



Supporting Information

for

A chemically contiguous hapten approach for a heroin–fentanyl vaccine

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NMR spectra of compounds 1–53

A chemically contiguous hapten approach for a heroin-fentanyl vaccine

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NMR Spectra of Compounds 1-53

¹ H NMR Spectra of Norheroin (1)	S1
¹³ C NMR Spectra of Norheroin (1)	S2
¹ H NMR Spectra of Compound 2	S3
¹³ C NMR Spectra of Compound 2	S4
¹ H NMR Spectra of Compound 3	S5
¹³ C NMR Spectra of Compound 3	S6
¹ H NMR Spectra of Compound 4	S7
¹³ C NMR Spectra of Compound 4	S8
¹ H NMR Spectra of Compound 5	S9
¹³ C NMR Spectra of Compound 5	S10
¹ H NMR Spectra of Compound 6	S11
¹³ C NMR Spectra of Compound 6	S12
¹ H NMR Spectra of Compound 7	S13
¹³ C NMR Spectra of Compound 7	S14
¹ H NMR Spectra of Compound 8	S15
¹³ C NMR Spectra of Compound 8	S16
¹ H NMR Spectra of Compound 10	S17
¹³ C NMR Spectra of Compound 10	S18
¹ H NMR Spectra of Compound 11	S19
¹³ C NMR Spectra of Compound 11	S20
¹ H NMR Spectra of Compound 13	S21
¹³ C NMR Spectra of Compound 13	S22

¹ H NMR Spectra of Compound 14	S23
¹³ C NMR Spectra of Compound 14	S24
¹ H NMR Spectra of Compound 15	S25
¹³ C NMR Spectra of Compound 15	S26
¹ H NMR Spectra of Compound 17	S27
¹³ C NMR Spectra of Compound 17	S28
¹ H NMR Spectra of HF-3 (18)	S29
¹³ C NMR Spectra of HF-3 (18)	S30
¹ H NMR Spectra of Compound 19	S31
¹³ C NMR Spectra of Compound 19	S32
¹ H NMR Spectra of Compound 20	S33
¹³ C NMR Spectra of Compound 20	S34
¹ H NMR Spectra of Compound 21	S35
¹³ C NMR Spectra of Compound 21	S36
¹ H NMR Spectra of Compound 22	S37
¹³ C NMR Spectra of Compound 22	S38
¹ H NMR Spectra of Compound 23	S39
¹³ C NMR Spectra of Compound 23	S40
¹ H NMR Spectra of Compound 24	S41
¹³ C NMR Spectra of Compound 24	S42
¹ H NMR Spectra of Compound 25	S43
¹³ C NMR Spectra of Compound 25	S44
¹ H NMR Spectra of Compound 26	S45
¹³ C NMR Spectra of Compound 26	S46
¹ H NMR Spectra of Compound 29	S47
¹³ C NMR Spectra of Compound 29	S48
¹ H NMR Spectra of Compound 30	S49
¹³ C NMR Spectra of Compound 30	S50
¹ H NMR Spectra of HF-5 (31)	S51
¹³ C NMR Spectra of HF-5 (31)	S52
¹ H NMR Spectra of Compound 32	S53
¹³ C NMR Spectra of Compound 32	S54
¹ H NMR Spectra of Compound 33	S55
¹³ C NMR Spectra of Compound 33	S56
¹ H NMR Spectra of Compound 34	S57
¹³ C NMR Spectra of Compound 34	S58
¹ H NMR Spectra of Compound 36	S59
¹³ C NMR Spectra of Compound 36	S60
¹ H NMR Spectra of Compound 37	S61
¹³ C NMR Spectra of Compound 37	S62
¹ H NMR Spectra of HF-6 (38)	S63
¹³ C NMR Spectra of HF-6 (38)	S64
¹ H NMR Spectra of Compound 39	S65
¹³ C NMR Spectra of Compound 39	S66

¹ H NMR Spectra of Compound 40	S67
¹³ C NMR Spectra of Compound 40	S68
¹ H NMR Spectra of Compound 41	S69
¹³ C NMR Spectra of Compound 41	S70
¹ H NMR Spectra of HF-7 (42)	S71
¹³ C NMR Spectra of HF-7 (42)	S72
¹ H NMR Spectra of Compound 43	S73
¹³ C NMR Spectra of Compound 43	S74
¹ H NMR Spectra of Compound 44	S75
¹³ C NMR Spectra of Compound 44	S76
¹ H NMR Spectra of HF-8 (45)	S77
¹³ C NMR Spectra of HF-8 (45)	S78
¹ H NMR Spectra of Compound 47	S79
¹³ C NMR Spectra of Compound 47	S80
¹ H NMR Spectra of Compound 48	S81
¹³ C NMR Spectra of Compound 48	S82
¹ H NMR Spectra of HF-9 (49)	S83
¹³ C NMR Spectra of HF-9 (49)	S84
¹ H NMR Spectra of Compound 50	S85
¹³ C NMR Spectra of Compound 50	S86
¹ H NMR Spectra of Compound 51	S87
¹³ C NMR Spectra of Compound 51	S88
¹ H NMR Spectra of Compound 52	S89
¹³ C NMR Spectra of Compound 52	S90
¹ H NMR Spectra of Fentanyl Hapten (53)	S91
¹³ C NMR Spectra of Fentanyl Hapten (53)	S92



















































































































































































