# A Novel TICT-based Molecular Rotor: Synthesis, Crystal structure and Application in High Resolution Imaging of Sweat Pores

Sanjeev Kumar[a], Balkaran Singh Sran[a], Dharmendra Gahalot[b], Prakash Chandra Mishra[b] and Prabhpreet Singh[*a]

[a]Department of Chemistry, UGC Centre for Advanced Studies-II, Guru Nanak Dev University, Amritsar 143001 (pb.)-India

[b]Department of Biotechnology, Guru Nanak Dev University, Amritsar 143001 (pb.)-India

E-mail: prabhpreet.chem@gndu.ac.in; M: +91 8427101534.
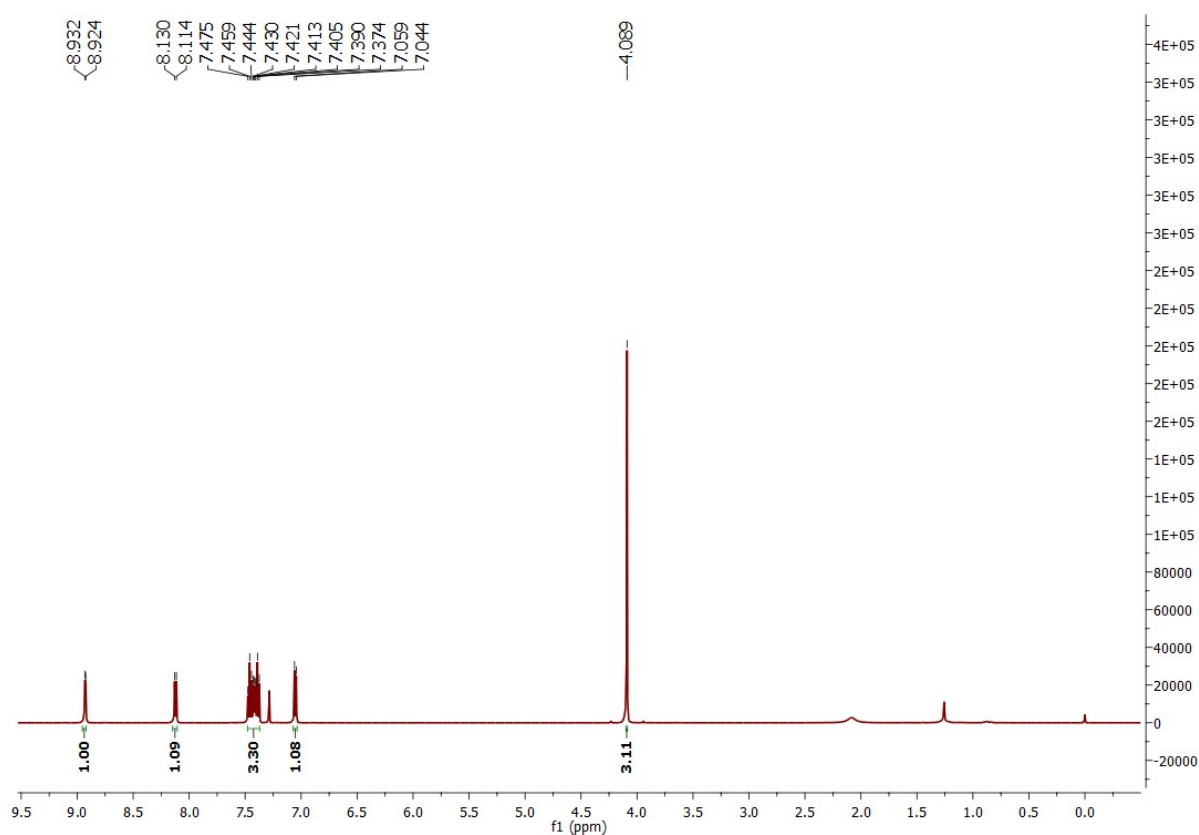
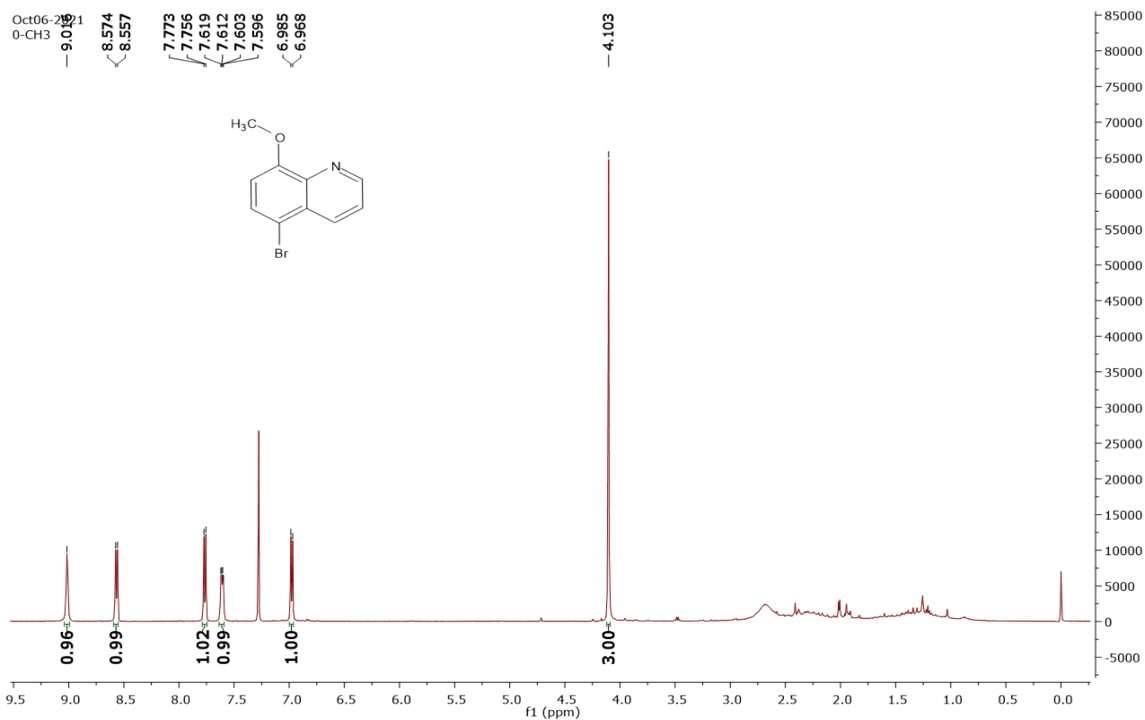**Figure S1:** ^{1}H NMR data of 8-methoxyquinoline.
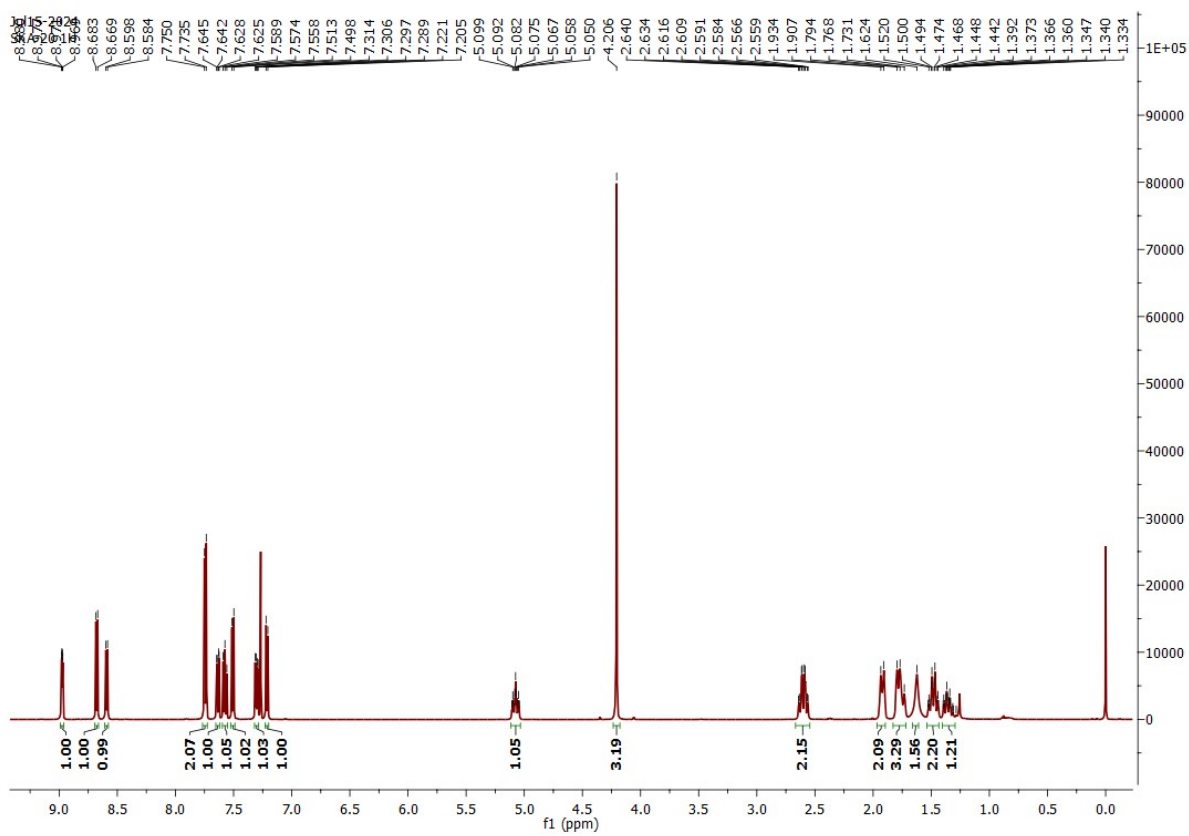
Figure S2: ¹H NMR data of Compound **2**.
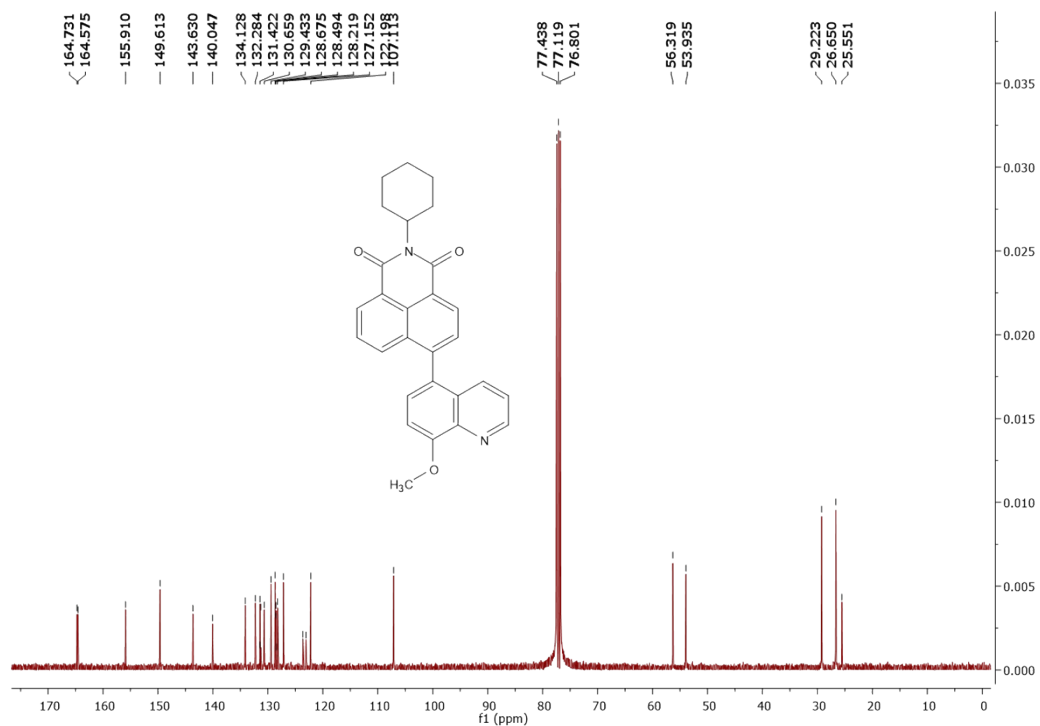

