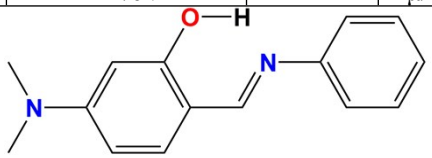
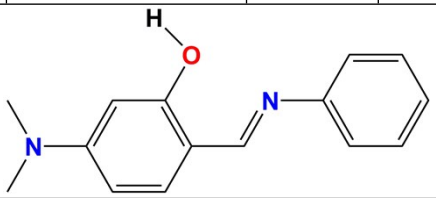
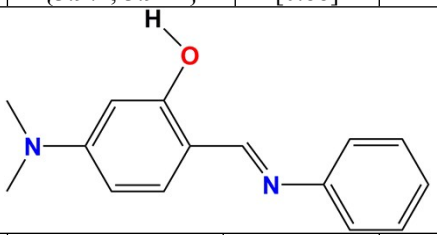
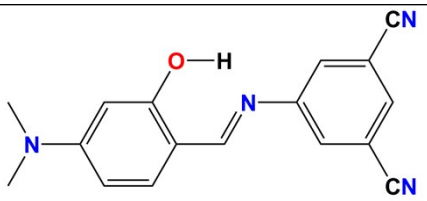
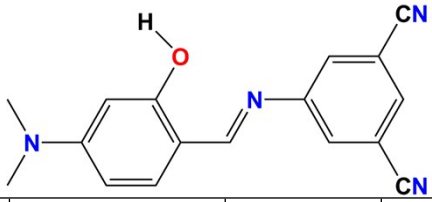
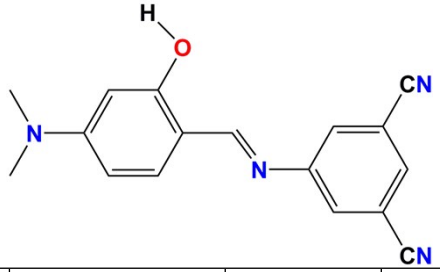
Electronic Supporting Information for "Photophysical Transformations Induced by Chemical Substitution to Salicylaldimines"

Cristina A. Barboza[a*], Pawel Gawrys[a*], Marzena Banasiewicz[a], Kinga Suwinska[b] and Andrzej L. Sobolewski[a]

[a] Physics Institute, Polish Academy of Sciences, Al. Lotników 32/46, Warsaw, Poland
[b] Faculty of Mathematics and Natural Sciences, Cardinal Stefan Wyszynski University in Warsaw, K. Woycickiego 1/3, Warsaw, Poland

Table S1. Vertical transition energy (ΔE), oscillator strength (f), dipole moment (μ), and leading electronic configurations computed with ADC(2)/cc-pVDZ method at the MP2/cc-pVDZ equilibrium geometry of the ground state computed for the compounds **1** and **4**. Excitation energies were also obtained at the ADC(2)/aug-cc-pVDZ, CC2/cc-pVDZ level of calculation and spin-scaled variants SCS-CC2 and SOS-CC2, besides on the CCSD(F12)/cc-pVDZ levels of theory. In braces are given excitation energies computed using the COSMO approximation with dielectric constant of two solvents, cyclohexane[§] and acetonitrile[§§] , respectively.

Molecule			ΔE/eV	f	μ/Debye	el. conf.
1	***enol***					
	S_0 $^1\pi\pi^*$	ADC(2)/cc-pVDZ	0.00 3.76{3.65[§]; 3.63[§§]}	- 0.87	3.43 8.93	$(64a)^2$ 0.93 (64a-65a)
		ADC(2)/aug-cc-pVDZ	3.65	0.88	9.45	
		CC2/cc-pVDZ	3.85	0.98	8.50	
		SCS-CC2/cc-pVDZ	3.97	0.90	7.45	
		SOS-CC2/cc-pVDZ	4.07	0.84	6.92	
		CCSD(F12)/cc-pVDZ	4.10			
	cis-open					
	S_0 $^1\pi\pi^*$		0.59 4.06 [4.13] {3.97[§]; 3.91[§§]}	- 0.77 [0.88]	5.28 4.90 [5.86]	$(64a)^2$ 0.86 (64a-65a)
	trans-open					
	S_0 $^1\pi\pi^*$		0.43 3.95 [4.03] {3.83[§]; 3.71[§§]}	- 0.86 [0.95]	5.40 8.33 [8.58]	$(64a)^2$ 0.90 (64a-65a)

4	***enol***					
	S_0 $^1\pi\pi^*$	ADC(2)/cc-pVDZ	0.00 3.46	- 0.93	9.04 19.76	$(76a)^2$ 0.82 (76a-77a)
		ADC(2)/aug-cc-pVDZ	3.36	0.91	20.64	
		CC2/cc-pVDZ	3.57	1.14	18.36	
		SCS-CC2/cc-pVDZ	3.71	1.11	16.68	
		SOS-CC2/cc-pVDZ	3.77	1.09	15.94	
		CCSD/cc-pVDZ	3.87			
	cis-open					
	S_0 $^1\pi\pi^*$		0.51 3.85	- 1.03	11.58 20.91	$(76a)^2$ 0.91 (76a-78a)
	trans-open					
	S_0 $^1\pi\pi^*$		0.36 3.71	- 0.97	11.61 21.23	$(76a)^2$ 0.80 (76a-77a)

***** Energy respective to the enol species of each derivative.

Table S2. Vertical transition energy (ΔE), oscillator strength (f), dipole moment (μ), and leading electronic configurations computed with ADC(2)/cc-pVDZ method at the MP2/cc-pVDZ equilibrium geometry of the ground state computed using two explicit methanol molecules for the compounds **1** and **4**.

Molecule		State	ΔE/eV	f	μ/Debye	el. conf.
1	***enol***	S_0 $^1\pi\pi^*$	0.00 3.80	- 0.81	2.92 9.18	$(82a)^2$ 0.93 (82a-83a)
	cis-open	S_0 $^1\pi\pi^*$	0.23 4.01*	- 0.92	8.13 14.09	$(82a)^2$ 0.91 (82a-83a)
	trans-open	S_0 $^1\pi\pi^*$	0.27 3.78*	- 0.95	7.27 11.28	$(82a)^2$ 0.92 (82a-83a)
4	***enol***	S_0 $^1\pi\pi^*$	0.00 3.70	- 0.88	9.96 22.01	$(94a)^2$ 0.70 (94a-96a)
	cis-open	S_0 $^1\pi\pi^*$	0.18* 3.82	- 0.99	13.57 23.06	$(94a)^2$ 0.92 (94a-95a)
	trans-open	S_0 $^1\pi\pi^*$	0.20* 3.56	- 0.95	13.84 23.27	$(94a)^2$ 0.93 (94a-95a)

***** Energy respective to the enol species of each derivative.

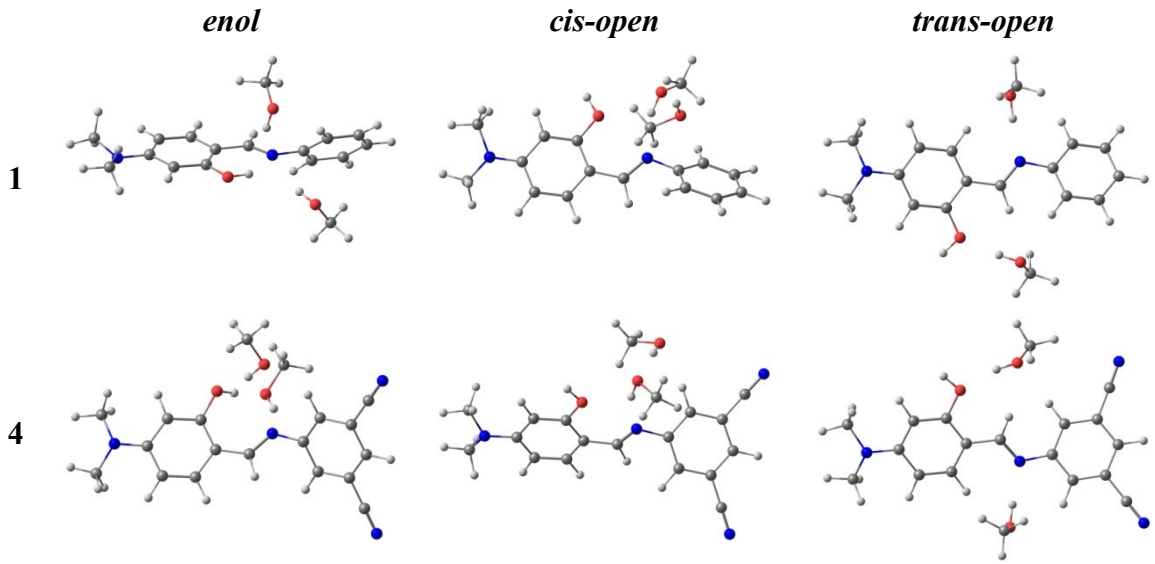
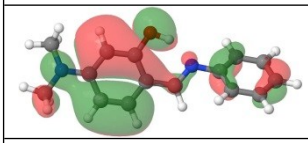
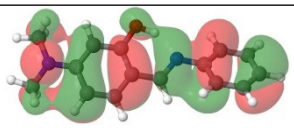
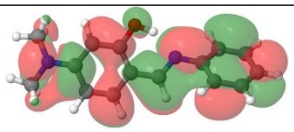
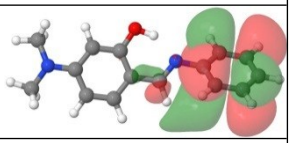
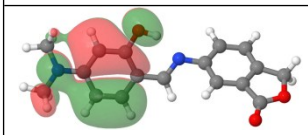
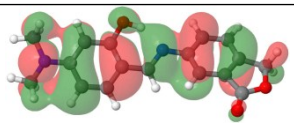
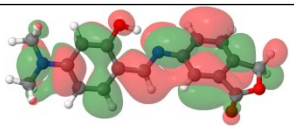
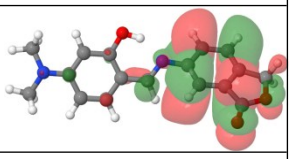
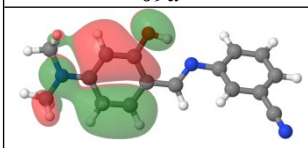
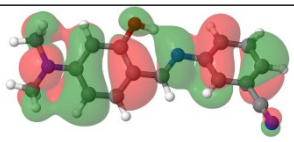
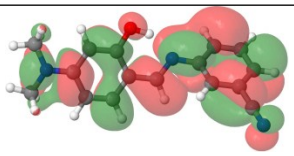
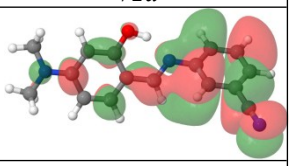
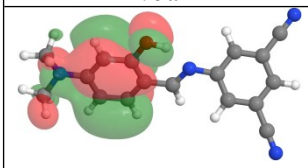
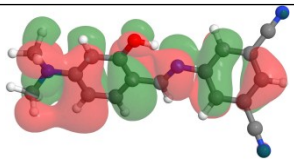
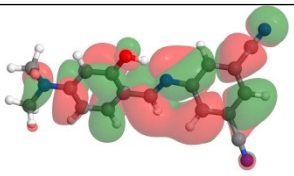
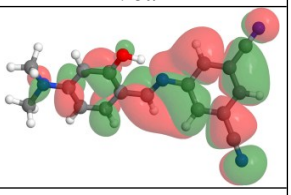
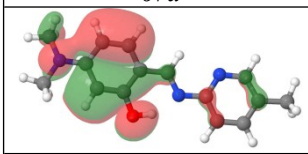
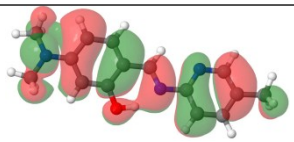
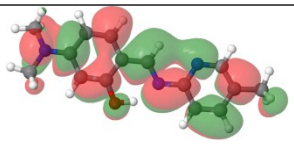
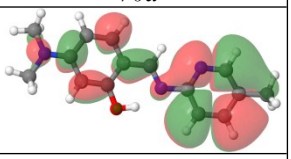
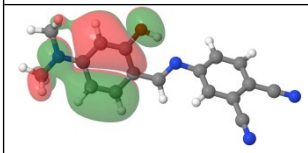
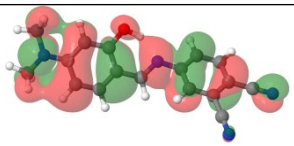
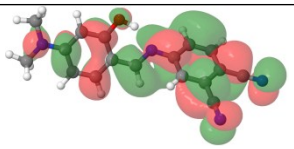
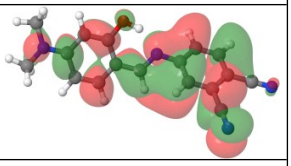
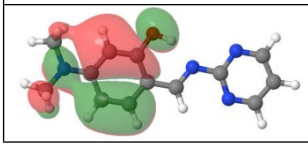
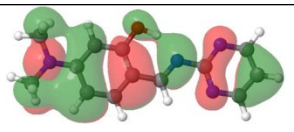
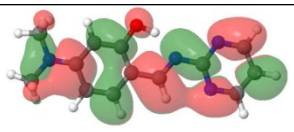
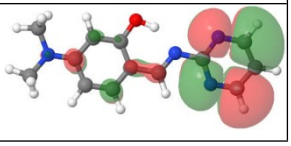


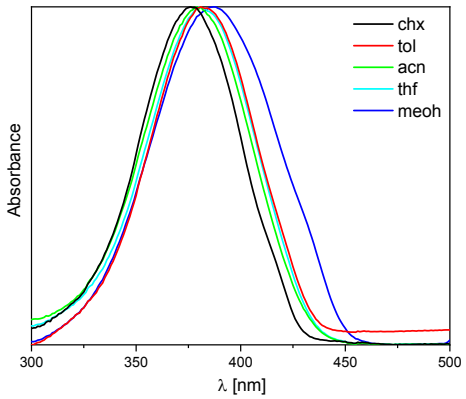
Figure S1. Ground state molecular structures of **1** and **4** optimized at MP2/cc-pVDZ level of calculation with two surrounding methanol molecules.

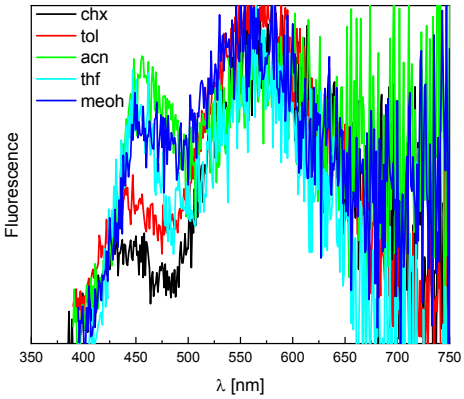
Table S3. Vertical transition energy (ΔE), oscillator strength (f), dipole moment (μ), and leading electronic configurations computed with ADC(2)/cc-pVDZ method at the MP2/cc-pVDZ equilibrium geometry of the ground state for **1**-**7**.

Molecule	State	ΔE/eV	f	μ/Debye	el. conf.
1	S_0	0.00	-	3.43	$(64a)^2$
	$^1\pi\pi^*$	3.76	0.87	8.93	0.93(64a-65a)
	$^1\pi\pi^*$	4.23	0.10	9.32	0.82(63a-65a)
	$^1\pi\pi^*$	4.60	0.00	2.41	0.67(62a-65a)
	$^1\pi\pi^*$	4.91	0.00	3.07	0.54(64a-66a)
	$^1\pi\pi^*$	5.07	0.07	7.51	0.73(64a-67a)
	$^1\pi\pi^*$	5.68	0.22	2.37	0.51(59a-65a)-0.50(62a-65a)
2	S_0	0.00	-	5.78	$(78a)^2$
	$^1\pi\pi^*$	3.63	0.94	13.09	0.97(78a-79a)
	$^1\pi\pi^*$	4.13	0.07	13.10	0.85(77a-79a)
	$^1\pi\pi^*$	4.50	0.02	11.54	0.71(78a-80a)
	$^1\pi\pi^*$	4.65	0.02	5.16	0.60(76a-79a)
	$^1n\pi^*$	4.84	0.00	3.95	0.64(73a-80a)
	$^1\pi\pi^*$	5.02	0.05	10.44	0.69(78a-82a)
3	S_0	0.00	-	6.21	$(70a)^2$
	$^1\pi\pi^*$	3.63	0.91	14.31	0.91(70a-71a)
	$^1\pi\pi^*$	4.12	0.06	13.89	0.82(69a-71a)
	$^1\pi\pi^*$	4.56	0.01	11.06	0.64(70a-72a)
	$^1n\pi^*$	4.66	0.02	5.23	0.59(65a-71a)
	$^1\pi\pi^*$	5.02	0.05	11.22	0.69(70a-74a)
	$^1\pi\pi^*$	5.31	0.02	24.05	0.61(70a-72a)
4	S_0	0.00	-	9.04	$(76a)^2$
	$^1\pi\pi^*$	3.46	0.93	19.76	0.82(76a-77a)
	$^1\pi\pi^*$	4.00	0.04	17.69	0.73(75a-77a)
	$^1\pi\pi^*$	4.18	0.02	23.98	0.75(76a-78a)
	$^1\pi\pi^*$	4.65	0.03	7.05	0.54(74a-77a)+ 0.52(71a-77a)
	$^1n\pi^*$	4.90	0.00	23.03	0.62(74a-78a)
	$^1\pi\pi^*$	4.95	0.03	15.81	0.73(76a-80a)
5	S_0	0.00	-	1.61	$(68a)^2$
	$^1\pi\pi^*$	3.52	0.99	8.26	0.93(68a-69a)
	$^1\pi\pi^*$	4.11	0.08	9.32	0.84(67a-69a)
	$^1n\pi^*$	4.60	0.00	1.11	0.78(63a-69a)
	$^1\pi\pi^*$	4.69	0.01	3.91	0.60(68a-70a)
	$^1n\pi^*$	4.85	0.00	4.17	0.82 (62a-69a)
	$^1\pi\pi^*$	5.04	0.03	5.25	0.75(68a-71a)
6	S_0	0.00	-	11.14	$(76a)^2$
	$^1\pi\pi^*$	3.38	1.02	22.91	0.86(76a-77a)
	$^1\pi\pi^*$	3.96	0.03	20.97	0.74(75a-77a)
	$^1\pi\pi^*$	4.35	0.01	22.09	0.74(76a-78a)
	$^1\pi\pi^*$	4.54	0.06	10.45	0.60(74a-77a)
	$^1n\pi^*$	4.86	0.01	22.58	0.51(76a-79a)+0.37(76a-80a)
	$^1\pi\pi^*$	4.99	0.06	21.05	0.68(76a-80a)
7	S_0	0.00	-	3.25	$(64a)^2$
	$^1\pi\pi^*$	3.45	0.88	9.95	0.96(64a-65a)
	$^1\pi\pi^*$	3.99	0.09	10.51	0.89(63a-65a)
	$^1\pi\pi^*$	4.23	0.00	3.32	0.85(61a-65a)
	$^1\pi\pi^*$	4.47	0.00	1.94	0.66(58a-65a)
	$^1n\pi^*$	4.53	0.00	1.49	0.66(58a-65a)
	$^1\pi\pi^*$	4.79	0.03	10.51	0.75(64a-66a)

Table S4. Relevant molecular π orbitals involved into the lowest electronic excitations of salicylideneaniline derivatives.

