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Live-cell Imaging of Lipid Droplets by Solvatochromic Styrylcoumarin Derivatives

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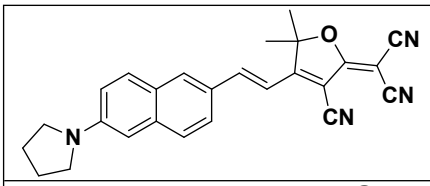
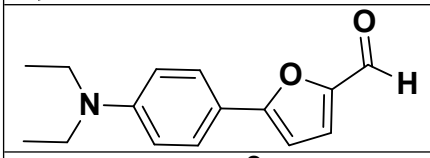
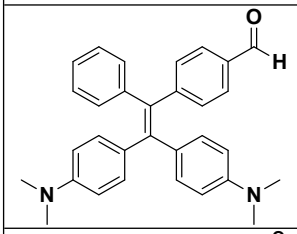
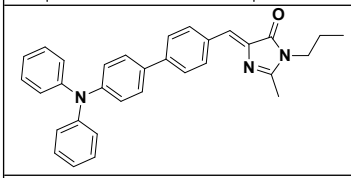
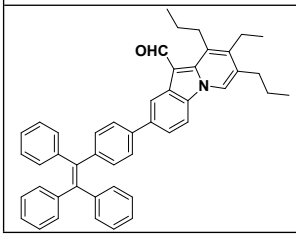
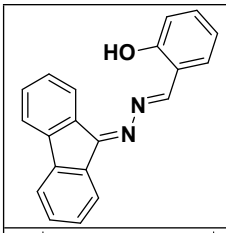
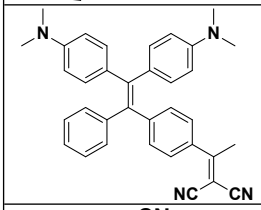
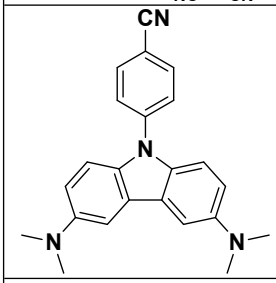
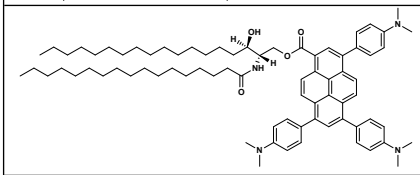
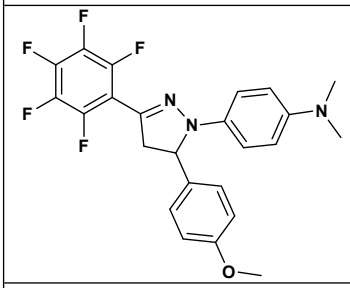
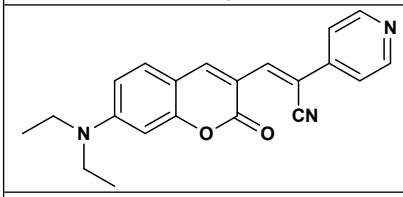
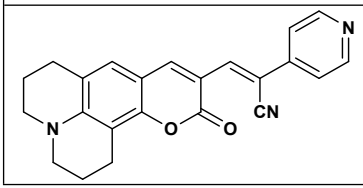
Table-S1: Some known structures that were used for imaging lipid droplets

	3 steps + synthesis of starting materials.	λ_{abs} 599 nm, λ_{em} 789 nm (DMSO)	5µM	Dyes Pigments 171 (2019) 107718
	1 step,	λ_{abs} .403nm, λ_{em} 520nm	2µM	Anal. Chem. 2019, 91, 1928−1935
	2 steps; Coupling Reaction	λ_{abs} . 405nm, λ_{em} . 520nm	10µM	**J. Mater. Chem. B,** 2014, **2**, 2013-2019
	3 steps; Heck Couling and synthesis of starting materials	λ_{abs} . 380nm, λ_{em} 620nm	5µM	**Chem. Sci.,** 2017,**8,** 5440-5446
	5 steps with Heck reaction	λ_{abs} . 383 nm, λ_{em} 470 nm.	100µM	Chem. Asian J. 2017, 12, 2501 – 2509

