The pharmacology of indole and indazole synthetic cannabinoid designer drugs AB-FUBINACA, ADB-FUBINACA, AB-PINACA, ADB-PINACA, 5F-AB-PINACA, 5F-ADB-PINACA, ADBICA and 5F-ADBICA

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Contents:

Table S1. IUPAC names, CAS numbers, and literature references for valinamide- and *tert*-leucinamide-derived indole and indazole synthetic cannabinoids.

	IUPAC	CAS	Notified to EMCDDA	Refs
AB-FUBINACA (**7**)	*N*-(1-amino-3-methyl-1-oxobutan-2-yl)-1-(4-fluorobenzyl)-1*H*-indazole-3-carboxamide	1629062-56-1 (racemate) 1185282-01-2 (*S*)	4 July 2013, Belgium	1–5
ADB-FUBINACA (**8**)	*N*-(1-amino-3,3-dimethyl-1-oxobutan-2-yl)-1-(4-fluorobenzyl)-1*H*-indazole-3-carboxamide	1445583-51-6 (racemate) 1185282-00-1 (*S*)	28 November 2013, Turkey and Germany	1, 4, 6–8
AB-PINACA (**9**)	*N*-(1-amino-3-methyl-1-oxobutan-2-yl)-1-pentyl-1*H*-indazole-3-carboxamide	1445583-20-9 (racemate) 1445752-09-9 (*S*)	21 May 2013, Sweden	2, 4, 5, 7
ADB-PINACA (**10**)	*N*-(1-amino-3,3-dimethyl-1-oxobutan-2-yl)-1-pentyl-1*H*-indazole-3-carboxamide	1633766-73-0 (racemate)	3 December 2013, United Kingdom[a]	3, 8, 9
5F-AB-PINACA (**11**)	*N*-(1-amino-3-methyl-1-oxobutan-2-yl)-1-(5-fluoropentyl-1*H*-indazole-3-carboxamide	-	5 July 2013, Belgium	10
5F-ADB-PINACA (**12**)	*N*-(1-amino-3,3-dimethyl-1-oxobutan-2-yl)-1-(5-fluoropentyl-1*H*-indazole-3-carboxamide	-	-	11
AB-FUBICA (**13**)	*N*-(1-amino-3-methyl-1-oxobutan-2-yl)-1-(4-fluorobenzyl)-1*H*-indole-3-carboxamide	-	-	-
ADB-FUBICA (**14**)	*N*-(1-amino-3,3-dimethyl-1-oxobutan-2-yl)-1-(4-fluorobenzyl)-1*H*-indole-3-carboxamide	-	-	-
AB-PICA (**15**)	*N*-(1-amino-3-methyl-1-oxobutan-2-yl)-1-pentyl-1*H*-indole-3-carboxamide	-	-	-
ADBICA (**16**)	*N*-(1-amino-3,3-dimethyl-1-oxobutan-2-yl)-1-pentyl-1*H*-indole-3-carboxamide	1445583-48-1 (racemate)	11 October 2013, Sweden	6
5F-AB-PICA (**17**)	*N*-(1-amino-3-methyl-1-oxobutan-2-yl)-1-(5-fluoropentyl-1*H*-indole-3-carboxamide	-	-	-
5F-ADBICA (**18**)	*N*-(1-amino-3,3-dimethyl-1-oxobutan-2-yl)-1-(5-fluoropentyl-1*H*-indole-3-carboxamide	-	September 2013, USA[a]	8

[a]An advisory was issued in September 2013 after information provided by law enforcement agencies in the United States, supplemented by information from the EMCDDA's monitoring of open source information, identified a series of non-fatal

intoxications in the United States associated with ADB-PINACA and 5F-ADBICA. These substances are known to be present on the EU drug market and have been reported by several Member States.

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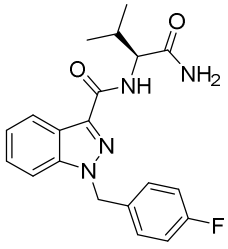
Figure S1. ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 300 K) of AB-FUBINACA (**7**).