HOMO		LUMO	
1			
63a	*64a*	*65a*	*66a*
			
2			
77a	*78a*	*79a*	*80a*
			
3			
69a	*70a*	*71a*	*72a*
			
4			
75a	*76a*	*77a*	*78a*
			
5			
67a	*68a*	*69a*	*70a*
			
6			
75a	*76a*	*77a*	*78a*
			
7			
63a	*64a*	*65a*	*66a*
			


chx
tol
acn
thf
meoh
Absorbance
λ [nm]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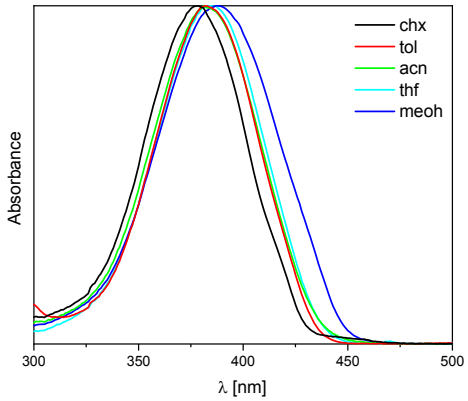
Fluorescence
λ [nm]

2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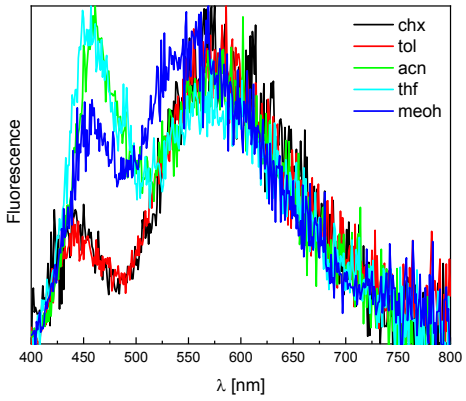
Absorbance
λ [nm]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tol
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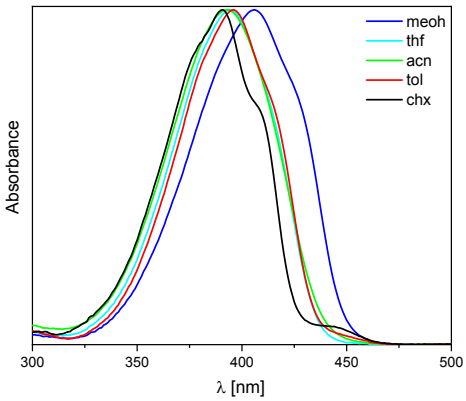
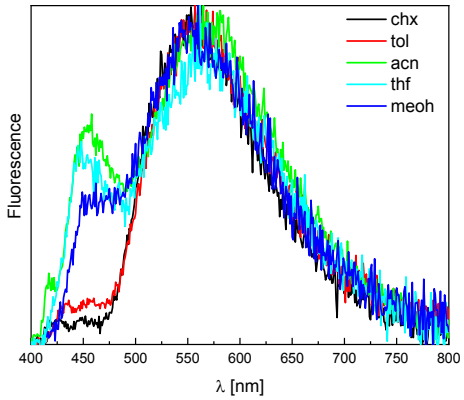
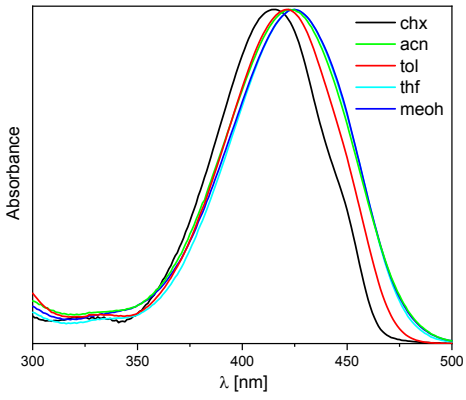
Fluorescence
λ [nm]

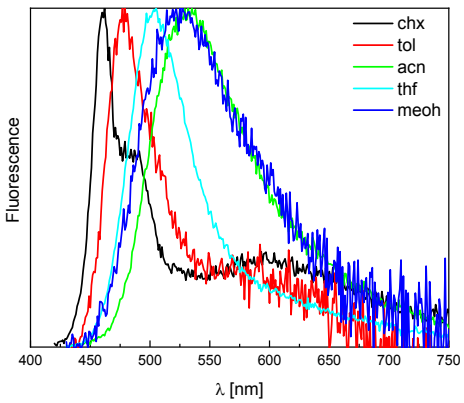
3


meoh
thf
acn
tol
chx
Absorbance
λ [nm]

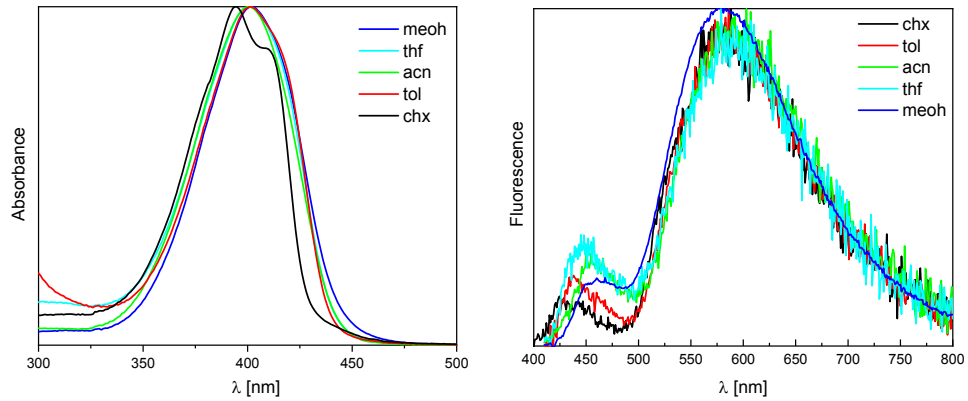

chx
tol
acn
thf
meoh
Fluorescence
λ [nm]

5


chx
acn
tol
thf
meoh
Absorbance
λ [nm]


chx
tol
acn
thf
meoh
Fluorescence
λ [nm]

6



7

Figure S2. Absorption and emission spectra measured in cyclohexane (chx), toluene (tol), acetonitrile (acn), tetrahydrofuran (thf) and methanol (meoh).

Table S5. Adiabatic energy of the fluorescing state (E(S_1))**,** vertical transition energy (ΔE), oscillator strength (*f*) and dipole moments (μ(S_1) and μ(S_0)), computed with ADC(2)/cc-pVDZ method at the equilibrium geometry of the S_1 state.

Conformer		**E(S_1)/eV**	**ΔE/eV**	***f***	**μ(S_1)/Debye**	**μ(S_0)/Debye**
1	*Open*	4.31	3.24	1.33	10.39	8.58
	Enol	3.32	2.90	0.96	7.32	4.72
	Keto	2.73	1.52	0.03	5.06	4.51
2	*Open*	4.15	3.18	1.33	14.76	10.38
	Enol	3.21	2.88	1.02	11.13	6.56
	Keto	2.67	1.45	0.02	8.39	1.46
3	*Open*	4.16	3.19	1.30	15.95	11.09
	Enol	3.22	2.88	0.98	13.26	7.27
	Keto	2.61	1.24	0.03	10.25	1.50
4	*Open*	3.95	3.11	1.23	21.05	13.71
	Enol	3.08	2.81	0.96	17.20	10.37
	Keto	2.58	1.33	0.01	12.57	7.14
5	*Open*	4.17	3.02	1.29	5.94	7.07
	Enol	3.23	2.85	1.04	5.92	1.04
	Keto	2.68	1.53	0.03	5.98	3.95
6	*Open*	3.85	2.98	1.41	23.20	16.73
	Enol	3.00	2.73	1.10	19.42	12.76
	Keto	2.51	1.12	0.02	13.14	6.66
7	*Open*	4.20	3.11	1.20	9.81	7.48
	Enol	3.02	2.80	0.75	10.16	3.99
	Keto	2.47	1.37	0.02	6.09	5.29

Table S6. Adiabatic energy of the fluorescing state (E(S_1))**,** vertical transition energy (ΔE), oscillator strength (*f*) and dipole moments (μ(S_1) and μ(S_0)), computed with ADC(2)/cc-pVDZ method at the equilibrium geometry of the S_1 state. Two molecules of cyclohexane, acetonitrile and methanol were used as explicit solvents of compound **1**.

Isomer	E(S_1)/eV	ΔE/eV	*f*	μ(S_1)/Debye	μ(S_0)/Debye
	Gas phase				
Cis-open	4.31	3.24	1.33	10.39	8.58
Enol	3.32	2.90	0.96	7.32	4.72
Keto	2.73	1.52	0.03	5.06	4.51
	Cyclohexane				
Cis-open	3.55	3.03	1.07	8.05	7.74
Enol	3.10	2.79	0.84	7.52	4.85
Keto	2.58	1.49	0.02	7.81	3.82
	Acetonitrile				
Cis-open	3.43	3.04	1.08	6.72	3.97
Enol	-	-	-	-	-
Keto	2.42	0.93 [1.64]	0.01	4.55	9.53
	Methanol				
Cis-open	3.54	2.92	1.13	10.90	9.78
Enol	3.05	2.71	0.91	7.50	5.67
Keto	2.29	1.72	0.01	5.39	8.12

Table S7. Vertical transition energy (ΔE), oscillator strength (*f*) and dipole moments (μ(S_1) and μ(S_0)), computed with ADC(2), CC2 and spin-scaled variants SCS-CC2[a] and SOS-CC2[b] , and CCSD/cc-pVDZ levels of theory of the compound **1**.

Isomer	Method	ΔE/eV	*f*	μ(S_1)/Debye	μ(S_0)/Debye
Cis-open	ADC2/cc-pVDZ	3.24	1.33	10.39	8.58
	ADC2/aug-cc-pVDZ	3.09	1.25	8.56	7.81
	CC2/cc-pVDZ	3.40	1.45	10.45	6.61
	SCS-CC2/cc-pVDZ	3.47[a]	1.40[a]	10.33	6.62
	SOS-CC2/cc-pVDZ	3.50	1.37	10.30	6.62
	CCSD/cc-pVDZ	3.59			
Enol	ADC2/cc-pVDZ	2.90	0.96	7.32	4.72
	ADC2/aug-cc-pVDZ	2.80	0.95	7.45	4.92
	CC2/cc-pVDZ	3.09	1.13	7.56	3.74
	SCS-CC2/cc-pVDZ	3.14	1.09	7.38	3.80
	SOS-CC2/cc-pVDZ	3.17	1.07	7.33	3.83
	CCSD/cc-pVDZ	3.25			
Keto	ADC2/cc-pVDZ	1.52	0.03	5.06	4.51
	ADC2/aug-cc-pVDZ	1.57	0.02	7.57	4.47
	CC2/cc-pVDZ	2.01	0.06	6.31	2.52
	SCS-CC2/cc-pVDZ	2.14	0.08	5.40	2.71
	SOS-CC2/cc-pVDZ	2.21	0.10	4.96	2.80
	CCSD/cc-pVDZ	2.38			

Table S8. Adiabatic energy of the fluorescing state (E(S_1))**,** vertical transition energy (ΔE), oscillator strength (*f*) and dipole moments (μ(S_1) and μ(S_0)), computed with ADC(2)/cc-pVDZ method at the equilibrium geometry of the S_1 state. Two molecules of cyclohexane, acetonitrile and methanol were used as explicit solvents of compound **4**.

Isomer	E(S_1)/eV	ΔE/eV	*f*	μ(S_1)/Debye	μ(S_0)/Debye
	Gas phase				
Cis-open	3.95	3.11	1.23	21.05	13.71

Enol	3.08	2.81	0.96	17.20	10.37
Keto	2.58	1.33	0.01	12.57	7.14
Cyclohexane					
Cis-open	3.25	2.96	1.00	22.13	13.67
Enol	2.89	2.71	0.80	20.44	10.43
Keto	2.45	1.30	0.01	15.93	7.40
Acetonitrile					
Cis-open	3.12	2.84	0.92	19.18	7.02
Enol	3.06	2.58	0.74	15.91	5.11
Keto	2.60	1.08	0.01	10.10	5.45
Methanol					
Cis-open	3.56	2.94	0.89	20.27	10.99
Enol	3.15	2.68	0.90	20.91	11.71
Keto	2.52	1.72	0.02	17.41	8.29

Table S9. Vertical transition energy (ΔE), oscillator strength (*f*) and dipole moments (μ(S_1) and μ(S_0)), computed with ADC(2), CC2 and spin-scaled variants SCS-CC2[a] and SOS-CC2[b] , and CCSD/cc-pVDZ levels of theory of the compound **4**.

Isomer	**Method**	**ΔE/eV**	***f***	**μ(S_1)/Debye**	**μ(S_0)/Debye**
Cis-open	ADC2/cc-pVDZ	3.11	1.23	21.05	13.71
	ADC2/aug-cc-pVDZ	2.99	1.15	22.56	14.24
	CC2/cc-pVDZ	3.24	1.40	21.65	12.94
	SCS-CC2/cc-pVDZ	3.33	1.38	20.71	12.74
	SOS-CC2/cc-pVDZ	3.38	1.36	20.29	12.66
	CCSD/cc-pVDZ	3.48			
Enol	ADC2/cc-pVDZ	2.81	0.96	17.20	10.37
	ADC2/aug-cc-pVDZ	2.71	0.92	20.32	10.85
	CC2/cc-pVDZ	2.98	1.22	17.72	10.01
	SCS-CC2/cc-pVDZ	3.06	1.19	16.73	9.80
	SOS-CC2/cc-pVDZ	3.09	1.18	16.35	9.71
	CCSD/cc-pVDZ	3.20			
Keto	ADC2/cc-pVDZ	1.33	0.01	12.57	7.14
	ADC2/aug-cc-pVDZ	1.36	0.01	15.97	7.51
	CC2/cc-pVDZ	1.84	0.03	14.67	7.76
	SCS-CC2/cc-pVDZ	2.00	0.04	13.48	7.60
	SOS-CC2/cc-pVDZ	2.08	0.05	12.89	7.53
	CCSD/cc-pVDZ	2.25			

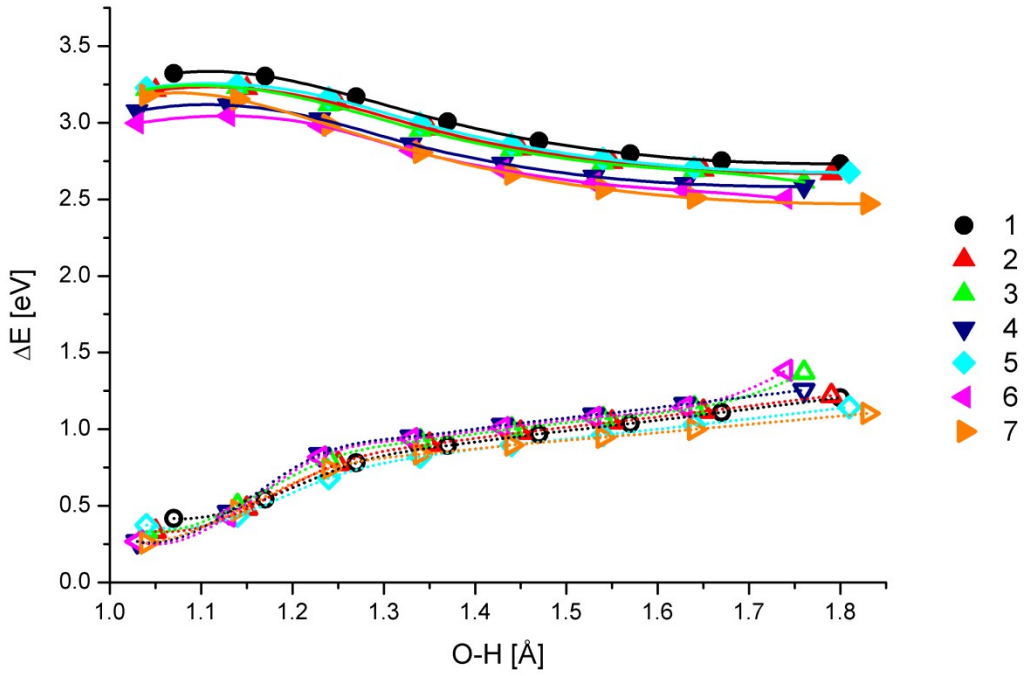


Figure S3. Minimum energy profiles for *enol* → *keto* reaction of the TSAN in the ground (S_0) and first excited singlet state (S_1) computed at MP2/ADC(2)/cc-pVDZ level of theory, respectively. Symbols connected by solid line denote energy profile optimized in the S_1 state, while dashed lines denotes vertical energy of the S_0.

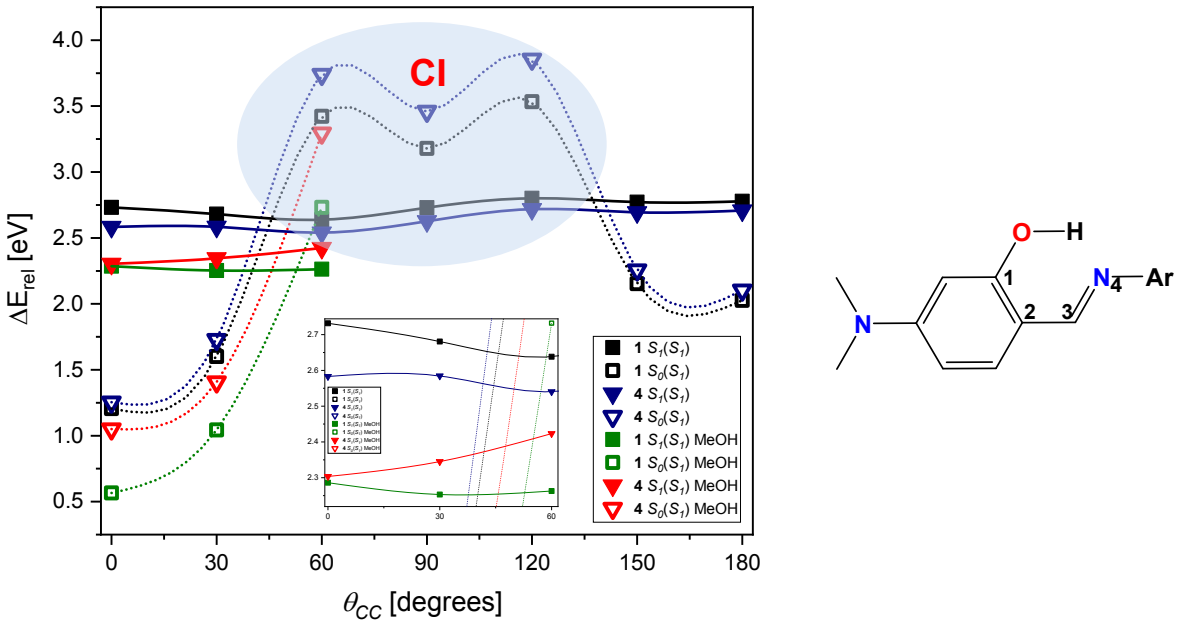


Figure S4. Left-panel - Minimum energy profiles for cis-keto → *trans-keto* reaction of the TSAN in the ground (S_0) and first excited singlet state (S_1) computed at MP2/ADC(2)/cc-pVDZ level of theory, respectively. Black and blue curves correspond to calculations performed in vacuum, while green and red ones were obtained using two explicit methanol molecules as solvent. Symbols connected by solid line denote energy profile optimized in the S_1 state, while dashed lines denotes vertical energy of the S_0. Right panel – molecular structure showing the labels for involved atoms in the C=C twist, for which the conical intersection is expected.

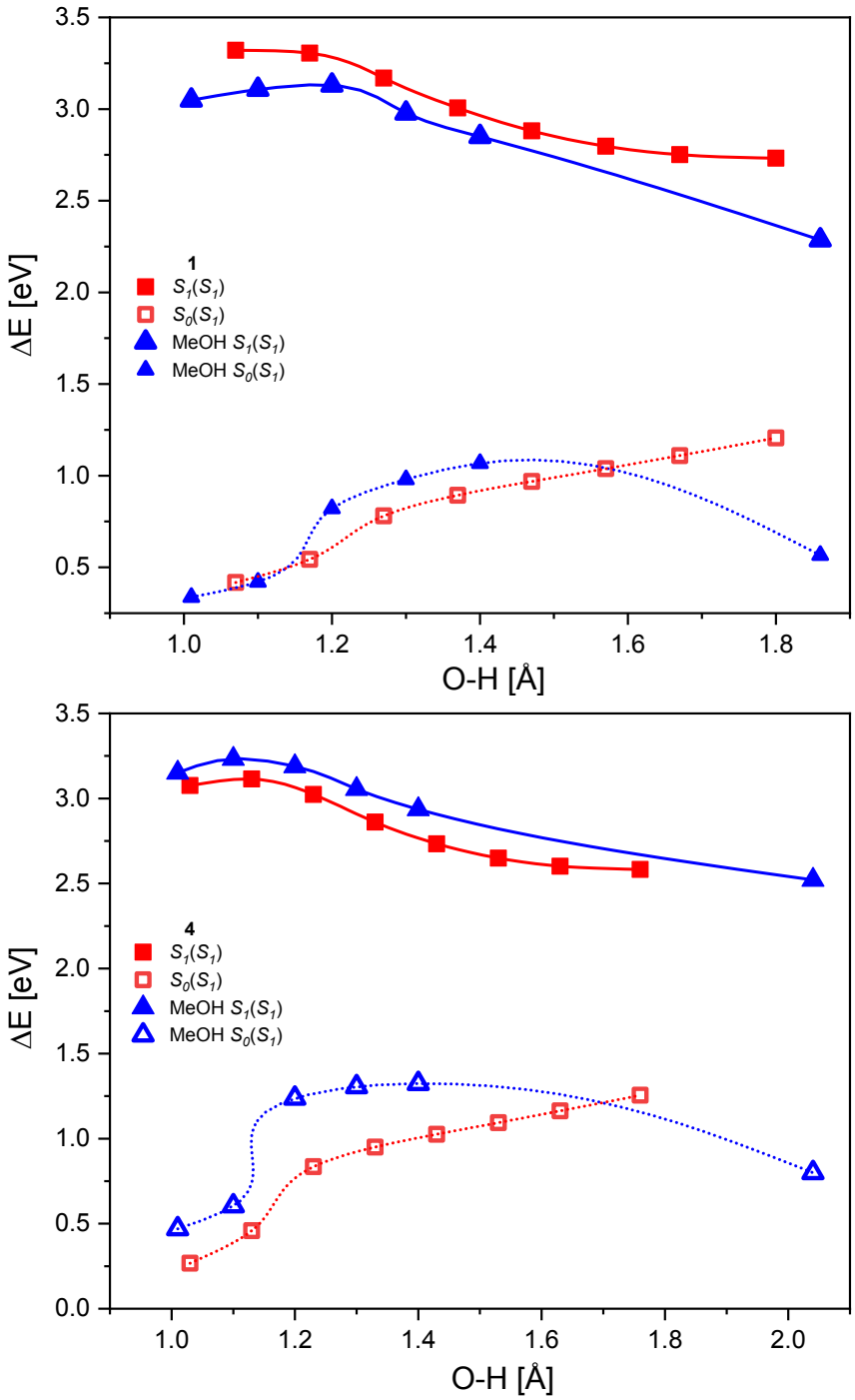


Figure S5. Minimum energy profiles for *enol* → *keto* reaction of the TSAN in the ground (S_0) and first excited singlet state (S_1) computed at MP2/ADC(2)/cc-pVDZ level of theory for **1** and **4**, respectively. Red (blue) symbols refers to calculations performed at vacuum (using two explicit methanol molecules as solvents). Symbols connected by solid line denote energy profile optimized in the S_1 state, while dashed lines denotes vertical energy of the S_0.

