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Dybek, M, Wallach, J, Kavanagh, PV, Colestock, T, Filbman, N, Dowling, G, Westphal, F, Elliott, SP, Adejare, A and Brandt, SD

Syntheses and analytical characterizations of the research chemical 1-[1-(2-fluorophenyl)-2-phenylethyl]pyrrolidine (fluorolintane) and five of its isomers

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Syntheses and analytical characterizations of the research chemical 1-[1-(2-fluorophenyl)-2-phenylethyl]pyrrolidine (fluorolintane) and five of its isomers

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^b Department of Pharmacology and Therapeutics, School of Medicine, Trinity Centre for Health Sciences, St. James's Hospital, James's Street, Dublin 8, D08W9RT, Ireland

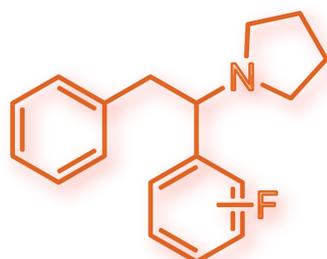
^c Department of Life Sciences, School of Science, Sligo Institute of Technology, Ash Lane, Sligo, F91YW50, Ireland

^d State Bureau of Criminal Investigation Schleswig-Holstein, Section Narcotics/Toxicology, Mühlenweg 166, D-24116 Kiel, Germany

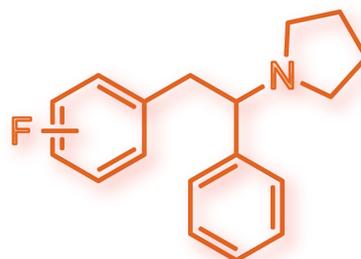
^e Elliott Forensic Consulting, Birmingham, UK

^f School of Pharmacy and Biomolecular Sciences, Liverpool John Moores University, Byrom Street, Liverpool, L3 3AF, UK

*Corresponding author: Simon D. Brandt, School of Pharmacy and Biomolecular Sciences, Liverpool John Moores University, Byrom Street, Liverpool, L3 3AF, UK. E-Mail: s.brandt@ljmu.ac.uk

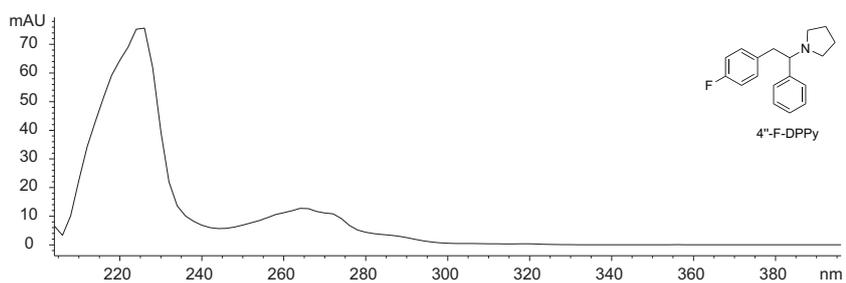
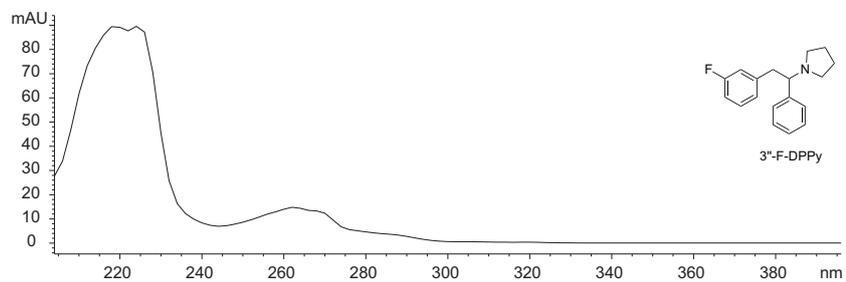
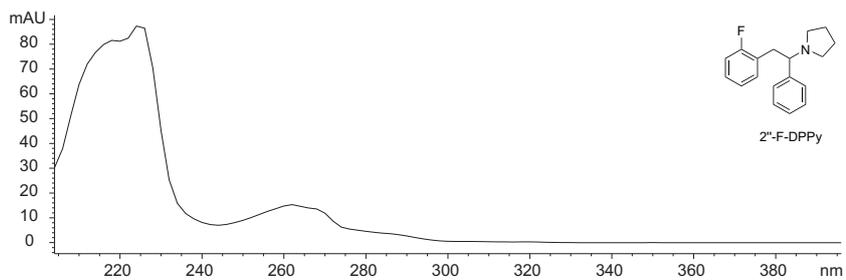
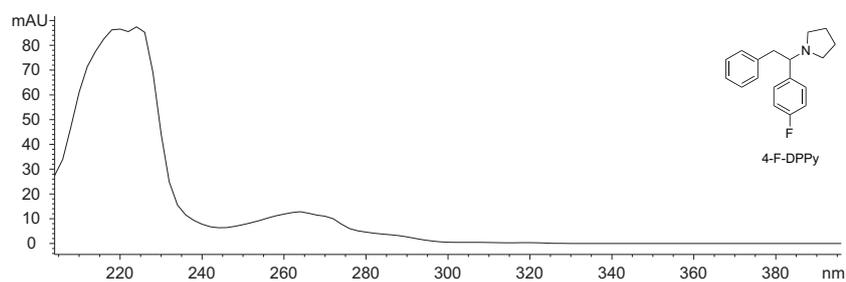
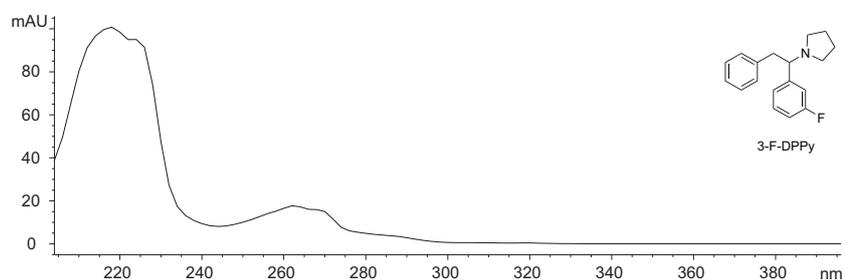
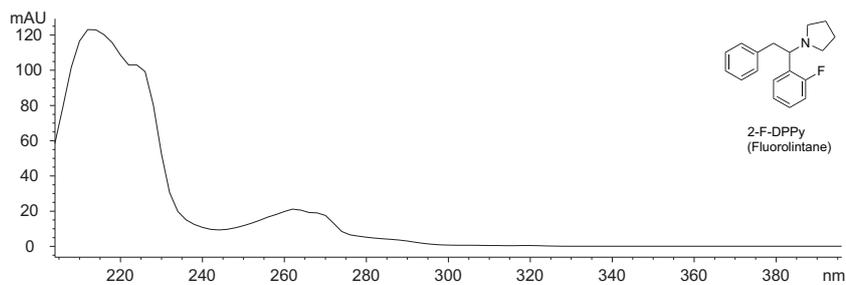


2-F: 2-F-DPPy (fluorolintane)
3-F: 3-F-DPPy
4-F: 4-F-DPPy



2-F: 2''-F-DPPy
3-F: 3''-F-DPPy
4-F: 4''-F-DPPy

Supporting Information – Drug Testing and Analysis

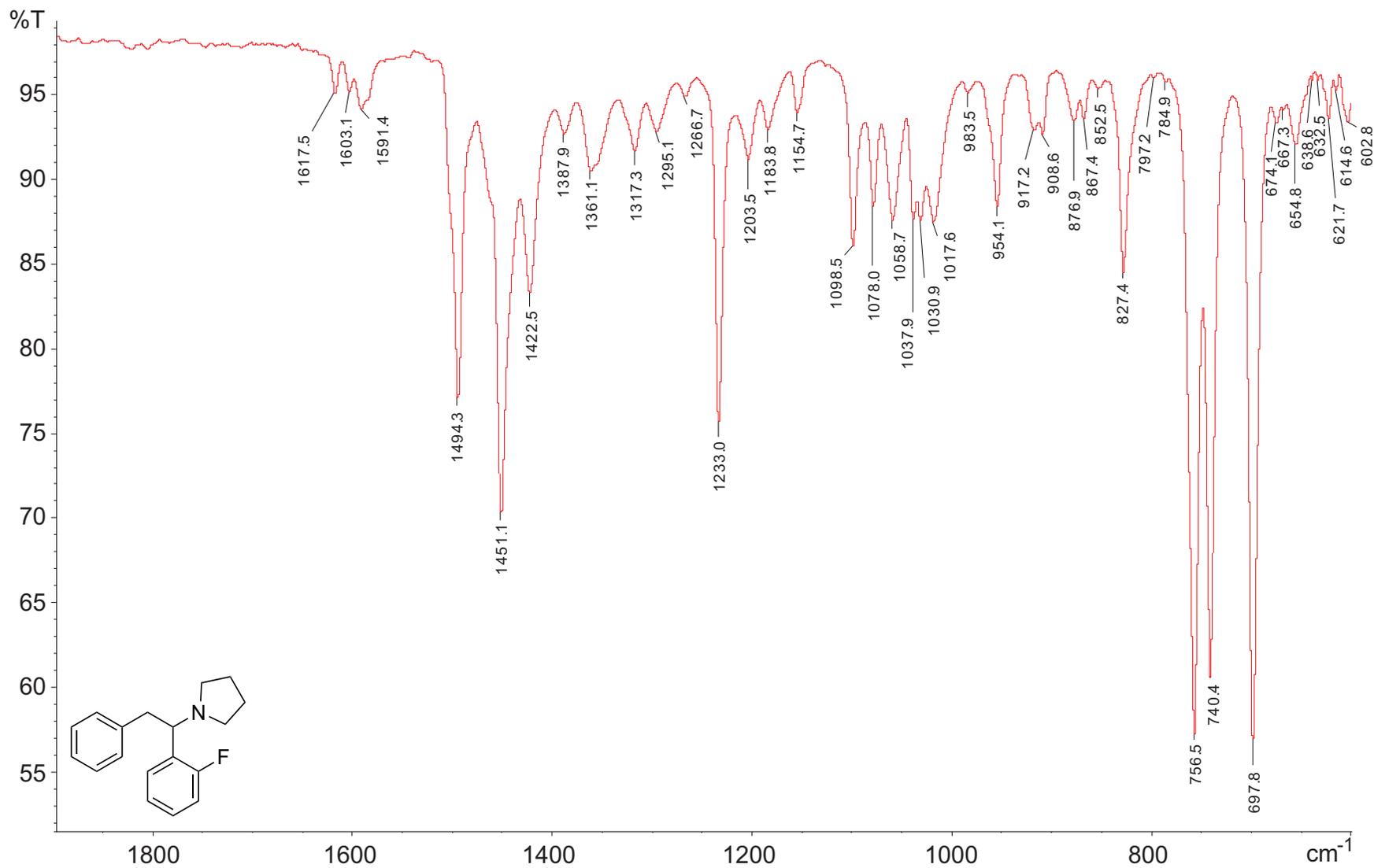


Supporting Information – Drug Testing and Analysis



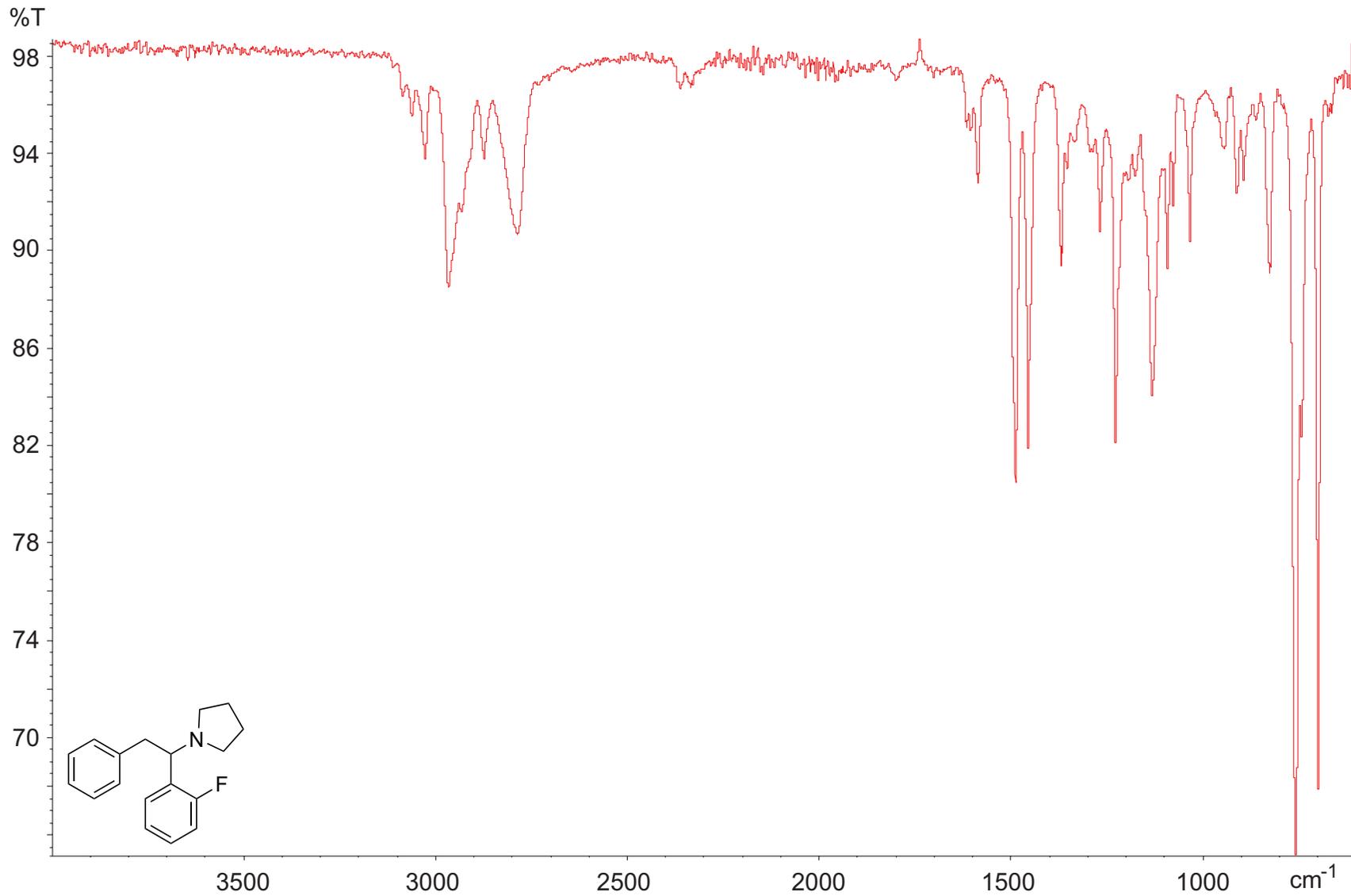
2-F-DPPy HCl (fluorolintane)
ATR-IR

Supporting Information – Drug Testing and Analysis



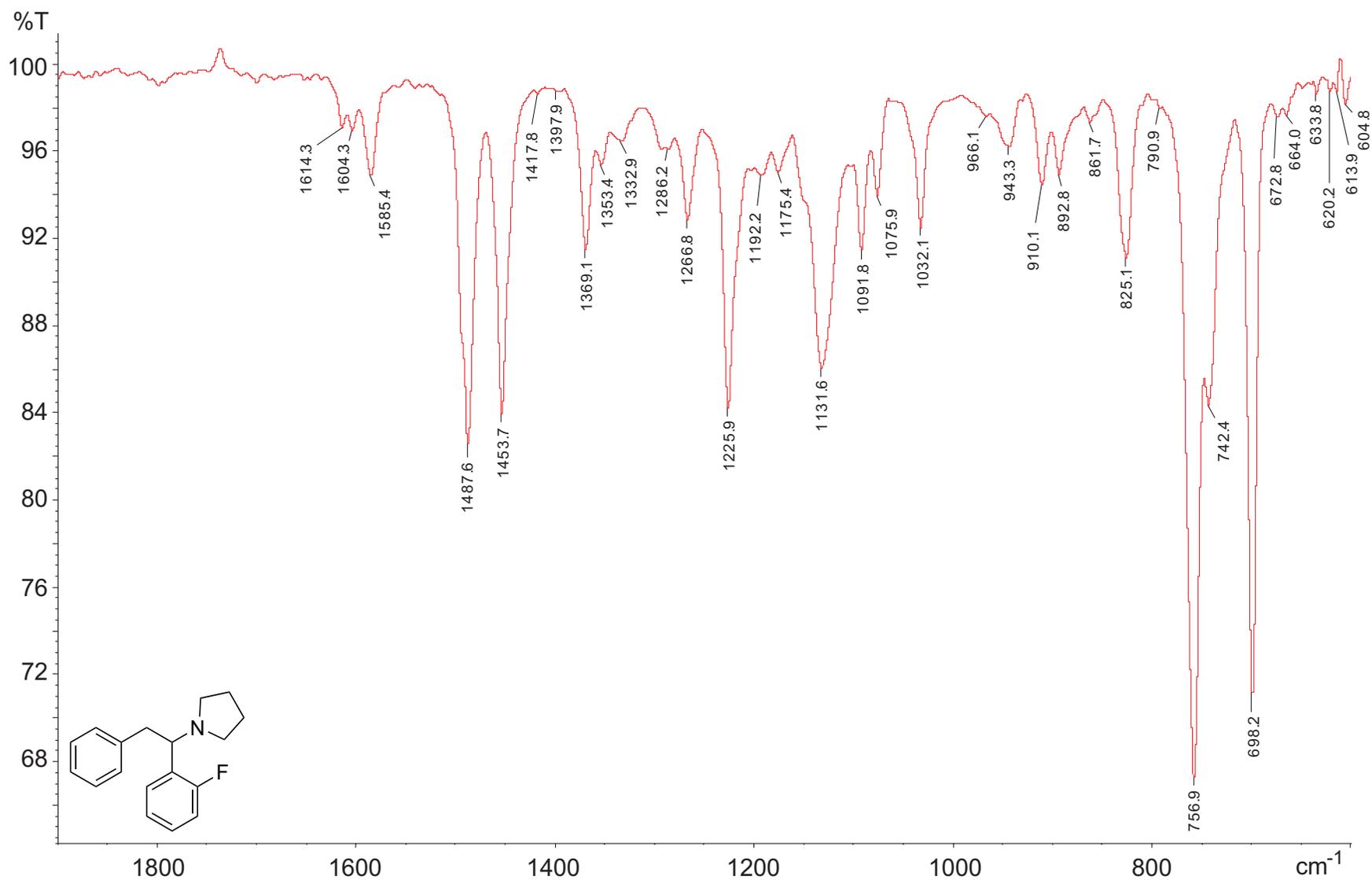
2-F-DPPy HCl (fluorolintane) (zoom)
ATR-IR

Supporting Information – Drug Testing and Analysis



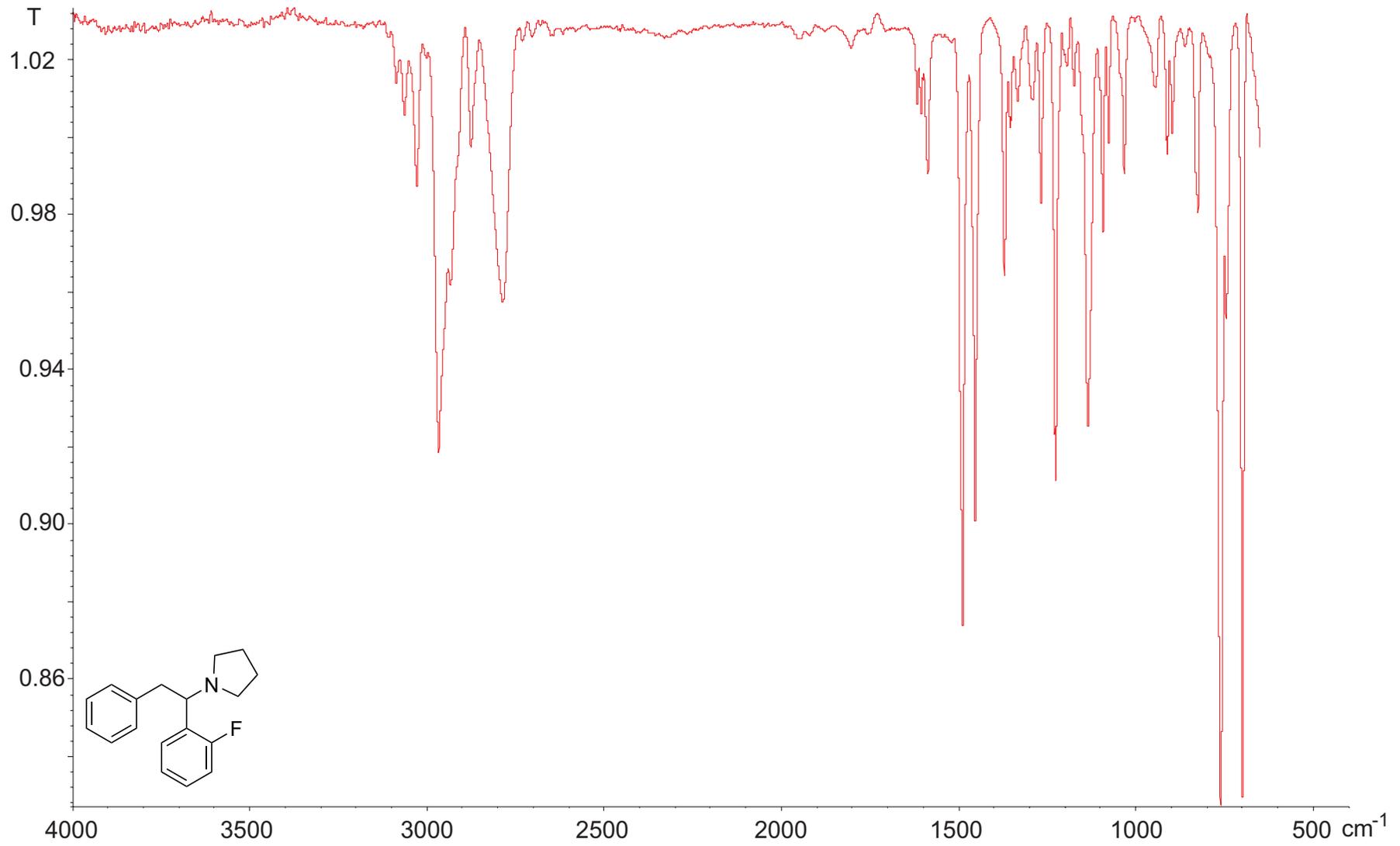
2-F-DPPy (fluorolintane) base
ATR-IR

Supporting Information – Drug Testing and Analysis



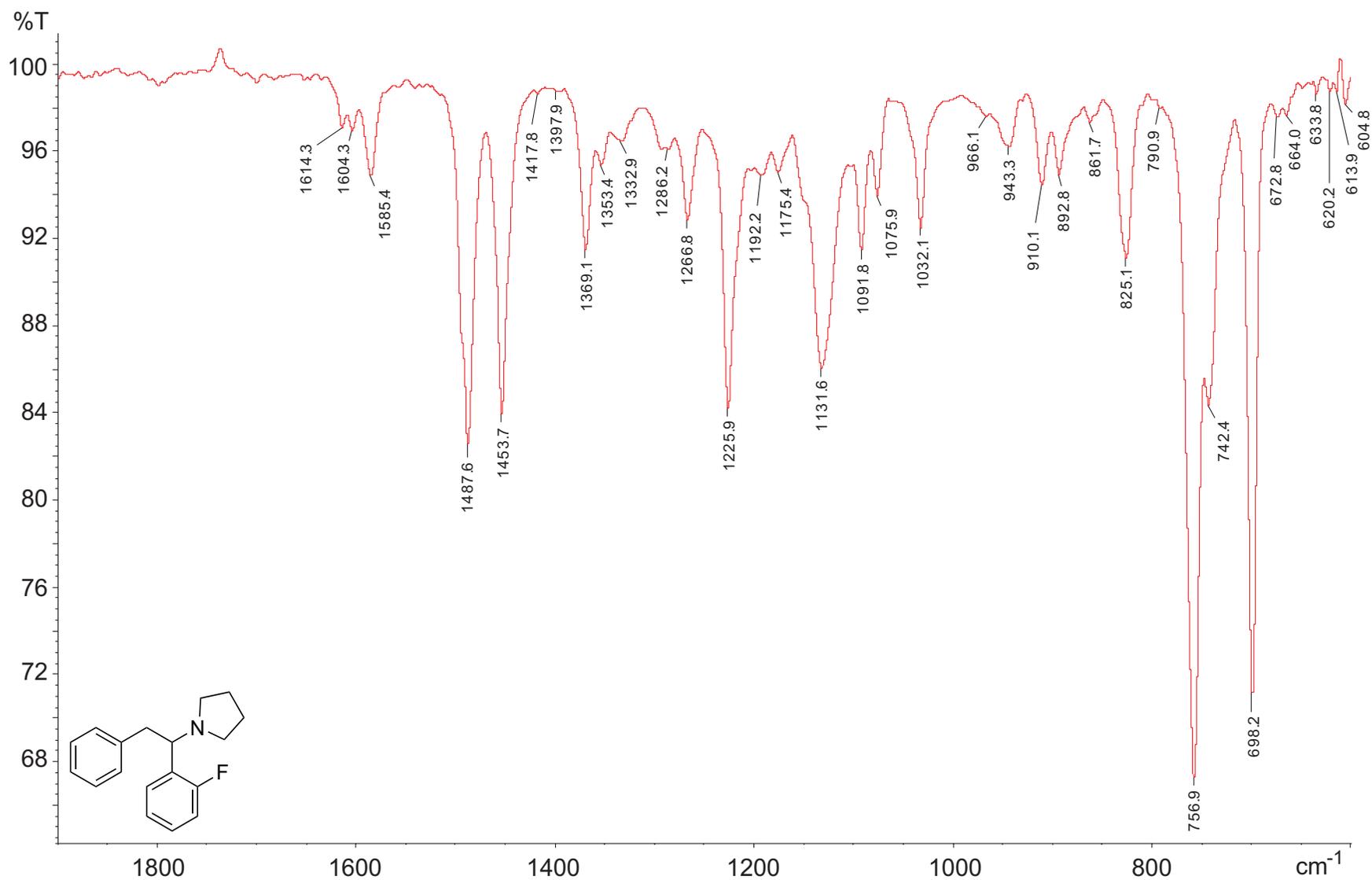
2-F-DPPy base (fluorolintane) (zoom)
ATR-IR

Supporting Information – Drug Testing and Analysis



2-F-DPPy (fluorolintane) GC-sIR

Supporting Information – Drug Testing and Analysis



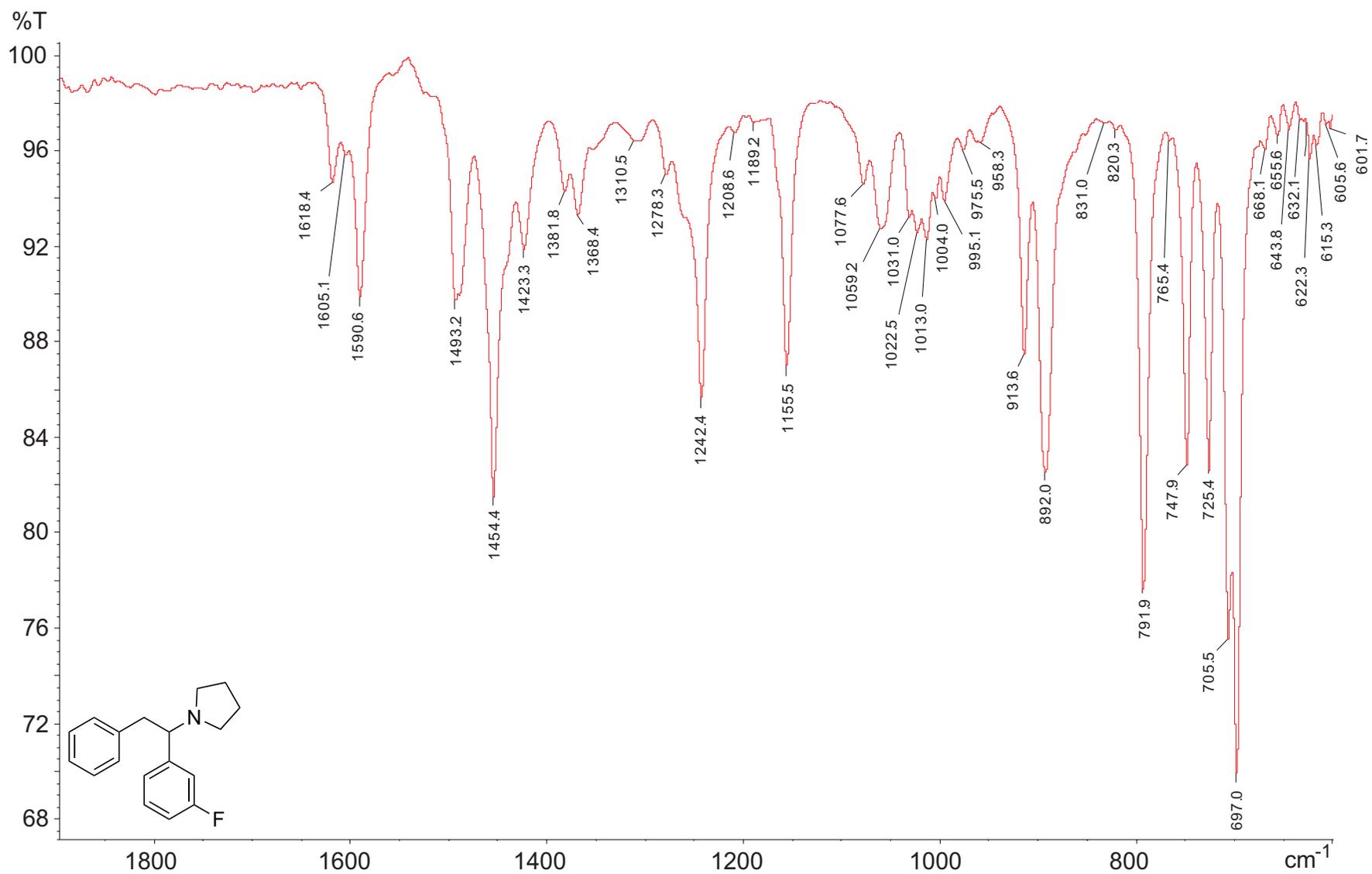
2-F-DPPy base (fluorolintane) (zoom)
ATR-IR

Supporting Information – Drug Testing and Analysis



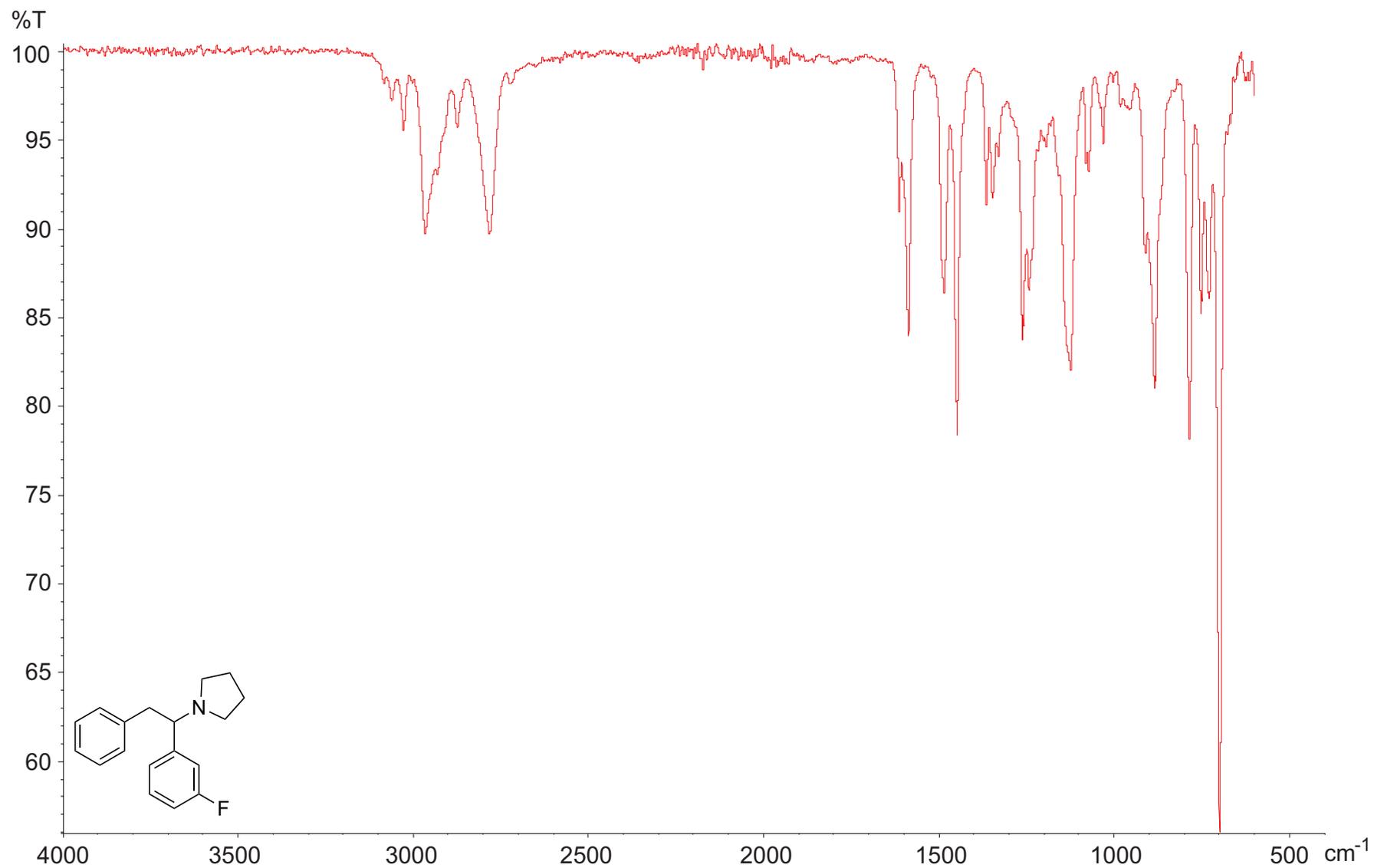
3-F-DPPy HCl
ATR-IR

Supporting Information – Drug Testing and Analysis



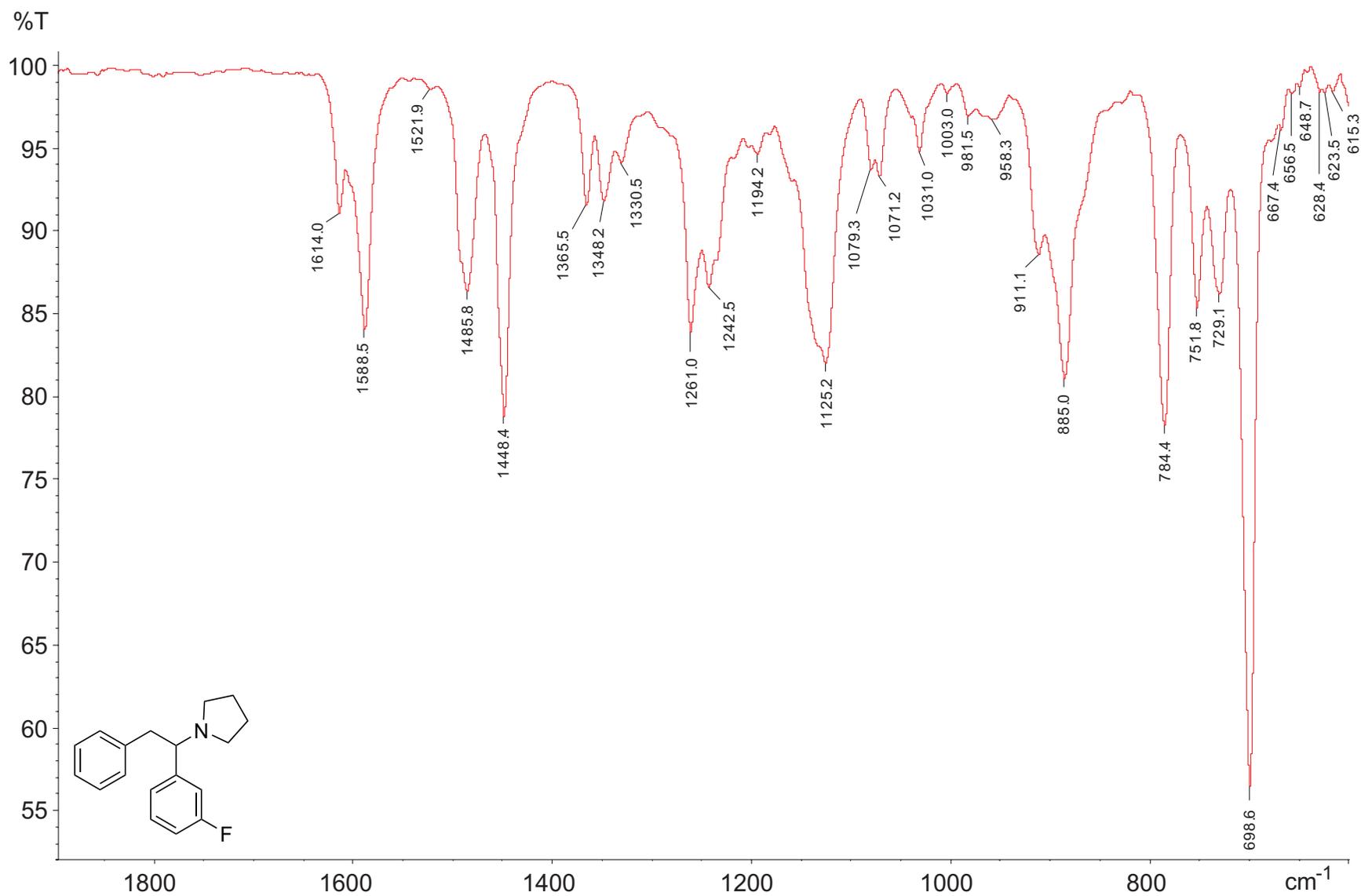
3-F-DPPy HCl (zoom)
ATR-IR

Supporting Information – Drug Testing and Analysis



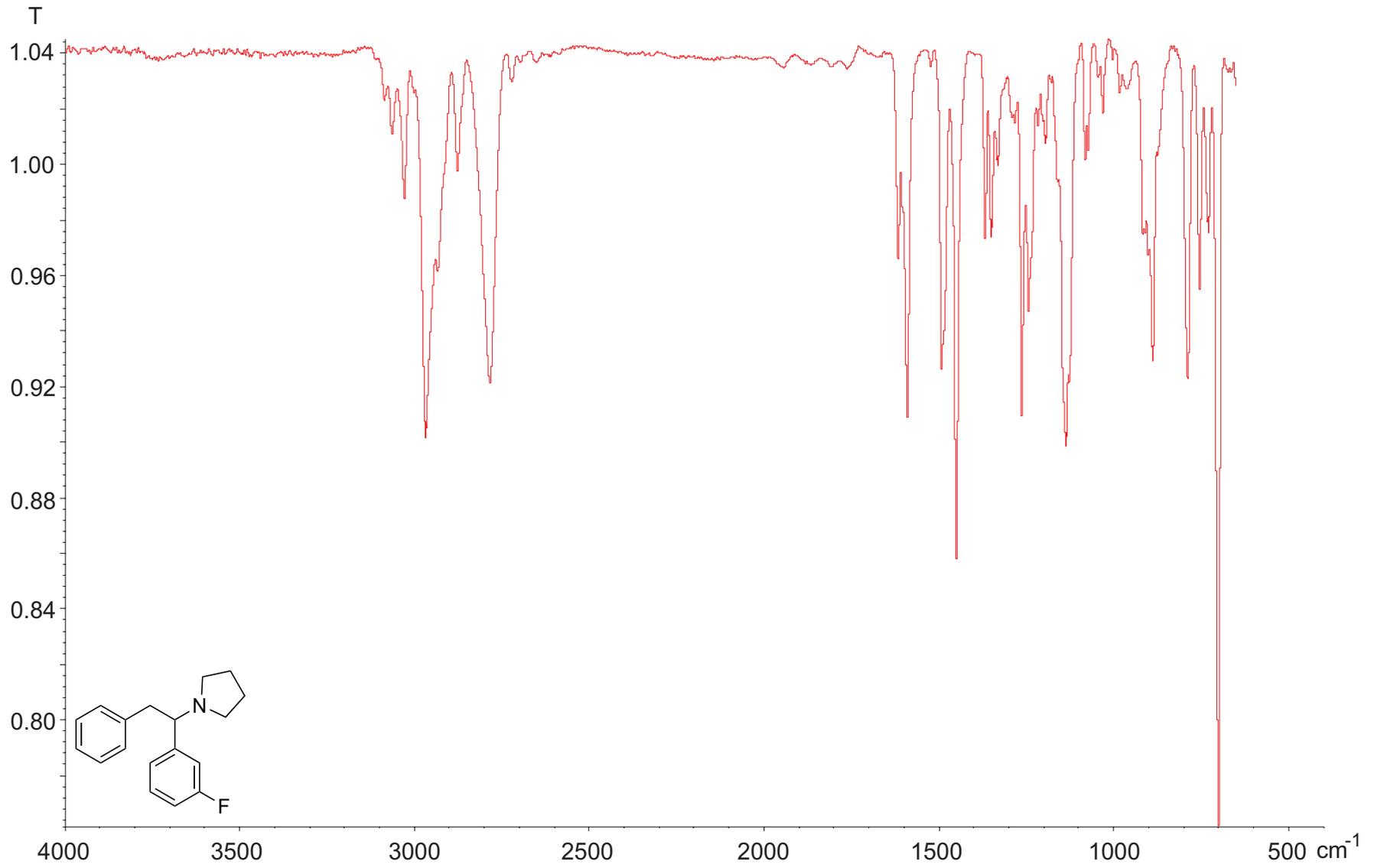
3-F-DPPy base
ATR-IR

Supporting Information – Drug Testing and Analysis



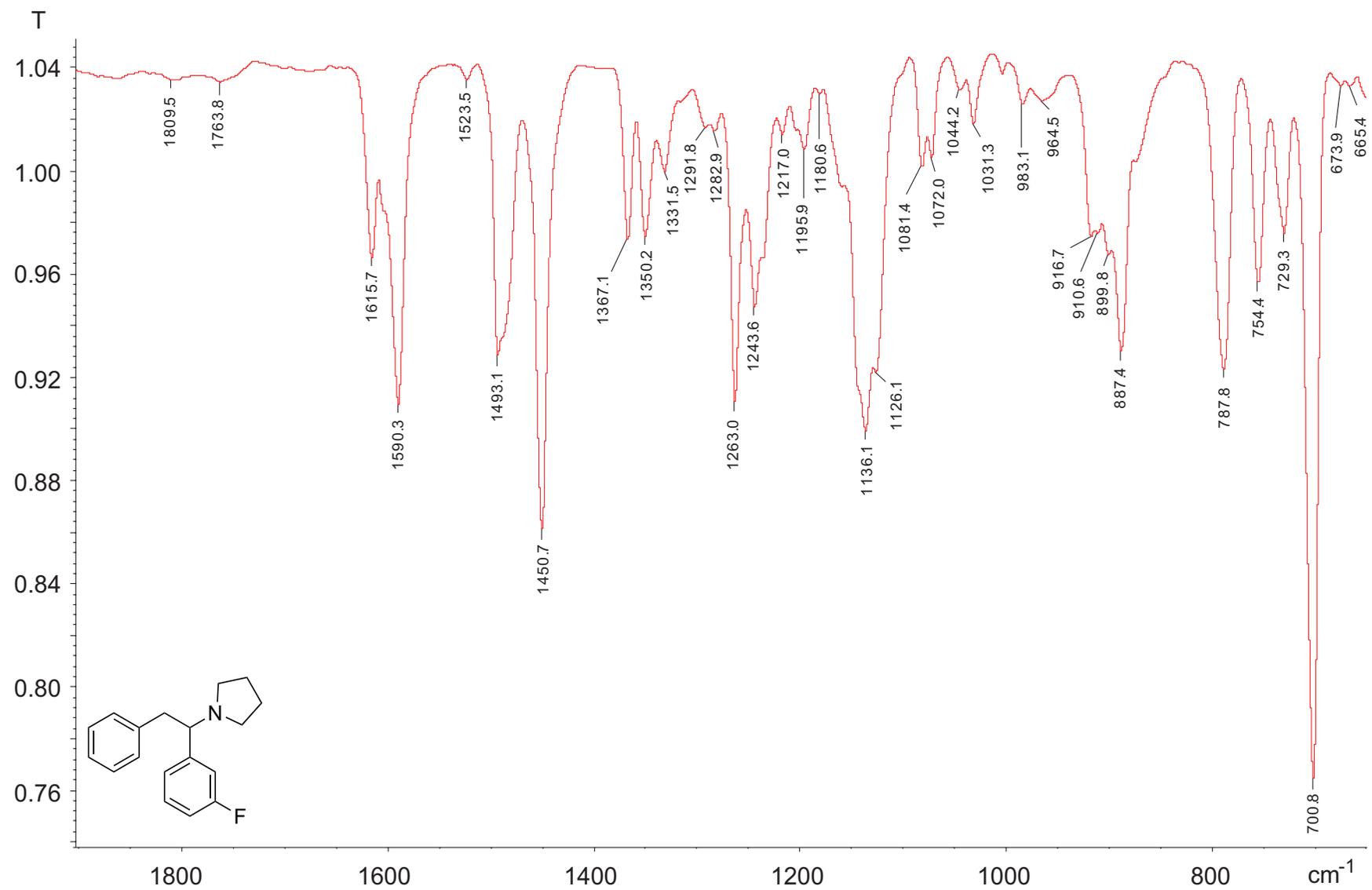
3-F-DPPy base (zoom)
ATR-IR

Supporting Information – Drug Testing and Analysis



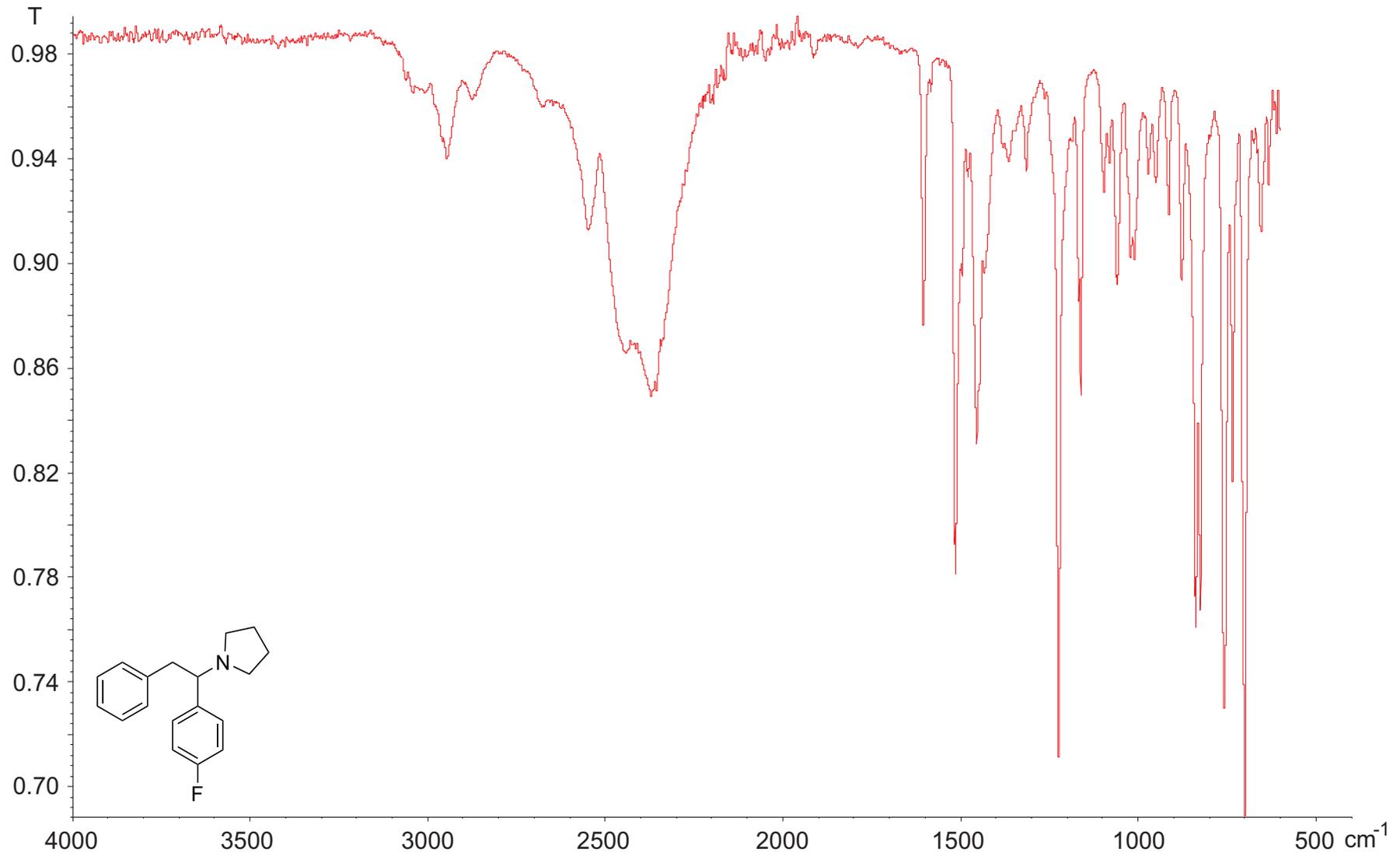
3-F-DPPy GC-sIR

Supporting Information – Drug Testing and Analysis



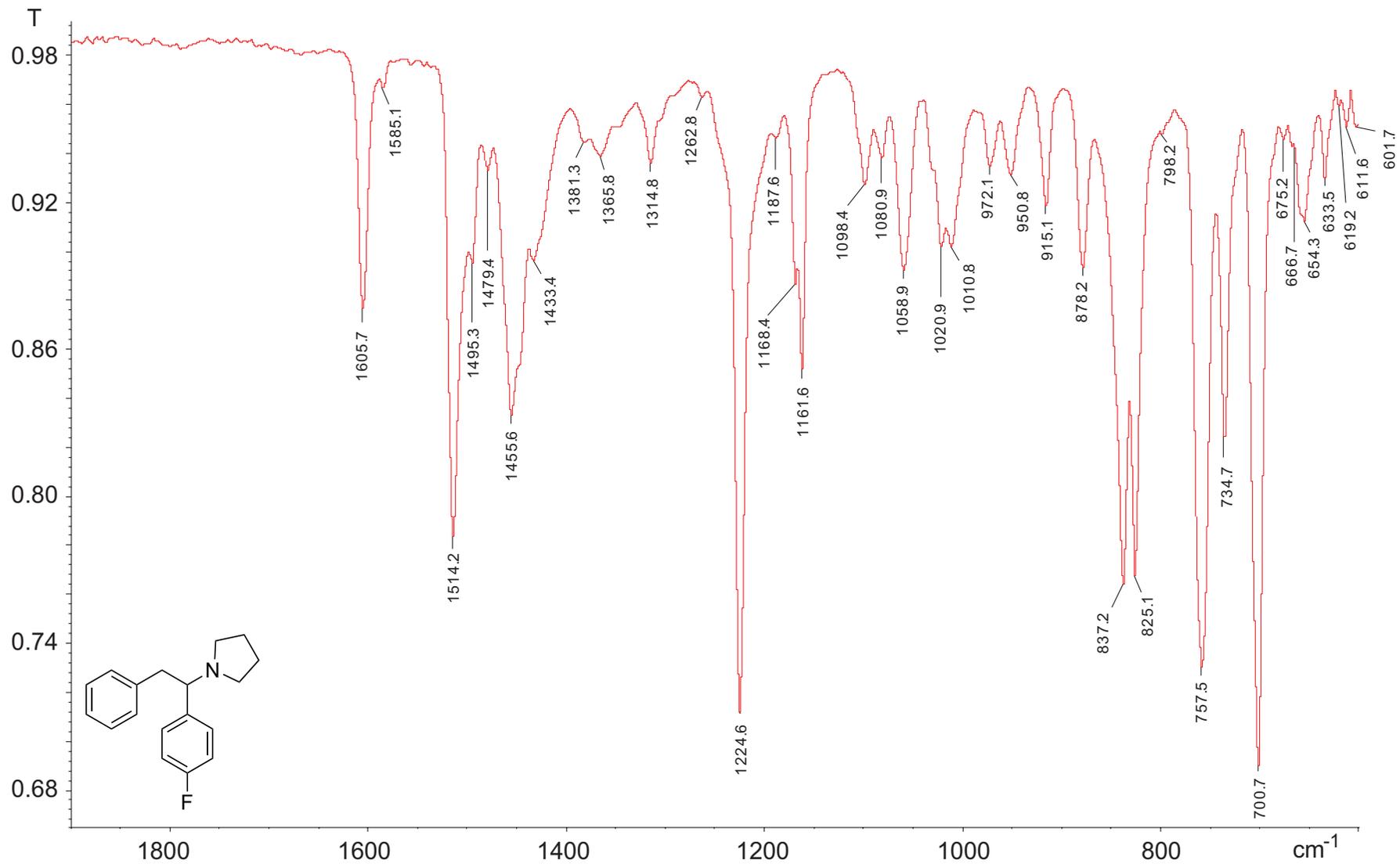
3-F-DPPy GC-sIR (zoom)

