

Selective enclathration of xylenols: Synergistic effects of mixed hosts

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Electronic Supplementary Information

Table S1: Torsion angles of the host molecules.

	τ_1	τ_2
Structure I	60	73
Structure II	41	79
Structure IIIa	58	60
IIIb	53	58
Structure IVa	59	59
IVb	56	60
IVc	55	59
IVd	60	66
Structure VH1a	42	70
VH1b	58	65
VH2a	42	46
VH2b	42	45

Table S2: Hydrogen bonding details for the structures obtained from the competition experiments

Compounds		
H1•34XYL		
O1-H1...O61	2.681	
O61-H61...O13	2.705	[-x+1, y-1/2, -z+1/2]
O13-H13...O1	2.705	[-x+2, y+1/2, -z+1/2]
H1•23XYL/26XYL		
O1-H1...O21	2.657	[x, y+1, z]
O13-H13...O33	2.711	[x, -y+2, z+1/2]
O21-H21...O61	2.653	
O33-H33...O71	2.729	
O61-H61...O1	2.686	
O71-H71...O13	2.727	[x, -y+1, z-1/2]
H1•23XYL/35XYL		
O1-H1...O28	2.676	[x+1, y+1, z]
O16-H16...O70	2.664	
O91-H91...O1	2.67	[x, y-1, z]
O31-H31...O81	2.643	
O81-O81...O59	2.674	[x, y-1, z]
O47-H47...O43	2.642	
O70-H70...O13	2.673	[x-1, y, z]
O43-H43...O62	2.667	
O28-H28...O91	2.651	
O59-H59...O31	2.630	[x-1, y+1, z]
O13-H13...O16	2.647	
O62-H62...O47	2.680	[x+1, y, z]

Table S3: Hydrogen bonding details for structure **V** containing mixed hosts

Compounds		
H1•H2•26XYL/35XYL		
O1-H1...O16	2.809	
O53-H53...O56	2.713	[x, y-1, z]
O41-H41...O81_a	3.002	
O41-H41...O91_b	2.573	
O81_a-H91...O1	2.912	
O91_b-H91...O1	2.587	
O13-H13...O53	2.762	[x, y+1, z]
O22-H22...O13	2.693	[x, -y+3/2, z+1/2]
O16-H16...O22	2.787	[x, -y+1/2, z-1/2]
O62-H62...O41	2.649	[x, -y+3/2, z-1/2]
O56-H56...O62	2.701	[x, -y+3/2, z+1/2]

Table S4: Results of competition experiments with mixed hosts (H1+H3) for mixtures of
23XYL/35XYL

Composition	H1	H3	2.3	3.5
Expt 1 Start	90	10	50	50
Expt 1 End	75	25	96	04
Expt 2 Start	80	20	50	50
Expt 2 End	67	33	94	06
Expt 3 Start	70	30	50	50
Expt 3 End	17	83	69	41
Expt 4 Start	60	40	50	50
Expt 4 End	14	86	49	51
Expt 5 Start	50	50	50	50
Expt 5 End	12	88	28	72

Table S5: Results of competition experiments with mixed hosts (H1+H3) for mixtures of
26XYL/35XYL

Composition	H1	H3	2.6	3.5
Expt 1 Start	90	10	50	50
Expt 1 End	100	0	0	100
Expt 2 Start	80	20	50	50
Expt 2 End	25	75	0	100
Expt 3 Start	70	30	50	50
Expt 3 End	16	84	0	100
Expt 4 Start	60	40	50	50
Expt 4 End	11	89	0	100
Expt 5 Start	50	50	50	50
Expt 5 End	13	87	0	100

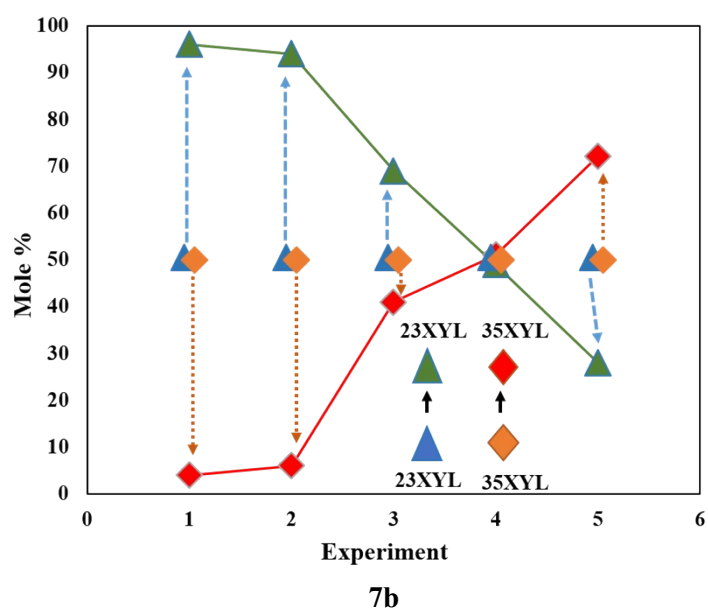
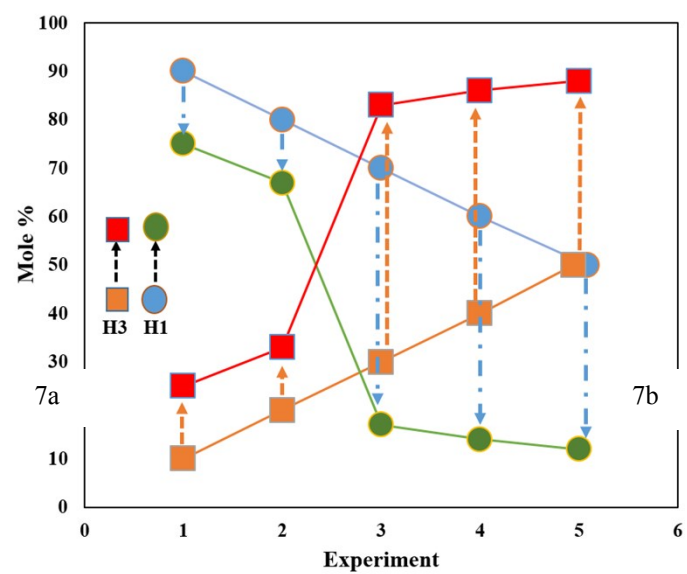


Figure S1: Trend followed by the hosts H1 and H3 (7a) and the guest 23XYL/35XYL (7b)