Figure S3: ¹H NMR data of **NI-HQ**.

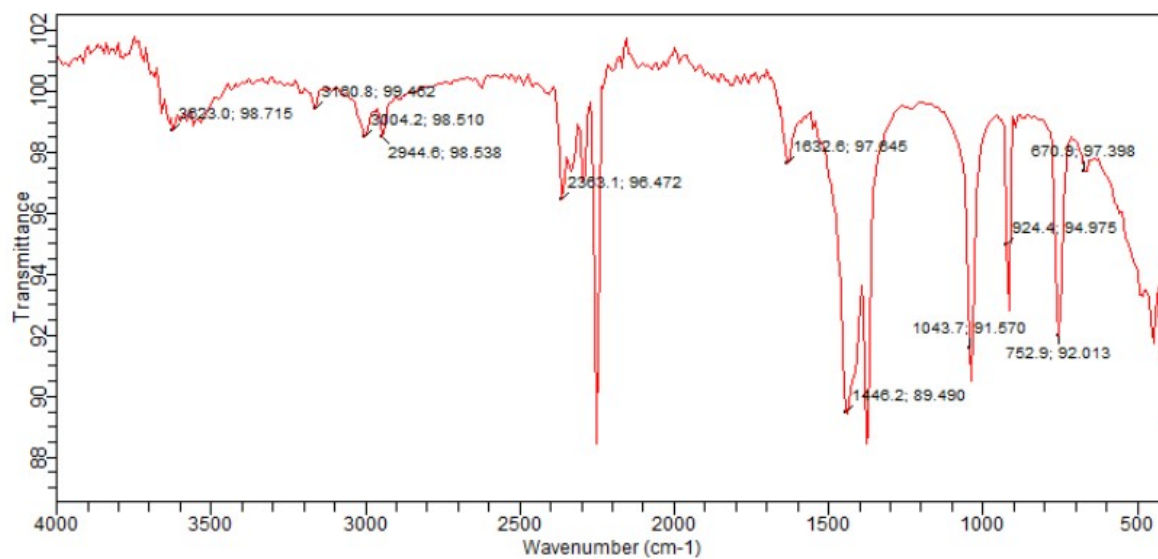**Figure S4:** ^{13}C NMR data of **NI-HQ**.
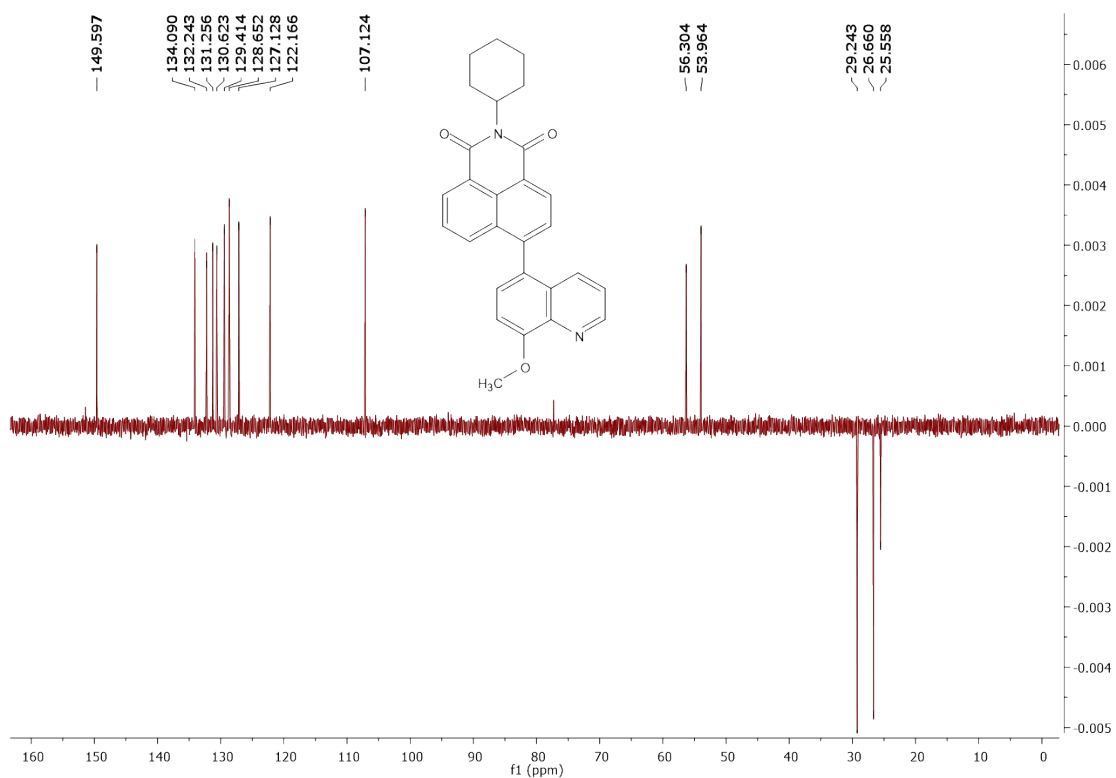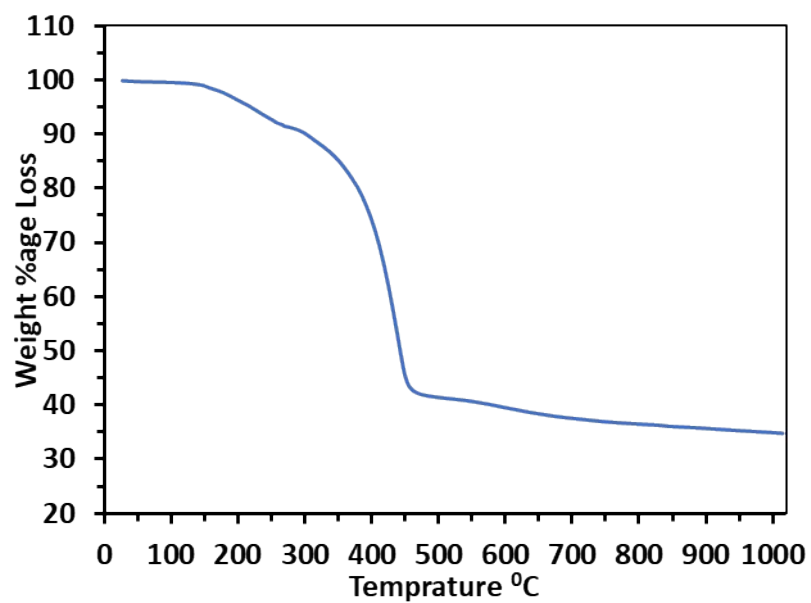