Supporting Information – Drug Testing and Analysis



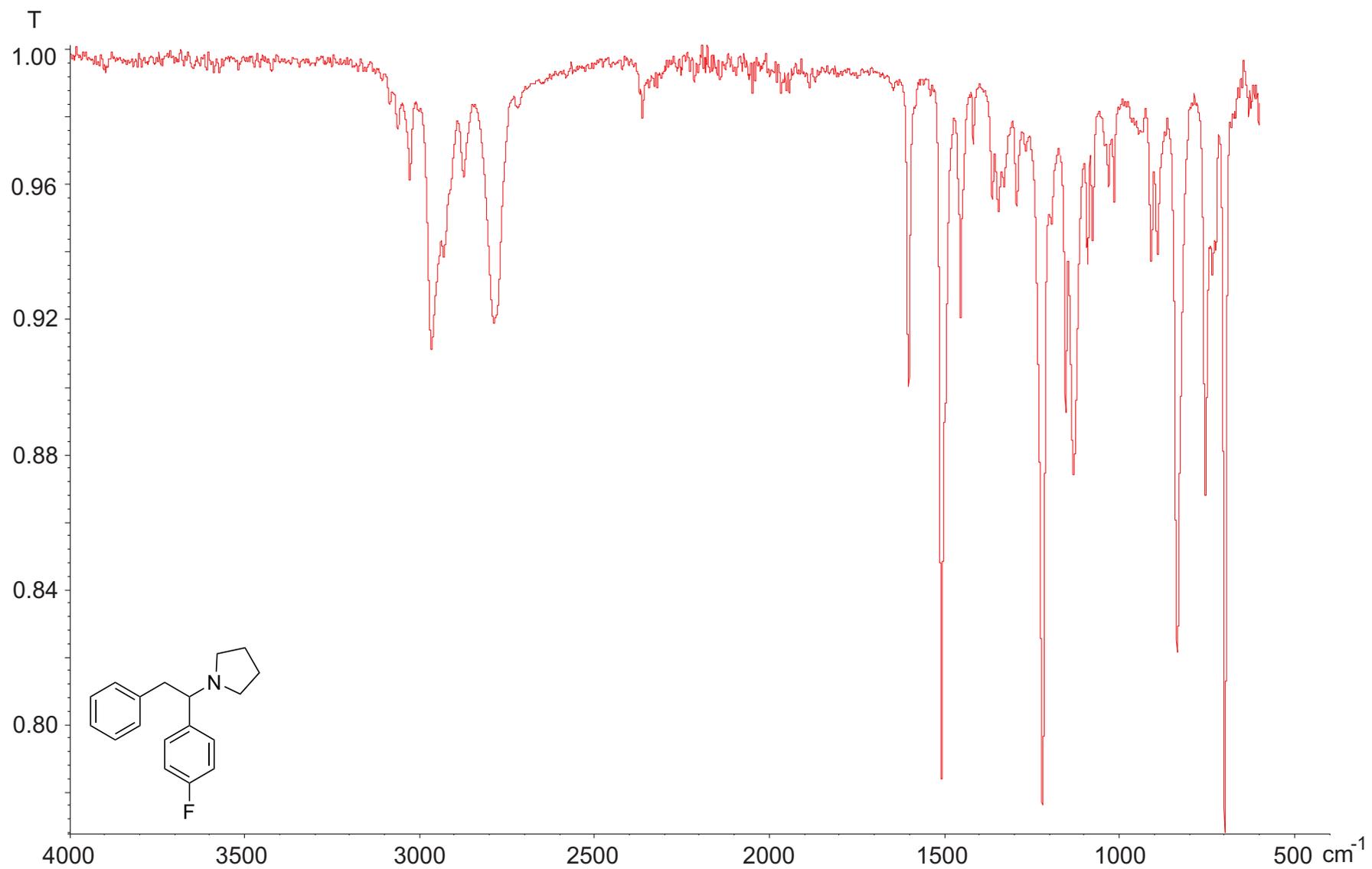
4-F-DPPy HCl
ATR-IR

Supporting Information – Drug Testing and Analysis



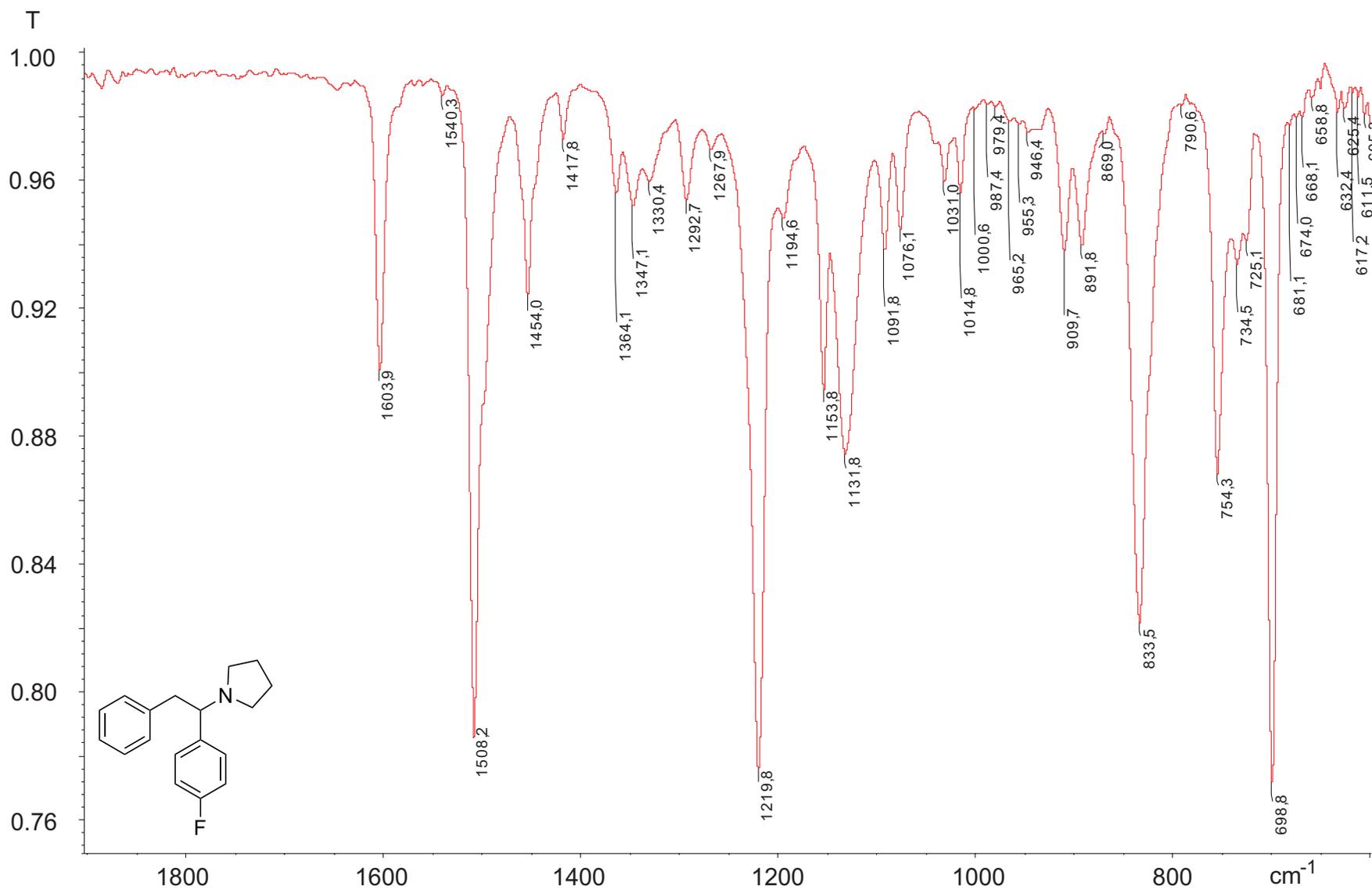
4-F-DPPy HCl (zoom)
ATR-IR

Supporting Information – Drug Testing and Analysis



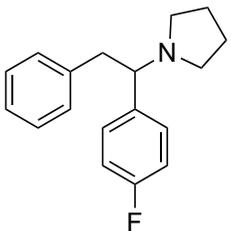
4-F-DPPy base
ATR-IR

Supporting Information – Drug Testing and Analysis



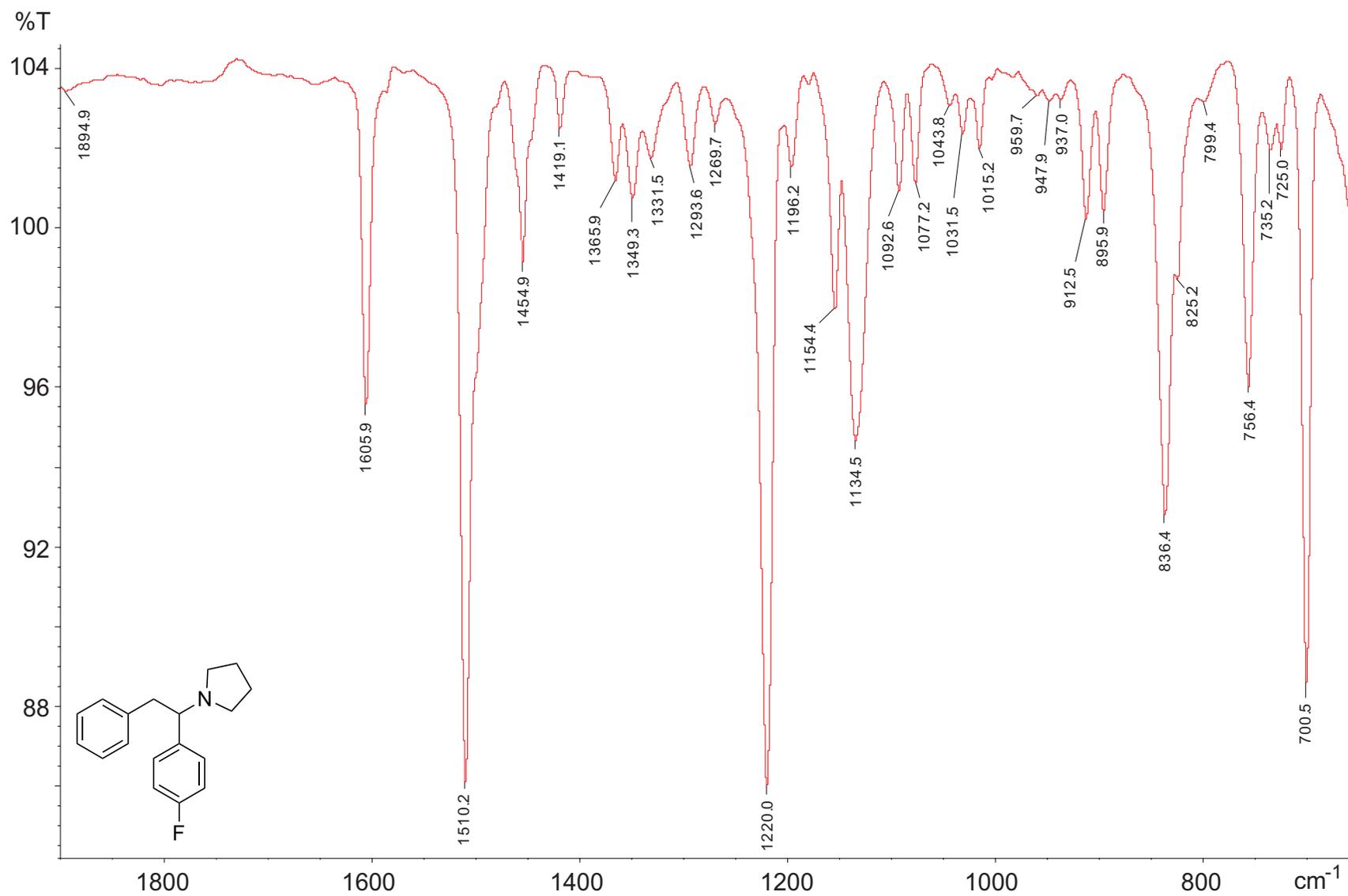
4-F-DPPy base (zoom)
ATR-IR

Supporting Information – Drug Testing and Analysis



4-F-DPPy GC-sIR

Supporting Information – Drug Testing and Analysis



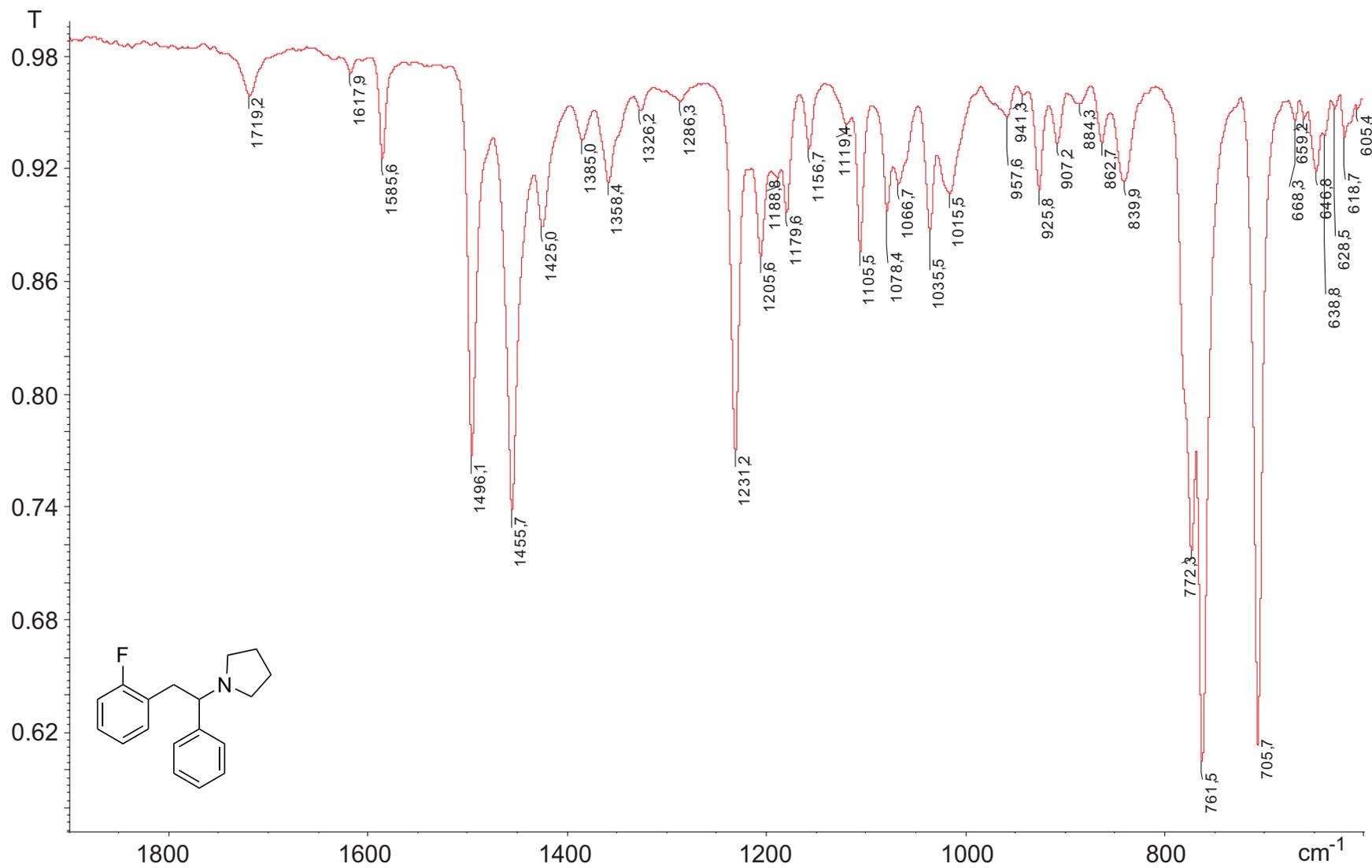
4-F-DPPy GC-sIR (zoom)

Supporting Information – Drug Testing and Analysis



2''-F-DPPy HCl
ATR-IR

Supporting Information – Drug Testing and Analysis



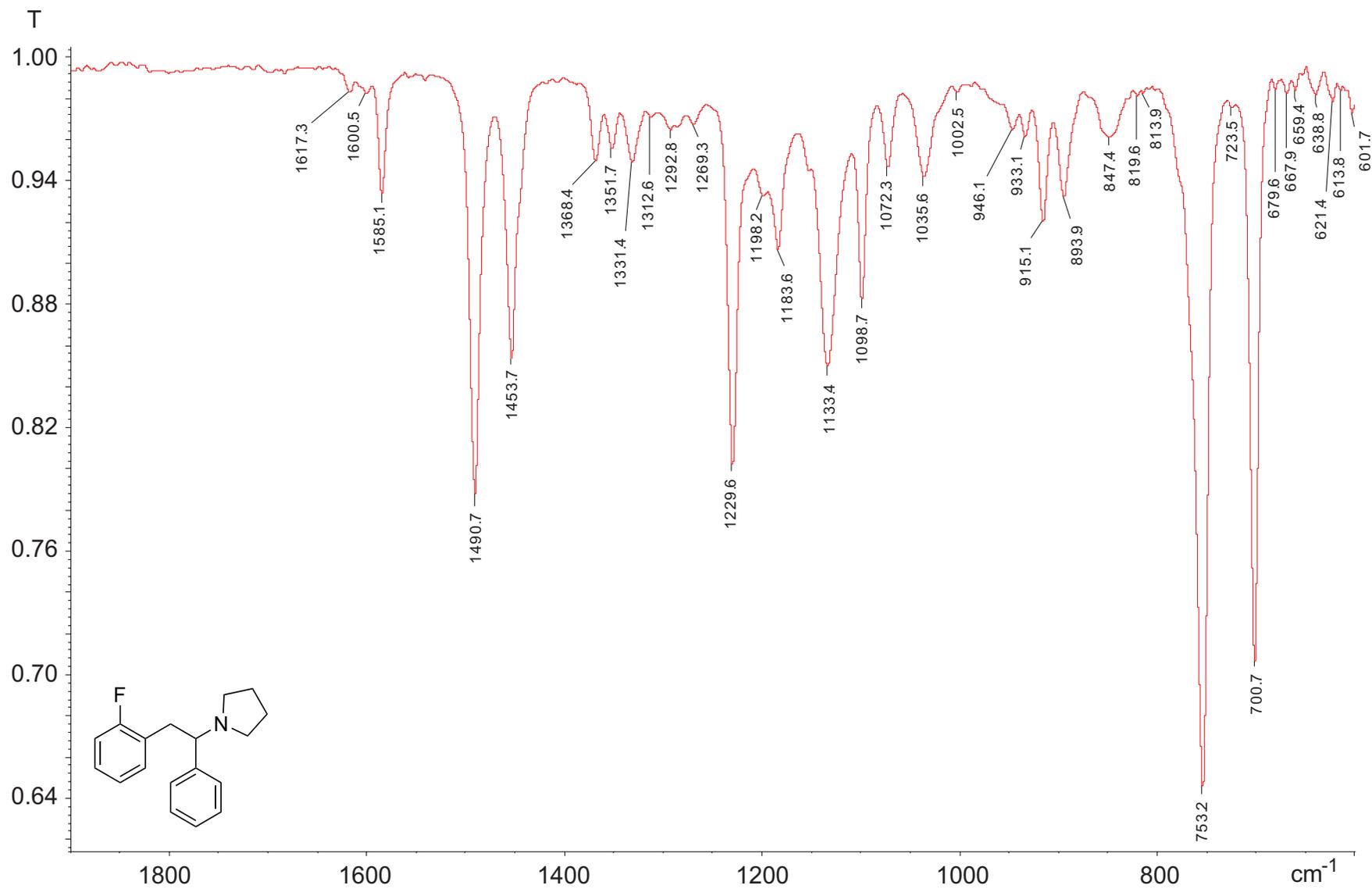
2''-F-DPPy HCl (zoom)
ATR-IR

Supporting Information – Drug Testing and Analysis



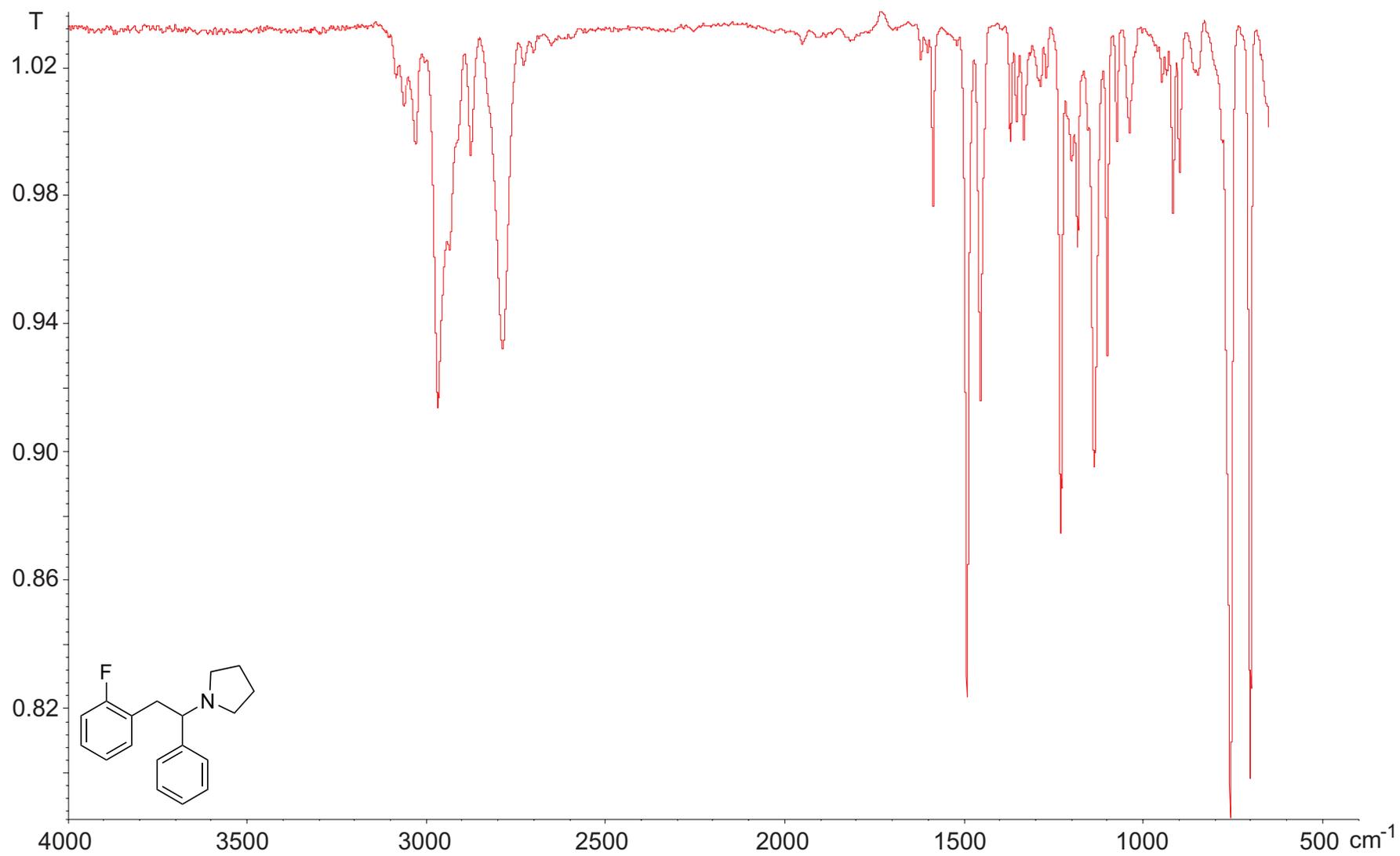
2''-F-DPPy base
ATR-IR

Supporting Information – Drug Testing and Analysis



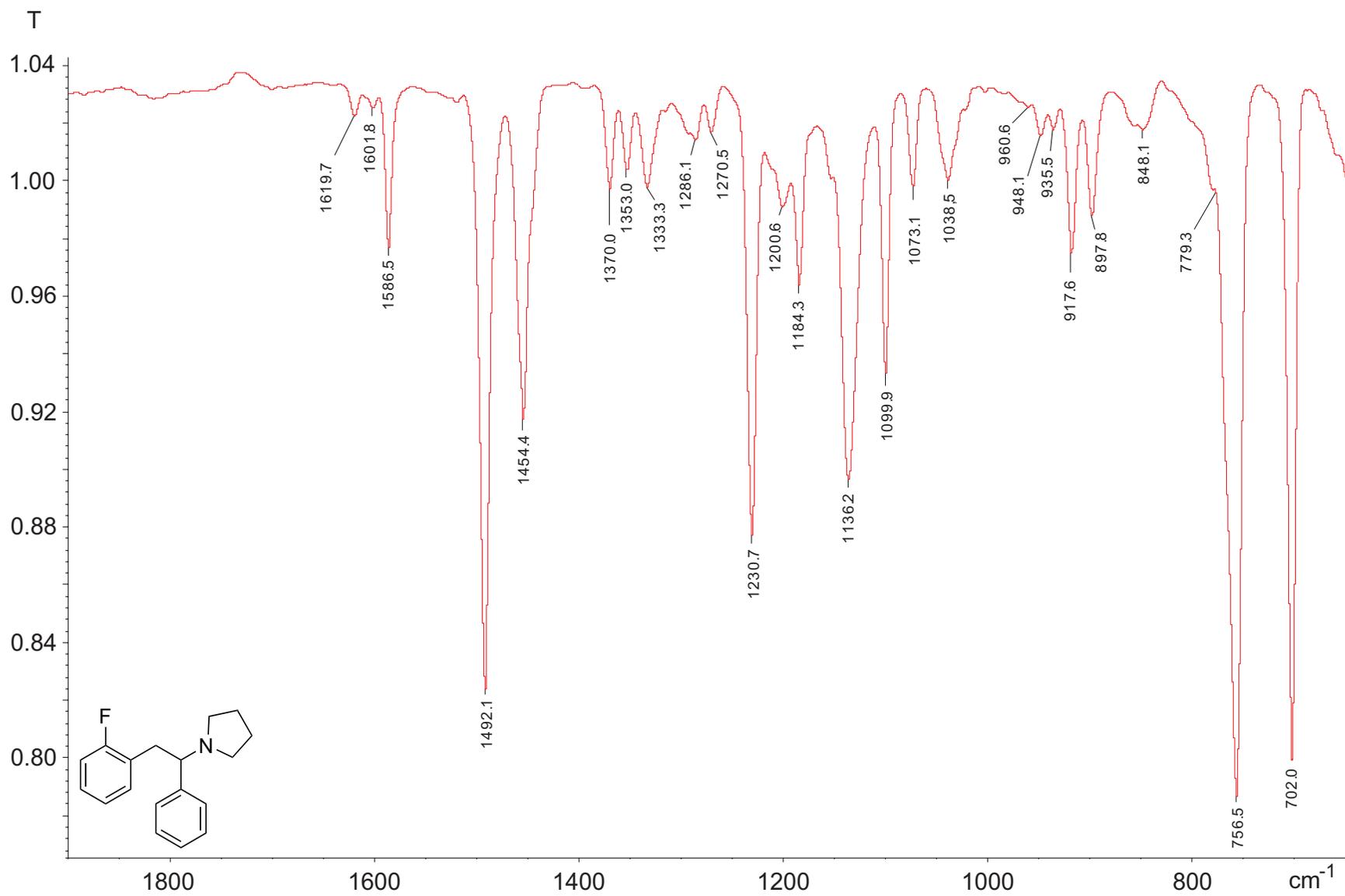
2''-F-DPPy base (zoom)
ATR-IR

Supporting Information – Drug Testing and Analysis



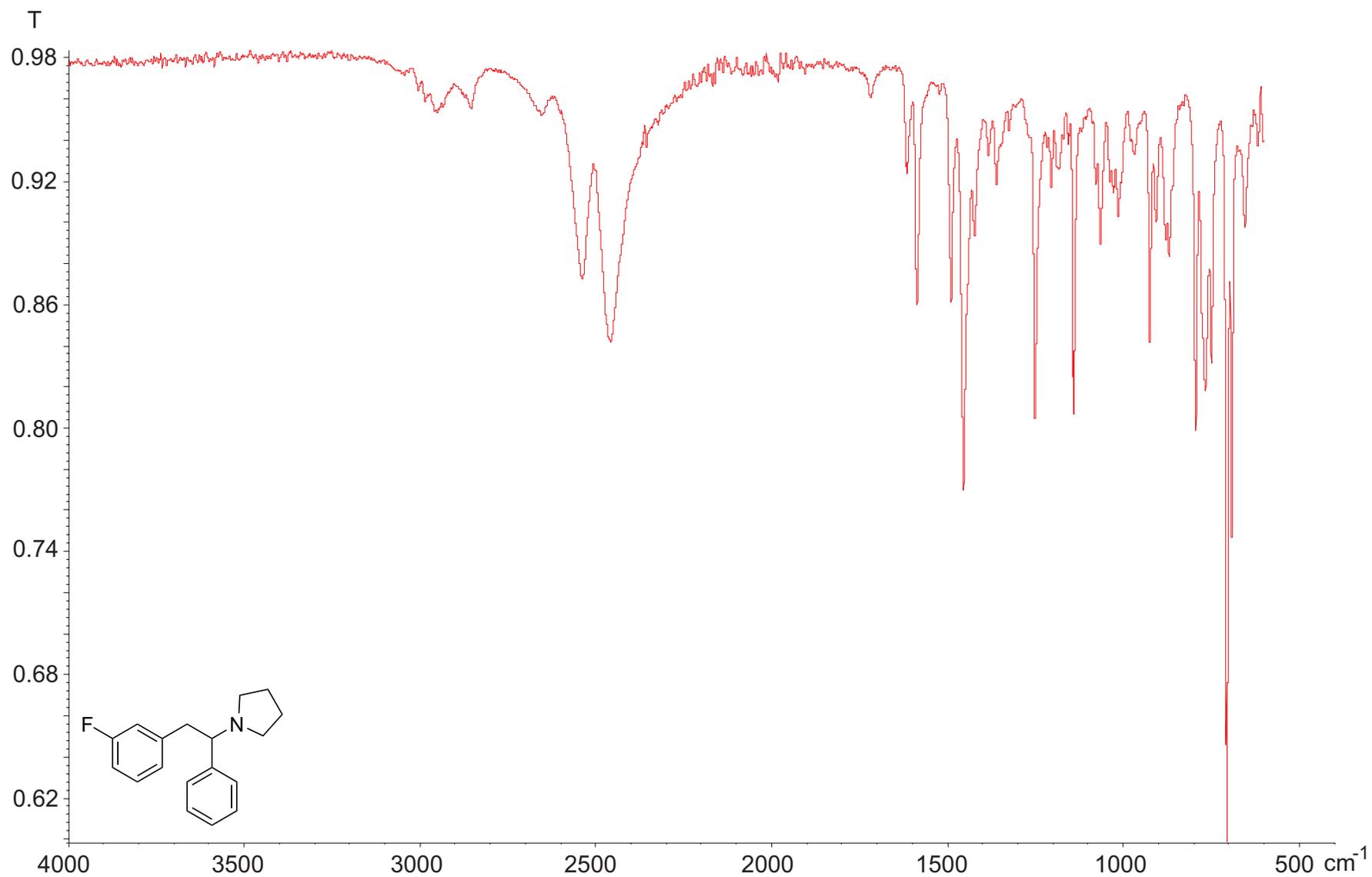
2''-F-DPPy GC-sIR

Supporting Information – Drug Testing and Analysis



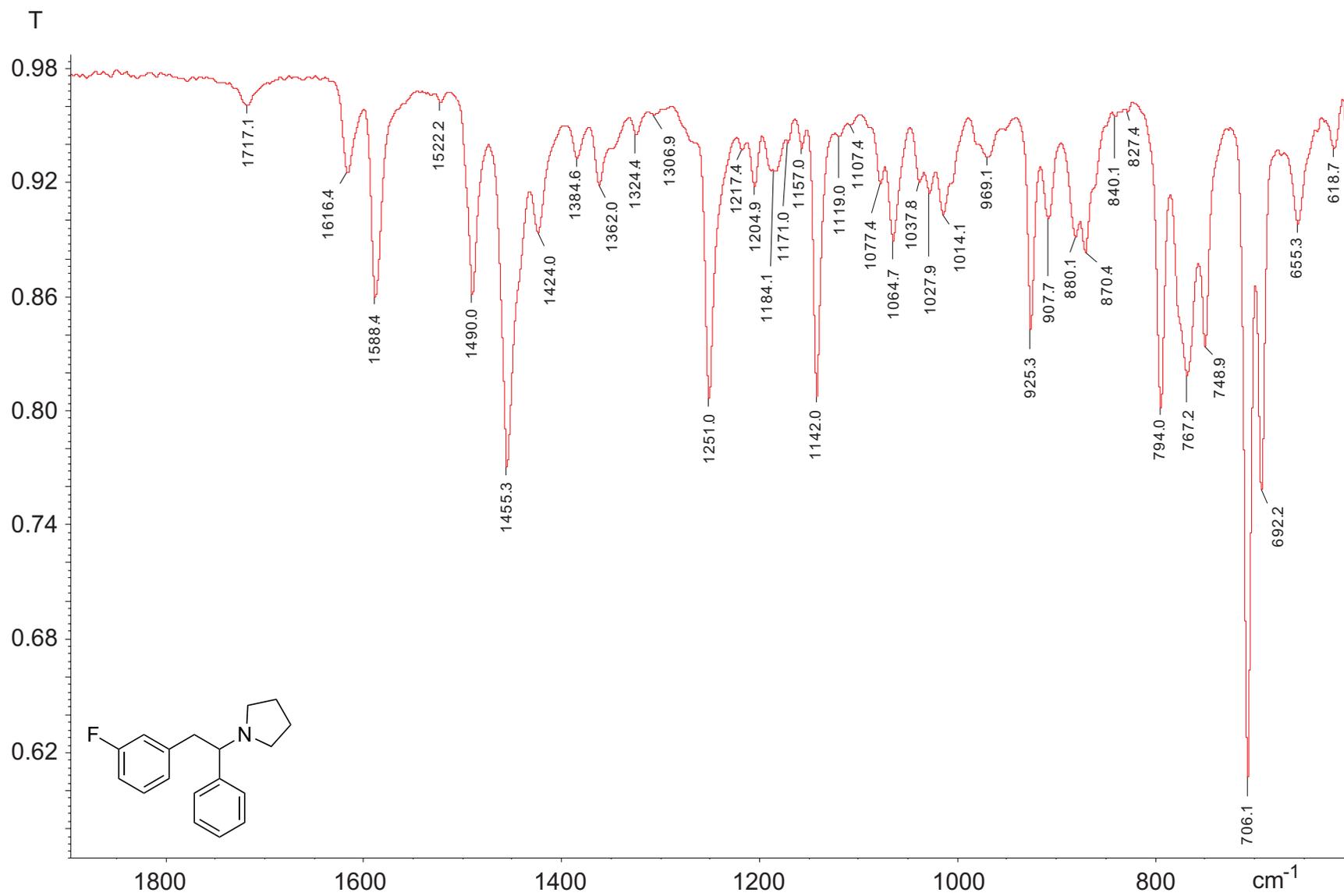
2''-F-DPPy GC-sIR (zoom)

Supporting Information – Drug Testing and Analysis



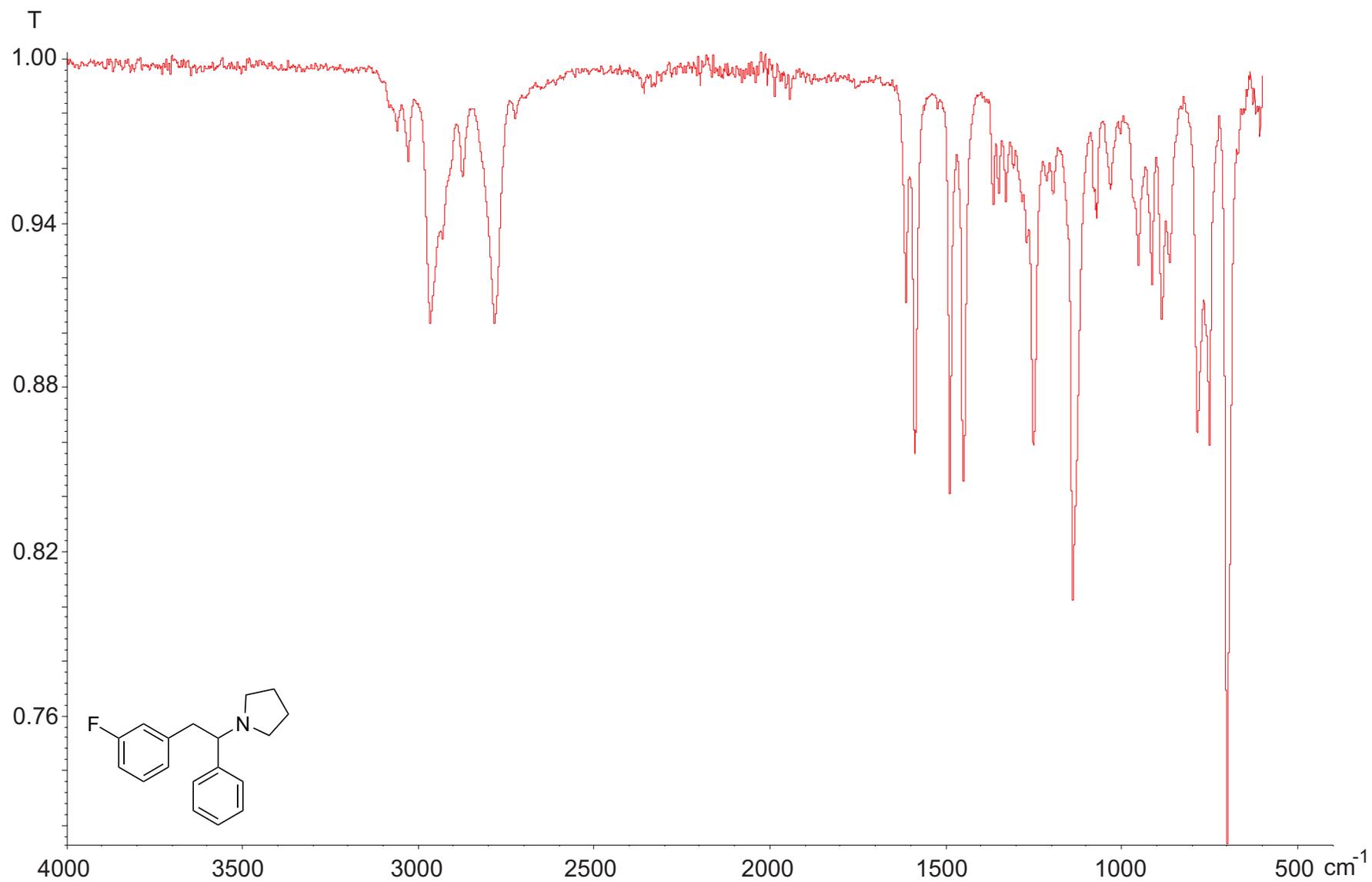
3''-F-DPPy HCl
ATR-IR

Supporting Information – Drug Testing and Analysis



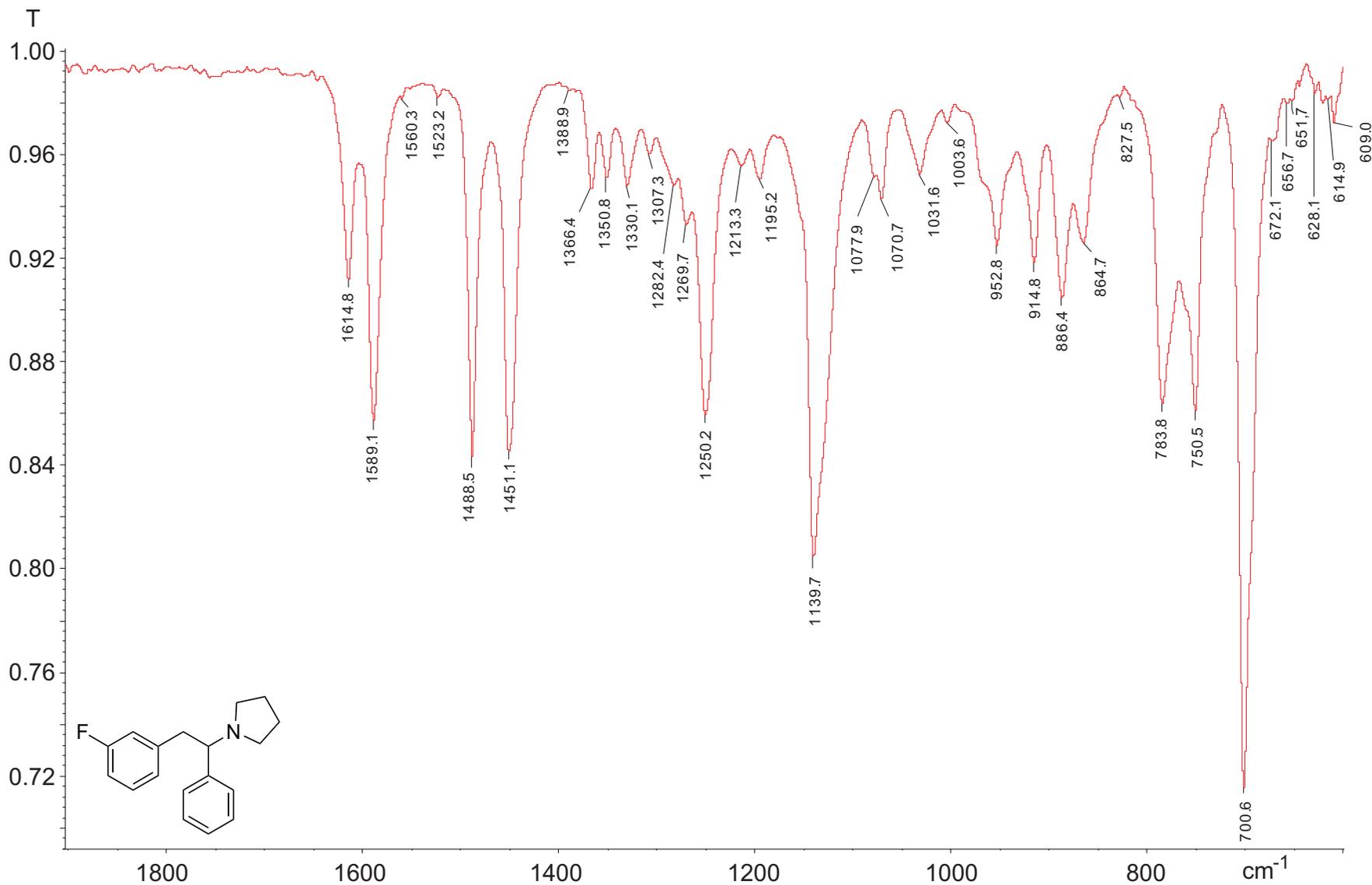
3''-F-DPPy HCl (zoom)
ATR-IR

Supporting Information – Drug Testing and Analysis



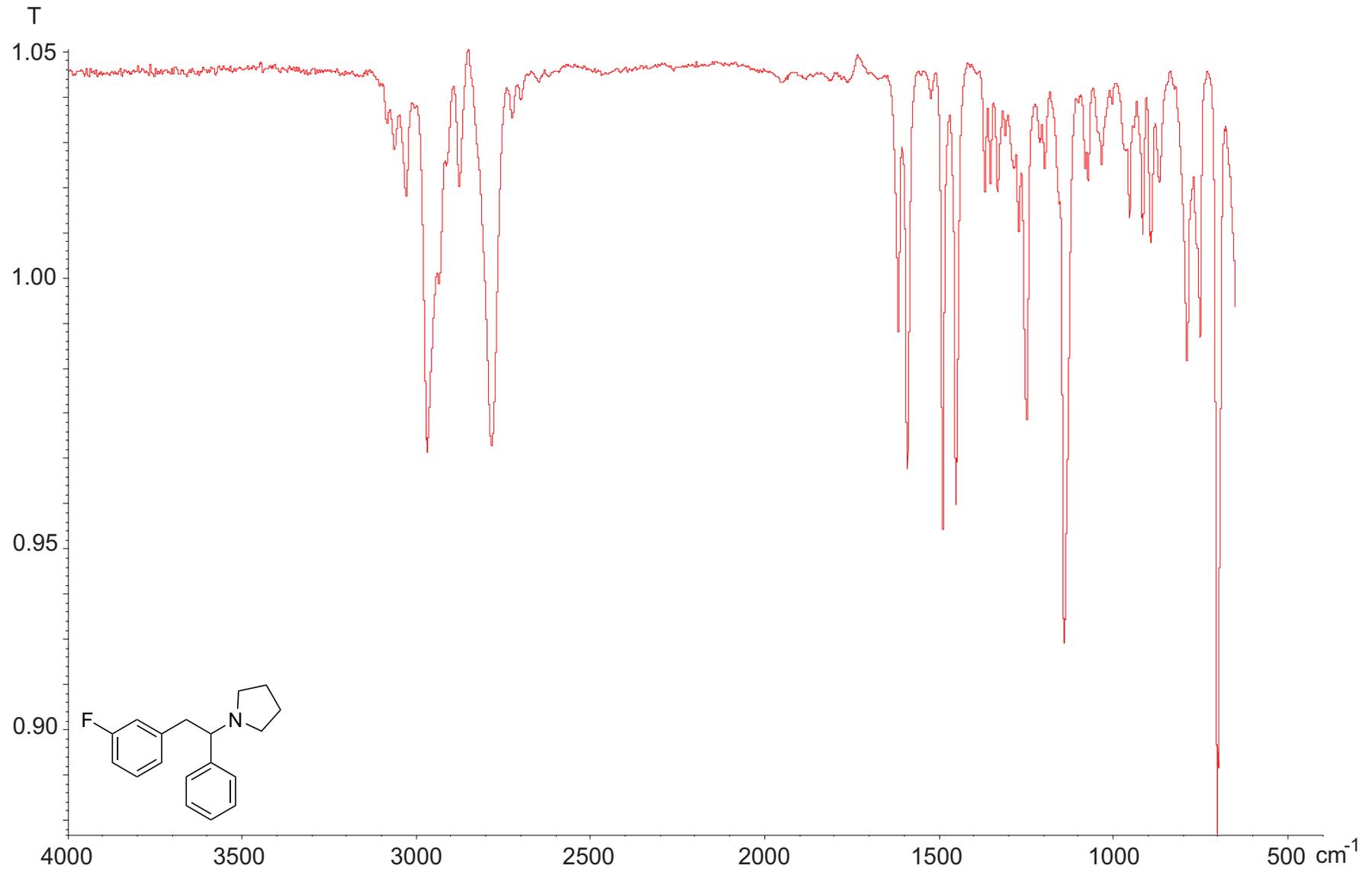
3''-F-DPPy base
ATR-IR

Supporting Information – Drug Testing and Analysis



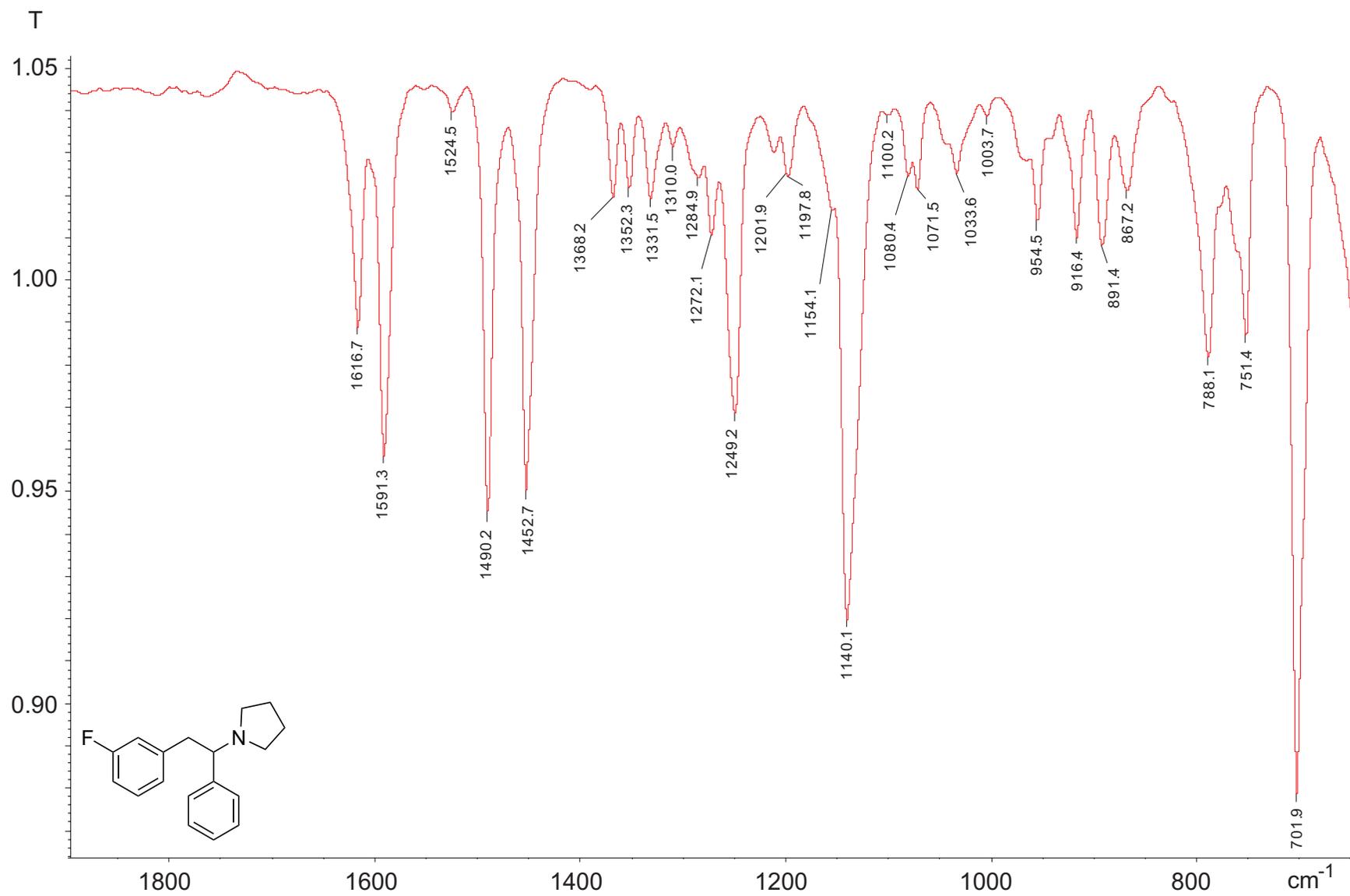
3'-F-DPPy base (zoom)
ATR-IR

Supporting Information – Drug Testing and Analysis



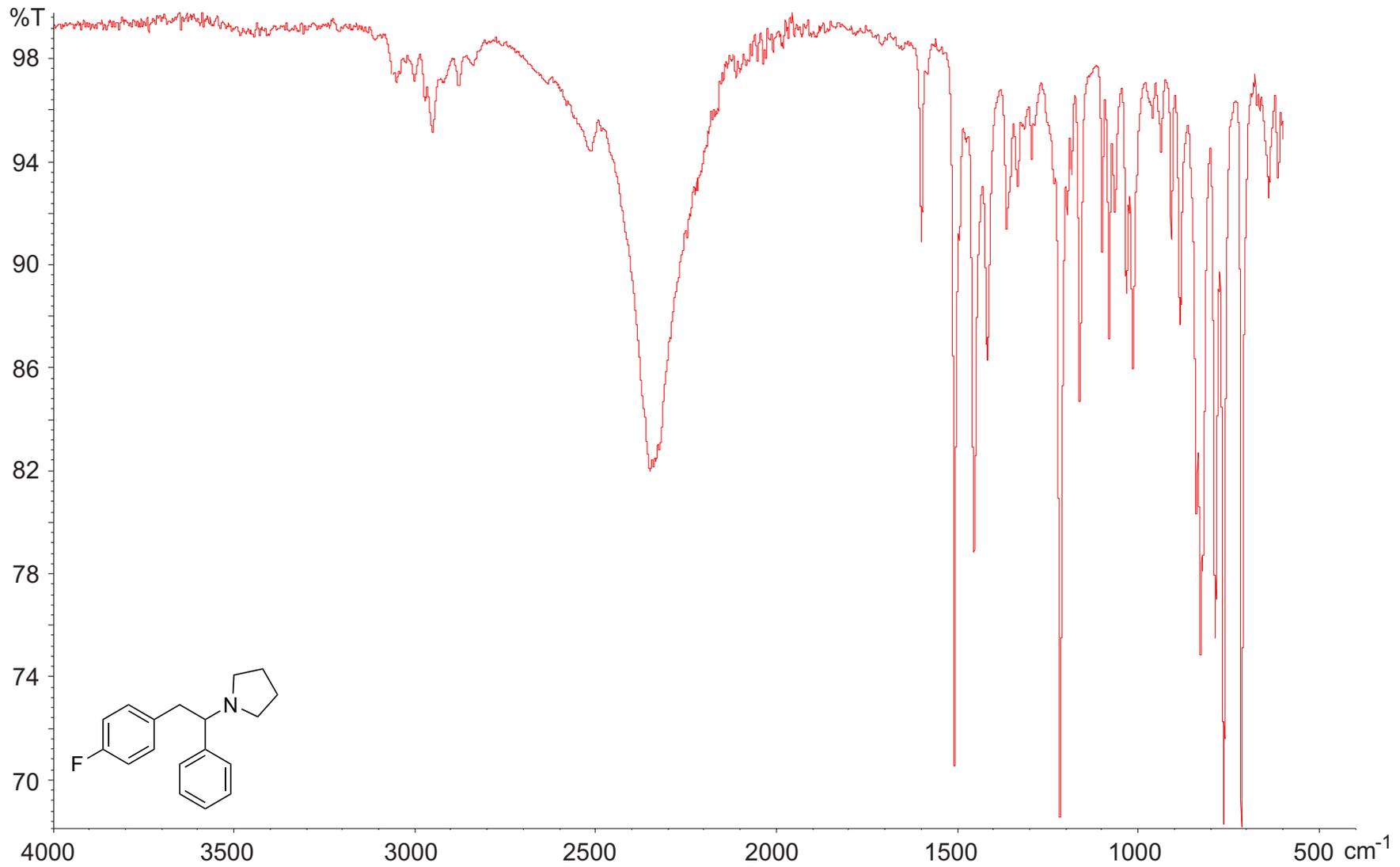
3''-F-DPPy GC-siR

Supporting Information – Drug Testing and Analysis



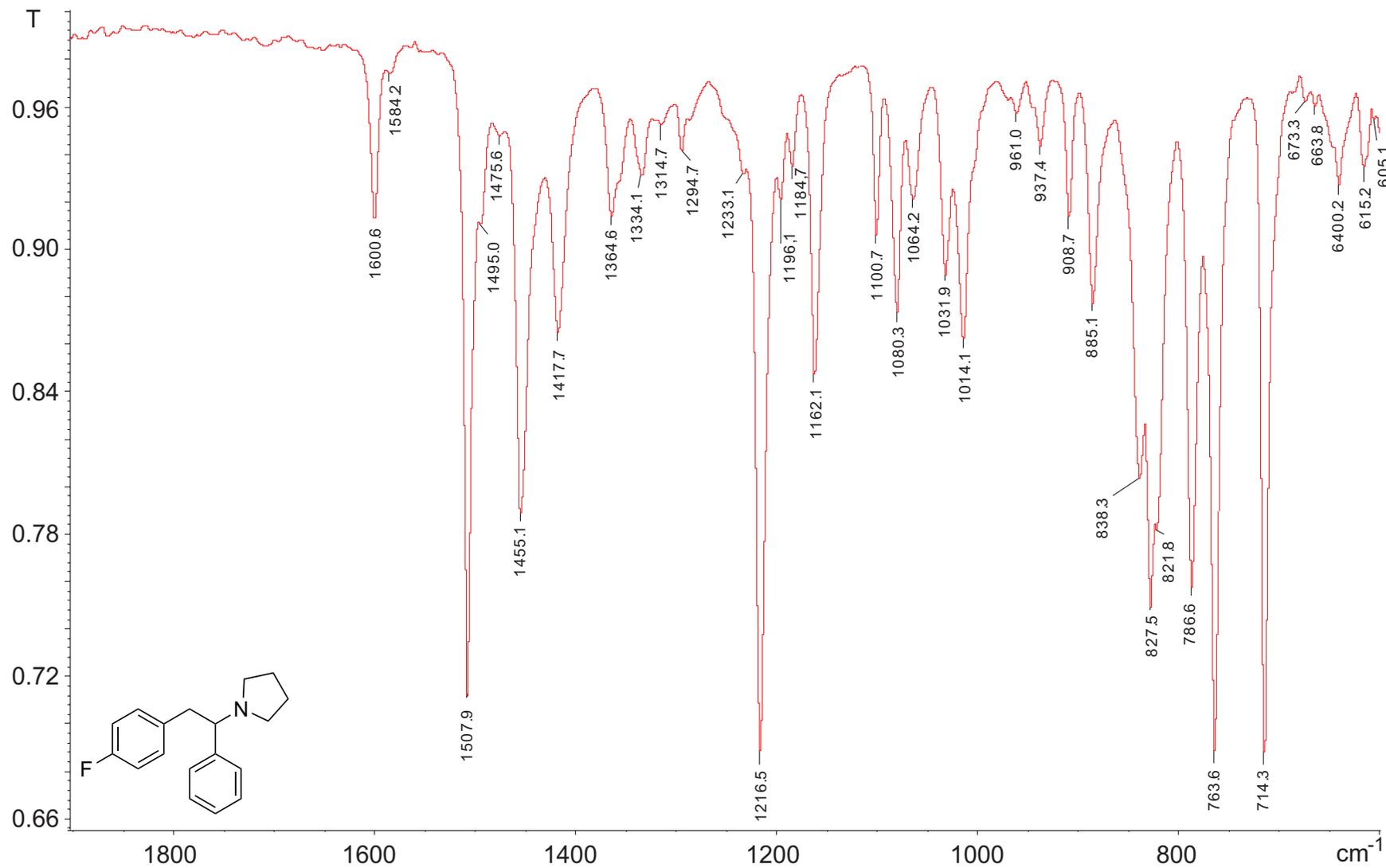
3''-F-DPPy GC-sIR (zoom)