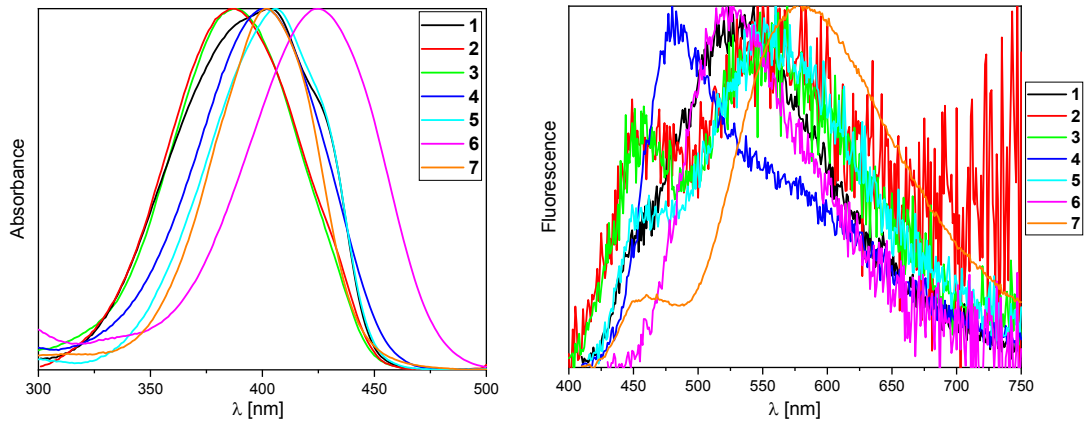


Figure S6. Absorption (left panel) and emission (right panel) spectra measured in methanol for compounds **1**-**7**.

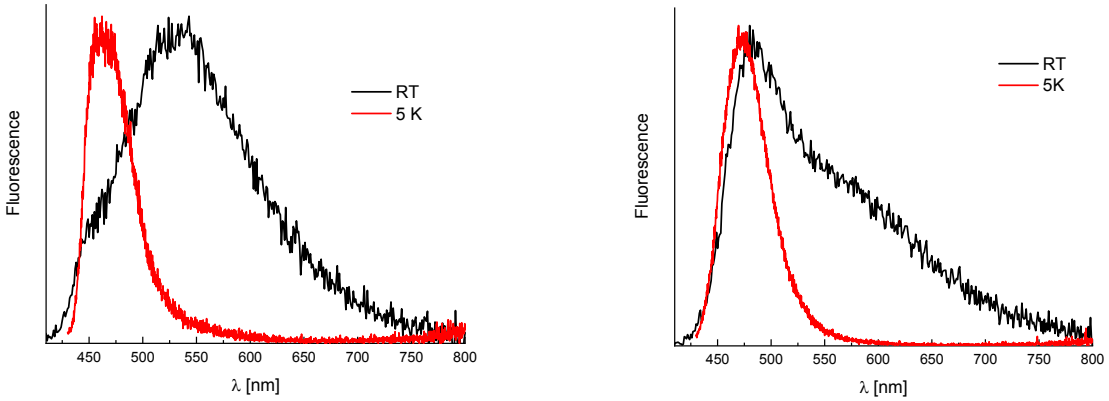


Figure S7. Fluorescence spectra of **1** and **4** measured in methanol at room temperature (RT) and 5 Kelvin.

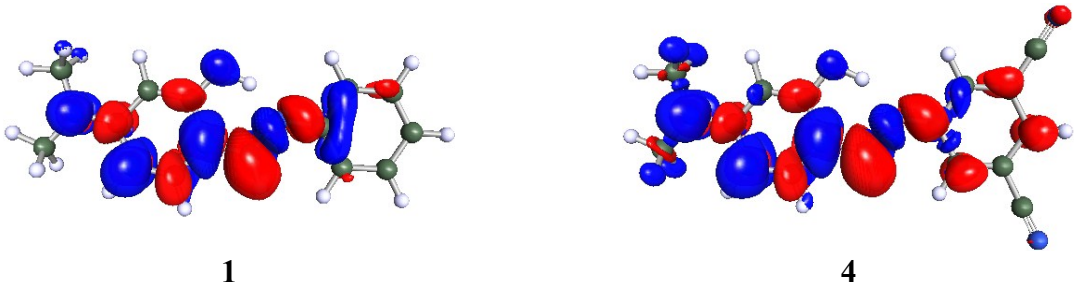


Figure S8. S_1 -S_0 electron density difference computed at ADC(2)/cc-pVDZ level of theory. Red (blue) indicates electron acceptor (donor) regions.

Crystal structure data

The X-ray data were collected on a Bruker D8 VENTURE DUO diffractometer using Cu$K\alpha$ radiation (λ = 1.54184 Å). Structures were solved by direct methods with SHELXT 2014/5 and refined against F^2 with full-matrix least-squares using SHELXL-2018/3. Hydrogen atoms were calculated at their idealized positions and were refined as riding atoms with isotropic thermal parameters based upon the corresponding bonded atom (U_{iso} = 1.2U_{eq}, U_{iso} = 1.5U_{eq} for CH_3 and OH hydrogens, respectively). Hydrogen atoms of methyl and hydroxyl groups were refined in geometric positions for which the calculated sum of the electron density is the highest (rotating group refinement). CCDC 1919005–1919010 contain the supplementary crystallographic data for this paper. These data can be obtained from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/structures.

Crystal data for 2 (CCDC 1919005): $C_{19}H_{20}N_2O_3$, M = 324.37, yellow plate, 0.405 × 0.151 × 0.040 mm, monoclinic, space group $C2/c$, V = 3267.0(8) Å^3, Z = 8, D_c = 1.319 g·cm^{-3}, F_{000} = 1376, T = 293(2) K, 2θ_{max} = 136.7º, 25438 reflections collected, 2988 unique (R_{int} = 0.215). Final *GooF* = 1.02, R = 0.070, wR = 0.139, R indices based on 1301 reflections with $I > 2\sigma(I)$, 220 parameters, 0 restraints. Lp and absorption corrections applied, μ = 0.730 mm^{-1}.

Crystal data for 3 (CCDC 1919006): $C_{18}H_{19}N_3O$, M = 293.36, yellow plate, 0.303 × 0.220 × 0.048 mm, monoclinic, space group $P2_1/c$, V = 1598.3(13) Å^3, Z = 4, D_c = 1.219 g·cm^{-3}, F_{000} = 624, T = 293(2) K, 2θ_{max} = 125.1º, 7642 reflections collected, 2471 unique (R_{int} = 0.068). Final *GooF* = 1.00, R = 0.061, wR = 0.117, R indices based on 1012 reflections with $I > 2\sigma(I)$, 203 parameters, 0 restraints. Lp and absorption corrections applied, μ = 0.614 mm^{-1}.

Crystal data for 4 (CCDC 1919007): $C_{19}H_{18}N_4O$, M = 318.37, yellow needle, 0.157 × 0.085 × 0.057 mm, monoclinic, space group $P2_1/c$, V = 1678(2) Å^3, Z = 4, D_c = 1.260 g·cm^{-3}, F_{000} = 672, T = 293(2) K, 2θ_{max} = 110.0º, 16345 reflections collected, 2093 unique (R_{int} = 0.144). Final *GooF* = 1.09, R = 0.087, wR = 0.159, R indices based on 1211 reflections with $I > 2\sigma(I)$, 221 parameters, 0 restraints. Lp and absorption corrections applied, μ = 0.648 mm^{-1}.

Crystal data for 5 (CCDC 1919008): $C_{17}H_{21}N_3O$, M = 283.37, yellow needle, 0.355 × 0.078 × 0.062 mm, monoclinic, space group $P2_1/c$, V = 1562.7(13) Å^3, Z = 4, D_c = 1.204 g·cm^{-3}, F_{000} = 608, T = 293(2) K, 2θ_{max} = 125.2º, 27810 reflections collected, 2491 unique (R_{int} = 0.060). Final *GooF* = 1.02, R = 0.052, wR = 0.131, R indices based on 1796 reflections with $I > 2\sigma(I)$, 214 parameters, 0 restraints. Lp and absorption corrections applied, μ = 0.605 mm^{-1}.

Crystal data for 6 (CCDC 1919009): $C_{19}H_{18}N_4O$, M = 318.37, yellow-orange needle, 0.254 × 0.076 × 0.044 mm, triclinic, space group $P1$, V = 859.1(16) Å^3, Z = 2, D_c = 1.231 g·cm^{-3}, F_{000} = 336, T = 274(2) K, 2θ_{max} = 118.4º, 21603 reflections collected, 2465 unique (R_{int} = 0.083). Final *GooF* = 1.04, R = 0.061, wR = 0.115, R indices based on 1362 reflections with $I > 2\sigma(I)$, 240 parameters, 0 restraints. Lp and absorption corrections applied, μ = 0.632 mm^{-1}.

Crystal data for 7 (CCDC 1919010): $C_{15}H_{18}N_4O$, M = 270.33, yellow-orange block, 0.121 × 0.099 × 0.055 mm, monoclinic, space group $P2_1/c$, V = 1433.2(16) Å^3, Z = 4, D_c = 1.253 g·cm^{-3}, F_{000} = 576, T = 293(2) K, 2θ_{max} = 120.5º, 29516 reflections collected, 2127 unique (R_{int} = 0.082). Final *GooF* = 1.05, R = 0.059, wR = 0.113, R indices based on 1363 reflections with $I > 2\sigma(I)$, 204 parameters, 0 restraints. Lp and absorption corrections applied, μ = 0.658 mm^{-1}.

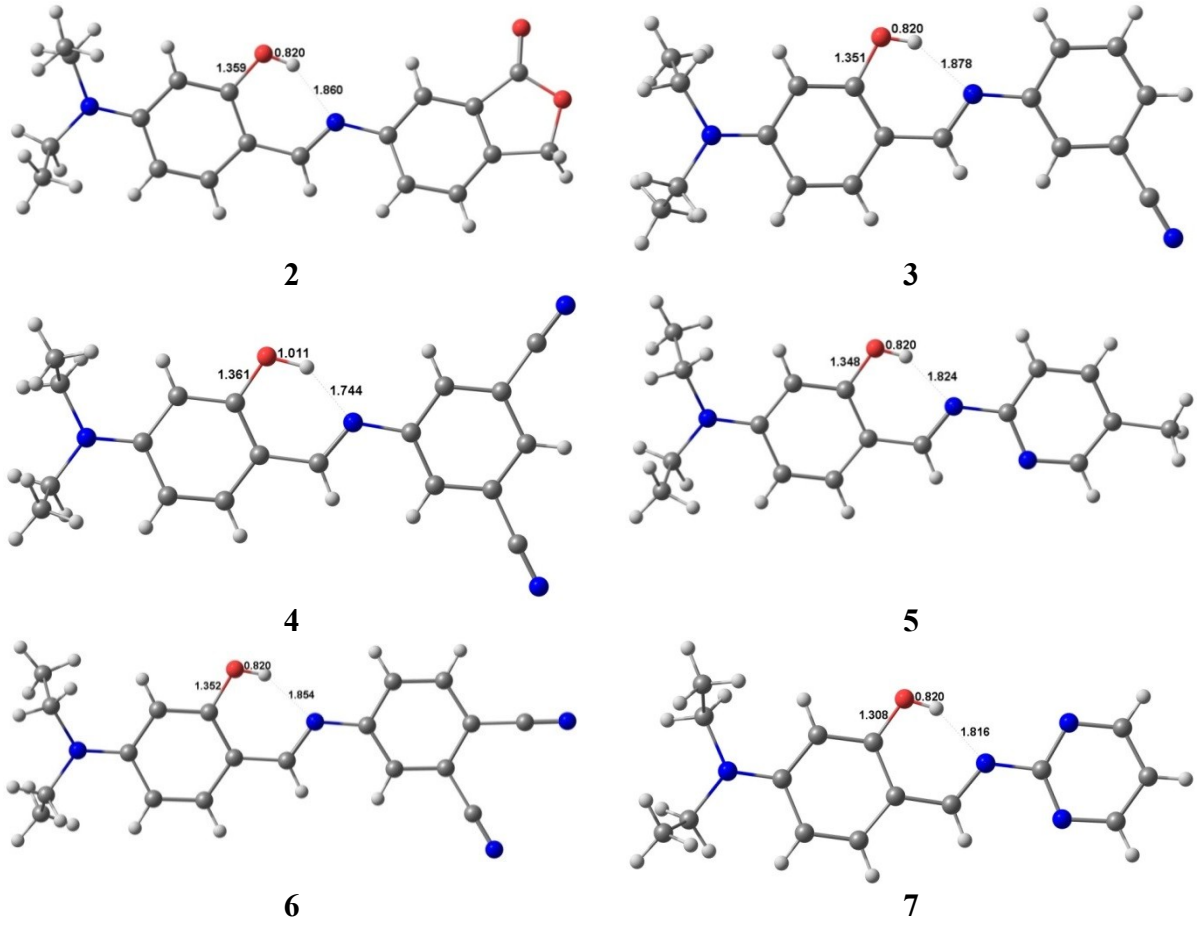


Figure S9. Molecular structures obtained by X-ray diffraction measurements.

Experimental and synthesis details

^{1}H FT-NMR and proton decoupled ^{13}C FT-NMR/DEPT 135 FT-NMR spectra were recorded using Bruker AVANCE 500 MHz or 300 MHz spectrometer respectively. The chemical shifts are given *vs.* TMS as an internal standard. The coupling constants were calculated by using chemical shifts reported in Hz unit. FT infrared spectra were recorded using Thermo-Nicolet Nexus 670 FTIR spectrometer. Mass spectra were recorded using Micromass LCT 4 spectrometer with positive ionisation method. Melting points were obtained with an A. KRÜSS Optronic KSP1N melting point meter. Absorption spectra at room temperature were measured with a Perkin-Elmer Lambda 35 spectrophotometer. Fluorescence spectra were collected with a spectrofluorimeter model FLS 1000, Edinburgh Instruments.

While all necessary substrates are purchasable (Fluorochem, UK) in the case of **4** and **2** it may be more economical to synthesise appropriate anilines using known methods (nitration of isophthalonitrile or phthalide respectively followed by dissolving metal reduction to aromatic amine). The reaction times were consistent with variable electron deficiency of the amine substrate. Compound **1** formed within several hours using boiling 2-propanol as a solvent. Noticeably, 4-(diethylamino)salicylaldehyde is much less reactive than unsubstituted salicylaldehyde as (diethylamino)group greatly diminishes electrophilicity of carbonyl carbon. For mildly electron poor amines (6-aminophthalide, 3-aminobenzonitrile), 1-propanol was a suitable choice to synthesise **2** and **3** because of its higher boiling point. For the same reason more electron deficient amines (3,5-dicyanoaniline, 2-amino-5-methylpyridine) required

using 1-butanol to synthesise **4** and **5** and for strongly deactivated aromatic amines (4,5-dicyanoaniline, 2-aminopyrimidine) reaction had to be run for at least 24 hours to obtain **6** and **7**. Generally using higher boiling alcohols than ethanol was mandatory to use the substrates at stoichiometric amounts and avoid using acidic catalysts. By using repetitive crystallisations from boiling alcohols followed by prolonged cooling in the freezer (crystallisations proceed poorly or very slowly in the fridge or ambient temperature) it was possible to isolate all compounds with good purity and significant mass recovery.

General procedure for synthesis and purification of salicylaldimines

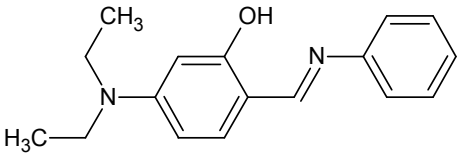
None of the reactions require using inert atmosphere or rigorously anhydrous conditions. In a typical procedure 4-(diethylamino)salicylaldehyde (10 mmol or 1 mmol) and appropriate aromatic amine (10 mmol or 1 mmol) were placed in a two-necked flask (100 ml) and appropriate solvent was added (40 ml, pure grade is sufficient but low water content solvents are preferable) (2-propanol for **1**; 1-propanol for **2**, **3**; 1-butanol for **4**, **5**, **6**, **7**). The reflux condenser with outlet connected to the gas bubbler was attached to the reaction flask (only to isolate the reaction system from surroundings). Attaching drying tube with anhydrous calcium chloride is optional. Flushing with inert gas is optional. In all examples here the reactions were carried out in air. The mixture was then vigorously refluxed for the time period depending on the reactivity of the amine (8 hours for **1**, 16-24 hours for **2**, **3**, **4**, **5**, 24-40 hours for **6**, **7**). The reaction may be conveniently monitored by TLC using dichloromethane as eluent - neat or mixed with hexane or ethyl acetate. The condensation product typically had lower retention factor that aldehyde and higher than amine. The spot ascribed to the salicylaldimine stained the TLC plate with intensive yellow colour (orange for **7**).

Next the reaction flask containing cherry-red solution was cooled below 60^{o}C and immediately diluted with solvent (60 ml) (methanol for **2**, **3**, **4**, **5**, **6**; 2-propanol for **7**; hexane for **1**) and placed in the freezer (-25^{o}C) for minimum 16 hours. (When methanol is used for **1** or **7** nothing happens or the yield of the crystallisations are very low.) This step is essential to remove most impurities as other methods like extraction will retain colour dyes side products. Next the heavy precipitate was filtered off while still cold on a sinter funnel under suction (G3, 1 inch wide) and quickly washed with chilled solvent (-25^{o}C) (3 x 25 ml) (methanol for **2**, **3**, **4**, **5**, **6**; 2-propanol for **7**; hexane for **1**). (The mother liquors may be evaporated to dryness and refluxed again for another 16 hours with some additional 4-(diethylamino)salicylaldehyde in 1-butanol to convert remaining unreacted amine. Additional 15-25% yield may be gained.)

