Supporting Information for

^{19}F Magic Angle Spinning NMR Spectroscopy and Density Functional Theory Calculations of Fluorosubstituted Tryptophans: Integrating Experiment and Theory for Accurate Determination of Chemical Shift Tensors

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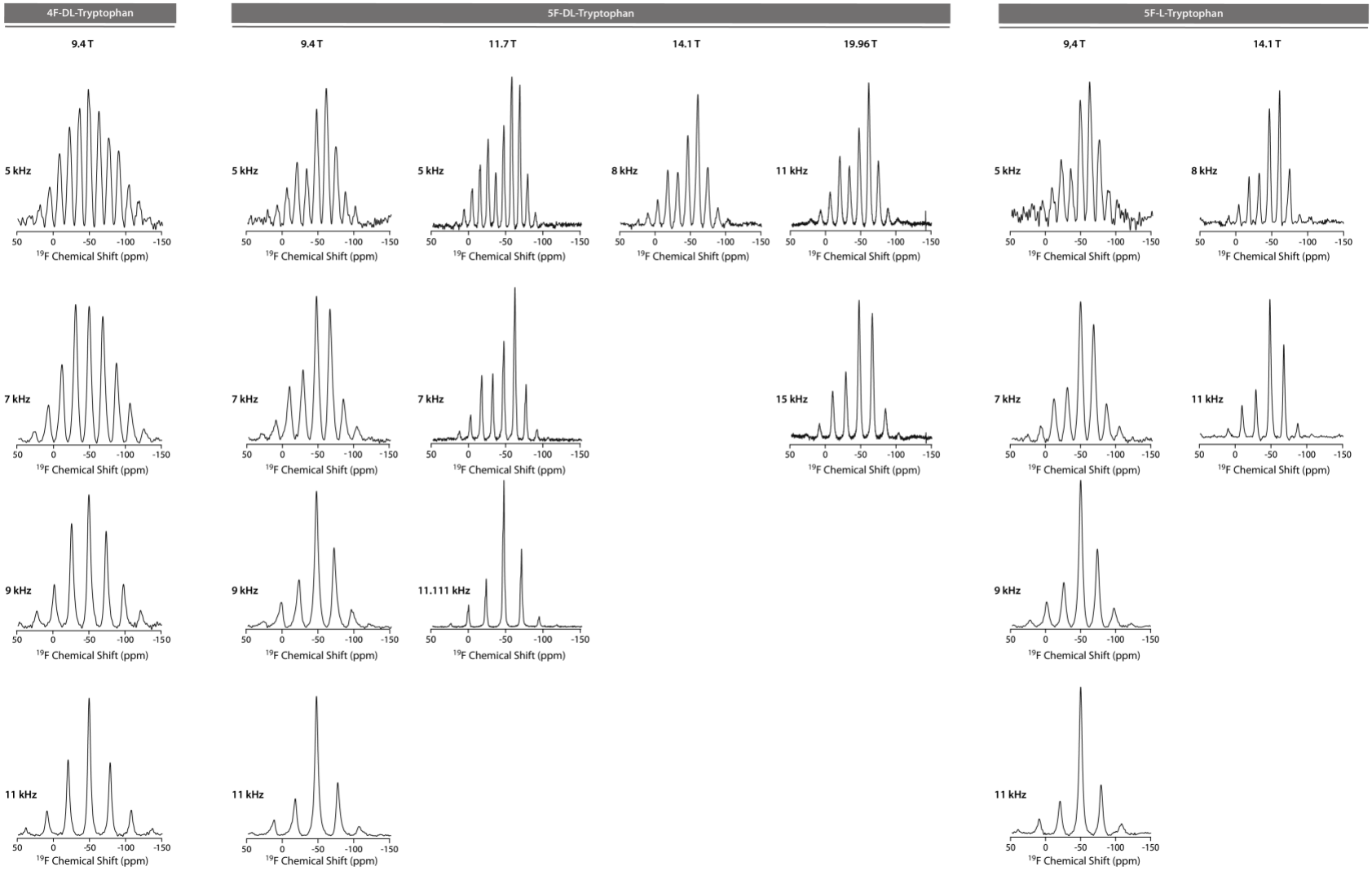

Figure S1: Summary of ^{19}F MAS NMR spectra of fluorosubstituted tryptophans (4F-DL-tryptophan, 5F-DL-tryptophan, 5F-L-tryptophan) acquired at several magnetic field strengths with different MAS frequencies.

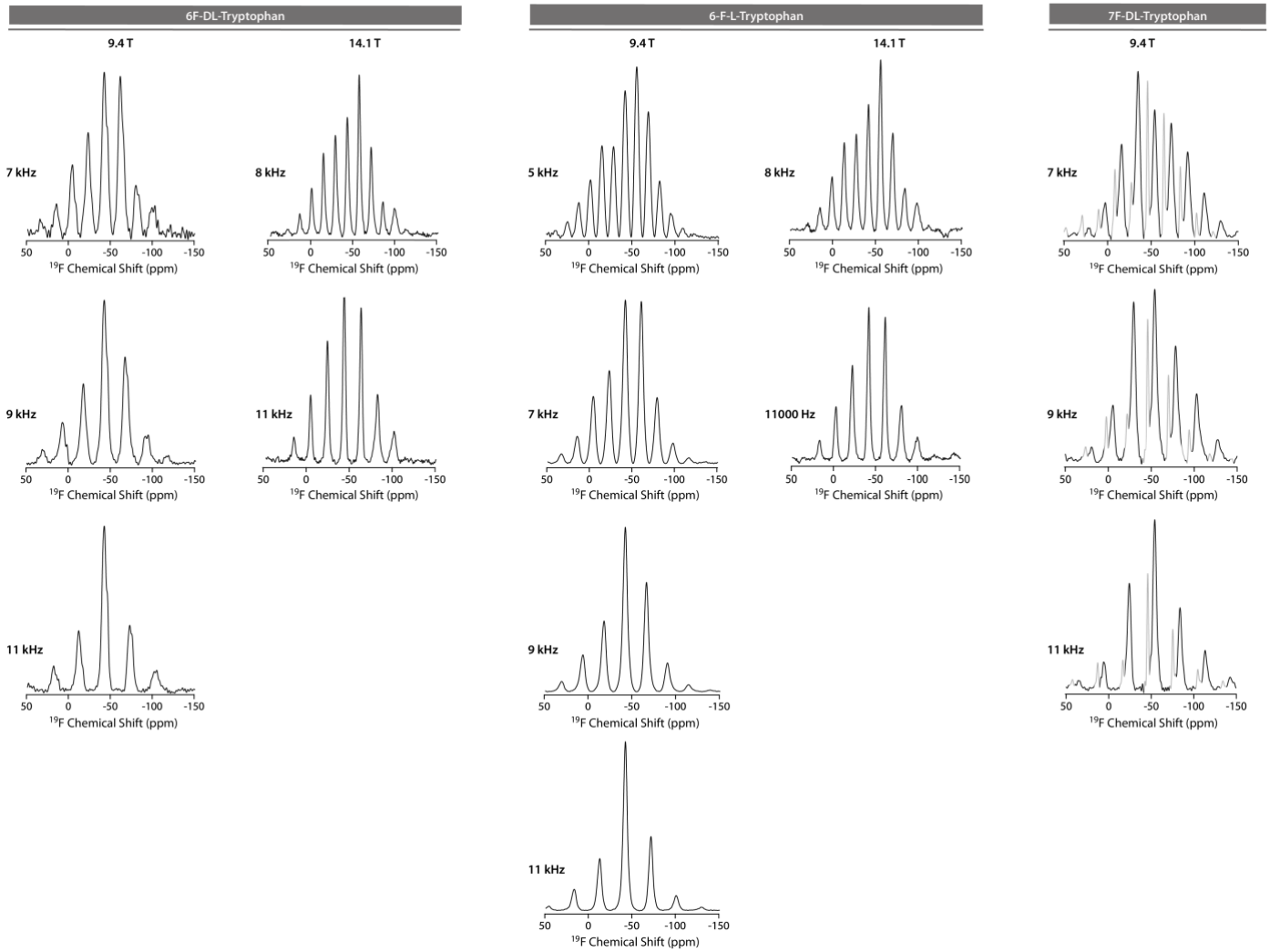

Figure S2: Summary of ^{19}F MAS NMR spectra of fluorosubstituted tryptophans (6F-DL-tryptophan, 6F-L-tryptophan, 7F-DL-tryptophan) acquired at various magnetic field strengths with various MAS frequencies.

