Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

New cyclic and acyclic imidazole-based sensitizers for achieving highly efficient photoanodes for dye-sensitized solar cells by potential assisted method

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1. Procedure for the synthesis of intermediate compounds

4-(4,5-bis(4-bromophenyl)-1H-imidazol-2-yl)benzaldehyde (7)

A mixture of compound **6** (1 g, 2.7 mmol, 1 equiv.), terephthalaldehyde (0.364 g, 2.7 mmol, 1 equiv.), ammonium acetate (0.837 g, 1.1 mmol, 4 equiv.) and glacial acetic acid (8 mL) were charged sequentially in a two-necked flask and heated to reflux for 12 h under N_2 atmosphere. After cooling, the product mixture was quenched with ice water. The obtained precipitate was collected via filtration and washed with water. The obtained solid was dried in the vacuum to get compound **7**. Yield = 57% (0.75 g); Greenish yellow color solid; mp = 222-224 °C; ^{1}H NMR (400 MHz $CDCl_3$) δ 10.0 (s, 1H), 8.07-7.96 (m, 4H), 7.48-7.40 (m, 8H), 4.67 (bs, NH, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.5, 132.0, 130.4, 129.4, 125.5; IR ($CHCl_3$): 3021, 2977, 2928, 2402, 1694, 1604, 1525, 1482, 1427, 1216, 1044, 929 cm^{-1}; HRMS (ESI): Calcd. For $C_{22}H_{14}Br_2N_2O$ $[M+H]^+$ 480.9551; found 480.9529.

4-(4,5-bis(4'-methoxy-[1,1'-biphenyl]-4-yl)-1H-imidazol-2-yl)benzaldehyde (8)

Compound **7** (0.500 g, 1.0 mmol, 1 equiv.), 4-methoxyphenyl boronic acid (0.346 g, 2.3 mmol, 2.2 equiv.), potassium phosphate tribasic (1.320 g, 6.2 mmol, 6 equiv.) were dissolved in 80 mL of toluene, 14 mL of tert-amyl alcohol and 7 mL of water. This solution was degassed for about 20 min under N_2 atmosphere and then Pd_2dba_3 (0.104 g, 0.11 equiv) and X-Phos (0.208 g, 0.42 equiv) were added simultaneously in one batch and heated to 85 °C for 12 h. The reaction mixture

was then cooled to the room temperature and plugged through a thin pad of Na_2SO_4 with DCM. The filtrate was concentrated and purified by the column chromatography (Hexanes: ethyl acetate, 7:3 v/v) yielded the target compound **8** (49%, 0.273 g) as yellow color solid; mp = 128-130 °C; ^{1}H NMR (400 MHz Acetone-d_6) δ 12.1 (s, NH, 1H), 10.08 (s, 1H), 8.37 (d, J = 8.4 Hz, 2H), 8.02 (d, J = 8.4 Hz, 2H), 7.79 (d, J = 8.4 Hz, 2H), 7.72-7.69 (m, 3H), 7.66-7.64 (m, 4H), 7.62-7.59 (m, 3H), 7.06-7.01 (m, 4H), 3.85-3.84 (m, 6H); ^{13}C NMR (125 MHz, Acetone-d_6) δ 191.4, 129.9, 128.9, 127.9, 127.8, 127.6, 126.5, 126.0, 125.4, 114.3, 114.2, 54.8, 54.7; IR ($CHCl_3$): 3445, 3021, 2974, 2926, 2402, 2364, 1695, 1609, 1517, 1216, 1040, 928 cm^{-1}; HRMS (ESI): Calcd. For $C_{36}H_{28}N_2O_3$ $[M+H]^+$ 537.2178; found 537.2161.

4-(4,5-bis(4-bromophenyl)-1-(4-methoxyphenyl)-1H-imidazol-2-yl)benzaldehyde (9)

A mixture of compound **6** (1 g, 2.7 mmol, 1 equiv.), terephthalaldehyde (0.364 g, 2.7 mmol, 1 equiv), p-anisidine (1.338 g, 1.1 mmol, 4 equiv.), ammonium acetate (0.837 g, 1.1 mmol, 4 equiv.) and glacial acetic acid (25 mL) were treated according to the similar procedure as that of compound **7** to give after column chromatography (Hexanes: ethyl acetate, 7:3 v/v), compound **9** (77%, 1.235 g) as light yellow color solid; mp = 190-192 °C; ^{1}H NMR (400 MHz $CDCl_3$) δ 9.97 (s, 1H), 7.76 (d, J = 8.4 Hz, 2H), 7.60 (d, J = 8.4 Hz, 2H), 7.42-7.38 (m, 6H), 6.99-

6.95 (m, 4H), 6.82 (d, J = 8.8 Hz, 2H), 3.81 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.6, 159.8, 138.2, 135.8, 135.5, 132.8, 132.4, 131.9, 131.4, 129.5, 129.2, 129.0, 128.9, 122.8, 121.1, 114.7, 55.4; IR ($CHCl_3$):3021, 2977, 2402, 2364, 1700, 1604, 1517, 1473, 1426, 1216, 1039, 929 cm^{-1}; HRMS (ESI): Calcd. For $C_{29}H_{20}Br_2N_2O_2$ $[M+H]^+$ 586.9970; found 586.9988.

4-(4,5-bis(4'-methoxy-[1,1'-biphenyl]-4-yl)-1-(4-methoxyphenyl)-1H-imidazol-2-yl)benzaldehyde (10)

Compound **9** (0.500 g, 0.85 mmol, 1 equiv.), 4-methoxyphenyl boronic acid (0.284 g, 1.8 mmol, 2.2 equiv.), potassium phosphate tribasic (1.082 g, 5.1 mmol, 6 equiv.), Pd_2dba_3 (0.088 g, 0.11 equiv) and X-Phos (0.170 g, 0.42 equiv) were treated according to the similar procedure to that of compound **8** to give after column chromatography (Hexanes: ethyl acetate, 9:1 v/v), compound **10** (93%, 0.51 g) as yellow color solid; mp = 118-120 °C; ^{1}H NMR (400 MHz $CDCl_3$) δ 9.97 (s, 1H), 7.78-7.75 (m, 2H), 7.71-7.64 (m, 3H), 7.57 (d, J = 8.4 Hz, 1H), 7.53 (d, J = 8.8 Hz, 4H), 7.49-7.44 (m, 4H), 7.23-7.18 (m, 2H), 7.04-7.03 (m, 2H), 6.98-6.91 (m, 4H), 6.82-6.78 (m, 2H), 3.84 (s, 3H), 3.83-3.82 (m, 3H), 3.79-3.78 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.7, 159.5, 159.4, 159.1, 136.3, 135.3, 132.6, 132.0, 131.44, 131.40, 129.5, 129.4, 129.0, 128.3, 127.9, 127.8, 127.6, 126.4, 122.2, 114.5, 114.4, 114.3, 114.1, 55.42, 55.40, 55.3; IR ($CHCl_3$): 3448, 3021,

2977, 2402, 2365, 1605, 1516, 1482, 1426, 1216, 1041, 929 cm^{-1}; HRMS (ESI): Calcd. For $C_{43}H_{34}N_2O_4$ $[M+H]^+$ 643.2597; found 643.2567.

4-(6,9-dibromo-1H-phenanthro[9,10-d]imidazol-2-yl)benzaldehyde (12)

A mixture of compound **11** (0.200 g, 0.54 mmol, 1 equiv.), terephthalaldehyde (0.073 g, 0.54 mmol, 1 equiv.), ammonium acetate (0.168 g, 2.2 mmol, 4 equiv.) and glacial acetic acid (8 mL) was followed the same procedure as that of compound **7**. Yield = 95% (0.250 g); pale-yellow color solid; mp = 230-232 °C; ^{1}H NMR (400 MHz DMSO-d_6) δ 11.96 (bs, NH, 1H), 10.08 (s, 1H), 9.09 (s, 2H), 8.45 (d, J = 8.4 Hz, 4H), 8.10 (d, J = 8.4 Hz, 2H), 7.93-7.88 (m, 2H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 192.9, 148.7, 137.6, 136.6, 135.5, 131.2, 131.1, 130.6, 129.0, 128.8, 128.5, 127.4, 127.1, 126.9, 126.2, 124.6, 124.4, 121.7, 119.9, 119.6; IR ($CHCl_3$): 3021, 2402, 1601, 1522, 1427, 1216, 1025, 929 cm^{-1}; HRMS (ESI): Calcd. For $C_{22}H_{12}Br_2N_2O$ $[M+H]^+$ 478.9395; found 478.9388.

4-(6,9-bis(4-methoxyphenyl)-1H-phenanthro[9,10-d]imidazol-2-yl)benzaldehyde (13)

Compound **12** (0.500 g, 1.0 mmol, 1 equiv.), 4-methoxyphenyl boronic acid (0.348 g, 2.3 mmol, 2.2 equiv.) and potassium phosphate tribasic (1.326 g, 6.2 mmol, 6 equiv.), Pd_2dba_3 (0.104 g, 0.11 equiv.) and X-Phos (0.208 g, 0.42 equiv.) were dissolved in 80 mL of toluene, 14 mL of tert-amyl alcohol and 7 mL of water were treated according to the similar procedure to that of compound **8** to give after

column chromatography (Hexanes: ethyl acetate, 8:2 v/v), compound **13**. Yield = 45% (0.250 g); orange color solid; mp = 206-208 °C; ^{1}H NMR (500 MHz Acetone-d_6) δ 12.6 (bs, NH, 1H), 10.08 (s, 1H), 9.08-9.05 (m, 2H), 8.70 (d, J = 8.5 Hz, 1H), 8.47 (d, J = 8.5 Hz, 2H), 8.38 (d, J = 8.5 Hz, 1H), 8.03 (d, J = 8.5 Hz, 2H), 7.95 (d, J = 8.0 Hz, 1H), 7.88 (d, J = 7.5 Hz, 1H), 7.85-7.82 (m, 4H), 7.08 (d, J = 7.5 Hz, 4H), 3.88 (s, 6H); ^{13}C NMR (125 MHz, Acetone-d_6) δ 192.4, 160.5, 160.4, 148.8, 139.1, 138.9, 138.7, 137.5, 136.7, 134.8, 134.4, 131.0, 130.8, 130.2, 129.7, 129.4, 129.3, 127.3, 126.9, 123.8, 123.4, 122.6, 122.3, 115.3, 115.2, 55.7; IR ($CHCl_3$): 3021, 2977, 2926, 2402, 2363, 1699, 1604, 1517, 1424, 1216, 1040, 929 cm^{-1}; HRMS (ESI): Calcd. For $C_{36}H_{26}N_2O_3$ $[M+H]^+$ 535.2022; found 535.2032.

4-(6,9-dibromo-1-(4-methoxyphenyl)-1H-phenanthro[9,10-d]imidazol-2-yl)benzaldehyde (14)

A mixture of compound **11** (1 g, 2.7 mmol, 1 equiv.), terephthalaldehyde (0.366 g, 2.7 mmol, 1 equiv), p-anisidine (1.345 g, 1.1 mmol, 4 equiv.), ammonium acetate (0.842 g, 1.1 mmol, 4 equiv.) and glacial acetic acid (25 mL) were treated according to the similar procedure as that of compound **9** to give after column chromatography (Hexanes: ethyl acetate, 9:1 v/v), compound **14** (87% , 1.394 g) as green color solid; mp = 216-218 °C; ^{1}H NMR (400 MHz $CDCl_3$) δ 9.98 (s, 1H), 8.69 (d, J = 1.6 Hz, 1H), 8.66-8.64 (m, 2H), 7.82-7.72 (m, 5H), 7.40-7.37 (m, 3H), 7.10 (d, J = 8.8 Hz, 2H), 7.04 (d, J = 8.8 Hz, 1H), 3.95 (s, 3H); ^{13}C NMR (100

MHz, $CDCl_3$) δ 191.6, 160.7, 137.3, 135.9, 135.7, 131.0, 130.3, 130.1, 129.8, 129.7, 129.5, 129.4, 128.7, 128.6, 126.9, 126.0, 125.9, 124.4, 122.4, 121.7, 120.2, 119.7, 115.6, 55.7; IR ($CHCl_3$): 3021, 2402, 1978, 1603, 1517, 1429, 1217, 1021 cm^{-1}; HRMS (ESI): Calcd. For $C_{29}H_{18}Br_2N_2O_2$ $[M+H]^+$ 584.9813; found 584.9819.

4-(1,6,9-tris(4-methoxyphenyl)-1H-phenanthro[9,10-d]imidazol-2-yl)benzaldehyde (15)

Compound **14** (0.500 g, 0.85 mmol, 1 equiv.), 4-methoxyphenyl boronic acid (0.285g, 1.8 mmol, 2.2 equiv.), potassium phosphate tribasic (1.086 g, 5.1 mmol, 6 equiv.), Pd_2dba_3 (0.085 g, 0.11 equiv) and X-Phos (0.170 g, 0.42 equiv) were treated according to the similar procedure as that of compound **10** to give after column chromatography (Hexanes: ethyl acetate, 7:3 v/v), compound **15** (36%, 0.2 g) as yellow color solid; mp = 132-134 °C; ^{1}H NMR (500 MHz $CDCl_3$) δ 9.98 (s, 1H), 8.93 (s, 1H), 8.87-8.86 (m, 2H), 7.94 (dd, *J* = 1.5, 7 Hz, 1H), 7.79 (s, 4H), 7.75 (d, *J* = 8.5 Hz, 2H), 7.65 (d, *J* = 8.5 Hz, 2H), 7.51 (dd, *J* = 2, 7 Hz, 1H), 7.44 (d, *J* = 8.5 Hz, 2H), 7.27 (d, *J* = 9 Hz, 1H), 7.11 (d, *J* = 9 Hz, 2H), 7.07 (d, *J* = 8.5 Hz, 2H), 7.02 (d, *J* = 8.5 Hz, 2H), 3.96 (s, 3H), 3.89 (s, 3H), 3.87 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 191.7, 160.6, 159.3, 159.2, 149.4, 138.3, 137.6, 137.5, 136.2, 135.7, 134.3, 133.6, 130.9, 129.9, 129.5, 129.4, 128.9, 128.8, 128.6, 128.4, 126.6, 125.9, 125.5, 125.0, 123.2, 121.9, 121.7, 121.4, 121.1, 115.4, 114.4, 114.4,

55.6, 55.43, 55.40; IR ($CHCl_3$): 3021, 2402, 1604, 1516, 1427, 1217, 1028, 928 cm^{-1}; HRMS (ESI): Calcd. For $C_{43}H_{32}N_2O_4$ $[M+H]^+$ 641.2440; found 641.2442.

4-(4,5-dimethyl-1H-imidazol-2-yl)benzaldehyde (16)

A mixture of terephthalaldehyde (1.56 g, 0.0116 mol, 1 equiv.) and ammonium acetate (3.58 g, 0.046 mol, 4 equiv.) in trifluoracetic acid at 0°C and 2,3-butadione (1g, 0.0116 mol, 1 equiv.) was slowly added to the above mixture and warmed to RT and reflux for 18 h. The reaction was monitored by the TLC. After completion of the reaction the solution was poured into water and extracted with dichloromethane. The organic layer was concentrated over the anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure. The crude product was subjected to the column chromatography (Hexanes: dichloromethane, 4:6 v/v) furnished the compound **16** (15%, 0.35 g) as colorless solid; mp = 136-138 °C; ^1H NMR (400 MHz $CDCl_3$) δ 10.03 (s, 1H), 8.13 (d, *J* = 8.0 Hz, 2H), 7.93 (d, *J* = 8.0 Hz, 2H), 2.34 (s, 3H), 2.18 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.5, 157.8, 144.8, 136.6, 133.0, 132.8, 130.1, 126.1, 11.2, 10.2; IR ($CHCl_3$): 3021, 2979, 2925, 2820, 2725, 2402, 1700,1639, 1606, 1518, 1421, 1297, 1216, 1079, 1041, 929 cm^{-1}; HRMS (ESI): Calcd. For $C_{12}H_{12}N_2O$ $[M+H]^+$ 201.1028; found 201.1023.

