Supporting Information

An expeditious $FeCl_3$-catalyzed cascade 1,4-conjugate addition/annulation/1,5-H shift sequence for modular access of all-pyrano-moiety-substituted chromenes

Xinwei He,[a,*] Ruxue Li,[a] Pui Ying Choy,[b,c] Jiahui Duan,[a] Zhenzhen Yin,[a] Keke Xu,[a] Qiang Tang,[a] Rong-Lin Zhong,[b] Yongjia Shang[a,*] and Fuk Yee Kwong[b,c,*]

[a]Key Laboratory of Functional Molecular Solids, Ministry of Education, College of Chemistry and Materials Science, Anhui Normal University, Wuhu 241000, P.R. China
[b]State Key Laboratory of Synthetic Chemistry and Department of Chemistry, The Chinese University of Hong Kong, New Territories, Shatin, Hong Kong SAR, P.R. China
[c]Shenzhen Center of Novel Functional Molecules, Shenzhen Municipal Key Laboratory of Chemical Synthesis of Medicinal Organic Molecules, CUHK Shenzhen Research Institute, No. 10. Second Yuexing Road, Shenzhen 518507, P.R. China

Email: xinweihe@mail.ahnu.edu.cn, shyj@mail.ahnu.edu.cn, fykwong@cuhk.edu.hk

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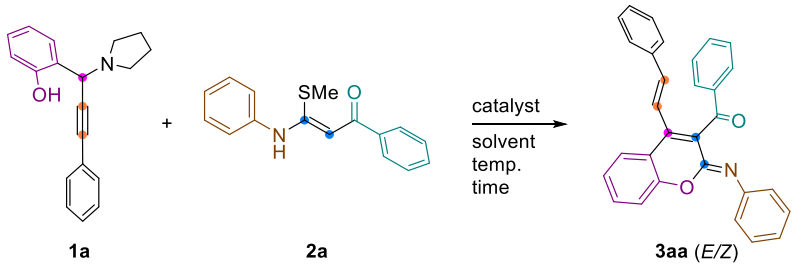
1. General consideration

Unless otherwise specified, all reagents and starting materials were purchased from commercial sources and used as received without purification. The solvents were used directly without purification unless stated. The dried acetonitrile used in screening was distilled from calcium hydride under nitrogen using standard procedures.[1] All cascade reactions were performed in a resealable screw-capped Schlenk flask (approximately 20 mL volume) in the presence of Teflon-coated magnetic stirrer bar (4.5 mm × 12 mm). Thin layer chromatography was conducted on precoated silica gel 60 F254 plates. Flash chromatography was performed using 200-300 mesh silica gel with the indicated solvent system according to standard techniques. Melting points were measured on an uncorrected Melting Point instrument. The ^{1}H and ^{13}C NMR spectra were recorded on a 400 MHz and 100 MHz NMR spectrometers, unless otherwise specified. Chemical shifts (δ) in parts per million were reported relative to the residual signals of chloroform (7.26 ppm for ^{1}H and 77.0 ppm for ^{13}C), and all ^{13}C NMR were recorded with proton broadband decoupling and indicated as $^{13}C\{^{1}H\}$ NMR. Multiplicities are described as s (singlet), d (doublet), t (triplet), q (quartet), or m (multiplet), and the coupling constants (J) are reported in Hertz (Hz). HRMS analysis with a quadrupole time-of-flight mass spectrometer yielded ion mass/charge (m/z) ratios in atomic mass units.

2. Reaction optimization

Table S1. Optimization of reaction conditions[a]

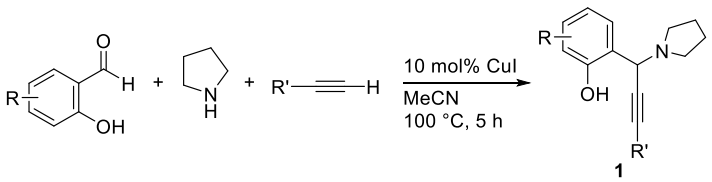


1a **2a** **3aa** (*E*/*Z*)

entry	Catalyst (mol%)	solvent	temp./ °C	yield/%[b]	*E*:*Z*
1	$FeCl_3$ (50)	MeCN	80	82	4:1
2	$Sc(OTf)_3$ (50)	MeCN	80	71	4:1
3	CuI (50)	MeCN	80	59	4:1
4	$AgNO_3$ (50)	MeCN	80	49	4:1
5	$CuBr_2$ (50)	MeCN	80	trace	4:1
6	ZnI_2 (50)	MeCN	80	45	4:1
7	$Fe(acac)_3$ (50)	MeCN	80	53	4:1
8	--	MeCN	80	trace	-
9[c]	$FeCl_3$ (50)	MeCN	80	72	4:1
10[d]	$FeCl_3$ (50)	MeCN	80	76	4:1
11	$FeCl_3$ (20)	MeCN	80	83	4:1
12	$FeCl_3$ (10)	MeCN	80	65	4:1
13	$FeCl_3$ (20)	DCE	80	nd	-
14	$FeCl_3$ (20)	THF	80	nd	-
15	$FeCl_3$ (20)	DMF	80	31	4:1
16	$FeCl_3$ (20)	EtOH	80	10	4:1
17	$FeCl_3$ (20)	toluene	80	15	4:1
18	$FeCl_3$ (20)	MeCN	rt	nr	-
19	$FeCl_3$ (20)	MeCN	60	32	9:5
20	$FeCl_3$ (20)	MeCN	100	72	>20:1
21	$FeCl_3$ (20)	MeCN	120	84	>20:1
22[e]	$FeCl_3$ (20)	MeCN	120	84	>20:1
23[f]	$FeCl_3$ (20)	MeCN	120	77	>20:1
24[g]	$FeCl_3$ (20)	MeCN	120	64	>20:1
25[h]	$FeCl_3$ (20)	MeCN	120	64	>20:1

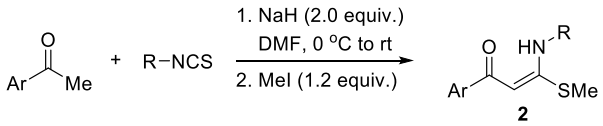
[a]Reaction conditions: 2-(3-Phenyl-1-(pyrrolidin-1-yl)prop-2-yn-1-yl)phenol (**1a**) (0.3 mmol), (*E*)-3-(methylthio)-1-phenyl-3-(phenylamino)prop-2-en-1-one (**2a**) (0.2 mmol), and catalyst (50 mol%) in undried solvent (2 mL) at indicated temperature for 12 h. [b]Isolated yields. [c]1.0 equivalent of **1a** was used. [d]2.0 equivalent of **1a** was used. [e]For 18 h. [f]For 8 h. [g]For 5 h. [h]Dried MeCN was used. nd = not detected. nr = no reaction.

3. General procedures for the synthesis of propargylamines 1



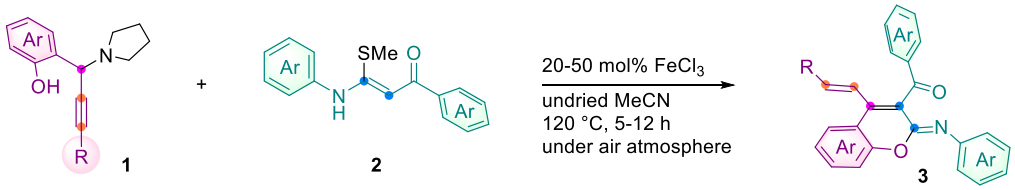
To a 25 mL round-bottom flask equipped with a magnetic stir bar were added pyrrolidine (1.2 mmol), aldehyde (1.0 mmol), acetylene (1.2 mmol), copper(I) iodide (10 mol%) and toluene (3 mL). The mixture was degassed and backfilled with nitrogen, and then stirred in an oil bath preheated to 100 °C for 5 h (monitored by TLC). After the reaction completed (as determined using TLC), the reaction mixture was cooled to room temperature, diluted with CH_2Cl_2 (10 mL) and filtered through a thin pad of silica gel. The filter cake was washed with CH_2Cl_2, and the combined filtrate was concentrated in vacuum. The crude product was purified by flash column chromatography on silica gel to afford the corresponding propargylamines[2].

4. General procedures for the synthesis of *N*,*S*-keteneacetals 2



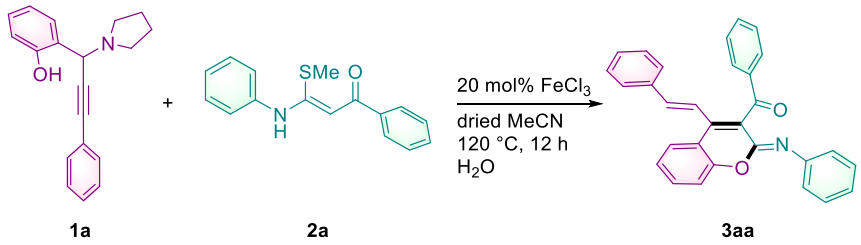
A mixture of acetophenone (0.24 mL, 2.0 mmol), sodium hydride (96 mg, 4.0 mmol), and *N*,*N*-dimethylformamide (5 mL) was stirred at room temperature for 30 minutes. Then, aryl isothiocyanates was added dropwise at 0 °C in an ice-water bath, and stirring was continued at room temperature for 1 h. Iodomethane (0.18 mL, 2.4 mmol) was then added dropwise, stirring for another 1 h. Upon completion of the reaction, the reaction mixture was extracted with CH_2Cl_2 (3 × 10 mL), and washed with brine. The organic layers were combined, dried over Na_2SO_4, filtered, and then evaporated under vacuum. The residue was purified using flash column chromatography with a silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:40, v/v) as the elution solvent to give corresponding *N*,*S*-keteneacetals **2**.

5. General procedures for the synthesis of alkenyl-iminochromene 3



A mixture of propargylamines **1** (0.3 mmol), *N*,*S*-keteneacetals **2** (0.2 mmol), and $FeCl_3$ (20-50 mol%) were added under air atmosphere to a resealable screw-capped Schlenk tube. Undried acetonitrile (2 mL) was then added. The tube sealed with a Teflon-coated cap and the resulting mixture was stirred in an oil bath preheated to 120 °C for 12 h (monitored by TLC). Upon completion of the reaction, the reaction mixture was cooled to room temperature, extracted with CH_2Cl_2 (3 × 10 mL), and washed with brine. The organic layers were combined, dried over Na_2SO_4, filtered, and then evaporated under a vacuum. The residue was purified using flash column chromatography with a silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:20, v/v) as the elution solvent to give desired products **3**.

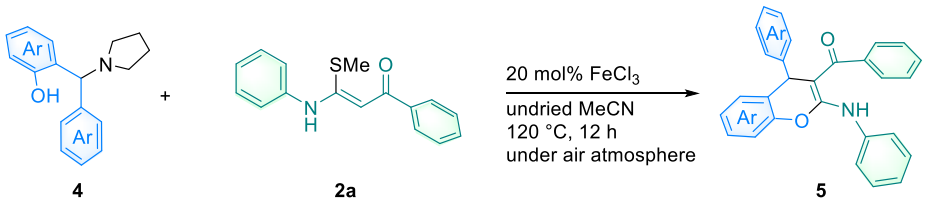
6. Large scale synthesis of compound 3aa



A mixture of **1a** (3.75 mmol), **2a** (2.5 mmol), and $FeCl_3$ (20 mol%) were added under air atmosphere to a resealable screw-capped Schlenk tube. Undried acetonitrile (10 mL) was then added. The tube sealed with a Teflon-coated cap and the resulting mixture was stirred in an oil bath preheated to 120 °C for 12 h (monitored by TLC). Upon completion of the reaction, the reaction mixture was cooled to room temperature, extracted with CH_2Cl_2 (3 × 20 mL), and washed with brine. The organic layers were combined, dried over Na_2SO_4, filtered, and then evaporated under a vacuum. The residue was purified using flash column chromatography with a silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:20, v/v) as the elution solvent to give

desired product **3aa** in 69% yield (736 mg).

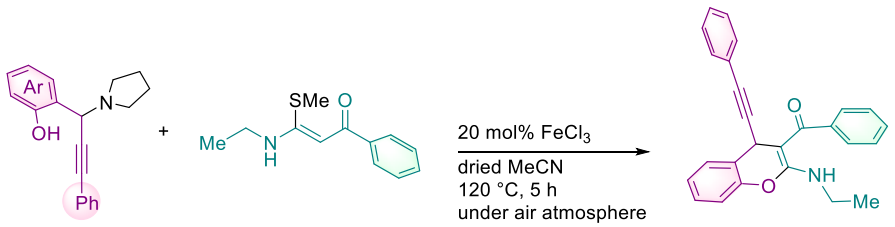
7. General procedures for the synthesis of aryl-iminochromene 5



4 **2a** **5**

A mixture of **4** (0.3 mmol), *N*,*S*-keteneacetals **2a** (0.2 mmol), and $FeCl_3$ (20 mol%) were added under air atmosphere to a resealable screw-capped Schlenk tube. Undried acetonitrile (2 mL) was then added. The tube sealed with a Teflon-coated cap and the resulting mixture was stirred in an oil bath preheated to 120 °C for 12 h (monitored by TLC). Upon completion of the reaction, the reaction mixture was cooled to room temperature, extracted with CH_2Cl_2 (3 × 10 mL), and washed with brine. The organic layers were combined, dried over Na_2SO_4, filtered, and then evaporated under a vacuum. The residue was purified using flash column chromatography with a silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:20, v/v) as the elution solvent to give desired products **5**.

8. General procedures for the synthesis of compound 6aq

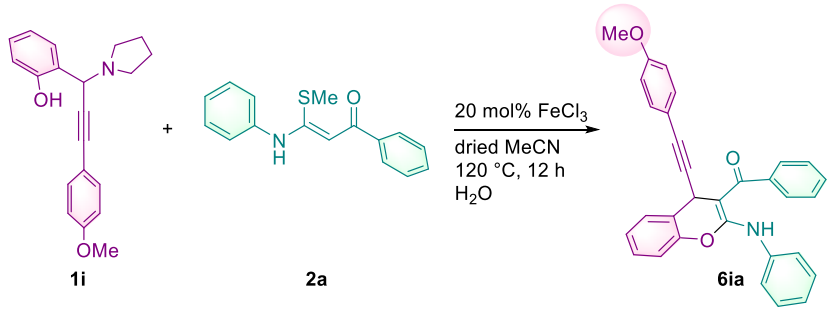


1a **2q** **6aq**, 46%

A mixture of **1a** (0.3 mmol), **2q** (0.2 mmol), and $FeCl_3$ (20 mol%) were added under air atmosphere to a resealable screw-capped Schlenk tube. Dried acetonitrile (2 mL) was then added. The tube sealed with a Teflon-coated cap and the resulting mixture was stirred in an oil bath preheated to 120 °C for 5 h (monitored by TLC). Upon completion of the reaction, the reaction mixture was cooled to room temperature, extracted with CH_2Cl_2 (3 × 10 mL), and washed with brine. The organic layers were

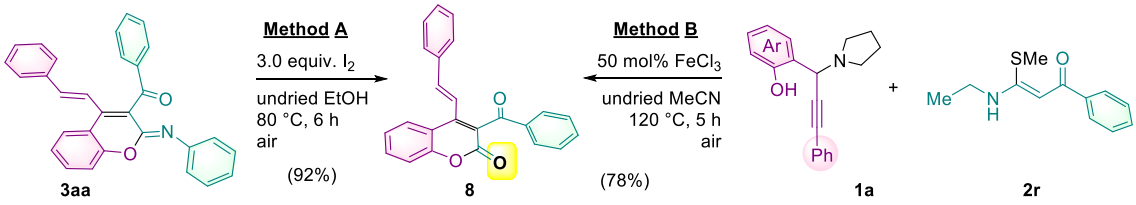
combined, dried over Na_2SO_4, filtered, and then evaporated under a vacuum. The residue was purified using flash column chromatography with a silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:20, v/v) as the elution solvent to give desired product **6aq** in 46% yield (35 mg).

9. General procedures for the synthesis of compound 6ia



A mixture of **1i** (0.3mmol), **2a** (0.2 mmol), and $FeCl_3$ (20 mol%) were added under air atmosphere to a resealable screw-capped Schlenk tube. Undried THF (2 mL) was then added. The tube sealed with a Teflon-coated cap and the resulting mixture was stirred in an oil bath preheated to 80 °C for 12 h (monitored by TLC). Upon completion of the reaction, the reaction mixture was cooled to room temperature, extracted with CH_2Cl_2 (3 × 10 mL), and washed with brine. The organic layers were combined, dried over Na_2SO_4, filtered, and then evaporated under a vacuum. The residue was purified using flash column chromatography with a silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:20, v/v) as the elution solvent to give desired product **6ia** in 70% yield (64 mg).

10. General procedures for the synthesis of compound 8

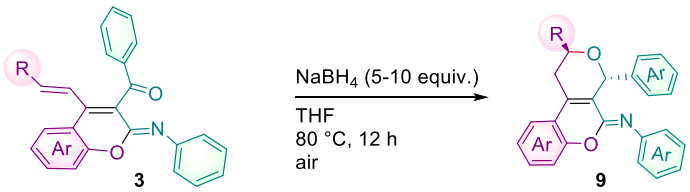


Method A: To a mixture of phenyl((*Z*)-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)methanone (**3aa**) (84 mg, 0.2 mmol) and I_2 (152 mg, 0.6 mmol) in undried ethanol (2 mL) under air atmosphere to a resealable screw-capped Schlenk tube. The tube sealed

with a Teflon-coated cap and the resulting mixture was stirred in an oil bath preheated to 80 °C for 6 h (monitored by TLC). Upon completion of the reaction, the reaction mixture was cooled to room temperature, and the solvent was removed under reduced pressure. The residue was purified using flash column chromatography with a silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:20, v/v) as the elution solvent to give desired product **8** in 92% yield (65 mg).

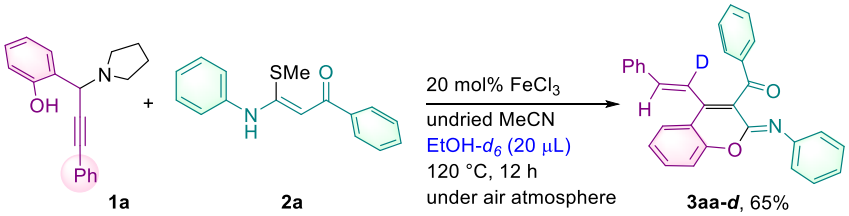
Method B: A mixture of **1a** (0.3 mmol), **2r** (0.2 mmol), and $FeCl_3$ (50 mol%) were added under air atmosphere to a resealable screw-capped Schlenk tube. Undried acetonitrile (2 mL) was then added. The tube sealed with a Teflon-coated cap and the resulting mixture was stirred in an oil bath preheated to 120 °C for 5 h (monitored by TLC). Upon completion of the reaction, the reaction mixture was cooled to room temperature, extracted with CH_2Cl_2 (3 × 10 mL), and washed with brine. The organic layers were combined, dried over Na_2SO_4, filtered, and then evaporated under a vacuum. The residue was purified using flash column chromatography with a silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:20, v/v) as the elution solvent to give desired product **8** in 78% yield (55 mg).

11. General procedures for the synthesis of compound 9



To a solution of 4-vinyliminochromene **3** (0.2 mmol), in THF (2 mL) was added solid sodium borohydride (5-10 equiv.) and the mixture was stirred in an oil bath preheated to 80 °C under air atmosphere for 12 h (monitored by TLC). Upon completion of the reaction, the reaction mixture was cooled to room temperature, extracted with CH_2Cl_2 (3 × 10 mL), and washed with brine. The combined organic layers were dried over Na_2SO_4, filtered and concentrated under reduced pressure. The residue was purified using flash column chromatography with a silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:20, v/v) as the elution solvent to give desired product **9**.

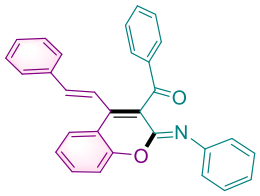
12. General procedures for deuterium-labelling experiment



A mixture of propargylamines **1a** (0.15 mmol), *N*,*S*-keteneacetals **2a** (0.1 mmol), and $FeCl_3$ (20 mol%) were added under air atmosphere to a resealable screw-capped Schlenk tube. Undried acetonitrile (2 mL) and ethanol-d_6 (20 μL) was then added. The tube sealed with a Teflon-coated cap and the resulting mixture was stirred in an oil bath preheated to 120 °C for 12 h (monitored by TLC). Upon completion of the reaction, the reaction mixture was cooled to room temperature, extracted with CH_2Cl_2 (3 × 10 mL), and washed with brine. The organic layers were combined, dried over Na_2SO_4, filtered, and then evaporated under a vacuum. The residue was purified using flash column chromatography with a silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:20, v/v) as the elution solvent to give desired products **3aa-*d*** in 65% yield.

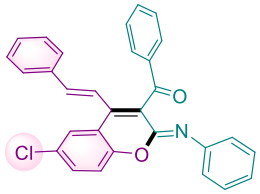
13. Characterization data for all compounds

Phenyl((*Z*)-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)methanone (Scheme 2, compound 3aa)



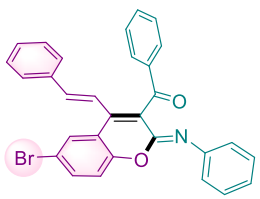
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.6) to afford a yellow solid in 84% yield (72 mg); mp 143-144 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08–7.97 (m, 2H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.58–7.53 (m, 1H), 7.47–7.40 (m, 3H), 7.36–7.30 (m, 4H), 7.30–7.26 (m, 3H), 7.23–7.18 (m, 1H), 7.17–7.14 (m, 1H), 7.13–7.09 (m, 2H), 7.08–7.04 (m, 1H), 6.95 (dd, *J* = 24.4 Hz, 16.4 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 194.0, 152.8, 147.6, 145.5, 139.8, 139.2, 136.7, 135.8, 133.5, 131.2, 129.3, 129.0, 128.8, 128.7, 128.7, 128.4, 127.0, 125.7, 124.1, 123.9, 123.1, 119.7, 119.4, 116.4; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{22}NO_2$ 428.1645; Found 428.1641.

((*Z*)-6-Chloro-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)(phenyl)methanone (Scheme 2, compound 3ba)



This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.5) to afford a yellow solid in 72% yield (66 mg); mp 196-197 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08–7.97 (m, 2H), 7.63 (d, *J* = 2.4 Hz, 1H), 7.60–7.55 (m, 1H), 7.48–7.43 (m, 2H), 7.38 (dd, J = 8.8 Hz, 2.4 Hz, 1H), 7.36–7.31 (m, 4H), 7.31–7.26 (m, 3H), 7.14–7.04 (m, 4H), 6.92 (dd, *J* = 50.0 Hz, 16.4 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 193.5, 151.2, 146.9, 145.2, 139.8, 138.7, 136.5, 135.6, 133.7, 130.9, 129.8, 129.2, 129.2, 128.8, 128.5, 127.1, 125.3, 124.4, 123.1, 120.9, 119.0, 117.7; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{21}ClNO_2$ 462.1255; Found 462.1249.

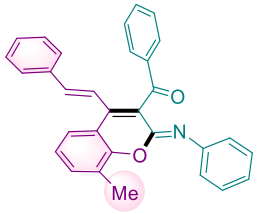
((*Z*)-6-Bromo-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)(phenyl)methanone (Scheme 2, compound 3ca)



This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.4) to afford a yellow solid in 69% yield (70 mg); mp 180-181 °C, ^{1}H NMR (400 MHz, $CDCl_3$)

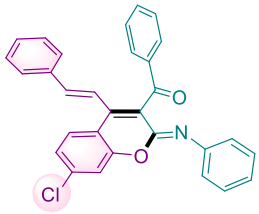
δ 8.05–7.98 (m, 2H), 7.76 (d, J = 2.4 Hz, 1H), 7.59–7.54 (m, 1H), 7.52 (dd, J = 8.8 Hz, 2.4 Hz, 1H), 7.48–7.43 (m, 2H), 7.37–7.32 (m, 4H), 7.31–7.26 (m, 3H), 7.13–7.06 (m, 3H), 7.04 (d, J = 8.8 Hz, 1H), 6.92 (dd, J = 50.8 Hz, 16.4 Hz, 2H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 193.4, 151.7, 146.8, 145.1, 139.8, 138.7, 136.5, 135.6, 133.8, 133.7, 129.8, 129.3, 129.2, 128.8, 128.8, 128.5, 128.2, 127.1, 124.4, 123.1, 121.4, 119.0, 118.0, 116.5; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{21}BrNO_2$ 506.0750; Found 506.0745.

((Z)-8-Methyl-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)(phenyl)methanone (Scheme 2, compound 3da)



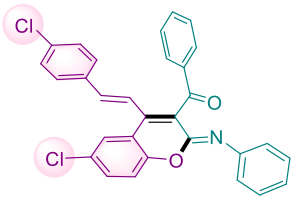
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.7) to afford a yellow solid in 58% yield (51 mg); mp 156-157 °C, ^1H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, J = 7.2 Hz, 2H), 7.58–7.51 (m, 2H), 7.45 (t, J = 7.6 Hz, 2H), 7.37–7.31 (m, 3H), 7.31–7.28 (m, 4H), 7.28–7.26 (m, 1H), 7.18–7.13 (m, 2H), 7.12–7.04 (m, 2H), 6.96 (dd, J = 19.6 Hz, 16.4 Hz, 2H), 2.27 (s, 3H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 194.1, 150.9, 147.8, 145.7, 140.3, 139.1, 136.8, 135.9, 133.5, 132.6, 129.3, 128.9, 128.8, 128.7, 128.7, 128.3, 127.0, 125.8, 124.1, 123.4, 123.3, 123.2, 120.1, 119.1, 15.5; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{24}NO_2$ 442.1802; Found 442.1811.

((*Z*)-7-Chloro-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)(phenyl)methanone (Scheme 2, compound 3ea)



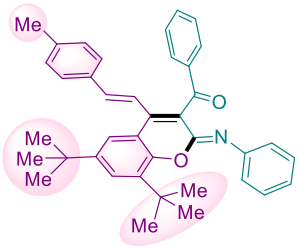
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.5) to afford a yellow solid in 76% yield (70 mg); mp 156-157 °C, ^1H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, J = 7.6 Hz, 2H), 7.65–7.49 (m, 3H), 7.45 (d, J = 7.6 Hz, 2H), 7.32–7.30 (m, 4H), 7.29–7.26 (m, 2H), 7.19–7.15 (m, 2H), 7.11–7.05 (m, 3H), 6.92 (dd, J = 22.4 Hz, 16.4 Hz, 2H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 193.6, 153.1, 146.8, 145.1, 139.6, 139.2, 136.9, 136.6, 135.6, 133.7, 132.0, 129.3, 129.2, 128.7, 128.5, 127.0, 126.6, 124.4, 124.2, 123.2, 123.0, 119.2, 118.2, 116.7; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{21}ClNO_2$ 462.1255; Found 462.1250.

((*Z*)-6-Chloro-4-((*E*)-4-chlorostyryl)-2-(phenylimino)-2*H*-chromen-3-yl)(phenyl)methanone (Scheme 2, compound 3fa)



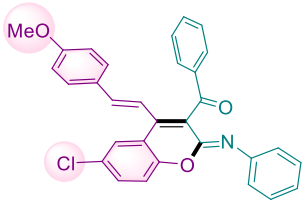
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.7) to afford a yellow solid in 78% yield (77 mg); mp 184-185 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08–7.91 (m, 2H), 7.62–7.53 (m, 2H), 7.45 (t, J = 8.0 Hz, 2H), 7.38 (d, J = 8.8 Hz, 1H), 7.32 – 7.27 (m, 4H), 7.26 – 7.22 (m, 2H), 7.15 – 7.01 (m, 4H), 6.86 (dd, J = 42.4 Hz, 16.4 Hz, 2H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 193.4, 151.2, 146.8, 145.1, 138.4, 136.5, 135.1, 134.0, 133.8, 131.0, 130.0, 129.2, 129.0, 128.8, 128.5, 128.2, 125.2, 124.4, 123.0, 120.7, 119.5, 117.7; HRMS (ESI-TOF) *m/z*: [M+H]$^+$ Calcd for $C_{30}H_{20}Cl_2NO_2$ 469.0866; Found 469.0859.

((*Z*)-6,8-Di-*tert*-butyl-4-((*E*)-4-methylstyryl)-2-(phenylimino)-2*H*-chromen-3-yl)(phenyl)methanone (Scheme 2, compound 3ga)



This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.6) to afford a yellow solid in 53% yield (59 mg); mp 146-147 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11–7.98 (m, 2H), 7.56–7.48 (m, 2H), 7.47–7.41 (m, 3H), 7.26–7.16 (m, 4H), 7.14–7.08 (m, 2H), 7.04–6.91 (m, 2H), 6.90–6.83 (m, 3H), 2.33 (s, 3H), 1.31 (s, 9H), 1.09 (s, 9H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 194.2, 147.6, 145.6, 141.7, 139.0, 136.9, 133.5, 133.3, 129.4, 128.6, 128.5, 127.1, 126.9, 126.4, 123.2, 121.4, 120.4, 119.4, 118.8, 34.7, 34.6, 31.4, 29.4, 21.3; HRMS (ESI-TOF) *m/z*: [M+H]$^+$ Calcd for $C_{39}H_{40}NO_2$ 554.3051; Found 554.3052.

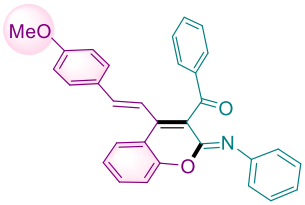
((*Z*)-6-Chloro-4-((*E*)-4-methoxystyryl)-2-(phenylimino)-2*H*-chromen-3-yl)(phenyl)methanone (Scheme 2, compound 3ha)



This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.5) to afford a yellow solid in 82% yield (81 mg); mp 175-176 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03–7.97 (m, 2H), 7.63 (d, J = 2.4 Hz, 1H), 7.58–7.53 (m, 1H), 7.47–7.42 (m, 2H), 7.39–7.35 (m, 1H), 7.31–7.25 (m, 4H), 7.10–7.04 (m, 4H), 6.93 (d, J = 16.4 Hz, 1H), 6.86–6.81 (m, 2H), 6.71 (d, J = 16.4 Hz, 1H), 3.80 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 193.7, 160.5, 151.2, 147.0,

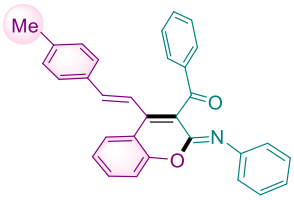
145.2, 139.3, 139.0, 136.6, 133.6, 130.8, 129.2, 129.2, 129.1, 128.7, 128.5, 128.4, 128.4, 125.3, 124.3, 123.0, 121.0, 117.6, 116.5, 114.2, 55.3; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{23}ClNO_3$ 492.1361; Found 492.1353.