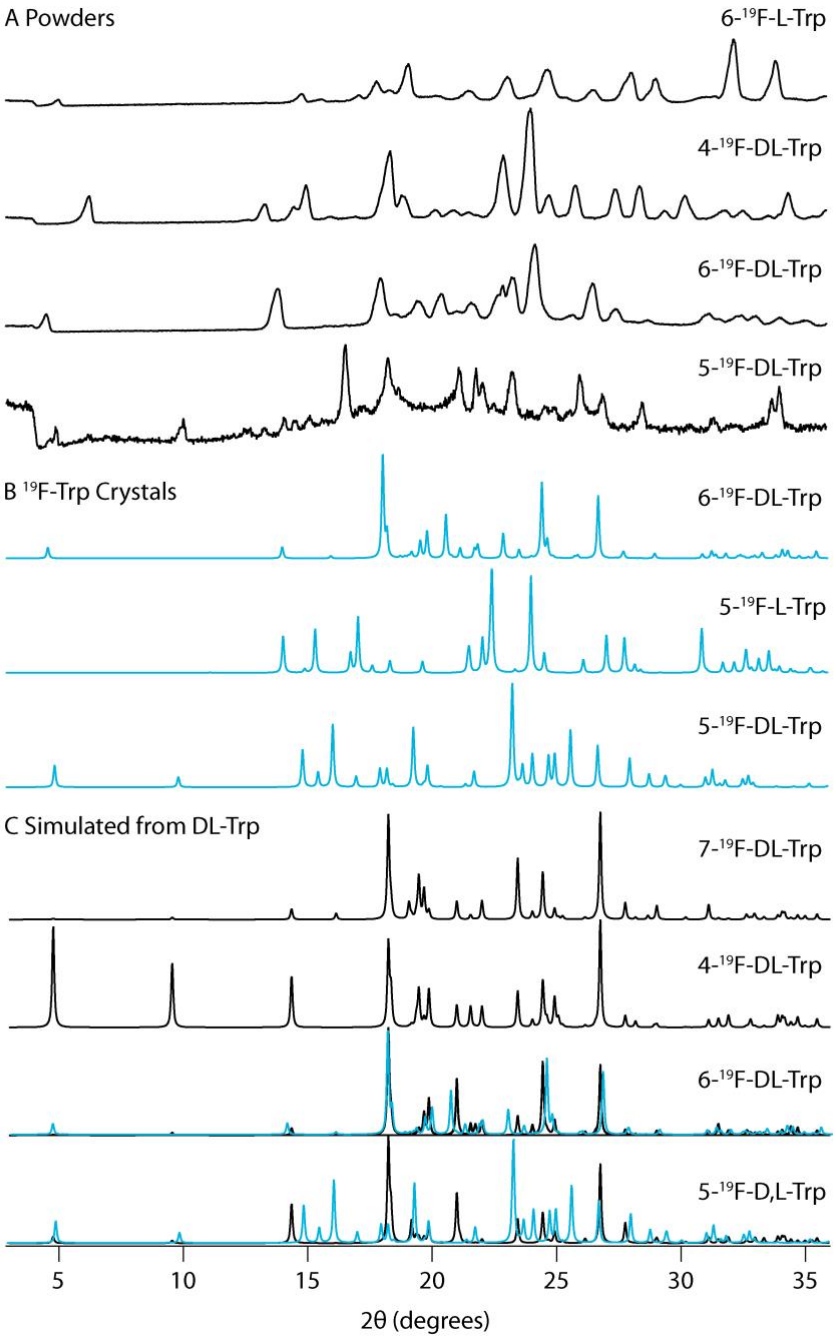

Figure S3. A. Experimental powder XRD patterns for fluorosubstituted tryptophan powders. B. Simulated powder XRD patterns of crystalline 6F-DL-tryptophan, 5F-L-tryptophan monohydrate, and 5F-DL-tryptophan. The patterns were generated in Mercury using the crystal structures. C. Black lines: simulated powder XRD patters for fluorosubstituted tryptophans, generated from the parent L- and DL-tryptophans. Crystal structure of the triclinic L-tryptophan (vixqok01.cif) and monoclinic DL-tryptophan (qqqbtp02.cif) were obtained from the Cambridge Crystallographic Data Centre (CCDC).[1] Blue lines: simulated powder XRD patterns for 6F-DL-tryptophan and 5F-L-tryptophan monohydrate crystals.

Table S1. MAS frequency and magnetic field dependence of the sensitivity of ^{19}F MAS NMR experiments for 5F-L/DL-tryptophan and 6F-L/DL-tryptophan.

Sample	Rotor size	Sample weight	Magnetic field strength	MAS frequency	Signal-to-noise ratio (normalized, per single scan)
6F-L-tryptophan	1.3 mm	2.2 mg	14.1 T	20 kHz	1.4
				30 kHz	1.9
				35 kHz	2.0
				40 kHz	2.0
				50 kHz	2.2
				60 kHz	2.2
6F-DL-tryptophan	1.3 mm	1.8 mg	14.1 T	20 kHz	1.0
				30 kHz	1.7
				35 kHz	2.0
				40 kHz	2.2
				50 kHz	2.2
				60 kHz	3.1
5F-L-tryptophan	1.3 mm	3.0 mg	14.1 T	20 kHz	4.1
				30 kHz	7.9
				35 kHz	10.1
				40 kHz	10.5
				50 kHz	11.7
				60 kHz	11.8
5F-DL-tryptophan	1.3 mm	3.0 mg	14.1 T	20 kHz	2.3
				30 kHz	3.1
				35 kHz	3.4
				40 kHz	3.9
				50 kHz	3.9
				60 kHz	4.0
	1.6 mm	7.6 mg	19.96 T	40 kHz	21.7
				40 kHz, ^{1}H decoupled	19.1

Table S2. Summary of experimental principal components of the chemical shift tensors, isotropic chemical shifts, reduced anisotropy, and asymmetry for the F-DL-tryptophan for various magnetic field strengths and various MAS frequencies.

