Supporting information for

Synthesis, characterization and chlorination of 4-(pentyloxy)-7-(prop-2-yn-1-yloxy)pteridin-2-amine

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Content

Table S1: Crystal data and structure refinement for **1**.

CCDC number	2264640
Empirical formula	C15 H18 Cl3 N5 O2
Formula weight	406.69
Temperature	170(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	$a = 11.569(2)$ Å alpha = 90°. $b = 10.294(2)$ Å beta = 94.14(3° $c = 15.764(3)$ Å gamma = 90°
Volume	$1872.5(7)$ Å^3
Z, Calculated density	4, 1.443 Mg/m^3
Absorption coefficient	0.509 mm^{-1}
F(000)	840
Crystal size	0.495 x 0.447 x 0.185 mm
Theta range for data collection	1.765° to 25.023°
Limiting indices	-13<=h<=13, -12<=k<=12, -18<=l<=17
Reflections collected / unique	13293 / 3306 [R(int) = 0.1182]
Completeness to theta = 25.023	99.9 %
Absorption correction	Numerical
Max. and min. transmission	0.9769 and 0.7965
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3306 / 96 / 288
Goodness-of-fit on F^2	0.987
Final R indices [I>2sigma(I)]	R1 = 0.0929, wR2 = 0.2431
R indices (all data)	R1 = 0.1398, wR2 = 0.2815
Extinction coefficient	0.027(6)
Largest diff. peak and hole	0.476 and -0.656 e$^-\cdot$Å^{-3}

Table S2: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **1**.
U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1)	1659(4)	5920(4)	2418(2)	33(1)
C(2)	661(4)	6029(4)	1131(3)	37(1)
C(3)	1028(4)	4012(4)	1670(3)	33(1)
C(4)	1625(4)	4542(4)	2380(3)	33(1)
C(5)	2007(5)	2539(5)	2925(3)	44(1)
C(6)	1400(4)	2005(4)	2199(3)	37(1)
C(7)	694(5)	118(4)	1449(3)	44(1)
C(8)	1329(4)	160(4)	679(3)	41(1)
C(9)	1794(5)	172(5)	26(3)	51(1)
C(10)	2203(4)	7831(4)	3228(3)	40(1)
C(11)	2774(4)	8114(4)	4088(3)	41(1)
C(12)	2784(4)	9564(4)	4275(3)	42(1)
C(13)	3322(5)	9908(5)	5150(3)	52(1)
C(14)	3351(6)	11364(6)	5306(4)	73(2)
N(1)	1190(3)	6663(3)	1821(2)	37(1)
N(2)	542(3)	4756(3)	1035(2)	36(1)
N(3)	2120(3)	3796(3)	3026(2)	39(1)
N(4)	906(3)	2705(3)	1577(2)	35(1)
N(5)	216(4)	6791(4)	497(2)	46(1)
O(1)	1339(3)	701(3)	2180(2)	43(1)
O(2)	2192(3)	6430(3)	3126(2)	40(1)
C(15)	4995(16)	4620(9)	3267(7)	103(5)
Cl(1)	5608(6)	3235(4)	3687(3)	96(2)
Cl(2)	4729(3)	4572(4)	2182(2)	102(1)
Cl(3)	5640(3)	5995(4)	3615(4)	131(2)
C(15')	4786(15)	4553(13)	3436(8)	66(4)
Cl(1')	5313(12)	3022(8)	3335(10)	174(6)
Cl(2')	5199(9)	5574(10)	2674(6)	166(5)
Cl(3')	5020(7)	5169(10)	4435(4)	153(4)