((*Z*)-4-((*E*)-4-Methoxystyryl)-2-(phenylimino)-2*H*-chromen-3-yl)(phenyl)methanone (Scheme 2, compound 3ia)



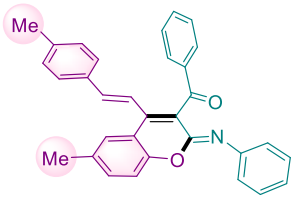
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.4) to afford a yellow solid in 65% yield (59 mg); mp 145-146 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10–7.94 (m, 2H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.57–7.52 (m, 1H), 7.48–7.38 (m, 3H), 7.30–7.27 (m, 2H), 7.26–7.13 (m, 4H), 7.11–7.03 (m, 3H), 6.94 (d, *J* = 16.4 Hz, 1H), 6.86–6.76 (m, 3H), 3.80 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 194.2, 160.4, 152.8, 147.7, 145.6, 140.1, 138.8, 136.8, 133.5, 131.1, 129.3, 128.6, 128.4, 128.4, 128.3, 125.7, 124.0, 123.8, 123.1, 119.6, 117.3, 116.3, 114.1, 55.3; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{24}NO_3$ 458.1751; Found 458.1756.

((*Z*)-4-((*E*)-4-Methylstyryl)-2-(phenylimino)-2*H*-chromen-3-yl)(phenyl)methanone (Scheme 2, compound 3ja)



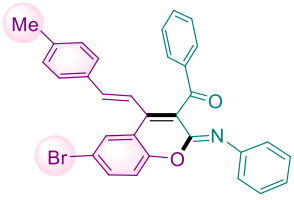
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.6) to afford a yellow solid in 68% yield (60 mg); mp 172-173 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10–7.98 (m, 2H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.57–7.53 (m, 1H), 7.48–7.40 (m, 3H), 7.29 (t, *J* = 7.8 Hz, 2H), 7.26–7.15 (m, 4H), 7.15–7.10 (m, 4H), 7.07 (d, *J* = 7.6 Hz, 1H), 6.93 (dd, *J* = 34.0 Hz, 16.4 Hz, 2H), 2.34 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 194.1, 152.8, 147.7, 145.6, 140.0, 139.2, 136.8, 133.5, 133.1, 131.2, 129.4, 129.3, 128.7, 128.4, 127.0, 125.8, 124.1, 123.9, 123.1, 119.5, 118.6, 116.3, 21.3; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{24}NO_2$ 442.1802; Found 442.1809.

((*Z*)-6-Methyl-4-((*E*)-4-methylstyryl)-2-(phenylimino)-2*H*-chromen-3-yl)(phenyl)methanone (Scheme 2, compound 3ka)



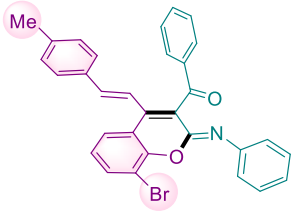
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.5) to afford a yellow solid in 65% yield (59 mg); mp 173-174 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11–7.94 (m, 2H), 7.57–7.52 (m, 1H), 7.47–7.39 (m, 3H), 7.30–7.27 (m, 2H), 7.26–7.20 (m, 3H), 7.16–7.08 (m, 4H), 7.08–7.01 (m, 2H), 6.90 (dd, *J* = 30.0 Hz, 16.4 Hz, 2H), 2.37 (s, 3H), 2.33 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 194.2, 150.8, 147.9, 145.7, 140.0, 139.1, 139.1, 136.8, 133.4, 133.4, 133.2, 131.9, 129.4, 129.3, 128.6, 128.5, 128.4, 126.9, 125.7, 124.0, 123.1, 119.2, 118.8, 116.0, 21.3, 20.9; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{32}H_{26}NO_2$ 456.1958; Found 456.1955.

((*Z*)-6-Bromo-4-((*E*)-4-methylstyryl)-2-(phenylimino)-2*H*-chromen-3-yl)(phenyl)methanone (Scheme 2, compound 3la)



This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.6) to afford a yellow solid in 68% yield (71 mg); mp 180-181 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04–7.95 (m, 2H), 7.76 (d, *J* = 1.6 Hz, 1H), 7.58–7.54 (m, 1H), 7.51 (d, *J* = 8.8 Hz, 1H), 7.44 (d, *J* = 8.0 Hz, 2H), 7.31–7.27 (m, 2H), 7.26–7.20 (m, 2H), 7.13 (s, 1H), 7.11 (s, 1H), 7.10–7.01 (m, 4H), 6.87 (dd, *J* = 59.2, 16.4 Hz, 2H), 2.34 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 193.5, 151.7, 146.9, 145.2, 139.7, 139.5, 138.8, 136.5, 133.8, 133.7, 132.9, 129.5, 129.2, 128.7, 128.5, 128.2, 127.0, 124.3, 123.0, 121.4, 118.0, 117.9, 116.5, 21.3; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{23}BrNO_2$ 520.0907; Found 520.0900.

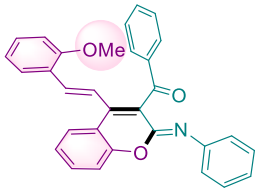
((*Z*)-8-Bromo-4-((*E*)-4-methylstyryl)-2-(phenylimino)-2*H*-chromen-3-yl)(phenyl)methanone (Scheme 2, compound 3ma)



This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.6) to afford a yellow solid in 74% yield (77 mg); mp 201-202 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 6.8 Hz, 2H), 7.63 (dd, *J* = 12.0 Hz, 7.6 Hz, 2H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.44 (t, *J* = 7.6

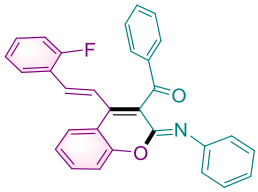
Hz, 2H), 7.37–7.26 (m, 4H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.15–7.02 (m, 4H), 6.88 (dd, *J* = 38.4 Hz, 16.4 Hz, 2H), 2.32 (s, 3H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 193.6, 149.6, 146.1, 144.5, 139.5, 139.4, 136.6, 134.6, 133.6, 133.0, 129.4, 129.4, 129.2, 128.7, 128.3, 128.3, 127.0, 124.9, 124.8, 124.4, 124.3, 121.3, 118.3, 110.2, 21.3; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{23}BrNO_2$ 520.0907; Found 520.0900.

((*Z*)-4-((*E*)-2-Methoxystyryl)-2-(phenylimino)-2*H*-chromen-3-yl)(phenyl)methanone (Scheme 2, compound 3na)



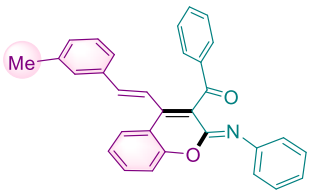
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.6) to afford a yellow solid in 75% yield (69 mg); mp 161-162 °C, ^1H NMR (400 MHz, $CDCl_3$) δ 8.12–8.00 (m, 2H), 7.74 (d, *J* = 7.6 Hz, 1H), 7.60–7.54 (m, 1H), 7.49–7.40 (m, 3H), 7.33–7.27 (m, 4H), 7.25–7.18 (m, 2H), 7.17–7.10 (m, 3H), 7.07 (t, *J* = 7.6 Hz, 1H), 7.03–6.98 (m, 1H), 6.90 (d, *J* = 7.2 Hz, 1H), 6.83 (d, *J* = 8.4 Hz, 1H), 3.73 (s, 3H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 194.1, 157.5, 152.8, 147.8, 145.7, 140.7, 137.0, 134.7, 133.4, 131.1, 130.1, 129.4, 128.6, 128.6, 128.4, 127.5, 126.0, 125.0, 124.0, 123.8, 123.1, 120.6, 120.3, 119.6, 116.3, 111.0, 55.4; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{24}NO_3$ 458.1751; Found 458.1760.

((*Z*)-4-((*E*)-2-Fluorostyryl)-2-(phenylimino)-2*H*-chromen-3-yl)(phenyl)methanone (Scheme 2, compound 3oa)



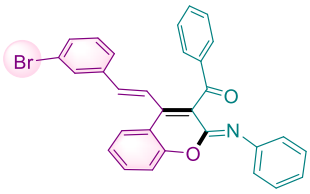
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.7) to afford a yellow solid in 84% yield (75 mg); mp 115-116 °C, ^1H NMR (400 MHz, $CDCl_3$) δ 8.09–7.99 (m, 2H), 7.71–7.66 (m, 1H), 7.59–7.54 (m, 1H), 7.48–7.41 (m, 3H), 7.36–7.31 (m, 1H), 7.30–7.27 (m, 2H), 7.25–7.18 (m, 2H), 7.17–7.09 (m, 4H), 7.08–6.98 (m, 4H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 193.9, 160.6 (d, $J_{C\text{-}F}$ = 250.5 Hz), 152.8, 147.5, 145.5, 139.9, 136.8, 133.6, 131.9 (d, $J_{C\text{-}F}$ = 2.8 Hz), 131.2, 130.3 (d, $J_{C\text{-}F}$ = 8.3 Hz), 128.9 (d, $J_{C\text{-}F}$ = 86.9 Hz), 129.1, 128.4, 128.1 (d, $J_{C\text{-}F}$ = 3.0 Hz), 125.8, 124.3, 124.3, 124.0 (d, $J_{C\text{-}F}$ = 21.3 Hz), 123.8, 123.7, 123.1, 122.5, 122.4, 119.3, 116.4, 116.0, 115.8; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{21}FNO_2$ 446.1551; Found 446.1545.

((*Z*)-4-((*E*)-3-Methylstyryl)-2-(phenylimino)-2*H*-chromen-3-yl)(phenyl)methanone (Scheme 2, compound 3pa)



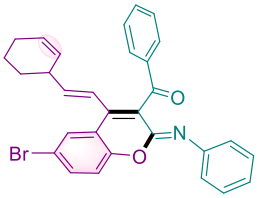
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.6) to afford a yellow solid in 79% yield (70 mg); mp 143-144 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14–7.94 (m, 2H), 7.69 (dd, J = 8.0 Hz, 1.6 Hz, 1H), 7.59–7.53 (m, 1H), 7.49–7.40 (m, 3H), 7.33–7.27 (m, 2H), 7.26–7.16 (m, 3H), 7.16–7.12 (m, 3H), 7.12–7.05 (m, 3H), 6.96 (dd, J = 22.0 Hz, 16.4 Hz, 2H), 2.33 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 194.0, 152.8, 147.6, 145.6, 139.9, 139.4, 138.4, 136.8, 135.8, 133.5, 131.2, 129.8, 129.3, 128.7, 128.7, 128.6, 128.4, 127.7, 125.8, 124.2, 124.1, 123.9, 123.1, 119.5, 119.5, 116.3, 21.3; HRMS (ESI-TOF) *m/z*: [M+H]$^+$ Calcd for $C_{31}H_{24}NO_2$ 442.1802; Found 442.1798.

((*Z*)-4-((*E*)-3-Bromostyryl)-2-(phenylimino)-2*H*-chromen-3-yl)(phenyl)methanone (Scheme 2, compound 3qa)



This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.7) to afford a yellow solid in 71% yield (72 mg); mp 158-159 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10–7.96 (m, 2H), 7.63 (dd, J = 8.0 Hz, 1.6 Hz, 1H), 7.59–7.55 (m, 1H), 7.50–7.41 (m, 4H), 7.41–7.37 (m, 1H), 7.33–7.26 (m, 2H), 7.26–7.20 (m, 2H), 7.19–7.14 (m, 2H), 7.14–7.03 (m, 3H), 6.91 (dd, J = 19.2 Hz, 16.4 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 193.7, 152.8, 147.4, 145.4, 139.3, 137.9, 137.6, 136.7, 133.6, 131.8, 131.3, 130.2, 129.6, 129.2, 128.7, 128.4, 125.7, 125.6, 124.2, 123.9, 123.1, 122.9, 121.2, 119.3, 116.4; HRMS (ESI-TOF) *m/z*: [M+H]$^+$ Calcd for $C_{30}H_{21}BrNO_2$ 506.0750; Found 506.0747.

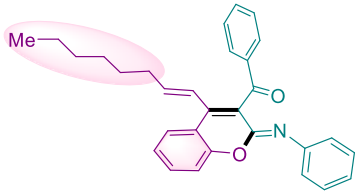
((*Z*)-6-Bromo-4-((*E*)-2-(cyclohex-1-en-1-yl)vinyl)-2-(phenylimino)-2*H*-chromen-3-yl)(phenyl)methanone (Scheme 2, compound 3ra)



This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.4) to afford a yellow solid in 72% yield (73 mg); mp 180-181 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02–7.96 (m, 2H), 7.70 (d, J = 2.4 Hz, 1H), 7.60–7.55 (m, 1H), 7.51–7.43 (m, 3H), 7.31–7.26 (m, 1H), 7.26–7.22 (m, 1H), 7.08–7.03 (m, 3H), 7.00 (d, J = 8.8 Hz, 1H), 6.35 (dd, J = 165.6 Hz, 16.0 Hz, 2H), 5.81 (d, J = 4.4 Hz, 1H), 2.16–2.09 (m, 2H), 2.08–2.02 (m, 2H), 1.69–1.62 (m, 2H),

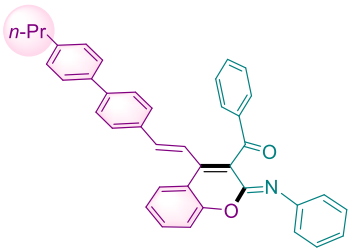
1.62–1.56 (m, 2H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 193.8, 151.7, 147.0, 145.3, 143.4, 139.5, 136.7, 135.7, 135.2, 133.6, 133.5, 129.2, 128.8, 128.6, 128.4, 128.3, 124.2, 123.0, 121.5, 117.9, 116.3, 114.7, 26.1, 23.9, 22.0, 22.0; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{25}BrNO_2$ 510.1063; Found 510.1057.

((*Z*)-4-((*E*)-Oct-1-en-1-yl)-2-(phenylimino)-2*H*-chromen-3-yl)(phenyl)methanone (Scheme 2, compound 3sa)



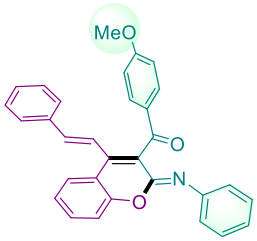
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.5) to afford a yellow liquid in 53% yield (46 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04–7.97 (m, 2H), 7.59–7.54 (m, 2H), 7.48–7.43 (m, 2H), 7.42–7.37 (m, 1H), 7.30–7.27 (m, 1H), 7.25–7.23 (m, 1H), 7.20–7.16 (m, 1H), 7.13–7.02 (m, 4H), 6.30–6.16 (m, 1H), 6.13–5.98 (m, 1H), 2.06 (d, *J* = 6.8 Hz, 2H), 1.27–1.20 (m, 4H), 1.19–1.12 (m, 4H), 0.85 (d, *J* = 6.8 Hz, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 194.0, 152.7, 147.7, 145.6, 142.7, 140.3, 136.7, 133.4, 131.0, 129.3, 128.6, 128.4, 128.2, 125.6, 123.9, 123.7, 123.0, 121.1, 119.6, 116.2, 33.5, 31.5, 28.5, 28.5, 22.5, 14.0; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{30}NO_2$ 436.2271; Found 436.2268.

Phenyl((*Z*)-2-(phenylimino)-4-((*E*)-2-(4'-propyl-[1,1'-biphenyl]-4-yl)vinyl)-2*H*-chromen-3-yl)methanone (Scheme 2, compound 3ta)



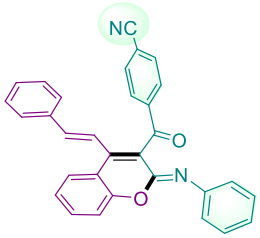
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.5) to afford a yellow solid in 76% yield (83 mg); mp 181-182 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 7.2 Hz, 2H), 7.73–7.68 (m, 1H), 7.59–7.54 (m, 2H), 7.54–7.47 (m, 4H), 7.46–7.43 (m, 2H), 7.43–7.35 (m, 2H), 7.32–7.26 (m, 3H), 7.25–7.19 (m, 2H), 7.16 (d, *J* = 8.0 Hz, 1H), 7.15–7.05 (m, 3H), 6.98 (dd, *J* = 16.4 Hz, 10.4 Hz, 2H), 2.63 (t, *J* = 7.6 Hz, 2H), 1.73–1.63 (m, 2H), 0.97 (t, *J* = 7.6 Hz, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 194.0, 152.8, 147.6, 145.5, 142.3, 141.8, 139.8, 138.9, 137.6, 136.8, 134.5, 133.5, 131.2, 129.3, 129.0, 128.7, 128.7, 128.4, 127.4, 127.2, 126.8, 125.7, 124.1, 123.9, 123.1, 119.5, 119.4, 116.4, 37.7, 24.5, 13.8; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{39}H_{32}NO_2$ 546.2428; Found 546.2424.

(4-Methoxyphenyl)((*Z*)-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)methanone (Scheme 2, compound 3ab)



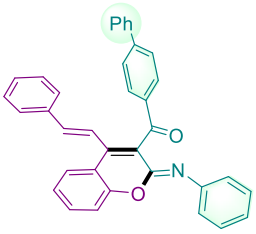
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.4) to afford a yellow solid in 82% yield (75 mg); mp 123-124 °C ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06–7.93 (m, 2H), 7.68 (dd, *J* = 8.0 Hz, 1.6 Hz, 1H), 7.45–7.39 (m, 1H), 7.36–7.30 (m, 4H), 7.29–7.26 (m, 3H), 7.22–7.17 (m, 1H), 7.16–7.13 (m, 1H), 7.13–7.09 (m, 2H), 7.08–7.04 (m, 1H), 7.03–6.88 (m, 4H), 3.85 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 192.5, 163.9, 152.8, 147.6, 145.7, 139.4, 139.0, 135.9, 131.7, 131.0, 129.8, 129.0, 128.9, 128.7, 128.4, 127.0, 125.7, 124.0, 123.8, 123.1, 119.8, 119.5, 116.3, 113.9, 55.5; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{24}NO_3$ 458.1751; Found 458.1758.

4-((*Z*)-2-(Phenylimino)-4-((*E*)-styryl)-2*H*-chromene-3-carbonyl)benzonitrile (Scheme 2, compound 3ac)



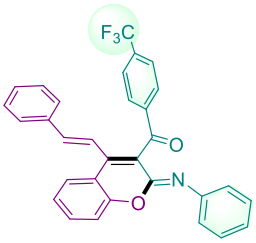
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.6) to afford a yellow solid in 92 % yield (83 mg); mp 155-156 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18–8.02 (m, 2H), 7.81–7.72 (m, 2H), 7.69 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.50–7.44 (m, 1H), 7.39–7.33 (m, 4H), 7.32–7.26 (m, 3H), 7.25–7.21 (m, 1H), 7.20–7.17 (m, 1H), 7.14–7.02 (m, 3H), 6.95 (s, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 192.5, 152.8, 147.4, 145.0, 141.0, 139.9, 139.8, 135.5, 132.6, 131.7, 129.4, 129.3, 128.8, 128.5, 127.6, 127.0, 125.9, 124.5, 124.1, 123.1, 119.2, 119.2, 118.0, 116.5; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{21}N2O_2$ 453.1598; Found 453.1603.

[1,1'-Biphenyl]-4-yl((*Z*)-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)methanone (Scheme 2, compound 3ad)



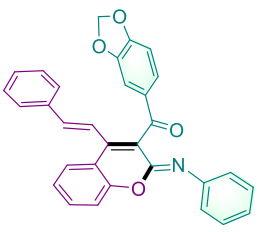
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.5) to afford a yellow solid in 92% yield (93 mg); mp 136-137 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19–8.04 (m, 2H), 7.73–7.65 (m, 3H), 7.65–7.60 (m, 2H), 7.49–7.42 (m, 3H), 7.42–7.38 (m, 1H), 7.38–7.32 (m, 3H), 7.32–7.27 (m, 4H), 7.24–7.20 (m, 1H), 7.20–7.06 (m, 4H), 6.98 (dd, J = 28.4 Hz, 16.4 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 193.5, 152.8, 147.6, 146.2, 145.6, 139.9, 139.8, 139.3, 135.9, 135.5, 131.2, 129.9, 129.0, 129.0, 128.9, 128.8, 128.7, 128.4, 128.2, 127.4, 127.3, 127.0, 125.8, 124.1, 123.9, 123.1, 119.7, 119.5, 116.4; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{36}H_{26}NO_2$ 504.1958; Found 504.1956.

((*Z*)-2-(Phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)(4-(trifluoromethyl)phenyl)methanone (Scheme 2, compound 3ae)



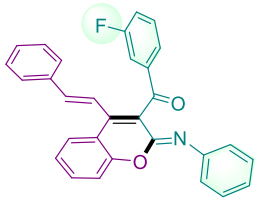
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.7) to afford a yellow solid in 76% yield (75 mg); mp 147-148 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, J = 8.0 Hz, 2H), 7.76–7.66 (m, 3H), 7.49–7.43 (m, 1H), 7.37–7.32 (m, 4H), 7.31–7.26 (m, 3H), 7.25–7.16 (m, 2H), 7.13–7.04 (m, 3H), 6.96 (dd, J = 20.8 Hz, 16.4 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 192.9, 152.8, 147.4, 145.2, 140.6, 139.7, 139.5, 135.6, 134.7, 134.4, 130.4 (d, $J_{C\text{-}F}$ = 227.5 Hz), 129.4, 129.2, 128.6 (d, $J_{C\text{-}F}$ = 30.2 Hz), 128.0, 127.0, 125.8 (q, $J_{C\text{-}F}$ = 3.5 Hz), 124.9, 124.2 (d, $J_{C\text{-}F}$ = 32.2 Hz), 123.1, 119.3, 119.3, 116.5; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{21}FNO_2$ 496.1519; Found 496.1525.

Benzo[*d*][1,3]dioxol-5-yl((*Z*)-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)methanone (Scheme 2, compound 3af)



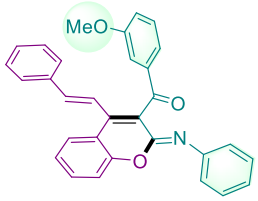
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.5) to afford a yellow solid in 89% yield (84 mg); mp 168-169 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (dd, J = 8.0 Hz, 1.6 Hz, 1H), 7.62 (dd, J = 8.4 Hz, 2.0 Hz, 1H), 7.51 (d, J = 1.6 Hz, 1H), 7.45–7.40 (m, 1H), 7.39–7.35 (m, 2H), 7.35–7.30 (m, 3H), 7.30–7.27 (m, 2H), 7.22–7.17 (m, 1H), 7.17–7.11 (m, 3H), 7.10–7.05 (m, 1H), 6.97 (dd, J = 34.8 Hz, 16.4 Hz, 2H), 6.82 (d, J = 8.2 Hz, 1H), 6.03 (s, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 192.0, 152.8, 152.3, 148.3, 147.6, 145.6, 139.5, 139.1, 135.9, 131.6, 131.1, 129.0, 128.7, 128.4, 127.0, 126.3, 125.7, 124.0, 123.8, 123.1, 119.7, 119.4, 116.3, 108.6, 108.1, 101.9; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{22}NO_4$ 472.1543; Found 472.1538.

(3-Fluorophenyl)((*Z*)-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)methanone (Scheme 2, compound 3ag)



This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.5) to afford a yellow solid in 90% yield (80 mg); mp 101-102 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, J = 7.6 Hz, 1H), 7.73–7.66 (m, 2H), 7.47–7.41 (m, 2H), 7.40–7.32 (m, 4H), 7.31–7.27 (m, 3H), 7.26–7.19 (m, 2H), 7.17 (d, J = 8.0 Hz, 1H), 7.13–7.05 (m, 3H), 6.96 (dd, J = 22.4 Hz, 16.4 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 192.7, 162.9 (d, $J_{C\text{-}F}$ = 246.4 Hz), 152.8, 147.4, 145.3, 140.3, 139.5, 138.8, 135.7, 130.4 (d, $J_{C\text{-}F}$ = 7.5 Hz), 130.3 (d, $J_{C\text{-}F}$ = 224.6 Hz), 128.8, 128.5, 127.0, 125.8, 125.0 (d, $J_{C\text{-}F}$ = 2.8 Hz), 124.1 (d, $J_{C\text{-}F}$ = 28.6 Hz), 123.1, 120.7, 120.4, 119.5, 119.3, 116.4, 115.6 (d, $J_{C\text{-}F}$ = 30.3 Hz); HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{21}FNO_2$ 446.1551; Found 446.1554.

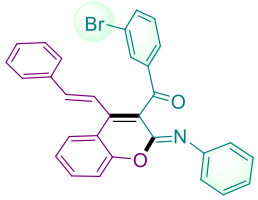
(3-Methoxyphenyl)((*Z*)-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)methanone (Scheme 2, compound 3ah)



This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.4) to afford a yellow solid in 76% yield (70 mg); mp 99-100 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (dd, J = 8.0 Hz, 1.6 Hz, 1H), 7.64–7.54 (m, 2H), 7.45–7.40 (m, 1H), 7.38–7.31 (m, 5H), 7.31–7.26 (m, 3H), 7.23–7.18 (m, 1H), 7.17–7.05 (m, 5H), 6.97 (dd, J = 26.8 Hz, 16.4 Hz, 2H), 3.83 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 193.8, 159.9, 152.8, 147.6, 145.6, 139.8, 139.2, 138.1, 135.9, 131.2, 129.7, 129.0, 128.8, 128.7, 128.4, 127.0, 125.7, 124.1, 123.9, 123.1, 122.3, 120.2, 119.7, 119.4, 116.3, 113.0, 55.4; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{24}NO_3$

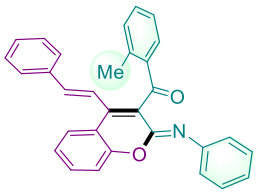
458.1751; Found 458.1755.

(3-Bromophenyl)((*Z*)-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)methanone (Scheme 2, compound 3ai)



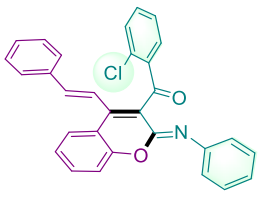
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.6) to afford a yellow solid in 65% yield (66 mg); m.p. 149-150 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30–8.03 (m, 1H), 7.94 (d, J = 8.0 Hz, 1H), 7.77–7.62 (m, 2H), 7.48–7.43 (m, 1H), 7.42–7.34 (m, 3H), 7.34–7.31 (m, 3H), 7.31–7.27 (m, 2H), 7.25–7.20 (m, 1H), 7.17 (dd, J = 8.4 Hz, 1.6 Hz, 1H), 7.14–7.05 (m, 3H), 6.97 (dd, J = 22.8 Hz, 16.4 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 192.5, 152.8, 147.4, 145.3, 140.4, 139.6, 138.6, 136.3, 135.7, 131.9, 131.4, 130.3, 129.2, 128.8, 128.5, 128.0, 127.8, 127.0, 125.8, 124.3, 124.0, 123.1, 123.0, 119.4, 119.3, 116.4; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{21}BrNO_2$ 506.0750; Found 506.0752.

((*Z*)-2-(Phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)(*o*-tolyl)methanone (Scheme 2, compound 3aj)



This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.7) to afford a yellow solid in 74% yield (65 mg); mp 180-181 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (dd, J = 8.0 Hz, 1.6 Hz, 1H), 7.67 (dd, J = 8.0 Hz, 1.6 Hz, 1H), 7.44–7.39 (m, 1H), 7.39–7.33 (m, 4H), 7.33–7.27 (m, 4H), 7.25–7.17 (m, 3H), 7.17–7.11 (m, 3H), 7.10–7.05 (m, 1H), 6.97 (dd, J = 31.6 Hz, 17.2 Hz, 2H), 2.63 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 195.7, 152.8, 147.5, 145.5, 140.4, 139.2, 139.0, 136.5, 135.9, 132.1, 132.0, 131.0, 130.6, 130.4, 129.0, 128.7, 128.4, 127.0, 125.8, 125.6, 124.1, 123.8, 123.3, 119.9, 119.6, 116.3, 21.5; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{24}NO_2$ 442.1802; Found 442.1796.

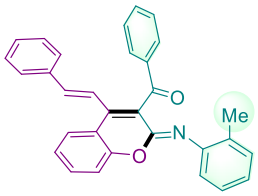
(2-Chlorophenyl)((*Z*)-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)methanone (Scheme 2, compound 3ak)



This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20,

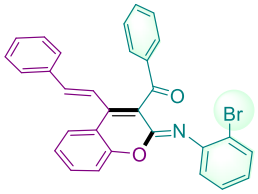
R_f = 0.6) to afford a yellow solid in 78% yield (72 mg); mp 174-175 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00–7.88 (m, 1H), 7.70 (dd, *J* = 8.0 Hz, 1.6 Hz, 1H), 7.48–7.42 (m, 2H), 7.41–7.38 (m, 3H), 7.37–7.32 (m, 3H), 7.32–7.27 (m, 3H), 7.22–7.18 (m, 1H), 7.15 (dd, *J* = 8.4 Hz, 1.2 Hz, 1H), 7.13–7.06 (m, 3H), 7.06–7.00 (m, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 192.1, 152.9, 147.3, 145.5, 140.6, 139.3, 136.6, 135.9, 133.4, 132.9, 131.7, 131.3, 131.1, 129.7, 129.0, 128.7, 128.5, 127.1, 126.8, 126.2, 124.1, 123.8, 123.2, 119.9, 119.6, 116.4; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{21}ClNO_2$ 462.1255; Found 462.1264.