Next the products were crystallised two times in a round bottom flask (100 ml) by dissolving in a boiling 1-propanol (20-40 ml) and cautiously diluting to the full volume of the flask while still hot with ambient temperature solvent (methanol for **2**, **3**, **4**, **5**, **6**; 2-propanol for **7**; hexane for **1**) and placing in the freezer (-25^{o}C) for minimum 16 hours (preferably overnight or over two nights). When the flask was removed from the freezer, the crystalline solids were immediately collected on a sinter funnel under suction (G3, 1 inch wide) and quickly washed with chilled (-25^{o}C) solvent (3 x 25 ml) (methanol for **2**, **3**, **4**, **5**, **6**; 2-propanol for **7**; hexane for **1**) so that losses by redissolving were negligible. (Mother liquors from these two crystallisations were kept and evaporated to dryness, as they mostly consisted of the target products.) Finally, the products were dried in air for at least 6 hours (after every crystallisation) in air, followed by drying for 24 hours in a vacuum desiccator (2 mbar) followed by dying in vacuum (2 mbar) at 50^{o}C for 4 hours. All compounds could be stored in

the sealed glass vials. No decomposition was noticed after storage for several months (ambient conditions, light exclusion).
In all cases very good spectral characteristics and measurements could be achieved without chromatography techniques, using crystallisation as a sole purification technique. In all cases the obtained solids contained crystals which were suitable for X-ray analysis with the exception of **6** which formed fluffy fibres. In this case crystals were obtained from slow evaporation from acetonitrile/2-propanol. The following salicylideneanilines were synthesised (yields given refer to the final crystallised crop):

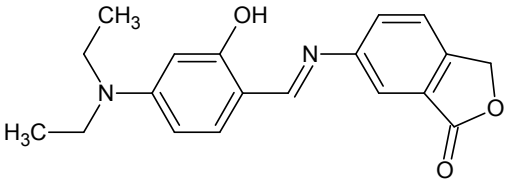
Compound 1. 4-(diethylamino)salicylaldehyde *N*-phenylimine. Yellow-orange crystals (68%).



Molecular Formula	= $C_{17}H_{20}N_2O$
Formula Weight	= 268.3535
Composition	= C(76.09%) H(7.51%) N(10.44%) O(5.96%)
Monoisotopic Mass	= 268.157563 Da
M+	= 268.157015 Da
[M+H]+	= 269.16484 Da

HRMS (ESI$^+$): calcd. for $C_{17}H_{21}N_2O$ $[M+H]^+$: 269.1648, found: 269.1663, error: 5.57 ppm.
FT-IR (KBr, cm^{-1}): 3074, 3035, 2974, 2931, 2893, 2871, 1633, 1605, 1585, 1553, 1521, 1486, 1449, 1424, 1386, 1373, 1350, 1343, 1304, 1256, 1246, 1224, 1199, 1168, 1155, 1137, 1094, 1083, 984, 911, 891, 855, 840, 825, 788, 762, 704, 694, 656, 524.
Melting point (1-propanol/hexane 1:3): 92-93^{o}C.

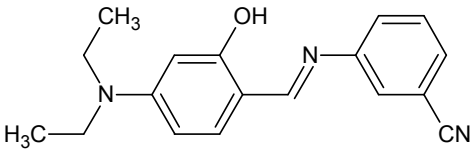
Compound 2. 4-(diethylamino)salicylaldehyde *N*-(6-phthalidyl)imine. Yellow thick crystals (43%).



Molecular Formula	= $C_{19}H_{20}N_2O_3$
Formula Weight	= 324.3737
Composition	= C(70.35%) H(6.21%) N(8.64%) O(14.80%)
Monoisotopic Mass	= 324.147393 Da
M+	= 324.146844 Da
[M+H]+	= 325.154669 Da

^{1}H FT-NMR (500 MHz, $CDCl_3$ + TMS, 298 K, ppm): 13.32 (broad s, 1H, OH), 8.48 (s, 1H, C-H imine), 7.73 (dd, J_{meta} = 2.0 Hz, J_{para} = 0.6 Hz, 1H, acceptor ring), 7.55 (dd, J_{ortho} = 8.1 Hz, J_{meta} = 1.8 Hz, 1H, acceptor ring), 7.47 (apparent doublet of quartets, J_{ortho} = 8.1 Hz, J_{para} = 0.8 Hz, 1H, acceptor ring), 7.18 (d, J_{ortho} = 9.0 Hz, 1H, donor ring), 6.28 (dd, J_{ortho} = 8.9 Hz, J_{meta} = 2.6 Hz, 1H, donor ring), 6.20 (d, J_{meta} = 2.5 Hz, 1H, donor ring), 5.33 (s, 2H, CH_2 phthalide), 3.42 (q, J = 7.2 Hz, 4H, N-CH_2), 1.22 (t, J = 7.2 Hz, 6H, -CH_3).
$^{13}C\{^1H\}$ FT-NMR / $^{13}C\{^1H\}$ DEPT135 FT-NMR (75 MHz, $CDCl_3$ + TMS, 298 K, ppm): 170.98 (C=O), 163.75 (C aromatic), 162.11 (C-H imine), 152.26 (C aromatic), 150.77 (C aromatic), 142.98 (C aromatic), 134.25 (C-H aromatic), 128.92 (C-H aromatic), 127.03 (C aromatic), 122.81 (C-H aromatic), 115.75 (C-H aromatic), 108.89 (C aromatic), 104.14 (C-H aromatic), 97.58 (C-H aromatic), 69.95 (CH_2 phthalide), 44.68 (N-CH_2), 12.70 (-CH_3).
HRMS (ESI$^+$): calcd. for $C_{19}H_{21}N_2O_3$ $[M+H]^+$: 325.1547, found: 325.1562, error: 4.61 ppm.
FT-IR (KBr, cm^{-1}): 3489, 3094, 3043, 2977, 2937, 2894, 2873, 1756 (νCO), 1636, 1592, 1557, 1520, 1487, 1448, 1424, 1386, 1377, 1352, 1300, 1283, 1258, 1244, 1228, 1194, 1136, 1084, 1045, 997, 978, 922, 897, 840, 821, 791, 773, 549.
Melting point (1-propanol/MeOH 1:3): 156-157^{o}C.

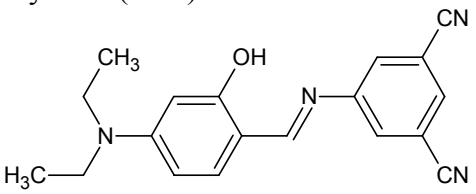
Compound 3. 4-(diethylamino)salicylaldehyde *N*-(3-cyanophenyl)imine. Yellow-orange flakes and crystals (47%).



Molecular Formula	= $C_{18}H_{19}N_3O$
Formula Weight	= 293.36296
Composition	= C(73.69%) H(6.53%) N(14.32%) O(5.45%)
Monoisotopic Mass	= 293.152812 Da
M+	= 293.152264 Da
[M+H]+	= 294.160089 Da

^{1}H FT-NMR (500 MHz, $CDCl_3$ + TMS, 298 K, ppm): 13.17 (broad s, 1H, OH), 8.40 (s, 1H, C-H imine), 7.47-7.48 (multiplet, 1H, acceptor ring), 7.42-7.47 (complicated multiplet, 1H+1H+1H, acceptor ring), 7.18 (d, J_{ortho} = 8.8 Hz, 1H, donor ring), 6.28 (dd, J_{ortho} = 8.8 Hz, J_{meta} = 2.4 Hz, 1H, donor ring), 6.19 (d, J_{meta} = 2.6 Hz, 1H, donor ring), 3.41 (q, J = 7.1 Hz, 4H, N-CH_2), 1.22 (t, J = 7.1 Hz, 6H, -CH_3).
$^{13}C\{^1H\}$ FT-NMR / $^{13}C\{^1H\}$ DEPT135 FT-NMR (75 MHz, $CDCl_3$ + TMS, 298 K, ppm): 163.73 (DEPT inactive), 162.26 (C-H imine), 152.37 (DEPT inactive), 150.23 (DEPT inactive), 134.31 (DEPT active), 130.13 (DEPT active), 128.59 (DEPT active), 125.84 (DEPT active), 124.20 (DEPT active), 118.68 (DEPT inactive), 113.25 (DEPT inactive), 108.81 (DEPT inactive), 104.18 (DEPT active), 97.57 (DEPT active), 44.69 (N-CH_2), 12.70 (-CH_3).
HRMS (ESI$^+$): calcd. for $C_{18}H_{20}N_3O$ $[M+H]^+$: 294.1601, found: 294.1613, error: 4.08 ppm.
FT-IR (KBr, cm^{-1}): 3063, 2972, 2931, 2890, 2231 (νCN), 1638, 1627, 1604, 1571, 1520, 1481, 1441, 1425, 1373, 1352, 1306, 1282, 1264, 1245, 1225, 1219, 1193, 1161, 1135, 1080, 1016, 950, 891, 823, 800, 697, 683.
Melting point (1-propanol/MeOH 1:3): 115-116°C.

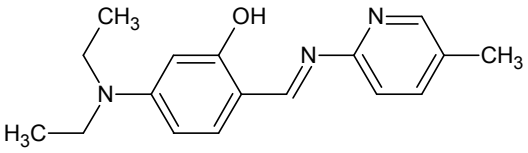
Compound 4. 4-(diethylamino)salicylaldehyde *N*-(3,5-dicyanophenyl)imine. Yellow thin crystals. (55%)



Molecular Formula	= $C_{19}H_{18}N_4O$
Formula Weight	= 318.37242
Composition	= C(71.68%) H(5.70%) N(17.60%) O(5.03%)
Monoisotopic Mass	= 318.148061 Da
M+	= 318.147513 Da
[M+H]+	= 319.155338 Da

^{1}H FT-NMR (500 MHz, $CDCl_3$ + TMS, 298 K, ppm): 12.68 (s, 1H, OH), 8.38 (s, 1H, C-H imine), 7.66-7.68 (multiplet, 1H + 2H, acceptor ring), 7.18 (d, J_{ortho} = 9.0 Hz, 1H, donor ring), 6.29 (dd, J_{ortho} = 8.9 Hz, J_{meta} = 2.4 Hz, 1H, donor ring), 6.18 (d, J_{meta} = 2.5 Hz, 1H, donor ring), 3.42 (q, J = 7.2 Hz, 4H, N-CH_2), 1.23 (t, J = 7.2 Hz, 6H, -CH_3).
$^{13}C\{^1H\}$ FT-NMR / $^{13}C\{^1H\}$ DEPT135 FT-NMR (75 MHz, $CDCl_3$ + TMS, 298 K, ppm): 163.84 (DEPT inactive), 163.32 (C-H imine), 153.05 (DEPT inactive), 151.49 (DEPT inactive), 134.92 (DEPT active), 130.69 (DEPT active), 128.50 (DEPT active), 116.67 (DEPT inactive), 114.84 (DEPT inactive), 108.62 (DEPT inactive), 104.70 (DEPT active), 97.38 (DEPT active), 44.78 (N-CH_2), 12.67 (-CH_3).
HRMS (ESI$^+$): calcd. for $C_{19}H_{19}N_4O$ $[M+H]^+$: 319.1553, found: 319.1551, error: -0.63 ppm.
FT-IR (KBr, cm^{-1}): 3073, 2978, 2933, 2902, 2870, 2239 (νCN), 1638, 1604, 1575, 1519, 1451, 1425, 1374, 1353, 1305, 1246, 1223, 1193, 1163, 1136, 1079, 1015, 1001, 978, 961, 888, 864, 822, 799, 786, 714, 677, 668.
Melting point (1-propanol/MeOH 1:3): 198-199°C.

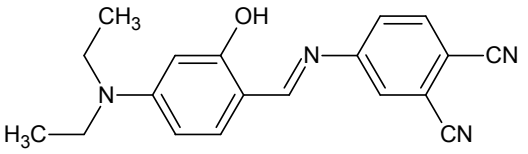
Compound 5. 4-(diethylamino)salicylaldehyde *N*-(5-methyl-2-pyridyl)imine. Orange thick needles (68%).



Molecular Formula	= $C_{17}H_{21}N_3O$
Formula Weight	= 283.36814
Composition	= C(72.06%) H(7.47%) N(14.83%) O(5.65%)
Monoisotopic Mass	= 283.168462 Da
M+	= 283.167914 Da
[M+H]+	= 284.175739 Da

^{1}H FT-NMR (500 MHz, $CDCl_3$ + TMS, 298 K, ppm): 14.42 (broad s, 1H, OH), 9.14 (s, 1H, C-H imine), 8.25 (doublet of triplets, J_{meta} = 1.5 Hz, J_{para} = 0.8 Hz, 1H, acceptor ring), 7.50 (apparent doublet of quartets, J_{ortho} = 8.1 Hz, J_{para} = 0.6 Hz, 1H, acceptor ring), 7.22 (d, J_{ortho} = 9.0 Hz, 1H, donor ring), 7.09 (d, J_{ortho} = 8.1 Hz, 1H, acceptor ring), 6.25 (dd, J_{ortho} = 8.9 Hz, J_{meta} = 2.6 Hz, 1H, donor ring), 6.14 (d, J_{meta} = 2.6 Hz, 1H, donor ring), 3.40 (q, J = 7.2 Hz, 4H, N-CH_2), 2.33 (s, 3H, -CH_3 pyridine ring), 1.21 (t, J = 7.2 Hz, 6H, -CH_3).
^{13}C{^{1}H} FT-NMR / ^{13}C{^{1}H} DEPT135 FT-NMR (75 MHz, $CDCl_3$ + TMS, 298 K, ppm): 166.44 (C aromatic), 160.04 (C-H imine), 155.49 (C aromatic), 152.56 (C aromatic), 148.79 (C-H aromatic), 138.81 (C-H aromatic), 134.95 (C-H aromatic), 130.29 (C aromatic), 118.39 (C-H aromatic), 104.34 (C-H aromatic), 97.78 (C-H aromatic), 44.64 (N-CH_2), 18.01 (-CH_3 pyridine ring). 12.77 (-CH_3).
HRMS (ESI$^+$): calcd. for $C_{17}H_{22}N_3O$ $[M+H]^+$: 284.1757, found: 284.1754, error: -1.06 ppm.
FT-IR (KBr, cm^{-1}): 3085, 3036, 2975, 2923, 2869, 1628, 1577, 1517, 1474, 1453, 1430, 1384, 1358, 1341, 1301, 1244, 1227, 1207, 1190, 1159, 1135, 1095, 1081, 1026, 993, 906, 840, 820, 796, 787, 695.
Melting point (1-propanol/MeOH 1:3): 127-128^{o}C.

Compound 6. 4-(diethylamino)salicylaldehyde *N*-(3,4-dicyanophenyl)imine. Yellow-orange fibres (36%). Long orange needles after slow evaporation.

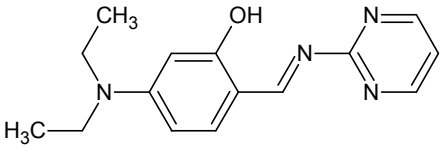


Molecular Formula	= $C_{19}H_{18}N_4O$
Formula Weight	= 318.37242
Composition	= C(71.68%) H(5.70%) N(17.60%) O(5.03%)
Monoisotopic Mass	= 318.148061 Da
M+	= 318.147513 Da
[M+H]+	= 319.155338 Da

^{1}H FT-NMR (500 MHz, $CDCl_3$ + TMS, 298 K, ppm): 12.82 (s, 1H, OH), 8.40 (s, 1H, C-H imine), 7.76 (d, J_{ortho} = 8.5 Hz, 1H, acceptor ring), 7.58 (d, J_{meta} = 2.1 Hz, 1H, acceptor ring), 7.49 (dd, J_{ortho} = 8.9 Hz, J_{meta} = 2.2 Hz, 1H, donor ring), 7.19 (d, J_{ortho} = 8.5 Hz, 1H, donor ring), 6.30 (dd, J_{ortho} = 8.9 Hz, J_{meta} = 2.5 Hz, 1H, donor ring), 6.18 (d, J_{meta} = 2.5 Hz, 1H, donor ring), 3.41 (q, J = 7.1 Hz, 4H, N-CH_2), 1.22 (t, J = 7.1 Hz, 6H, -CH_3), 3.43 (q, J = 7.2 Hz, 4H, N-CH_2), 1.23 (t, J = 7.2 Hz, 6H, -CH_3).
^{13}C{^{1}H} FT-NMR / ^{13}C{^{1}H} DEPT135 FT-NMR (75 MHz, $CDCl_3$ + TMS, 298 K, ppm): 164.18 (weak, DEPT inactive), 163.17 (C-H imine), 153.68 (DEPT inactive), 153.29 (DEPT inactive), 135.10 (DEPT active), 134.70 (DEPT active), 125.94 (DEPT active), 125.58 (DEPT active), 117.03 (DEPT inactive), 115.83 (DEPT inactive), 115.39 (DEPT inactive), 110.66 (DEPT inactive), 108.85 (weak, broad, DEPT inactive), 104.94 (DEPT active), 97.37 (DEPT active), 44.84 (N-CH_2), 12.69 (-CH_3).
HRMS (ESI$^+$): calcd. for $C_{19}H_{19}N_4O$ $[M+H]^+$: 319.1553, found: 319.1570, error: 5.33 ppm.

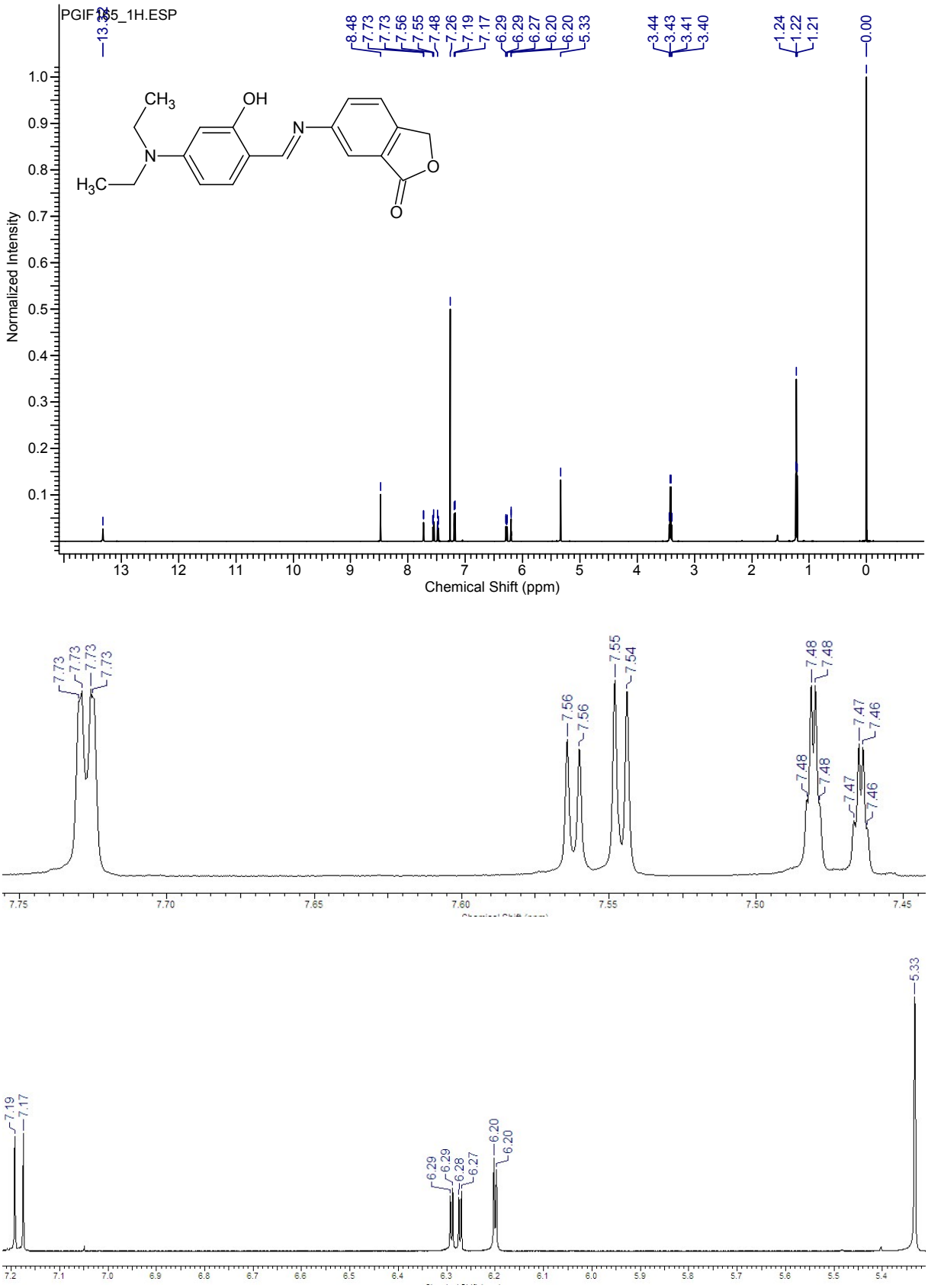
FT-IR (KBr, cm^{-1}): 3102, 3075, 3036, 2970, 2931, 2890, 2869, 2234 (νCN), 2225 (νCN), 1630, 1571, 1517, 1488, 1424, 1371, 1347, 1307, 1281, 1259, 1241, 1229, 1218, 1205, 1190, 1165, 1134, 1089, 1082, 1013, 978, 952, 887, 844, 822, 782, 751, 693, 654, 523.
Melting point (1-propanol/MeOH 1:4): 169-170°C.