¹H NMR spectra for the different studies

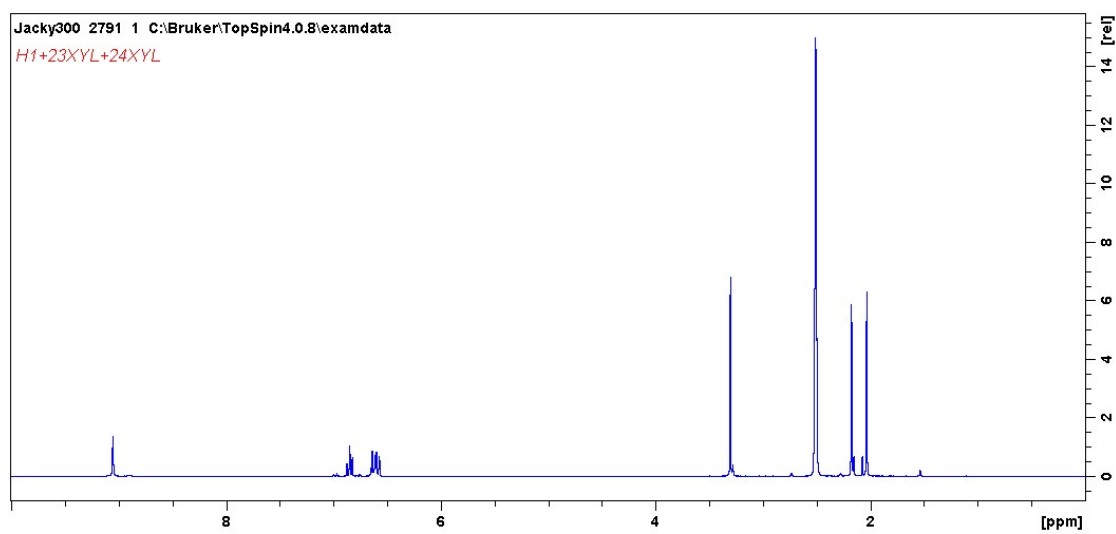


Figure S2: ¹H NMR spectrum for H1+ 23XYL+24XYL

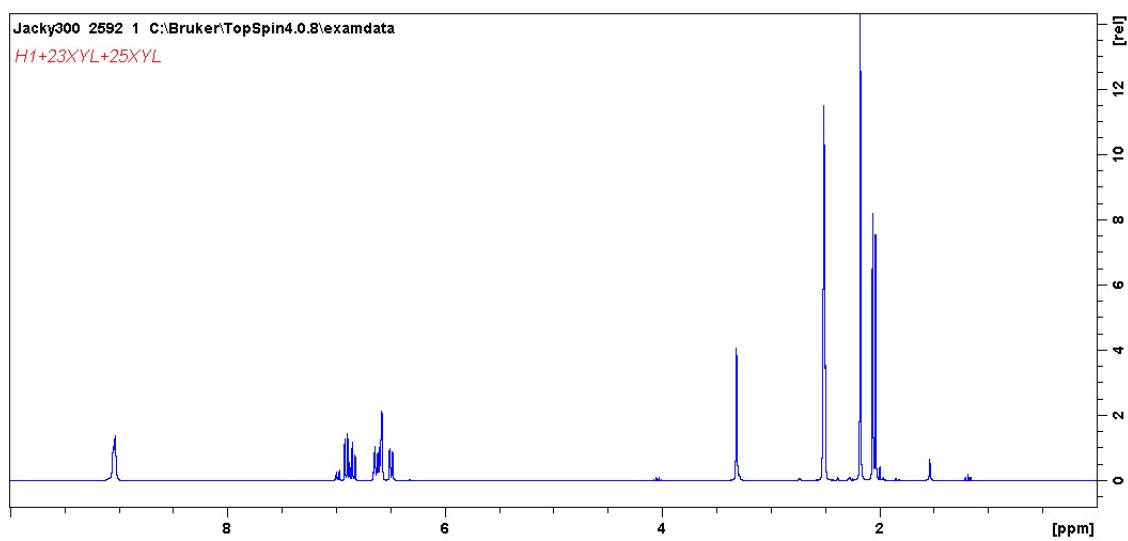


Figure S3: ¹H NMR spectrum for H1+ 23XYL+25XYL

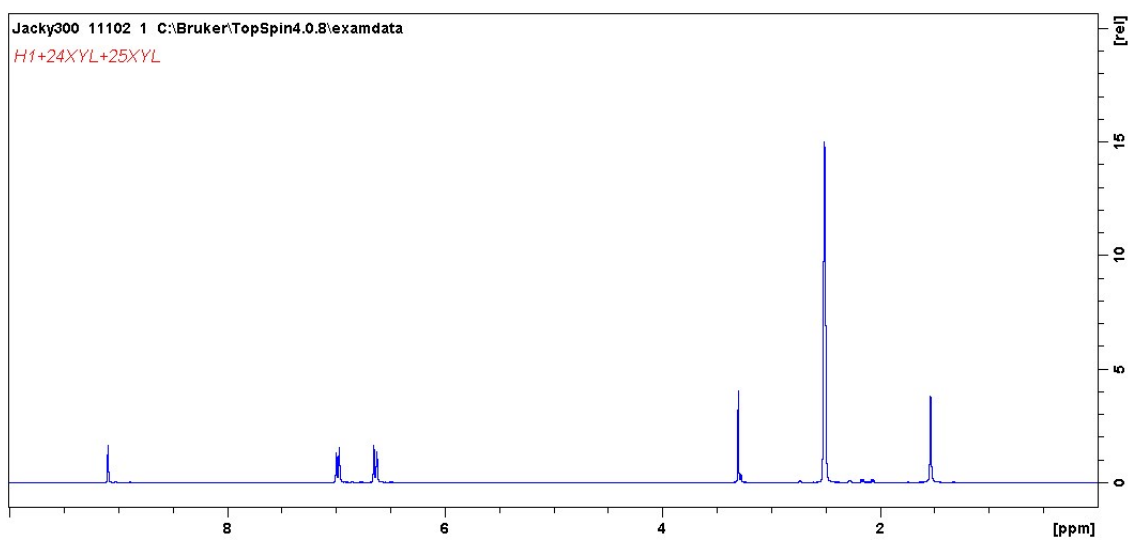


Figure S4: ¹H NMR spectrum for H1+ 24XYL+25XYL

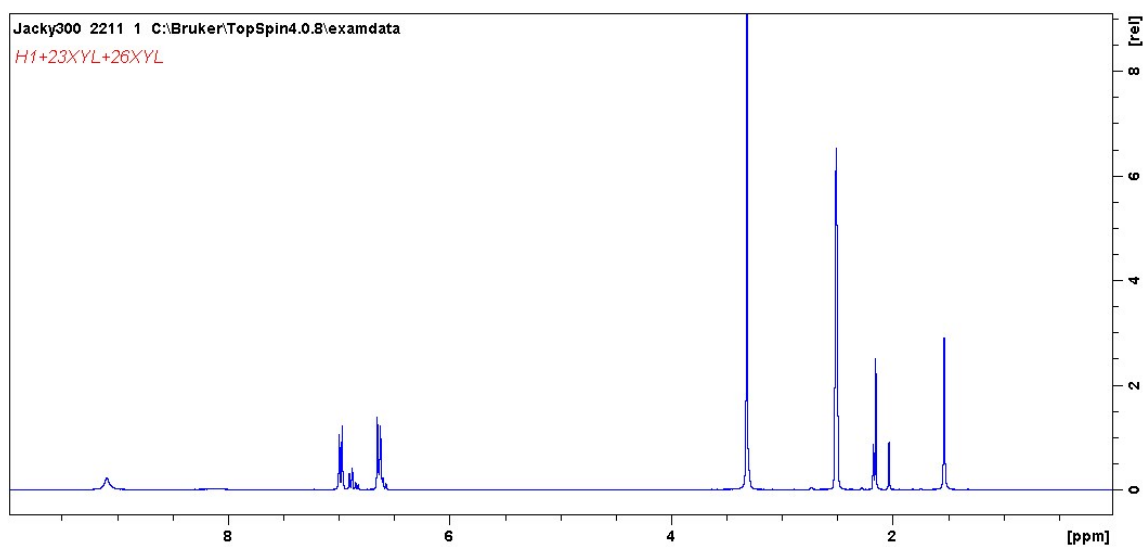


Figure S5: ¹H NMR spectrum for H1+ 23XYL+26XYL

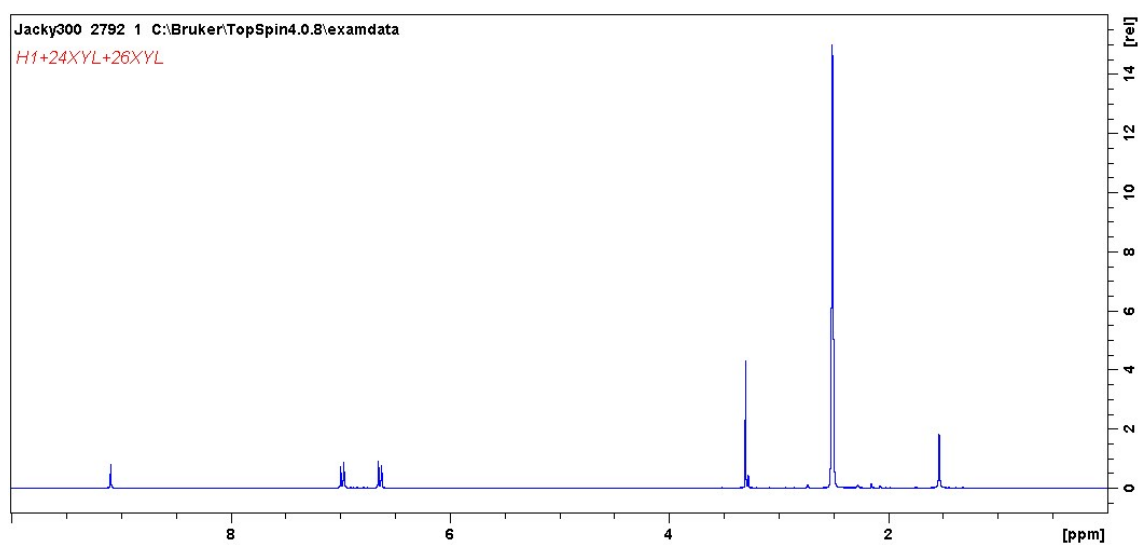


Figure S6: ¹H NMR spectrum for H1+ 24XYL+26XYL

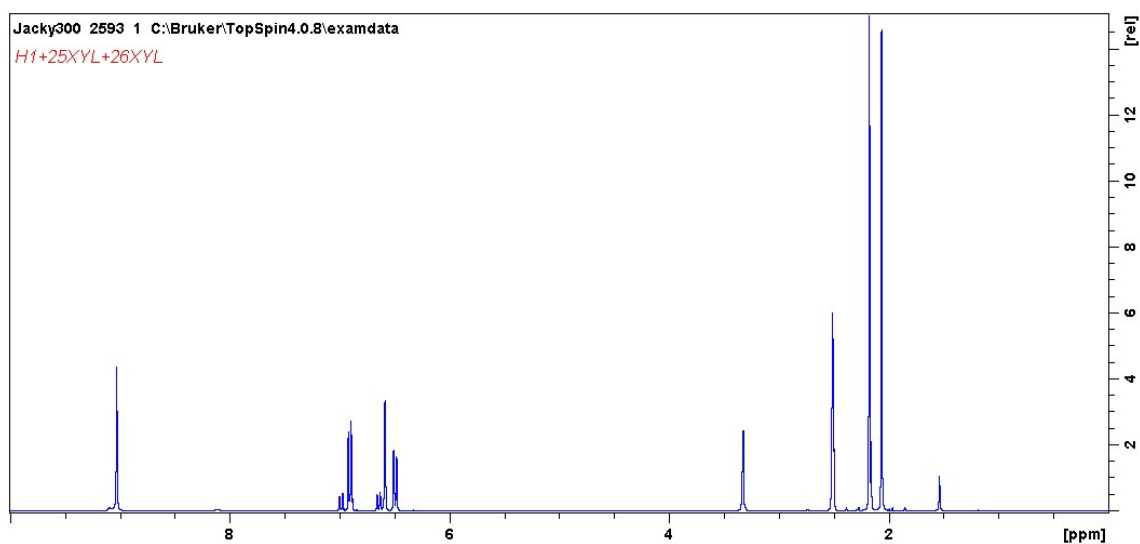