Phenyl((*Z*)-4-((*E*)-styryl)-2-(*o*-tolylimino)-2*H*-chromen-3-yl)methanone (Scheme 2, compound 3al)



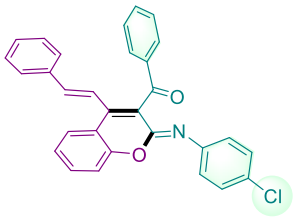
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.6) to afford a yellow solid in 60% yield (52 mg); mp 162-163 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12–8.00 (m, 2H), 7.70 (dd, *J* = 8.0 Hz, 1.6 Hz, 1H), 7.59–7.54 (m, 1H), 7.48–7.44 (m, 2H), 7.43–7.39 (m, 1H), 7.37–7.34 (m, 2H), 7.33–7.26 (m, 3H), 7.23–7.19 (m, 1H), 7.17–7.09 (m, 2H), 7.07–6.99 (m, 2H), 6.99–6.93 (m, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 194.0, 152.9, 147.1, 144.3, 139.7, 139.2, 136.8, 135.9, 133.6, 131.3, 131.2, 130.1, 129.3, 129.0, 128.7, 128.7, 127.0, 125.8, 125.7, 123.9, 123.8, 121.3, 119.7, 119.4, 116.4, 18.0; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{24}NO_2$ 442.1802; Found 442.1799.

((*Z*)-2-((2-Bromophenyl)imino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)(phenyl)methanone (Scheme 2, compound 3am)



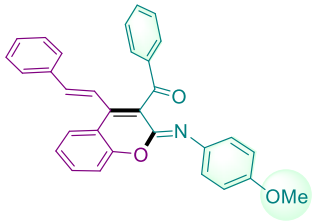
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.5) to afford a yellow solid in 65% yield (66 mg); mp 163-164 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15–8.03 (m, 2H), 7.73–7.68 (m, 1H), 7.58–7.54 (m, 1H), 7.51 (dd, *J* = 8.0 Hz, 1.6 Hz, 1H), 7.48–7.41 (m, 3H), 7.36–7.27 (m, 5H), 7.26–7.18 (m, 2H), 7.14–7.07 (m, 2H), 7.01 (dd, *J* = 29.6 Hz, 16.4 Hz, 2H), 6.93–6.87 (m, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 193.8, 152.7, 148.8, 145.2, 140.8, 139.6, 136.6, 135.8, 133.7, 132.6, 131.3, 129.7, 129.1, 128.8, 128.7, 128.7, 128.1, 127.5, 127.0, 125.8, 124.7, 124.1, 123.0, 119.5, 119.3, 116.9, 116.5; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{21}BrNO_2$ 506.0750; Found506.0744.

((*Z*)-2-((4-Chlorophenyl)imino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)(phenyl)methanone (Scheme 2, compound 3an)



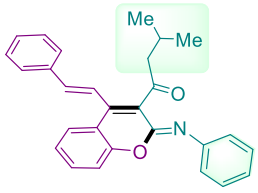
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.7) to afford a yellow solid in 72% yield (66 mg); mp 187-188 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09–7.96 (m, 2H), 7.70 (dd, J = 8.0 Hz, 1.6 Hz, 1H), 7.59–7.54 (m, 1H), 7.49–7.43 (m, 3H), 7.35–7.31 (m, 3H), 7.31–7.27 (m, 2H), 7.26–7.19 (m, 3H), 7.17 (dd, J = 8.4 Hz, 1.2 Hz, 1H), 7.10–7.04 (m, 2H), 6.96 (dd, J = 27.2 Hz, 16.4 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 193.9, 152.6, 148.1, 144.1, 140.2, 139.5, 136.7, 135.8, 133.7, 131.4, 129.3, 129.2, 129.1, 128.7, 128.5, 128.5, 127.0, 125.8, 124.6, 124.1, 119.6, 119.4, 116.3; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{21}ClNO_2$ 462.1255; Found 462.1260.

((*Z*)-2-((4-Methoxyphenyl)imino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)(phenyl)methanone (Scheme 2, compound 3ao)



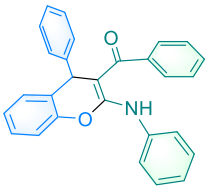
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.4) to afford a yellow solid in 70% yield (64 mg); mp 160-161 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05–7.88 (m, 2H), 7.65 (dd, J = 8.4 Hz, 2.0 Hz, 1H), 7.55–7.50 (m, 1H), 7.42 (d, J = 8.0 Hz, 3H), 7.36–7.26 (m, 4H), 7.25–7.08 (m, 5H), 7.03–6.89 (m, 2H), 6.88–6.72 (m, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 194.1, 156.6, 152.9, 146.7, 139.0, 138.4, 136.9, 135.9, 133.5, 131.0, 129.3, 129.2, 128.9, 128.7, 128.7, 127.2, 127.0, 125.7, 125.2, 123.8, 119.8, 119.6, 116.3, 113.6, 55.4; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{24}NO_3$ 458.1751; Found 458.1759.

3-Methyl-1-((*Z*)-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)butan-1-one (Scheme 2, compound 3ap)



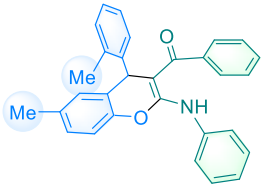
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.5) to afford a yellow solid in 60% yield (48 mg); mp 100-101 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (dd, J = 8.0 Hz, 1.6 Hz, 1H), 7.53–7.49 (m, 2H), 7.43–7.38 (m, 3H), 7.37–7.33 (m, 3H), 7.28–7.27 (m, 1H), 7.26–7.24 (m, 1H), 7.19–7.10 (m, 3H), 7.02 (s, 2H), 2.74 (d, J = 6.4 Hz, 2H), 2.35–2.25 (m, 1H), 0.94 (d, J = 6.4 Hz, 6H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 203.3, 152.5, 147.0, 145.5, 139.2, 137.9, 135.8, 131.1, 131.0, 129.1, 128.9, 128.5, 127.0, 125.8, 124.2, 123.8, 123.3, 119.5, 119.4, 116.2, 52.2, 23.7, 22.7; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{28}H_{26}NO_2$ 408.1958; Found 408.1960.

Phenyl(4-phenyl-2-(phenylamino)-4*H*-chromen-3-yl)methanone (Scheme 3, compound 5aa)



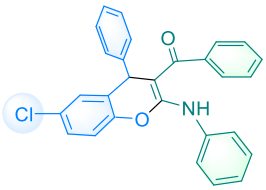
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.6) to afford a white solid in 88% yield (71 mg); mp 188-190 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.36 (s, 1H), 7.53 (d, J = 7.6 Hz, 2H), 7.46–7.38 (m, 3H), 7.37–7.32 (m, 2H), 7.25–7.17 (m, 4H), 7.16–7.11 (m, 3H), 7.12–7.04 (m, 3H), 6.86–6.81 (m, 2H), 5.03 (s, 1H); ^{13}C NMR (100MHz, $CDCl_3$) δ 194.4, 160.0, 148.4, 146.7, 141.3, 137.2, 129.1, 129.0, 128.9, 128.4, 128.0, 127.6, 126.9, 126.4, 126.3, 125.2, 124.6, 122.4, 116.2, 89.9, 42.3; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{28}H_{22}NO_2$ 404.1645; Found 404.1648.

(6-Methyl-2-(phenylamino)-4-(*o*-tolyl)-4*H*-chromen-3-yl)(phenyl)methanone (Scheme 3, compound 5ba)



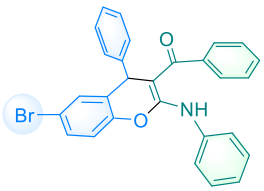
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.5) to afford a white solid in 82% yield (70 mg); mp 101-102 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.30 (s, 1H), 7.57 – 7.50 (m, 2H), 7.47 – 7.28 (m, 5H), 7.20 (t, J = 7.4 Hz, 1H), 7.10 – 7.01 (m, 3H), 7.02 – 6.98 (m, 3H), 6.97 – 6.92 (m, 1H), 6.93 – 6.82 (m, 2H), 5.23 (s, 1H), 2.19 (s, 3H), 1.74 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 195.1, 160.1, 146.0, 145.8, 141.8, 137.4, 134.8, 134.0, 130.3, 129.2, 128.8, 128.7, 128.3, 128.3, 126.6, 126.5, 126.1, 126.0, 124.5, 122.5, 116.1, 90.4, 37.9, 20.8, 19.0; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{26}NO_2$ 432.1958; Found 432.1965.

(6-Chloro-4-phenyl-2-(phenylamino)-4*H*-chromen-3-yl)(phenyl)methanone (Scheme 3, compound 5ca)



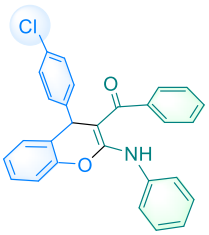
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.6) to afford a white solid in 75% yield (65 mg); mp 178-179 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.28 (s, 1H), 7.50–7.46 (m, 2H), 7.46–7.37 (m, 3H), 7.36–7.30 (m, 2H), 7.25–7.18 (m, 1H), 7.19–7.12 (m, 4H), 7.13–7.04 (m, 3H), 6.82–6.77 (m, 2H), 4.97 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.5, 159.7, 146.9, 146.0, 141.0, 137.0, 130.1, 129.2, 129.1, 128.7, 128.6, 128.1, 127.7, 126.8, 126.6, 126.3, 124.8, 122.6, 117.6, 89.3, 42.3; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{28}H_{21}ClNO_2$ 438.1255; Found 438.1248.

(6-Bromo-4-phenyl-2-(phenylamino)-4*H*-chromen-3-yl)(phenyl)methanone (Scheme 3, compound 5da)



This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.6) to afford a white solid in 70% yield (65 mg); mp 183-184 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.27 (s, 1H), 7.51–7.47 (m, 2H), 7.46–7.38 (m, 3H), 7.37–7.28 (m, 3H), 7.27–7.19 (m, 2H), 7.19–7.15 (m, 2H), 7.15–7.07 (m, 3H), 7.01 (d, *J* = 8.6 Hz, 1H), 6.84–6.76 (m, 2H), 4.97 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.5, 159.6, 147.5, 146.0, 141.0, 137.0, 131.6, 130.6, 129.2, 129.1, 129.0, 128.6, 128.1, 126.8, 126.6, 126.3, 124.8, 122.6, 118.0, 117.6, 89.3, 42.2; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{28}H_{21}BrNO_2$ 482.0750; Found482.0745.

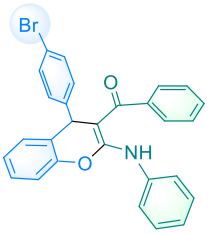
(4-(4-Chlorophenyl)-2-(phenylamino)-4*H*-chromen-3-yl)(phenyl)methanone (Scheme 3, compound 5ea)



This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.6) to afford a white solid in 70% yield (61 mg); mp 170-171 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.32 (s, 1H), 7.54–7.49 (m, 2H), 7.48–7.39 (m, 3H), 7.38–7.32 (m, 2H), 7.25–7.17 (m, 4H), 7.14 (d, *J* = 8.0 Hz, 1H), 7.11–7.04 (m, 4H), 6.77–6.69 (m, 2H), 5.02 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.4, 159.9, 148.3, 145.2, 141.2, 137.1, 132.0, 129.1, 129.1, 128.9, 128.5, 128.2, 128.2, 127.9, 126.3, 126.3, 125.3, 124.7, 122.5, 116.4, 89.5, 41.8; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd

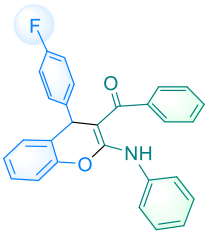
for $C_{28}H_{21}ClNO_2$ 438.1255; Found 438.1263.

(4-(4-bromophenyl)-2-(phenylamino)-4H-chromen-3-yl)(phenyl)methanone (Scheme 3, compound 5fa)



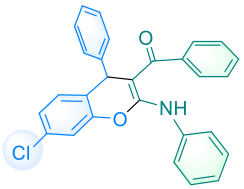
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.6) to afford a white solid in 68% yield (65 mg); mp 155-156 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.31 (s, 1H), 7.50 (d, J = 7.8 Hz, 2H), 7.42 (q, J = 7.4 Hz, 3H), 7.35 (t, J = 7.4 Hz, 2H), 7.22 (d, J = 8.2 Hz, 4H), 7.18 (d, J = 7.6 Hz, 2H), 7.13 (d, J = 8.1 Hz, 1H), 7.07 (d, J = 4.2 Hz, 2H), 6.66 (d, J = 8.3 Hz, 2H), 5.00 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.4, 159.9, 148.3, 145.7, 141.2, 137.0, 131.5, 129.2, 129.1, 128.9, 128.6, 128.2, 127.9, 126.3, 126.2, 125.3, 124.7, 122.5, 120.1, 116.4, 89.4, 41.8; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{28}H_{21}BrNO_2$ 482.0750; Found 482.0746.

(4-(4-Fluorophenyl)-2-(phenylamino)-4*H*-chromen-3-yl)(phenyl)methanone (Scheme 3, compound 5ga)



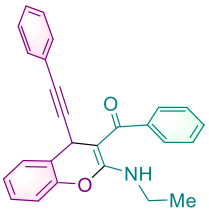
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.6) to afford a white solid in 62% yield (52 mg); mp 158-159 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.30 (s, 1H), 7.52–7.48 (m, 2H), 7.45–7.32 (m, 5H), 7.20 (m, 4H), 7.13 (d, J = 8.0 Hz, 1H), 7.09–7.05 (m, 2H), 5.02 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.5, 162.5, 161.3 (d, J_{C-F} = 243.4 Hz), 148.3, 142.6 (d, J_{C-F} = 3.1 Hz), 141.3, 137.1, 129.1, 129.1, 128.9, 128.4 (d, J_{C-F} = 8.0 Hz), 128.1, 127.8, 126.6, 126.3, 125.3, 124.7, 122.5, 116.4, 115.2 (d, J_{C-F} = 21.3 Hz), 89.8, 41.6; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{28}H_{21}FNO_2$ 422.1551; Found 422.1556.

(4-(3-Chlorophenyl)-2-(phenylamino)-4*H*-chromen-3-yl)(phenyl)methanone (Scheme 3, compound 5ha)



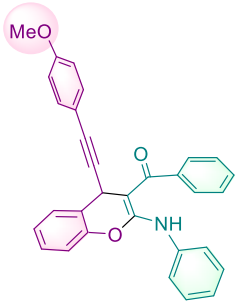
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.6) to afford a white solid in 60% yield (52 mg); mp 143-144 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.29 (s, 1H), 7.50–7.47 (m, 2H), 7.47–7.37 (m, 3H), 7.36–7.30 (m, 2H), 7.25–7.20 (m, 1H), 7.18–7.13 (m, 3H), 7.13–7.09 (m, 2H), 7.04 (d, *J* = 1.1 Hz, 2H), 6.82–6.77 (m, 2H), 4.99 (s, 1H); ^{13}C NMR (100MHz, $CDCl_3$) δ 194.6, 159.5, 148.6, 146.2, 141.1, 136.9, 132.8, 129.9, 129.2, 129.1, 128.5, 128.1, 126.8, 126.5, 126.3, 125.5, 125.4, 124.8, 122.6, 116.6, 89.5, 41.9; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{28}H_{21}ClNO_2$ 438.1255; Found 438.1258.

(2-(Ethylamino)-4-(phenylethynyl)-4*H*-chromen-3-yl)(phenyl)methanone (Scheme 3, compound 6aq)



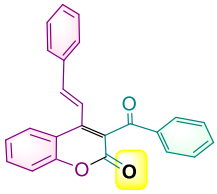
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.4) to afford a yellow solid in 46% yield (35 mg). mp 114-115 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.35 (d, *J* = 6.0 Hz, 1H), 7.62–7.57 (m, 2H), 7.47–7.42 (m, 3H), 7.33–7.27 (m, 2H), 7.26–7.20 (m, 5H), 7.17–7.09 (m, 2H), 4.81 (s, 1H), 3.62 (dq, *J* = 7.2 Hz, 5.6 Hz, 2H), 1.37 (d, *J* = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 191.9, 162.9, 149.0, 141.8, 131.5, 128.8, 128.7, 128.3, 128.1, 128.1, 127.8, 126.5, 125.1, 123.8, 123.4, 116.3, 92.4, 86.0, 81.5, 35.8, 29.3, 15.4; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{26}H_{22}NO_2$ 380.1645; Found 380.1647.

(4-((4-Methoxyphenyl)ethynyl)-2-(phenylamino)-4*H*-chromen-3-yl)(phenyl)methanone (Scheme 3, compound 6ia)



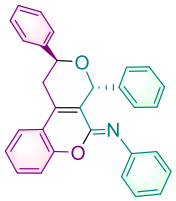
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.7) to afford a white solid in 70% yield (64 mg); mp 133-134 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.40 (s, 1H), 7.70–7.64 (m, 2H), 7.53–7.50 (m, 1H), 7.50–7.48 (m, 2H), 7.48–7.46 (m, 2H), 7.44–7.39 (m, 2H), 7.33–7.27 (m, 2H), 7.24–7.16 (m, 4H), 7.15–7.12 (m, 1H), 6.80–6.75 (m, 2H), 4.92 (s, 1H), 3.78 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 193.2, 160.3, 159.3, 148.8, 141.2, 137.0, 132.9, 129.3, 129.1, 128.7, 128.4, 128.2, 126.6, 125.4, 124.8, 123.7, 122.6, 116.5, 115.3, 113.7, 90.4, 87.9, 81.8, 55.2, 29.3; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{31}H_{24}NO_3$ 458.1751; Found 458.1743.

(*E*)-3-Benzoyl-4-styryl-2*H*-chromen-2-one (Scheme 5, compound 8)



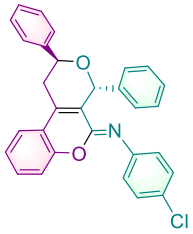
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.3) to afford a white solid in 78% yield (55 mg); mp 150-151 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97–7.87 (m, 2H), 7.84 (dd, *J* = 8.0 Hz, 1.6 Hz, 1H), 7.66–7.61 (m, 1H), 7.59–7.55 (m, 1H), 7.47–7.41 (m, 3H), 7.40–7.33 (m, 2H), 7.32–7.30 (m, 4H), 7.03 (dd, *J* = 18.0 Hz, 16.4 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 192.9, 159.0, 153.4, 148.8, 141.1, 136.3, 135.3, 134.1, 132.7, 129.6, 129.3, 128.9, 128.8, 127.2, 126.3, 124.7, 124.2, 119.1, 118.6, 117.5; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{24}H_{17}O_3$ 353.1172; Found 353.1181.

(*Z*)-*N*,2,4-Triphenyl-1,4-dihydro-2*H*,5*H*-pyrano[3,4-*c*]chromen-5-imine (Scheme 5, compound 9aa)



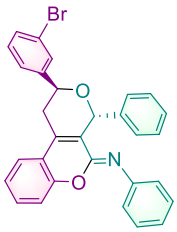
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.7) to afford a yellow solid in 51% yield (44 mg); mp 191-192 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51–7.48 (m, 2H), 7.48–7.45 (m, 1H), 7.42–7.37 (m, 5H), 7.37–7.31 (m, 4H), 7.31–7.27 (m, 2H), 7.26–7.25 (m, 1H), 7.21–7.17 (m, 1H), 7.13–7.10 (m, 1H), 7.08–6.99 (m, 3H), 6.21 (s, 1H), 4.77 (dd, *J* = 10.4 Hz, 4.0 Hz, 1H), 3.05 (dd, *J* = 17.6 Hz, 4.4 Hz, 1H), 2.96 (dd, *J* = 17.6 Hz, 10.4 Hz, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 152.4, 146.7, 146.0, 141.7, 139.8, 138.1, 130.2, 128.9, 128.5, 128.4, 128.0, 127.8, 127.7, 126.0, 125.7, 123.6, 122.8, 122.8, 119.8, 115.9, 74.4, 68.2, 31.5; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{24}NO_2$ 430.1802; Found 430.1809.

(*Z*)-*N*-(4-Chlorophenyl)-2,4-diphenyl-1,4-dihydro-2*H*,5*H*-pyrano[3,4-*c*]chromen-5-imine (Scheme 5, compound 9an)



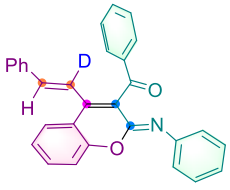
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.7) to afford a yellow solid in 55% yield (51 mg); mp 179-180 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, J = 7.8 Hz, 3H), 7.44–7.37 (m, 6H), 7.35–7.30 (m, 3H), 7.25–7.21 (m, 3H), 7.15 (d, J = 8.2 Hz, 1H), 6.97 (d, J = 8.2 Hz, 2H), 6.19 (s, 1H), 4.76 (dd, J = 10.4 Hz, 4.0 Hz, 1H), 3.03 (dd, J = 18.0 Hz, 4.4 Hz, 1H), 2.96 (dd, J = 17.6 Hz, 10.4 Hz, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 152.6, 147.6, 144.9, 142.0, 139.0, 130.7, 129.2, 129.0, 128.9, 128.8, 128.5, 128.2, 126.3, 125.9, 124.6, 124.2, 123.3, 120.1, 116.3, 74.7, 68.6, 31.9; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{23}ClNO_2$ 464.1412; Found 464.1414.

(*Z*)-2-(3-Bromophenyl)-*N*,4-diphenyl-1,4-dihydro-2*H*,5*H*-pyrano[3,4-*c*]chromen-5-imine (Scheme 5, compound 9qa)



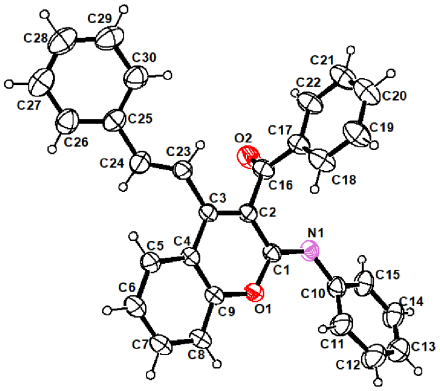
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.7) to afford a yellow solid in 50% yield (51 mg); mp 192-193 °C, ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56–7.55 (m, 1H), 7.48–7.46 (m, 3H), 7.44–7.36 (m, 2H), 7.35–7.31 (m, 3H), 7.30–7.28 (m, 3H), 7.25–7.19 (m, 2H), 7.12–7.10 (m, 1H), 7.05–7.02 (m, 1H), 7.01-6.98 (m, 2H), 6.20 (s, 1H), 4.73 (dd, J = 10.8 Hz, 4.0 Hz, 1H), 3.04 (dd, J = 17.6 Hz, 4.0 Hz, 1H), 2.89 (dd, J = 18.0 Hz, 10.8 Hz, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 152.3, 146.5, 145.9, 144.1, 139.5, 137.7, 130.8, 130.3, 130.1, 129.0, 128.8, 128.4, 128.1, 127.9, 125.6, 124.5, 123.6, 122.8, 122.6, 119.6, 116.0, 74.4, 67.6, 31.5; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{23}BrNO_2$ 508.0907; Found 508.0914.

Phenyl((*Z*)-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)methanone (Scheme 4, compound 3aa-*d*)



This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:20, R_f = 0.6) to afford a yellow solid in 65% yield (27 mg); mp 138-140 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, J = 7.0 Hz, 2H), 7.69 (d, J = 7.8 Hz, 1H), 7.56 (t, J = 7.4 Hz, 1H), 7.46-7.41 (m, 3H), 7.31-7.28 (m, 6H), 7.20-7.14 (m, 2H), 7.11-7.04 (m, 3H), 7.01-6.90 (m, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 194.1, 152.9, 147.7, 145.6, 139.9, 139.8, 139.7, 139.2, 139.1, 136.8, 135.9, 133.6, 131.3, 129.4, 129.1, 128.9, 128.8, 128.5, 127.1, 125.8, 124.2, 124.0, 123.2, 119.8, 119.5, 116.6; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{30}H_{21}DNO_2$ 429.1708; Found 429.1706.

14. X-ray crystallographic data of compound 3aa



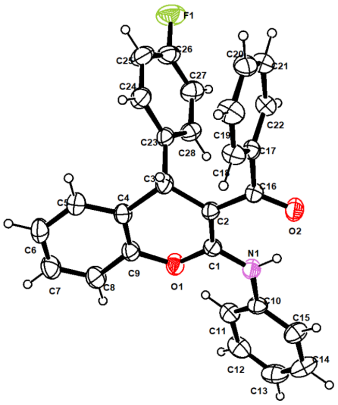
The purified compound **3aa** is dissolved in a mixed solvent of ethyl acetate and petroleum ether, and placed in a dark cabinet to slowly evaporate. After several days, a colourless bulk crystal was obtained. The X-ray crystal-structure determinations were obtained on a Bruker Smart CCDC APEX-2 diffractometer (graphite-monochromated Mo *Kα* radiation, *λ*=0.71073 nm) at 296(2) K.

Figure S1. ORTEP drawing of compound **3aa** (30% probability for the thermal ellipsoid).

Table S2. Crystal data and structure refinement for compound **3aa**.

CCDC number	2184624
Identification code	20200616h
Empirical formula	C30 H21 N O2
Formula weight	427.48
Temperature	298.15 K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 13.4932(16) Å α= 90°.
	b = 9.8466(12) Å β= 102.184(4)°.
	c = 17.378(2) Å γ= 90°.
Volume	2256.9(5) $Å^3$
Z	4
Density (calculated)	1.258 g/cm^3
Absorption coefficient	0.078 mm^{-1}
F(000)	896.0
Crystal size	0.15 × 0.11 × 0.1 mm^3
Theta range for data collection	5.962 to 49.998°.
Index ranges	-16<=h<=15, -11<=k<=11, -20<=l<=20
Reflections collected	44868
Independent reflections	3960 [R(int) = 0.1377, R(sigma) = 0.0596]
Max. and min. transmission	0.746 and 0.703
Data / restraints / parameters	3960 / 691 / 489
Goodness-of-fit on F^2	1.017
Final R indices [I>2sigma(I)]	R1 = 0.0688, wR2 = 0.1680
Final R indices (all data)	R1 = 0.1615, wR2 = 0.2281
Largest diff. peak and hole	0.20 and -0.22 $e.Å^{-3}$

15. X-ray crystallographic data of compound 5ga



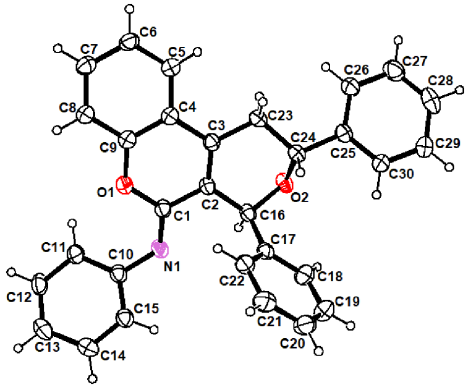
The purified compound **5ga** is dissolved in a mixed solvent of ethyl acetate and petroleum ether, and placed in a dark cabinet to slowly evaporate. After several days, a colourless bulk crystal was obtained. The X-ray crystal-structure determinations were obtained on a Bruker Smart CCDC APEX-2 diffractometer (graphite-monochromated Mo *Kα* radiation, *λ*=0.71073 nm) at 296(2) K.

Figure S2. ORTEP drawing of compound **5ga** (30% probability for the thermal ellipsoid).

Table S3. Crystal data and structure refinement for compound **5ga**.

CCDC number	2184624
Identification code	20210930a
Empirical formula	C28 H20 F N O2
Formula weight	421.45
Temperature	300.00 K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 9.5747(19) Å α= 101.581(6)°. b = 9.6132(18) Å β= 95.065(7)°. c = 12.847(3) Å γ= 111.403(6)°.
Volume	1061.5(4) $Å^3$
Z	2
Density (calculated)	1.319 g/cm^3
Absorption coefficient	0.089 mm^{-1}
F(000)	440.0
Crystal size	0.13 × 0.12 × 0.11 mm^3
Theta range for data collection	5.192 to 55.336°.
Index ranges	-12<=h<=12, -12<=k<=12, -16<=l<=16
Reflections collected	16838
Independent reflections	4695 [R(int) = 0.1059, R(sigma) = 0.1007]
Goodness-of-fit on F^2	0.995
Max. and min. transmission	0.746 and 0.703
Data / restraints / parameters	4695 / 0 / 290
Final R indices [I>2sigma(I)]	R1 = 0.0686, wR2 = 0.1612
Final R indices (all data)	R1 = 0.1646, wR2 = 0.2094
Largest diff. peak and hole	0.24 and -0.22 $e.Å^{-3}$

16. X-ray crystallographic data of compound 9aa



The purified compound **9aa** is dissolved in a mixed solvent of ethyl acetate and petroleum ether, and placed in a dark cabinet to slowly evaporate. After several days, a colourless bulk crystal was obtained. The X-ray crystal-structure determinations were obtained on a Bruker Smart CCDC APEX-2 diffractometer (graphite-monochromated Mo *Kα* radiation, *λ*=0.71073 nm) at 296(2) K.

Figure S3. ORTEP drawing of compound **9aa** (30% probability for the thermal ellipsoid).

Table S4. Crystal data and structure refinement for compound **9aa**.