Supporting Information – Drug Testing and Analysis



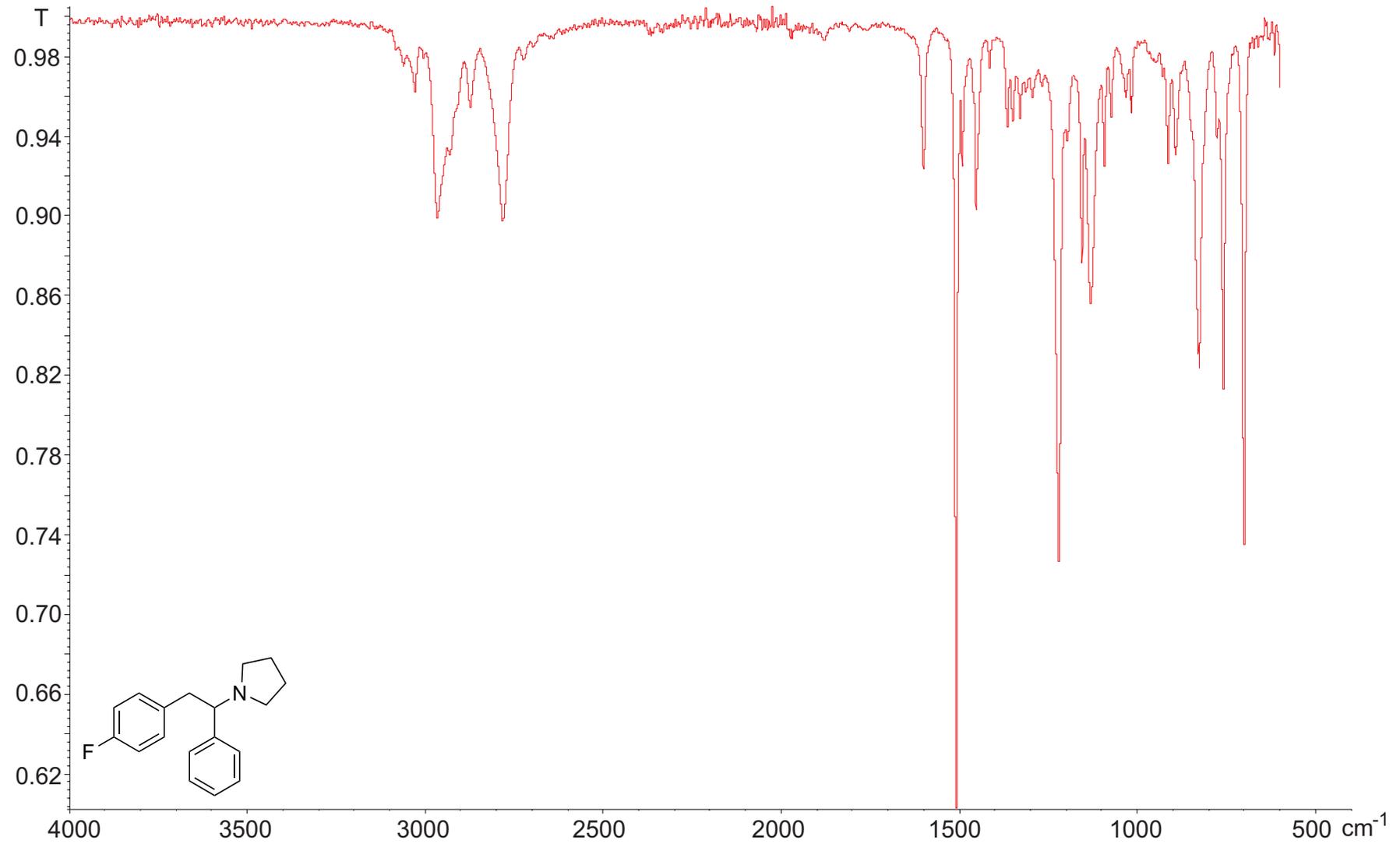
4'-F-DPPy HCl
ATR-IR

Supporting Information – Drug Testing and Analysis



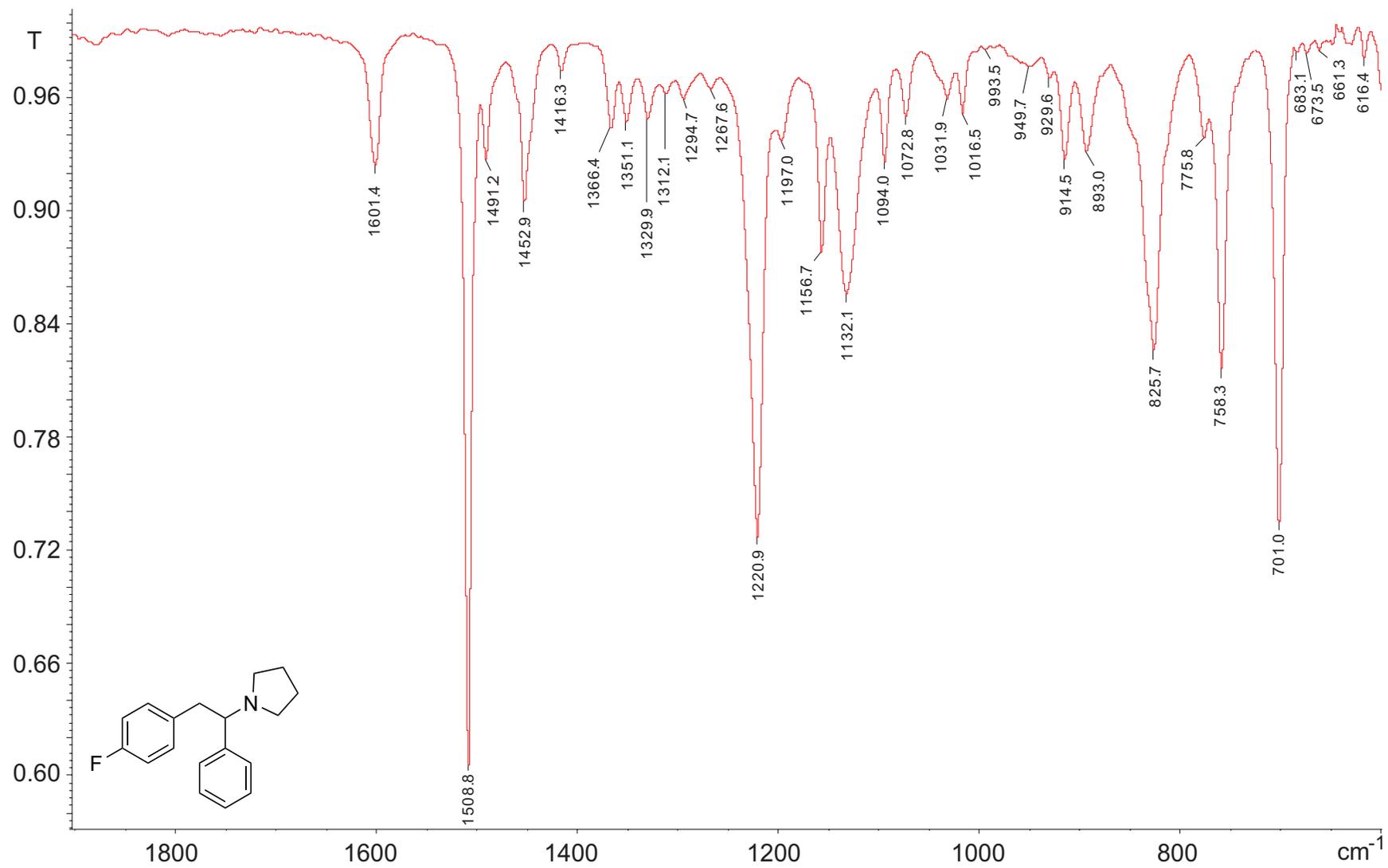
4'-F-DPPy HCl (zoom)
ATR-IR

Supporting Information – Drug Testing and Analysis



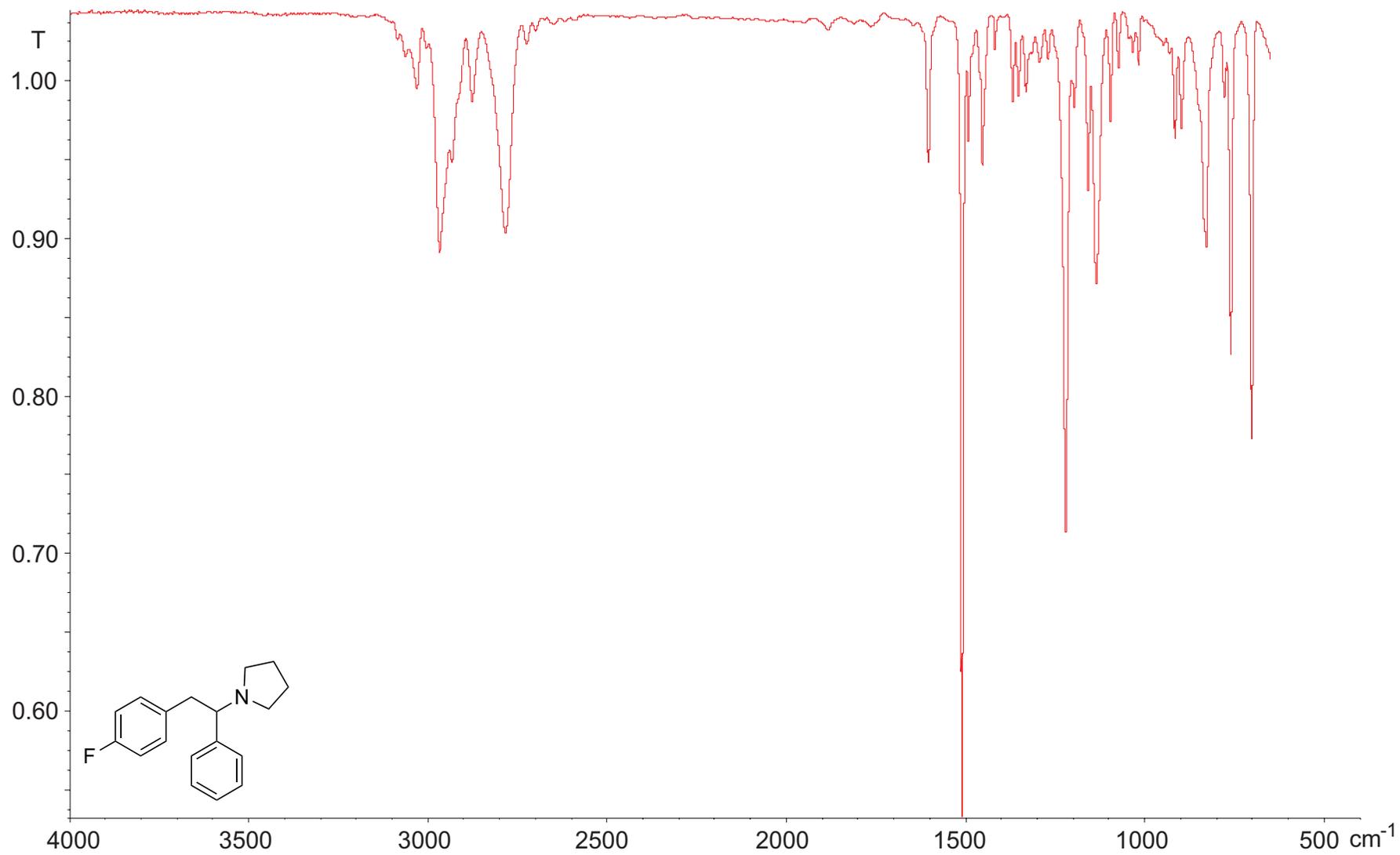
4''-F-DPPy base
ATR-IR

Supporting Information – Drug Testing and Analysis



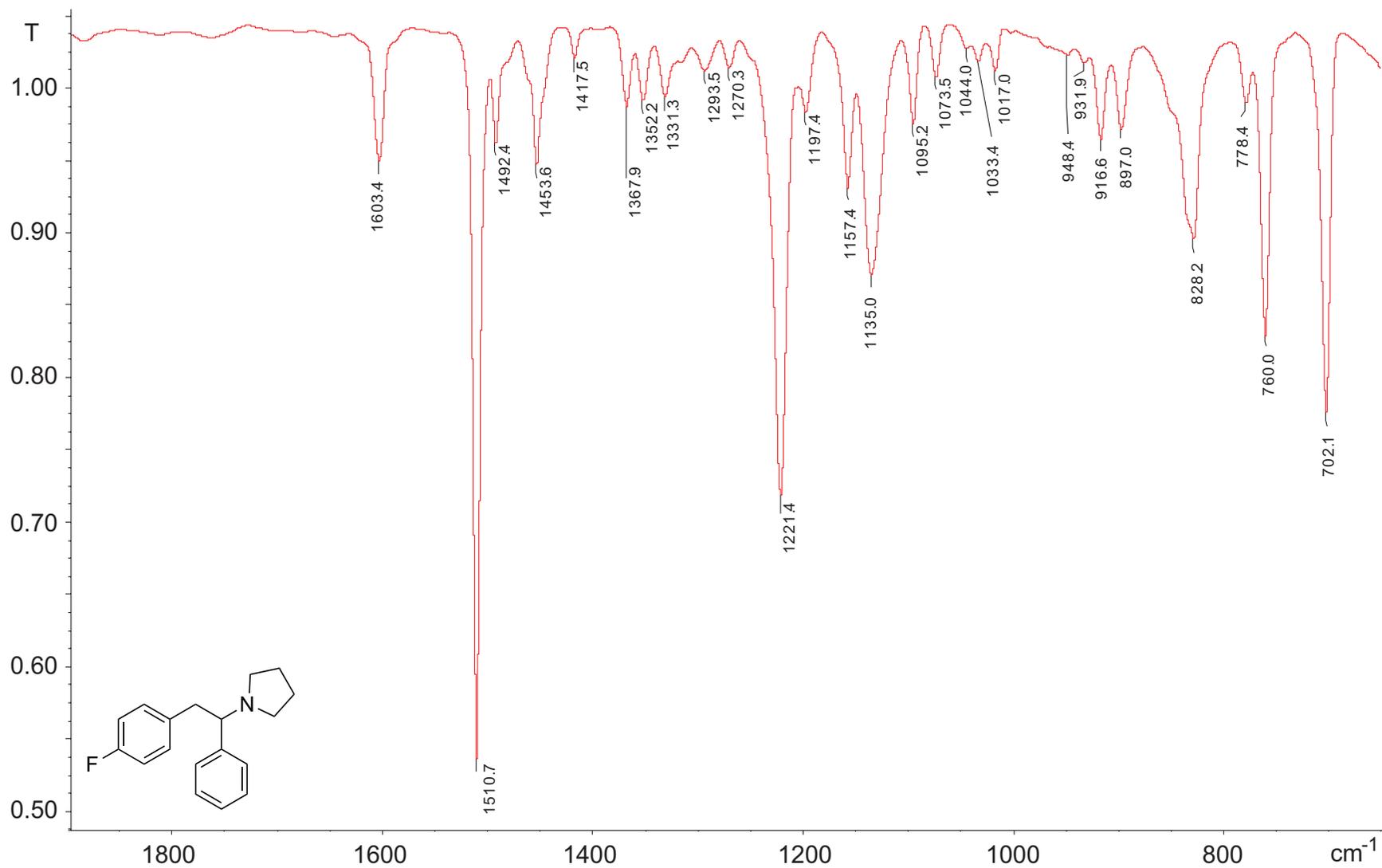
4''-F-DPPy base (zoom)
ATR-IR

Supporting Information – Drug Testing and Analysis



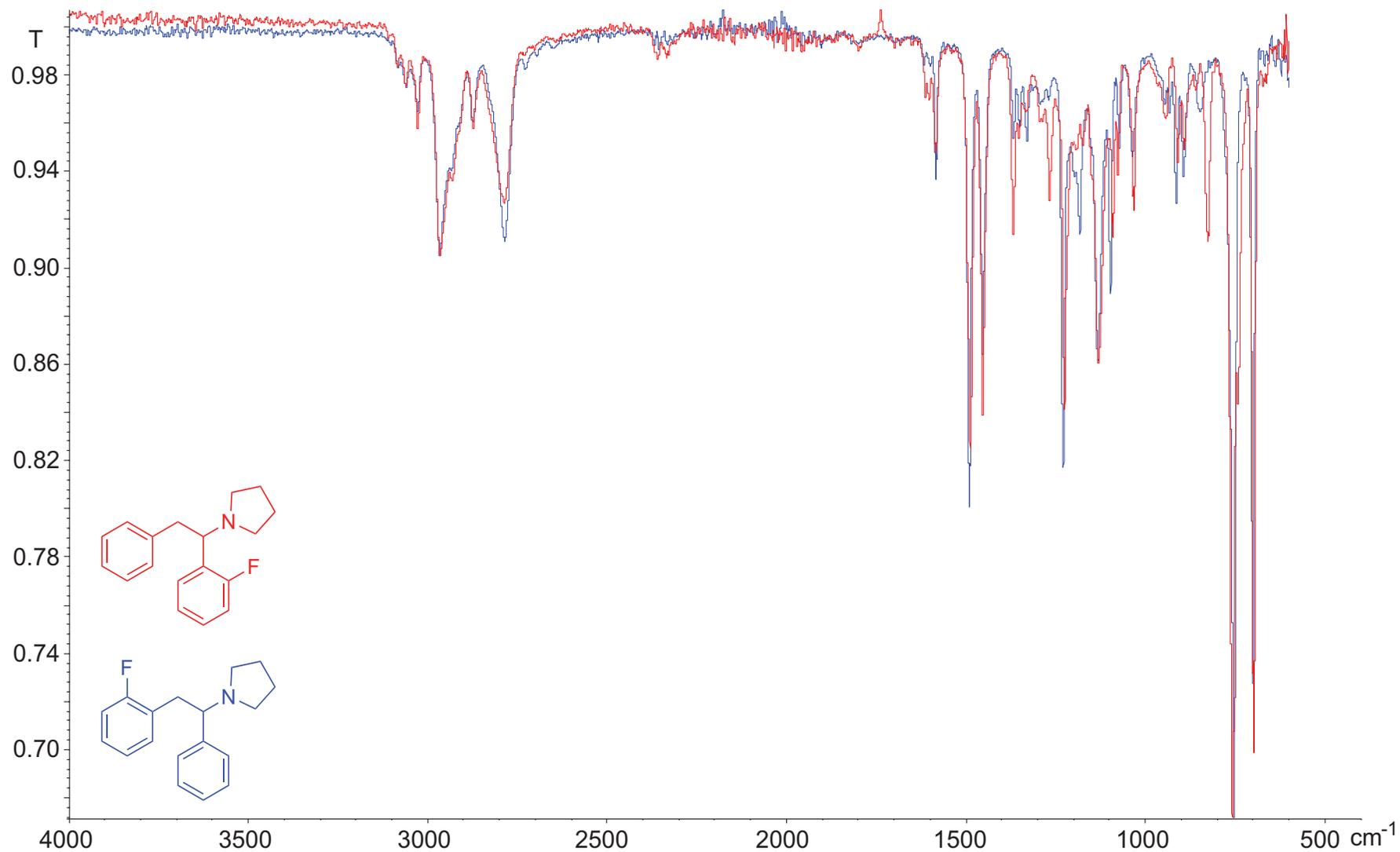
4''-F-DPPy GC-sIR

Supporting Information – Drug Testing and Analysis



4'-F-DPPy GC-sIR (zoom)

Supporting Information – Drug Testing and Analysis

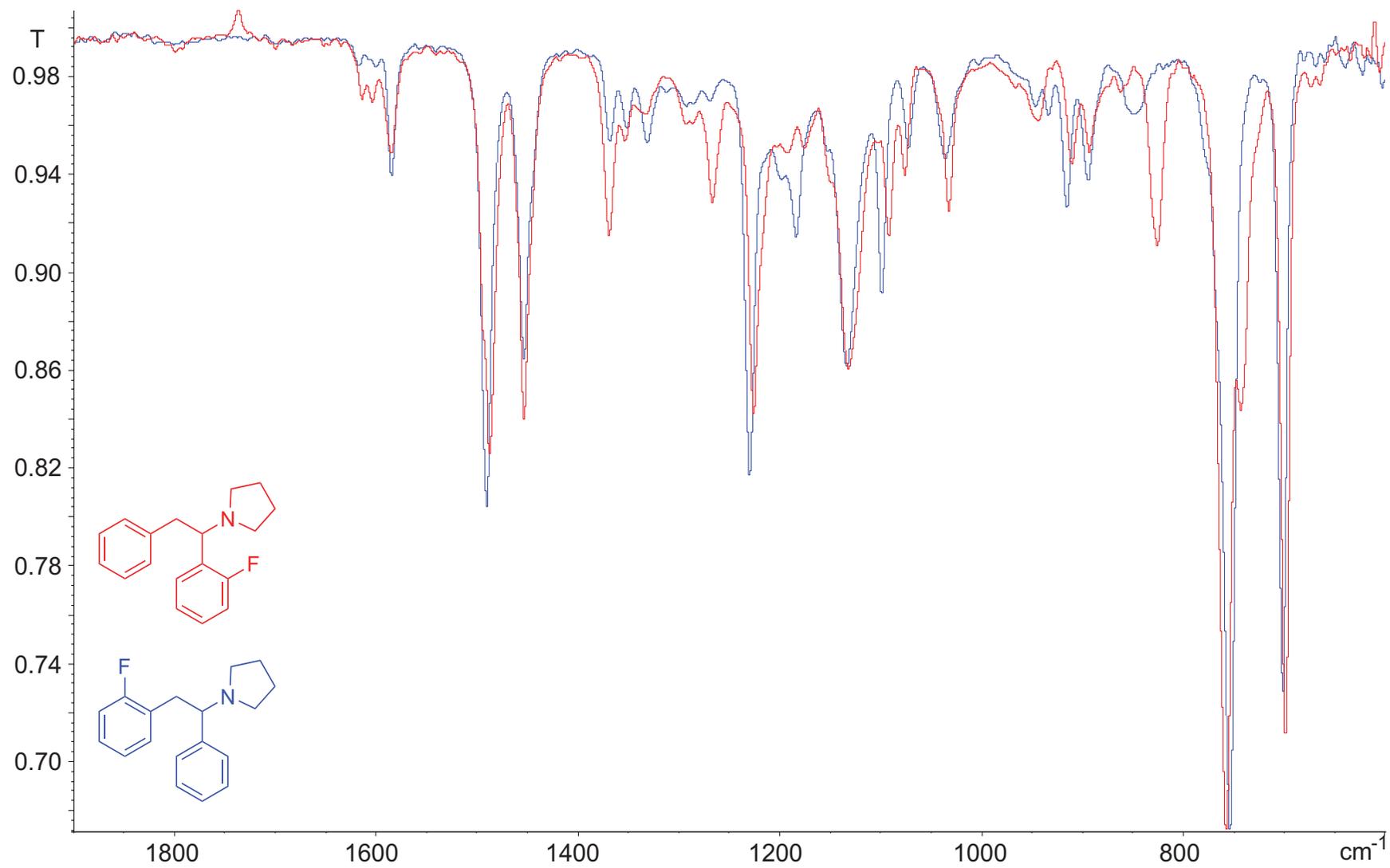


2-F-DPPy (fluorolintane) base

2''-F-DPPy base

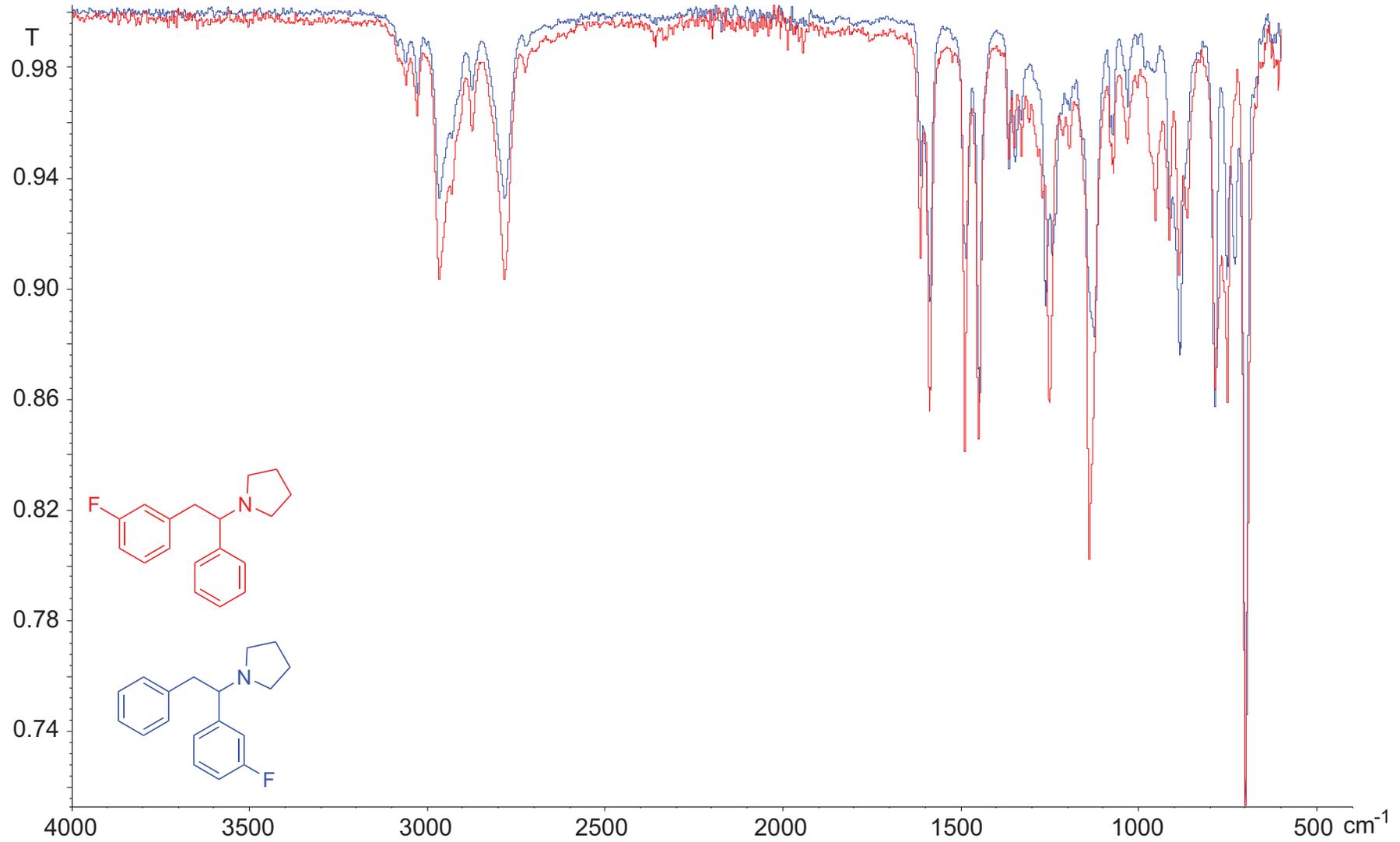
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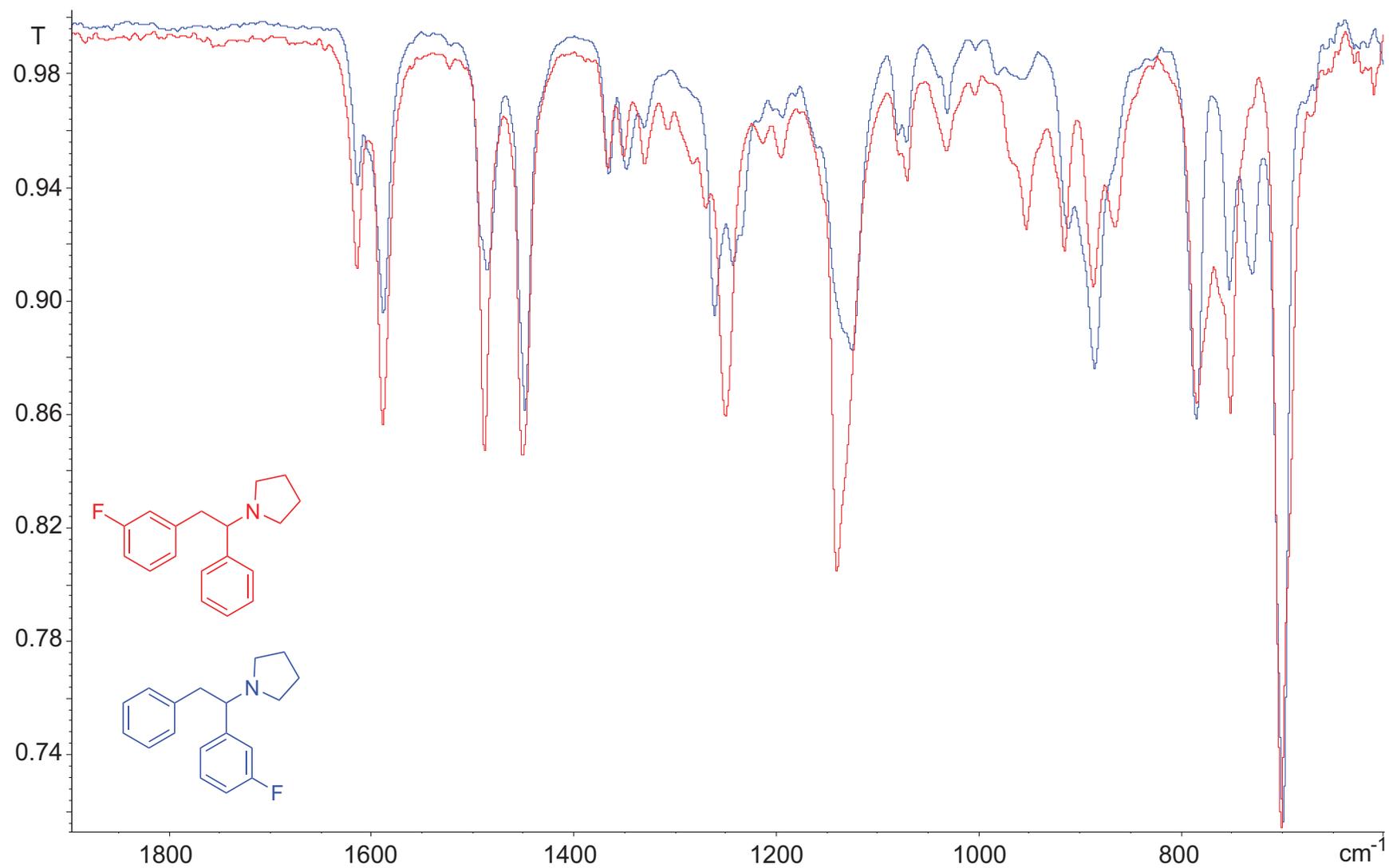
2-F-DPPy base (zoom)
2''-F-DPPy base (zoom)
ATR-IR

Supporting Information – Drug Testing and Analysis



3''-F-DPPy base
3-F-DPPy base
ATR-IR

Supporting Information – Drug Testing and Analysis

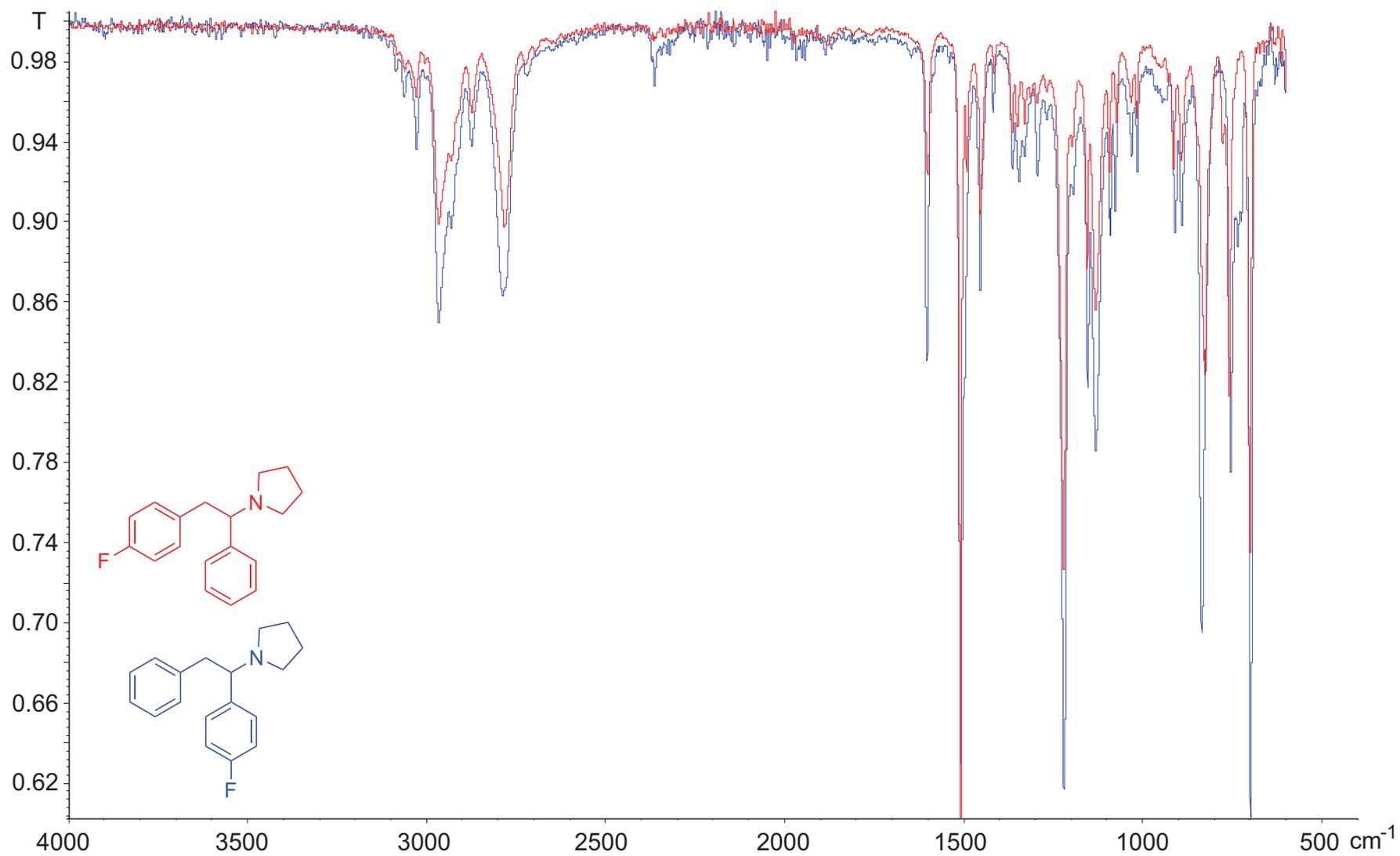


3''-F-DPPy base (zoom)

3-F-DPPy base (zoom)

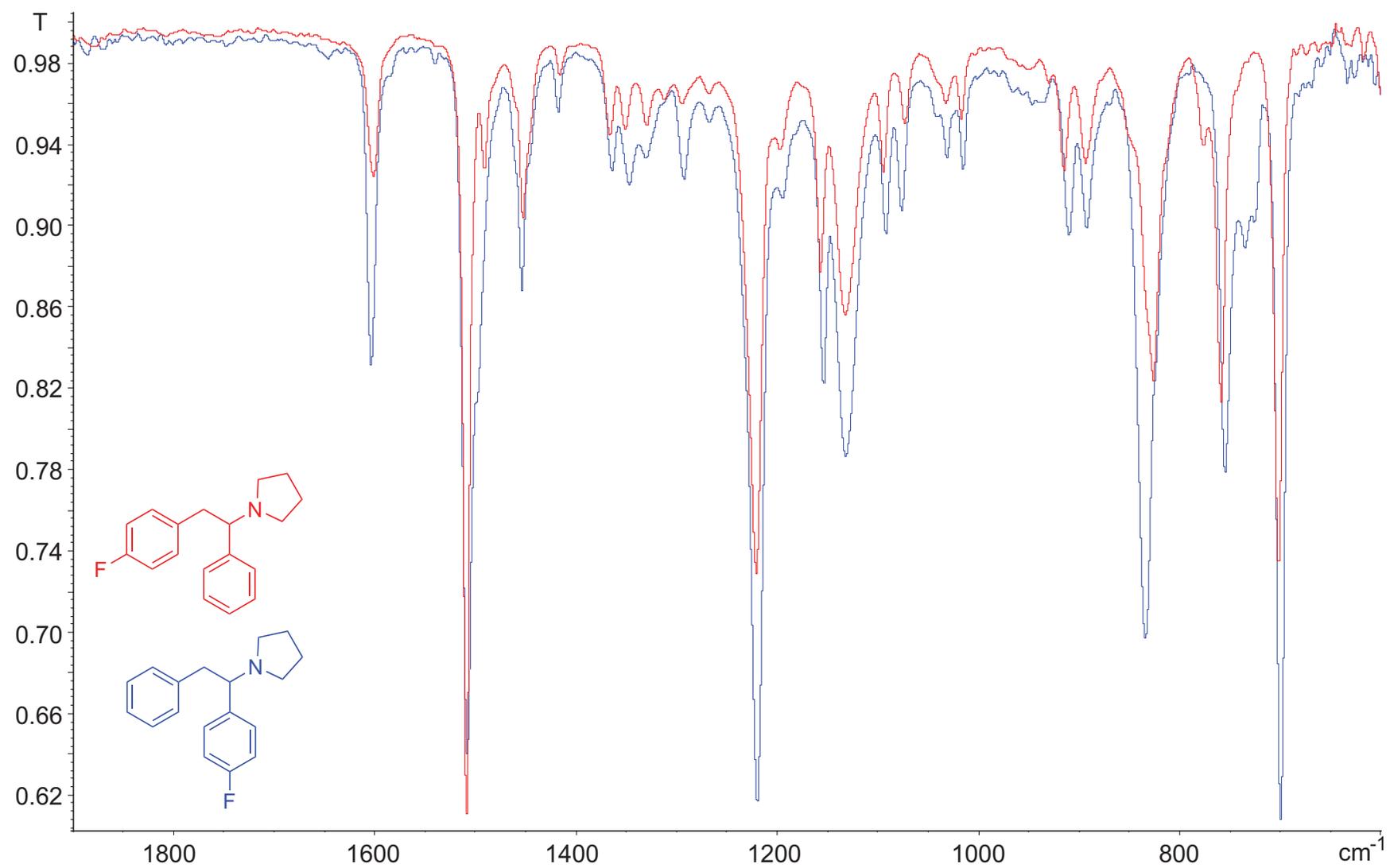
ATR-IR

Supporting Information – Drug Testing and Analysis



4''-F-DPPy base
4-F-DPPy base
ATR-IR

Supporting Information – Drug Testing and Analysis



4''-F-DPPy base (zoom)

4-F-DPPy base (zoom)

ATR-IR

Supporting Information – Drug Testing and Analysis

400 MHz ¹ H NMR for 2-F-DPPy (fluorolintane) freebase. 20 mg/mL in d ₆ -DMSO. Shifts in ppm and set to solvent reference (2.50 ppm).	
¹ H [δ / ppm]	2-F-DPPy
H ₁	3.89 (dd, <i>J</i> = 10.1, 4.9 Hz, 1H)
H ₂	3.29 (dd, <i>J</i> = 13.2, 4.8 Hz, 1H) 2.91 (dd, <i>J</i> = 12.9, 10.4 Hz, 1H)
H _α	2.60–2.47 (m, 2H) *coalescing with solvent DMSO solvent peak 2.42–2.30 (m, 2H)
H _β	1.69–1.60 (m, 4H)
H _{1'}	–
H _{2'}	–
H _{3'}	7.00–6.89 (m, 1H) *overlap with C _{2''} ,6''
H _{4'}	7.22–7.15 (m, 1H)
H _{5'}	7.15–7.00 *overlap with H _{4''} and H _{3''} ,5''
H _{6'}	7.45 (td, <i>J</i> = 7.4, 1.9 Hz, 1H)
H _{1''}	–
H _{2''}	6.94 (d, <i>J</i> = 7.0 Hz, 1H) *overlap with C _{3'}
H _{3''}	7.15–7.00 (m, 2H) *overlap with H _{4''} and H _{5'}
H _{4''}	7.15–7.00 *overlap with H _{5'} and H _{3''} ,5''
H _{5''}	7.15–7.00 (m, 2H) *overlap with H _{4''} and H _{5'}
H _{6''}	6.94 (d, <i>J</i> = 7.0 Hz, 1H) *overlap with C _{3'}

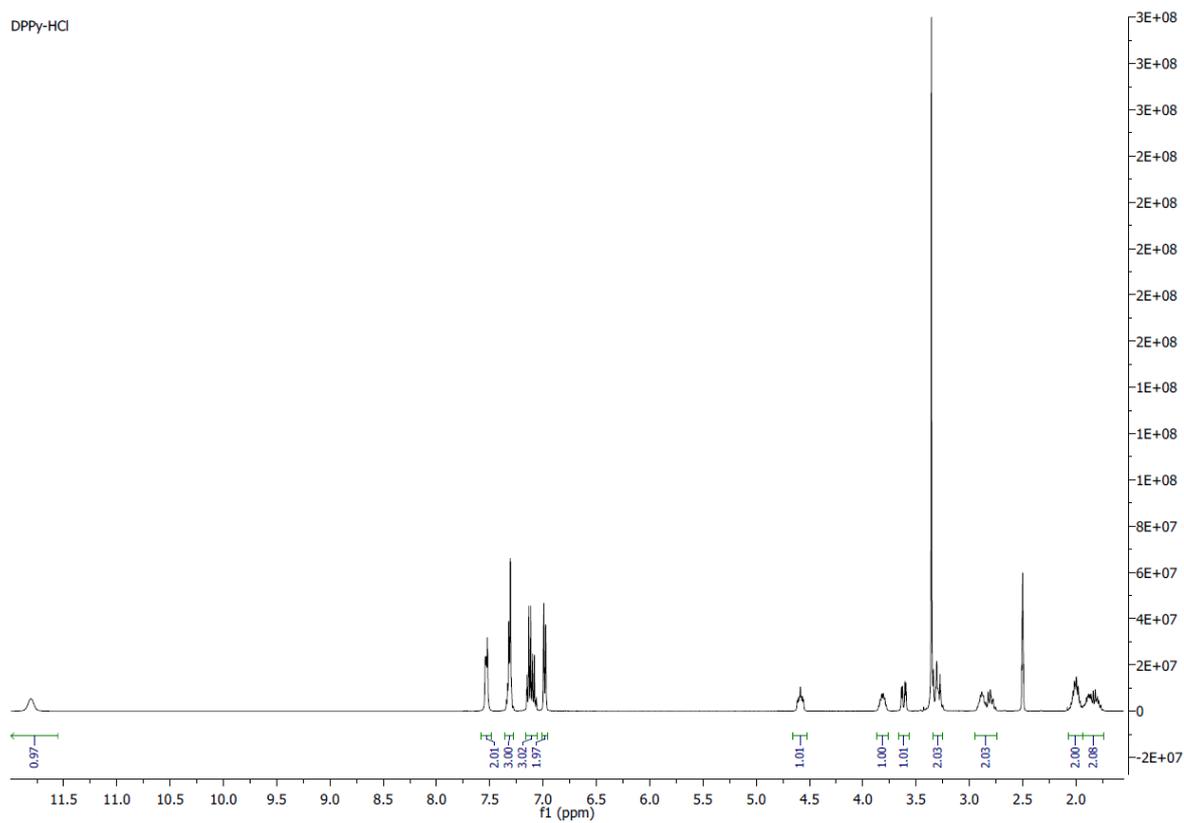
Supporting Information – Drug Testing and Analysis

101 MHz ^{13}C NMR for 2-F-DPPy (fluorolintane) freebase. 20 mg/mL in d_6 -DMSO. Shifts in ppm, and set to solvent reference (39.52 ppm).	
^{13}C [δ / ppm]	2-F-DPPy (^{13}C)
C ₁	62.28
C ₂	40.39
C _{α}	51.41
C _{β}	22.88
C _{1'}	127.96 127.83 *overlap with C _{3'',5''}
C _{2'}	161.48 159.06
C _{3'}	114.99 114.76
C _{4'}	128.60 128.52
C _{5'}	124.11 124.07
C _{6'}	129.78 129.73
C _{1''}	138.66
C _{2''}	129.16
C _{3''}	127.86
C _{4''}	125.87
C _{5''}	127.86
C _{6''}	129.16

376.5 MHz ^{19}F NMR. 20 mg/mL for fluorolintane freebase in d_6 -DMSO. Reference CFCl_3 (0.00 ppm).
^{19}F NMR
117.78

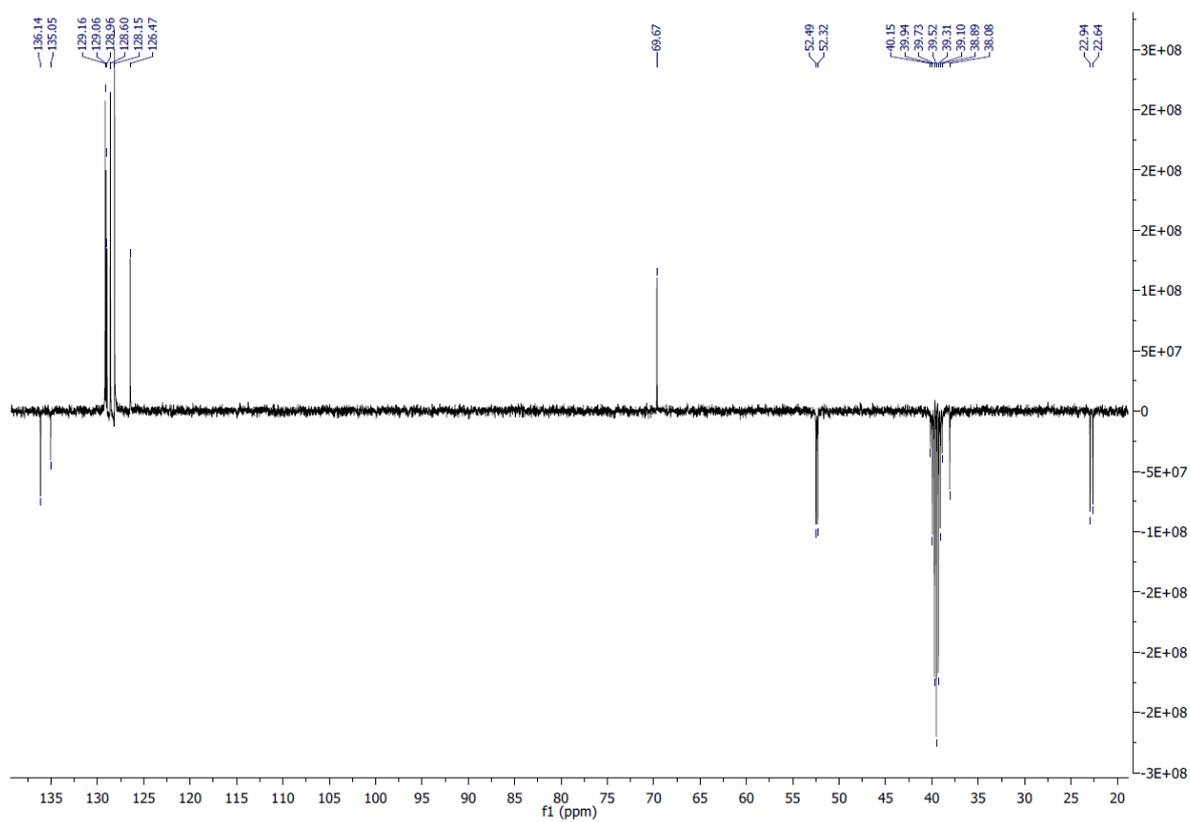
Compound	^{19}F NMR
2-F-DPPy	-116.32
3-F-DPPy	-111.59
4-F-DPPy	-112.06
2''-F-DPPy	-117.11
3''-F-DPPy	-113.10
4''-F-DPPy	-115.80

Supporting Information – Drug Testing and Analysis

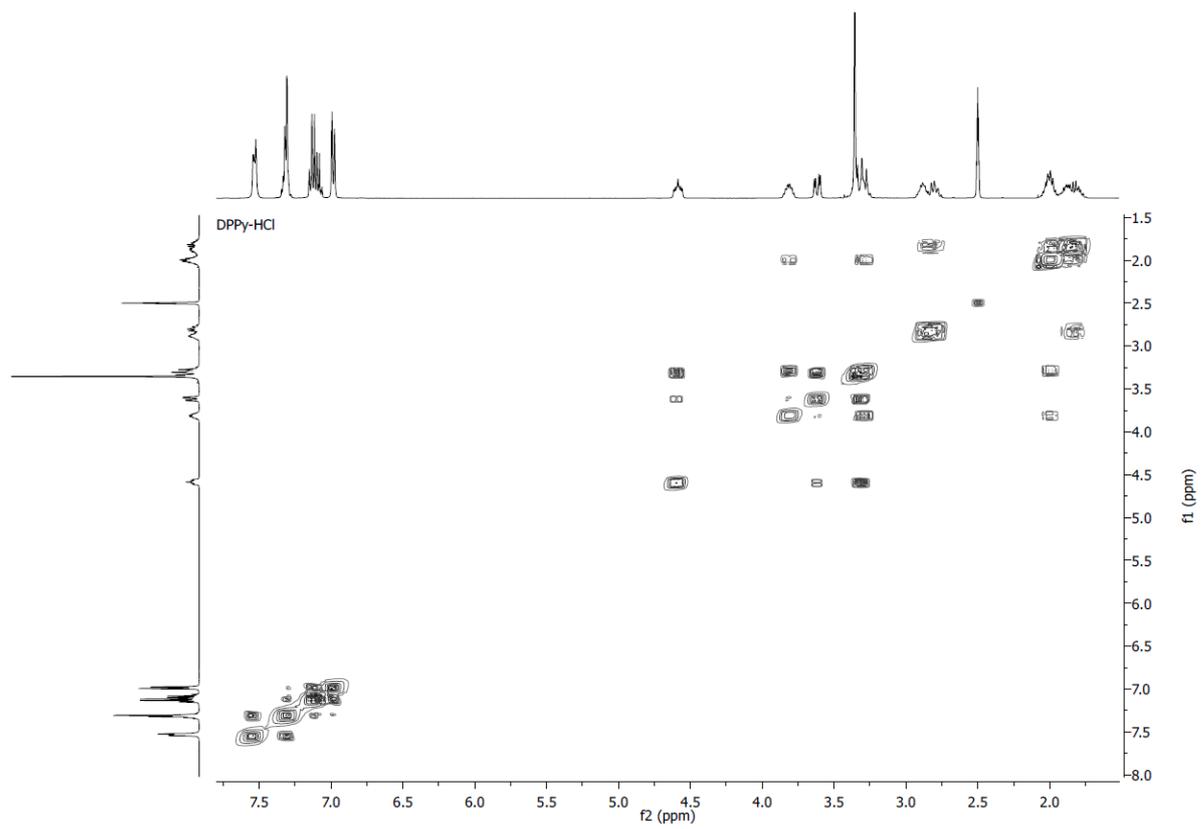


^1H NMR of DPPy HCl (400 MHz, $\text{d}_6\text{-DMSO}$)

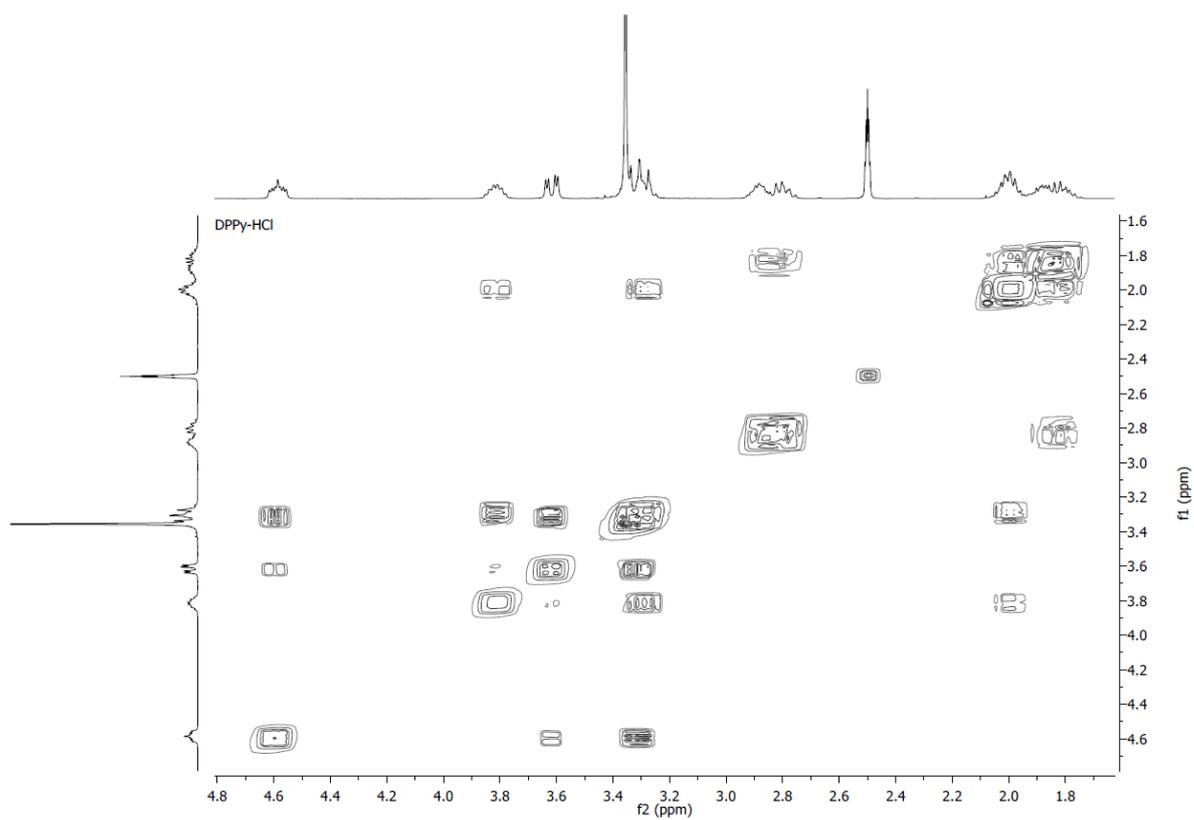
Supporting Information – Drug Testing and Analysis



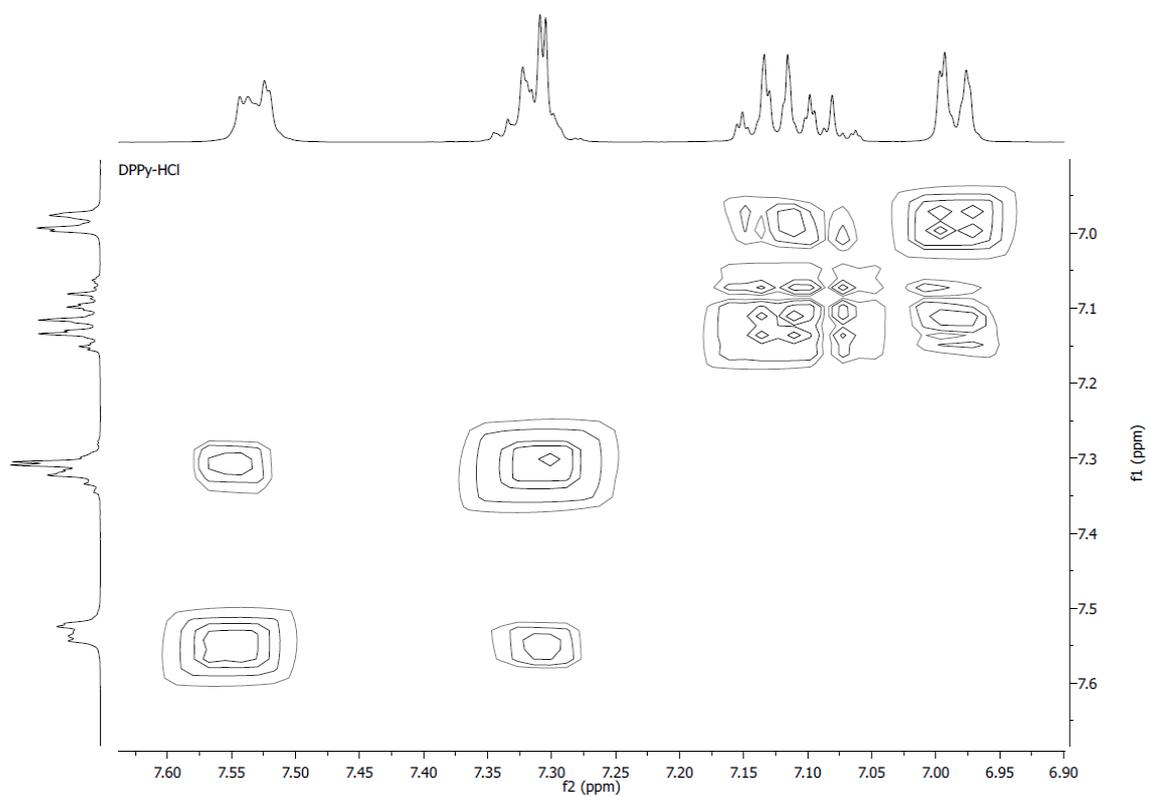
^{13}C PENDANT NMR of DPPy HCl (101 MHz, d_6 -DMSO)



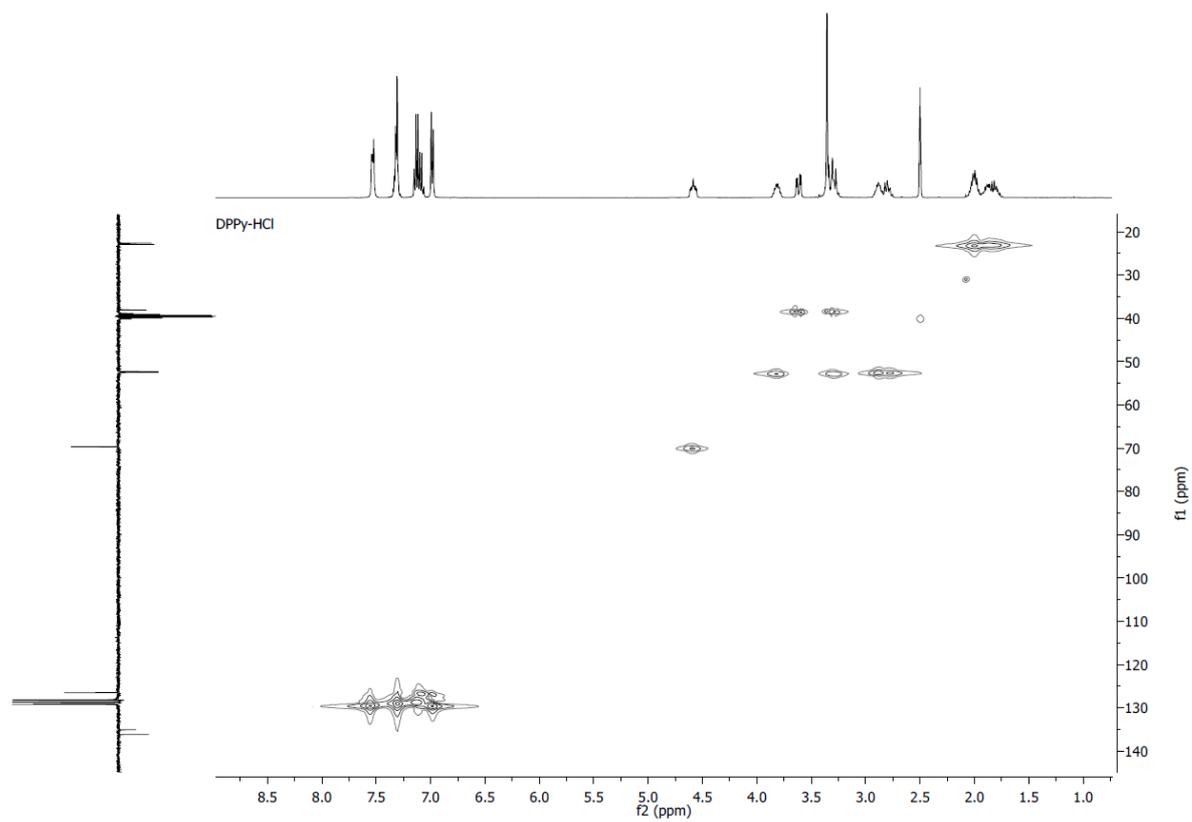
COSY-45 2-D NMR of DPPy HCl (d_6 -DMSO)



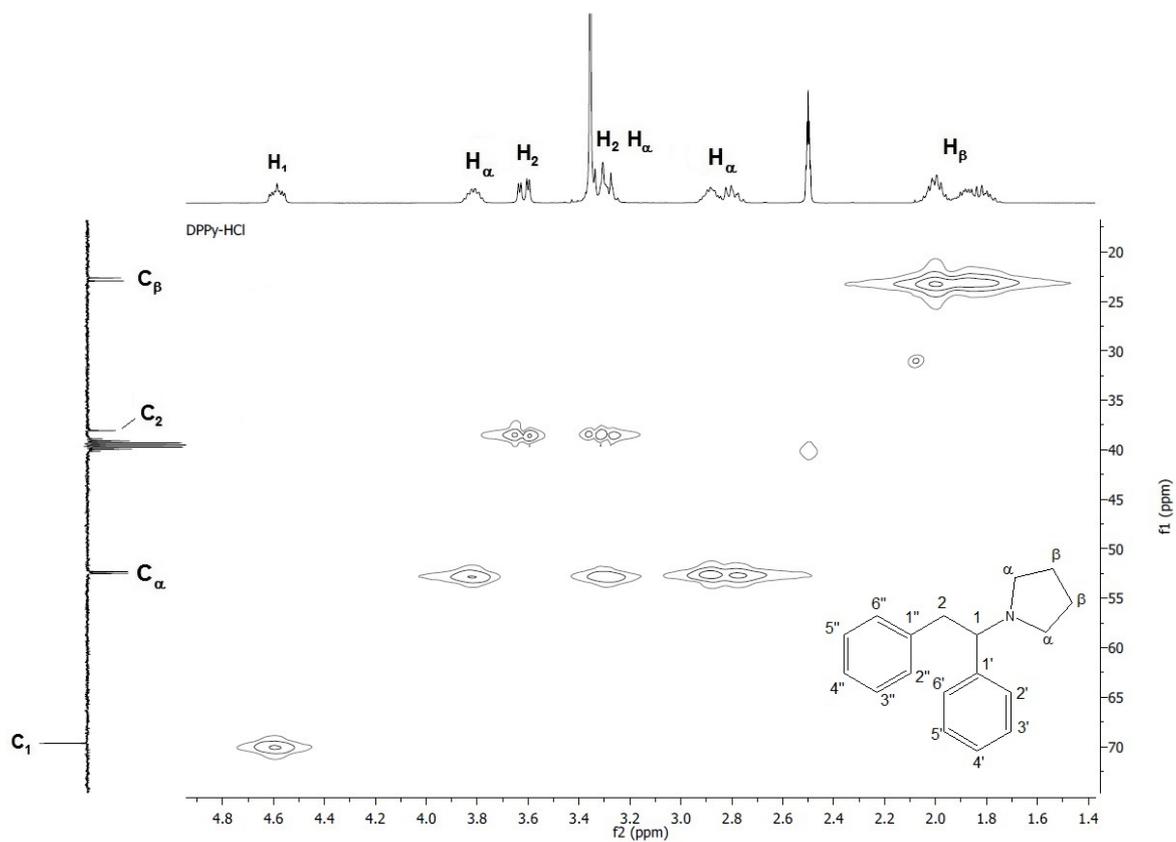
COSY-45 2-D NMR of DPPy HCl, zoomed in on aliphatic section (d_6 -DMSO)



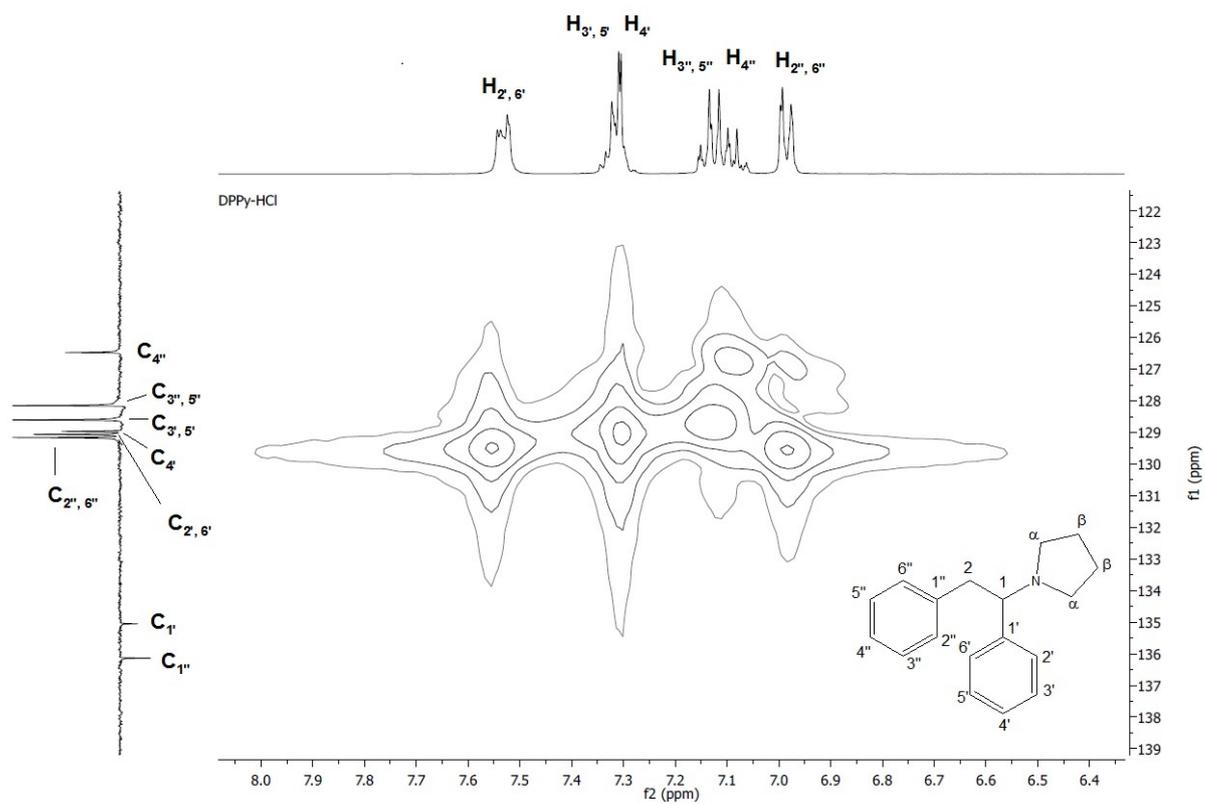
COSY-45 2-D NMR of DPPy HCl, zoomed in on aromatic section (d_6 -DMSO)



HMQC 2-D NMR of DPPy HCl (d_6 -DMSO)