2. Optoelectronic properties of imidazole dyes

Figure S1. UV-Vis spectra of imidazole dyes and their corresponding aldehydes

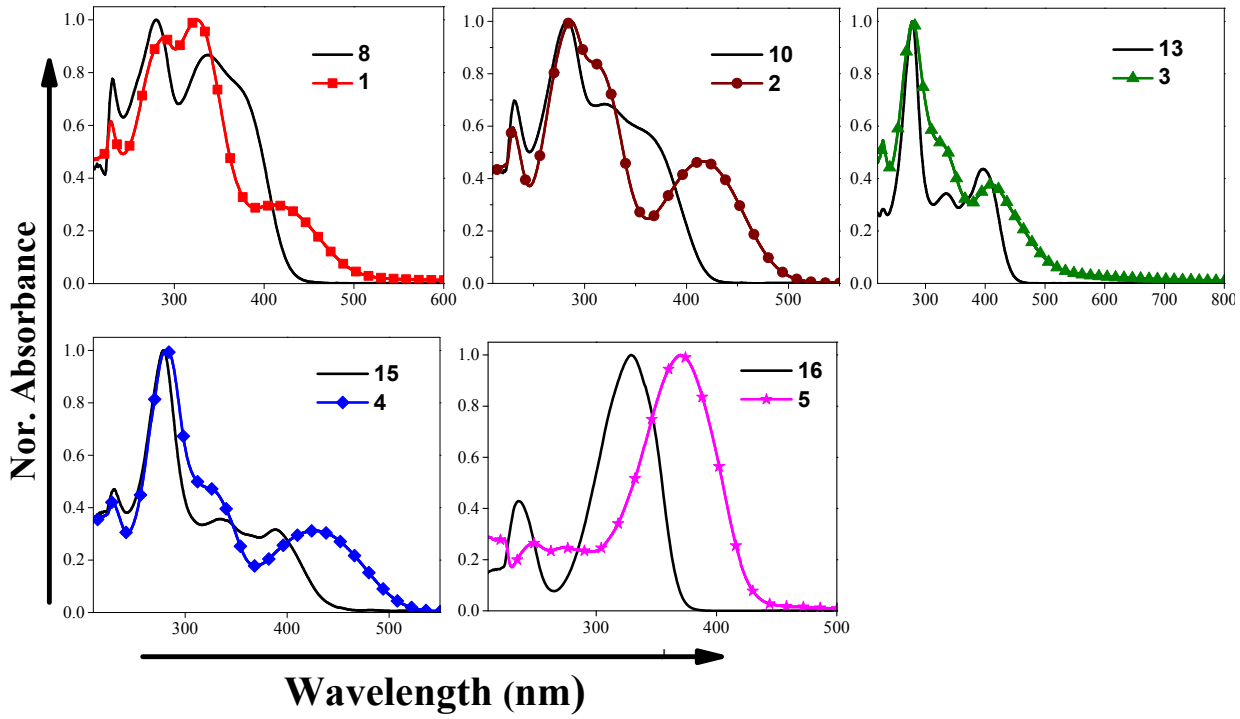


Figure S2. Cyclic voltammogram of imidazole sensitizers in DMF solution at a scan rate of 50mV/s

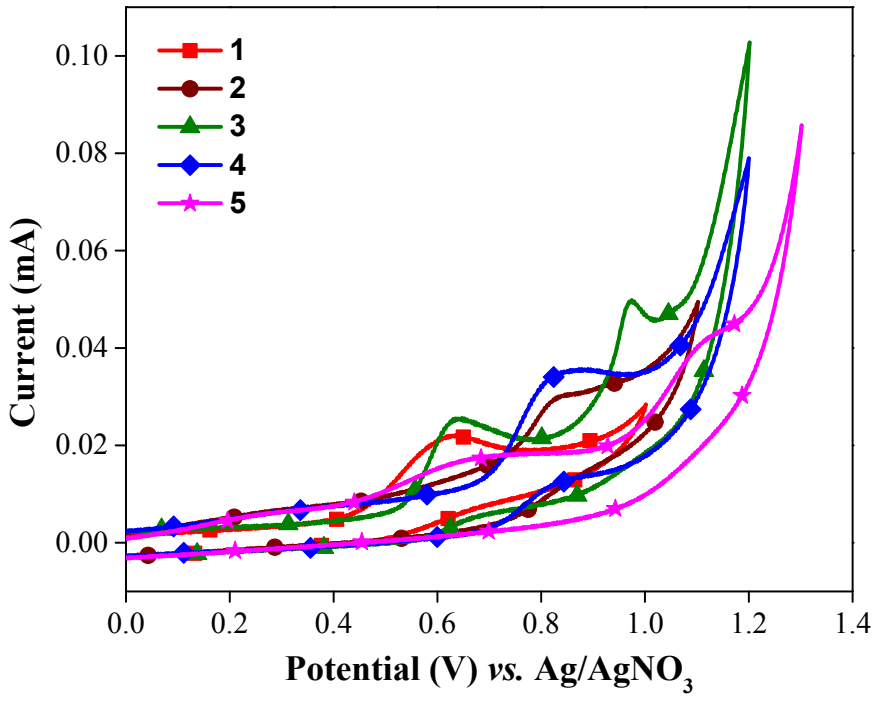


Figure S3. Cyclic voltammograms of 0.1 mM of dye **1** in DMF solution at different scan rates

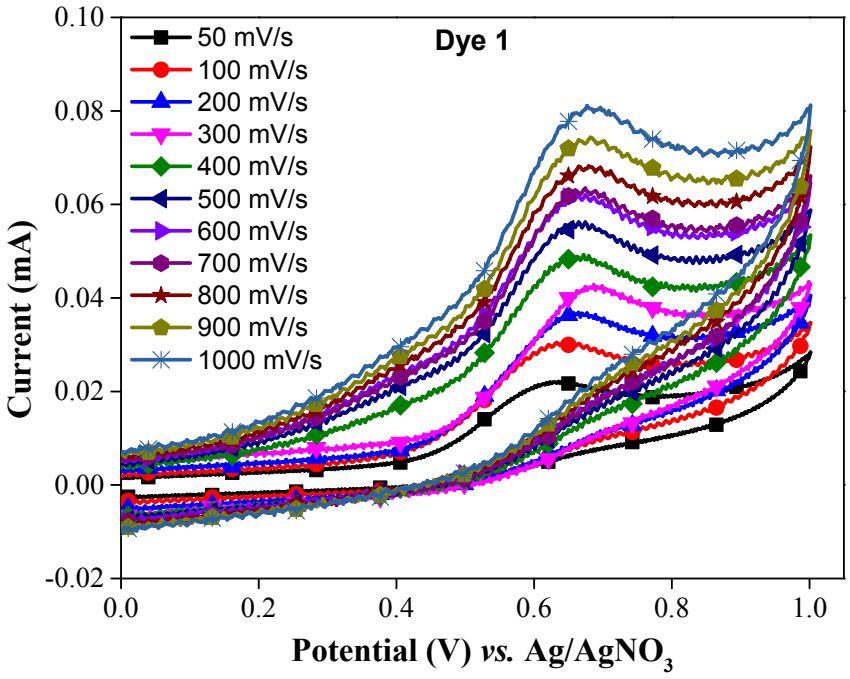


Figure S4. Cyclic voltammograms of 0.1 mM of dye **2** in DMF solution at different scan rates

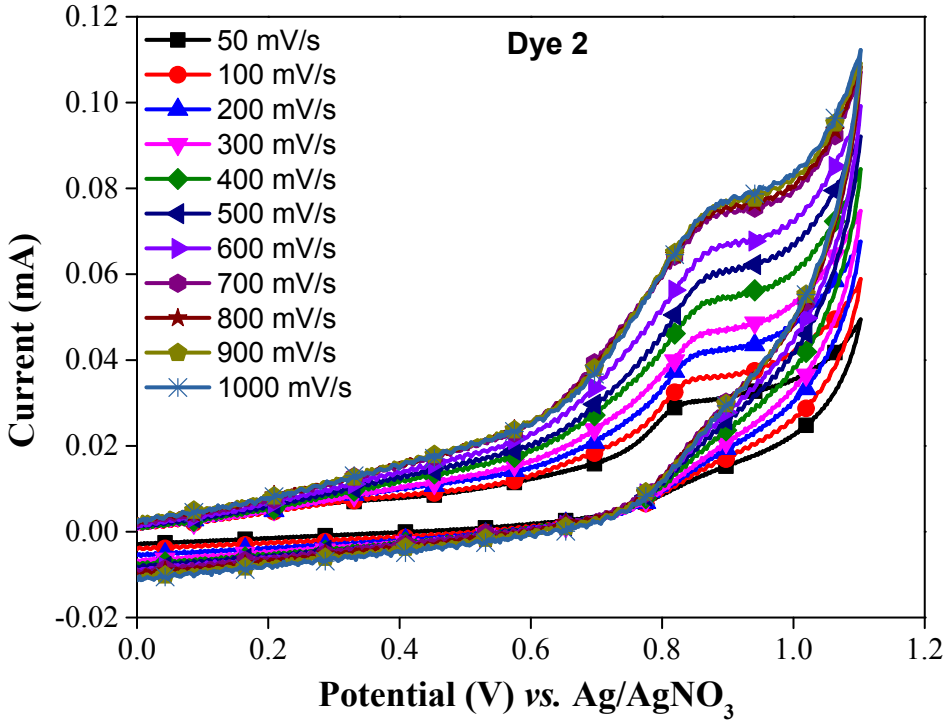


Figure S5. Cyclic voltammograms of 0.1 mM of dye **3** in DMF solution at different scan rates

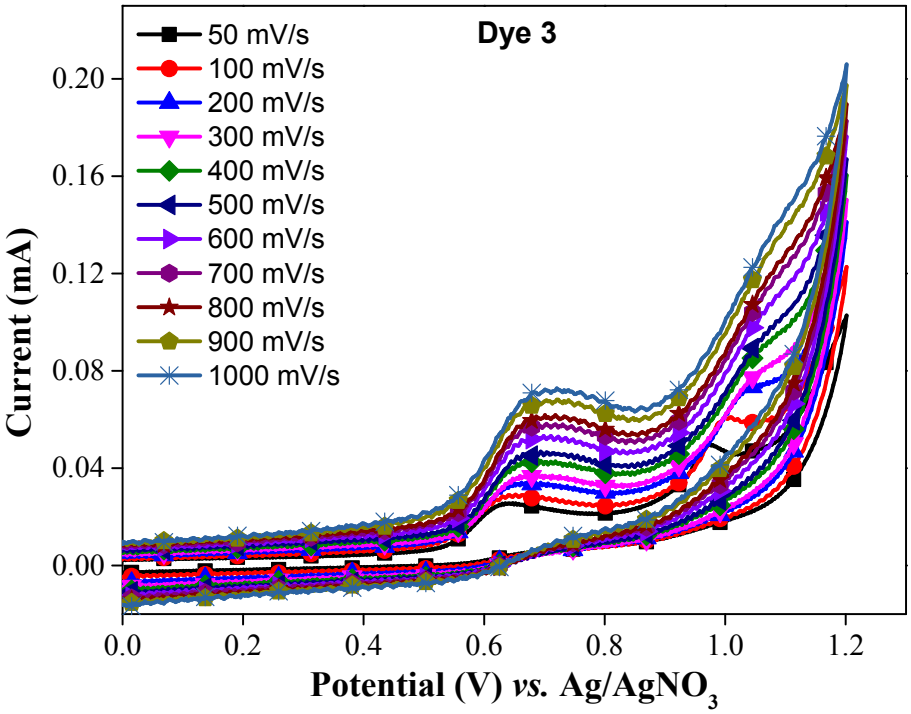


Figure S6. Cyclic voltammograms of 0.1 mM of dye **4** in DMF solution at different scan rates

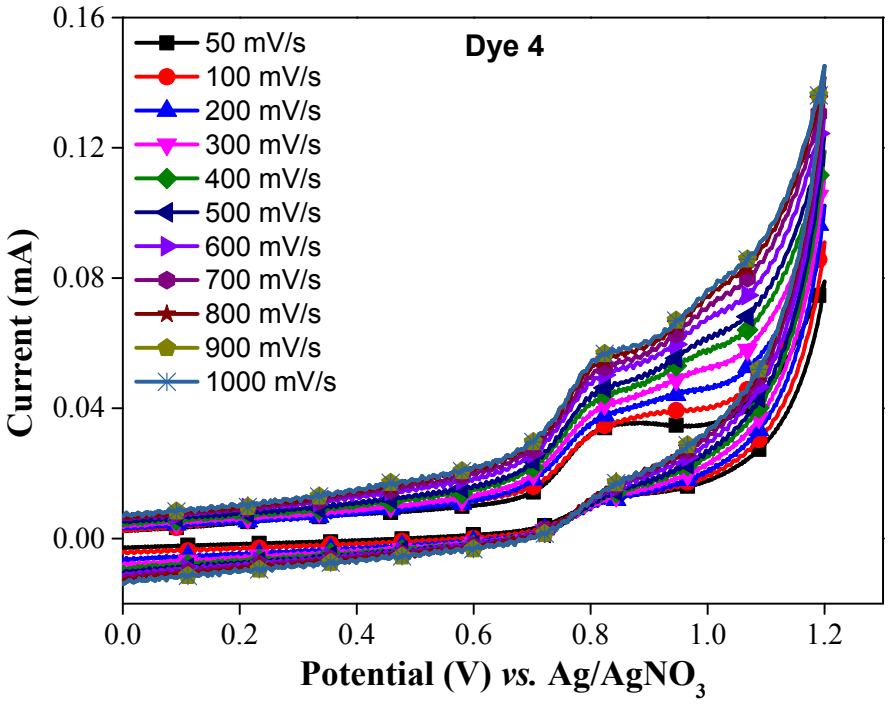


Figure S7. Cyclic voltammograms of 0.1 mM of dye **5** in DMF solution at different scan rates