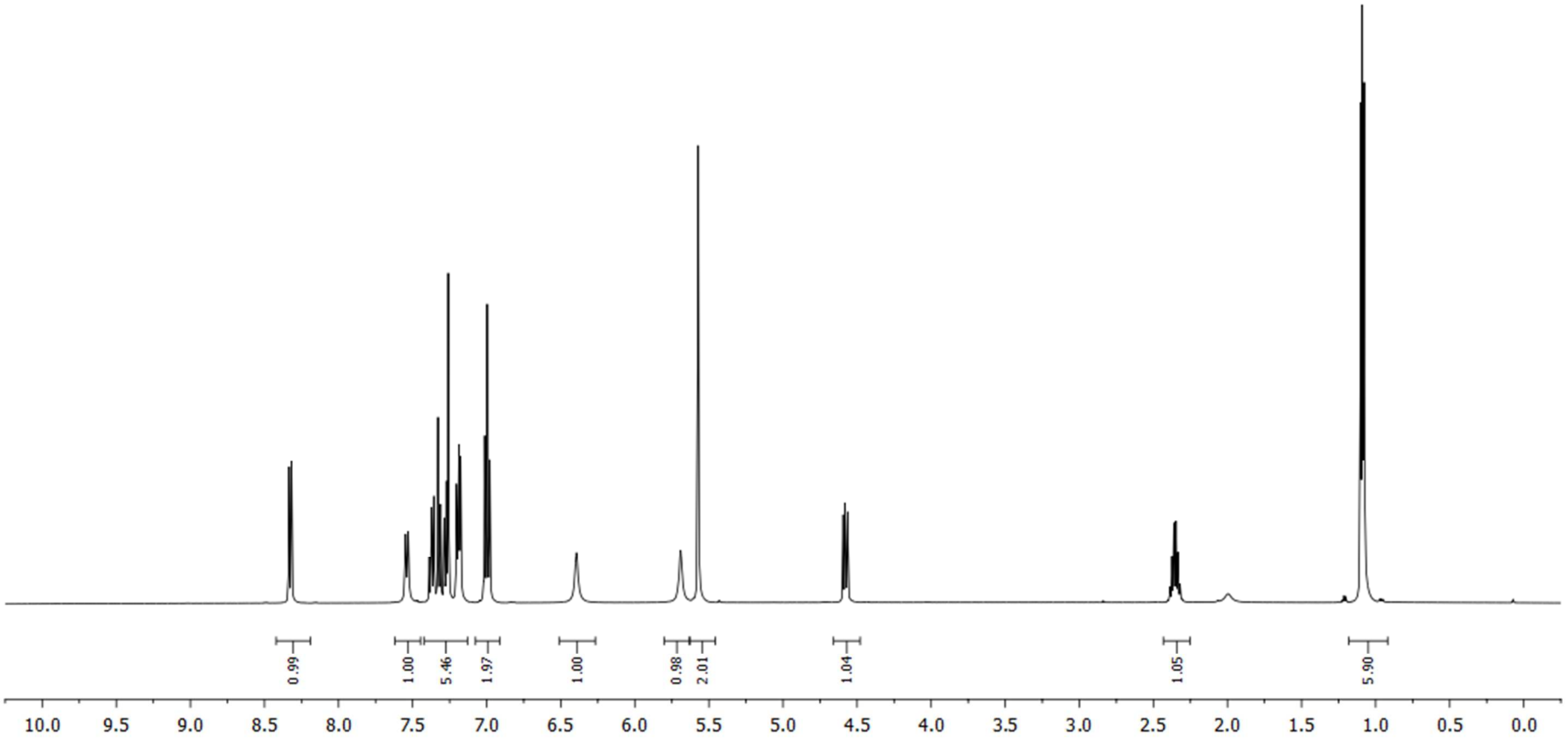


Figure S2. ^{13}C NMR spectrum (125 MHz, $CDCl_3$, 300 K) of AB-FUBINACA (**7**).

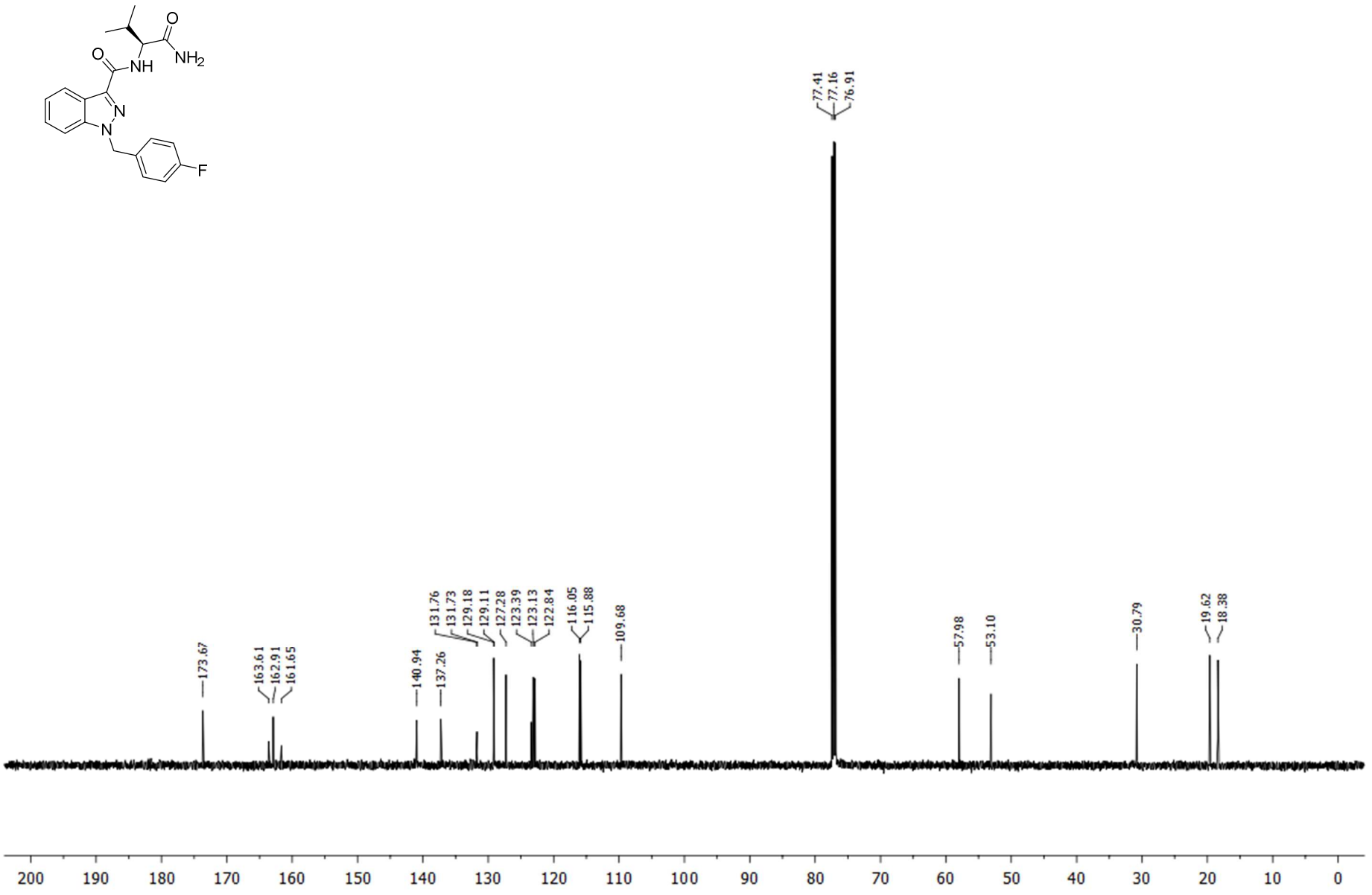


Figure S3. ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 300 K) of AB-PINACA (**9**).