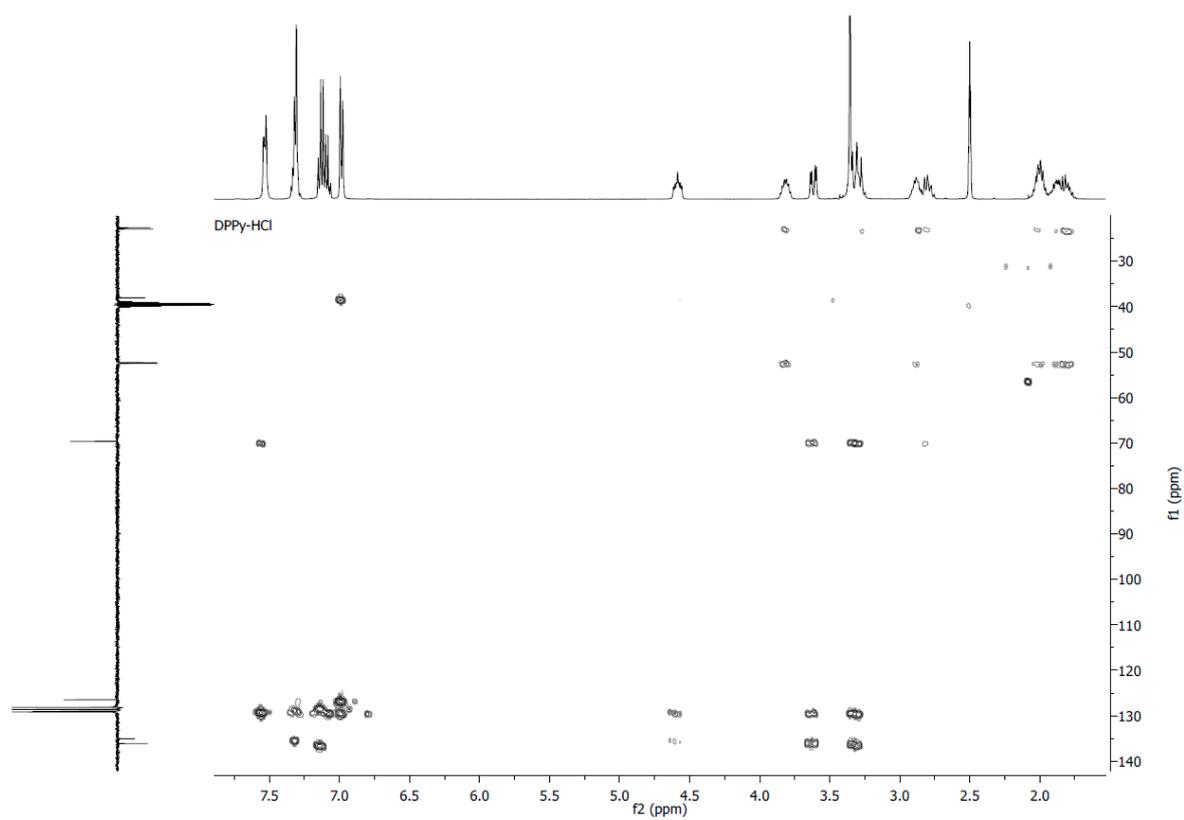


HMQC 2-D NMR of DPPy HCl, zoomed in on aliphatic section (d₆-DMSO)



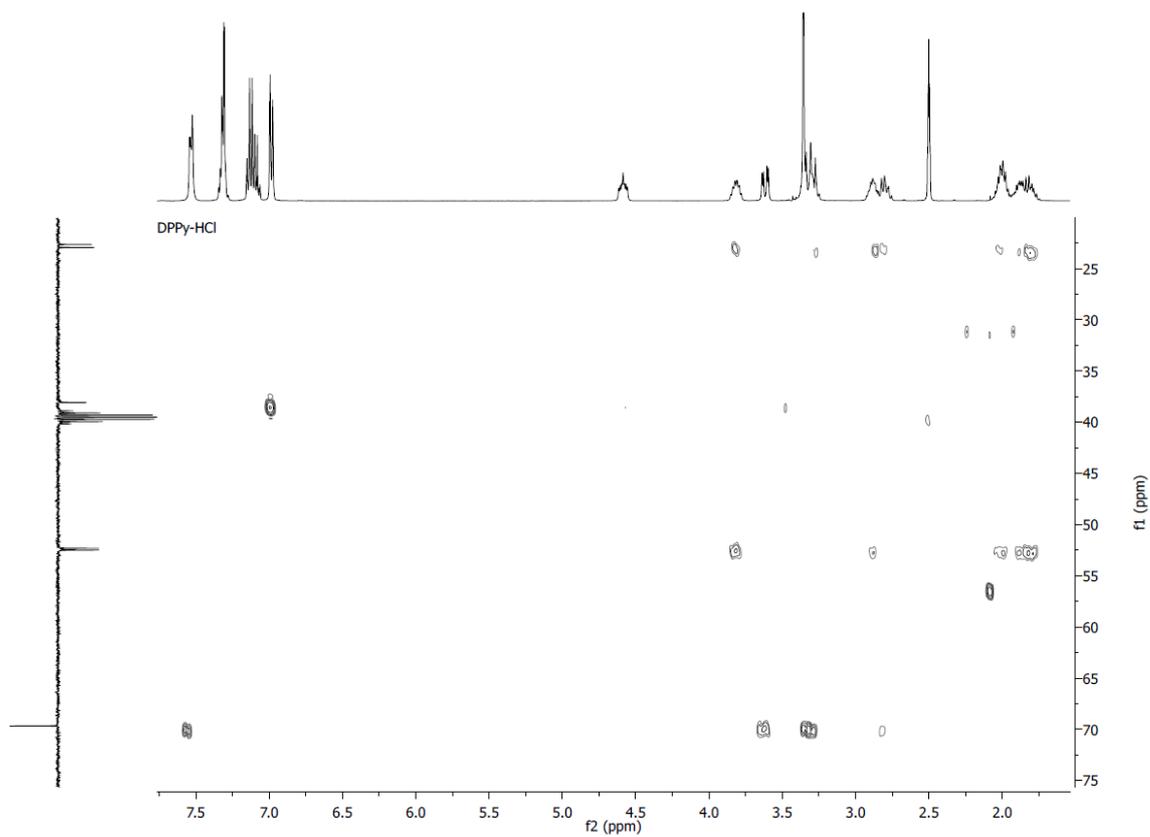
HMQC 2-D NMR of DPPy HCl, zoomed in on aromatic section (d_6 -DMSO)

Supporting Information – Drug Testing and Analysis



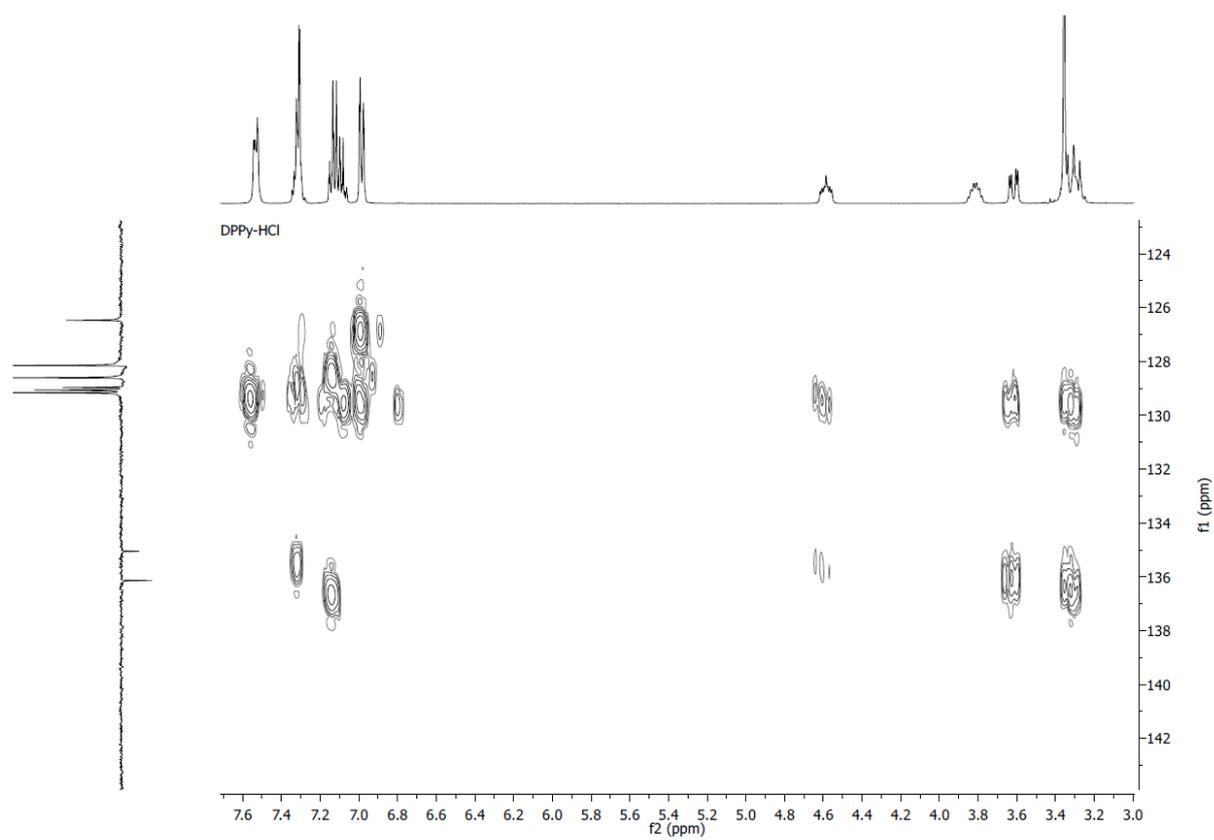
HMBC 2-D NMR of DPPy HCl (d_6 -DMSO)

Supporting Information – Drug Testing and Analysis



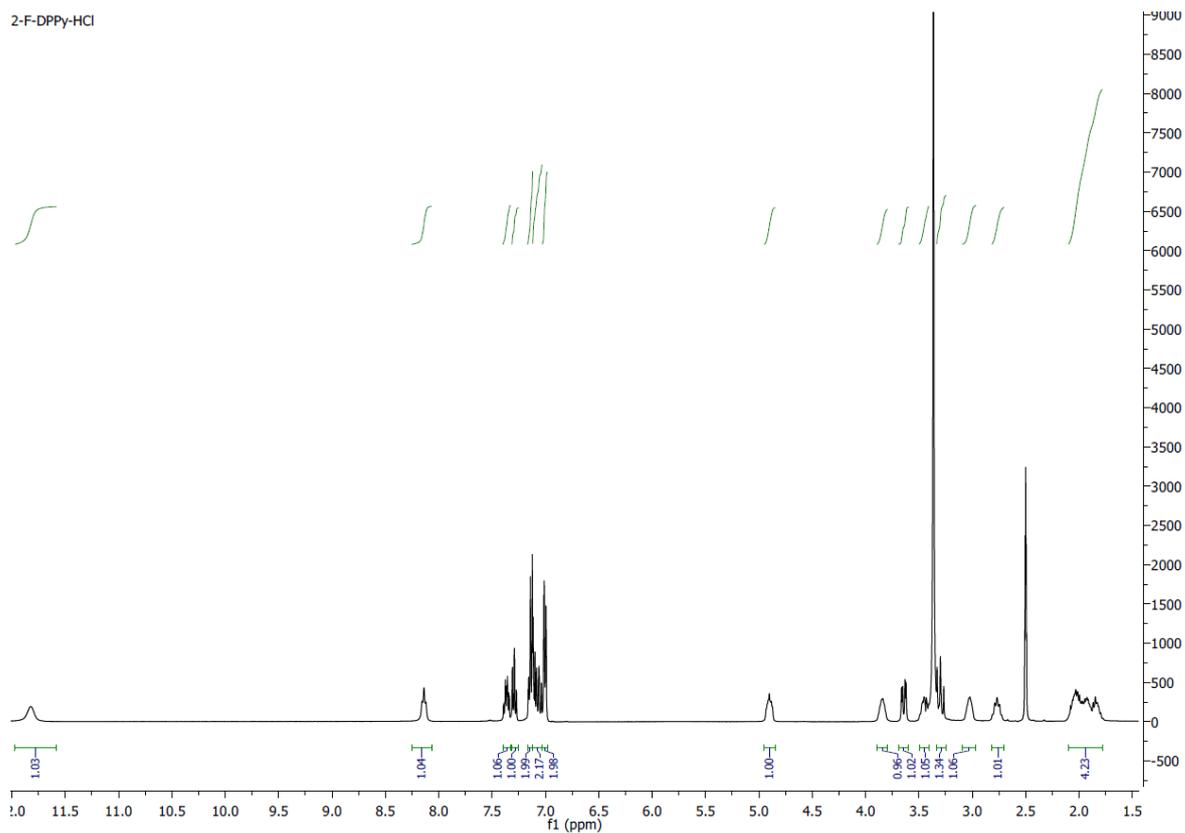
HMBC 2-D NMR of DPPy HCl, zoomed in on aliphatic section (d_6 -DMSO)

Supporting Information – Drug Testing and Analysis



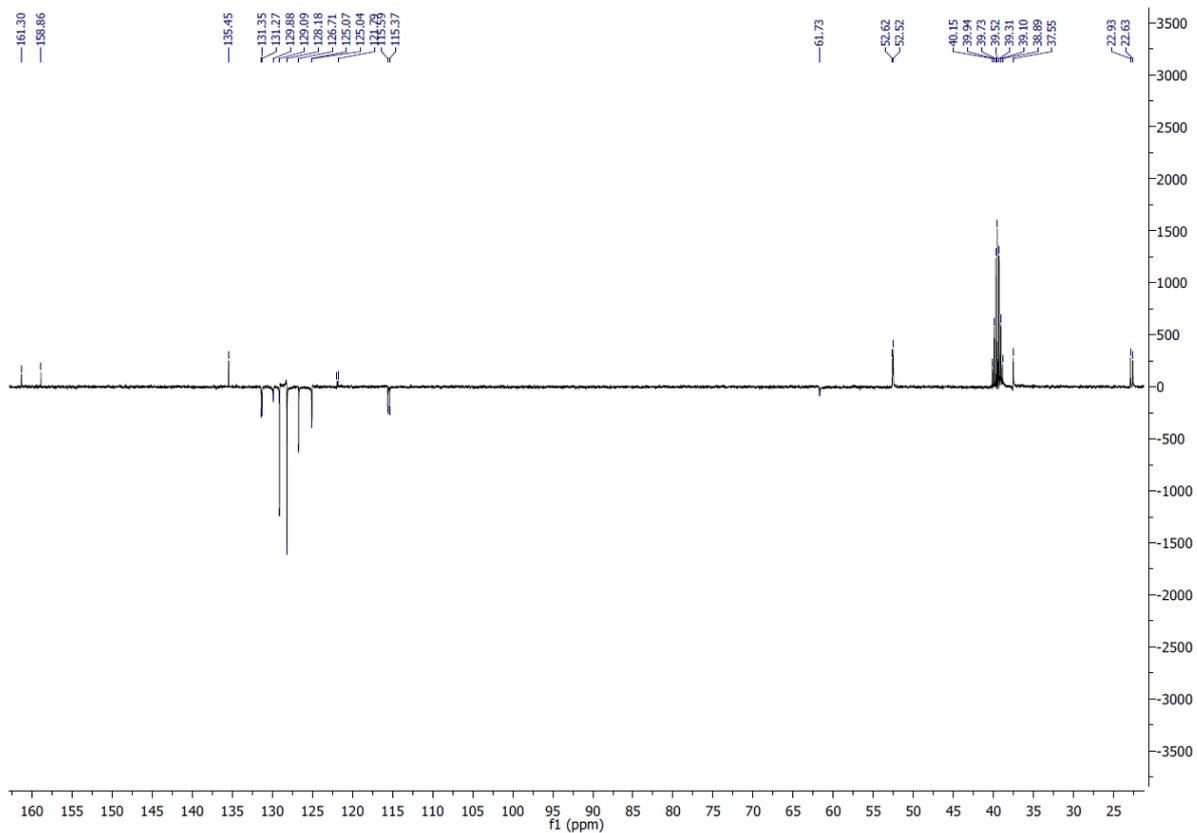
HMBC 2-D NMR of DPPy HCl, zoomed in on aromatic section (d₆-DMSO)

Supporting Information – Drug Testing and Analysis

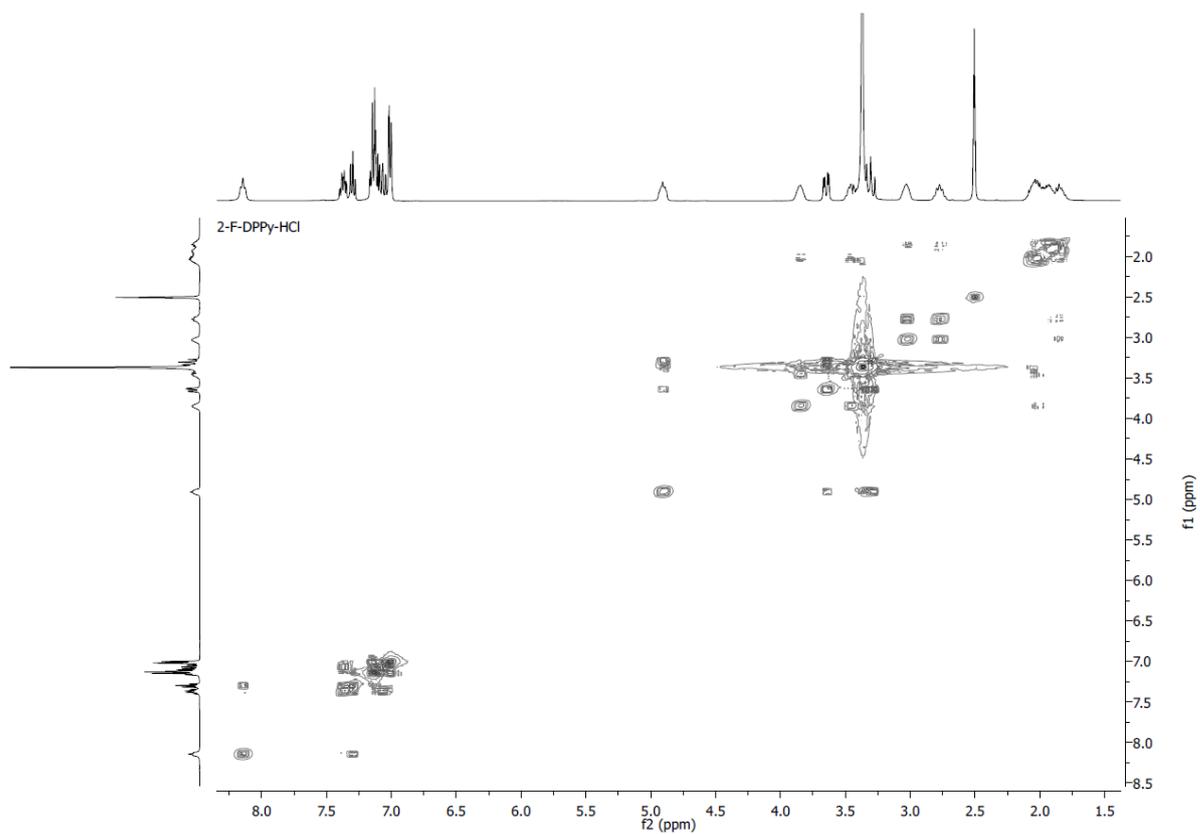


^1H NMR of 2-F-DPPy HCl (400 MHz, d_6 -DMSO)

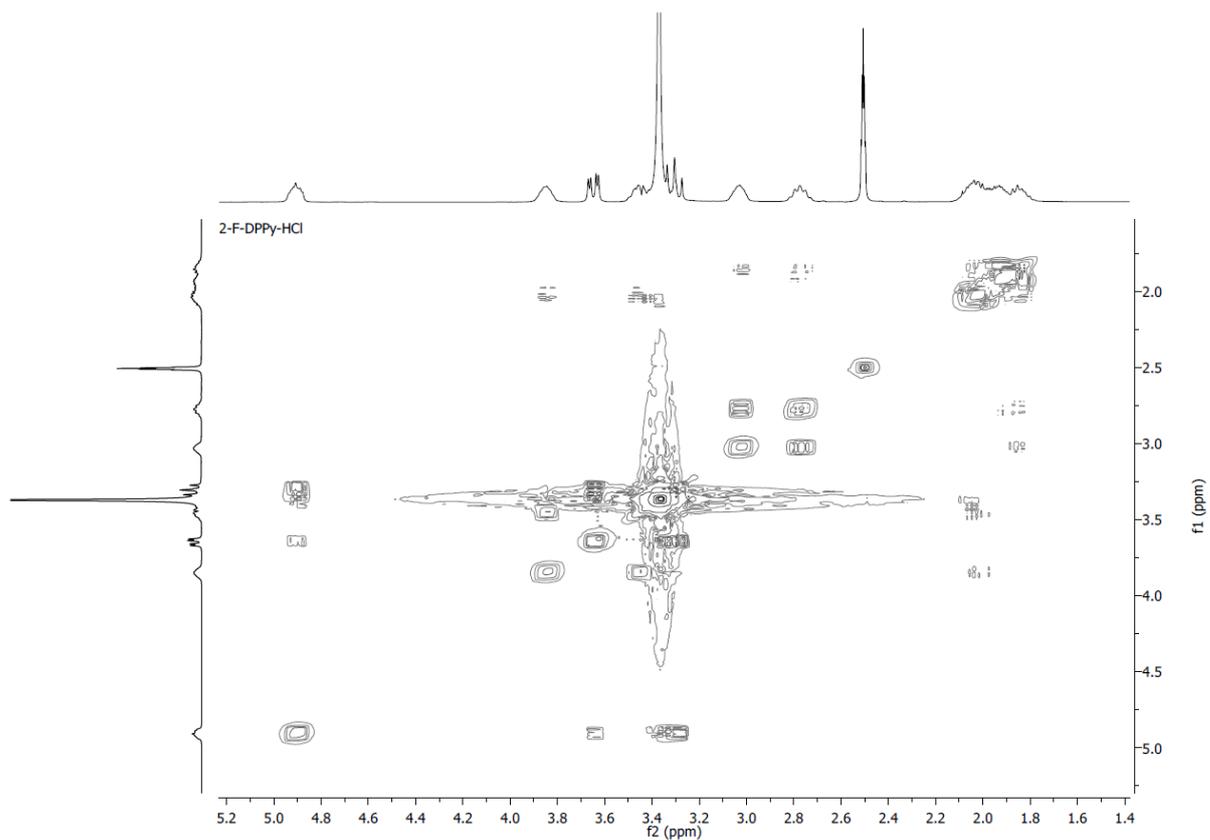
Supporting Information – Drug Testing and Analysis



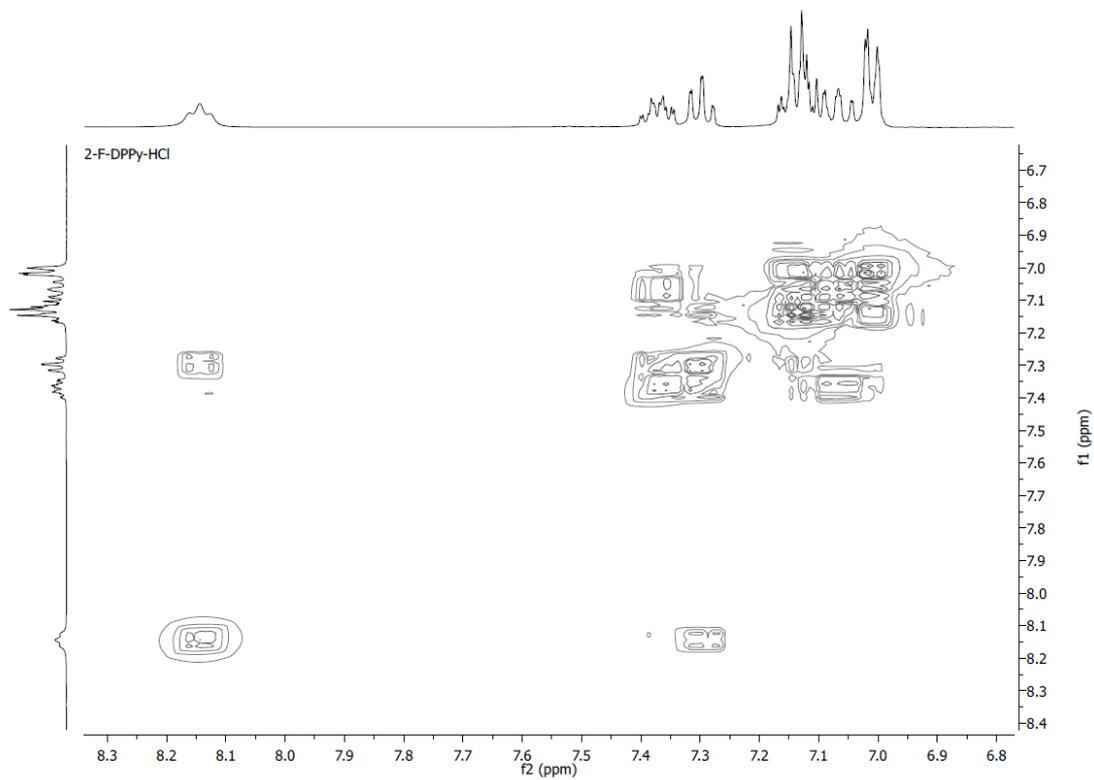
^{13}C PENDANT NMR of 2-F-DPPy HCl (101 MHz, $\text{d}_6\text{-DMSO}$)



COSY-45 2-D NMR of 2-F-DPPy HCl (d_6 -DMSO)

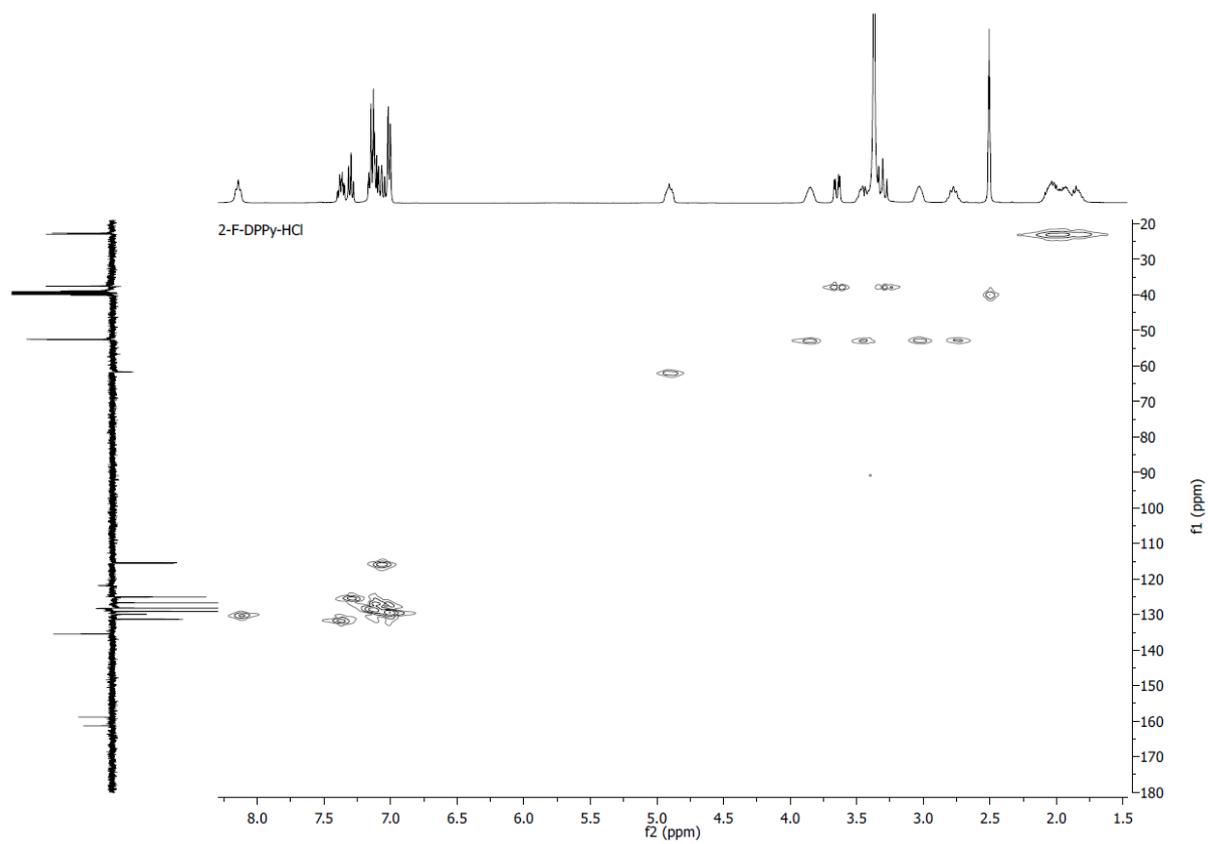


COSY-45 2-D NMR of 2-F-DPPy HCl, zoomed in on aliphatic section (d_6 -DMSO)



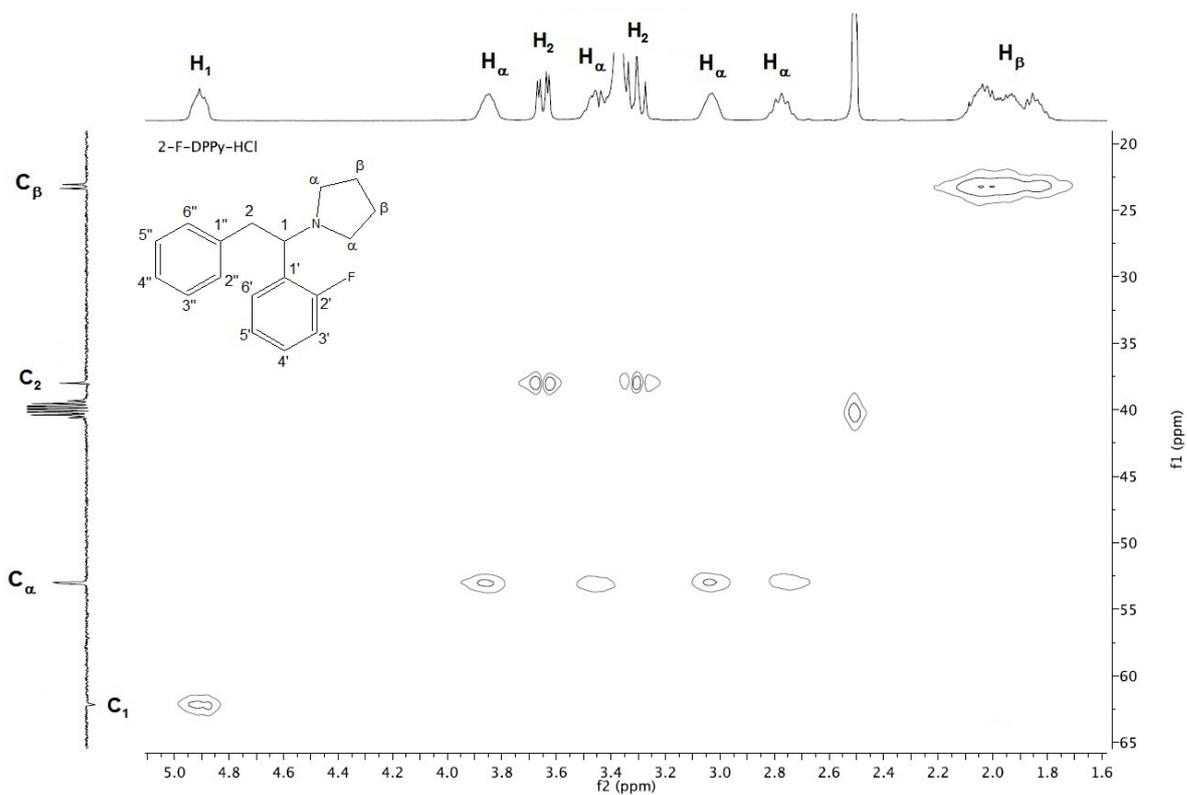
COSY-45 2-D NMR of 2-F-DPPy HCl, zoomed in on aromatic section (d_6 -DMSO)

Supporting Information – Drug Testing and Analysis



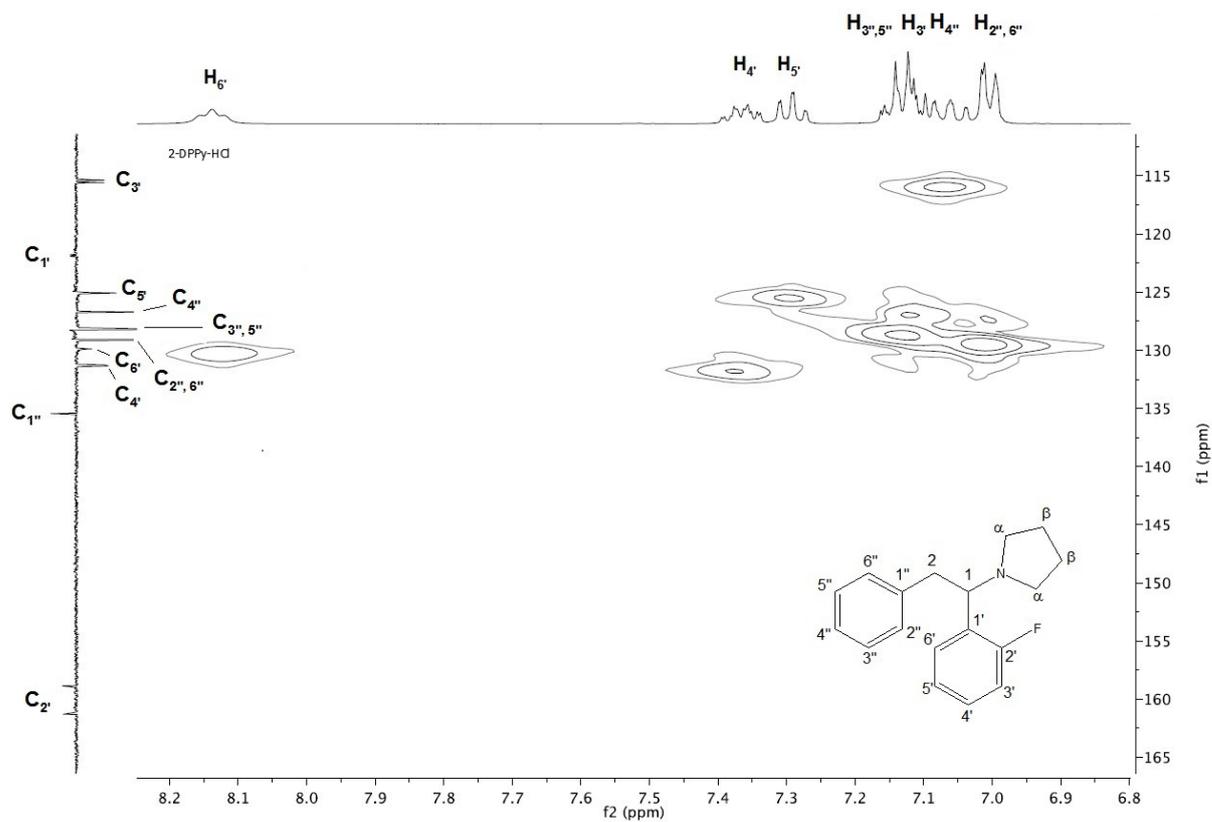
HMQC 2-D NMR of 2-F-DPPy HCl (d_6 -DMSO)

Supporting Information – Drug Testing and Analysis



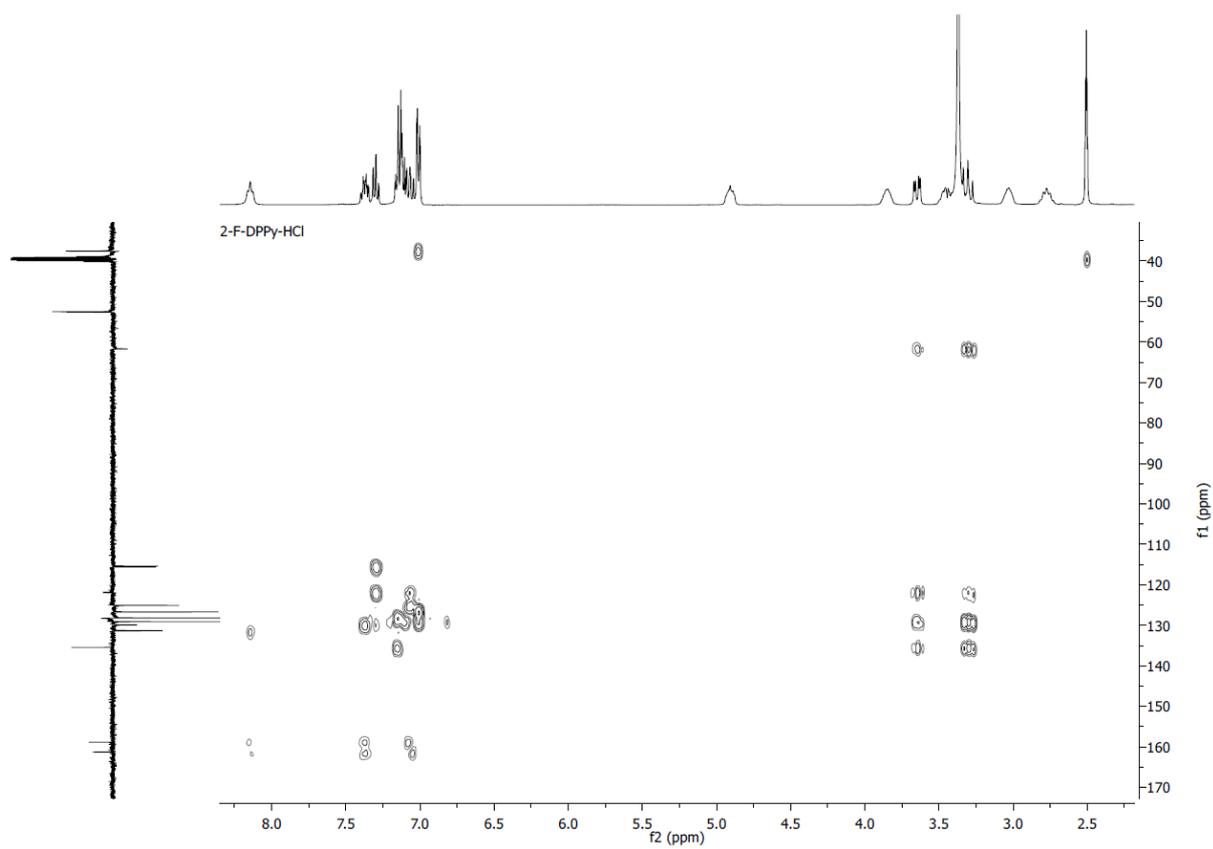
HMQC 2-D NMR of 2-F-DPPy HCl, zoomed in on the aliphatic section (d_6 -DMSO)

Supporting Information – Drug Testing and Analysis



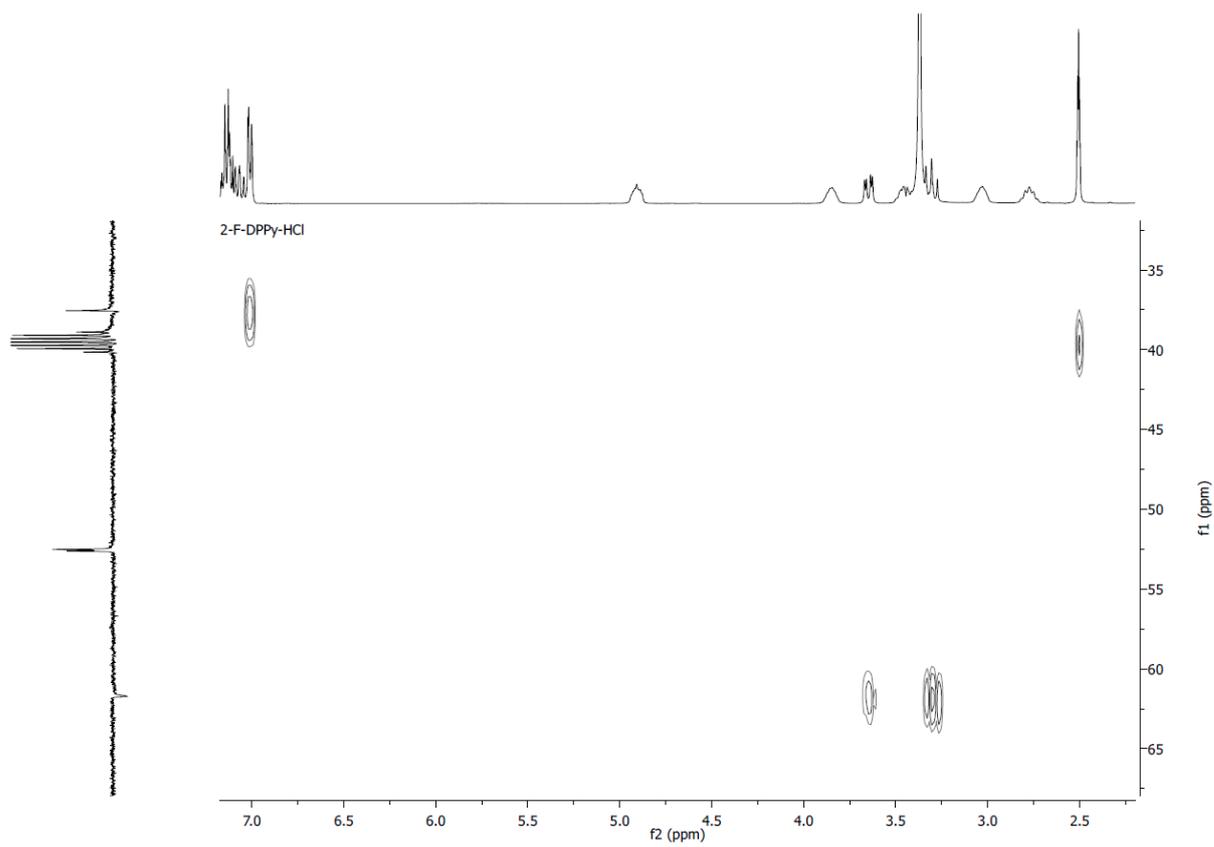
HMQC 2-D NMR of 2-F-DPPy HCl, zoomed in on the aromatic section (d_6 -DMSO)

Supporting Information – Drug Testing and Analysis

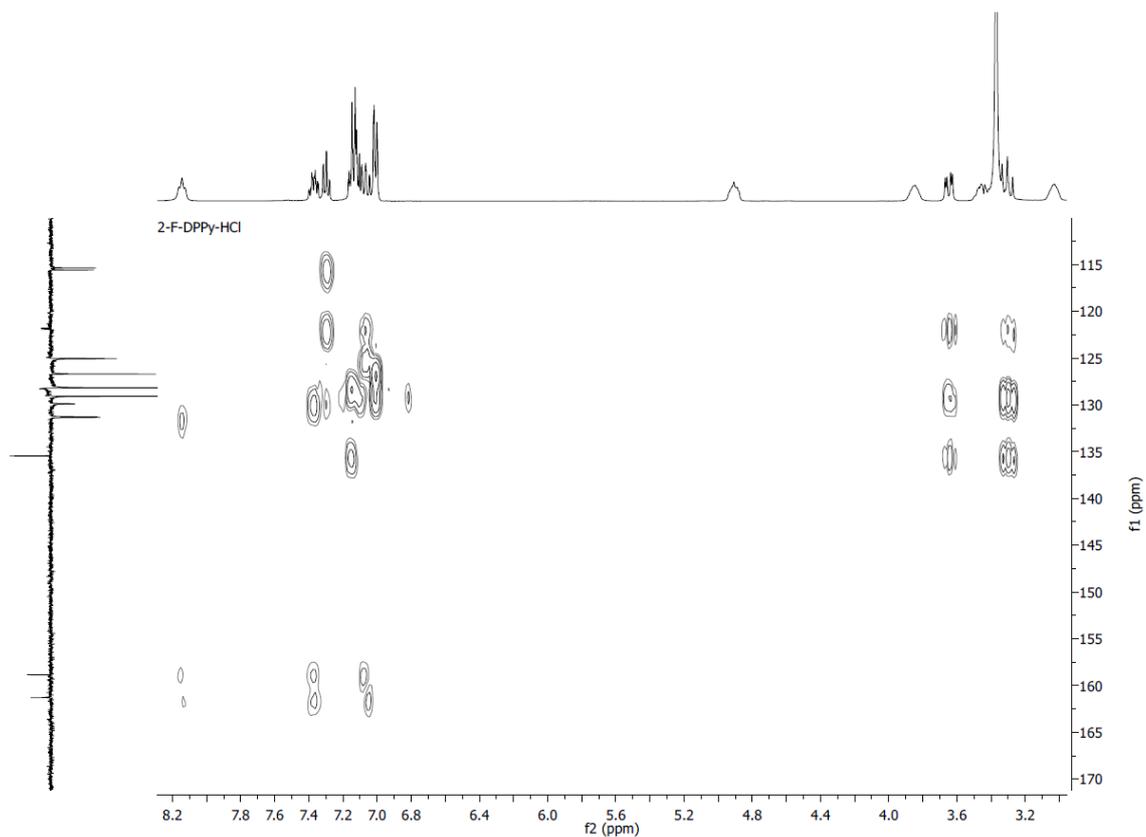


HMBC 2-D NMR of 2-F-DPPy HCl (d_6 -DMSO)

Supporting Information – Drug Testing and Analysis

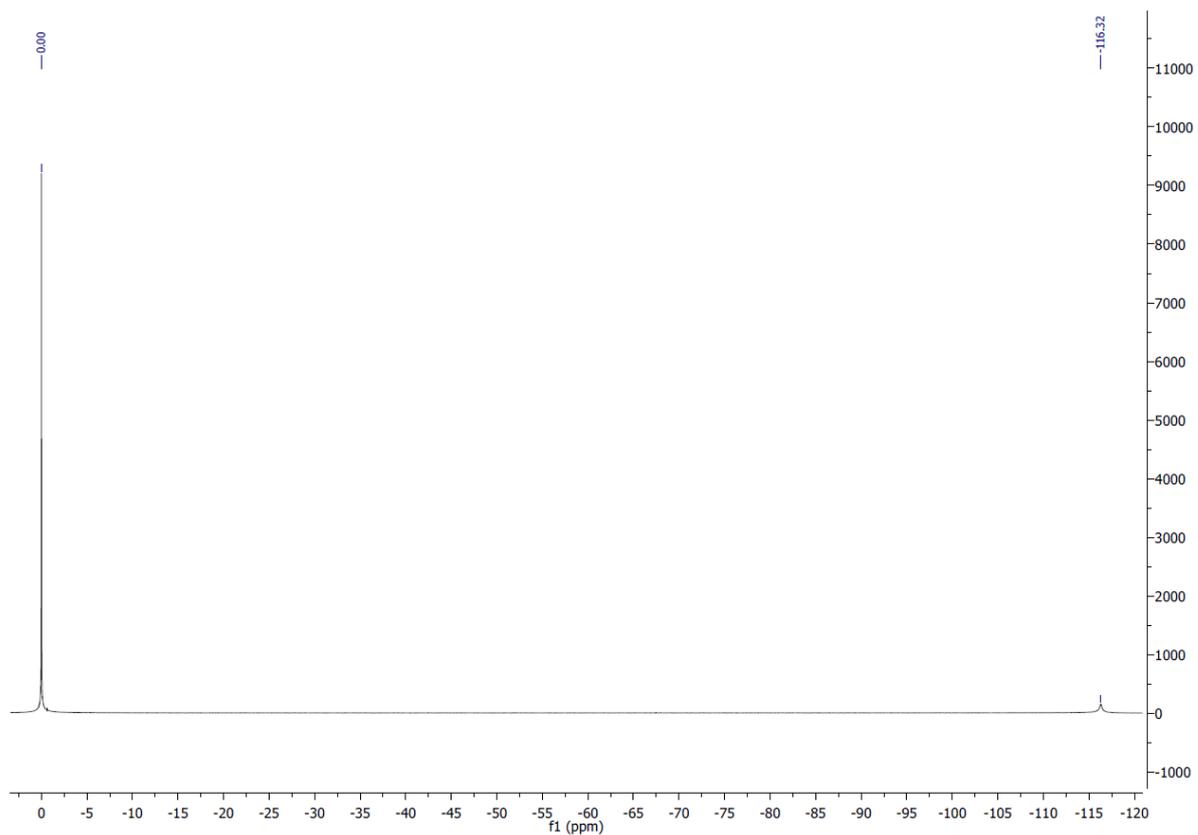


HMBC 2-D NMR of 2-F-DPPy HCl, zoomed in on the aliphatic section (d_6 -DMSO)



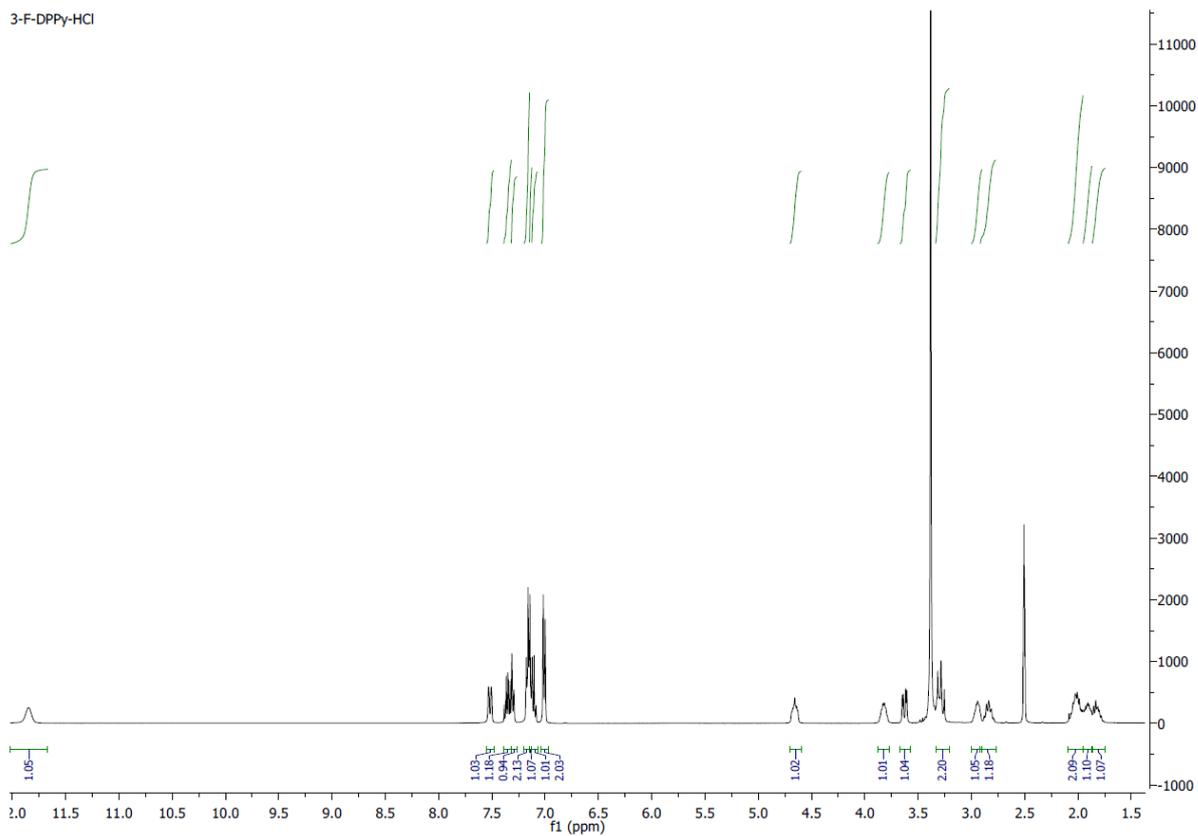
HMBC 2-D NMR of 2-F-DPPy HCl, zoomed in on the aromatic section (d_6 -DMSO)

Supporting Information – Drug Testing and Analysis



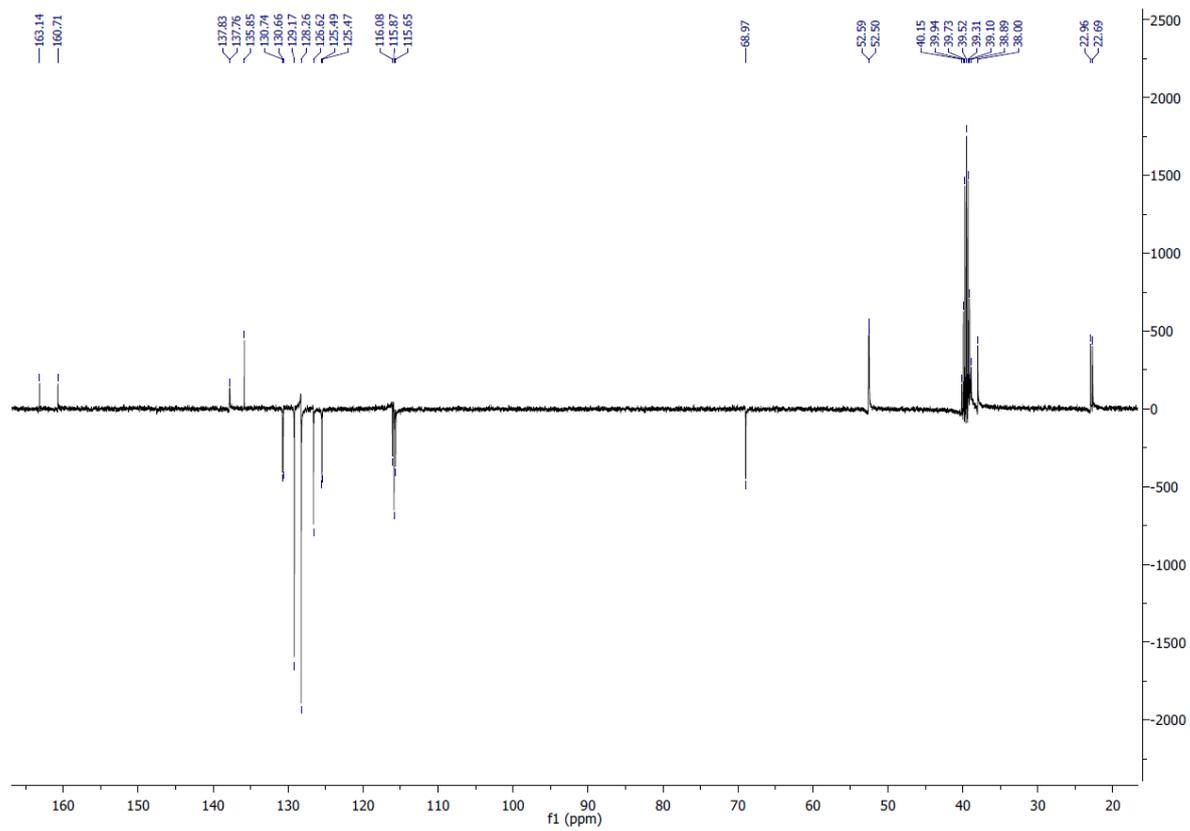
^{19}F NMR of 2-F-DPPy HCl with CFCl_3 as internal reference (376.5 MHz, d_6 -DMSO)

Supporting Information – Drug Testing and Analysis

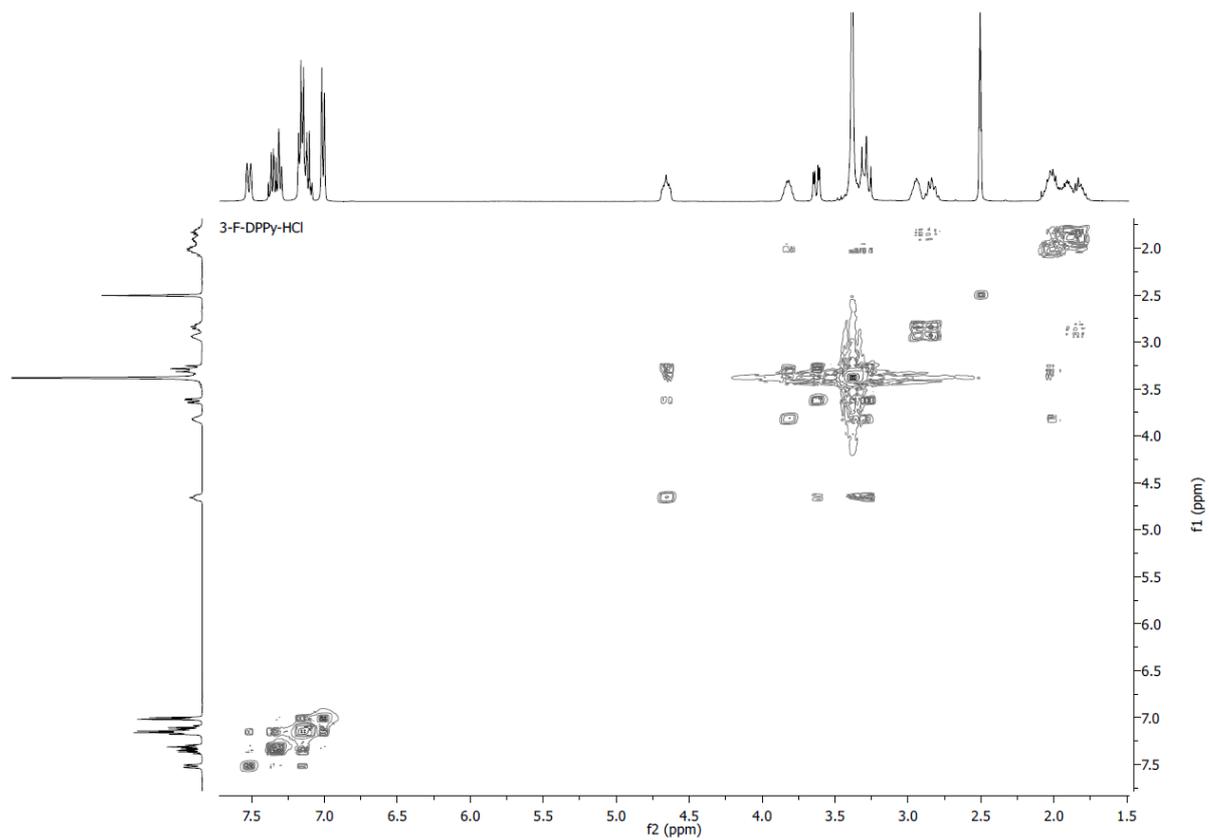


^1H NMR of 3-F-DPPy HCl (400 MHz, $\text{d}_6\text{-DMSO}$)