Compound	Field Strength	Spinning Frequency	δ_{iso} (ppm)	δ (ppm)	η	δ_{11} (ppm)	δ_{22} (ppm)	δ_{33} (ppm)
4F-DL-tryptophan	9.4 T	*5 kHz	-50.0	-62.0	1.0	10.8	-48.9	-112.0
		7 kHz	-50.0	-63.4	1.0	12.1	-48.7	-113.4
		9 kHz	-50.0	-62.2	0.9	10.2	-48.0	-112.2
		*11 kHz	-50.0	61.6	1.0	11.6	-50.8	-110.8
	Average		-50.0	-62.8	1.0	11.2	-48.3	-112.8
	Standard Deviation		0.0	0.8	0.0	1.4	0.5	0.8
5F-DL-tryptophan	9.4 T	*5 kHz	-47.2	55.4	0.6	8.2	-57.2	-92.6
		7 kHz	-47.2	51.7	0.6	4.5	-58.6	-87.4
		9 kHz	-47.2	54.7	0.5	7.5	-61.3	-87.7
		*11 kHz	-47.2	55.8	0.6	8.6	-59.2	-91.0
		Average	-47.2	53.2	0.6	6.0	-60.0	-87.6
		STD	0.0	2.1	0.1	2.1	1.9	0.2
	11.7 T	5 kHz	-47.2	52.0	0.5	4.8	-61.4	-85.0
		7 kHz	-47.2	51.7	0.5	4.5	-59.7	-86.4
		11 kHz	-47.2	51.4	0.5	4.1	-60.9	-85.1
		Average	-47.2	51.7	0.5	4.4	-60.7	-85.5
		STD	0.0	0.3	0.0	0.3	0.9	0.8
	14.1 T	8 kHz	-47.2	51.8	0.5	4.6	-59.4	-86.8
	19.96 T	11 kHz	-47.2	50.6	0.5	4.8	-61.4	-85.0
		15 kHz	-47.2	50.5	0.5	4.5	-59.7	-86.4
		Average	-47.2	50.6	0.5	4.1	-60.9	-85.1
		STD	0.0	0.1	0.0	0.2	1.2	1.0
	Average		-47.2	51.8	0.5	4.8	-60.5	-86.1
	Standard Deviation		0.0	1.3	0.1	1.3	1.0	1.2
5F-L-tryptophan	9.4 T	*5 kHz	-48.4	55.3	0.6	5.9	-60.6	-93.4
		7 kHz	-48.4	50.1	0.5	0.8	-62.2	-86.6
		9 kHz	-48.4	52.7	0.5	3.4	-62.5	-89.0
		*11 kHz	-48.4	53.5	0.5	4.1	-62.1	-90.1
		Average	-48.4	51.4	0.5	2.1	-62.4	-87.8
		STD	0.0	1.8	0.1	1.8	0.2	1.7
	14.1 T	8 kHz	-47.1	44.4	0.4	-5.0	-62.1	-81.1
		11 kHz	-47.1	47.0	0.3	-2.4	-65.0	-80.8
		Average	-47.1	45.7	0.4	-3.7	-63.5	-80.9
		STD	0.0	1.9	0.1	1.9	2.1	0.2
	Average		-47.7	48.6	0.4	-0.8	-62.9	-84.4
	Standard Deviation		0.8	3.7	0.1	3.7	1.4	4.1

Compound	Field Strength	Spinning Frequency	δ_{iso} (ppm)	δ (ppm)	η	δ_{11} (ppm)	δ_{22} (ppm)	δ_{33} (ppm)
6F-DL-tryptophan	9.4 T	7 kHz	-43.3	55.2	0.7	11.9	-51.7	-90.1
		9 kHz	-43.3	57.4	0.7	14.2	-51.2	-92.8
		*11 kHz	-43.3	56.0	0.9	12.7	-45.9	-96.8
		Average	-43.3	56.3	0.8	13.1	-51.5	-91.5
		STD	0.0	1.5	0.1	1.6	0.3	1.9
	14.1 T	8 kHz	-43.3	57.4	0.7	14.1	-51.2	-92.8
		11 kHz	-43.3	54.8	0.7	11.5	-50.5	-90.8
		Average	-43.3	56.1	0.7	12.8	-50.9	-91.8
		STD	0.0	1.8	0.0	1.8	0.5	1.4
	Average		-43.3	56.2	0.8	12.9	-51.2	-91.6
	Standard Deviation		0.0	1.4	0.1	1.4	0.5	1.4
6F-L-tryptophan	9.4 T	*5 kHz	-43.2	58.9	0.7	15.7	-52.1	-93.2
		7 kHz	-43.2	55.4	0.7	12.2	-52.3	-89.5
		9 kHz	-43.2	57.5	0.6	14.3	-53.5	-90.3
		*11 kHz	-43.2	59.3	0.6	16.1	-53.9	-91.8
		Average	-43.2	56.4	0.7	13.2	-52.9	-89.9
		STD	0.0	1.5	0.1	1.5	0.9	0.6
	14.1 T	8 kHz	-43.2	55.1	0.8	12.1	-49.7	-91.4
		11 kHz	-43.2	55.0	0.9	12.0	-47.2	-93.8
		Average	-42.0	55.0	0.8	12.0	-48.4	-92.6
		STD	0.0	0.1	0.1	0.1	1.8	1.7
	Average		-43.2	55.7	0.8	12.6	-50.7	-91.3
	Standard Deviation		0.0	1.2	0.1	1.1	2.8	1.9
7F-DL-tryptophan	9.4 T	7 kHz	-55.7	-68.7	0.8	5.9	-48.7	-124.4
		9 kHz	-55.7	-66.6	0.8	3.2	-48.0	-122.3
		*11 kHz	-55.7	-68.1	0.8	4.7	-48.0	-123.8
	Average		-55.7	-67.6	0.8	4.6	-48.3	-123.3
	Standard Deviation		0.0	1.4	0.0	1.9	0.5	1.4

*At 9.4 T, the spectra acquired with 5 kHz spinning exhibit lower sensitivity, and the spectra acquired with 11 kHz spinning have fewer spinning side bands than those obtained with 7 kHz and 9 kHz spinning. Due to the lower accuracy, the values obtained with 5 kHz and 11 kHz spinning at 9.4 T were not included in the calculation of the average values of the CST parameters.

X-ray structure determination

Crystals were mounted using viscous oil onto a plastic mesh and cooled to 200 K, the data collection temperature. Data were collected on a Bruker-AXS APEX II DUO CCD diffractometer with Cu-Kα radiation (λ = 1.54178 Å) focused with Goebel mirrors. Unit cell parameters were obtained from 36 data frames, 0.5º ω, i.e. three different sections of the Ewald sphere. The systematic absences in the diffraction data are consistent with $P2_1$ and $P2_1/m$ for 5F-L-Trp hydrate; $P2_1/c$ for 6F-DL-Trp; and $P2_12_12_1$ for 5F-L-Trp. The non-centrosymmetric space group option, $P2_1$, is consistent with the chirally resolved 5F-L-Trp and refinement yielded chemically reasonable and computationally stable results. The data were treated with multi-scan absorption corrections.[2] Structures were solved using intrinsic phasing methods[3] and refined with full-matrix, least-squares procedures on F^2.[4] The Flack parameters refined yielding ambiguous results since the low anomalous dispersion resulted in high standard errors. However, the handedness which resulted in values closest to zero, regardless of standard deviation for the two 5F-DL-Trp structures: 0.1(5) for the anhydrate and -0.03(13) for the hydrate, coincided with the chirality reported by the chemical supplier. Non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms bound to nitrogen and all hydrogen atoms in the hydrate were located from the difference map and refined with isotropic parameters. The ammonium hydrogen atoms in 6F-DL-Trp were restrained with a refined average N-H distance of 1.01(3) Å. The remaining hydrogen atoms were treated as idealized contributions with geometrically calculated positions and with U_{iso} equal to 1.2 U_{eq} of the attached carbon atom. Atomic scattering factors are contained in the SHELXTL program library.[4] The structures have been deposited at the CCDC: 5F-L-Trp: 1839071; 5F-L-Trp hydrate: 1839072 and 6F-DL-Trp: 1839073.