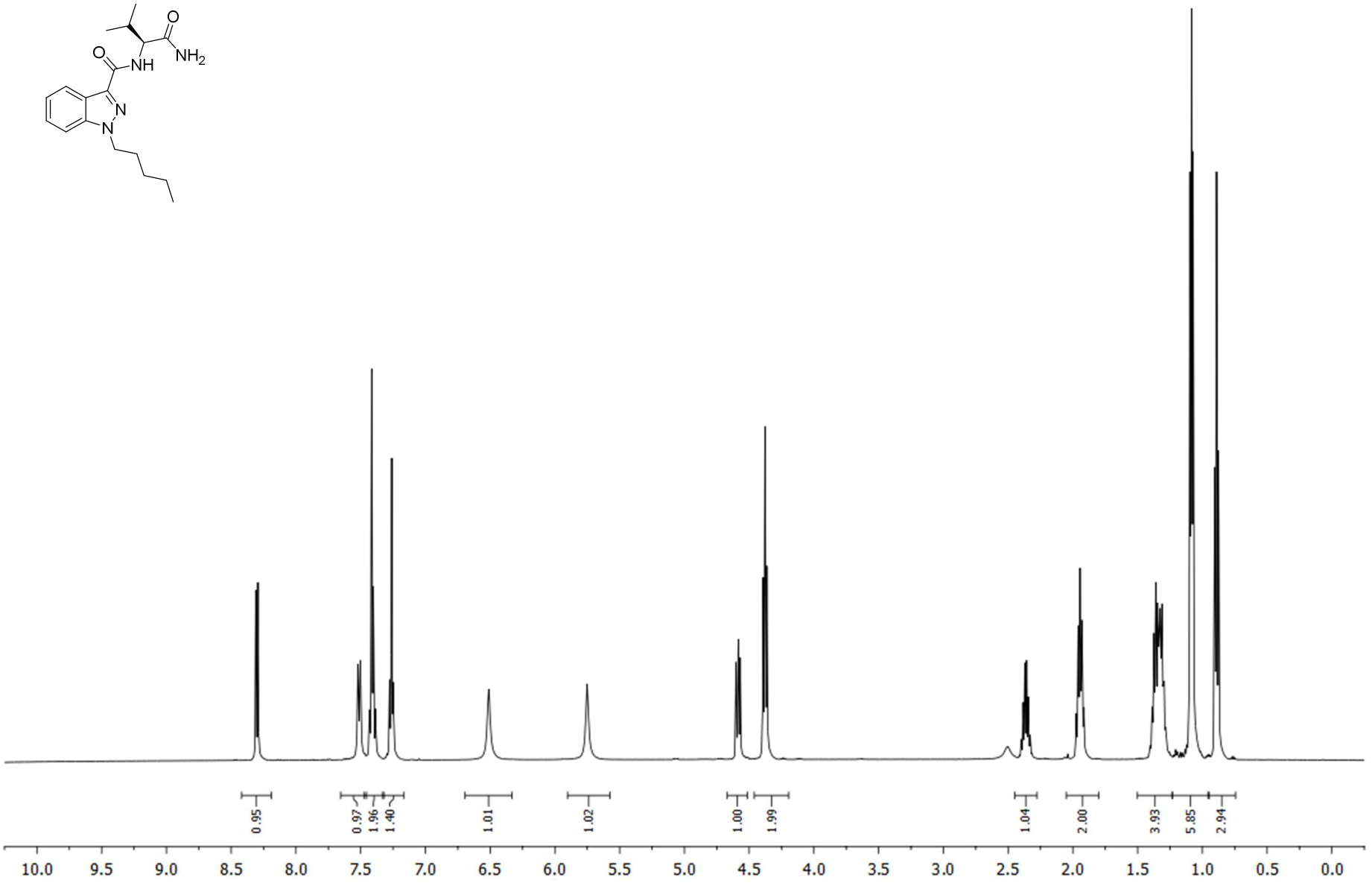


Figure S4. ^{13}C NMR spectrum (125 MHz, $CDCl_3$, 300 K) of AB-PINACA (**9**).

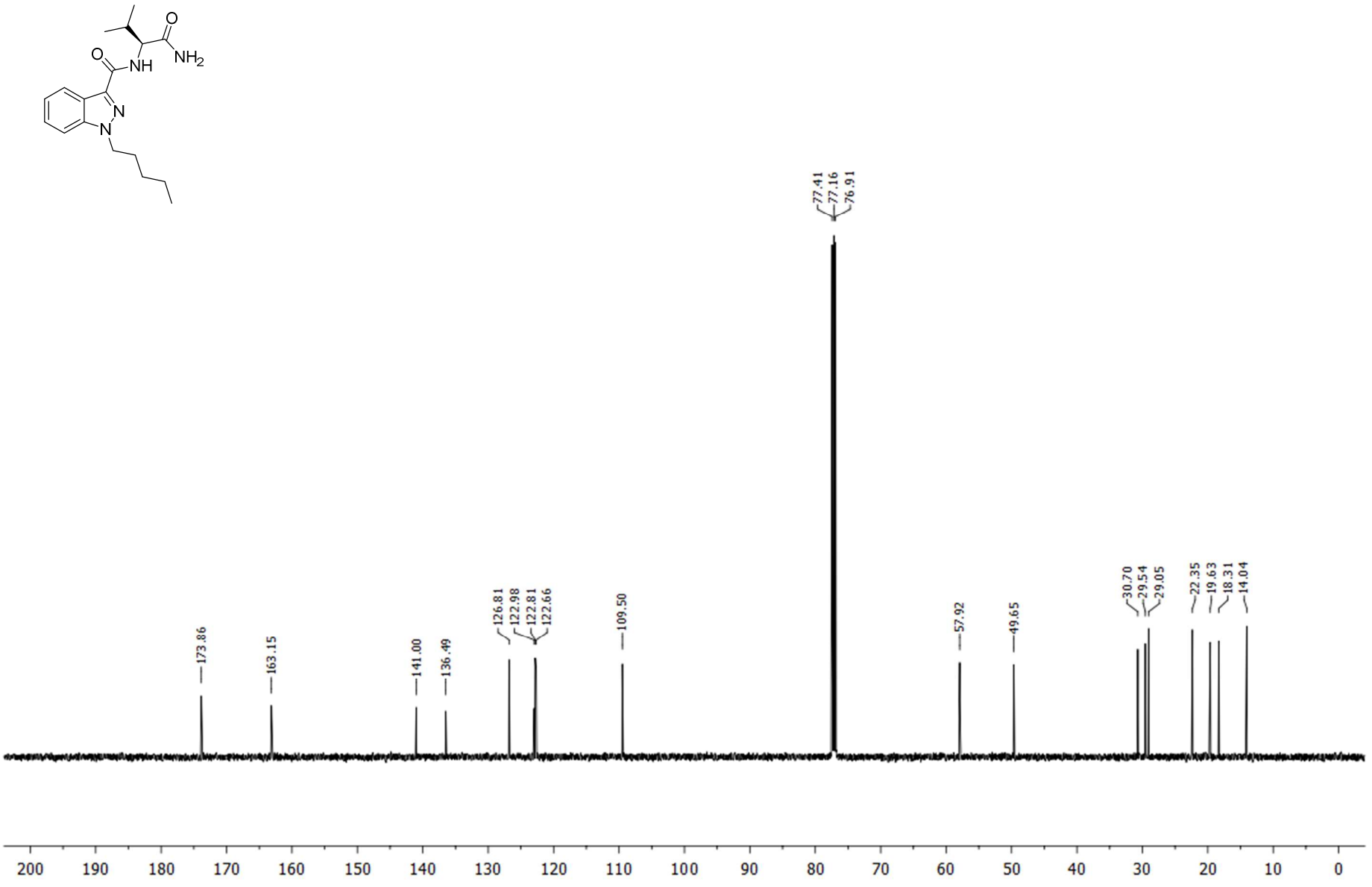


Figure S5. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 300 K) of ADB-PINACA (**10**).