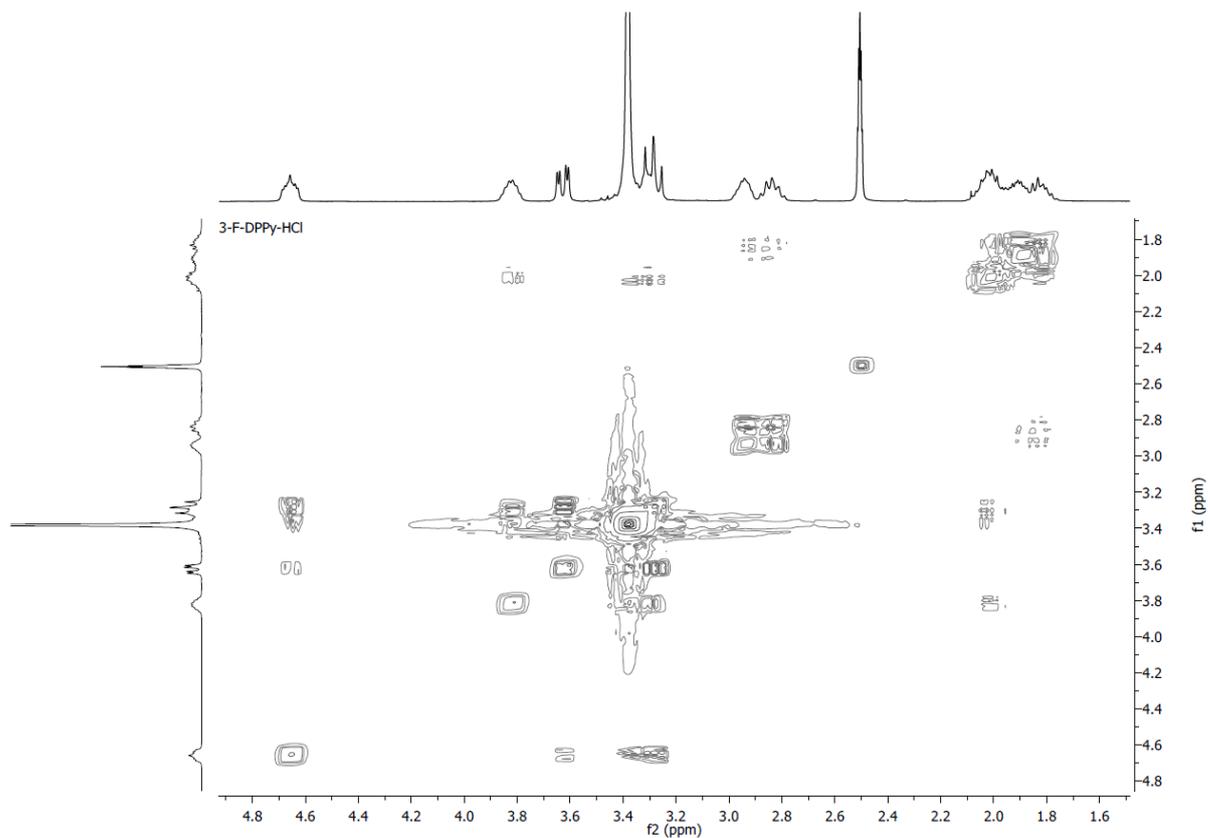
Supporting Information – Drug Testing and Analysis



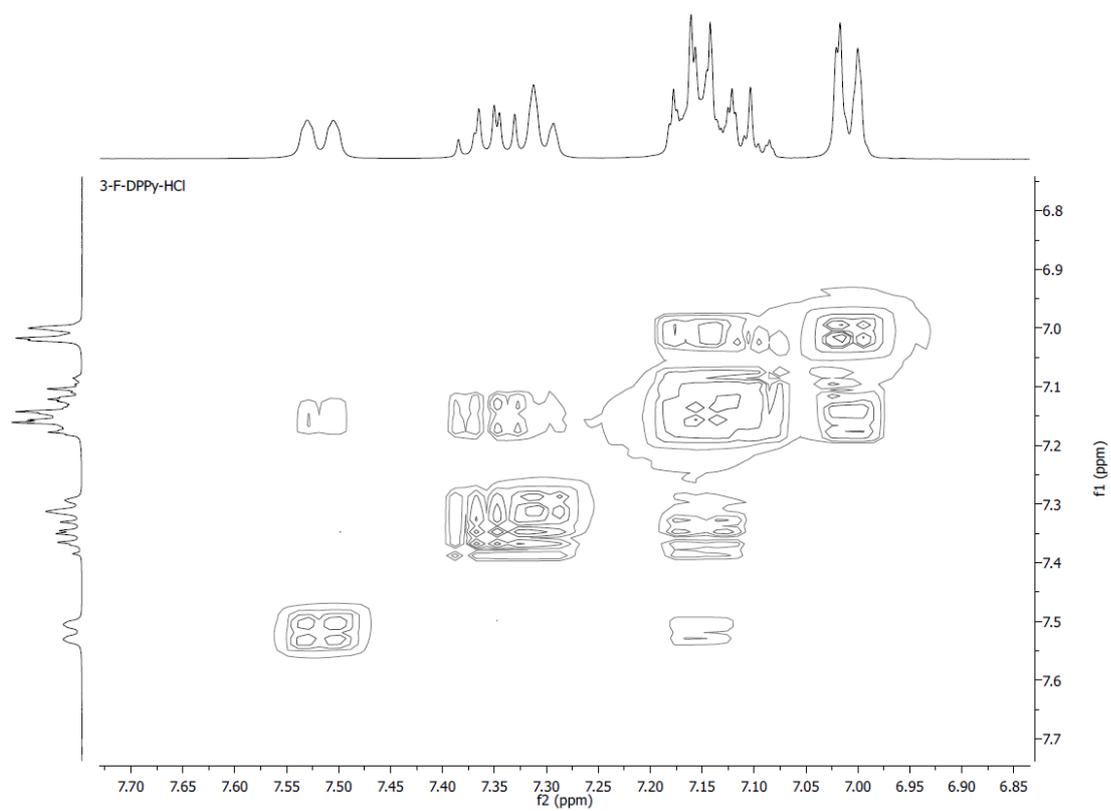
^{13}C PENDANT NMR of 3-F-DPPy HCl (101 MHz, $\text{d}_6\text{-DMSO}$)



COSY-45 2-D NMR of 3-F-DPPy HCl (d₆-DMSO)

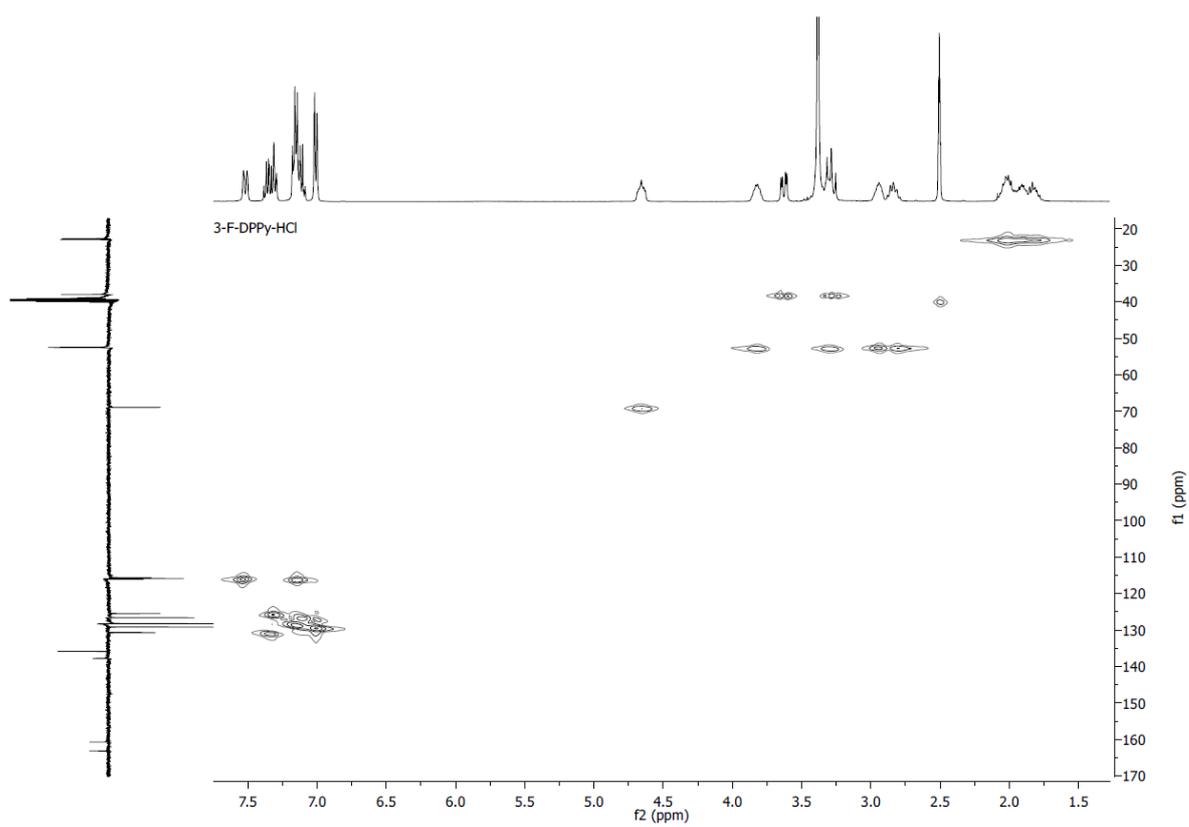


COSY-45 2-D NMR of 3-F-DPPy HCl, zoomed in on aliphatic section (d₆-DMSO)

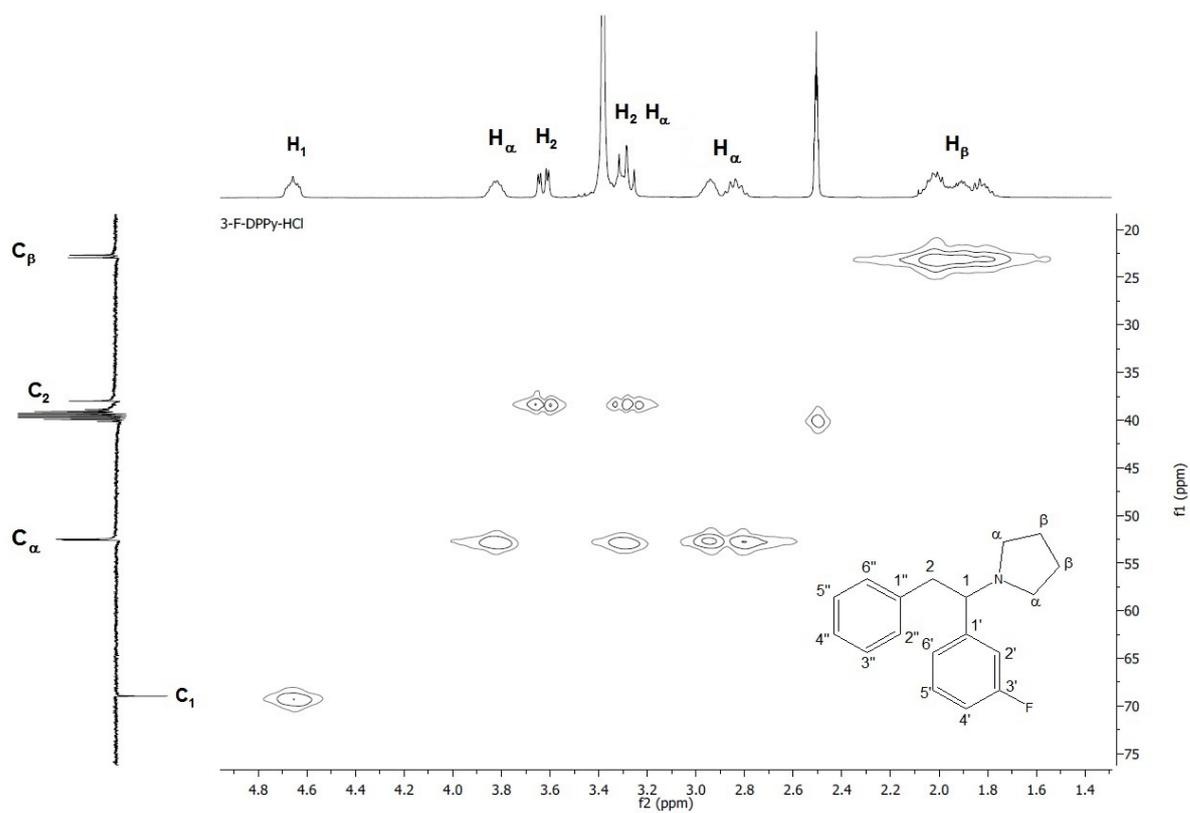


COSY-45 2-D NMR of 3-F-DPPy HCl, zoomed in on aromatic section (d_6 -DMSO)

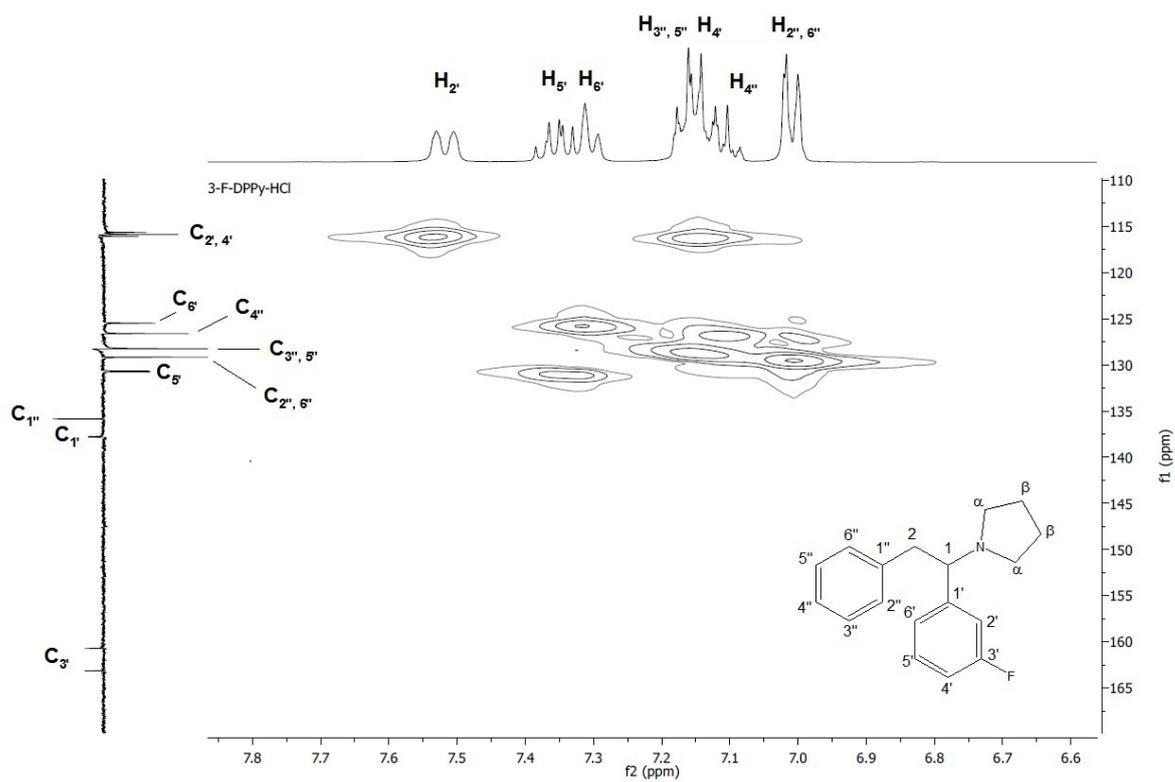
Supporting Information – Drug Testing and Analysis



HMQC 2-D NMR of 3-F-DPPy HCl (d_6 -DMSO)

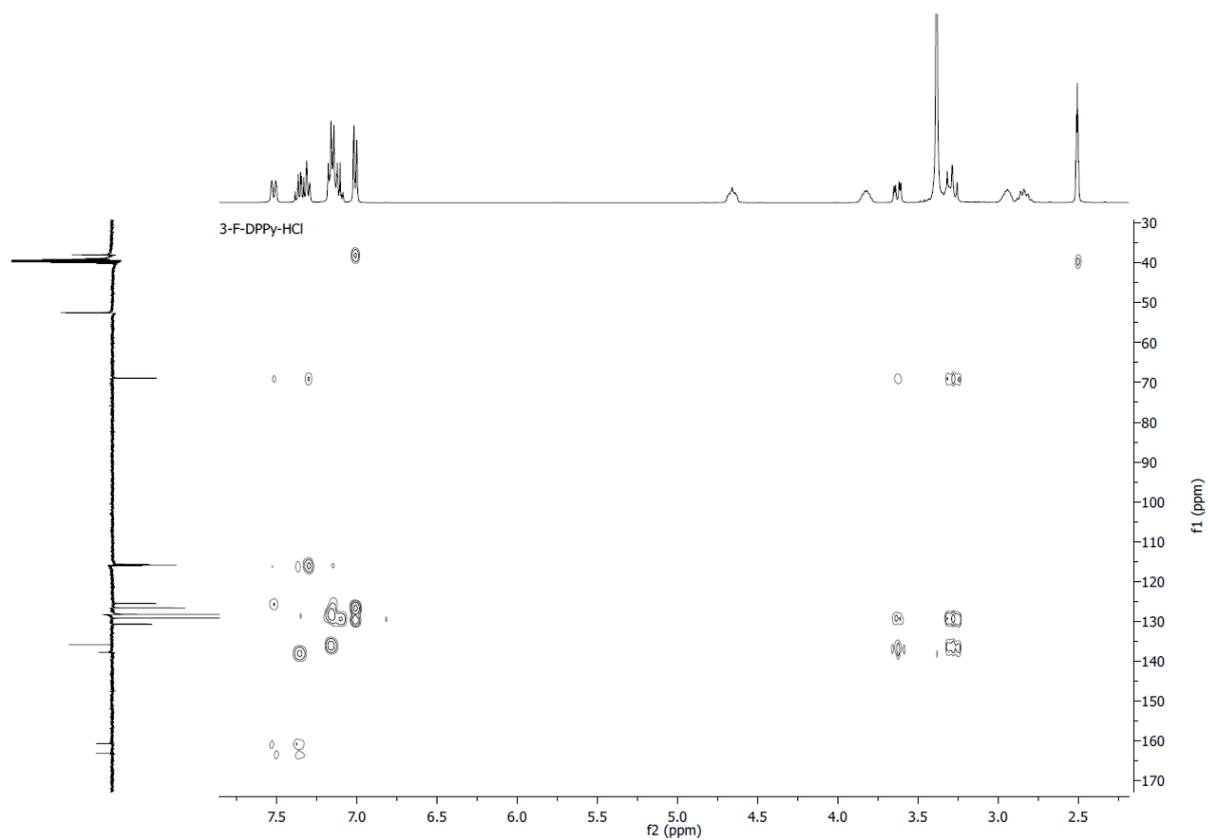


HMQC 2-D NMR of 3-F-DPPy HCl, zoomed in on aliphatic section (d_6 -DMSO)



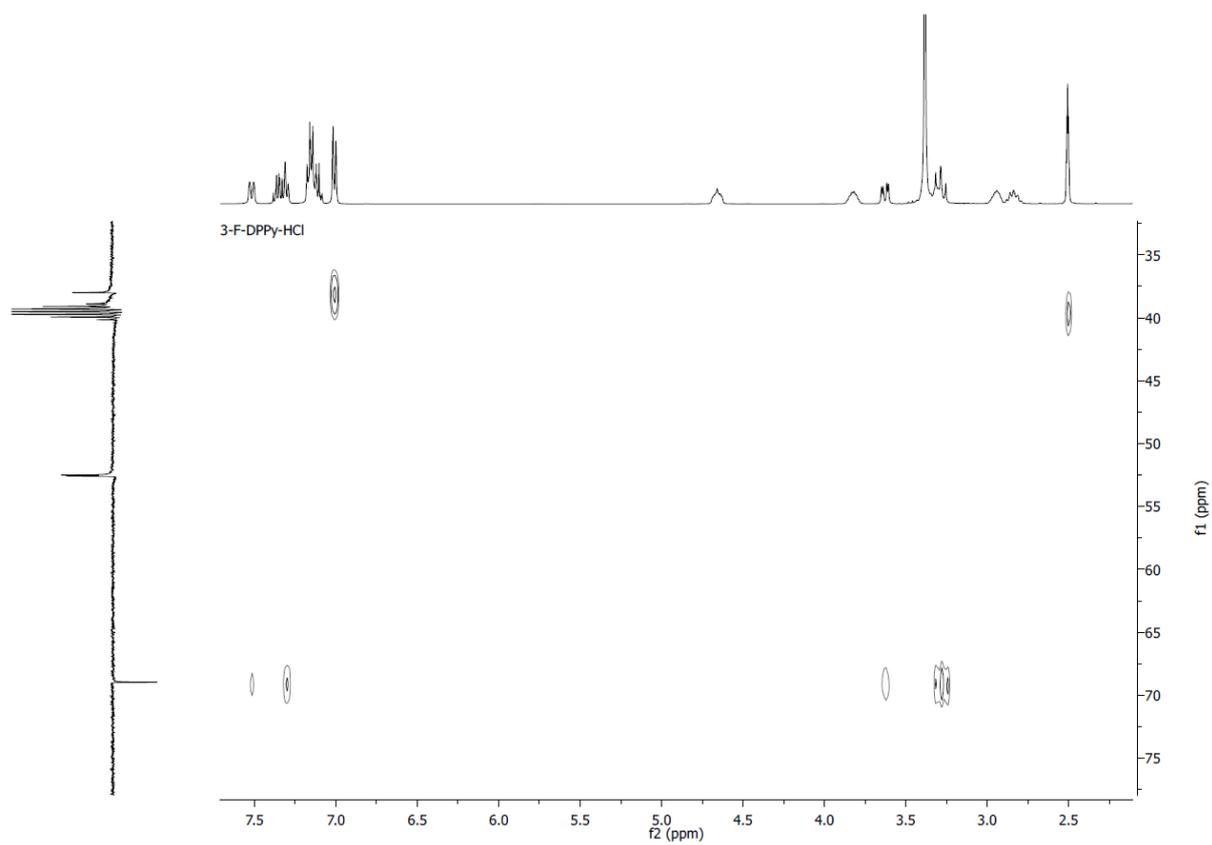
HMQC 2-D NMR of 3-F-DPPy HCl, zoomed in on aromatic section (d_6 -DMSO)

Supporting Information – Drug Testing and Analysis

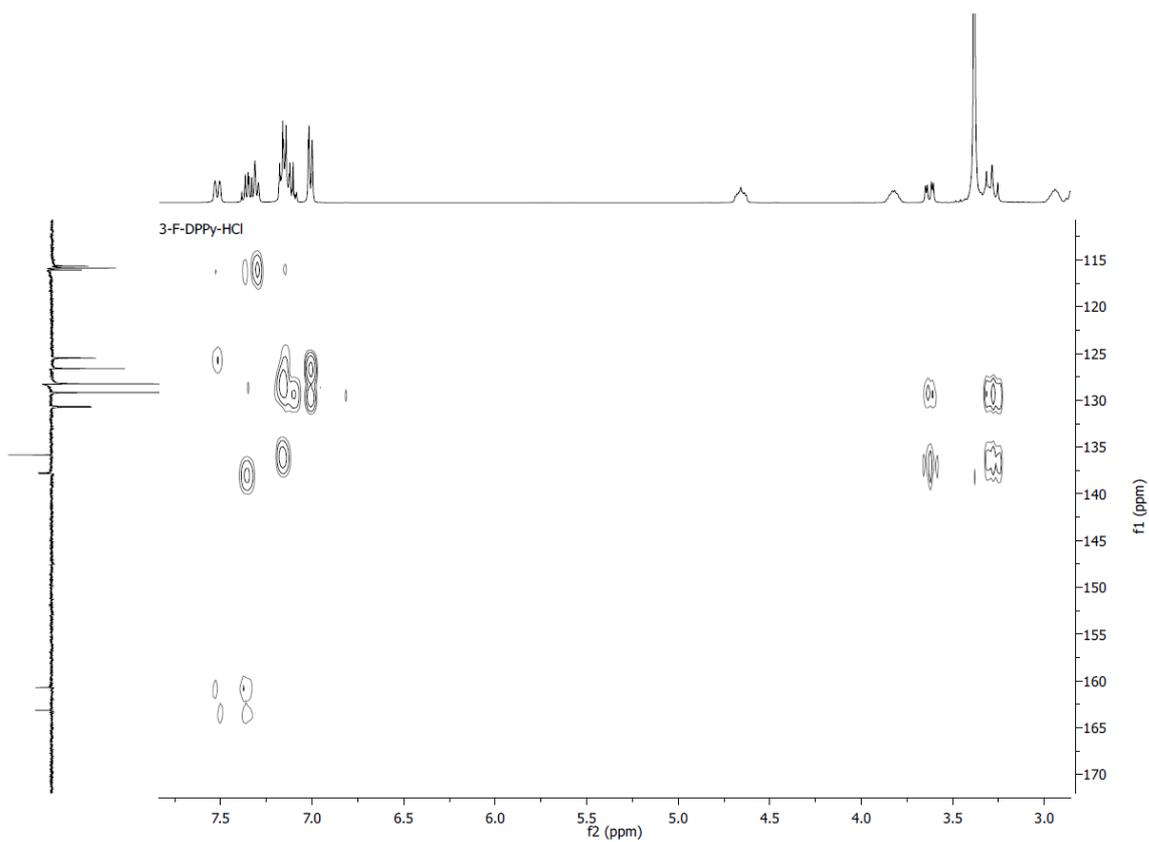


HMBC 2-D NMR of 3-F-DPPy HCl (d_6 -DMSO)

Supporting Information – Drug Testing and Analysis

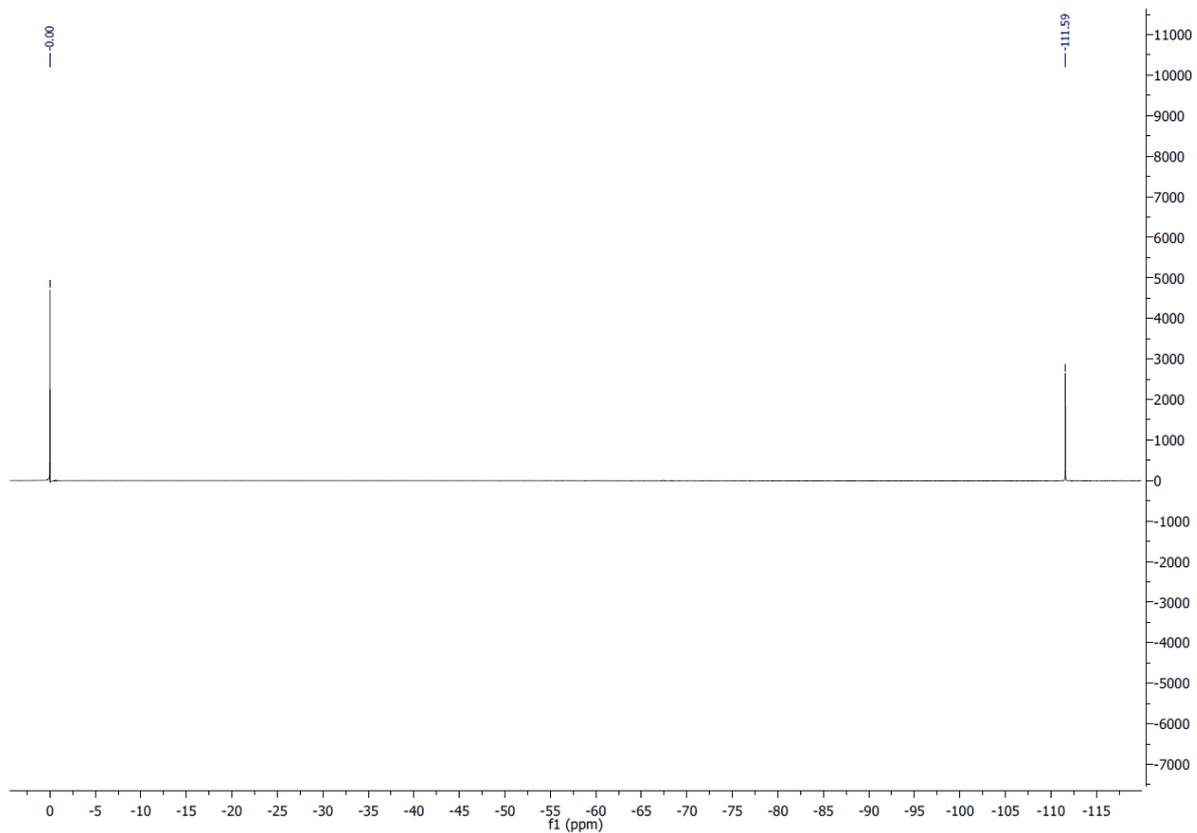


HMBC 2-D NMR of 3-F-DPPy HCl, zoomed in on the aliphatic section (d_6 -DMSO)



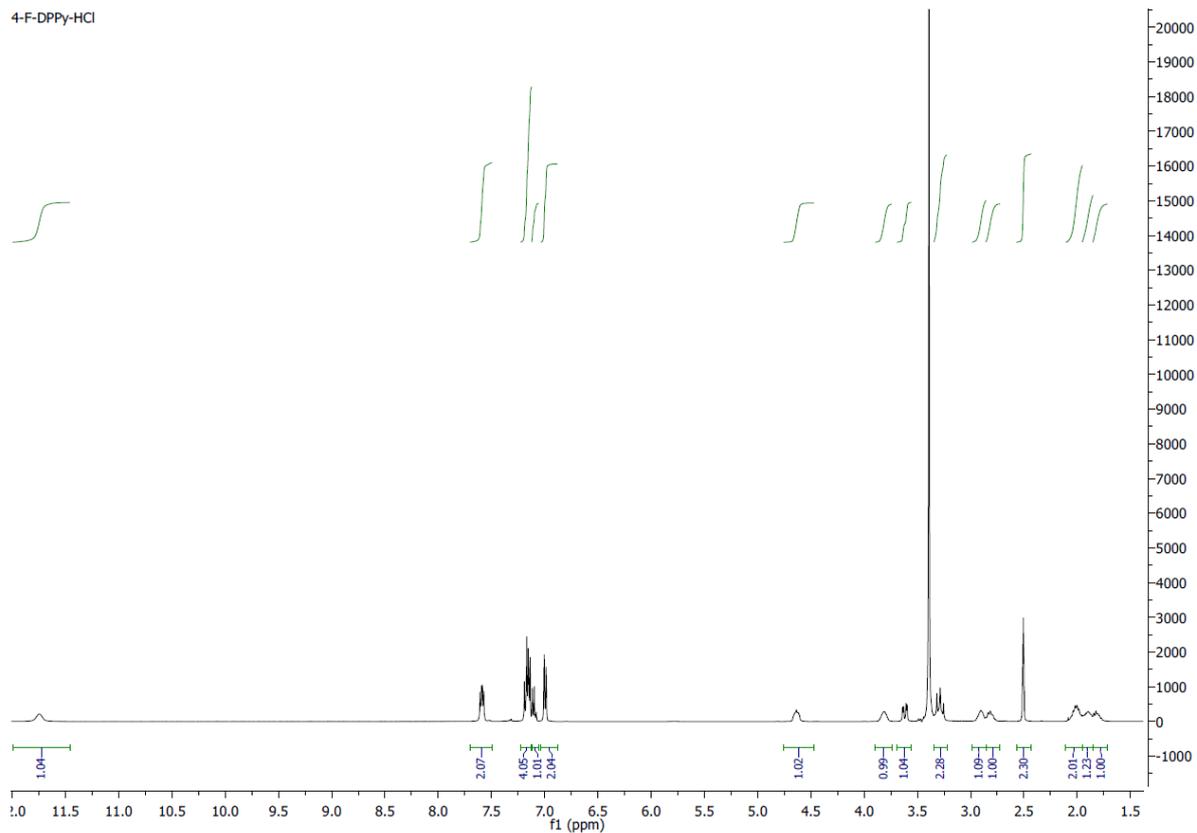
HMBC 2-D NMR of 3-F-DPPy HCl, zoomed in on the aromatic section (d₆-DMSO)

Supporting Information – Drug Testing and Analysis



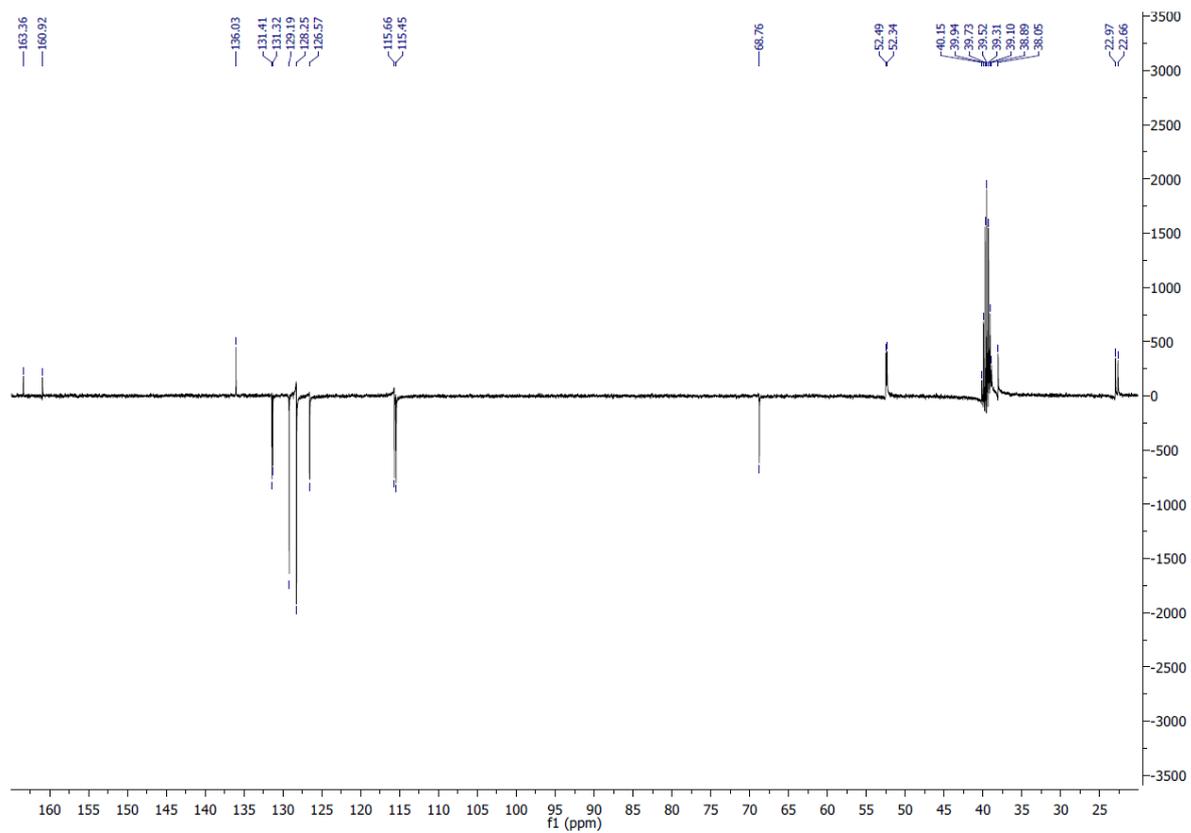
^{19}F NMR of 3-F-DPPy HCl with CFCl_3 as internal reference (376.5 MHz, d_6 -DMSO)

Supporting Information – Drug Testing and Analysis



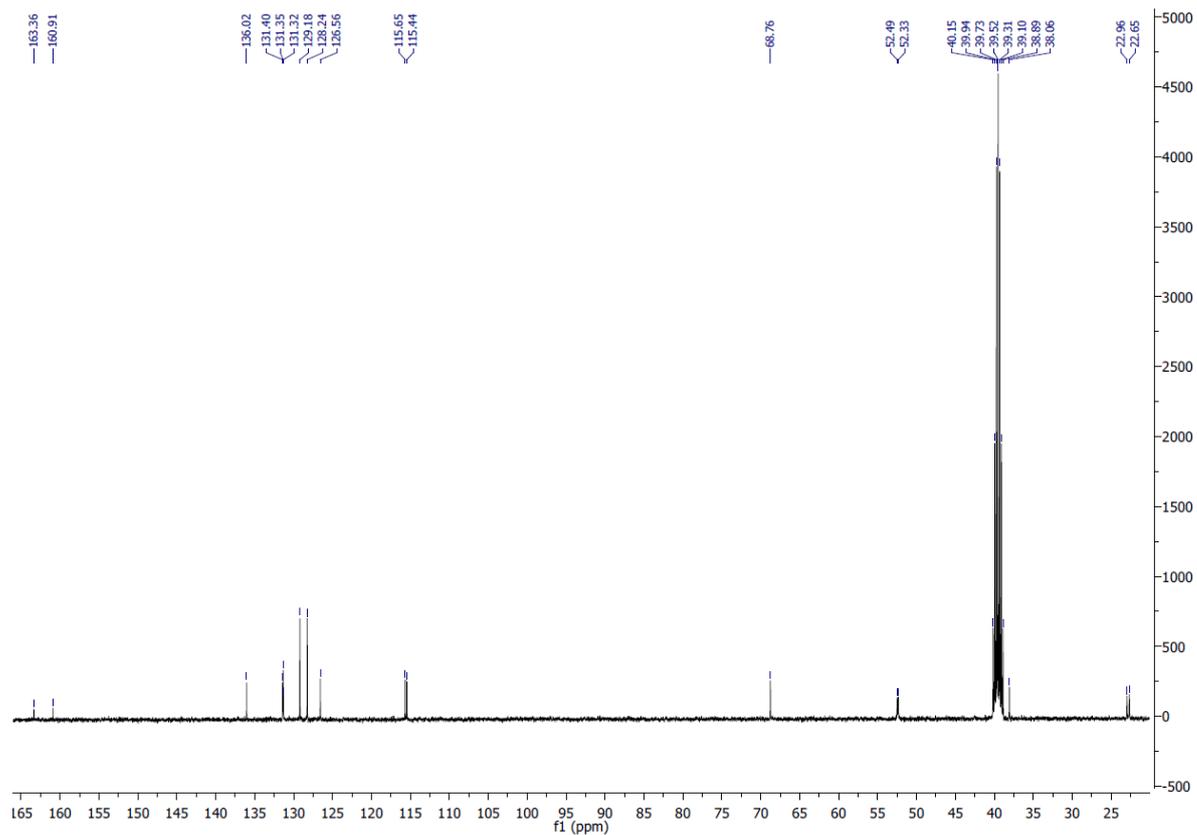
^1H NMR of 4-F-DPPy HCl (400 MHz, $\text{d}_6\text{-DMSO}$)

Supporting Information – Drug Testing and Analysis



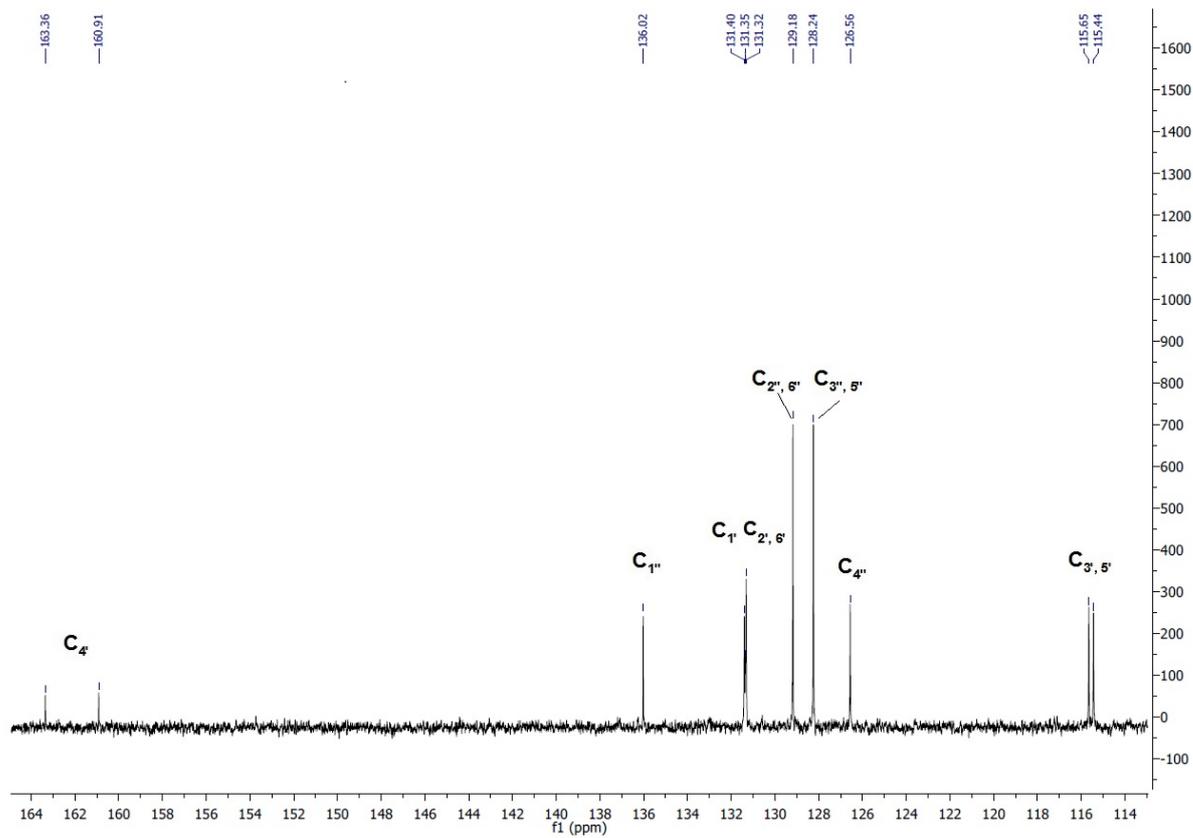
^{13}C PENDANT NMR of 4-F-DPPy HCl (101 MHz, $\text{d}_6\text{-DMSO}$)

Supporting Information – Drug Testing and Analysis



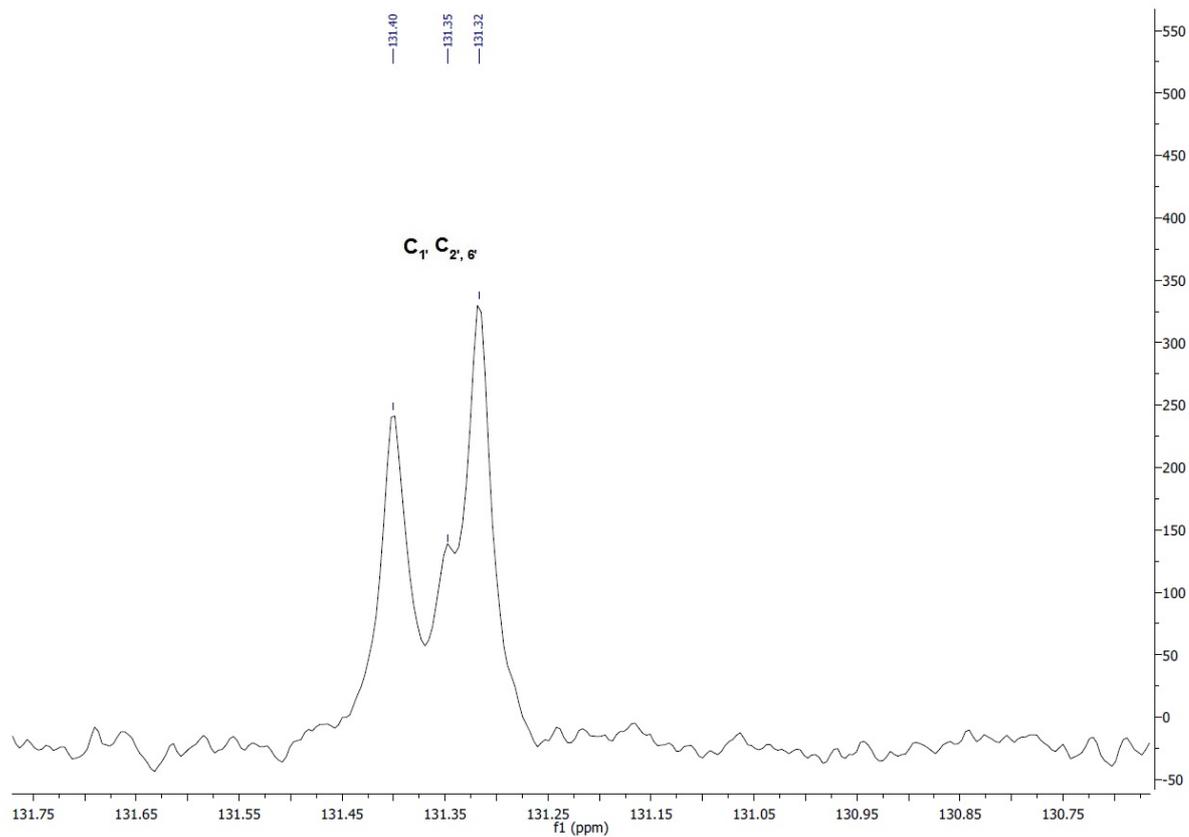
^{13}C NMR of 4-F-DPPy HCl (101 MHz, $\text{d}_6\text{-DMSO}$)

Supporting Information – Drug Testing and Analysis

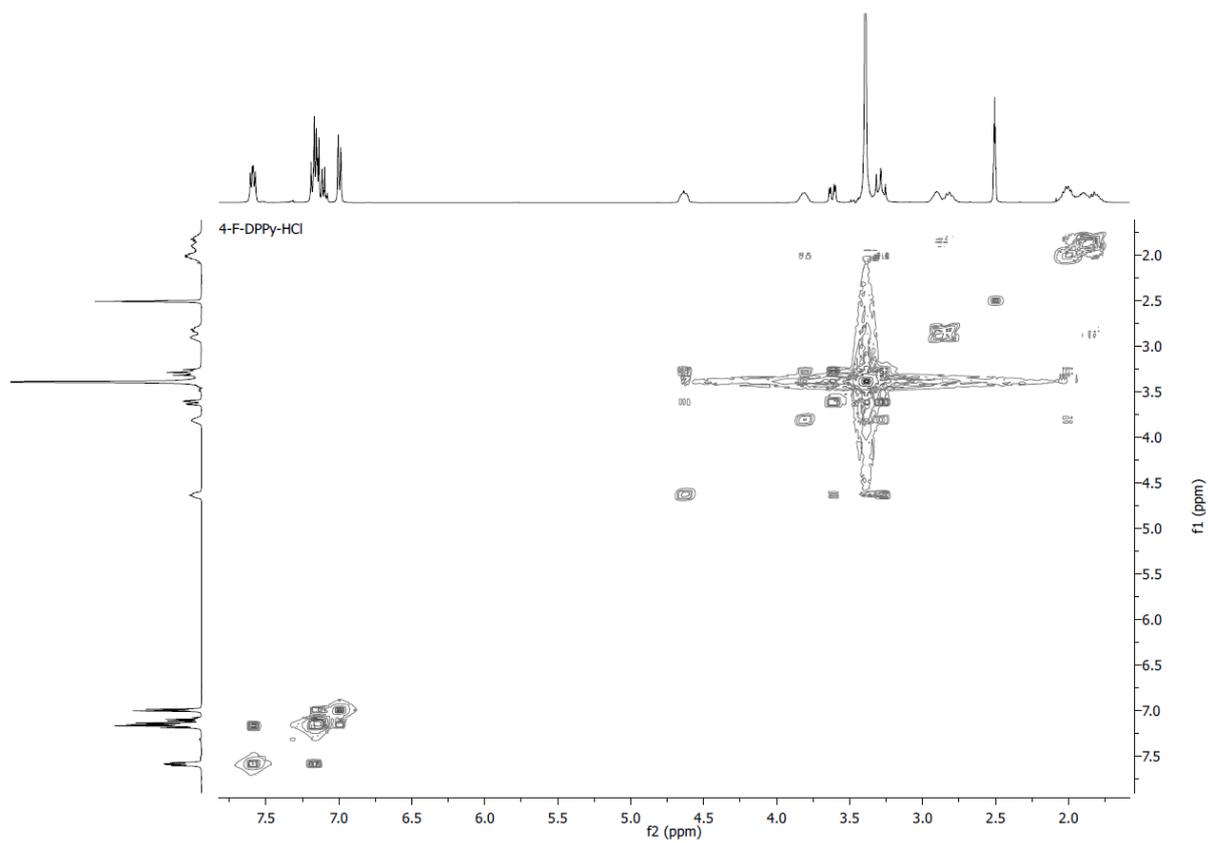


^{13}C NMR of 4-F-DPPy HCl, zoomed in on the aromatic section (101 MHz, d_6 -DMSO)

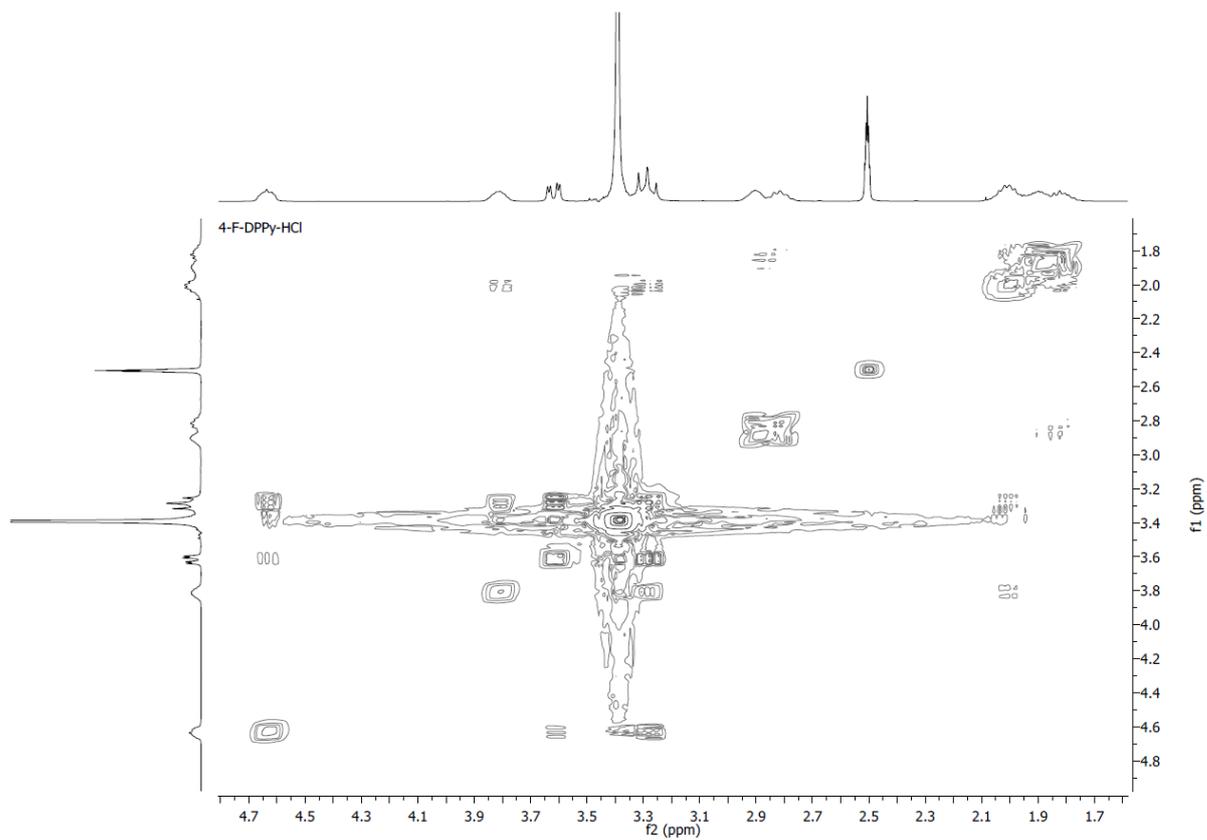
Supporting Information – Drug Testing and Analysis



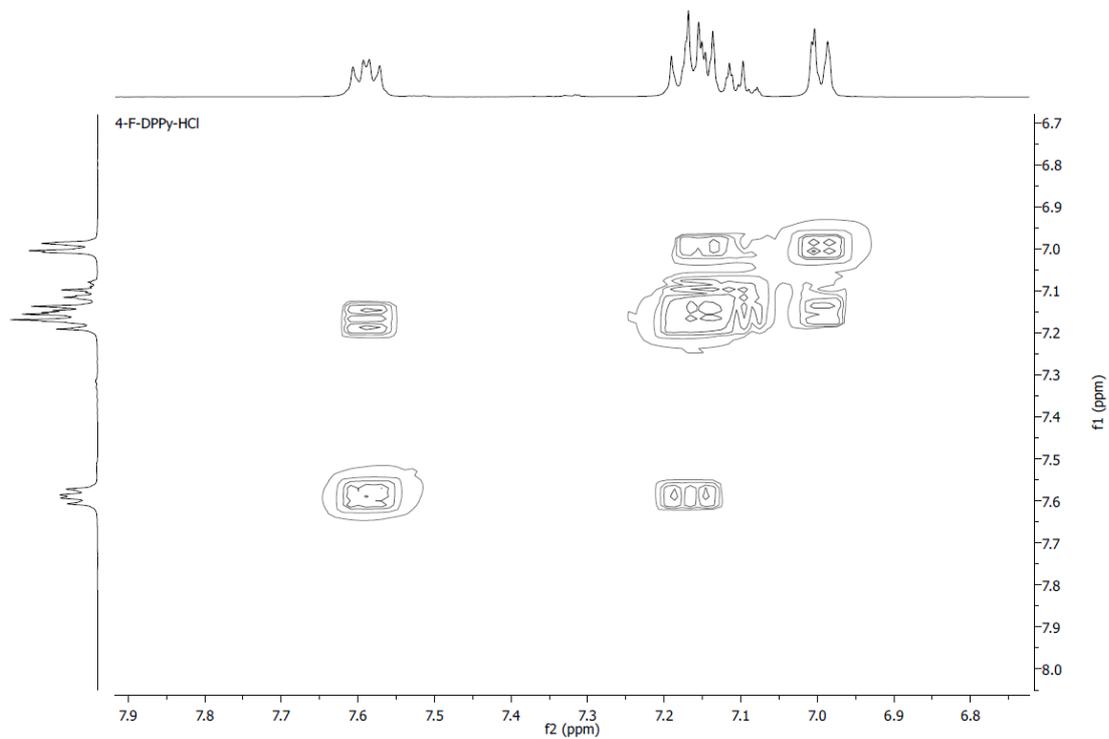
^{13}C NMR of 4-F-DPPy HCl, zoomed in to display $\text{C}_1, \text{C}_2, \text{C}_6$ overlap (101 MHz, d_6 -DMSO)



COSY-45 2-D NMR of 4-F-DPPy HCl (d₆-DMSO)

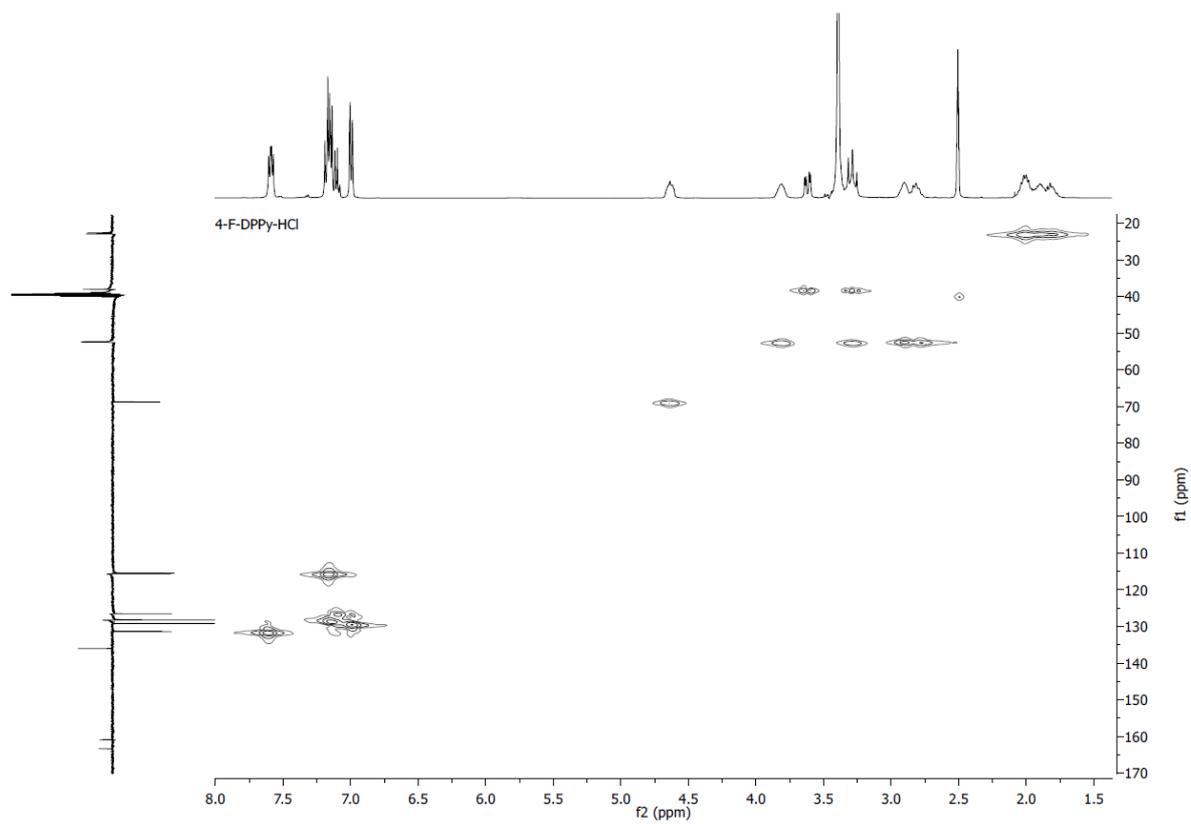


COSY-45 2-D NMR of 4-F-DPPy HCl, zoomed in on aliphatic section (d_6 -DMSO)

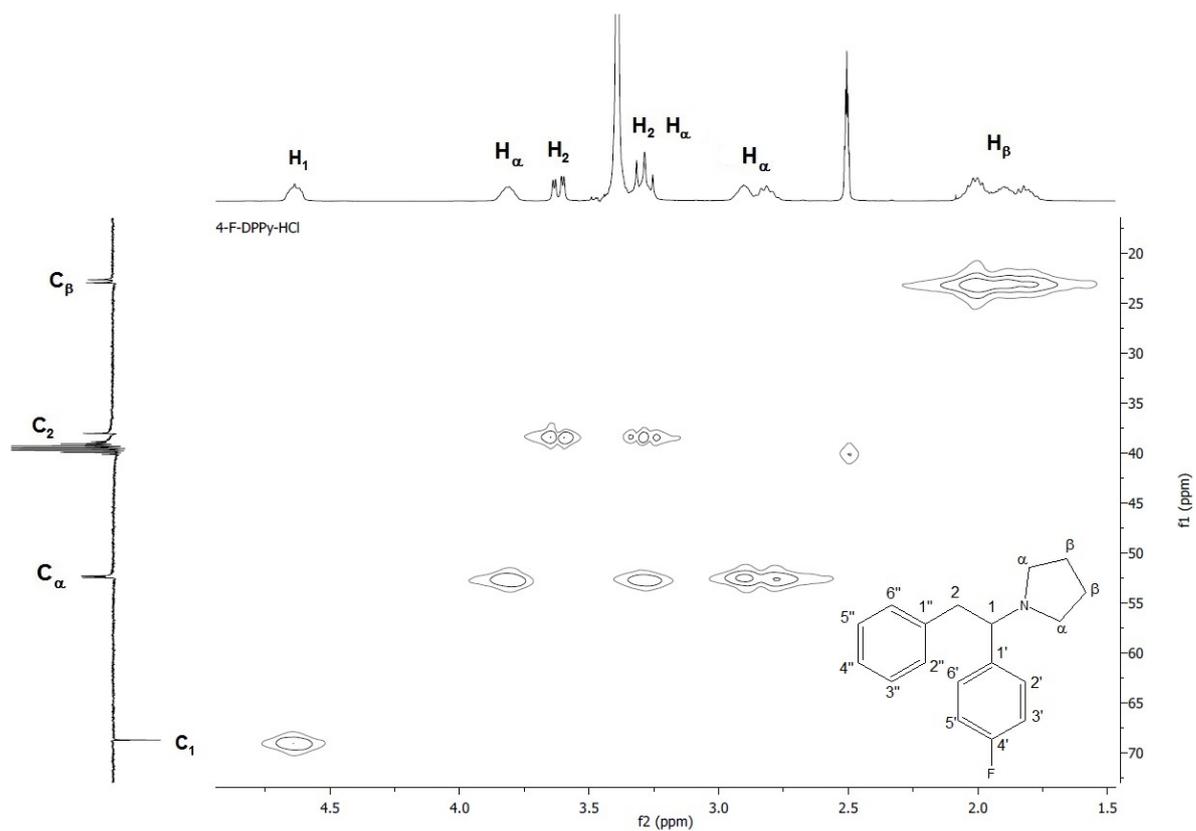


COSY-45 2-D NMR of 4-F-DPPy HCl, zoomed in on aromatic section (d_6 -DMSO)