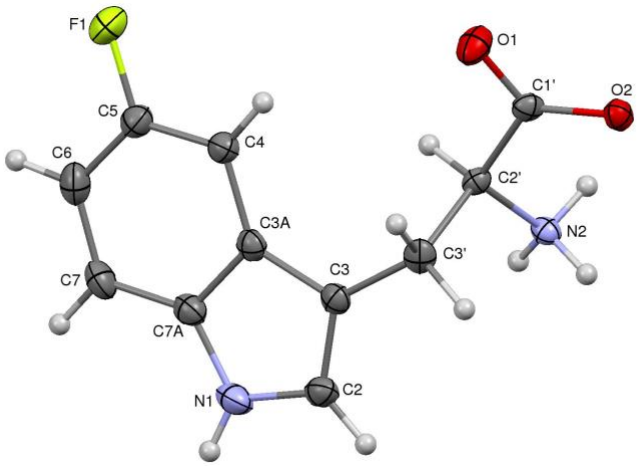

Figure S6. Molecular structure of 5F-L-tryptophan (5F-L-tryp) with 30% probability thermal ellipsoids. H-atoms are depicted with arbitrary radii.

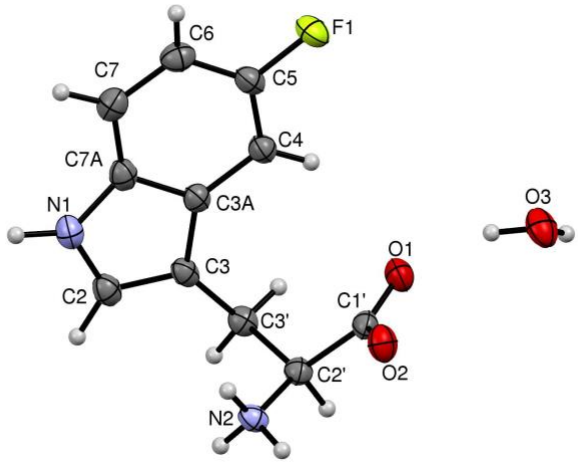

Figure S7. Molecular structure of 5F-L-tryptophan (5F-L-Trp) hydrate with 30% probability thermal ellipsoids. H-atoms are depicted with arbitrary radii.

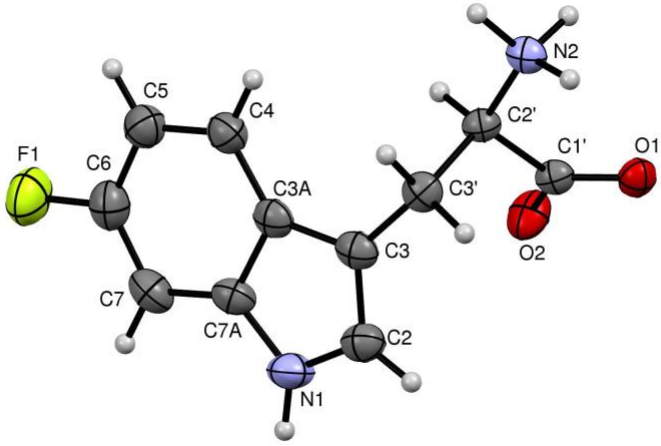

Figure S8. Molecular structure of 6F-L-tryptophan (6F-L-Trp) with 30% probability thermal ellipsoids. H-atoms are depicted with arbitrary radii.

Table S5. Crystal data and structure refinement for 5F-L-tryptophan (5F-L-Trp).

Identification code	5F-L-tryp	
Empirical formula	C11 H11 F N2 O2	
Formula weight	222.22	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 4.9666(4) Å	α= 90º.
	b = 5.7741(4) Å	β= 90º.
	c = 35.618(2) Å	γ= 90º.
Volume	1021.45(13) $Å^3$	
Z	4	
Density (calculated)	1.445 g/cm^3	
Absorption coefficient	0.959 mm^{-1}	
F(000)	464	
Crystal size	0.274 x 0.212 x 0.042 mm^3	
Theta range for data collection	2.481 to 75.019º.	
Index ranges	-5<=h<=5, -7<=k<=6, -43<=l<=36	
Reflections collected	4387	
Independent reflections	1964 [R(int) = 0.0317]	
Completeness to theta = 67.679º	98.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7526 and 0.7173	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1964 / 0 / 162	
Goodness-of-fit on F^2	1.023	
Final R indices [I>2sigma(I)]	R1 = 0.0548, wR2 = 0.1401	
R indices (all data)	R1 = 0.0572, wR2 = 0.1418	
Absolute structure parameter	0.1(5)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.219 and -0.200 e.$Å^{-3}$	

Table S6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 5F-L-tryptophan (5F-L-Trp). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
F(1)	129(6)	1883(5)	2982(1)	56(1)
O(1)	3370(8)	-809(6)	4367(1)	46(1)
O(2)	4574(6)	557(5)	4929(1)	32(1)
N(1)	7769(8)	7923(8)	3474(1)	44(1)
C(2)	8534(9)	6838(9)	3801(1)	38(1)
C(3)	7066(8)	4864(8)	3849(1)	32(1)
C(3A)	5318(8)	4696(7)	3530(1)	32(1)
C(4)	3400(9)	3036(8)	3420(1)	35(1)
C(5)	2065(9)	3459(8)	3093(1)	38(1)
C(6)	2484(10)	5384(10)	2865(1)	47(1)
C(7)	4391(10)	6998(9)	2966(1)	45(1)
C(7A)	5793(9)	6638(8)	3303(1)	37(1)
N(2)	4541(8)	5005(6)	4679(1)	28(1)
C(1')	4119(8)	750(8)	4582(1)	29(1)
C(2')	4536(8)	3113(7)	4397(1)	26(1)
C(3')	7139(8)	3164(9)	4164(1)	34(1)

Table S7. Bond lengths [Å] and angles [º] for 5F-L-tryptophan (5F-L-Trp).

F(1)-C(5)	1.382(5)
O(1)-C(1')	1.239(5)
O(2)-C(1')	1.263(4)
N(1)-C(7A)	1.374(6)
N(1)-C(2)	1.376(6)
N(1)-H(1)	0.84(6)
C(2)-C(3)	1.364(6)
C(2)-H(2)	0.9500
C(3)-C(3A)	1.431(6)
C(3)-C(3')	1.491(6)
C(3A)-C(7A)	1.404(6)
C(3A)-C(4)	1.408(6)
C(4)-C(5)	1.362(6)
C(4)-H(4)	0.9500
C(5)-C(6)	1.391(7)
C(6)-C(7)	1.377(7)
C(6)-H(6)	0.9500
C(7)-C(7A)	1.400(6)
C(7)-H(7)	0.9500
N(2)-C(2')	1.485(5)
N(2)-H(2A)	0.98(5)
N(2)-H(2B)	0.88(6)
N(2)-H(2C)	0.87(5)
C(1')-C(2')	1.529(6)
C(2')-C(3')	1.536(5)
C(2')-H(2')	1.0000
C(3')-H(3'A)	0.9900
C(3')-H(3'B)	0.9900

C(7A)-N(1)-C(2)	109.2(4)
C(7A)-N(1)-H(1)	126(4)
C(2)-N(1)-H(1)	125(4)
C(3)-C(2)-N(1)	109.8(4)
C(3)-C(2)-H(2)	125.1
N(1)-C(2)-H(2)	125.1
C(2)-C(3)-C(3A)	106.4(4)
C(2)-C(3)-C(3')	129.1(4)
C(3A)-C(3)-C(3')	124.5(4)
C(7A)-C(3A)-C(4)	119.7(4)
C(7A)-C(3A)-C(3)	107.6(4)
C(4)-C(3A)-C(3)	132.7(4)
C(5)-C(4)-C(3A)	116.5(4)
C(5)-C(4)-H(4)	121.7

