Novel julonidine-based polypyridyl derivative as hydrogen bonding-induced fluorescence smart sensor for detecting impurity methanol in biodiesel

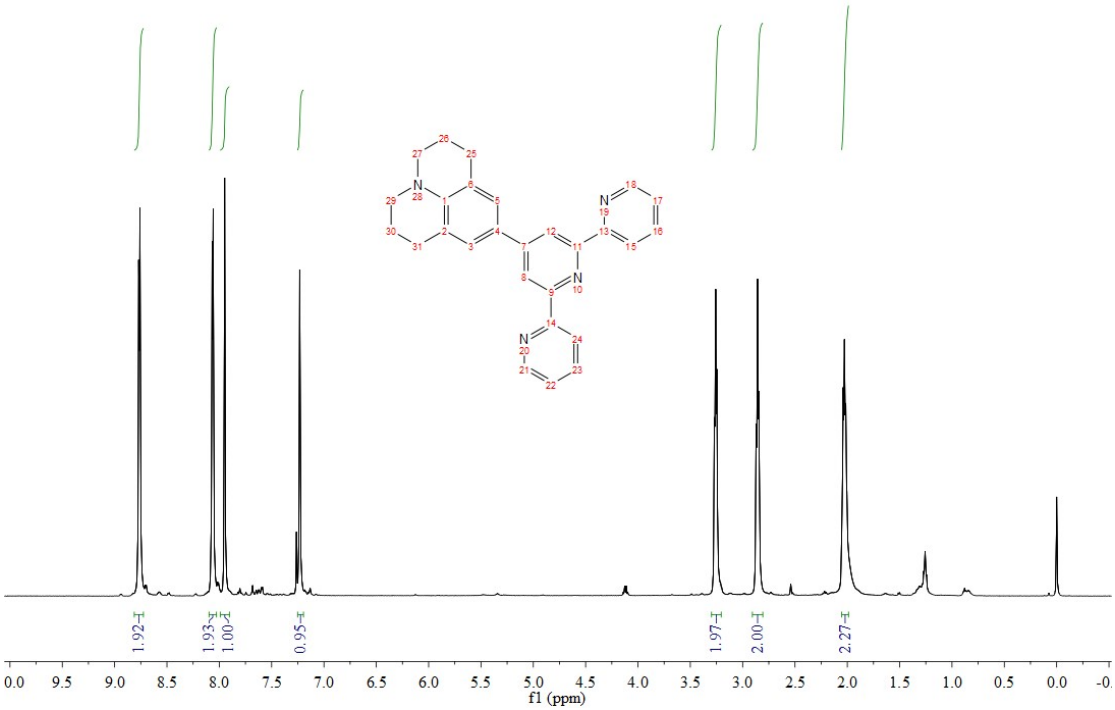