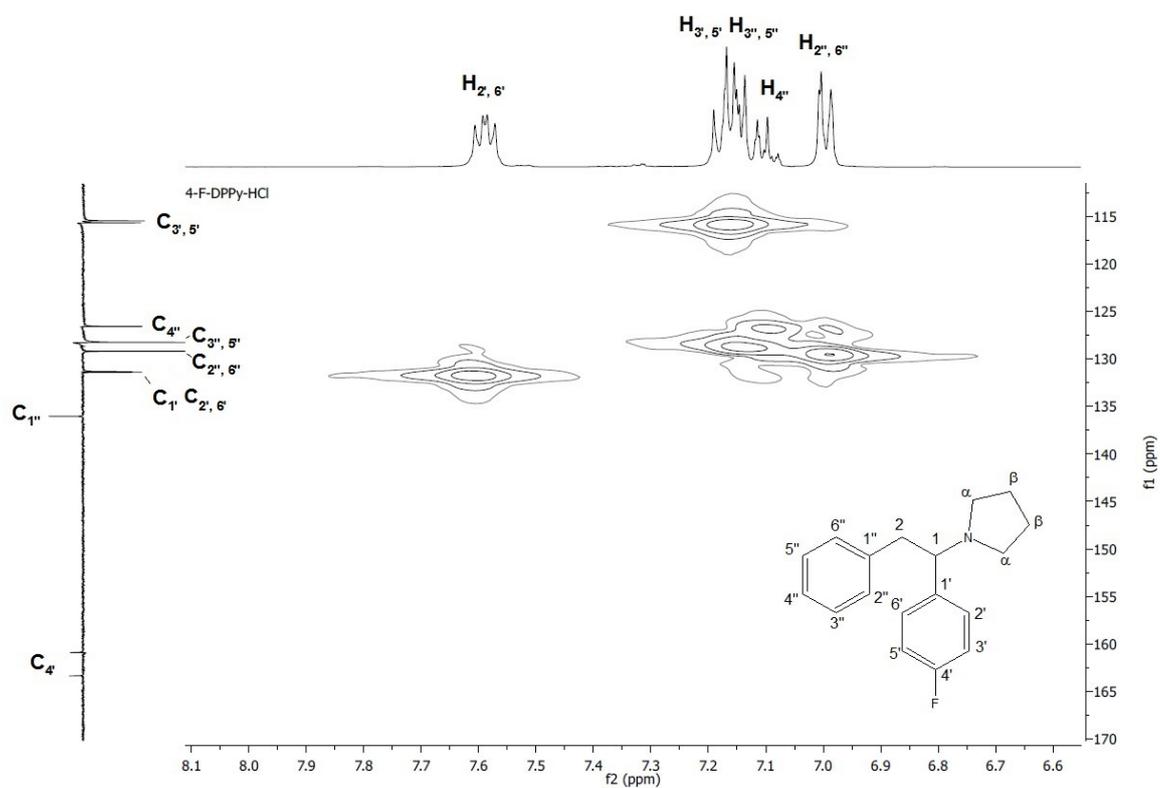
Supporting Information – Drug Testing and Analysis



HMQC 2-D NMR of 4-F-DPPy HCl (d_6 -DMSO)

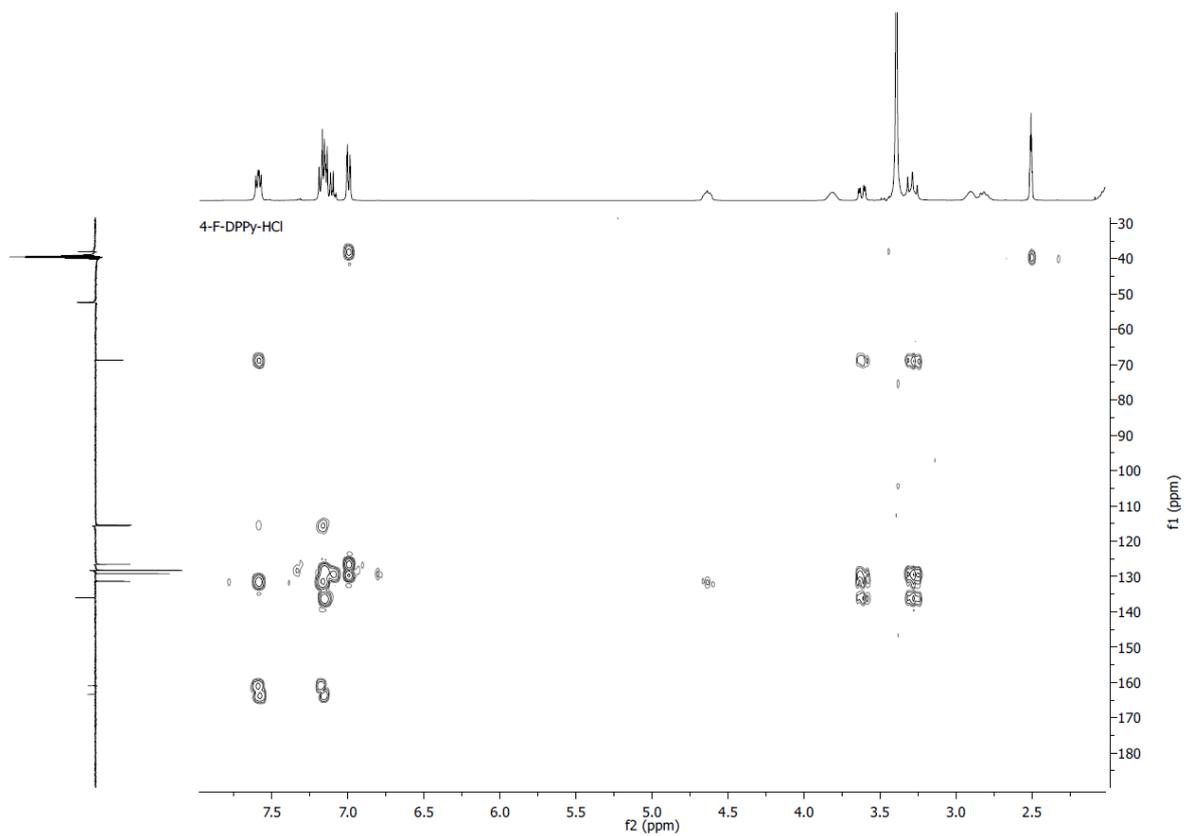


HMQC 2-D NMR of 4-F-DPPy HCl, zoomed in on aliphatic section (d_6 -DMSO)

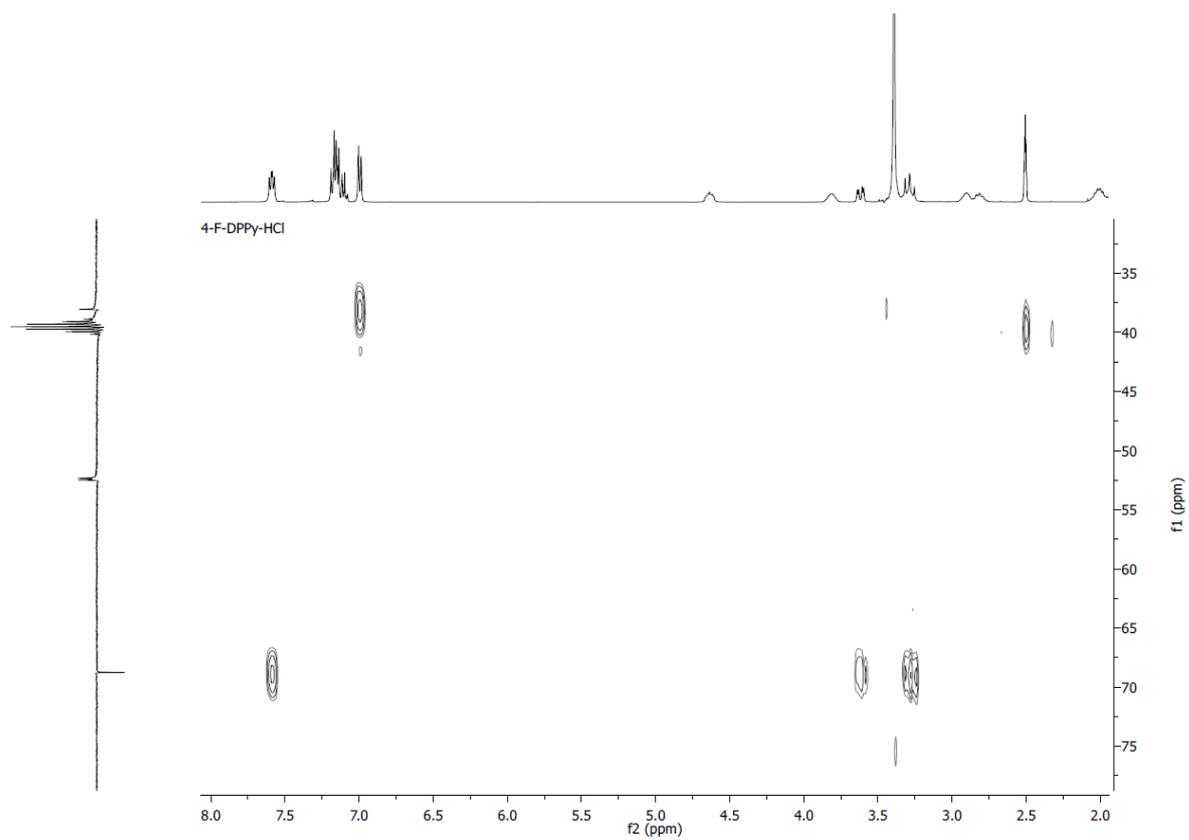


HMQC 2-D NMR of 4-F-DPPy HCl, zoomed in on aromatic section (d_6 -DMSO)

Supporting Information – Drug Testing and Analysis

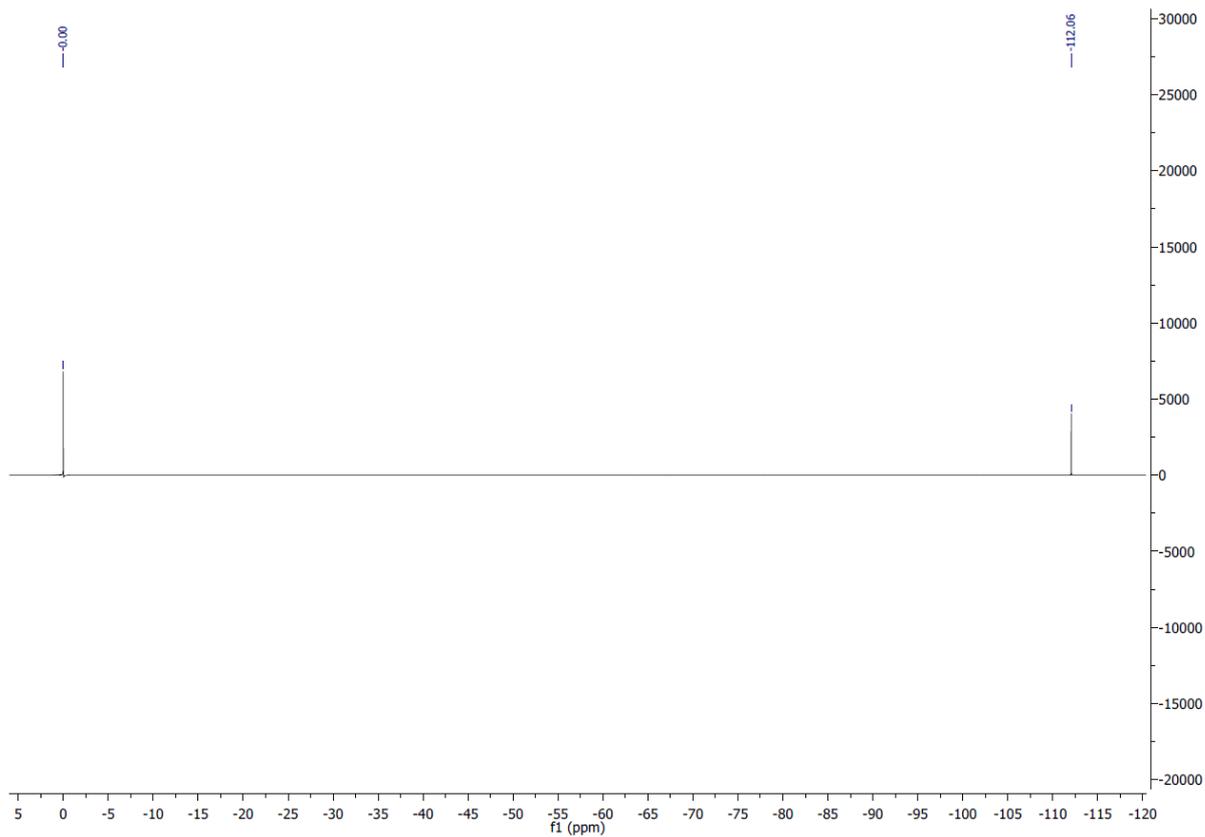


HMBC 2-D NMR of 4-F-DPPy HCl (d_6 -DMSO)



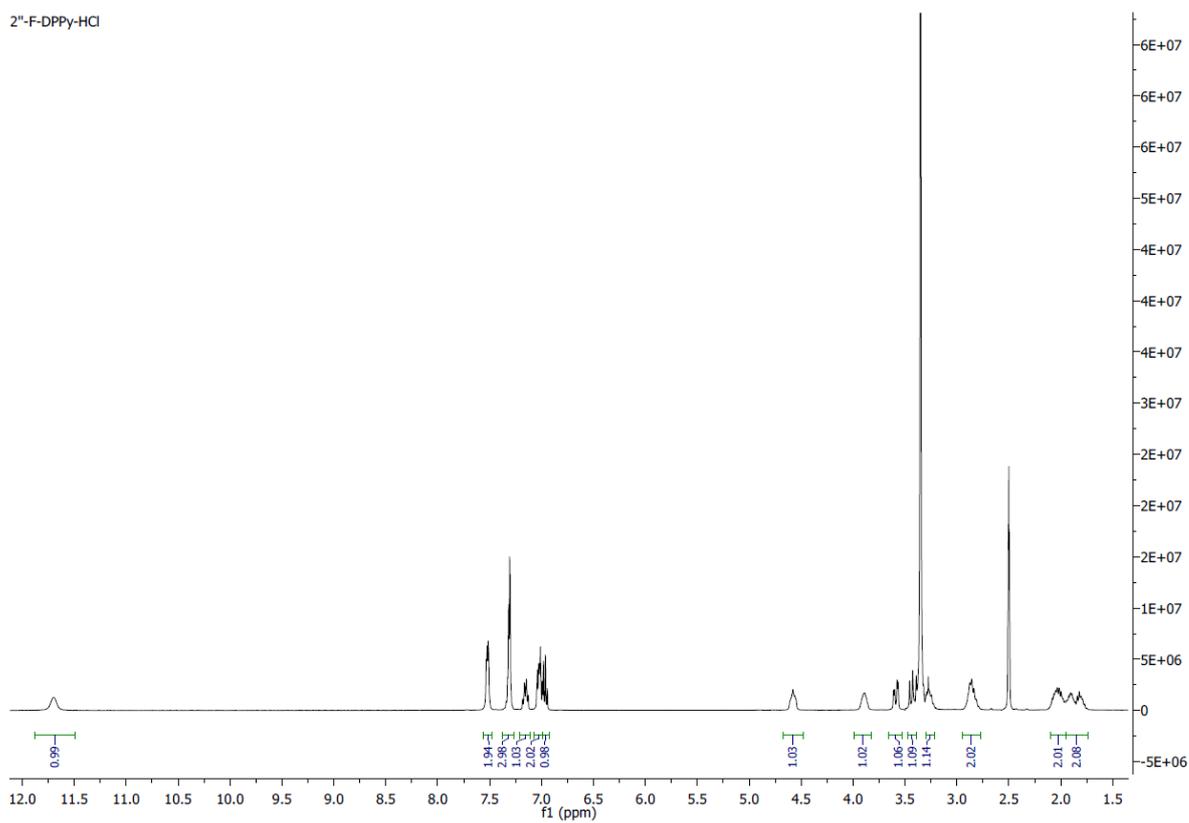
HMBC 2-D NMR of 4-F-DPPy HCl, zoomed in on aliphatic section (d_6 -DMSO)

Supporting Information – Drug Testing and Analysis



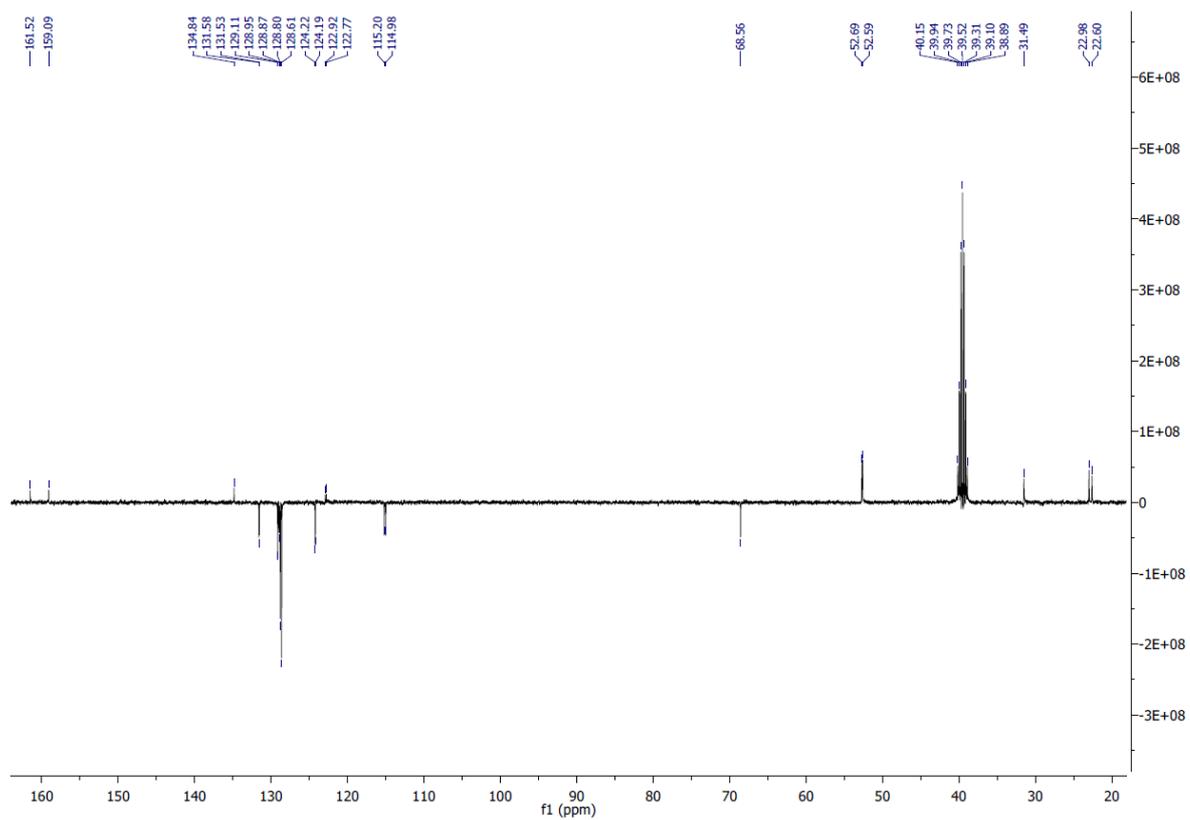
^{19}F NMR of 4-F-DPPy HCl with CFCl_3 as internal reference (376.5 MHz, $\text{d}_6\text{-DMSO}$)

Supporting Information – Drug Testing and Analysis

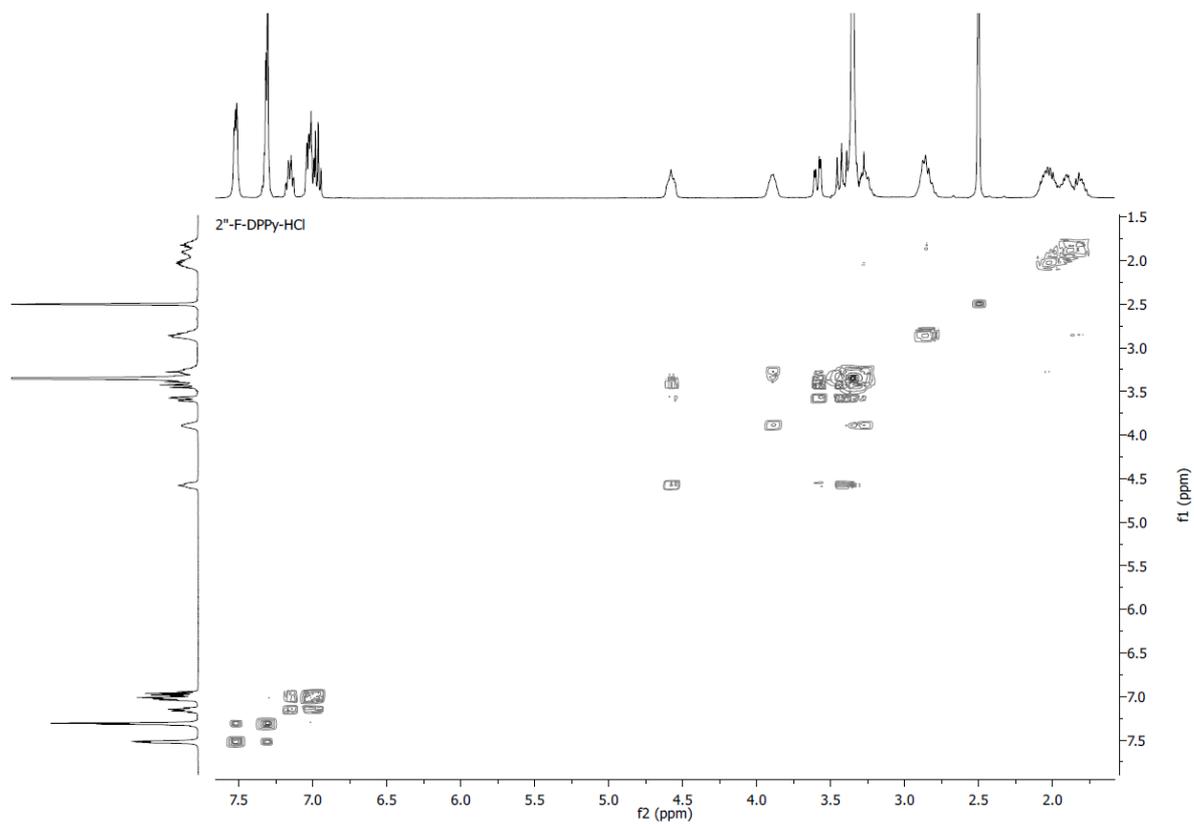


¹H NMR of 2''-F-DPPy HCl (400 MHz, d₆-DMSO)

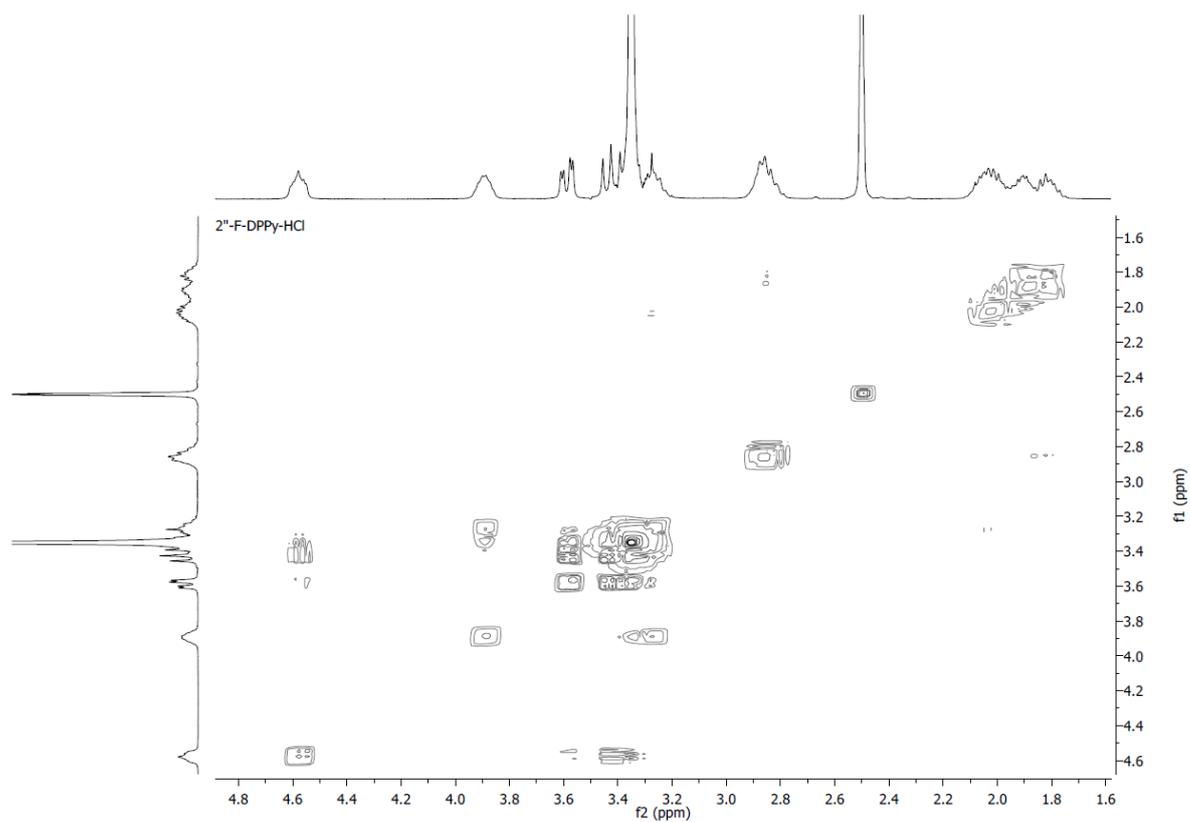
Supporting Information – Drug Testing and Analysis



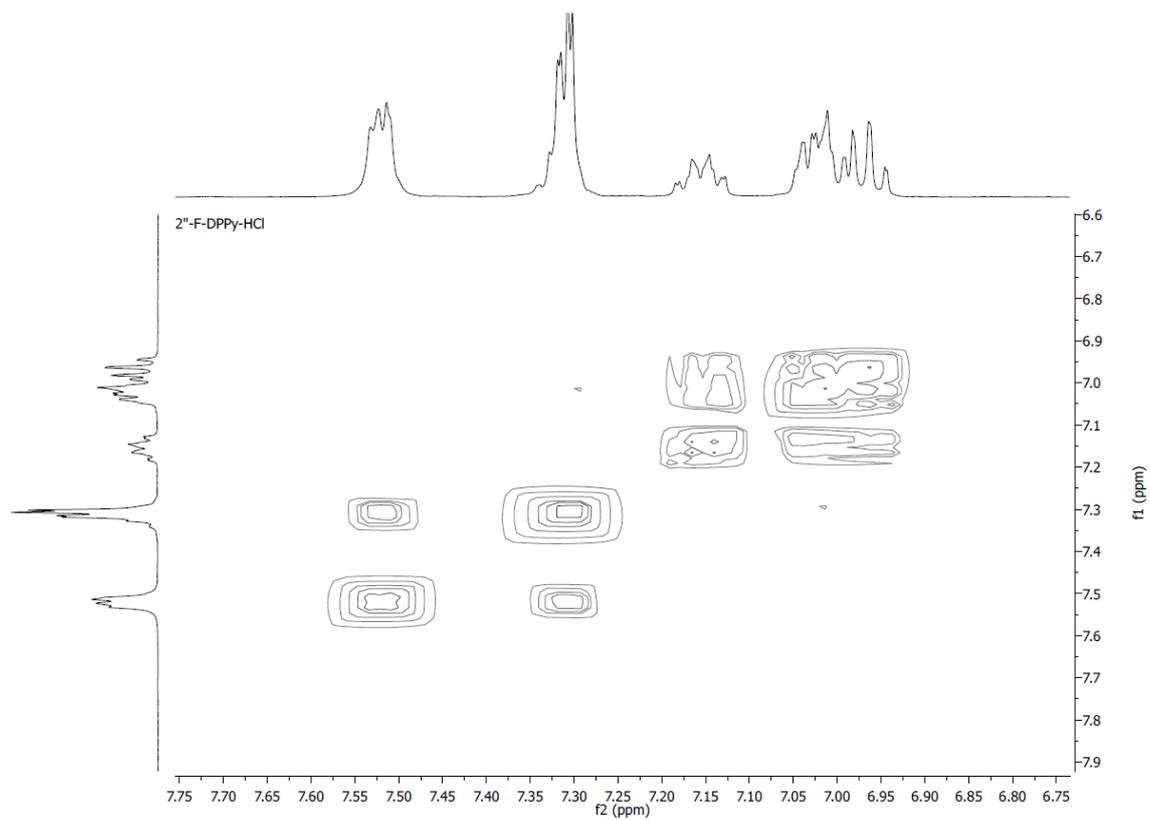
^{13}C PENDANT NMR of 2''-F-DPPy HCl (101 MHz, d_6 -DMSO)



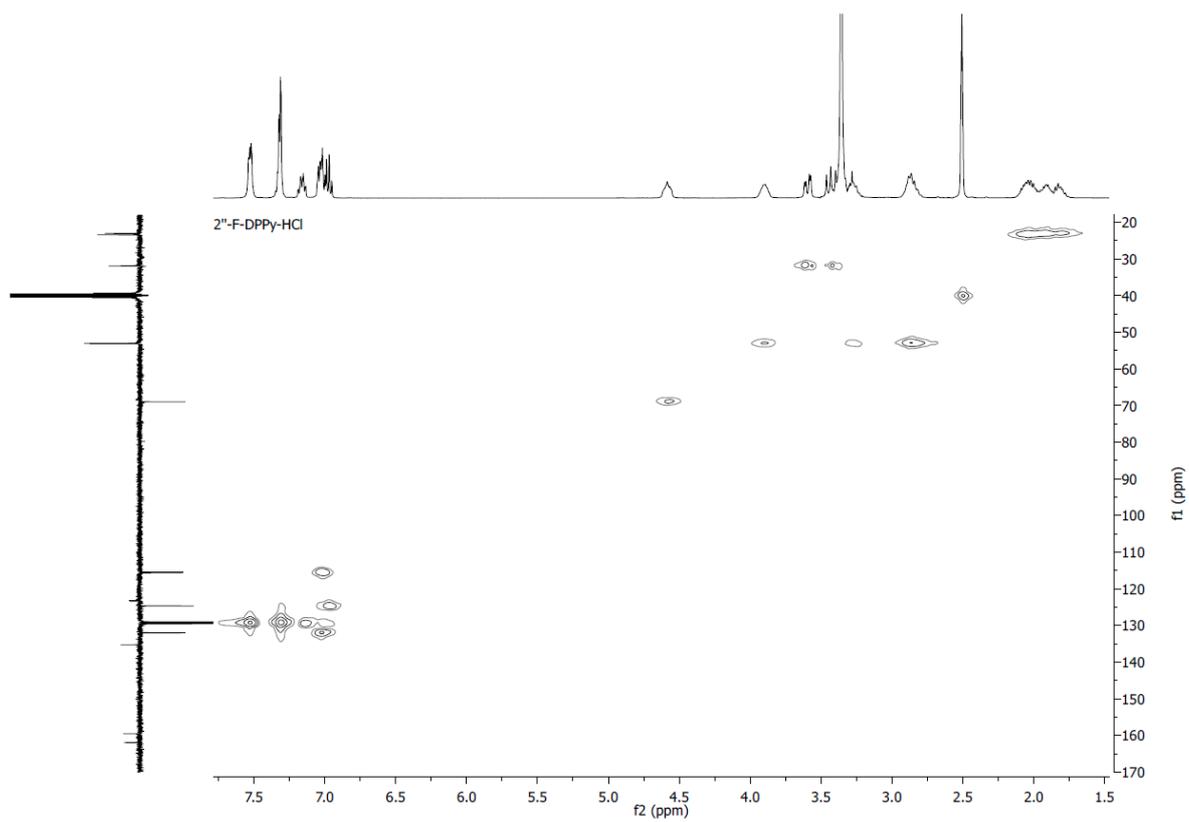
COSY-45 2-D NMR of 2''-F-DPPy HCl (d₆-DMSO)



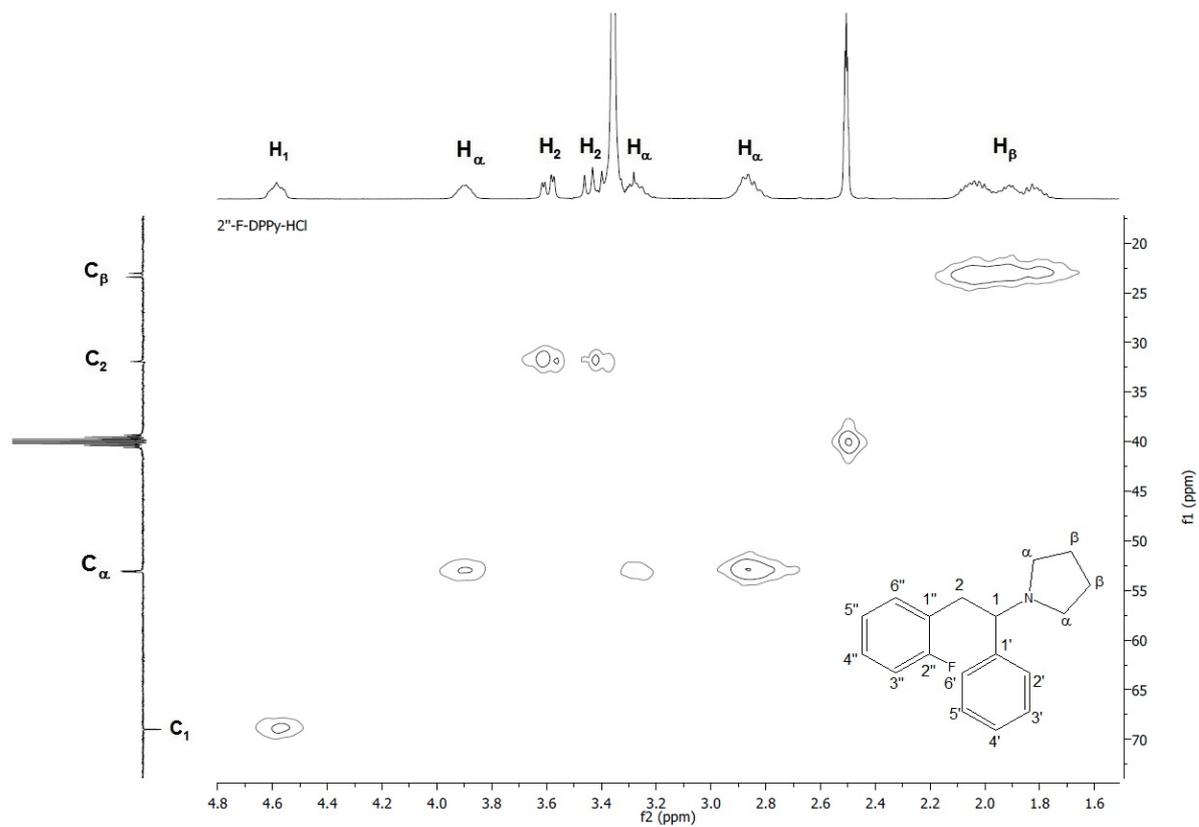
COSY-45 2-D NMR of 2''-F-DPPy HCl, zoomed in on aliphatic section (d_6 -DMSO)



COSY-45 2-D NMR of 2''-F-DPPy HCl, zoomed in on aromatic section (d_6 -DMSO)

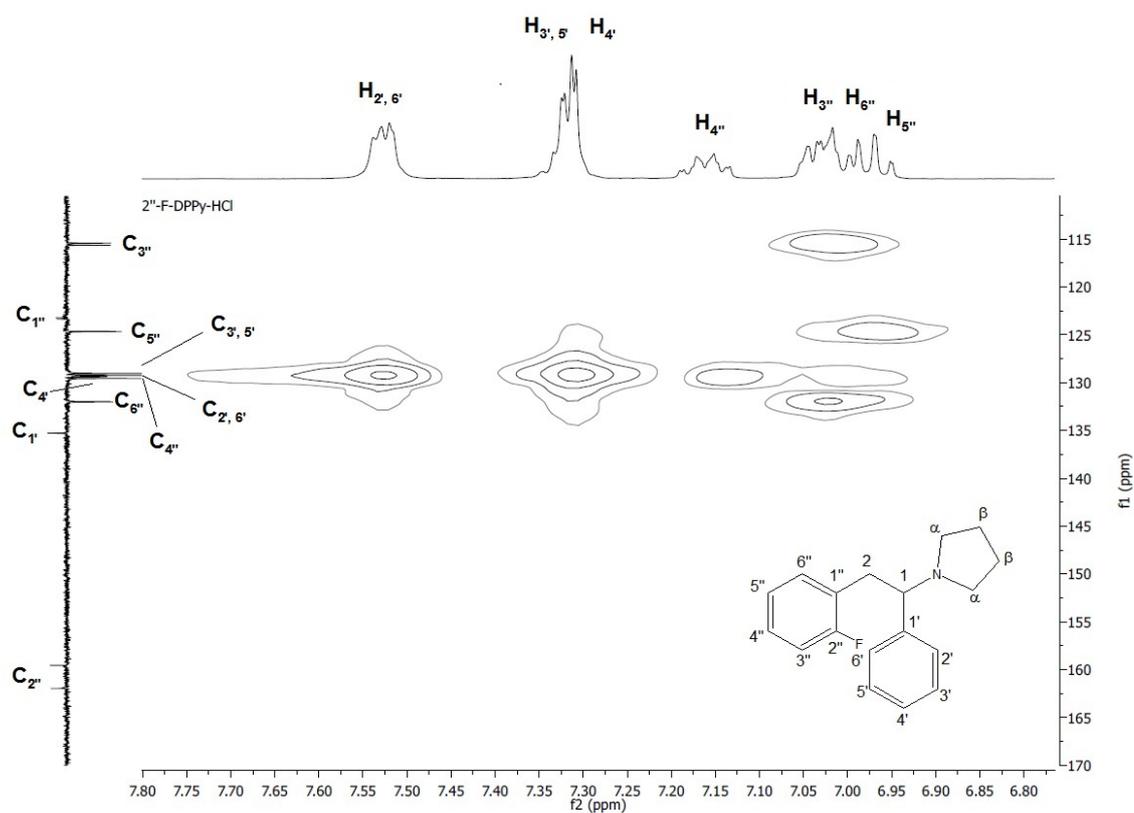


HMQC 2-D NMR of 2''-F-DPPy HCl (d_6 -DMSO)



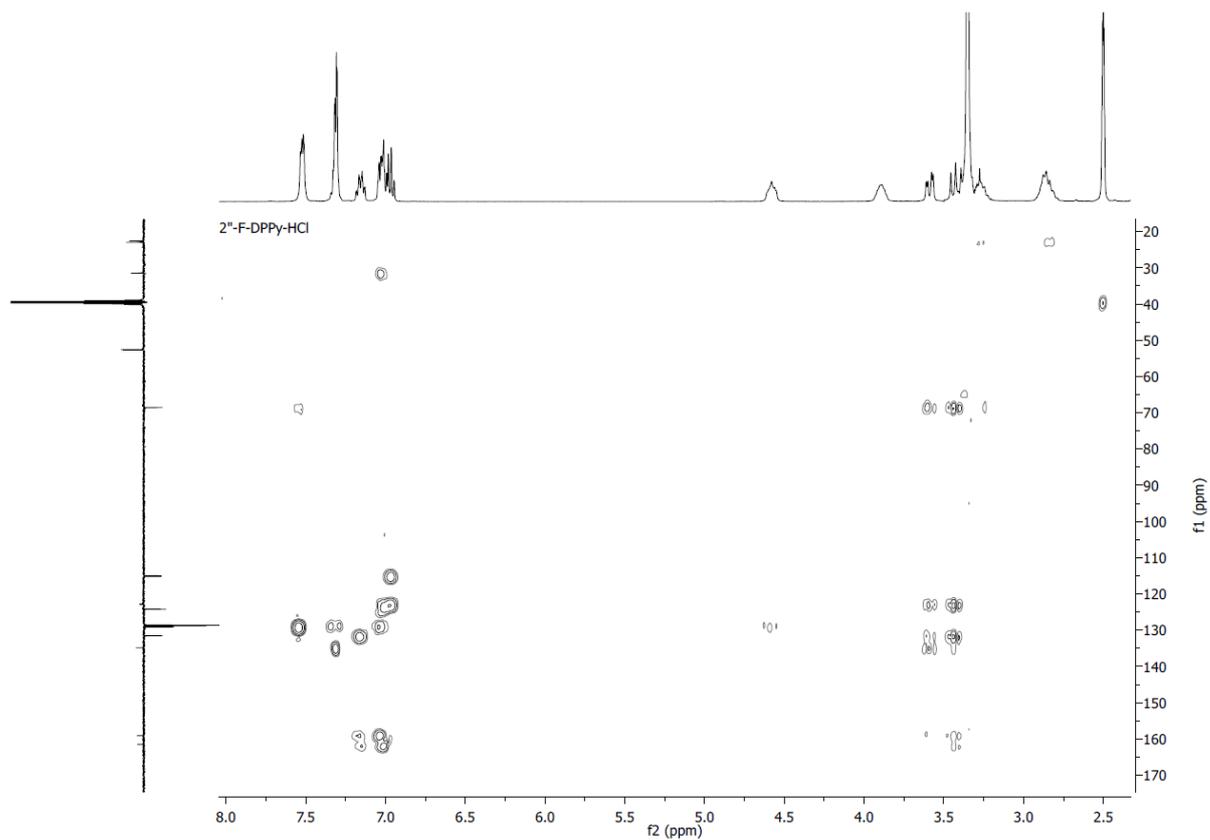
HMQC 2-D NMR of 2''-F-DPPy HCl, zoomed in on aliphatic section (d_6 -DMSO)

Supporting Information – Drug Testing and Analysis



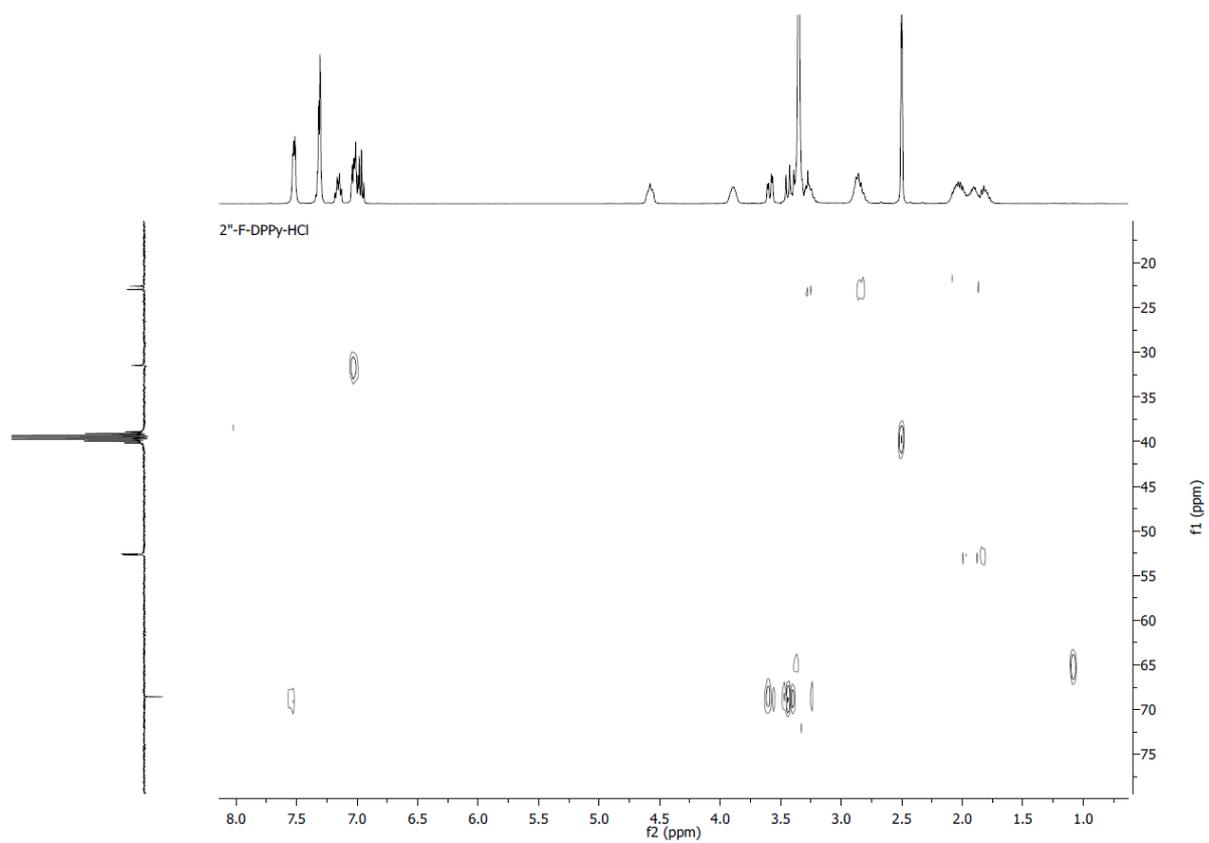
HMQC 2-D NMR of 2''-F-DPPy HCl, zoomed in on aromatic section (d_6 -DMSO)

Supporting Information – Drug Testing and Analysis



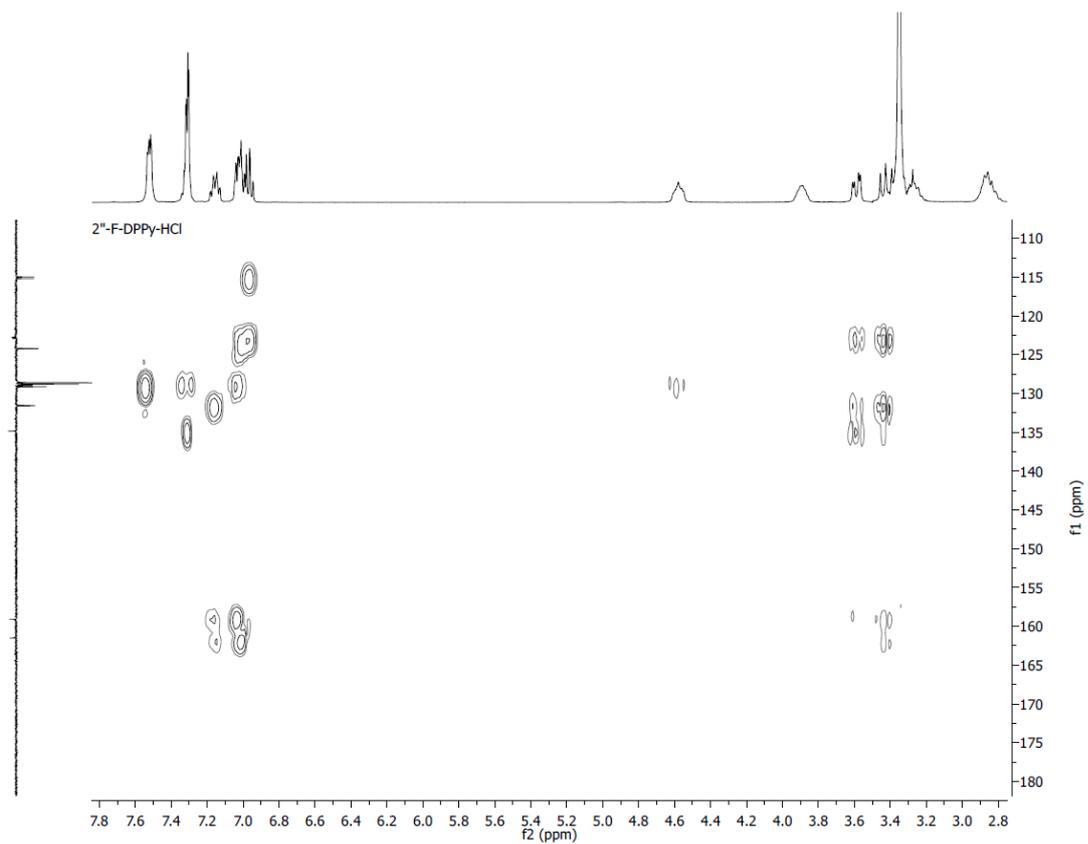
HMBC 2-D NMR of 2''-F-DPPy HCl (d_6 -DMSO)

Supporting Information – Drug Testing and Analysis



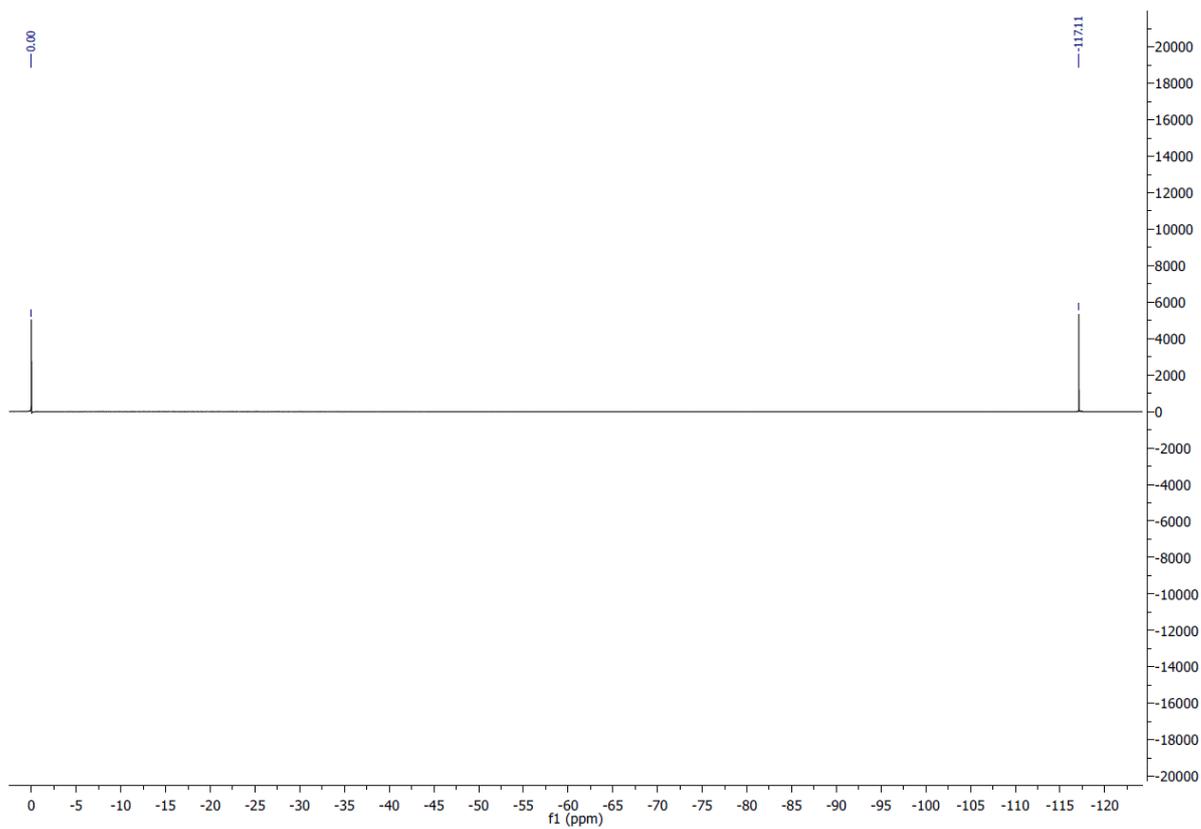
HMBC 2-D NMR of 2''-F-DPPy HCl, zoomed in on aliphatic section (d_6 -DMSO)

Supporting Information – Drug Testing and Analysis



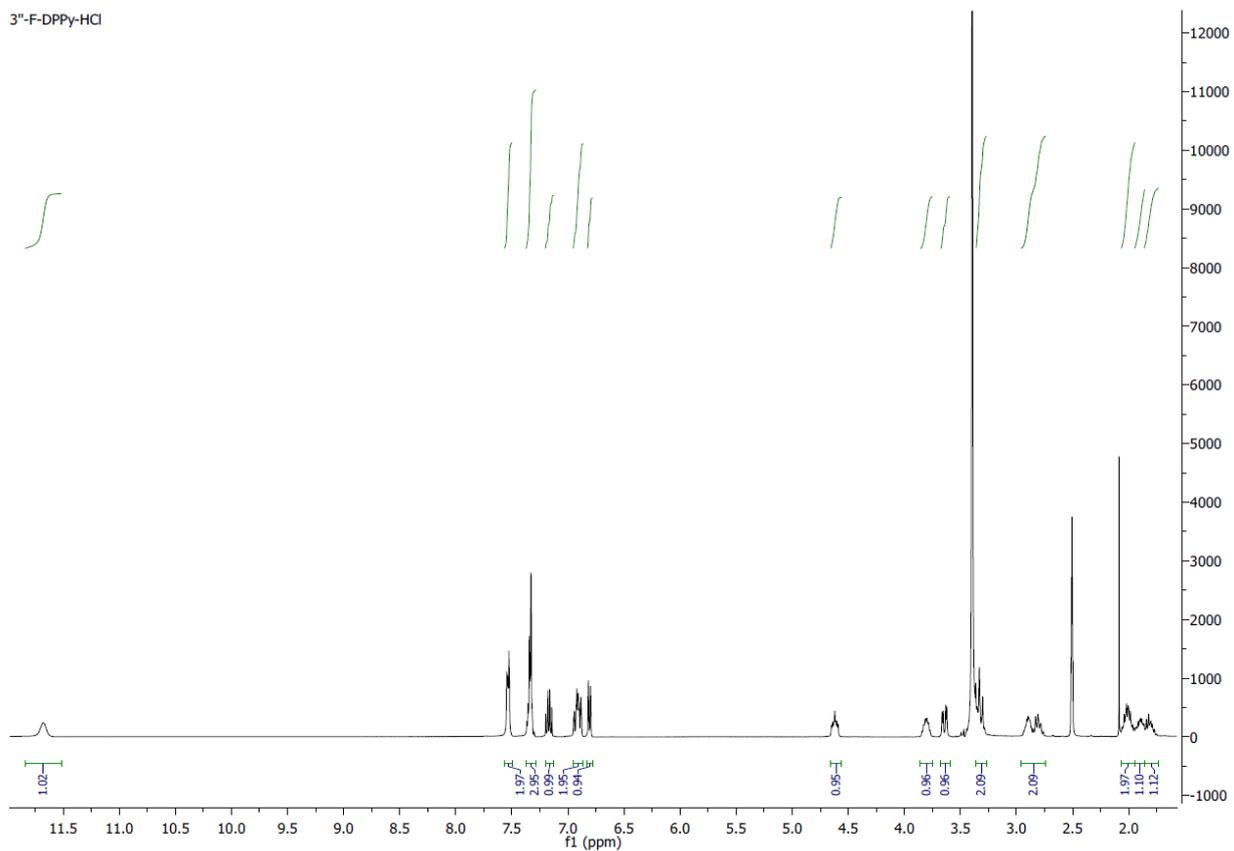
HMBC 2-D NMR of 2''-F-DPPy HCl, zoomed in on aromatic section (d_6 -DMSO)

Supporting Information – Drug Testing and Analysis



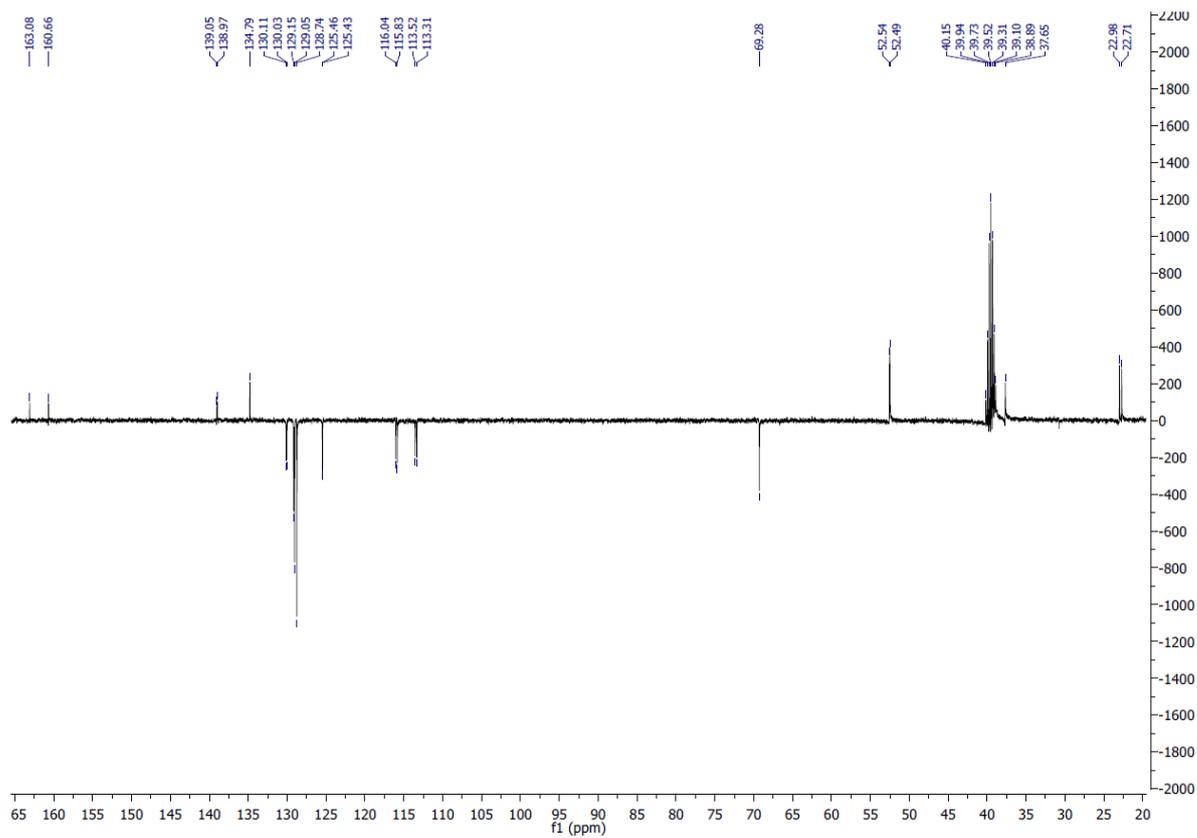
^{19}F NMR of 2''-F-DPPy HCl with CFCl_3 as internal reference (376.5 MHz, d_6 -DMSO)