Table S3: Bond lengths [Å] and angles [°] for **1**.
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C(1)-N(1)            1.301(6)
C(1)-O(2)            1.343(5)
C(1)-C(4)            1.420(6)
C(2)-N(2)            1.325(6)
C(2)-N(5)            1.343(6)
C(2)-N(1)            1.373(6)
C(3)-N(2)            1.350(5)
C(3)-N(4)            1.359(5)
C(3)-C(4)            1.384(6)
C(4)-N(3)            1.368(5)
C(5)-N(3)            1.309(6)
C(5)-C(6)            1.410(7)
C(6)-N(4)            1.314(6)
C(6)-O(1)            1.345(5)
C(7)-O(1)            1.456(6)
C(7)-C(8)            1.464(7)
C(8)-C(9)            1.197(7)
C(10)-O(2)           1.451(5)
C(10)-C(11)          1.494(6)
C(11)-C(12)          1.522(6)
C(12)-C(13)          1.514(7)
C(13)-C(14)          1.518(8)
C(15)-Cl(3)          1.674(11)
C(15)-Cl(1)          1.704(11)
C(15)-Cl(2)          1.717(11)
C(15')-Cl(2')        1.690(12)
C(15')-Cl(3')        1.701(12)
C(15')-Cl(1')        1.701(12)
Cl(3')-Cl(3')#1      1.818(16)

N(1)-C(1)-O(2)       121.0(4)
N(1)-C(1)-C(4)       123.2(4)
O(2)-C(1)-C(4)       115.8(4)
N(2)-C(2)-N(5)       117.4(4)
N(2)-C(2)-N(1)       126.7(4)
N(5)-C(2)-N(1)       115.8(4)
N(2)-C(3)-N(4)       116.6(4)
N(2)-C(3)-C(4)       122.2(4)
N(4)-C(3)-C(4)       121.2(4)
N(3)-C(4)-C(3)       122.6(4)
N(3)-C(4)-C(1)       121.3(4)
C(3)-C(4)-C(1)       116.0(4)
N(3)-C(5)-C(6)       121.6(4)
N(4)-C(6)-O(1)       120.7(4)
N(4)-C(6)-C(5)       123.8(4)
O(1)-C(6)-C(5)       115.5(4)
O(1)-C(7)-C(8)       112.6(4)
C(9)-C(8)-C(7)       176.4(5)
O(2)-C(10)-C(11)     107.1(3)
C(10)-C(11)-C(12)    111.3(4)
C(13)-C(12)-C(11)    113.8(4)
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C(12)-C(13)-C(14)          112.4(5)
C(1)-N(1)-C(2)             115.6(4)
C(2)-N(2)-C(3)             116.2(4)
C(5)-N(3)-C(4)             115.5(4)
C(6)-N(4)-C(3)             115.3(4)
C(6)-O(1)-C(7)             116.9(4)
C(1)-O(2)-C(10)            118.7(3)
Cl(3)-C(15)-Cl(1)          114.6(8)
Cl(3)-C(15)-Cl(2)          113.2(7)
Cl(1)-C(15)-Cl(2)          113.7(7)
Cl(2')-C(15')-Cl(3')       113.1(9)
Cl(2')-C(15')-Cl(1')       112.8(9)
Cl(3')-C(15')-Cl(1')       113.5(9)
C(15')-Cl(3')-Cl(3')#1     145.3(11)
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Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1