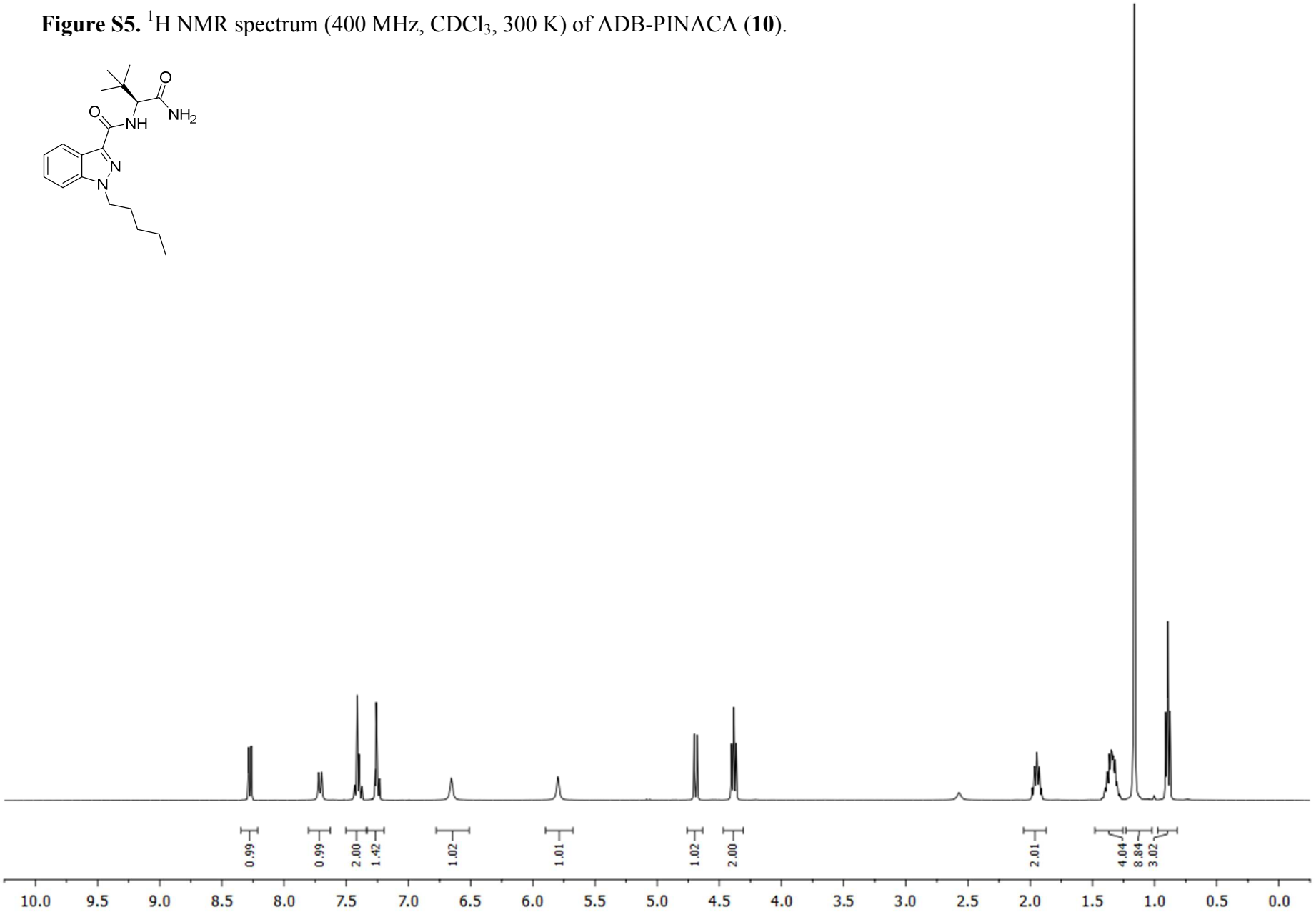


Figure S6. ^{13}C NMR spectrum (100 MHz, $CDCl_3$, 300 K) of ADB-PINACA (**10**).

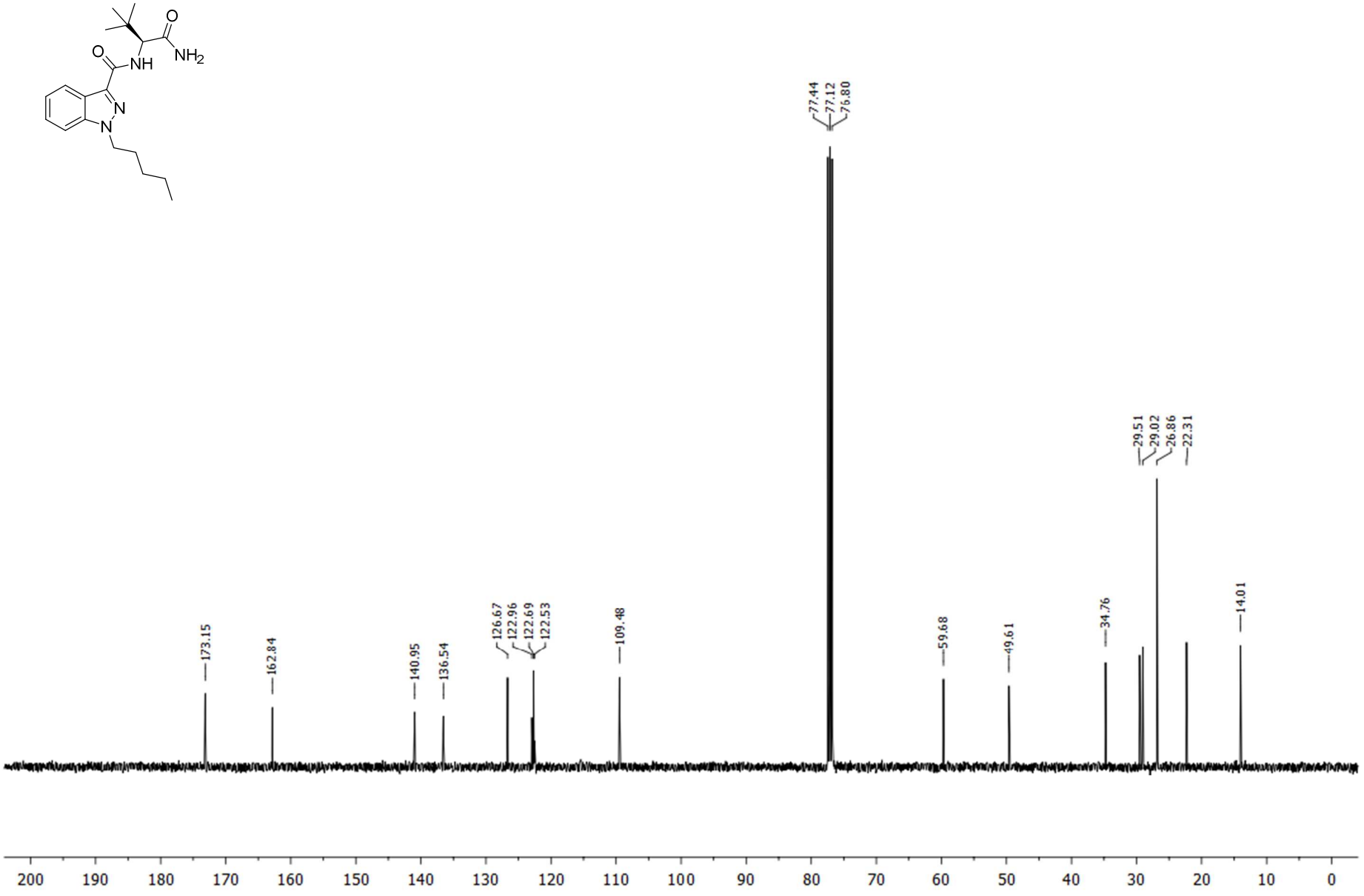
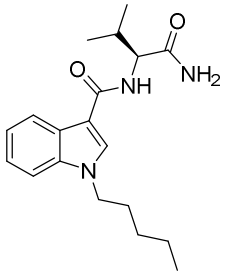


