Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary information for

A new heterocyclic skeleton with highly tunable absorbtion/emission wavelength via H-bonding

Olesya A. Tomashenko, Alexander F. Khlebnikov,* Ivan P. Mosiagin, Mikhail S. Novikov, Elena V. Grachova, Julia R. Shakirova, Sergey P. Tunik*

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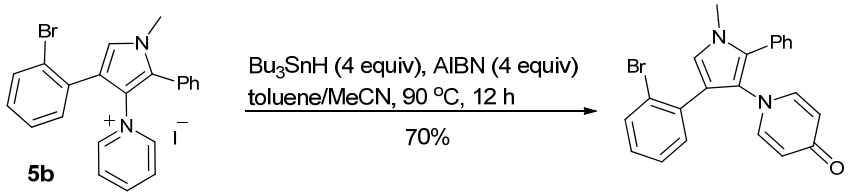
EXPERIMENTAL DETAILS

Numerous attempts to cyclize salts **3a,b**, ylides **4a**,**b** and **6** either by radical reactions (Bu_3SnH, AIBN, toluene or mixture acetonitrile/toluene, heating up to 90 °C, normal or slow addition of reagents) or by palladium-catalyzed reactions failed. Typical procedure for the cyclization under radical conditions is presented below. Typical procedure for the cyclization under palladium-catalysis is presented in the article (synthesis of the compounds **8**, **9a-c**).

Cyclization of 1-(4-(2-bromophenyl)-1-methyl-2-phenyl-1*H*-pyrrol-3-yl)pyridin-1-ium iodide (5b).



The pyridinium iodide **5b** didn't give any desired product under radical conditions. We were only able to isolate the unexpected product 1-(4-(2-bromophenyl)-1-methyl-2-phenyl-1*H*-pyrrol-3-yl)pyridin-4(1*H*)-one, which was shown to be the oxidized substrate **5b**. Traces of oxygen in the reaction mixture are the most probable oxidizer. Interestingly the iodide **5b** didn't give pyridin-4(1*H*)-one under reflux with AIBN in toluene/acetonitrile mixture in air.

To the solution of **5b** (245 mg, 0.47 mmol) in dry acetonitrile (20 mL) solution of Bu_3SnH (276 mg, 0.95 mmol, 2 equiv) and AIBN (156 mg, 0.95 mmol, 2 equiv) in toluene (10 mL) was added through syringe pump for 6 h at the atmosphere of argon at 90 °C. As TLC (DCM/MeOH 10:1) showed that there was still starting material, addition of Bu_3SnH and AIBN was repeated in the same manner. Then reaction mixture was filtered, evaporated to dryness and purified by column chromatography on silica gel (DCM/MeOH from 60:1 to 20:1) to obtain 1-(4-(2-bromophenyl)-1-methyl-2-phenyl-1*H*-pyrrol-3-yl)pyridin-4(1*H*)-one as solid, yield 133 mg, 70% (there are still some Bu_3Sn-species and it is difficult to remove them). ^{1}H NMR ($CDCl_3$): δ 3.32 (s, 3H), 6.16 (d, *J* = 7.7 Hz, 2H), 6.83 (s, 1H), 7.07 (d, *J* = 7.7 Hz, 2H), 7.12–7.19 (m, 2H), 7.19–7.30 (m, 3H), 7.37–7.44 (m, 3H), 7.57–7.64 (m, 1H). ^{13}C NMR ($CDCl_3$): δ 35.5 (CH_3), 118.2 (CH), 118.4 (C), 121.2 (CH), 124.3 (C), 124.7 (C), 127.6 (CH), 128.2 (C), 128.5 (C), 128.7 (CH), 129.1 (CH), 129.1 (CH), 129.8 (CH), 131.8 (CH), 133.1 (C), 133.2 (CH), 141.8 (CH), 178.8 (C). HRMS (ESI) m/z: 405.0597 calcd for $C_{22}H_{18}BrN_2O^+$ $[M + H]^+$, found 405.0609.

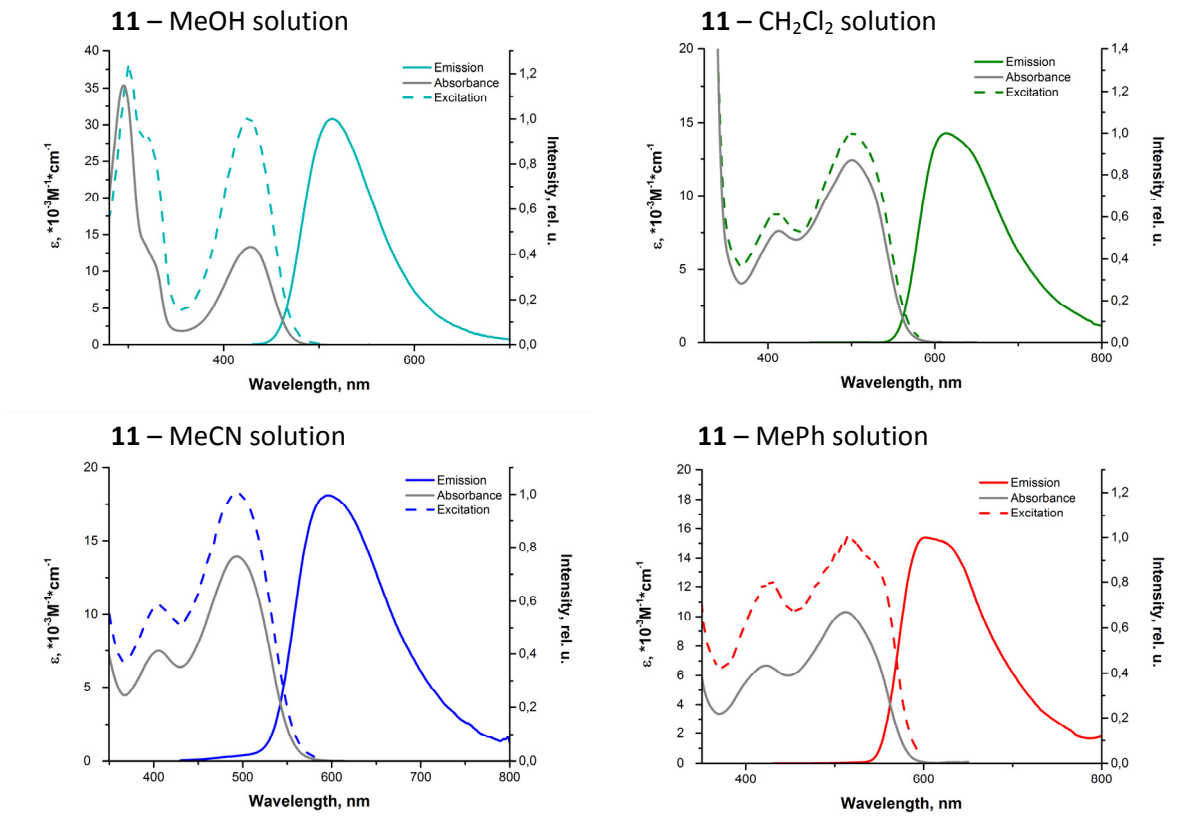
PHOTOPHISICAL DATA

All the photophysical measurements in solution were carried out in freshly distilled solvents (dichloromethane, acetonitrile, methanol, toluene). UV/Vis spectra were recorded on a UV-spectrometr. The emission and excitation spectra in solutions were measured with a spectrofluorimeter. The absolute emission quantum yields of the solutions were determined by a comparative method by using LED pumping and using coumarin 102 in ethanol ($\Phi_r = 0.764$) as the reference with the refraction coefficients of dichloromethane, acetonitrile, methanol, toluene and ethanol equal to 1.42, 1.34, 1.33, 1.49 and 1.36, respectively. The following equation

$$\Phi_s = \Phi_r \frac{\eta_s^2 A_r I_s}{\eta_r^2 A_s I_r}$$

was used to calculate the quantum yield, where Φ_s is the quantum yield of the sample, Φ_r is the quantum yield of the reference, η is the refractive index of the solvent, A_s and A_r are the absorbance of the sample and the reference at the wavelength of excitation, respectively, and I_s and I_r are the integrated areas of emission bands[1]. Fluorescence lifetimes were determined by the TCSPC (Time-Correlated Single Photon Counting) method. The lifetime data were fit using the Jobin-Yvon software package and the Origin 8.1 program.

Figure S1 Absorption, Excitation and Emission spectra of **11** in different solvents.



[1] K. Rurack and M. Spieles, *Anal. Chem.*, 2011, **83**, 1232–1242

Figure S2 Absorption, Excitation and Emission spectra of **12** in different solvents.

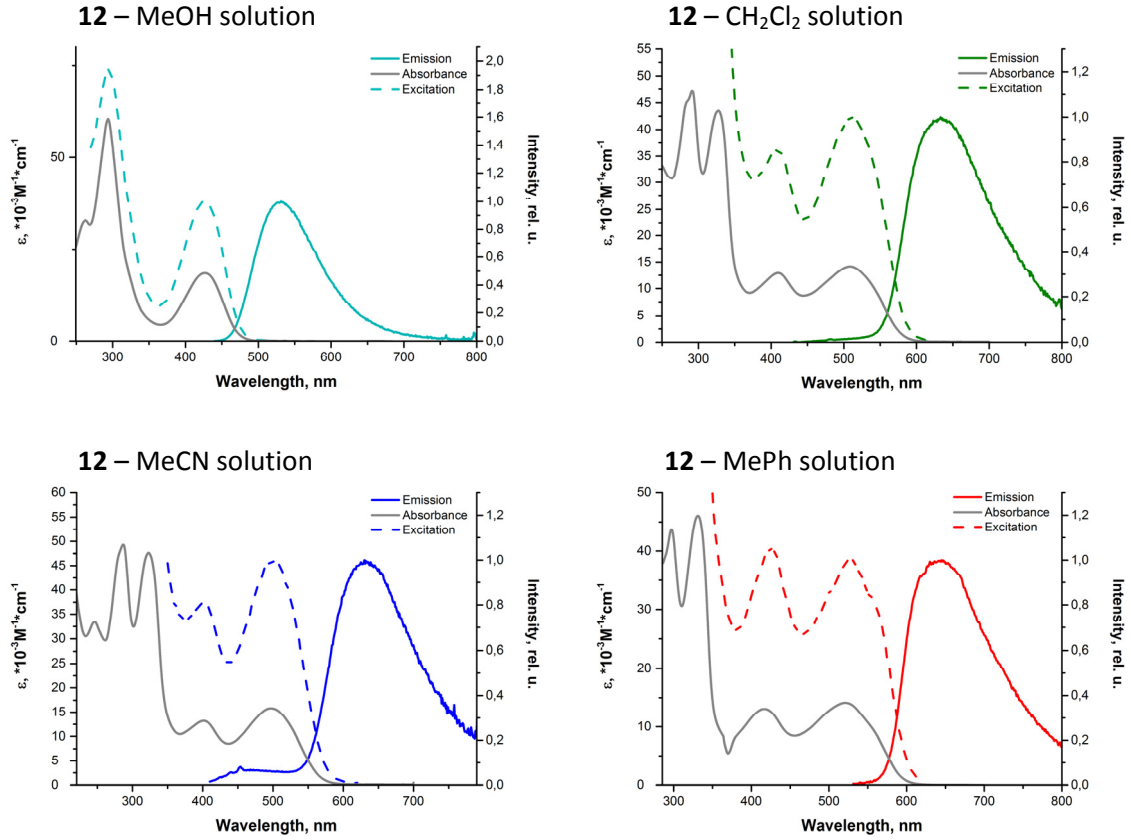


Figure S3 Absorption, Excitation and Emission spectra of **13** in different solvents.

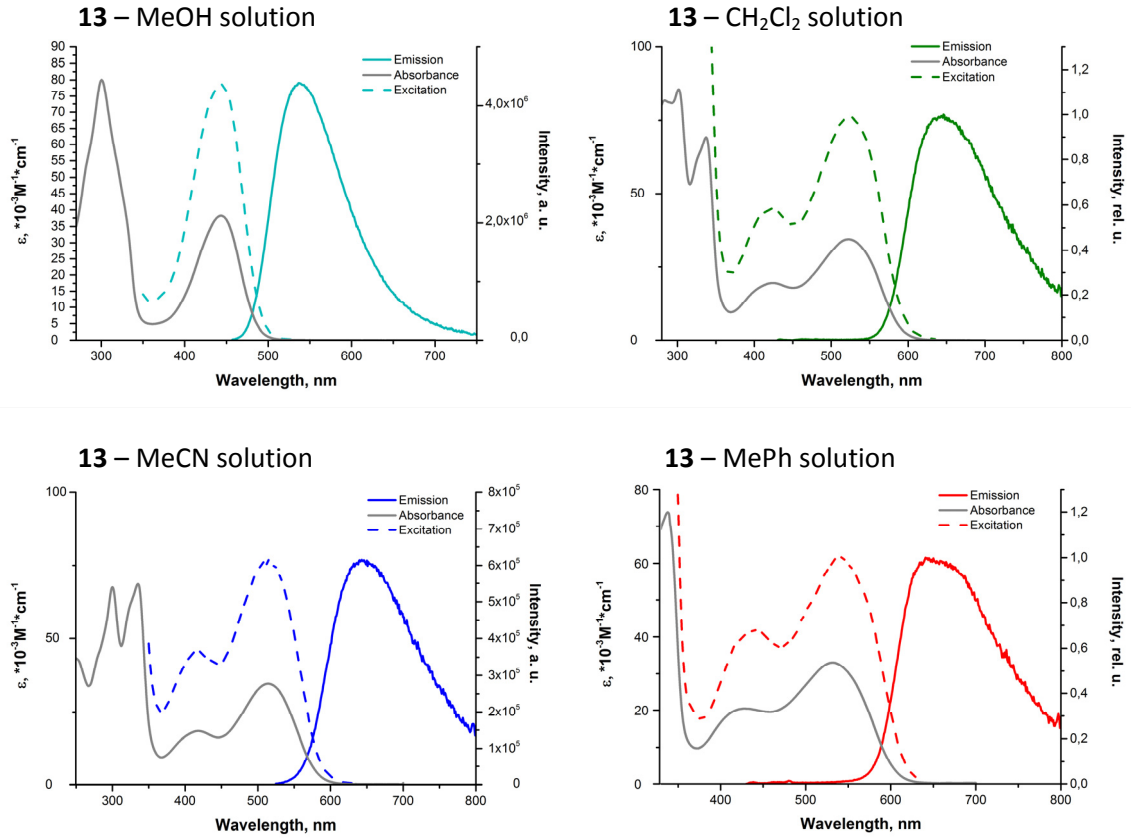


Figure S4 Absorbance and FL intensity of **11** in acetonitrile solution with different amounts of HCOOH (amount of **11** is $6.4*10^{-5}$ mmol)

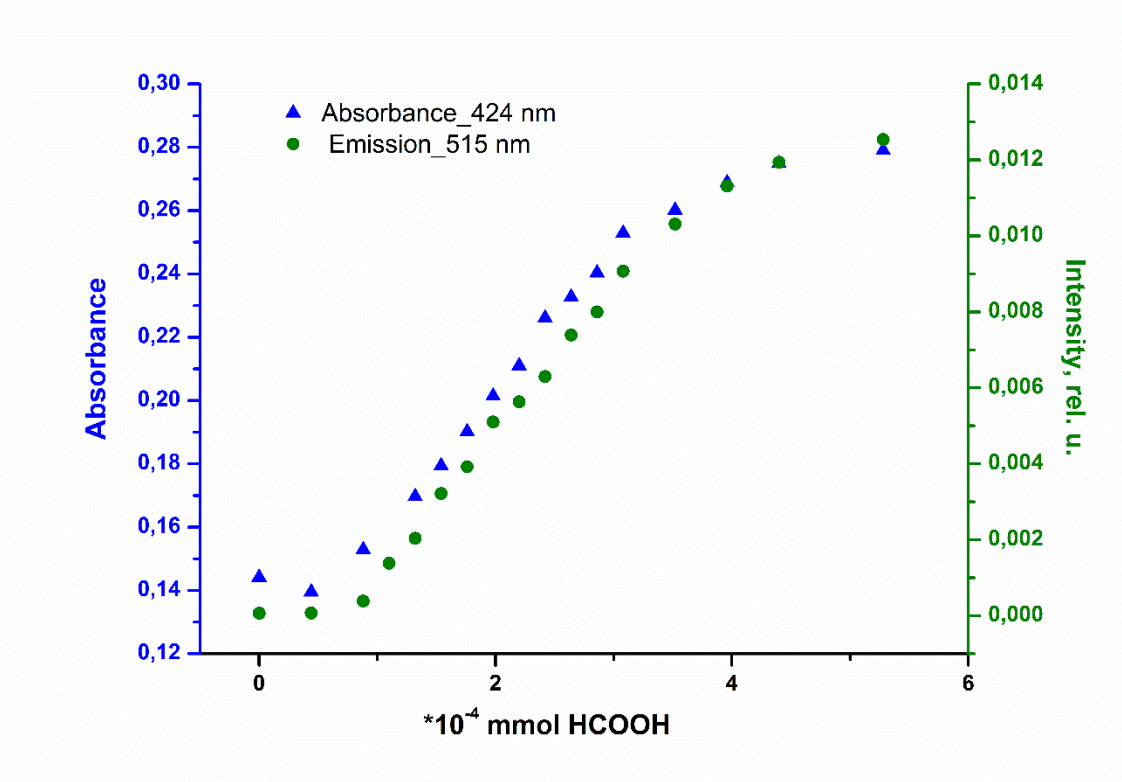
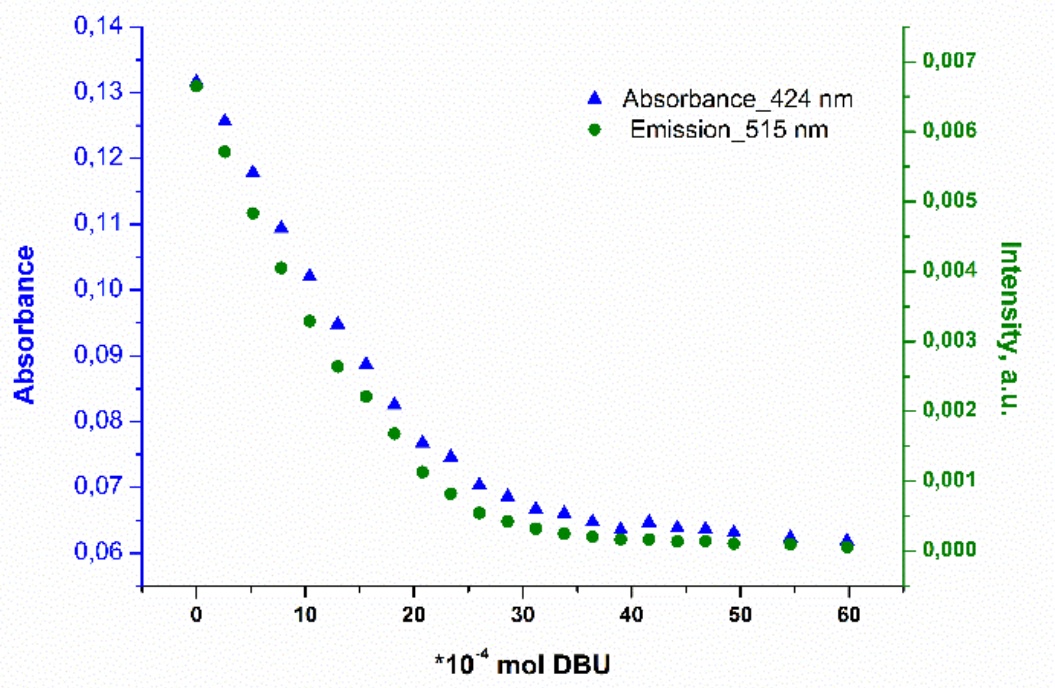


Figure S5 Titration of **11•HCl** in acetonitrile solution with different amounts of DBU (1,8-Diazabicycloundec-7-ene) (amount of **11•HCl** is $5.29*10^{-5}$ mmol)

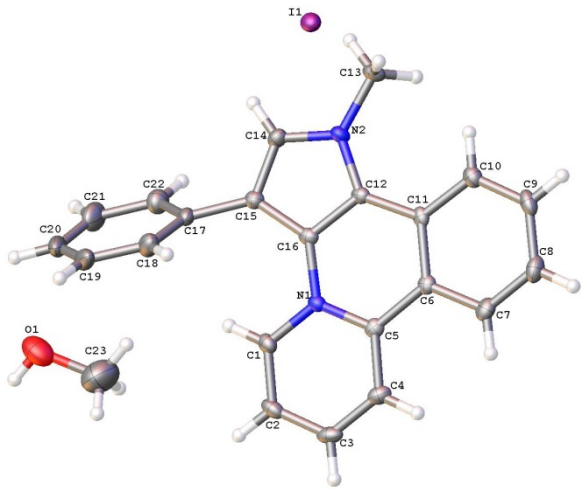


X-RAY DIFFRACTION EXPERIMENTS

Crystal structures of **8, 9a, 11, 13** were determined by single crystal X-ray diffraction analysis. A suitable crystal was selected and fixed on micro-mounts and the diffraction data were collected on a SuperNova, Dual, Cu at zero, Atlas diffractometer. The crystal was measured at a temperature of 100(2) K using monochromated MoKα radiation. The unit cell parameters and refinement characteristics of the crystal structures of **8, 9a, 11, 13** are given below. Using Olex2[2], the structures were solved with the ShelXS[3] structure solution program using Direct Methods and refined with the ShelXL[2] refinement package using Least Squares minimisation.

1-Methyl-3-phenyl-1*H*-pyrido[2,1-a]pyrrolo[3,2-c]isoquinolin-4-ium iodide **(8)**

Single crystals of **8** were growth from methanol/diethyl ether. CCDC for **8** is **1407108**.



Molecular structure of compound **8**, displacement parameters are drawn at 50% probability level.

Table S1 Crystal data and structure refinement for 8

Empirical formula	$C_{23}H_{21}IN_2O$
Formula weight	468.32
Temperature/K	100(2)
Crystal system	monoclinic
Space group	C2/c
a/Å	26.5184(9)
b/Å	8.2523(2)
c/Å	18.6675(5)
α/°	90
β/°	106.173(3)
γ/°	90

[2] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Cryst.*, 2009, **42,** 339-341.
[3] G.M. Sheldrick, *Acta Cryst. A,* 2008, **64**, 112-122.

Volume/Å^3	3923.5(2)
Z	8
ρ_{calc}g/cm^3	1.586
μ/mm^{-1}	1.647
F(000)	1872.0
Crystal size/mm^3	0.24 × 0.18 × 0.09
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.188 to 55
Index ranges	$-34 \leq h \leq 32$, $-10 \leq k \leq 9$, $-24 \leq l \leq 21$
Reflections collected	11477
Independent reflections	4420 [R_{int} = 0.0279, R_{sigma} = 0.0364]
Data/restraints/parameters	4420/0/247
Goodness-of-fit on F^2	1.046
Final R indexes [I>=2σ (I)]	R_1 = 0.0274, wR_2 = 0.0565
Final R indexes [all data]	R_1 = 0.0343, wR_2 = 0.0598
Largest diff. peak/hole / e Å^{-3}	0.49/-0.45

Table S2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 8. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
N1	6752.8(8)	1780(2)	3934.7(10)	13.9(4)
N2	6897.7(8)	-449(3)	5606.1(10)	16.5(4)
C1	6346.4(10)	2666(3)	3488.6(13)	18.0(5)
C2	6407.5(10)	3549(3)	2900.7(13)	20.2(5)
C3	6891.0(11)	3541(3)	2748.4(13)	21.2(6)
C4	7297.6(10)	2667(3)	3195.3(13)	19.2(5)
C5	7239.2(10)	1767(3)	3804.2(13)	15.2(5)
C6	7666.5(9)	868(3)	4301.0(12)	15.0(5)
C7	8166.1(10)	825(3)	4166.2(14)	20.1(5)
C8	8571.1(10)	-46(3)	4616.7(14)	23.7(6)
C9	8498.8(10)	-894(3)	5225.9(14)	22.4(6)
C10	8023.2(10)	-852(3)	5386.1(13)	18.7(5)
C11	7598.4(9)	30(3)	4933.0(12)	14.3(5)
C12	7087.2(9)	133(3)	5039.7(12)	14.0(5)
C13	7163.6(10)	-1421(3)	6257.7(13)	20.0(5)
C14	6375.8(9)	-89(3)	5442.7(12)	17.7(5)
C15	6204.7(10)	710(3)	4778.4(12)	16.0(5)
C16	6666.4(9)	888(3)	4532.2(12)	14.6(5)
C17	5645.8(10)	1123(3)	4432.3(13)	18.0(5)
C18	5379.7(11)	522(4)	3730.2(14)	28.1(6)
C19	4854.2(11)	886(4)	3418.6(15)	37.4(8)

C20	4591.7(12)	1848(4)	3793.9(18)	39.0(8)
C21	4848.5(12)	2411(4)	4497.1(18)	38.5(8)
C22	5371.9(11)	2050(3)	4818.9(16)	27.2(6)
O1	4373.3(9)	5807(3)	3530.2(12)	45.3(6)
C23	4888.9(17)	6051(6)	3487(2)	70.2(13)
I1	6508.1(2)	1576.2(2)	7634.1(2)	20.11(6)

Table S3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 8. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1	16.6(11)	11.3(10)	12.2(9)	-0.6(8)	1.4(8)	-1.3(8)
N2	18.4(11)	17.0(11)	12.8(9)	2.2(8)	2.1(8)	1.3(9)
C1	18.2(13)	15.2(13)	17.1(11)	-0.8(10)	-0.9(10)	-1.6(10)
C2	26.1(15)	14.1(13)	15.3(11)	0.1(10)	-2.7(10)	0(1)
C3	33.5(16)	16.1(14)	14.0(11)	-0.6(10)	6.3(11)	-7.6(11)
C4	27.0(15)	15.3(13)	17.5(12)	-3.4(10)	9.9(11)	-4.3(11)
C5	18.7(13)	11.1(12)	15.6(11)	-5.5(9)	4.4(10)	-2.2(9)
C6	16.6(13)	11.3(12)	16.2(11)	-4.7(9)	3.2(10)	-3.0(9)
C7	19.2(14)	16.5(13)	25.3(13)	-5.2(11)	7.5(11)	-5.2(10)
C8	15.9(13)	21.6(15)	33.9(14)	-6.9(12)	7.6(11)	-1.5(11)
C9	16.3(14)	17.3(14)	27.6(13)	-4.4(11)	-4.0(11)	1.6(10)
C10	18.8(14)	16.5(13)	18.6(12)	-2.8(10)	1.4(10)	-0.6(10)
C11	13.9(12)	11.1(12)	15.5(11)	-5.2(9)	0.0(9)	-1.5(9)
C12	17.7(13)	11.1(12)	12(1)	-2.3(9)	2.2(9)	-3.3(9)
C13	25.2(14)	18.3(14)	14.2(11)	3.9(10)	2(1)	0.4(11)
C14	17.8(13)	19.5(14)	16.9(11)	-1.2(10)	6.5(10)	-2.9(10)
C15	18.4(13)	13.4(13)	15.8(11)	-1.4(9)	4.2(10)	-1.2(10)
C16	19.4(13)	11.0(12)	12.2(10)	-2.9(9)	2.1(9)	-2.3(9)
C17	13.6(13)	19.2(13)	20.7(12)	4.3(10)	4.1(10)	-1.4(10)
C18	21.1(15)	40.7(18)	21.3(13)	-0.3(12)	3.9(11)	-7.1(13)
C19	22.5(16)	62(2)	22.4(14)	12.8(15)	-2.2(12)	-16.3(15)
C20	15.5(15)	54(2)	44.8(18)	28.2(17)	4.5(13)	1.6(14)
C21	24.4(17)	40(2)	54(2)	8.7(16)	16.5(15)	9.3(14)
C22	23.3(15)	26.8(16)	31.8(14)	0.6(12)	8.2(12)	2.0(12)
O1	50.4(16)	33.9(14)	42.8(13)	5.1(11)	-1.7(11)	4.2(11)
C23	67(3)	79(3)	72(3)	17(2)	31(2)	-3(2)
I1	20.35(10)	18.53(10)	20.08(9)	2.04(7)	3.35(7)	-3.43(7)

Table S4 Bond Lengths for 8.

Atom	Atom	Length/Å	Atom	Atom	Length/Å

N1	C1	1.375(3)	C9	C10	1.375(3)
N1	C5	1.378(3)	C10	C11	1.409(3)
N1	C16	1.407(3)	C11	C12	1.427(3)
N2	C12	1.377(3)	C12	C16	1.393(3)
N2	C13	1.463(3)	C14	C15	1.366(3)
N2	C14	1.364(3)	C15	C16	1.430(3)
C1	C2	1.364(3)	C15	C17	1.482(3)
C2	C3	1.389(4)	C17	C18	1.395(4)
C3	C4	1.370(4)	C17	C22	1.388(4)
C4	C5	1.402(3)	C18	C19	1.385(4)
C5	C6	1.452(3)	C19	C20	1.370(5)
C6	C7	1.416(3)	C20	C21	1.380(5)
C6	C11	1.422(3)	C21	C22	1.383(4)
C7	C8	1.369(4)	O1	C23	1.406(4)
C8	C9	1.393(4)			

Table S5 Bond Angles for 8.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	N1	C5	120.8(2)	C10	C11	C6	119.0(2)
C1	N1	C16	119.0(2)	C10	C11	C12	125.4(2)
C5	N1	C16	120.2(2)	N2	C12	C11	130.6(2)
C12	N2	C13	129.4(2)	N2	C12	C16	106.5(2)
C14	N2	C12	108.46(19)	C16	C12	C11	122.9(2)
C14	N2	C13	121.9(2)	N2	C14	C15	111.6(2)
C2	C1	N1	121.5(2)	C14	C15	C16	104.1(2)
C1	C2	C3	119.0(2)	C14	C15	C17	123.1(2)
C4	C3	C2	119.5(2)	C16	C15	C17	132.7(2)
C3	C4	C5	121.8(2)	N1	C16	C15	130.7(2)
N1	C5	C4	117.3(2)	C12	C16	N1	119.8(2)
N1	C5	C6	119.6(2)	C12	C16	C15	109.3(2)
C4	C5	C6	123.1(2)	C18	C17	C15	120.7(2)
C7	C6	C5	120.1(2)	C22	C17	C15	120.3(2)
C7	C6	C11	118.5(2)	C22	C17	C18	118.9(2)
C11	C6	C5	121.4(2)	C19	C18	C17	120.3(3)
C8	C7	C6	121.1(2)	C20	C19	C18	120.4(3)
C7	C8	C9	120.2(2)	C19	C20	C21	119.7(3)
C10	C9	C8	120.5(2)	C20	C21	C22	120.7(3)
C9	C10	C11	120.7(2)	C21	C22	C17	120.0(3)
C6	C11	C12	115.6(2)				

Table S6 Torsion Angles for 8.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N1	C1	C2	C3	0.5(4)	C9	C10	C11	C12	178.9(2)
N1	C5	C6	C7	179.0(2)	C10	C11	C12	N2	5.6(4)
N1	C5	C6	C11	-1.6(3)	C10	C11	C12	C16	-173.3(2)
N2	C12	C16	N1	172.2(2)	C11	C6	C7	C8	2.2(4)
N2	C12	C16	C15	-2.2(3)	C11	C12	C16	N1	-8.7(3)
N2	C14	C15	C16	-1.8(3)	C11	C12	C16	C15	176.9(2)
N2	C14	C15	C17	174.6(2)	C12	N2	C14	C15	0.5(3)
C1	N1	C5	C4	-1.0(3)	C13	N2	C12	C11	-3.0(4)
C1	N1	C5	C6	177.7(2)	C13	N2	C12	C16	176.0(2)
C1	N1	C16	C12	-172.8(2)	C13	N2	C14	C15	-174.8(2)
C1	N1	C16	C15	0.3(4)	C14	N2	C12	C11	-177.9(2)
C1	C2	C3	C4	-0.9(4)	C14	N2	C12	C16	1.1(3)
C2	C3	C4	C5	0.4(4)	C14	C15	C16	N1	-171.1(2)
C3	C4	C5	N1	0.6(3)	C14	C15	C16	C12	2.5(3)
C3	C4	C5	C6	-178.1(2)	C14	C15	C17	C18	-119.6(3)
C4	C5	C6	C7	-2.3(4)	C14	C15	C17	C22	57.2(4)
C4	C5	C6	C11	177.0(2)	C15	C17	C18	C19	178.6(3)
C5	N1	C1	C2	0.5(3)	C15	C17	C22	C21	-179.0(3)
C5	N1	C16	C12	6.9(3)	C16	N1	C1	C2	-179.8(2)
C5	N1	C16	C15	180.0(2)	C16	N1	C5	C4	179.4(2)
C5	C6	C7	C8	-178.4(2)	C16	N1	C5	C6	-1.9(3)
C5	C6	C11	C10	178.6(2)	C16	C15	C17	C18	55.6(4)
C5	C6	C11	C12	0.2(3)	C16	C15	C17	C22	-127.6(3)
C6	C7	C8	C9	-0.8(4)	C17	C15	C16	N1	13.0(4)
C6	C11	C12	N2	-176.1(2)	C17	C15	C16	C12	-173.4(3)
C6	C11	C12	C16	5.0(3)	C17	C18	C19	C20	0.4(4)
C7	C6	C11	C10	-2.1(3)	C18	C17	C22	C21	-2.2(4)
C7	C6	C11	C12	179.5(2)	C18	C19	C20	C21	-2.2(5)
C7	C8	C9	C10	-0.7(4)	C19	C20	C21	C22	1.7(5)
C8	C9	C10	C11	0.8(4)	C20	C21	C22	C17	0.5(5)
C9	C10	C11	C6	0.6(4)	C22	C17	C18	C19	1.7(4)

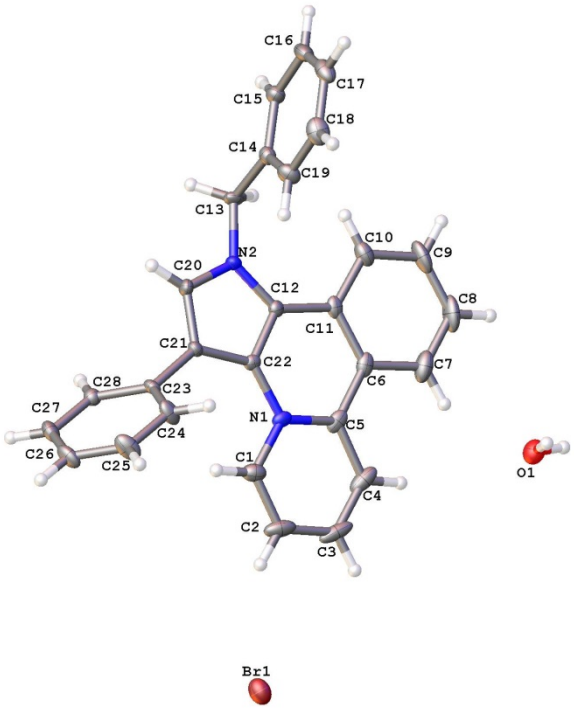
Table S7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 8.

Atom	*x*	*y*	*z*	U(eq)
H1	6022	2662	3590	22
H2	6129	4149	2606	24
H3	6939	4124	2346	25
H4	7621	2672	3092	23

H7	8220	1397	3765	24
H8	8895	-71	4516	28
H9	8774	-1492	5527	27
H10	7982	-1413	5798	22
H13A	7228	-2489	6100	30
H13B	6946	-1492	6590	30
H13C	7491	-918	6511	30
H14	6163	-354	5746	21
H18	5556	-126	3470	34
H19	4679	475	2952	45
H20	4242	2120	3576	47
H21	4667	3039	4757	46
H22	5540	2430	5294	33
H1A	4179	6488	3274	68
H23A	4891	6048	2973	105
H23B	5111	5197	3749	105
H23C	5017	7074	3708	105

1-Benzyl-3-phenyl-1*H*-pyrido[2,1-a]pyrrolo[3,2-c]isoquinolin-4-ium bromide **(9a)**

Single crystals of **9a** were growth from chloroform/diethyl ether. CCDC for **9a** is **1407107**.



Molecular structure of compound **9a**, displacement parameters are drawn at 50% probability level.

Table S8 Crystal data and structure refinement for 9a.

Empirical formula	$C_{28}H_{22}BrN_2O_{0.5}$
Formula weight	474.89

Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	9.9409(5)
b/Å	10.7823(5)
c/Å	11.4682(6)
α/°	67.893(5)
β/°	76.899(5)
γ/°	87.268(4)
Volume/Å^3	1108.25(10)
Z	2
ρ_{calc}g/cm^3	1.423
μ/mm^{-1}	1.875
F(000)	487.0
Crystal size/mm^3	0.23 × 0.17 × 0.10
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.636 to 53.988
Index ranges	-12 ≤ h ≤ 12, -13 ≤ k ≤ 13, -14 ≤ l ≤ 14
Reflections collected	9310
Independent reflections	4771 [R_{int} = 0.0223, R_{sigma} = 0.0427]
Data/restraints/parameters	4771/2/292
Goodness-of-fit on F^2	1.091
Final R indexes [I>=2σ (I)]	R_1 = 0.0423, wR_2 = 0.1037
Final R indexes [all data]	R_1 = 0.0545, wR_2 = 0.1109
Largest diff. peak/hole / e Å^{-3}	0.45/-0.73

Table S9 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 9a. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
N1	3056(2)	4597(2)	4979(2)	15.2(5)
N2	2418(2)	7745(2)	5273(2)	14.7(5)
C9	3662(3)	5246(4)	9002(3)	32.8(8)
C23	1678(3)	6841(3)	2687(3)	14.1(5)
C22	2618(3)	5893(3)	4846(3)	12.9(5)
C21	2088(3)	6878(3)	3843(2)	13.3(5)
C12	2779(3)	6433(3)	5742(3)	13.7(5)
C20	2012(3)	7993(3)	4145(3)	16.1(6)
C26	914(3)	6841(3)	497(3)	24.7(7)
C14	1149(3)	8825(3)	6768(3)	16.8(6)
C3	3981(3)	2100(3)	5143(4)	32.4(8)
C1	3047(3)	4143(3)	4007(3)	21.7(6)
C28	2406(3)	7649(3)	1455(3)	15.8(5)

C5	3549(3)	3820(3)	6045(3)	19.4(6)
C10	3268(3)	6094(3)	7903(3)	23.4(6)
C8	4036(3)	3951(4)	9130(3)	36.2(9)
C17	-1218(3)	9042(3)	8525(3)	26.3(7)
C7	3997(3)	3493(3)	8175(3)	30.3(8)
C24	560(3)	6036(3)	2804(3)	23.8(7)
C6	3593(3)	4329(3)	7036(3)	19.6(6)
C15	1148(3)	9691(3)	7408(3)	19.7(6)
C27	2017(3)	7650(3)	366(3)	21.1(6)
C2	3496(3)	2914(3)	4071(4)	28.8(7)
C13	2450(3)	8796(3)	5784(3)	17.5(6)
C11	3217(3)	5657(3)	6901(3)	16.7(6)
C16	-31(3)	9805(3)	8278(3)	24.0(7)
C25	187(3)	6035(4)	1707(3)	28.2(7)
C19	-46(3)	8059(3)	7020(3)	22.8(6)
C4	4019(3)	2548(3)	6093(4)	29.3(8)
C18	-1222(3)	8172(3)	7905(3)	28.2(7)
Br1	4831.7(3)	751.0(3)	2406.6(3)	28.44(12)
O1	4355(5)	545(5)	9646(4)	28.3(10)

Table S10 Anisotropic Displacement Parameters ($Å^2×10^3$) for 9a. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1	11.4(11)	12.7(11)	21.8(12)	-7.5(10)	-2.0(9)	-1.4(9)
N2	20.3(12)	12.9(11)	12.4(11)	-6.6(9)	-2.9(9)	-0.8(9)
C9	23.4(16)	59(2)	13.7(15)	-8.4(15)	-7.5(12)	-3.4(15)
C23	15.2(13)	18.7(14)	11.2(13)	-8.5(11)	-3.9(10)	2.7(10)
C22	10.0(12)	12.6(13)	15.8(13)	-5.6(11)	-1.4(10)	-2(1)
C21	14.5(12)	15.1(13)	10.1(12)	-5.3(11)	-1.3(10)	-0.5(10)
C12	12.9(12)	13.9(13)	12.9(13)	-3.8(11)	-1.7(10)	-1.4(10)
C20	21.7(14)	13.1(13)	12.5(13)	-3.1(11)	-5.2(11)	1.7(11)
C26	20.8(15)	42.0(19)	17.4(15)	-16.4(14)	-7.9(12)	4.5(13)
C14	17.1(13)	19.0(14)	14.2(13)	-5.8(11)	-4.7(11)	2.3(11)
C3	12.5(14)	16.0(15)	69(3)	-19.4(17)	-2.7(15)	0.5(12)
C1	16.6(14)	23.5(15)	28.6(17)	-15.2(13)	-2.3(12)	-1.2(11)
C28	14.7(13)	17.1(13)	15.5(13)	-6.3(11)	-2.8(10)	1.1(10)
C5	9.3(12)	15.4(14)	28.9(16)	-2.5(12)	-4.7(11)	-2.2(10)
C10	19.0(14)	34.5(17)	16.0(14)	-8.2(13)	-3.6(11)	-2.8(12)
C8	24.6(17)	51(2)	19.8(16)	5.9(15)	-12.0(13)	-3.2(15)
C17	21.3(15)	38.3(18)	18.1(15)	-10.4(14)	-4.6(12)	10.7(13)
C7	20.0(15)	29.4(17)	29.2(18)	5.3(14)	-9.4(13)	-1.4(13)

C24	17.9(14)	35.9(18)	15.5(14)	-9.4(13)	1.9(11)	-9.6(13)
C6	11.8(13)	20.4(14)	20.4(15)	0.2(12)	-4.5(11)	-3.7(11)
C15	23.8(15)	19.2(14)	17.9(14)	-8.4(12)	-5.7(11)	1.0(11)
C27	20.3(14)	28.9(16)	12.4(14)	-7.4(12)	-1.4(11)	3.1(12)
C2	16.5(14)	24.5(16)	53(2)	-25.6(16)	-2.0(14)	-1.4(12)
C13	21.5(14)	15.1(13)	18.8(14)	-10.9(12)	-1.7(11)	-2.3(11)
C11	10.5(12)	22.2(14)	13.6(13)	-2.0(11)	-2.1(10)	-4.2(10)
C16	31.0(17)	26.7(16)	16.4(15)	-11.0(13)	-6.1(12)	10.5(13)
C25	18.6(15)	46(2)	25.3(17)	-18.9(15)	-3.8(12)	-8.4(14)
C19	21.5(15)	29.5(16)	22.9(15)	-14.4(13)	-7.2(12)	-0.1(12)
C4	14.9(14)	15.6(15)	52(2)	-5.0(15)	-9.4(14)	1.0(11)
C18	15.8(14)	39.7(19)	27.1(17)	-9.0(15)	-6.5(12)	-1.7(13)
Br1	24.71(18)	38.0(2)	23.11(18)	-10.77(14)	-7.26(12)	-0.51(13)
O1	29(2)	26(2)	29(2)	-7(2)	-9.6(19)	4(2)

Table S11 Bond Lengths for 9a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	C22	1.406(3)	C14	C13	1.518(4)
N1	C1	1.378(4)	C14	C19	1.391(4)
N1	C5	1.378(4)	C3	C2	1.390(5)
N2	C12	1.373(3)	C3	C4	1.356(5)
N2	C20	1.368(3)	C1	C2	1.359(4)
N2	C13	1.463(3)	C28	C27	1.388(4)
C9	C10	1.378(4)	C5	C6	1.445(4)
C9	C8	1.390(6)	C5	C4	1.413(4)
C23	C21	1.488(4)	C10	C11	1.408(4)
C23	C28	1.396(4)	C8	C7	1.369(5)
C23	C24	1.394(4)	C17	C16	1.384(5)
C22	C21	1.425(4)	C17	C18	1.375(5)
C22	C12	1.398(4)	C7	C6	1.413(4)
C21	C20	1.365(4)	C24	C25	1.390(4)
C12	C11	1.430(4)	C6	C11	1.422(4)
C26	C27	1.380(4)	C15	C16	1.390(4)
C26	C25	1.378(4)	C19	C18	1.398(4)
C14	C15	1.389(4)	O1	O1[1]	1.816(9)

[1]1-X,-Y,2-Z

Table S12 Bond Angles for 9a.