Table S4: Anisotropic displacement parameters (Å^2 x 10^3) for **1**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	48(2)	30(2)	20(2)	−1(2)	5(2)	−1(2)
C(2)	53(3)	28(2)	30(2)	1(2)	6(2)	4(2)
C(3)	46(2)	25(2)	27(2)	0(2)	8(2)	0(2)
C(4)	47(2)	29(2)	25(2)	2(2)	5(2)	2(2)
C(5)	73(3)	30(2)	29(2)	1(2)	0(2)	2(2)
C(6)	60(3)	24(2)	29(2)	2(2)	11(2)	0(2)
C(7)	78(3)	24(2)	30(2)	−5(2)	11(2)	−11(2)
C(8)	61(3)	28(2)	33(2)	−4(2)	0(2)	−2(2)
C(9)	66(3)	48(3)	39(3)	−9(2)	8(2)	1(2)
C(10)	63(3)	22(2)	35(2)	−3(2)	3(2)	−1(2)
C(11)	63(3)	24(2)	36(2)	−2(2)	1(2)	−1(2)
C(12)	61(3)	25(2)	41(3)	−3(2)	4(2)	−3(2)
C(13)	61(3)	48(3)	49(3)	−15(2)	11(2)	−8(2)
C(14)	89(4)	59(4)	74(4)	−35(3)	18(3)	−19(3)
N(1)	56(2)	29(2)	25(2)	−1(2)	3(2)	2(2)
N(2)	54(2)	26(2)	28(2)	−1(1)	2(2)	2(2)
N(3)	57(2)	29(2)	30(2)	5(2)	2(2)	0(2)
N(4)	54(2)	26(2)	25(2)	−1(1)	7(2)	1(2)
N(5)	83(3)	24(2)	30(2)	0(2)	−8(2)	5(2)
O(1)	78(2)	22(2)	29(2)	2(1)	4(2)	−2(1)
O(2)	63(2)	24(2)	32(2)	−1(1)	−3(1)	0(1)
C(15)	170(16)	52(6)	94(7)	3(6)	56(8)	−14(6)
Cl(1)	141(4)	63(2)	82(2)	3(2)	0(2)	6(2)
Cl(2)	99(2)	120(3)	88(2)	13(2)	25(2)	−3(2)
Cl(3)	96(3)	67(2)	223(7)	−37(3)	−29(3)	−7(2)
C(15')	29(7)	87(9)	83(9)	−14(7)	12(8)	−3(7)
Cl(1')	136(8)	70(4)	326(17)	−40(7)	89(11)	−13(4)
Cl(2')	189(9)	175(9)	143(8)	58(8)	80(7)	20(8)
Cl(3')	130(6)	229(10)	97(4)	−46(5)	−16(4)	57(6)

Table S5: Hydrogen coordinates (x 10^4) and isotropic
displacement parameters (Å^2 x 10^3) for **1**.

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	x	y	z	U(eq)
H(10A)	1402	8176	3182	48
H(10B)	2640	8241	2781	48
H(11A)	3580	7785	4119	49
H(11B)	2356	7654	4525	49
H(12A)	3219	10014	3843	51
H(12B)	1978	9891	4221	51
H(13A)	4122	9563	5214	63
H(13B)	2873	9487	5586	63
H(14A)	3705	11539	5878	110
H(14B)	3809	11785	4884	110
H(14C)	2559	11708	5256	110
H(1N5)	-80(40)	6400(40)	10(30)	32(11)
H(2N5)	340(40)	7680(60)	520(30)	41(13)
H(3C5)	2320(40)	1960(50)	3380(30)	45(13)
H(4C7)	-170(40)	660(50)	1340(30)	52(14)
H(5C7)	570(40)	-720(60)	1650(30)	51(14)
H(6C9)	2290(60)	200(60)	-550(50)	81(19)
H(15)	4209	4650	3492	124
H(15')	3926	4473	3336	79

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Table S6:   Hydrogen bonds for 1 [Å and °].
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Nr Donor --- H....Acceptor [  ARU ]    D - H   H...A   D...A    D - H...A  A..H..A* A'..H..A"
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1  N5   --H1N5  ..N2   [ 3565.01]  0.91(5)  2.07(5)  2.973(5)   170(4)

2  C9   --H6C9  ..N3   [ 4554.01]  1.13(8)  2.45(8)  3.374(6)   138(5)

3  C14  --H14A  ..Cl3A [ 3676.02]   0.98     2.75    3.371(8)    122

4  C14  --H14A  ..Cl2A [ 4565.02]   0.98     2.57    3.397(7)    142'     94'         358
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Translation of ARU-Code to CIF and Equivalent Position Code

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 [ 3565.] =        -x,1-y,-z
 [ 4554.] =        x,1/2-y,-1/2+z
 [ 4565.] =        x,3/2-y,1/2+z
 [ 3676.] =        1-x,2-y,1-z
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Figure S1: Molecular structure of compound **1** showing the disordered co-crystalized solvent molecule. The Ellipsoids are shown at the 50% level. The hydrogen atoms on N5, C5, C7 and C9 were found and refined freely.