Figure S7. ^{1}H NMR spectrum (400 MHz, DMSO-d_6, 300 K) of AB-PICA (**15**).



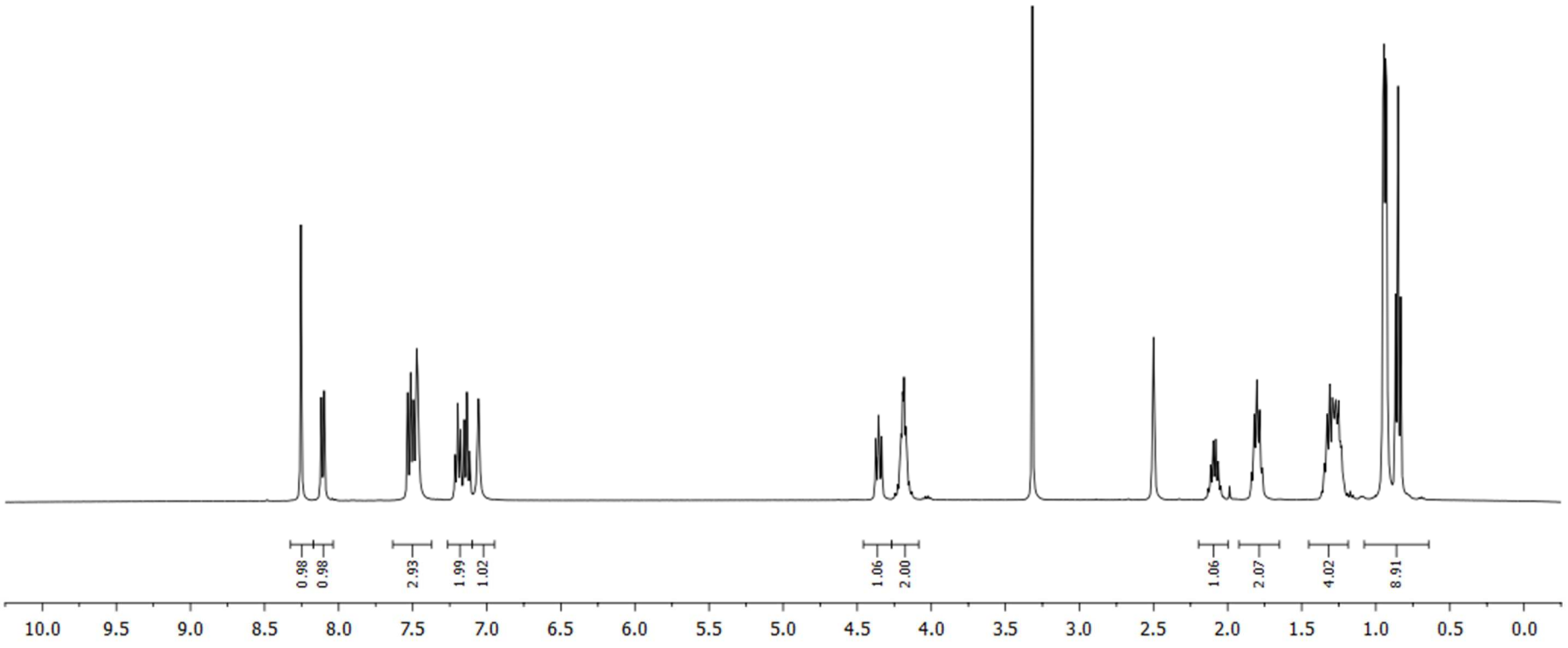


Figure S8. ^{13}C NMR spectrum (100 MHz, DMSO-d_6, 300 K) of AB-PICA (**15**).