Figure S7: ¹H NMR spectrum for H1+ 25XYL+26XYL

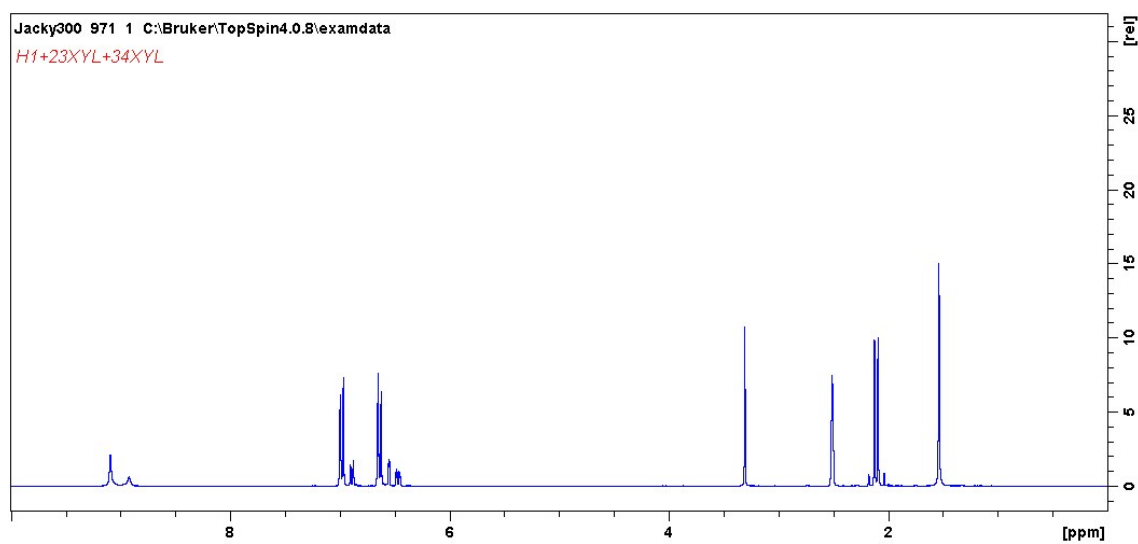


Figure S8: ¹H NMR spectrum for H1+ 23XYL+34XYL

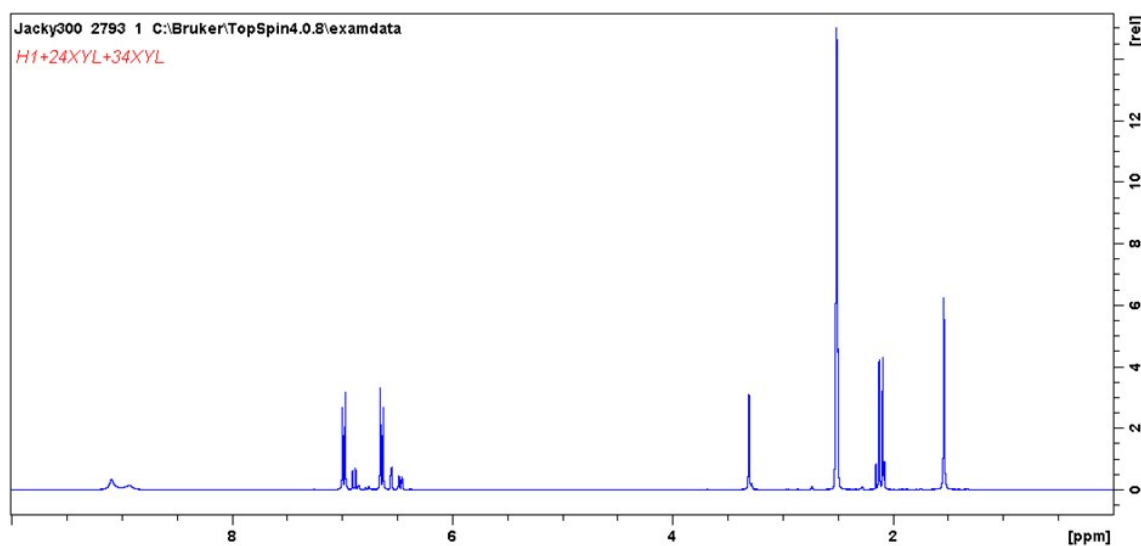


Figure S9: ¹H NMR spectrum for H1+ 24XYL+34XYL

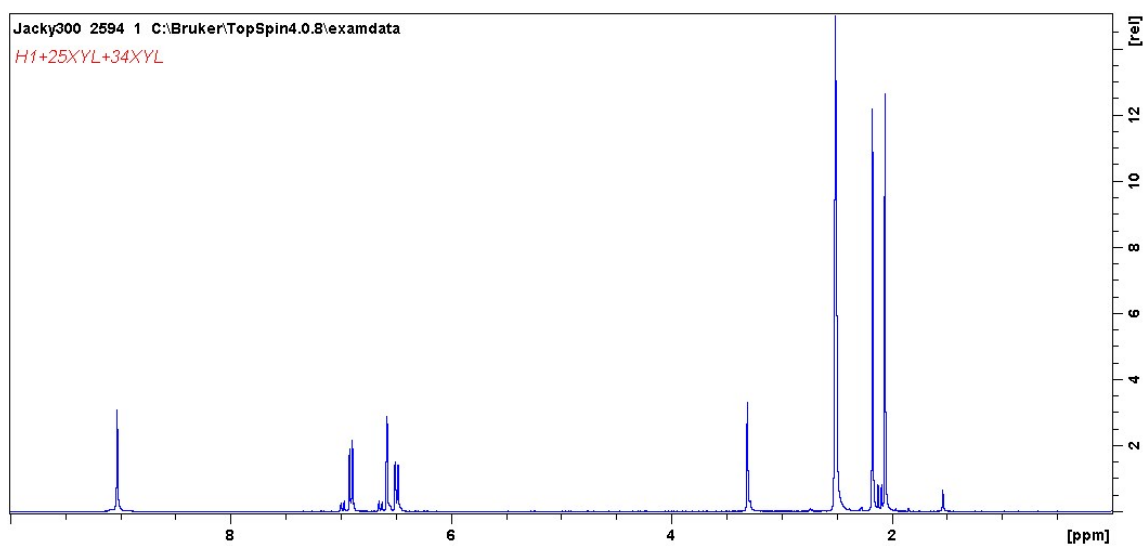


Figure S10: ¹H NMR spectrum for H1+ 25XYL+34XYL

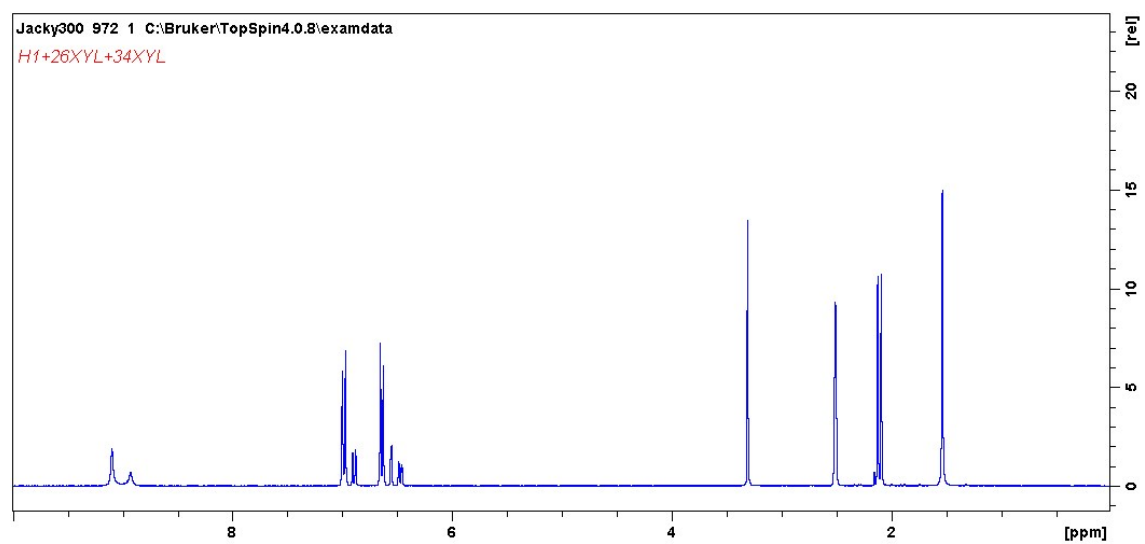


Figure S11: ¹H NMR spectrum for H1+ 26XYL+34XYL

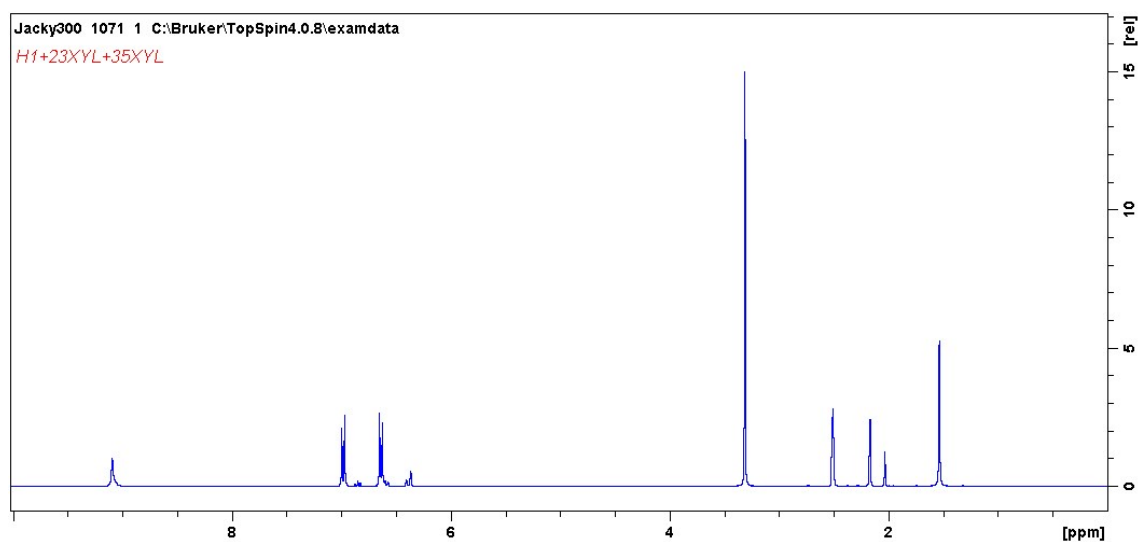


Figure S12: ¹H NMR spectrum for H1+ 23XYL+35XYL