Figure S2: Crystal structure of compound **1** with the major occupancy component of the co-crystallized solvent molecule. The Ellipsoids are shown at the 50% level. The hydrogen atoms on N5, C5, C7 and C9 were found and refined freely.
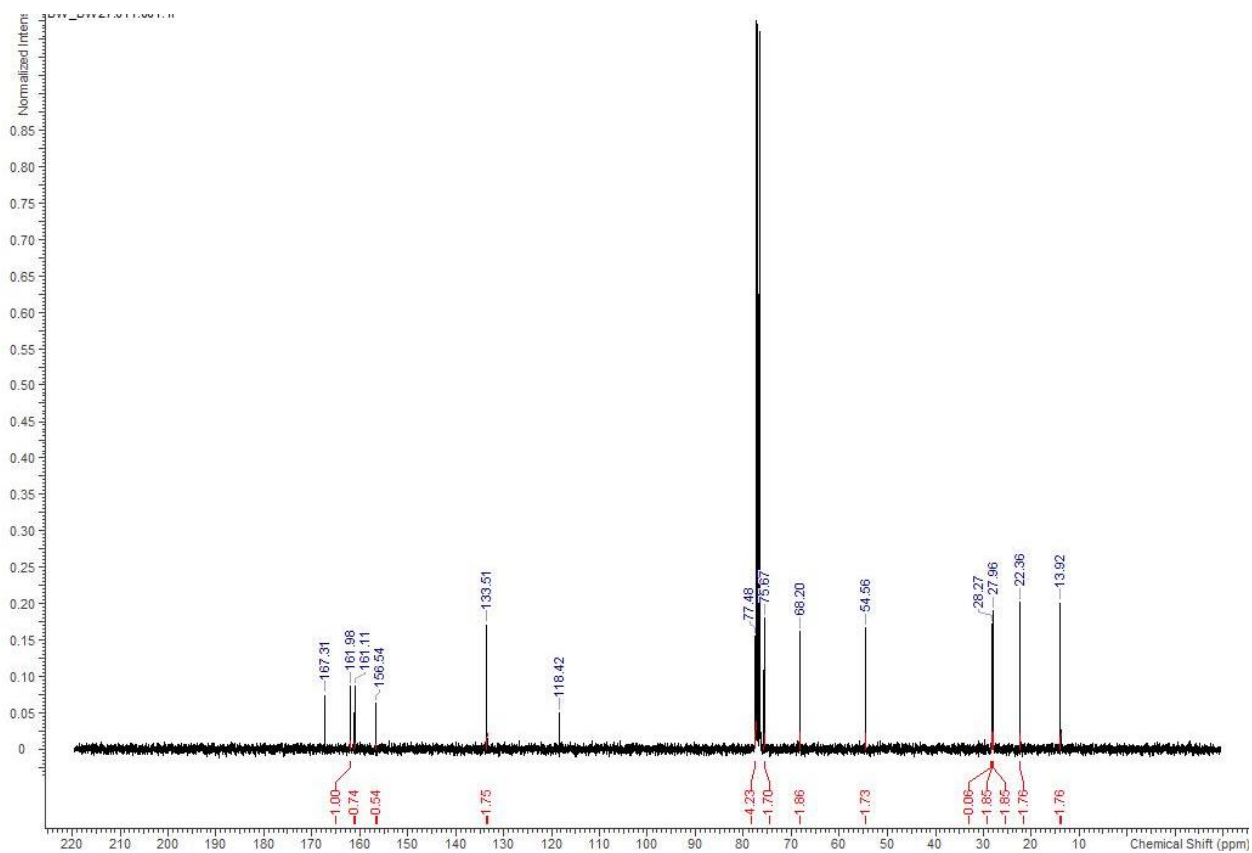