Figure S1. ^{1}H NMR spectra of compound **A1** in $CDCl_3$

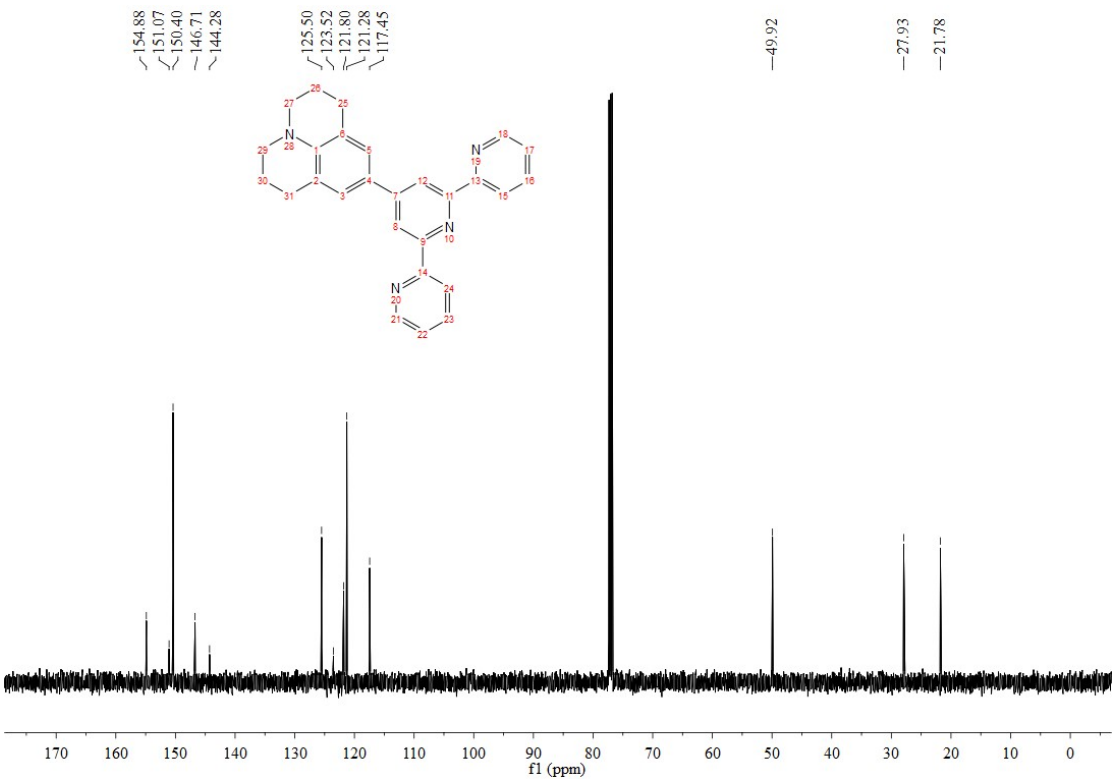

Figure S2. ^{13}C NMR spectra of compound **A1** in $CDCl_3$

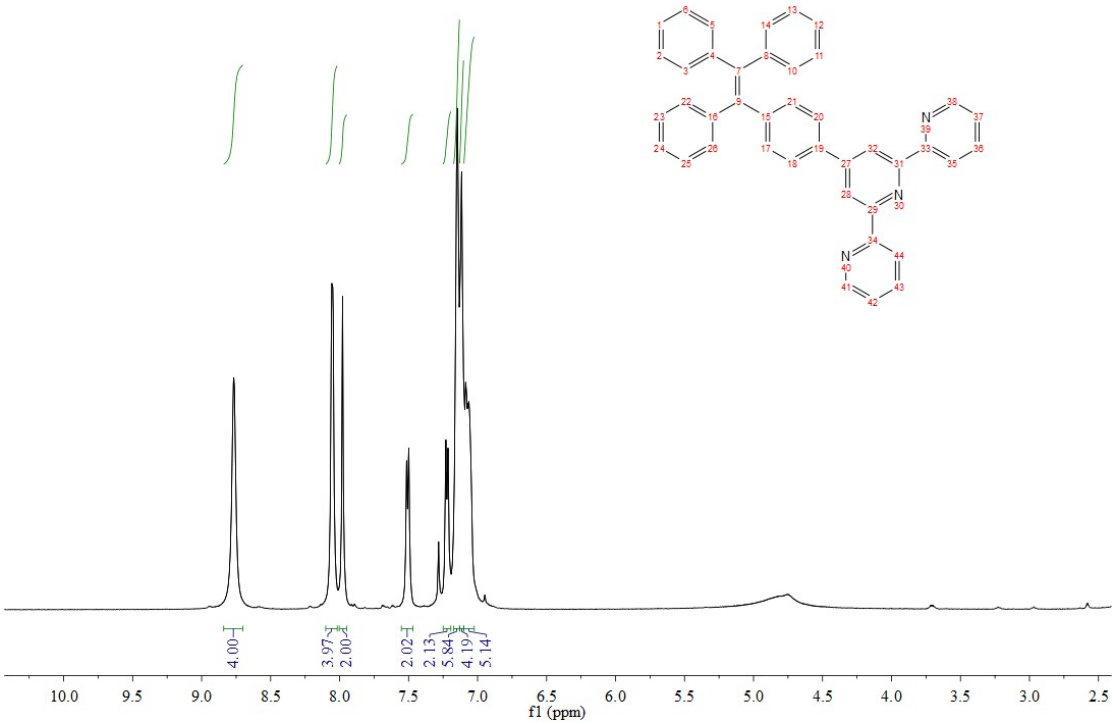