Atom Atom Atom Angle/° Atom Atom Atom Angle/°

C1	N1	C22	119.3(2)	C2	C1	N1	121.6(3)
C1	N1	C5	120.7(2)	C27	C28	C23	120.4(3)
C5	N1	C22	119.9(2)	N1	C5	C6	120.0(2)
C12	N2	C13	130.0(2)	N1	C5	C4	116.9(3)
C20	N2	C12	108.6(2)	C4	C5	C6	123.1(3)
C20	N2	C13	121.4(2)	C9	C10	C11	120.6(3)
C10	C9	C8	120.5(3)	C7	C8	C9	120.4(3)
C28	C23	C21	119.6(2)	C18	C17	C16	119.5(3)
C24	C23	C21	121.5(2)	C8	C7	C6	120.8(3)
C24	C23	C28	118.9(2)	C25	C24	C23	120.3(3)
N1	C22	C21	130.4(2)	C7	C6	C5	119.8(3)
C12	C22	N1	120.1(2)	C7	C6	C11	118.8(3)
C12	C22	C21	109.3(2)	C11	C6	C5	121.3(3)
C22	C21	C23	132.4(2)	C14	C15	C16	120.7(3)
C20	C21	C23	123.3(2)	C26	C27	C28	120.0(3)
C20	C21	C22	104.3(2)	C1	C2	C3	119.0(3)
N2	C12	C22	106.3(2)	N2	C13	C14	114.2(2)
N2	C12	C11	131.3(3)	C10	C11	C12	125.4(3)
C22	C12	C11	122.4(2)	C10	C11	C6	118.8(3)
C21	C20	N2	111.3(2)	C6	C11	C12	115.8(3)
C25	C26	C27	120.3(3)	C17	C16	C15	120.2(3)
C15	C14	C13	118.0(2)	C26	C25	C24	120.1(3)
C15	C14	C19	118.9(3)	C14	C19	C18	119.9(3)
C19	C14	C13	123.0(3)	C3	C4	C5	122.0(3)
C4	C3	C2	119.8(3)	C17	C18	C19	120.7(3)

Table S13 Torsion Angles for 9a.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N1	C22	C21	C23	7.6(5)	C1	N1	C5	C6	178.0(2)
N1	C22	C21	C20	-172.3(3)	C1	N1	C5	C4	-0.8(4)
N1	C22	C12	N2	172.9(2)	C28	C23	C21	C22	-116.1(3)
N1	C22	C12	C11	-8.2(4)	C28	C23	C21	C20	63.7(4)
N1	C1	C2	C3	-0.3(4)	C28	C23	C24	C25	0.5(4)
N1	C5	C6	C7	175.1(2)	C5	N1	C22	C21	179.4(3)
N1	C5	C6	C11	-4.0(4)	C5	N1	C22	C12	4.9(4)
N1	C5	C4	C3	-0.5(4)	C5	N1	C1	C2	1.2(4)
N2	C12	C11	C10	5.4(5)	C5	C6	C11	C12	1.0(4)
N2	C12	C11	C6	-176.3(3)	C5	C6	C11	C10	179.4(2)
C9	C10	C11	C12	177.7(3)	C10	C9	C8	C7	-1.0(5)
C9	C10	C11	C6	-0.6(4)	C8	C9	C10	C11	1.0(5)
C9	C8	C7	C6	0.8(5)	C8	C7	C6	C5	-179.5(3)

C23	C21	C20	N2	178.5(2)	C8	C7	C6	C11	-0.4(4)
C23	C28	C27	C26	-0.6(4)	C7	C6	C11	C12	-178.2(2)
C23	C24	C25	C26	-0.7(5)	C7	C6	C11	C10	0.3(4)
C22	N1	C1	C2	178.2(3)	C24	C23	C21	C22	65.4(4)
C22	N1	C5	C6	1.0(4)	C24	C23	C21	C20	-114.8(3)
C22	N1	C5	C4	-177.7(2)	C24	C23	C28	C27	0.1(4)
C22	C21	C20	N2	-1.7(3)	C6	C5	C4	C3	-179.2(3)
C22	C12	C11	C10	-173.2(3)	C15	C14	C13	N2	173.0(2)
C22	C12	C11	C6	5.1(4)	C15	C14	C19	C18	0.1(4)
C21	C23	C28	C27	-178.5(3)	C27	C26	C25	C24	0.2(5)
C21	C23	C24	C25	179.0(3)	C2	C3	C4	C5	1.4(5)
C21	C22	C12	N2	-2.7(3)	C13	N2	C12	C22	-177.0(3)
C21	C22	C12	C11	176.2(2)	C13	N2	C12	C11	4.2(5)
C12	N2	C20	C21	0.1(3)	C13	N2	C20	C21	178.9(2)
C12	N2	C13	C14	-87.0(3)	C13	C14	C15	C16	177.2(3)
C12	C22	C21	C23	-177.5(3)	C13	C14	C19	C18	-177.7(3)
C12	C22	C21	C20	2.7(3)	C16	C17	C18	C19	-0.6(5)
C20	N2	C12	C22	1.6(3)	C25	C26	C27	C28	0.4(5)
C20	N2	C12	C11	-177.2(3)	C19	C14	C15	C16	-0.7(4)
C20	N2	C13	C14	94.5(3)	C19	C14	C13	N2	-9.2(4)
C14	C15	C16	C17	0.6(4)	C4	C3	C2	C1	-1.0(5)
C14	C19	C18	C17	0.6(5)	C4	C5	C6	C7	-6.2(4)
C1	N1	C22	C21	2.4(4)	C4	C5	C6	C11	174.7(3)
C1	N1	C22	C12	-172.1(2)	C18	C17	C16	C15	0.0(4)

Table S14 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 9a.

Atom	*x*	*y*	*z*	U(eq)
H9	3678	5543	9662	39
H20	1721	8815	3649	19
H26	659	6840	-235	30
H3	4279	1250	5209	39
H1	2726	4692	3288	26
H28	3155	8189	1364	19
H10	3034	6963	7823	28
H8	4315	3391	9869	43
H17	-2008	9118	9106	32
H7	4239	2620	8276	36
H24	61	5497	3619	29
H15	1945	10201	7254	24
H27	2500	8197	-452	25

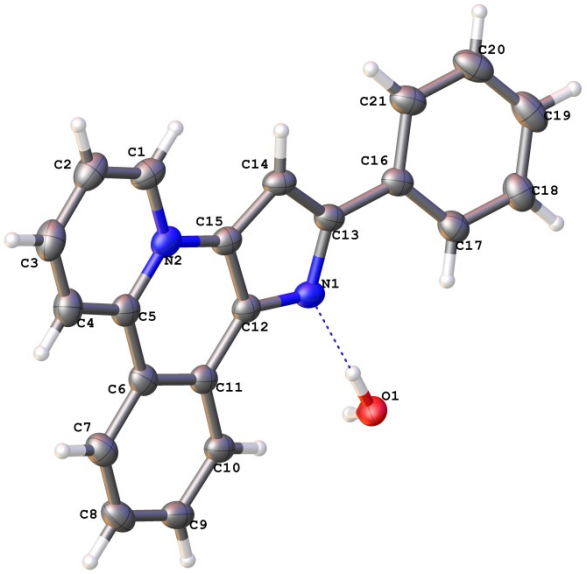
H2	3479	2622	3407	35
H13A	2590	9658	5070	21
H13B	3234	8672	6183	21
H16	-22	10395	8694	29
H25	-554	5490	1789	34
H19	-62	7473	6600	27
H4	4364	2002	6797	35
H18	-2017	7652	8077	34
H1A	3528	588	9703	43
H1B	4794	244	10245	43

Table S15 Atomic Occupancy for 9a.

Atom	***Occupancy***	**Atom**	***Occupancy***	**Atom**	***Occupancy***
O1	0.5	H1A	0.5	H1B	0.5

2-Phenylpyrido[2,1-a]pyrrolo[3,2-c]isoquinoline **(11)**

Single crystals of **11** were growth from chloroform/hexane. CCDC for **11** is **1407277**



Molecular structure of compound **11**, displacement parameters are drawn at 50% probability level.

Table S16 Crystal data and structure refinement for 11

Empirical formula	$C_{21}H_{15}N_2O_{0.5}$
Formula weight	303.35
Temperature/K	100(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	17.5157(6)

b/Å	8.5175(2)
c/Å	19.8322(5)
α/°	90.00
β/°	95.754(3)
γ/°	90.00
Volume/Å^3	2943.85(15)
Z	8
ρ_{calc}mg/mm^3	1.369
m/mm^{-1}	0.651
F(000)	1272.0
Crystal size/mm^3	0.24 × 0.16 × 0.08
2Θ range for data collection	6.42 to 144.98°
Index ranges	$-21 \le h \le 21$, $-10 \le k \le 10$, $-23 \le l \le 24$
Reflections collected	45149
Independent reflections	5846[R(int) = 0.0632]
Data/restraints/parameters	5846/0/440
Goodness-of-fit on F^2	1.037
Final R indexes [I>=2σ (I)]	R_1 = 0.0489, wR_2 = 0.1266
Final R indexes [all data]	R_1 = 0.0769, wR_2 = 0.1499
Largest diff. peak/hole / e Å^{-3}	0.23/-0.19

Table S17 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 11. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C11	5551.6(10)	6237(2)	754.0(9)	33.0(4)
N2	5030.7(9)	7791.6(19)	-482.5(7)	35.5(4)
N1	4428.4(9)	7605.0(18)	1191.7(7)	34.0(3)
C6	5913.8(10)	5984(2)	155.0(9)	35.9(4)
C15	4658.2(11)	8029(2)	95.7(9)	33.3(4)
C7	6543.4(11)	4948(2)	183.2(10)	42.2(5)
C1	4781.3(12)	8604(2)	-1065.1(9)	41.3(5)
C5	5639.2(11)	6754(2)	-473.6(9)	36.5(4)
C12	4901.3(10)	7255(2)	709.7(9)	32.2(4)
C8	6807.1(11)	4206(2)	775.4(11)	44.5(5)
C14	4005.8(11)	8898(2)	203.0(9)	35.9(4)
C10	5831.3(11)	5462(2)	1357.5(10)	36.8(4)
C4	5960.9(12)	6518(3)	-1088.8(10)	44.7(5)
C16	3245.2(10)	9186(2)	1234.1(9)	34.8(4)
C9	6450.4(11)	4472(2)	1365.5(10)	41.6(5)
C21	2788.4(12)	10430(2)	962.5(10)	42.1(5)
C13	3883.2(10)	8598(2)	878.2(9)	34.0(4)
C2	5114.3(13)	8396(3)	-1648.4(10)	47.5(5)

C19	1997.9(12)	10280(3)	1885.8(11)	51.6(6)
C20	2172.7(12)	10969(3)	1286.7(11)	49.7(5)
C3	5710.3(12)	7314(3)	-1663.5(10)	49.8(6)
C17	3071.3(11)	8529(3)	1839.0(9)	39.7(4)
C18	2452.1(11)	9061(3)	2162.3(10)	46.5(5)
N2A	6.3(9)	7806.7(19)	427.0(7)	36.9(4)
N1A	617.7(9)	7631.7(18)	-1244.5(7)	35.1(4)
C6A	-872.2(11)	6004(2)	-221.8(9)	35.4(4)
C12A	143.1(10)	7282(2)	-766.4(9)	33.8(4)
C5A	-611.2(11)	6782(2)	407.6(9)	38.2(4)
C11A	-507.7(10)	6271(2)	-817.6(9)	33.5(4)
C10A	-786.8(11)	5510(2)	-1426.6(9)	36.1(4)
C15A	388.1(11)	8040(2)	-149.9(9)	36.4(4)
C9A	-1400.4(11)	4508(2)	-1441.8(10)	40.8(4)
C8A	-1754.4(12)	4215(2)	-853.2(11)	44.1(5)
C7A	-1496.3(11)	4944(2)	-257.1(10)	42.4(5)
C13A	1165.2(11)	8615(2)	-923.0(9)	36.3(4)
C4A	-954.6(12)	6572(3)	1011.7(10)	46.5(5)
C14A	1042.1(11)	8901(2)	-247.4(9)	38.6(4)
C1A	247.7(12)	8615(2)	1009.4(9)	43.2(5)
C16A	1800.4(11)	9204(2)	-1279.5(10)	39.0(4)
C2A	-100.5(13)	8431(3)	1584.7(10)	48.3(5)
C21A	1960.1(11)	8568(3)	-1891.8(10)	44.4(5)
C20A	2580.6(12)	9088(3)	-2214.6(12)	52.7(6)
C3A	-711.5(13)	7376(3)	1591.9(10)	51.2(6)
C17A	2270.6(12)	10426(3)	-1001.5(11)	47.9(5)
C19A	3048.3(13)	10269(3)	-1934.9(13)	59.1(7)
C18A	2883.6(13)	10946(3)	-1328.5(13)	58.1(7)
O1	4667.9(11)	6358(2)	2516.1(8)	33.9(5)
O1A	344(3)	6359(6)	-2533(2)	56.0(13)

Table S18 Anisotropic Displacement Parameters ($Å^2×10^3$) for 11. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka×b×U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C11	29.3(8)	28.1(10)	40.2(9)	-0.5(7)	-3.6(7)	-7.5(7)
N2	38.6(8)	32.6(9)	34.1(7)	-1.2(6)	-2.9(6)	-10.2(7)
N1	33.7(8)	28.7(9)	38.1(7)	2.4(6)	-4.3(6)	-2.7(6)
C6	30.4(9)	33.0(11)	43.1(9)	-5.4(8)	-1.9(7)	-7.5(8)
C15	36.2(9)	28.2(10)	34.1(8)	-0.7(7)	-3.7(7)	-5.5(7)
C7	34.8(10)	42.2(12)	48.7(10)	-7.4(9)	-1.1(8)	-1.4(9)
C1	48.6(11)	35.8(11)	37.2(9)	2.3(8)	-7.1(8)	-10.4(9)
C5	33.2(9)	33.4(11)	41.7(9)	-3.5(8)	-1.4(7)	-9.9(8)
C12	32.2(9)	28.3(10)	35.2(8)	-0.2(7)	-1.5(7)	-5.3(7)
C8	32.9(9)	38.6(12)	60.5(12)	-7.8(9)	-2.8(9)	2.3(9)
C14	39.2(10)	28.4(10)	37.8(9)	2.1(7)	-8.1(7)	-1.1(8)

C10	33.1(9)	31(1)	44.7(9)	1.7(8)	-3.9(7)	-5.2(8)
C4	37.5(10)	51.2(13)	45.4(10)	-5.3(9)	4.6(8)	-12.0(9)
C16	32.0(9)	29.4(10)	40.8(9)	-4.0(7)	-7.3(7)	-2.9(7)
C9	35.3(10)	31.5(11)	54.9(11)	4.8(9)	-10.2(8)	-4.1(8)
C21	40.3(10)	35.1(11)	48.3(10)	-5.6(9)	-8.3(8)	2.8(9)
C13	31.9(9)	26.9(10)	41.6(9)	-1.4(7)	-3.9(7)	-2.5(7)
C2	54.3(12)	51.9(14)	34.8(9)	2.7(9)	-3.5(8)	-19.2(11)
C19	33.2(10)	59.1(15)	60.6(13)	-25.7(11)	-4.2(9)	2.1(10)
C20	40.9(11)	44.6(14)	60.0(12)	-13(1)	-12.8(9)	8.3(10)
C3	46.2(11)	63.7(15)	39.7(10)	-1.5(10)	5.5(9)	-16.7(11)
C17	31.7(9)	42.4(12)	43.7(9)	-3.4(9)	-2.8(8)	-0.3(8)
C18	35.1(10)	55.8(15)	48.1(10)	-11.2(10)	0.6(8)	-4.0(9)
N2A	41.3(8)	28.7(9)	38.1(8)	-2.3(6)	-8.3(6)	8.5(7)
N1A	35.3(8)	26.8(9)	41.6(8)	-1.5(6)	-4.2(6)	1.2(6)
C6A	33.3(9)	29.1(10)	41.8(9)	1.0(7)	-6.2(7)	7.6(7)
C12A	35.4(9)	24.1(10)	39.5(9)	-2.0(7)	-7.6(7)	5.0(7)
C5A	35.7(9)	35.9(11)	41.7(9)	2.7(8)	-2.3(8)	13.5(8)
C11A	32.6(9)	25(1)	41.2(9)	2.1(7)	-4.2(7)	7.1(7)
C10A	34.9(9)	30.2(10)	41.6(9)	-1.2(8)	-4.4(7)	3.2(8)
C15A	40.5(10)	28.5(10)	38.0(9)	1.6(7)	-6.4(8)	6.6(8)
C9A	37.8(10)	32.7(11)	49.1(10)	-2.2(8)	-9.1(8)	3.4(8)
C8A	35(1)	36.6(12)	58.3(12)	3.2(9)	-8.0(9)	-1.2(8)
C7A	36.1(10)	41.3(12)	48.5(10)	7.6(9)	-1.4(8)	5.3(9)
C13A	37.4(10)	26(1)	42.5(9)	-0.8(8)	-11.1(8)	3.5(8)
C4A	40.9(11)	48.6(13)	49.4(11)	-2.9(9)	0.9(9)	11.1(9)
C14A	41.7(10)	26.3(10)	44.2(10)	-0.1(8)	-12.8(8)	2.0(8)
C1A	52.2(12)	35.8(11)	38.8(9)	-1.7(8)	-8.8(8)	11.2(9)
C16A	34.0(9)	30.3(11)	49.7(10)	6.9(8)	-11.2(8)	2.1(8)
C2A	57.1(13)	46.0(13)	39.3(10)	-5.8(9)	-8.0(9)	17.9(11)
C21A	35.4(10)	42.4(12)	53.7(11)	2.7(10)	-4.3(8)	-0.4(9)
C20A	37.5(11)	59.3(16)	60.0(12)	12.5(11)	-0.8(9)	3.2(10)
C3A	50.3(12)	59.9(15)	43.4(10)	0.5(10)	4.5(9)	19.6(11)
C17A	44.5(11)	36.5(12)	58.0(12)	7.8(9)	-18.0(9)	-5.1(9)
C19A	37.8(11)	62.9(17)	73.6(15)	29.7(13)	-8.8(10)	-7.2(11)
C18A	46.5(12)	45.5(15)	76.8(15)	20.5(12)	-21.1(11)	-14.2(10)
O1	35.9(10)	42.7(12)	23.0(8)	4.2(8)	2.1(7)	0.4(9)
O1A	53(3)	64(3)	49(2)	-1(2)	-7(2)	-4(2)

Table S19 Bond Lengths for 11.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C11	C6	1.418(3)	N2A	C5A	1.387(3)
C11	C12	1.427(3)	N2A	C15A	1.396(2)
C11	C10	1.411(3)	N2A	C1A	1.374(2)
N2	C15	1.390(2)	N1A	C12A	1.355(2)
N2	C1	1.379(2)	N1A	C13A	1.380(2)

N2	C5	1.383(3)	C6A	C5A	1.447(3)
N1	C12	1.359(2)	C6A	C11A	1.417(3)
N1	C13	1.377(2)	C6A	C7A	1.414(3)
C6	C7	1.409(3)	C12A	C11A	1.424(3)
C6	C5	1.448(3)	C12A	C15A	1.411(2)
C15	C12	1.412(2)	C5A	C4A	1.405(3)
C15	C14	1.396(3)	C11A	C10A	1.414(2)
C7	C8	1.372(3)	C10A	C9A	1.371(3)
C1	C2	1.358(3)	C15A	C14A	1.390(3)
C5	C4	1.409(3)	C9A	C8A	1.398(3)
C8	C9	1.399(3)	C8A	C7A	1.371(3)
C14	C13	1.401(2)	C13A	C14A	1.400(3)
C10	C9	1.372(3)	C13A	C16A	1.465(3)
C4	C3	1.361(3)	C4A	C3A	1.370(3)
C16	C21	1.402(3)	C1A	C2A	1.356(3)
C16	C13	1.468(3)	C16A	C21A	1.384(3)
C16	C17	1.385(3)	C16A	C17A	1.405(3)
C21	C20	1.388(3)	C2A	C3A	1.398(3)
C2	C3	1.395(3)	C21A	C20A	1.388(3)
C19	C20	1.386(3)	C20A	C19A	1.378(3)
C19	C18	1.387(3)	C17A	C18A	1.382(3)
C17	C18	1.390(3)	C19A	C18A	1.390(4)

Table S20 Bond Angles for 11.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C6	C11	C12	117.53(16)	C5A	N2A	C15A	120.20(16)
C10	C11	C6	119.51(18)	C1A	N2A	C5A	120.79(18)
C10	C11	C12	122.94(17)	C1A	N2A	C15A	119.01(18)
C1	N2	C15	118.86(17)	C12A	N1A	C13A	104.88(15)
C1	N2	C5	120.66(17)	C11A	C6A	C5A	121.08(18)
C5	N2	C15	120.48(16)	C7A	C6A	C5A	120.75(18)
C12	N1	C13	105.13(15)	C7A	C6A	C11A	118.17(17)
C11	C6	C5	120.94(18)	N1A	C12A	C11A	128.74(16)
C7	C6	C11	118.43(18)	N1A	C12A	C15A	110.55(17)
C7	C6	C5	120.62(18)	C15A	C12A	C11A	120.68(18)
N2	C15	C12	121.18(17)	N2A	C5A	C6A	119.36(17)
N2	C15	C14	131.47(17)	N2A	C5A	C4A	117.11(18)
C14	C15	C12	107.26(16)	C4A	C5A	C6A	123.5(2)
C8	C7	C6	121.15(19)	C6A	C11A	C12A	117.53(17)
C2	C1	N2	121.4(2)	C10A	C11A	C6A	119.52(18)
N2	C5	C6	119.32(17)	C10A	C11A	C12A	122.93(17)
N2	C5	C4	117.05(18)	C9A	C10A	C11A	120.49(18)
C4	C5	C6	123.63(19)	N2A	C15A	C12A	121.06(18)
N1	C12	C11	128.95(16)	C14A	C15A	N2A	131.18(18)
N1	C12	C15	110.60(17)	C14A	C15A	C12A	107.71(17)

C15	C12	C11	120.42(16)	C10A	C9A	C8A	120.35(18)
C7	C8	C9	120.07(19)	C7A	C8A	C9A	120.24(19)
C15	C14	C13	104.80(16)	C8A	C7A	C6A	121.21(19)
C9	C10	C11	120.27(18)	N1A	C13A	C14A	112.41(17)
C3	C4	C5	122.1(2)	N1A	C13A	C16A	120.73(17)
C21	C16	C13	120.36(18)	C14A	C13A	C16A	126.83(18)
C17	C16	C21	118.14(19)	C3A	C4A	C5A	122.0(2)
C17	C16	C13	121.49(18)	C15A	C14A	C13A	104.45(17)
C10	C9	C8	120.56(19)	C2A	C1A	N2A	121.5(2)
C20	C21	C16	120.8(2)	C21A	C16A	C13A	121.29(18)
N1	C13	C14	112.20(16)	C21A	C16A	C17A	118.2(2)
N1	C13	C16	121.29(16)	C17A	C16A	C13A	120.53(19)
C14	C13	C16	126.47(17)	C1A	C2A	C3A	119.5(2)
C1	C2	C3	119.3(2)	C16A	C21A	C20A	121.1(2)
C20	C19	C18	119.2(2)	C19A	C20A	C21A	120.6(2)
C19	C20	C21	120.4(2)	C4A	C3A	C2A	119.1(2)
C4	C3	C2	119.4(2)	C18A	C17A	C16A	120.4(2)
C16	C17	C18	121.1(2)	C20A	C19A	C18A	119.0(2)
C19	C18	C17	120.3(2)	C17A	C18A	C19A	120.8(2)

Table S21 Torsion Angles for 11.

A	B	C	D	Angle/°
C11	C6	C7	C8	-0.5(3)
C11	C6	C5	N2	2.2(3)
C11	C6	C5	C4	-178.23(18)
C11	C10	C9	C8	-0.7(3)
N2	C15	C12	C11	1.6(3)
N2	C15	C12	N1	-176.84(16)
N2	C15	C14	C13	176.12(19)
N2	C1	C2	C3	1.4(3)
N2	C5	C4	C3	2.6(3)
C6	C11	C12	N1	175.23(17)
C6	C11	C12	C15	-2.9(3)
C6	C11	C10	C9	0.2(3)
C6	C7	C8	C9	0.0(3)
C6	C5	C4	C3	-177.03(19)
C15	N2	C1	C2	-178.74(18)
C15	N2	C5	C6	-3.6(3)
C15	N2	C5	C4	176.81(16)
C15	C14	C13	N1	0.5(2)
C15	C14	C13	C16	-177.26(18)
C7	C6	C5	N2	-178.58(17)
C7	C6	C5	C4	1.0(3)
C7	C8	C9	C10	0.6(3)
C1	N2	C15	C12	-178.53(17)

C1	N2	C15	C14	5.4(3)
C1	N2	C5	C6	176.70(16)
C1	N2	C5	C4	-2.9(3)
C1	C2	C3	C4	-1.8(3)
C5	N2	C15	C12	1.7(3)
C5	N2	C15	C14	-174.35(19)
C5	N2	C1	C2	1.0(3)
C5	C6	C7	C8	-179.76(18)
C5	C4	C3	C2	-0.3(3)
C12	C11	C6	C7	-178.22(17)
C12	C11	C6	C5	1.1(3)
C12	C11	C10	C9	178.71(17)
C12	N1	C13	C14	-0.5(2)
C12	N1	C13	C16	177.44(16)
C12	C15	C14	C13	-0.4(2)
C14	C15	C12	C11	178.54(16)
C14	C15	C12	N1	0.1(2)
C10	C11	C6	C7	0.4(3)
C10	C11	C6	C5	179.68(17)
C10	C11	C12	N1	-3.3(3)
C10	C11	C12	C15	178.51(17)
C16	C21	C20	C19	-0.2(3)
C16	C17	C18	C19	-0.6(3)
C21	C16	C13	N1	167.03(17)
C21	C16	C13	C14	-15.3(3)
C21	C16	C17	C18	1.3(3)
C13	N1	C12	C11	-178.04(18)
C13	N1	C12	C15	0.2(2)
C13	C16	C21	C20	178.43(18)
C13	C16	C17	C18	-178.04(18)
C20	C19	C18	C17	-0.5(3)
C17	C16	C21	C20	-0.9(3)
C17	C16	C13	N1	-13.6(3)
C17	C16	C13	C14	164.01(19)
C18	C19	C20	C21	0.9(3)
N2A	C5A	C4A	C3A	2.1(3)
N2A	C15A	C14A	C13A	176.86(19)
N2A	C1A	C2A	C3A	1.1(3)
N1A	C12A	C11A	C6A	174.89(17)
N1A	C12A	C11A	C10A	-3.6(3)
N1A	C12A	C15A	N2A	-177.39(16)
N1A	C12A	C15A	C14A	0.1(2)
N1A	C13A	C14A	C15A	0.4(2)
N1A	C13A	C16A	C21A	-12.9(3)
N1A	C13A	C16A	C17A	167.85(17)
C6A	C5A	C4A	C3A	-177.37(19)
C6A	C11A	C10A	C9A	-0.7(3)

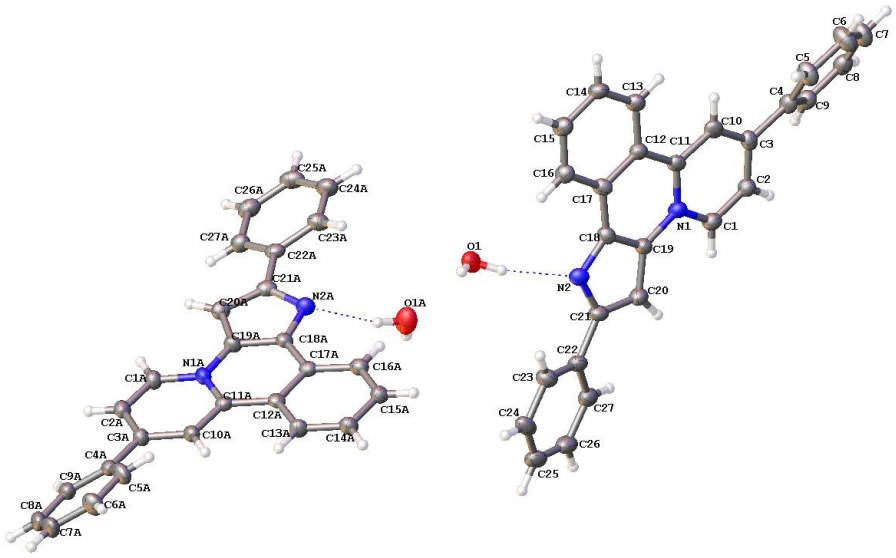
C12A	N1A	C13A	C14A	-0.3(2)
C12A	N1A	C13A	C16A	177.95(16)
C12A	C11A	C10A	C9A	177.81(18)
C12A	C15A	C14A	C13A	-0.3(2)
C5A	N2A	C15A	C12A	1.9(3)
C5A	N2A	C15A	C14A	-174.93(19)
C5A	N2A	C1A	C2A	0.7(3)
C5A	C6A	C11A	C12A	2.5(3)
C5A	C6A	C11A	C10A	-178.92(17)
C5A	C6A	C7A	C8A	179.16(18)
C5A	C4A	C3A	C2A	-0.4(3)
C11A	C6A	C5A	N2A	0.0(3)
C11A	C6A	C5A	C4A	179.43(18)
C11A	C6A	C7A	C8A	-1.3(3)
C11A	C12A	C15A	N2A	0.8(3)
C11A	C12A	C15A	C14A	178.24(17)
C11A	C10A	C9A	C8A	-0.5(3)
C10A	C9A	C8A	C7A	0.8(3)
C15A	N2A	C5A	C6A	-2.2(3)
C15A	N2A	C5A	C4A	178.31(17)
C15A	N2A	C1A	C2A	-179.82(18)
C15A	C12A	C11A	C6A	-2.9(3)
C15A	C12A	C11A	C10A	178.59(17)
C9A	C8A	C7A	C6A	0.2(3)
C7A	C6A	C5A	N2A	179.51(17)
C7A	C6A	C5A	C4A	-1.1(3)
C7A	C6A	C11A	C12A	-177.01(17)
C7A	C6A	C11A	C10A	1.6(3)
C13A	N1A	C12A	C11A	-177.83(18)
C13A	N1A	C12A	C15A	0.1(2)
C13A	C16A	C21A	C20A	-177.46(19)
C13A	C16A	C17A	C18A	177.99(18)
C14A	C13A	C16A	C21A	165.13(19)
C14A	C13A	C16A	C17A	-14.2(3)
C1A	N2A	C5A	C6A	177.23(17)
C1A	N2A	C5A	C4A	-2.2(3)
C1A	N2A	C15A	C12A	-177.59(17)
C1A	N2A	C15A	C14A	5.6(3)
C1A	C2A	C3A	C4A	-1.2(3)
C16A	C13A	C14A	C15A	-177.77(18)
C16A	C21A	C20A	C19A	-0.8(3)
C16A	C17A	C18A	C19A	-0.3(3)
C21A	C16A	C17A	C18A	-1.3(3)
C21A	C20A	C19A	C18A	-0.8(3)
C20A	C19A	C18A	C17A	1.4(3)
C17A	C16A	C21A	C20A	1.8(3)

Table S22 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 11.

Atom	*x*	*y*	*z*	U(eq)
H7	6784	4763	-206	51
H1	4376	9308	-1058	50
H8	7223	3526	785	53
H14	3716	9536	-106	43
H10	5595	5622	1751	44
H4	6357	5795	-1103	54
H9	6635	3975	1767	50
H21	2899	10900	560	50
H2	4947	8970	-2034	57
H19	1581	10631	2100	62
H20	1876	11797	1101	60
H3	5934	7139	-2063	60
H17	3374	7717	2032	48
H18	2342	8598	2566	56
H10A	-552	5692	-1820	43
H9A	-1582	4019	-1846	49
H8A	-2167	3523	-866	53
H7A	-1736	4737	131	51
H4A	-1359	5867	1018	56
H14A	1333	9526	66	46
H1A	659	9305	1009	52
H2A	66	9001	1972	58
H21A	1647	7779	-2090	53
H20A	2681	8636	-2623	63
H3A	-950	7223	1985	61
H17A	2169	10887	-595	58
H19A	3468	10607	-2149	71
H18A	3189	11759	-1141	70
H1B	4981	6885	2782	51
H1C	4596	6821	2135	51
H1AA	433	6697	-2131	84
H1AB	33	6977	-2759	84

2,7-Diphenylpyrido[2,1-a]pyrrolo[3,2-c]isoquinoline **(13)**

Single crystals of **13** were growth from acetone/pentane. CCDC for **13** is **1412486**



Molecular structure of compound **13**, displacement parameters are drawn at 50% probability level.

Table S23 Crystal data and structure refinement for 13

Formula	$2(C_{27}H_{18}N_2)$, $2(H_2O)$
Crystal System	Monoclinic
a (Å)	16.6795(12)
b (Å)	8.7264(8)
c (Å)	26.906(2)
β (°)	101.297(7)
V (Å^3)	3840.4(5)
Molecular weight	776.90
Space group	*P2/c*
μ (mm^{-1})	0.644
Temperature (K)	100(2)
Z	4
D_{calc} (g/cm^3)	1.344
Crystal size (mm^3)	0.25×0.18×0.14
Radiation	Cu$K\alpha$
Total reflections	30214
Unique reflections	7285
Angle range 2θ (°)	6.7-139.992
F(000)	1632.0
Index ranges	$-20 \le h \le 19$, $-10 \le k \le 10$, $-32 \le l \le 32$
Reflections with $\|F_o\| \ge 4\sigma_F$	2956
R_{int}	0.1615
R_σ	0.1578
R_1 ($\|F_o\| \ge 4\sigma_F$)	0.0723
wR_2 ($\|F_o\| \ge 4\sigma_F$)	0.1604
R_1 (all data)	0.1812

wR_2 (all data)	0.2400
S	1.010
ρ_{min}, ρ_{max}, e/Å^3	0.34/-0.30

$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$;
$w = 1/[\sigma^2(F_o^2)+(aP)^2 + bP]$, where $P = (F_o^2 + 2F_c^2)/3$; $s = \{\Sigma[w(F_o^2 - F_c^2)]/(n - p)\}^{1/2}$
where n is the number of reflections and p is the number of refinement parameters.

Table S24 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 13. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
N(1)	2628(2)	3210(5)	7767.9(15)	25.8(9)
N(2)	3085(2)	3018(5)	6516.4(15)	26.8(9)
C(1)	2942(3)	4025(6)	8203.2(18)	29.8(11)
C(2)	2646(3)	3809(6)	8636.8(17)	27.4(11)
C(3)	2029(3)	2705(6)	8651.1(17)	27.1(10)
C(4)	1731(3)	2358(7)	9123.2(17)	29.0(11)
C(5)	1519(4)	861(7)	9220.9(19)	37.0(13)
C(6)	1239(4)	528(8)	9667(2)	44.8(15)
C(7)	1161(4)	1689(7)	10006(2)	41.8(14)
C(8)	1378(3)	3181(7)	9909.9(19)	33.4(12)
C(9)	1674(3)	3514(6)	9475.3(18)	29.6(11)
C(10)	1709(3)	1951(6)	8210.1(18)	27.0(11)
C(11)	1987(3)	2192(6)	7752.1(18)	25(1)
C(12)	1643(3)	1424(6)	7286.7(18)	26.2(10)
C(13)	961(3)	415(6)	7258.9(18)	28.6(11)
C(14)	615(3)	-279(7)	6813.7(19)	31.7(12)
C(15)	931(3)	-8(7)	6370.8(18)	32.7(12)
C(16)	1590(3)	933(6)	6384.0(18)	29.2(11)
C(17)	1955(3)	1672(6)	6837.8(18)	25.9(10)
C(18)	2643(3)	2667(6)	6873.8(17)	26(1)
C(19)	2964(3)	3434(6)	7333.6(17)	27.4(11)
C(20)	3638(3)	4312(6)	7256.1(18)	29.6(11)
C(21)	3681(3)	4005(6)	6748.1(19)	29.9(11)
C(22)	4277(3)	4636(7)	6468.2(19)	31.0(12)
C(23)	4377(3)	3963(7)	6016(2)	34.0(12)
C(24)	4938(3)	4567(7)	5738(2)	37.8(13)
C(25)	5396(3)	5856(7)	5918(2)	41.5(14)
C(26)	5296(3)	6526(7)	6369(2)	40.8(14)
C(27)	4747(3)	5925(7)	6650(2)	34.1(12)
N(1A)	2389(2)	2465(5)	2194.6(14)	25.9(9)
N(2A)	1944(2)	2301(5)	3447.4(15)	27.2(9)
C(1A)	2076(3)	3238(6)	1756.9(17)	27.5(11)
C(2A)	2363(3)	3037(6)	1319.7(18)	30.3(11)
C(3A)	3006(3)	1987(6)	1307.5(17)	27.0(11)
C(4A)	3320(3)	1645(6)	842.7(17)	26.5(11)
C(5A)	3617(4)	204(7)	773.8(18)	37.8(13)
C(6A)	3947(4)	-110(7)	347.9(19)	39.2(14)

$C^{(7A)}$	3947(3)	1020(8)	-18.0(19)	42.1(16)
$C^{(8A)}$	3646(3)	2458(8)	49.0(18)	38.5(14)
$C^{(9A)}$	3321(3)	2779(7)	479.0(17)	32.1(12)
$C^{(10A)}$	3328(3)	1243(6)	1757.5(17)	26.6(11)
$C^{(11A)}$	3036(3)	1460(6)	2211.7(17)	23.9(10)
$C^{(12A)}$	3383(3)	689(6)	2678.6(17)	22.3(9)
$C^{(13A)}$	4042(3)	-358(6)	2701.4(17)	27.7(11)
$C^{(14A)}$	4376(3)	-1080(7)	3146.4(18)	30.4(12)
$C^{(15A)}$	4055(3)	-837(6)	3588.6(18)	28.7(11)
$C^{(16A)}$	3409(3)	151(6)	3574.5(17)	27.6(11)
$C^{(17A)}$	3060(3)	921(6)	3127.5(17)	22.7(10)
$C^{(18A)}$	2380(3)	1928(6)	3085.6(17)	23.1(10)
$C^{(19A)}$	2051(3)	2693(6)	2623.8(17)	25.6(10)
$C^{(20A)}$	1376(3)	3550(6)	2699.6(18)	27.2(10)
$C^{(21A)}$	1339(3)	3274(6)	3211.1(18)	25.1(10)
$C^{(22A)}$	745(3)	3945(6)	3486.1(18)	27.7(11)
$C^{(23A)}$	617(3)	3298(7)	3941.0(19)	31.8(12)
$C^{(24A)}$	75(3)	3950(7)	4213(2)	36.9(13)
$C^{(25A)}$	-376(3)	5242(7)	4028(2)	35.3(12)
$C^{(26A)}$	-252(3)	5882(7)	3578(2)	35.0(12)
$C^{(27A)}$	295(3)	5234(6)	3304.2(18)	30.5(11)
$O^{(1)}$	2150(2)	3540(6)	5483.3(15)	45.4(11)
$O^{(1A)}$	2746(3)	2680(5)	4523.6(15)	47.1(11)

Table S25 Anisotropic Displacement Parameters ($Å^2×10^3$) for 13. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
$N^{(1)}$	21.8(19)	28(2)	27.7(19)	-3.2(17)	6.0(15)	0.1(18)
$N^{(2)}$	25(2)	25(2)	31(2)	-2.0(18)	8.8(15)	2.3(19)
$C^{(1)}$	24(2)	34(3)	31(2)	-1(2)	5.7(18)	-1(2)
$C^{(2)}$	26(2)	30(3)	26(2)	-2(2)	4.8(18)	1(2)
$C^{(3)}$	31(2)	27(3)	24(2)	3(2)	7.5(18)	7(2)
$C^{(4)}$	28(2)	36(3)	24(2)	-6(2)	7.7(18)	4(2)
$C^{(5)}$	52(3)	34(3)	29(3)	-4(2)	15(2)	2(3)
$C^{(6)}$	65(4)	39(4)	36(3)	-1(3)	24(3)	-3(3)
$C^{(7)}$	54(4)	46(4)	30(3)	-2(3)	18(2)	3(3)
$C^{(8)}$	28(3)	43(4)	29(2)	-4(2)	5.8(19)	7(3)
$C^{(9)}$	29(2)	29(3)	31(2)	-4(2)	6.6(19)	3(2)
$C^{(10)}$	23(2)	29(3)	30(2)	1(2)	10.1(18)	9(2)
$C^{(11)}$	21(2)	26(3)	29(2)	0(2)	8.3(17)	4(2)
$C^{(12)}$	22(2)	29(3)	28(2)	0(2)	6.1(17)	1(2)
$C^{(13)}$	25(2)	34(3)	29(2)	-3(2)	10.8(17)	2(2)
$C^{(14)}$	23(2)	38(3)	35(3)	-1(2)	8.2(18)	-4(2)
$C^{(15)}$	28(3)	42(3)	29(2)	-8(2)	7.4(19)	-1(2)
$C^{(16)}$	28(2)	32(3)	28(2)	-5(2)	7.7(18)	1(2)

$C^{(17)}$	26(2)	25(3)	30(2)	-4(2)	12.2(18)	1(2)
$C^{(18)}$	26(2)	27(3)	26(2)	-1(2)	9.6(17)	3(2)
$C^{(19)}$	24(2)	35(3)	24(2)	2(2)	7.6(17)	-2(2)
$C^{(20)}$	26(2)	32(3)	31(2)	2(2)	4.1(18)	-4(2)
$C^{(21)}$	23(2)	32(3)	36(3)	5(2)	7.6(19)	-4(2)
$C^{(22)}$	22(2)	39(3)	33(2)	4(2)	7.9(18)	1(2)
$C^{(23)}$	31(3)	36(3)	37(3)	3(2)	13(2)	1(3)
$C^{(24)}$	32(3)	46(4)	41(3)	14(3)	19(2)	11(3)
$C^{(25)}$	24(2)	53(4)	49(3)	13(3)	10(2)	3(3)
$C^{(26)}$	28(3)	44(4)	49(3)	13(3)	5(2)	-6(3)
$C^{(27)}$	26(2)	38(3)	38(3)	7(2)	4.1(19)	3(2)
$N^{(1A)}$	25(2)	33(3)	20.1(18)	2.8(17)	5.7(14)	-1.5(19)
$N^{(2A)}$	25(2)	30(2)	27.3(19)	-1.7(18)	8.6(15)	2.5(19)
$C^{(1A)}$	29(2)	30(3)	23(2)	3(2)	4.8(17)	2(2)
$C^{(2A)}$	29(2)	35(3)	27(2)	8(2)	3.7(18)	-3(2)
$C^{(3A)}$	26(2)	32(3)	23(2)	3(2)	5.7(17)	0(2)
$C^{(4A)}$	23(2)	36(3)	21(2)	4(2)	3.5(16)	-5(2)
$C^{(5A)}$	45(3)	48(4)	22(2)	2(2)	12(2)	-5(3)
$C^{(6A)}$	46(3)	46(4)	30(3)	-2(2)	18(2)	4(3)
$C^{(7A)}$	35(3)	71(5)	22(2)	9(3)	10(2)	2(3)
$C^{(8A)}$	32(3)	61(4)	21(2)	12(3)	0.6(19)	-5(3)
$C^{(9A)}$	24(2)	48(4)	24(2)	6(2)	4.4(18)	-2(2)
$C^{(10A)}$	23(2)	36(3)	21(2)	2(2)	5.2(17)	-2(2)
$C^{(11A)}$	20(2)	25(3)	27(2)	1(2)	4.7(16)	-3(2)
$C^{(12A)}$	21(2)	20(2)	26(2)	1.2(19)	6.2(16)	-4(2)
$C^{(13A)}$	26(2)	32(3)	27(2)	1(2)	9.3(17)	6(2)
$C^{(14A)}$	27(2)	38(3)	28(2)	2(2)	9.8(19)	3(2)
$C^{(15A)}$	26(2)	32(3)	28(2)	5(2)	6.6(18)	0(2)
$C^{(16A)}$	25(2)	32(3)	27(2)	-3(2)	8.2(17)	-3(2)
$C^{(17A)}$	21(2)	22(3)	25(2)	-2.0(19)	5.0(17)	-3(2)
$C^{(18A)}$	21(2)	23(3)	25(2)	4.2(19)	6.8(16)	-1(2)
$C^{(19A)}$	24(2)	30(3)	24(2)	1(2)	8.9(17)	2(2)
$C^{(20A)}$	27(2)	24(3)	30(2)	1(2)	5.8(18)	2(2)
$C^{(21A)}$	23(2)	21(2)	32(2)	-4(2)	8.1(17)	-3(2)
$C^{(22A)}$	21(2)	31(3)	32(2)	-3(2)	6.3(18)	-6(2)
$C^{(23A)}$	29(3)	33(3)	36(3)	-1(2)	13(2)	-2(2)
$C^{(24A)}$	29(3)	50(4)	35(3)	-2(3)	12(2)	-1(3)
$C^{(25A)}$	28(2)	40(3)	42(3)	-12(3)	15(2)	-3(3)
$C^{(26A)}$	25(2)	36(3)	43(3)	-4(2)	5(2)	2(2)
$C^{(27A)}$	26(2)	37(3)	29(2)	-3(2)	6.4(18)	2(2)
$O^{(1)}$	34(2)	62(3)	41(2)	22(2)	9.9(16)	11(2)
$O^{(1A)}$	49(2)	59(3)	33.0(19)	-5.3(19)	8.2(17)	16(2)

Table S26 Bond Lengths for 13.