Figure S3: ¹H NMR spectrum of compound **1**.
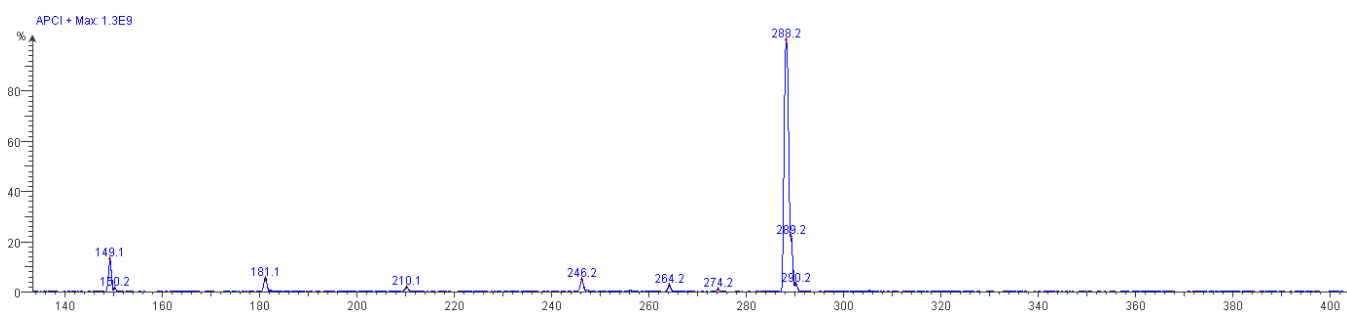
Figure S4: ¹³C NMR spectrum of compound **1**.