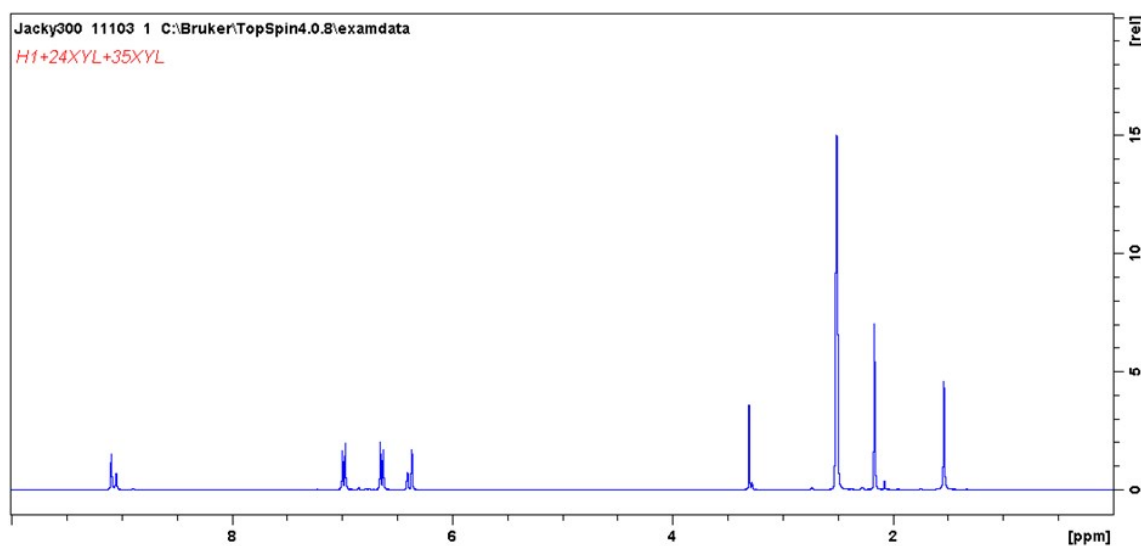


Figure S13: ¹H NMR spectrum for H1+ 24XYL+35XYL

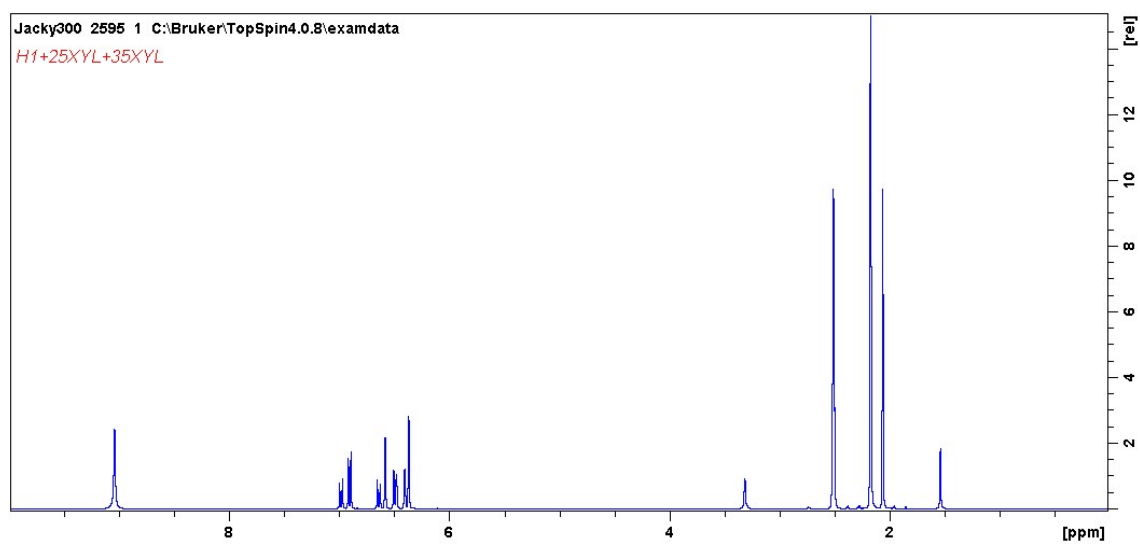


Figure S14: ¹H NMR spectrum for H1+ 25XYL+35XYL

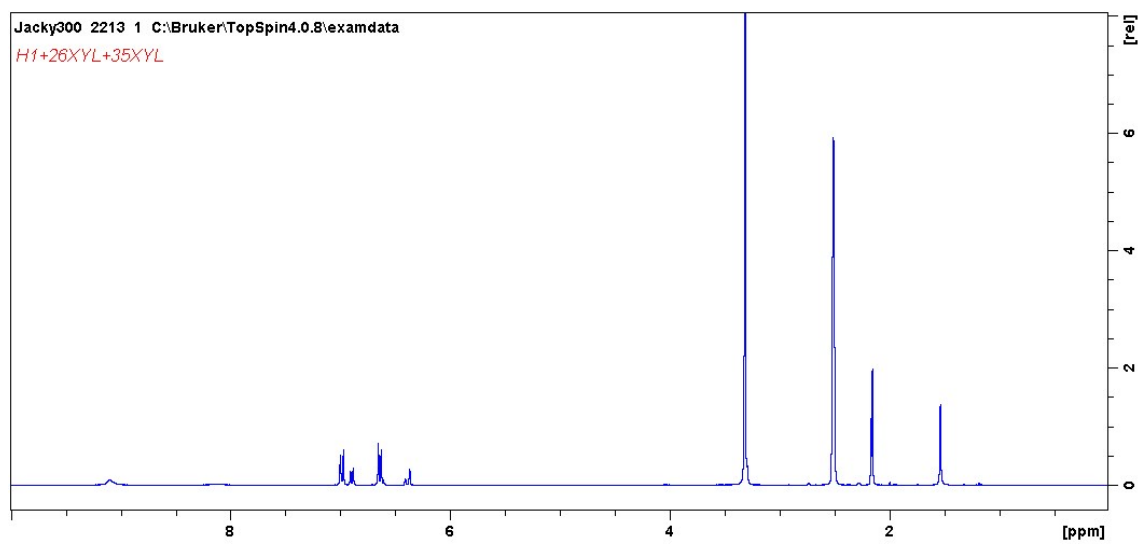


Figure S15: ¹H NMR spectrum for H1+ 26XYL+35XYL

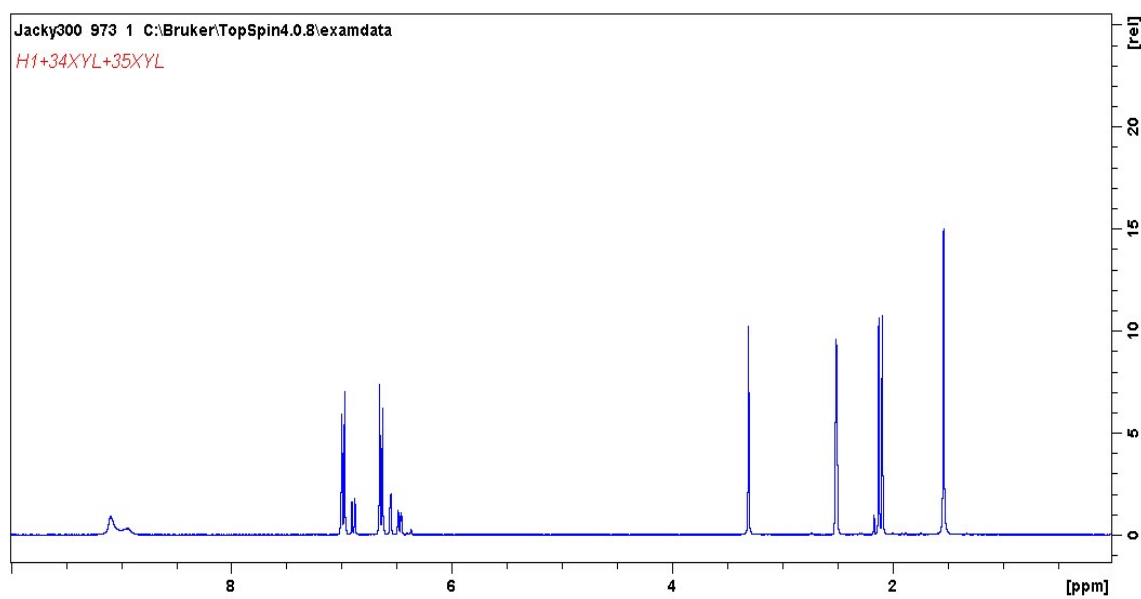


Figure S16: ¹H NMR spectrum for H1+ 34XYL+35XYL

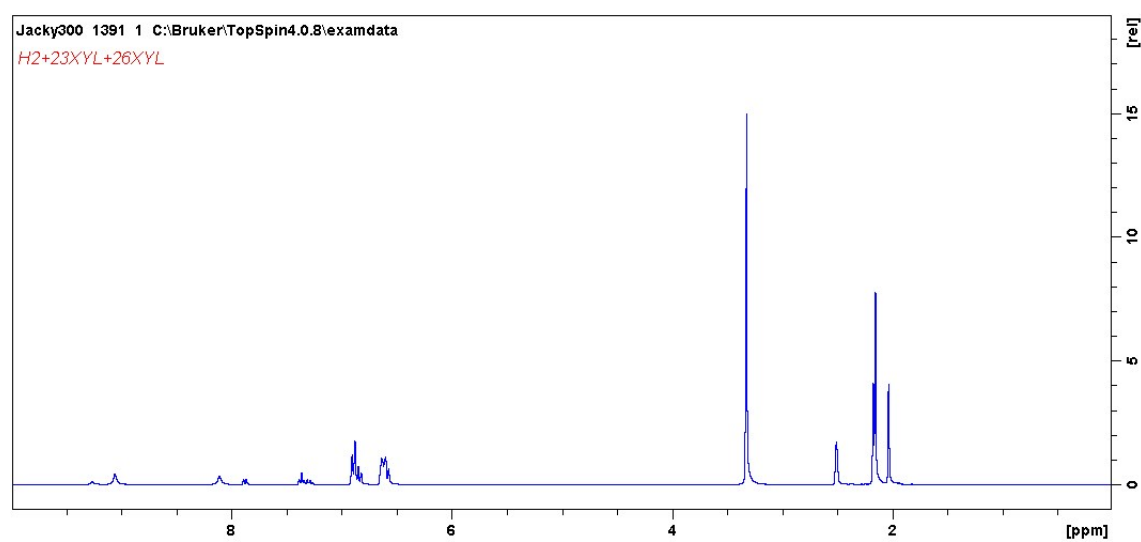


Figure S17: NMR spectrum for H2+ 23XYL+26XYL

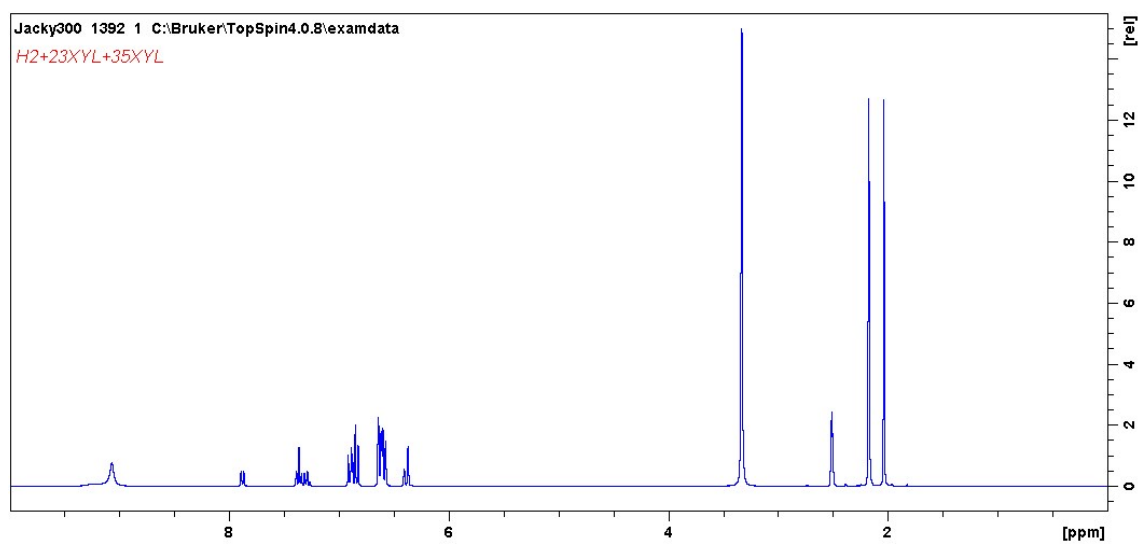