Figure S5: ^{13}C-DEPT NMR data of **NI-HQ**.
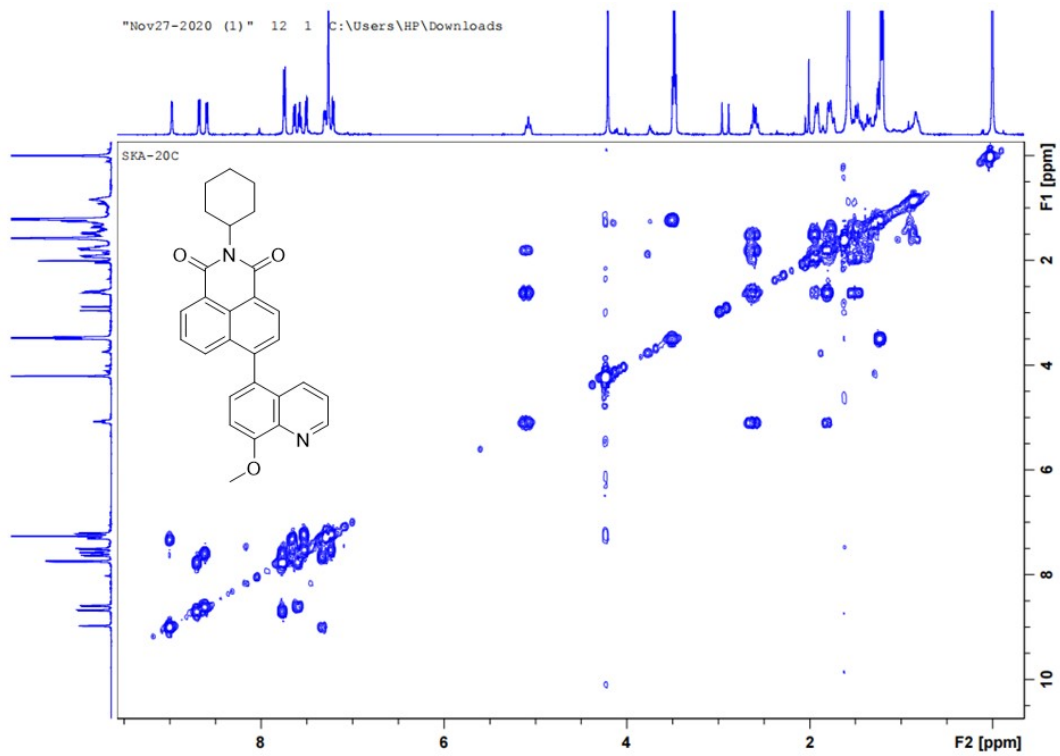
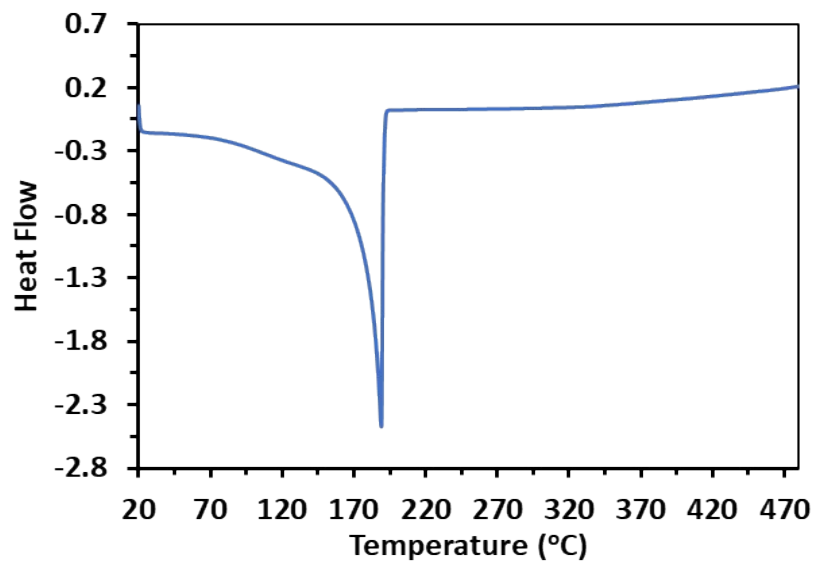**Figure S6:** ^{1}H-^{1}H COSY NMR data of **NI-HQ**.
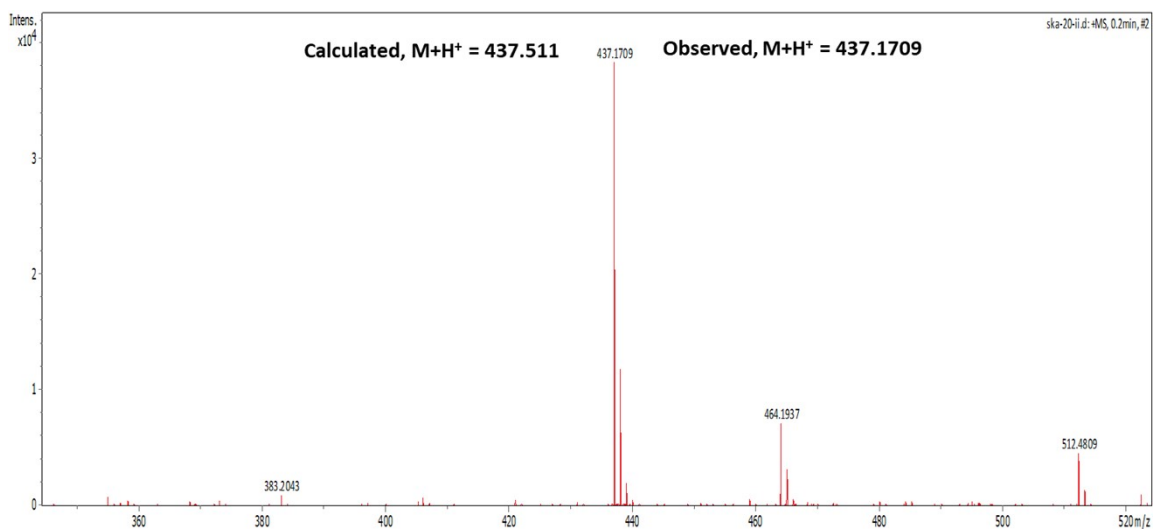
Figure S7: HRMS data of **NI-HQ**.