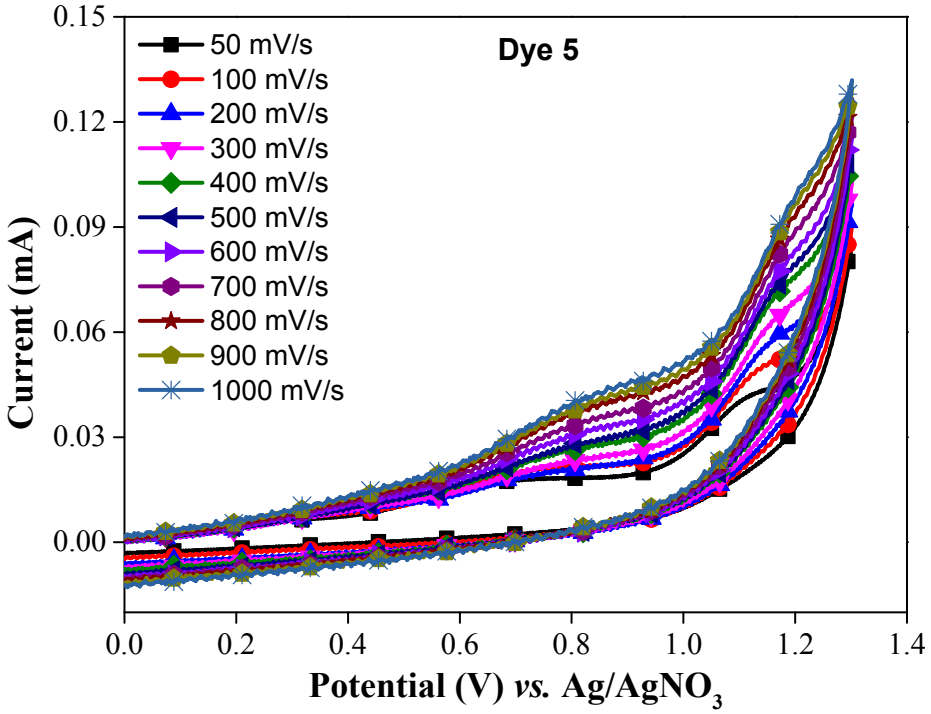
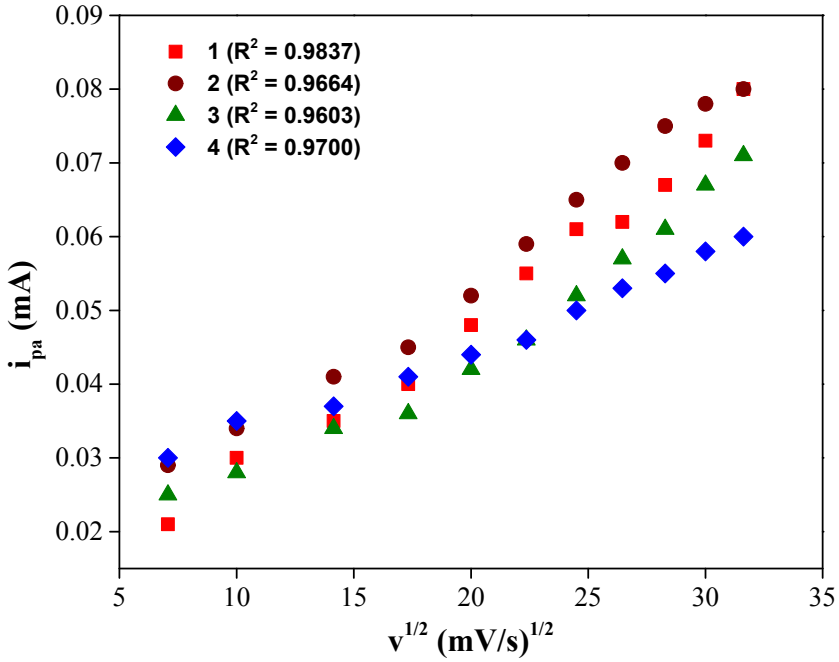


Figure S8. A plot of anodic peak current versus square root of the scan rate for the imidazole sensitizers in DMF solution



3. Figure S9: Optimized structure, HOMO and LUMO orbitals of imidazole sensitizers 1 to 5 using UB3LYP/6-31G (d, p) basis set.

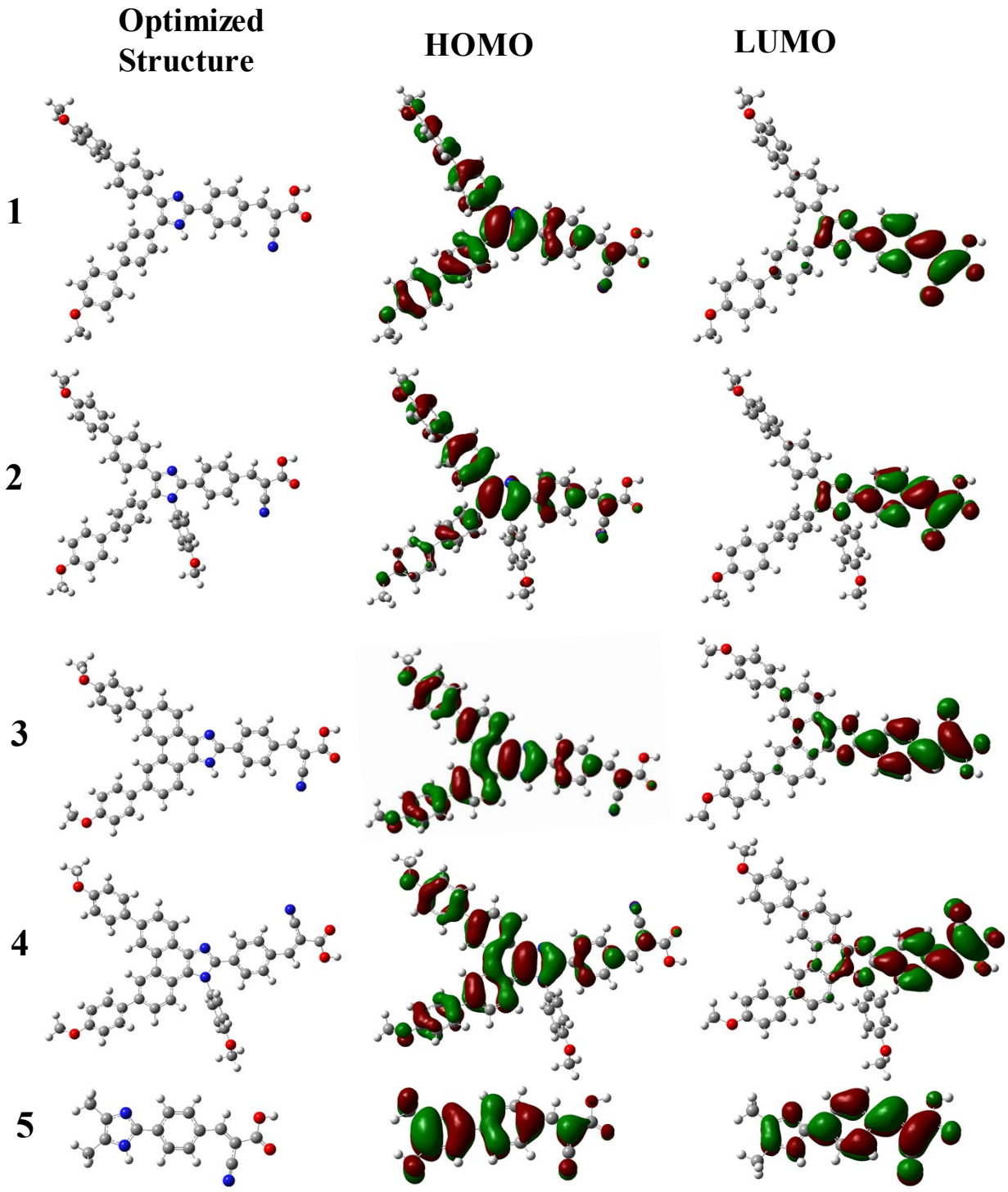


Figure S10. Box chart of J_{SC}, V_{OC}, FF and η of the optimized DSSC based on imidazole sensitizers 1 to 5.

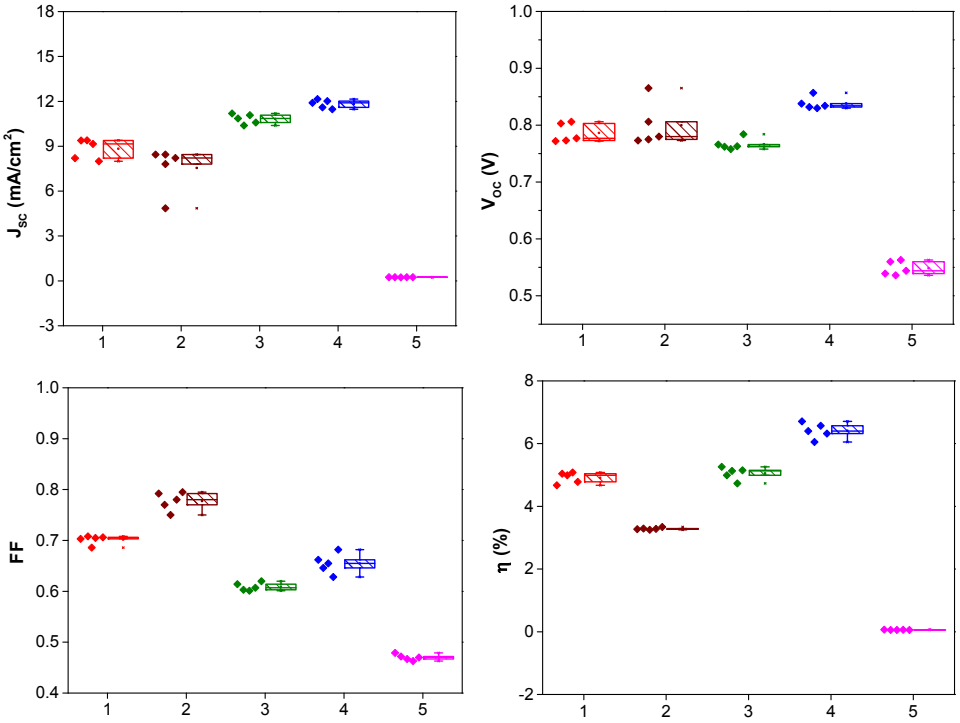


Figure S11. Box chart of J_{SC}, V_{OC}, FF and η of the optimized DSSC based on imidazole sensitizers 1 to 5 with CDCA.

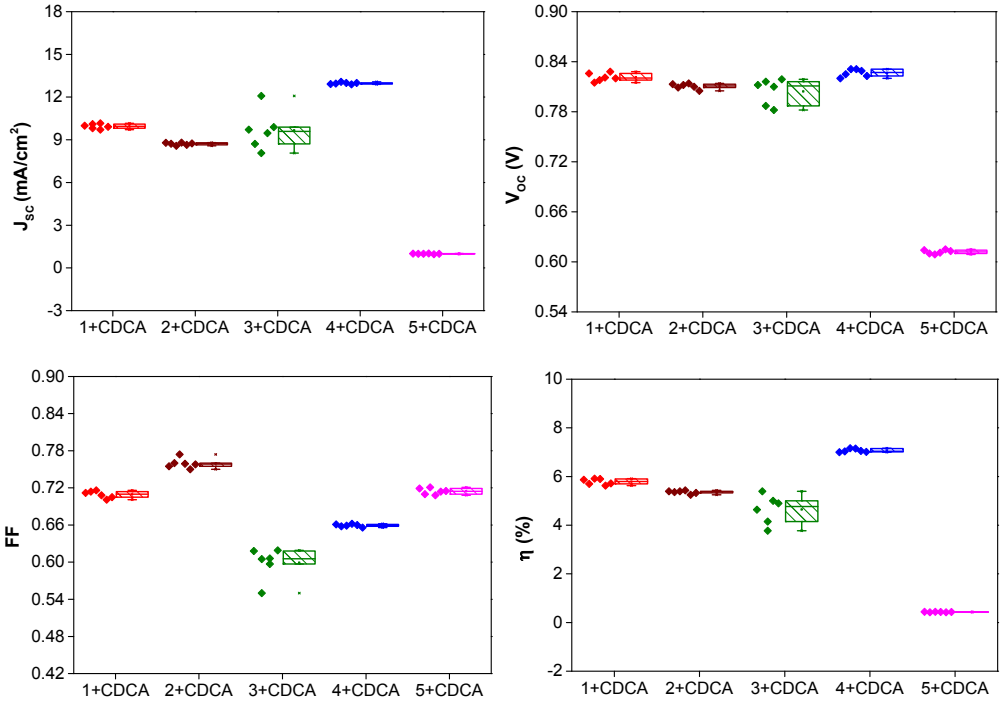


Figure S12. Nyquist and Bode phase plots of dye 5 in the absence and presence of CDCA.

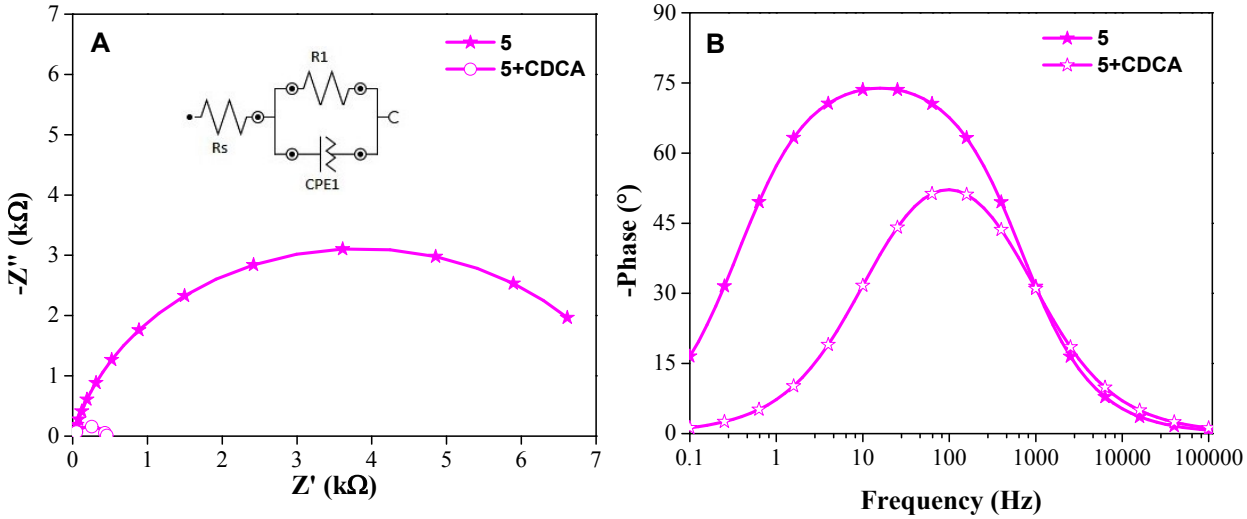
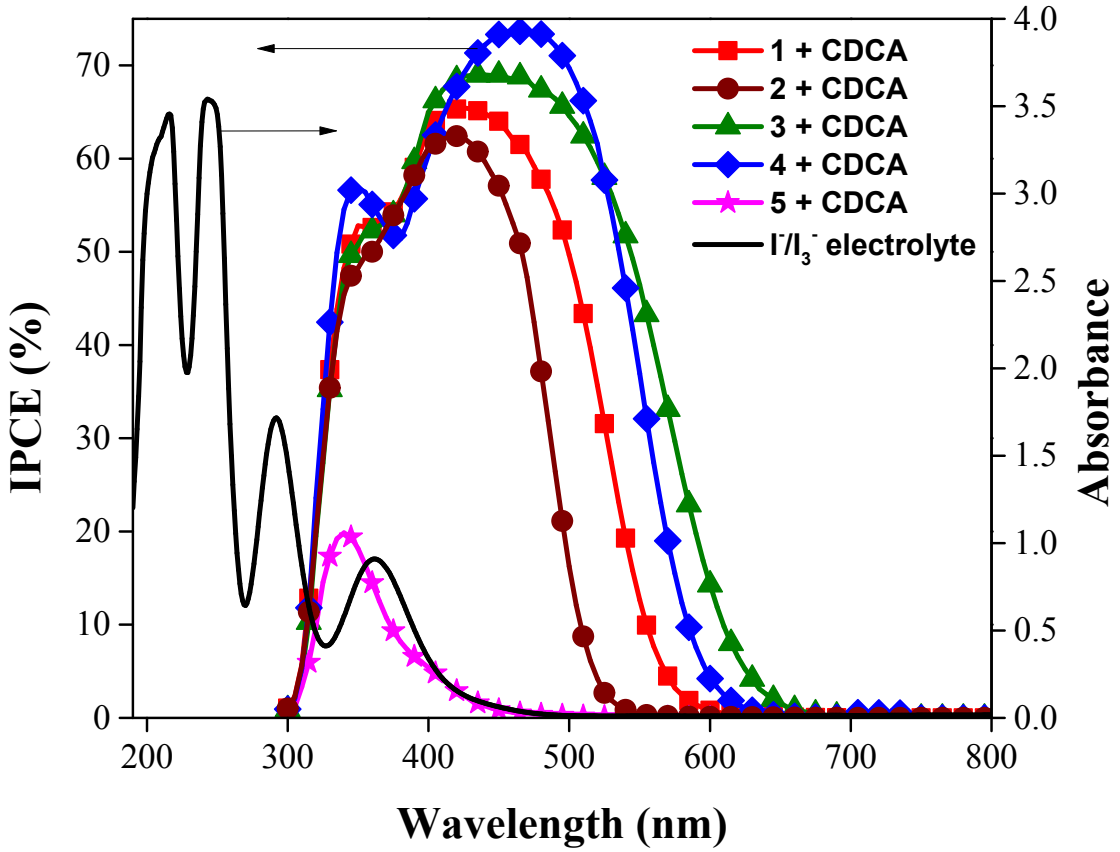


Figure S13. IPCE curves of dye 1 to 5 in the presence of CDCA and absorbance spectrum of I^-/I_3^- electrolyte.