Atom	Atom	Length/Å	Atom	Atom	Length/Å

$N^{(1)}$	$C^{(1)}$	1.383(6)	$N^{(1A)}$	$C^{(1A)}$	1.369(6)
$N^{(1)}$	$C^{(11)}$	1.384(6)	$N^{(1A)}$	$C^{(11A)}$	1.385(6)
$N^{(1)}$	$C^{(19)}$	1.405(6)	$N^{(1A)}$	$C^{(19A)}$	1.395(6)
$N^{(2)}$	$C^{(18)}$	1.356(6)	$N^{(2A)}$	$C^{(18A)}$	1.363(6)
$N^{(2)}$	$C^{(21)}$	1.370(7)	$N^{(2A)}$	$C^{(21A)}$	1.376(6)
$C^{(1)}$	$C^{(2)}$	1.366(7)	$C^{(1A)}$	$C^{(2A)}$	1.366(7)
$C^{(2)}$	$C^{(3)}$	1.415(7)	$C^{(2A)}$	$C^{(3A)}$	1.416(7)
$C^{(3)}$	$C^{(4)}$	1.483(7)	$C^{(3A)}$	$C^{(4A)}$	1.477(6)
$C^{(3)}$	$C^{(10)}$	1.370(7)	$C^{(3A)}$	$C^{(10A)}$	1.386(7)
$C^{(4)}$	$C^{(5)}$	1.392(8)	$C^{(4A)}$	$C^{(5A)}$	1.378(8)
$C^{(4)}$	$C^{(9)}$	1.400(7)	$C^{(4A)}$	$C^{(9A)}$	1.392(7)
$C^{(5)}$	$C^{(6)}$	1.401(7)	$C^{(5A)}$	$C^{(6A)}$	1.392(7)
$C^{(6)}$	$C^{(7)}$	1.386(8)	$C^{(6A)}$	$C^{(7A)}$	1.394(8)
$C^{(7)}$	$C^{(8)}$	1.389(8)	$C^{(7A)}$	$C^{(8A)}$	1.376(9)
$C^{(8)}$	$C^{(9)}$	1.386(7)	$C^{(8A)}$	$C^{(9A)}$	1.399(7)
$C^{(10)}$	$C^{(11)}$	1.415(7)	$C^{(10A)}$	$C^{(11A)}$	1.414(6)
$C^{(11)}$	$C^{(12)}$	1.437(7)	$C^{(11A)}$	$C^{(12A)}$	1.442(6)
$C^{(12)}$	$C^{(13)}$	1.429(7)	$C^{(12A)}$	$C^{(13A)}$	1.422(7)
$C^{(12)}$	$C^{(17)}$	1.422(7)	$C^{(12A)}$	$C^{(17A)}$	1.430(6)
$C^{(13)}$	$C^{(14)}$	1.365(7)	$C^{(13A)}$	$C^{(14A)}$	1.371(7)
$C^{(14)}$	$C^{(15)}$	1.413(7)	$C^{(14A)}$	$C^{(15A)}$	1.413(7)
$C^{(15)}$	$C^{(16)}$	1.367(7)	$C^{(15A)}$	$C^{(16A)}$	1.375(7)
$C^{(16)}$	$C^{(17)}$	1.409(7)	$C^{(16A)}$	$C^{(17A)}$	1.401(7)
$C^{(17)}$	$C^{(18)}$	1.427(7)	$C^{(17A)}$	$C^{(18A)}$	1.422(7)
$C^{(18)}$	$C^{(19)}$	1.416(7)	$C^{(18A)}$	$C^{(19A)}$	1.422(6)
$C^{(19)}$	$C^{(20)}$	1.411(7)	$C^{(19A)}$	$C^{(20A)}$	1.399(7)
$C^{(20)}$	$C^{(21)}$	1.408(7)	$C^{(20A)}$	$C^{(21A)}$	1.410(7)
$C^{(21)}$	$C^{(22)}$	1.467(7)	$C^{(21A)}$	$C^{(22A)}$	1.469(6)
$C^{(22)}$	$C^{(23)}$	1.390(7)	$C^{(22A)}$	$C^{(23A)}$	1.402(7)
$C^{(22)}$	$C^{(27)}$	1.403(8)	$C^{(22A)}$	$C^{(27A)}$	1.387(7)
$C^{(23)}$	$C^{(24)}$	1.409(7)	$C^{(23A)}$	$C^{(24A)}$	1.390(7)
$C^{(24)}$	$C^{(25)}$	1.392(9)	$C^{(24A)}$	$C^{(25A)}$	1.391(8)
$C^{(25)}$	$C^{(26)}$	1.388(9)	$C^{(25A)}$	$C^{(26A)}$	1.387(8)
$C^{(26)}$	$C^{(27)}$	1.397(7)	$C^{(26A)}$	$C^{(27A)}$	1.399(7)

Table S27 Bond Angles for 13.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
$C^{(1)}$	$N^{(1)}$	$C^{(11)}$	121.2(4)	$C^{(1A)}$	$N^{(1A)}$	$C^{(11A)}$	120.3(4)
$C^{(1)}$	$N^{(1)}$	$C^{(19)}$	119.1(4)	$C^{(1A)}$	$N^{(1A)}$	$C^{(19A)}$	119.6(4)
$C^{(11)}$	$N^{(1)}$	$C^{(19)}$	119.7(4)	$C^{(11A)}$	$N^{(1A)}$	$C^{(19A)}$	120.1(4)
$C^{(18)}$	$N^{(2)}$	$C^{(21)}$	105.5(4)	$C^{(18A)}$	$N^{(2A)}$	$C^{(21A)}$	105.2(4)
$C^{(2)}$	$C^{(1)}$	$N^{(1)}$	120.7(5)	$C^{(2A)}$	$C^{(1A)}$	$N^{(1A)}$	122.6(5)
$C^{(1)}$	$C^{(2)}$	$C^{(3)}$	120.3(5)	$C^{(1A)}$	$C^{(2A)}$	$C^{(3A)}$	119.9(5)
$C^{(2)}$	$C^{(3)}$	$C^{(4)}$	122.0(5)	$C^{(2A)}$	$C^{(3A)}$	$C^{(4A)}$	123.1(4)
$C^{(10)}$	$C^{(3)}$	$C^{(2)}$	117.7(4)	$C^{(10A)}$	$C^{(3A)}$	$C^{(2A)}$	116.6(4)

$C^{(10)}$	$C^{(3)}$	$C^{(4)}$	120.3(5)	$C^{(10A)}$	$C^{(3A)}$	$C^{(4A)}$	120.3(5)
$C^{(5)}$	$C^{(4)}$	$C^{(3)}$	119.6(5)	$C^{(5A)}$	$C^{(4A)}$	$C^{(3A)}$	119.7(5)
$C^{(5)}$	$C^{(4)}$	$C^{(9)}$	119.7(5)	$C^{(5A)}$	$C^{(4A)}$	$C^{(9A)}$	120.3(5)
$C^{(9)}$	$C^{(4)}$	$C^{(3)}$	120.8(5)	$C^{(9A)}$	$C^{(4A)}$	$C^{(3A)}$	120.1(5)
$C^{(4)}$	$C^{(5)}$	$C^{(6)}$	119.7(5)	$C^{(4A)}$	$C^{(5A)}$	$C^{(6A)}$	120.1(5)
$C^{(7)}$	$C^{(6)}$	$C^{(5)}$	120.1(6)	$C^{(5A)}$	$C^{(6A)}$	$C^{(7A)}$	119.8(6)
$C^{(6)}$	$C^{(7)}$	$C^{(8)}$	120.1(5)	$C^{(8A)}$	$C^{(7A)}$	$C^{(6A)}$	120.1(5)
$C^{(9)}$	$C^{(8)}$	$C^{(7)}$	120.1(5)	$C^{(7A)}$	$C^{(8A)}$	$C^{(9A)}$	120.1(5)
$C^{(8)}$	$C^{(9)}$	$C^{(4)}$	120.2(5)	$C^{(4A)}$	$C^{(9A)}$	$C^{(8A)}$	119.6(6)
$C^{(3)}$	$C^{(10)}$	$C^{(11)}$	122.9(5)	$C^{(3A)}$	$C^{(10A)}$	$C^{(11A)}$	123.6(5)
$N^{(1)}$	$C^{(11)}$	$C^{(10)}$	116.9(4)	$N^{(1A)}$	$C^{(11A)}$	$C^{(10A)}$	117.0(4)
$N^{(1)}$	$C^{(11)}$	$C^{(12)}$	120.0(4)	$N^{(1A)}$	$C^{(11A)}$	$C^{(12A)}$	120.1(4)
$C^{(10)}$	$C^{(11)}$	$C^{(12)}$	123.1(5)	$C^{(10A)}$	$C^{(11A)}$	$C^{(12A)}$	122.9(5)
$C^{(13)}$	$C^{(12)}$	$C^{(11)}$	120.7(4)	$C^{(13A)}$	$C^{(12A)}$	$C^{(11A)}$	120.8(4)
$C^{(17)}$	$C^{(12)}$	$C^{(11)}$	121.3(5)	$C^{(13A)}$	$C^{(12A)}$	$C^{(17A)}$	118.1(4)
$C^{(17)}$	$C^{(12)}$	$C^{(13)}$	118.0(5)	$C^{(17A)}$	$C^{(12A)}$	$C^{(11A)}$	121.1(4)
$C^{(14)}$	$C^{(13)}$	$C^{(12)}$	121.0(4)	$C^{(14A)}$	$C^{(13A)}$	$C^{(12A)}$	120.8(4)
$C^{(13)}$	$C^{(14)}$	$C^{(15)}$	120.2(5)	$C^{(13A)}$	$C^{(14A)}$	$C^{(15A)}$	120.7(5)
$C^{(16)}$	$C^{(15)}$	$C^{(14)}$	120.6(5)	$C^{(16A)}$	$C^{(15A)}$	$C^{(14A)}$	119.7(5)
$C^{(15)}$	$C^{(16)}$	$C^{(17)}$	120.4(4)	$C^{(15A)}$	$C^{(16A)}$	$C^{(17A)}$	121.1(4)
$C^{(12)}$	$C^{(17)}$	$C^{(18)}$	117.3(4)	$C^{(16A)}$	$C^{(17A)}$	$C^{(12A)}$	119.7(5)
$C^{(16)}$	$C^{(17)}$	$C^{(12)}$	119.9(5)	$C^{(16A)}$	$C^{(17A)}$	$C^{(18A)}$	123.7(4)
$C^{(16)}$	$C^{(17)}$	$C^{(18)}$	122.9(4)	$C^{(18A)}$	$C^{(17A)}$	$C^{(12A)}$	116.6(4)
$N^{(2)}$	$C^{(18)}$	$C^{(17)}$	129.1(5)	$N^{(2A)}$	$C^{(18A)}$	$C^{(17A)}$	128.3(4)
$N^{(2)}$	$C^{(18)}$	$C^{(19)}$	110.4(5)	$N^{(2A)}$	$C^{(18A)}$	$C^{(19A)}$	110.1(4)
$C^{(19)}$	$C^{(18)}$	$C^{(17)}$	120.5(4)	$C^{(17A)}$	$C^{(18A)}$	$C^{(19A)}$	121.6(4)
$N^{(1)}$	$C^{(19)}$	$C^{(18)}$	121.1(5)	$N^{(1A)}$	$C^{(19A)}$	$C^{(18A)}$	120.4(4)
$N^{(1)}$	$C^{(19)}$	$C^{(20)}$	131.2(5)	$N^{(1A)}$	$C^{(19A)}$	$C^{(20A)}$	131.6(5)
$C^{(20)}$	$C^{(19)}$	$C^{(18)}$	107.7(4)	$C^{(20A)}$	$C^{(19A)}$	$C^{(18A)}$	107.9(4)
$C^{(21)}$	$C^{(20)}$	$C^{(19)}$	103.5(4)	$C^{(19A)}$	$C^{(20A)}$	$C^{(21A)}$	104.0(4)
$N^{(2)}$	$C^{(21)}$	$C^{(20)}$	113.0(4)	$N^{(2A)}$	$C^{(21A)}$	$C^{(20A)}$	112.8(4)
$N^{(2)}$	$C^{(21)}$	$C^{(22)}$	120.5(5)	$N^{(2A)}$	$C^{(21A)}$	$C^{(22A)}$	121.3(4)
$C^{(20)}$	$C^{(21)}$	$C^{(22)}$	126.5(5)	$C^{(20A)}$	$C^{(21A)}$	$C^{(22A)}$	125.9(5)
$C^{(23)}$	$C^{(22)}$	$C^{(21)}$	120.0(5)	$C^{(23A)}$	$C^{(22A)}$	$C^{(21A)}$	120.9(5)
$C^{(23)}$	$C^{(22)}$	$C^{(27)}$	119.2(5)	$C^{(27A)}$	$C^{(22A)}$	$C^{(21A)}$	121.1(5)
$C^{(27)}$	$C^{(22)}$	$C^{(21)}$	120.7(5)	$C^{(27A)}$	$C^{(22A)}$	$C^{(23A)}$	118.1(5)
$C^{(22)}$	$C^{(23)}$	$C^{(24)}$	120.8(6)	$C^{(24A)}$	$C^{(23A)}$	$C^{(22A)}$	121.4(5)
$C^{(25)}$	$C^{(24)}$	$C^{(23)}$	119.6(6)	$C^{(23A)}$	$C^{(24A)}$	$C^{(25A)}$	120.4(5)
$C^{(26)}$	$C^{(25)}$	$C^{(24)}$	119.5(5)	$C^{(26A)}$	$C^{(25A)}$	$C^{(24A)}$	118.4(5)
$C^{(25)}$	$C^{(26)}$	$C^{(27)}$	121.2(6)	$C^{(25A)}$	$C^{(26A)}$	$C^{(27A)}$	121.4(5)
$C^{(26)}$	$C^{(27)}$	$C^{(22)}$	119.6(5)	$C^{(22A)}$	$C^{(27A)}$	$C^{(26A)}$	120.4(5)

Table S28 Torsion Angles for 13.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
$N^{(1)}$	$C^{(1)}$	$C^{(2)}$	$C^{(3)}$	2.1(8)	$N^{(1A)}$	$C^{(1A)}$	$C^{(2A)}$	$C^{(3A)}$	0.4(8)

N(1) C(11) C(12) C(13)	-177.6(5)	N(1A) C(11A) C(12A) C(13A)	179.4(5)
N(1) C(11) C(12) C(17)	0.9(8)	N(1A) C(11A) C(12A) C(17A)	1.0(7)
N(1) C(19) C(20) C(21)	177.4(6)	N(1A) C(19A) C(20A) C(21A)	178.3(6)
N(2) C(18) C(19) N(1)	-177.6(5)	N(2A) C(18A) C(19A) N(1A)	-178.8(5)
N(2) C(18) C(19) C(20)	0.3(6)	N(2A) C(18A) C(19A) C(20A)	-1.1(6)
N(2) C(21) C(22) C(23)	-16.2(8)	N(2A) C(21A) C(22A) C(23A)	-18.8(8)
N(2) C(21) C(22) C(27)	163.3(5)	N(2A) C(21A) C(22A) C(27A)	161.1(5)
C(1) N(1) C(11) C(10)	-4.2(7)	C(1A) N(1A) C(11A) C(10A)	-2.3(7)
C(1) N(1) C(11) C(12)	176.5(5)	C(1A) N(1A) C(11A) C(12A)	177.8(5)
C(1) N(1) C(19) C(18)	-177.7(5)	C(1A) N(1A) C(19A) C(18A)	-178.5(5)
C(1) N(1) C(19) C(20)	5.0(9)	C(1A) N(1A) C(19A) C(20A)	4.4(9)
C(1) C(2) C(3) C(4)	175.7(5)	C(1A) C(2A) C(3A) C(4A)	176.6(5)
C(1) C(2) C(3) C(10)	-4.2(8)	C(1A) C(2A) C(3A) C(10A)	-1.9(8)
C(2) C(3) C(4) C(5)	-143.8(5)	C(2A) C(3A) C(4A) C(5A)	-148.1(5)
C(2) C(3) C(4) C(9)	35.1(8)	C(2A) C(3A) C(4A) C(9A)	32.5(8)
C(2) C(3) C(10) C(11)	2.2(8)	C(2A) C(3A) C(10A) C(11A)	1.4(8)
C(3) C(4) C(5) C(6)	179.9(5)	C(3A) C(4A) C(5A) C(6A)	-177.2(5)
C(3) C(4) C(9) C(8)	178.6(5)	C(3A) C(4A) C(9A) C(8A)	177.8(5)
C(3) C(10) C(11) N(1)	1.9(7)	C(3A) C(10A) C(11A) N(1A)	0.7(8)
C(3) C(10) C(11) C(12)	-178.8(5)	C(3A) C(10A) C(11A) C(12A)	-179.4(5)
C(4) C(3) C(10) C(11)	-177.7(5)	C(4A) C(3A) C(10A) C(11A)	-177.2(5)
C(4) C(5) C(6) C(7)	0.9(10)	C(4A) C(5A) C(6A) C(7A)	-2.4(9)
C(5) C(4) C(9) C(8)	-2.5(8)	C(5A) C(4A) C(9A) C(8A)	-1.6(8)
C(5) C(6) C(7) C(8)	-1.4(10)	C(5A) C(6A) C(7A) C(8A)	2.0(9)
C(6) C(7) C(8) C(9)	-0.1(9)	C(6A) C(7A) C(8A) C(9A)	-1.5(9)
C(7) C(8) C(9) C(4)	2.1(8)	C(7A) C(8A) C(9A) C(4A)	1.3(8)
C(9) C(4) C(5) C(6)	1.0(9)	C(9A) C(4A) C(5A) C(6A)	2.2(8)
C(10) C(3) C(4) C(5)	36.2(7)	C(10A) C(3A) C(4A) C(5A)	30.4(7)
C(10) C(3) C(4) C(9)	-145.0(5)	C(10A) C(3A) C(4A) C(9A)	-149.0(5)
C(10) C(11) C(12) C(13)	3.1(8)	C(10A) C(11A) C(12A) C(13A)	-0.6(7)
C(10) C(11) C(12) C(17)	-178.4(5)	C(10A) C(11A) C(12A) C(17A)	-178.9(5)
C(11) N(1) C(1) C(2)	2.3(8)	C(11A) N(1A) C(1A) C(2A)	1.8(8)
C(11) N(1) C(19) C(18)	1.8(8)	C(11A) N(1A) C(19A) C(18A)	1.6(7)
C(11) N(1) C(19) C(20)	-175.6(5)	C(11A) N(1A) C(19A) C(20A)	-175.5(5)
C(11) C(12) C(13) C(14)	177.9(5)	C(11A) C(12A) C(13A) C(14A)	179.4(5)
C(11) C(12) C(17) C(16)	-178.3(5)	C(11A) C(12A) C(17A) C(16A)	179.8(5)
C(11) C(12) C(17) C(18)	2.3(8)	C(11A) C(12A) C(17A) C(18A)	0.8(7)
C(12) C(13) C(14) C(15)	0.1(8)	C(12A) C(13A) C(14A) C(15A)	2.0(8)
C(12) C(17) C(18) N(2)	175.5(5)	C(12A) C(17A) C(18A) N(2A)	177.5(5)
C(12) C(17) C(18) C(19)	-3.5(8)	C(12A) C(17A) C(18A) C(19A)	-1.5(7)
C(13) C(12) C(17) C(16)	0.2(8)	C(13A) C(12A) C(17A) C(16A)	1.5(7)
C(13) C(12) C(17) C(18)	-179.2(5)	C(13A) C(12A) C(17A) C(18A)	-177.5(4)
C(13) C(14) C(15) C(16)	0.9(9)	C(13A) C(14A) C(15A) C(16A)	-0.9(8)
C(14) C(15) C(16) C(17)	-1.3(9)	C(14A) C(15A) C(16A) C(17A)	0.2(8)
C(15) C(16) C(17) C(12)	0.7(8)	C(15A) C(16A) C(17A) C(12A)	-0.5(8)
C(15) C(16) C(17) C(18)	-179.9(5)	C(15A) C(16A) C(17A) C(18A)	178.5(5)
C(16) C(17) C(18) N(2)	-3.8(9)	C(16A) C(17A) C(18A) N(2A)	-1.5(8)

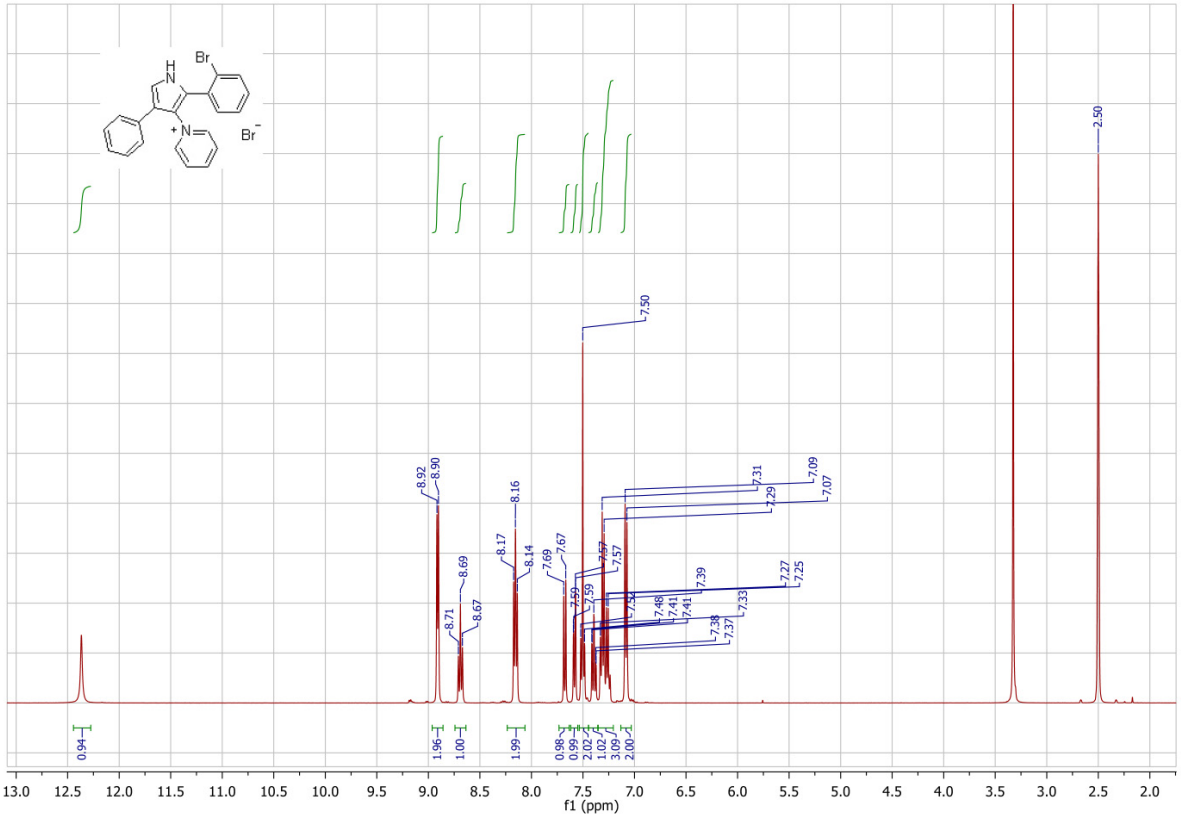
$C^{(16)}C^{(17)}C^{(18)}C^{(19)}$	177.2(5)	$C^{(16A)}C^{(17A)}C^{(18A)}C^{(19A)}$	179.6(5)
$C^{(17)}C^{(12)}C^{(13)}C^{(14)}$	-0.6(8)	$C^{(17A)}C^{(12A)}C^{(13A)}C^{(14A)}$	-2.2(8)
$C^{(17)}C^{(18)}C^{(19)}N^{(1)}$	1.5(8)	$C^{(17A)}C^{(18A)}C^{(19A)}N^{(1A)}$	0.3(8)
$C^{(17)}C^{(18)}C^{(19)}C^{(20)}$	179.4(5)	$C^{(17A)}C^{(18A)}C^{(19A)}C^{(20A)}$	178.0(5)
$C^{(18)}N^{(2)}C^{(21)}C^{(20)}$	-0.1(6)	$C^{(18A)}N^{(2A)}C^{(21A)}C^{(20A)}$	-0.3(6)
$C^{(18)}N^{(2)}C^{(21)}C^{(22)}$	-179.7(5)	$C^{(18A)}N^{(2A)}C^{(21A)}C^{(22A)}$	-179.1(5)
$C^{(18)}C^{(19)}C^{(20)}C^{(21)}$	-0.3(6)	$C^{(18A)}C^{(19A)}C^{(20A)}C^{(21A)}$	0.9(6)
$C^{(19)}N^{(1)}C^{(1)}C^{(2)}$	-178.3(5)	$C^{(19A)}N^{(1A)}C^{(1A)}C^{(2A)}$	-178.1(5)
$C^{(19)}N^{(1)}C^{(11)}C^{(10)}$	176.4(5)	$C^{(19A)}N^{(1A)}C^{(11A)}C^{(10A)}$	177.7(5)
$C^{(19)}N^{(1)}C^{(11)}C^{(12)}$	-2.9(7)	$C^{(19A)}N^{(1A)}C^{(11A)}C^{(12A)}$	-2.3(7)
$C^{(19)}C^{(20)}C^{(21)}N^{(2)}$	0.2(6)	$C^{(19A)}C^{(20A)}C^{(21A)}N^{(2A)}$	-0.4(6)
$C^{(19)}C^{(20)}C^{(21)}C^{(22)}$	179.8(5)	$C^{(19A)}C^{(20A)}C^{(21A)}C^{(22A)}$	178.4(5)
$C^{(20)}C^{(21)}C^{(22)}C^{(23)}$	164.2(5)	$C^{(20A)}C^{(21A)}C^{(22A)}C^{(23A)}$	162.5(5)
$C^{(20)}C^{(21)}C^{(22)}C^{(27)}$	-16.2(9)	$C^{(20A)}C^{(21A)}C^{(22A)}C^{(27A)}$	-17.6(8)
$C^{(21)}N^{(2)}C^{(18)}C^{(17)}$	-179.2(5)	$C^{(21A)}N^{(2A)}C^{(18A)}C^{(17A)}$	-178.2(5)
$C^{(21)}N^{(2)}C^{(18)}C^{(19)}$	-0.1(6)	$C^{(21A)}N^{(2A)}C^{(18A)}C^{(19A)}$	0.8(6)
$C^{(21)}C^{(22)}C^{(23)}C^{(24)}$	179.0(5)	$C^{(21A)}C^{(22A)}C^{(23A)}C^{(24A)}$	177.9(5)
$C^{(21)}C^{(22)}C^{(27)}C^{(26)}$	-178.4(5)	$C^{(21A)}C^{(22A)}C^{(27A)}C^{(26A)}$	-178.3(5)
$C^{(22)}C^{(23)}C^{(24)}C^{(25)}$	-0.2(8)	$C^{(22A)}C^{(23A)}C^{(24A)}C^{(25A)}$	2.2(8)
$C^{(23)}C^{(22)}C^{(27)}C^{(26)}$	1.1(8)	$C^{(23A)}C^{(22A)}C^{(27A)}C^{(26A)}$	1.6(8)
$C^{(23)}C^{(24)}C^{(25)}C^{(26)}$	0.3(8)	$C^{(23A)}C^{(24A)}C^{(25A)}C^{(26A)}$	-2.0(8)
$C^{(24)}C^{(25)}C^{(26)}C^{(27)}$	0.4(9)	$C^{(24A)}C^{(25A)}C^{(26A)}C^{(27A)}$	1.7(8)
$C^{(25)}C^{(26)}C^{(27)}C^{(22)}$	-1.1(8)	$C^{(25A)}C^{(26A)}C^{(27A)}C^{(22A)}$	-1.5(8)
$C^{(27)}C^{(22)}C^{(23)}C^{(24)}$	-0.5(8)	$C^{(27A)}C^{(22A)}C^{(23A)}C^{(24A)}$	-2.0(8)

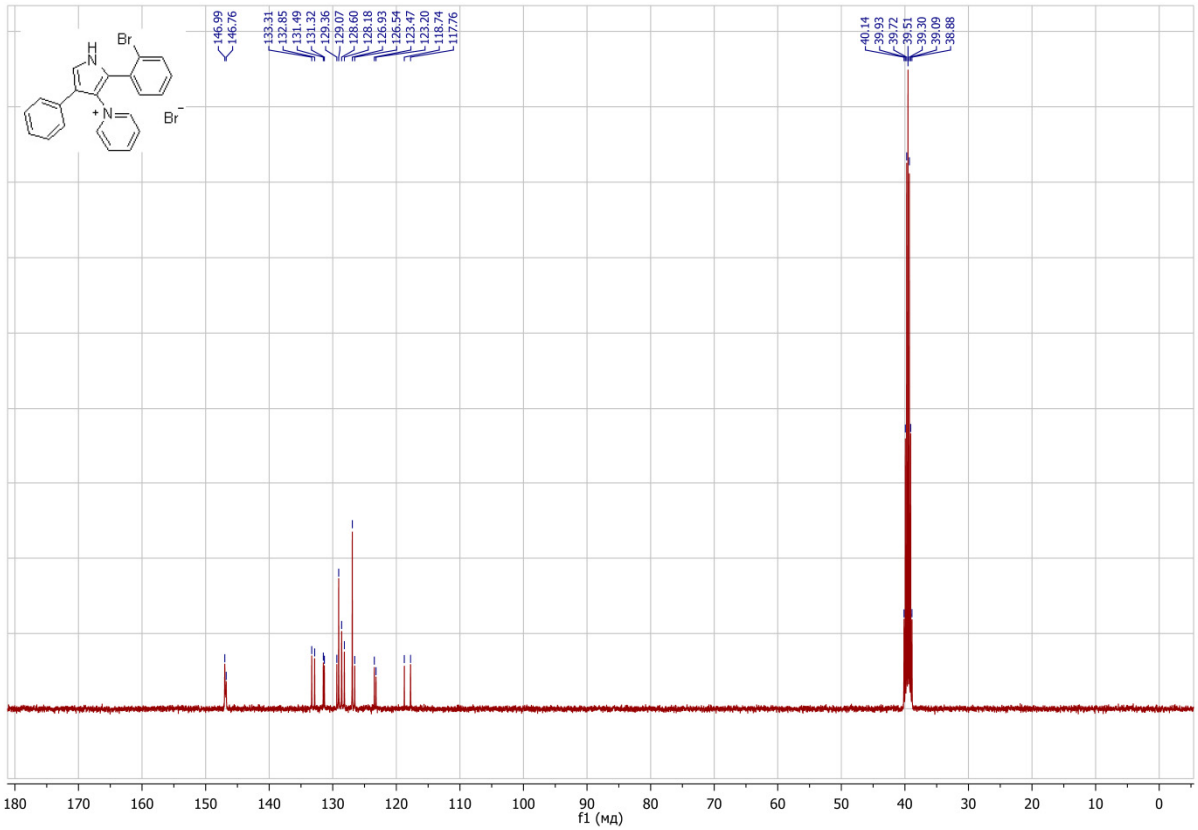
Table S29 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 13.

Atom	*x*	*y*	*z*	U(eq)
$H^{(1)}$	3360	4730	8201	36
$H^{(2)}$	2850	4388	8924	33
$H^{(5)}$	1564	85	8991	44
$H^{(6)}$	1104	-474	9736	54
$H^{(7)}$	963	1468	10298	50
$H^{(8)}$	1324	3958	10138	40
$H^{(9)}$	1835	4508	9418	36
$H^{(10)}$	1290	1249	8212	32
$H^{(13)}$	750	229	7548	34
$H^{(14)}$	172	-932	6802	38
$H^{(15)}$	687	-474	6068	39
$H^{(16)}$	1798	1087	6092	35
$H^{(20)}$	3975	4944	7486	36
$H^{(23)}$	4070	3104	5896	41
$H^{(24)}$	5001	4106	5437	45
$H^{(25)}$	5765	6266	5736	50
$H^{(26)}$	5600	7391	6487	49

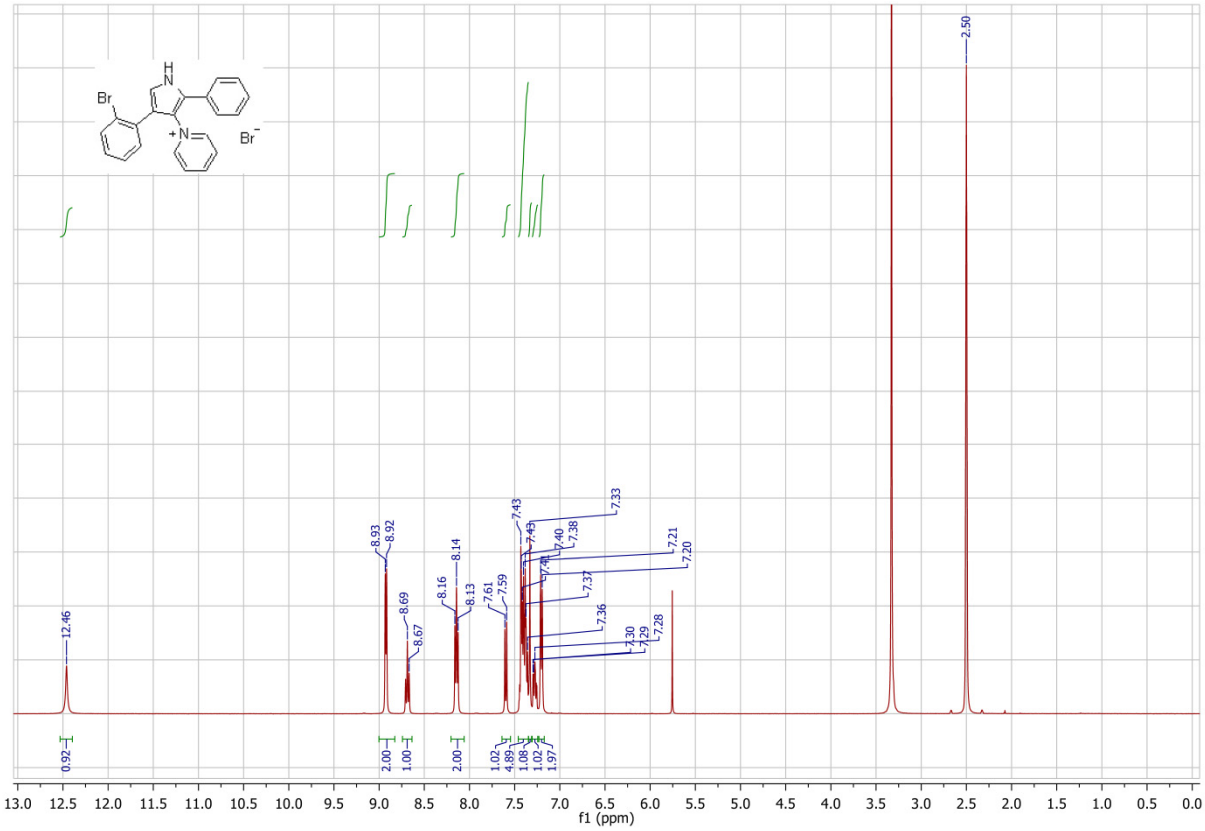
$H^{(27)}$	4694	6377	6954	41
$H^{(1A)}$	1651	3928	1757	33
$H^{(2A)}$	2137	3589	1030	36
$H^{(5A)}$	3598	-560	1012	45
$H^{(6A)}$	4166	-1072	307	47
$H^{(7A)}$	4152	802	-308	51
$H^{(8A)}$	3659	3217	-192	46
$H^{(9A)}$	3108	3744	522	38
$H^{(10A)}$	3758	564	1761	32
$H^{(13A)}$	4249	-555	2411	33
$H^{(14A)}$	4818	-1737	3157	36
$H^{(15A)}$	4280	-1343	3888	34
$H^{(16A)}$	3200	311	3866	33
$H^{(20A)}$	1031	4159	2467	33
$H^{(23A)}$	899	2414	4064	38
$H^{(24A)}$	14	3521	4520	44
$H^{(25A)}$	-752	5665	4203	42
$H^{(26A)}$	-539	6761	3455	42
$H^{(27A)}$	358	5671	2999	37
$H^{(1B)}$	2297	2920	5275	68
$H^{(1C)}$	2469	3456	5770	68
$H^{(1AA)}$	2607	2599	4204	71
$H^{(1AB)}$	2892	3597	4601	71

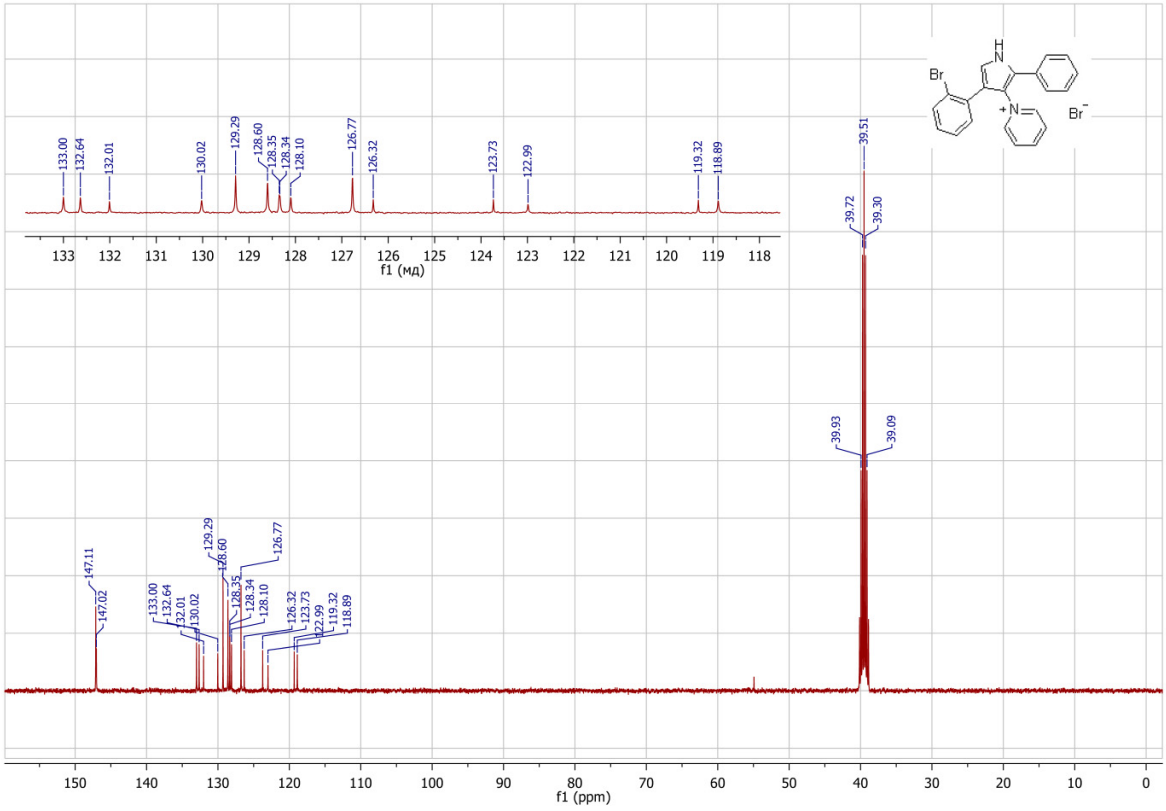
1-(2-(2-Bromophenyl)-4-phenyl-1*H*-pyrrol-3-yl)pyridin-1-ium bromide **(3a)**, DMSO-d_6



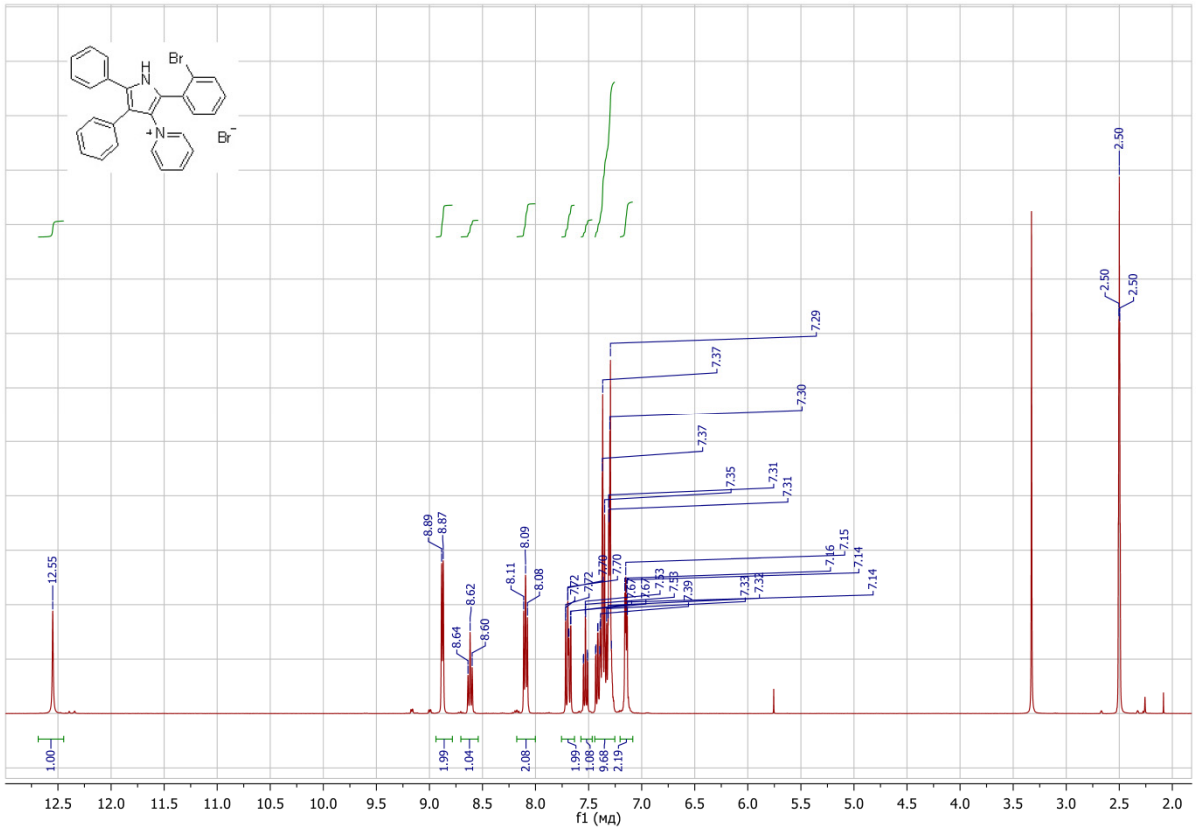


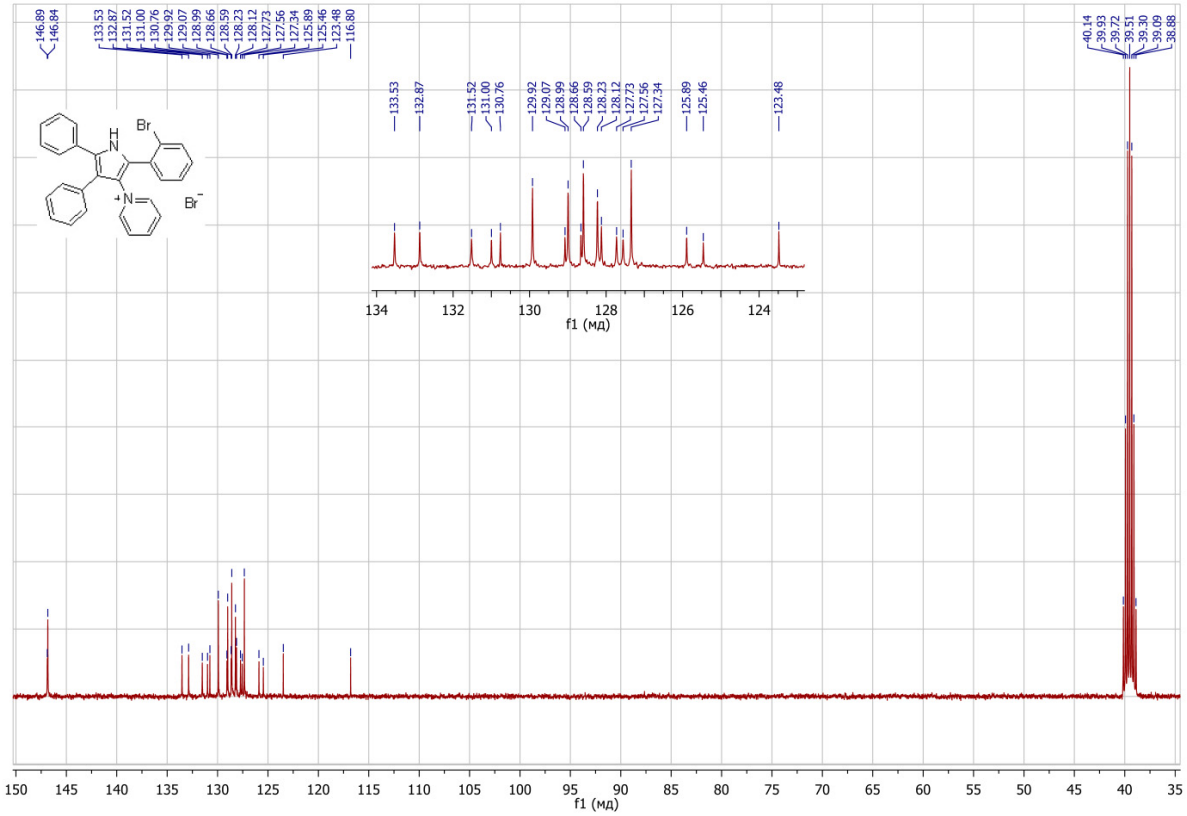
1-(4-(2-Bromophenyl)-2-phenyl-1*H*-pyrrol-3-yl)pyridin-1-ium bromide **(3b)**, DMSO-d_6



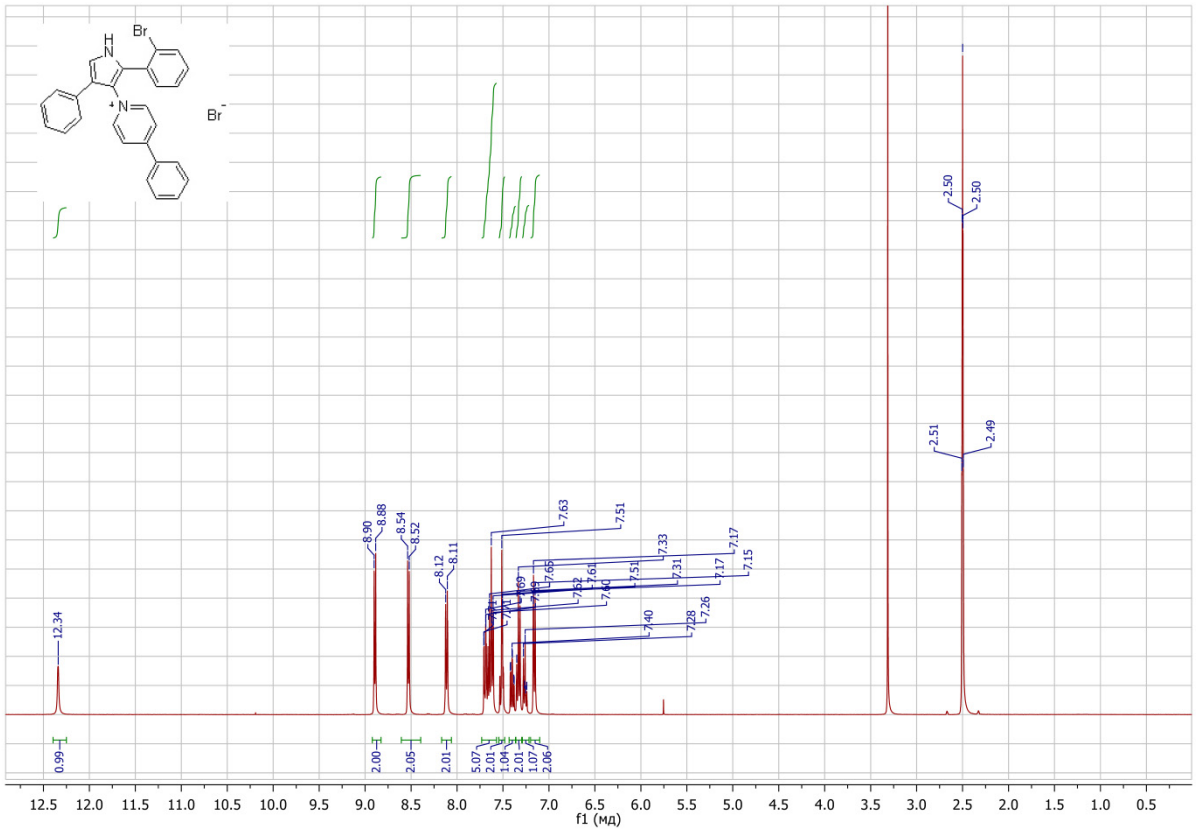


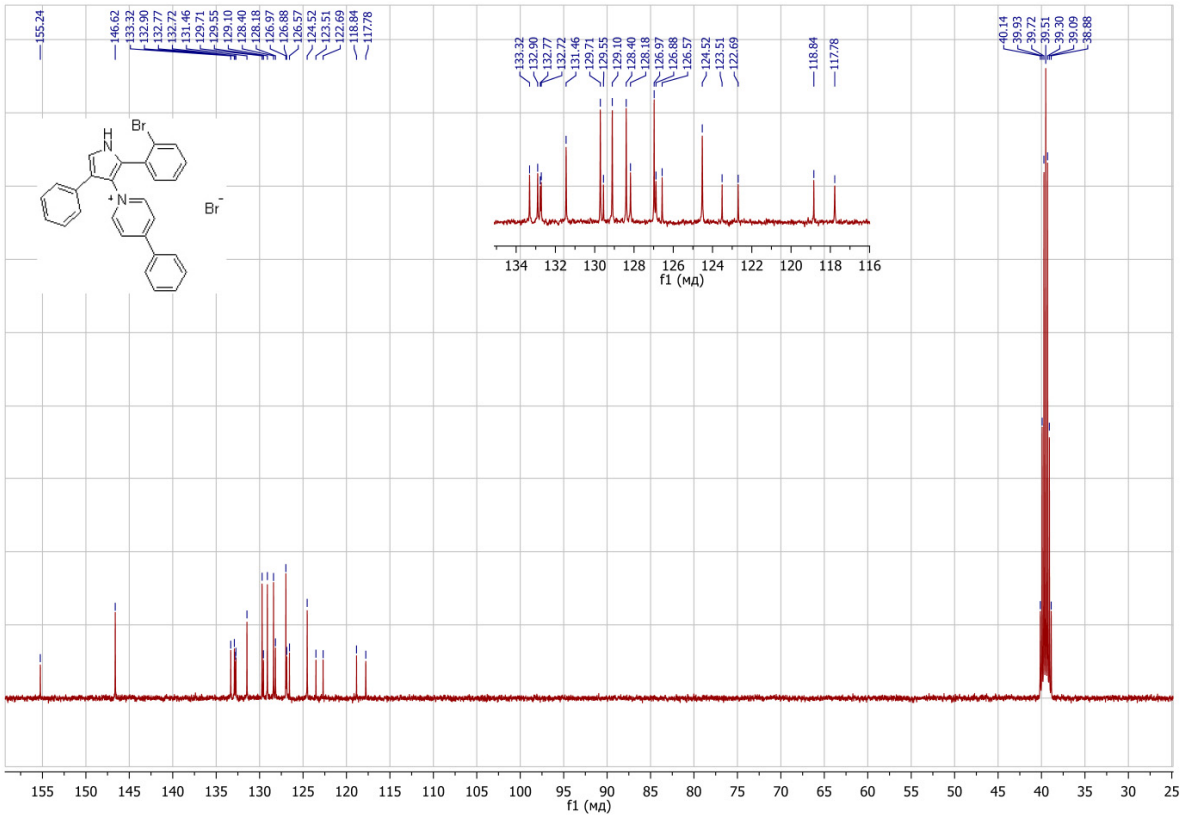
1-(2-(2-Bromophenyl)-4,5-diphenyl-1*H*-pyrrol-3-yl)pyridin-1-ium bromide **(3c)**, DMSO-d_6