Supporting Information – Drug Testing and Analysis

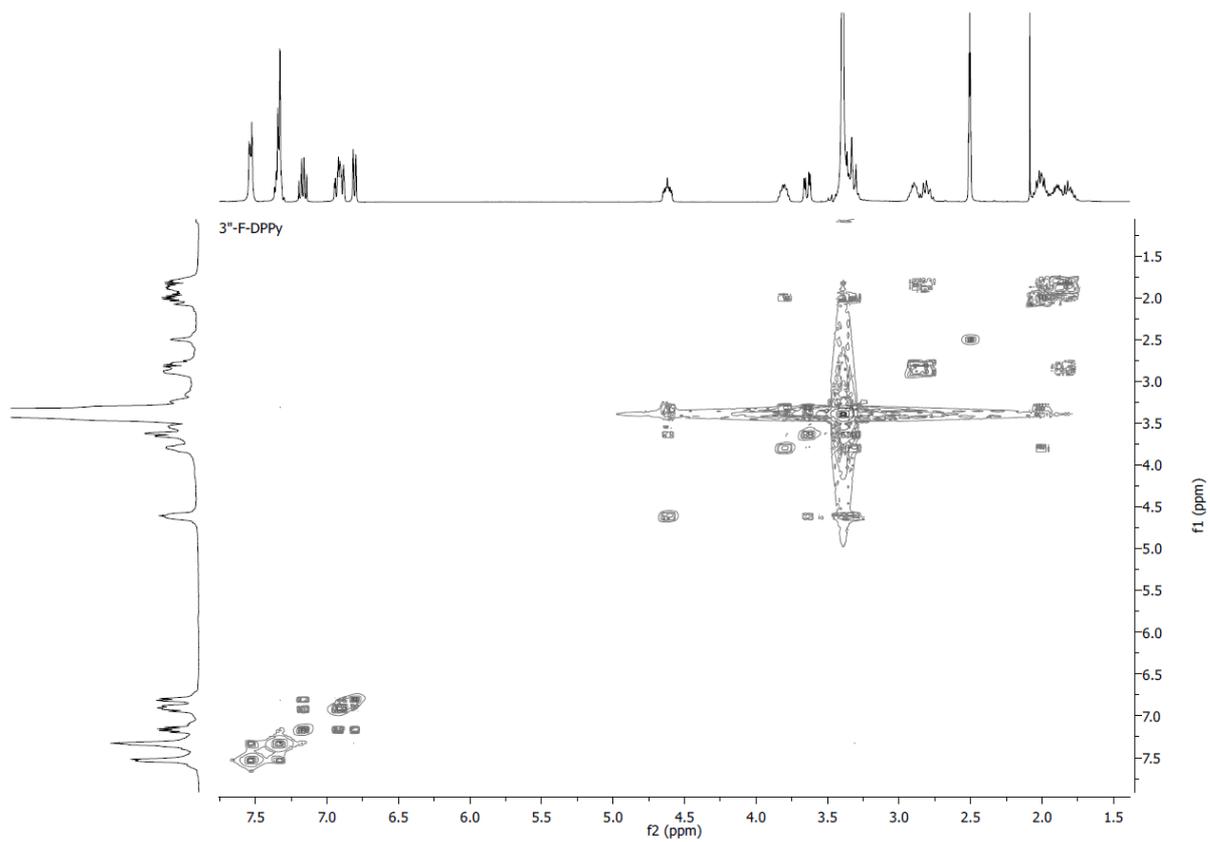


^1H NMR of 3''-F-DPPy HCl (400 MHz, $\text{d}_6\text{-DMSO}$)

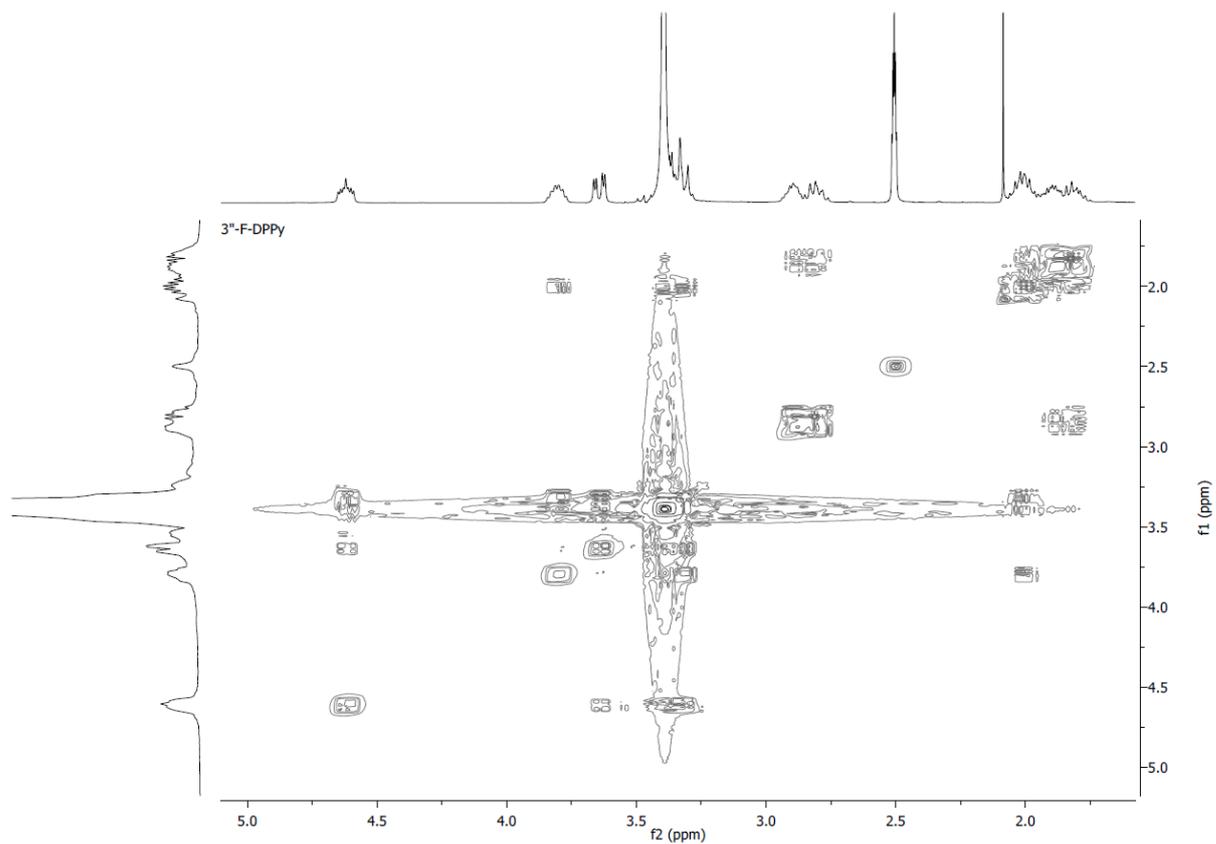
Supporting Information – Drug Testing and Analysis



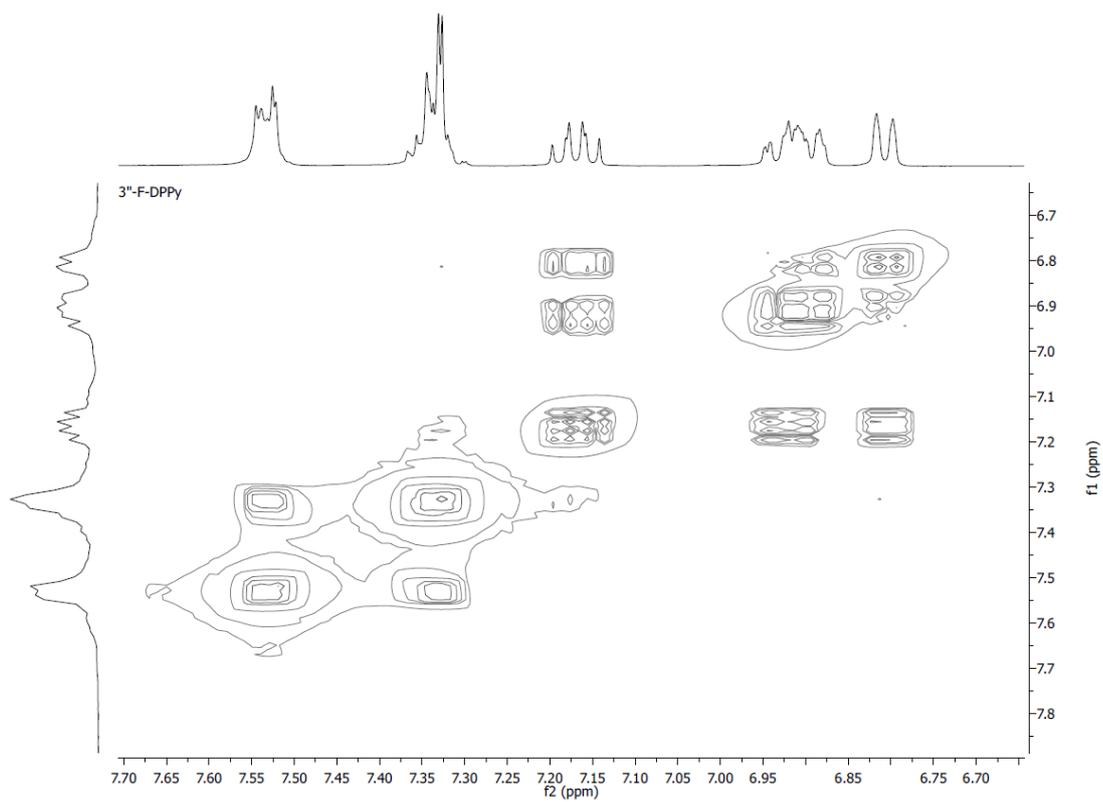
^{13}C PENDANT NMR of $3''\text{-F-DPPy HCl}$ (101 MHz, $\text{d}_6\text{-DMSO}$)



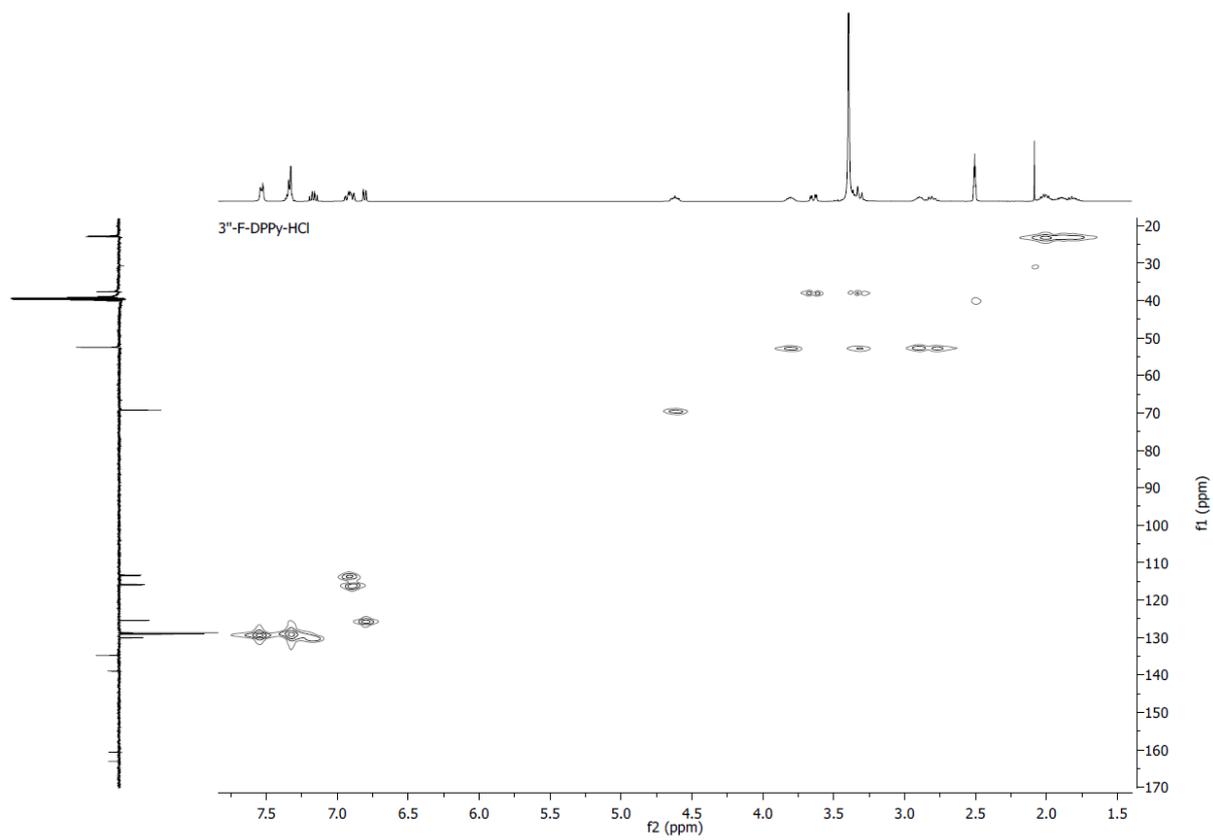
COSY-45 2-D NMR of 3''-F-DPPy HCl (d₆-DMSO)



COSY-45 2-D NMR of 3''-F-DPPy HCl, zoomed in on aliphatic section (d_6 -DMSO)

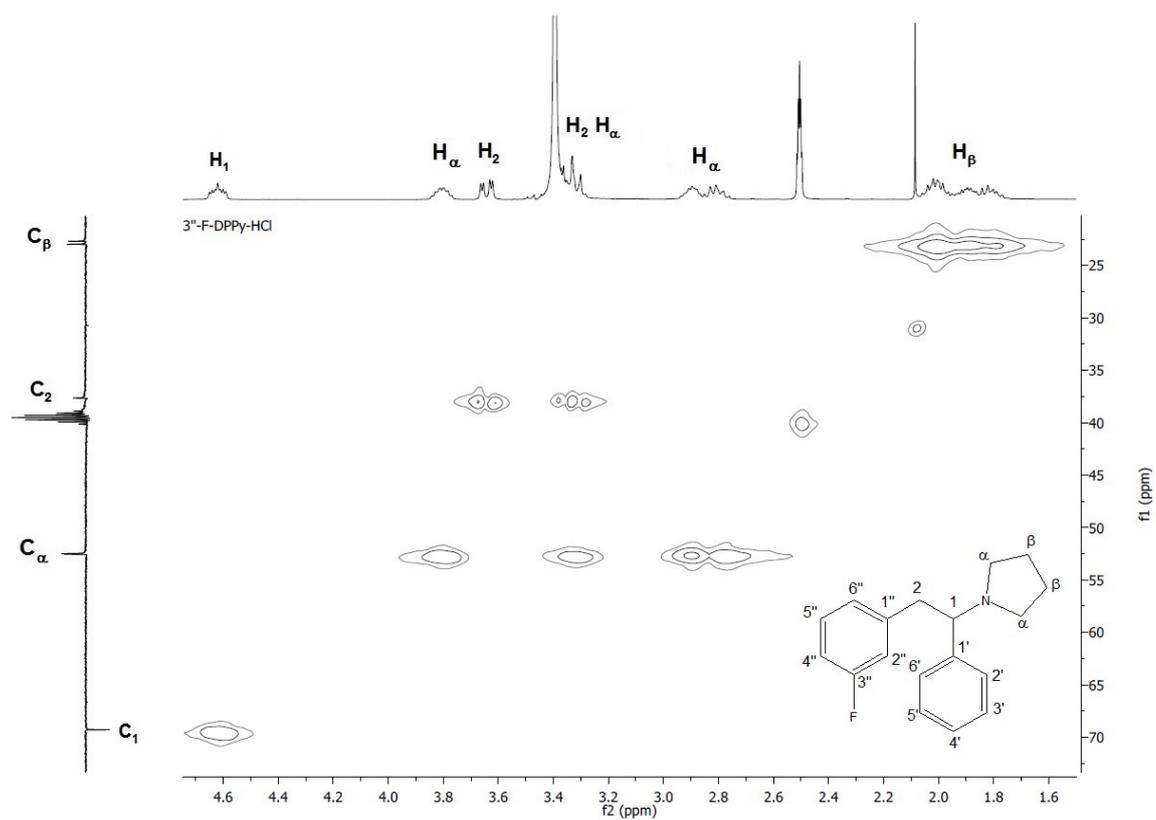


COSY-45 2-D NMR of 3''-F-DPPy HCl, zoomed in on aromatic section (d_6 -DMSO)

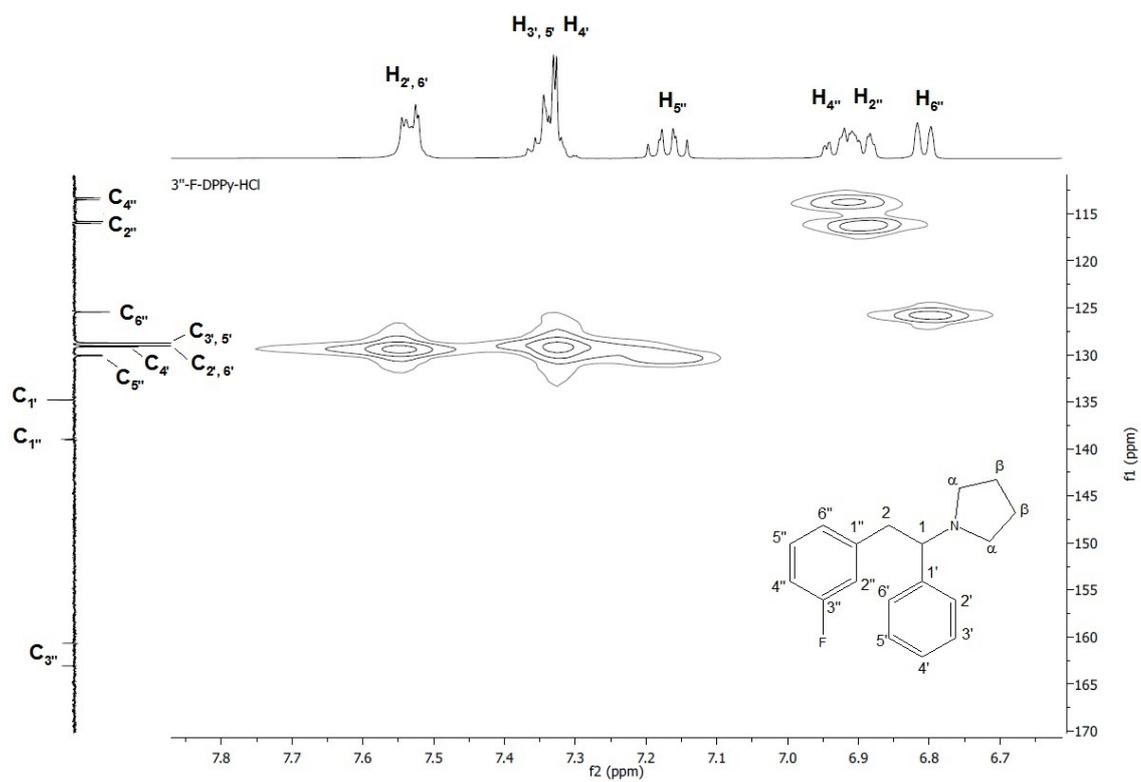


HMQC 2-D NMR of 3''-F-DPPy HCl (d_6 -DMSO)

Supporting Information – Drug Testing and Analysis

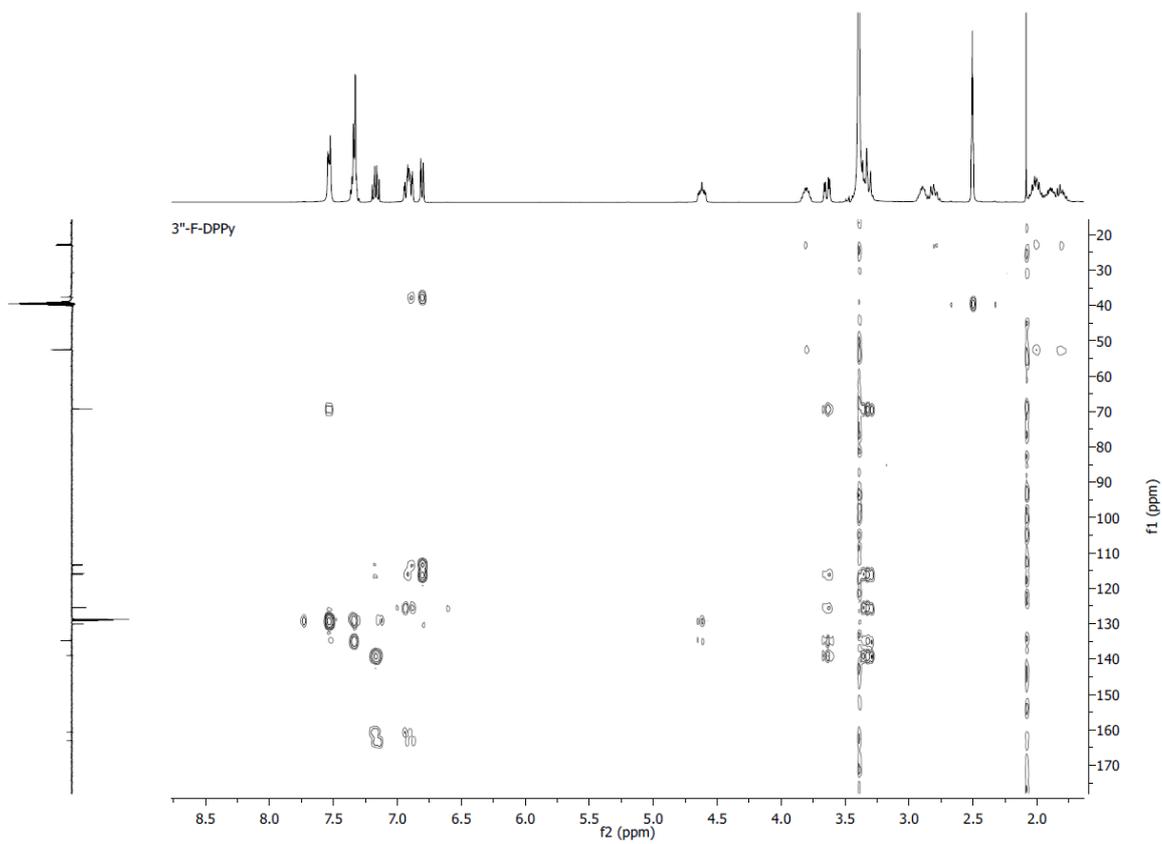


HMQC 2-D NMR of 3''-F-DPPy HCl, zoomed in on aliphatic section; acetone integration value of 0.64; 2% (w/w) based on peak area (d₆-DMSO)

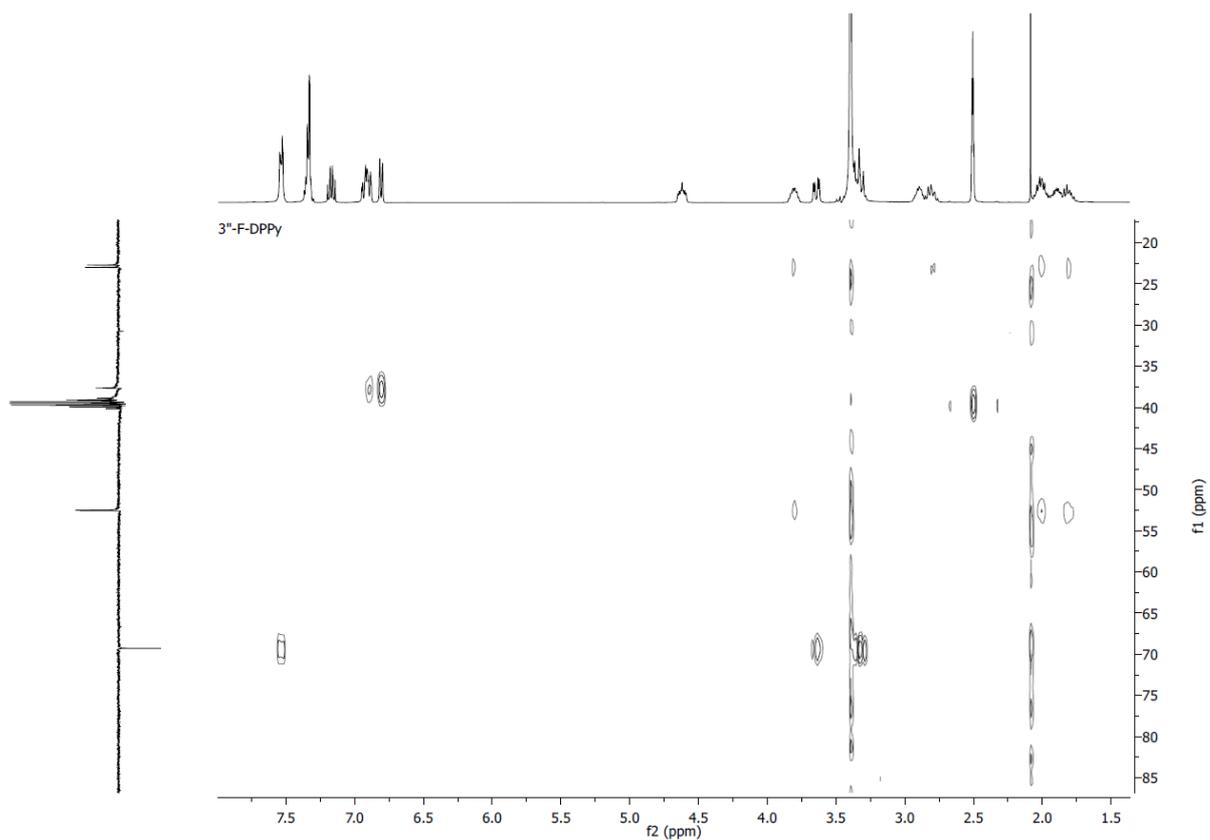


HMQC 2-D NMR of 3''-F-DPPy HCl, zoomed in on aromatic section (d_6 -DMSO)

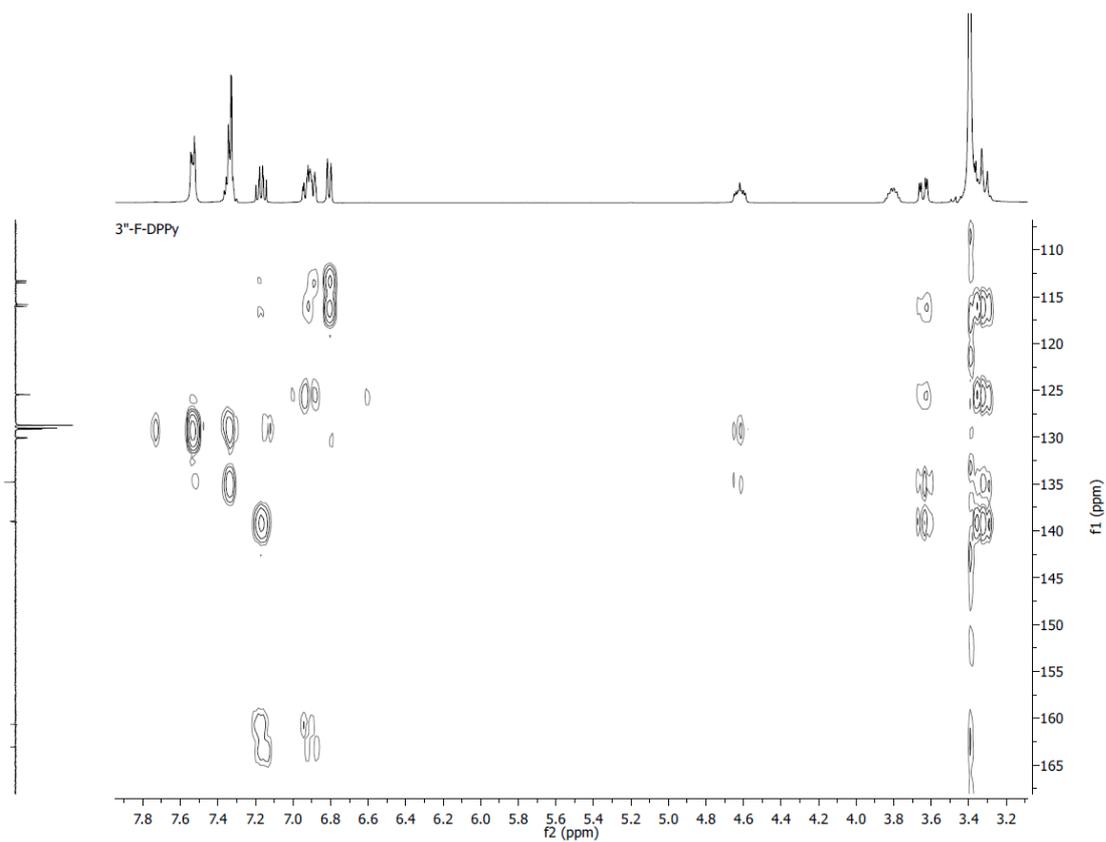
Supporting Information – Drug Testing and Analysis



HMBC 2-D NMR of 3''-F-DPPy HCl (d_6 -DMSO)

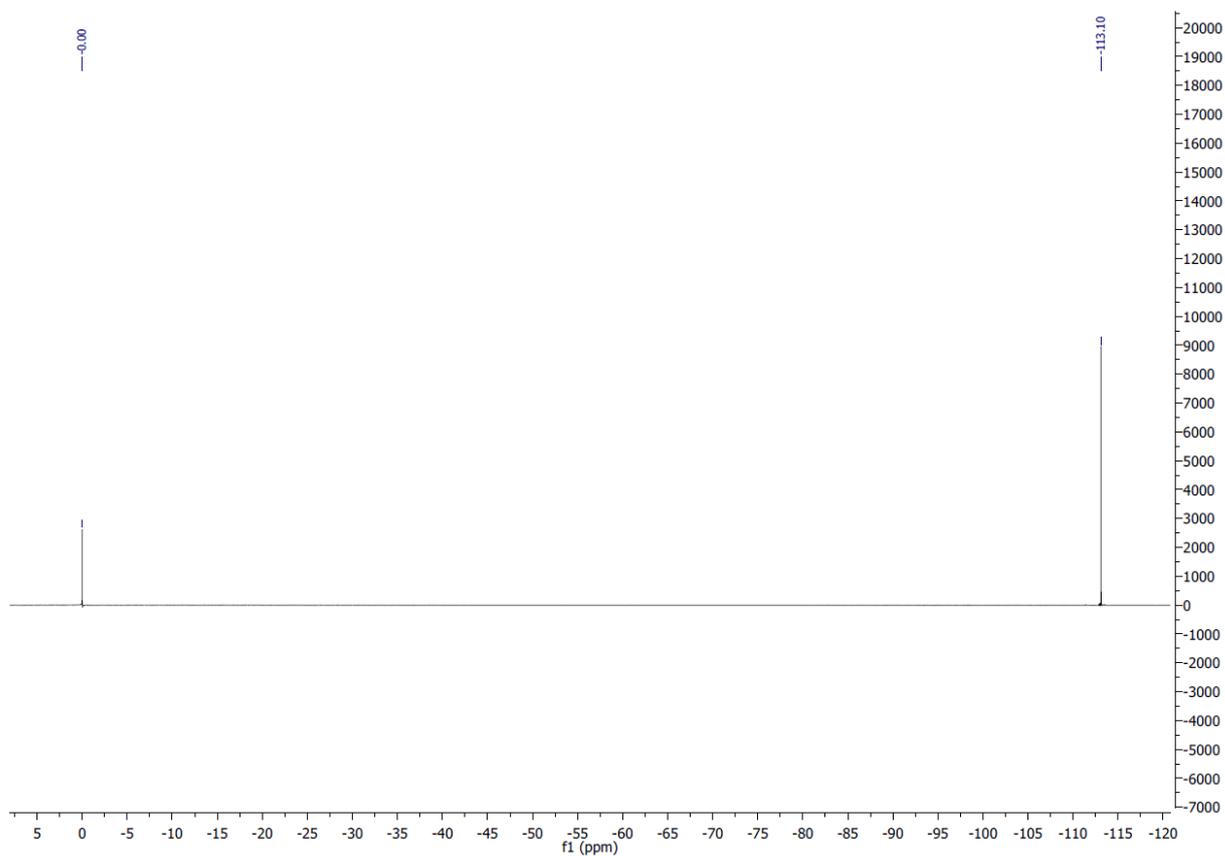


HMBC 2-D NMR of 3''-F-DPPy HCl, zoomed in on the aliphatic section (d_6 -DMSO)



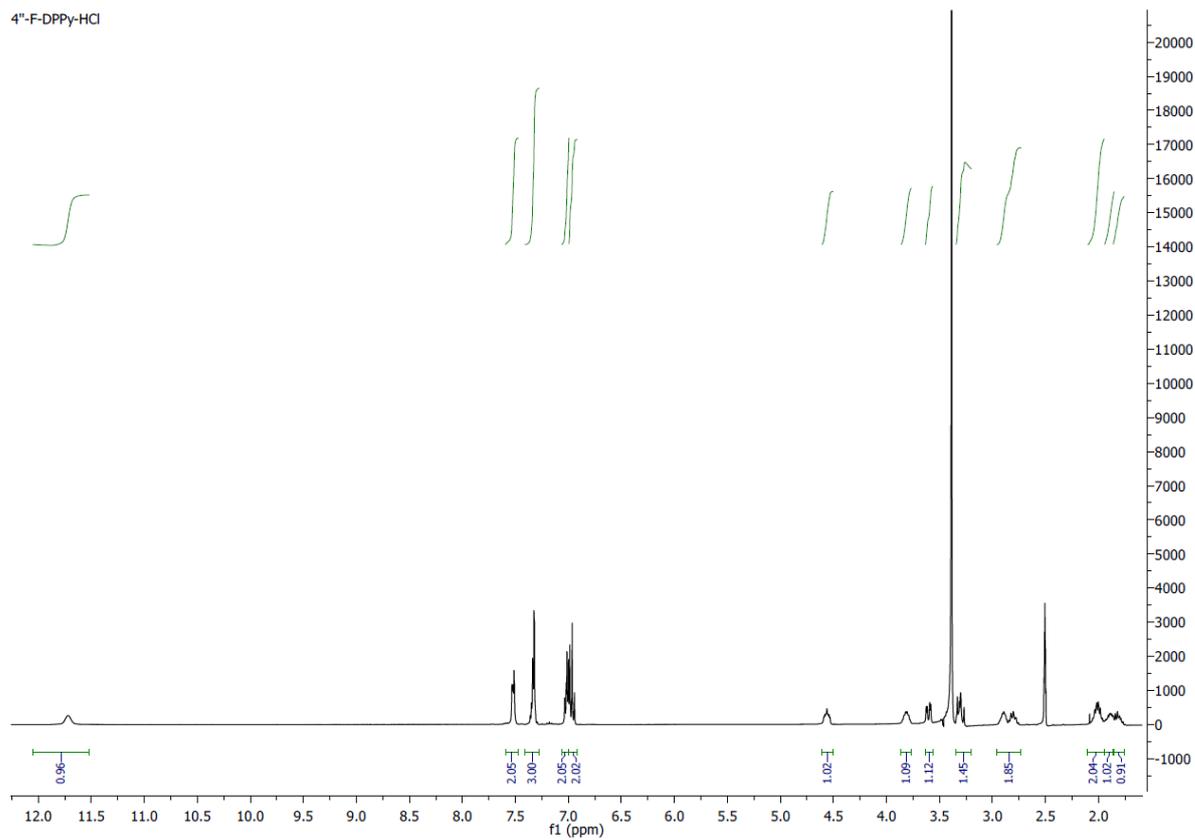
HMBC 2-D NMR of 3^F-F-DPPy HCl, zoomed in on the aromatic section (d₆-DMSO)

Supporting Information – Drug Testing and Analysis



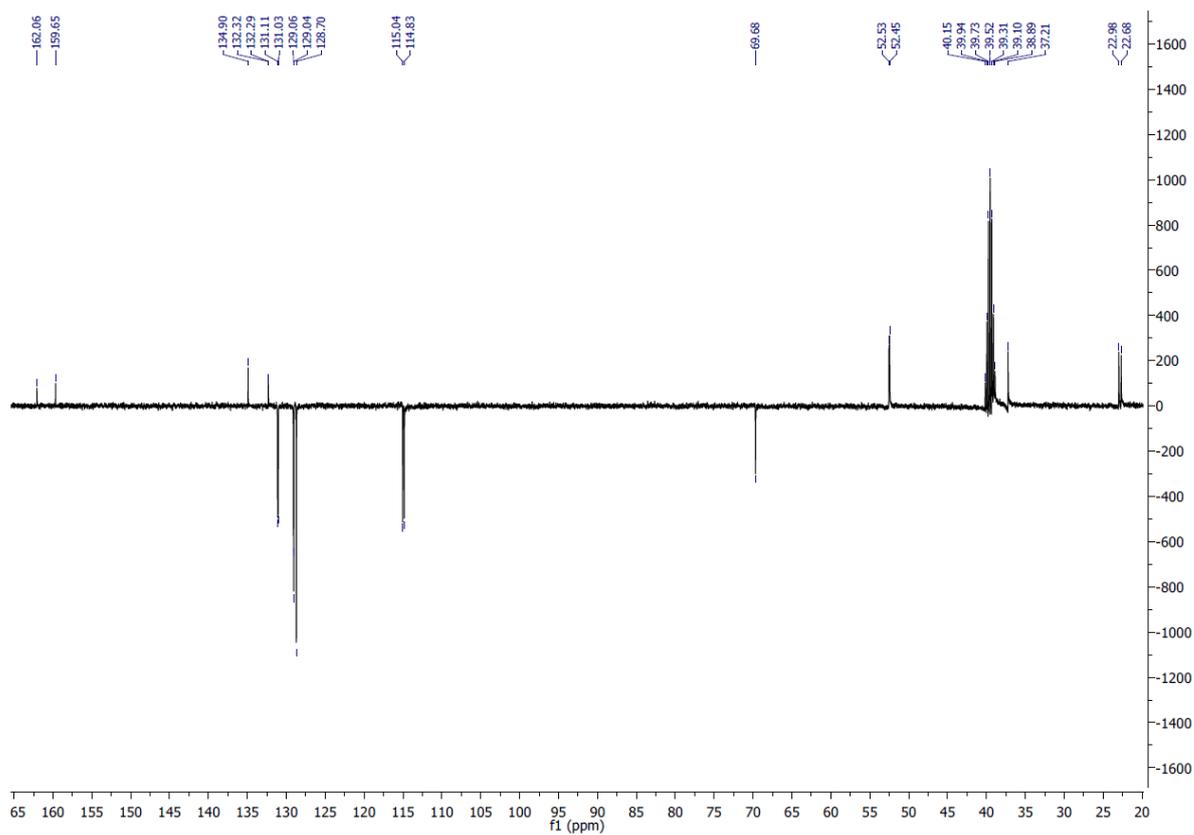
^{19}F NMR of 3''-F-DPPy HCl with CFCl_3 as internal reference (376.5 MHz, d_6 -DMSO)

Supporting Information – Drug Testing and Analysis



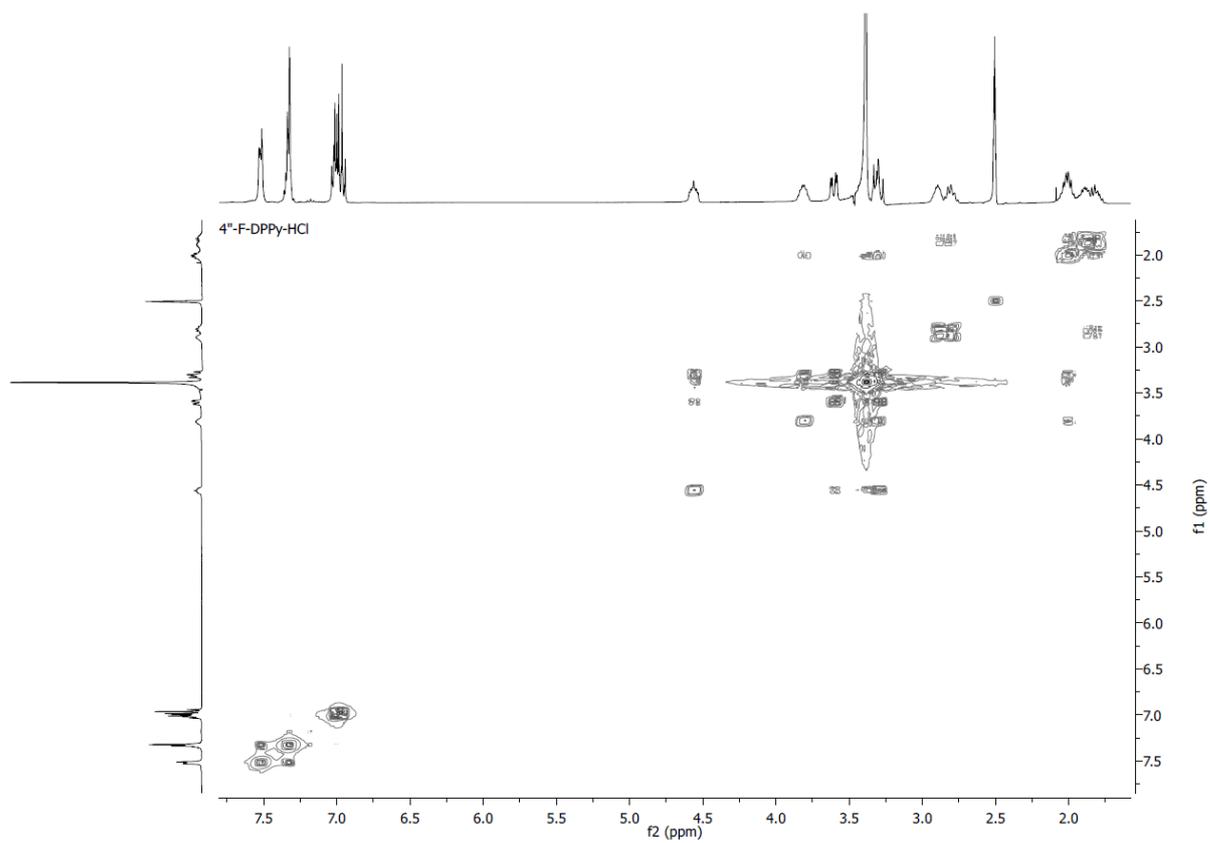
^1H NMR of 4''-F-DPPy HCl (400 MHz, $\text{d}_6\text{-DMSO}$)

Supporting Information – Drug Testing and Analysis



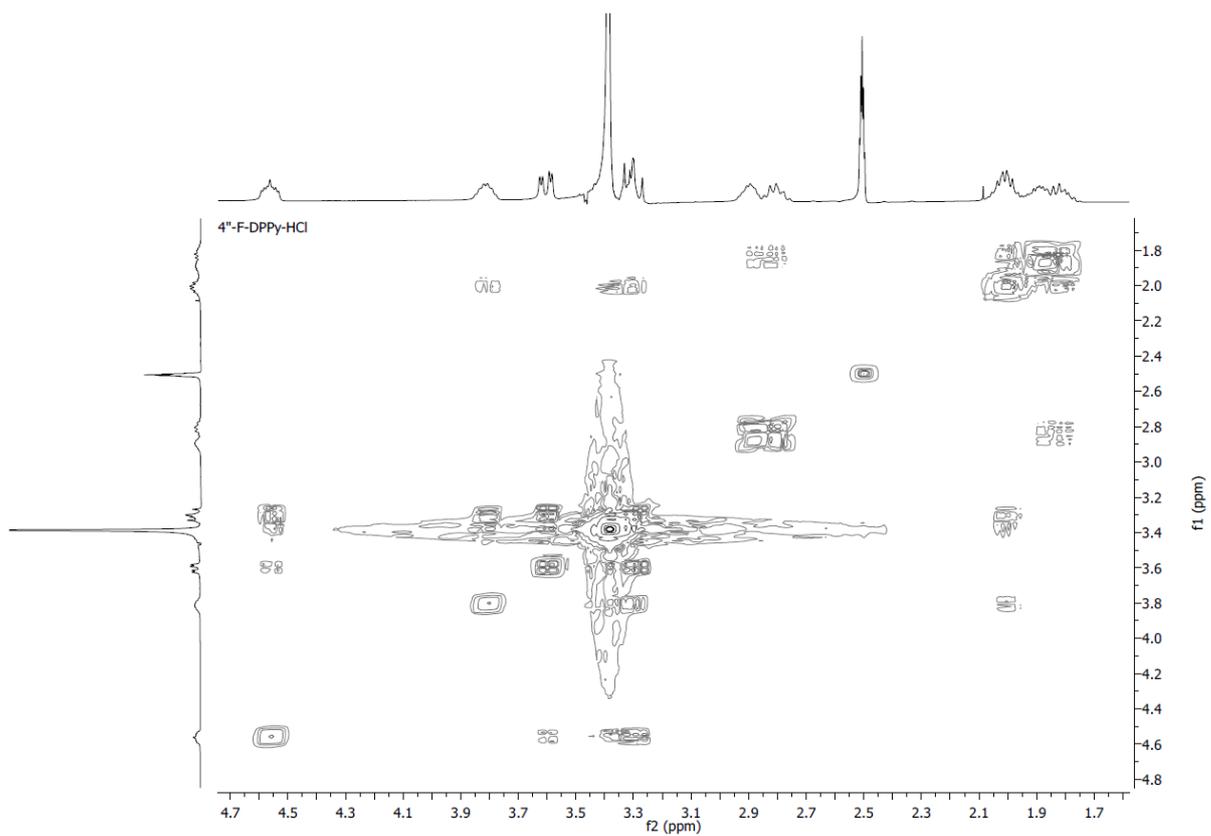
^{13}C PENDANT NMR of 4''-F-DPPy HCl (101 MHz, $\text{d}_6\text{-DMSO}$)

Supporting Information – Drug Testing and Analysis

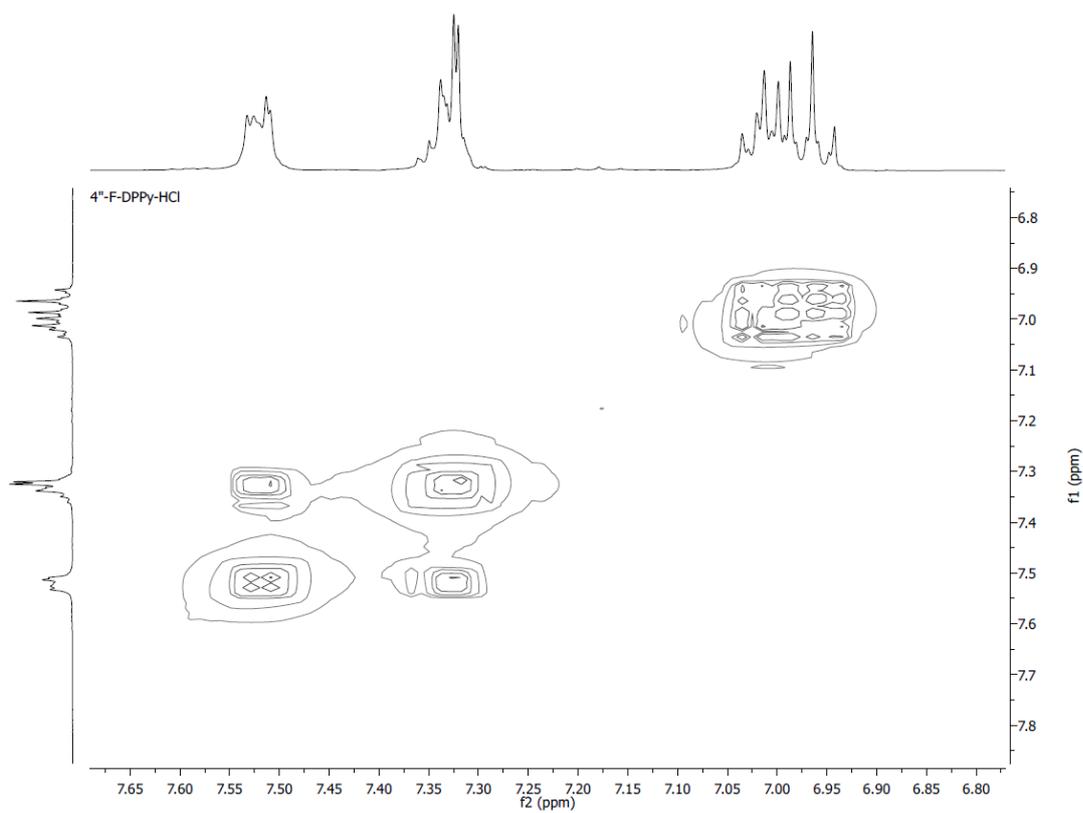


COSY-45 2-D NMR of 4''-F-DPPy HCl (d₆-DMSO)

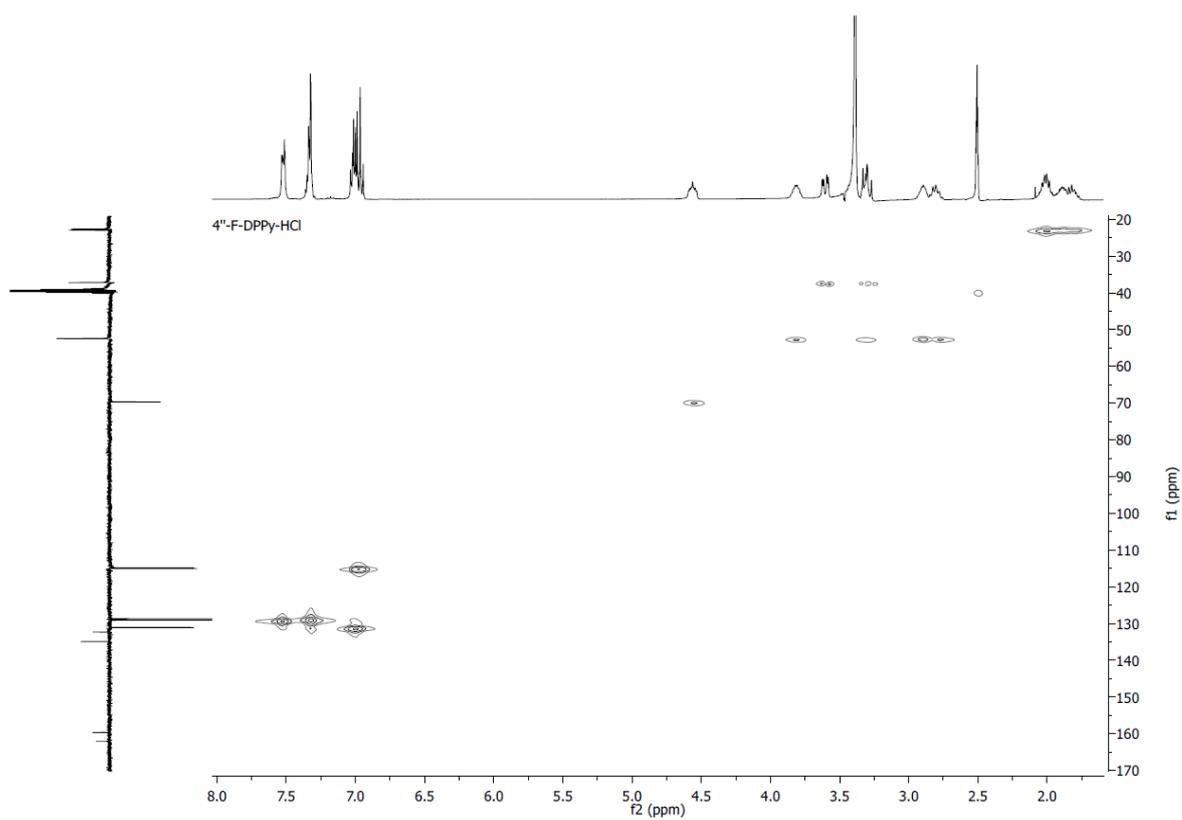
Supporting Information – Drug Testing and Analysis



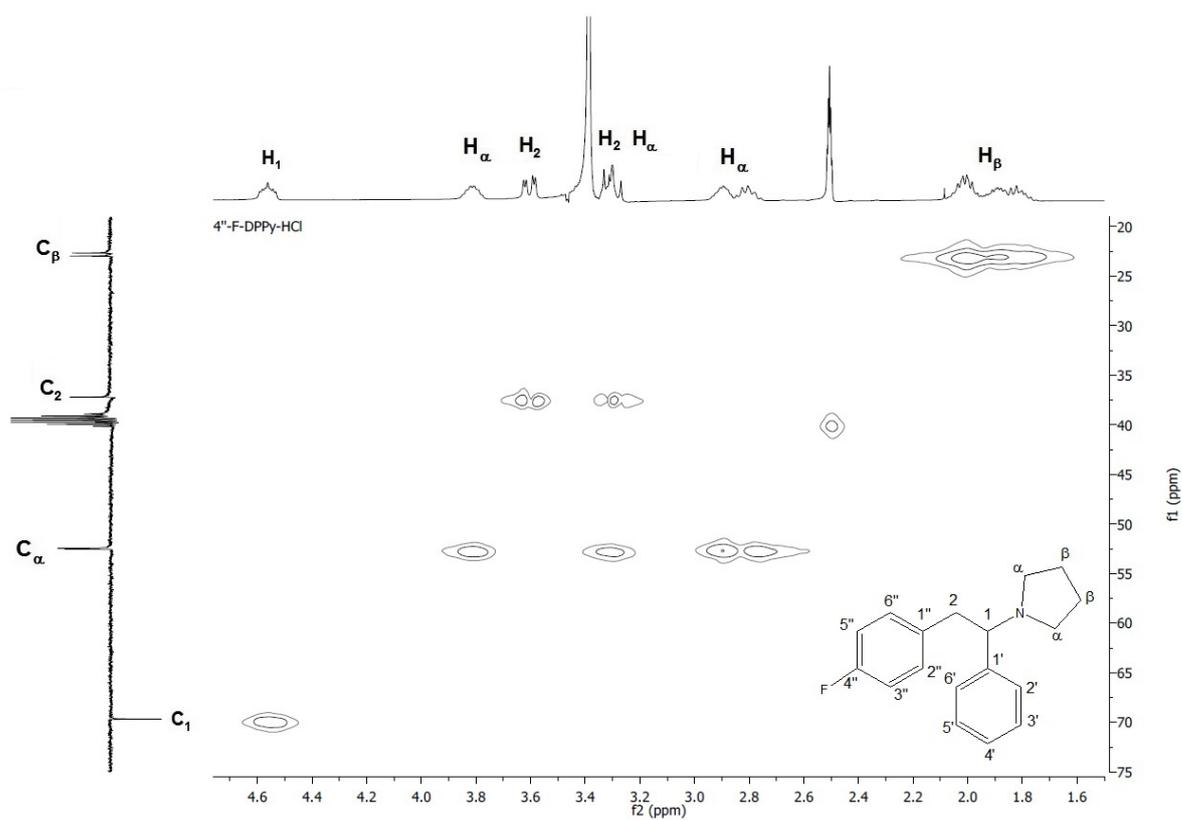
COSY-45 2-D NMR of 4''-F-DPPy HCl, zoomed in on the aliphatic section (d₆-DMSO)



COSY-45 2-D NMR of 4''-F-DPPy HCl, zoomed in on the aromatic section (d_6 -DMSO)

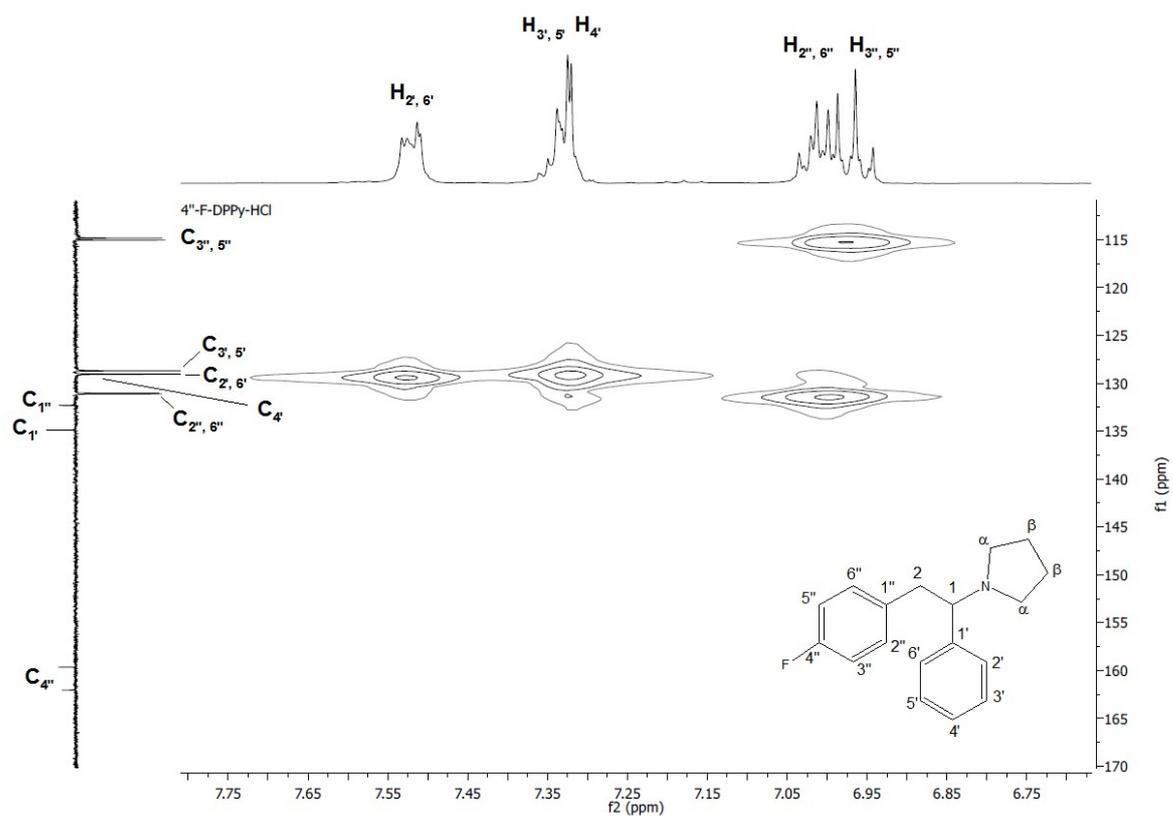


HMQC 2-D NMR of 4''-F-DPPy HCl (d_6 -DMSO)

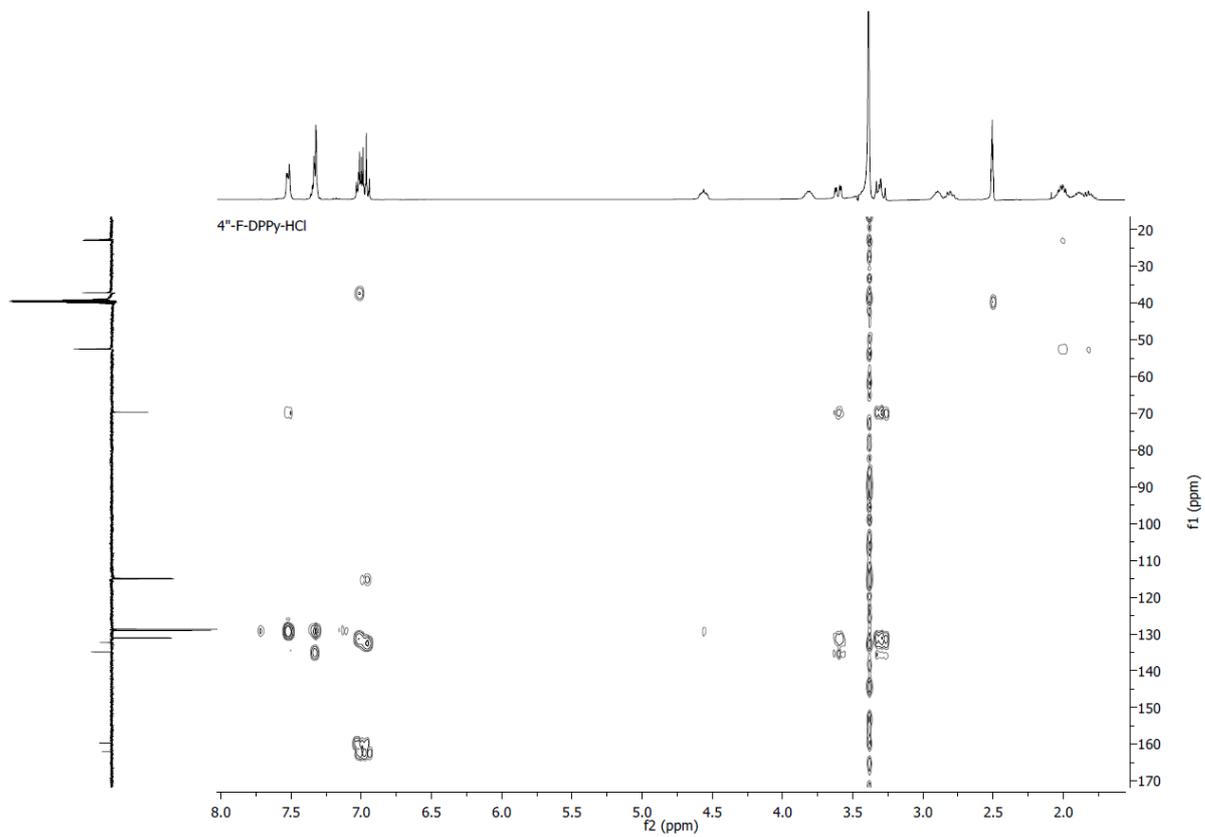


HMQC 2-D NMR of 4''-F-DPPy HCl, zoomed in on the aliphatic section (d_6 -DMSO)