4. New dye adsorption technique based on electrosorption method

Open circuit potential (OCP) measurement

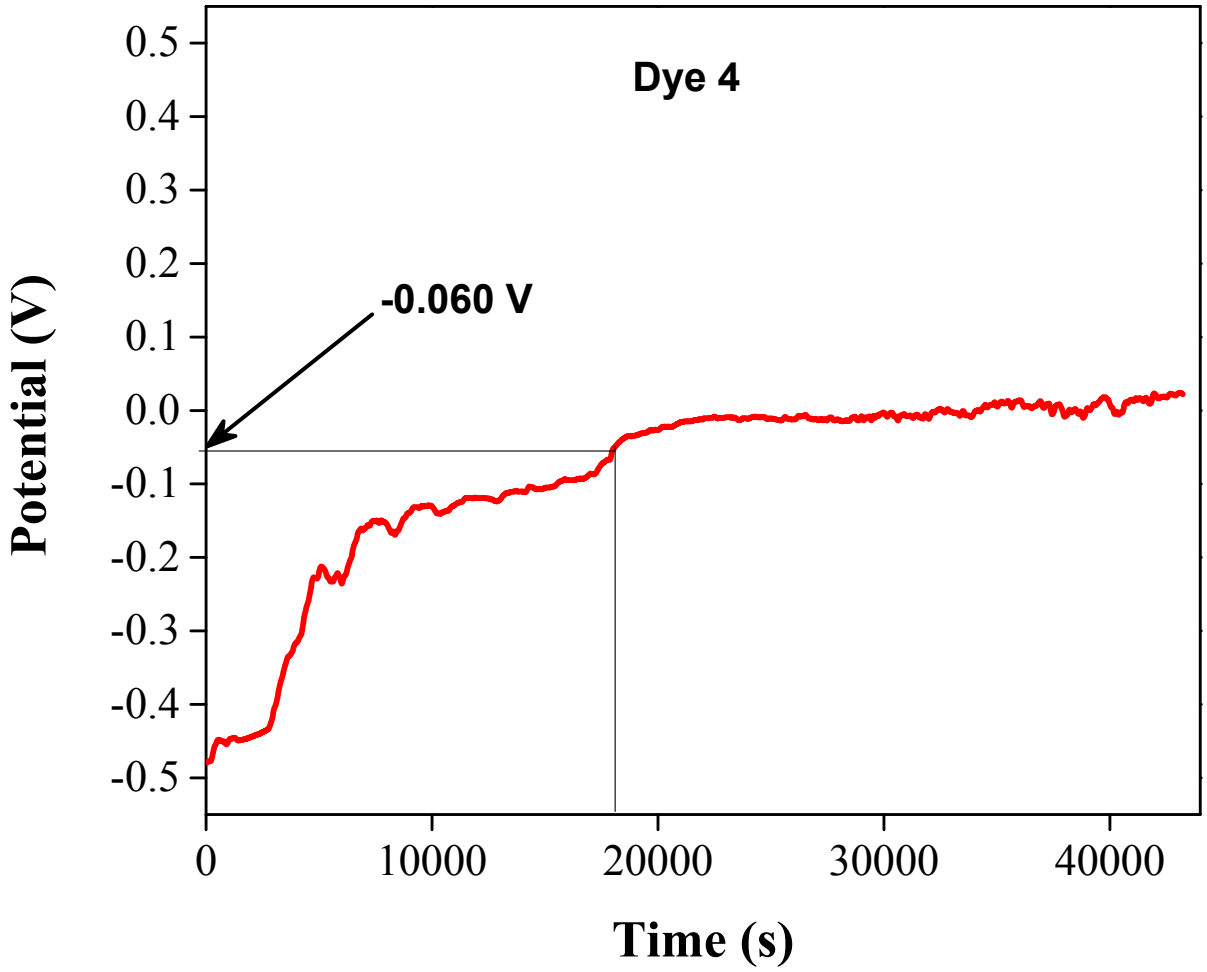
To carry out the TiO_2 dye staining by potential assisted method, an appropriate potential value has to be chosen for the dyes under investigation instead of choosing potential arbitrarily. This value has been measured by recording the potential difference between working electrode (FTO/TiO_2) and reference electrode (Ag/Ag^+) in 0.5 mM of dye **4** in tert-butyl alcohol: acetonitrile (1:1, v/v) for 12 h and the obtained data is displayed in **figure S14**. As seen in the figure, the potential value is changing in the first few hours and attains a stable value after several hours and this value is noted and applied as open circuit potential[1] on a fresh FTO/TiO_2 electrode (chronoamperometry) for dye loading as discussed in the manuscript. This applied potential accelerates the dye adsorption and the resultant dye loading on the electrode exceeds that of the conventional dyeing process within 1 h of potential applied. At this applied potential there was no charge transfer process which is evident from the very low current observed, which his due to capacitive nature of the FTO/TiO_2 – dye solution interface.[2,3]

1 P. Ponthiaux, R. Bayon, F. Wenger and J.-P. Celis, in *Woodhead Publishing Series in Biomaterials*, ed. Y. B. T.-B.-T. in B. and M. I. Yan, Woodhead Publishing, 2013, pp. 372–394.

2 Y. Jin, M. Wu, G. Zhao and M. Li, *Chem. Eng. J.*, 2011, **168**, 1248–1255.

3 H. Seo, M. K. Son, H. J. Kim and M. Shiratani, *Thin Solid Films*, 2014, **554**, 118–121.

Figure S14. OCP measurements of dye **4** in the presence of CDCA.



Scheme S1: (A) Open circuit potential of FTO/TiO_2 electrode in 0.5 mM dye 1 to 4 solution and (B) Electrosorption carried out on fresh FTO/TiO_2 electrode applying potential noted after 12 h from the experiment (A).

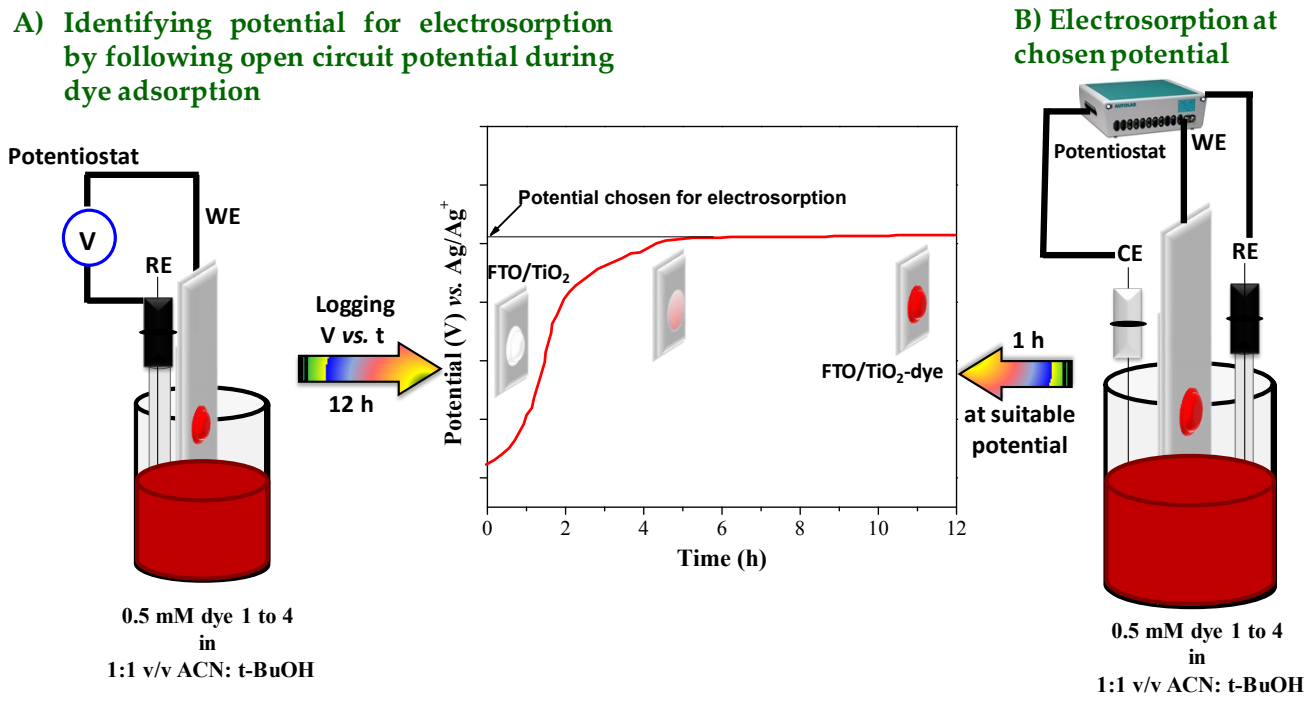


Table S1: HOMO, LUMO, and energy gap values of Imidazole sensitizers obtained from computational methods.

Dyes	E_g (eV)	HOMO/LUMO (eV)
1	2.59	-5.24/-2.65
2	2.64	-5.14/-2.50
3	2.89	-5.56/-2.67
4	2.55	-5.11/-2.56
5	3.14	-5.69/-2.55

Table S2: Photovoltaic parameters of imidazole sensitizers recorded on 1st, 30th, and 60th day

Dyes	1st day				30th day				60th day			
	J_{SC} (mA/cm^2)	V_{OC} (V)	FF	η[a] (%)	J_{SC} (mA/cm^2)	V_{OC} (V)	FF	η[a] (%)	J_{SC} (mA/cm^2)	V_{OC} (V)	FF	η[a] (%)
1*	10.10	0.818	0.716	5.91	8.01	0.828	0.713	4.72	5.21	0.803	0.673	2.81
2*	8.80	0.814	0.759	5.43	5.39	0.829	0.768	3.44	3.36	0.770	0.717	1.85
3*	12.08	0.812	0.550	5.39	11.28	0.803	0.574	5.20	6.31	0.796	0.612	3.07
4*	13.07	0.831	0.659	7.16	11.72	0.832	0.631	6.16	8.49	0.810	0.711	4.88
5*	1.01	0.611	0.708	0.436	0.42	0.602	0.605	0.15	0.07	0.363	0.400	0.01

***** With chenodeoxycholic acid. [a] TiO_2 film has a 5 μm scattering layer and 6 μm transparent layer. Electrolyte composition: 0.05 M iodine, 0.1 M lithium iodide, 0.6 M 1-butyl-3-methylimidazolium iodide, and 0.5 M of t-butyl pyridine in 15:85 v/v % of valeronitrile and acetonitrile.