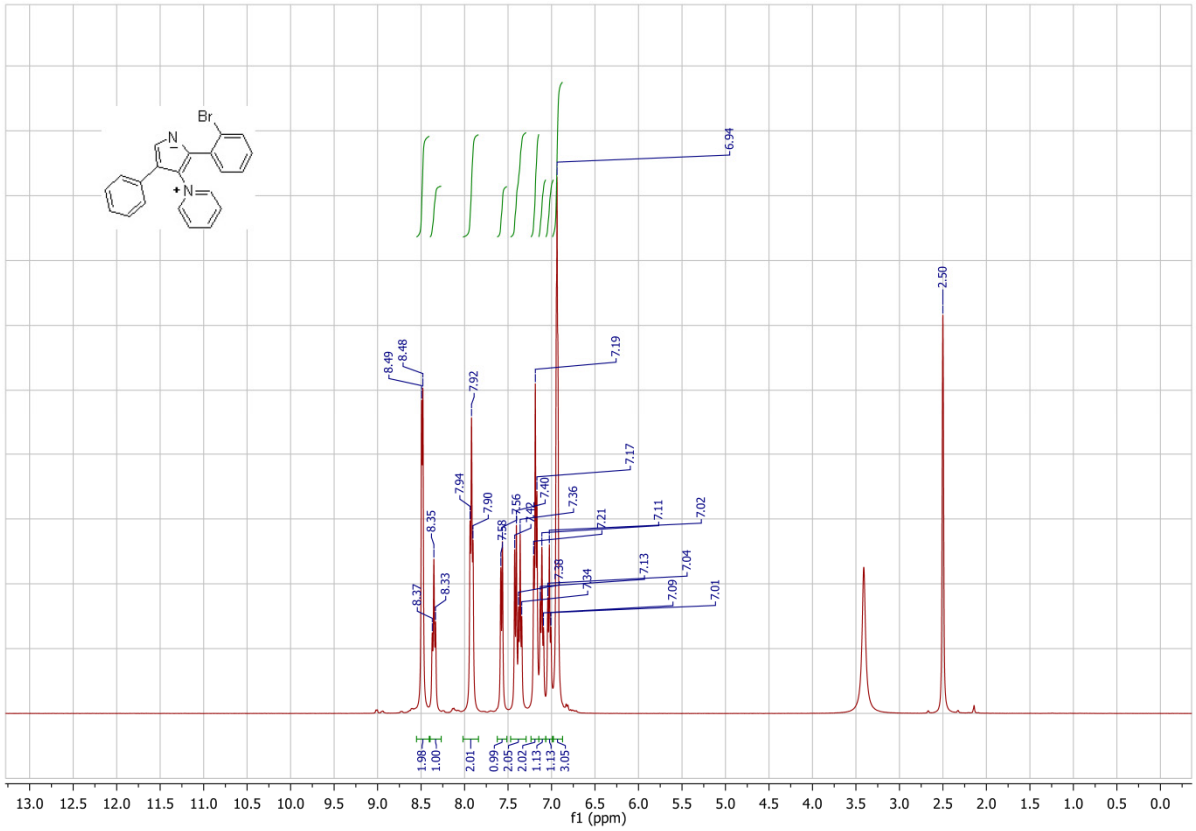


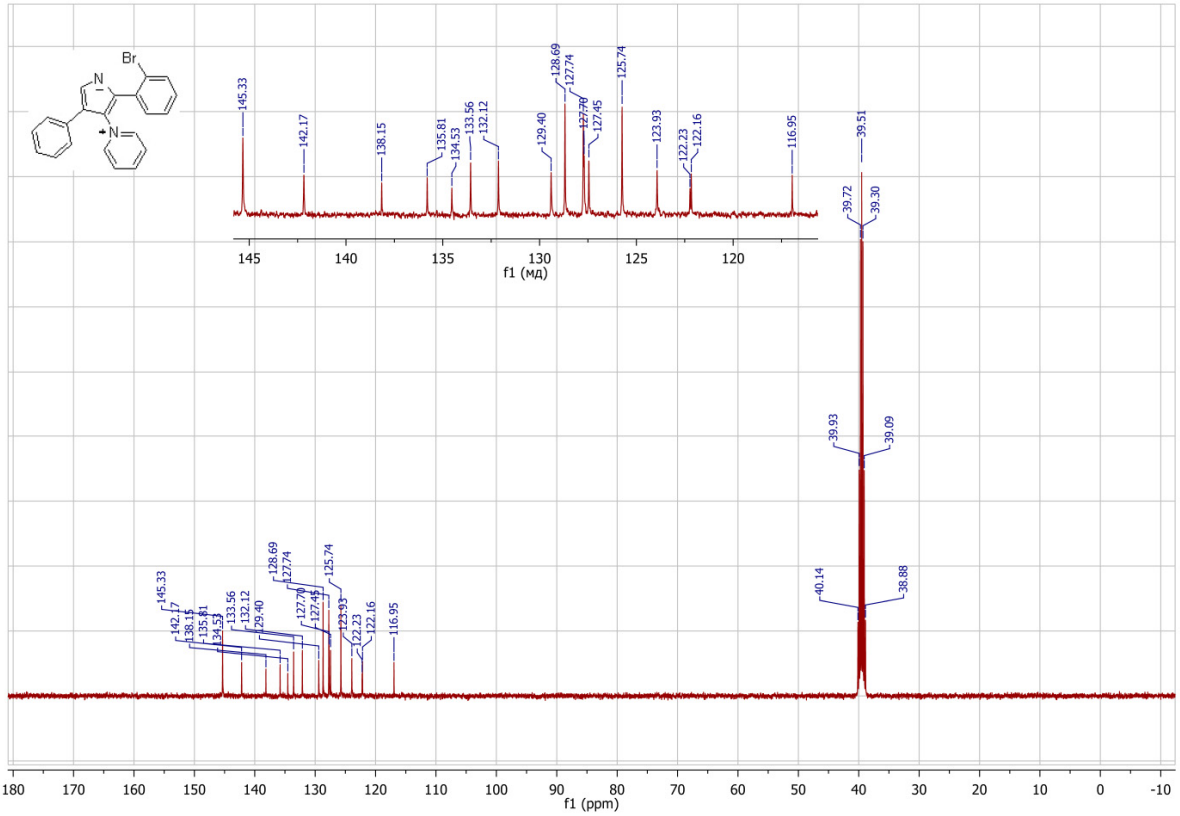
1-(2-(2-Bromophenyl)-4-phenyl-1*H*-pyrrol-3-yl)-4-phenylpyridin-1-ium bromide **(3d)**, DMSO-d_6



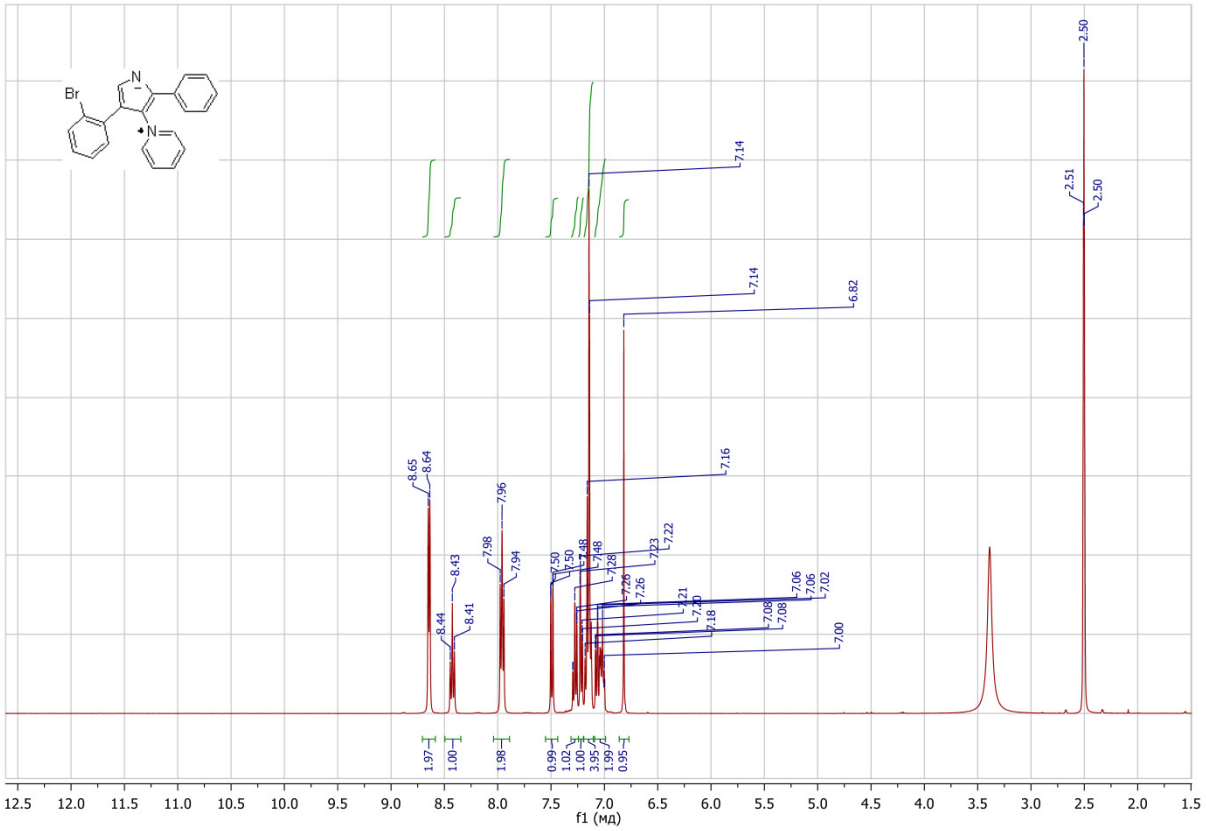


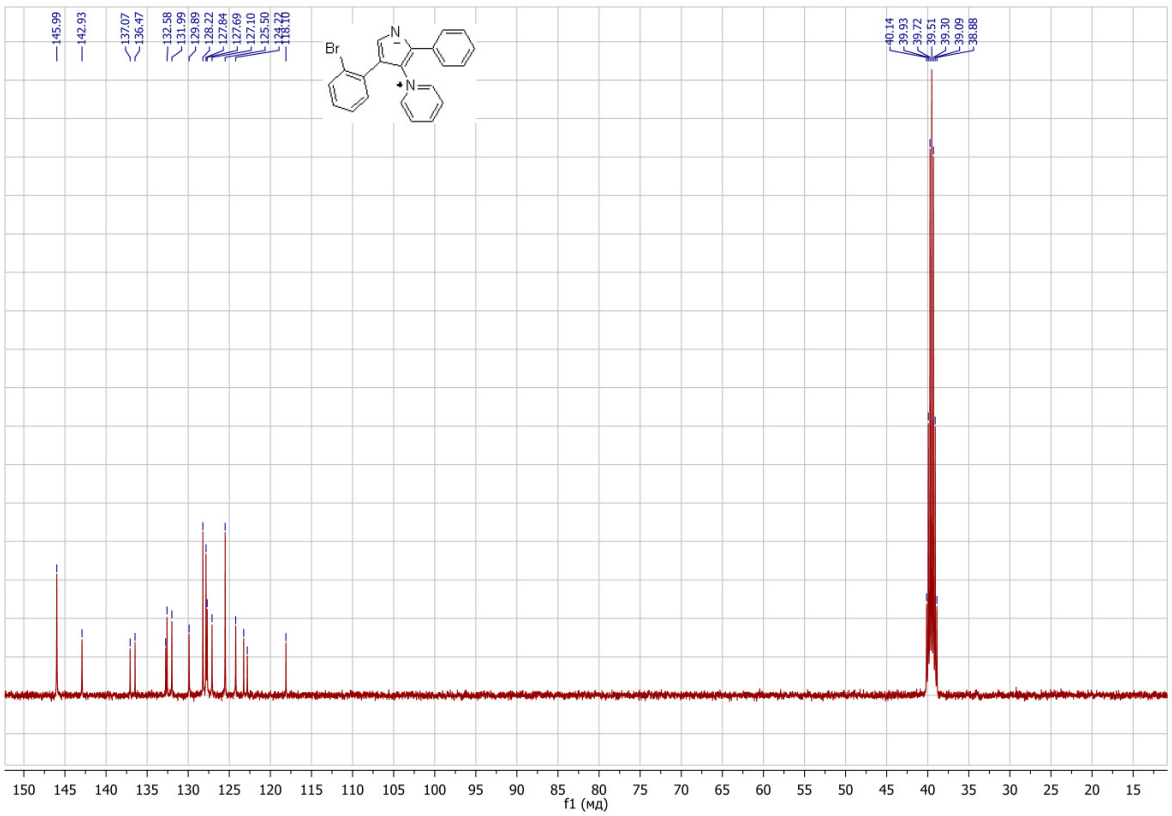
2-(2-Bromophenyl)-4-phenyl-3-(pyridin-1-ium-1-yl)pyrrol-1-ide **(4a)**, DMSO-d_6



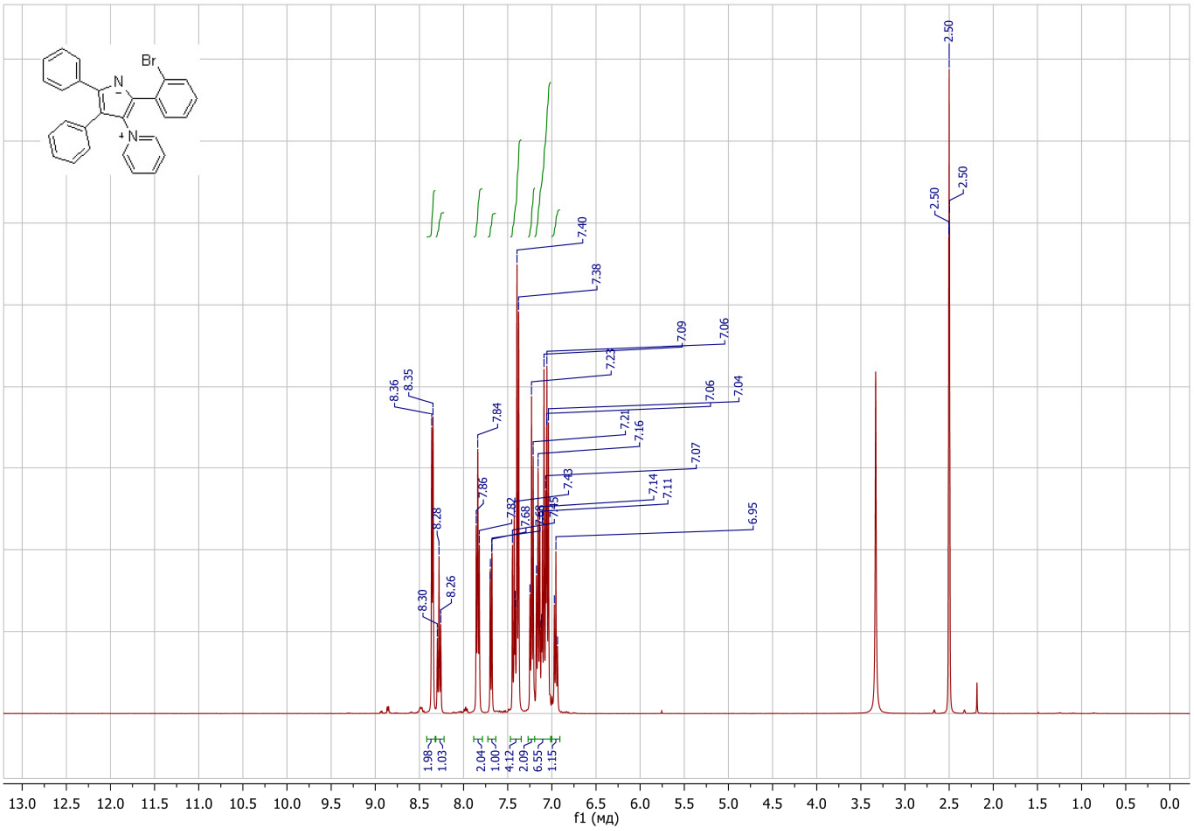


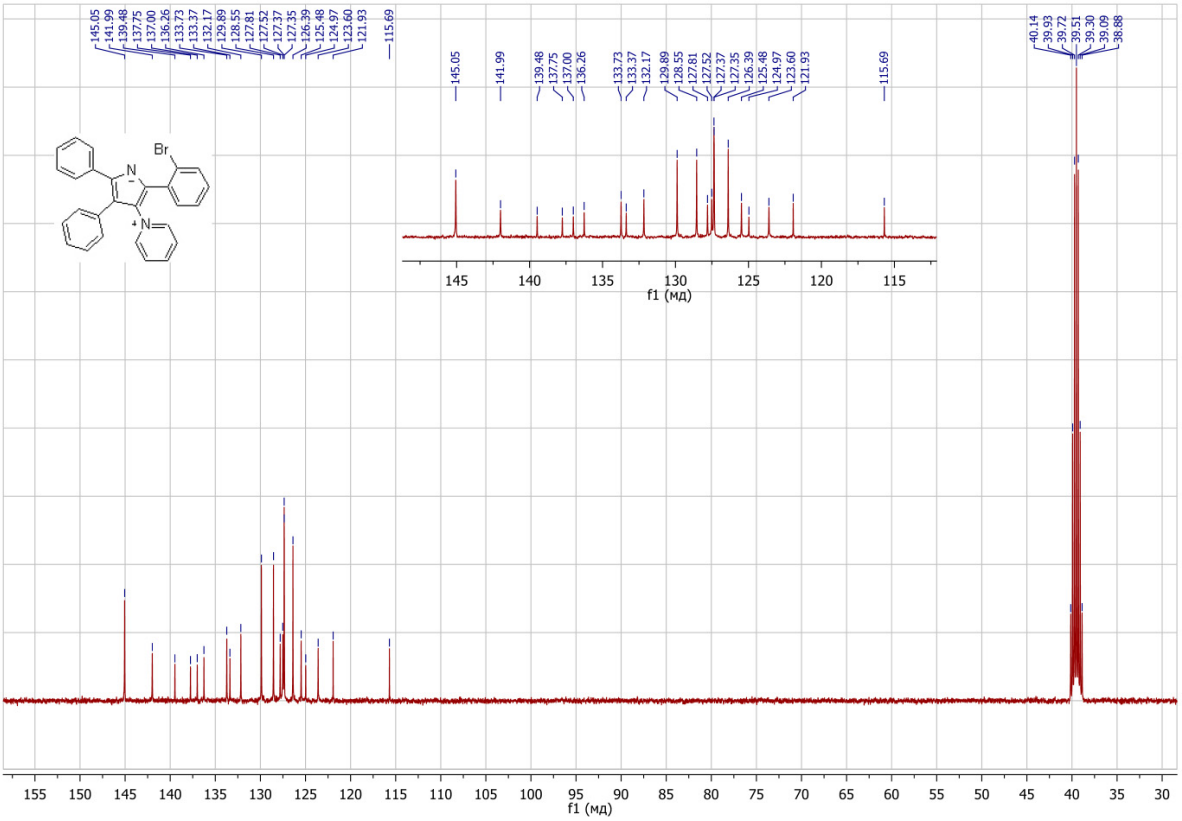
4-(2-Bromophenyl)-2-phenyl-3-(pyridin-1-ium-1-yl)pyrrol-1-ide **(4b)**, DMSO-d_6



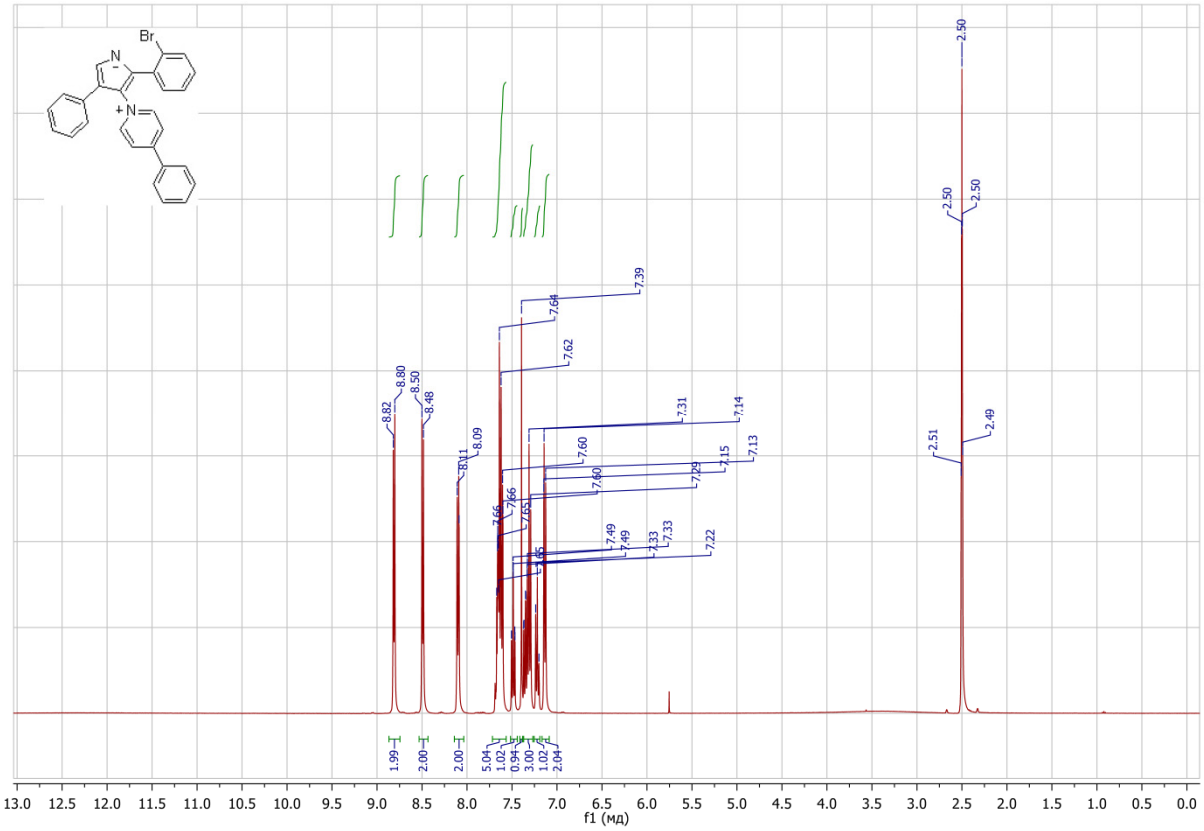


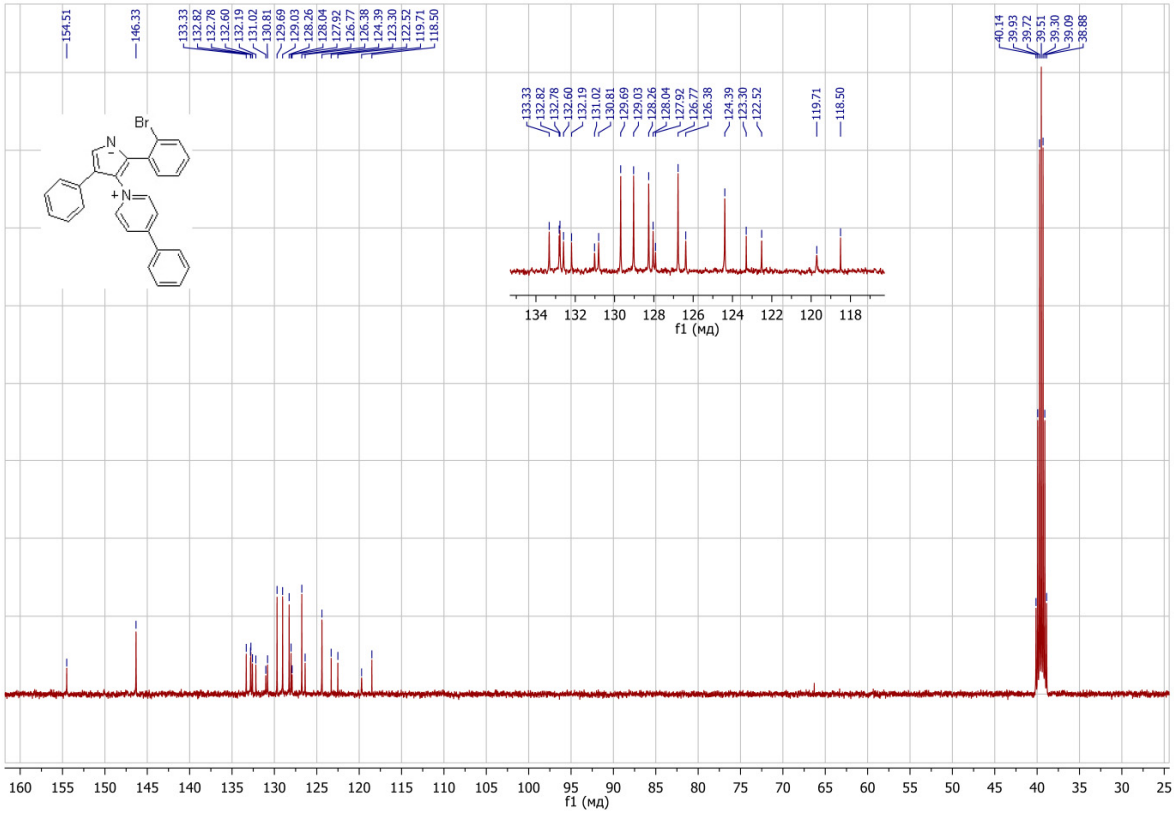
2-(2-Bromophenyl)-4,5-diphenyl-3-(pyridin-1-ium-1-yl)pyrrol-1-ide **(4c)**, DMSO-d_6



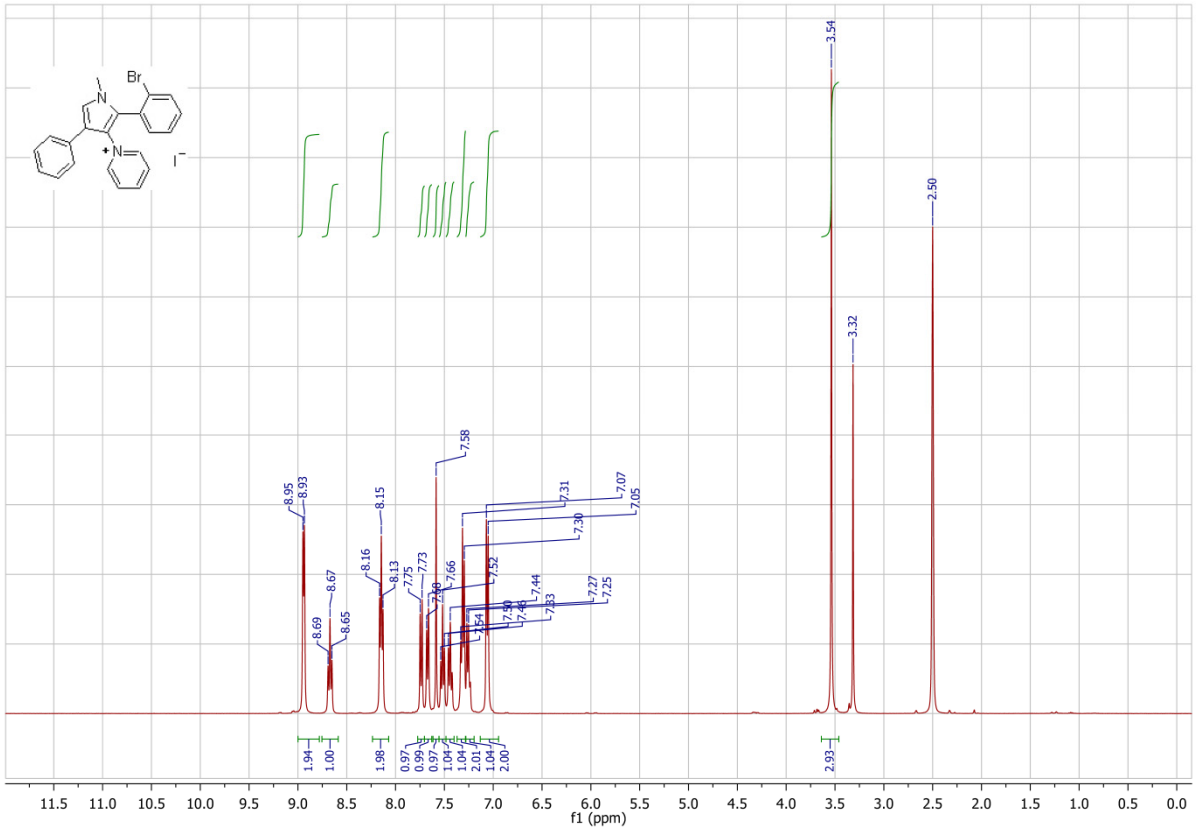


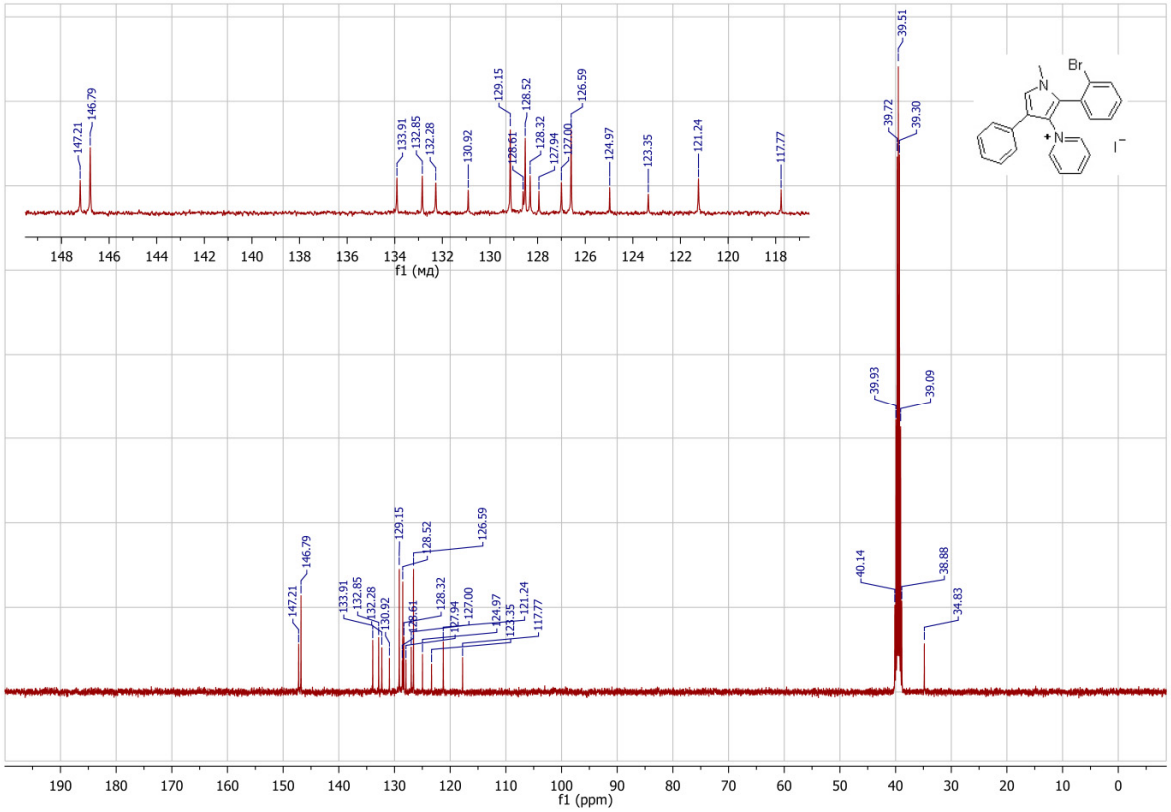
2-(2-Bromophenyl)-4-phenyl-3-(4-phenylpyridin-1-ium-1-yl)pyrrol-1-ide **(4d)**, DMSO-d_6





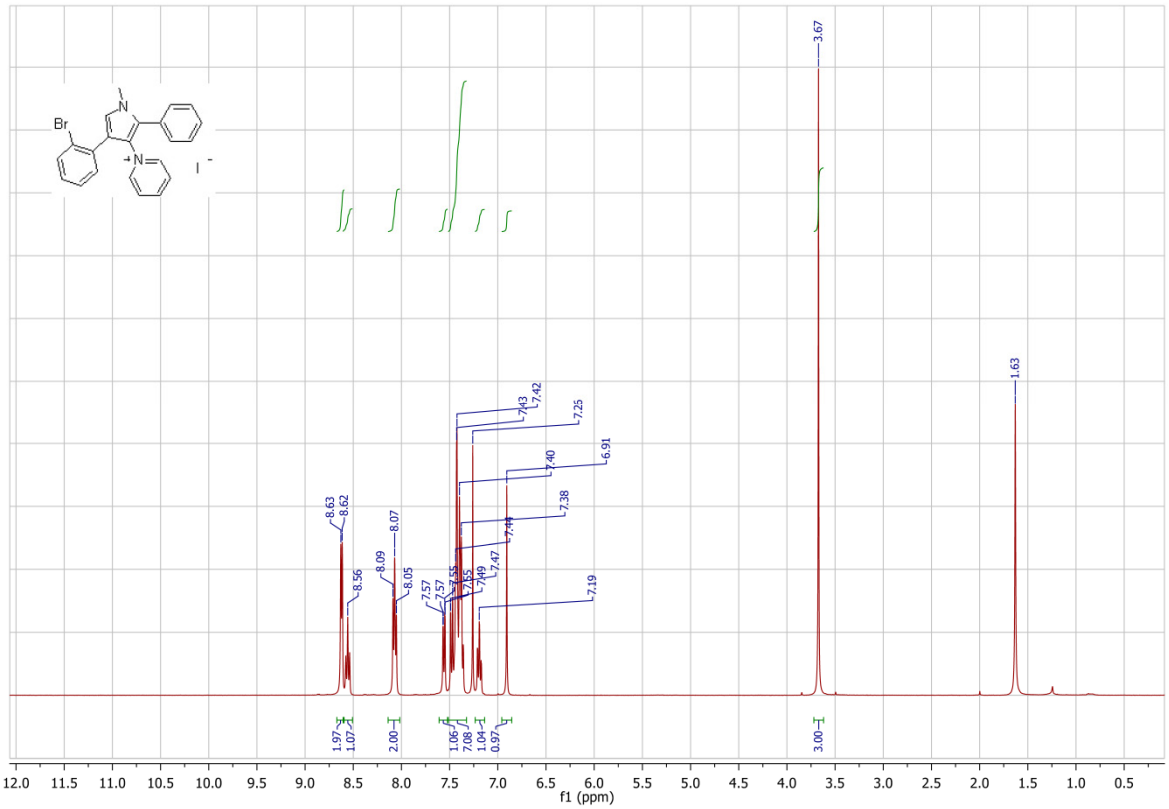
1-(2-(2-Bromophenyl)-1-methyl-4-phenyl-1*H*-pyrrol-3-yl)pyridin-1-ium iodide **(5a)**, DMSO-d_6

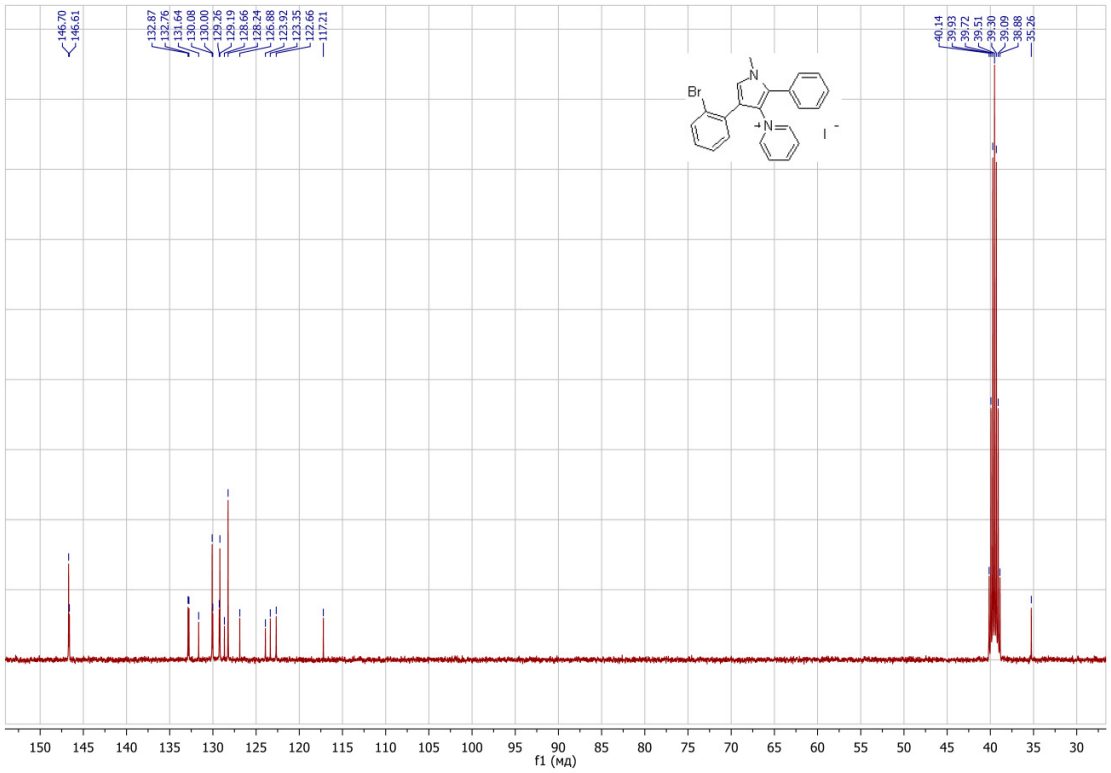




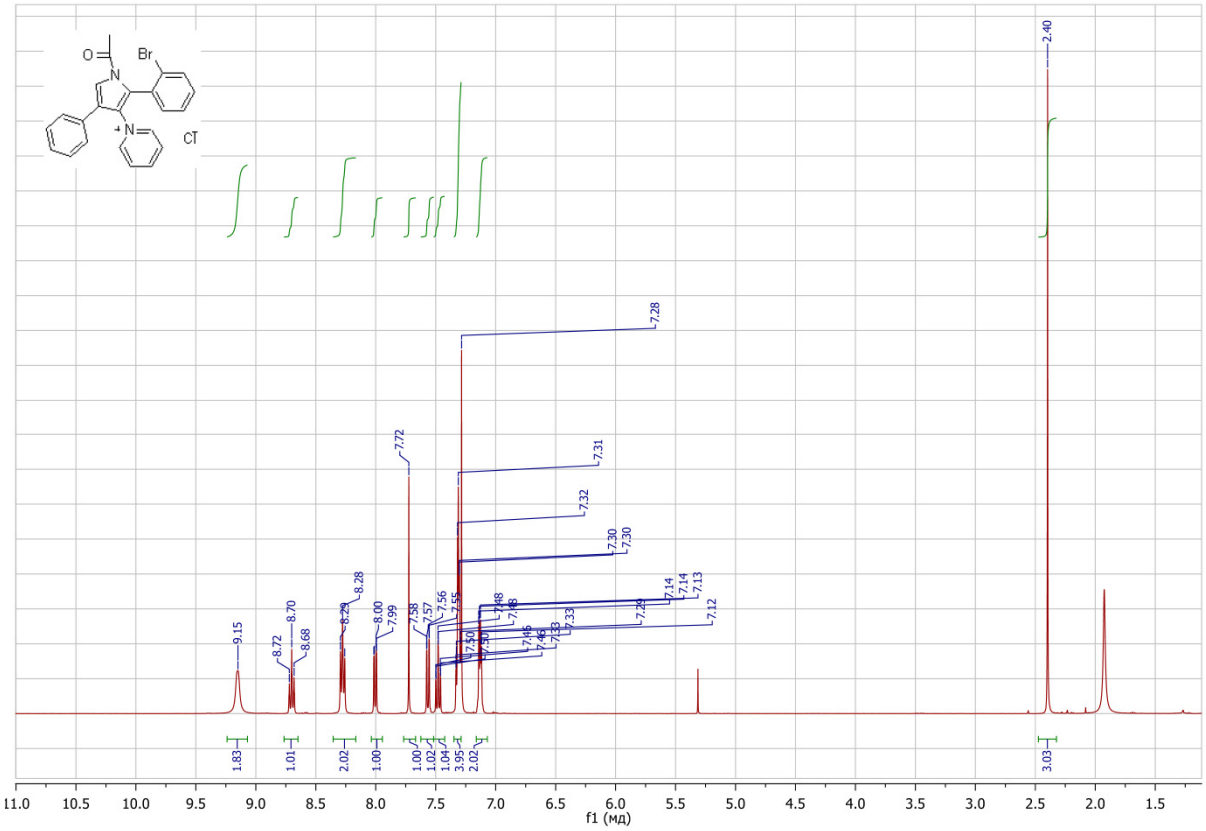
1-(4-(2-Bromophenyl)-1-methyl-2-phenyl-1*H*-pyrrol-3-yl)pyridin-1-ium iodide **(5b)**,

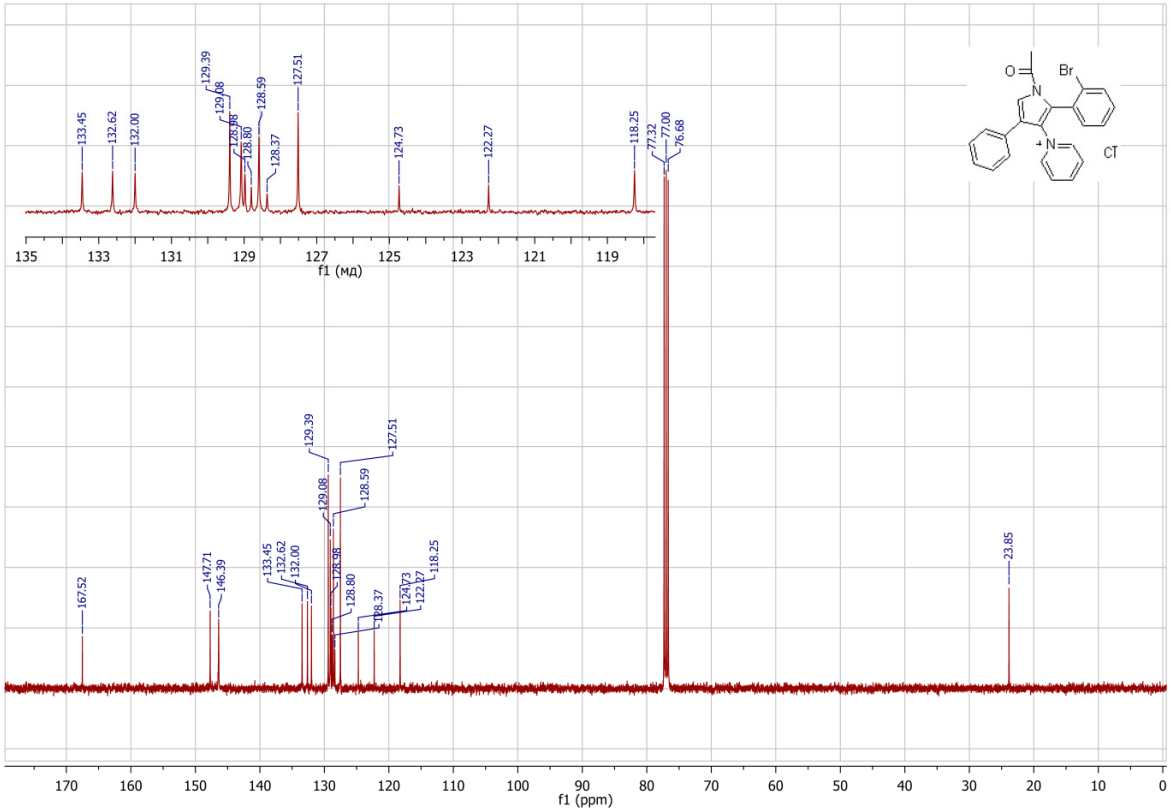
^{1}H NMR ($CDCl_3$), ^{13}C NMR (DMSO-d_6)



