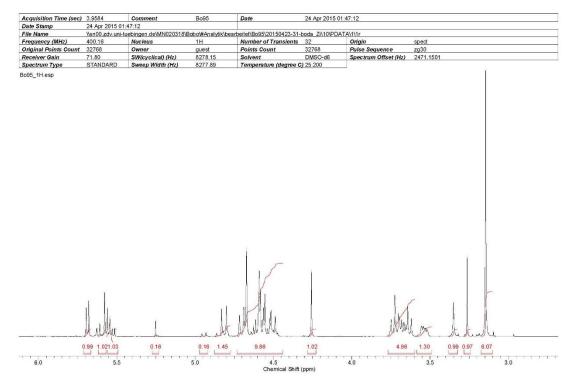


Figure S32. Compound 4b ¹H-NMR Zoom.

Acquisition Time (sec)	1.2059	Comment	Bo121	Date	22 Aug 2015	15:07:12		
Date Stamp	22 Aug 2015 1	5:07:12		File Name	C:\#Uni\#Ana	alytik\20150822-25-boda_Zi\11\pdata\1\1	Frequency (MHz)	100.62
Nucleus	13C	Number of Transients	2048	Origin	spect	Original Points Count 32768	Owner	guest
Points Count	32768	Pulse Sequence	zgpg30	Receiver Gain	18390.40	SW(cyclical) (Hz) 27173.91	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	12045.0283	Spectrum Type	STANDARD	Sweep Width (Hz)	27173.08	Temperature (degree C) 26.200		
Spectrum Offset (Hz) Bo121_13C.esp	12045.0283	Spectrum Type	STANDARD	Sweep Width (Hz)	27173.08	Temperature (degree C) 26.200		
D0121_100.00p						1		

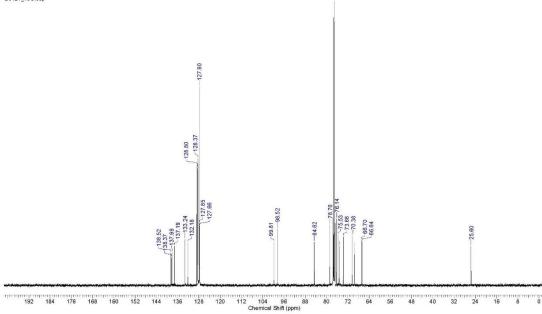


Figure S33. Compound 4c ¹³C-NMR.

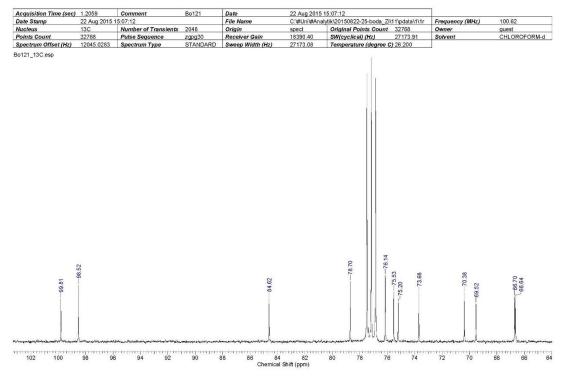


Figure S34. Compound **4c** ¹³C-NMR Zoom.

Acquisition Time (sec)	3.9584	Comment	Bo121	Date	22 Aug 2015 13:48:16			Date Stamp	22 Aug 2015 13:48:16
File Name	C:\#Uni\#Analy	ytik\20150822-25-boda_Zi	\10\PDATA\1\1r	Frequency (MHz)	400.16	Nucleus	1H	Number of Transients	64
Origin	spect	Original Points Count	32768	Owner	guest	Points Count	32768	Pulse Sequence	zg30
Receiver Gain	114.00	SW(cyclical) (Hz)	8278.15	Solvent	CHLOROFO	RM-d		Spectrum Offset (Hz)	2462.9351

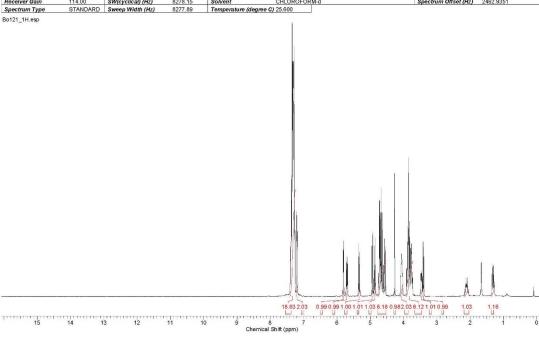


Figure S35. Compound **4c** ¹H-NMR.