	2 steps	λ_{abs} 380nm, λ_{em} 595nm	7.5µM	ACS Appl. Mater. Interfaces 2016, 8, 16, 10193-10200
	3 steps ,	λ_{abs} 450nm, λ_{em} 705nm	10µM	***Chem. Commun.***, 2016,**52**, 5957-5960
	4 steps, 65% yield	λ_{abs} 384nm, λ_{em} 578nm	12µM	J. Org. Chem. 2019, 84, 5535−5547
	4 steps and synthesis of starting materials– 8.5% yield	λ_{abs} 405, λ_{em} 540nm	2µM	Analyst, 2019, 144, 1608–1621
	3 steps	λ_{abs} 395 nm, λ_{em} 560nm	0.5 µM	Chem. Sci., 2019, 10, 9009–9016
	3 steps 85% yield	λ_{abs} 485nm, λ_{em} 580nm	0.2 µM	This work
	3 step 90% yield	λ_{abs} 512nm, λ_{em} 605nm	0.2 µM	This work

Highlights

1. Easy synthetic steps with high yields
2. Coumarin and pyridine functionality provides greater biocompatibility

3. Nanomolar concentration of probes used for live cell lipid droplet imaging
4. High photostability with red emission

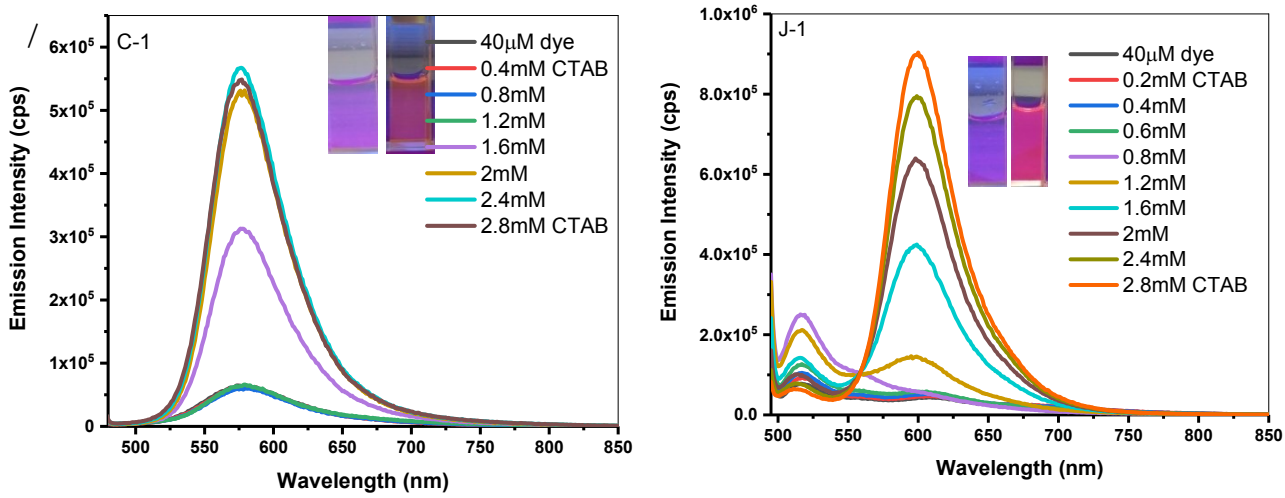


Fig S1: Effect of surfactant (CTAB) concentration on the emission of C-1 and J-1. With increase in concentration, notable emission intensity shifts were noted along with distinct color changes indicating localization preferences.