5. NMR and Mass spectra of imidazole dyes

Figure S15. ^{1}H and ^{13}C NMR of 7

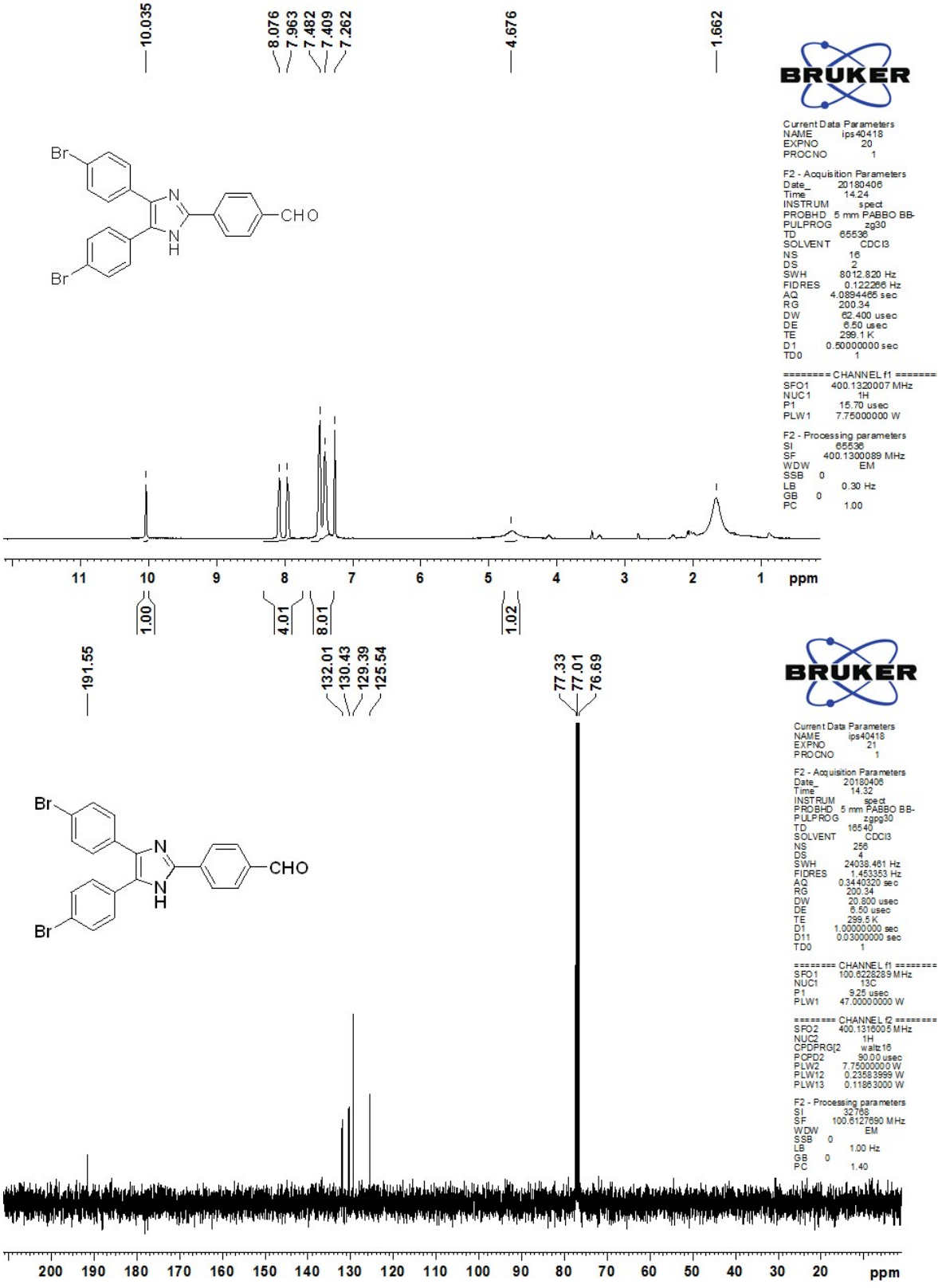


Figure S16. ^{1}H and ^{13}C NMR of 8

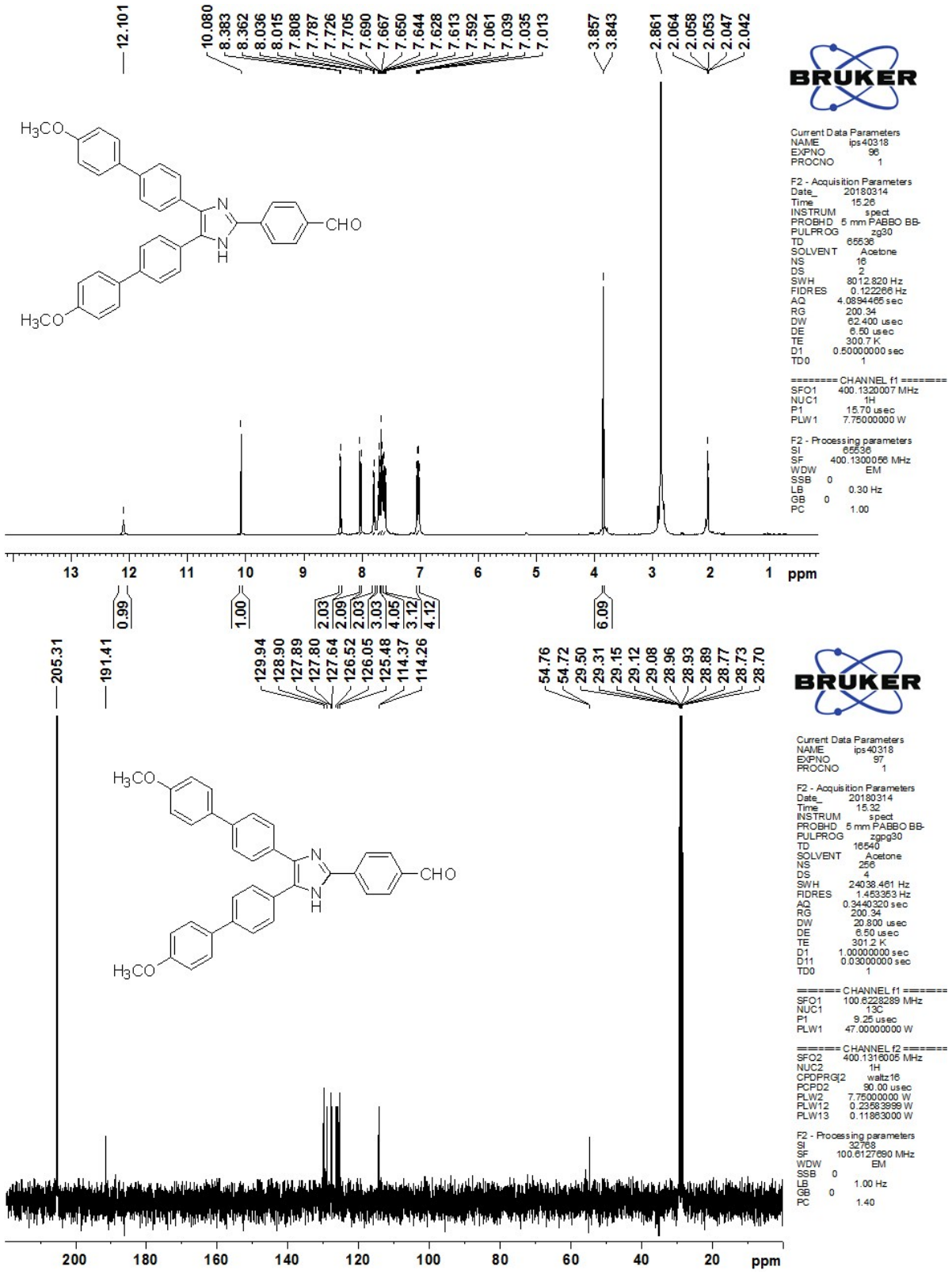
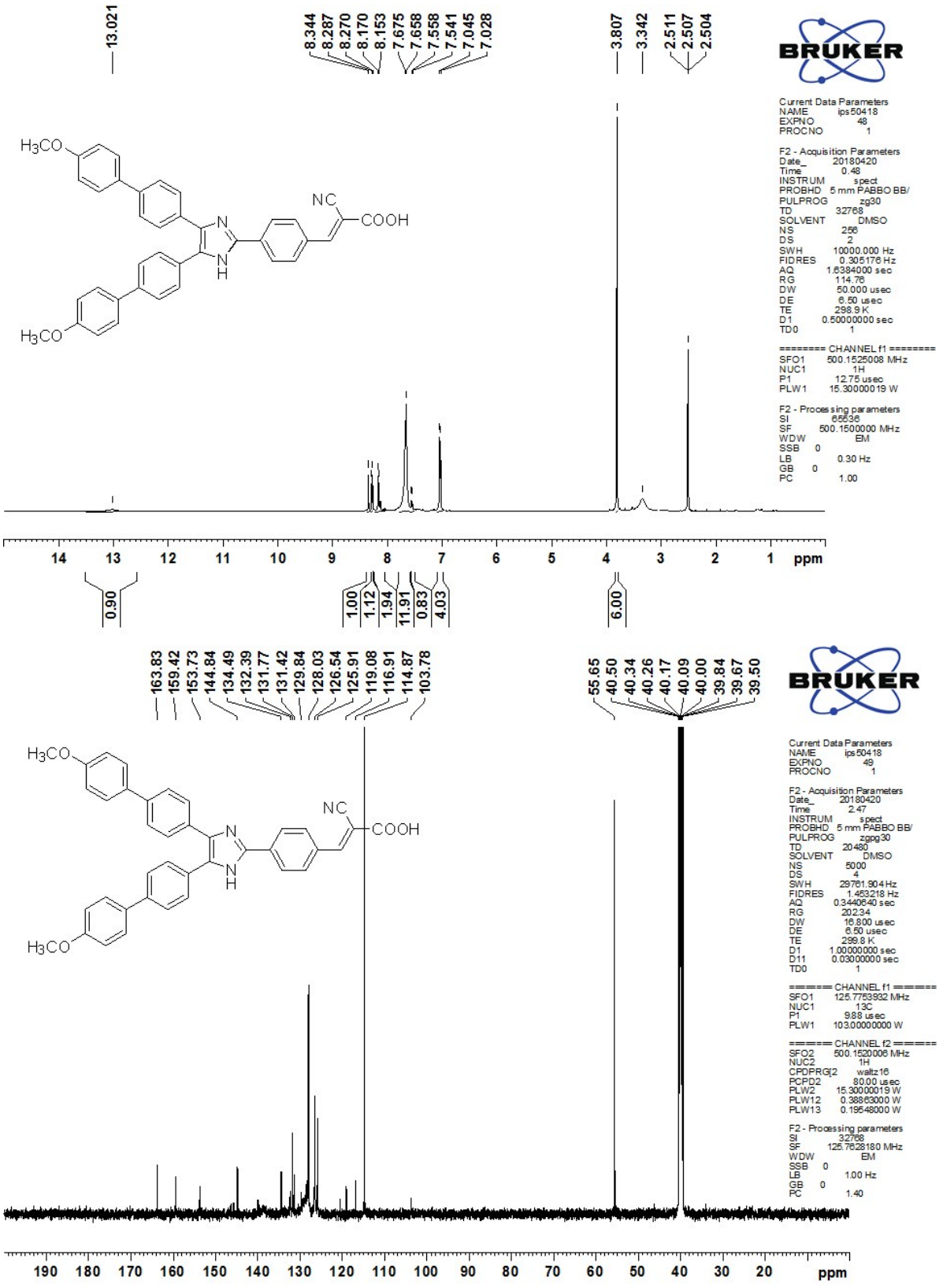


Figure S17. ^{1}H, ^{13}C NMR and mass spectrum of 1



Qualitative Compound Identification Report

Data File	SJE-B5.d	**Sample Name**	220518-16-KRR-SJE-B5
Sample Type	Sample	**Position**	P2-B5
Instrument Name	Instrument 1	**User Name**	
Acq Method	Direct Infusion_HPLC.m	**Acquired Time**	22-05-2018 12:11:09 (UTC+05:30)
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition Time (Local)**	22-05-2018 12:11:09 (UTC+05:30)
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)	**QTOF Driver Version**	8.00.00
QTOF Firmware Version	20.698	**Tune Mass Range Max.**	3200

Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	Hits (DB)
Cpd 1: C39 H29 N3 O4; 0.420	0.42	603.2142	970016	C39 H29 N3 O4	603.2158	-2.74	1