C(3A)-C(4)-H(4)	121.7
C(4)-C(5)-F(1)	117.8(4)
C(4)-C(5)-C(6)	124.6(4)
F(1)-C(5)-C(6)	117.6(4)
C(7)-C(6)-C(5)	119.4(4)
C(7)-C(6)-H(6)	120.3
C(5)-C(6)-H(6)	120.3
C(6)-C(7)-C(7A)	117.7(4)
C(6)-C(7)-H(7)	121.1
C(7A)-C(7)-H(7)	121.1
N(1)-C(7A)-C(7)	131.0(4)
N(1)-C(7A)-C(3A)	107.1(4)
C(7)-C(7A)-C(3A)	122.0(4)
C(2')-N(2)-H(2A)	116(3)
C(2')-N(2)-H(2B)	120(4)
H(2A)-N(2)-H(2B)	105(5)
C(2')-N(2)-H(2C)	105(3)
H(2A)-N(2)-H(2C)	109(4)
H(2B)-N(2)-H(2C)	100(4)
O(1)-C(1')-O(2)	126.5(4)
O(1)-C(1')-C(2')	115.0(3)
O(2)-C(1')-C(2')	118.5(4)
N(2)-C(2')-C(1')	111.4(3)
N(2)-C(2')-C(3')	110.5(3)
C(1')-C(2')-C(3')	111.3(3)
N(2)-C(2')-H(2')	107.8
C(1')-C(2')-H(2')	107.8
C(3')-C(2')-H(2')	107.8
C(3)-C(3')-C(2')	113.5(3)
C(3)-C(3')-H(3'A)	108.9
C(2')-C(3')-H(3'A)	108.9
C(3)-C(3')-H(3'B)	108.9
C(2')-C(3')-H(3'B)	108.9
H(3'A)-C(3')-H(3'B)	107.7

Table S8. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 5F-L-tryptophan (5F-L-Trp). The anisotropic displacement factor exponent takes the form:

$-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
F(1)	56(2)	64(2)	48(2)	-6(1)	-14(1)	-13(2)
O(1)	64(2)	31(2)	43(2)	-2(1)	-15(2)	1(2)
O(2)	31(2)	34(2)	30(1)	5(1)	-1(1)	1(1)
N(1)	45(2)	39(2)	47(2)	4(2)	11(2)	-10(2)
C(2)	32(2)	44(3)	39(2)	-5(2)	6(2)	-8(2)
C(3)	28(2)	38(2)	29(2)	-2(2)	5(1)	1(2)
C(3A)	30(2)	36(2)	29(2)	-1(2)	6(2)	1(2)
C(4)	36(2)	36(2)	34(2)	-1(2)	2(2)	-4(2)
C(5)	37(2)	41(3)	36(2)	-5(2)	-3(2)	-1(2)
C(6)	51(3)	59(3)	30(2)	3(2)	-1(2)	8(2)
C(7)	55(3)	43(3)	36(2)	11(2)	8(2)	-1(2)
C(7A)	39(2)	36(2)	37(2)	1(2)	8(2)	-3(2)
N(2)	30(2)	24(2)	31(2)	1(1)	2(2)	0(2)
C(1')	21(2)	31(2)	34(2)	3(2)	-4(1)	1(2)
C(2')	24(2)	28(2)	28(2)	-2(2)	-3(2)	0(2)
C(3')	24(2)	45(3)	34(2)	0(2)	1(2)	9(2)

Table S9. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for 5F-L-tryptophan (5F-L-Trp).

	x	y	z	U(eq)
H(1)	8540(120)	9080(110)	3382(15)	59(17)
H(2)	9881	7383	3969	46
H(4)	3054	1691	3566	42
H(6)	1462	5584	2642	56
H(7)	4744	8311	2814	54
H(2A)	4160(110)	6560(90)	4584(14)	46(14)
H(2B)	5920(120)	5180(100)	4831(16)	54(16)
H(2C)	3310(100)	4620(80)	4842(13)	31(12)
H(2')	2993	3388	4222	32
H(3'A)	8665	3550	4331	41
H(3'B)	7468	1599	4060	41

Table S10. Torsion angles [º] for 5F-L-tryptophan (5F-L-Trp).

C(7A)-N(1)-C(2)-C(3)	-0.6(5)
N(1)-C(2)-C(3)-C(3A)	0.9(5)
N(1)-C(2)-C(3)-C(3')	-178.4(4)
C(2)-C(3)-C(3A)-C(7A)	-0.8(4)
C(3')-C(3)-C(3A)-C(7A)	178.5(4)
C(2)-C(3)-C(3A)-C(4)	178.6(4)
C(3')-C(3)-C(3A)-C(4)	-2.1(7)
C(7A)-C(3A)-C(4)-C(5)	-1.1(6)
C(3)-C(3A)-C(4)-C(5)	179.5(4)
C(3A)-C(4)-C(5)-F(1)	-178.7(4)
C(3A)-C(4)-C(5)-C(6)	0.4(7)
C(4)-C(5)-C(6)-C(7)	0.9(8)
F(1)-C(5)-C(6)-C(7)	179.9(4)
C(5)-C(6)-C(7)-C(7A)	-1.4(7)
C(2)-N(1)-C(7A)-C(7)	-179.6(5)
C(2)-N(1)-C(7A)-C(3A)	0.0(5)
C(6)-C(7)-C(7A)-N(1)	-179.8(4)
C(6)-C(7)-C(7A)-C(3A)	0.6(7)
C(4)-C(3A)-C(7A)-N(1)	-179.0(4)
C(3)-C(3A)-C(7A)-N(1)	0.5(5)
C(4)-C(3A)-C(7A)-C(7)	0.6(6)
C(3)-C(3A)-C(7A)-C(7)	-179.9(4)
O(1)-C(1')-C(2')-N(2)	161.3(4)
O(2)-C(1')-C(2')-N(2)	-19.2(5)
O(1)-C(1')-C(2')-C(3')	-74.8(5)
O(2)-C(1')-C(2')-C(3')	104.6(4)
C(2)-C(3)-C(3')-C(2')	113.3(5)
C(3A)-C(3)-C(3')-C(2')	-65.8(5)
N(2)-C(2')-C(3')-C(3)	-82.4(4)
C(1')-C(2')-C(3')-C(3)	153.3(3)

Table S11. Hydrogen bonds for 5F-L-tryptophan (5F-L-Trp) [Å and º].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2A)...O(1)#1	0.98(5)	1.75(6)	2.723(5)	174(5)
N(2)-H(2A)...O(2)#1	0.98(5)	2.62(5)	3.327(4)	129(4)
N(2)-H(2B)...O(2)#2	0.88(6)	2.05(6)	2.880(5)	157(5)
N(2)-H(2C)...O(2)#3	0.87(5)	2.03(5)	2.852(5)	157(4)

Symmetry transformations used to generate equivalent atoms:

#1 x,y+1,z #2 x+1/2,-y+1/2,-z+1 #3 x-1/2,-y+1/2,-z+1

Table S12. Crystal data and structure refinement for 5F-L-tryptophan hydrate (5F-L-Trp.hydrate).