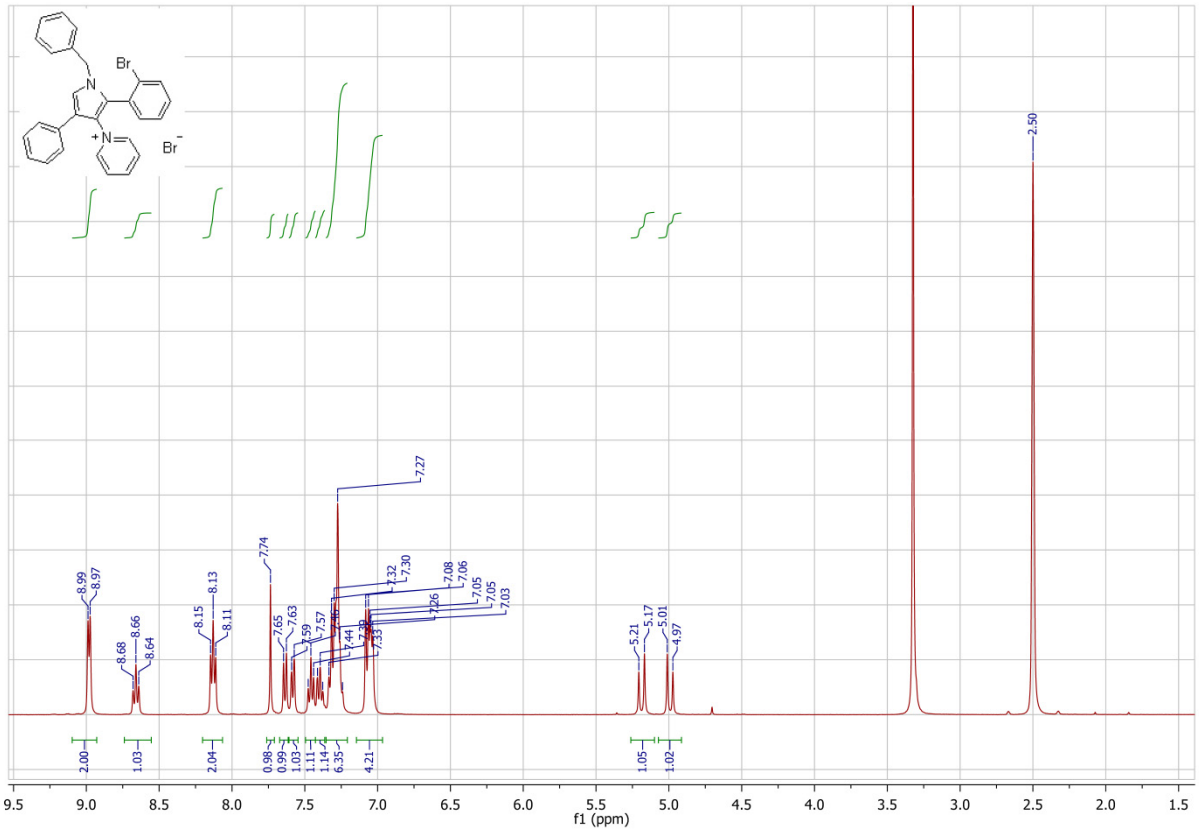


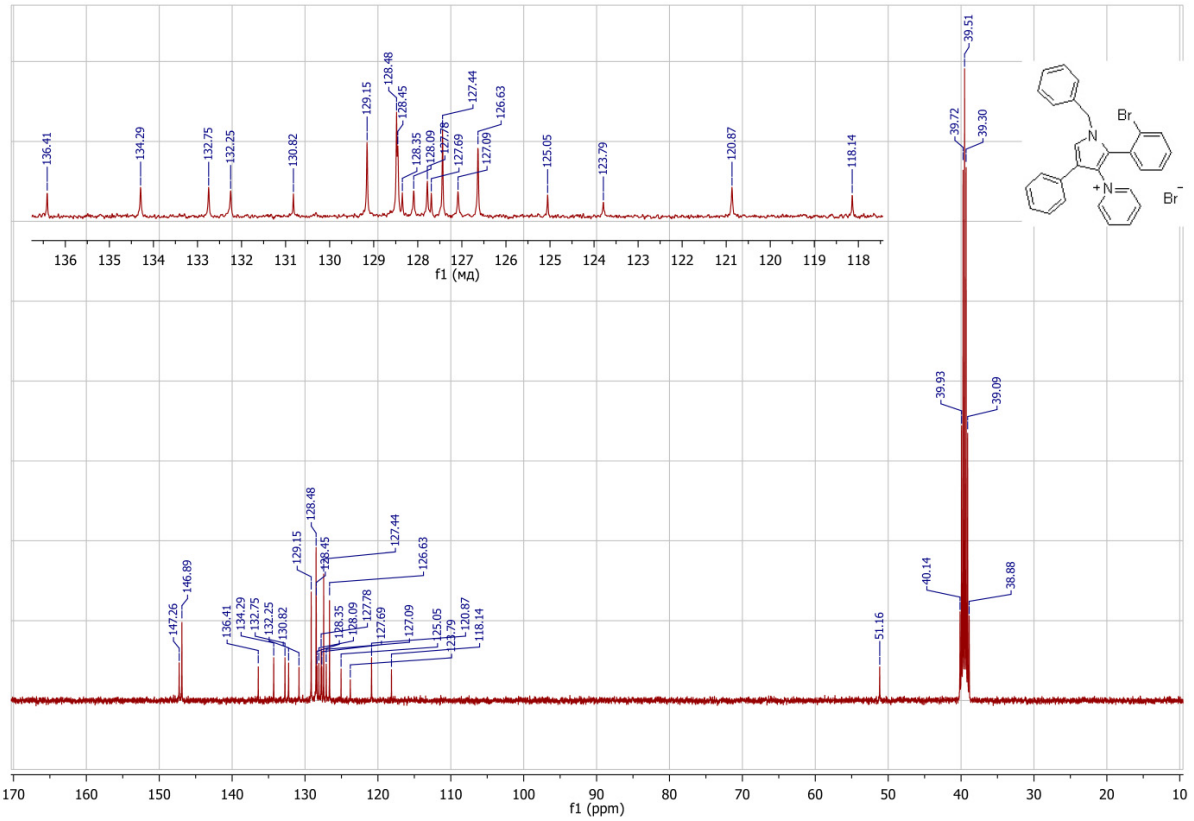
1-(1-Acetyl-2-(2-bromophenyl)-4-phenyl-1*H*-pyrrol-3-yl)pyridin-1-ium chloride **(6)**, $CDCl_3$



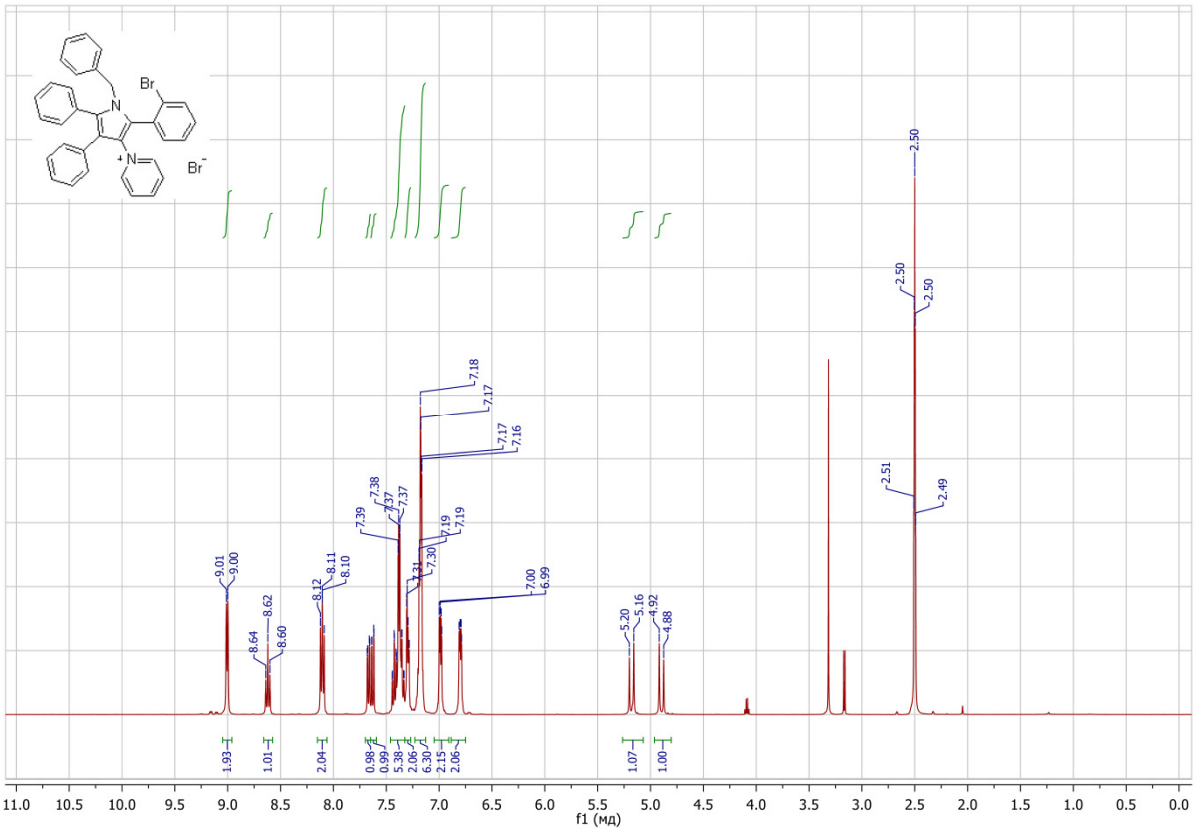


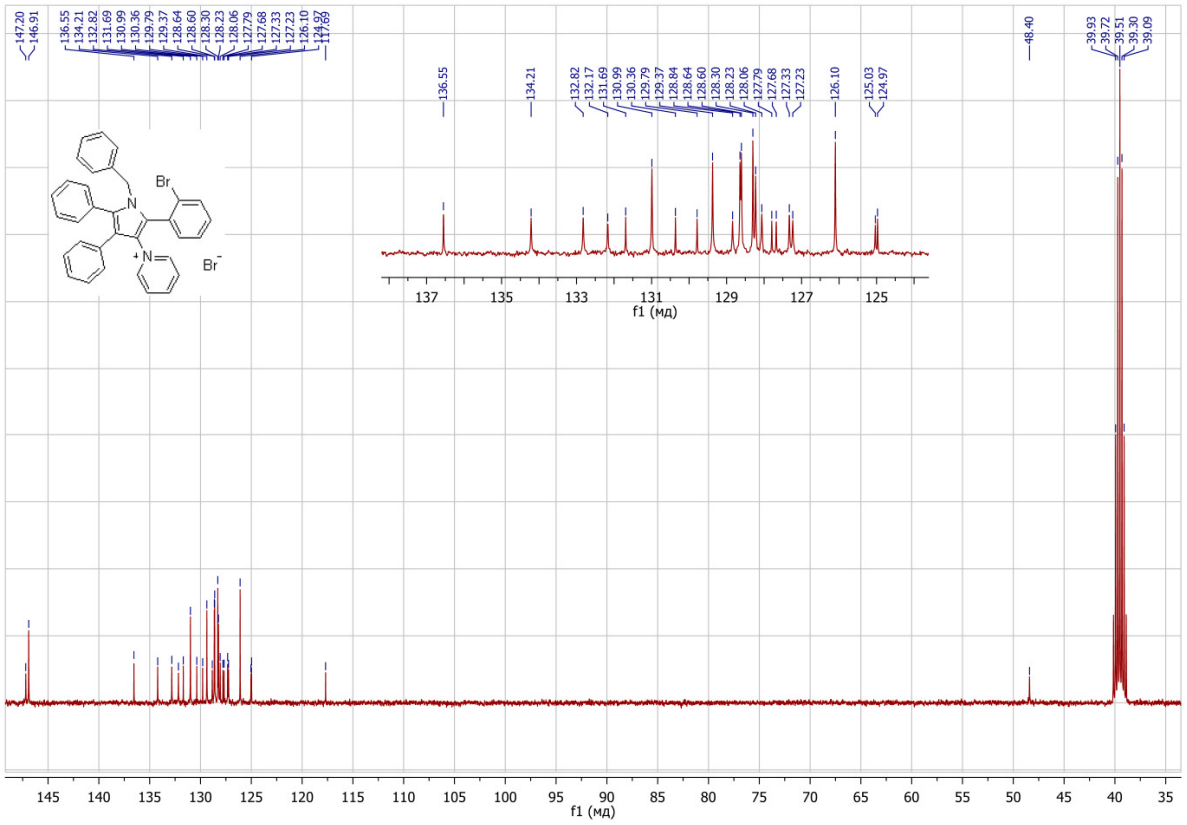
1-(1-Benzyl-2-(2-bromophenyl)-4-phenyl-1*H*-pyrrol-3-yl)pyridin-1-ium bromide **(7a)**, DMSO-d_6



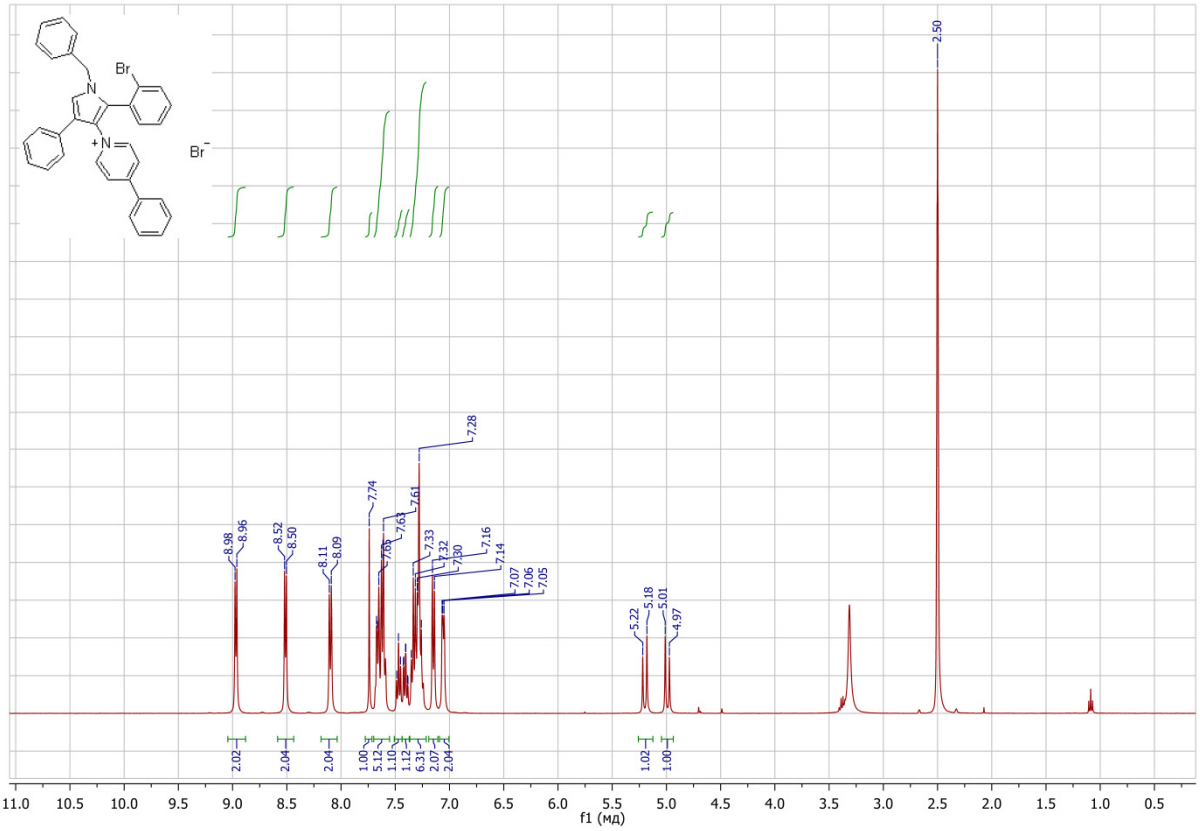


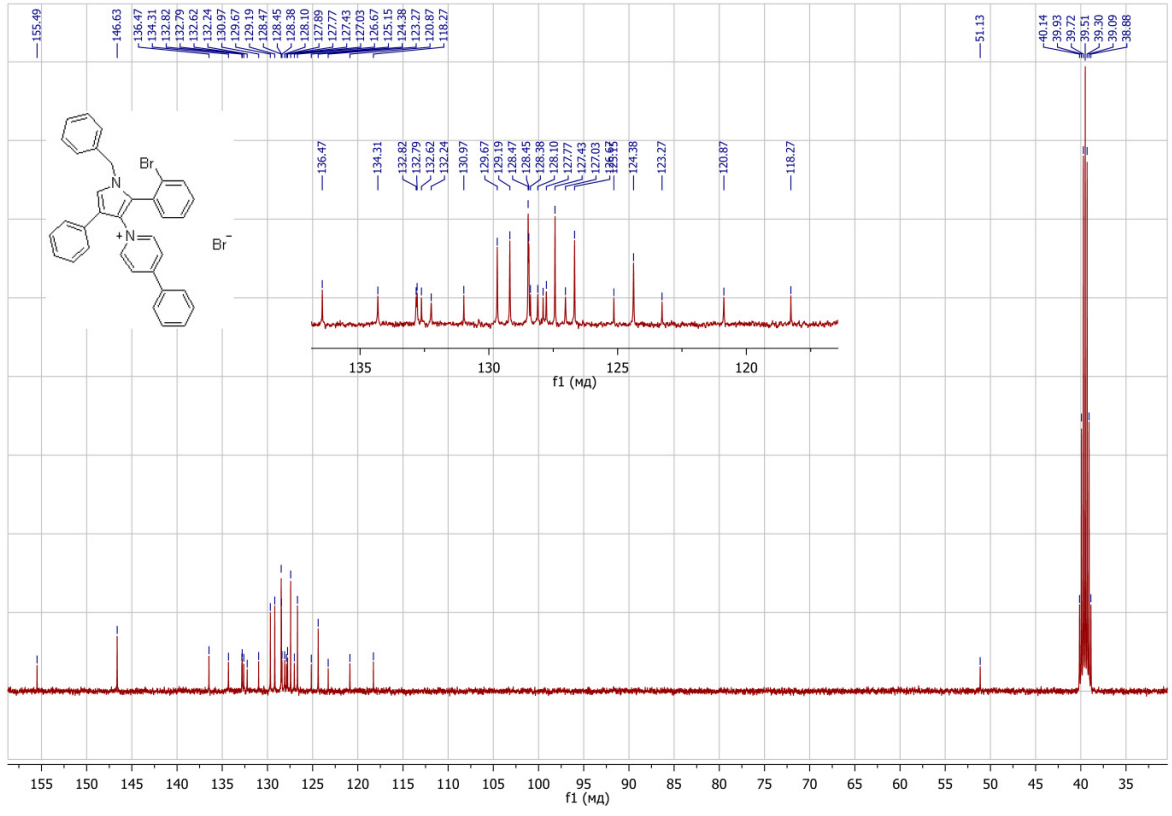
1-(1-Benzyl-2-(2-bromophenyl)-4,5-diphenyl-1*H*-pyrrol-3-yl)pyridin-1-ium bromide **(7b)**, DMSO-d_6



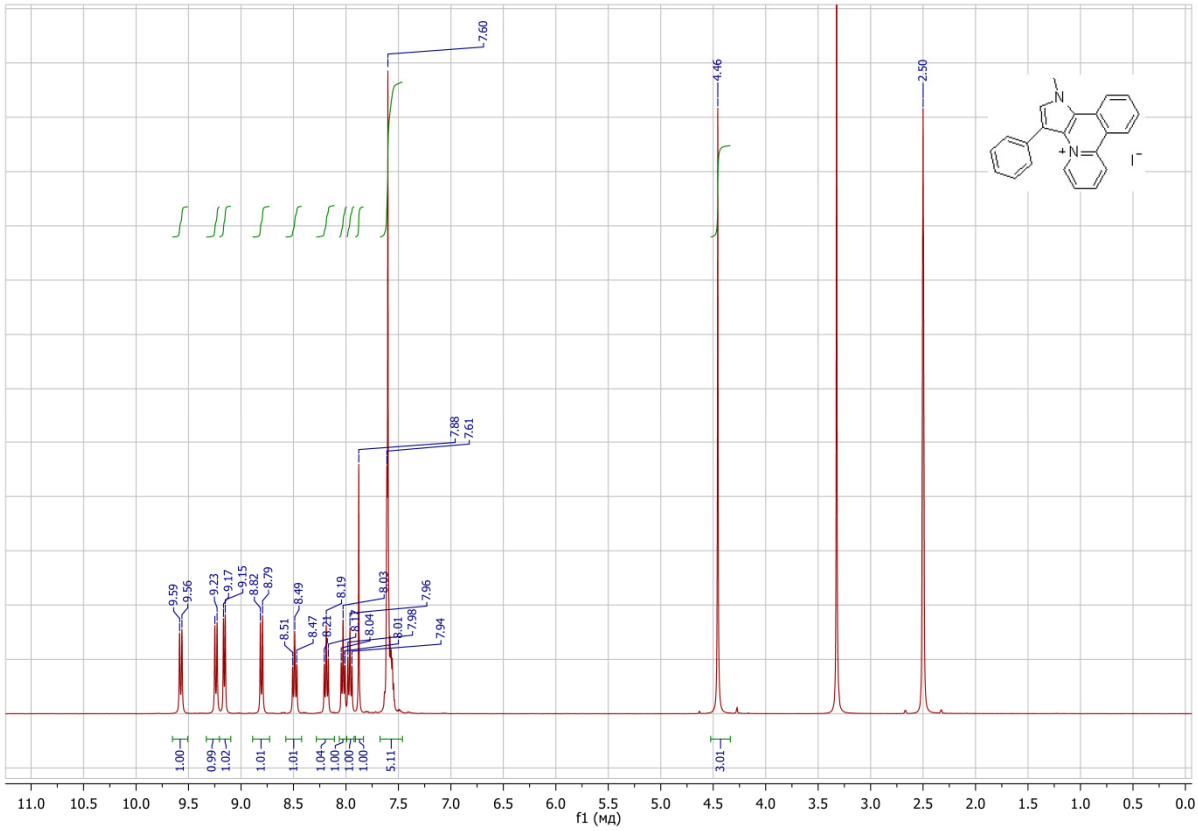


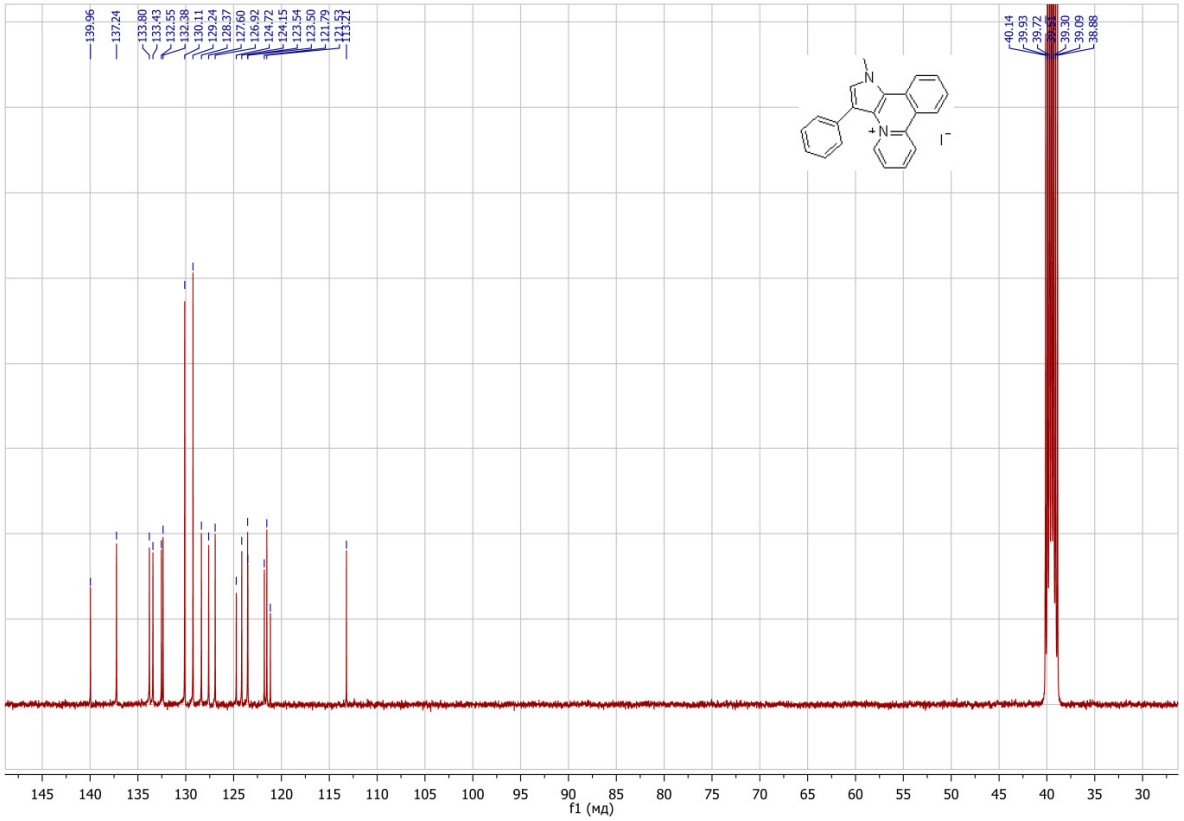
1-(1-Benzyl-2-(2-bromophenyl)-4-phenyl-1*H*-pyrrol-3-yl)-4-phenylpyridin-1-ium bromide **(7c)**, DMSO-d_6



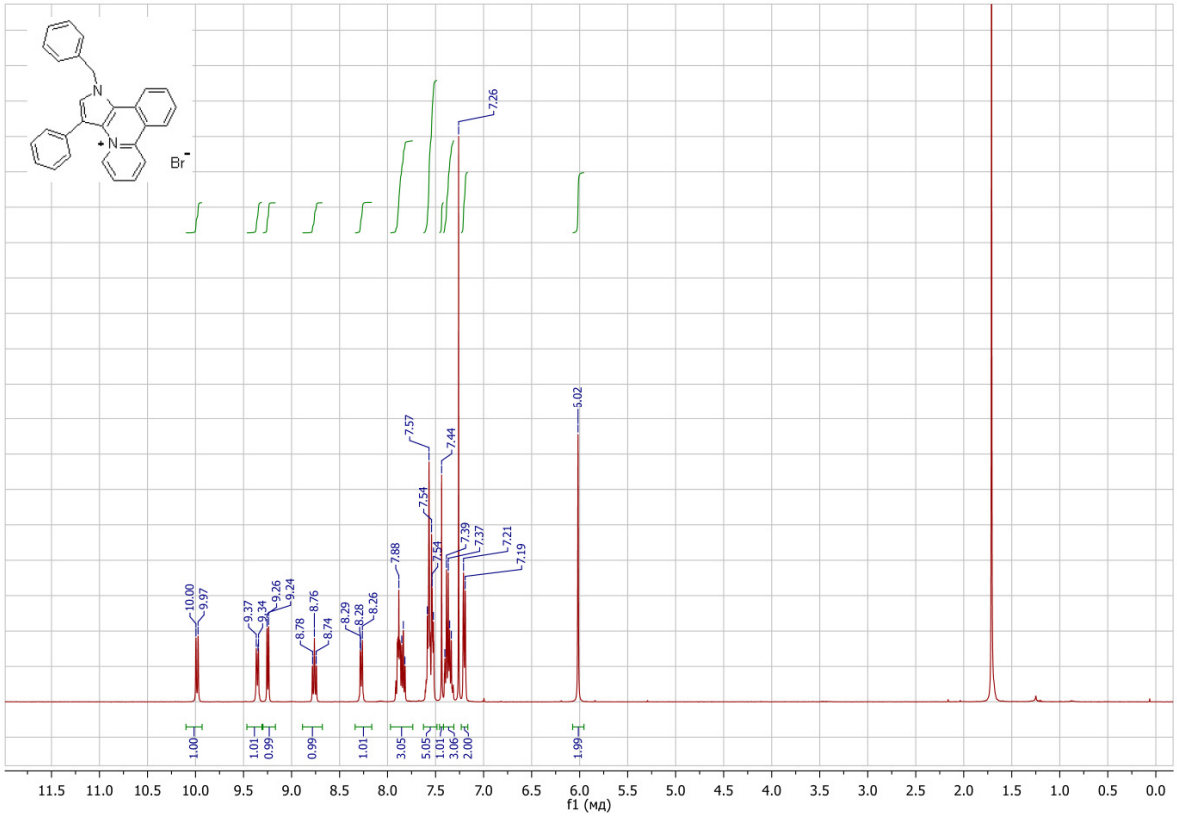


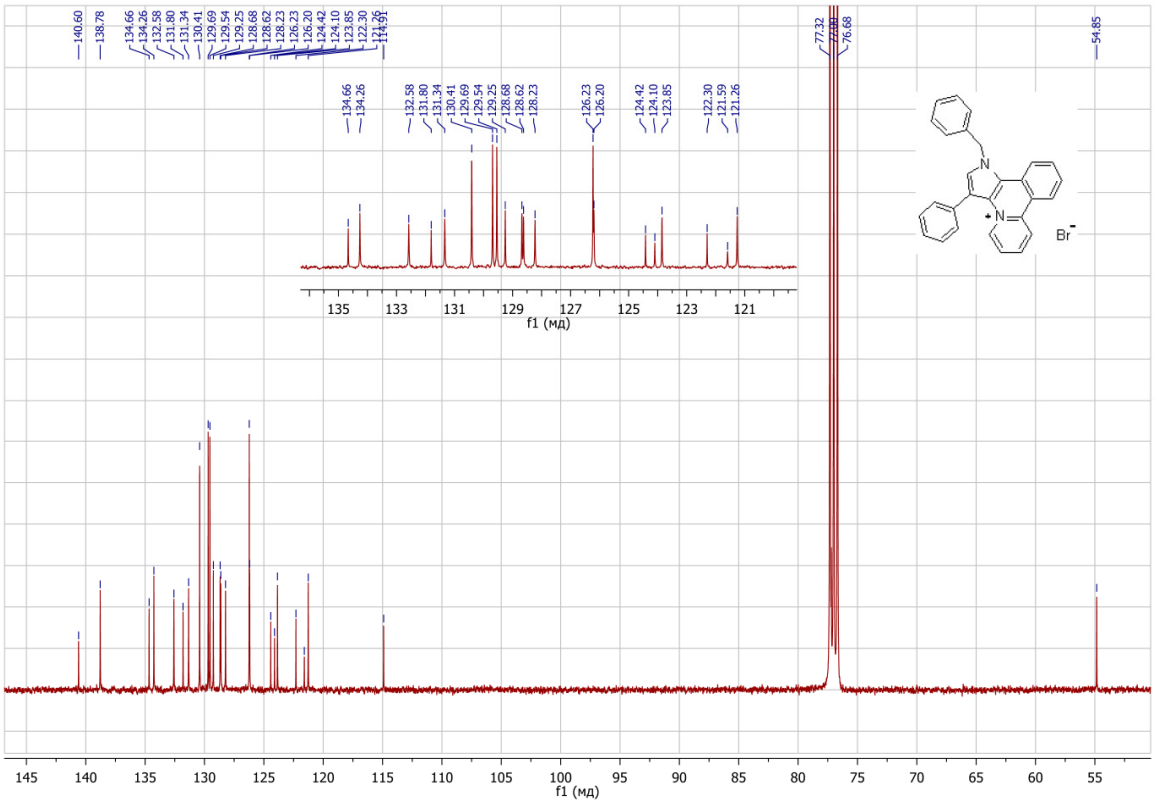
1-Methyl-3-phenyl-1*H*-pyrido[2,1-a]pyrrolo[3,2-c]isoquinolin-4-ium iodide **(8)**, DMSO-d_6



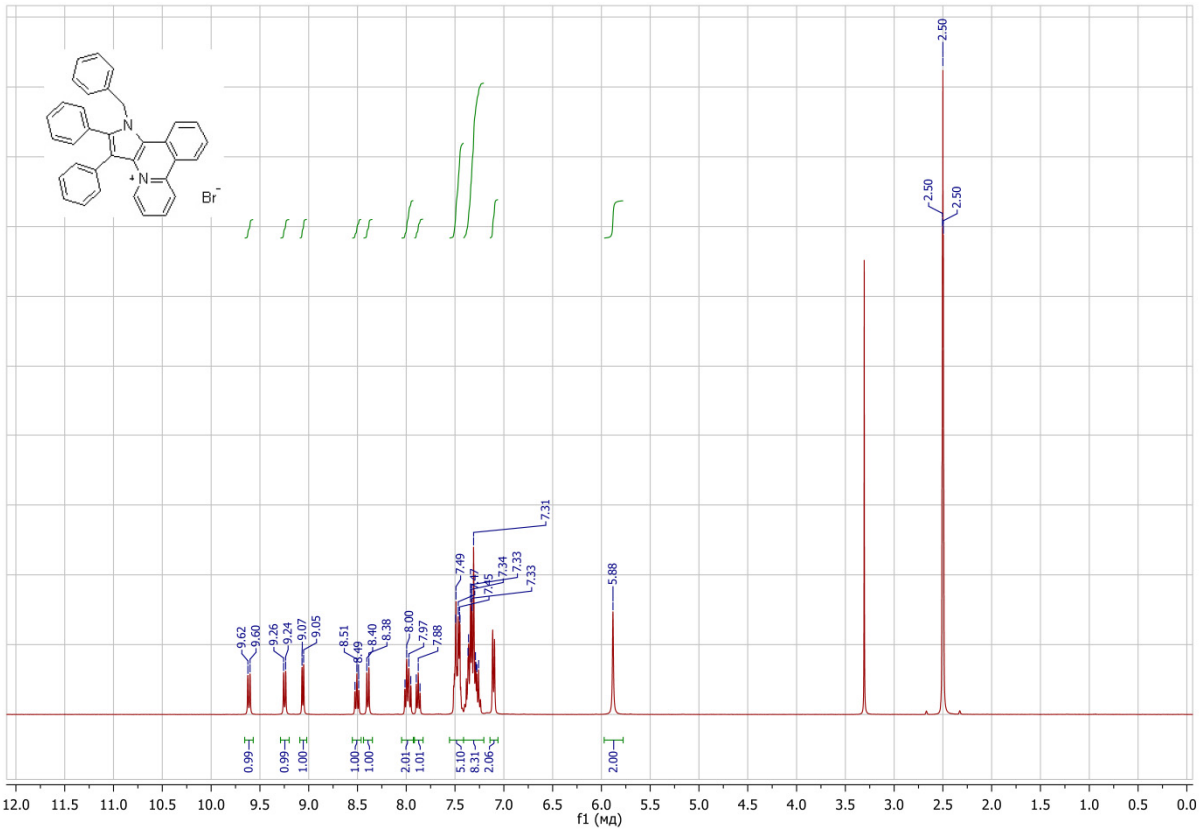


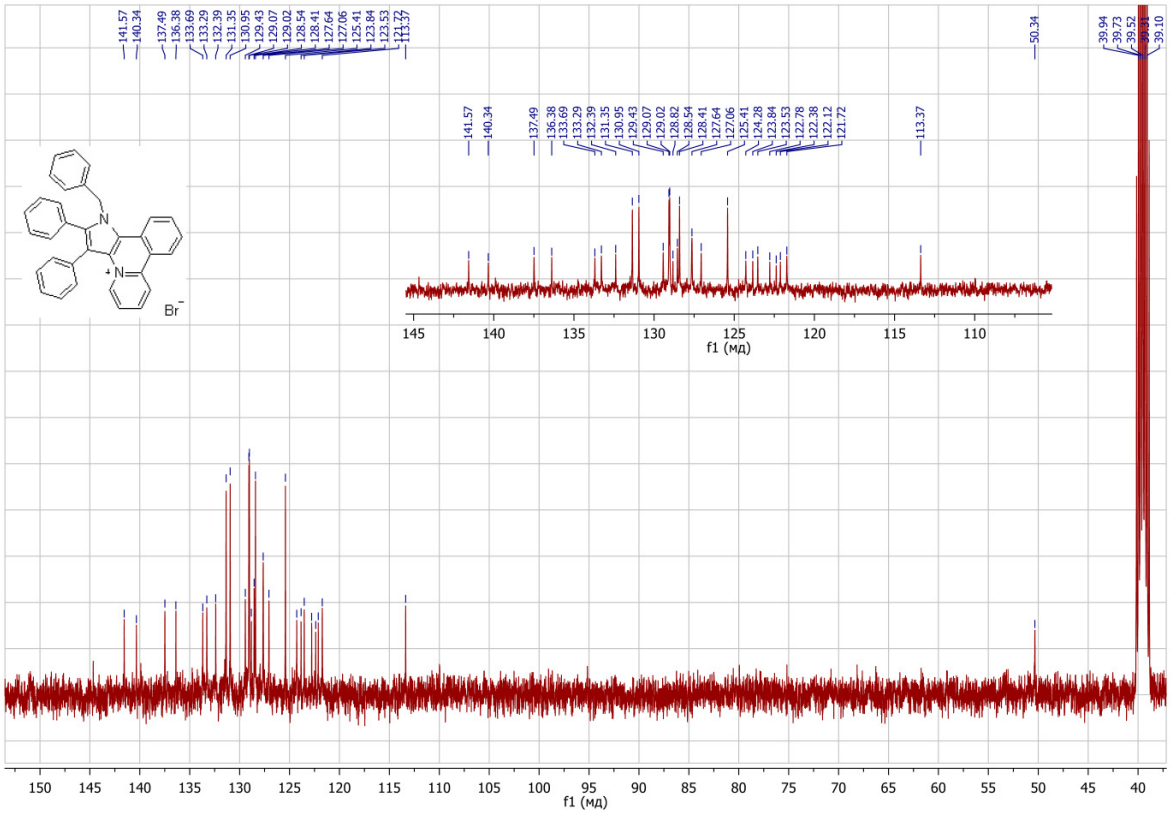
1-Benzyl-3-phenyl-1*H*-pyrido[2,1-a]pyrrolo[3,2-c]isoquinolin-4-ium bromide **(9a)**, $CDCl_3$



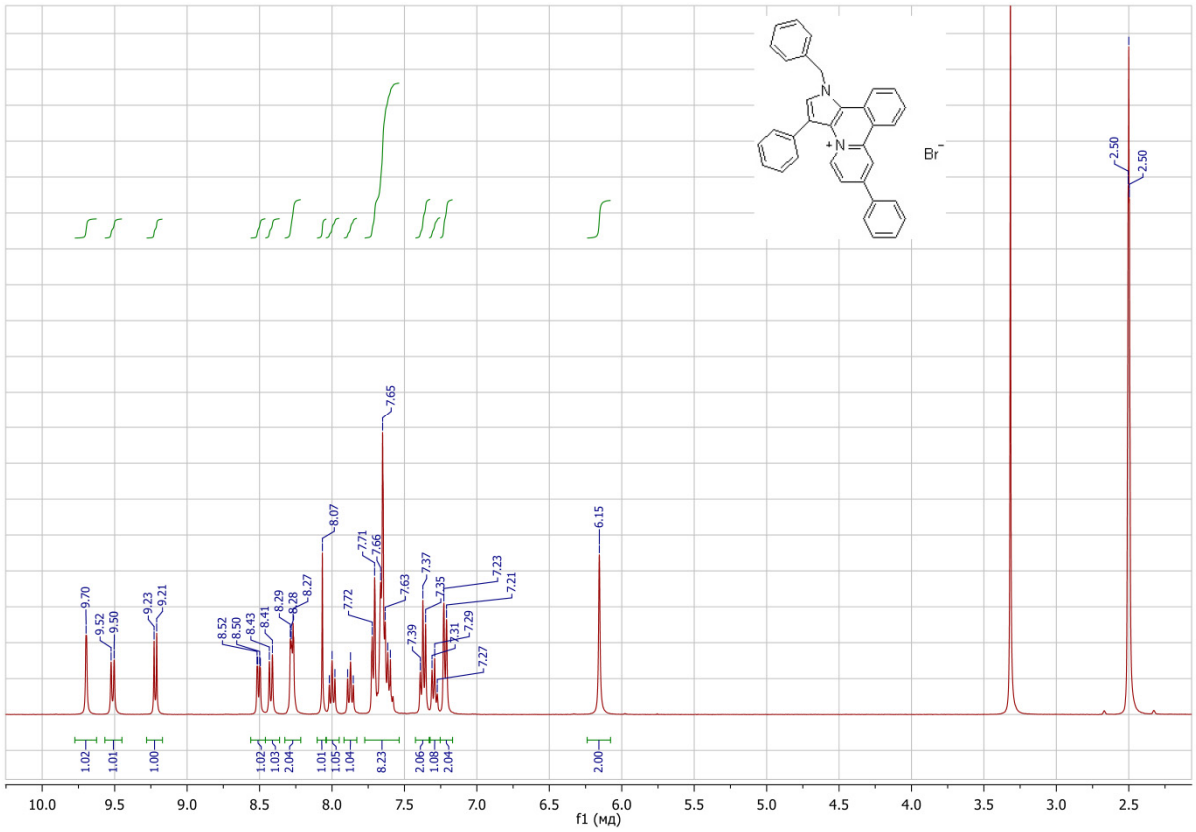


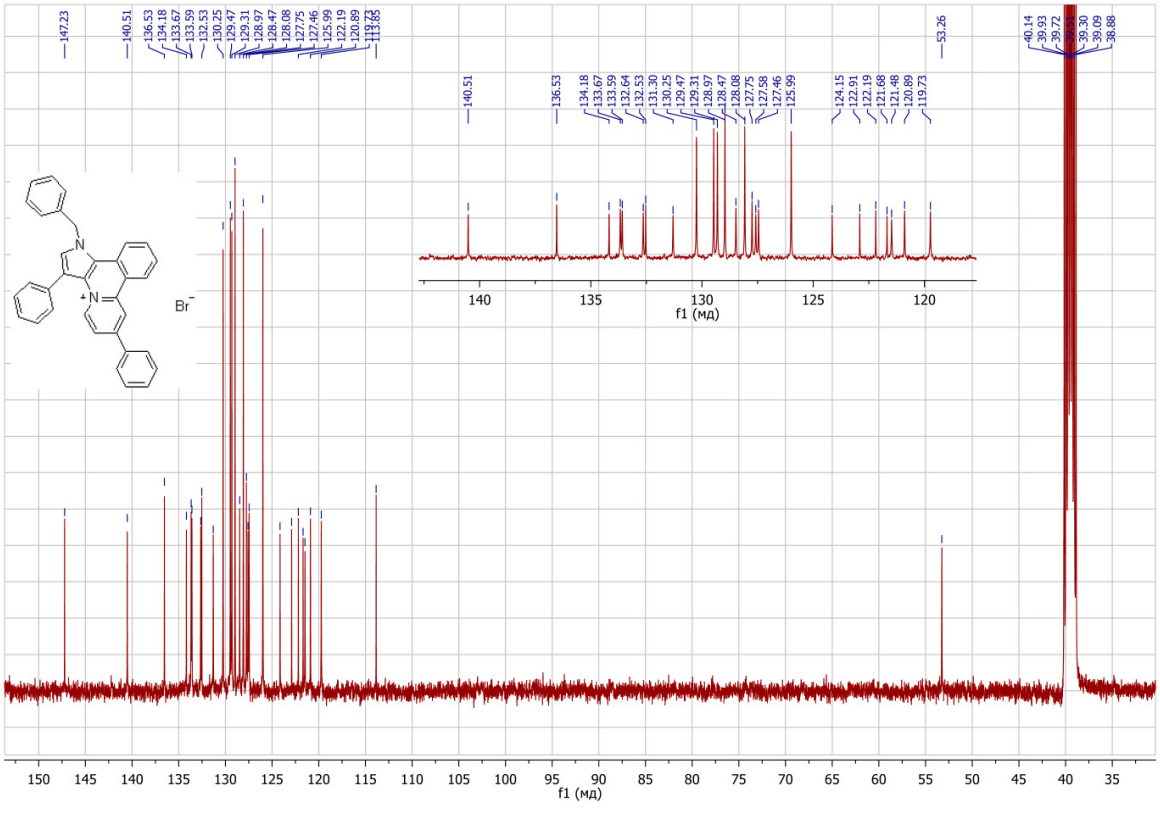
1-Benzyl-2,3-diphenyl-1*H*-pyrido[2,1-a]pyrrolo[3,2-c]isoquinolin-4-ium bromide **(9b)**, DMSO-d_6



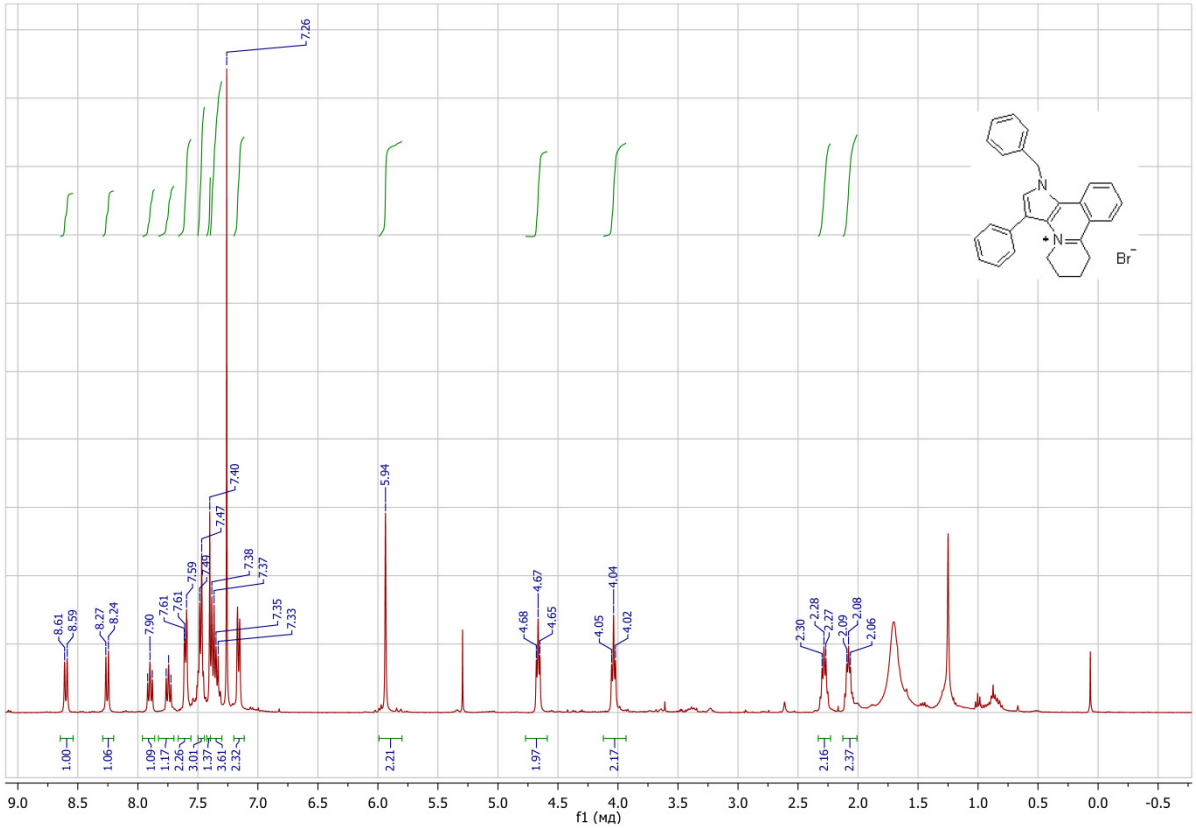


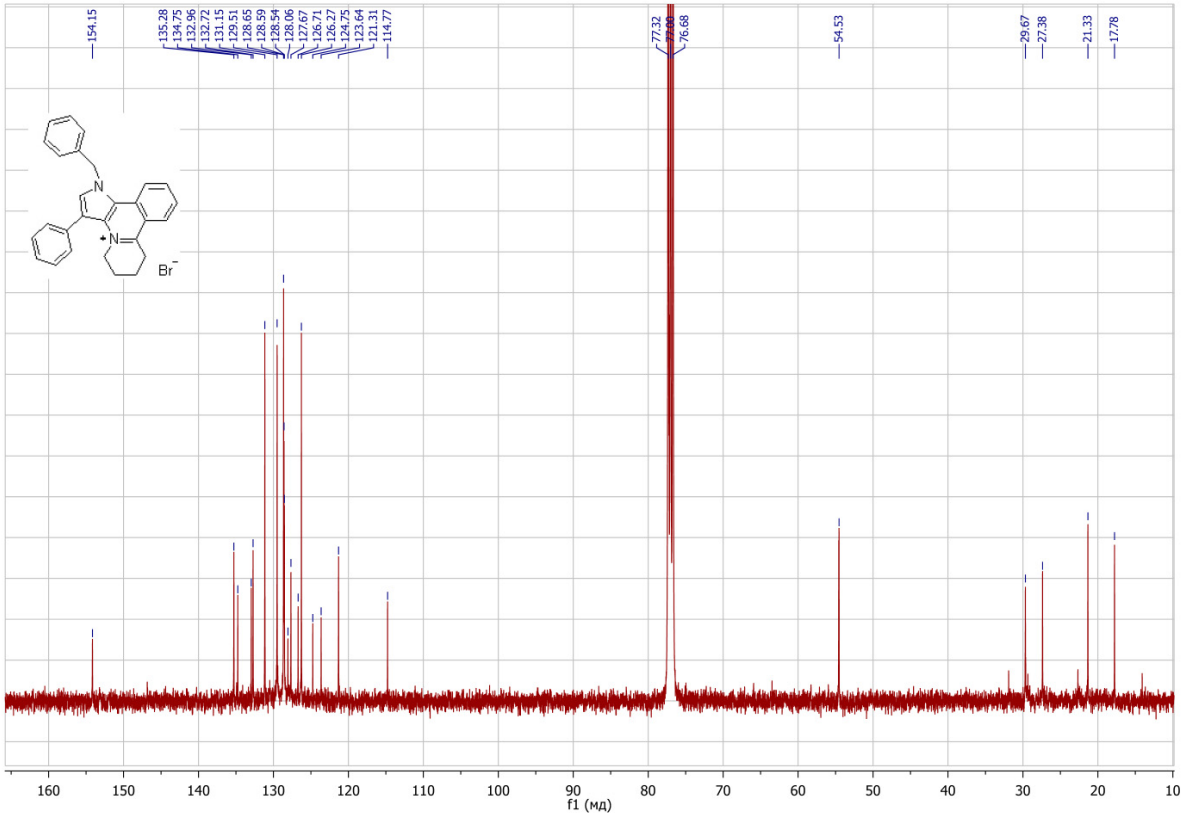
1-Benzyl-3,7-diphenyl-1*H*-pyrido[2,1-a]pyrrolo[3,2-c]isoquinolin-4-ium bromide **(9c)**, DMSO-d_6