Figure S18: ¹H NMR spectrum for H2+ 23XYL+35XYL

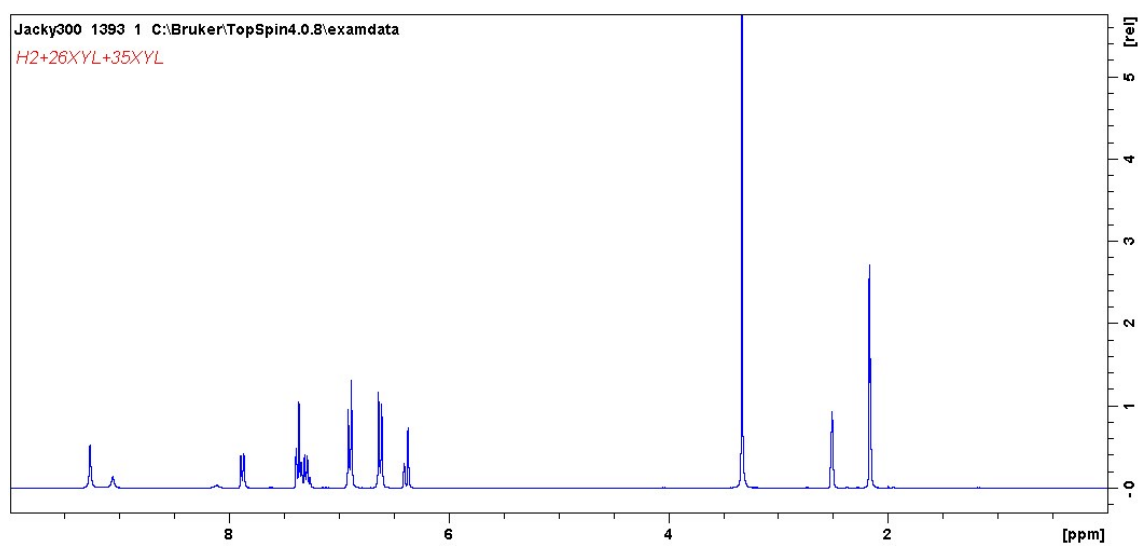


Figure S19: ¹H NMR spectrum for H2+ 26XYL+35XYL

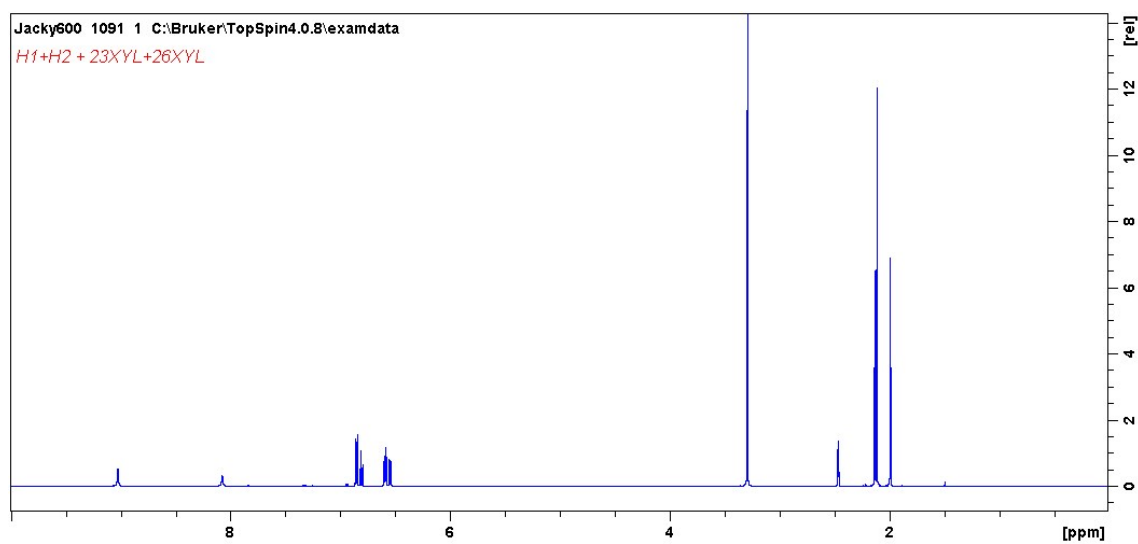


Figure S20: ^1H NMR spectrum for H1+H2+ 23XYL+26XYL

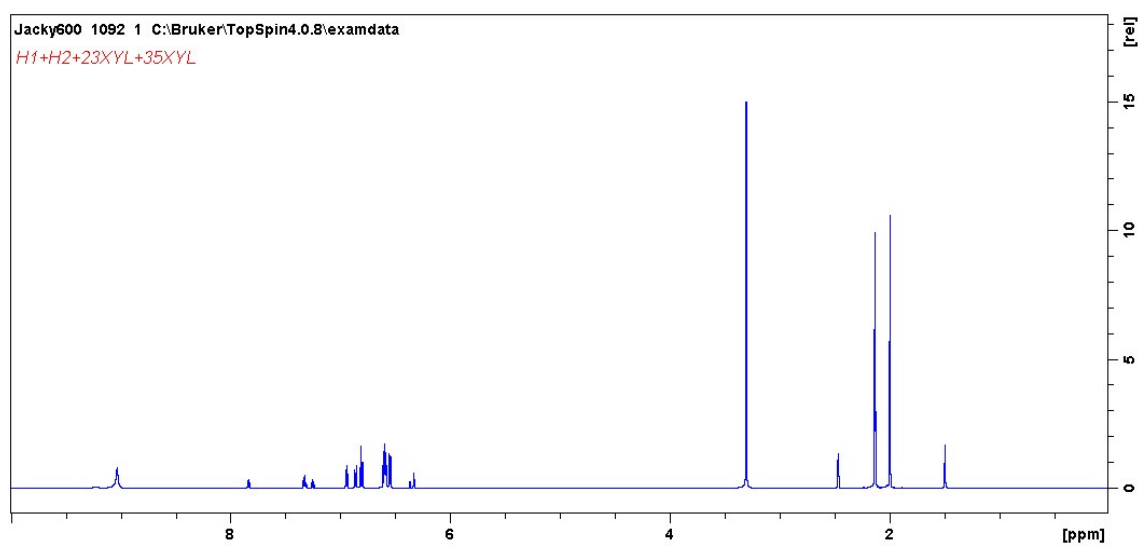


Figure S21: ^1H NMR spectrum for H1+H2+ 23XYL+35XYL

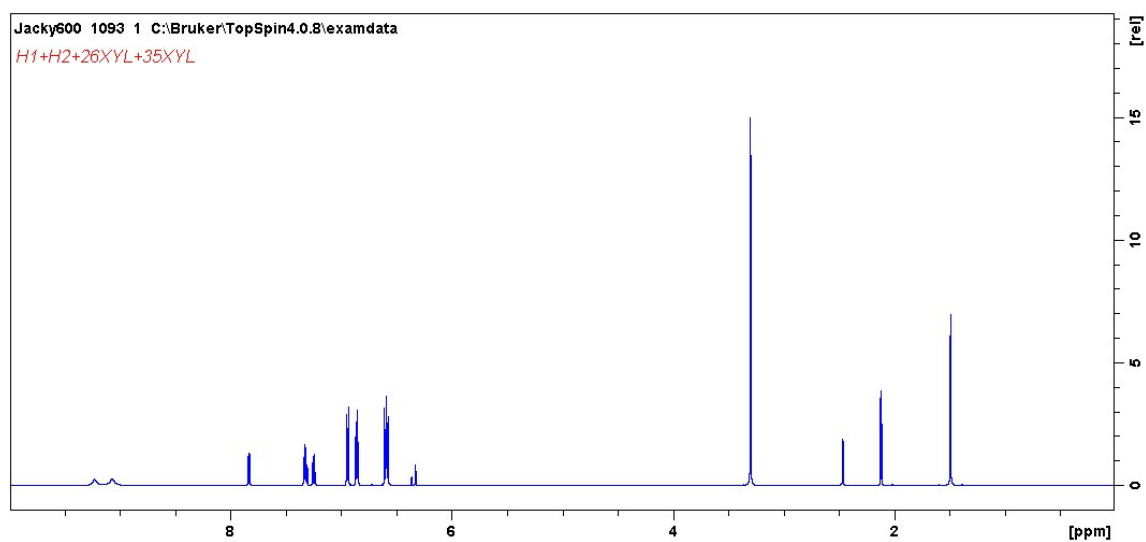


Figure S22: ^1H NMR spectrum for H1+H2+ 26XYL+35XYL

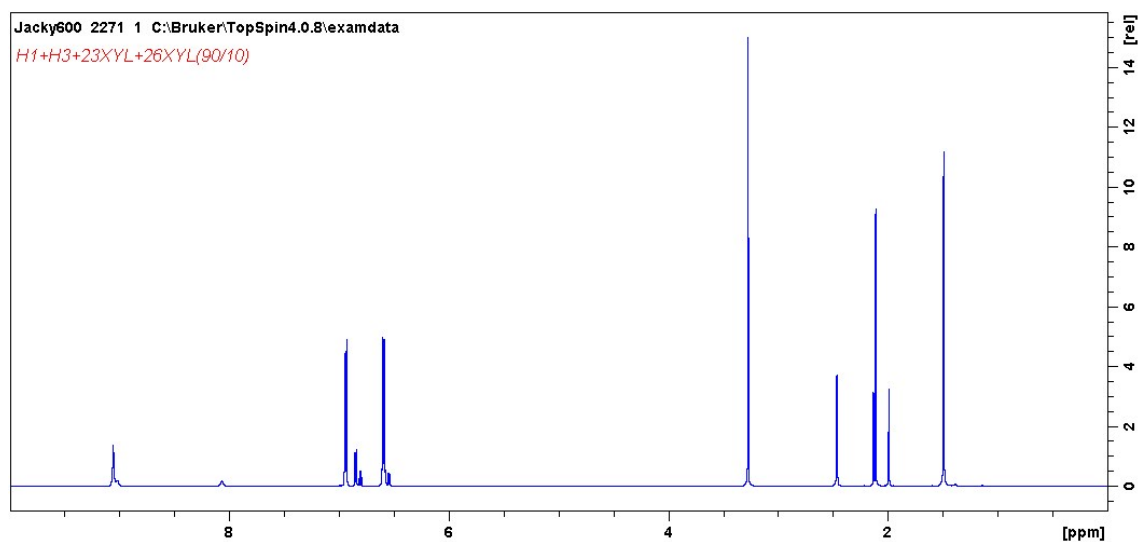


Figure S23: ^1H NMR spectrum for H1+H3+23XY+26XYL (ratio H1:H3 90/10)