Identification code	5F-L-Trp.hydrate	
Empirical formula	C11 H13 F N2 O3	
Formula weight	240.23	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 6.2680(2) Å	α= 90º.
	b = 5.4718(2) Å	β= 92.294(2)º.
	c = 15.7972(6) Å	γ = 90º.
Volume	541.37(3) $Å^3$	
Z	2	
Density (calculated)	1.474 g/cm^3	
Absorption coefficient	1.017 mm^{-1}	
F(000)	252	
Crystal size	0.334 x 0.146 x 0.064 mm^3	
Theta range for data collection	5.605 to 74.926º.	
Index ranges	-7<=h<=7, -6<=k<=6, -19<=l<=18	
Reflections collected	6218	
Independent reflections	2189 [R(int) = 0.0260]	
Completeness to theta = 67.679º	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7539 and 0.6320	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2189 / 1 / 206	
Goodness-of-fit on F^2	1.055	
Final R indices [I>2sigma(I)]	R1 = 0.0379, wR2 = 0.0982	
R indices (all data)	R1 = 0.0380, wR2 = 0.0985	
Absolute structure parameter	-0.03(13)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.258 and -0.206 $e.Å^{-3}$	

Table S13. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 5F-L-tryptophan hydrate (5F-L-Trp.hydrate). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
F(1)	9448(2)	6199(3)	3835(1)	37(1)
O(1)	4984(3)	7627(3)	1421(1)	32(1)
O(2)	6092(2)	4456(3)	663(1)	34(1)
O(3)	8384(2)	10218(4)	875(1)	38(1)
N(1)	2823(3)	-225(4)	3617(1)	31(1)
N(2)	2548(3)	1795(4)	880(1)	26(1)
C(1')	4750(3)	5569(4)	1085(1)	25(1)
C(2)	1583(3)	838(4)	2986(1)	28(1)
C(2')	2531(3)	4382(4)	1162(1)	24(1)
C(3)	2531(3)	2926(4)	2703(1)	25(1)
C(3')	1581(3)	4604(4)	2041(1)	25(1)
C(4)	6150(3)	4930(4)	3220(1)	26(1)
C(3A)	4505(3)	3176(4)	3197(1)	24(1)
C(5)	7810(3)	4533(4)	3798(1)	28(1)
C(6)	7966(3)	2552(5)	4352(1)	31(1)
C(7)	6347(4)	822(4)	4343(1)	31(1)
C(7A)	4627(3)	1171(4)	3761(1)	28(1)

Table S14. Bond lengths [Å] and angles [º] for 5F-L-tryptophan hydrate (5F-L-Trp.hydrate).

F(1)-C(5)	1.373(2)
O(1)-C(1')	1.250(3)
O(2)-C(1')	1.253(3)
O(3)-H(12)	0.88(5)
O(3)-H(13)	0.86(4)
N(1)-C(2)	1.369(3)
N(1)-C(7A)	1.376(3)
N(1)-H(1)	0.96(4)
N(2)-C(2')	1.485(3)
N(2)-H(6)	0.86(3)
N(2)-H(7)	0.87(3)
N(2)-H(8)	0.85(4)
C(1')-C(2')	1.544(3)
C(2)-C(3)	1.371(3)
C(2)-H(2)	1.02(3)
C(2')-C(3')	1.538(3)
C(2')-H(11)	1.00(3)
C(3)-C(3A)	1.442(3)
C(3)-C(3')	1.497(3)
C(3')-H(9)	0.97(3)
C(3')-H(10)	0.99(3)
C(4)-C(5)	1.374(3)
C(4)-C(3A)	1.408(3)
C(4)-H(3)	0.92(3)
C(3A)-C(7A)	1.414(3)
C(5)-C(6)	1.394(3)
C(6)-C(7)	1.388(3)
C(6)-H(4)	0.90(3)
C(7)-C(7A)	1.401(3)
C(7)-H(5)	0.96(3)
H(12)-O(3)-H(13)	106(4)
C(2)-N(1)-C(7A)	108.90(18)
C(2)-N(1)-H(1)	123.8(18)

C(7A)-N(1)-H(1)	126.9(18)
C(2')-N(2)-H(6)	114.9(19)
C(2')-N(2)-H(7)	114(2)
H(6)-N(2)-H(7)	106(3)
C(2')-N(2)-H(8)	107(2)
H(6)-N(2)-H(8)	108(3)
H(7)-N(2)-H(8)	107(3)
O(1)-C(1')-O(2)	126.41(19)
O(1)-C(1')-C(2')	115.86(18)
O(2)-C(1')-C(2')	117.62(19)
N(1)-C(2)-C(3)	110.48(19)
N(1)-C(2)-H(2)	121.7(17)
C(3)-C(2)-H(2)	127.7(18)
N(2)-C(2')-C(3')	110.76(17)
N(2)-C(2')-C(1')	111.10(16)
C(3')-C(2')-C(1')	114.83(16)
N(2)-C(2')-H(11)	108(2)
C(3')-C(2')-H(11)	107.7(18)
C(1')-C(2')-H(11)	103.5(19)
C(2)-C(3)-C(3A)	106.08(18)
C(2)-C(3)-C(3')	124.96(19)
C(3A)-C(3)-C(3')	128.90(18)
C(3)-C(3')-C(2')	115.14(16)
C(3)-C(3')-H(9)	108(2)
C(2')-C(3')-H(9)	109.2(17)
C(3)-C(3')-H(10)	110.1(16)
C(2')-C(3')-H(10)	104.2(15)
H(9)-C(3')-H(10)	110(3)
C(5)-C(4)-C(3A)	116.34(19)
C(5)-C(4)-H(3)	121.7(18)
C(3A)-C(4)-H(3)	122.0(18)
C(4)-C(3A)-C(7A)	119.44(19)
C(4)-C(3A)-C(3)	133.65(19)
C(7A)-C(3A)-C(3)	106.90(18)
F(1)-C(5)-C(4)	117.9(2)
F(1)-C(5)-C(6)	117.11(19)

C(4)-C(5)-C(6)	124.94(19)
C(7)-C(6)-C(5)	119.39(19)
C(7)-C(6)-H(4)	122(2)
C(5)-C(6)-H(4)	118(2)
C(6)-C(7)-C(7A)	117.2(2)
C(6)-C(7)-H(5)	124.3(18)
C(7A)-C(7)-H(5)	118.4(18)
N(1)-C(7A)-C(7)	129.7(2)
N(1)-C(7A)-C(3A)	107.63(19)
C(7)-C(7A)-C(3A)	122.7(2)

Table S15. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 5F-L-tryptophan hydrate (5F-L-Trp.hydrate). The anisotropic displacement factor exponent takes the form:
$-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
F(1)	29(1)	40(1)	41(1)	-3(1)	-4(1)	-10(1)
O(1)	31(1)	28(1)	39(1)	2(1)	2(1)	-6(1)
O(2)	27(1)	34(1)	40(1)	3(1)	10(1)	-1(1)
O(3)	23(1)	37(1)	55(1)	6(1)	2(1)	-4(1)
N(1)	31(1)	27(1)	35(1)	3(1)	5(1)	-5(1)
N(2)	20(1)	28(1)	28(1)	-4(1)	2(1)	-3(1)
C(1')	23(1)	26(1)	25(1)	6(1)	0(1)	-2(1)
C(2)	26(1)	28(1)	31(1)	-3(1)	7(1)	-4(1)
C(2')	21(1)	26(1)	26(1)	2(1)	0(1)	0(1)
C(3)	21(1)	26(1)	26(1)	-5(1)	5(1)	-4(1)
C(3')	21(1)	27(1)	28(1)	-3(1)	3(1)	1(1)
C(4)	25(1)	25(1)	27(1)	-1(1)	2(1)	-3(1)
C(3A)	24(1)	25(1)	24(1)	-2(1)	4(1)	-1(1)
C(5)	24(1)	29(1)	30(1)	-6(1)	3(1)	-5(1)
C(6)	27(1)	37(1)	28(1)	-2(1)	0(1)	4(1)
C(7)	35(1)	29(1)	28(1)	2(1)	4(1)	4(1)
C(7A)	29(1)	26(1)	28(1)	-2(1)	7(1)	-2(1)

Table S16. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 5F-L-tryptophan hydrate (5F-L-Trp.hydrate).

	x	y	z	U(eq)
H(1)	2520(50)	-1790(70)	3864(19)	34(7)
H(2)	120(40)	150(60)	2804(17)	31(7)
H(3)	6130(40)	6250(60)	2865(17)	26(6)
H(4)	9180(50)	2370(60)	4674(18)	30(7)
H(5)	6340(50)	-590(60)	4706(18)	33(7)
H(6)	3340(40)	840(60)	1191(16)	19(5)
H(7)	2960(50)	1610(60)	370(20)	34(7)
H(8)	1270(60)	1280(70)	890(20)	41(8)
H(9)	50(50)	4300(70)	1992(18)	36(8)
H(10)	1840(40)	6320(60)	2205(16)	23(6)
H(11)	1600(50)	5340(70)	750(20)	39(8)
H(12)	7530(70)	9250(110)	1150(30)	75(13)
H(13)	7680(60)	11550(80)	780(20)	43(9)

Table S17. Torsion angles [º] for 5F-L-tryptophan hydrate (5F-L-Trp.hydrate).