CCDC number	2184629
Identification code	mo_20201230a_0m_a
Empirical formula	C30 H23 N O2
Formula weight	429.49
Temperature	300.01 K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 4.8767(3) Å α= 89.426(3)°.
	b = 9.4727(7) Å β= 89.496(3)°.
	c = 24.3972(19) Å γ= 77.542(3)°.
Volume	1100.42(14) $Å^3$
Z	2
Density (calculated)	1.296 g/cm^3
Absorption coefficient	0.081 mm^{-1}
F(000)	452.0
Crystal size	0.12 × 0.11 × 0.1 mm^3
Theta range for data collection	6.644 to 55.05°.
Index ranges	-6<=h<=6, -12<=k<=12, -31<=l<=31
Reflections collected	48049
Independent reflections	5071 [R(int) = 0.0607, R(sigma) = 0.0333]
Max. and min. transmission	0.746 and 0.701
Data / restraints / parameters	5071 / 77 / 384
Goodness-of-fit on F^2	1.016
Final R indices [I>2sigma(I)]	R1 = 0.0673, wR2 = 0.1576
R indices (all data)	R1 = 0.1128, wR2 = 0.1837
Largest diff. peak and hole	0.39 and -0.43 $e.Å^{-3}$

17. Computational Details

Geometry optimizations were performed by DFT calculation with the with the B3PW91-D3 functional,[3,4] where the Stuttgart-Dresden-Bonn basis sets[5] were used for Fe with the effective core potentials employed for representing core electrons and the 6-31G(d) basis sets were used for all other atoms. We performed single-point calculations using 6-311+G(d,p) basis sets for non-metal atoms. Solvation effects of acetonitrile were evaluated with the PCM method.[6] All these calculations were carried out with Gaussian16 program.[7]

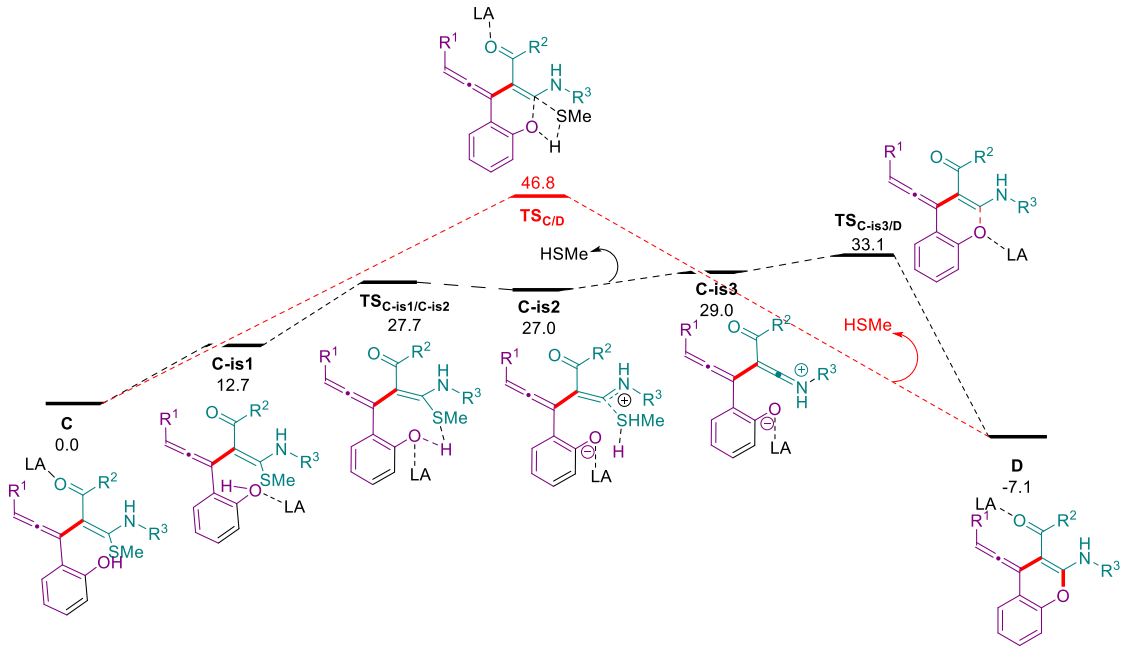


Figure S4. DFT energy profile of possible reaction mechanism from intermediate **C** to **D**

Coordination

C, B3PW91-D3/BSII=-3303.730947

C -2.796217	-0.949539	2.927755
C -1.716185	-1.567923	2.305096
C -0.886355	-0.848803	1.442061
C -1.125554	0.517505	1.201165
C -2.224298	1.110503	1.833147
C-3.058991	0.396536	2.685293
H -3.427277	-1.523752	3.600986
H -1.514223	-2.623969	2.481329
C -0.217040	1.343658	0.358361
H -2.394118	2.169703	1.668269
H -3.893119	0.893376	3.171833
C 1.257247	1.185775	0.548233
C 2.045003	0.640617	-0.460577
C 1.814749	1.427638	1.865820
N 3.372506	0.421403	-0.264421
H 3.642123	0.745323	0.684215
C -0.711475	2.216671	-0.492934
C -1.176964	3.054231	-1.389181
O 0.160283	-1.450248	0.805121
H 0.195298	-2.377144	1.079907
S 1.301709	0.272077	-2.028387
C 2.703935	0.402576	-3.182815
H 3.263930	-0.530793	-3.267835
H 2.262435	0.657451	-4.150264
H 3.374575	1.207278	-2.873312
H -1.242031	2.703606	-2.422234

C 4.114992	-0.678978	-0.755377
C 5.477345	-0.499873	-1.010329
C 3.532377	-1.938554	-0.938923
C 6.247704	-1.566997	-1.463921
H 5.916857	0.482684	-0.861009
C 4.304859	-2.993418	-1.416471
H 2.480572	-2.074545	-0.708230
C 5.663111	-2.814548	-1.680677
H 7.306267	-1.418561	-1.660626
H 3.844983	-3.966924	-1.567081
H 6.262810	-3.643386	-2.046752
C -1.606105	4.437870	-1.134681
C -0.734492	5.498328	-1.418073
C -2.875789	4.737477	-0.614855
C -1.111738	6.817185	-1.175832
H 0.250208	5.282989	-1.827675
C -3.250485	6.052794	-0.370832
H -3.568385	3.926491	-0.409409
C -2.369903	7.100868	-0.648083
H -0.419824	7.625111	-1.400601
H -4.238536	6.264483	0.031127
H -2.666017	8.129504	-0.459790
C 2.101068	0.233319	2.726005
C 1.065428	-0.614287	3.127116
C 3.407329	-0.023336	3.145177
C 1.338890	-1.724422	3.922217
H 0.048361	-0.402445	2.809510
C 3.683522	-1.147948	3.917997
H 4.204288	0.647926	2.838595
C 2.650999	-2.001745	4.305921
H 0.526878	-2.374937	4.238678
H 4.706621	-1.359492	4.217719
H 2.867909	-2.878433	4.910971
O 2.057168	2.567096	2.341676
Fe 1.999191	4.543714	2.016782
Cl 3.596004	5.494788	3.097591
Cl 0.112923	5.325618	2.689922
Cl 2.226446	4.931380	-0.085732

$TS_{C/D}$, B3PW91-D3/BSII=-3303.6561246

C -1.611265	-0.869520	4.048050
C -0.700221	-1.424319	3.152083
C -0.461375	-0.751450	1.963750
C -1.059334	0.461626	1.630057
C -1.969819	0.998922	2.547702
C -2.247851	0.335546	3.739036
H -1.821074	-1.376493	4.985124
H -0.193311	-2.362651	3.353506
C -0.661811	1.130568	0.368853
H -2.446969	1.946269	2.312139
H -2.955674	0.768024	4.440386
C 0.769392	0.943314	0.007921
C 1.215063	-0.434301	-0.031024
C 1.632033	1.981421	-0.279154
N 2.508596	-0.766195	-0.014455
H 3.094706	0.070712	-0.149877
C -1.551454	1.836584	-0.296433
C -2.501459	2.554618	-0.845223
O 0.386890	-1.369988	1.022854
H -0.112869	-1.863373	0.164421
S -0.065689	-1.466217	-1.554373
C 1.077239	-2.479885	-2.537367
H 1.404635	-3.375847	-2.008107
H 0.544034	-2.752381	-3.453329
H 1.939962	-1.866531	-2.807634
H -3.140414	2.079076	-1.591682
C 3.115633	-2.028982	-0.210082
C 4.242811	-2.074765	-1.038209
C 2.644792	-3.196775	0.398313
C 4.874477	-3.289279	-1.278637
H 4.603799	-1.163514	-1.506354
C 3.278322	-4.410462	0.134881
H 1.802951	-3.160273	1.076926
C 4.389610	-4.465184	-0.704164
H 5.743444	-3.313797	-1.930133
H 2.903371	-5.316556	0.603580
H 4.880004	-5.414275	-0.901491
C -2.755022	3.974911	-0.561190
C -3.727934	4.663767	-1.297770
C-2.034827	4.668051	0.423289
C -3.973291	6.014309	-1.060059
H -4.290195	4.137302	-2.066148
C -2.280058	6.014142	0.658525
H -1.252086	4.153908	0.974650
C -3.250729	6.694105	-0.080741
H -4.728455	6.535629	-1.642625
H -1.699436	6.539735	1.411734
H -3.439004	7.748534	0.103463
C 1.190930	3.371792	-0.546342
C 0.485347	3.655014	-1.719785

C 1.643856	4.415087	0.268402
C 0.212667	4.976465	-2.062090
H 0.187609	2.839165	-2.370411
C 1.355060	5.732860	-0.071057
H 2.233534	4.186257	1.151693
C 0.640549	6.013513	-1.236551
H -0.333911	5.194129	-2.974717
H 1.701386	6.542928	0.565073
H 0.419162	7.043404	-1.502093
O 2.937051	1.797097	-0.364209
Fe 3.887889	2.093890	-2.023468
Cl 3.968604	4.185718	-2.626031
Cl 2.665646	0.814373	-3.365475
Cl 5.861410	1.205873	-1.613244

C-is1, B3PW91-D3/BSII =-3303.7176356

C -1.379097	-1.088223	3.182831
C -0.605537	-1.554842	2.133348
C -0.252935	-0.740698	1.017840
C -0.753532	0.609709	1.078151
C -1.533617	1.072801	2.156743
C -1.842337	0.236196	3.210413
H -1.614683	-1.754955	4.010630
H -0.233572	-2.583002	2.128024
C -0.273996	1.540894	0.046378
H -1.832970	2.118190	2.170289
H -2.427084	0.601010	4.050151
C 1.212298	1.687896	0.076737
C 1.956074	0.784459	-0.644070
C 1.860130	2.404276	1.165620
O 3.080402	2.330217	1.397420
N 3.307752	0.620140	-0.577222
H 3.666060	1.248402	0.164034
C -1.034913	2.134701	-0.867809
C -1.799730	2.757110	-1.745802
H -0.163159	0.795453	-2.014274
S 1.137065	-0.090184	-2.009988
C 1.572376	1.166926	-3.345953
H 2.655488	1.258106	-3.457576
H 1.131873	0.803483	-4.278095
H 1.135903	2.135494	-3.054816
H -1.930562	2.303937	-2.733943
C 4.004251	-0.595883	-0.796429
C 5.337143	-0.518124	-1.232470
C 3.408381	-1.838438	-0.548286
C 6.064549	-1.675784	-1.440462
H 5.781322	0.457268	-1.413872
C 4.152346	-2.998652	-0.784292
H 2.388750	-1.884174	-0.173026
C 5.481256	-2.929784	-1.221625
H 7.104147	-1.613544	-1.772878
H 3.700430	-3.964245	-0.585831
H 6.048414	-3.840872	-1.382526
C -2.492019	4.027889	-1.510084
C -2.874791	4.818872	-2.601976
C -2.793789	4.475412	-0.215441
C -3.519901	6.037363	-2.405583
H -2.658544	4.476840	-3.612137
C -3.436623	5.692720	-0.020813
H -2.531820	3.851451	0.633700
C -3.799392	6.481614	-1.114002
H -3.806483	6.640058	-3.263676
H -3.670532	6.019688	0.989421
H -4.307242	7.429994	-0.959981
C 1.016871	3.247458	2.053818
C 0.157331	4.223559	1.542047
C 1.141373	3.089550	3.437625
C -0.577991	5.028570	2.409150
H 0.067044	4.360361	0.468634
C 0.381150	3.871603	4.300278
H 1.820469	2.334954	3.822144
C -0.478695	4.844058	3.787617
H -1.231391	5.794757	2.001084
H 0.460268	3.724768	5.374133
H -1.066471	5.460929	4.462782
O 0.455902	-1.209770	0.032496
Fe -0.024627	-3.024714	-0.287612
Cl -2.187163	-3.047417	-0.674534
Cl 0.555350	-4.376168	1.319692
Cl 1.062478	-3.455904	-2.220040

TS$_{C\text{-}is1/C\text{-}is2}$, B3PW91-D3/BSII=-3303.6852276

C -0.729802	-0.979628	3.492095
C -0.202624	-1.503961	2.316345
C -0.143019	-0.713347	1.163828
C -0.582389	0.625220	1.218745
C -1.119209	1.133906	2.402217
C -1.197934	0.333797	3.539581
H -0.780734	-1.608803	4.376781
H 0.139328	-2.532617	2.265515

C	-0.378766	1.469894	0.004055
H	-1.454127	2.166843	2.430954
H	-1.615170	0.736824	4.457880
C	1.030203	1.940443	-0.206140
C	1.892922	1.236275	-1.023093
C	1.593046	2.995628	0.643349
O	2.807557	3.256992	0.667237
N	3.210644	1.465711	-1.155479
H	3.519840	2.239403	-0.544027
C	-1.348671	1.689071	-0.857349
C	-2.335754	1.905019	-1.696414
H	-0.023159	0.045453	-1.624274
S	1.257065	-0.100184	-2.059988
C	1.183029	0.767601	-3.655207
H	2.208148	0.923448	-3.998186
H	0.652398	0.096131	-4.335132
H	0.654620	1.716036	-3.541129
H	-2.458307	1.222551	-2.539813
C	4.138313	0.674820	-1.881057
C	4.959297	1.298417	-2.826195
C	4.236925	-0.701757	-1.653626
C	5.864138	0.535002	-3.558372
H	4.873166	2.370251	-2.983928
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C	5.938231	-0.845588	-3.363296
H	6.503181	1.018098	-4.292389
H	5.172304	-2.532173	-2.248645
H	6.634747	-1.439492	-3.948360
C	-3.306551	3.005760	-1.576250
C	-3.996394	3.456148	-2.709466
C	-3.567376	3.612138	-0.338264
C	-4.904888	4.507320	-2.613481
H	-3.814942	2.981272	-3.671156
C	-4.474167	4.661862	-0.245115
H	-3.067652	3.238215	0.550986
C	-5.142720	5.117642	-1.382873
H	-5.430623	4.847772	-3.501666
H	-4.675278	5.114126	0.722921
H	-5.855944	5.933989	-1.307199
C	0.680623	3.779678	1.523655
C	-0.481542	4.383266	1.032495
C	1.035191	3.944457	2.866786
C	-1.290857	5.130406	1.884684
H	-0.750693	4.278827	-0.013856
C	0.207355	4.663237	3.722861
H	1.950432	3.487123	3.230103
C	-0.957464	5.256309	3.233165
H	-2.183218	5.608280	1.490323
H	0.471878	4.765112	4.771807
H	-1.600386	5.823760	3.901023
O	0.321820	-1.187198	-0.012389
Fe	0.106733	-2.866955	-0.816272
Cl	2.153769	-3.618598	-1.141167
Cl	-0.842941	-2.321331	-2.784743
Cl	-1.159497	-4.209564	0.324031

C-is2, B3PW91-D3/BSII=-3303.6852276

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C	0.175157	-1.333718	2.357272
C	0.200499	-0.629538	1.146123
C	-0.453212	0.618456	1.056864
C	-1.157120	1.102931	2.163170
C	-1.196701	0.387455	3.355202
H	-0.539126	-1.395417	4.377274
H	0.676414	-2.295347	2.402740
C	-0.321243	1.426936	-0.192286
H	-1.648653	2.067993	2.088389
H	-1.745357	0.781515	4.205727
C	1.065259	1.942124	-0.422762
C	1.917426	1.362469	-1.331244
C	1.638436	2.901959	0.541946
O	2.852060	3.149007	0.604076
N	3.242838	1.608347	-1.452207
H	3.538721	2.290283	-0.733332
C	-1.346213	1.642916	-0.982711
C	-2.390683	1.827273	-1.758151
H	0.128857	-0.201911	-2.123615
S	1.312685	0.290490	-2.665685
C	0.614222	1.540608	-3.783365
H	1.446731	2.140864	-4.155150
H	0.144757	0.998076	-4.608096
H	-0.113693	2.153497	-3.249956
H	-2.547575	1.117401	-2.572845
C	4.199018	0.654226	-1.902103
C	5.272674	1.093825	-2.679261
C	4.078831	-0.693195	-1.547845
C	6.222784	0.174102	-3.113639
H	5.348796	2.145706	-2.941226
C	5.016497	-1.608959	-2.015542

H 3.259058	-1.019710	-0.911677
C 6.090368	-1.178156	-2.792977
H 7.060611	0.512570	-3.717132
H 4.897770	-2.658384	-1.764332
H 6.825293	-1.894764	-3.148900
C -3.379616	2.907257	-1.610009
C -4.167310	3.283773	-2.706010
C -3.561136	3.572016	-0.388126
C -5.094174	4.317067	-2.591785
H -4.048645	2.763299	-3.653922
C -4.486061	4.603405	-0.275671
H -2.984074	3.256995	0.475793
C -5.253085	4.984597	-1.378381
H -5.696154	4.598529	-3.451850
H -4.622968	5.100869	0.681419
H -5.979885	5.787353	-1.287623
C 0.721047	3.632543	1.461848
C -0.413708	4.294741	0.982905
C 1.050146	3.707490	2.818743
C -1.221545	5.013456	1.860593
H -0.664690	4.252164	-0.072496
C 0.221823	4.396130	3.698414
H 1.943929	3.203441	3.173430
C -0.914872	5.050224	3.220680
H -2.092584	5.538108	1.477766
H 0.464396	4.427180	4.757065
H -1.557061	5.595211	3.907639
O 0.832910	-1.142943	0.068938
Fe 0.168793	-2.637791	-0.801938
Cl 1.777774	-3.263802	-2.164379
Cl -1.437138	-1.627042	-2.069919
Cl -0.606137	-4.210651	0.475493

C-is3, B3PW91-D3/BSII=-2865.0208612

C-2.681608	-1.581897	3.479310
C -1.622945	-2.026874	2.696254
C -1.032571	-1.160521	1.769165
C -1.464592	0.178663	1.689071
C -2.524950	0.610379	2.490870
C -3.145720	-0.267921	3.372004
H -3.147433	-2.268634	4.180778
H -1.262454	-3.047735	2.769099
C-0.728008	1.101752	0.801683
H-2.849459	1.644989	2.414074
H-3.974979	0.072505	3.985306
C 0.758976	1.036818	0.982897
C 1.538441	0.271023	0.270954
C 1.368785	1.660693	2.247705
O 1.850590	0.939289	3.095844
N 2.304375	-0.481477	-0.428629
H 2.144996	-1.500304	-0.363039
C -1.290228	1.974389	0.000335
C -1.832252	2.880144	-0.779860
H -2.062456	2.601451	-1.809973
C 3.198569	-0.046862	-1.456960
C 3.833508	1.189066	-1.361072
C 3.434509	-0.910699	-2.525220
C 4.714465	1.570858	-2.368241
H 3.650990	1.836812	-0.511348
C 4.318434	-0.513433	-3.524843
H 2.911866	-1.860897	-2.581271
C 4.957246	0.724450	-3.450663
H 5.217819	2.531000	-2.298725
H 4.499837	-1.174668	-4.366918
H 5.646785	1.027789	-4.233373
C -2.084521	4.276335	-0.397783
C -2.536088	5.186522	-1.362929
C -1.824034	4.741565	0.900343
C -2.714823	6.530514	-1.042679
H -2.741663	4.836855	-2.372513
C -2.001213	6.081257	1.218088
H -1.459100	4.046046	1.651137
C -2.445437	6.983080	0.247778
H -3.064893	7.224162	-1.802804
H -1.785446	6.427303	2.225458
H-2.582769	8.031575	0.498751
C1.270782	3.132042	2.385178
C1.098178	3.970796	1.277663
C 1.360088	3.679755	3.673989
C 0.987133	5.345943	1.463485
H 1.042774	3.549179	0.276985
C 1.238532	5.050893	3.853075
H 1.508496	3.010110	4.515868
C 1.043485	5.883946	2.748002
H 0.839347	5.995919	0.605965
H 1.284871	5.474415	4.852376
H 0.928749	6.954797	2.891498
O -0.042789	-1.552528	0.940589
Fe 0.463613	-3.294097	0.359307
Cl 1.175987	-3.088160	-1.708761

Cl -1.122334	-4.774484	0.557941
Cl 2.231777	-3.730503	1.695403

$TS_{C\text{-}is3/D}$, B3PW91-D3/BSII=-2865.0193129

C -2.681608	-1.581897	3.479310
C -1.622945	-2.026874	2.696254
C -1.032571	-1.160521	1.769165
C -1.464592	0.178663	1.689071
C -2.524950	0.610379	2.490870
C -3.145720	-0.267921	3.372004
H -3.147433	-2.268634	4.180778
H -1.262454	-3.047735	2.769099
C -0.728008	1.101752	0.801683
H -2.849459	1.644989	2.414074
H -3.974979	0.072505	3.985306
C 0.758976	1.036818	0.982897
C 1.456892	-0.053365	0.823885
C 1.462924	2.214911	1.673825
O 1.938119	2.060514	2.779380
N 2.527511	-0.732899	0.638583
H 2.649635	-1.579592	1.218159
C -1.290228	1.974389	0.000335
C -1.832252	2.880144	-0.779860
H -2.062456	2.601451	-1.809973
C 3.452850	-0.566343	-0.439353
C 3.683780	0.696483	-0.979541
C 4.131566	-1.694379	-0.897546
C 4.607197	0.825929	-2.012394
H 3.159762	1.563709	-0.594517
C 5.051917	-1.547799	-1.931886
H 3.918081	-2.668658	-0.468154
C 5.290318	-0.292447	-2.491526
H 4.797078	1.808056	-2.436000
H 5.577118	-2.422649	-2.303412
H 6.010697	-0.184801	-3.297491
C -2.084521	4.276335	-0.397783
C -2.536088	5.186522	-1.362929
C-1.824034	4.741565	0.900343
C -2.714823	6.530514	-1.042679
H -2.741663	4.836855	-2.372513
C -2.001213	6.081257	1.218088
H-1.459100	4.046046	1.651137
C -2.445437	6.983080	0.247778
H -3.064893	7.224162	-1.802804
H -1.785446	6.427303	2.225458
H -2.582769	8.031575	0.498751
C 1.461247	3.511594	0.958295
C 1.289646	3.593370	-0.428700
C 1.642659	4.680084	1.713756
C 1.271308	4.838968	-1.050020
H 1.162910	2.688056	-1.017369
C 1.613287	5.919395	1.089167
H 1.788298	4.590198	2.786099
C 1.419073	5.999557	-0.292521
H 1.124373	4.903816	-2.124197
H 1.731038	6.826195	1.675656
H 1.376556	6.971001	-0.777255
O -0.042789	-1.552528	0.940589
Fe 0.463613	-3.294097	0.359307
Cl 1.175987	-3.088160	-1.708761
Cl -1.122334	-4.774484	0.557941
Cl 2.231777	-3.730503	1.695403

D, B3PW91-D3/BSII=-2865.0872217

C -2.382709	-1.978572	-1.451024
C -1.130226	-1.869395	-0.858913
C -0.688223	-0.619541	-0.436580
C -1.453966	0.537918	-0.590294
C -2.713443	0.399009	-1.188161
C -3.176438	-0.839801	-1.612133
H -2.738936	-2.949655	-1.782928
H -0.486931	-2.730410	-0.706231
C-0.901499	1.836449	-0.148481
H -3.322959	1.289575	-1.314668
H-4.157535	-0.919250	-2.071793
C 0.481166	1.791929	0.362310
C 1.084686	0.580155	0.557966
C 1.123622	3.058655	0.789659
N 2.257970	0.379218	1.244472
H 2.540427	1.160082	1.819851
C -1.602167	2.947654	-0.288661
C -2.392645	3.986260	-0.411439
O 0.544681	-0.601892	0.179087
H -2.407196	4.537477	-1.355720
C -3.266317	4.498764	0.658828
C -4.345984	5.334829	0.344886
C -3.031246	4.170618	2.002590
C -5.188876	5.811716	1.345922
H -4.527786	5.605652	-0.693405
C -3.873464	4.648294	2.999770

H	-2.163013	3.565154	2.247371
C	-4.958295	5.466464	2.676685
H	-6.025827	6.455316	1.085976
H	-3.677234	4.391465	4.037996
H	-5.613119	5.840893	3.459505
C	3.323558	-0.445387	0.835074
C	3.371213	-1.066240	-0.418953
C	4.398440	-0.598607	1.719464
C	4.476385	-1.839044	-0.764853
H	2.551496	-0.948485	-1.118300
C	5.502678	-1.360484	1.356025
H	4.362200	-0.116236	2.693641
C	5.548023	-1.991216	0.113038
H	4.499968	-2.318017	-1.740425
H	6.329924	-1.465067	2.053145
H	6.408104	-2.592322	-0.167719
C	2.595531	3.260854	0.578503
C	3.302569	2.631650	-0.455003
C	3.267068	4.150549	1.426534
C	4.662323	2.870480	-0.622374
H	2.781732	1.952884	-1.124124
C	4.629262	4.382323	1.263837
H	2.699061	4.650467	2.205847
C	5.329034	3.740966	0.240581
H	5.202521	2.373273	-1.423175
H	5.146536	5.065134	1.932849
H	6.393460	3.921419	0.113824
O	0.439656	3.980201	1.305909
Fe	0.127203	5.510252	2.561802
Cl	2.108657	6.340459	2.886112
Cl	-0.775785	4.557364	4.313448
Cl	-1.253438	6.810633	1.468755

HSMe, B3PW91-D3/BSII=-438.6351064

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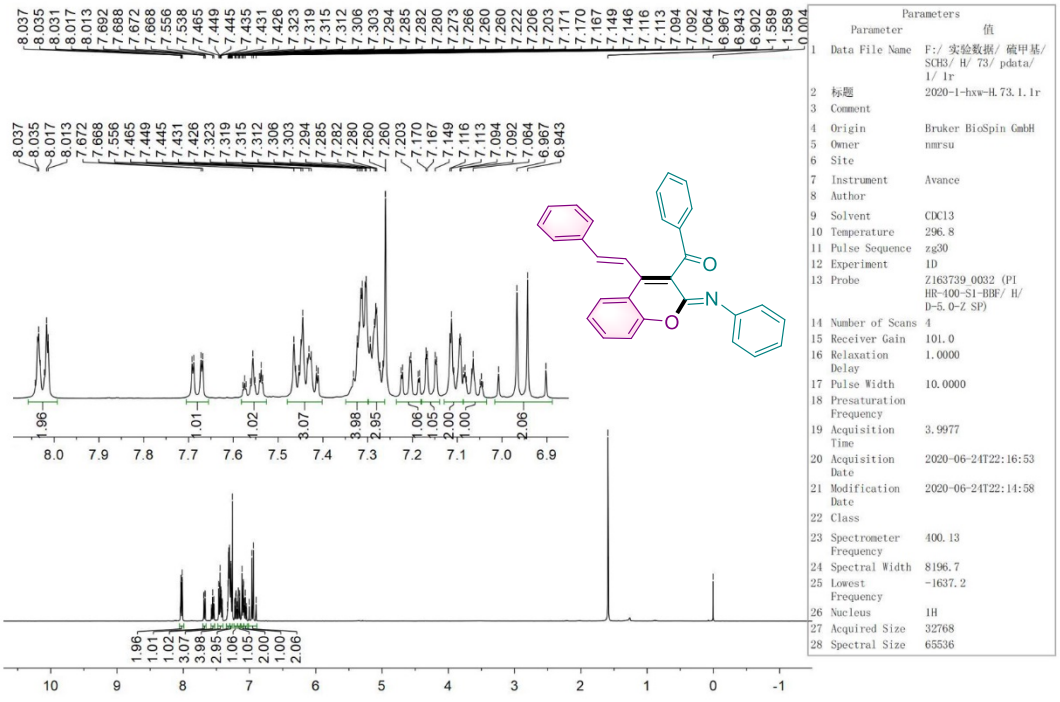
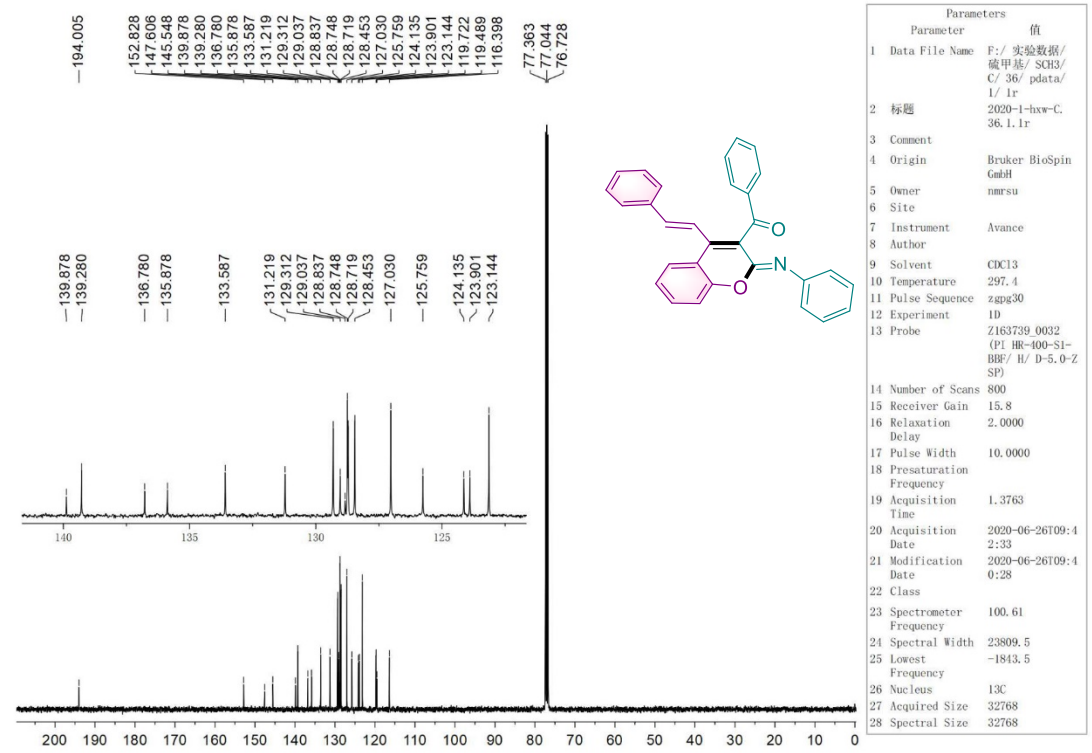
H	-1.446865	1.740072	-0.079557
C	0.770421	0.505214	-0.081951
H	1.127087	-0.503590	-0.081951
H	1.127087	1.009617	-0.955602
H	1.127088	1.009617	0.791699