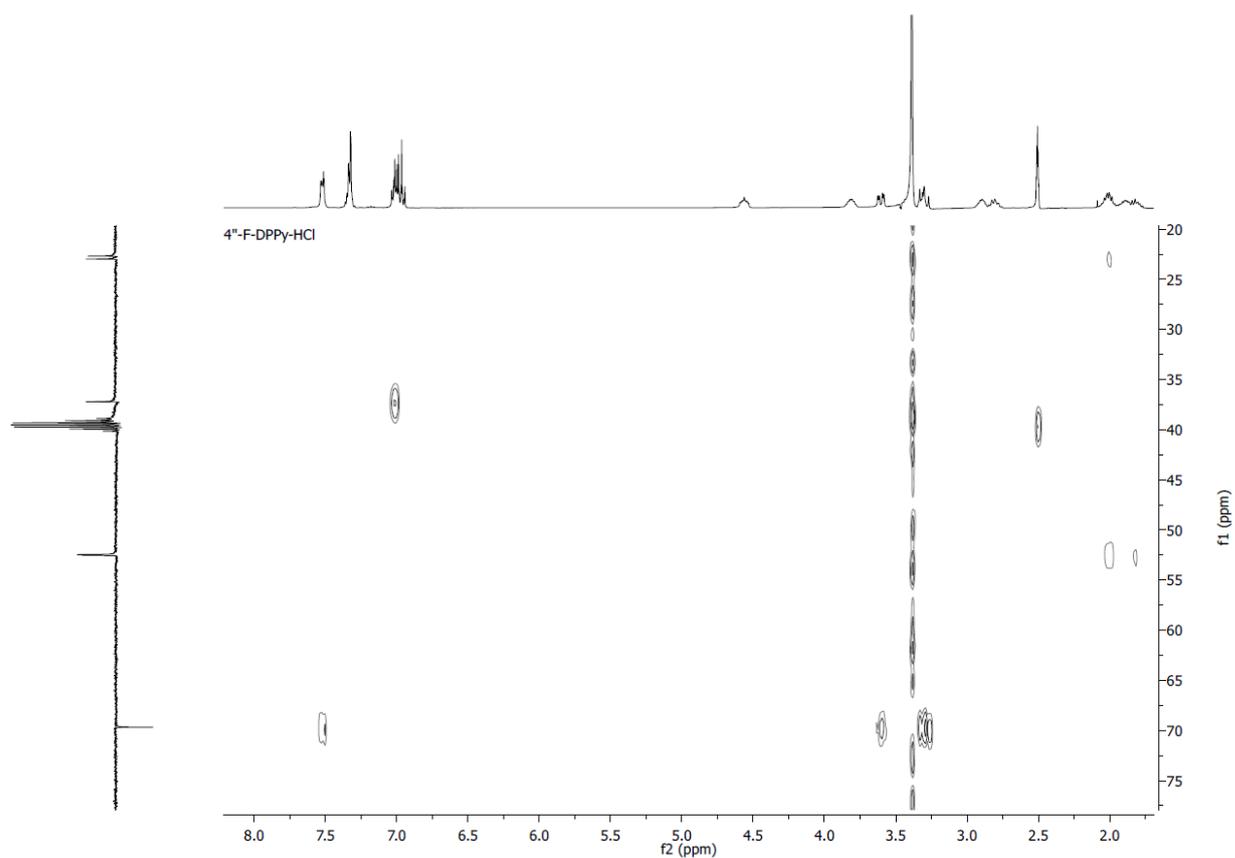
Supporting Information – Drug Testing and Analysis



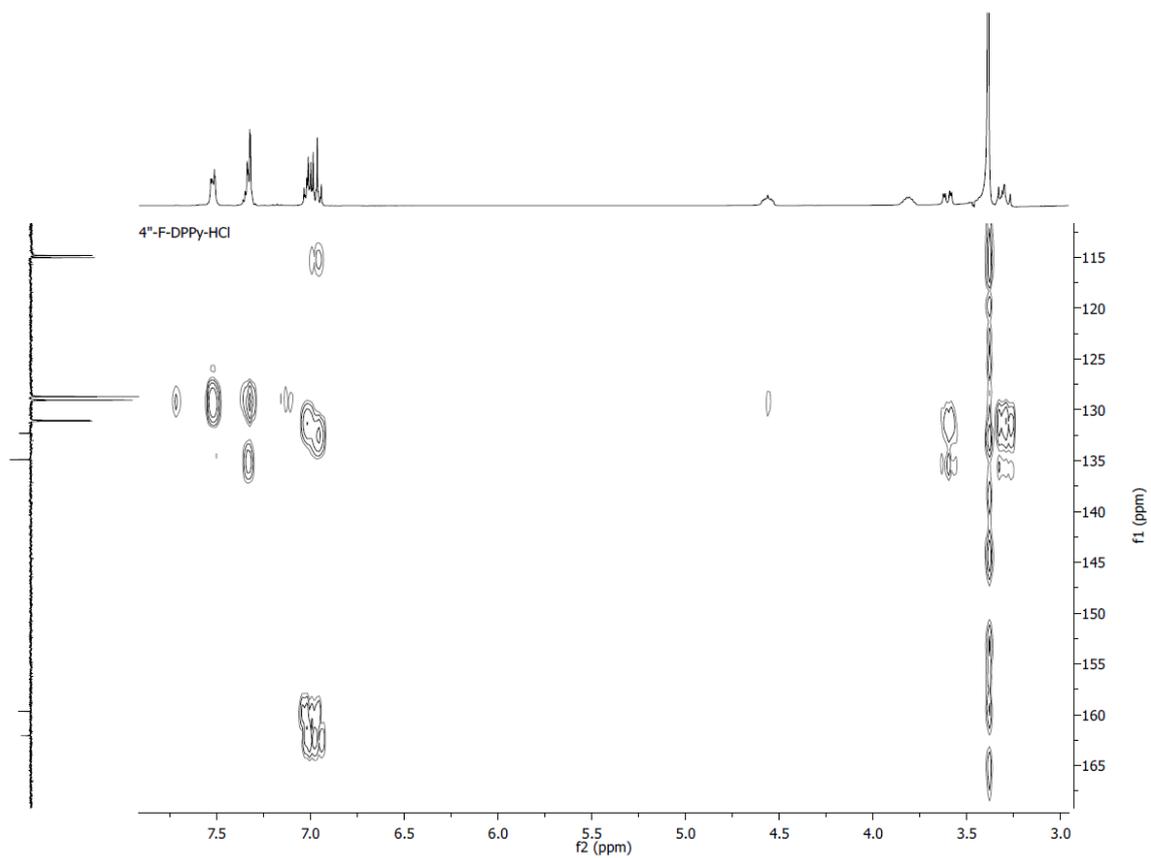
HMQC 2-D NMR of 4''-F-DPPy HCl, zoomed in on the aromatic section (d_6 -DMSO)



HMBC 2-D NMR of 4''-F-DPPy HCl (d₆-DMSO)

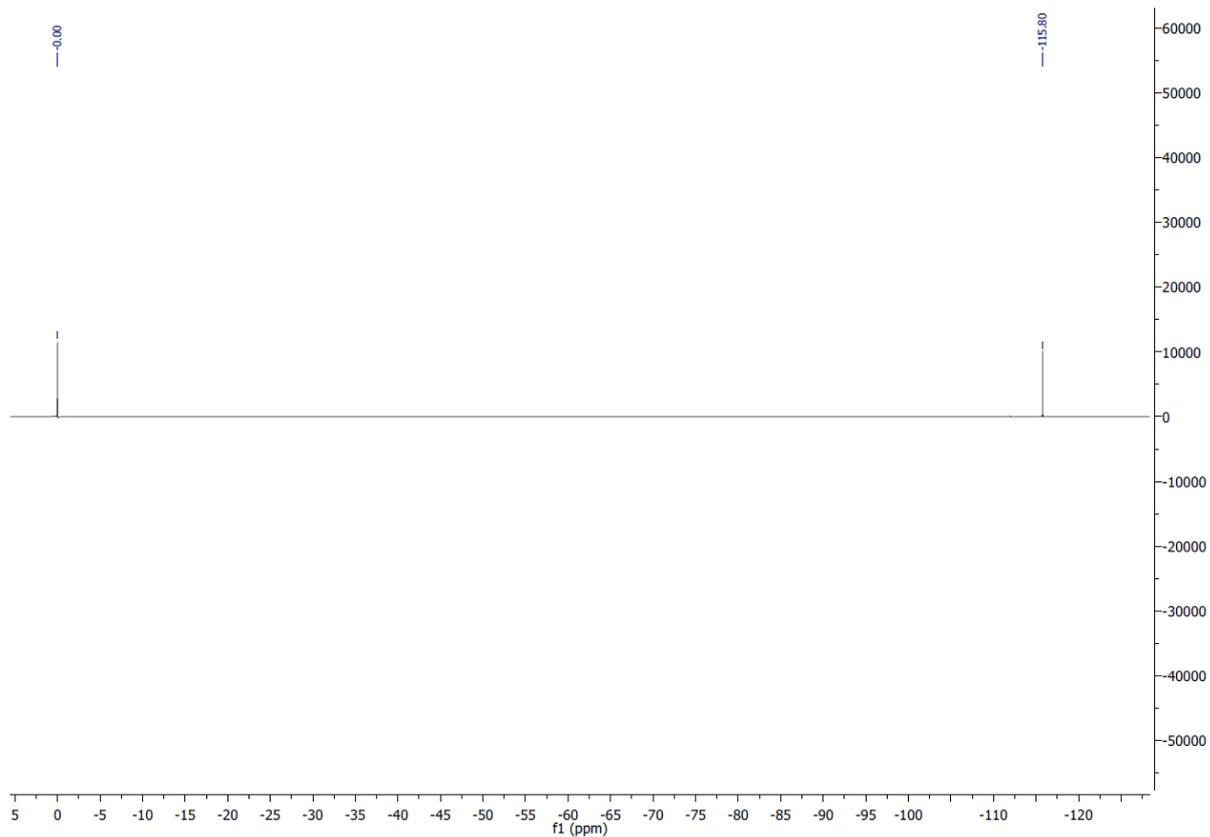


HMBC 2-D NMR of 4''-F-DPPy HCl, zoomed in on the aliphatic section (d₆-DMSO)



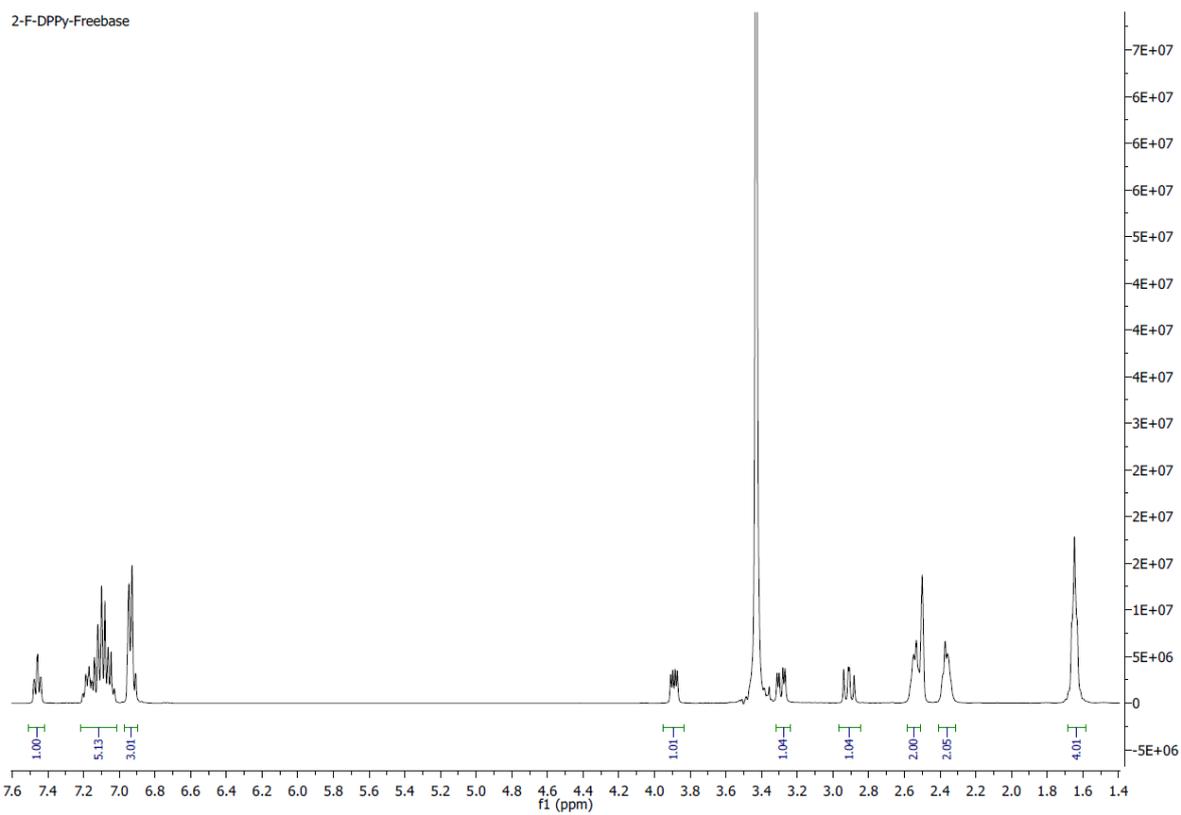
HMBC 2-D NMR of 4'-F-DPPy HCl, zoomed in on the aromatic section (d_6 -DMSO)

Supporting Information – Drug Testing and Analysis



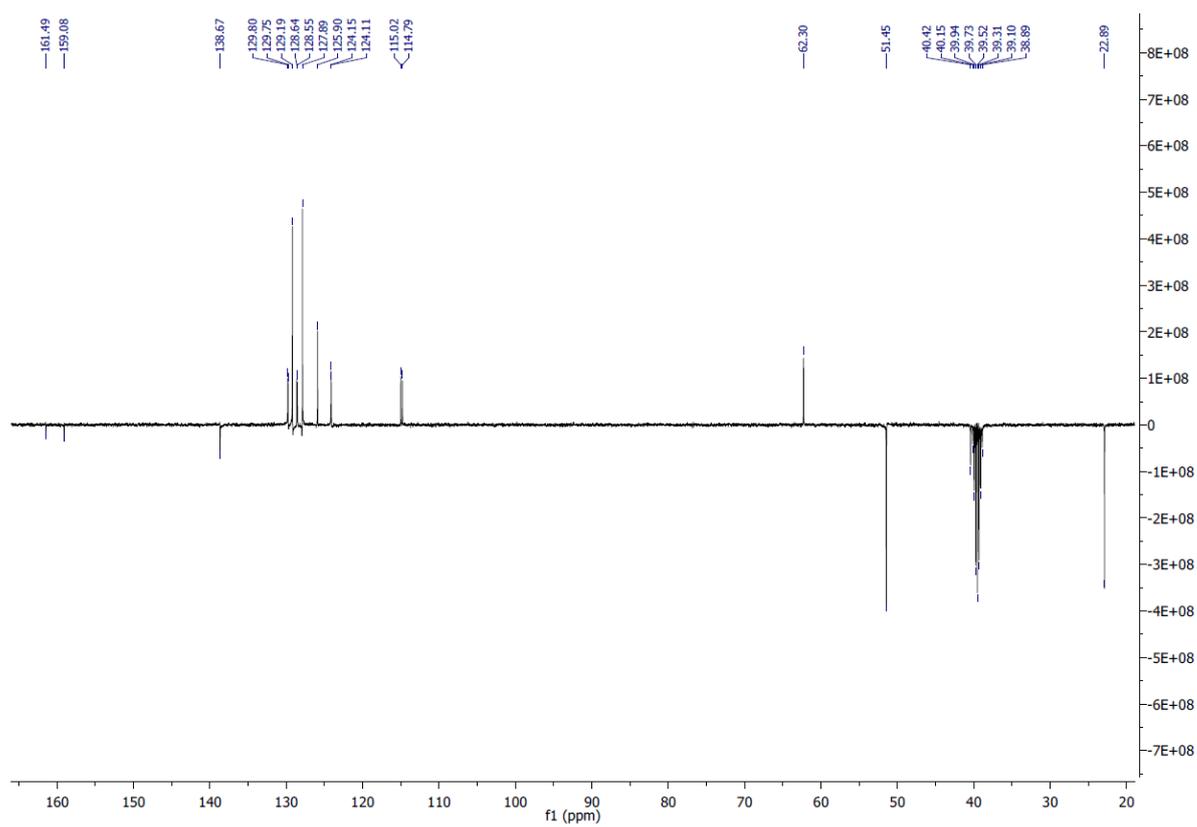
^{19}F NMR of 4-F-DPPy HCl with CFCl_3 as internal reference (376.5 MHz, d_6 -DMSO)

Supporting Information – Drug Testing and Analysis



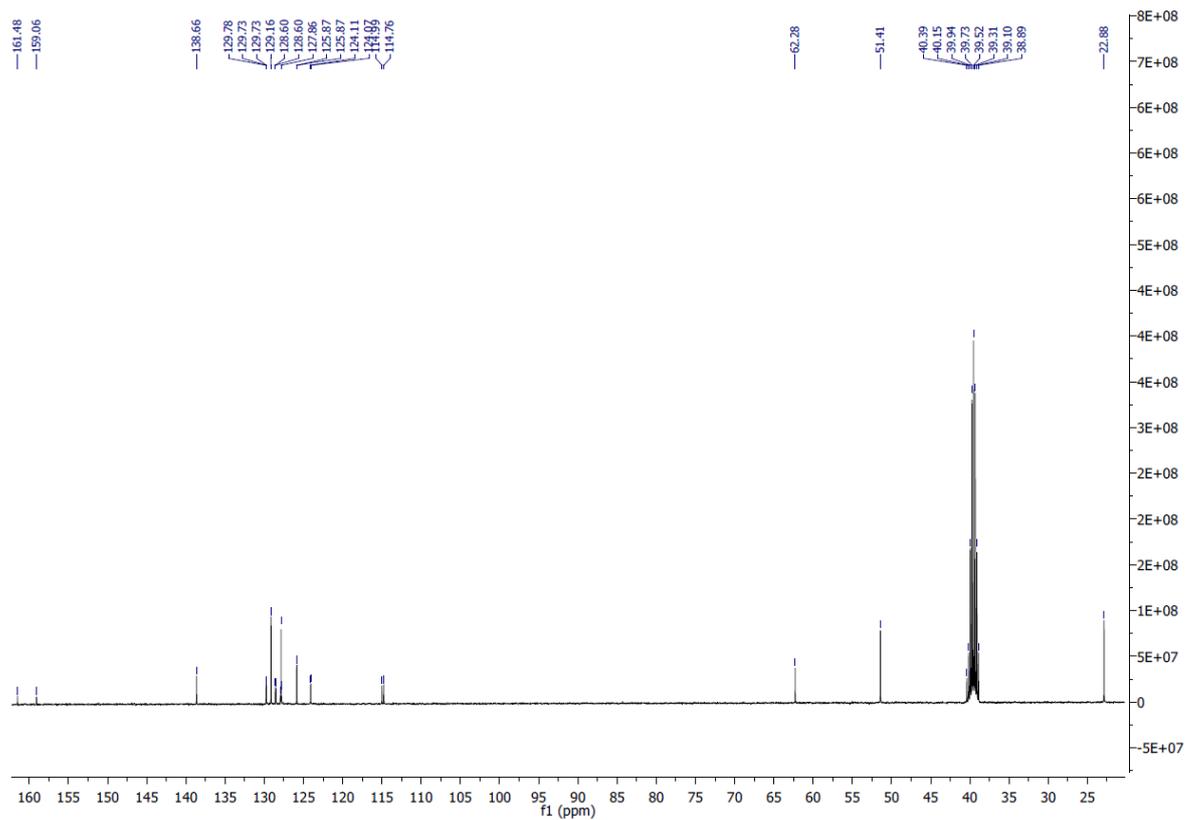
^1H NMR of 2-F-DPPy freebase (400 MHz, d_6 -DMSO)

Supporting Information – Drug Testing and Analysis



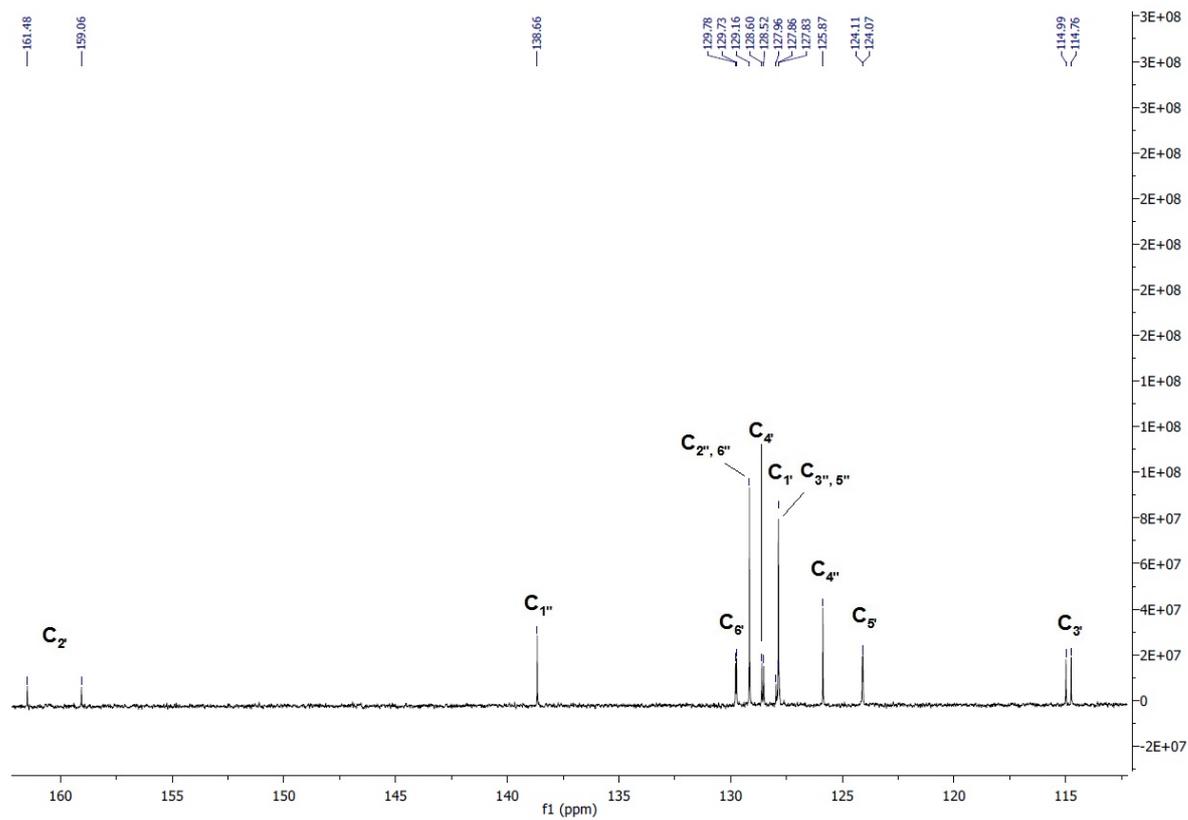
^{13}C PENDANT NMR of 2-F-DPPy freebase (101 MHz, $\text{d}_6\text{-DMSO}$)

Supporting Information – Drug Testing and Analysis



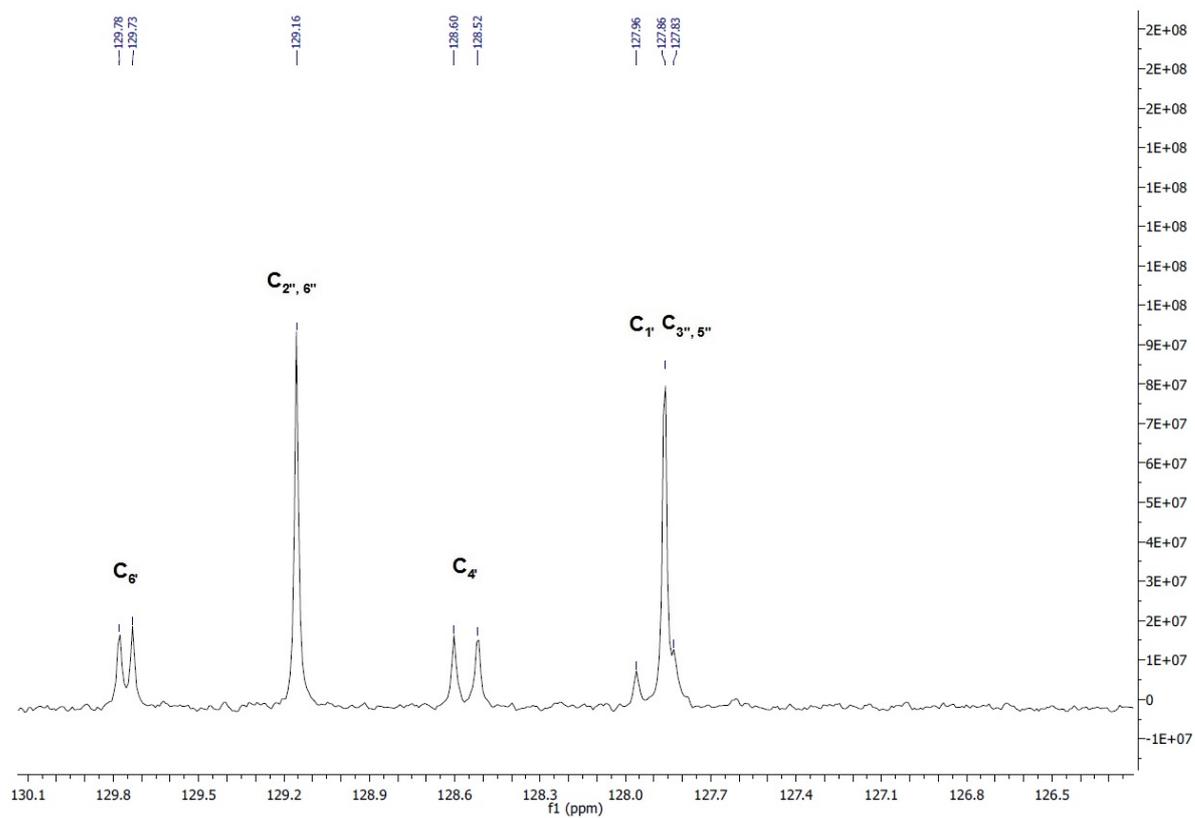
¹³C NMR of 2-F-DPPy freebase (101 MHz, d₆-DMSO)

Supporting Information – Drug Testing and Analysis

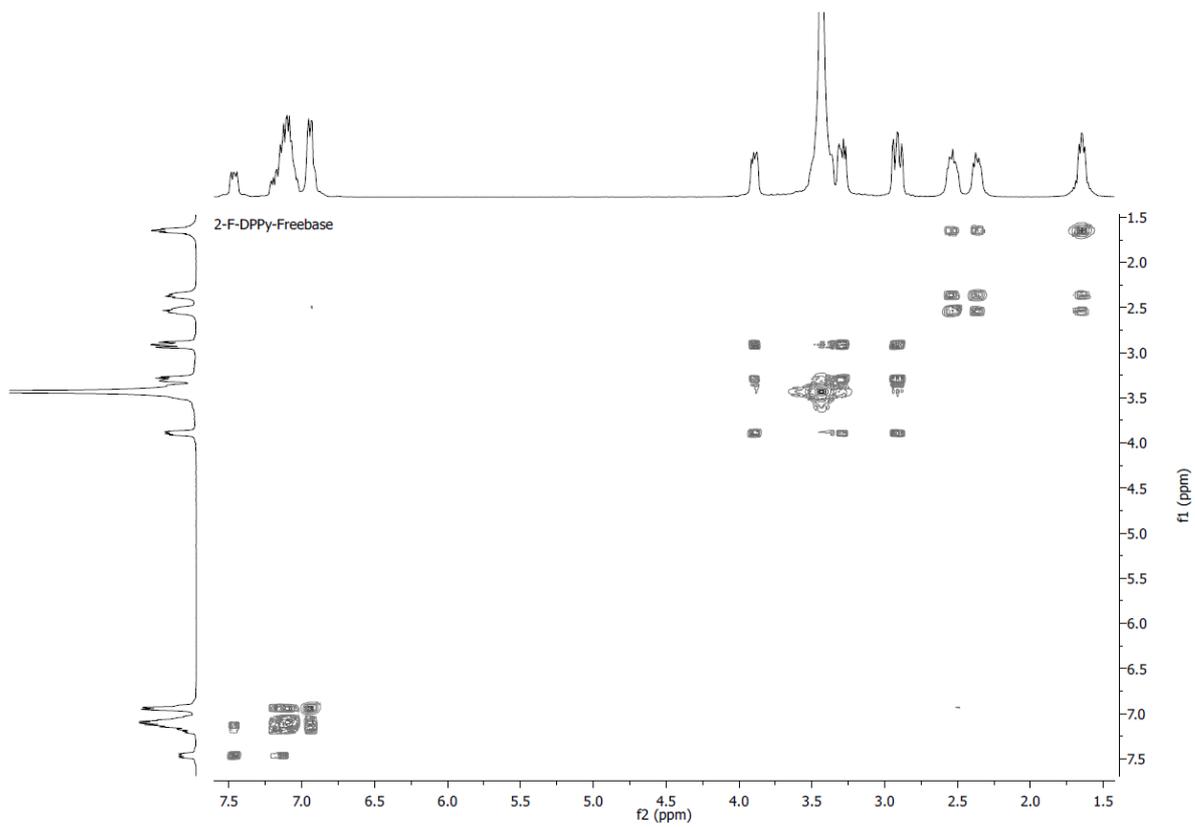


¹³C NMR of 2-F-DPPy freebase, zoomed in on the aromatic section (101 MHz, d₆-DMSO)

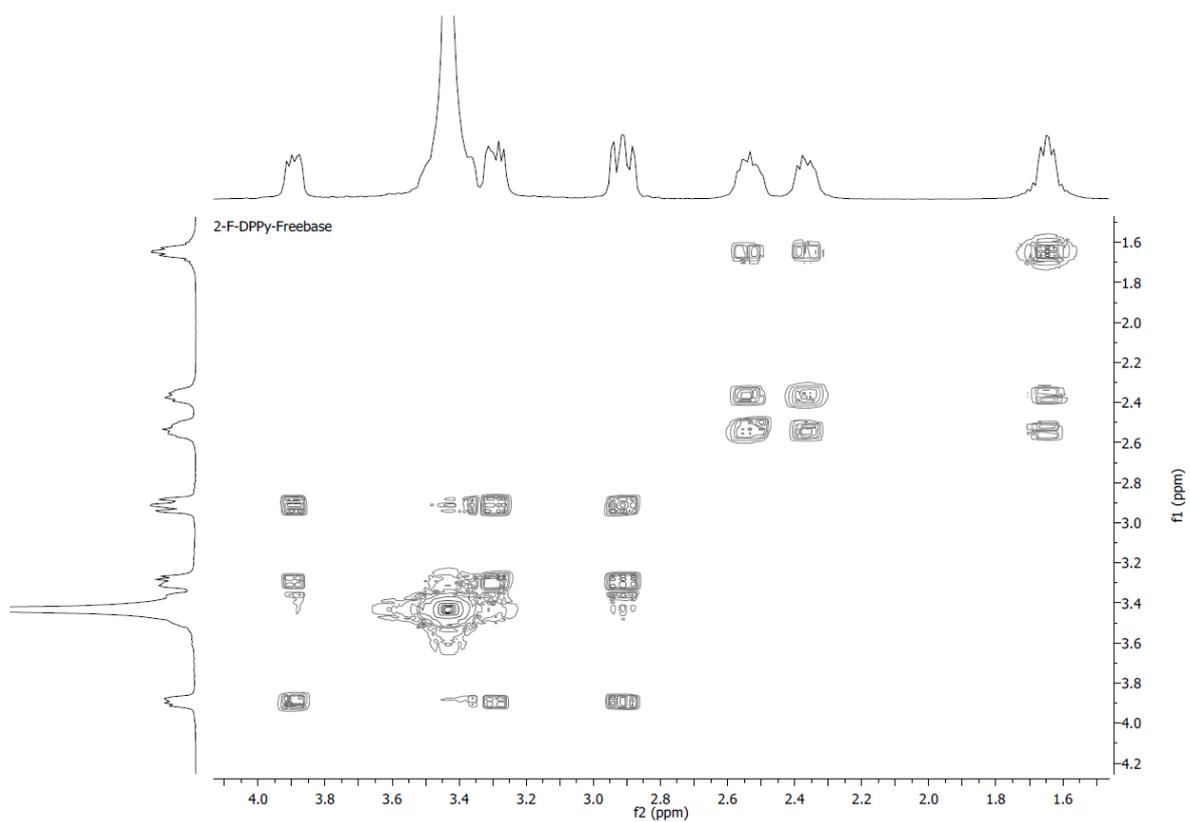
Supporting Information – Drug Testing and Analysis



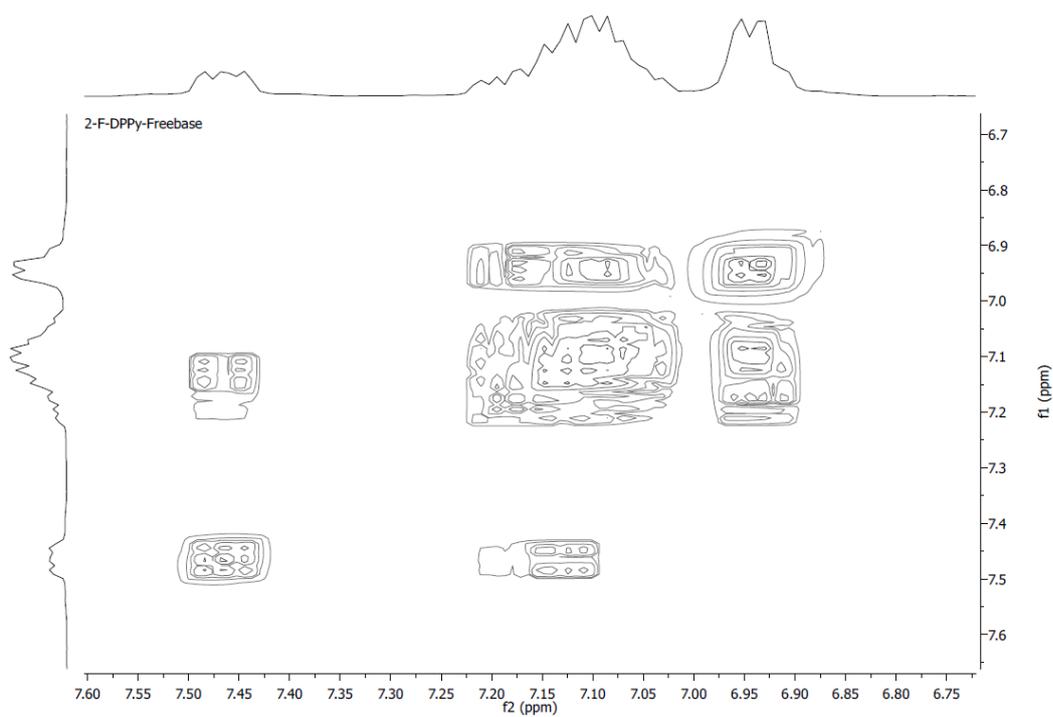
^{13}C NMR of 2-F-DPPy freebase, zoomed in to display $\text{C}_{1'}$, $\text{C}_{3''}$, $\text{C}_{5''}$ overlap (101 MHz, $\text{d}_6\text{-DMSO}$)



COSY-45 2-D NMR of 2-F-DPPy freebase (d_6 -DMSO)

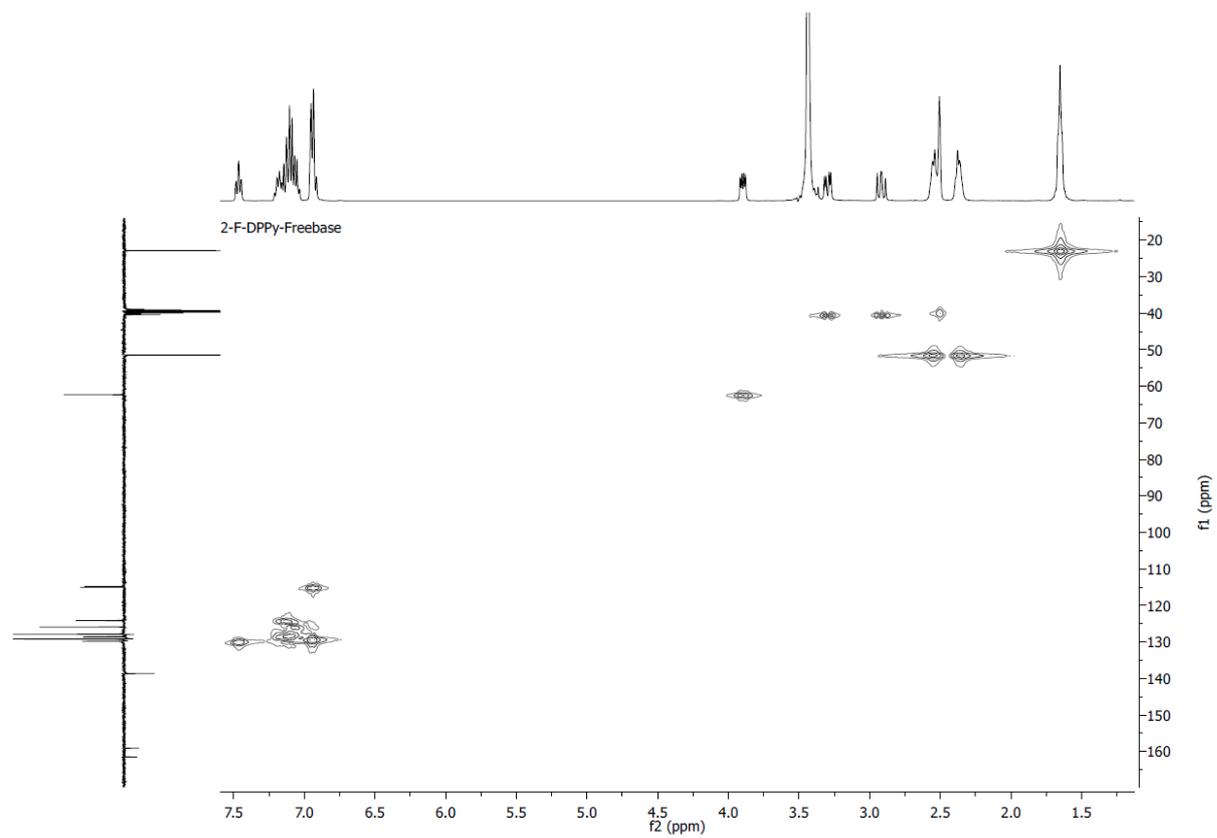


COSY-45 2-D NMR of 2-F-DPPy freebase, zoomed in on aliphatic section (d_6 -DMSO)

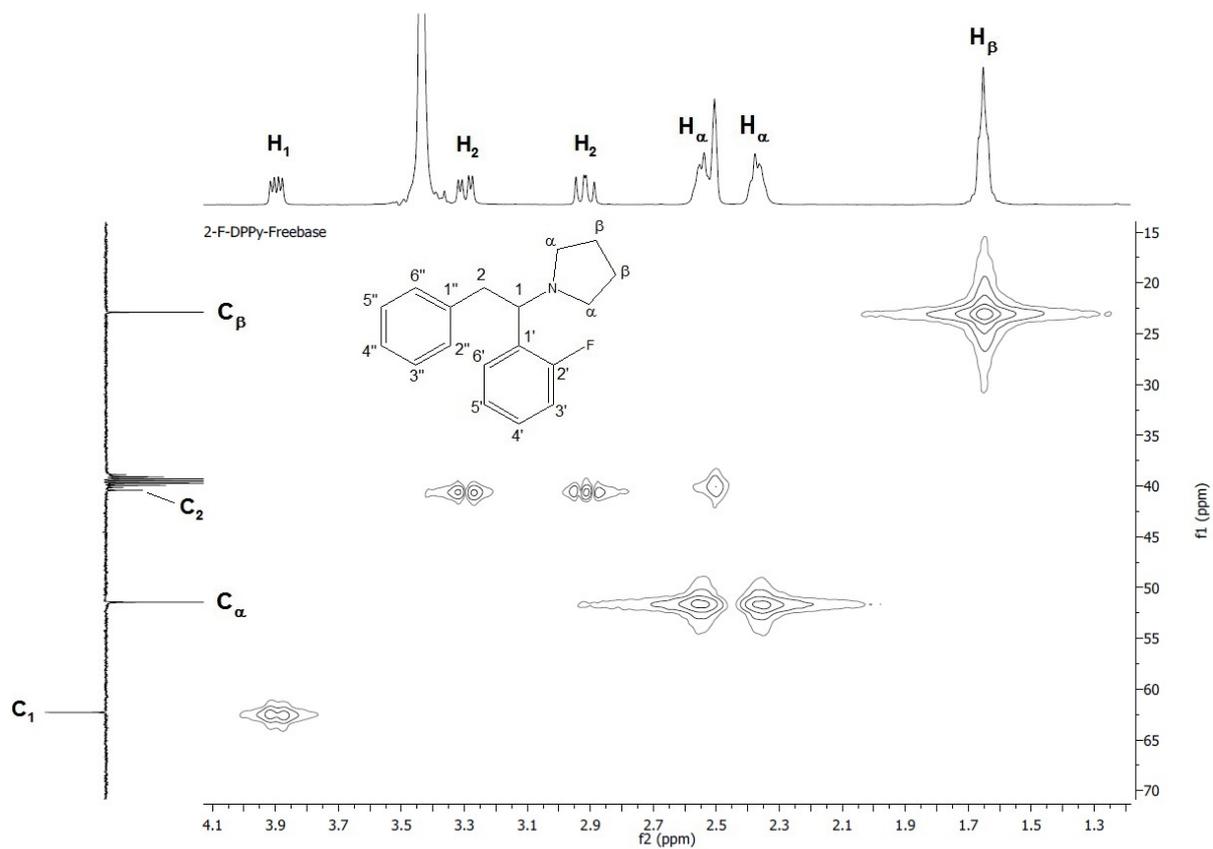


COSY-45 2-D NMR of 2-F-DPPy freebase, zoomed in on aromatic section (d_6 -DMSO)

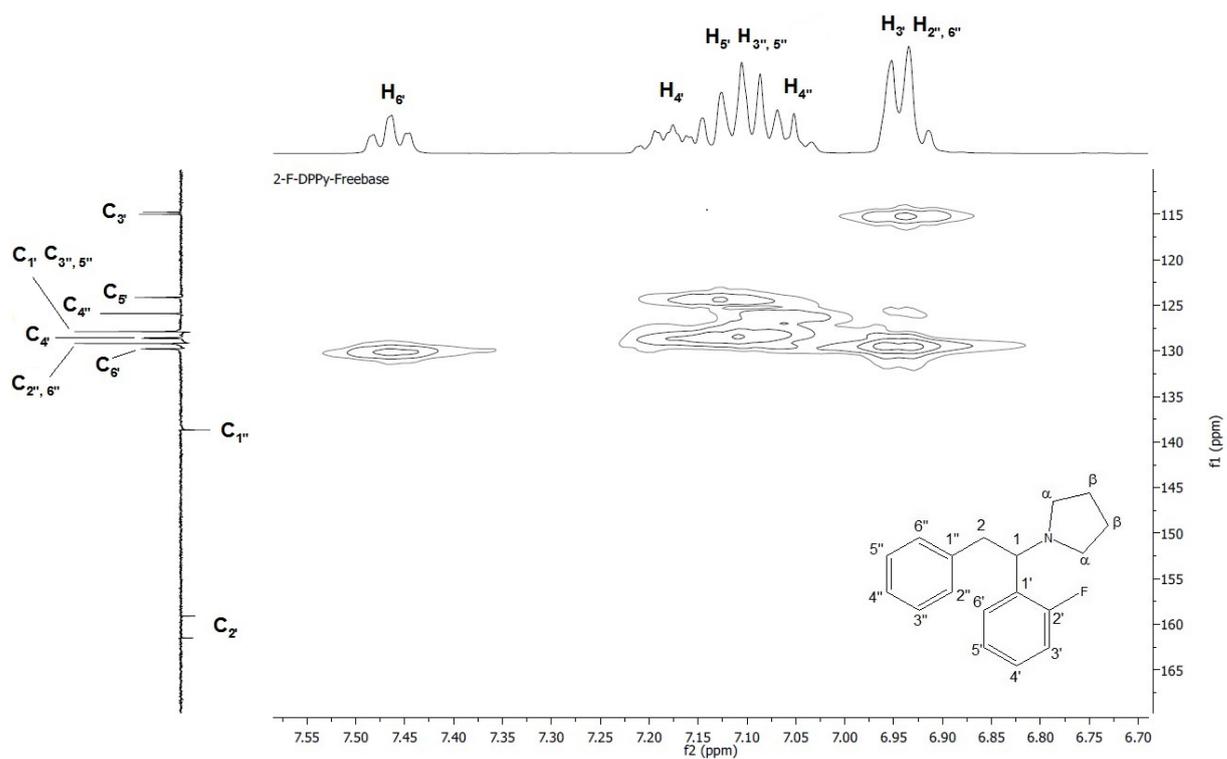
Supporting Information – Drug Testing and Analysis



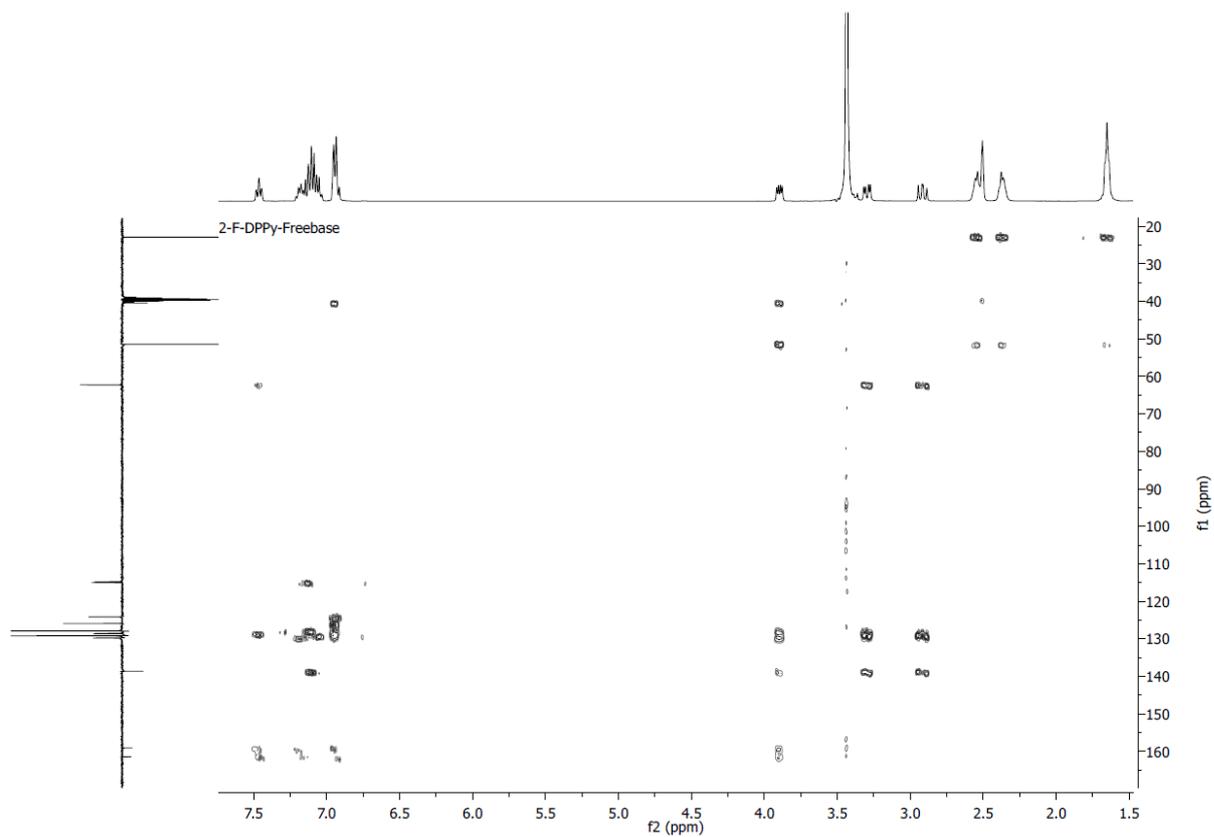
HMQC 2-D NMR of 2-F-DPPy freebase (d_6 -DMSO)



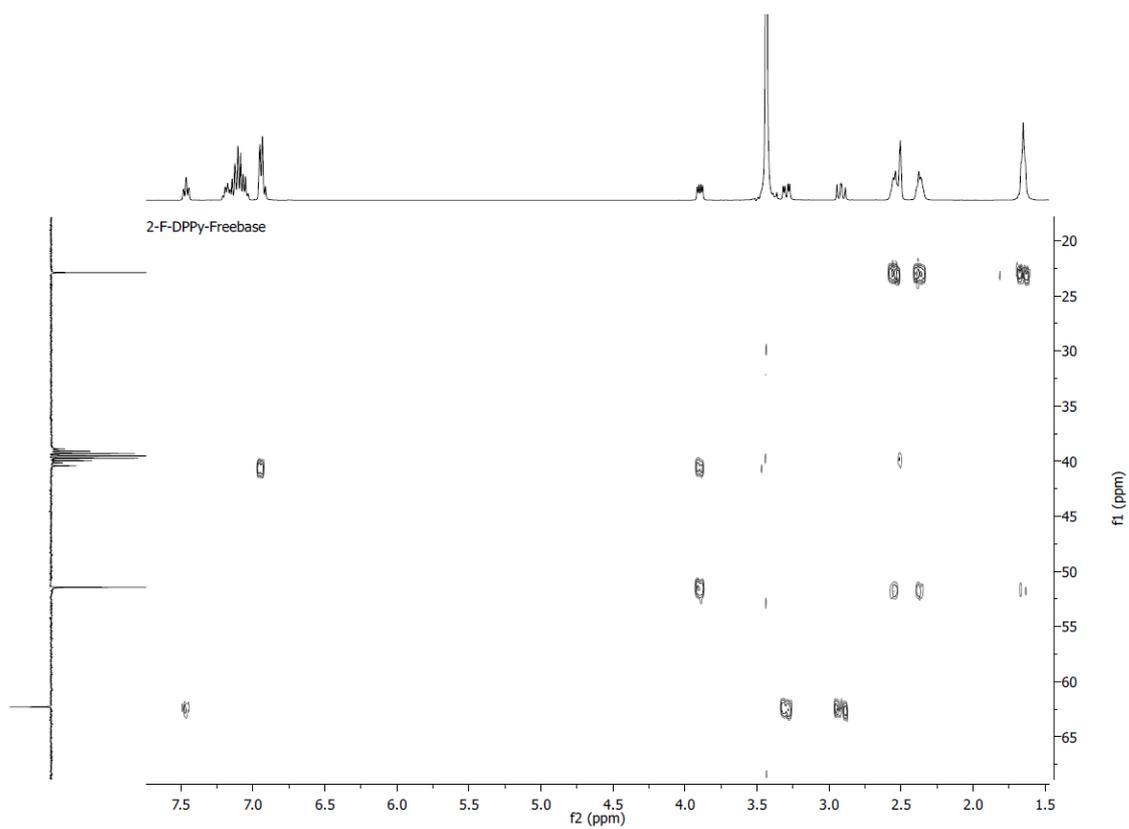
HMQC 2-D NMR of 2-F-DPPy freebase, zoomed in on aliphatic section (d_6 -DMSO)



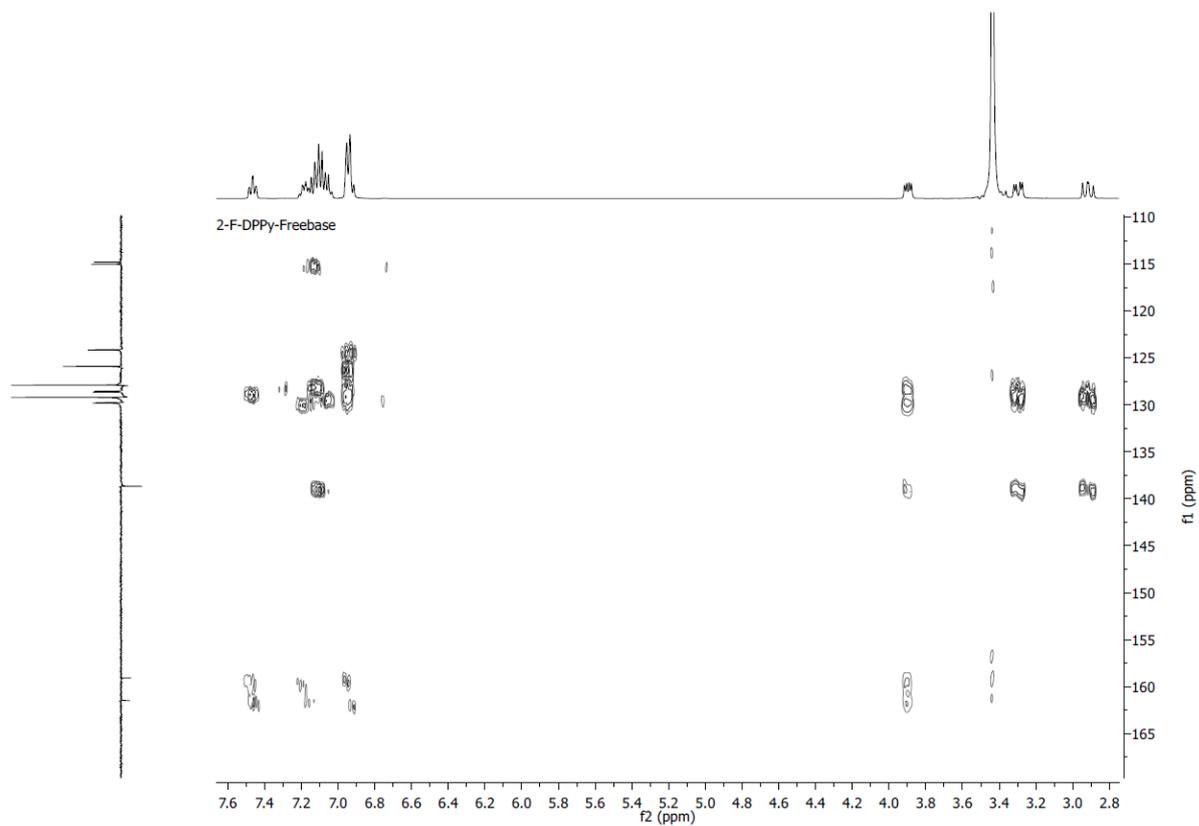
HMQC 2-D NMR of 2-F-DPPy freebase, zoomed in on aromatic section (d_6 -DMSO)



HMBC 2-D NMR of 2-F-DPPy freebase (d_6 -DMSO)

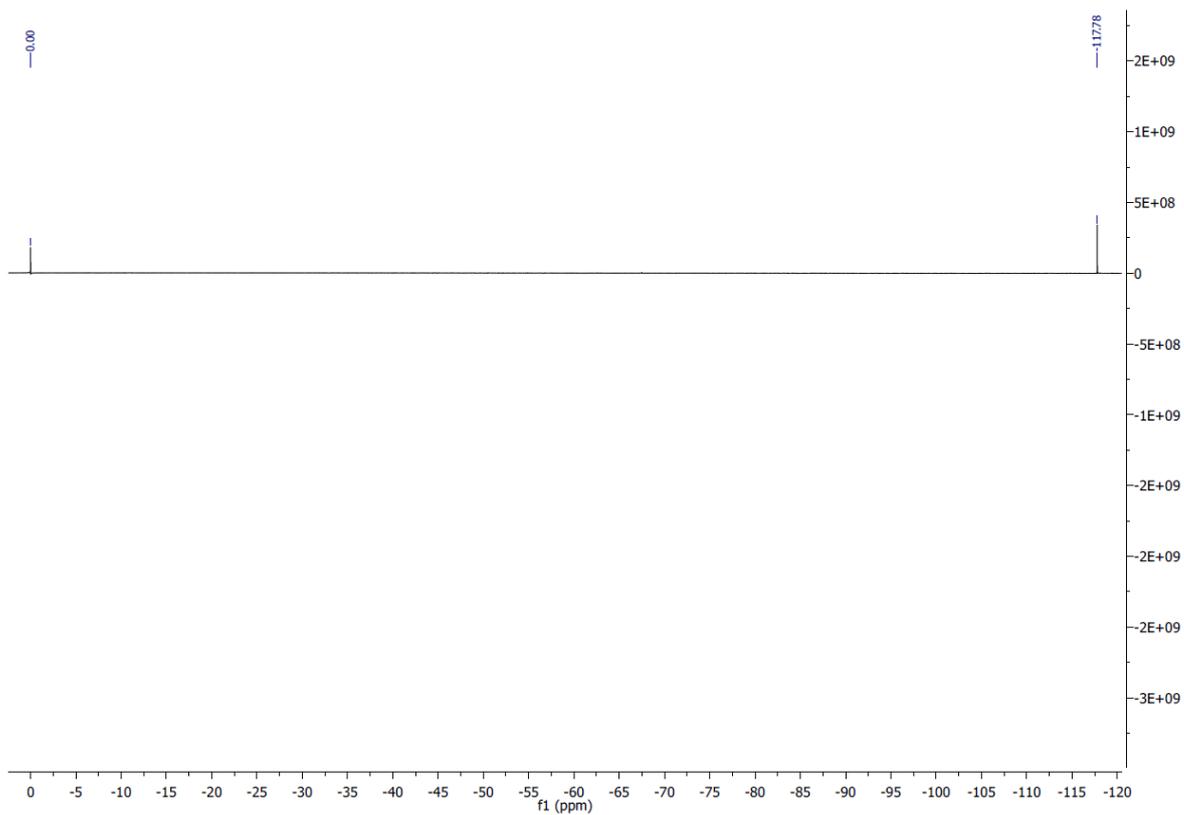


HMBC 2-D NMR of 2-F-DPPy freebase, zoomed in on aliphatic section (d_6 -DMSO)



HMBC 2-D NMR of 2-F-DPPy freebase, zoomed in on aromatic section (d₆-DMSO)

Supporting Information – Drug Testing and Analysis



^{19}F NMR of 2-F-DPPy freebase with CFCl_3 as internal reference (376.5 MHz, d_6 -DMSO)