Figure S5: Mass (APCI) spectrum of compound **1**.
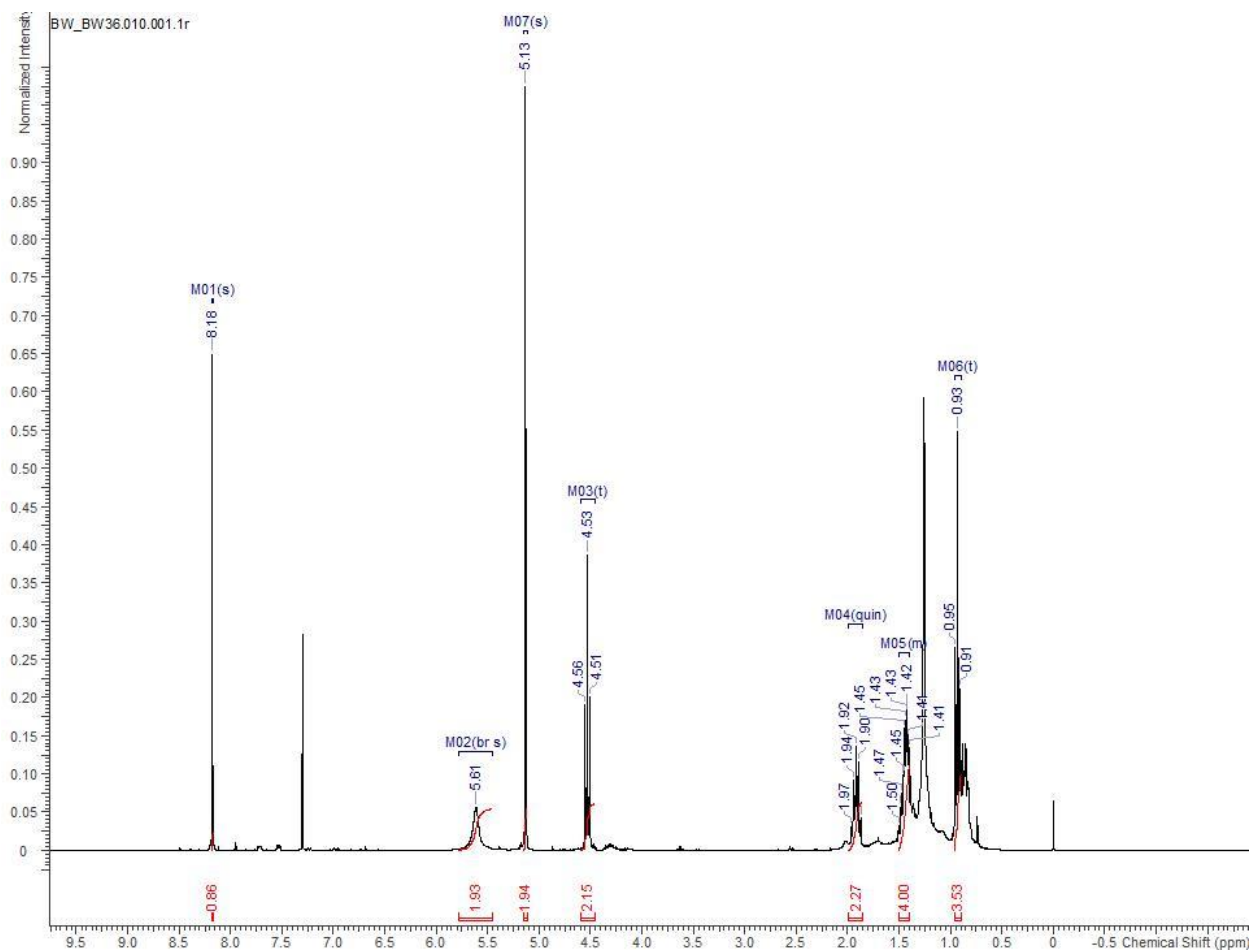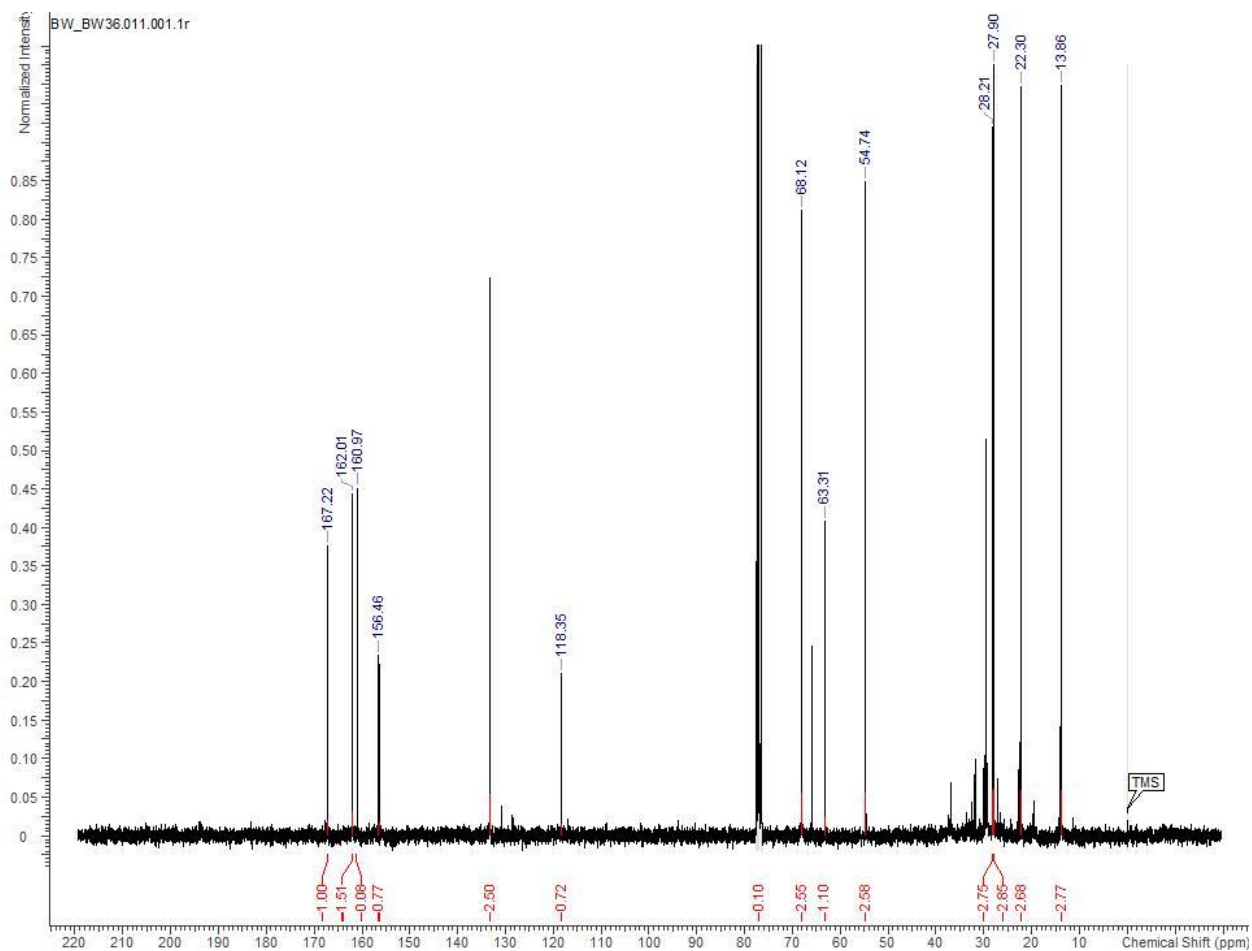
10