Figure S8: FTIR data of **NQ-OCH₃**.
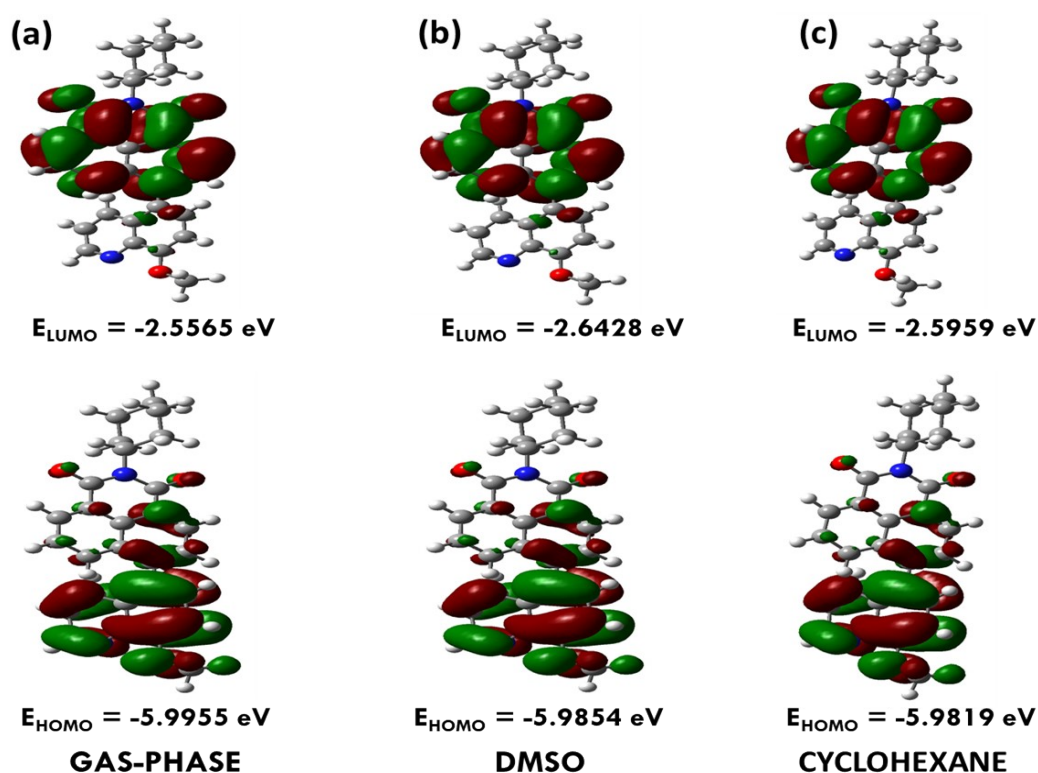

Figure S9: TGA data of **NI-HQ**.

Figure S10: DSC data of **NI-HQ**.

Table S1: Crystal data and structure refinement for NI-HQ.

| Identification code	**NI-HQ**
CCDC Number	2094838
Empirical formula	$C_{28}H_{24}N_2O_3$
Formula weight	436.49
Temperature/K	296.15
Crystal system	Triclinic
Space group	P-1
a/Å	8.698(4)
b/Å	10.218(4)
c/Å	17.020(8)
α/°	99.167(8)
β/°	98.646(7)
γ/°	108.563(16)
Volume/Å^3	1382.6(11)
Z	2
ρ_{calc} [gcm^{-3}]	1.048
μ [mm^{-1}]	0.069
$F(000)$	460.0
Crystal size/mm^3	0.21×0.18×0.11
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	5.374 to 56.1
Index ranges	-10 ≤ h ≤ 11, -13 ≤ k ≤ 13, -22 ≤ l ≤ 22
Reflections collected	21322
Independent reflections	6606 [R_{int} = 0.0910, R_{sigma} = 0.1263]
Data/restraints/parameters	6606/0/300
Goodness-of-fit on F^2	0.880
Final R indexes [$I{\geq}2\sigma(I)$]	R_1 = 0.0694, wR_2 = 0.1813
Final R indexes [all data]	R_1 = 0.1982, wR_2 = 0.2495
Largest peak/hole [eÅ^{-3}]	0.23/-0.18

Table S2: Photophysical parameters of NI-HQ in different solvents.

Solvent	E_T (30)	ν_a (cm^{-1})	ν_f (cm^{-1})	$\Delta\nu$ (cm^{-1})	Φ	τ (ns)	K_rx10^7 s^{-1}	K_{nr}x10^8 s^{-1}	E_f	Δf
Cyclohexane	30.8	29851	22935	6916	0.37	1.58	23.4	7.7	0.28	0.406
Hexane	30.9	30030	22935	7095	0.36	ND	ND	ND	ND	0.374
Toluene	33.9	29586	21505	8081	0.28	ND	ND	ND	ND	0.466
Benzene	34.3	29326	20920	8406	0.29	ND	ND	ND	ND	0.457
Diethyl ether	34.5	29674	21052	8622	0.23	ND	ND	ND	ND	0.523
THF	37.5	29674	20202	9472	0.22	2.34	9.4	9.1	0.15	0.605
EA	38.0	29155	19920	9235	0.26	3.03	8.6	9.1	0.18	0.570
CHCl$_3$	39.1	29070	20920	8150	0.25	1.81	13.8	8.3	0.18	0.569
DCM	40.7	29070	20162	8908	0.25	ND	ND	ND	ND	0.623
DMSO	45.1	28902	17793	11109	0.10	2.52	4.0	9.6	0.06	0.705
CH$_3$CN	45.6	28985	18621	10364	0.23	4.97	4.6	9.5	0.15	0.655
EtOH	51.8	29069	17985	11084	0.041	0.98	4.1	9.8	0.03	0.651
MeOH	55.4	28901	17985	10916	0.013	0.33	4.0	9.6	0.01	0.646