18. ^{1}H, and ^{13}C NMR spectra for all compounds

Phenyl((*Z*)-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)methanone (Figure 2, compound 3aa)

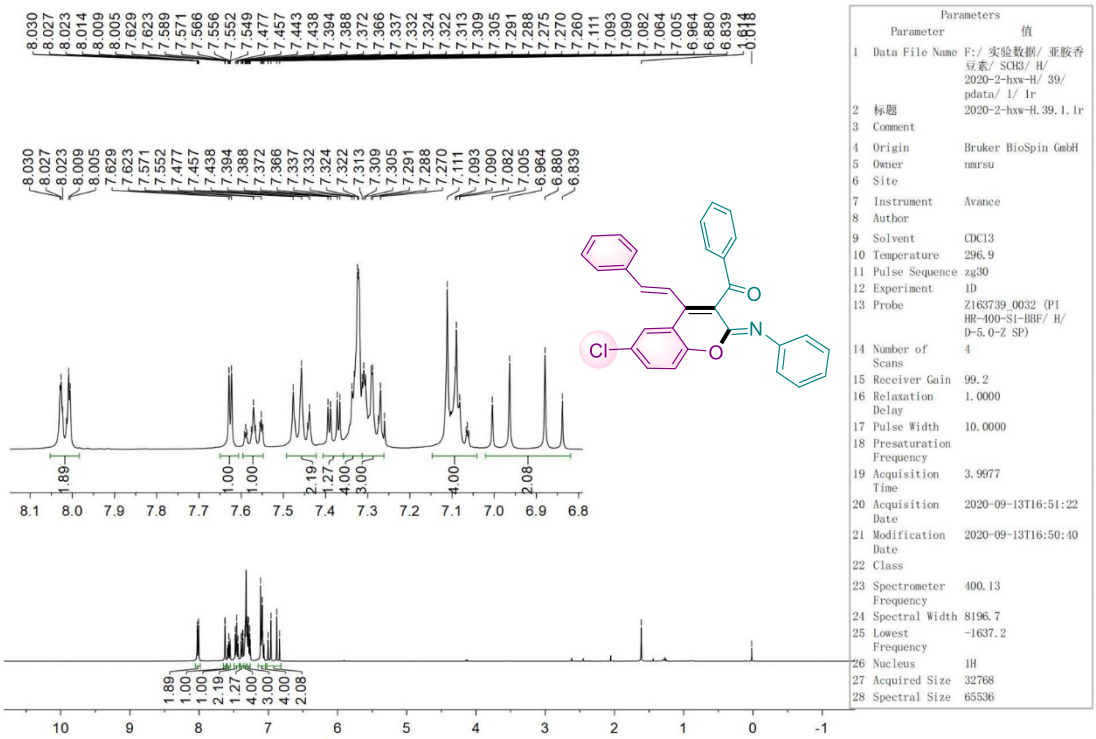


^{1}H NMR Spectra of compound 3aa



^{13}C NMR Spectra of compound 3aa

((*Z*)-6-Chloro-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)(phenyl)methanone (Figure 2, compound 3ba)



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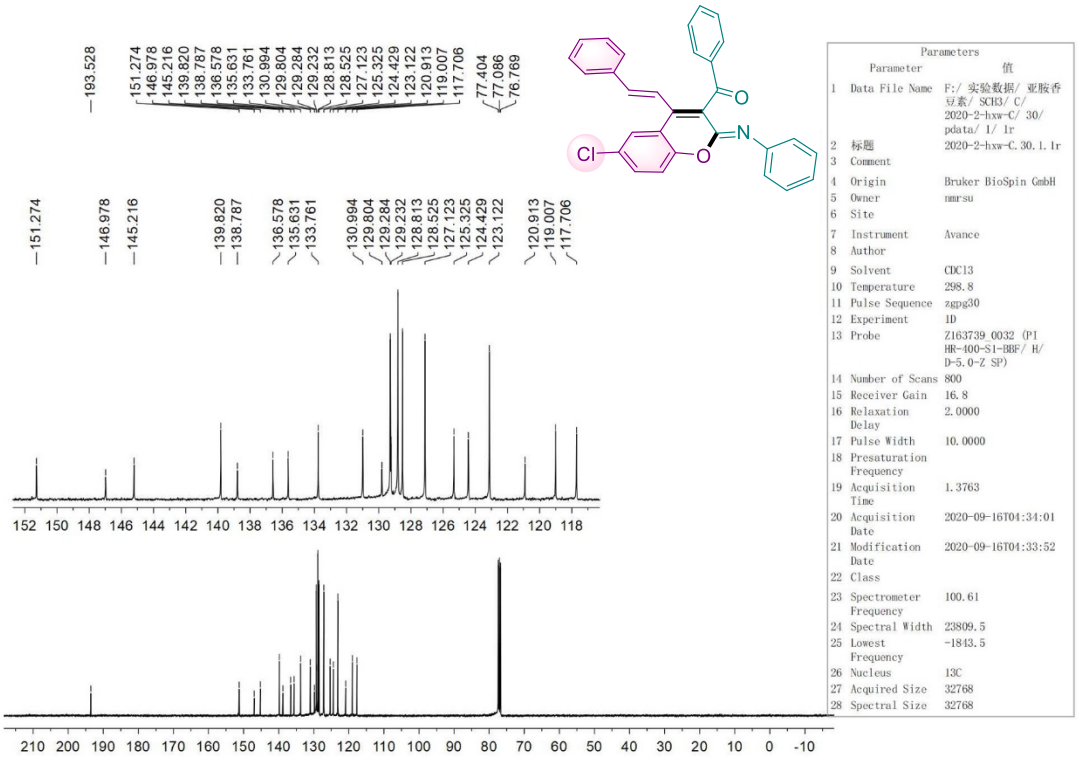
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	296.9
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14	Number of Scans	4
15	Receiver Gain	99.2
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	3.9977
20	Acquisition Date	2020-09-13T16:51:22
21	Modification Date	2020-09-13T16:50:40
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8196.7
25	Lowest Frequency	-1637.2
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

^{1}H NMR Spectra of compound 3ba



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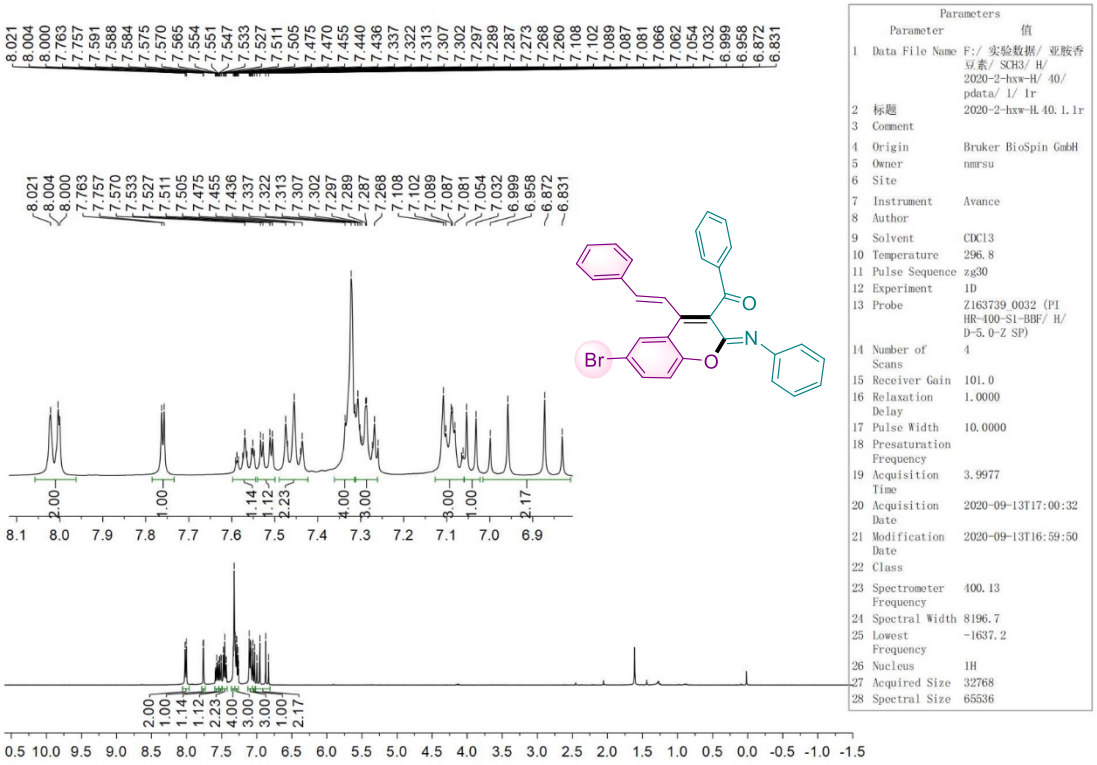
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	298.8
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14	Number of Scans	800
15	Receiver Gain	16.8
16	Relaxation Delay	2.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	1.3763
20	Acquisition Date	2020-09-16T04:34:01
21	Modification Date	2020-09-16T04:33:52
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	23809.5
25	Lowest Frequency	-1843.5
26	Nucleus	13C
27	Acquired Size	32768
28	Spectral Size	32768

^{13}C NMR Spectra of compound 3ba

((*Z*)-6-Bromo-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)(phenyl)methanone (Figure 2, compound 3ca)



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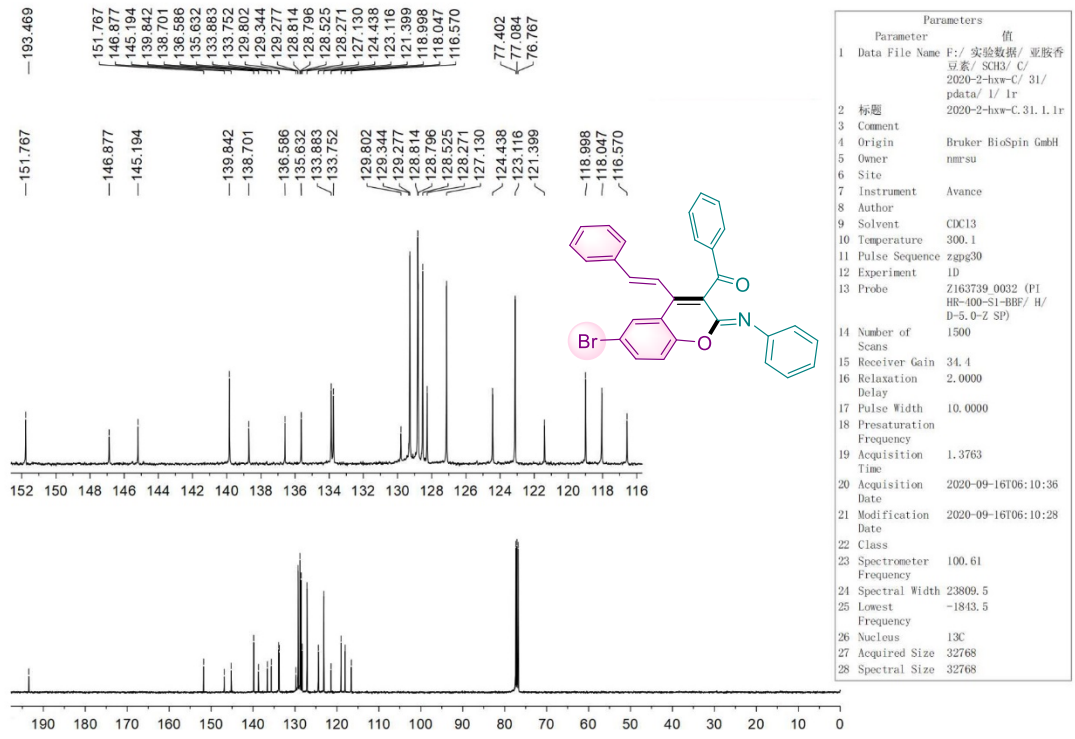
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	296.8
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14	Number of Scans	4
15	Receiver Gain	101.0
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	3.9977
20	Acquisition Date	2020-09-13T17:00:32
21	Modification Date	2020-09-13T16:59:50
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8196.7
25	Lowest Frequency	-1637.2
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

^{1}H NMR Spectra of compound 3ca



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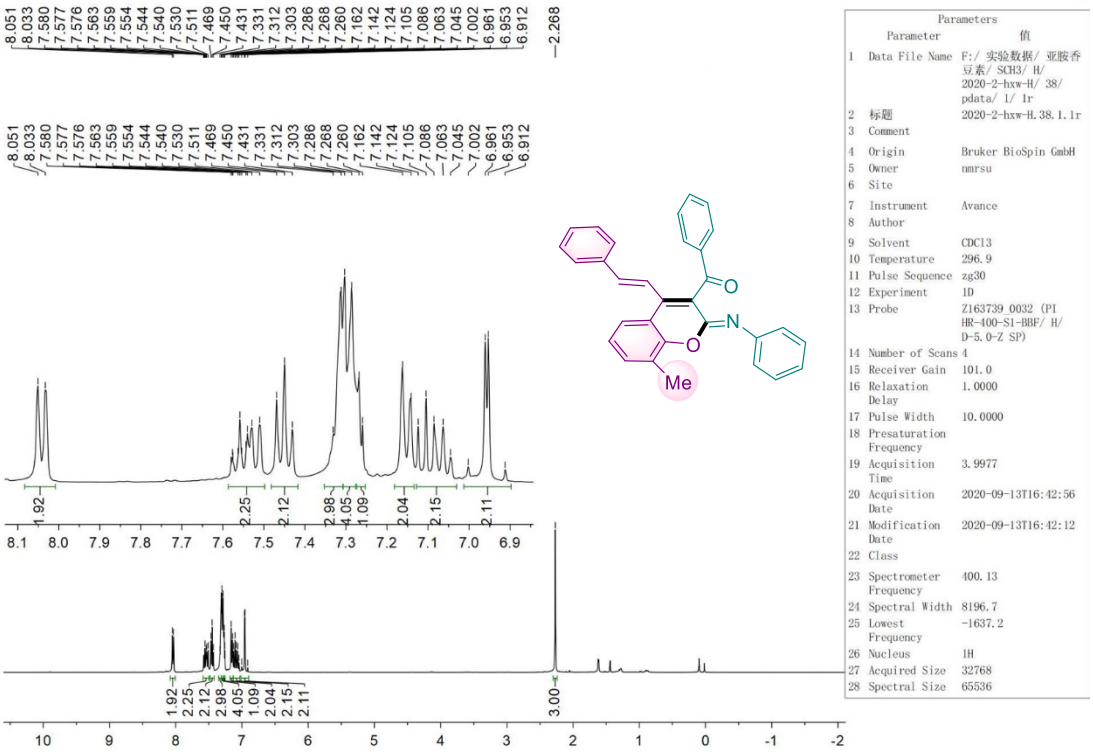
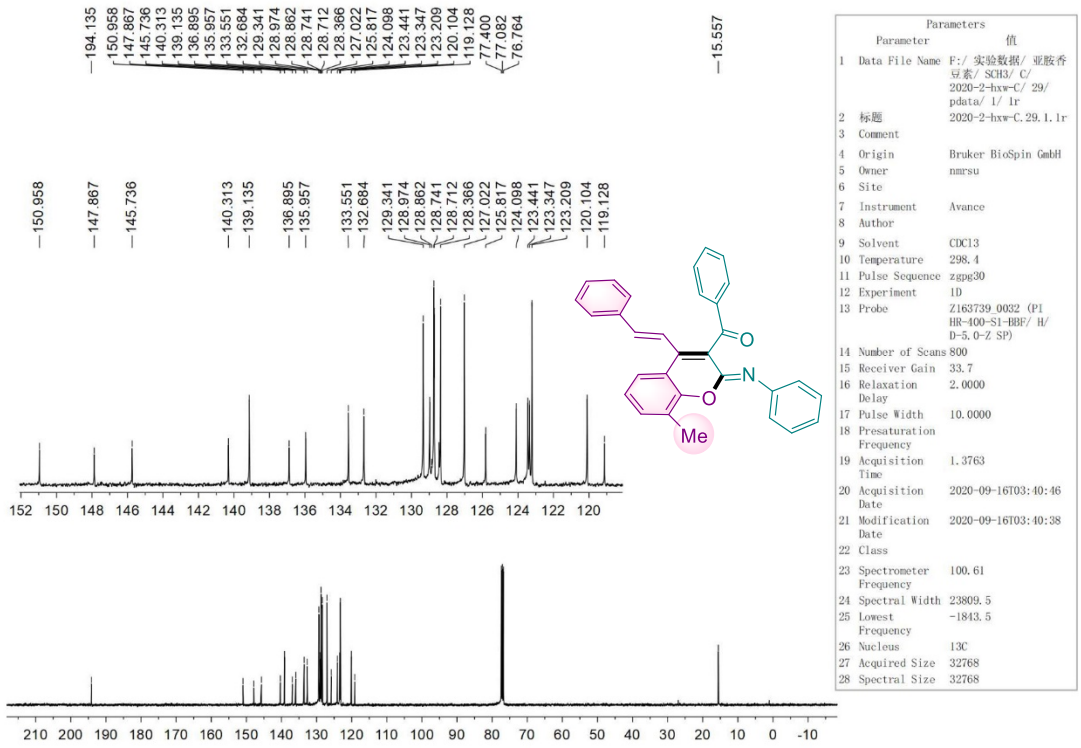
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	300.1
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14	Number of Scans	1500
15	Receiver Gain	34.4
16	Relaxation Delay	2.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	1.3763
20	Acquisition Date	2020-09-16T06:10:36
21	Modification Date	2020-09-16T06:10:28
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	23809.5
25	Lowest Frequency	-1843.5
26	Nucleus	13C
27	Acquired Size	32768
28	Spectral Size	32768

^{13}C NMR Spectra of compound 3ca

((Z)-8-Methyl-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)(phenyl)methanone (Figure 2, compound 3da)

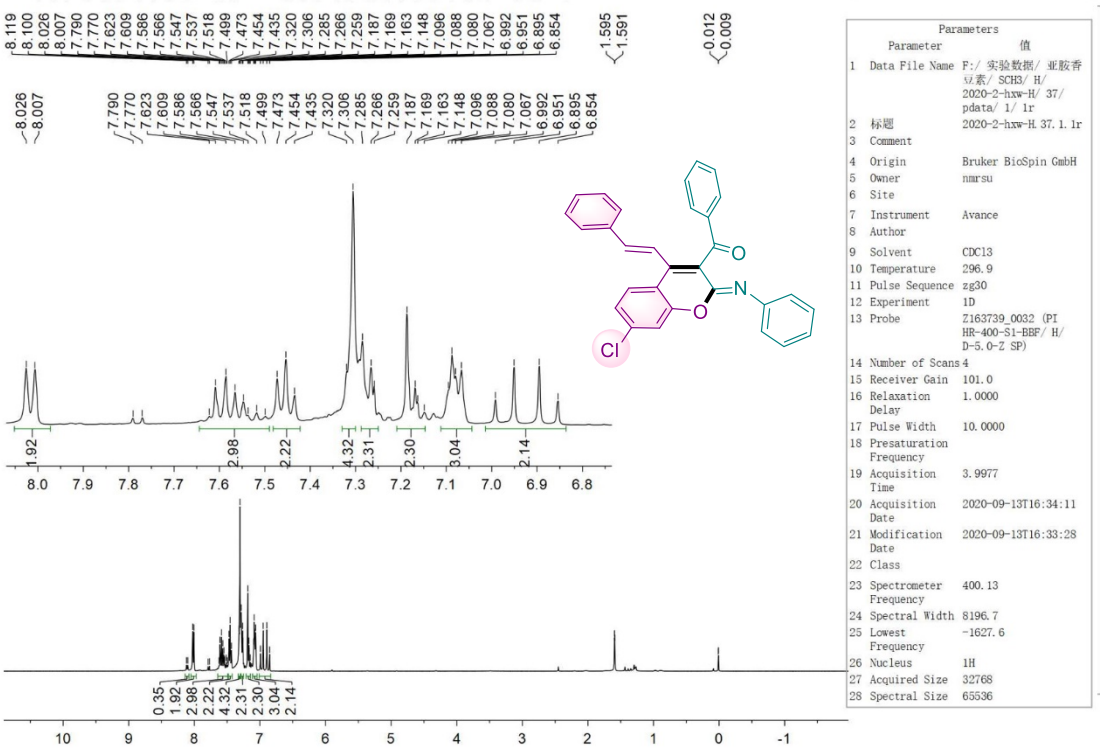


^{1}H NMR Spectra of compound 3da



^{13}C NMR Spectra of compound 3da

((*Z*)-7-Chloro-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)(phenyl)methanone (Figure 2, compound 3ea)



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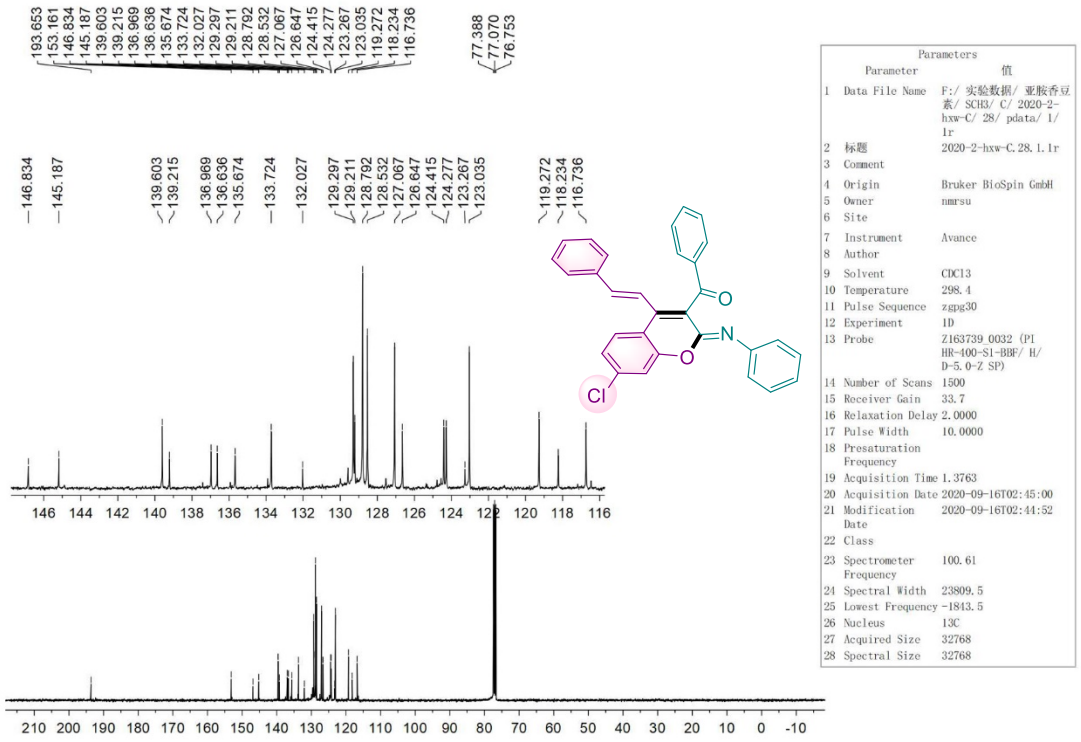
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	296.9
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14	Number of Scans	4
15	Receiver Gain	101.0
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	3.9977
20	Acquisition Date	2020-09-13T16:34:11
21	Modification Date	2020-09-13T16:33:28
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8196.7
25	Lowest Frequency	-1627.6
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

^{1}H NMR Spectra of compound 3ea



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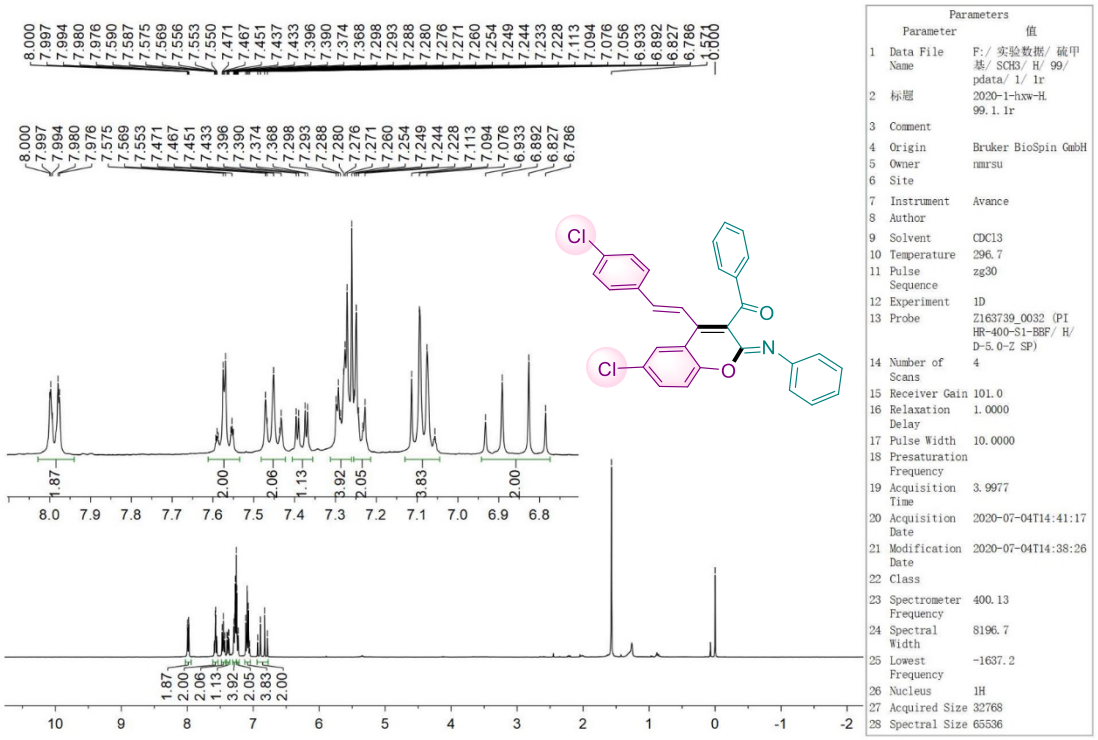
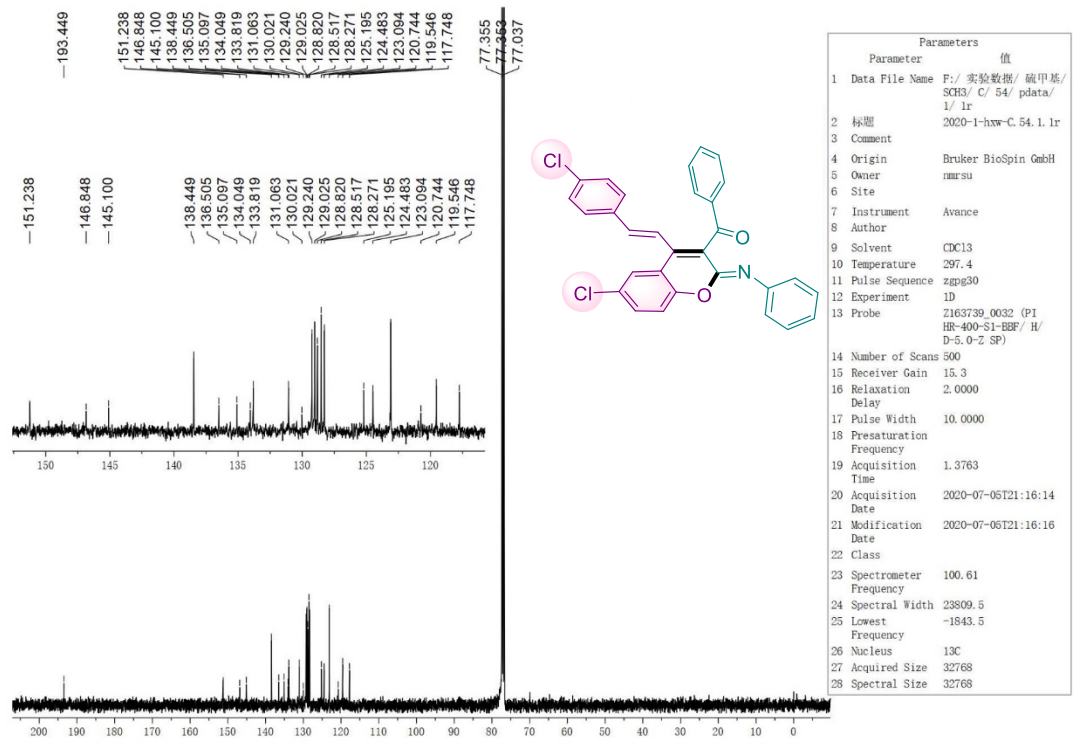
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	298.4
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14	Number of Scans	1500
15	Receiver Gain	33.7
16	Relaxation Delay	2.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	1.3763
20	Acquisition Date	2020-09-16T02:45:00
21	Modification Date	2020-09-16T02:44:52
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	23809.5
25	Lowest Frequency	-1843.5
26	Nucleus	13C
27	Acquired Size	32768
28	Spectral Size	32768

^{13}C NMR Spectra of compound 3ea

((*Z*)-6-Chloro-4-((*E*)-4-chlorostyryl)-2-(phenylimino)-2*H*-chromen-3-yl)(phenyl)methanone (Figure 2, compound 3fa)