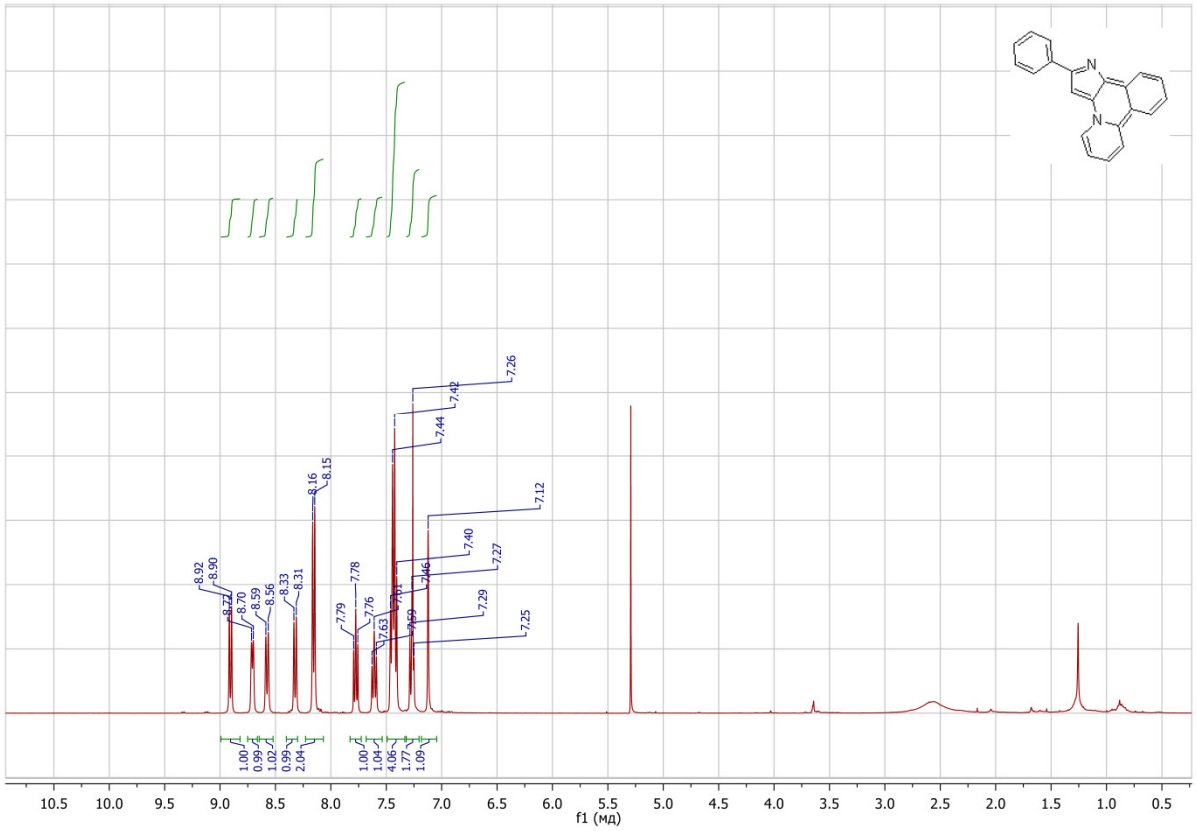


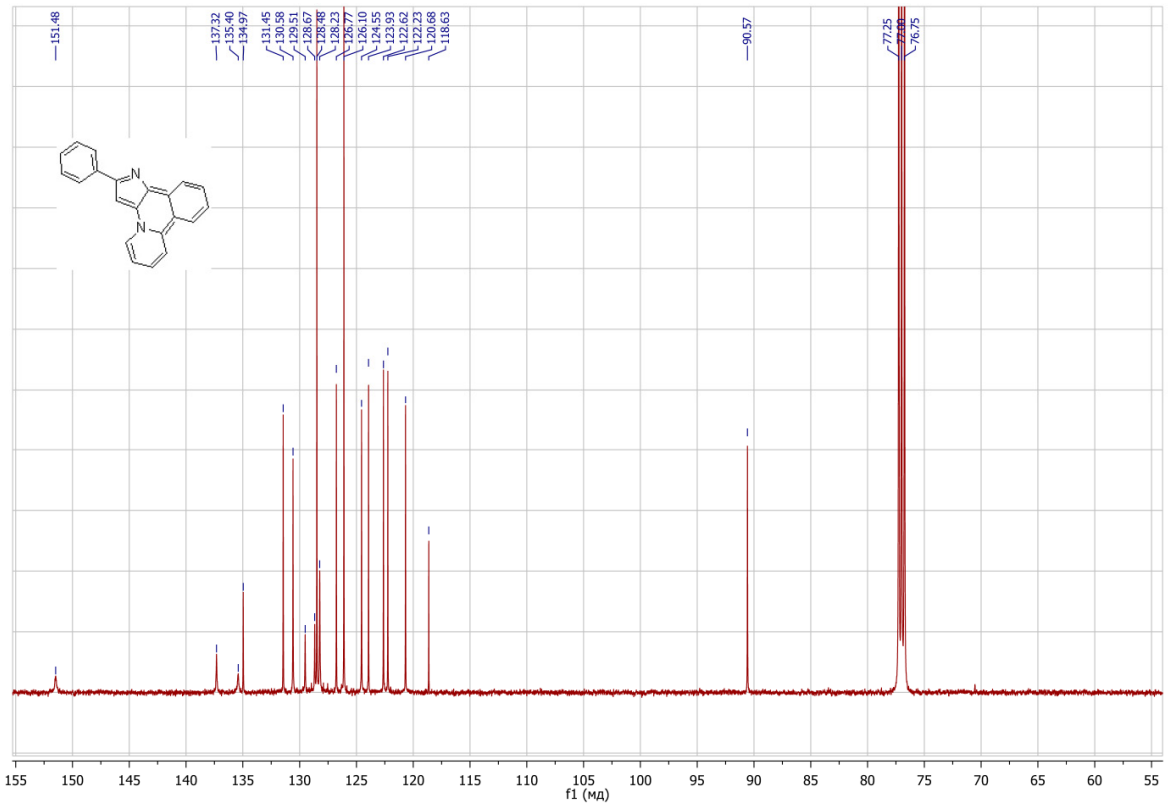
1-Benzyl-3-phenyl-5,6,7,8-tetrahydro-1*H*-pyrido[2,1-a]pyrrolo[3,2-c]isoquinolin-4-ium bromide **(10)**, $CDCl_3$



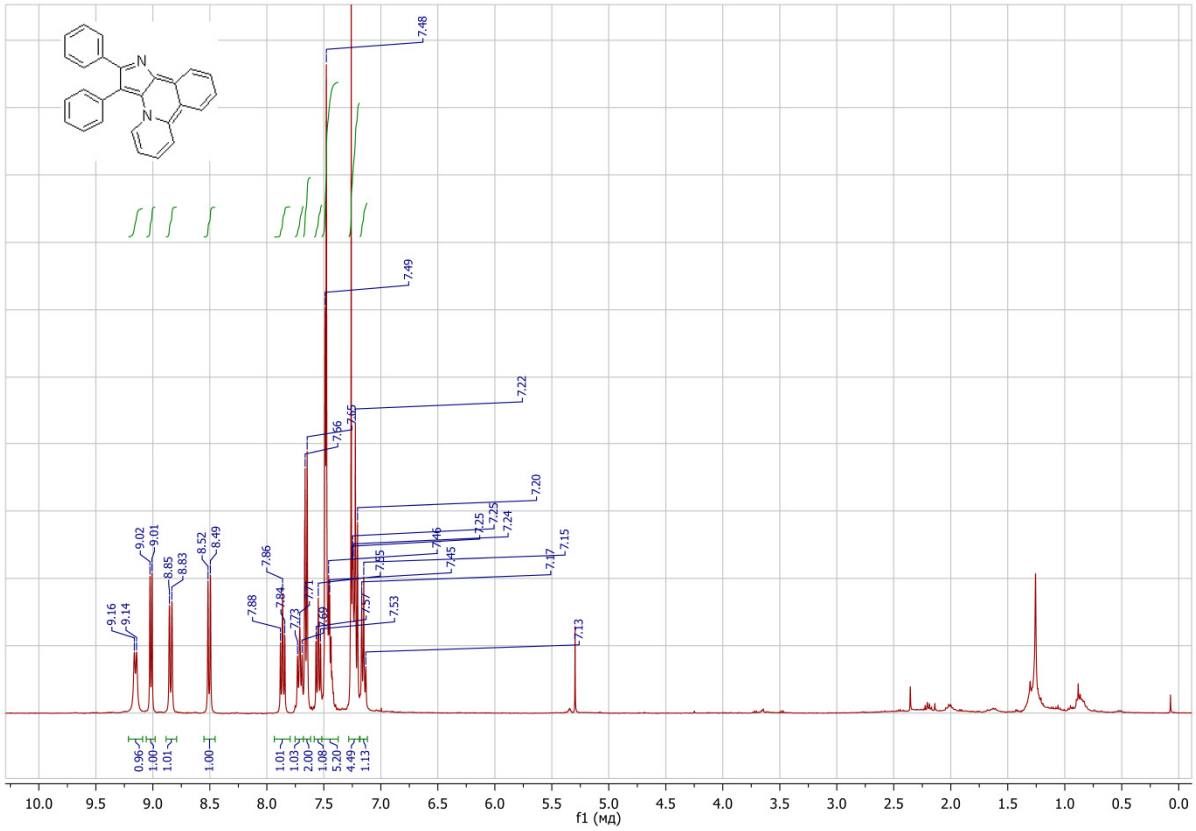


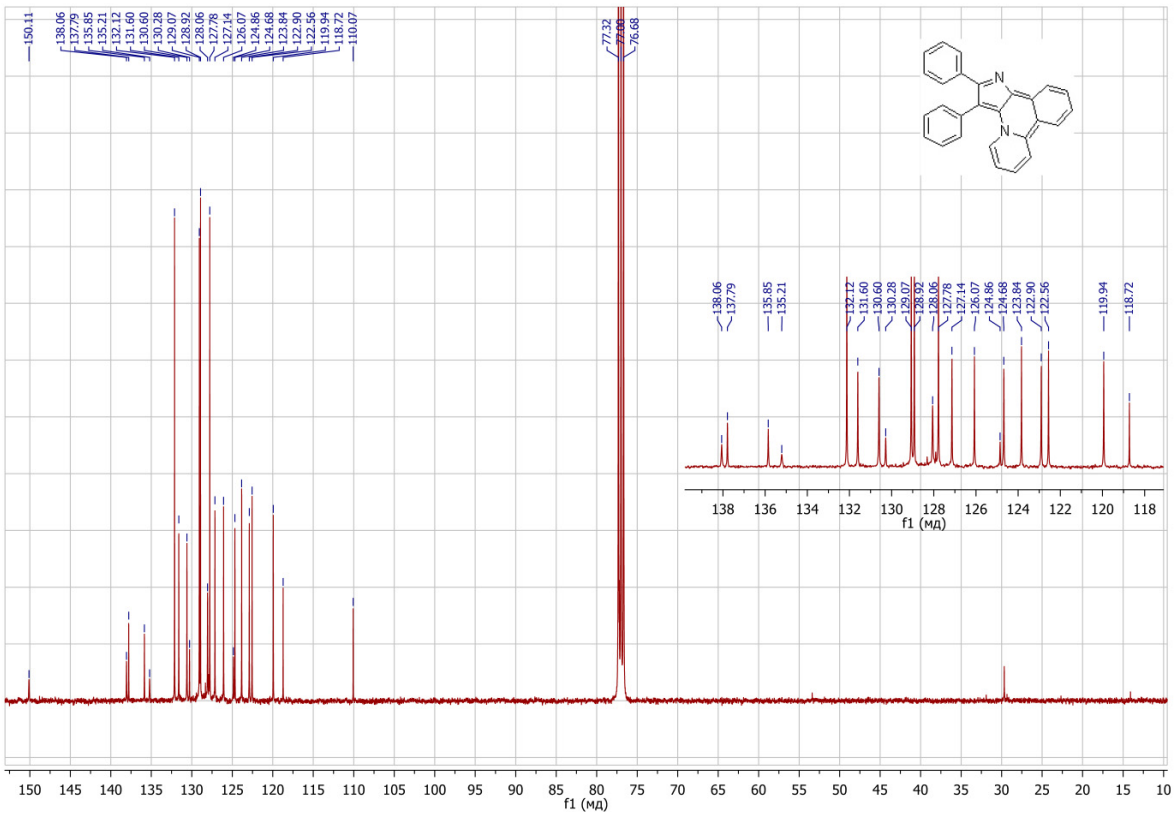
2-Phenylpyrido[2,1-a]pyrrolo[3,2-c]isoquinoline **(11)**, $CDCl_3$



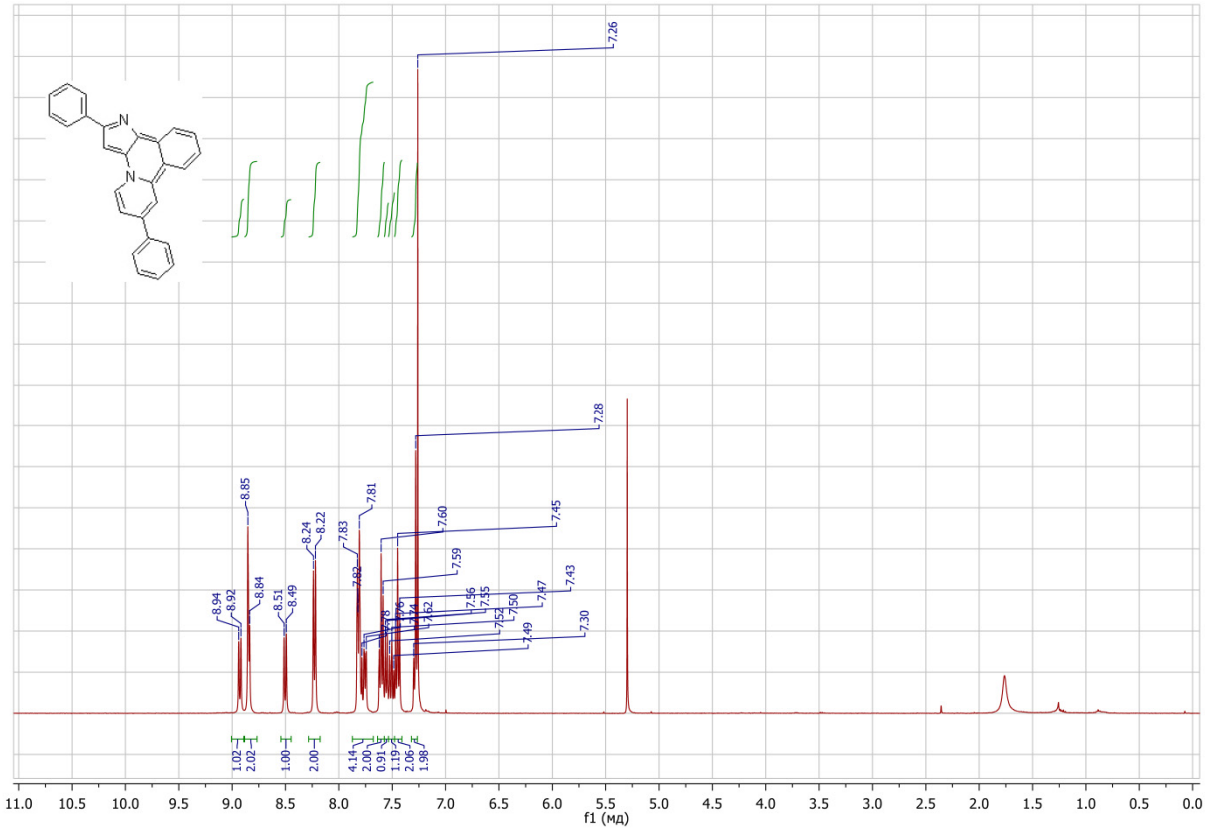


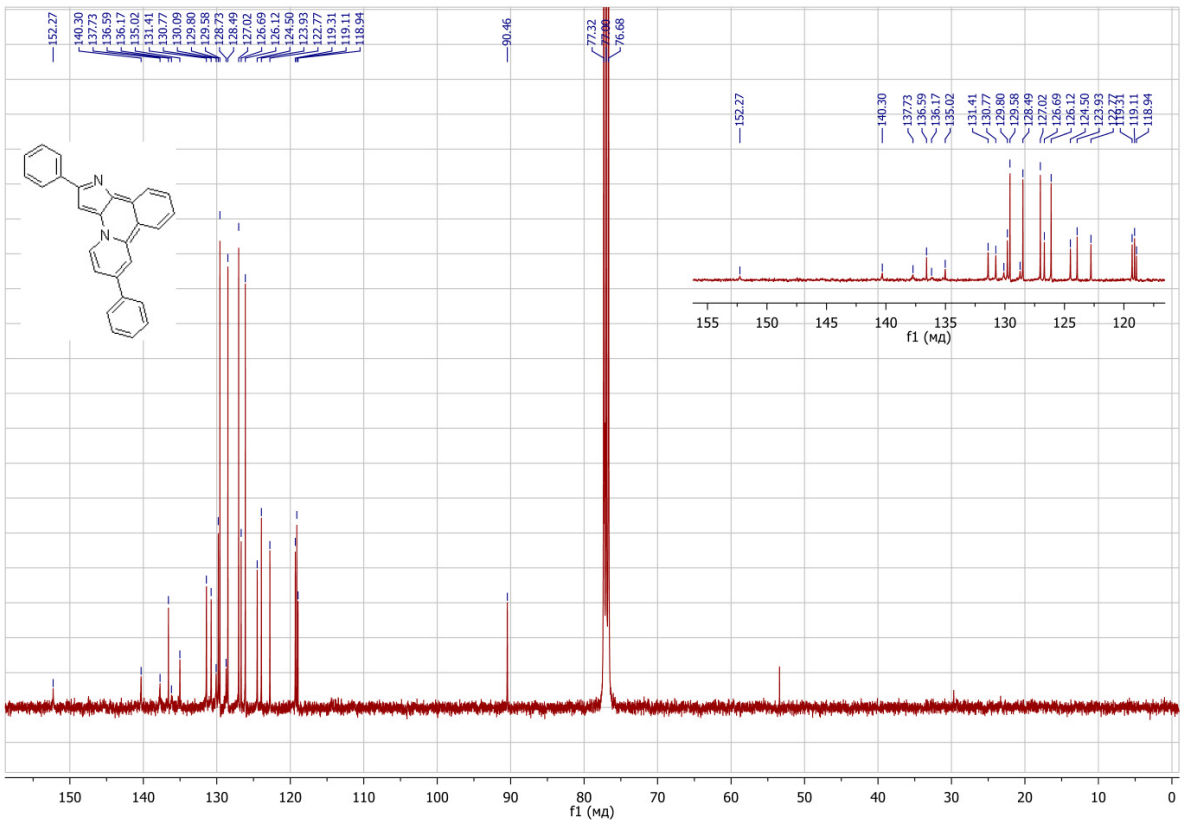
2,3-Diphenylpyrido[2,1-a]pyrrolo[3,2-c]isoquinoline **(12)**, $CDCl_3$



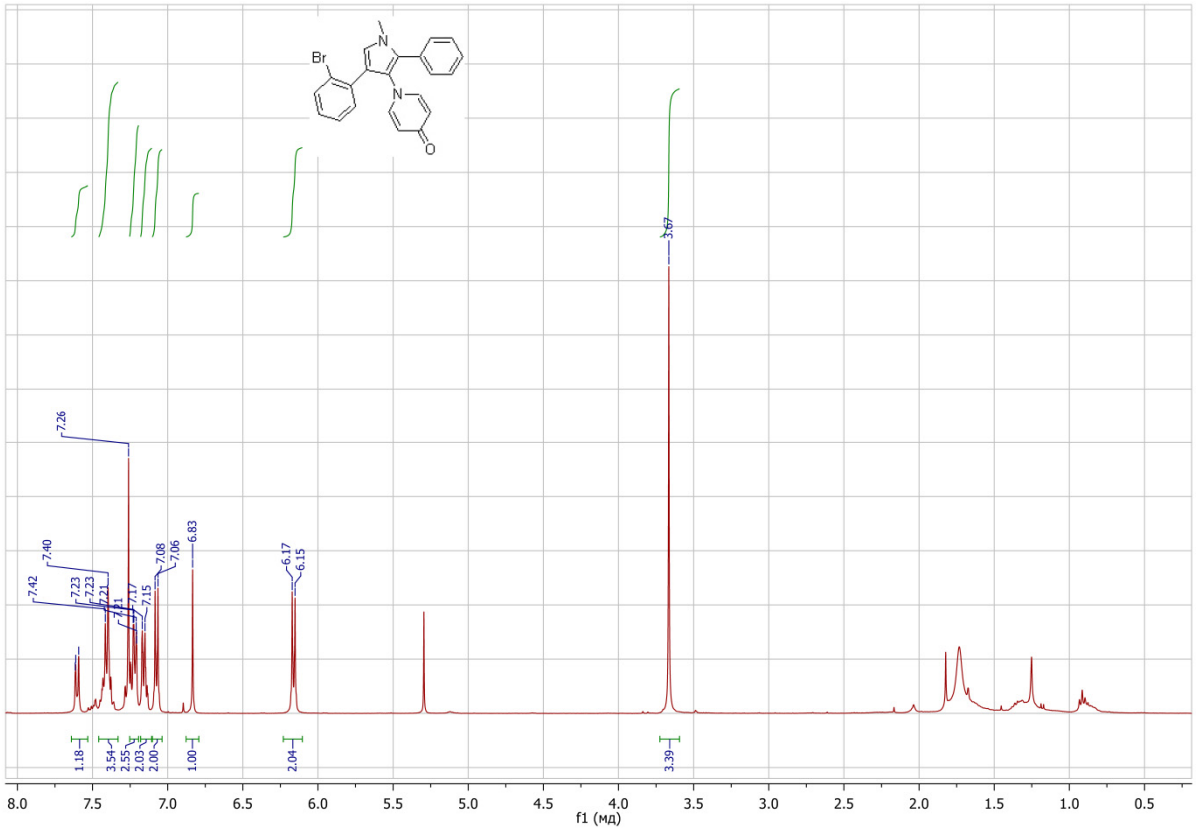


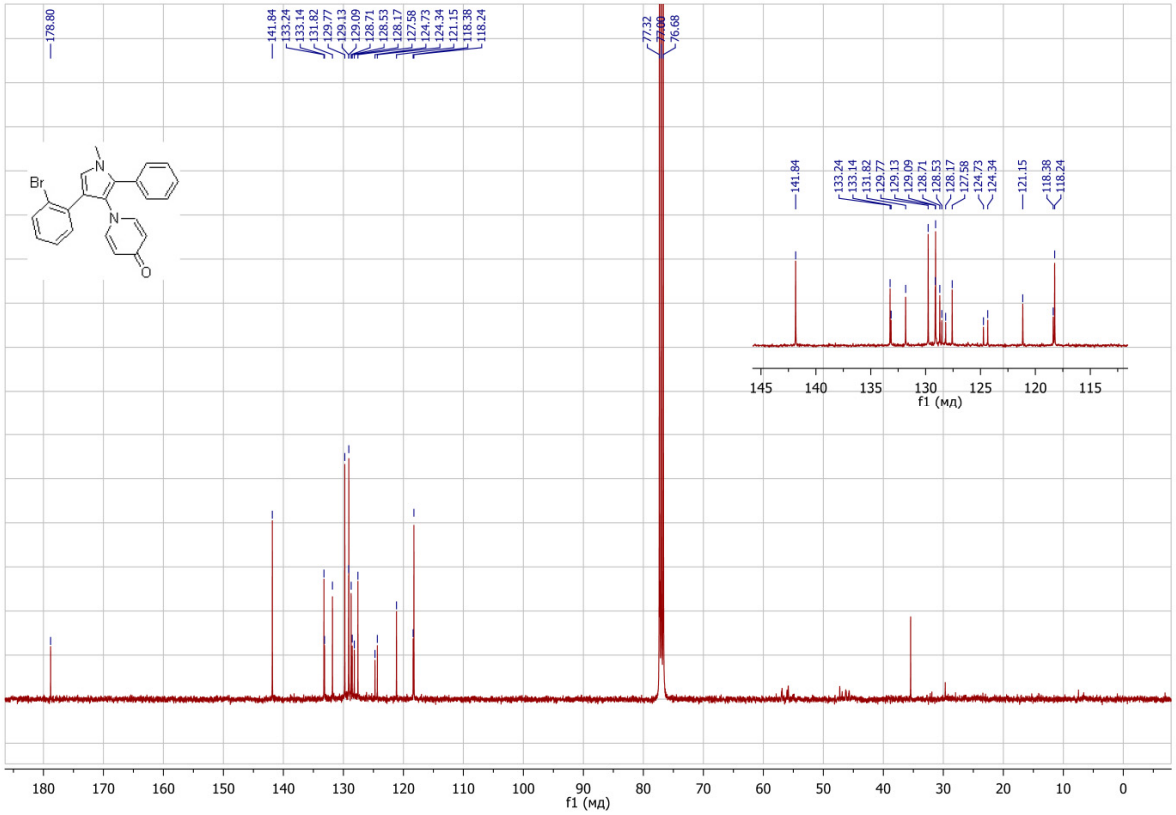
2,7-Diphenylpyrido[2,1-a]pyrrolo[3,2-c]isoquinoline **(13)**, $CDCl_3$





1-(4-(2-Bromophenyl)-1-methyl-2-phenyl-1*H*-pyrrol-3-yl)pyridin-4(1*H*)-one, $CDCl_3$





Computational Details

All calculations were performed with the B3LYP density functional method[4] by using the Gaussian 09 suite of quantum chemical programs[5] at Resource center "Computer center of Saint Petersburg State University". Geometry optimizations of molecules were performed at the B3LYP/6-31G+(d,p) level with PCM solvent model for the solvents. The vertical excitation energies and oscillator strengths were obtained for the 10 lowest S0-S1 transitions at the optimized ground state equilibrium geometries by using the TD-DFT B3LYP/6-31G+(d,p). The emissions were calculated at the same level of theory as implemented in the Gaussian 09: Step 1: Ground state geometry optimization and frequencies (equilibrium solvation); Step 2: Vertical excitation with linear response solvation; Step 3: State-specific solvation of the vertical excitation; Step 4: Relaxation of the excited state geometry; Step 5: Vibrational frequencies of the excited state structure; Step 6: Emission state-specific solvation (part 1); Step 7: Emission to final ground state (part 2).

Table S30. Bond Lengths for compound 11 and 11·H_2O (Å)

Atom	Atom	X-Ray	Calcd 11*	Calcd 11·H_2O*	Atom	Atom	X-Ray
C11	C6	1.418(3)	1.431	1.433	C6A	C11A	1.417(3)
C11	C12	1.427(3)	1.421	1.424	C12A	C11A	1.424(3)
C11	C10	1.411(3)	1.418	1.420	C11A	C10A	1.414(2)
N2	C15	1.390(2)	1.386	1.387	N2A	C15A	1.396(2)
N2	C1	1.379(2)	1.384	1.383	N2A	C1A	1.374(2)
N2	C5	1.383(3)	1.403	1.400	N2A	C5A	1.387(3)
N1	C12	1.359(2)	1.343	1.350	N1A	C12A	1.355(2)
N1	C13	1.377(2)	1.369	1.371	N1A	C13A	1.380(2)
C6	C7	1.409(3)	1.424	1.423	C6A	C7A	1.414(3)
C6	C5	1.448(3)	1.446	1.445	C6A	C5A	1.447(3)
C15	C12	1.412(2)	1.431	1.426	C12A	C15A	1.411(2)
C15	C14	1.396(3)	1.402	1.403	C15A	C14A	1.390(3)
C7	C8	1.372(3)	1.379	1.379	C8A	C7A	1.371(3)
C1	C2	1.358(3)	1.365	1.365	C1A	C2A	1.356(3)
C5	C4	1.409(3)	1.413	1.414	C5A	C4A	1.405(3)
C8	C9	1.399(3)	1.416	1.414	C9A	C8A	1.398(3)
C14	C13	1.401(2)	1.416	1.410	C13A	C14A	1.400(3)
C10	C9	1.372(3)	1.377	1.378	C10A	C9A	1.371(3)
C4	C3	1.361(3)	1.378	1.377	C4A	C3A	1.370(3)
C16	C21	1.402(3)	1.408	1.408	C16A	C21A	1.384(3)
C16	C13	1.468(3)	1.470	1.471	C13A	C16A	1.465(3)
C16	C17	1.385(3)	1.409	1.408	C16A	C17A	1.405(3)
C21	C20	1.388(3)	1.395	1.395	C21A	C20A	1.388(3)
C2	C3	1.395(3)	1.412	1.412	C2A	C3A	1.398(3)
C19	C20	1.386(3)	1.399	1.399	C20A	C19A	1.378(3)
C19	C18	1.387(3)	1.399	1.398	C19A	C18A	1.390(4)
C17	C18	1.390(3)	1.394	1.395	C17A	C18A	1.382(3)

[4] (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648. (b) Becke, A. D. *Phys. Rev. A* **1988**, *38*, 3098. (c) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785.

[5] **Gaussian 09, Revision D.01**, Frisch, M. J.; Trucks, G.W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ő.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc.; Wallingford CT, **2013**.

Table S31. Bond Angles for compound for compound 11 and 11·H_2O (˚)									
Atom	**Atom**	**Atom**	**X-Ray**	**Calcd 11***	**Calcd 11·H_2O***	**Atom**	**Atom**	**Atom**	**X-Ray**
C6	C11	C12	117.53(16)	117.92	117.48	C6A	C11A	C12A	117.53(17)
C10	C11	C6	119.51(18)	119.92	119.67	C10A	C11A	C6A	119.52(18)
C10	C11	C12	122.94(17)	122.16	122.86	C10A	C11A	C12A	122.93(17)
C1	N2	C15	118.86(17)	119.19	119.19	C1A	N2A	C15A	119.01(18)
C1	N2	C5	120.66(17)	120.32	120.51	C1A	N2A	C5A	120.79(18)
C5	N2	C15	120.48(16)	120.50	120.38	C5A	N2A	C15A	120.20(16)
C12	N1	C13	105.13(15)	105.65	106.12	C12A	N1A	C13A	104.88(15)
C11	C6	C5	120.94(18)	120.59	120.85	C11A	C6A	C5A	121.08(18)
C7	C6	C11	118.43(18)	117.85	118.09	C7A	C6A	C11A	118.17(17)
C7	C6	C5	120.62(18)	121.56	121.06	C7A	C6A	C5A	120.75(18)
N2	C15	C12	121.18(17)	120.89	121.10	N2A	C15A	C12A	121.06(18)
N2	C15	C14	131.47(17)	132.33	131.67	C14A	C15A	N2A	131.18(18)
C14	C15	C12	107.26(16)	106.78	107.22	C14A	C15A	C12A	107.71(17)
C8	C7	C6	121.15(19)	121.21	121.19	C8A	C7A	C6A	121.21(19)
C2	C1	N2	121.4(2)	122.19	122.13	C2A	C1A	N2A	121.5(2)
N2	C5	C6	119.32(17)	119.51	119.50	N2A	C5A	C6A	119.36(17)
N2	C5	C4	117.05(18)	116.82	116.76	N2A	C5A	C4A	117.11(18)
C4	C5	C6	123.63(19)	123.67	123.74	C4A	C5A	C6A	123.5(2)
N1	C12	C11	128.95(16)	128.51	129.18	N1A	C12A	C11A	128.74(16)
N1	C12	C15	110.60(17)	110.90	110.14	N1A	C12A	C15A	110.55(17)
C15	C12	C11	120.42(16)	120.60	120.68	C15A	C12A	C11A	120.68(18)
C7	C8	C9	120.07(19)	120.38	120.21	C7A	C8A	C9A	120.24(19)
C15	C14	C13	104.80(16)	104.15	104.36	C15A	C14A	C13A	104.45(17)
C9	C10	C11	120.27(18)	120.56	120.39	C9A	C10A	C11A	120.49(18)
C3	C4	C5	122.1(2)	122.78	122.78	C3A	C4A	C5A	122.0(2)
C21	C16	C13	120.36(18)	121.84	121.85	C21A	C16A	C13A	121.29(18)
C17	C16	C21	118.14(19)	118.16	118.24	C21A	C16A	C17A	118.2(2)
C17	C16	C13	121.49(18)	120.00	120.91	C17A	C16A	C13A	120.53(19)
C10	C9	C8	120.56(19)	120.08	120.45	C10A	C9A	C8A	120.35(18)
C20	C21	C16	120.8(2)	120.97	120.99	C16A	C21A	C20A	121.1(2)
N1	C13	C14	112.20(16)	112.53	112.16	N1A	C13A	C14A	112.41(17)
N1	C13	C16	121.29(16)	120.37	121.58	N1A	C13A	C16A	120.73(17)
C14	C13	C16	126.47(17)	127.10	126.26	C14A	C13A	C16A	126.83(18)
C1	C2	C3	119.3(2)	119.29	119.20	C1A	C2A	C3A	119.5(2)
C20	C19	C18	119.2(2)	119.33	119.37	C20A	C19A	C18A	119.0(2)
C19	C20	C21	120.4(2)	120.28	120.21	C19A	C20A	C21A	120.6(2)
C4	C3	C2	119.4(2)	118.61	118.70	C4A	C3A	C2A	119.1(2)
C16	C17	C18	121.1(2)	120.80	120.65	C18A	C17A	C16A	120.4(2)
C19	C18	C17	120.3(2)	120.45	120.53	C17A	C18A	C19A	120.8(2)

*Geometry optimizations of **11** and **11**·H_2O in the gas phase were performed at the B3LYP/6-31G+(d,p) level.

Figure S6. Frontier MO of **11** and complexes of **11** with MeOH (DFT B3LYP/6-31+G(d,p), PCM for MeOH).

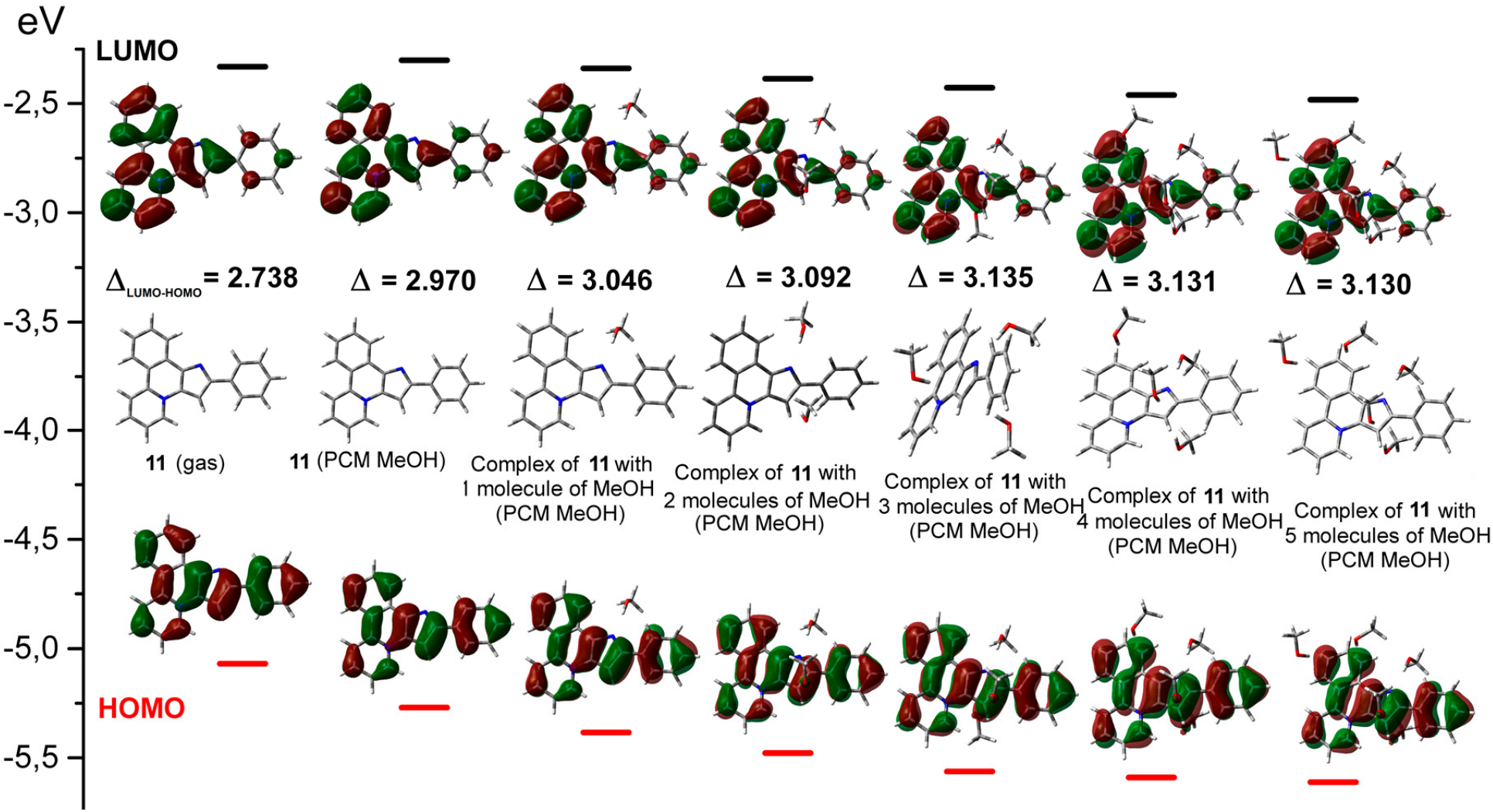
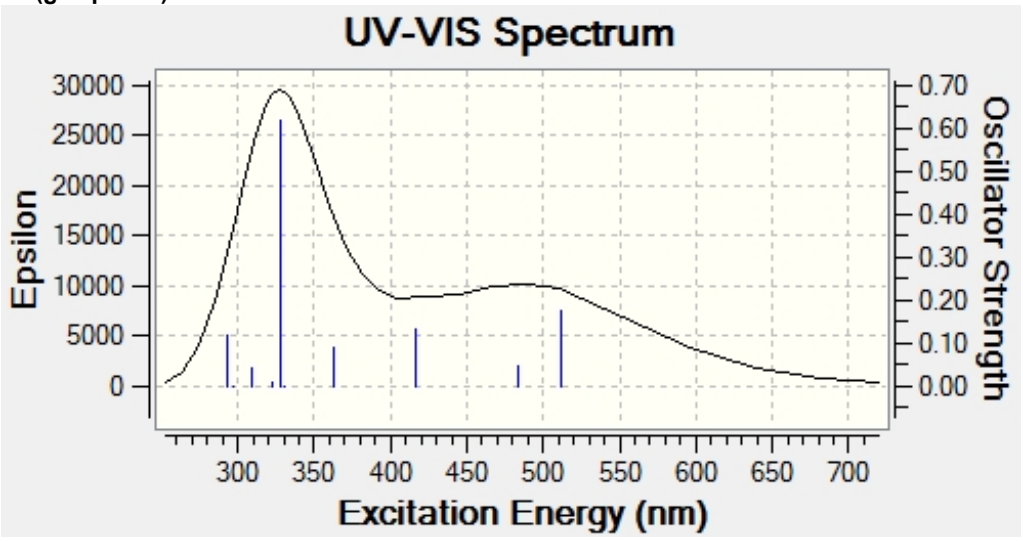


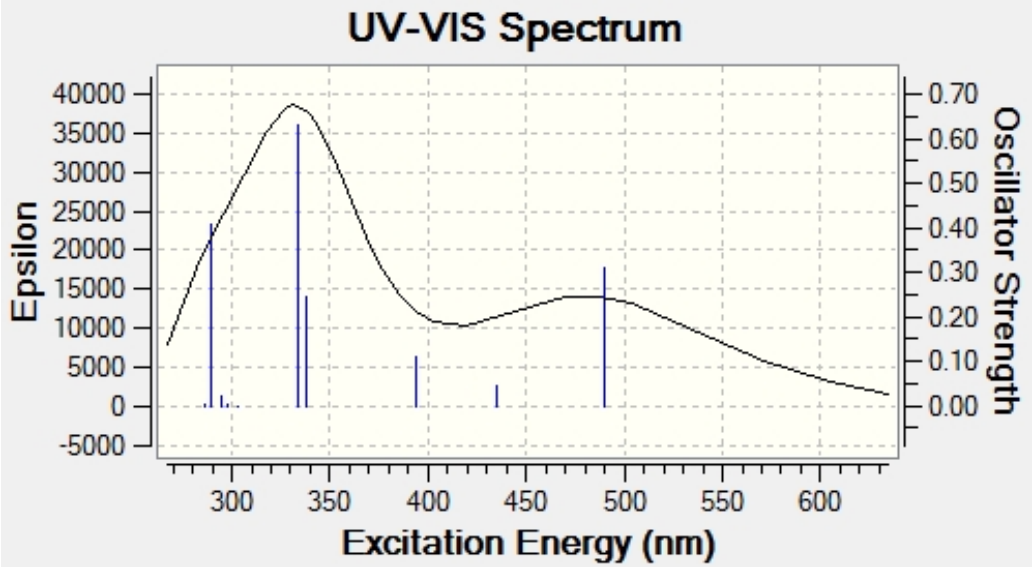
Table S32. Calculated UV-VIS spectra and excited states for 11 and H-complexes 11

11 (gas phase)



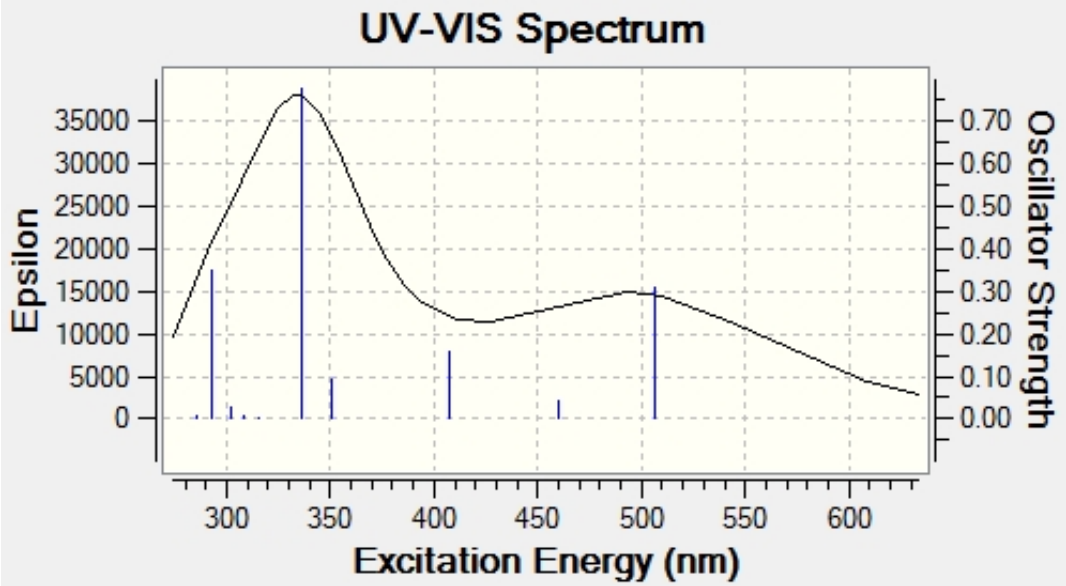
Excited State 1: Singlet-A 2.4249 eV 511.31 nm f=0.1772 <S**2>=0.000
76 -> 78 -0.24406
77 -> 78 0.62199
77 -> 79 -0.21526
Excited State 2: Singlet-A 2.5650 eV 483.37 nm f=0.0471 <S**2>=0.000
77 -> 78 0.24126
77 -> 79 0.65296
Excited State 3: Singlet-A 2.9742 eV 416.87 nm f=0.1313 <S**2>=0.000
76 -> 78 0.62673
76 -> 79 -0.11992
77 -> 78 0.18133
77 -> 79 -0.13626
77 -> 80 0.17827
Excited State 4: Singlet-A 3.4136 eV 363.20 nm f=0.0886 <S**2>=0.000
72 -> 78 0.12104
76 -> 79 0.67079
77 -> 78 0.10434
Excited State 5: Singlet-A 3.7518 eV 330.47 nm f=0.0000 <S**2>=0.000
73 -> 78 0.70513
Excited State 6: Singlet-A 3.7741 eV 328.51 nm f=0.6168 <S**2>=0.000
72 -> 78 0.10745
74 -> 78 -0.10714
76 -> 78 -0.15801
77 -> 80 0.65016
Excited State 7: Singlet-A 3.8466 eV 322.32 nm f=0.0096 <S**2>=0.000
75 -> 78 0.69244
Excited State 8: Singlet-A 4.0140 eV 308.88 nm f=0.0426 <S**2>=0.000
72 -> 78 0.12193
74 -> 78 0.65882
77 -> 82 -0.12895
Excited State 9: Singlet-A 4.1646 eV 297.71 nm f=0.0000 <S**2>=0.000
77 -> 81 0.69739
Excited State 10: Singlet-A 4.2362 eV 292.68 nm f=0.1186 <S**2>=0.000
72 -> 78 0.52711
74 -> 79 0.33600
75 -> 79 0.11586
76 -> 79 -0.10244
76 -> 80 0.10606
77 -> 80 -0.10046
77 -> 84 -0.14143
77 -> 85 -0.11863

11 (CH_2Cl_2)