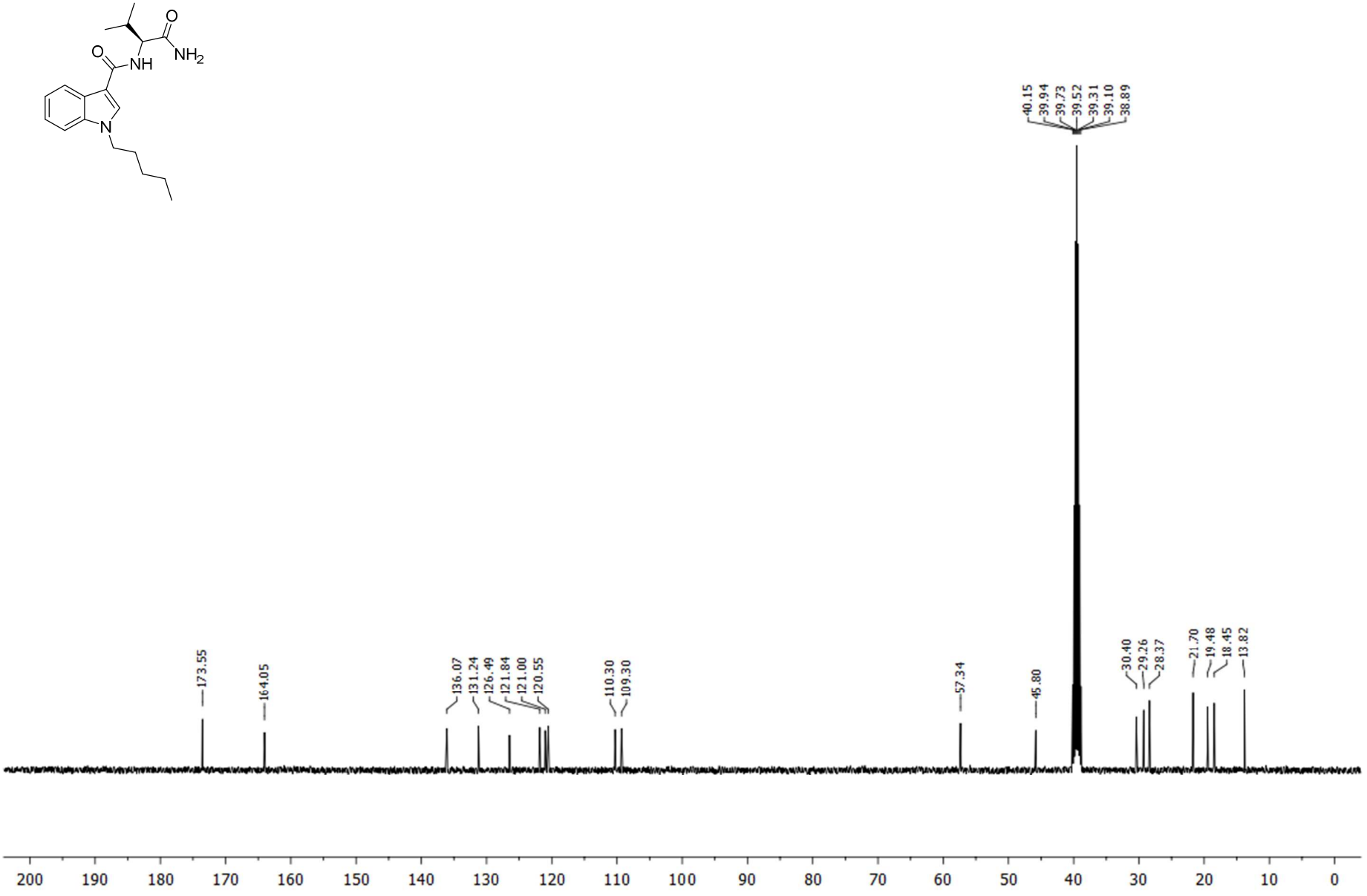


Figure S9. ^{1}H NMR spectrum (400 MHz, DMSO-d_6, 300 K) of 5F-AB-PICA (**17**).

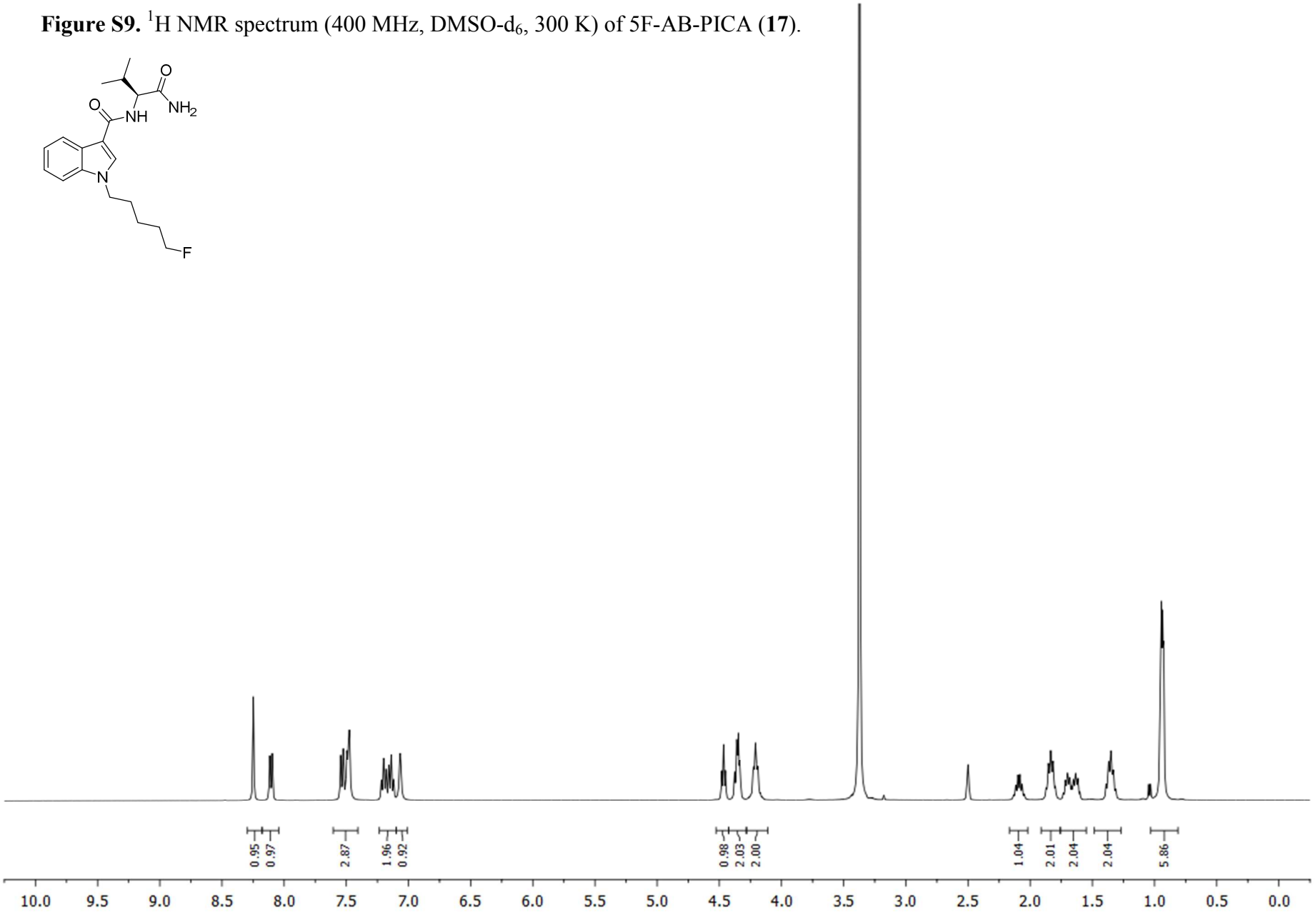
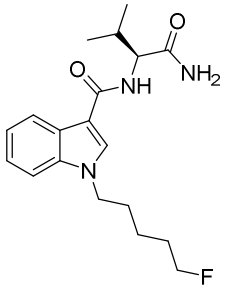


Figure S10. ^{13}C NMR spectrum (100 MHz, DMSO-d_6, 300 K) of 5F-AB-PICA (**17**).