(a) E_{LUMO} = -2.5565 eV

(b) E_{LUMO} = -2.6428 eV

(c) E_{LUMO} = -2.5959 eV

E_{HOMO} = -5.9955 eV
GAS-PHASE

E_{HOMO} = -5.9854 eV
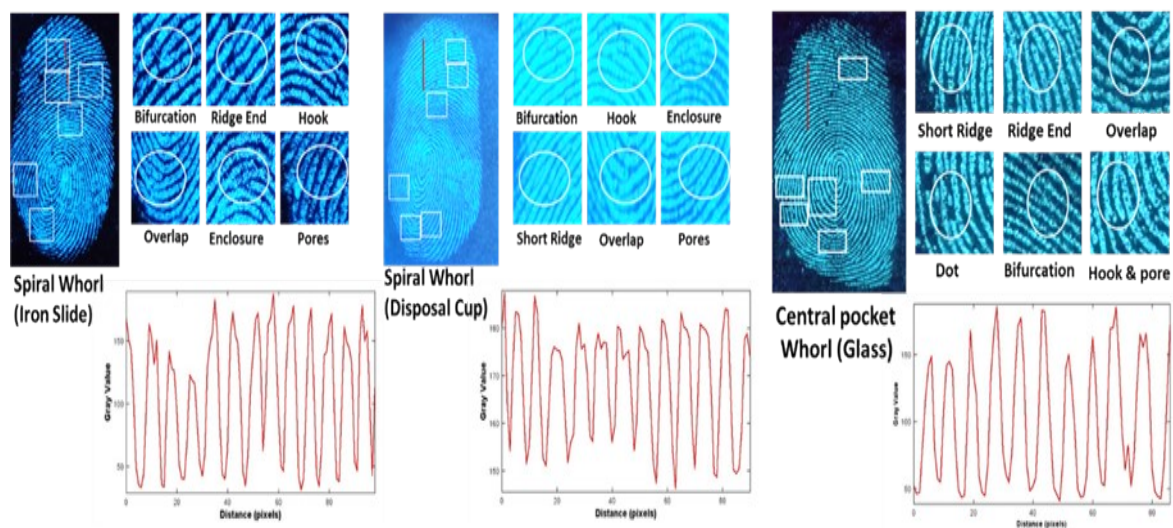**DMSO**

E_{HOMO} = -5.9819 eV
CYCLOHEXANE

Figure S11: The optimized geometries of **NI-HQ** showing HOMO/LUMO contours in (a) gas-phase; (b) DMSO; (c) cyclohexane; and (d) absorbance spectrum of **NI-HQ** in gas-phase, DMSO and cyclohexane predicted by TD-DFT.
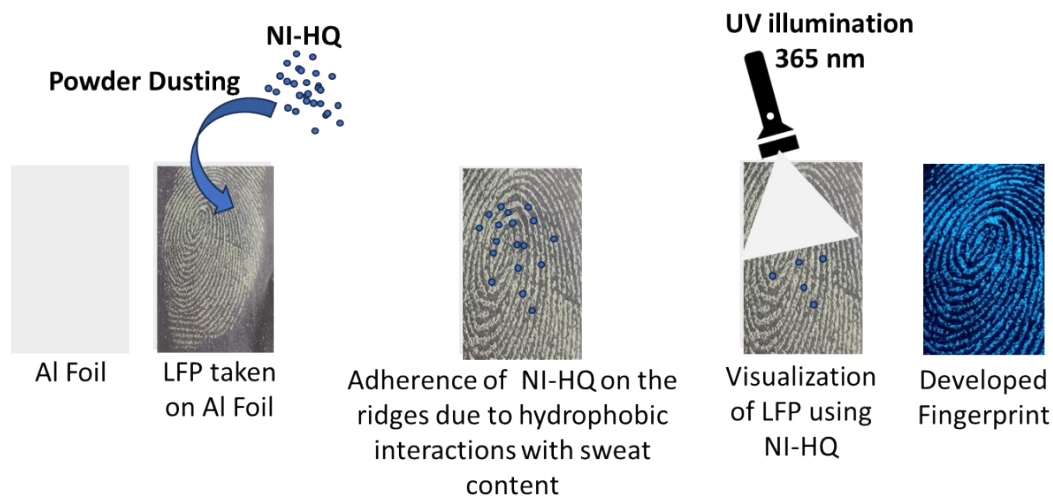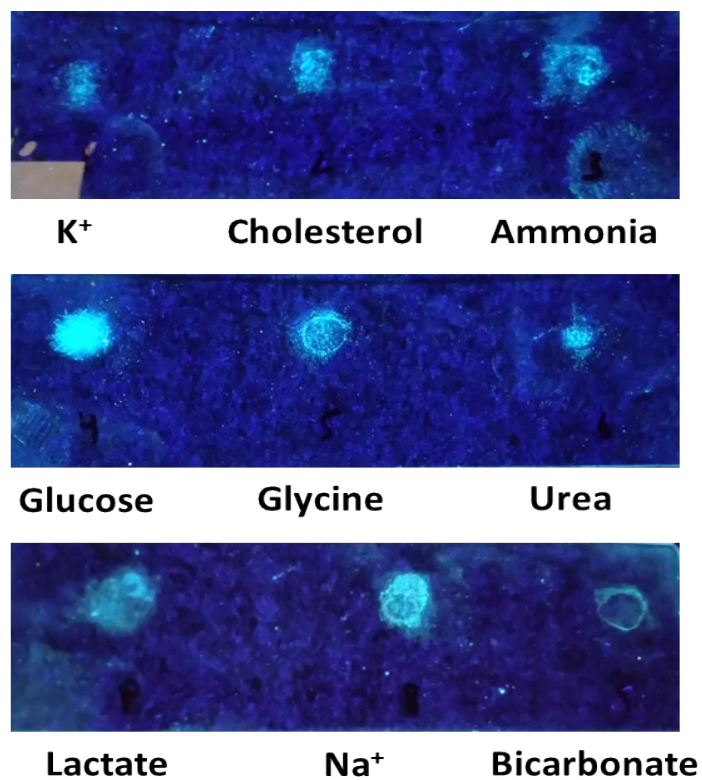
Figure S12: The mechanism for staining of LFPs with NI-HQ using powder dusting method.


Figure S13: Level 1–3 details of developed FPs on the iron slide, disposal cup and glass slide and the variations of the fluorescence intensity between the fingerprint ridges and furrows across the red line.

K⁺　　　　**Cholesterol**　　　**Ammonia**

Glucose　　　**Glycine**　　　**Urea**

Lactate　　　　**Na⁺**　　　**Bicarbonate**

Figure S14: The interaction of **NI-HQ** with different components of the sweat using powder dusting method.