Figure S18. ^{1}H and ^{13}C NMR of 9

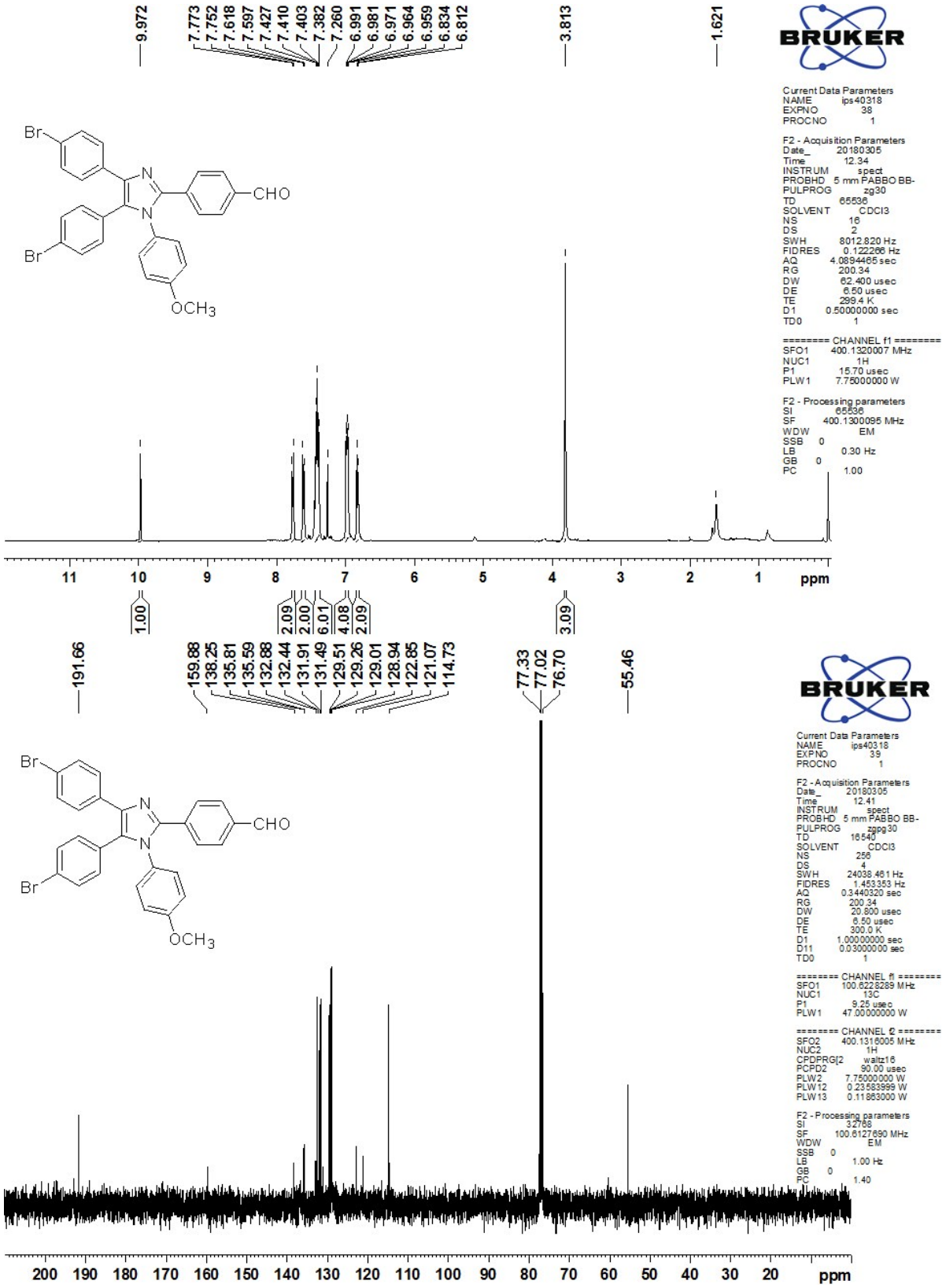


Figure S19. ^{1}H and ^{13}C NMR of 10

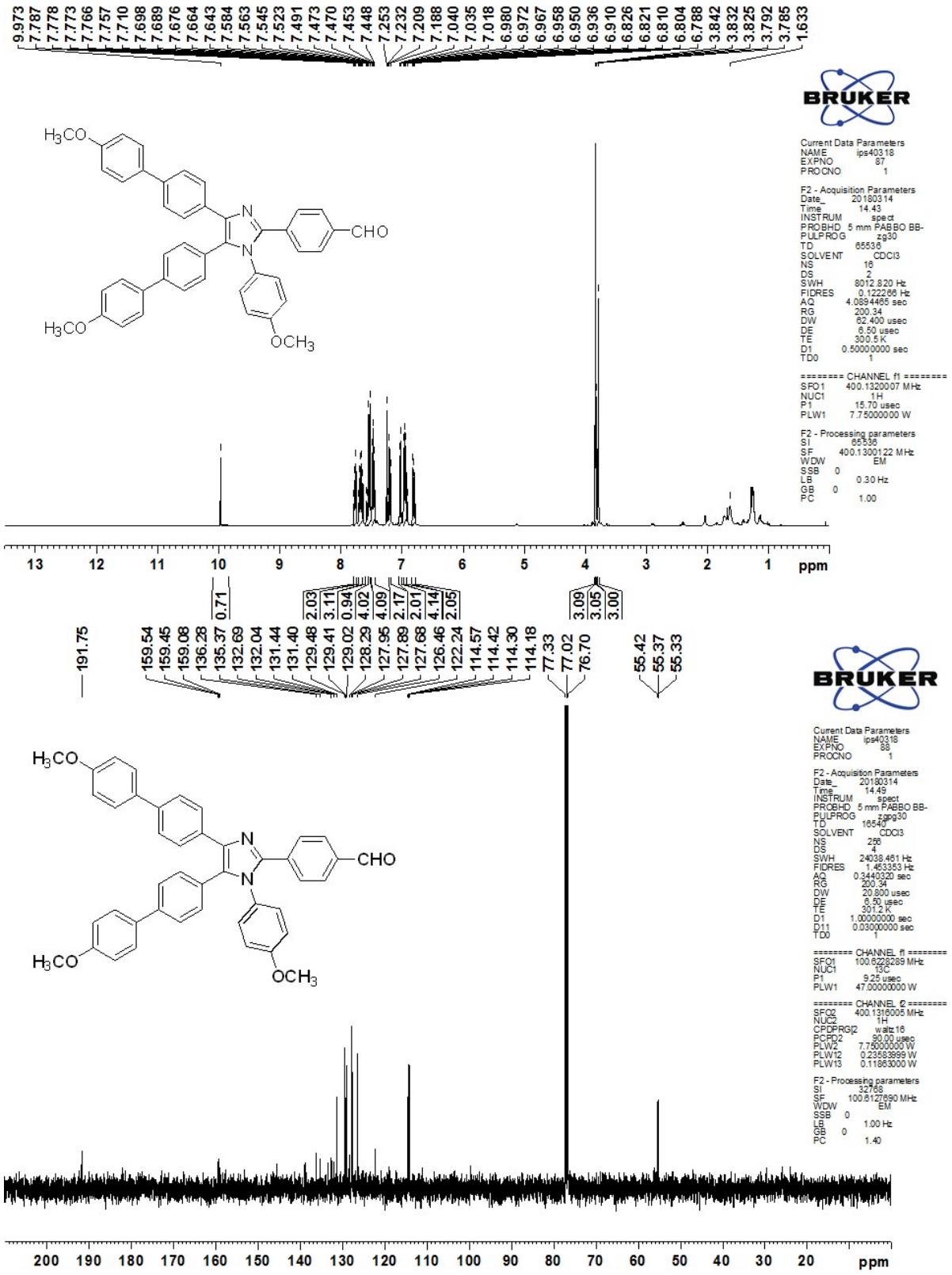
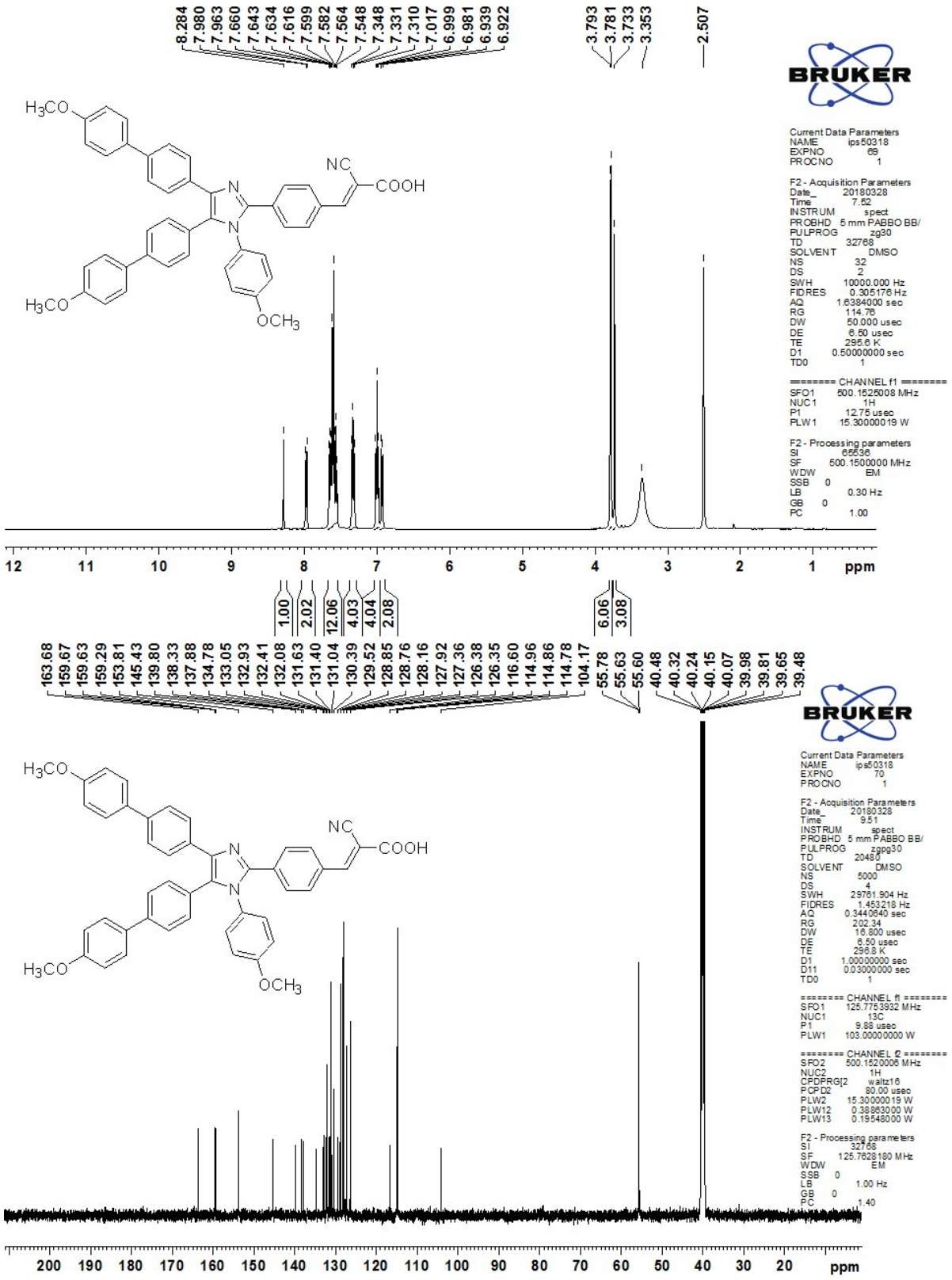


Figure S20. ^{1}H, ^{13}C NMR and mass spectrum of 2



Qualitative Compound Identification Report

Data File	SJE-B5A.d	**Sample Name**	290618-3-KRR-SJE-B5A
Sample Type	Sample	**Position**	P2-F3
Instrument Name	Instrument 1	**User Name**	
Acq Method	Direct Infusion_HPLC.m	**Acquired Time**	29-06-2018 11:39:03 (UTC+05:30)
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			
Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition Time (Local)**	29-06-2018 11:39:03 (UTC+05:30)
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)	**QTOF Driver Version**	8.00.00
QTOF Firmware Version	20.698	**Tune Mass Range Max.**	3200

Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	Hits (DB)
Cpd 1: C46 H35 N3 O5; 0.301	0.301	709.2586	14316	C46 H35 N3 O5	709.2577	1.38	1

Figure S21. ^{1}H and ^{13}C NMR of 12

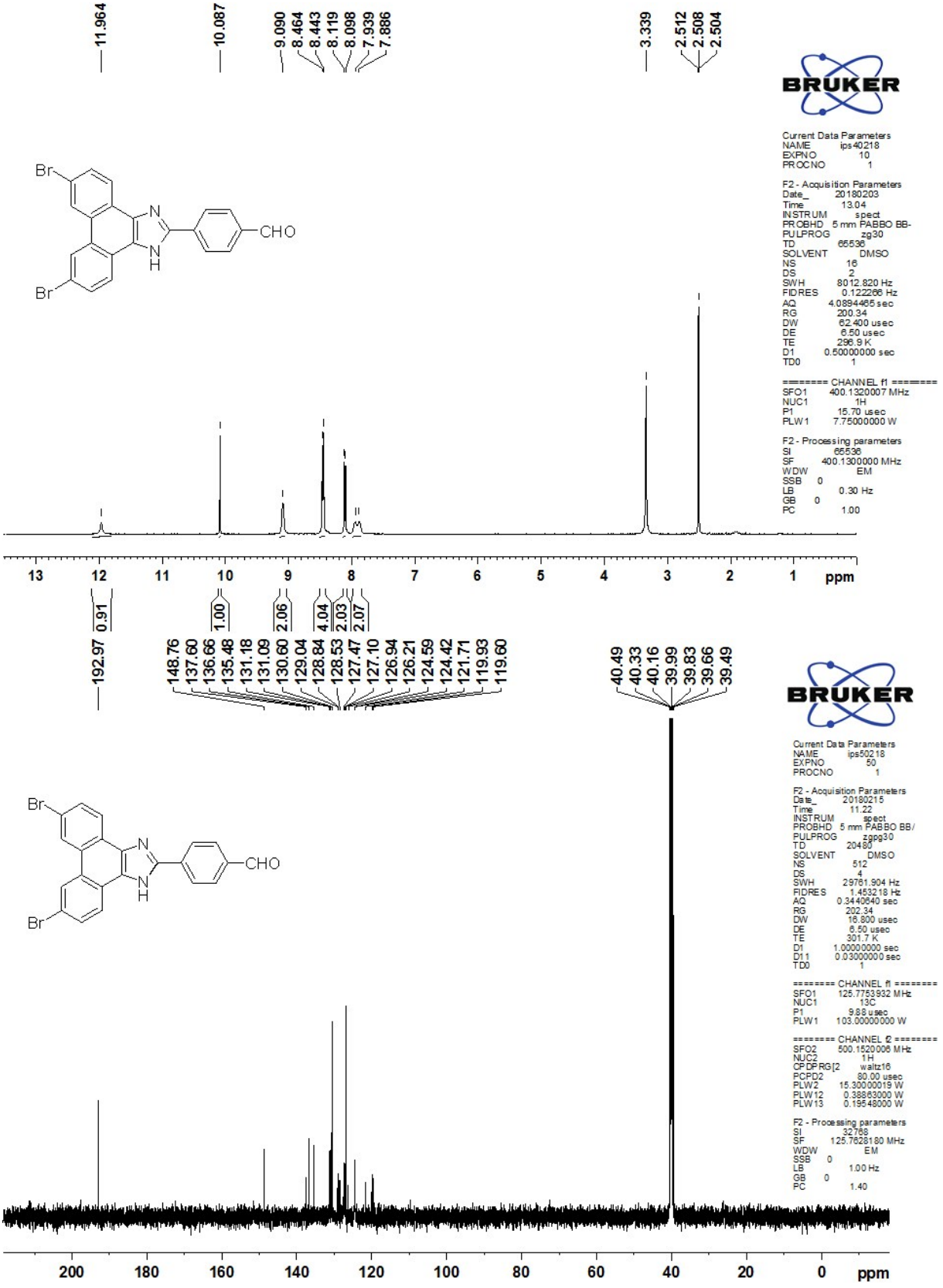


Figure S22. ^{1}H and ^{13}C NMR of 13

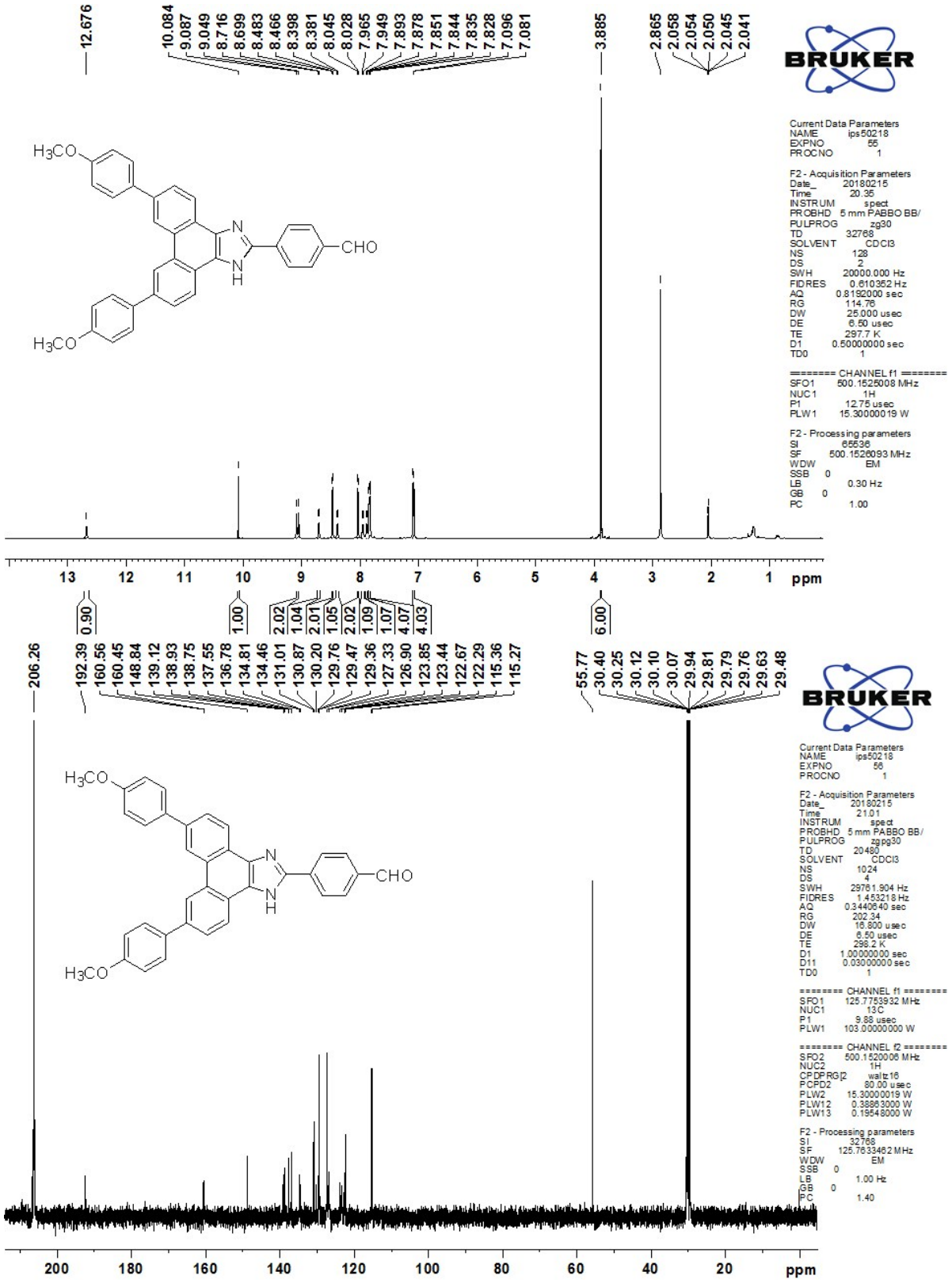
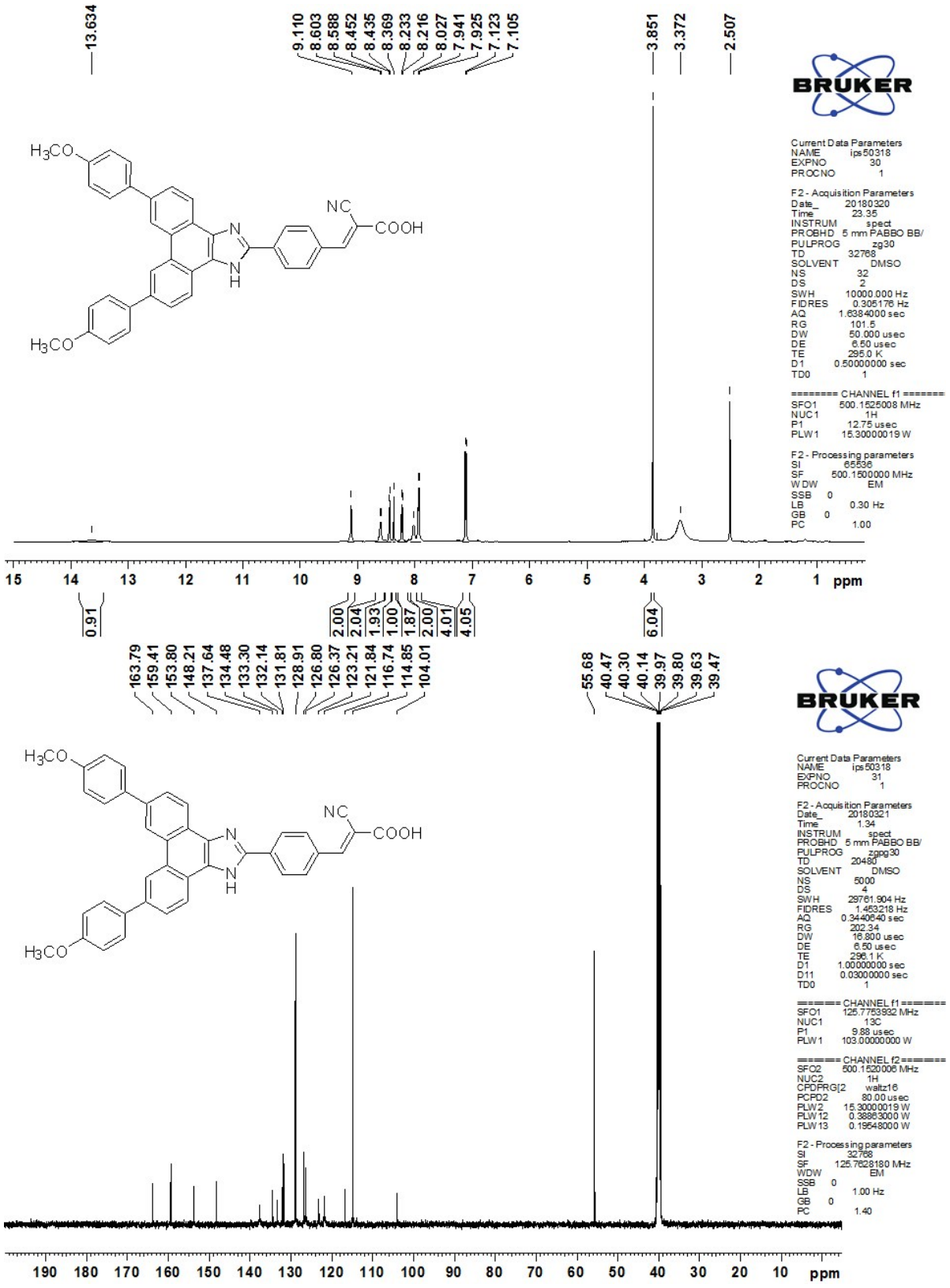