C(7A)-N(1)-C(2)-C(3)	0.1(2)
O(1)-C(1')-C(2')-N(2)	-170.02(17)
O(2)-C(1')-C(2')-N(2)	13.5(2)
O(1)-C(1')-C(2')-C(3')	-43.3(2)
O(2)-C(1')-C(2')-C(3')	140.15(19)
N(1)-C(2)-C(3)-C(3A)	-0.1(2)
N(1)-C(2)-C(3)-C(3')	-177.45(18)
C(2)-C(3)-C(3')-C(2')	-103.5(2)
C(3A)-C(3)-C(3')-C(2')	79.7(3)
N(2)-C(2')-C(3')-C(3)	51.0(2)
C(1')-C(2')-C(3')-C(3)	-75.9(2)
C(5)-C(4)-C(3A)-C(7A)	0.8(3)
C(5)-C(4)-C(3A)-C(3)	179.5(2)
C(2)-C(3)-C(3A)-C(4)	-178.8(2)
C(3')-C(3)-C(3A)-C(4)	-1.6(3)
C(2)-C(3)-C(3A)-C(7A)	0.0(2)
C(3')-C(3)-C(3A)-C(7A)	177.23(18)
C(3A)-C(4)-C(5)-F(1)	179.66(16)
C(3A)-C(4)-C(5)-C(6)	-0.1(3)
F(1)-C(5)-C(6)-C(7)	179.71(19)
C(4)-C(5)-C(6)-C(7)	-0.6(3)
C(5)-C(6)-C(7)-C(7A)	0.4(3)
C(2)-N(1)-C(7A)-C(7)	179.9(2)
C(2)-N(1)-C(7A)-C(3A)	-0.1(2)
C(6)-C(7)-C(7A)-N(1)	-179.7(2)
C(6)-C(7)-C(7A)-C(3A)	0.3(3)
C(4)-C(3A)-C(7A)-N(1)	179.06(17)
C(3)-C(3A)-C(7A)-N(1)	0.1(2)
C(4)-C(3A)-C(7A)-C(7)	-0.9(3)
C(3)-C(3A)-C(7A)-C(7)	-179.93(19)

Table S18. Hydrogen bonds for 5F-L-tryptophan hydrate (5F-L-Trp.hydrate) [Å and º].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...F(1)#1	0.96(4)	2.22(3)	2.912(2)	128(2)
N(2)-H(6)...O(1)#2	0.86(3)	2.06(3)	2.856(3)	153(2)
N(2)-H(7)...O(2)#3	0.87(3)	2.11(3)	2.910(2)	153(3)
N(2)-H(8)...O(3)#1	0.85(4)	1.90(4)	2.749(2)	178(4)
C(2')-H(11)...O(3)#3	1.00(3)	2.57(3)	3.277(3)	127(2)
O(3)-H(12)...O(1)	0.88(5)	1.89(5)	2.728(2)	159(4)
O(3)-H(13)...O(2)#4	0.86(4)	1.88(4)	2.741(3)	176(3)

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y-1,z #2 x,y-1,z #3 -x+1,y-1/2,-z

#4 x,y+1,z

Table S19. Crystal data and structure refinement for 6F-DL-tryptophan (6F-DL-Trp).

Identification code	6F-DL-Trp	
Empirical formula	C11 H11 F N2 O2	
Formula weight	222.22	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 19.1378(18) Å	α= 90º.
	b = 5.7720(5) Å	β= 100.245(5)º.
	c = 9.3448(8) Å	γ = 90º.
Volume	1015.80(16) $Å^3$	
Z	4	
Density (calculated)	1.453 g/cm^3	
Absorption coefficient	0.964 mm^{-1}	
F(000)	464	
Crystal size	0.538 x 0.281 x 0.032 mm^3	
Theta range for data collection	2.346 to 75.408º.	
Index ranges	-23<=h<=23, -7<=k<=7, -11<=l<=10	
Reflections collected	9881	
Independent reflections	1994 [R(int) = 0.1196]	
Completeness to theta = 67.679º	97.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7539 and 0.5147	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1994 / 3 / 161	
Goodness-of-fit on F^2	1.079	
Final R indices [I>2sigma(I)]	R1 = 0.0885, wR2 = 0.2456	
R indices (all data)	R1 = 0.1249, wR2 = 0.2779	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.373 and -0.380 $e.Å^{-3}$	

Table S20. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 6F-DL-tryptophan (6F-DL-Trp). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
F(1)	5133(2)	5555(6)	2813(3)	63(1)
O(1)	9808(2)	3388(5)	6331(3)	33(1)
O(2)	8785(2)	1982(5)	5137(3)	43(1)
N(1)	6864(2)	2276(7)	6677(4)	42(1)
N(2)	9396(2)	7787(6)	5836(4)	31(1)
C(2)	7531(3)	3035(8)	7263(5)	39(1)
C(3)	7698(2)	4960(8)	6562(4)	34(1)
C(3A)	7086(2)	5472(7)	5467(4)	33(1)
C(4)	6915(2)	7227(8)	4439(5)	39(1)
C(5)	6253(2)	7249(9)	3555(5)	42(1)
C(6)	5774(3)	5496(9)	3704(5)	45(1)
C(7)	5909(2)	3733(9)	4691(5)	43(1)
C(7A)	6572(2)	3741(8)	5572(4)	35(1)
C(1')	9167(2)	3585(7)	5716(4)	28(1)
C(2')	8834(2)	5979(7)	5657(4)	28(1)
C(3')	8375(2)	6292(7)	6844(4)	33(1)

Table S21. Bond lengths [Å] and angles [º] for 6F-DL-tryptophan (6F-DL-Trp).