(a)　　　　　　　**(b)**
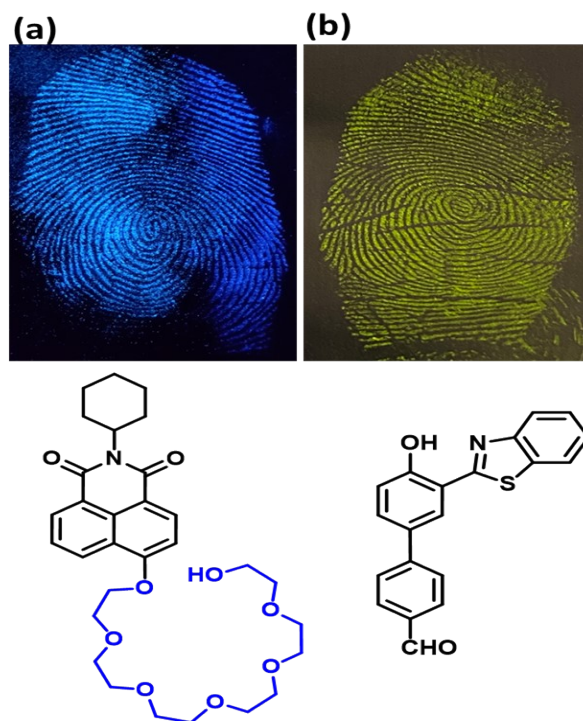
Figure S15: The LFPs developed using other organic-based luminophores (a) naphthalimide-hexaethylene glycol and (b) substituted hydroxyphenyl benzothiazole.
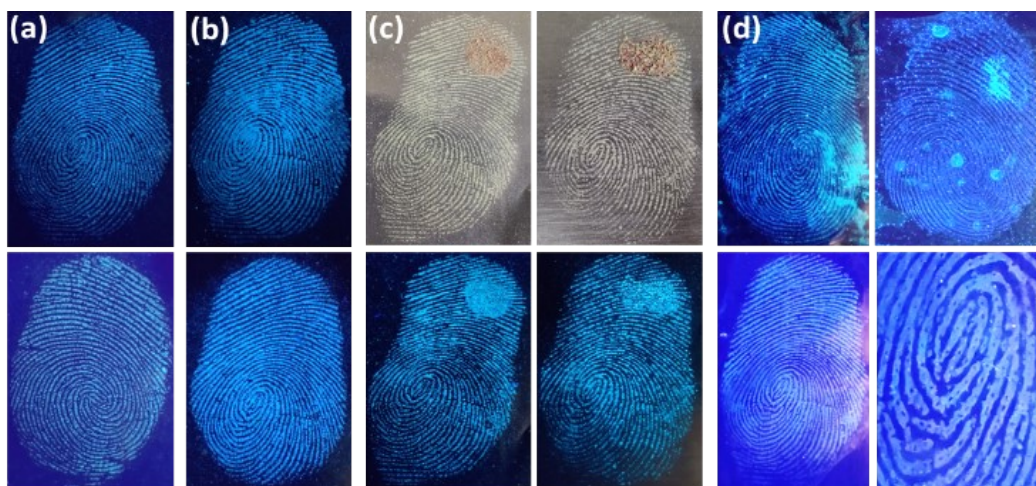
Figure S16. (a) Photographs of developed FPs on aluminium foil visualized after keeping for 3 months at room temperature; photographs of (b) 20 days aged LFPs and (c) stained LFPs taken on aluminium foil and developed using **NI-HQ** powder; (top) daylight images and (bottom) after illumination under 365 nm UV lamp and (d) photographs of LFPs taken on aluminium foil and developed using 1 mM solution of **NI-HQ** in 70% H_2O–CH_3CN mixture.
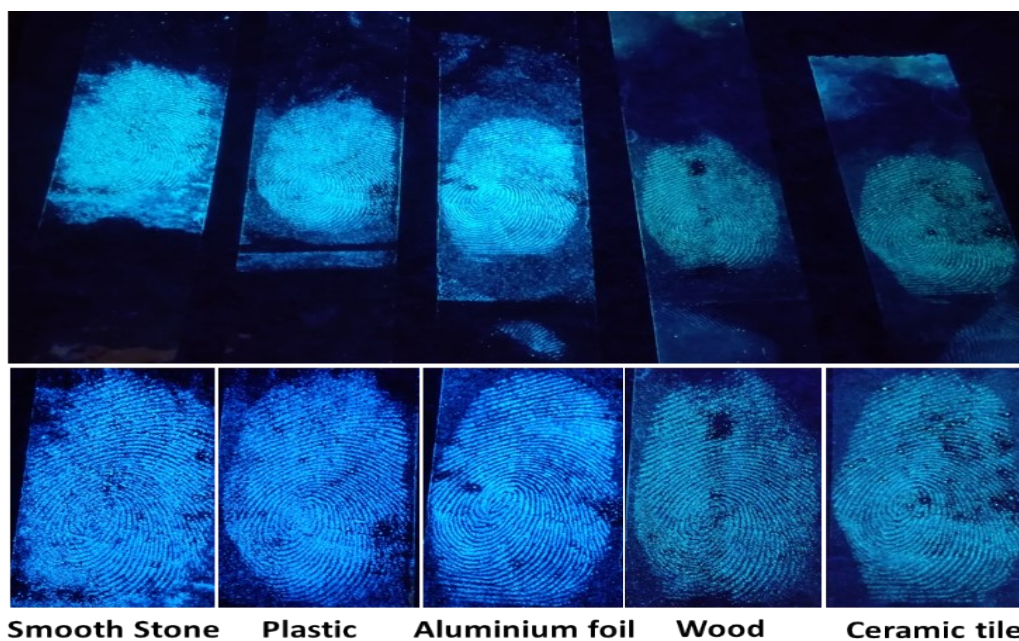