Compound 7. 4-(diethylamino)salicylaldehyde *N*-(2-pyrimidinyl)imine. Orange crystalline solid (37%).

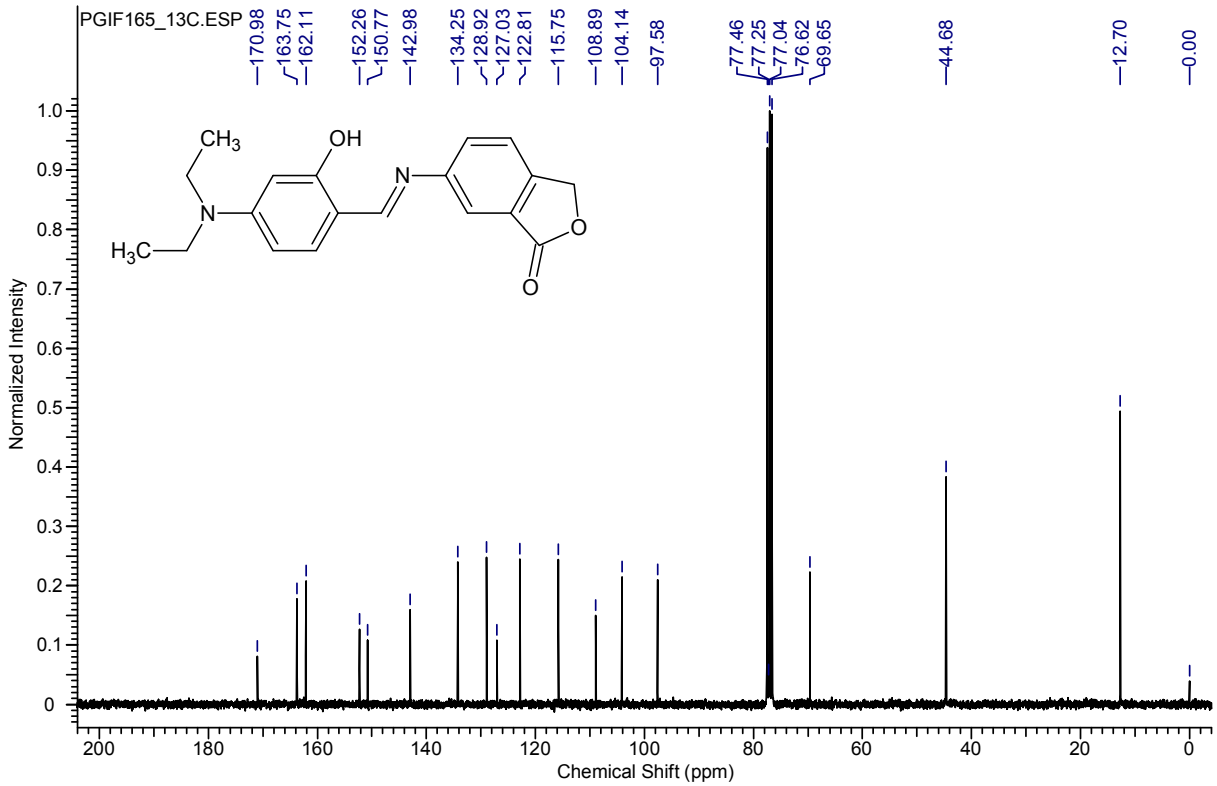


Molecular Formula	= $C_{15}H_{18}N_4O$
Formula Weight	= 270.32962
Composition	= C(66.64%) H(6.71%) N(20.73%) O(5.92%)
Monoisotopic Mass	= 270.148061 Da
M+	= 270.147513 Da
[M+H]+	= 271.155338 Da

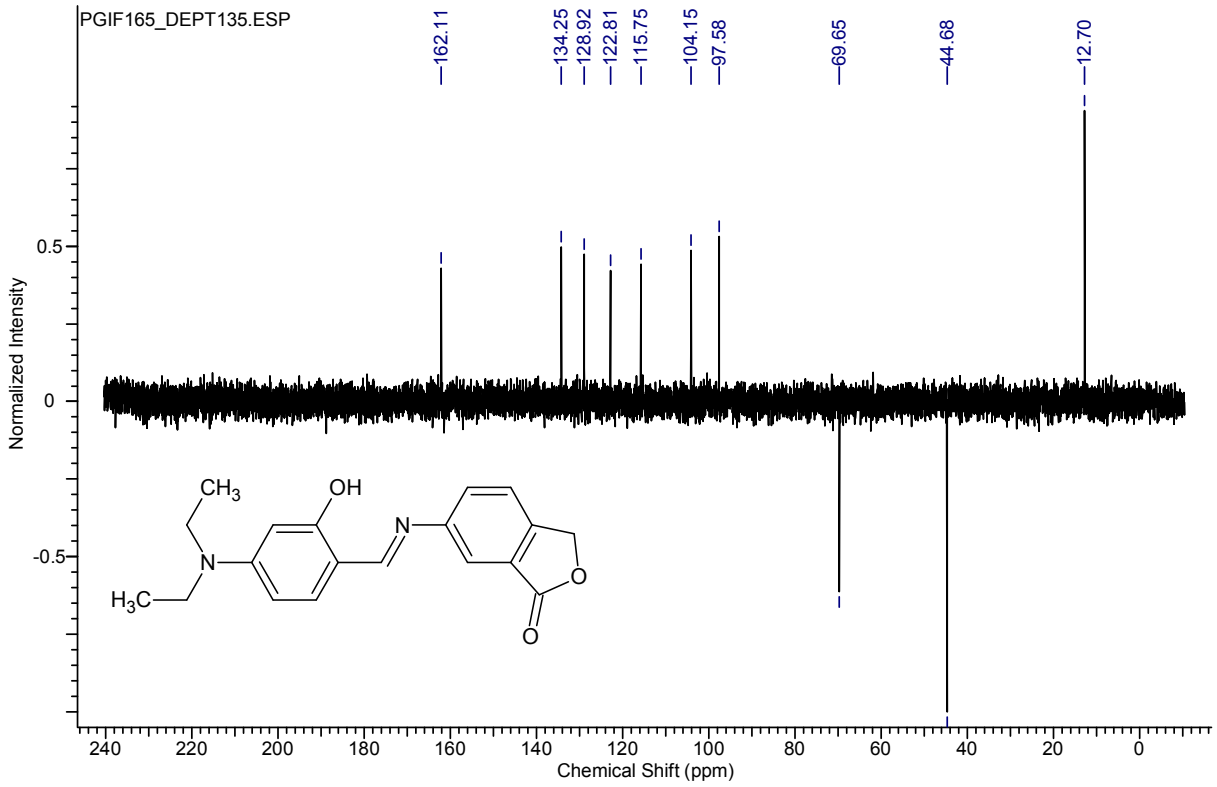
^{1}H FT-NMR (500 MHz, $CDCl_3$ + TMS, 298 K, ppm): 14.00 (s, 1H, OH), 9.07 (s, 1H, C-H imine), 8.66 (d, J_{ortho} = 4.8 Hz, 2H, acceptor ring), 7.16 (d, J_{ortho} = 9.0 Hz, 1H, donor ring), 7.03 (t, J_{ortho} = 4.8 Hz, 1H, acceptor ring), 6.27 (dd, J_{ortho} = 9.2 Hz, J_{meta} = 2.6 Hz, 1H, donor ring), 6.08 (d, J_{meta} = 2.5 Hz, 1H, donor ring), 3.42 (q, J = 7.2 Hz, 4H, N-CH_2), 1.22 (t, J = 7.2 Hz, 6H, -CH_3).
$^{13}C\{^{1}H\}$ FT-NMR / $^{13}C\{^{1}H\}$ DEPT135 FT-NMR (75 MHz, $CDCl_3$ + TMS, 298 K, ppm): 170.64 (C aromatic), 162.42 (C aromatic), 160.28 (C-H imine), 158.50 (C-H aromatic), 154.11 (C aromatic), 135.84 (C-H aromatic), 116.97 (C-H aromatic), 109.79 (C aromatic), 105.90 (C-H aromatic), 98.08 (C-H aromatic), 44.77 (N-CH_2), 12.85 (-CH_3).
HRMS (ESI^+): calcd. for $C_{15}H_{19}N_4O$ $[M+H]^+$: 271.1553, found: 271.1566, error: 4.79 ppm.
FT-IR (KBr, cm^{-1}): 3075, 3031, 2968, 2930, 2895, 2870, 1635, 1624, 1564, 1513, 1486, 1439, 1396, 1373, 1349,1301, 1263, 1245, 1223, 1198, 1142, 1097, 1076, 1007, 988, 963, 913, 824, 814, 795, 695, 638, 515.
Melting point (1-propanol/2-propanol 1:3): 177-178°C.



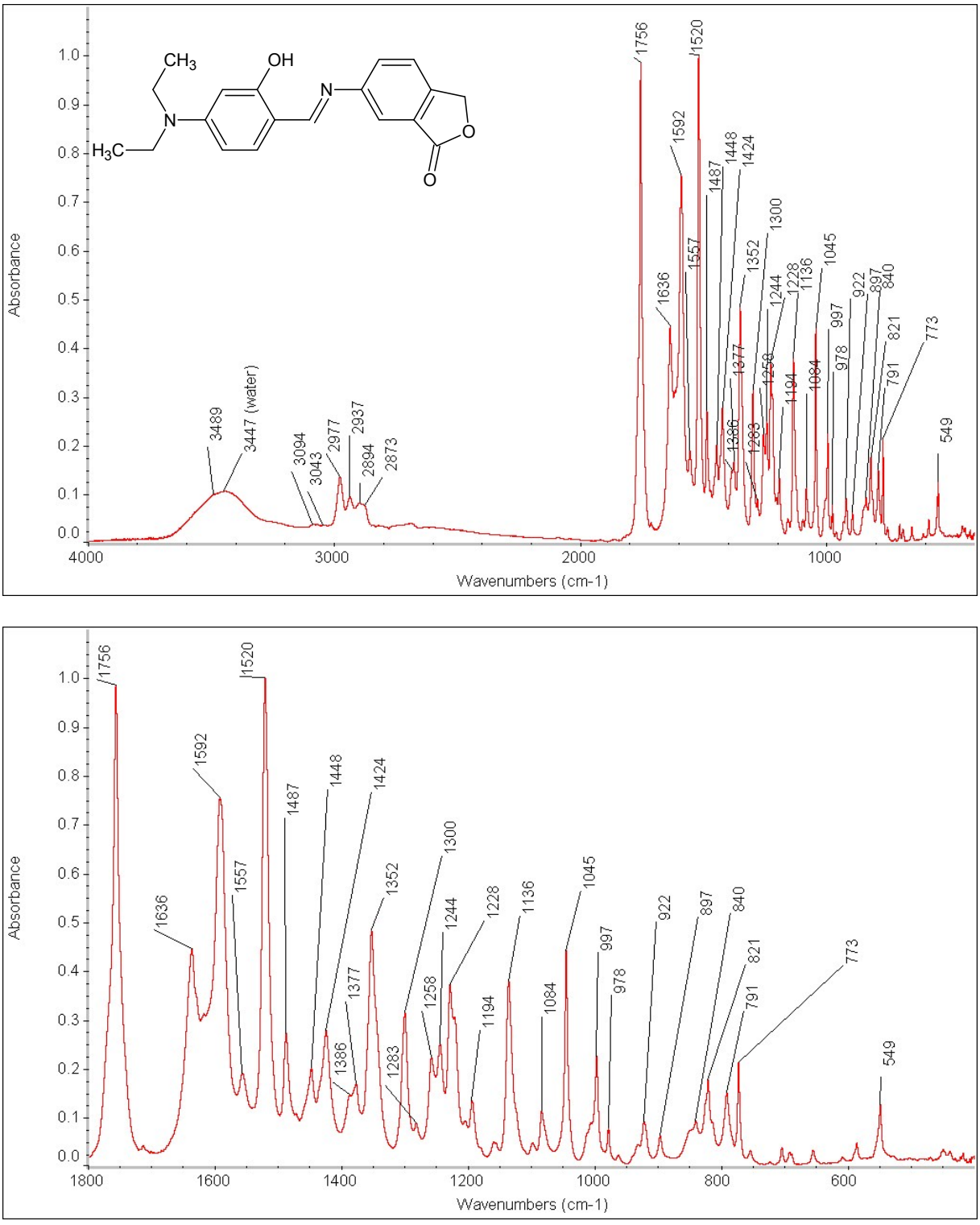
Spectrum S1. 1H FT-NMR spectrum of **2** (with extended aromatic region)



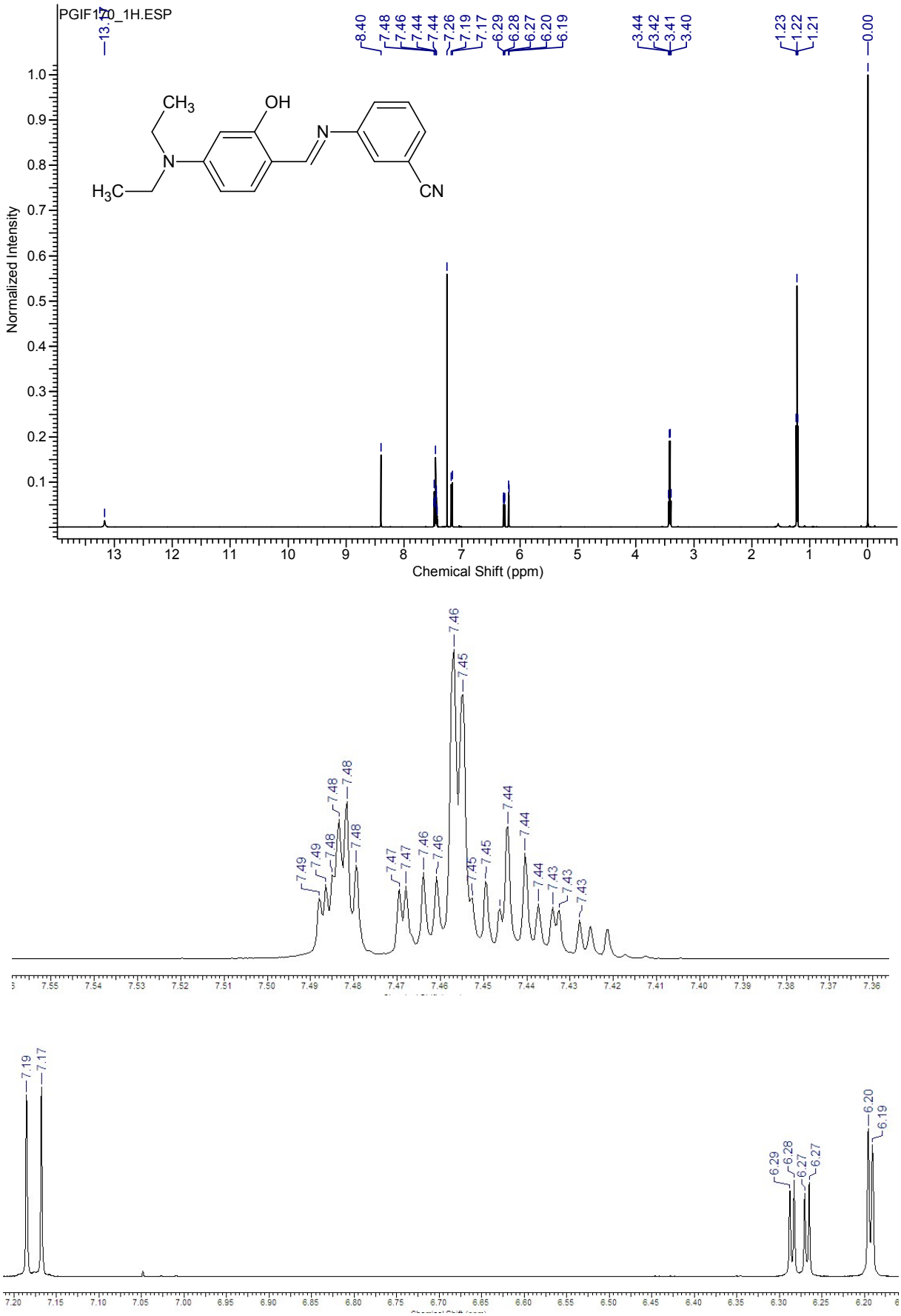
Spectrum S2. 13C{1H} FT-NMR spectrum of **2**



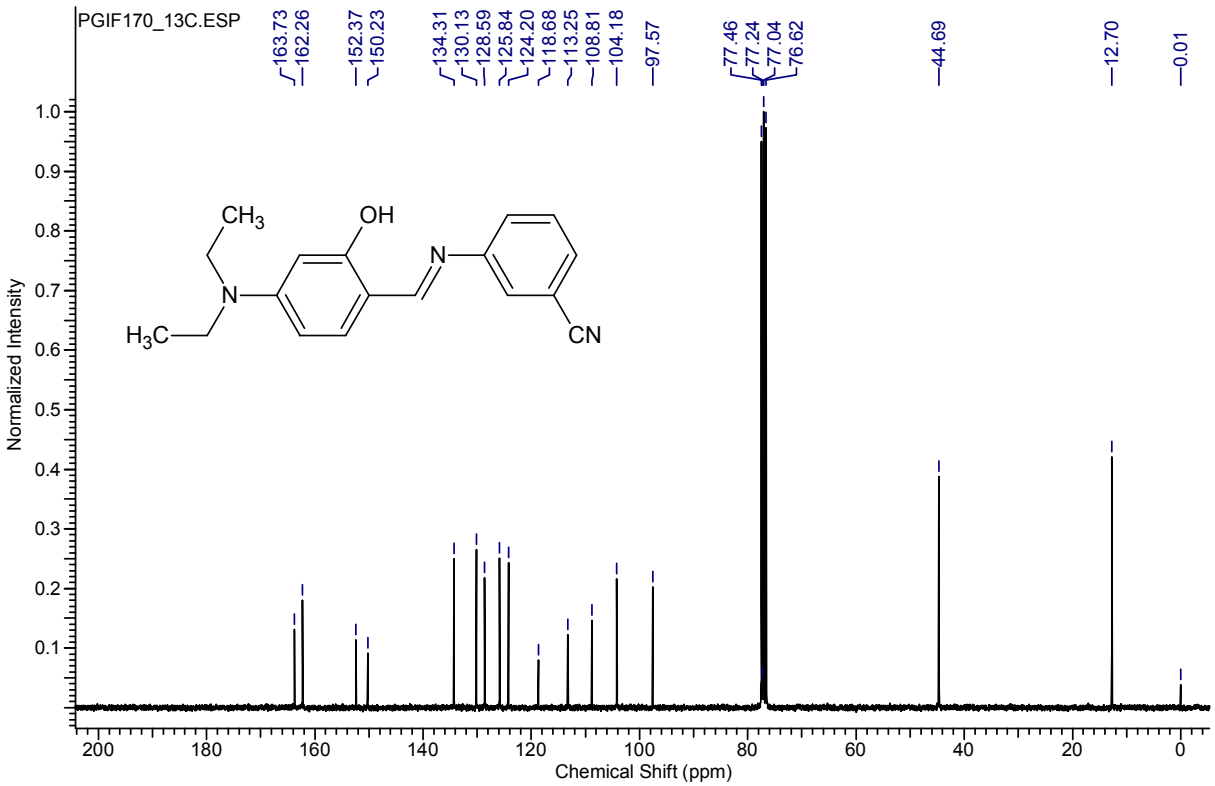
Spectrum S3. 13C{1H} DEPT135 FT-NMR spectrum of **2**