F(1)-C(6)	1.356(5)
O(1)-C(1')	1.264(5)
O(2)-C(1')	1.242(5)
N(1)-C(2)	1.369(6)
N(1)-C(7A)	1.374(6)
N(1)-H(1)	0.90(6)
N(2)-C(2')	1.487(5)
N(2)-H(2A)	1.01(3)
N(2)-H(2B)	1.01(3)
N(2)-H(2C)	1.02(3)
C(2)-C(3)	1.356(6)
C(2)-H(2)	0.9500
C(3)-C(3A)	1.441(6)
C(3)-C(3')	1.490(6)
C(3A)-C(4)	1.394(6)
C(3A)-C(7A)	1.418(6)
C(4)-C(5)	1.384(6)
C(4)-H(4)	0.9500
C(5)-C(6)	1.389(7)
C(5)-H(5)	0.9500
C(6)-C(7)	1.367(7)
C(7)-C(7A)	1.385(6)
C(7)-H(7)	0.9500
C(1')-C(2')	1.518(5)
C(2')-C(3')	1.543(5)
C(2')-H(2')	1.0000
C(3')-H(3'A)	0.9900
C(3')-H(3'B)	0.9900
C(2)-N(1)-C(7A)	109.2(4)
C(2)-N(1)-H(1)	122(4)
C(7A)-N(1)-H(1)	129(4)
C(2')-N(2)-H(2A)	107(2)
C(2')-N(2)-H(2B)	116(4)

H(2A)-N(2)-H(2B)	104(4)
C(2')-N(2)-H(2C)	110(3)
H(2A)-N(2)-H(2C)	109(4)
H(2B)-N(2)-H(2C)	110(5)
C(3)-C(2)-N(1)	110.6(4)
C(3)-C(2)-H(2)	124.7
N(1)-C(2)-H(2)	124.7
C(2)-C(3)-C(3A)	106.3(4)
C(2)-C(3)-C(3')	127.5(4)
C(3A)-C(3)-C(3')	126.2(4)
C(4)-C(3A)-C(7A)	118.6(4)
C(4)-C(3A)-C(3)	134.4(4)
C(7A)-C(3A)-C(3)	107.0(4)
C(5)-C(4)-C(3A)	119.7(4)
C(5)-C(4)-H(4)	120.1
C(3A)-C(4)-H(4)	120.1
C(4)-C(5)-C(6)	118.9(4)
C(4)-C(5)-H(5)	120.5
C(6)-C(5)-H(5)	120.5
F(1)-C(6)-C(7)	118.3(5)
F(1)-C(6)-C(5)	117.5(4)
C(7)-C(6)-C(5)	124.2(4)
C(6)-C(7)-C(7A)	116.2(4)
C(6)-C(7)-H(7)	121.9
C(7A)-C(7)-H(7)	121.9
N(1)-C(7A)-C(7)	130.7(4)
N(1)-C(7A)-C(3A)	106.9(4)
C(7)-C(7A)-C(3A)	122.4(4)
O(2)-C(1')-O(1)	125.4(4)
O(2)-C(1')-C(2')	116.9(4)
O(1)-C(1')-C(2')	117.8(3)
N(2)-C(2')-C(1')	110.1(3)
N(2)-C(2')-C(3')	109.3(3)
C(1')-C(2')-C(3')	111.7(3)
N(2)-C(2')-H(2')	108.6
C(1')-C(2')-H(2')	108.6

C(3')-C(2')-H(2')	108.6
C(3)-C(3')-C(2')	113.7(3)
C(3)-C(3')-H(3'A)	108.8
C(2')-C(3')-H(3'A)	108.8
C(3)-C(3')-H(3'B)	108.8
C(2')-C(3')-H(3'B)	108.8
H(3'A)-C(3')-H(3'B)	107.7

Table S22. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 6F-DL-tryptophan (6F-DL-Trp)
The anisotropic displacement factor exponent takes the form:
$-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}	
F(1)46(2)	67(2)	69(2)	5(2)	-10(1)	2(2)	
O(1)34(2)	37(2)	27(2)	1(1)	4(1)	4(1)	
O(2)46(2)	26(2)	53(2)	-8(1)	-2(1)	3(1)	
N(1)47(2)	39(2)	42(2)	9(2)	12(2)	-6(2)	
N(2)36(2)	29(2)	28(2)	-3(1)	9(1)	-1(2)	
C(2)45(3)	37(2)	36(2)	2(2)	12(2)	0(2)	
C(3)40(2)	32(2)	32(2)	-4(2)	14(2)	-1(2)	
C(3A)	36(2)	34(2)	32(2)	-4(2)	15(2)	2(2)
C(4)37(2)	41(3)	40(2)	2(2)	13(2)	0(2)	
C(5)42(3)	45(3)	41(2)	3(2)	11(2)	6(2)	
C(6)37(3)	52(3)	43(3)	-4(2)	4(2)	4(2)	
C(7)37(3)	46(3)	48(3)	-4(2)	13(2)	-9(2)	
C(7A)	39(2)	36(2)	33(2)	-1(2)	12(2)	-5(2)
C(1')34(2)	26(2)	23(2)	-2(1)	7(1)	1(2)	
C(2')32(2)	26(2)	25(2)	-1(1)	5(1)	-1(2)	
C(3')39(2)	34(2)	28(2)	-4(2)	8(2)	3(2)	

Table S23. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 6F-DL-tryptophan (6F-DL-Trp).

	x	y	z	U(eq)
H(1)	6670(30)	1000(110)	7000(60)	66(18)
H(2A)	9709(19)	7460(70)	5100(40)	29(11)
H(2B)	9740(30)	7800(110)	6790(50)	73(19)
H(2C)	9170(30)	9380(70)	5640(70)	80(20)
H(2)	7836	2313	8050	47
H(4)	7252	8402	4346	46
H(5)	6129	8444	2857	50
H(7)	5566	2569	4768	52
H(2')	8525	6185	4684	33
H(3'A)	8654	5798	7790	40
H(3'B)	8264	7958	6921	40

Table S24. Torsion angles [º] for 6F-DL-tryptophan (6F-DL-Trp).

C(7A)-N(1)-C(2)-C(3)	-0.8(5)
N(1)-C(2)-C(3)-C(3A)	0.8(5)
N(1)-C(2)-C(3)-C(3')	-178.7(4)
C(2)-C(3)-C(3A)-C(4)	177.7(4)
C(3')-C(3)-C(3A)-C(4)	-2.7(7)
C(2)-C(3)-C(3A)-C(7A)	-0.5(4)
C(3')-C(3)-C(3A)-C(7A)	179.0(4)
C(7A)-C(3A)-C(4)-C(5)	0.2(6)
C(3)-C(3A)-C(4)-C(5)	-177.9(4)
C(3A)-C(4)-C(5)-C(6)	-0.6(7)
C(4)-C(5)-C(6)-F(1)	-179.4(4)
C(4)-C(5)-C(6)-C(7)	0.8(7)
F(1)-C(6)-C(7)-C(7A)	179.7(4)
C(5)-C(6)-C(7)-C(7A)	-0.5(7)
C(2)-N(1)-C(7A)-C(7)	-178.0(5)
C(2)-N(1)-C(7A)-C(3A)	0.4(5)
C(6)-C(7)-C(7A)-N(1)	178.3(5)
C(6)-C(7)-C(7A)-C(3A)	0.1(6)
C(4)-C(3A)-C(7A)-N(1)	-178.5(4)
C(3)-C(3A)-C(7A)-N(1)	0.1(5)
C(4)-C(3A)-C(7A)-C(7)	0.1(6)
C(3)-C(3A)-C(7A)-C(7)	178.7(4)
O(2)-C(1')-C(2')-N(2)	-157.5(3)
O(1)-C(1')-C(2')-N(2)	21.6(4)
O(2)-C(1')-C(2')-C(3')	80.8(4)
O(1)-C(1')-C(2')-C(3')	-100.0(4)
C(2)-C(3)-C(3')-C(2')	107.5(5)
C(3A)-C(3)-C(3')-C(2')	-71.9(5)
N(2)-C(2')-C(3')-C(3)	166.1(3)
C(1')-C(2')-C(3')-C(3)	-71.8(4)

Table S25. Hydrogen bonds for 6F-DL-tryptophan (6F-DL-Trp) [Å and º].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2A)...O(1)#1	1.01(3)	1.82(3)	2.823(4)	173(4)
N(2)-H(2B)...O(1)#2	1.01(3)	1.84(3)	2.831(4)	165(5)
N(2)-H(2C)...O(2)#3	1.02(3)	1.71(3)	2.718(5)	174(6)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1,-z+1 #2 -x+2,y+1/2,-z+3/2 #3 x,y+1,z

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