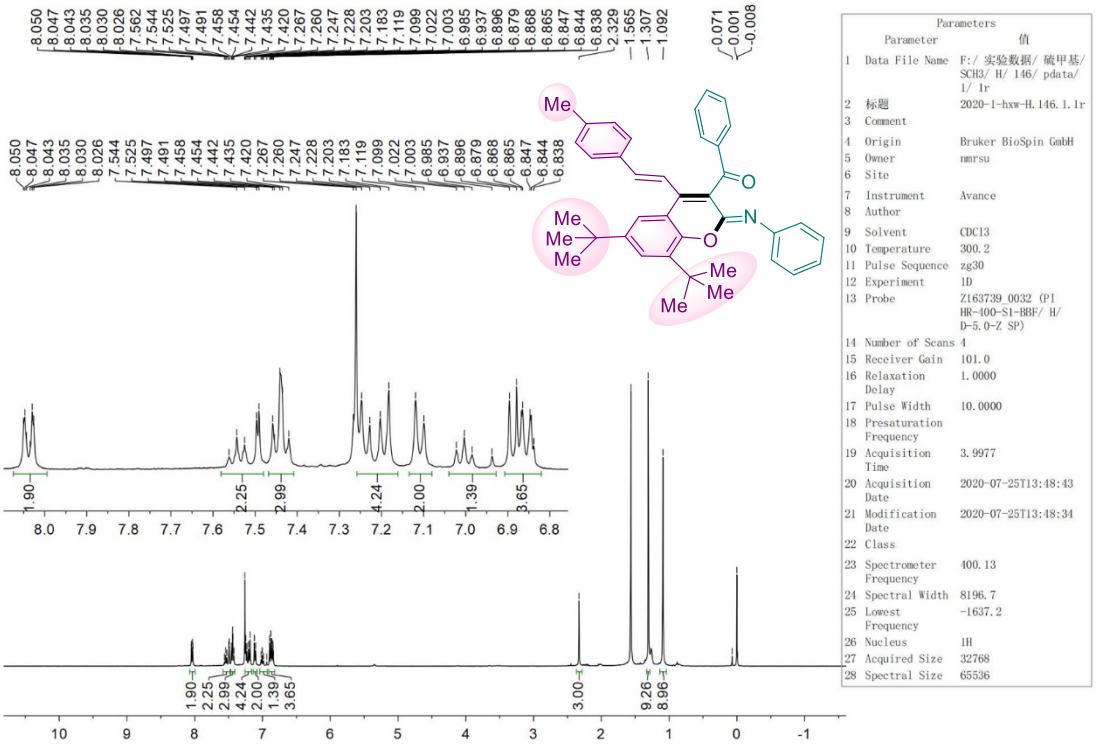


^{1}H NMR Spectra of compound 3fa

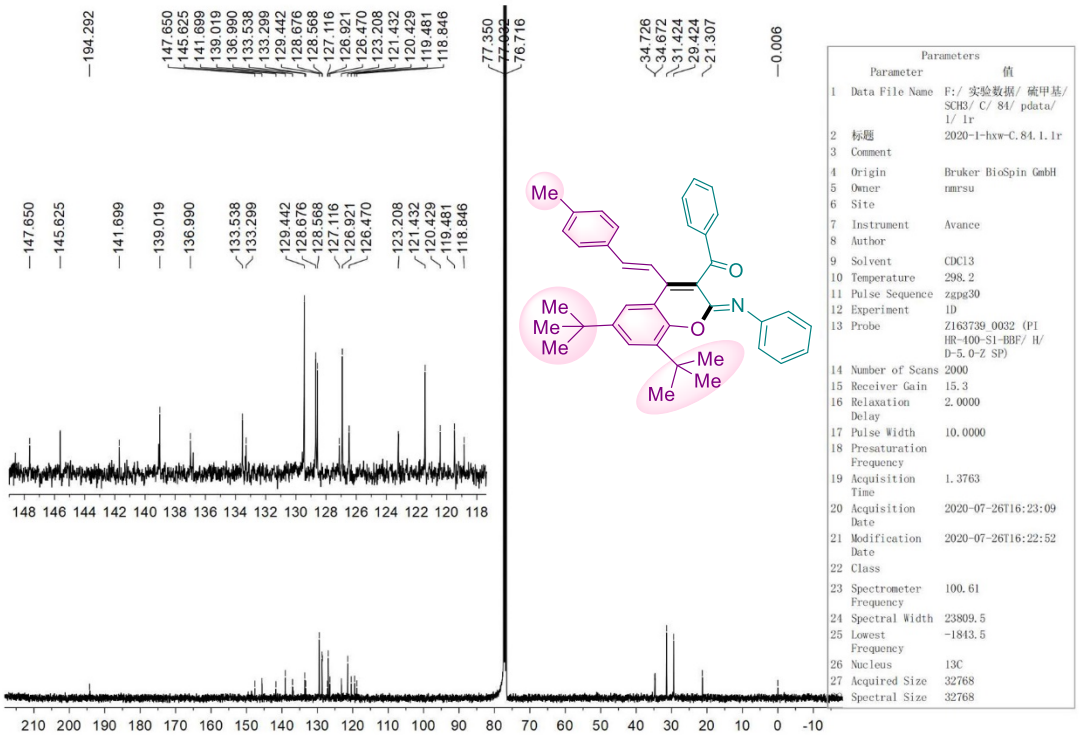


^{13}C NMR Spectra of compound 3fa

((*Z*)-6,8-Di-*tert*-butyl-4-((*E*)-4-methylstyryl)-2-(phenylimino)-2*H*-chromen-3-yl)(phenyl)methanone (Figure 2, compound 3ga)

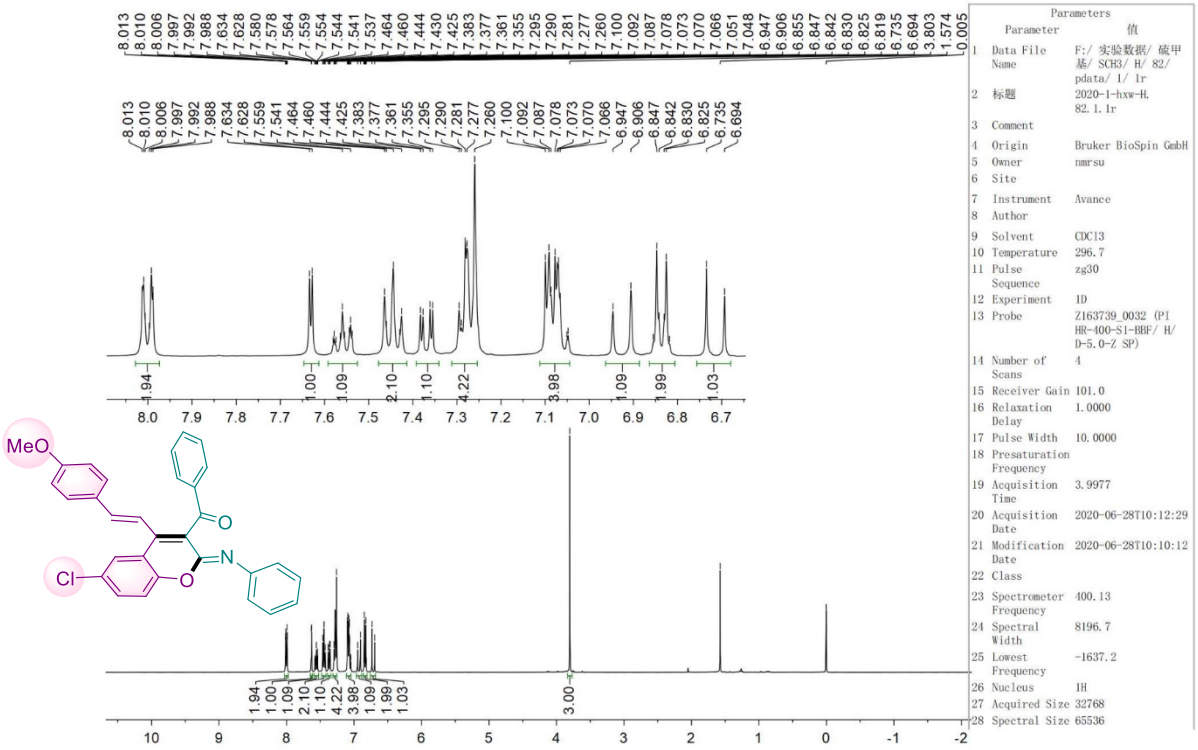


^{1}H NMR Spectra of compound 3ga

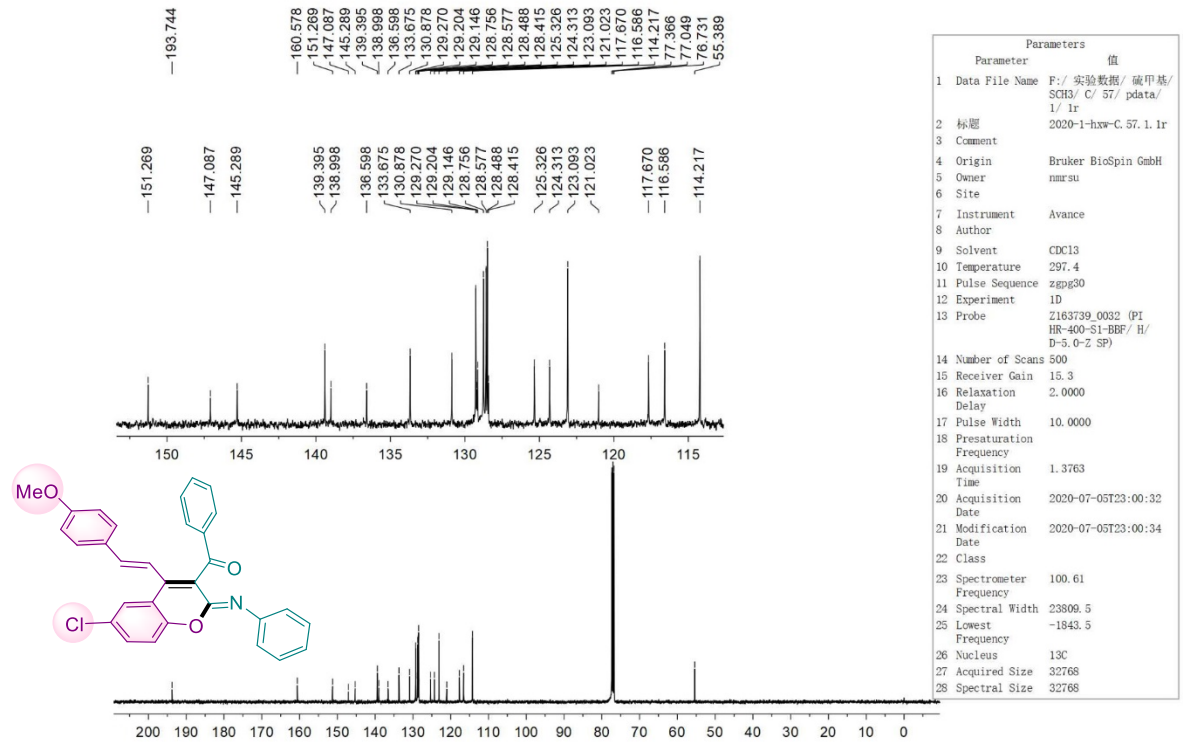


^{13}C NMR Spectra of compound 3ga

((*Z*)-6-Chloro-4-((*E*)-4-methoxystyryl)-2-(phenylimino)-2*H*-chromen-3-yl)(phenyl)methanone (Figure 2, compound 3ha)

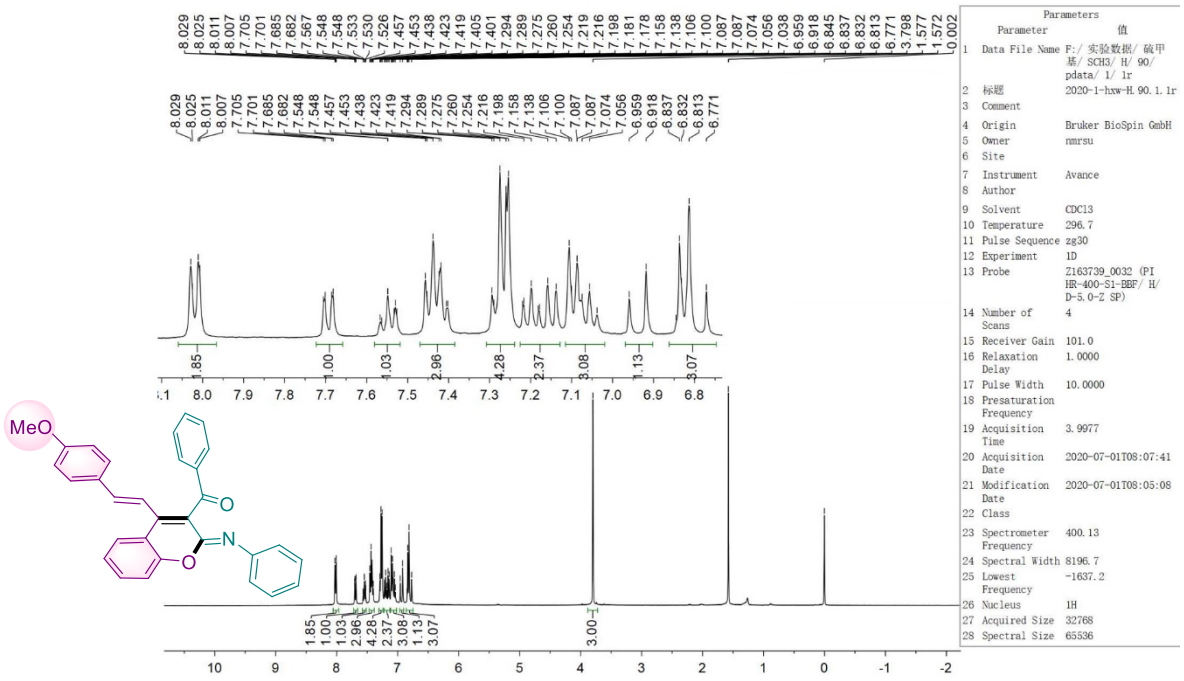


^{1}H NMR Spectra of compound 3ha

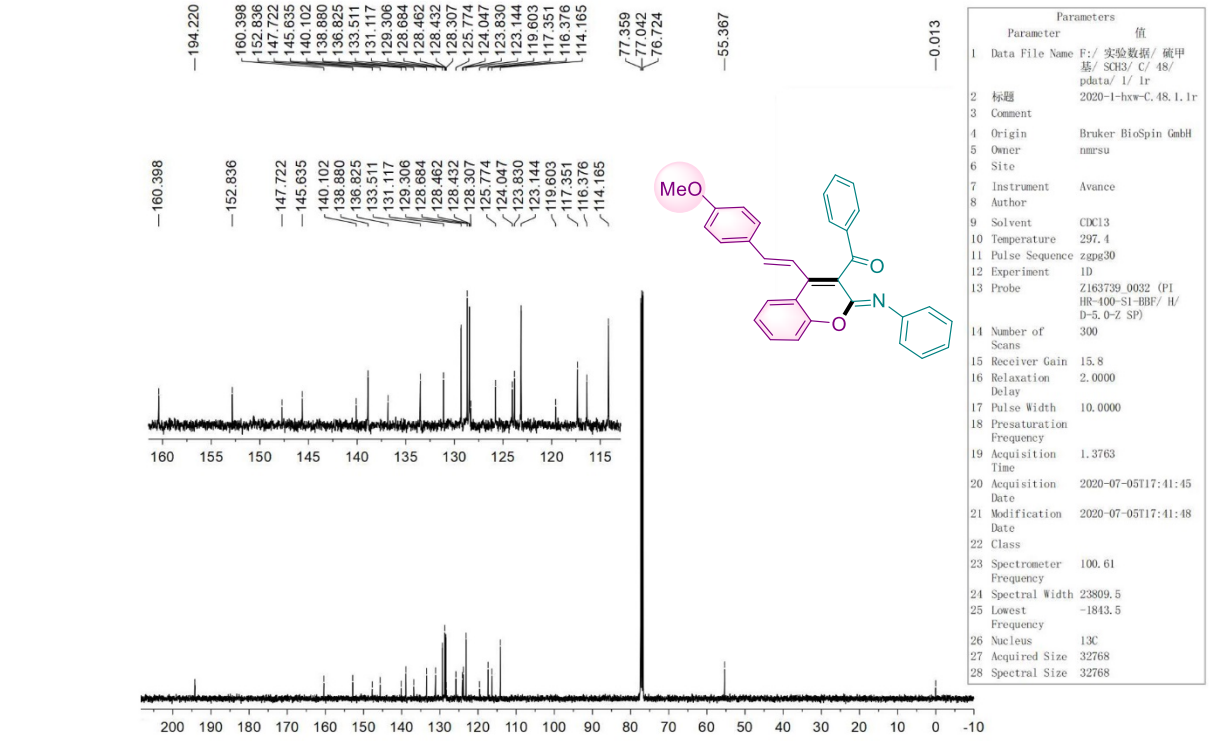


^{13}C NMR Spectra of compound 3ha

((*Z*)-4-((*E*)-4-Methoxystyryl)-2-(phenylimino)-2*H*-chromen-3-yl)(phenyl)methanone (Figure 2, compound 3ia)

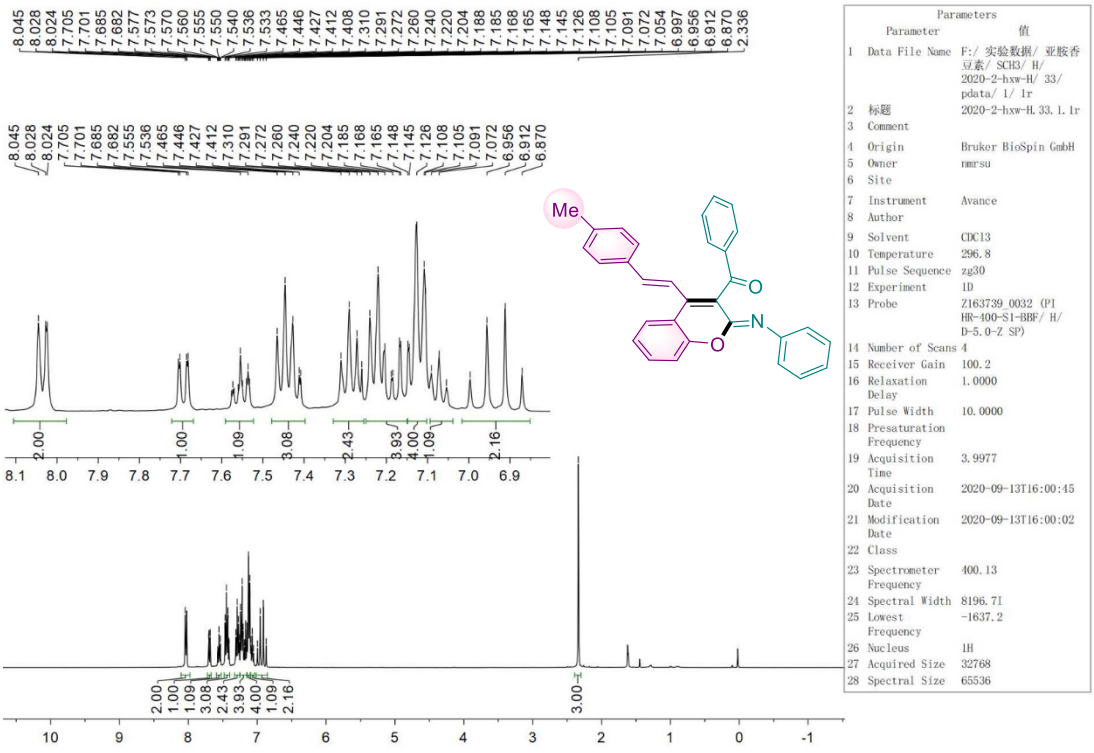


^{1}H NMR Spectra of compound 3ia

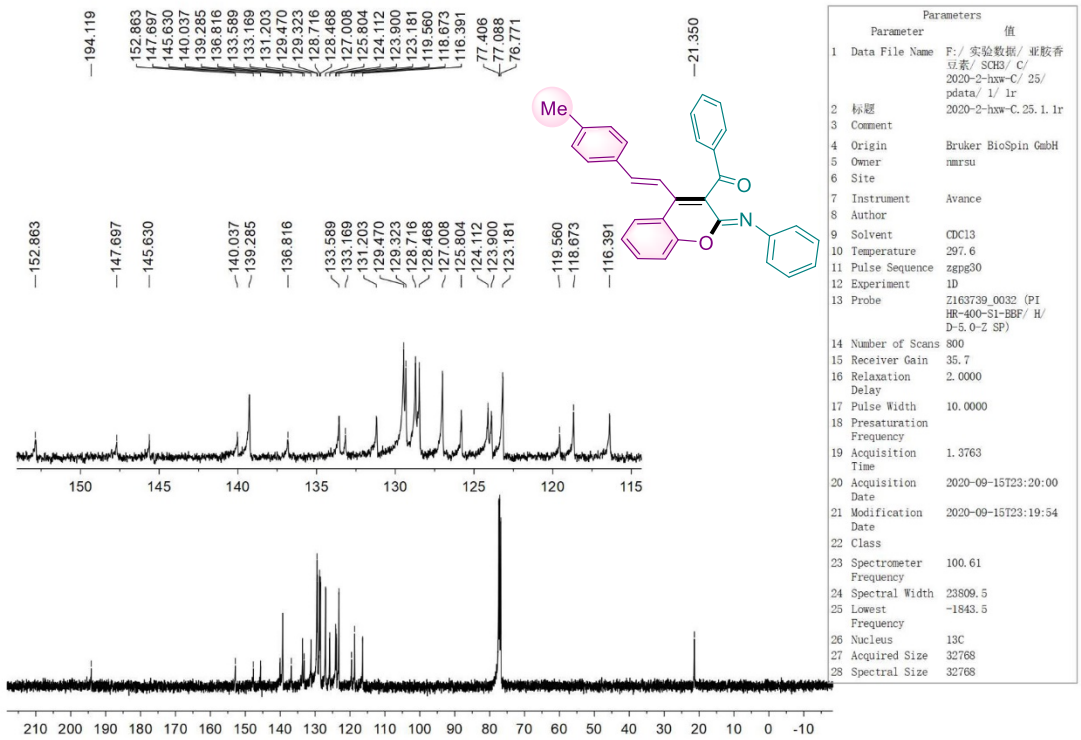


^{13}C NMR Spectra of compound 3ia

((*Z*)-4-((*E*)-4-Methylstyryl)-2-(phenylimino)-2*H*-chromen-3-yl)(phenyl)methanone (Figure 2, compound 3ja)

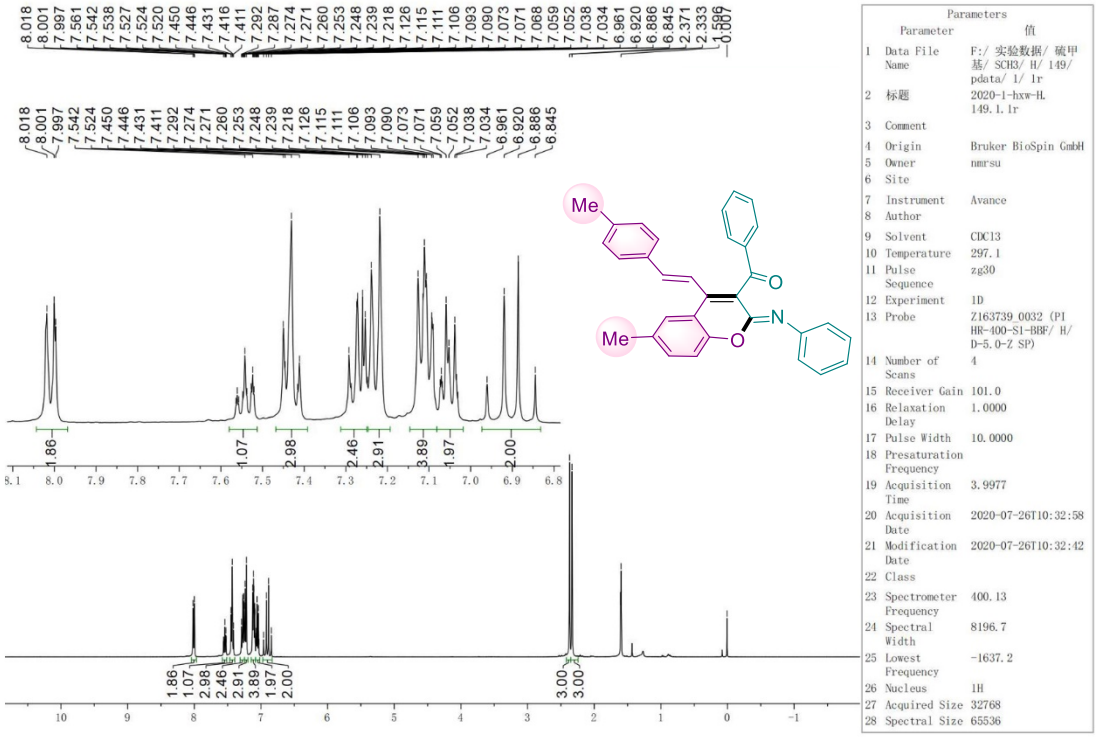


^{1}H NMR Spectra of compound 3ja

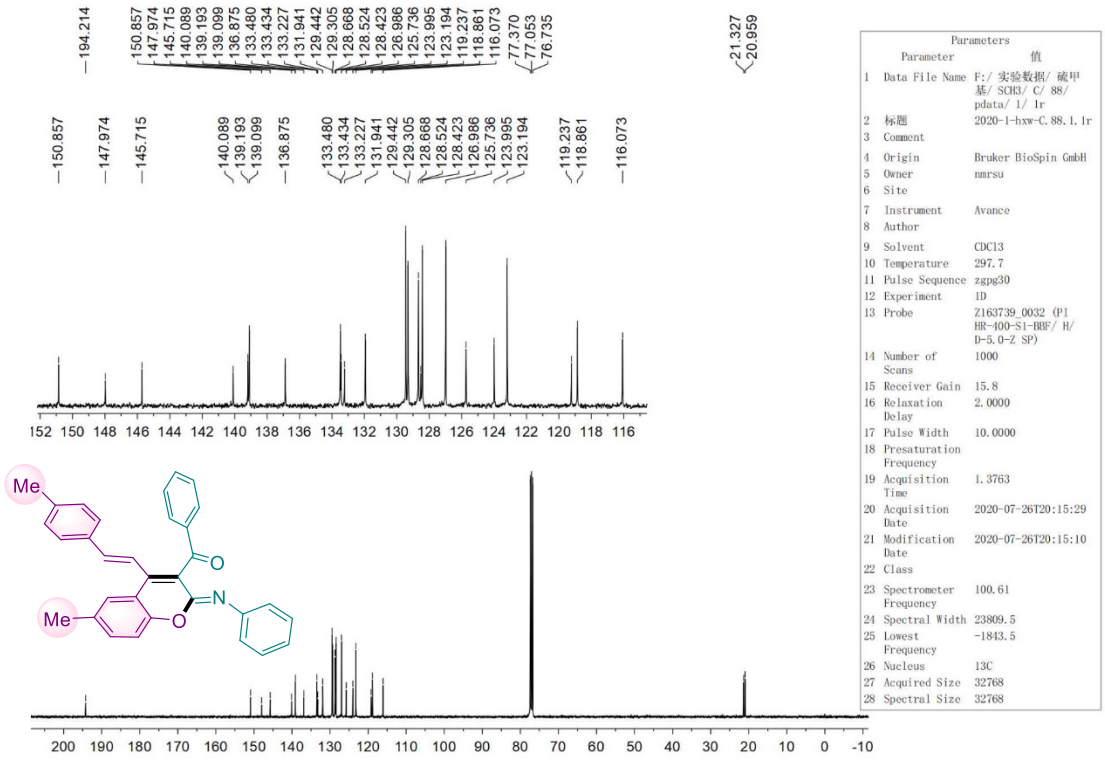


^{13}C NMR Spectra of compound 3ja

((*Z*)-6-Methyl-4-((*E*)-4-methylstyryl)-2-(phenylimino)-2*H*-chromen-3-yl)(phenyl)methanone (Figure 2, compound 3ka)