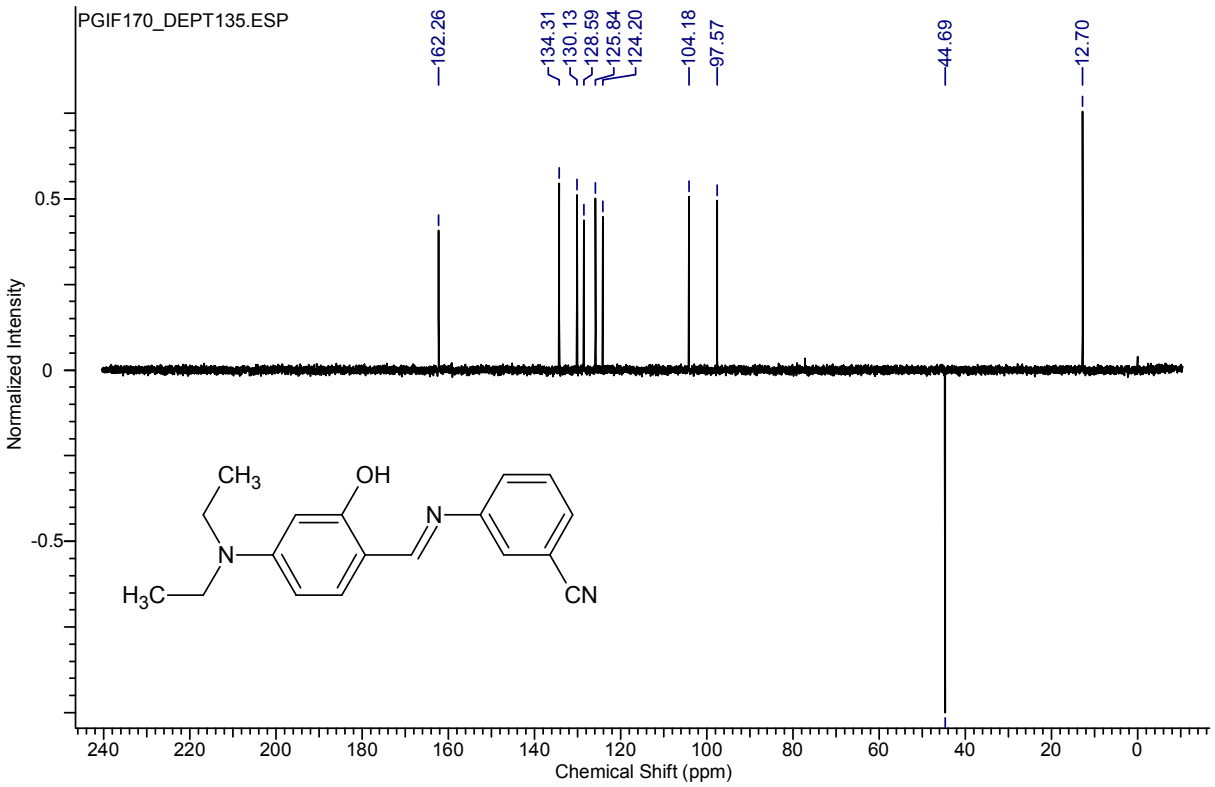
Spectrum S4. FT-IR spectrum of **2**



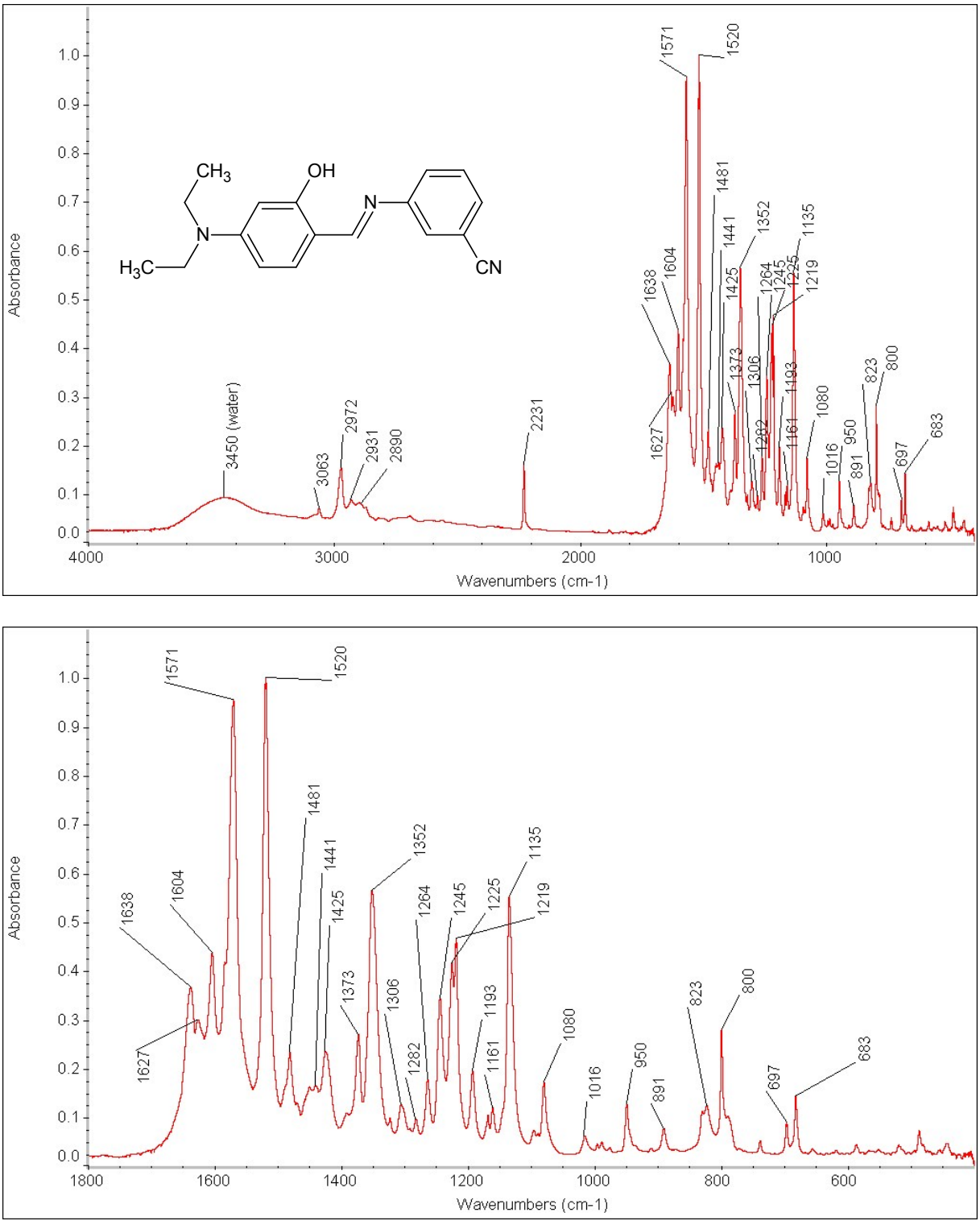
Spectrum S5. 1H FT-NMR spectrum of **3** (with extended aromatic region)



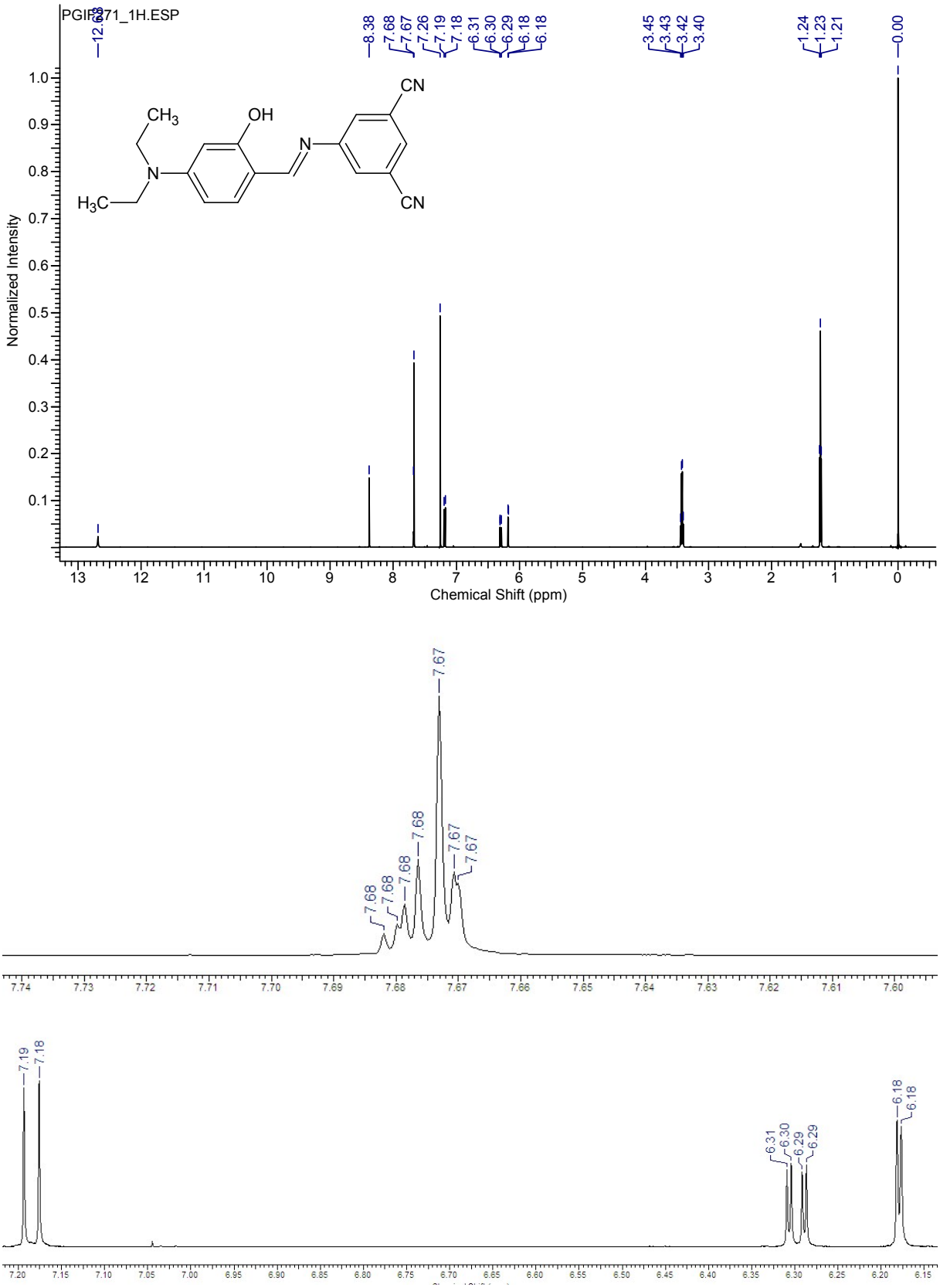
Spectrum S6. 13C{1H} FT-NMR spectrum of **3**



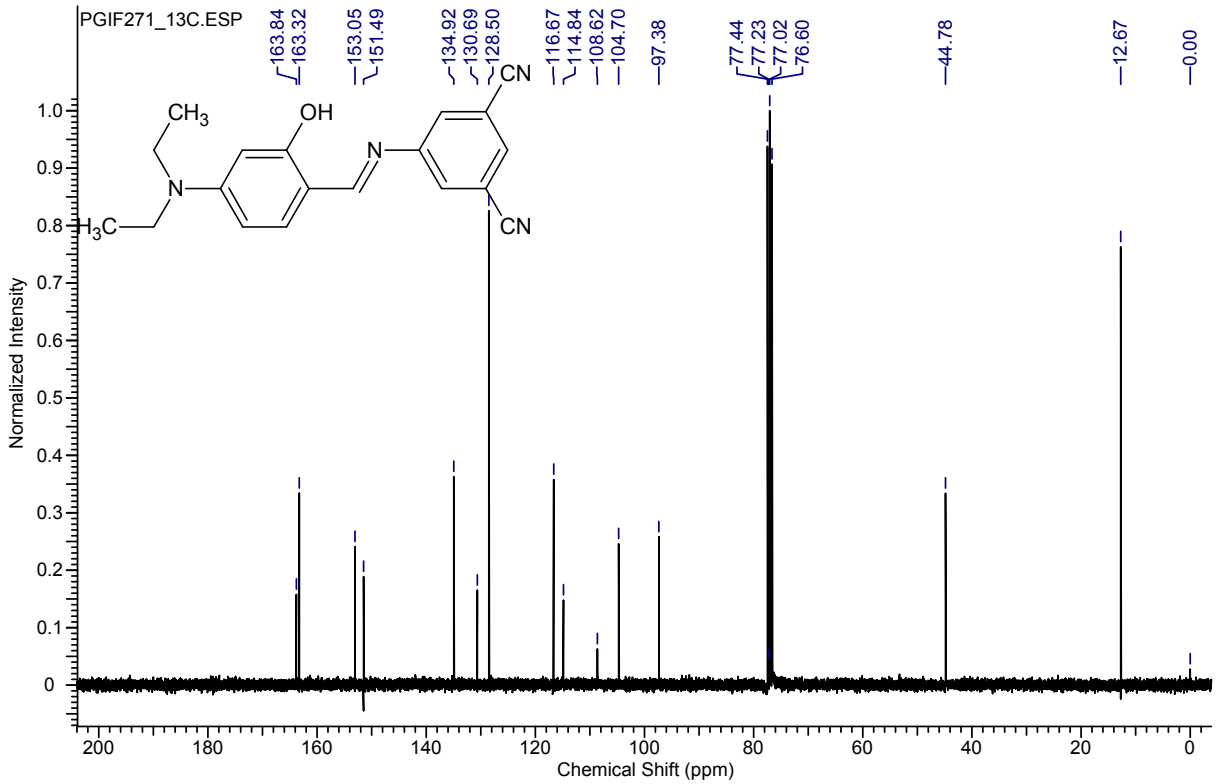
Spectrum S7. 13C{1H} DEPT135 FT-NMR spectrum of **3**



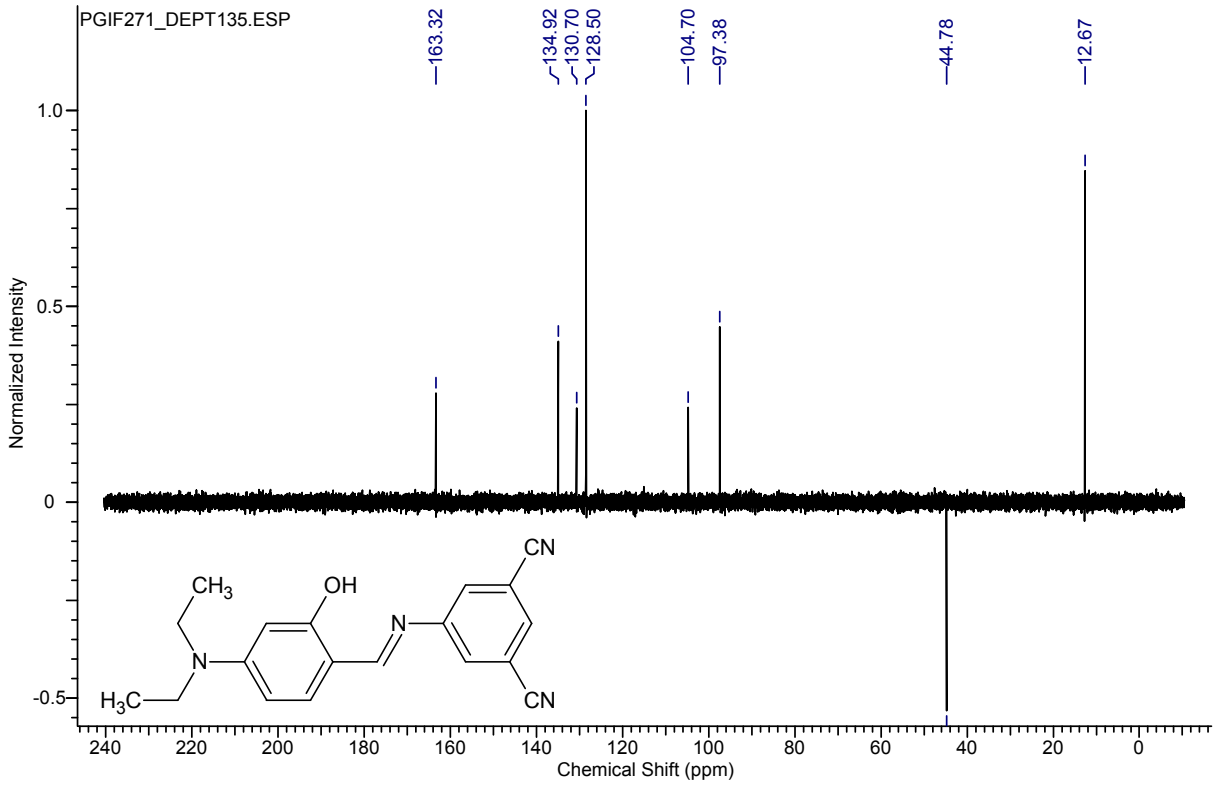
Spectrum S8. FT-IR spectrum of **3**



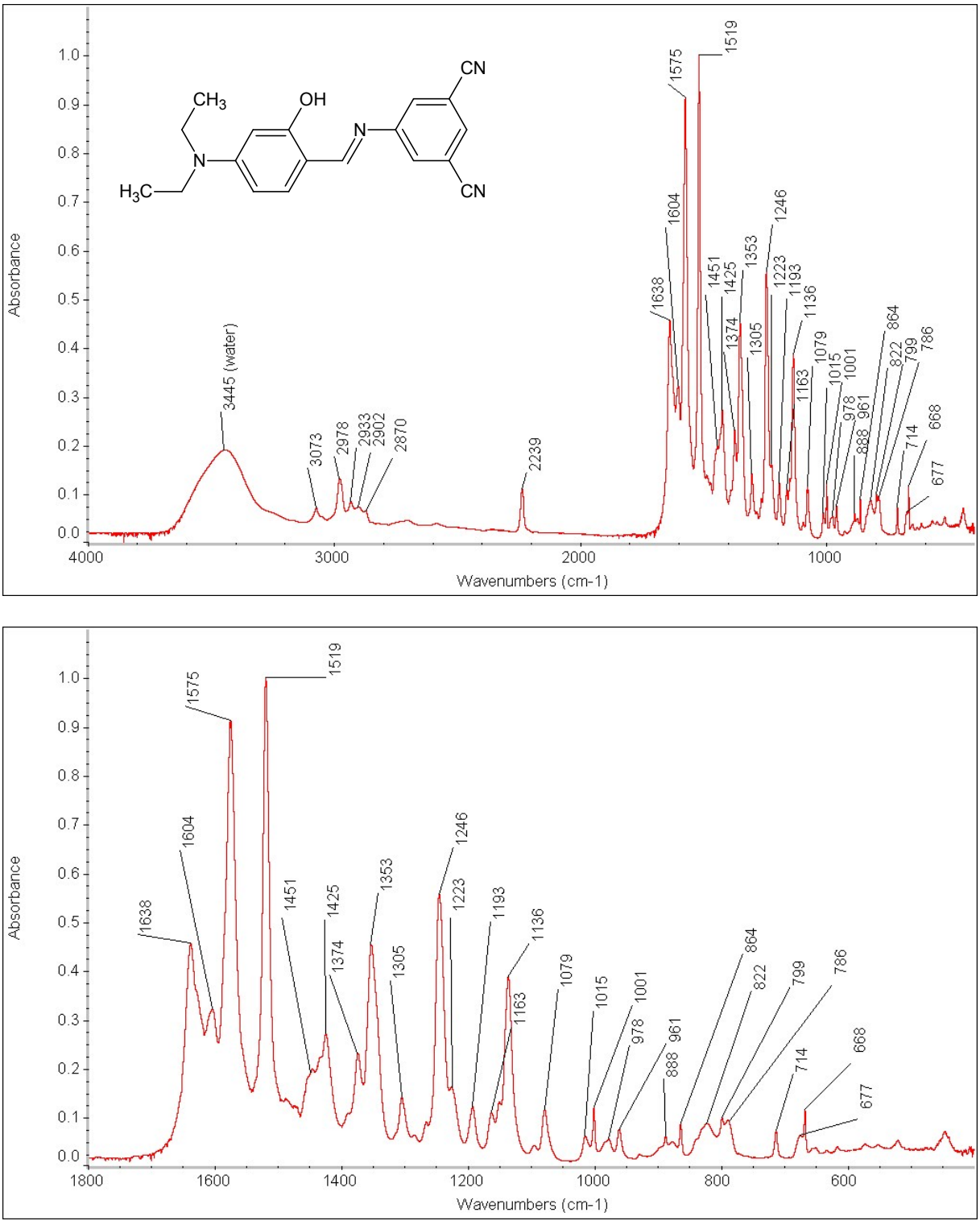
Spectrum S9. 1H FT-NMR spectrum of **4** (with extended aromatic region)