Figure S23. ^{1}H, ^{13}C NMR and mass spectrum of 3

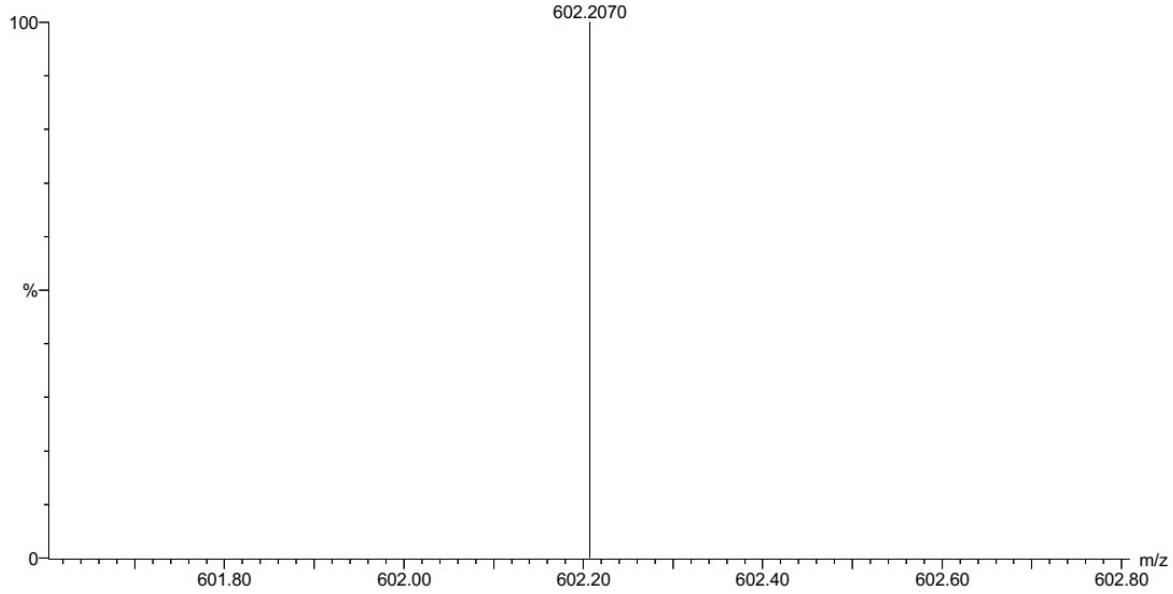


Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-39 H: 0-28 N: 0-3 O: 0-4

KRR-SJE-P5R
17072018-15-KRR-SJE-P5R 14 (0.353) AM (Cen,5, 80.00, Ar,5000.0,0.00,1.00); Sb (1,40.00); Sm (Mn, 1x0.00); Cm (7:14) TOF MS ES+
1.32e+003



Minimum:				-1.5		
Maximum:		5.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
602.2070	602.2080	-1.0	-1.7	27.5	n/a	C39 H28 N3 O4

Figure S24. ^{1}H and ^{13}C NMR of 14

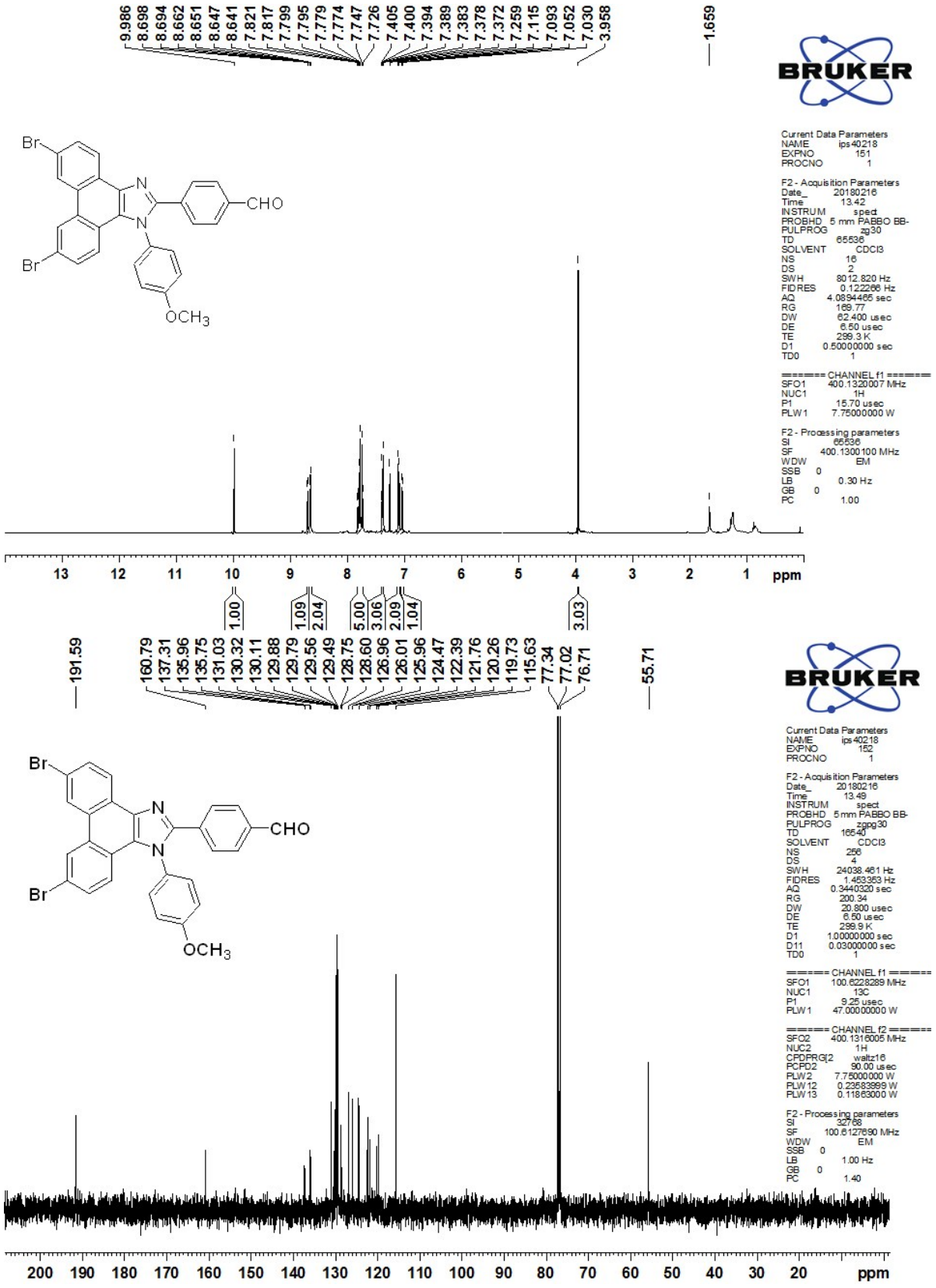


Figure S25. ^{1}H and ^{13}C NMR of 15

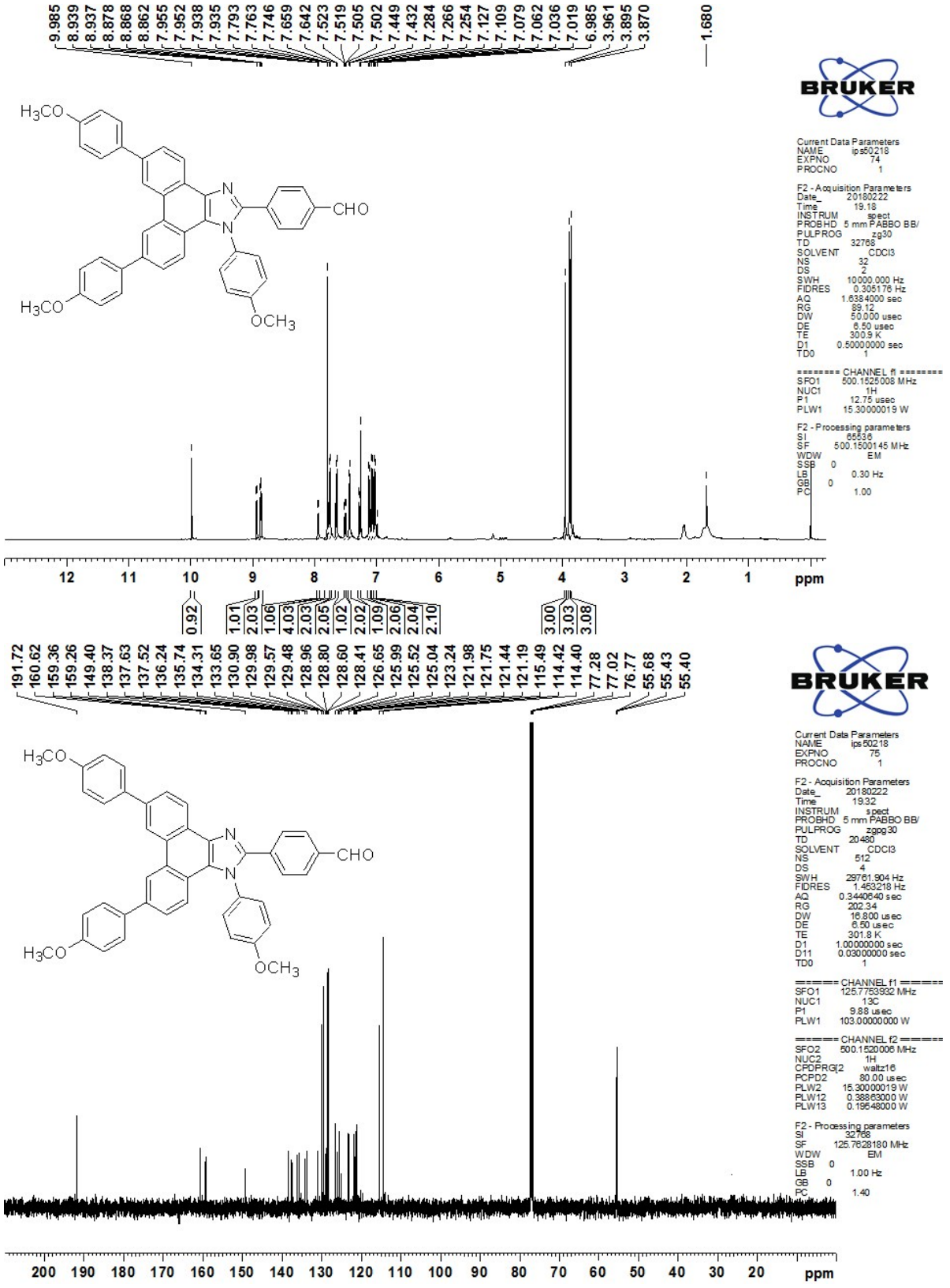
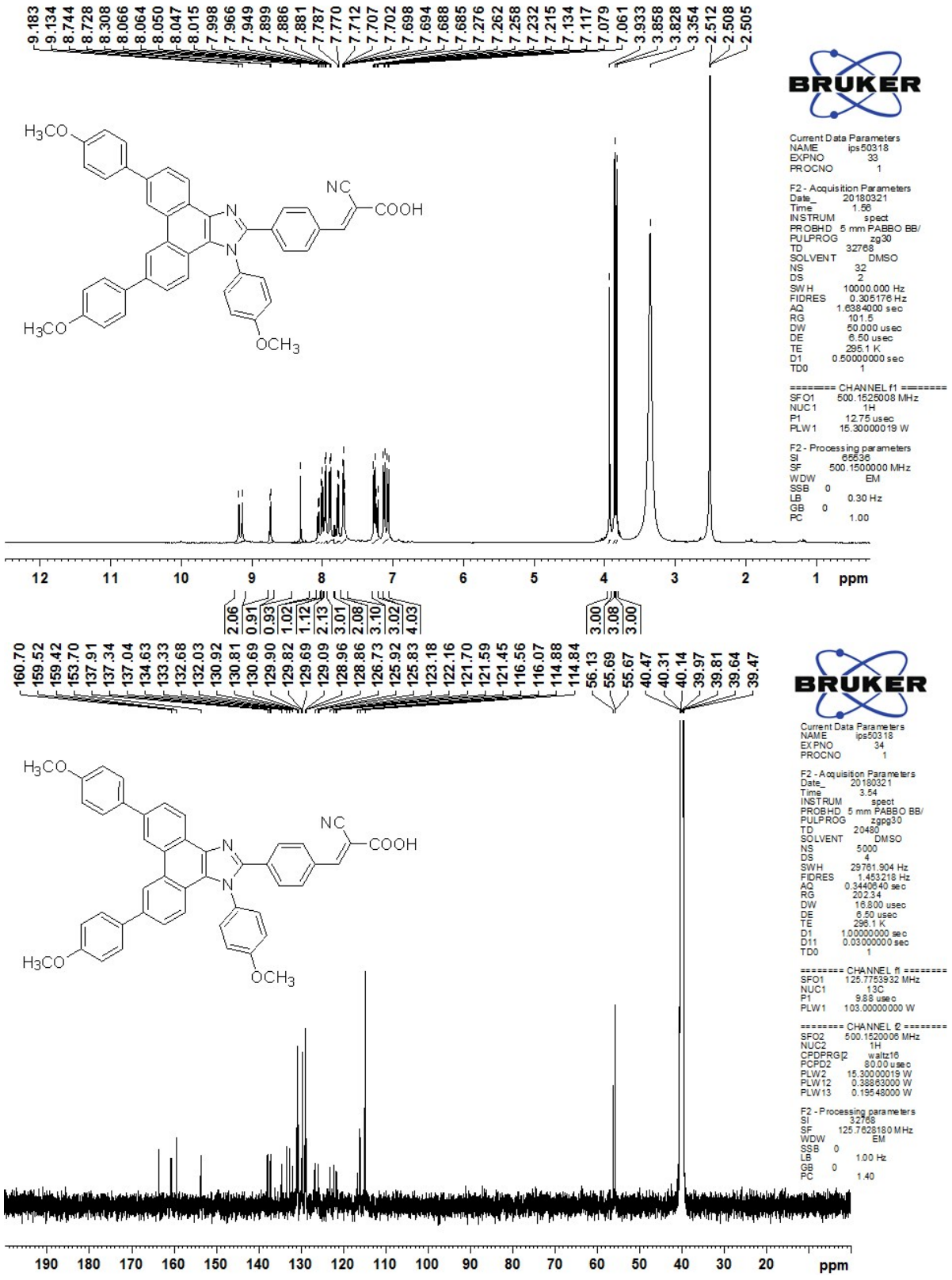