Excited State 1: Singlet-A **2.5356 eV 488.97 nm f=0.3109** <S**2>=0.000
76 -> 78 -0.14721
77 -> 78 0.67958
77 -> 79 -0.10010
Excited State 2: Singlet-A 2.8470 eV 435.48 nm f=0.0413 <S**2>=0.000
76 -> 78 0.14302
77 -> 78 0.12653
77 -> 79 0.67447
Excited State 3: Singlet-A 3.1557 eV 392.89 nm f=0.1166 <S**2>=0.000
76 -> 78 0.64848
77 -> 78 0.10951
77 -> 79 -0.15955
77 -> 80 0.16644
Excited State 4: Singlet-A 3.6711 eV 337.73 nm f=0.1974 <S**2>=0.000
73 -> 78 -0.17515
76 -> 79 0.44893
77 -> 80 0.49862
Excited State 5: Singlet-A 3.7157 eV 333.67 nm f=0.6819 <S**2>=0.000
76 -> 78 0.13162
76 -> 79 0.50947
77 -> 80 -0.45387
Excited State 6: Singlet-A 4.1170 eV 301.15 nm f=0.0003 <S**2>=0.000
72 -> 78 0.68852
75 -> 78 0.13511
Excited State 7: Singlet-A 4.1590 eV 298.11 nm f=0.0054 <S**2>=0.000
72 -> 78 -0.14722
75 -> 78 0.52271
77 -> 81 -0.39569
77 -> 82 0.17240
Excited State 8: Singlet-A 4.2060 eV 294.78 nm f=0.0217 <S**2>=0.000
73 -> 78 -0.23903
74 -> 78 0.60509
75 -> 78 -0.11559
77 -> 81 -0.14561
77 -> 82 -0.12584
Excited State 9: Singlet-A 4.2792 eV 289.73 nm f=0.4031 <S**2>=0.000
73 -> 78 0.59137
74 -> 78 0.23452
74 -> 79 0.13002
76 -> 79 0.14265
76 -> 80 -0.11590
77 -> 80 0.10045
77 -> 84 0.10623

11 (Toluene)



Excited State 1: Singlet-A 2.4493 eV 506.19 nm f=0.3106 <S**2>=0.000
76 -> 78 -0.16787
77 -> 78 0.67326
77 -> 79 -0.11337

Excited State 2: Singlet-A 2.6926 eV 460.46 nm f=0.0440 <S**2>=0.000
76 -> 78 0.12029
77 -> 78 0.13982
77 -> 79 0.67678

Excited State 3: Singlet-A 3.0439 eV 407.32 nm f=0.1590 <S**2>=0.000
76 -> 78 0.65199
77 -> 78 0.13069
77 -> 79 -0.14578
77 -> 80 0.14956

Excited State 4: Singlet-A 3.5360 eV 350.63 nm f=0.0941 <S**2>=0.000
72 -> 78 0.12663
76 -> 79 0.68070

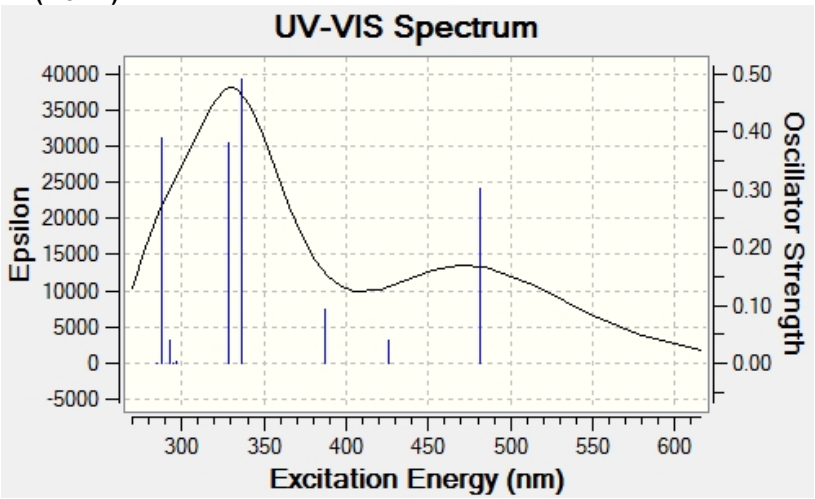
Excited State 5: Singlet-A 3.6903 eV 335.97 nm f=0.7762 <S**2>=0.000
76 -> 78 -0.13871
77 -> 80 0.67377

Excited State 6: Singlet-A 3.9238 eV 315.98 nm f=0.0001 <S**2>=0.000
73 -> 78 0.70072
Excited State 7: Singlet-A 4.0272 eV 307.87 nm f=0.0054 <S**2>=0.000
75 -> 78 0.67157
77 -> 81 -0.12232
77 -> 83 0.13660

Excited State 8: Singlet-A 4.1075 eV 301.85 nm f=0.0281 <S**2>=0.000
72 -> 78 0.10399
74 -> 78 0.66353
77 -> 81 0.13730

Excited State 9: Singlet-A 4.2377 eV 292.57 nm f=0.3490 <S**2>=0.000
72 -> 78 0.63417
74 -> 79 0.16214
76 -> 79 -0.11615
77 -> 84 -0.12789

11 (MeCN)



Excited State 1: Singlet-A 2.5754 eV 481.41 nm f=0.3026 <S**2>=0.000
76 -> 78 -0.14179
77 -> 78 0.68057

Excited State 2: Singlet-A 2.9094 eV 426.15 nm f=0.0395 <S**2>=0.000
76 -> 78 0.15311
77 -> 78 0.12465
77 -> 79 0.67214

Excited State 3: Singlet-A 3.2034 eV 387.04 nm f=0.0942 <S**2>=0.000
76 -> 78 0.64377
77 -> 78 0.10164
77 -> 79 -0.16683
77 -> 80 0.18018

Excited State 4: Singlet-A 3.6871 eV 336.26 nm f=0.4916 <S**2>=0.000
74 -> 78 0.14028
76 -> 78 -0.13857
76 -> 79 0.22080
77 -> 80 0.62896

Excited State 5: Singlet-A 3.7713 eV 328.76 nm f=0.3807 <S**2>=0.000
74 -> 78 0.10439
76 -> 79 0.63656
77 -> 80 -0.23233

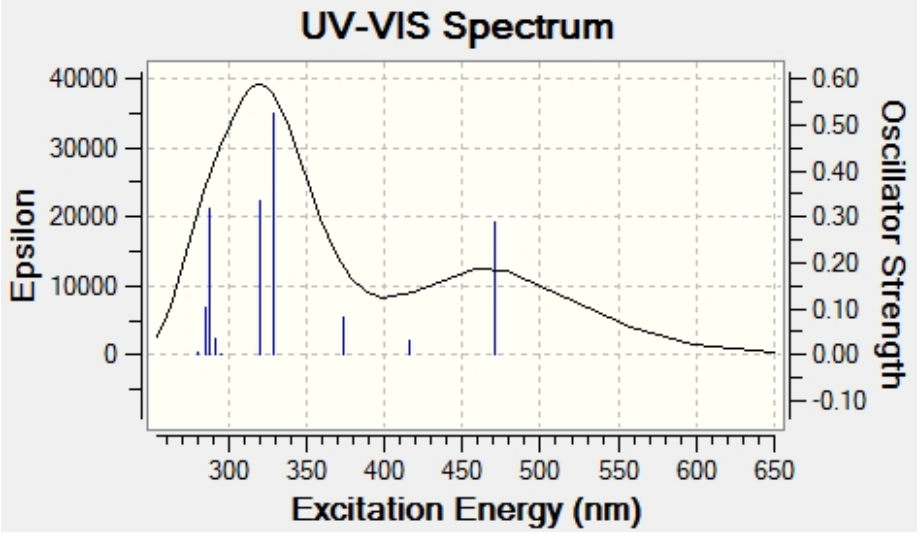
Excited State 6: Singlet-A 4.1749 eV 296.97 nm f=0.0027 <S**2>=0.000
74 -> 78 0.16223
75 -> 78 -0.38188
77 -> 81 0.52743
77 -> 82 0.16084

Excited State 7: Singlet-A 4.2000 eV 295.20 nm f=0.0000 <S**2>=0.000
72 -> 78 0.70502

Excited State 8: Singlet-A 4.2412 eV 292.33 nm f=0.0386 <S**2>=0.000
73 -> 78 0.55732
74 -> 78 0.24728
75 -> 78 0.25123
77 -> 81 0.10478
77 -> 82 -0.15973

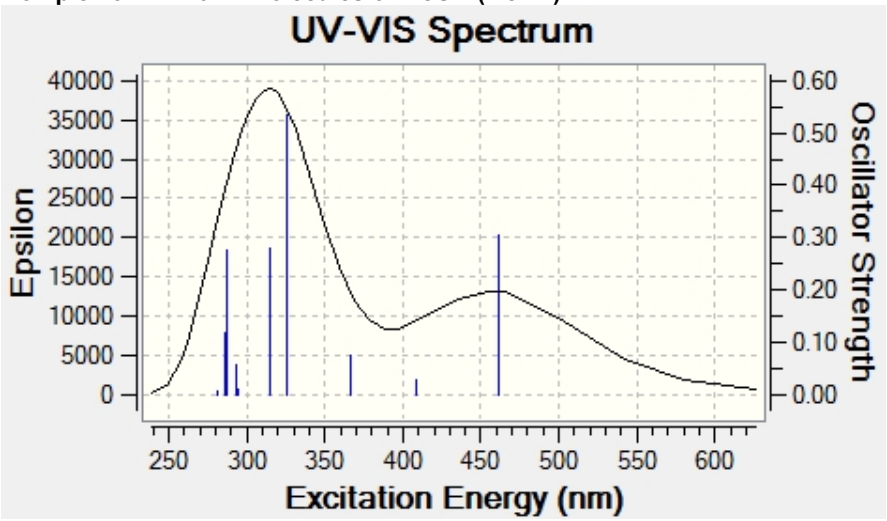
Excited State 9: Singlet-A 4.3046 eV 288.03 nm f=0.3878 <S**2>=0.000
73 -> 78 -0.31926
74 -> 78 0.48564
75 -> 78 0.23526
76 -> 79 -0.15047
76 -> 80 0.14376
77 -> 80 -0.10149
77 -> 84 -0.10085

Complex of 11 with 1 molecule of MeOH (MeCN)



Excited State 1: Singlet-A 2.6364 eV 470.27 nm f=0.2876 <S**2>=0.000
85 -> 87 0.12681
86 -> 87 0.68489
Excited State 2: Singlet-A 2.9804 eV 416.00 nm f=0.0315 <S**2>=0.000
85 -> 87 0.14176
86 -> 87 -0.10863
86 -> 88 0.67720
Excited State 3: Singlet-A 3.3219 eV 373.23 nm f=0.0816 <S**2>=0.000
85 -> 87 0.64470
86 -> 88 -0.14783
86 -> 89 0.19483
Excited State 4: Singlet-A 3.7657 eV 329.25 nm f=0.5236 <S**2>=0.000
83 -> 87 -0.17843
85 -> 87 -0.15332
85 -> 88 -0.18559
86 -> 89 0.63100
Excited State 5: Singlet-A 3.8707 eV 320.31 nm f=0.3329 <S**2>=0.000
83 -> 87 0.17075
85 -> 88 0.63175
86 -> 89 0.21041
Excited State 6: Singlet-A 4.1981 eV 295.33 nm f=0.0021 <S**2>=0.000
84 -> 87 0.57796
86 -> 90 -0.35866
86 -> 91 -0.13567
Excited State 7: Singlet-A 4.2423 eV 292.25 nm f=0.0337 <S**2>=0.000
82 -> 87 0.58790
83 -> 87 -0.28664
86 -> 90 0.15870
Excited State 8: Singlet-A 4.3134 eV 287.44 nm f=0.3171 <S**2>=0.000
81 -> 87 -0.14372
82 -> 87 0.23125
83 -> 87 0.54518
85 -> 88 -0.18588
86 -> 90 0.17261
Excited State 9: Singlet-A 4.3381 eV 285.80 nm f=0.1042 <S**2>=0.000
80 -> 87 -0.10154
81 -> 87 -0.32641
82 -> 87 -0.19710
83 -> 87 -0.12426
84 -> 87 0.30674
86 -> 90 0.43960

Complex of 11 with 2 molecules of MeOH (MeCN)



Excited State 1: Singlet-A 2.6887 eV 461.13 nm f=0.3055 <S**2>=0.000
94 -> 96 -0.11408
95 -> 96 0.68706

Excited State 2: Singlet-A 3.0337 eV 408.69 nm f=0.0290 <S**2>=0.000
94 -> 96 -0.15218
95 -> 96 -0.10546
95 -> 97 0.67479

Excited State 3: Singlet-A 3.3789 eV 366.94 nm f=0.0757 <S**2>=0.000
94 -> 96 0.64428
95 -> 97 0.15499
95 -> 98 -0.19481

Excited State 4: Singlet-A 3.8112 eV 325.31 nm f=0.5341 <S**2>=0.000
92 -> 96 0.16320
94 -> 96 0.15707
94 -> 97 0.14064
95 -> 98 0.63939

Excited State 5: Singlet-A 3.9335 eV 315.20 nm f=0.2800 <S**2>=0.000
92 -> 96 0.19555
94 -> 97 0.62946
95 -> 98 -0.17937

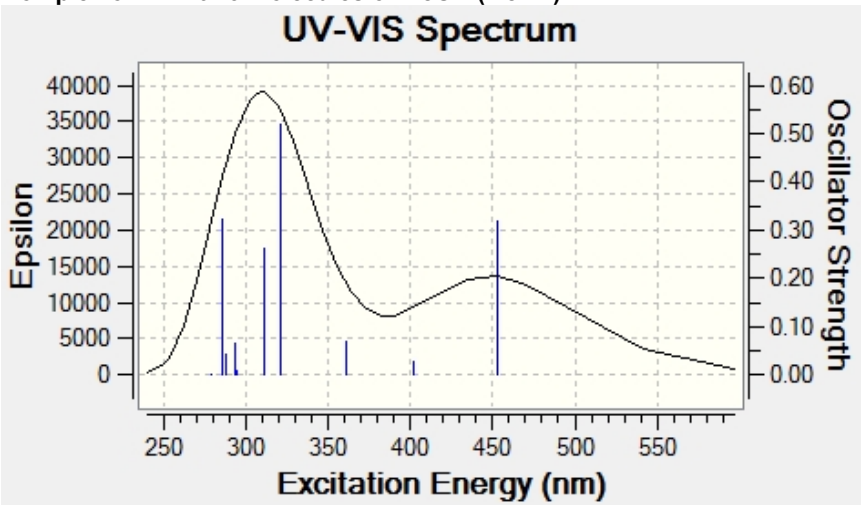
Excited State 6: Singlet-A 4.2116 eV 294.39 nm f=0.0079 <S**2>=0.000
92 -> 96 0.12790
93 -> 96 0.60671
95 -> 99 0.26794
95 ->100 -0.16134

Excited State 7: Singlet-A 4.2328 eV 292.91 nm f=0.0552 <S**2>=0.000
91 -> 96 0.48461
92 -> 96 -0.44904
94 -> 97 0.12594
95 -> 99 -0.10548

Excited State 8: Singlet-A 4.3202 eV 286.99 nm f=0.2739 <S**2>=0.000
90 -> 96 -0.27757
91 -> 96 0.41893
92 -> 96 0.38679
94 -> 97 -0.19126

Excited State 9: Singlet-A 4.3401 eV 285.67 nm f=0.1161 <S**2>=0.000
90 -> 96 0.61898
91 -> 96 0.15471
92 -> 96 0.15804
93 -> 96 -0.10235
94 -> 97 -0.11213
95 -> 99 0.13500

Complex of 11 with 3 molecules of MeOH (MeCN)



Excited State 1: Singlet-A 2.7363 eV 453.10 nm f=0.3184 <S**2>=0.000
103 ->105 -0.10188
104 ->105 0.68900

Excited State 2: Singlet-A 3.0811 eV 402.40 nm f=0.0265 <S**2>=0.000
103 ->105 0.16156
104 ->105 0.10162
104 ->106 0.67260

Excited State 3: Singlet-A 3.4328 eV 361.17 nm f=0.0704 <S**2>=0.000
103 ->105 0.64312
104 ->106 -0.16096
104 ->107 -0.19550

Excited State 4: Singlet-A 3.8576 eV 321.40 nm f=0.5181 <S**2>=0.000
101 ->105 0.17185
103 ->105 0.15646
103 ->106 -0.11802
104 ->107 0.63928

Excited State 5: Singlet-A 3.9894 eV 310.78 nm f=0.2624 <S**2>=0.000
101 ->105 -0.23217
103 ->106 0.61479
104 ->107 0.17352

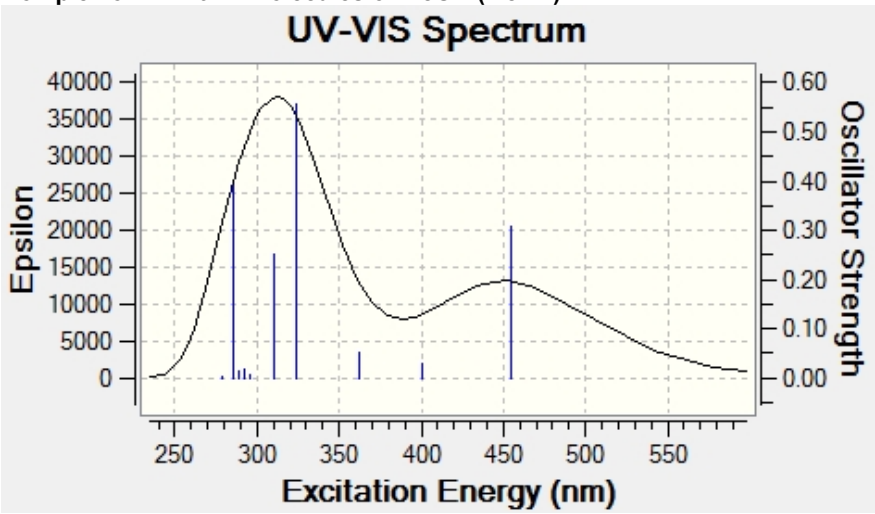
Excited State 6: Singlet-A 4.2023 eV 295.04 nm f=0.0069 <S**2>=0.000
101 ->105 -0.16720
102 ->105 0.63362
104 ->108 -0.18499
104 ->109 -0.14842

Excited State 7: Singlet-A 4.2235 eV 293.56 nm f=0.0663 <S**2>=0.000
99 ->105 0.17371
100 ->105 0.41382
101 ->105 0.47372
102 ->105 0.11916
103 ->106 0.16284

Excited State 8: Singlet-A 4.3014 eV 288.24 nm f=0.0427 <S**2>=0.000
99 ->105 0.46988
100 ->105 -0.45235
101 ->105 0.19449
104 ->108 -0.10848

Excited State 9: Singlet-A 4.3341 eV 286.07 nm f=0.3211 <S**2>=0.000
99 ->105 0.46503
100 ->105 0.26068
101 ->105 -0.30195
101 ->106 -0.12065
103 ->106 -0.23186
104 ->107 0.11188

Complex of 11 with 4 molecules of MeOH (MeCN)



Excited State 1: Singlet-A 2.7284 eV 454.42 nm f=0.3093 <S**2>=0.000
112 ->114 -0.10083
113 ->114 0.68841

Excited State 2: Singlet-A 3.0916 eV 401.04 nm f=0.0305 <S**2>=0.000
112 ->114 0.16032
113 ->114 0.10674
113 ->115 0.67207

Excited State 3: Singlet-A 3.4223 eV 362.29 nm f=0.0513 <S**2>=0.000
112 ->114 0.63846
113 ->115 -0.15970
113 ->116 -0.21656

Excited State 4: Singlet-A 3.8262 eV 324.04 nm f=0.5554 <S**2>=0.000
110 ->114 0.17199
112 ->114 0.18171
112 ->115 -0.10746
113 ->116 0.64162

Excited State 5: Singlet-A 4.0000 eV 309.96 nm f=0.2529 <S**2>=0.000
110 ->114 -0.23447
112 ->115 0.62484
113 ->116 0.15030

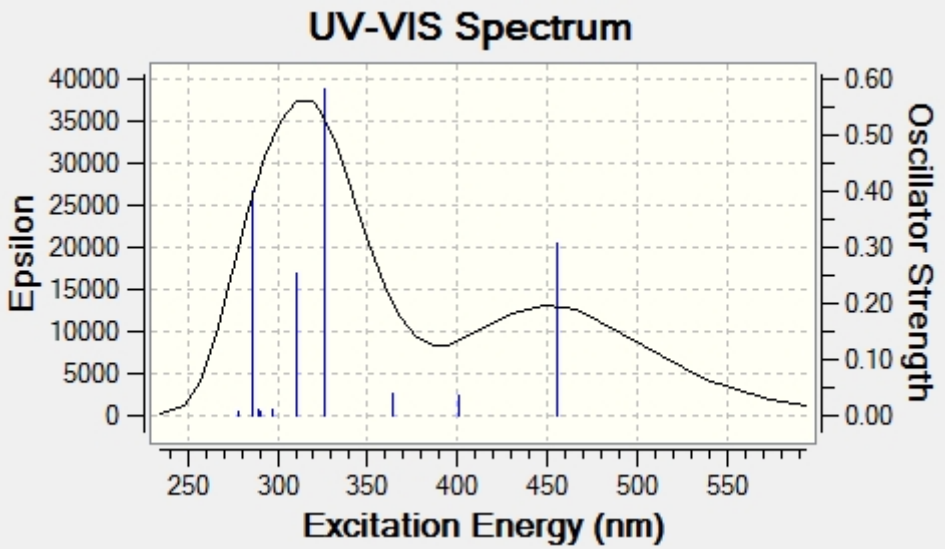
Excited State 6: Singlet-A 4.1881 eV 296.04 nm f=0.0079 <S**2>=0.000
111 ->114 0.65908
113 ->117 -0.14799
113 ->118 -0.15586

Excited State 7: Singlet-A 4.2452 eV 292.06 nm f=0.0182 <S**2>=0.000
108 ->114 -0.18482
109 ->114 0.56519
110 ->114 -0.30899
113 ->117 -0.11487

Excited State 8: Singlet-A 4.2989 eV 288.41 nm f=0.0129 <S**2>=0.000
108 ->114 0.61359
109 ->114 0.29132
110 ->114 0.16036

Excited State 9: Singlet-A 4.3361 eV 285.94 nm f=0.3930 <S**2>=0.000
108 ->114 -0.26891
109 ->114 0.20355
110 ->114 0.50222
110 ->115 0.10202
112 ->115 0.26329
113 ->116 -0.10516

Complex of 11 with 5 molecules of MeOH (MeCN)



Excited State 1: Singlet-A 2.7238 eV 455.19 nm f=0.3044 <S**2>=0.000
122 ->123 0.68791

Excited State 2: Singlet-A 3.0940 eV 400.73 nm f=0.0338 <S**2>=0.000
121 ->123 -0.16195
122 ->123 0.11131
122 ->124 0.67089

Excited State 3: Singlet-A 3.4100 eV 363.58 nm f=0.0382 <S**2>=0.000
121 ->123 0.63297
122 ->124 0.16124
122 ->125 0.23462

Excited State 4: Singlet-A 3.7971 eV 326.53 nm f=0.5828 <S**2>=0.000
119 ->123 -0.17218
121 ->123 -0.20165
121 ->124 0.10205
122 ->125 0.63946

Excited State 5: Singlet-A 3.9995 eV 310.00 nm f=0.2531 <S**2>=0.000
119 ->123 -0.23539
121 ->124 0.63046
122 ->125 -0.13783

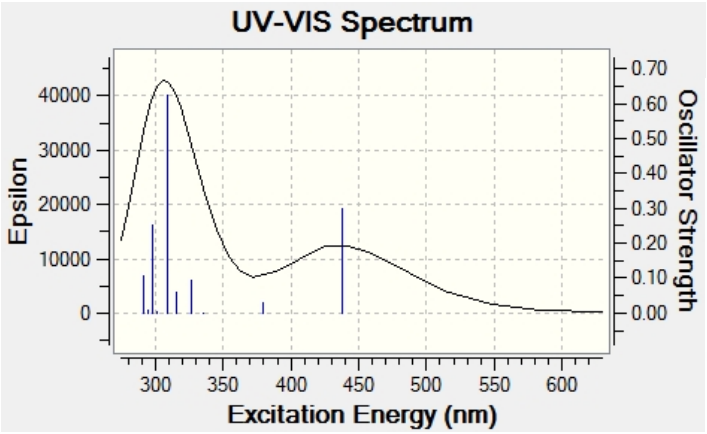
Excited State 6: Singlet-A 4.1740 eV 297.04 nm f=0.0078 <S**2>=0.000
120 ->123 0.66678
122 ->126 -0.11350
122 ->127 -0.15762

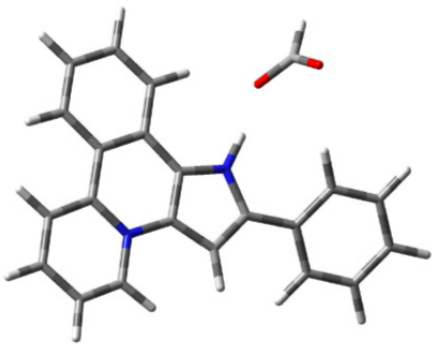
Excited State 7: Singlet-A 4.2625 eV 290.87 nm f=0.0049 <S**2>=0.000
117 ->123 0.53199
118 ->123 0.40005
122 ->126 -0.15175

Excited State 8: Singlet-A 4.2894 eV 289.05 nm f=0.0100 <S**2>=0.000
117 ->123 -0.39677
118 ->123 0.52621
119 ->123 -0.22724

Excited State 9: Singlet-A 4.3361 eV 285.93 nm f=0.4000 <S**2>=0.000
117 ->123 -0.10366
118 ->123 0.20171
119 ->123 0.56495
121 ->124 0.26316

Complex of 11 with formic acid (MeCN)





Excited State 1: Singlet-A 2.8343 eV 437.45 nm f=0.2999 <S**2>=0.000
89 -> 90 0.69788

Excited State 2: Singlet-A 3.2638 eV 379.87 nm f=0.0286 <S**2>=0.000
86 -> 90 -0.12950
89 -> 91 0.68312

Excited State 3: Singlet-A 3.6959 eV 335.47 nm f=0.0000 <S**2>=0.000
88 -> 90 0.70508

Excited State 4: Singlet-A 3.7929 eV 326.88 nm f=0.0932 <S**2>=0.000
85 -> 90 -0.12130
86 -> 90 0.34737
87 -> 90 0.22343
89 -> 92 0.53805

Excited State 5: Singlet-A 3.9253 eV 315.86 nm f=0.0591 <S**2>=0.000
86 -> 90 -0.16651
87 -> 90 0.66074
89 -> 92 -0.17390

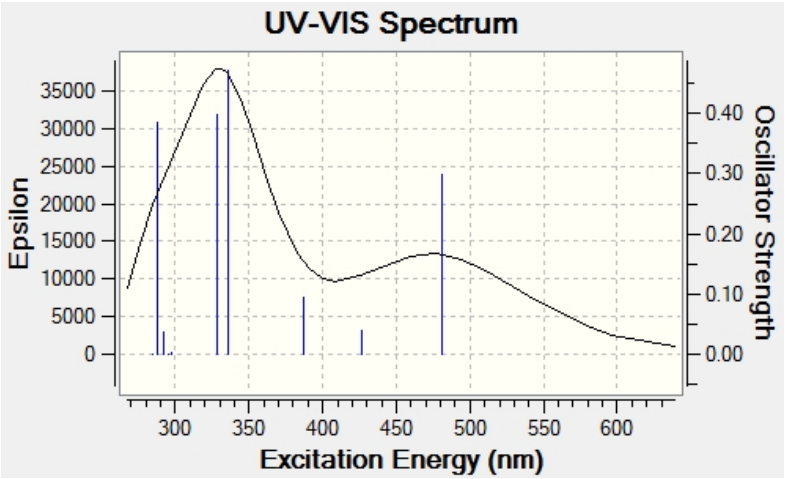
Excited State 6: Singlet-A 4.0064 eV 309.46 nm f=0.6252 <S**2>=0.000
82 -> 90 -0.21130
83 -> 90 -0.21217
84 -> 90 -0.10872
86 -> 90 0.45985
89 -> 92 -0.38527
89 -> 93 0.10174

Excited State 7: Singlet-A 4.1088 eV 301.75 nm f=0.0032 <S**2>=0.000
84 -> 90 0.14792
85 -> 90 0.65628
86 -> 90 0.18708

Excited State 8: Singlet-A 4.1586 eV 298.14 nm f=0.2507 <S**2>=0.000
82 -> 90 0.37548
83 -> 90 0.14066
84 -> 90 0.39747
85 -> 90 -0.14696
85 -> 91 0.10265
86 -> 90 0.18777
86 -> 91 -0.24170
89 -> 91 0.10208
89 -> 92 -0.12686

Excited State 9: Singlet-A 4.2124 eV 294.33 nm f=0.0082 <S**2>=0.000
82 -> 90 -0.33379
83 -> 90 -0.21967
84 -> 90 0.53893
86 -> 90 -0.13241
86 -> 91 0.10998

11 (MeOH)



Excited State 1: Singlet-A 2.5758 eV 481.34 nm f=0.2991 <S**2>=0.000
76 -> 78 -0.14319
77 -> 78 0.68007

Excited State 2: Singlet-A 2.9077 eV 426.40 nm f=0.0394 <S**2>=0.000
76 -> 78 0.15242
77 -> 78 0.12583
77 -> 79 0.67203

Excited State 3: Singlet-A 3.2024 eV 387.16 nm f=0.0936 <S**2>=0.000
76 -> 78 0.64345
77 -> 78 0.10255
77 -> 79 -0.16653
77 -> 80 0.18082

Excited State 4: Singlet-A 3.6887 eV 336.12 nm f=0.4711 <S**2>=0.000
74 -> 78 0.14472
76 -> 78 -0.13662
76 -> 79 0.23482
77 -> 80 0.62336

Excited State 5: Singlet-A 3.7705 eV 328.82 nm f=0.3975 <S**2>=0.000
74 -> 78 0.10223
76 -> 79 0.63149
77 -> 80 -0.24590

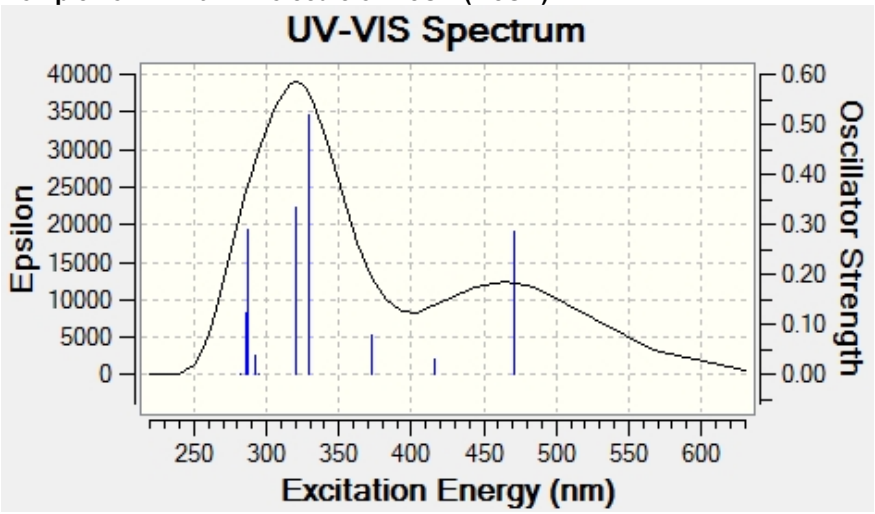
Excited State 6: Singlet-A 4.1748 eV 296.98 nm f=0.0027 <S**2>=0.000
74 -> 78 0.15592
75 -> 78 -0.38931
77 -> 81 0.52367
77 -> 82 0.16187

Excited State 7: Singlet-A 4.1972 eV 295.40 nm f=0.0000 <S**2>=0.000
72 -> 78 0.70503

Excited State 8: Singlet-A 4.2403 eV 292.39 nm f=0.0365 <S**2>=0.000
73 -> 78 0.56063
74 -> 78 0.24798
75 -> 78 0.24305
77 -> 81 0.10555
77 -> 82 -0.15953

Excited State 9: Singlet-A 4.3060 eV 287.94 nm f=0.3846 <S**2>=0.000
73 -> 78 -0.31311
74 -> 78 0.49299
75 -> 78 0.22573
76 -> 79 -0.15078
76 -> 80 0.14381
77 -> 80 -0.10230
77 -> 84 -0.10289

Complex of 11 with 1 molecule of MeOH (MeOH)



Excited State 1: Singlet-A 2.6359 eV 470.37 nm f=0.2862 <S**2>=0.000
85 -> 87 0.12745
86 -> 87 0.68467

Excited State 2: Singlet-A 2.9767 eV 416.52 nm f=0.0310 <S**2>=0.000
85 -> 87 0.14095
86 -> 87 -0.10897
86 -> 88 0.67729

Excited State 3: Singlet-A 3.3215 eV 373.28 nm f=0.0808 <S**2>=0.000
85 -> 87 0.64436
86 -> 88 -0.14709
86 -> 89 0.19602

Excited State 4: Singlet-A 3.7648 eV 329.32 nm f=0.5185 <S**2>=0.000
83 -> 87 -0.17570
85 -> 87 -0.15377
85 -> 88 -0.18786
86 -> 89 0.62980

Excited State 5: Singlet-A 3.8694 eV 320.42 nm f=0.3336 <S**2>=0.000
83 -> 87 0.16831
85 -> 88 0.63096
86 -> 89 0.21243

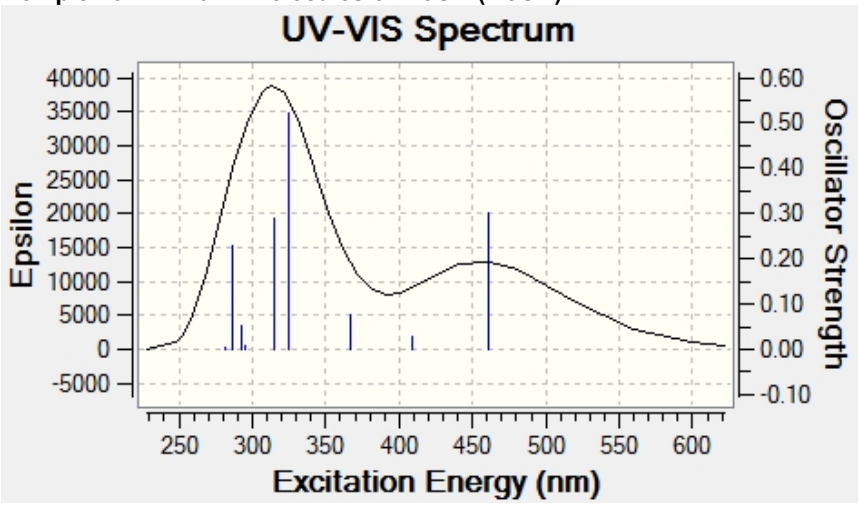
Excited State 6: Singlet-A 4.2015 eV 295.10 nm f=0.0022 <S**2>=0.000
84 -> 87 0.56049
86 -> 90 -0.38010
86 -> 91 -0.13657

Excited State 7: Singlet-A 4.2417 eV 292.30 nm f=0.0376 <S**2>=0.000
82 -> 87 0.57532
83 -> 87 -0.31895
84 -> 87 0.10882
86 -> 90 0.11742
86 -> 91 -0.11247

Excited State 8: Singlet-A 4.3141 eV 287.39 nm f=0.2886 <S**2>=0.000
81 -> 87 -0.18647
82 -> 87 0.26776
83 -> 87 0.52118
85 -> 88 -0.17700
86 -> 90 0.17022

Excited State 9: Singlet-A 4.3371 eV 285.87 nm f=0.1242 <S**2>=0.000
81 -> 87 -0.37813
82 -> 87 -0.18678
83 -> 87 -0.13753
84 -> 87 0.30649
86 -> 90 0.40007

Complex of 11 with 2 molecules of MeOH (MeOH)



Excited State 1: Singlet-A 2.6891 eV 461.06 nm f=0.3023 <S**2>=0.000
94 -> 96 -0.11511
95 -> 96 0.68674

Excited State 2: Singlet-A 3.0322 eV 408.90 nm f=0.0288 <S**2>=0.000
94 -> 96 -0.15184
95 -> 96 -0.10628
95 -> 97 0.67469

Excited State 3: Singlet-A 3.3779 eV 367.04 nm f=0.0752 <S**2>=0.000
94 -> 96 0.64406
95 -> 97 0.15486
95 -> 98 -0.19524

Excited State 4: Singlet-A 3.8130 eV 325.16 nm f=0.5226 <S**2>=0.000
92 -> 96 0.16592
94 -> 96 0.15619
94 -> 97 0.14774
95 -> 98 0.63701

Excited State 5: Singlet-A 3.9327 eV 315.27 nm f=0.2871 <S**2>=0.000
92 -> 96 0.19328
94 -> 97 0.62818
95 -> 98 -0.18633

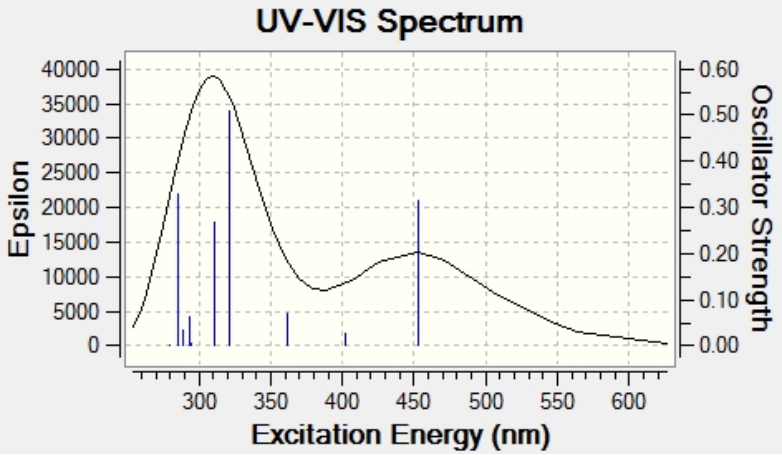
Excited State 6: Singlet-A 4.2100 eV 294.50 nm f=0.0075 <S**2>=0.000
92 -> 96 0.12372
93 -> 96 0.61001
95 -> 99 0.26348
95 ->100 -0.16051

Excited State 7: Singlet-A 4.2319 eV 292.97 nm f=0.0524 <S**2>=0.000
91 -> 96 0.48679
92 -> 96 -0.44799
94 -> 97 0.12318
95 -> 99 -0.10396

Excited State 8: Singlet-A 4.3198 eV 287.01 nm f=0.2285 <S**2>=0.000
90 -> 96 -0.34837
91 -> 96 0.39726
92 -> 96 0.36646
94 -> 97 -0.17667

Excited State 9: Singlet-A 4.3379 eV 285.81 nm f=0.1593 <S**2>=0.000
90 -> 96 0.58493
91 -> 96 0.19769
92 -> 96 0.20654
93 -> 96 -0.10044
94 -> 97 -0.13439
95 -> 99 0.11780

Complex of 11 with 3 molecules of MeOH (MeOH)



Excited State 1: Singlet-A 2.7370 eV 453.00 nm f=0.3153 <S**2>=0.000
103 ->105 -0.10284
104 ->105 0.68872

Excited State 2: Singlet-A 3.0796 eV 402.60 nm f=0.0263 <S**2>=0.000
103 ->105 0.16134
104 ->105 0.10239
104 ->106 0.67249

Excited State 3: Singlet-A 3.4318 eV 361.28 nm f=0.0701 <S**2>=0.000
103 ->105 0.64296
104 ->106 -0.16092
104 ->107 -0.19572

Excited State 4: Singlet-A 3.8595 eV 321.24 nm f=0.5077 <S**2>=0.000
101 ->105 0.17421
103 ->105 0.15553
103 ->106 -0.12399
104 ->107 0.63726

Excited State 5: Singlet-A 3.9885 eV 310.85 nm f=0.2677 <S**2>=0.000
101 ->105 -0.22916
103 ->106 0.61439
104 ->107 0.17942

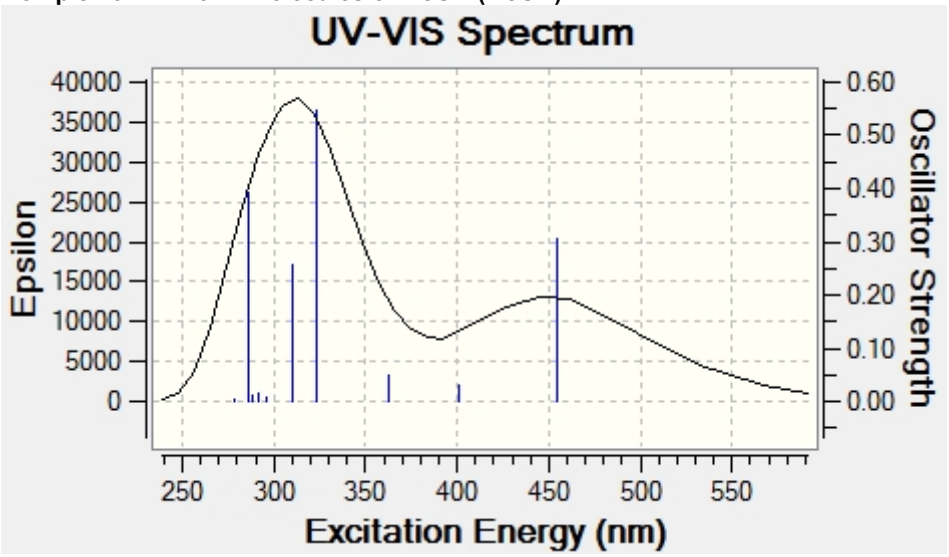
Excited State 6: Singlet-A 4.2004 eV 295.17 nm f=0.0066 <S**2>=0.000
101 ->105 -0.16288
102 ->105 0.63605
104 ->108 -0.18151
104 ->109 -0.14737

Excited State 7: Singlet-A 4.2225 eV 293.63 nm f=0.0634 <S**2>=0.000
99 ->105 0.21489
100 ->105 -0.39597
101 ->105 0.47397
102 ->105 0.11544
103 ->106 0.15970

Excited State 8: Singlet-A 4.2978 eV 288.48 nm f=0.0323 <S**2>=0.000
99 ->105 0.44215
100 ->105 0.48782
101 ->105 0.18325
104 ->108 -0.10808

Excited State 9: Singlet-A 4.3345 eV 286.04 nm f=0.3297 <S**2>=0.000
99 ->105 0.47004
100 ->105 -0.23081
101 ->105 -0.31161
101 ->106 -0.12435
103 ->106 -0.23582
104 ->107 0.11516

Complex of 11 with 4 molecules of MeOH (MeOH)



Excited State 1: Singlet-A 2.7284 eV 454.42 nm f=0.3093 <S**2>=0.000
112 ->114 -0.10083
113 ->114 0.68841

Excited State 2: Singlet-A 3.0916 eV 401.04 nm f=0.0305 <S**2>=0.000
112 ->114 0.16032
113 ->114 0.10674
113 ->115 0.67207

Excited State 3: Singlet-A 3.4223 eV 362.29 nm f=0.0513 <S**2>=0.000
112 ->114 0.63846
113 ->115 -0.15970
113 ->116 -0.21656

Excited State 4: Singlet-A 3.8262 eV 324.04 nm f=0.5554 <S**2>=0.000
110 ->114 0.17199
112 ->114 0.18171
112 ->115 -0.10746
113 ->116 0.64162

Excited State 5: Singlet-A 4.0000 eV 309.96 nm f=0.2529 <S**2>=0.000
110 ->114 -0.23447
112 ->115 0.62484
113 ->116 0.15030

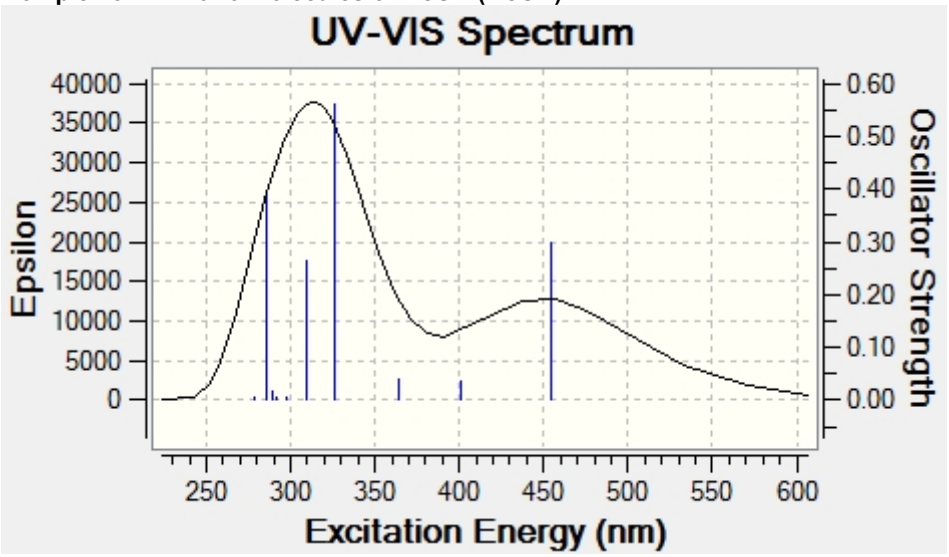
Excited State 6: Singlet-A 4.1881 eV 296.04 nm f=0.0079 <S**2>=0.000
111 ->114 0.65908
113 ->117 -0.14799
113 ->118 -0.15586

Excited State 7: Singlet-A 4.2452 eV 292.06 nm f=0.0182 <S**2>=0.000
108 ->114 -0.18482
109 ->114 0.56519
110 ->114 -0.30899
113 ->117 -0.11487

Excited State 8: Singlet-A 4.2989 eV 288.41 nm f=0.0129 <S**2>=0.000
108 ->114 0.61359
109 ->114 0.29132
110 ->114 0.16036

Excited State 9: Singlet-A 4.3361 eV 285.94 nm f=0.3930 <S**2>=0.000
108 ->114 -0.26891
109 ->114 0.20355
110 ->114 0.50222
110 ->115 0.10202
112 ->115 0.26329
113 ->116 -0.10516

Complex of 11 with 5 molecules of MeOH (MeOH)



Excited State 1: Singlet-A 2.7269 eV 454.67 nm f=0.2984 <S**2>=0.000
121 ->123 0.10154
122 ->123 0.68736

Excited State 2: Singlet-A 3.0953 eV 400.56 nm f=0.0339 <S**2>=0.000
121 ->123 -0.16231
122 ->123 0.11283
122 ->124 0.67047

Excited State 3: Singlet-A 3.4104 eV 363.55 nm f=0.0406 <S**2>=0.000
121 ->123 0.63411
122 ->124 0.16205
122 ->125 0.23031

Excited State 4: Singlet-A 3.8085 eV 325.55 nm f=0.5627 <S**2>=0.000
119 ->123 -0.17059
121 ->123 -0.19558
121 ->124 0.11312
122 ->125 0.63801

Excited State 5: Singlet-A 3.9991 eV 310.03 nm f=0.2653 <S**2>=0.000
119 ->123 -0.22300
121 ->124 0.62935
122 ->125 -0.14925

Excited State 6: Singlet-A 4.1652 eV 297.67 nm f=0.0060 <S**2>=0.000
120 ->123 0.67120
122 ->126 -0.10304
122 ->127 -0.14474

Excited State 7: Singlet-A 4.2563 eV 291.29 nm f=0.0043 <S**2>=0.000
117 ->123 0.37340
118 ->123 0.53768
119 ->123 -0.13154
122 ->126 -0.15089

Excited State 8: Singlet-A 4.2891 eV 289.07 nm f=0.0157 <S**2>=0.000
117 ->123 0.53745
118 ->123 -0.30540
119 ->123 0.30903

Excited State 9: Singlet-A 4.3399 eV 285.68 nm f=0.3944 <S**2>=0.000
117 ->123 -0.18111
118 ->123 0.27515
119 ->123 0.51368
121 ->124 0.25951

Table S33. B3LYP/6-31G+(d,p) Absolute Energies (au), Cartesian Coordinates of stationary points

Compound **11** (gas phase)

E = -918.22282813, **H (0K)** = -917.931203,
H (298K) = -917.914961, **G (298K)** = -917.976036 au.
Imaginary frequency = 0.