Figure S3. ^{1}H NMR spectra of compound **A2** in $CDCl_3$

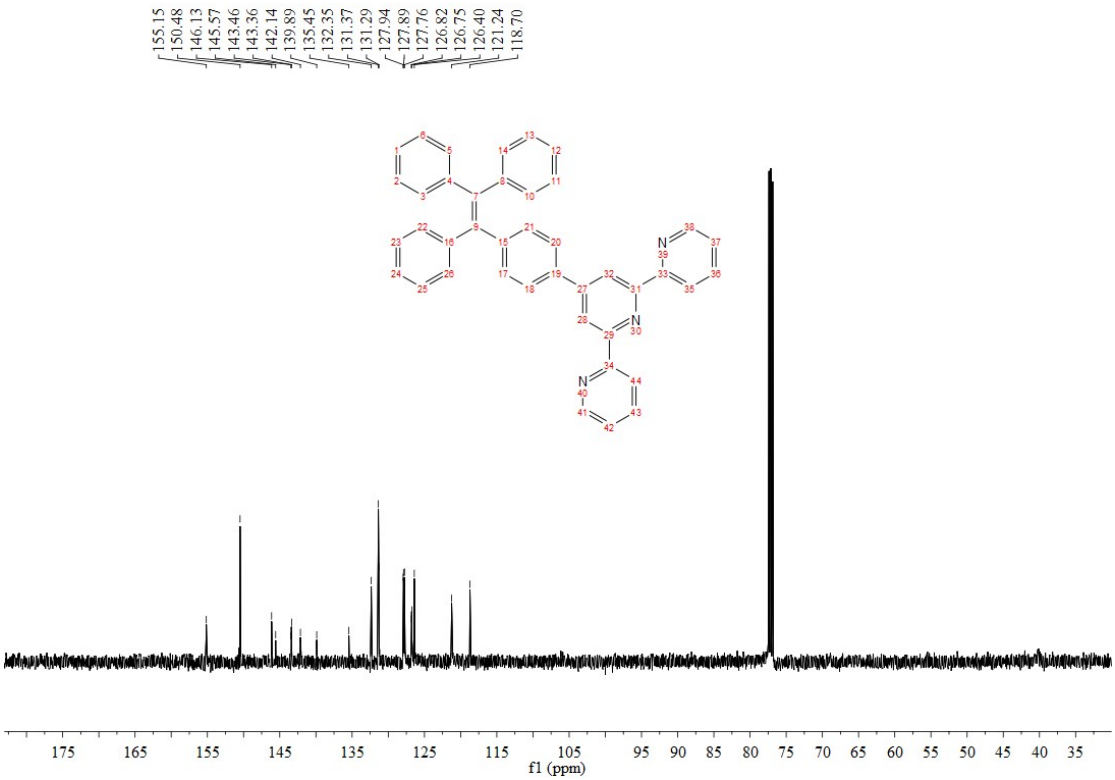

Figure S4. ^{13}C NMR spectra of compound **A2** in $CDCl_3$

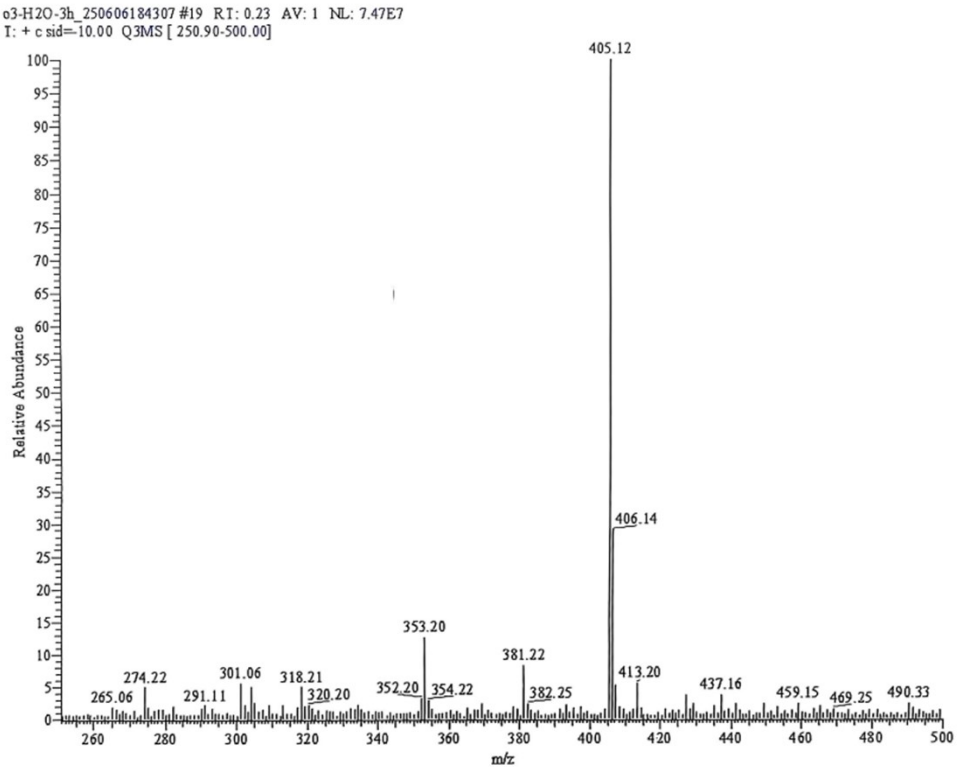