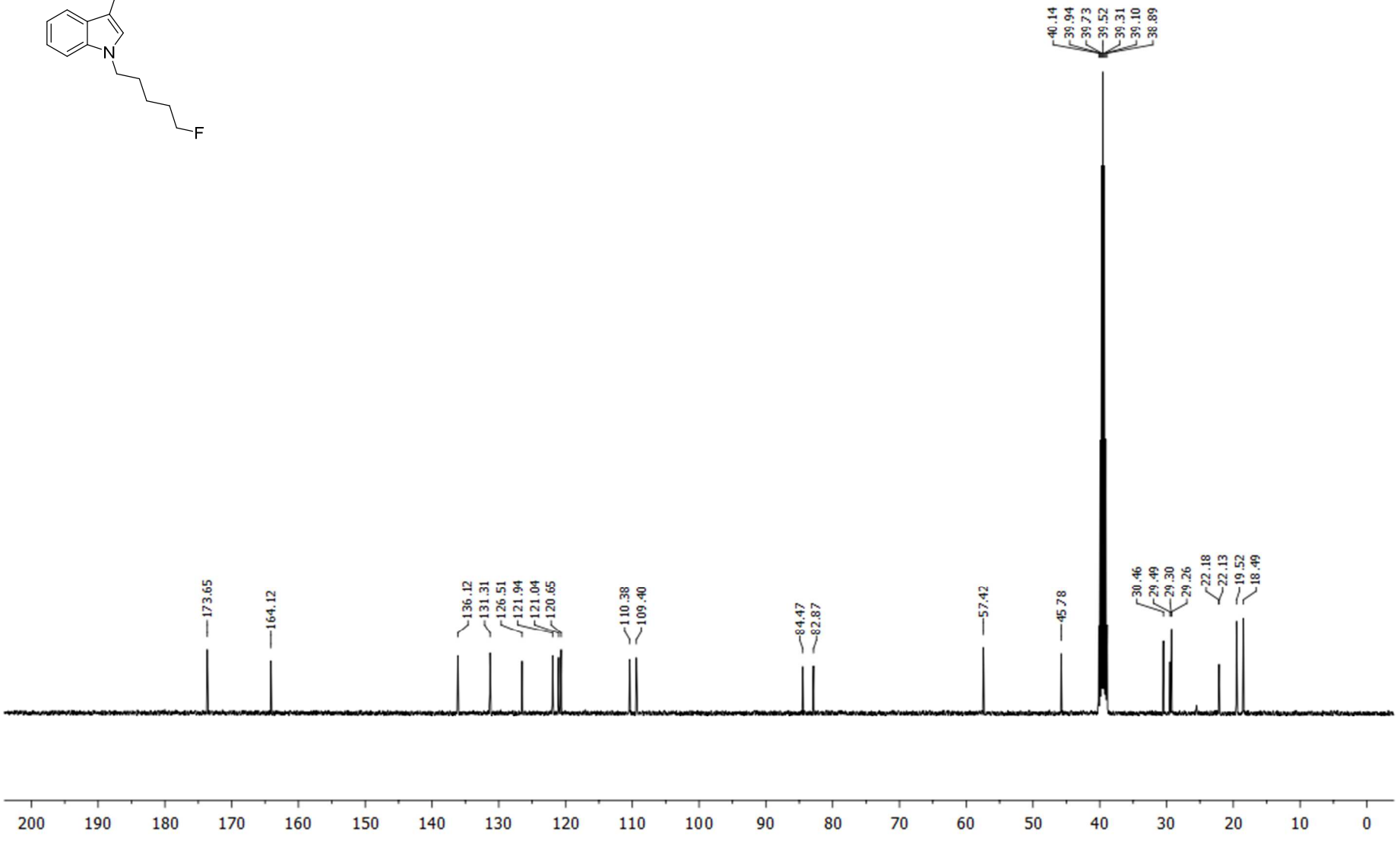


Figure S11. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 300 K) of 5F-ADBICA (**18**).