Figure S17. Photographs of developed FPs lifted with tape from different surfaces and pasted on the paper for documentation purposes.
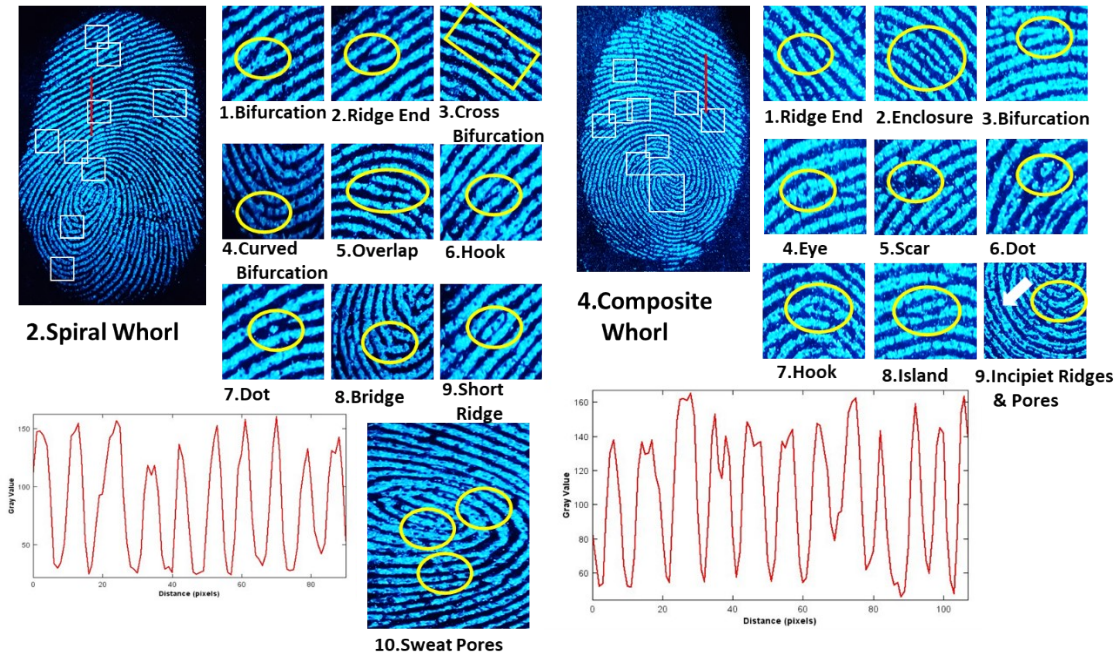
Figure S18: Comparing developed FPs of subjects S2 and S4 on the basis of minutiae points (level 2). The images captured under of 365 nm UV illumination lamp.
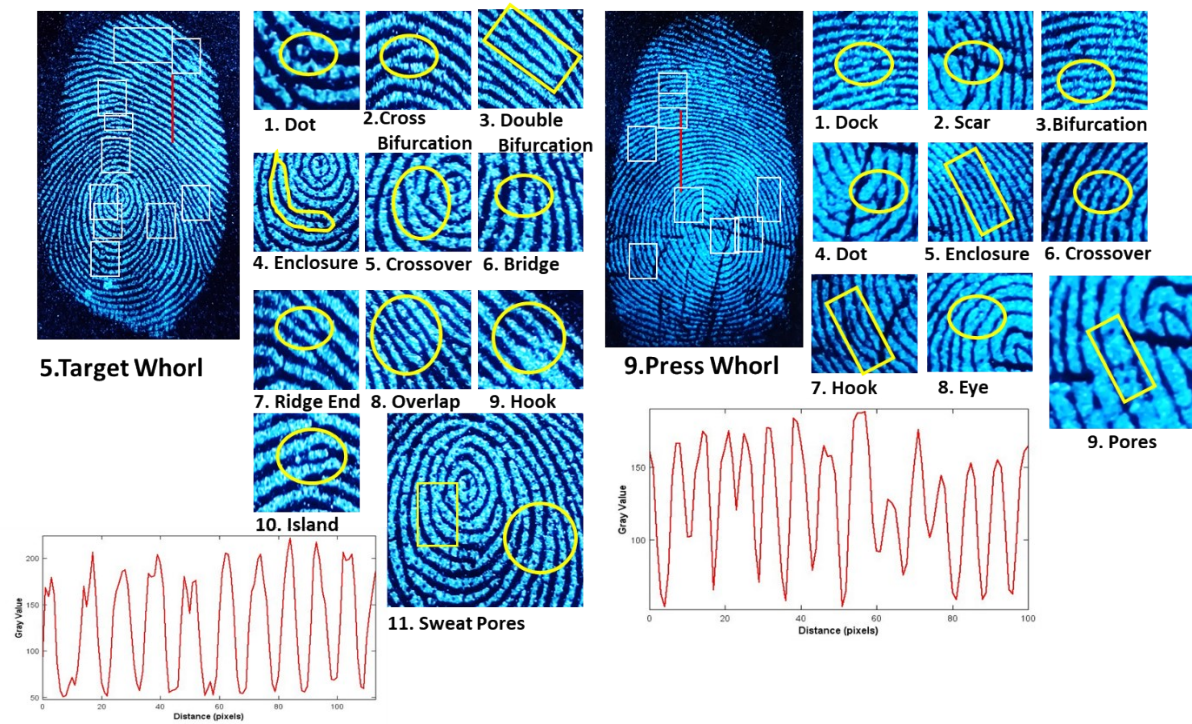
Figure S19: Comparing developed FPs of subjects S5 and S9 on the basis of minutiae points (level 2). The images captured under of 365 nm UV illumination lamp.
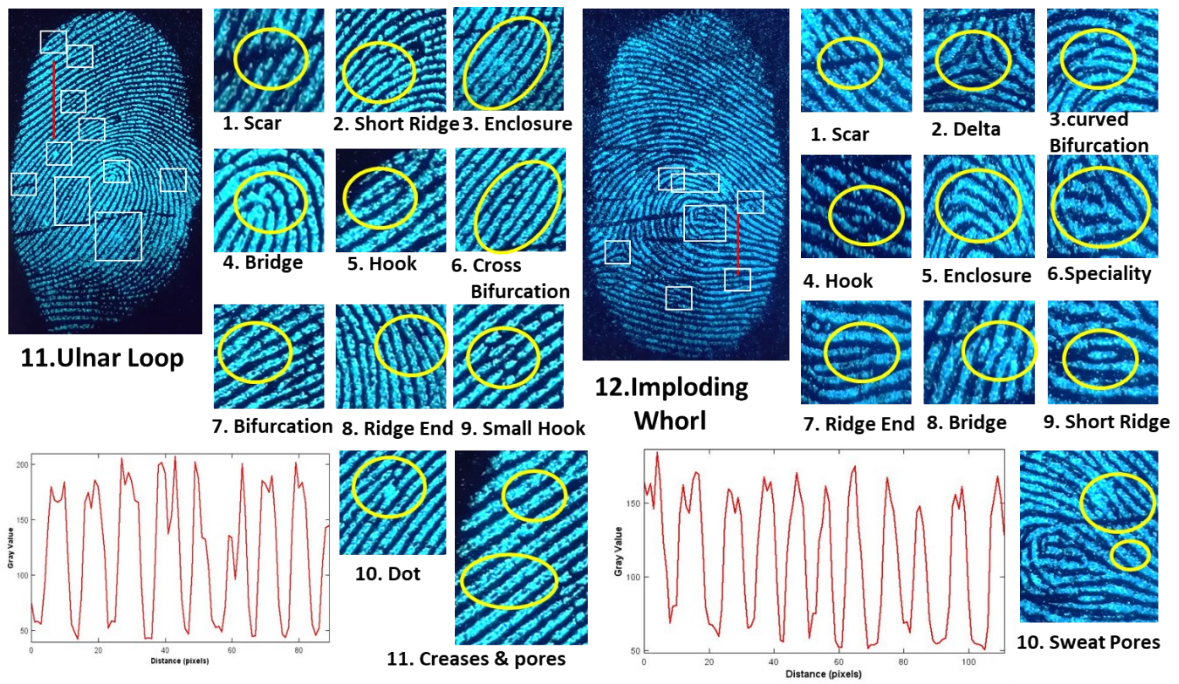
Figure S20: Comparing developed FPs of subjects S11 and S12 on the basis of minutiae points (level 2). The images captured under of 365 nm UV illumination lamp.