Acquisition Time (sec)	3.9584	Comment	Bo121	Date	22 Aug 2015	13:48:16		Date Stamp	22 Aug 2015 13:48:16
File Name	C:\#Uni\#Anal	lytik\20150822-25-boda_Z	1\10\PDATA\1\1	Frequency (MHz)	400.16	Nucleus	1H	Number of Transients	64
Origin	spect	Original Points Count	32768	Owner	guest	Points Count	32768	Pulse Sequence	zg30
Receiver Gain	114.00	SW(cyclical) (Hz)	8278.15	Solvent	CHLOROFOR	RM-d		Spectrum Offset (Hz)	2462.9351
Spectrum Type	STANDARD	Sween Width (Hz)	8277 89	Temperature (degree C	1.25.600				

Bo121_1H.esp

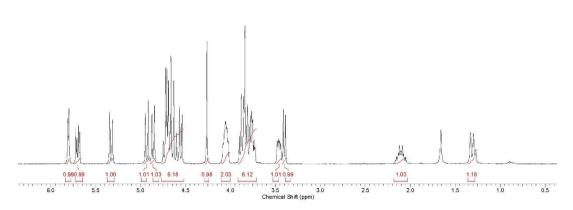


Figure S36. Compound 4c ¹H-NMR Zoom.

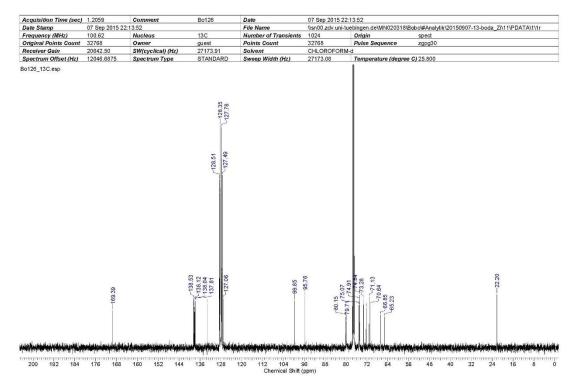


Figure S37. Compound 4d ¹³C-NMR.

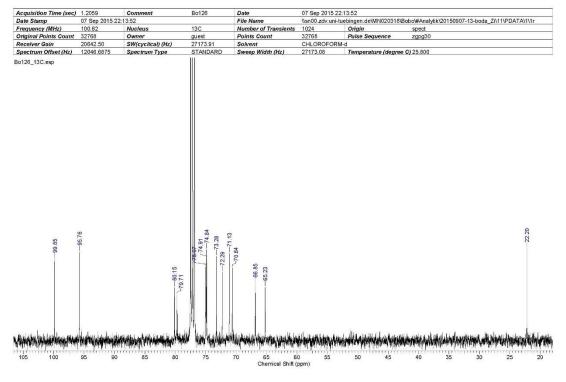


Figure S38. Compound 4d ¹³C-NMR Zoom.

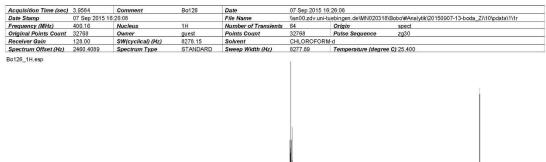


Figure S39. Compound 4d ¹H-NMR.

	r e
	2.05 0.99 1.00 1.000.97 0.993.18 3.04 5.08 4.07 1.09 2.95
15 14 13 12 11 10 9 8 Chemical Shift (i	7 6 5 4 3 2 1 0 oppm)

Acquisition Time (sec)		Comment	Bo126	Date	07 Sep 2015			
Date Stamp	07 Sep 2015 1	6:26:08		File Name	\\sn00.zdv.ur	ni-tuebingen.de\MN020318	\Bobo\#Analytik\2015090	7-13-boda_Zi\10\pdata\1\1r
requency (MHz)	400.16	Nucleus	1H	Number of Transients	64	Origin	spect	
Original Points Count		Owner	guest	Points Count	32768	Pulse Seguence	zg30	
Receiver Gain	128.00	SW(cyclical) (Hz)	8278.15	Solvent	CHLOROFO			
pectrum Offset (Hz)	2460.4089	Spectrum Type	STANDARD	Sweep Width (Hz)	8277.89	Temperature (degree	e C) 25.400	
1	n l							
					M. M.			<u> </u>
0.99	1.001.00	0.97	0.99 3.18 3.	045.08 4.0	7 1.09		-	2.95

Figure S40. Compound 4d ¹H-NMR Zoom.