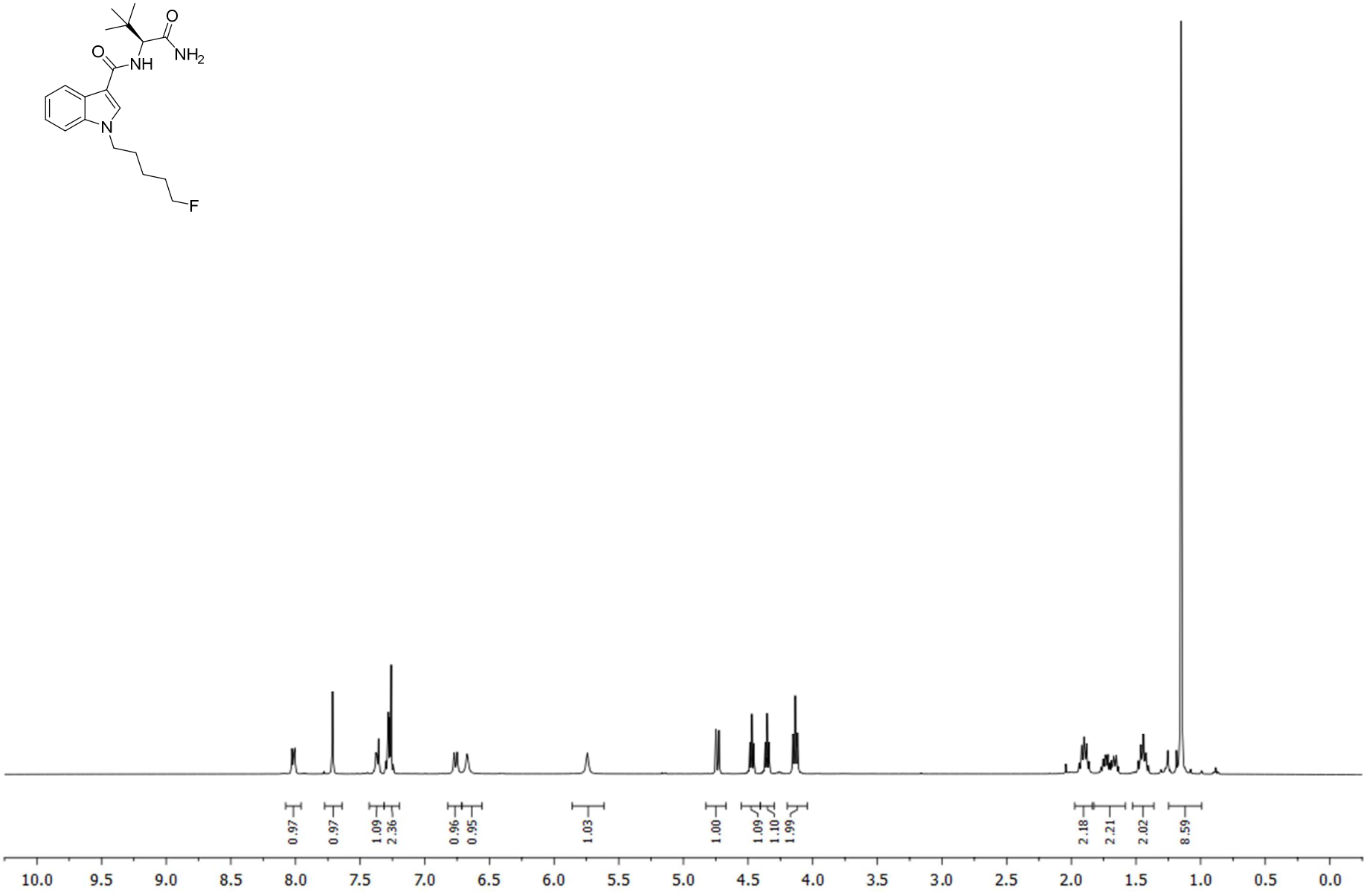


Figure S12. ^{13}C NMR spectrum (100 MHz, $CDCl_3$, 300 K) of 5F-ADBICA (**18**).

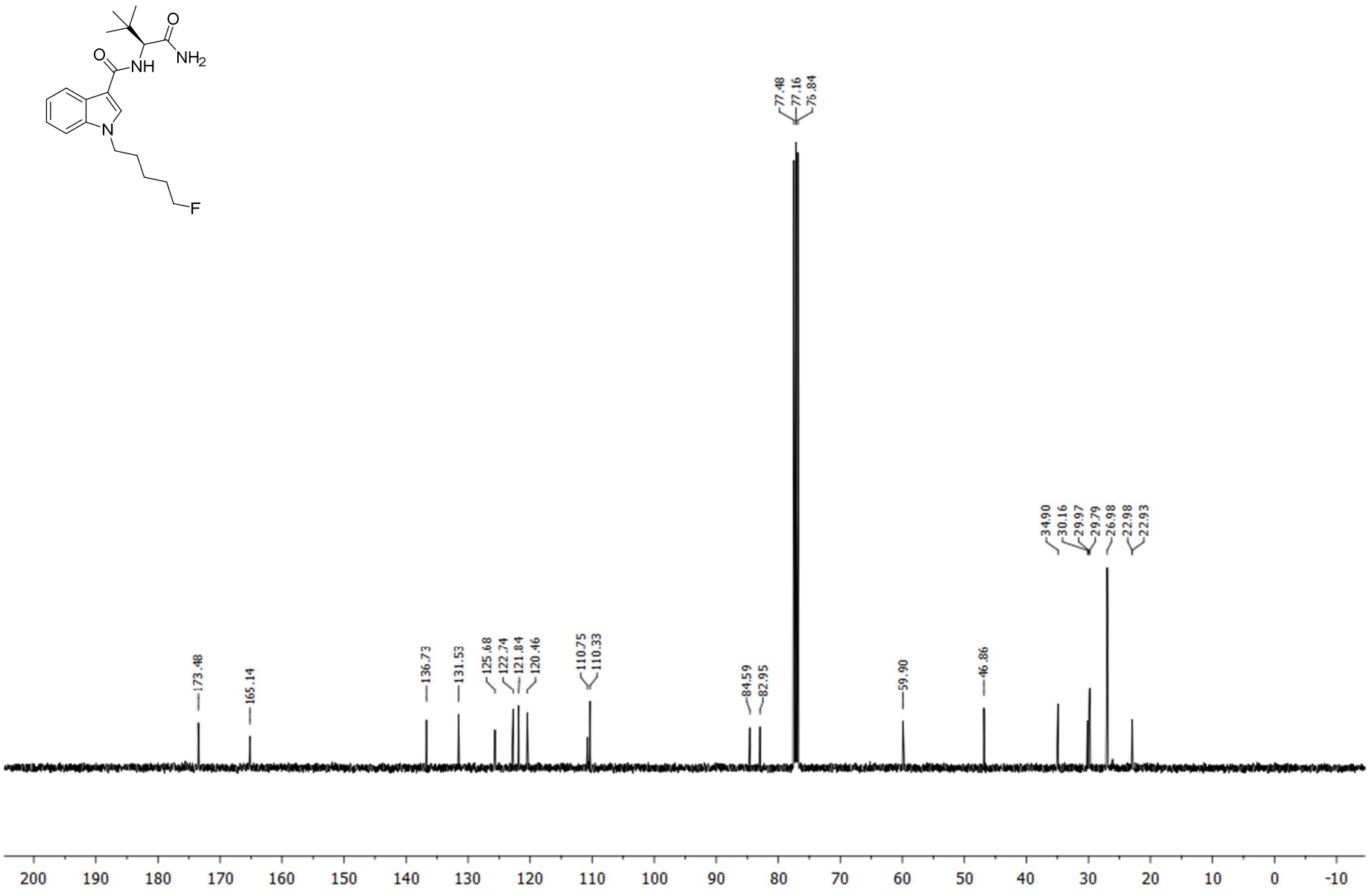


Figure S13. Mean area under the vehicle-vehicle baseline curve (AUC ± SEM) for body temperature for (A) AB-PINACA and (B) AB-FUBINACA (3 mg/kg), following pretreatment with vehicle, rimonabant (CB_1 antagonist, 3 mg/kg), or SR144528 (CB_2 antagonist, 3 mg/kg). The area was significantly reduced for both AB-PINACA and AB-FUBINACA by rimonabant but not SR144528. * $p < .05$ compared to vehicle.