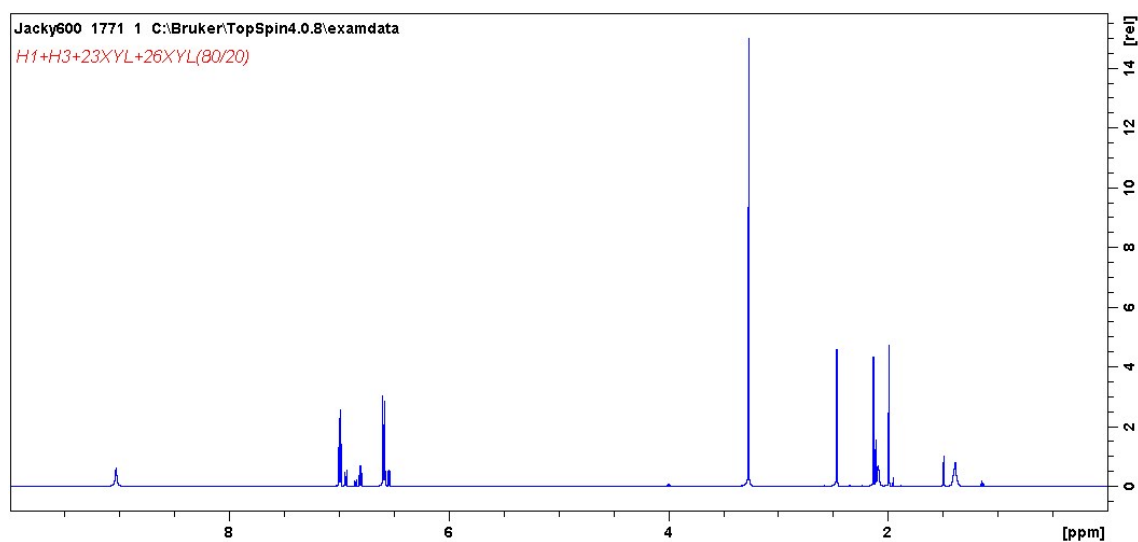


Figure S24: ^1H NMR spectrum for H1+H3+23XY+26XYL (ratio H1:H3 80/20)

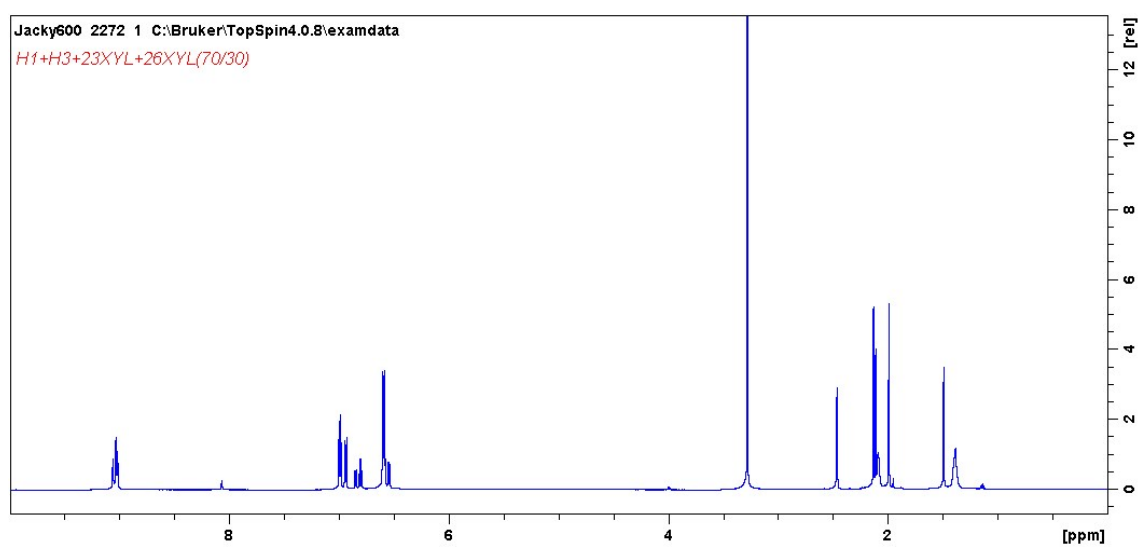


Figure S25: ^1H NMR spectrum for H1+H3+23XY+26XYL (ratio H1:H3 70/30)

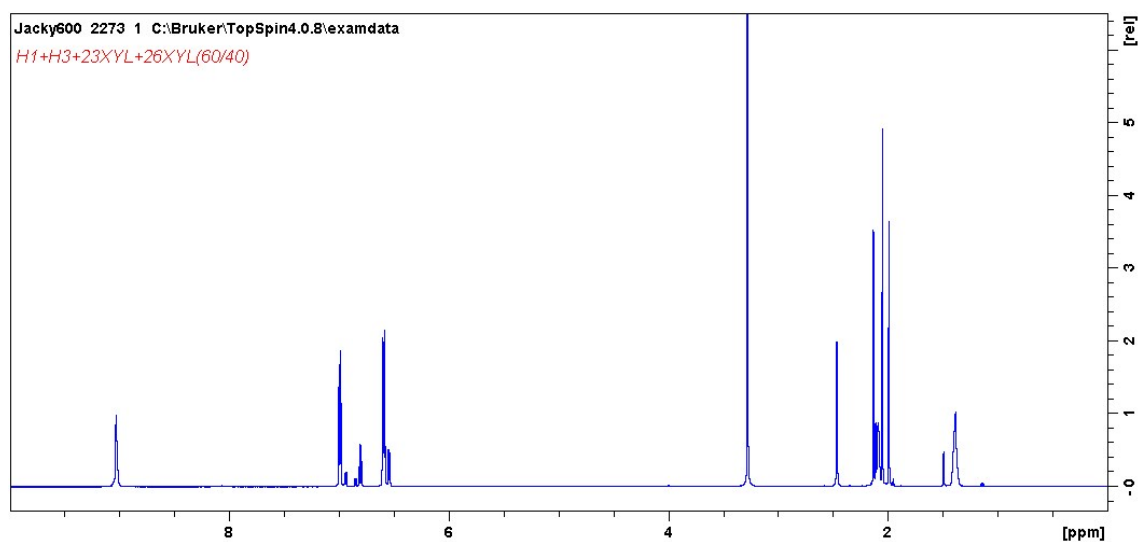
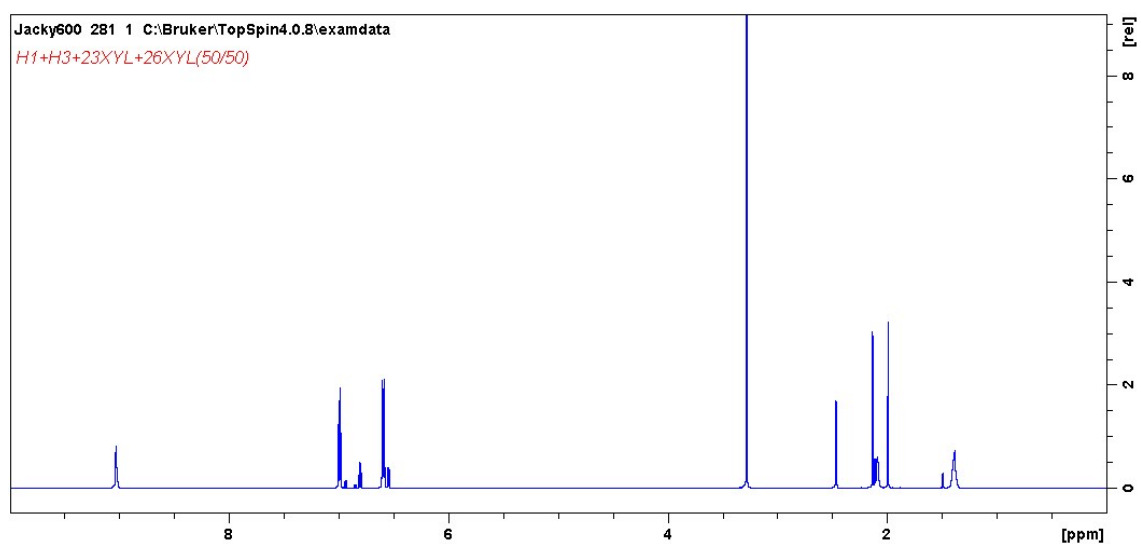


Figure S26: ^1H NMR spectrum for H1+H3+23XY+26XYL (ratio H1:H3 60/40)



e S27: ^1H NMR spectrum for H1+H3+23XY+26XYL (ratio H1:H3 50/50)

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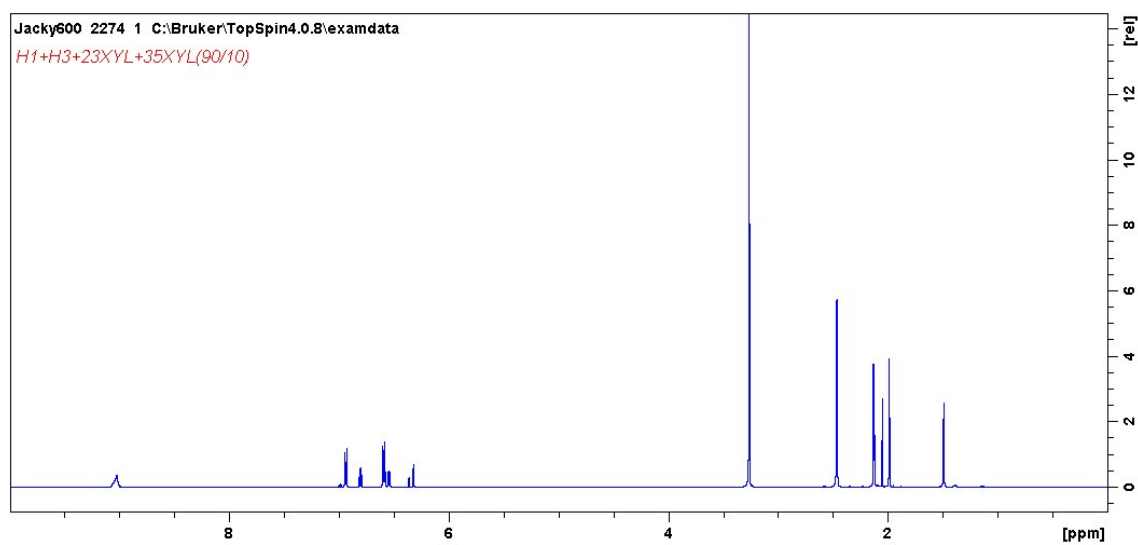