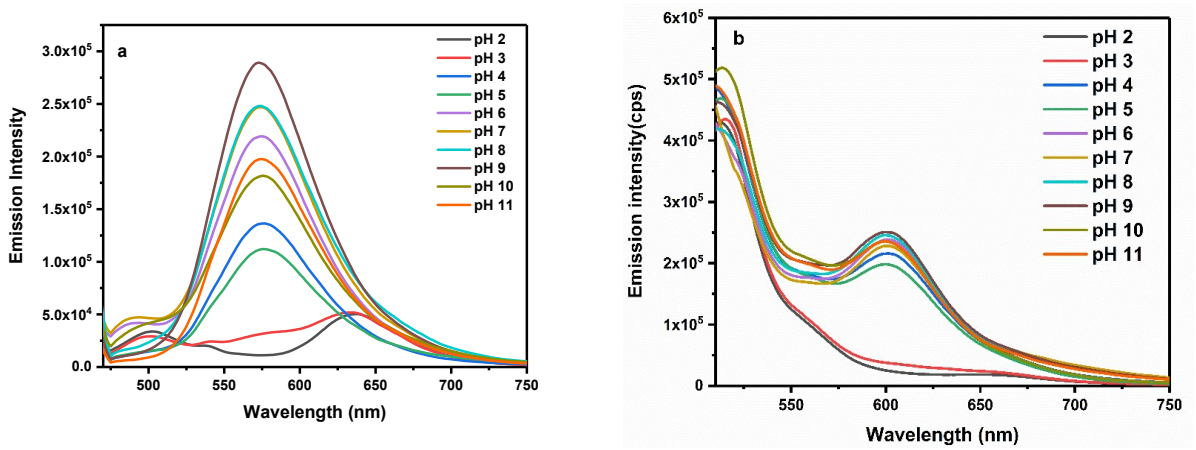


Fig S2: Effect of pH on the emission of C-1 and J-1 (C-1 Ex.wl 450 nm and J-1 Ex Wl 510 nm)

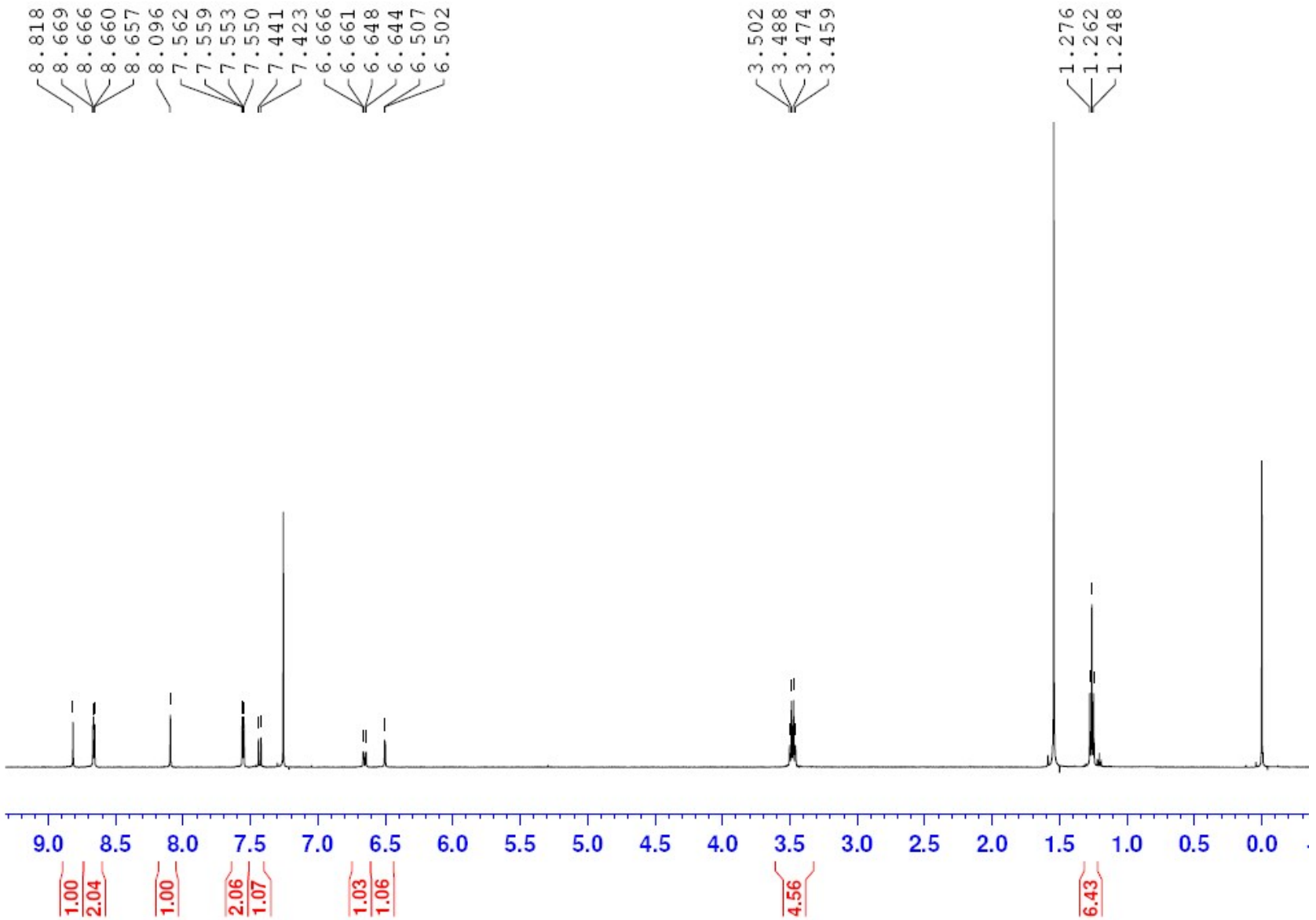
Supporting Information

3-(7-Diethylamino-2-oxo-2*H*-chromen-3-yl)-2-pyridin-4-yl-acrylonitrile (C-1)