Figure S5. Mass spectrum of compound **A1**

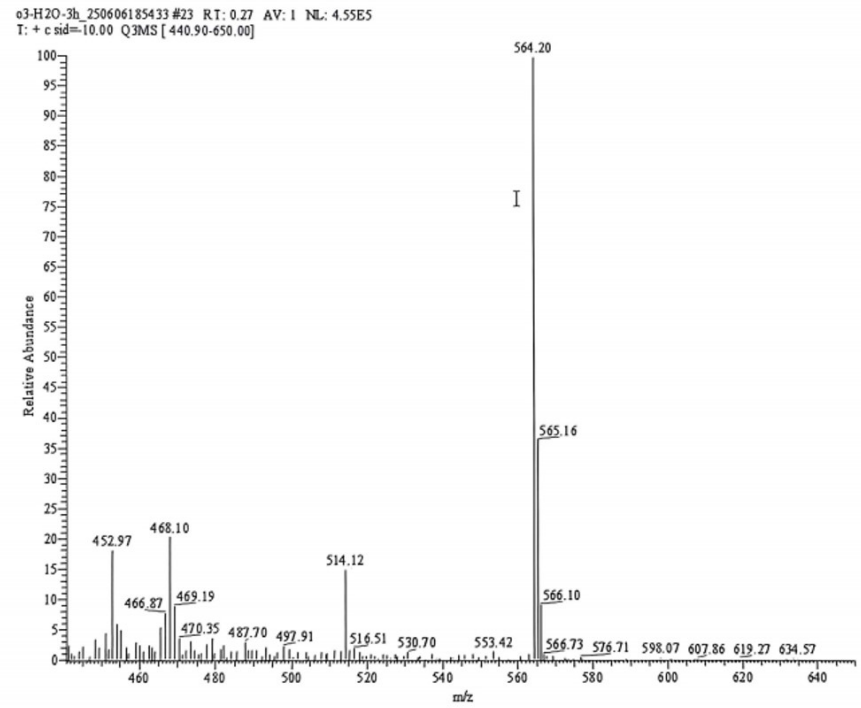

Figure S6. Mass spectrum of compound **A2**

Table S1. Fluorescence quantum yield (Φ_f) of compound **A1** in various solvents