Figure S28: ^1H NMR spectrum for H1+H3+23XY+35XYL (ratio H1:H3 90/10)

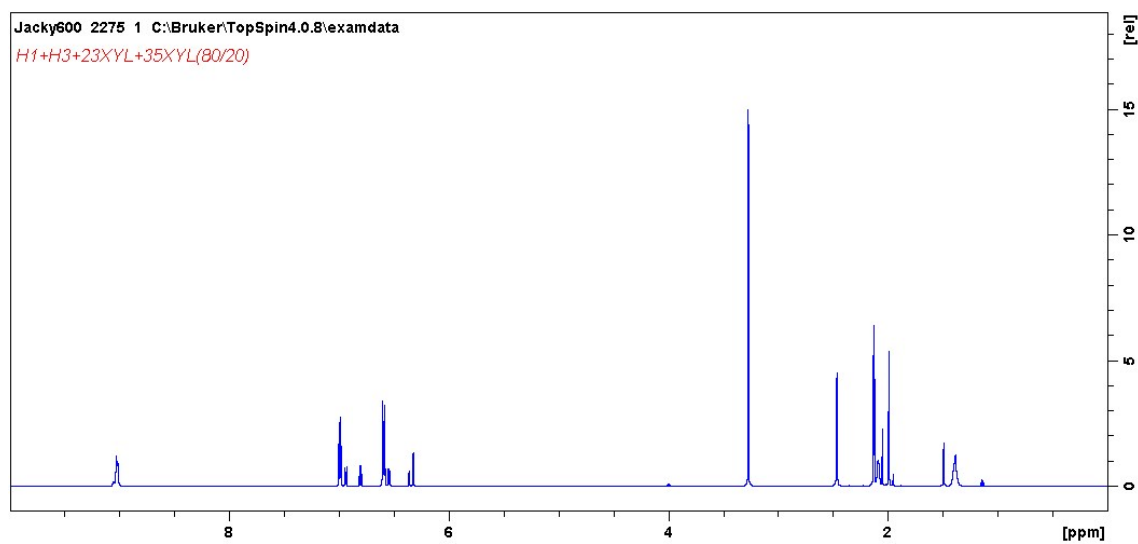


Figure S29: ^1H NMR spectrum for H1+H3+23XY+35XYL (ratio H1:H3 80/20)

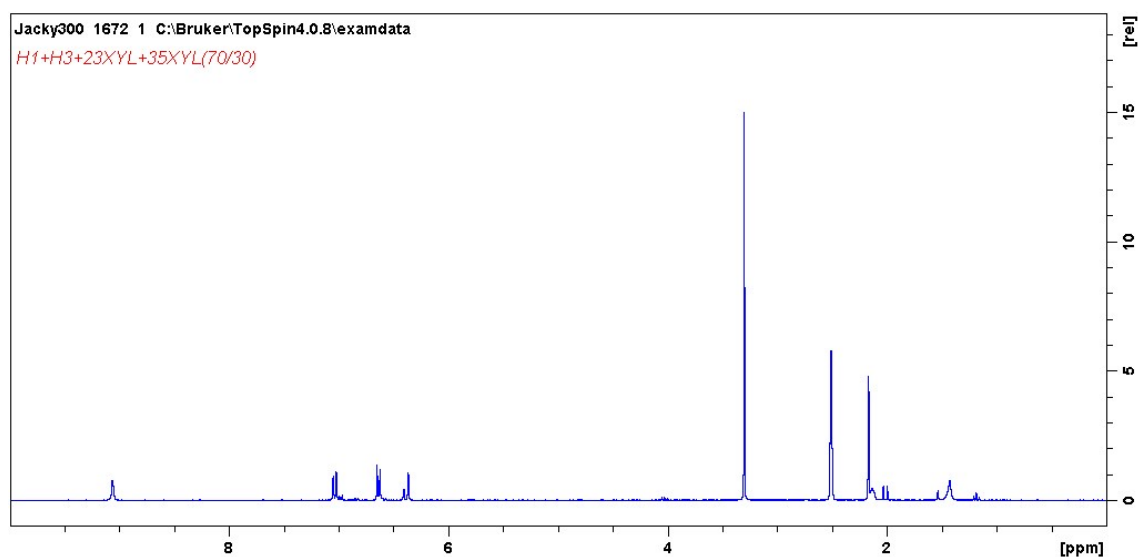
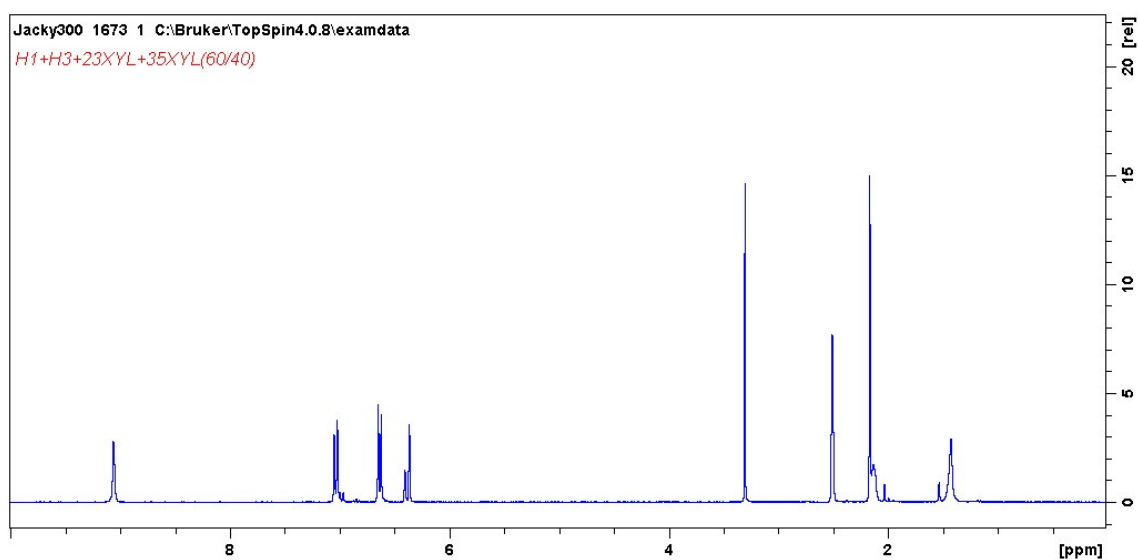


Figure S30: ^1H NMR spectrum for H1+H3+23XY+35XYL (ratio H1:H3 70/30)



e S31: ^1H NMR spectrum for H1+H3+23XY+35XYL (ratio H1:H3 60/40)

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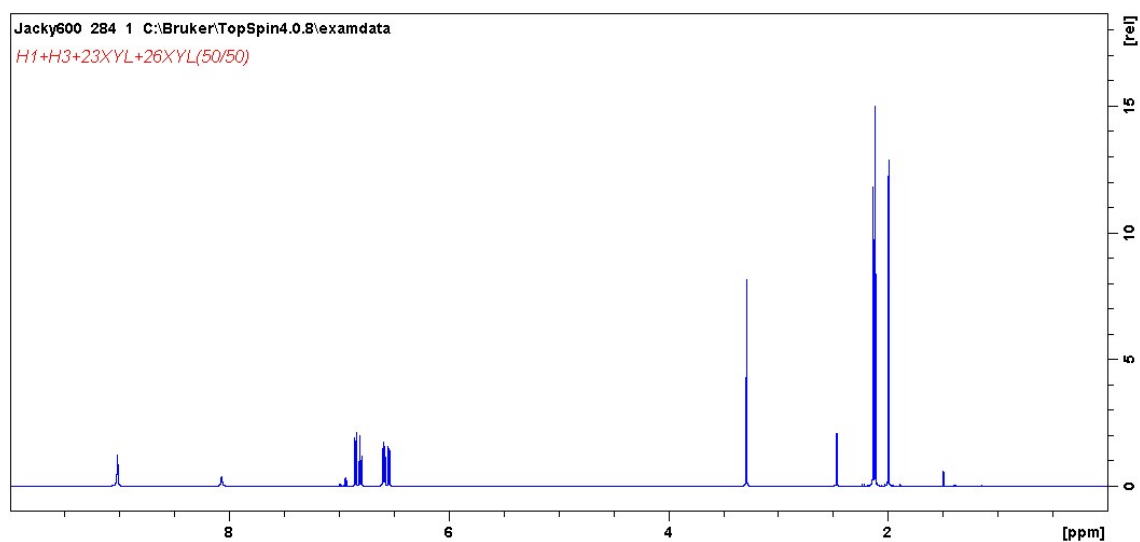


Figure S32: ^1H NMR spectrum for H1+H3+23XY+35XYL (ratio H1:H3 50/50)