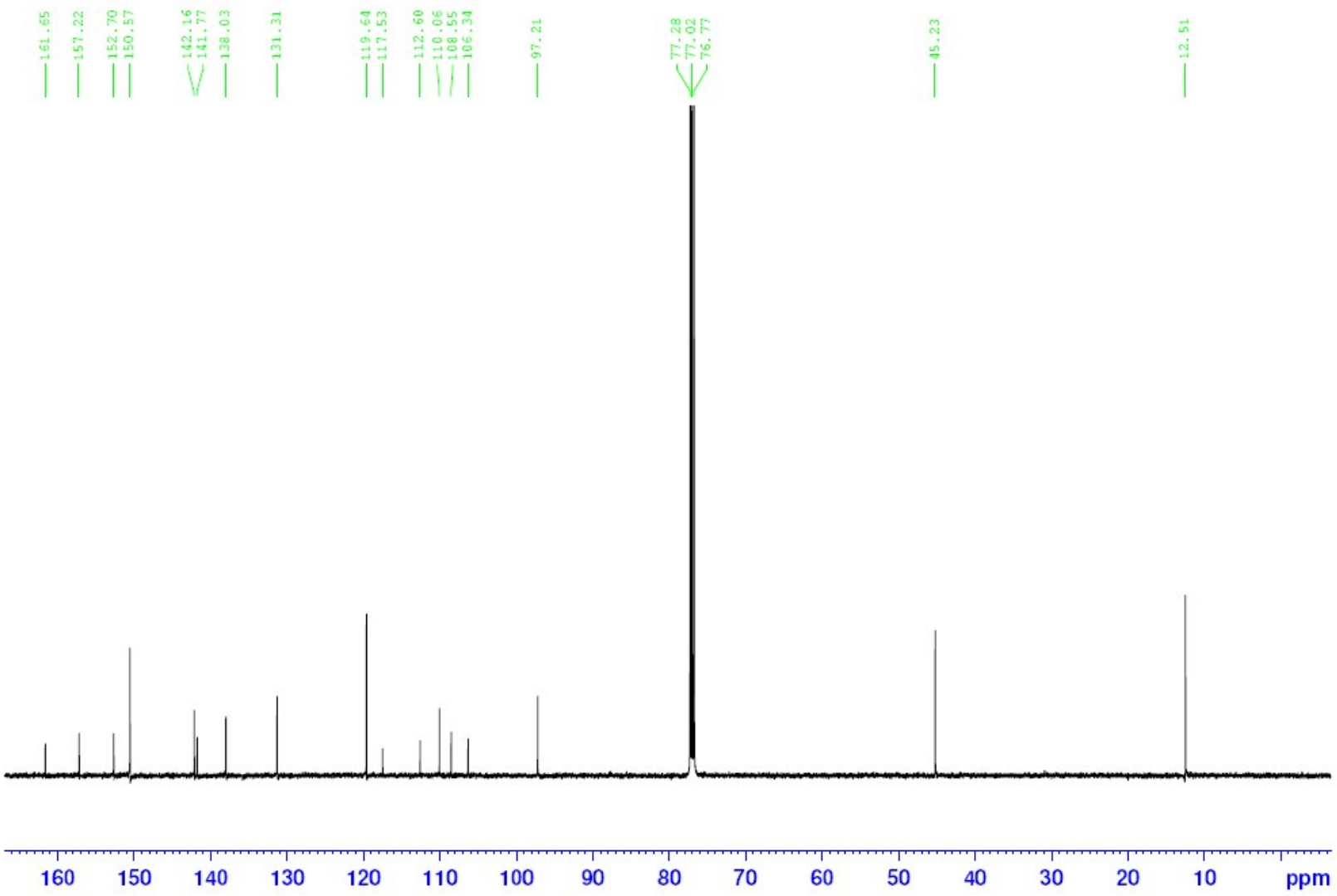
Yield 85 %, (110 mg) ^{1}H-NMR (500 MHz, $CDCl_3$) δ (ppm): 8.81 (s, 1H), 8.66–8.65 (d, 2H), 8.09 (s, 1H), 7.56–7.55 (d, 2H), 7.44–7.42 (d, 1H), 6.66–6.64 (d, 1H), 6.50 (s, 1H), 3.50–3.45 (q, 4H), 1.27–1.24 (t, 6H). ^{13}C-NMR (125 MHz, DMSO-d_6): δ (ppm) 160.69, 157.59, 153.36, 148.30, 143.71, 132.27, 120.81, 117.33, 112, 111, 108.37, 97.13, 55.38, 45.04, 31.16, 22.65, 12.88 HRMS (ESI-Q-TOF): $C_{21}H_{23}N_2O_2$ $[M + H]^+$: cal. *m*/*z* 346.1585, found, *m*/*z* 346.1593 (error 2.3ppm)