Solvent	CYH	DCM	THF	EA	MeCN	DMSO	MeOH	biodiesel
Φ_f(%)	31.5	39.5	19.5	17.4	8.5	5.2	–	36.7

Table S2. XYZ coordinates optimized molecular geometry of **A1**

C	-4.01456505	-0.06178474	-0.06051062
C	-3.30006455	0.91928101	-0.76443793
C	-1.92079449	0.92099713	-0.73873002
H	-1.39782206	1.67658548	-1.29323296
C	-1.19832859	-0.03323812	-0.03940617
C	-1.91174856	-1.00149824	0.64955192
C	-3.29122741	-1.03089783	0.65052923
H	-1.38200131	-1.74195320	1.21784178
N	-5.40405448	-0.05941882	-0.04852962
C	-4.01695587	-2.12215440	1.42047599
H	-4.08793954	-3.01509751	0.80520784
H	-3.44812997	-2.37918423	2.30650585
C	-5.42968127	-1.66666670	1.80596524
H	-5.37415782	-0.85629201	2.52258695
H	-5.98795422	-2.48391917	2.24766466
C	-6.14460174	-1.16873211	0.54686761
H	-7.13524600	-0.81026415	0.79774690
H	-6.25751875	-1.99255662	-0.15691083
C	-6.15594577	0.84372092	-0.91618752
H	-6.27776840	0.42367812	-1.91390346
H	-7.14279122	0.97059797	-0.48845457
C	-5.44683497	2.19702892	-1.01521777
H	-5.38624878	2.63618062	-0.02686545
H	-6.01227780	2.86241023	-1.65728170
C	-4.03677165	1.97269915	-1.57507260
H	-3.47372783	2.89870519	-1.56243581
H	-4.11310200	1.64859865	-2.60950020
C	0.28526066	-0.01630891	-0.02504975
C	0.98688272	1.17510047	0.11009331
C	1.01581977	-1.19168333	-0.14636767
C	2.36972908	1.14980266	0.11524586
H	0.48684590	2.11028682	0.22899551
C	2.39763305	-1.13546463	-0.12476107
H	0.53918123	-2.13780092	-0.27466524
N	3.04844609	0.01459965	0.00160109
C	3.20473679	-2.37295271	-0.25363729
C	4.59059389	-2.32311056	-0.24886764
C	3.23067491	-4.65953834	-0.49163565
C	5.29907440	-3.50133030	-0.37152424

H	5.07462091	-1.37763864	-0.15104599
C	4.61123047	-4.69746644	-0.49596664
H	2.65404781	-5.55667206	-0.58526323
H	6.37066637	-3.48887573	-0.37066166
H	5.12896334	-5.62907928	-0.59333134
C	3.14630139	2.40504806	0.25911884
C	4.53274548	2.38617169	0.28177866
C	3.11645939	4.69160566	0.49694077
C	5.21217841	3.57991896	0.41792216
H	5.03960527	1.45175068	0.19392869
C	4.49547216	4.76037814	0.52835851
H	2.51821510	5.57563565	0.57885646
H	6.28358983	3.59140552	0.43817816
H	4.99024299	5.70331988	0.63555563
N	2.46520406	3.54105243	0.36523735
N	2.55141447	-3.52385808	-0.37293298