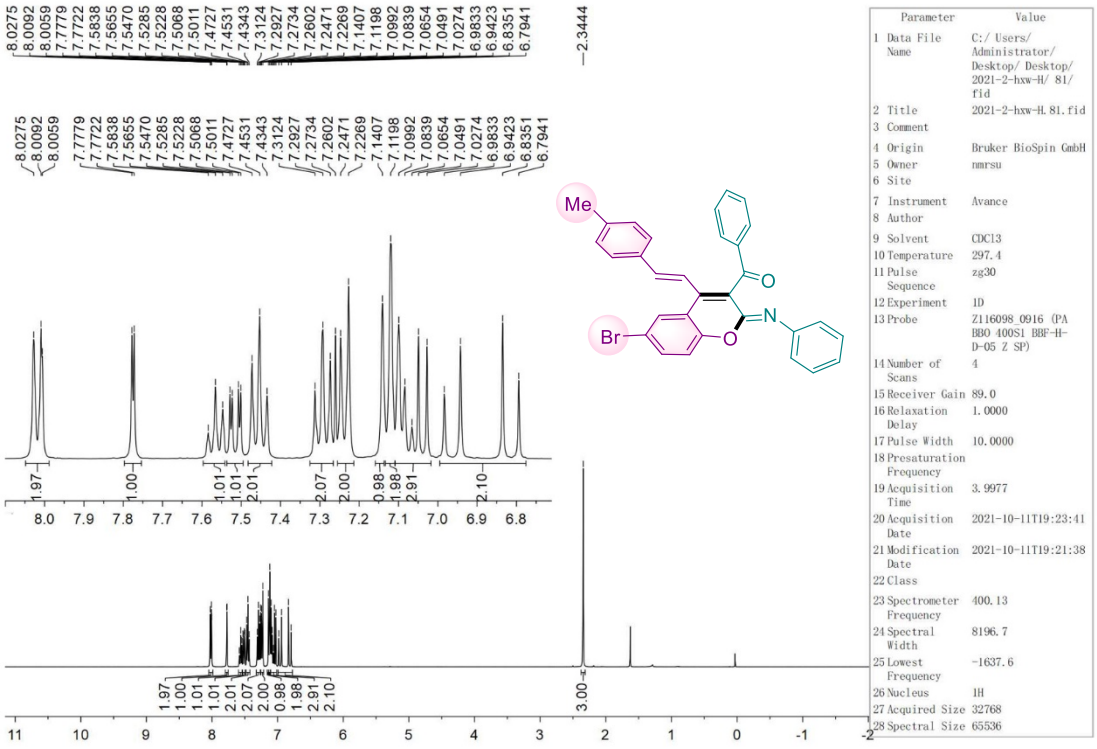


^{1}H NMR Spectra of compound 3ka

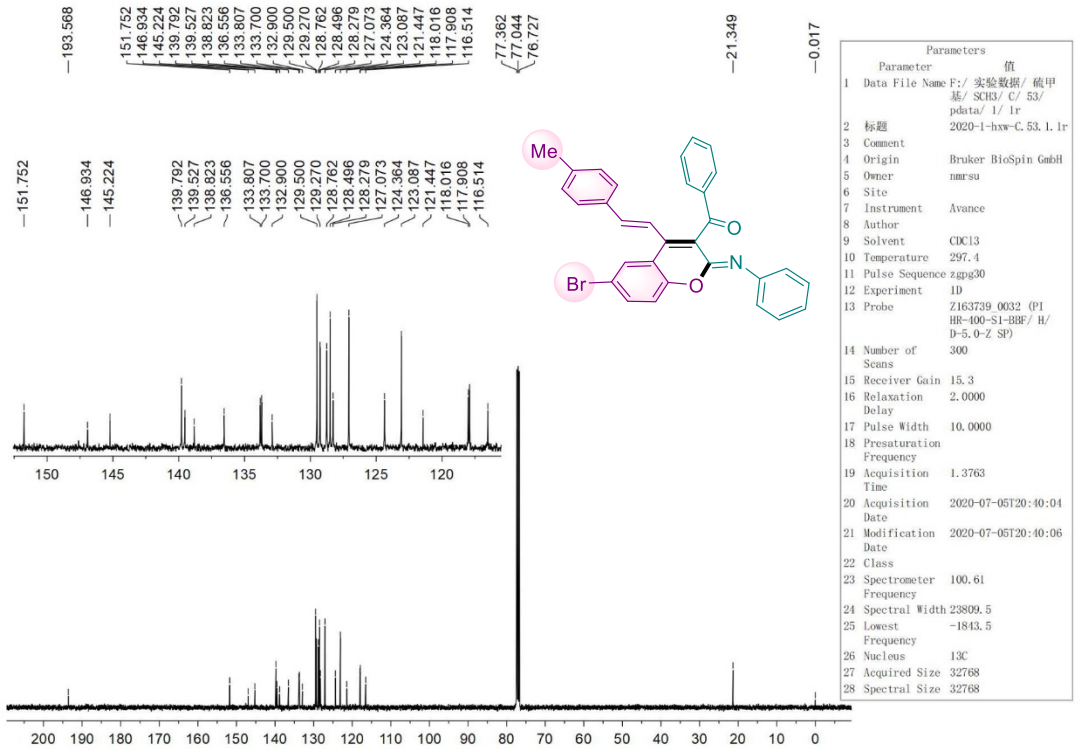


^{13}C NMR Spectra of compound 3ka

((*Z*)-6-Bromo-4-((*E*)-4-methylstyryl)-2-(phenylimino)-2*H*-chromen-3-yl)(phenyl)methanone (Figure 2, compound 3la)

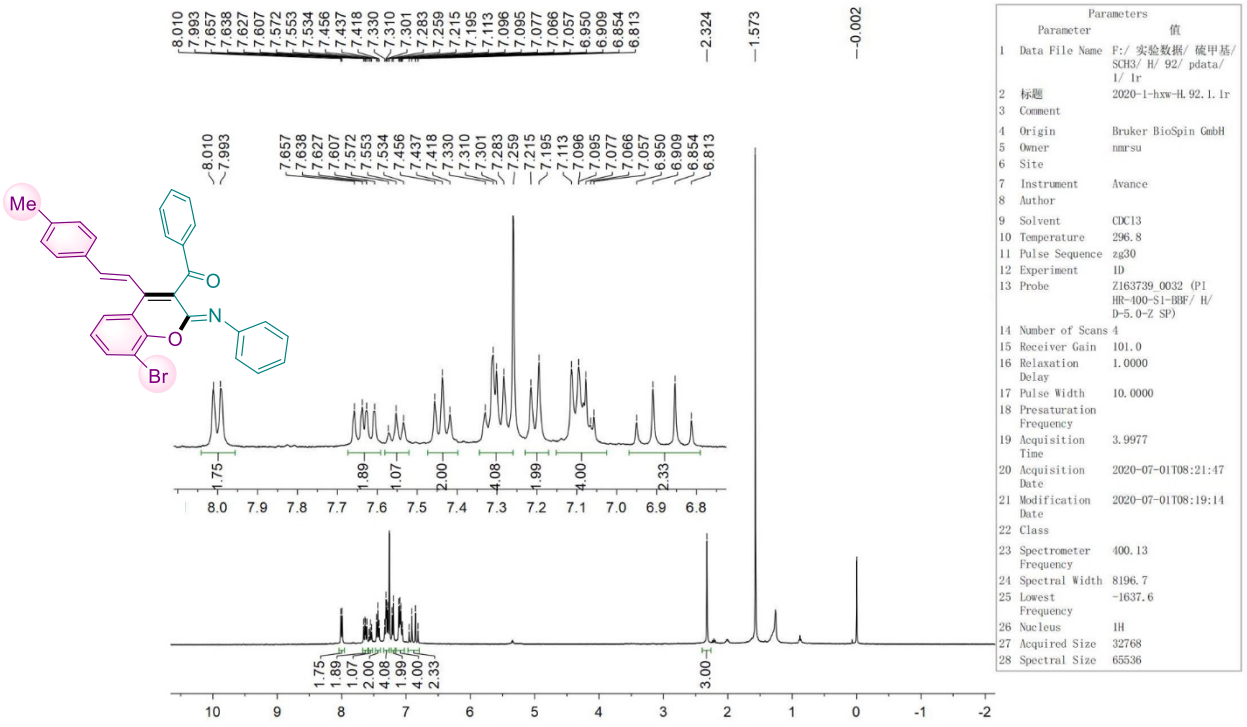


^{1}H NMR Spectra of compound 3la

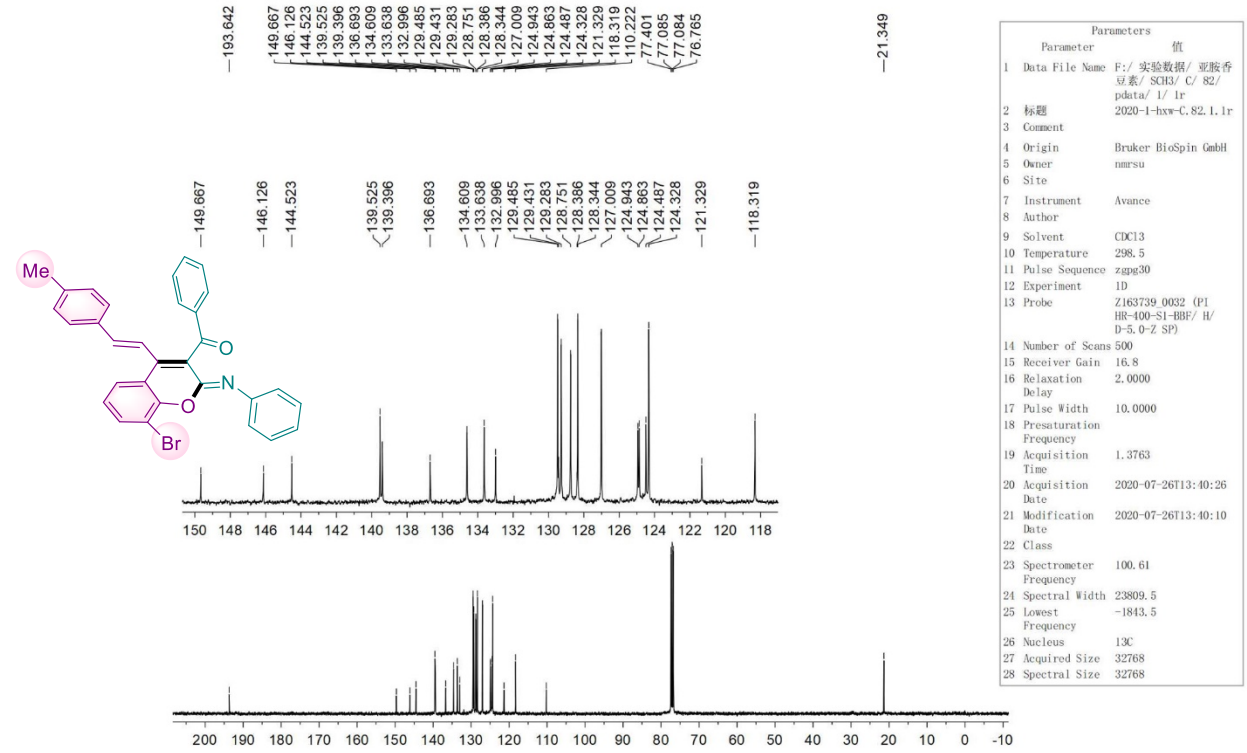


^{13}C NMR Spectra of compound 3la

((*Z*)-8-Bromo-4-((*E*)-4-methylstyryl)-2-(phenylimino)-2*H*-chromen-3-yl)(phenyl)methanone (Figure 2, compound 3ma)

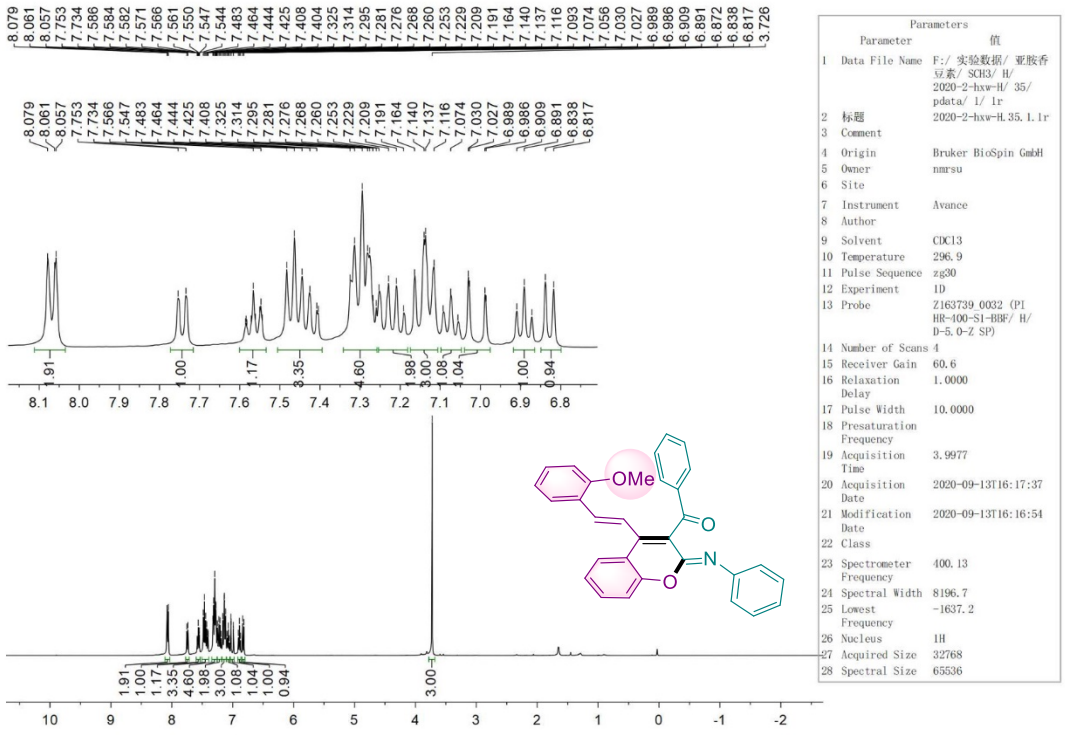


^{1}H NMR Spectra of compound 3ma



^{13}C NMR Spectra of compound 3ma

((*Z*)-4-((*E*)-2-Methoxystyryl)-2-(phenylimino)-2*H*-chromen-3-yl)(phenyl)methanone (Figure 2, compound 3na)



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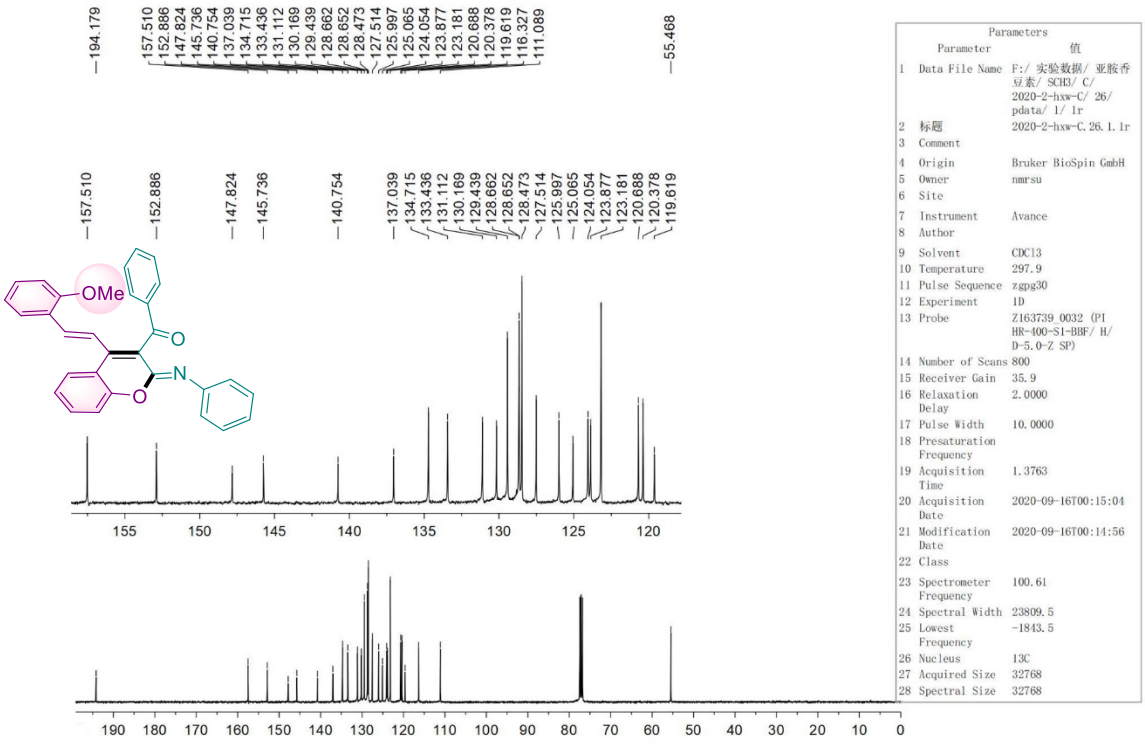
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	296.9
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14	Number of Scans	4
15	Receiver Gain	60.6
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	3.9977
20	Acquisition Date	2020-09-13T16:17:37
21	Modification Date	2020-09-13T16:16:54
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8196.7
25	Lowest Frequency	-1637.2
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

^{1}H NMR Spectra of compound 3na



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3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	297.9
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
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15	Receiver Gain	35.9
16	Relaxation Delay	2.0000
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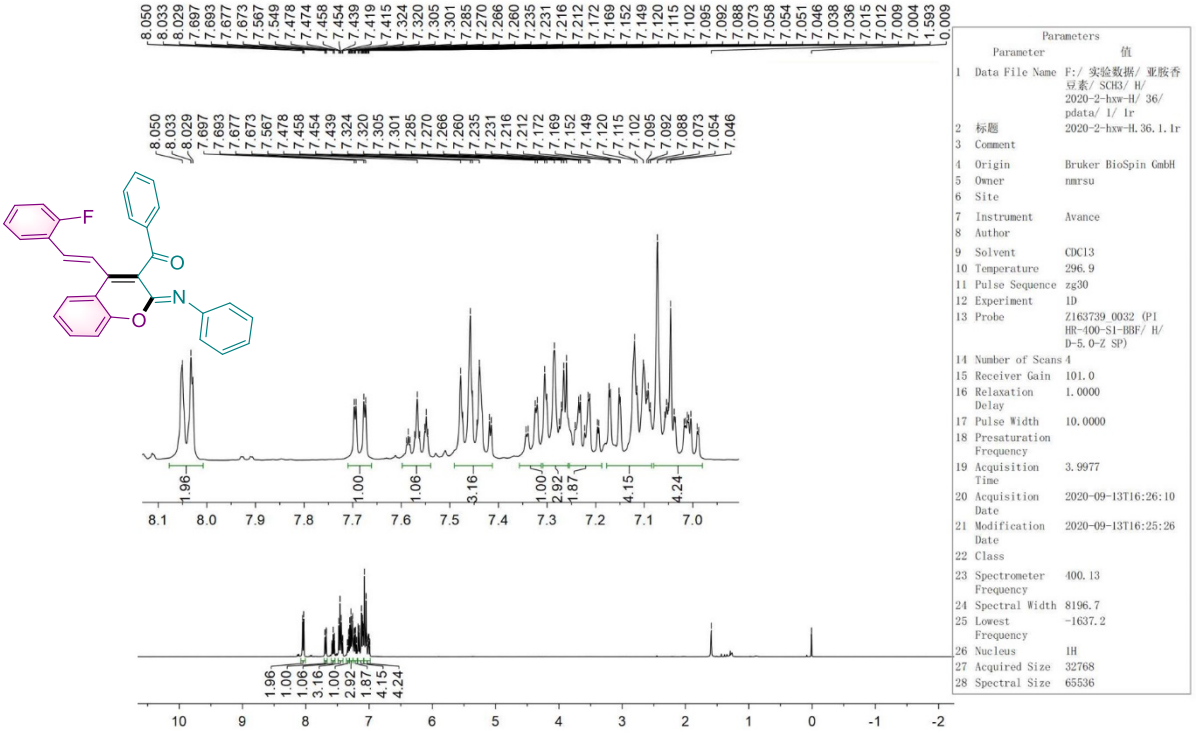
21	Modification Date	2020-09-16T00:14:56
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	23809.5
25	Lowest Frequency	-1843.5
26	Nucleus	13C
27	Acquired Size	32768
28	Spectral Size	32768

^{13}C NMR Spectra of compound 3na

((*Z*)-4-((*E*)-2-Fluorostyryl)-2-(phenylimino)-2*H*-chromen-3-yl)(phenyl)methanone (Figure 2, compound 3oa)



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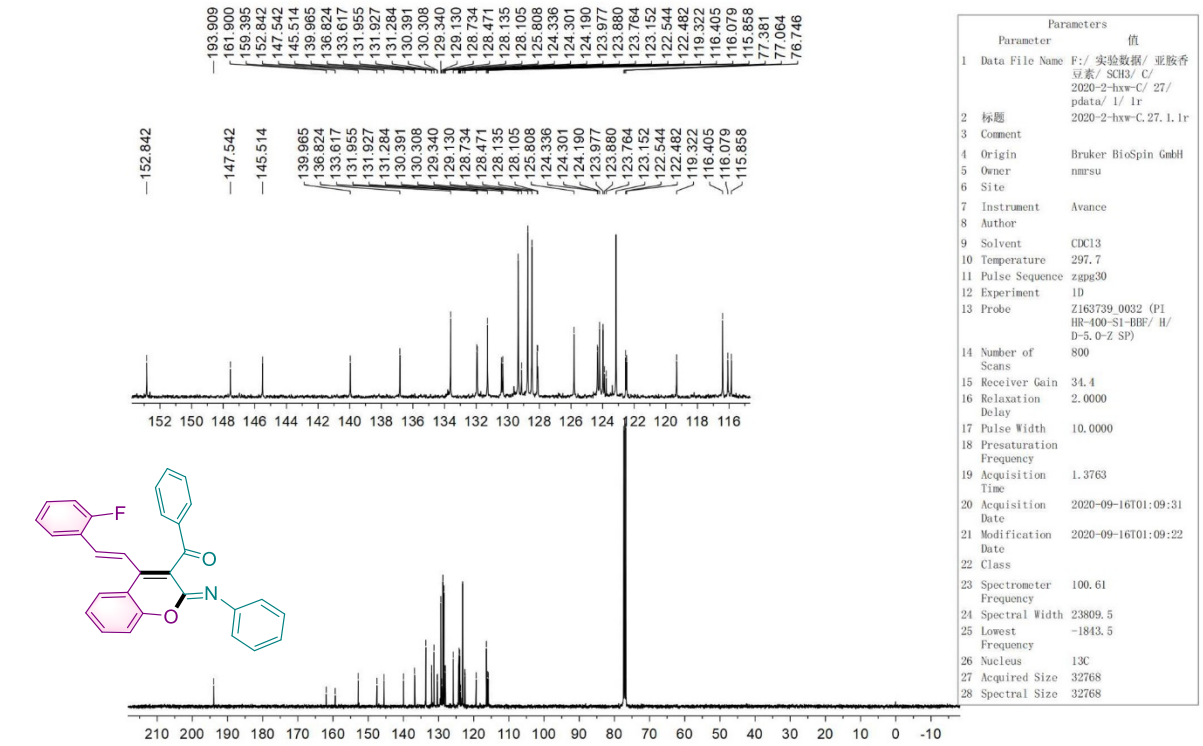
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	296.9
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14	Number of Scans	4
15	Receiver Gain	101.0
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	3.9977
20	Acquisition Date	2020-09-13T16:26:10
21	Modification Date	2020-09-13T16:25:26
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8196.7
25	Lowest Frequency	-1637.2
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

^{1}H NMR Spectra of compound 3oa



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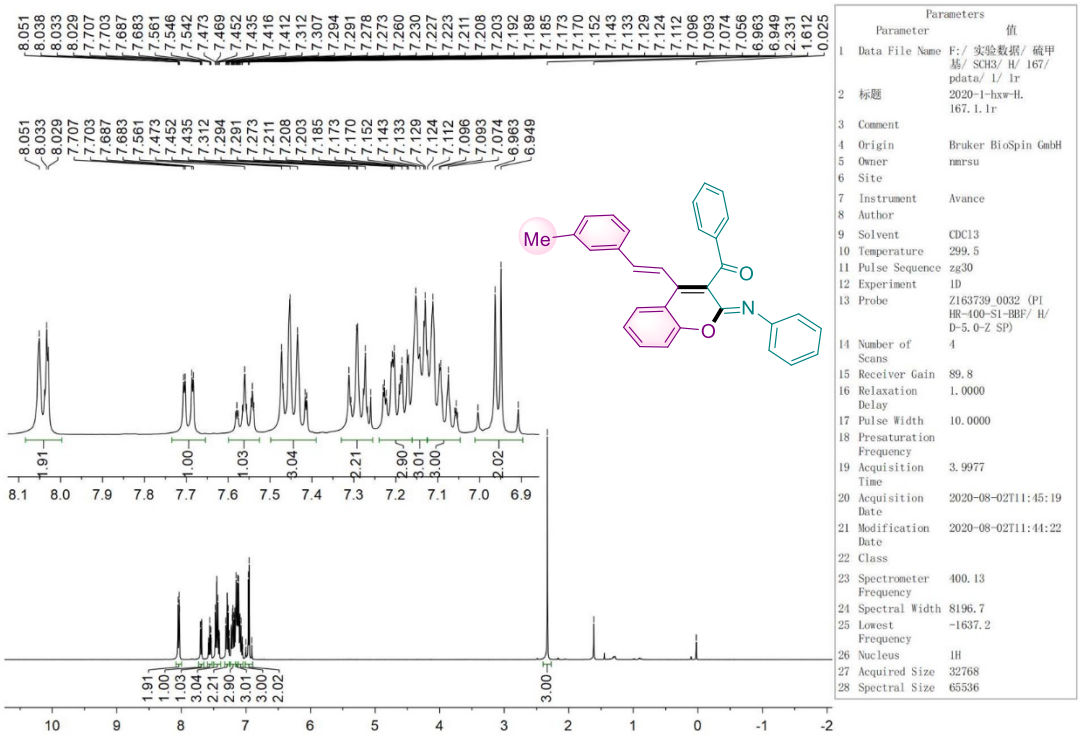
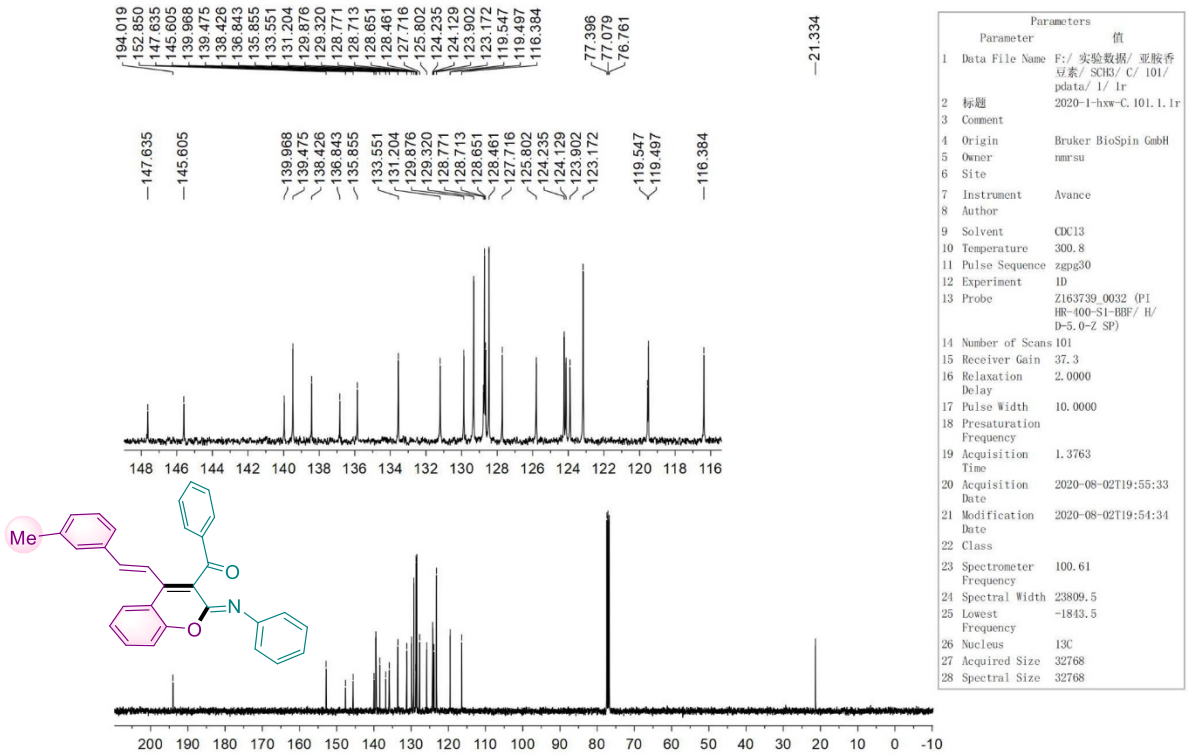
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	297.7
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14	Number of Scans	800
15	Receiver Gain	34.4
16	Relaxation Delay	2.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	1.3763
20	Acquisition Date	2020-09-16T01:09:31
21	Modification Date	2020-09-16T01:09:22
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	23809.5
25	Lowest Frequency	-1843.5
26	Nucleus	13C
27	Acquired Size	32768
28	Spectral Size	32768

^{13}C NMR Spectra of compound 3oa

((*Z*)-4-((*E*)-3-Methylstyryl)-2-(phenylimino)-2*H*-chromen-3-yl)(phenyl)methanone (Figure 2, compound 3pa)

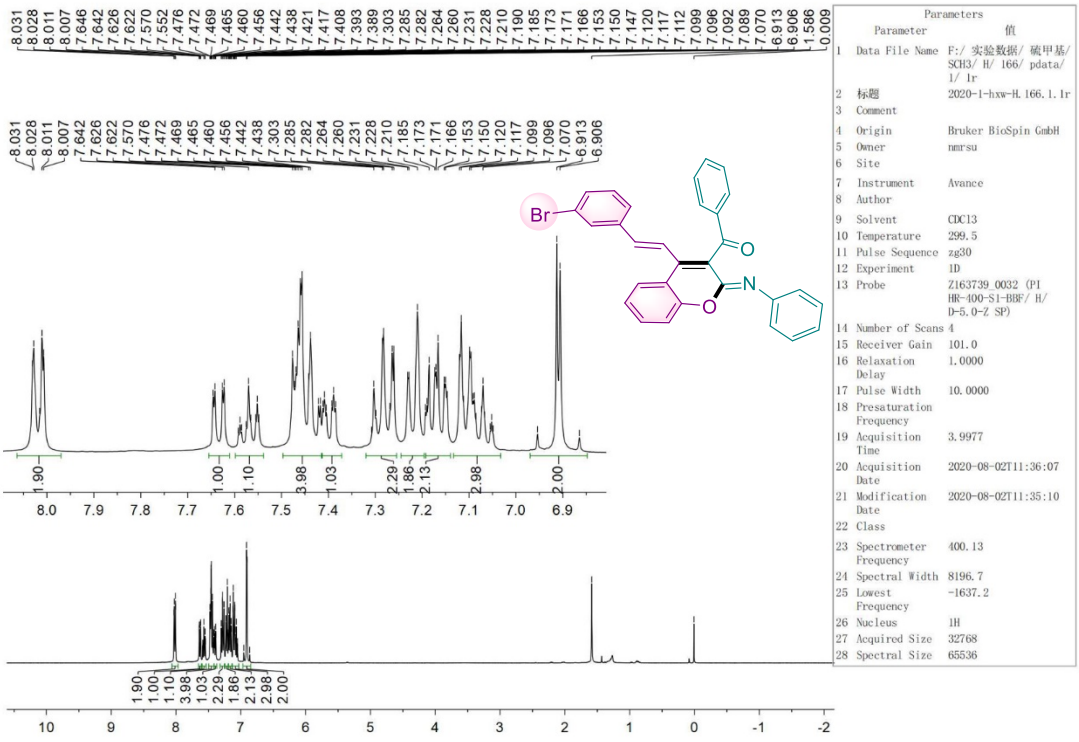


^{1}H NMR Spectra of compound 3pa

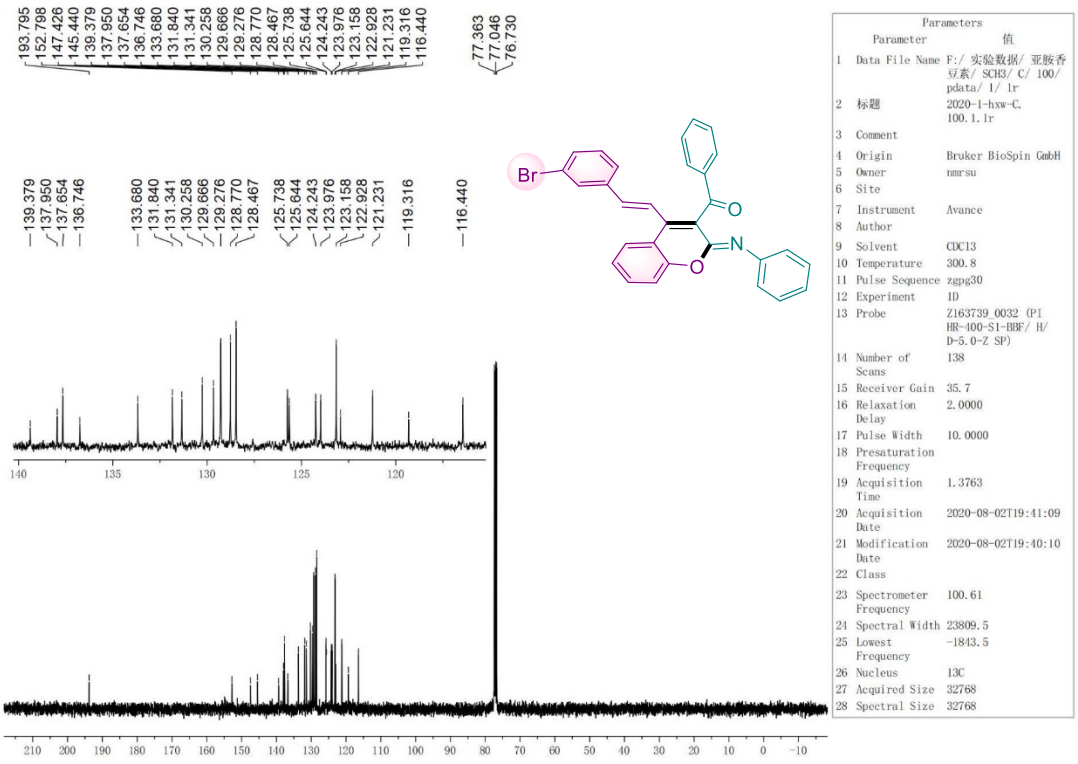


^{13}C NMR Spectra of compound 3pa

((*Z*)-4-((*E*)-3-Bromostyryl)-2-(phenylimino)-2*H*-chromen-3-yl)(phenyl)methanone (Figure 2, compound 3qa)