3-(10-Oxo-2,3,5,6-tetrahydro-1*H*,4*H*,10*H*-11-oxa-3*a*-aza-benzo[*de*]anthracen-9-yl)-2-pyridin-4-yl-acrylonitrile (J-1)

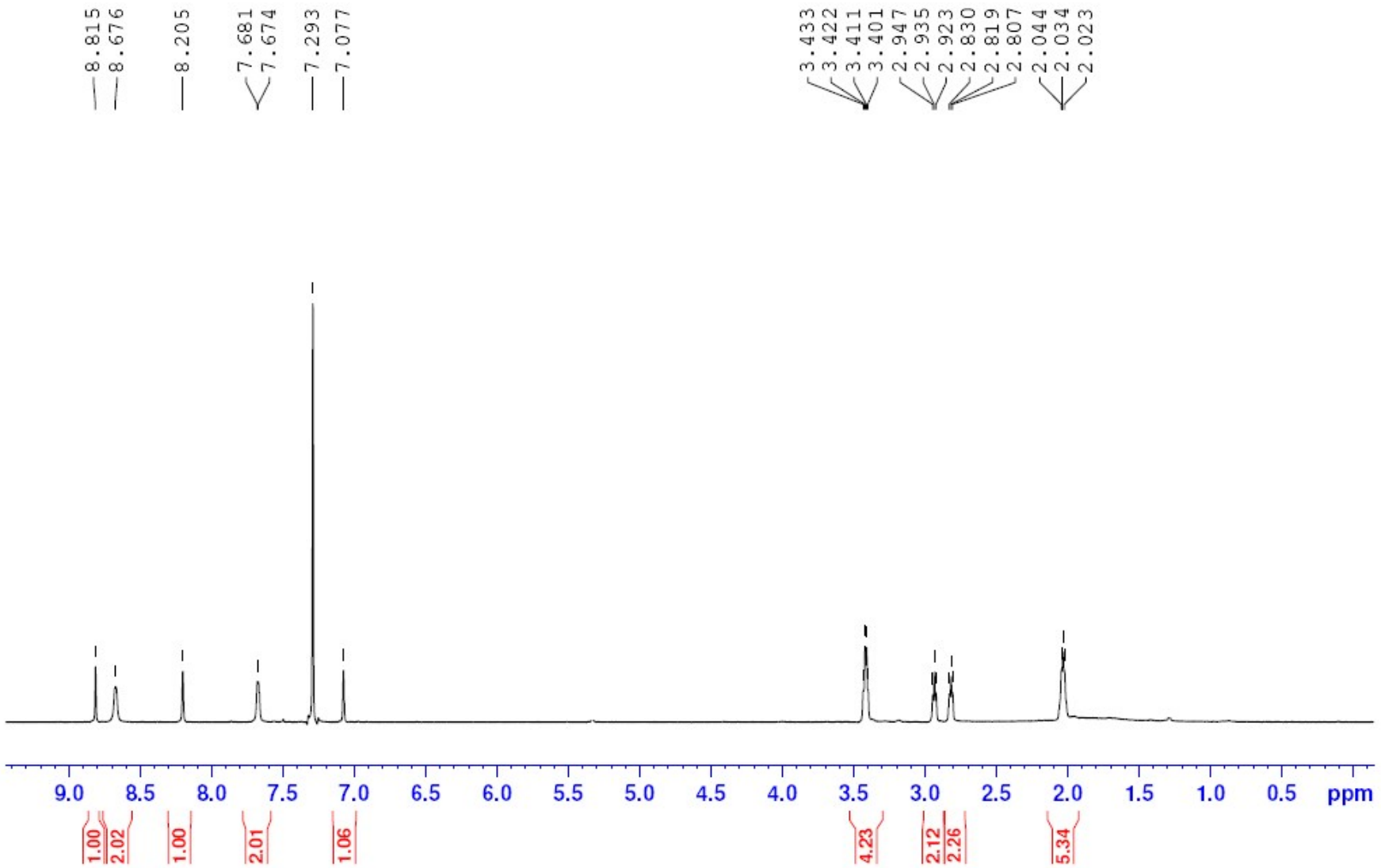
Yield 90%. ^{1}H-NMR (500 MHz, $CDCl_3$) δ (ppm): 8.81 (s, 1H), 8.67–8.66 (d, 2H), 8.2 (s, 1H), 7.68–7.67 (d, 2H), 7.68–7.67 (d, 2H), 7.0 (s, 1H), 3.43–3.40 (t, 4H), 2.94–2.92 (m, 2H), 2.83–2.80 (m, 2H), 2.04–2.02 (t, 4H) ^{13}C-NMR (125 MHz, $CDCl_3$): δ (ppm) 161.92, 152.24, 150.14, 148.54, 142.17, 138.53, 127.40, 119.78, 119.61, 117.76, 111.23, 108.54, 106.31,104.90, 96.14, 50.42, 27.38, 21.16, 20.19, 19.99. HRMS (ESI-Q-TOF): $C_{21}H_{23}N_2O_2$ $[M+ H]^+$: cal. *m*/*z* 370.1598, found, *m*/*z* 370.1601 (error 0.8pm)