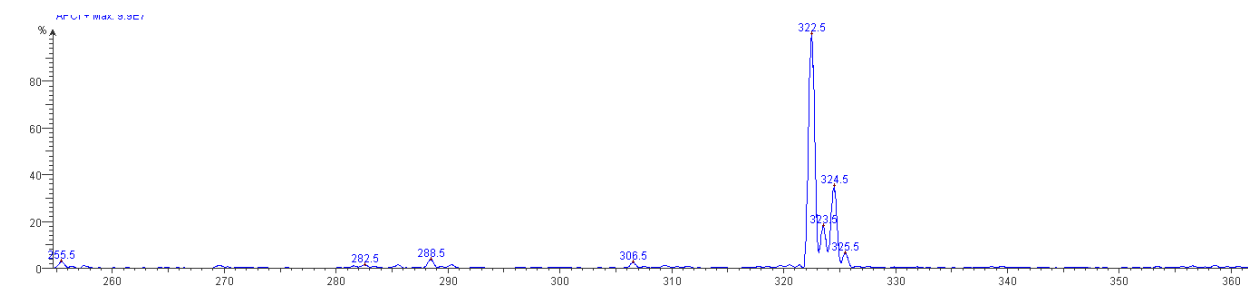Figure S6: ^{1}H NMR spectrum of compound **2**.

Figure S7: ^{13}C NMR spectrum of compound **2**.

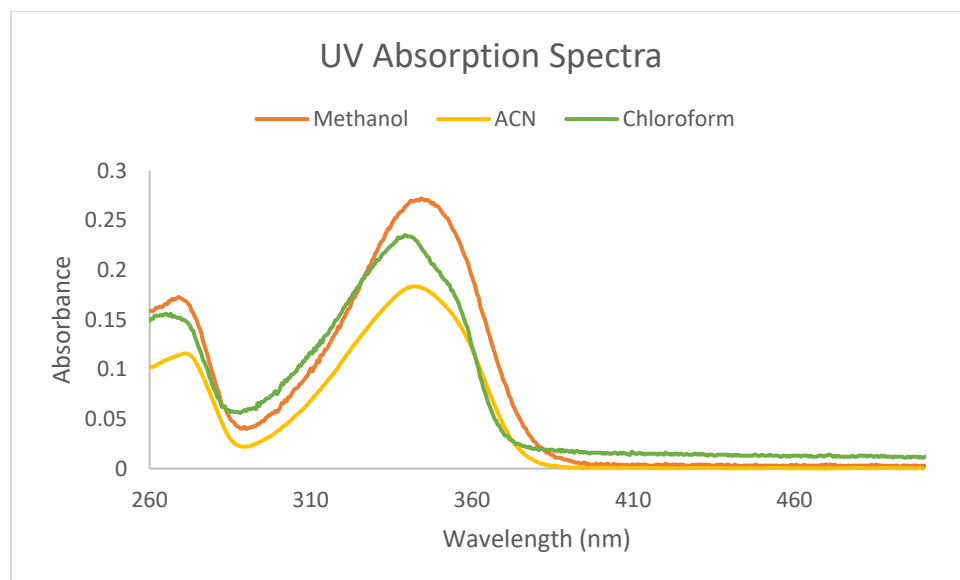Figure S8: Mass (APCI) spectrum of compound **2**.