C	-2.7886430	-3.4683810	0.0000590
C	-1.6027360	-2.7921720	-0.0000520
C	-2.7217110	-0.6496520	0.0000440
C	-3.9409700	-1.3640820	0.0001860
C	-0.3043560	-0.7874810	-0.0000250
C	-2.6384720	0.7936450	-0.0000150
C	-1.3664930	1.4498320	-0.0000370
C	-0.1997420	0.6392610	-0.0000160
C	-1.3014040	2.8666390	-0.0000790
H	-0.3189190	3.3259850	-0.0000920
C	-2.4540210	3.6205440	-0.0001100
C	-3.7187930	2.9836300	-0.0001070
C	-3.8066000	1.6072960	-0.0000600
H	-2.7759370	-4.5523010	0.0000270
H	-0.6430550	-3.2876190	-0.0001860
H	-4.8616980	-0.7971250	0.0002890
H	-2.3968330	4.7051940	-0.0001450
H	-4.6261620	3.5797640	-0.0001520
H	-4.7916720	1.1557630	-0.0000820
C	1.8188330	-0.1314420	-0.0000320
N	1.0861770	1.0251760	0.0000230
N	-1.5424620	-1.4099810	-0.0000110
C	3.2875270	-0.0807160	-0.0000230
C	3.9491530	1.1626940	0.0004080
C	4.0712460	-1.2505100	-0.0004320
C	5.3415800	1.2304580	0.0004370
H	3.3478640	2.0649270	0.0007140
C	5.4641910	-1.1810570	-0.0004030
H	3.5908370	-2.2242860	-0.0008010
C	6.1084320	0.0603460	0.0000340
H	5.8316920	2.2004010	0.0007800
H	6.0480800	-2.0975190	-0.0007320
H	7.1933950	0.1144160	0.0000550
C	1.0045500	-1.2892240	-0.0000070
H	1.3363730	-2.3169210	0.0000330
C	-3.9990370	-2.7404970	0.0002080
H	-4.9551700	-3.2518170	0.0003390

Compound **11** (PCM toluene)

E = -918.22961087, **H (0K)** = -917.937949,
H (298K) = -917.921671, **G (298K)** = -917.982973 au.
Imaginary frequency = 0.

C	-2.7710600	-3.4747190	0.0183400
C	-1.5885510	-2.7913020	0.0112580
C	-2.7186580	-0.6573900	0.0041900
C	-3.9354540	-1.3760870	0.0128000
C	-0.3018900	-0.7778940	0.0002380
C	-2.6430730	0.7886370	-0.0043560
C	-1.3753670	1.4525880	-0.0067920
C	-0.2038950	0.6451900	-0.0027980
C	-1.3227740	2.8693930	-0.0138520
H	-0.3471820	3.3428830	-0.0157090
C	-2.4820050	3.6152660	-0.0190390
C	-3.7411520	2.9697320	-0.0179110
C	-3.8172060	1.5917760	-0.0108000
H	-2.7529120	-4.5582700	0.0232690
H	-0.6270130	-3.2828060	0.0105280
H	-4.8603590	-0.8164690	0.0147770
H	-2.4318360	4.7001950	-0.0246950
H	-4.6532120	3.5583750	-0.0231110
H	-4.7981850	1.1322030	-0.0114090
C	1.8208910	-0.1190480	-0.0023140
N	1.0850040	1.0357480	-0.0033180
N	-1.5390300	-1.4103340	0.0049650
C	3.2908720	-0.0699700	-0.0017040
C	3.9596010	1.1683830	0.0615330
C	4.0712750	-1.2411790	-0.0632880
C	5.3529470	1.2305970	0.0651570
H	3.3656690	2.0743440	0.1082470
C	5.4648920	-1.1777780	-0.0595720
H	3.5872660	-2.2114620	-0.1188620
C	6.1155790	0.0590300	0.0051690
H	5.8464230	2.1975560	0.1155860
H	6.0441690	-2.0958520	-0.1089500
H	7.2007090	0.1084360	0.0078880
C	1.0088780	-1.2776430	0.0001310
H	1.3408490	-2.3052290	0.0074180
C	-3.9837340	-2.7529580	0.0197720
H	-4.9368940	-3.2695590	0.0265250

Compound **11** (PCM CH_2Cl_2)

E = -918.23645305, **H (0K)** = -917.944674,
H (298K) = -917.928415, **G (298K)** = -917.989583 au.
Imaginary frequency = 0.

C	-2.7581460	-3.4795840	0.0200990
C	-1.5778710	-2.7907590	0.0126700
C	-2.7167770	-0.6639140	0.0045960
C	-3.9314970	-1.3851420	0.0139850
C	-0.3002660	-0.7703580	0.0008570
C	-2.6470980	0.7850030	-0.0049720
C	-1.3830720	1.4548390	-0.0069050
C	-0.2077130	0.6493120	-0.0023170
C	-1.3394590	2.8713590	-0.0144170
H	-0.3688910	3.3552640	-0.0156540
C	-2.5038950	3.6116760	-0.0208180
C	-3.7583330	2.9595080	-0.0207460
C	-3.8255250	1.5799090	-0.0130760
H	-2.7356190	-4.5628190	0.0254580

Compound **11** (PCM MeCN)

E = -918.23913726, **H (0K)** = -917.947427,
H (298K) = -917.932057, **G (298K)** = -917.990264 au.
Imaginary frequency = 0.

C	2.7525620	-3.4818790	-0.0000810
C	1.5732120	-2.7908480	-0.0000150
C	2.7160750	-0.6666690	-0.0000250
C	3.9297320	-1.3892870	-0.0001330
C	0.2997050	-0.7674370	0.0000190
C	2.6488510	0.7832080	0.0000360
C	1.3865050	1.4556560	-0.0000040
C	0.2090940	0.6514530	-0.0000270
C	1.3463010	2.8723680	0.0000090
H	0.3772220	3.3594450	-0.0000310
C	2.5126960	3.6105710	0.0000840
C	3.7653480	2.9553910	0.0001670
C	3.8290980	1.5751820	0.0001460
H	2.7280560	-4.5650300	-0.0000890

H	-0.6151100	-3.2796500	0.0121950	H	0.6098320	-3.2785150	0.0000150
H	-4.8595420	-0.8311690	0.0163420	H	4.8589480	-0.8373750	-0.0002240
H	-2.4592140	4.6967920	-0.0267510	H	2.4707320	4.6958010	0.0000940
H	-4.6740220	3.5421950	-0.0272370	H	4.6824570	3.5358110	0.0002600
H	-4.8033400	1.1143900	-0.0148290	H	4.8056840	1.1073080	0.0002470
C	1.8228600	-0.1096610	-0.0017280	C	-1.8236520	-0.1053640	0.0000010
N	1.0836600	1.0443010	-0.0031420	N	-1.0826600	1.0485410	-0.0000370
N	-1.5369580	-1.4110510	0.0057550	N	1.5356160	-1.4113540	-0.0000010
C	3.2939000	-0.0616750	-0.0014160	C	-3.2949670	-0.0578970	0.0000030
C	3.9688150	1.1736820	0.0682540	C	-3.9729970	1.1784490	-0.0003100
C	4.0717760	-1.2352710	-0.0699470	C	-4.0713310	-1.2349590	0.0003150
C	5.3630230	1.2317480	0.0711820	C	-5.3675230	1.2342050	-0.0003200
H	3.3816920	2.0838270	0.1212440	H	-3.3888820	2.0921740	-0.0005530
C	5.4660010	-1.1762540	-0.0665690	C	-5.4659160	-1.1782190	0.0003050
H	3.5855770	-2.2040650	-0.1305830	H	-3.5839850	-2.2049970	0.0005850
C	6.1220770	0.0579230	0.0042930	C	-6.1246450	0.0568470	-0.0000130
H	5.8592440	2.1970040	0.1268000	H	-5.8655850	2.2001080	-0.0005700
H	6.0414990	-2.0963240	-0.1212840	H	-6.0394950	-2.1010700	0.0005540
H	7.2072800	0.1034640	0.0065810	H	-7.2098910	0.1004780	-0.0000210
C	1.0122300	-1.2684010	0.0008750	C	-1.0136470	-1.2641530	0.0000310
H	1.3437910	-2.2960650	0.0080760	H	-1.3452620	-2.2919050	0.0000510
C	-3.9722080	-2.7626960	0.0215230	C	3.9674870	-2.7671720	-0.0001560
H	-4.9231860	-3.2830810	0.0288060	H	4.9175420	-3.2892240	-0.0002430

Compound **11** (PCM MeOH)

E = -918.23904461, **H (0K)** = -917.947339,
H (298K) = -917.931967, **G (298K)** = -917.990181 au.
Imaginary frequency = 0.

C	2.7527550	-3.4818060	0.0000170
C	1.5733720	-2.7908540	0.0000420
C	2.7160990	-0.6665740	-0.0000040
C	3.9297950	-1.3891500	-0.0000550
C	0.2997280	-0.7675430	0.0000210
C	2.6487850	0.7832650	0.0000060
C	1.3863850	1.4556280	-0.0000250
C	0.2090350	0.6513890	-0.0000220
C	1.3460630	2.8723440	-0.0000430
H	0.3769240	3.3592970	-0.0000740
C	2.5123890	3.6106210	-0.0000170
C	3.7651070	2.9555350	0.0000390
C	3.8289740	1.5753470	0.0000520
H	2.7283180	-4.5649620	0.0000330
H	0.6100100	-3.2785590	0.0000710
H	4.8589660	-0.8371570	-0.0001190
H	2.4703450	4.6958480	-0.0000320
H	4.6821660	3.5360360	0.0000790
H	4.8055990	1.1075460	0.0001150
C	-1.8236240	-0.1055090	0.0000020
N	-1.0826920	1.0484080	-0.0000340
N	1.5356540	-1.4113420	0.0000230
C	-3.2949260	-0.0580280	0.0000000
C	-3.9728560	1.1783580	0.0000220
C	-4.0713350	-1.2350430	-0.0000240
C	-5.3673700	1.2341890	0.0000220
H	-3.3886200	2.0920010	0.0000400
C	-5.4659120	-1.1782280	-0.0000230
H	-3.5840170	-2.2050960	-0.0000470
C	-6.1245550	0.0568770	0.0000000
H	-5.8653800	2.2001200	0.0000400
H	-6.0395550	-2.1010400	-0.0000420
H	-7.2098000	0.1005720	0.0000000

Compound **11*H_2O** (gas phase)

E = -994.67124022, **H (0K)** = -994.354665,
H (298K) = -994.335392, **G (298K)** = -994.403096 au.
Imaginary frequency = 0.

C	3.0343690	-3.5441200	-0.0350600
C	1.8261810	-2.9089910	-0.0181860
C	2.8681450	-0.7293670	-0.0234120
C	4.1126490	-1.4005230	-0.0412190
C	0.4601630	-0.9506200	-0.0002780
C	2.7321000	0.7096270	-0.0146800
C	1.4378630	1.3255570	0.0022550
C	0.3013430	0.4669460	0.0036160
C	1.3335400	2.7414210	0.0120580
H	0.3491320	3.1970810	0.0355310
C	2.4678300	3.5242660	0.0018250
C	3.7501550	2.9279970	-0.0166220
C	3.8767470	1.5553650	-0.0239420
H	3.0597740	-4.6277090	-0.0380450
H	0.8844930	-3.4373310	-0.0069290
H	5.0134380	-0.8030580	-0.0501240
H	2.3752780	4.6063180	0.0092620
H	4.6397240	3.5503540	-0.0245020
H	4.8737070	1.1316750	-0.0369100
C	-1.6930640	-0.4010780	-0.0008550
N	-1.0102810	0.7878190	0.0021110
N	1.7201770	-1.5304470	-0.0136570
C	-3.1631030	-0.4449510	-0.0254730
C	-3.9119290	0.6551120	-0.4854710
C	-3.8584960	-1.5942830	0.3976070
C	-5.3055960	0.6017520	-0.5216130
H	-3.3962940	1.5482910	-0.8200330
C	-5.2514160	-1.6460910	0.3576250
H	-3.3047170	-2.4462000	0.7809930
C	-5.9835700	-0.5471860	-0.1029990
H	-5.8632470	1.4611120	-0.8835540
H	-5.7663690	-2.5415330	0.6948140
H	-7.0687540	-0.5856770	-0.1327450

C	-1.0135980	-1.2642940	0.0000370
H	-1.3452160	-2.2920480	0.0000730
C	3.9676560	-2.7670240	-0.0000430
H	4.9177420	-3.2890220	-0.0000850

Complex of **11** with 1 molecule of MeOH (PCM MeCN)

E = -1033.98948794, **H (0K)** = -1033.644451, **H (298K)** = -1033.623564, **G (298K)** = -1033.697242 au.
Imaginary frequency = 0.

C	3.2786830	-3.5370010	0.2986700
C	2.0435600	-2.9578640	0.2119400
C	2.9944010	-0.7527930	-0.0046520
C	4.2670880	-1.3589210	0.0860780
C	0.5977370	-1.0688160	-0.0198530
C	2.7977830	0.6768990	-0.1603460
C	1.4809560	1.2310640	-0.2401690
C	0.3810150	0.3245130	-0.1688830
C	1.3195700	2.6310740	-0.3926600
H	0.3153000	3.0377690	-0.4432990
C	2.4196330	3.4625740	-0.4656980
C	3.7234640	2.9247820	-0.3889550
C	3.9052650	1.5634690	-0.2392260
H	3.3494380	-4.6116380	0.4159820
H	1.1270780	-3.5266720	0.2564650
H	5.1442600	-0.7298710	0.0377250
H	2.2830420	4.5336740	-0.5820370
H	4.5871450	3.5793660	-0.4471600
H	4.9181900	1.1850960	-0.1840960
C	-1.5793850	-0.6271320	-0.1268410
N	-0.9491320	0.5886630	-0.2337290
N	1.8863700	-1.5957330	0.0623960
C	-3.0458600	-0.7457690	-0.1827900
C	-3.8336840	0.2569590	-0.7814980
C	-3.7020160	-1.8753730	0.3471210
C	-5.2230430	0.1350430	-0.8456010
H	-3.3478670	1.1295060	-1.2035920
C	-5.0905520	-1.9984740	0.2782140
H	-3.1226540	-2.6558740	0.8311650
C	-5.8605620	-0.9930840	-0.3177580
H	-5.8087230	0.9208740	-1.3147630
H	-5.5726130	-2.8770300	0.6979450
H	-6.9413250	-1.0875260	-0.3690690
C	-0.6631240	-1.6887180	0.0102630
H	-0.9006560	-2.7397650	0.0806110
C	4.4251240	-2.7200730	0.2343640
H	5.4171650	-3.1519100	0.3009220
O	-2.0374470	3.1100850	0.3727290
H	-1.6890500	2.2080390	0.1458860
C	-1.9844650	3.2753470	1.7841830
H	-0.9564070	3.2061610	2.1684580
H	-2.3720390	4.2704740	2.0215780
H	-2.6009110	2.5318850	2.3093600

C	-0.8253540	-1.5127050	0.0001400
H	-1.1149960	-2.5521500	-0.0397600
C	4.2175810	-2.7736060	-0.0476980
H	5.1910040	-3.2510800	-0.0617130
O	-1.9145640	3.4498520	0.3406610
H	-1.6734590	2.4939140	0.2583680
H	-2.4083220	3.5284560	1.1651600

Complex of **11** with 2 molecules of MeOH (PCM MeCN)

E = -1149.73329275, **H (0K)** = -1149.335845, **H (298K)** = -1149.309755, **G (298K)** = -1149.398458 au.
Imaginary frequency = 0.

C	-3.3716490	-3.3016900	-0.9937710
C	-2.1373920	-2.7267160	-0.8730860
C	-3.0927290	-0.5733150	-0.3599370
C	-4.3643690	-1.1750360	-0.4850670
C	-0.6964200	-0.8681980	-0.4463710
C	-2.8981320	0.8294950	-0.0404440
C	-1.5827120	1.3807960	0.0717870
C	-0.4802150	0.4962730	-0.1368650
C	-1.4246390	2.7542920	0.3819140
H	-0.4223570	3.1619430	0.4569880
C	-2.5274880	3.5627020	0.5773520
C	-3.8295870	3.0276530	0.4697870
C	-4.0080020	1.6915300	0.1670170
H	-3.4405660	-4.3541940	-1.2407580
H	-1.2200110	-3.2777710	-1.0149750
H	-5.2431100	-0.5651080	-0.3327650
H	-2.3932960	4.6140890	0.8140260
H	-4.6949580	3.6642520	0.6235930
H	-5.0199070	1.3144630	0.0907710
C	1.4855570	-0.4258320	-0.3491950
N	0.8518580	0.7599240	-0.0772120
N	-1.9837130	-1.3923650	-0.5604010
C	2.9543620	-0.5414600	-0.3678630
C	3.7704060	0.4076180	0.2783670
C	3.5837990	-1.6179730	-1.0254180
C	5.1610810	0.2834970	0.2667000
H	3.3099490	1.2429800	0.7934450
C	4.9737190	-1.7427500	-1.0328670
H	2.9831300	-2.3556890	-1.5485430
C	5.7719610	-0.7920990	-0.3867720
H	5.7688040	1.0272860	0.7746840
H	5.4340680	-2.5797370	-1.5503550
H	6.8537750	-0.8878110	-0.3940940
C	0.5674460	-1.4738300	-0.5794250
H	0.8049910	-2.4998550	-0.8195180
C	-4.5193580	-2.5093810	-0.7938930
H	-5.5107220	-2.9388870	-0.8820660
O	1.9320200	3.3561620	0.0351720
H	1.5835210	2.4275850	-0.0137100
C	0.7013890	-1.4867330	3.5430440
H	0.7125580	-1.9657030	4.5248410
H	-0.2097940	-0.8813640	3.4579500
H	1.5755850	-0.8286750	3.4633310
O	0.7348560	-2.5318800	2.5666900
H	0.7310590	-2.1301400	1.6818060
C	2.2744430	3.7842360	-1.2773080
H	1.4053710	3.7806730	-1.9509090
H	2.6509010	4.8091200	-1.2096700
H	3.0601320	3.1568970	-1.7217870

Complex of **11** with 3 molecules of MeOH (PCM MeCN)			
E = -1265.47639819, **H (0K)** = -1265.026861, **H (298K)** = -1264.995398, **G (298K)** = -1265.099452 au. Imaginary frequency = 0.			
C	-3.3458490	-3.3283220	0.0587460
C	-2.1290930	-2.7053590	0.0687900
C	-3.1484290	-0.5203700	0.0418500
C	-4.4016630	-1.1712480	0.0320150
C	-0.7452490	-0.7567820	0.0722170
C	-2.9954530	0.9236880	0.0341570
C	-1.6972290	1.5235900	0.0458690
C	-0.5695250	0.6458060	0.0698770
C	-1.5777930	2.9346150	0.0374910
H	-0.5871870	3.3759860	0.0355660
C	-2.7038020	3.7349380	0.0206780
C	-3.9896560	3.1525720	0.0106010
C	-4.1298800	1.7780200	0.0163830
H	-3.3835460	-4.4109170	0.0657690
H	-1.1955490	-3.2474130	0.0833050
H	-5.2982500	-0.5685210	0.0176570
H	-2.6002230	4.8159220	0.0136990
H	-4.8730250	3.7828430	-0.0028000
H	-5.1304470	1.3648720	0.0069620
C	1.4251100	-0.2374640	0.1159330
N	0.7543510	0.9562100	0.0975100
N	-2.0159680	-1.3312180	0.0603750
C	2.8958410	-0.3062400	0.1741570
C	3.6572740	0.7898550	0.6239350
C	3.5793230	-1.4795920	-0.2029280
C	5.0496860	0.7139830	0.6922680
H	3.1518970	1.7008000	0.9241750
C	4.9708670	-1.5551480	-0.1306000
H	3.0208970	-2.3355210	-0.5693430
C	5.7151880	-0.4580100	0.3170790
H	5.6157930	1.5716110	1.0450200
H	5.4745700	-2.4694920	-0.4312180
H	6.7983370	-0.5157130	0.3713380
C	0.5388920	-1.3406960	0.0970550
H	0.8076610	-2.3867500	0.1309930
C	-4.5164110	-2.5448740	0.0398920
H	-5.4946810	-3.0117590	0.0316780
O	1.7794620	3.5119120	-0.5213230
H	1.4515680	2.6019830	-0.3027360
C	0.8267320	-0.4827010	4.1853590
H	0.7919850	-0.7622300	5.2408020
H	0.0433200	0.2609080	3.9927010
H	1.8049500	-0.0340870	3.9725330
O	0.6174780	-1.6793090	3.4291240
H	0.6494570	-1.4598060	2.4839040
C	0.7879860	-2.7397780	-3.6688790
H	0.7467780	-2.7636080	-4.7602080
H	0.0048230	-3.3994740	-3.2743010
H	1.7673260	-3.1155040	-3.3467390
O	0.5854510	-1.3806500	-3.2724490
H	0.6182580	-1.3336640	-2.3030040
C	2.1644500	3.5393610	-1.8907410
H	1.3225480	3.3093120	-2.5591970
H	2.5182910	4.5487320	-2.1199940
H	2.9787300	2.8318610	-2.1018040

Complex of **11** with 4 molecules of MeOH (PCM MeCN)			
E = -1381.21868249, **H (0K)** = -1380.716819, **H (298K)** = -1380.680026, **G (298K)** = -1380.799136 au. Imaginary frequency = 0.			
C	-2.8064480	-3.9522060	1.0283680
C	-1.6679520	-3.2153120	0.8557880
C	-2.9056650	-1.3522930	-0.0433010
C	-4.0772120	-2.1189870	0.1386490
C	-0.5040740	-1.2382280	0.1840300
C	-2.9062180	-0.0063920	-0.5891020
C	-1.6872700	0.7273610	-0.7324120
C	-0.4793980	0.0792300	-0.3291630
C	-1.7212960	2.0425400	-1.2607970
H	-0.7895970	2.5866530	-1.3756350
C	-2.9204250	2.6164700	-1.6422130
C	-4.1281040	1.8980540	-1.5064780
C	-4.1176770	0.6162700	-0.9912950
H	-2.7302370	-4.9496680	1.4439110
H	-0.6882350	-3.5851670	1.1179510
H	-5.0276860	-1.6878280	-0.1406040
H	-2.9328050	3.6225380	-2.0510580
H	-5.0676390	2.3500090	-1.8071530
H	-5.0611410	0.0931180	-0.9018450
C	1.5857950	-0.4554770	0.1295310
N	0.7959100	0.5515460	-0.3573800
N	-1.7002990	-1.9403850	0.3318380
C	3.0453110	-0.3090120	0.2737150
C	3.6509110	0.9621720	0.3083210
C	3.8738760	-1.4422930	0.4007060
C	5.0322770	1.0928750	0.4639990
H	3.0345850	1.8493700	0.2179770
C	5.2539060	-1.3096880	0.5595300
H	3.4398580	-2.4366890	0.3627810
C	5.8422840	-0.0404890	0.5917430
H	5.4760050	2.0842350	0.4911560
H	5.8706160	-2.1992030	0.6516150
H	6.9164760	0.0631020	0.7136290
C	0.8269440	-1.5975270	0.4801880
H	1.2025030	-2.5160310	0.9075110
C	-4.0464160	-3.3939900	0.6617470
H	-4.9650600	-3.9552290	0.7887980
C	2.0403930	2.7031450	-2.9107040
H	2.2686000	3.6626150	-3.3838280
H	1.3030150	2.1780660	-3.5345620
H	2.9616420	2.1042650	-2.8834370
O	1.5399820	2.9678370	-1.6053660
H	1.3172130	2.1054570	-1.1685280
C	-1.4923940	4.9194960	1.8662730
H	-1.5956220	5.3446430	2.8670140
H	-1.7928710	5.6755760	1.1303050
H	-0.4401750	4.6574010	1.7016280
O	-2.3390130	3.7662260	1.8155190
H	-2.2576620	3.3625010	0.9391100
C	0.5923600	0.6128580	4.0423940
H	0.5517340	0.6962340	5.1308310
H	-0.3284930	1.0366490	3.6227950
H	1.4503190	1.1908010	3.6772230
O	0.7226340	-0.7786060	3.7347990
H	0.7731560	-0.8806300	2.7707970
C	1.7011330	-2.2971740	-3.5610860

H	1.7882700	-2.9501950	-4.4324770
H	2.6925000	-1.8905270	-3.3260800
H	1.0247990	-1.4694980	-3.8086210
O	1.1897200	-3.0960510	-2.4898710
H	1.1222320	-2.5443420	-1.6936590

Complex of **11** with 5 molecules of MeOH (PCM MeCN)

E = -1496.96004198, **H (0K)** = -1496.406448, **H (298K)** = -1496.363961, **G (298K)** = -1496.502007 au.
Imaginary frequency = 0.

C	1.5247800	4.5018440	1.2265290
C	0.5697710	3.5372870	1.0632060
C	2.0793790	2.1302420	-0.1823040
C	3.0606060	3.1303290	-0.0094770
C	-0.1904970	1.4246890	0.2433900
C	2.3170660	0.8897720	-0.8993020
C	1.2845310	-0.0896090	-1.0342870
C	0.0177600	0.2068600	-0.4447130
C	1.5491660	-1.2931260	-1.7369850
H	0.7519470	-2.0209910	-1.8489220
C	2.7933380	-1.5246870	-2.2927100
C	3.8182720	-0.5606060	-2.1683740
C	3.5812930	0.6195290	-1.4881810
H	1.2753210	5.4020810	1.7749470
H	-0.4304360	3.6333870	1.4577500
H	4.0431000	2.9713980	-0.4297580
H	2.9823780	-2.4471650	-2.8335590
H	4.7907860	-0.7381020	-2.6163290
H	4.3854830	1.3412610	-1.4195890
C	-2.0482790	0.1868310	0.2566380
N	-1.1171190	-0.5429070	-0.4325180
N	0.8265720	2.3699010	0.3762620
C	-3.4163580	-0.3081540	0.4928850
C	-3.7332630	-1.6737250	0.3565150
C	-4.4450570	0.5765870	0.8749720
C	-5.0299670	-2.1344660	0.5924840
H	-2.9590150	-2.3747820	0.0667320
C	-5.7395120	0.1138540	1.1139650
H	-4.2373160	1.6375680	0.9724900
C	-6.0406100	-1.2454080	0.9734180
H	-5.2497410	-3.1928010	0.4827510
H	-6.5151670	0.8172000	1.4032750
H	-7.0485570	-1.6057200	1.1569770
C	-1.5236680	1.4245610	0.7009180
H	-2.0394490	2.1741040	1.2836270
C	2.8056510	4.2978700	0.6777990
H	3.5825030	5.0450660	0.7927560
C	-2.0622140	-2.5105350	-3.2444210
H	-2.1472040	-3.4211190	-3.8444340
H	-1.4596920	-1.7826500	-3.8065240
H	-3.0695980	-2.0937190	-3.1053350
O	-1.4557550	-2.8590870	-2.0051710
H	-1.3777690	-2.0422310	-1.4479670
C	1.7114800	-4.6604890	0.8372380
H	1.9301730	-5.2725780	1.7149480
H	1.9627080	-5.2344560	-0.0633450
H	0.6395180	-4.4291150	0.8271410
O	2.5077150	-3.4758360	0.9488810
H	2.3224340	-2.9064960	0.1880570
C	6.1162160	-2.2176720	1.3065680
H	6.7341130	-2.1922270	2.2068760

Complex of **11** with 1 molecule of MeOH (PCM MeOH)

E = -1033.98938872, **H (0K)** = -1033.644346, **H (298K)** = -1033.623437, **G (298K)** = -1033.697829 au.
Imaginary frequency = 0.

C	3.3207450	-3.5171120	0.2665400
C	2.0810600	-2.9463400	0.1905580
C	3.0144510	-0.7315120	-0.0005640
C	4.2919950	-1.3290800	0.0786040
C	0.6204050	-1.0657500	-0.0152470
C	2.8062430	0.6984890	-0.1363480
C	1.4849860	1.2437150	-0.2068500
C	0.3919670	0.3275460	-0.1474610
C	1.3132220	2.6447990	-0.3373830
H	0.3061700	3.0455450	-0.3799100
C	2.4072000	3.4852430	-0.3993040
C	3.7151300	2.9562810	-0.3326050
C	3.9070520	1.5943170	-0.2034080
H	3.3999800	-4.5925680	0.3701120
H	1.1690340	-3.5225750	0.2303950
H	5.1642650	-0.6928890	0.0354210
H	2.2623860	4.5569780	-0.4988380
H	4.5738730	3.6180650	-0.3819850
H	4.9227680	1.2226080	-0.1546900
C	-1.5606190	-0.6414770	-0.1145240
N	-0.9405720	0.5808110	-0.2084240
N	1.9131440	-1.5836590	0.0584150
C	-3.0261210	-0.7743370	-0.1679970
C	-3.8281350	0.2319300	-0.7414040
C	-3.6674520	-1.9225910	0.3398850
C	-5.2162820	0.0950310	-0.8028310
H	-3.3555140	1.1207400	-1.1437300
C	-5.0546680	-2.0604480	0.2736070
H	-3.0777080	-2.7067810	0.8049210
C	-5.8387690	-1.0516190	-0.2976190
H	-5.8128040	0.8843390	-1.2521180
H	-5.5246640	-2.9534880	0.6761130
H	-6.9185680	-1.1575110	-0.3469000
C	-0.6349190	-1.6964940	0.0091410
H	-0.8630150	-2.7502840	0.0682160
C	4.4607810	-2.6907410	0.2090320
H	5.4562440	-3.1158970	0.2669700
O	-2.0614170	3.1189460	0.2440620
H	-1.6998990	2.2085130	0.0781940
C	-2.2324840	3.2907310	1.6452140
H	-1.2822460	3.1964010	2.1906750
H	-2.6261890	4.2970720	1.8159620
H	-2.9455280	2.5665960	2.0645430

H	6.7123980	-2.6308770	0.4831590
H	5.2502260	-2.8651500	1.4853930
O	5.7162640	-0.8673560	1.0408010
H	5.1283560	-0.8653810	0.2722110
C	-0.6402940	-1.1521000	3.8873880
H	-0.3680700	-1.3484610	4.9269300
H	0.1542020	-1.5380000	3.2368290
H	-1.5747090	-1.6813110	3.6627250
O	-0.7900560	0.2649100	3.7554410
H	-1.0224540	0.4687910	2.8351640
C	-2.9217250	2.4675470	-3.1200290
H	-3.1823590	3.1997660	-3.8876500
H	-3.7988660	1.8391930	-2.9216900
H	-2.1079980	1.8363190	-3.4981550
O	-2.5244730	3.2035200	-1.9590180
H	-2.2801720	2.5756780	-1.2599400

Complex of **11** with 2 molecules of MeOH (PCM MeOH)

E = -1149.73318514, **H (0K)** = -1149.335732, **H (298K)** = -1149.309645, **G (298K)** = -1149.398311 au.
Imaginary frequency = 0.

C	-3.3722730	-3.3011080	-0.9938160
C	-2.1379310	-2.7263390	-0.8731350
C	-3.0929100	-0.5727370	-0.3600670
C	-4.3646480	-1.1742810	-0.4852040
C	-0.6966480	-0.8680680	-0.4464430
C	-2.8980890	0.8300110	-0.0405730
C	-1.5825690	1.3810860	0.0717050
C	-0.4802220	0.4964130	-0.1369740
C	-1.4242450	2.7545480	0.3818910
H	-0.4218880	3.1620030	0.4570340
C	-2.5269480	3.5631280	0.5773270
C	-3.8291540	3.0283200	0.4697020
C	-4.0078130	1.6922560	0.1668870
H	-3.4413570	-4.3536160	-1.2407470
H	-1.2206330	-3.2775490	-1.0149580
H	-5.2432800	-0.5641900	-0.3329150
H	-2.3925680	4.6144750	0.8140690
H	-4.6944080	3.6650820	0.6235070
H	-5.0197890	1.3153760	0.0906070
C	1.4853880	-0.4259820	-0.3492960
N	0.8518530	0.7598620	-0.0773870
N	-1.9840050	-1.3919880	-0.5605010
C	2.9541760	-0.5417770	-0.3680040
C	3.7703430	0.4074420	0.2778490
C	3.5834450	-1.6185800	-1.0252270
C	5.1609960	0.2831420	0.2661510
H	3.3100140	1.2430540	0.7926340
C	4.9733430	-1.7435220	-1.0327140
H	2.9826560	-2.3563910	-1.5480790
C	5.7717140	-0.7927440	-0.3869820
H	5.7688250	1.0270460	0.7738380
H	5.4335760	-2.5807360	-1.5499400
H	6.8535180	-0.8885870	-0.3943200
C	0.5671320	-1.4738770	-0.5794810
H	0.8045620	-2.4999660	-0.8194090
C	-4.5198680	-2.5086000	-0.7939860
H	-5.5113030	-2.9379540	-0.8821410
O	1.9323160	3.3560790	0.0356130
H	1.5837410	2.4275690	-0.0134450
C	0.7040060	-1.4877980	3.5436880

Complex of **11** with 3 molecules of MeOH (PCM MeOH)

E = -1265.47625673, **H (0K)** = -1265.026713, **H (298K)** = -1264.995254, **G (298K)** = -1265.099270 au.
Imaginary frequency = 0.

C	-3.3457650	-3.3284560	0.0580750
C	-2.1290630	-2.7054260	0.0683170
C	-3.1485110	-0.5204660	0.0413790
C	-4.4017060	-1.1714610	0.0313570
C	-0.7453240	-0.7567790	0.0718270
C	-2.9956270	0.9235690	0.0339390
C	-1.6974310	1.5235470	0.0460580
C	-0.5696870	0.6458520	0.0699460
C	-1.5780580	2.9345890	0.0381220
H	-0.5874730	3.3760080	0.0365290
C	-2.7040930	3.7348420	0.0212740
C	-3.9899280	3.1524150	0.0106920
C	-4.1300960	1.7778760	0.0160780
H	-3.3834050	-4.4110550	0.0650980
H	-1.1954860	-3.2474180	0.0830740
H	-5.2983180	-0.5687710	0.0170000
H	-2.6005630	4.8158320	0.0146320
H	-4.8733150	3.7826630	-0.0027960
H	-5.1306410	1.3646860	0.0062470
C	1.4249870	-0.2372600	0.1158310
N	0.7541380	0.9563350	0.0977850
N	-2.0159810	-1.3312570	0.0599230
C	2.8957250	-0.3058360	0.1741860
C	3.6568690	0.7902750	0.6244210
C	3.5794750	-1.4789100	-0.2032120
C	5.0492750	0.7146370	0.6929280
H	3.1512620	1.7010250	0.9248620
C	4.9710200	-1.5542290	-0.1307160
H	3.0212680	-2.3347970	-0.5700590
C	5.7150510	-0.4571070	0.3174580
H	5.6151680	1.5722650	1.0460220
H	5.4749500	-2.4683620	-0.4315960
H	6.7982050	-0.5146160	0.3718520
C	0.5388540	-1.3405850	0.0965200
H	0.8077370	-2.3866130	0.1303940
C	-4.5163890	-2.5450770	0.0390930
H	-5.4946270	-3.0120300	0.0307240
O	1.7786280	3.5126030	-0.5204310
H	1.4511110	2.6024990	-0.3021350
C	0.8279220	-0.4857250	4.1861520

H	0.7118590	-1.9676810	4.5250750	H	0.7888220	-0.7660130	5.2412450
H	-0.2028030	-0.8757980	3.4592460	H	0.0488330	0.2620360	3.9920130
H	1.5828960	-0.8359760	3.4644040	H	1.8089830	-0.0418650	3.9764600
O	0.7298150	-2.5323410	2.5664810	O	0.6147160	-1.6805720	3.4282660
H	0.7287600	-2.1298940	1.6819160	H	0.6505470	-1.4604010	2.4833480
C	2.2774430	3.7833130	-1.2764010	C	0.7938610	-2.7391740	-3.6688930
H	1.4095110	3.7805450	-1.9514940	H	0.7490080	-2.7643760	-4.7600500
H	2.6549810	4.8077830	-1.2084480	H	0.0171230	-3.4045010	-3.2710220
H	3.0631530	3.1549200	-1.7193540	H	1.7771550	-3.1072220	-3.3499060
				O	0.5823810	-1.3813200	-3.2730440
				H	0.6178940	-1.3331360	-2.3037610
				C	2.1642220	3.5404550	-1.8896480
				H	1.3227700	3.3100130	-2.5585400
				H	2.5175910	4.5500690	-2.1185810
				H	2.9790040	2.8334510	-2.1004460

Complex of **11** with 4 molecules of MeOH (PCM MeOH)

E = -1381.21855240, **H (0K)** = -1380.716700,
H (298K) = -1380.679894, **G (298K)** = -1380.799179 au.
Imaginary frequency = 0.

C	-2.8050440	-3.9528600	1.0273190
C	-1.6667300	-3.2156100	0.8551190
C	-2.9047950	-1.3527460	-0.0438520
C	-4.0761520	-2.1198320	0.1377180
C	-0.5032680	-1.2380730	0.1840150
C	-2.9056380	-0.0067420	-0.5893320
C	-1.6868720	0.7274140	-0.7321200
C	-0.4788960	0.0795170	-0.3289100
C	-1.7211210	2.0428290	-1.2599080
H	-0.7895180	2.5871800	-1.3742130
C	-2.9203060	2.6165490	-1.6414060
C	-4.1278070	1.8976750	-1.5063780
C	-4.1171650	0.6157050	-0.9916810
H	-2.7286280	-4.9503870	1.4426750
H	-0.6869480	-3.5852320	1.1173800
H	-5.0266870	-1.6888550	-0.1416190
H	-2.9328980	3.6228220	-2.0497400
H	-5.0673840	2.3494740	-1.8071600
H	-5.0605020	0.0922350	-0.9027230
C	1.5863560	-0.4546250	0.1299890
N	0.7962340	0.5522140	-0.3568730
N	-1.6993150	-1.9405700	0.3314320
C	3.0457940	-0.3077030	0.2743490
C	3.6508900	0.9636970	0.3095580
C	3.8747580	-1.4407330	0.4008690
C	5.0321920	1.0948380	0.4653640
H	3.0342220	1.8506970	0.2196070
C	5.2547260	-1.3076870	0.5598180
H	3.4410860	-2.4352620	0.3624410
C	5.8426090	-0.0382820	0.5926370
H	5.4755470	2.0863520	0.4929860
H	5.8717700	-2.1970090	0.6515330
H	6.9167560	0.0656600	0.7146290
C	0.8278230	-1.5970020	0.4803150
H	1.2035930	-2.5153140	0.9078720
C	-4.0451100	-3.3949250	0.6605660
H	-4.9636220	-3.9564480	0.7873320
C	2.0402690	2.7020800	-2.9118200
H	2.2678760	3.6610900	-3.3861660
H	1.3029820	2.1758820	-3.5348480
H	2.9618190	2.1036870	-2.8840520

Complex of **11** with 5 molecules of MeOH (PCM MeOH)

E = -1496.95995619, **H (0K)** = -1496.406503,
H (298K) = -1496.363946, **G (298K)** = -1496.502995 au.
Imaginary frequency = 0.

C	1.4142350	4.5250180	1.1470540
C	0.4685260	3.5487220	1.0000870
C	2.0012470	2.1223670	-0.1946360
C	2.9727580	3.1345250	-0.0382900
C	-0.2665350	1.4085050	0.2299830
C	2.2556700	0.8669500	-0.8790940
C	1.2315290	-0.1227830	-1.0002000
C	-0.0409640	0.1753490	-0.4246280
C	1.5093360	-1.3389640	-1.6753120
H	0.7172120	-2.0736200	-1.7783810
C	2.7595100	-1.5739160	-2.2160590
C	3.7773850	-0.6008690	-2.1026110
C	3.5271330	0.5919030	-1.4500970
H	1.1524410	5.4371360	1.6694640
H	-0.5357790	3.6462340	1.3837700
H	3.9602030	2.9729400	-0.4457190
H	2.9586280	-2.5057760	-2.7368980
H	4.7547140	-0.7815480	-2.5386640
H	4.3263810	1.3198860	-1.3900070
C	-2.1087800	0.1488090	0.2688850
N	-1.1664410	-0.5877430	-0.3967170
N	0.7410990	2.3660480	0.3459400
C	-3.4676640	-0.3628780	0.5200400
C	-3.7465540	-1.7422660	0.4673630
C	-4.5222200	0.5165020	0.8374610
C	-5.0327880	-2.2224230	0.7207930
H	-2.9491690	-2.4377790	0.2319010
C	-5.8064420	0.0346710	1.0941950
H	-4.3418670	1.5865510	0.8707590
C	-6.0699980	-1.3383850	1.0366550
H	-5.2234410	-3.2911080	0.6768690
H	-6.6033470	0.7332920	1.3327500
H	-7.0697960	-1.7134430	1.2346630
C	-1.6026330	1.4052450	0.6802230
H	-2.1315660	2.1629010	1.2404070
C	2.7019490	4.3173840	0.6158780
H	3.4715770	5.0737950	0.7184600
C	-2.0865300	-2.5109620	-3.2416640
H	-2.1597230	-3.4086760	-3.8622990
H	-1.4648460	-1.7753400	-3.7718880
H	-3.0952470	-2.0913210	-3.1219500

O	1.5400680	2.9681400	-1.6066850	O	-1.5160980	-2.8880160	-1.9938010
H	1.3175720	2.1061930	-1.1689690	H	-1.4369920	-2.0805970	-1.4236010
C	-1.4934560	4.9186320	1.8630680	C	1.7677440	-4.5735270	1.0240800
H	-1.6012720	5.3521190	2.8597450	H	2.0251500	-5.1472740	1.9170510
H	-1.7855100	5.6703370	1.1192610	H	1.9405970	-5.2009790	0.1409180
H	-0.4413990	4.6503830	1.7074920	H	0.7052830	-4.3058710	1.0712030
O	-2.3451010	3.7690000	1.8157920	O	2.6058430	-3.4128020	1.0205850
H	-2.2615640	3.3590890	0.9424670	H	2.3878490	-2.8768880	0.2442800
C	0.5933300	0.6111510	4.0445930	C	6.6738640	-2.0002510	1.0080910
H	0.5479920	0.6928930	5.1329700	H	7.4887620	-1.8730570	1.7239530
H	-0.3226000	1.0418790	3.6212960	H	7.0983050	-2.2939470	0.0401080
H	1.4569140	1.1839580	3.6846140	H	6.0106240	-2.7967610	1.3662760
O	0.7157260	-0.7806080	3.7351620	O	5.9938160	-0.7426320	0.9271850
H	0.7697670	-0.8813220	2.7712220	H	5.2673970	-0.8232460	0.2932550
C	1.7022400	-2.2996720	-3.5609870	C	-0.2770670	-0.9284810	3.8727820
H	1.7880860	-2.9534430	-4.4319480	H	-0.0671100	-1.1115860	4.9290390
H	2.6944440	-1.8949600	-3.3261480	H	0.6705010	-0.9336210	3.3199800
H	1.0277110	-1.4707020	-3.8091620	H	-0.9150940	-1.7374040	3.4958530
O	1.1890080	-3.0967410	-2.4893460	O	-0.9303830	0.3420370	3.7908030
H	1.1225910	-2.5443980	-1.6934950	H	-1.1286630	0.5290290	2.8591270
				C	-2.9767240	2.3557560	-3.1801930
				H	-3.2635510	3.0716210	-3.9538610
				H	-3.8317270	1.7001850	-2.9736230
				H	-2.1431810	1.7486380	-3.5546950
				O	-2.6015790	3.1153190	-2.0271030
				H	-2.3458440	2.5022430	-1.3191330

Complex of **11** with formic acid (PCM MeCN)

E = -1108.04750210, **H (0K)** = -1107.719995,
H (298K) = -1107.699192, **G (298K)** = -1107.771786 au.
Imaginary frequency = 0.

C	-3.6629650	-3.3967530	0.3175590
C	-2.3892750	-2.9077410	0.2261070
C	-3.1800510	-0.6368300	0.0602920
C	-4.4921770	-1.1476520	0.1565060
C	-0.8139750	-1.1246850	0.0138330
C	-2.8824190	0.7790170	-0.0755920
C	-1.5321170	1.2391680	-0.1593330
C	-0.5186920	0.2392050	-0.0998910
C	-1.2599150	2.6203730	-0.2952250
H	-0.2283820	2.9502630	-0.3688900
C	-2.2987750	3.5311100	-0.3430550
C	-3.6357500	3.0907420	-0.2590280
C	-3.9205160	1.7440660	-0.1294270
H	-3.8116120	-4.4650520	0.4154500
H	-1.5177110	-3.5439280	0.2482520
H	-5.3217110	-0.4563290	0.1309660
H	-2.0840940	4.5901390	-0.4476980
H	-4.4481090	3.8090070	-0.2977200
H	-4.9583320	1.4424870	-0.0713680
C	1.4118810	-0.8969340	-0.0742130
N	0.8420930	0.3584940	-0.1452820
N	-2.1396640	-1.5594620	0.1003710
C	2.8635200	-1.1173360	-0.0907370
C	3.7618810	-0.1308450	0.3590940
C	3.3793130	-2.3467950	-0.5458990
C	5.1371430	-0.3746100	0.3503700
H	3.3925910	0.8210920	0.7296830
C	4.7534080	-2.5857980	-0.5463110
H	2.7035220	-3.1108970	-0.9173140
C	5.6399070	-1.5996190	-0.0991320
H	5.8169790	0.3951620	0.7041710

H	5.1322220	-3.5383390	-0.9050910	
H	6.7100610	-1.7842270	-0.1026590	
C	0.3992210	-1.8487060	0.0275480	
H	0.5503850	-2.9116090	0.1309750	
C	-4.7447410	-2.4969630	0.2828350	
H	-5.7648180	-2.8565690	0.3545580	
H	1.3593970	1.2653650	-0.2802410	
C	2.7162430	3.4284440	0.1806830	
O	2.9738150	3.1172920	1.3668290	
O	2.0309270	2.7630730	-0.6609360	
H	3.1277710	4.3921530	-0.1977380	