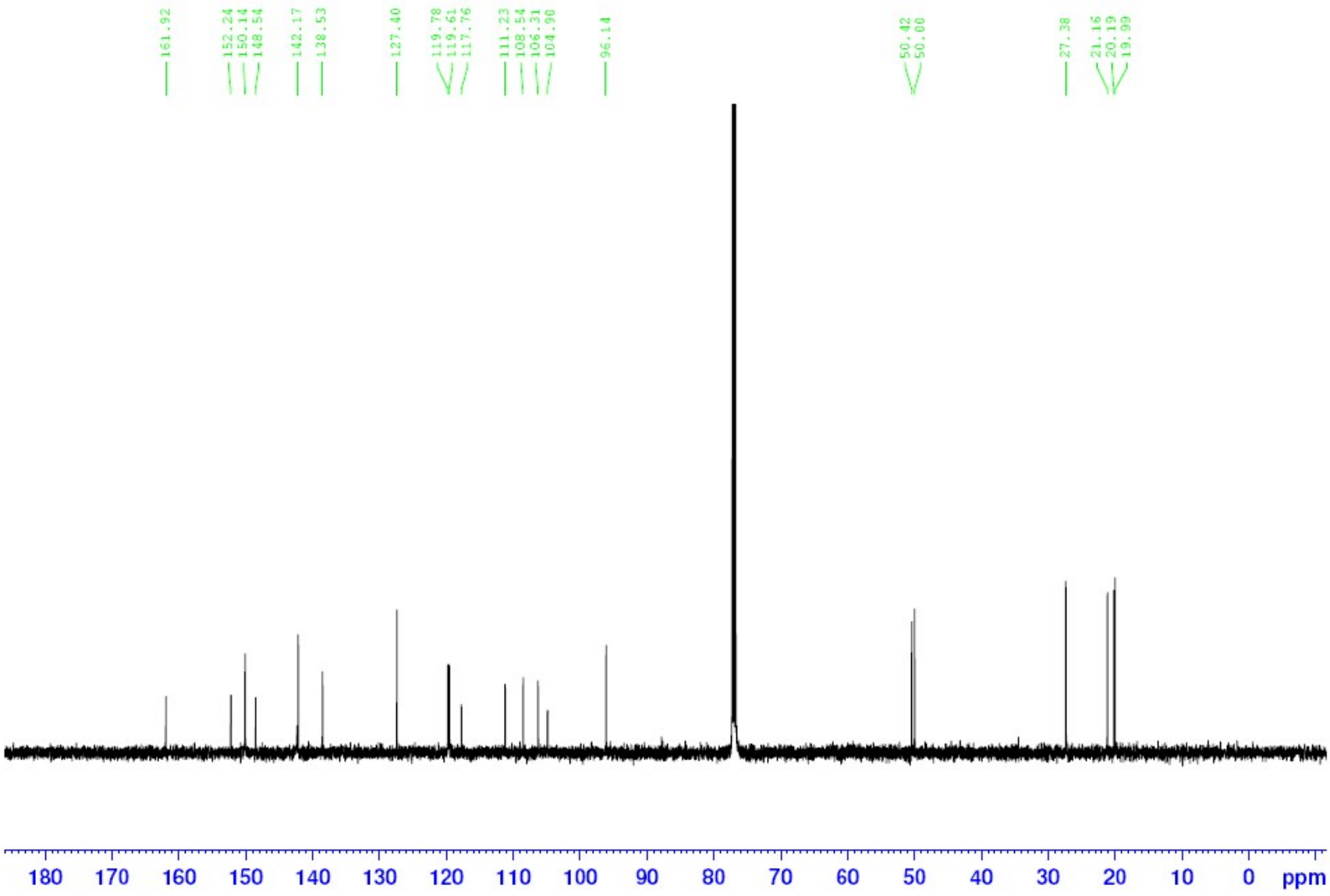
[1]H-NMR spectrum of compound C-1



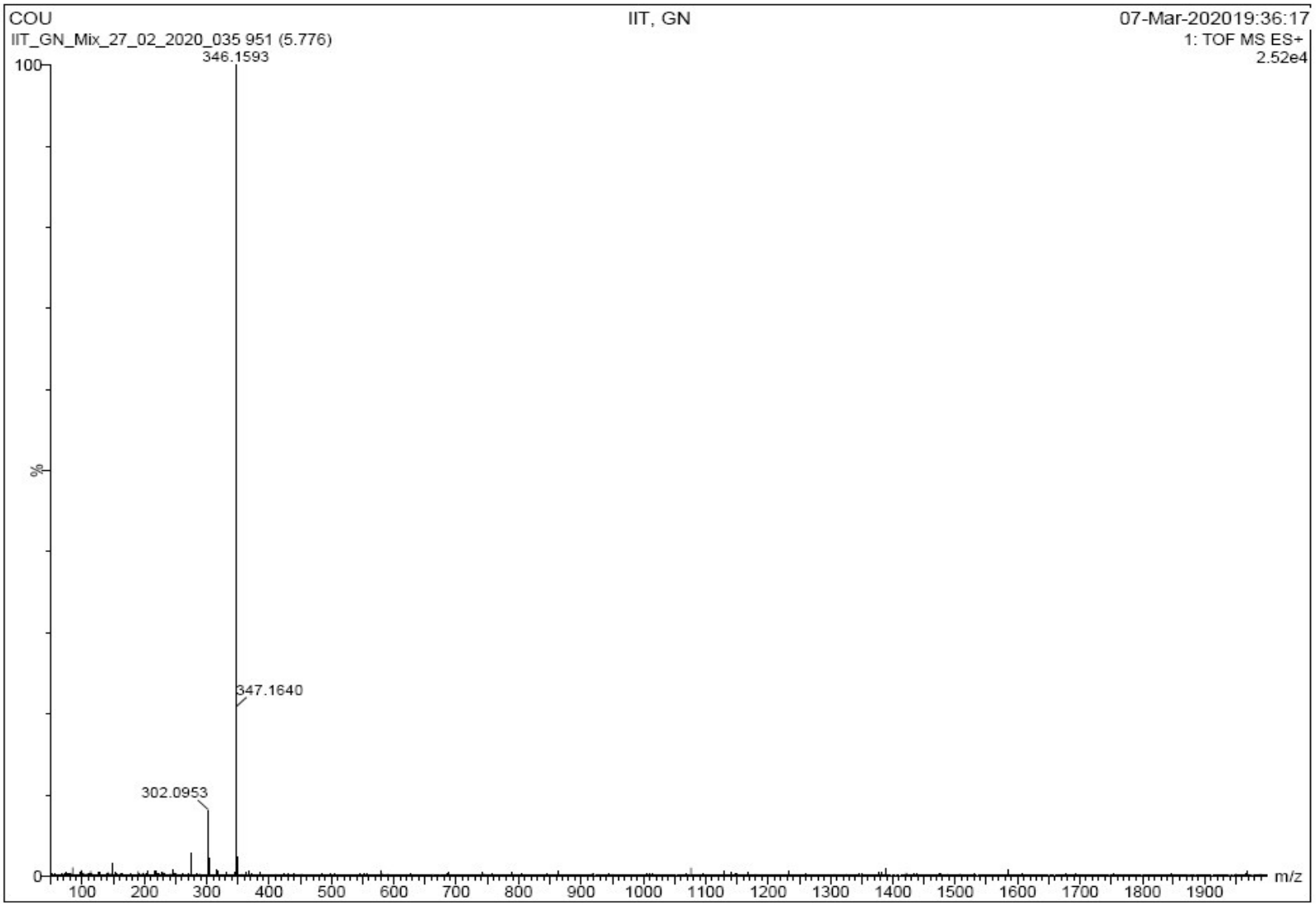