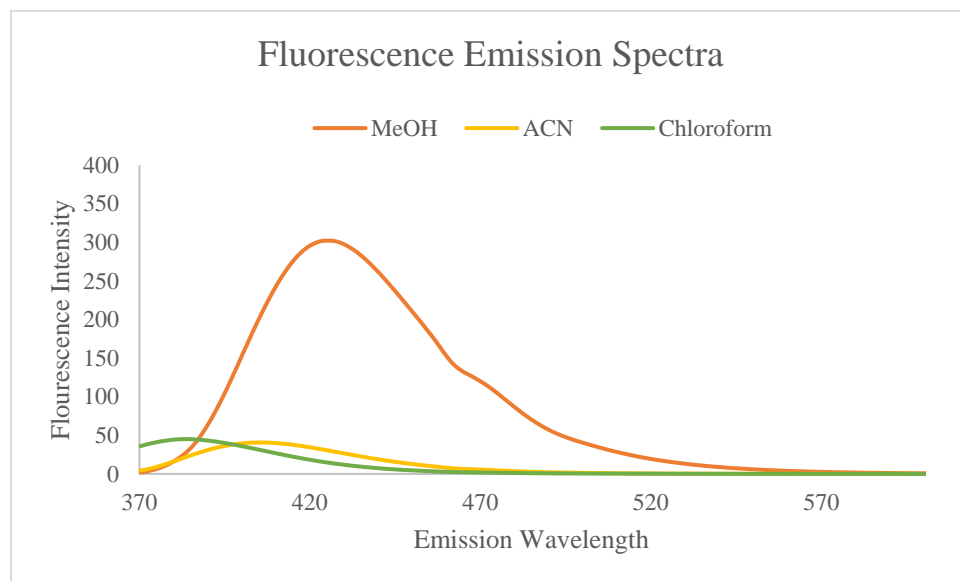Figure S9: UV Absorption spectra for compound **1** in protic and aprotic solvents.

Figure S10: Fluorescence emission spectra for compound **1** in protic and aprotic solvents.
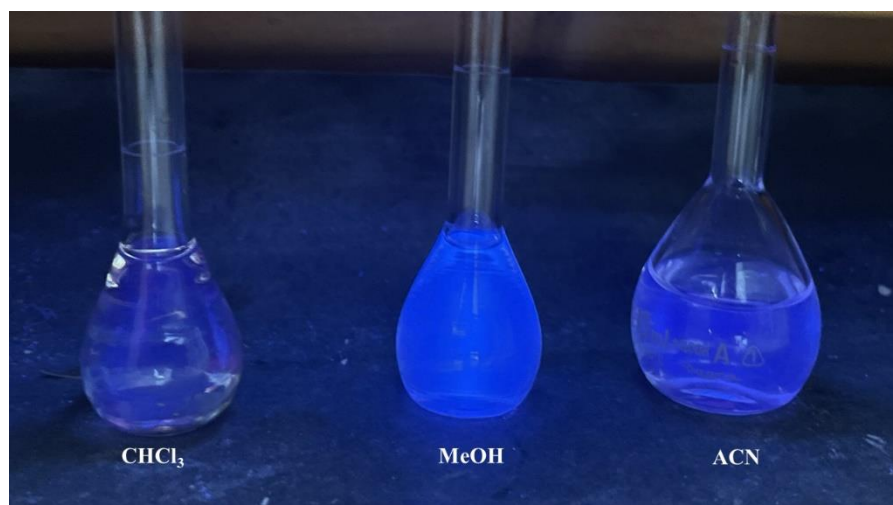
Figure S11: A photo showing fluorescence of 10 μM solutions of compound **1** in chloroform, methanol and acetonitrile respectively.