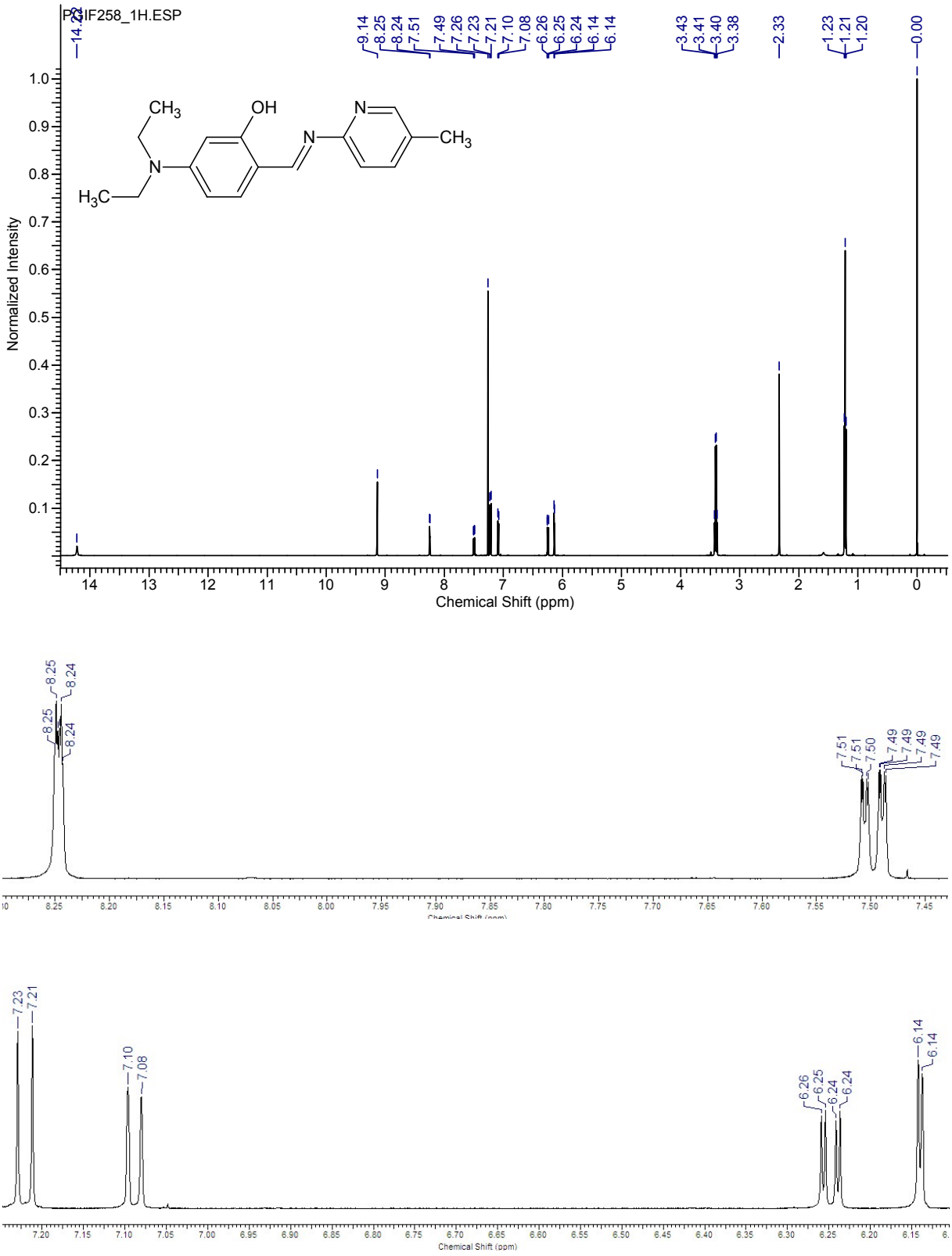
Spectrum S10. 13C{1H} FT-NMR spectrum of **4**



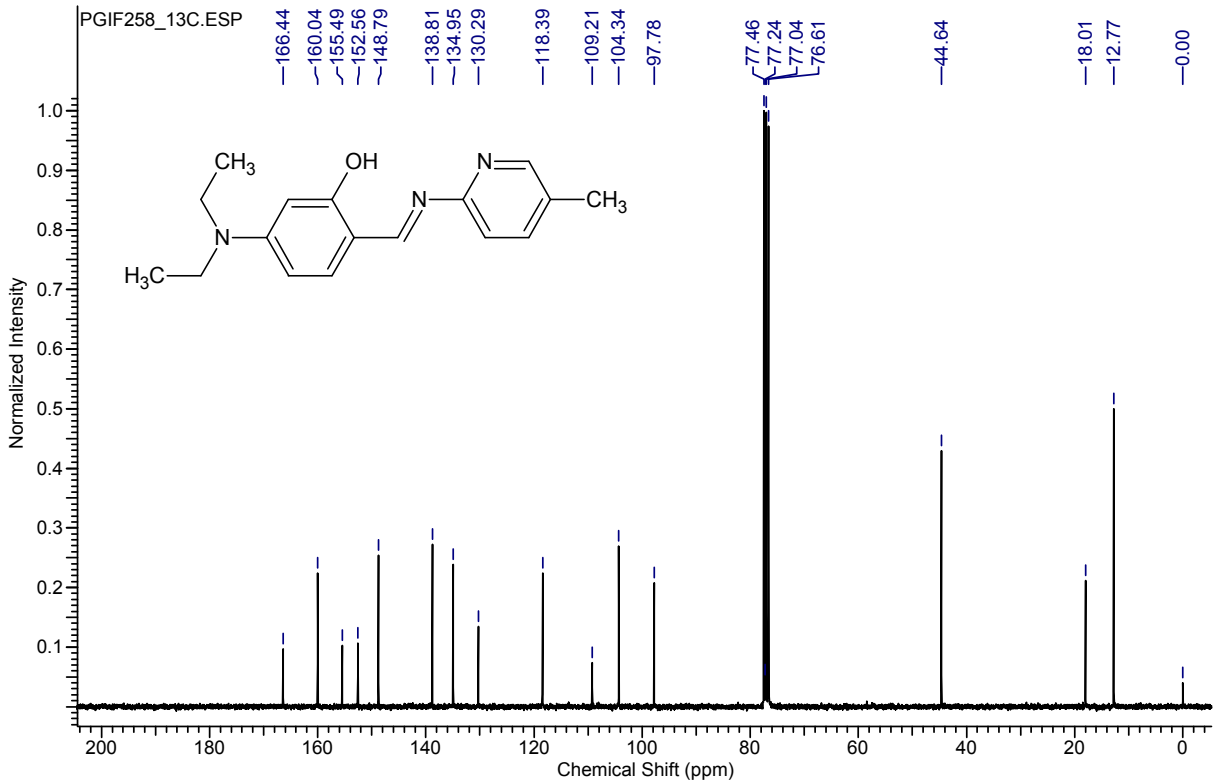
Spectrum S11. 13C{1H} DEPT135 FT-NMR spectrum of **4**



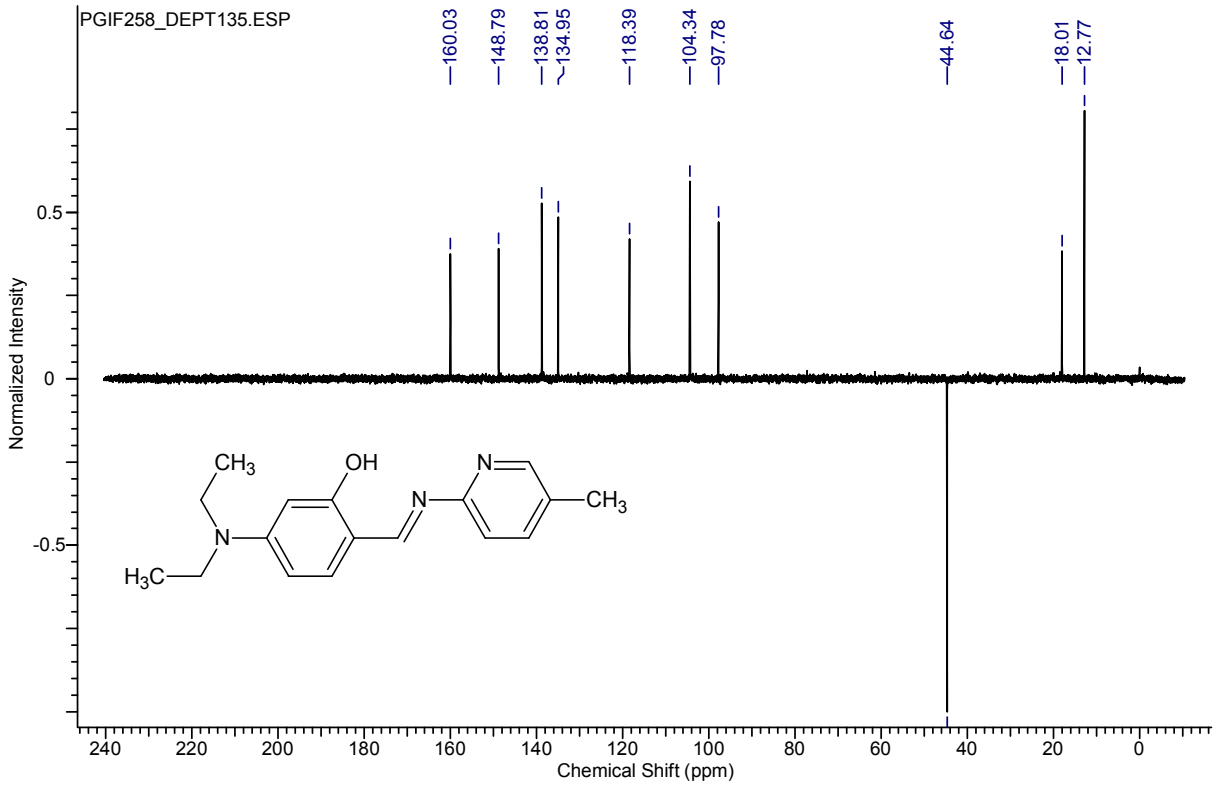
Spectrum S12. FT-IR spectrum of **4**



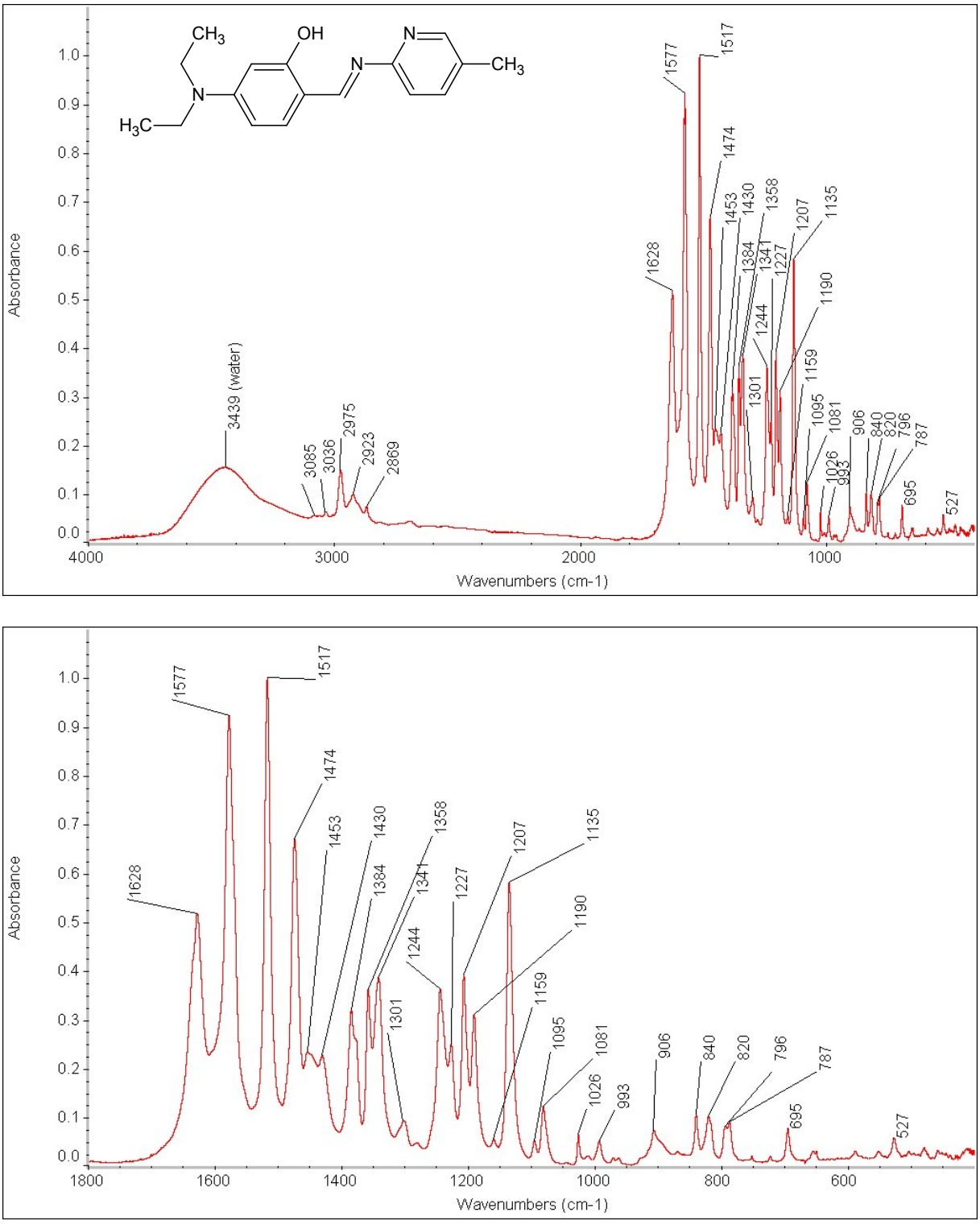
Spectrum S13. 1H FT-NMR spectrum of **5** (with extended aromatic region)



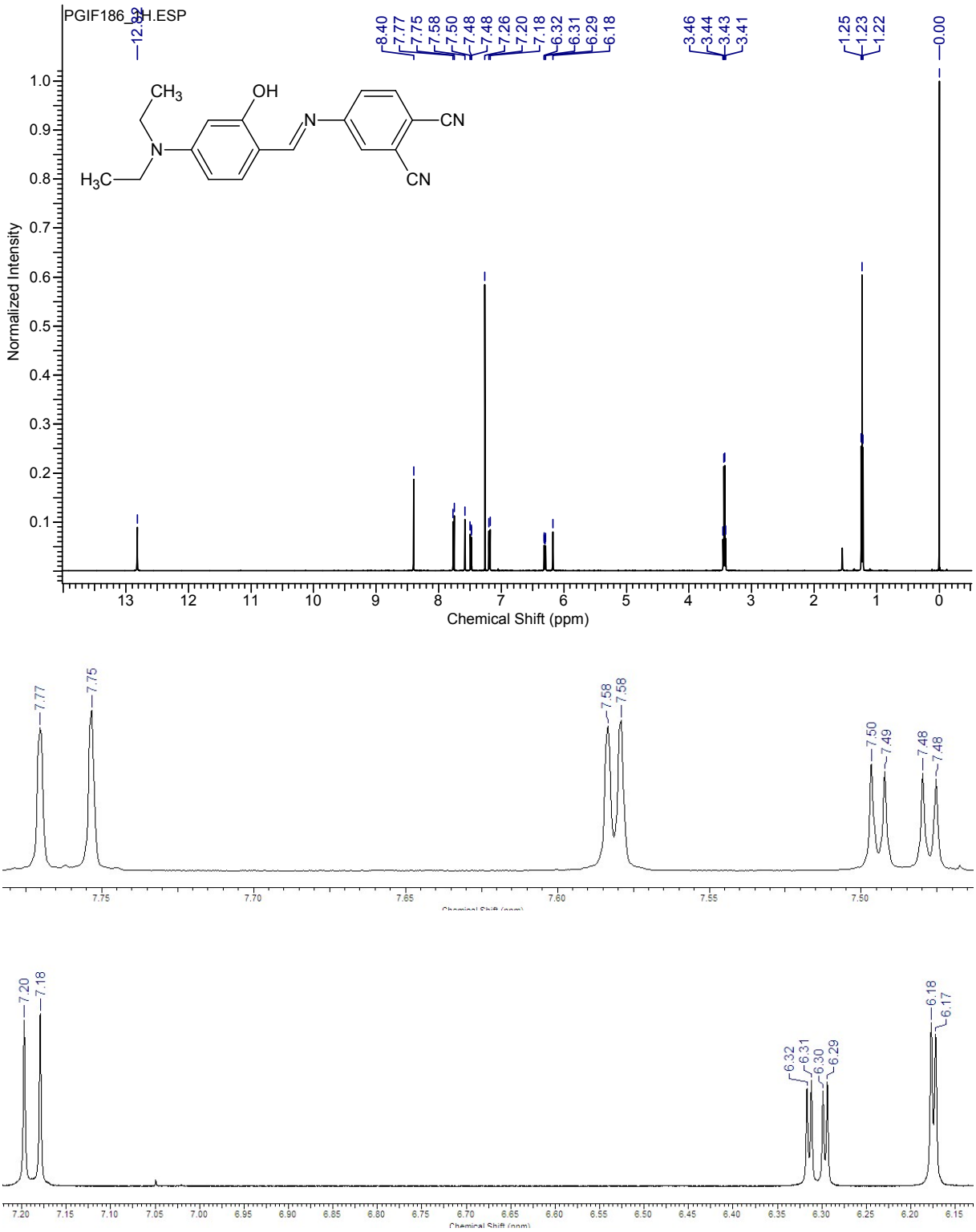
Spectrum S14. 13C{1H} FT-NMR spectrum of **5**



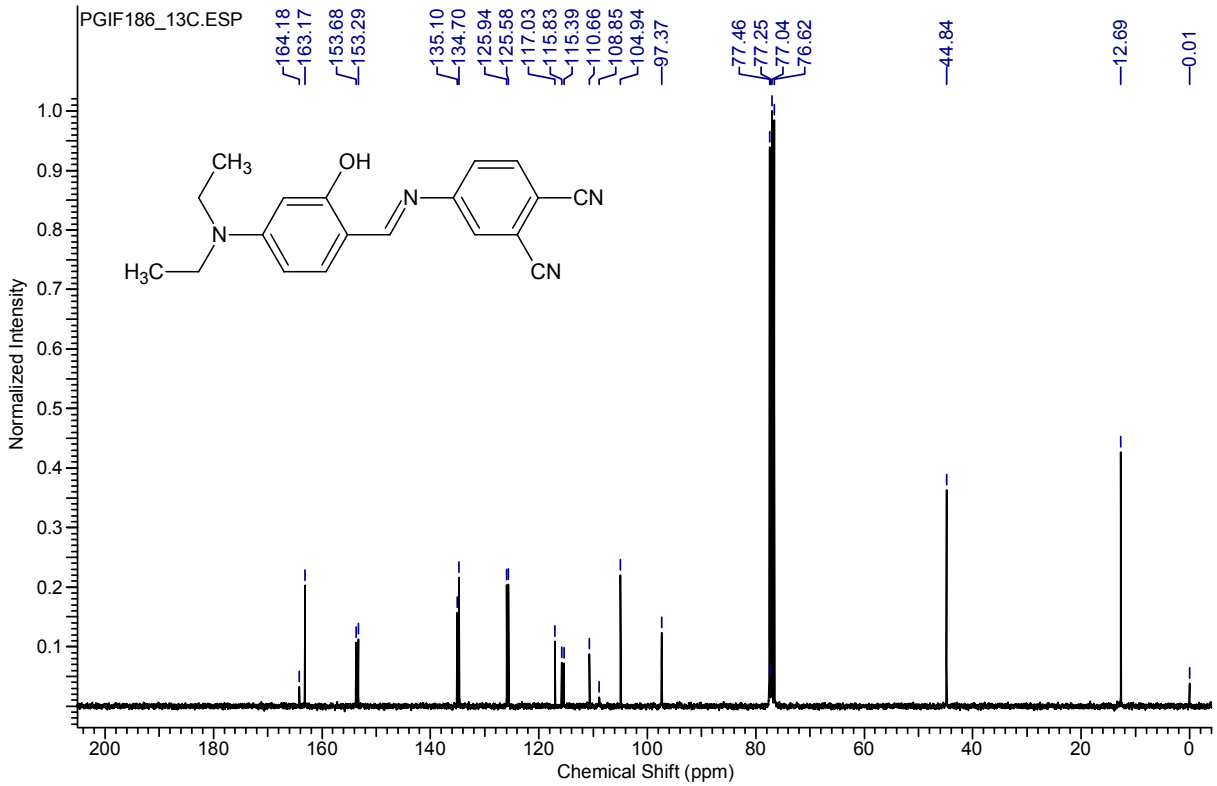
Spectrum S15. 13C{1H} DEPT135 FT-NMR spectrum of **5**