^{13}C-NMR spectrum of compound C-1



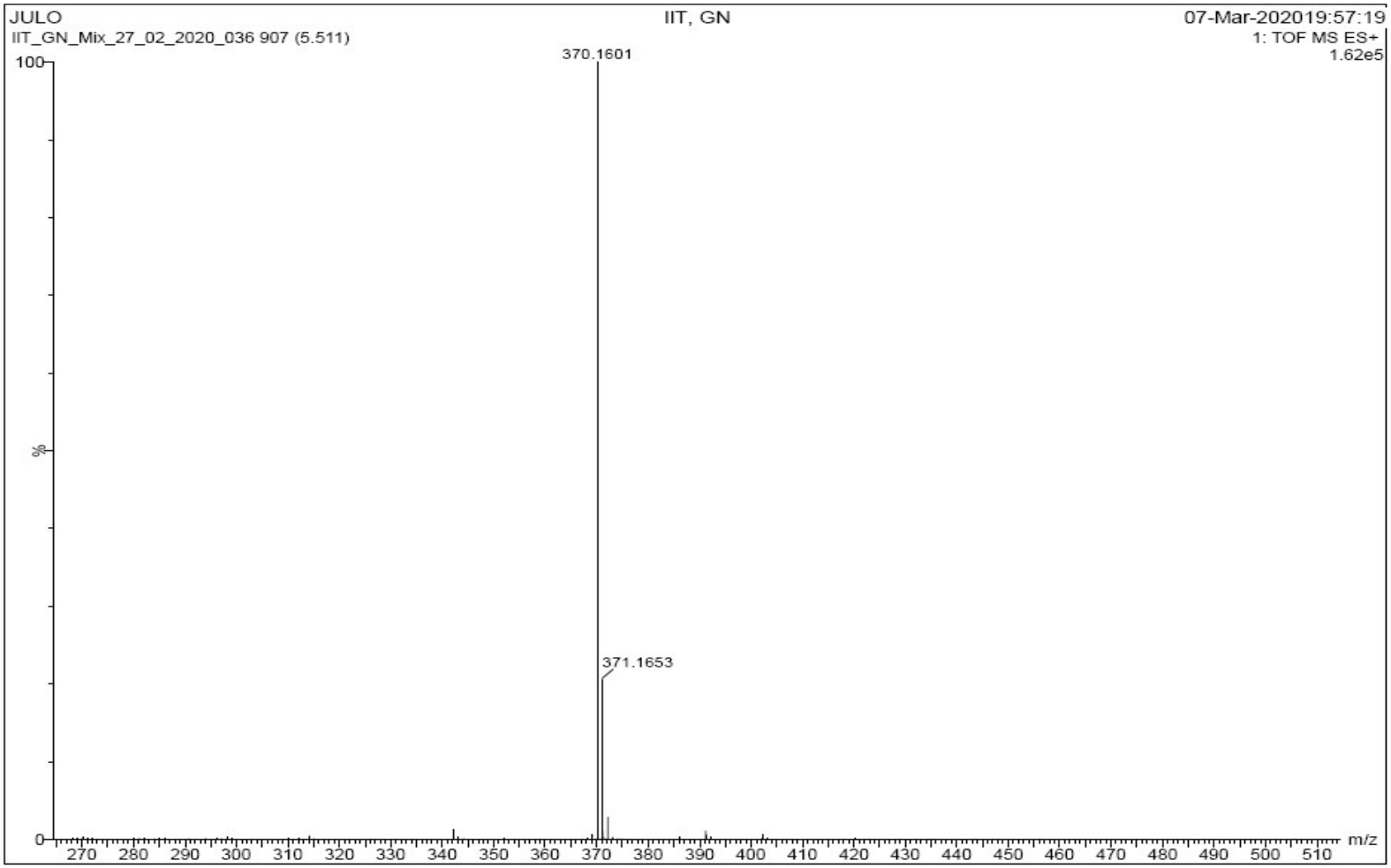
^{1}H-NMR spectrum of compound J-1



^{13}C-NMR spectrum of compound J-1



HRMS spectrum of compound C-1



HRMS spectrum of compound J-1