Table S3. XYZ coordinates optimized molecular geometry of **A2**

C	1.79620616	0.17496238	-0.34307276
C	1.12711828	0.65315874	0.77496664
C	-0.25380930	0.63689004	0.83129468
H	-0.75294875	0.99867521	1.70803249
C	-1.00002307	0.13512917	-0.22670527
C	-0.33115670	-0.33976478	-1.34884151
C	1.04780119	-0.30935431	-1.40974864
H	-0.89239976	-0.71135904	-2.18297787
C	-2.48511833	0.11177909	-0.16412924
C	-3.19646378	1.21439319	0.28735472
C	-3.19570278	-1.01399837	-0.55584152
C	-4.57812713	1.15255982	0.33237251
H	-2.70838542	2.11545123	0.58541260
C	-4.57749397	-0.99721374	-0.48457644
H	-2.70520491	-1.89906113	-0.89503457
N	-5.23996241	0.06690328	-0.04824348
C	-5.36741965	-2.18398130	-0.89200622
C	-6.75155333	-2.18080147	-0.81259616
C	-5.36036455	-4.33192392	-1.71100967
C	-7.44232962	-3.31009556	-1.20412004
H	-7.24861720	-1.30865890	-0.45183190
C	-6.73851420	-4.41128920	-1.66344719
H	-4.77201356	-5.15611401	-2.05817563
H	-8.51244360	-3.33274919	-1.15222324
H	-7.24232369	-5.30274117	-1.97463851
C	-5.36915286	2.31368960	0.80613263

C	-6.75422557	2.26560449	0.84316613
C	-5.36285089	4.46206650	1.62398739
C	-7.44587262	3.37262288	1.29252870
H	-7.25135881	1.37729063	0.52439465
C	-6.74198613	4.49674072	1.69234074
H	-4.77438999	5.30542034	1.92134456
H	-8.51673978	3.36060536	1.33062248
H	-7.24648149	5.37197354	2.04561318
N	-4.70008303	3.39502237	1.19143788
N	-4.69843151	-3.24354656	-1.33384000
H	1.68881762	1.02649811	1.60610681
H	1.54996062	-0.65119455	-2.29244810
C	3.29114859	0.21681182	-0.43648123
C	4.09485162	-0.30303023	0.49440523
C	3.59122751	-1.11211088	1.65150829
C	3.96296444	-0.77080980	2.94731073
C	2.78960702	-2.22831121	1.45443900
C	3.52060490	-1.51583469	4.02432023
H	4.60324468	0.07412427	3.10478854
C	2.35596775	-2.98043501	2.53219661
H	2.50136740	-2.50063027	0.45992600
C	2.71565049	-2.62406417	3.81951702
H	3.80687241	-1.23622652	5.01892895
H	1.73826724	-3.84050214	2.36534034
H	2.37673969	-3.20516252	4.65409855
C	5.58397745	-0.13199688	0.47864919
C	6.16334562	1.12793541	0.41284387
C	6.40864357	-1.24744347	0.57613983
C	7.53987715	1.26950863	0.43071319
H	5.53623952	1.99259613	0.34047682
C	7.78369324	-1.10638033	0.58249224
H	5.96790718	-2.22126185	0.65386325
C	8.35369508	0.15374017	0.51069853
H	7.97356918	2.24865157	0.38176178
H	8.40793617	-1.97544471	0.64918091
H	9.41993395	0.26398931	0.52211973
C	3.79965931	0.89483724	-1.67312955
C	4.68436356	0.25621699	-2.53151255
C	3.34827767	2.16931093	-1.99821348
C	5.11970271	0.88416612	-3.68536308
H	5.03501859	-0.72620255	-2.29045724
C	3.79172107	2.80050851	-3.14527432
H	2.64530711	2.65820746	-1.35359332
C	4.67880492	2.15872056	-3.99327320

H	5.80107855	0.37833604	-4.34038984
H	3.44202144	3.78645934	-3.37970231
H	5.01789587	2.64529458	-4.88623620

Table S2 Fluorescence excitation and emission wavelength (nm) information of compound **A1**

Solvent	CYH	DCM	THF	EA	MeCN	DMSO	MeOH	biodiesel	solid
λ_{em}	441	523	548	528	417	590	–	540	560
λ_{ex}	310	330	330	330	300	330	330	380	330