Figure S26. ^{1}H, ^{13}C NMR and mass spectrum of 4

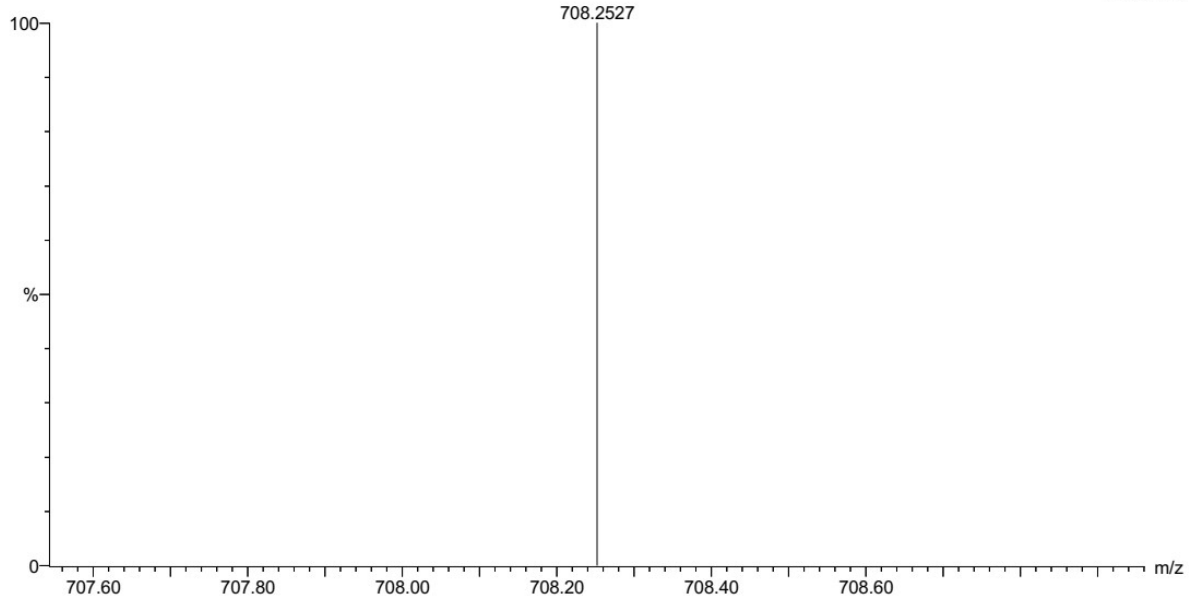


Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
24 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-46 H: 0-34 N: 0-3 O: 0-5 S: 0-1

IPS-SJE-P5
040518-13-IPS-SJE-P5 13 (0.327) AM (Cen,5, 80.00, Ar,5000.0,0.00,1.00); Sb (1,40.00); Sm (Mn, 1x0.00); Cm (9:13) TOF MS ES+
2.43e+005



Minimum:				-1.5		
Maximum:		5.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
708.2527	708.2498	2.9	4.1	31.5	n/a	C46 H34 N3 O5

Figure S27. ^{1}H and ^{13}C NMR of 16

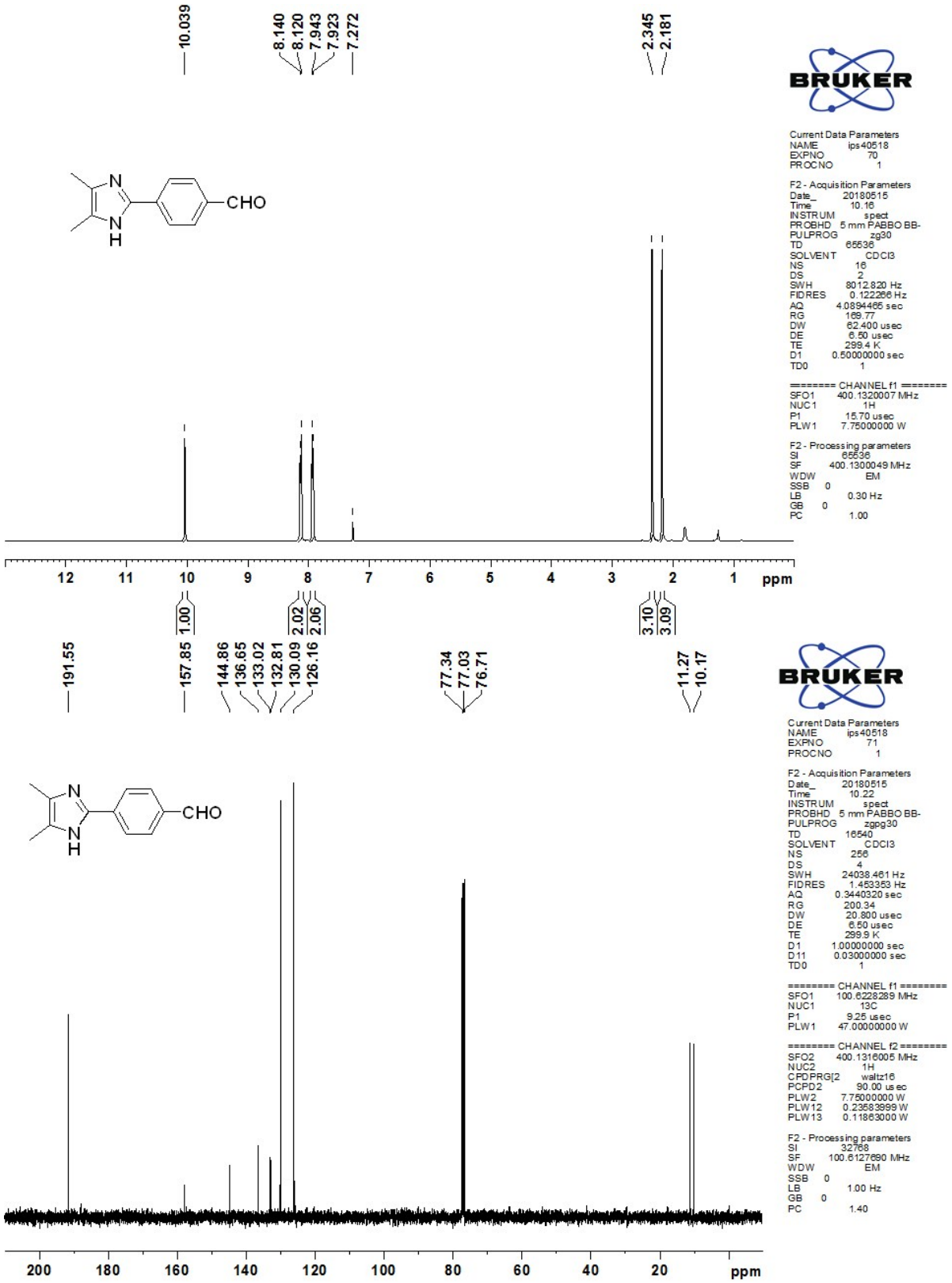
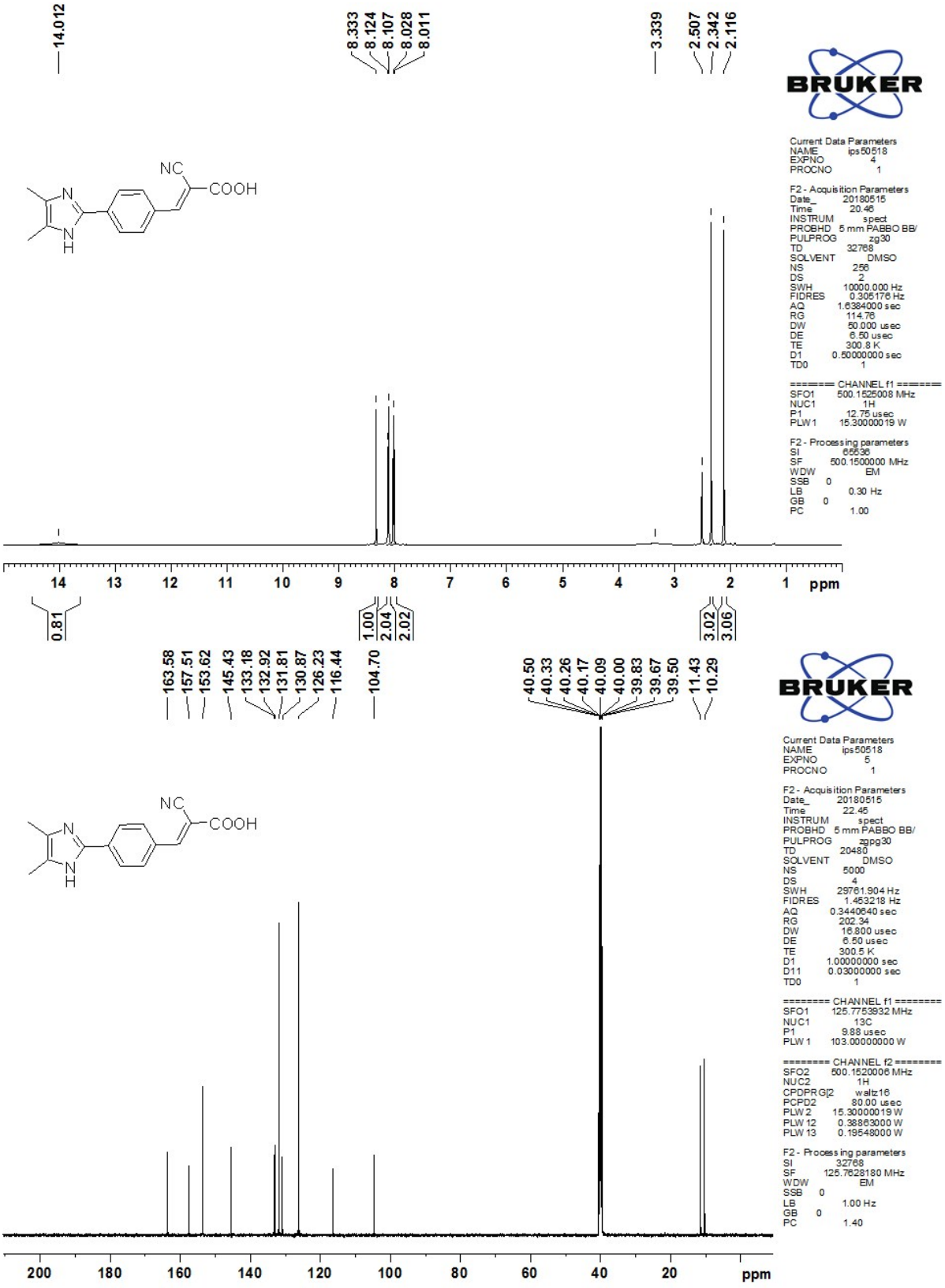


Figure S28. ^{1}H, ^{13}C NMR and mass spectrum of 5

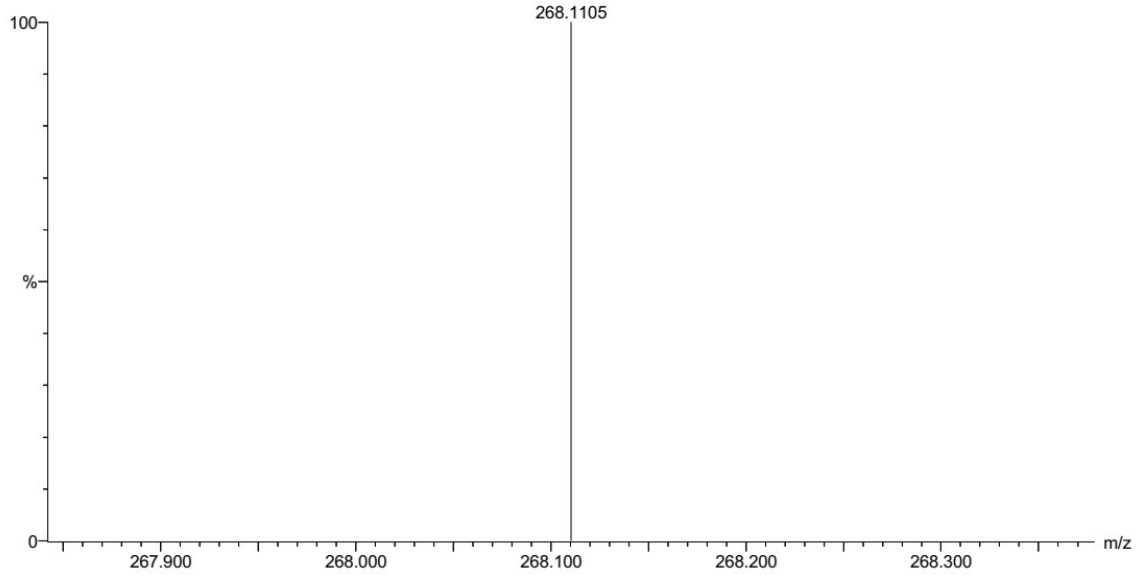


Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
8 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-15 H: 0-14 N: 0-3 O: 0-2

KRR-SJE-M3R
18072018-01-KRR-SJE-M3R 20 (0.504) AM (Cen,5, 80.00, Ar,5000.0,0.00,1.00); Sb (1,40.00); Sm (Mn, 1x0.00); Cm (5:20) TOF MS ES+
1.68e+005



Minimum:				-1.5		
Maximum:		5.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
268.1105	268.1086	1.9	7.1	10.5	n/a	C15 H14 N3 O2