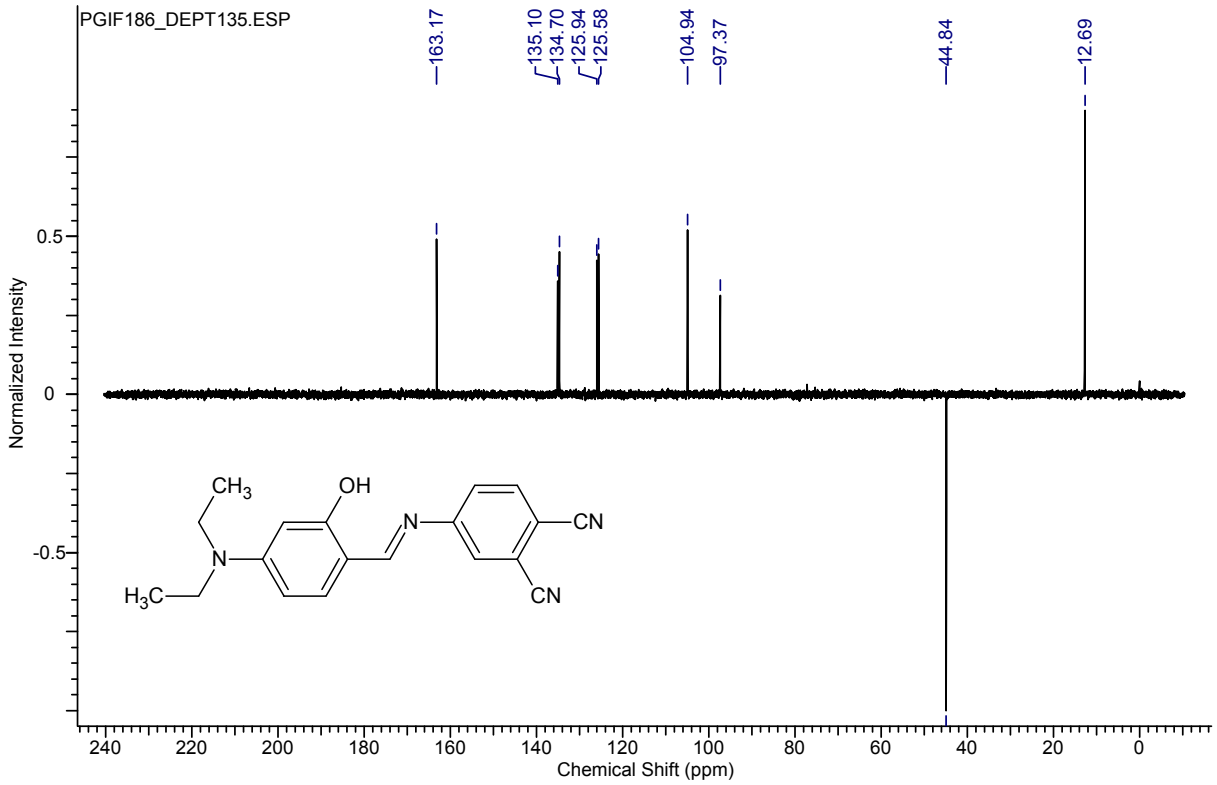
Spectrum S16. FT-IR spectrum of **5**



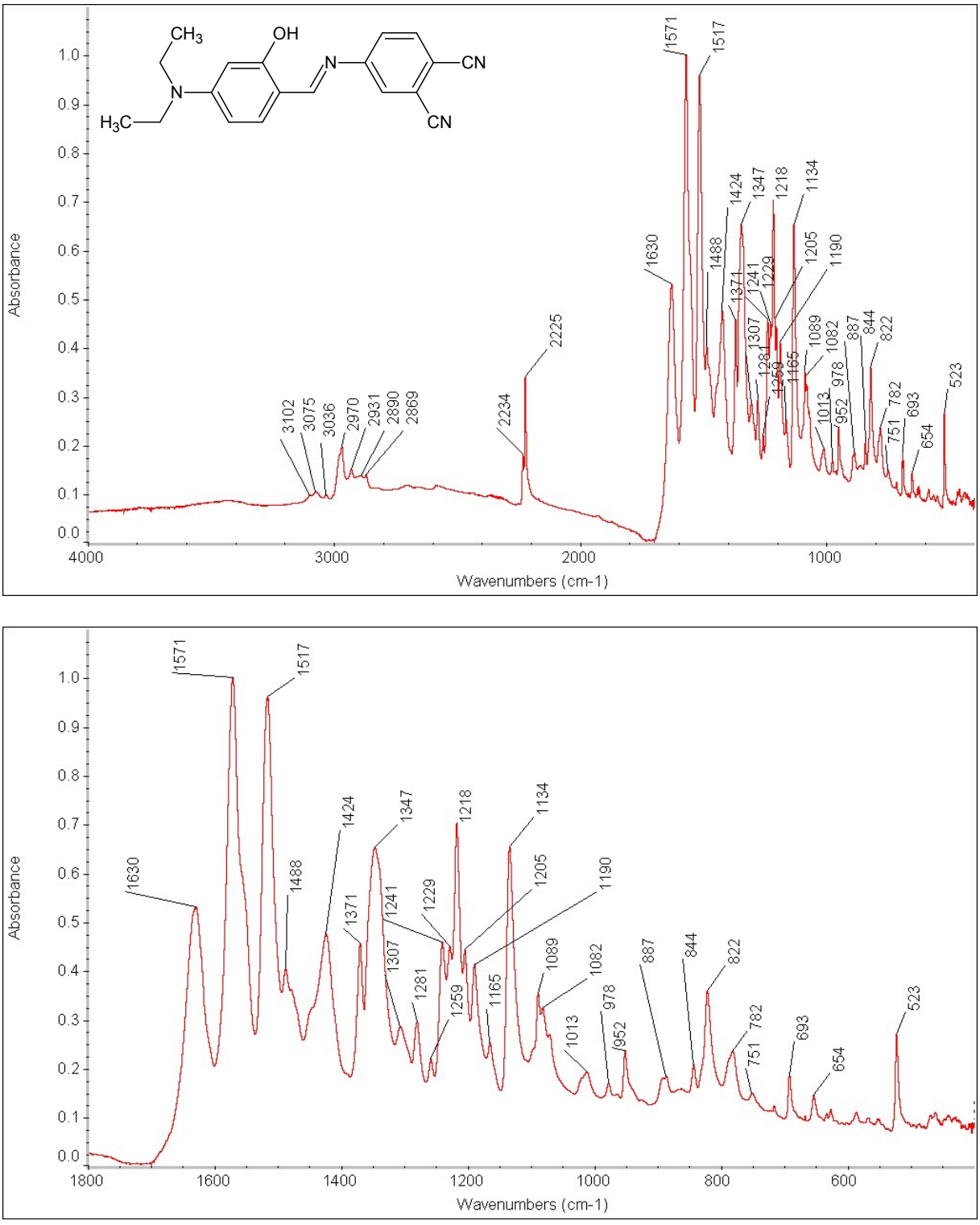
Spectrum S17. 1H FT-NMR spectrum of **6** (with extended aromatic region)



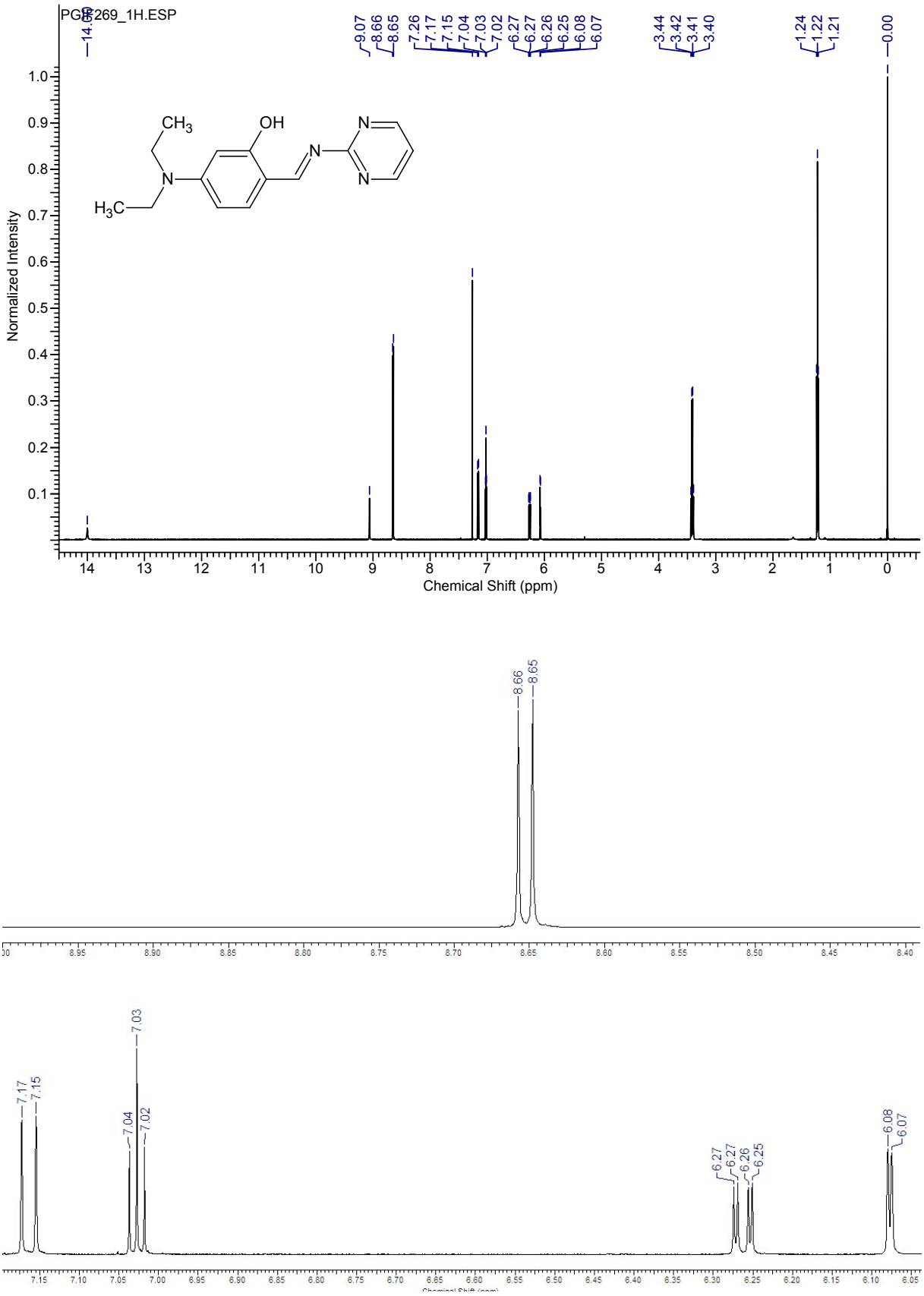
Spectrum S18. 13C{1H} FT-NMR spectrum of **6**



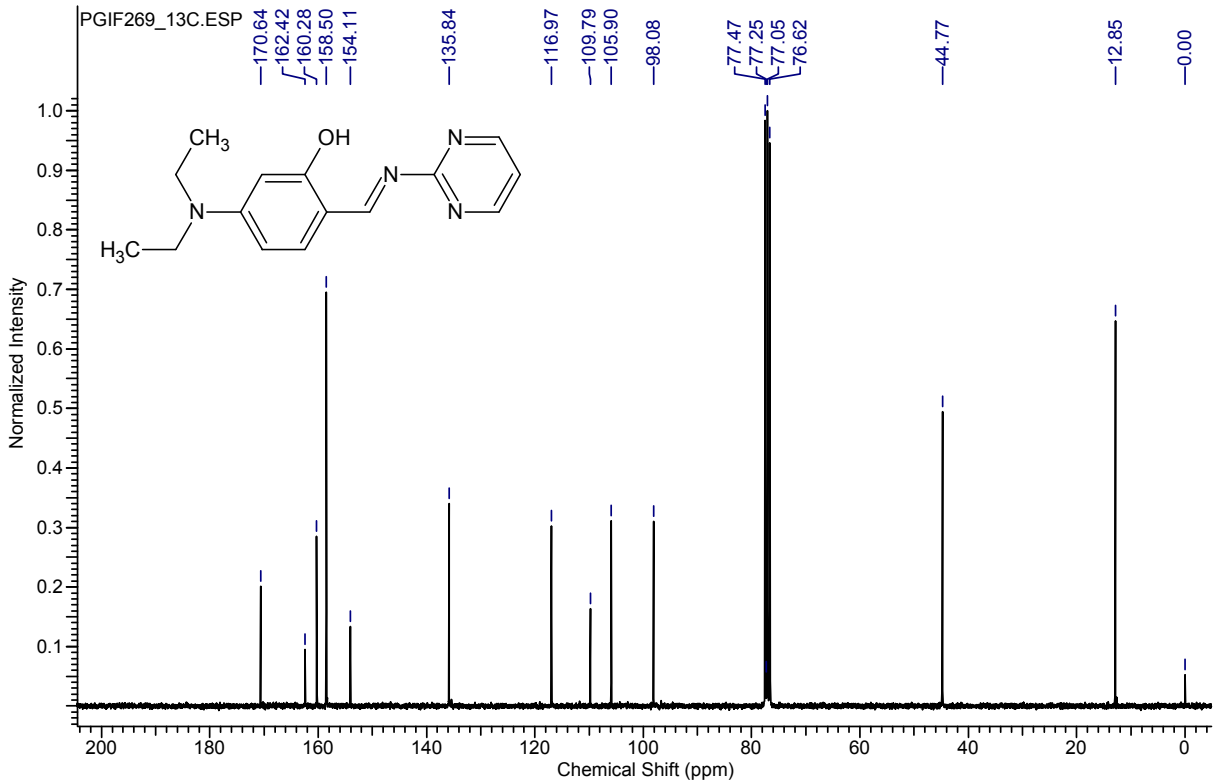
Spectrum S19. 13C{1H} DEPT135 FT-NMR spectrum of **6**



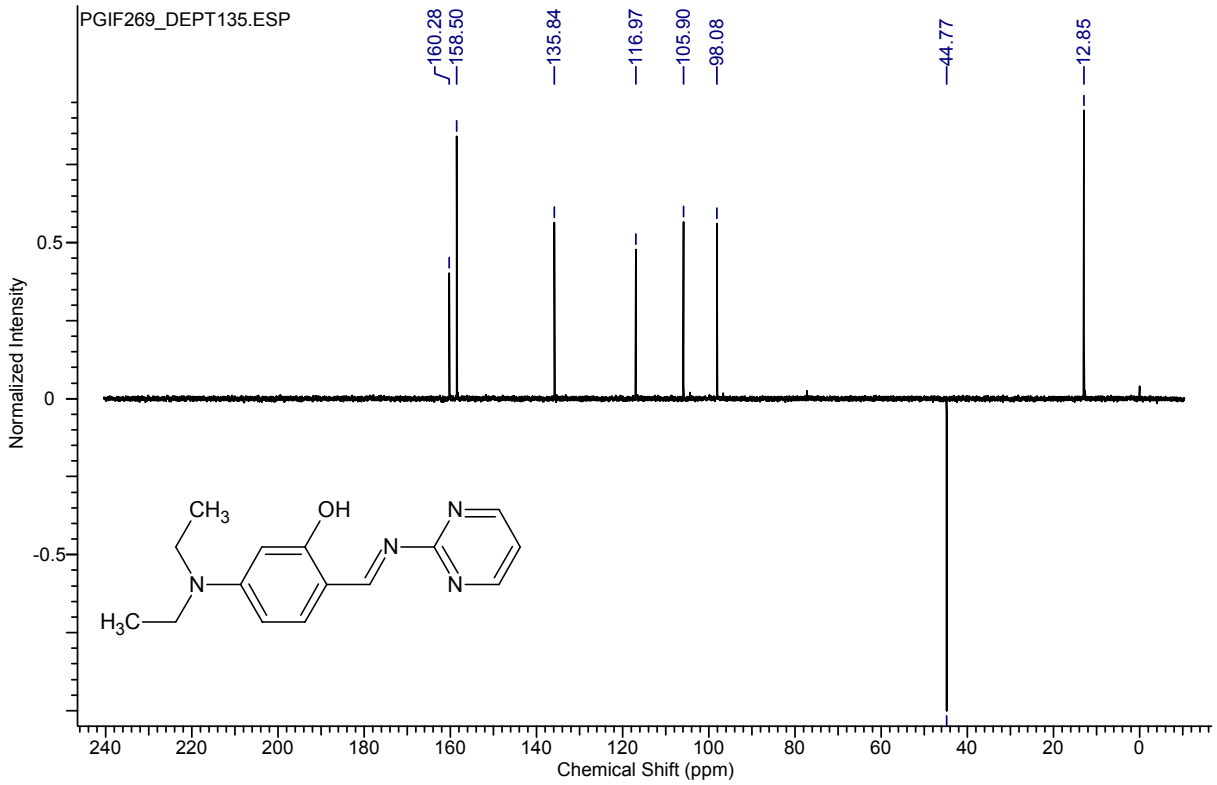
Spectrum S20. FT-IR spectrum of **6**



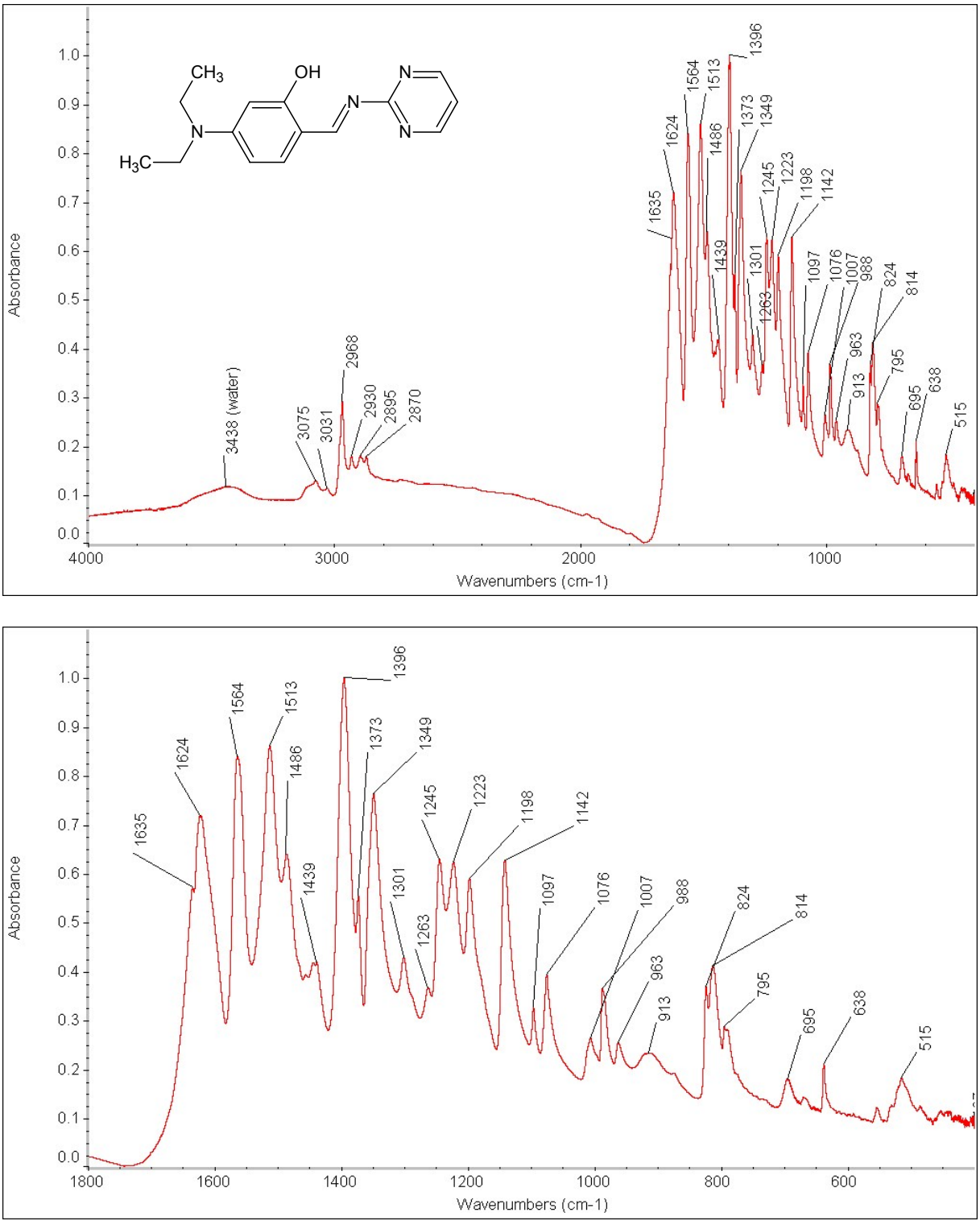
Spectrum S21. 1H FT-NMR spectrum of **7** (with extended aromatic region)



Spectrum S22. 13C{1H} FT-NMR spectrum of **7**



Spectrum S23. 13C{1H} DEPT135 FT-NMR spectrum of **7**



Spectrum S24. FT-IR spectrum of **7**