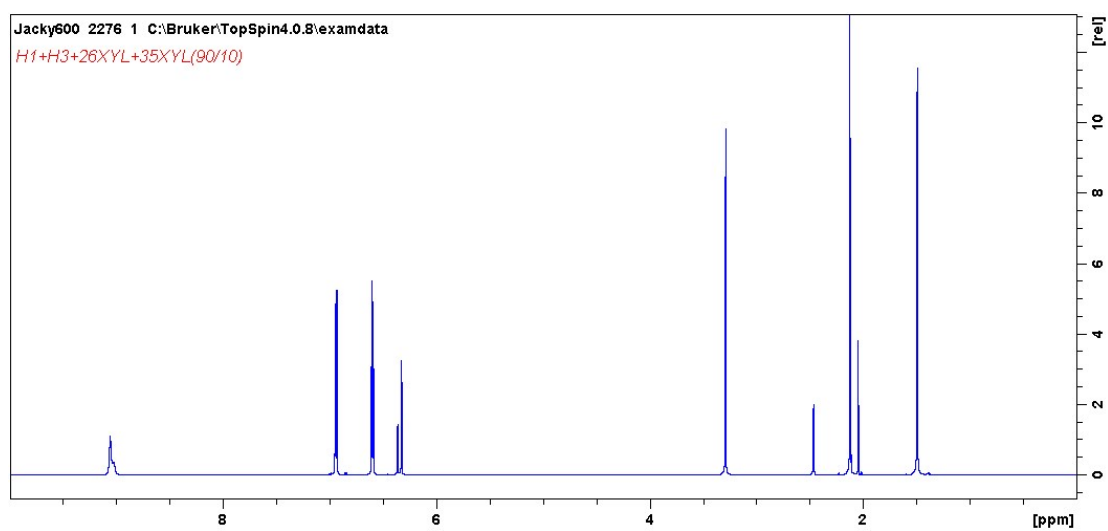


Figure S33: ^1H NMR spectrum for H1+H3+26XY+35XYL (ratio H1:H3 90/10)

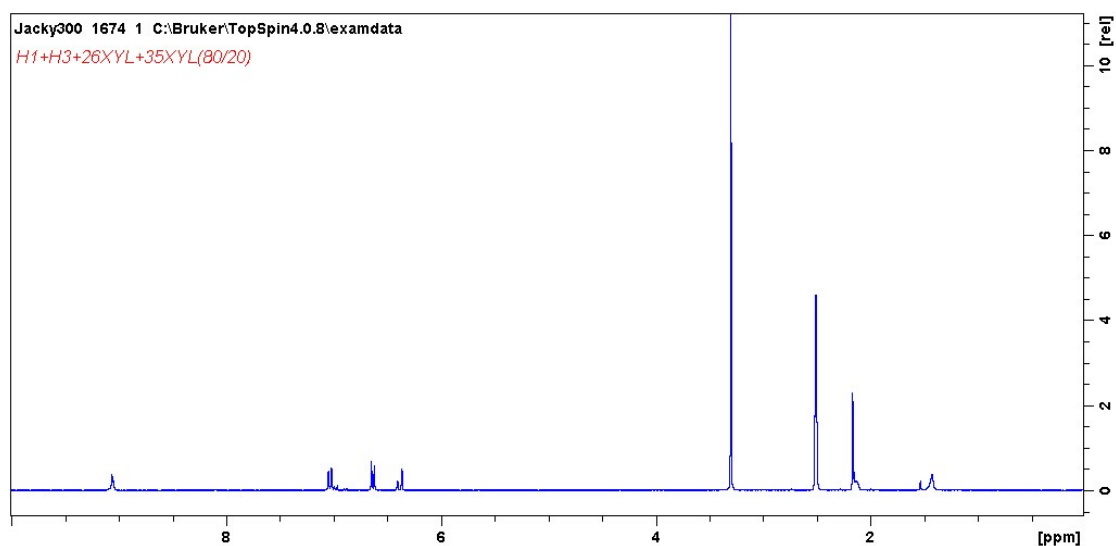


Figure S34: ^1H NMR spectrum for H1+H3+26XY+35XYL (ratio H1:H3 80/20)

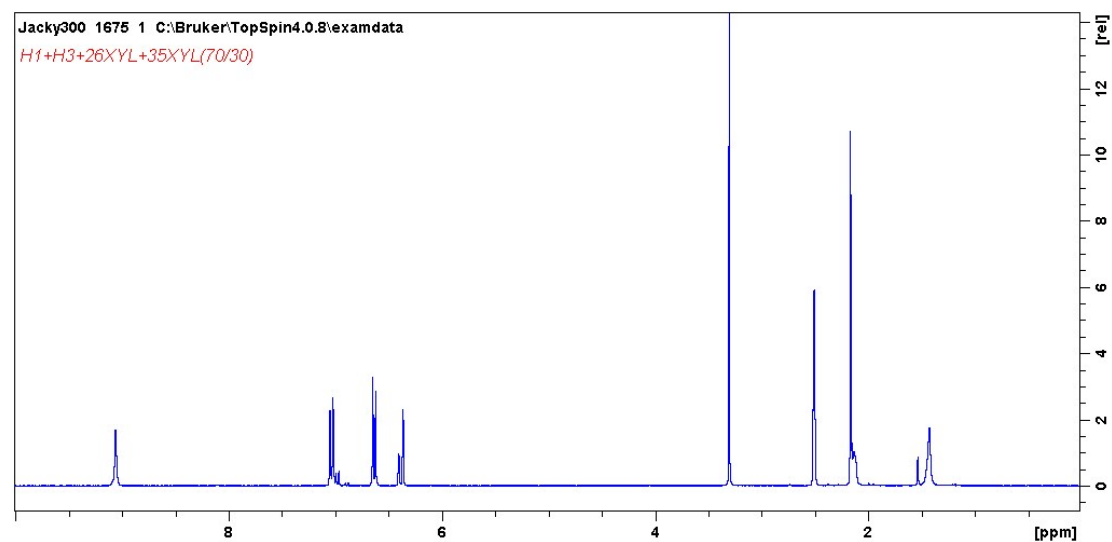


Figure S35: ^1H NMR spectrum for H1+H3+26XY+35XYL (ratio H1:H3 70/30)

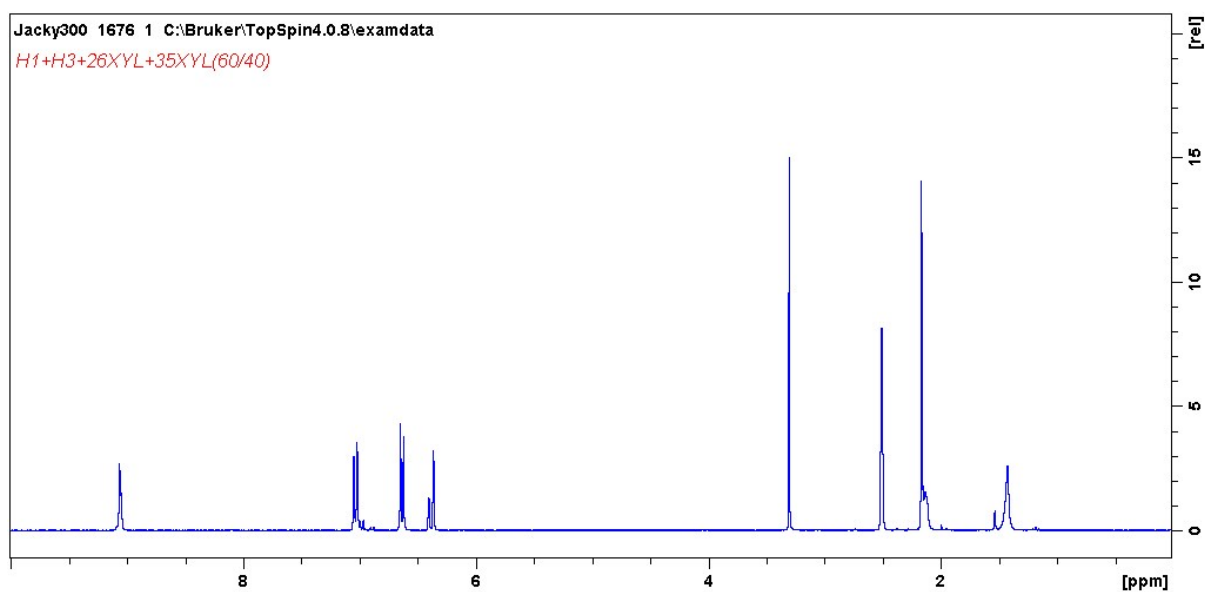


Figure S36: ^1H NMR spectrum for H1+H3+26XY+35XYL (ratio H1:H3 60/40)

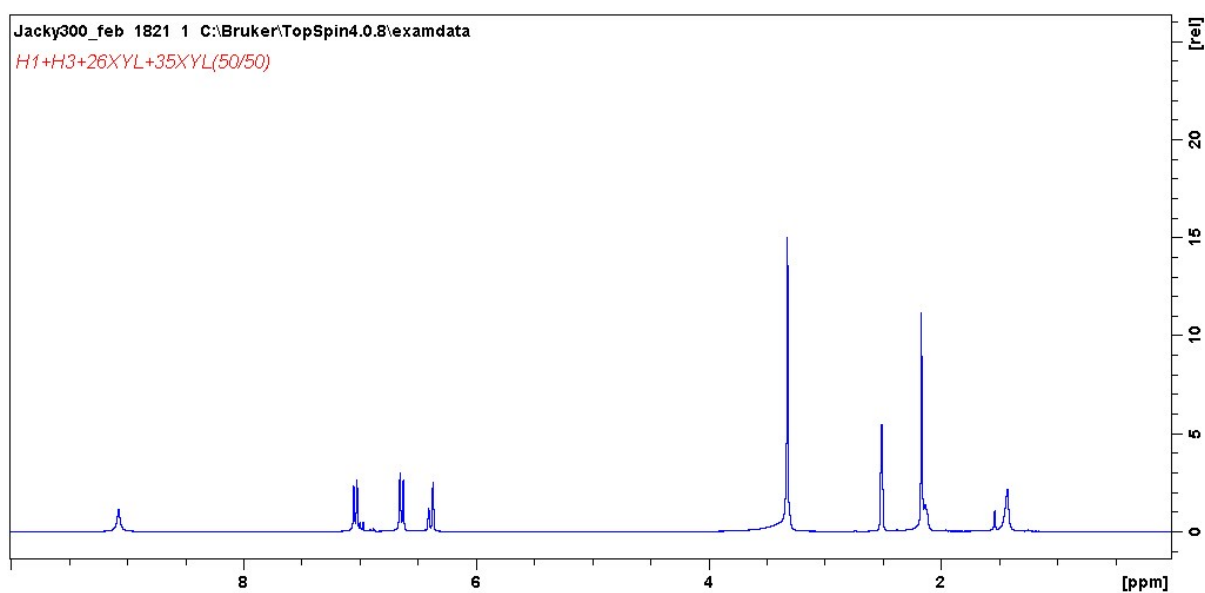


Figure S37: ^1H NMR spectrum for H1+H3+26XY+35XYL (ratio H1:H3 50/50)