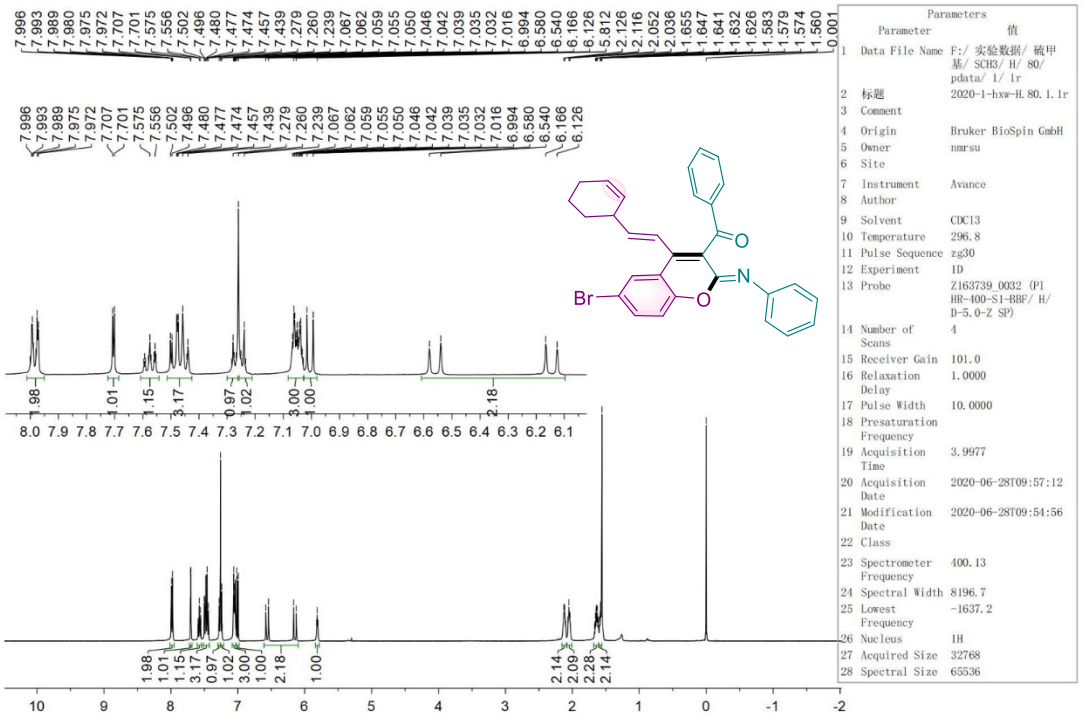


^{1}H NMR Spectra of compound 3qa

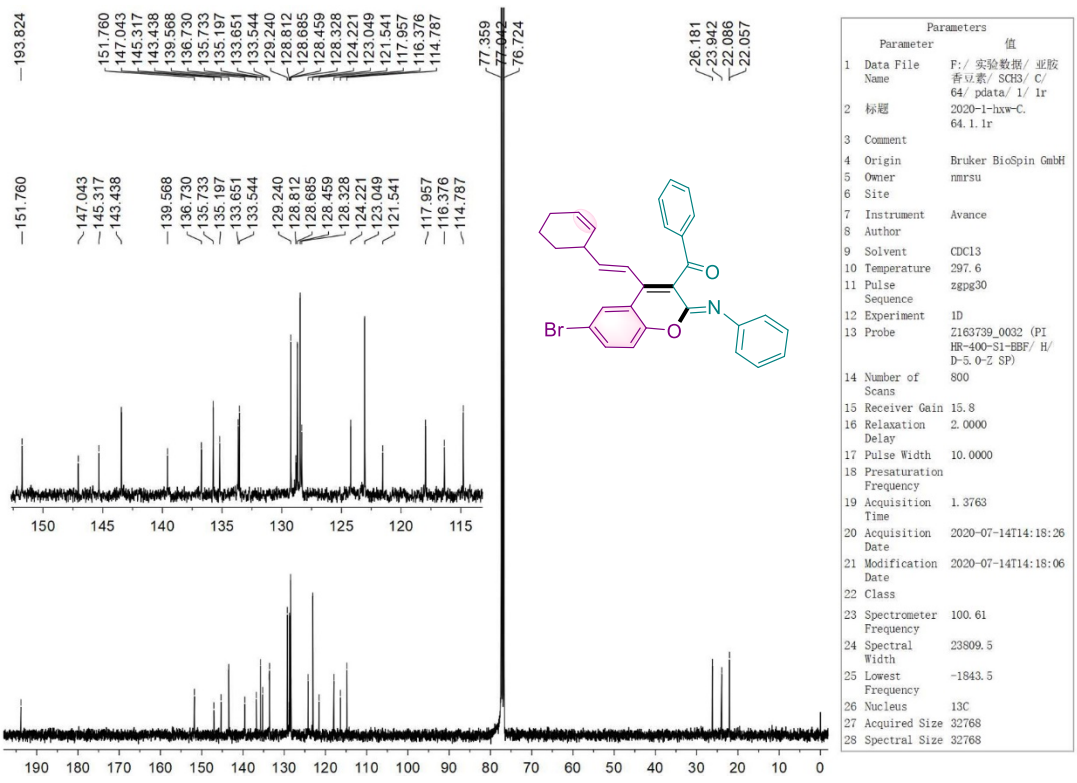


^{13}C NMR Spectra of compound 3qa

((*Z*)-6-Bromo-4-((*E*)-2-(cyclohex-1-en-1-yl)vinyl)-2-(phenylimino)-2*H*-chromen-3-yl)(phenyl)methanone (Figure 2, compound 3ra)

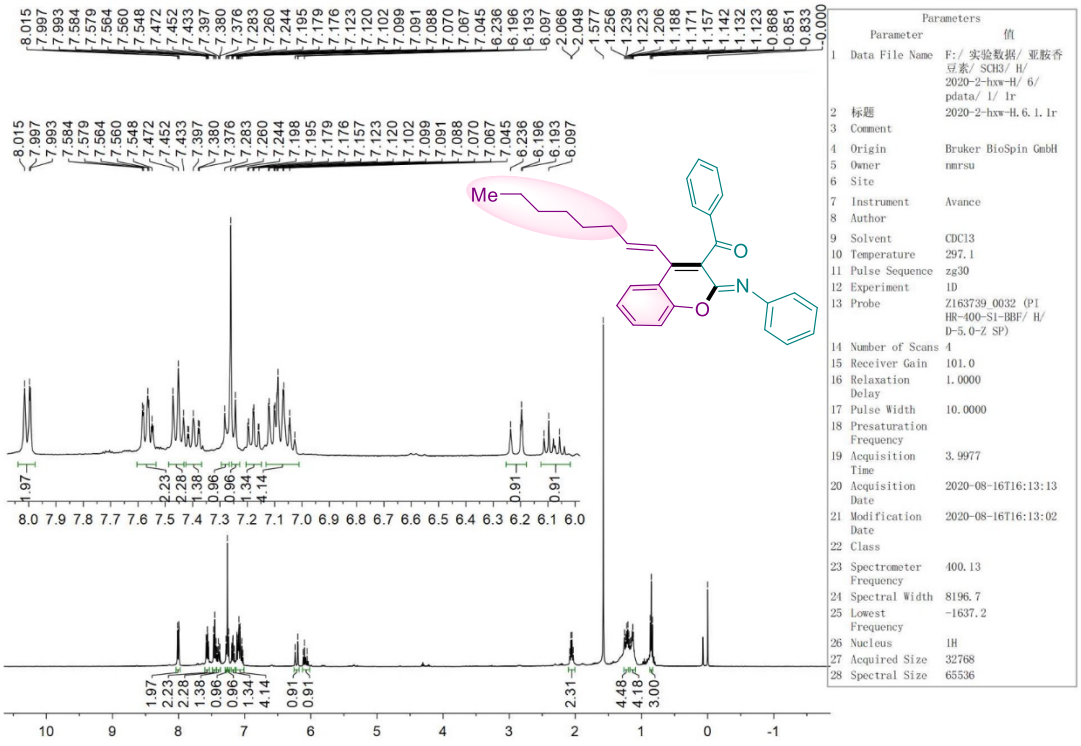


^{1}H NMR Spectra of compound 3ra

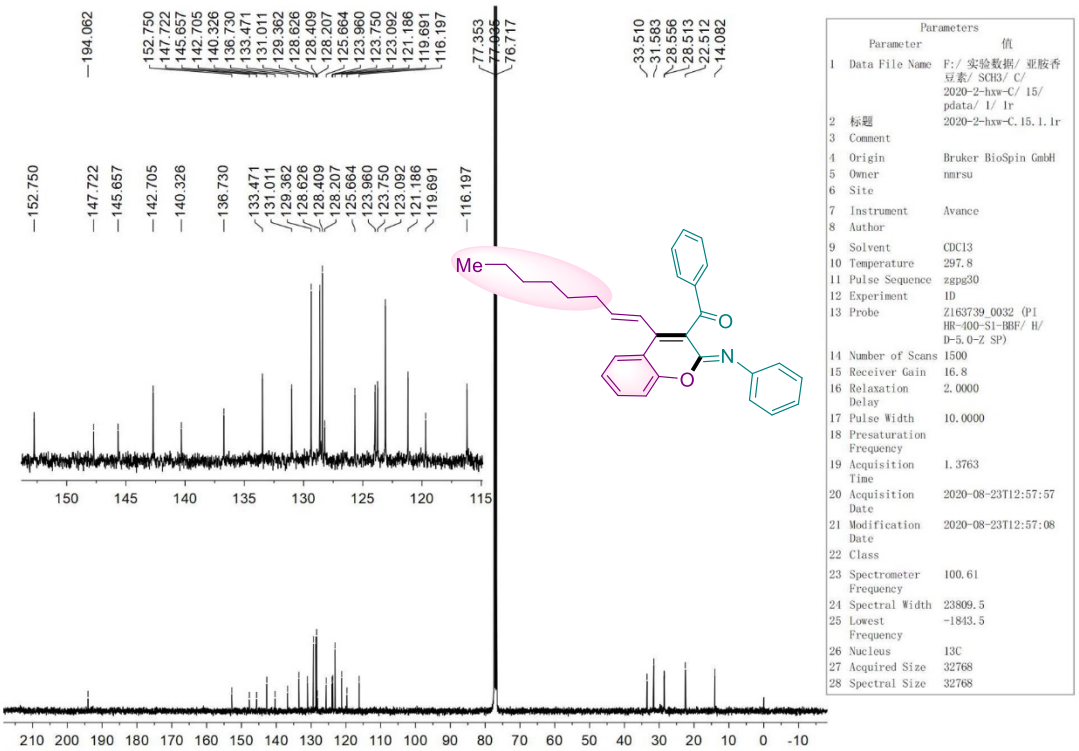


^{13}C NMR Spectra of compound 3ra

((*Z*)-4-((*E*)-Oct-1-en-1-yl)-2-(phenylimino)-2*H*-chromen-3-yl)(phenyl)methanone (Figure 2, compound 3sa)

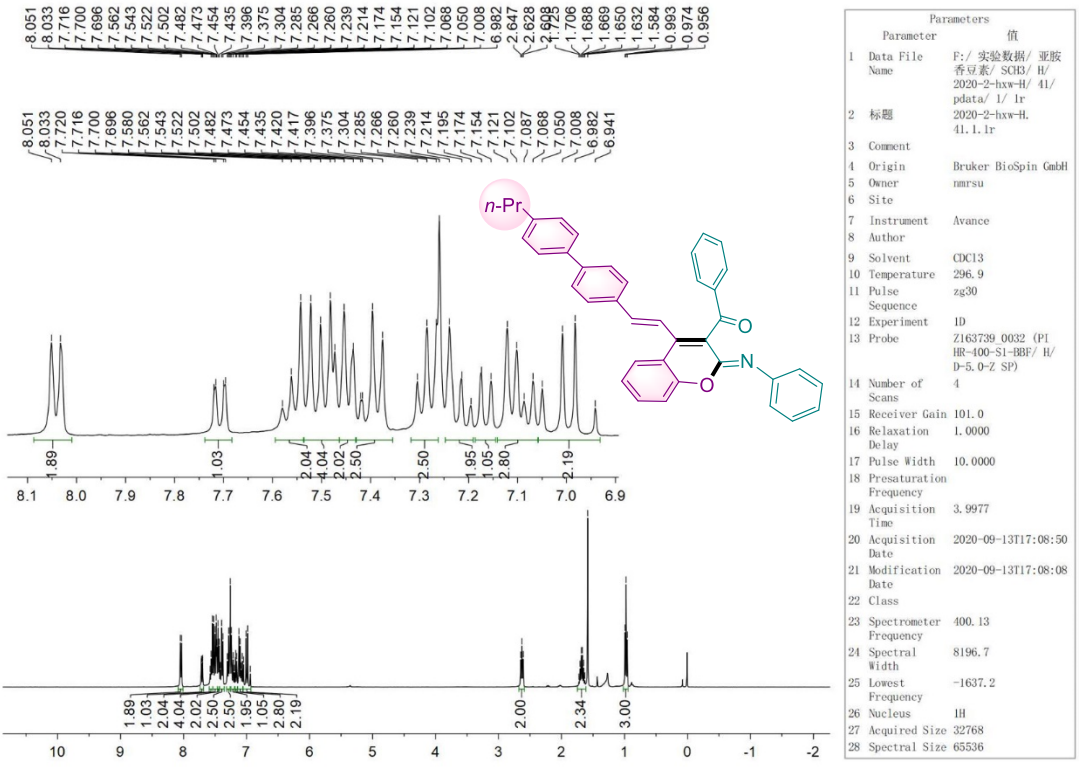


^{1}H NMR Spectra of compound 3sa



^{13}C NMR Spectra of compound 3sa

Phenyl((*Z*)-2-(phenylimino)-4-((*E*)-2-(4'-propyl-[1,1'-biphenyl]-4-yl)vinyl)-2*H*-chromen-3-yl)methanone (Figure 2, compound 3ta)



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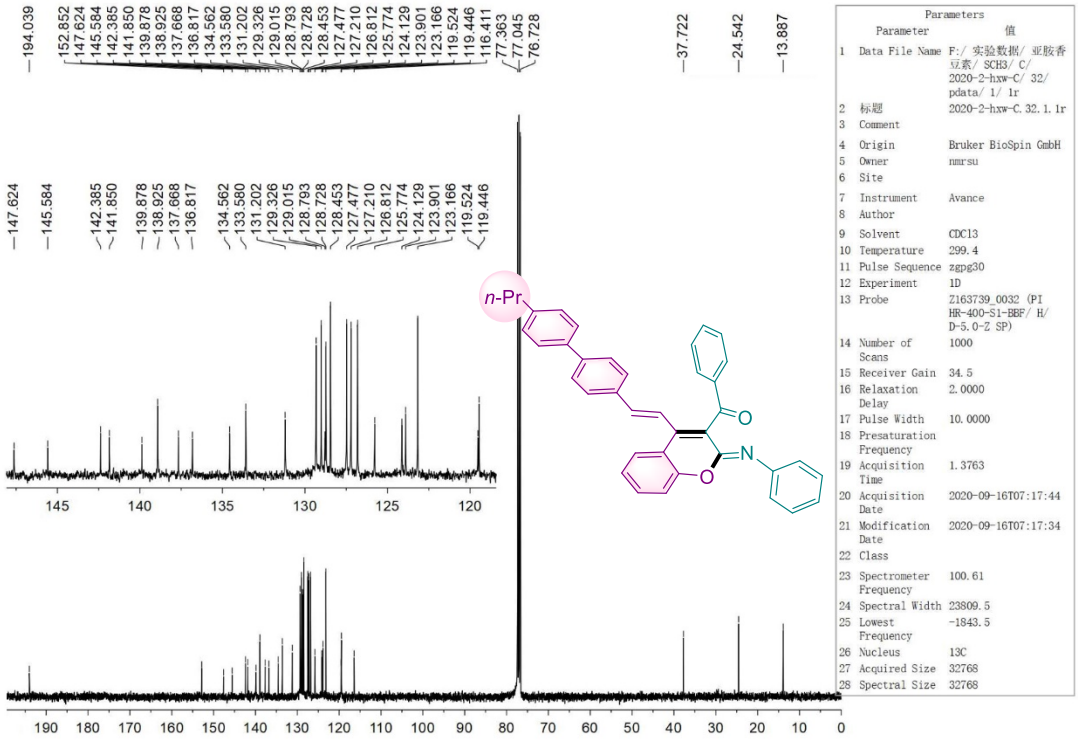
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	296.9
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14	Number of Scans	4
15	Receiver Gain	101.0
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	3.9977
20	Acquisition Date	2020-09-13T17:08:50
21	Modification Date	2020-09-13T17:08:08
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8196.7
25	Lowest Frequency	-1637.2
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

^{1}H NMR Spectra of compound 3ta



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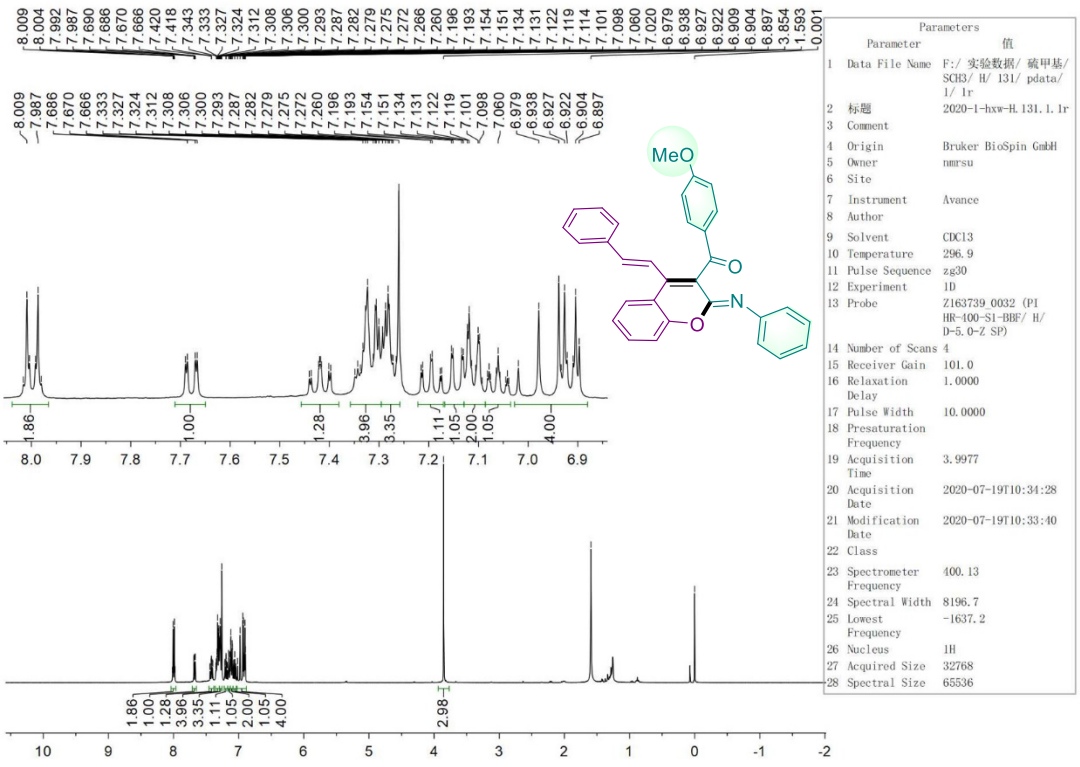
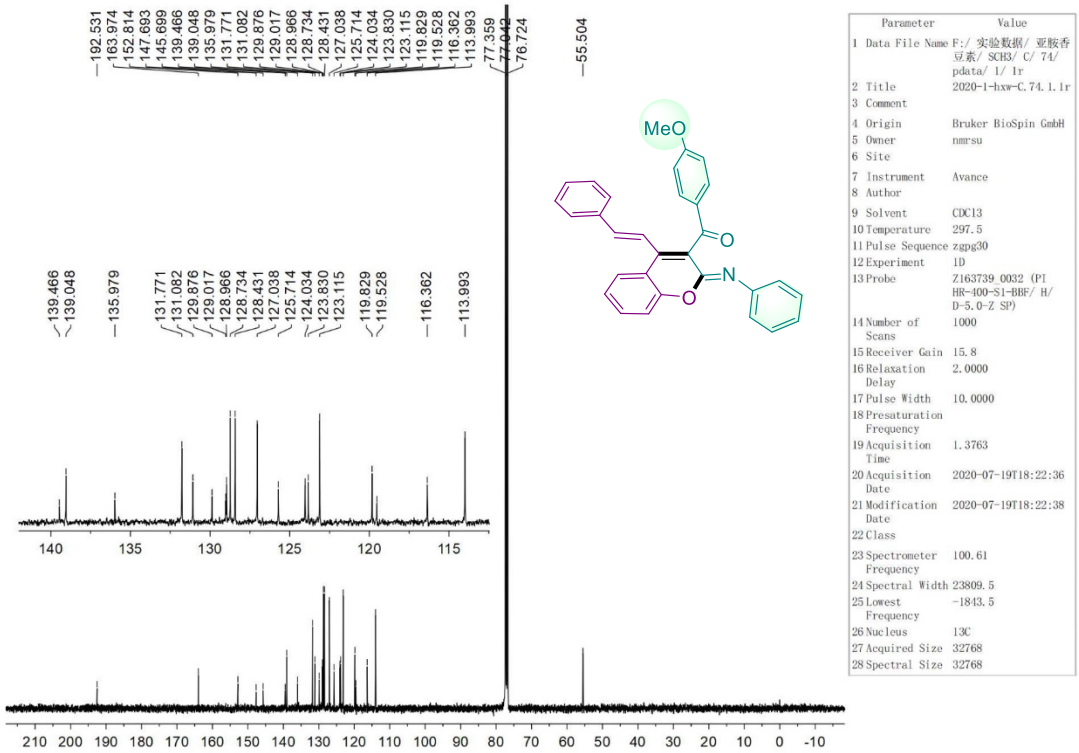
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	299.4
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14	Number of Scans	1000
15	Receiver Gain	34.5
16	Relaxation Delay	2.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	1.3763
20	Acquisition Date	2020-09-16T07:17:44
21	Modification Date	2020-09-16T07:17:34
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	23809.5
25	Lowest Frequency	-1843.5
26	Nucleus	13C
27	Acquired Size	32768
28	Spectral Size	32768

^{13}C NMR Spectra of compound 3ta

(4-Methoxyphenyl)((*Z*)-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)methanone (Figure 2, compound 3ab)

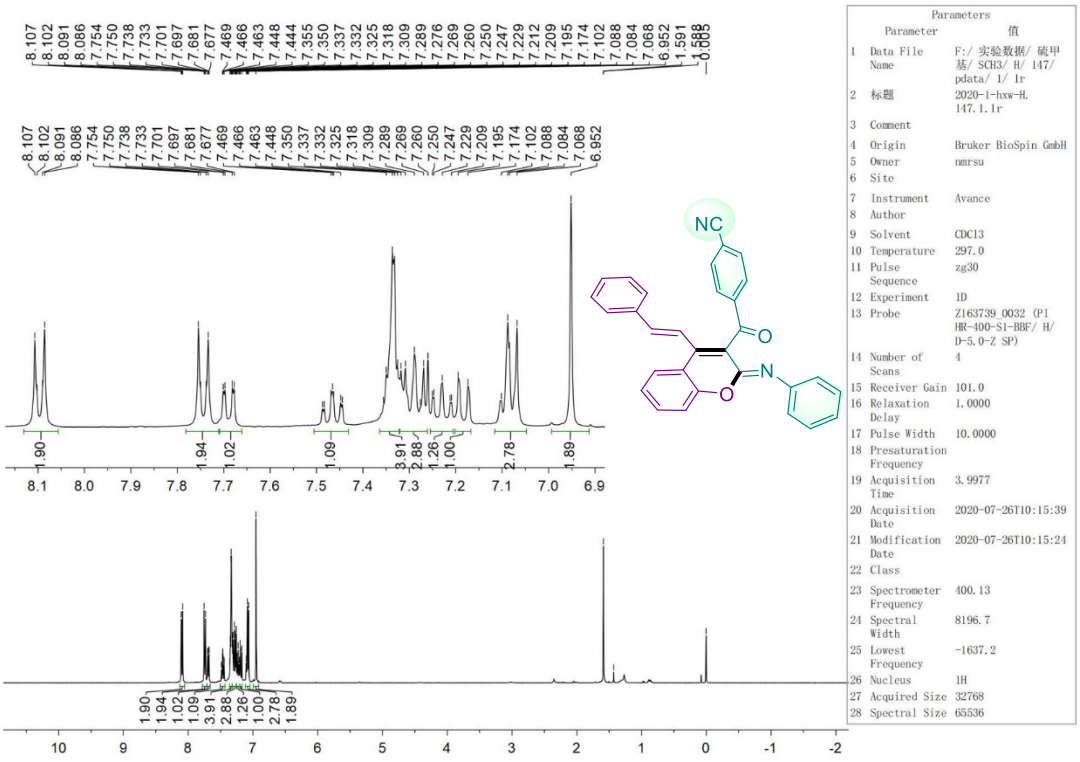


^{1}H NMR Spectra of compound 3ab

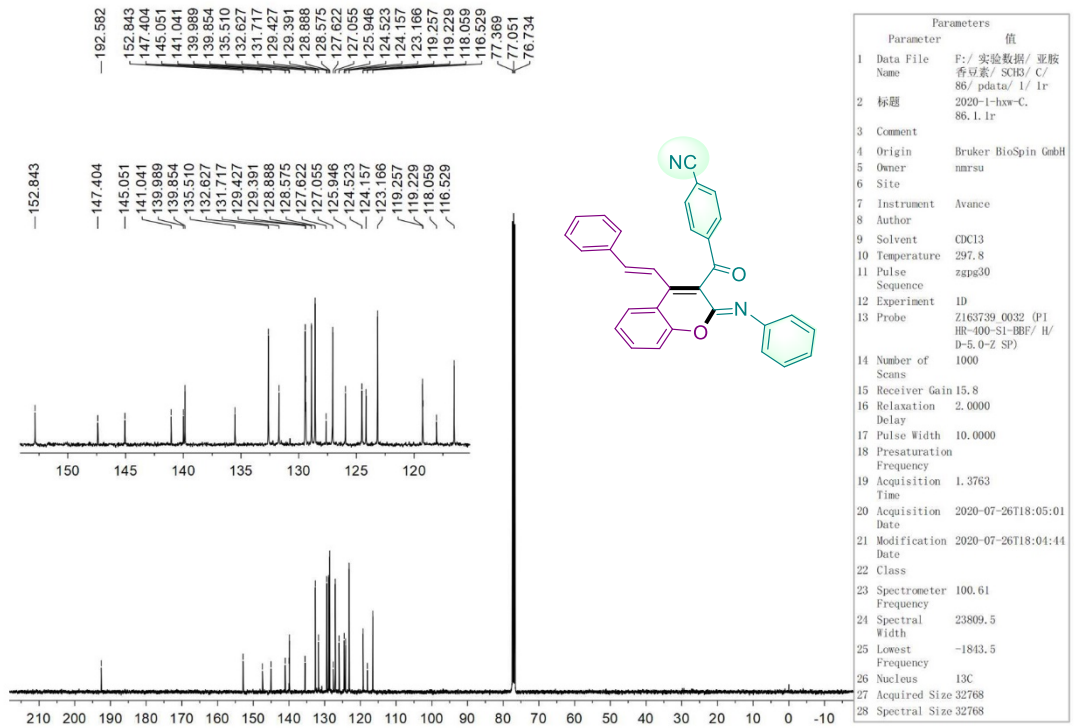


^{13}C NMR Spectra of compound 3ab

4-((*Z*)-2-(Phenylimino)-4-((*E*)-styryl)-2*H*-chromene-3-carbonyl)benzonitrile (Figure 2, compound 3ac)

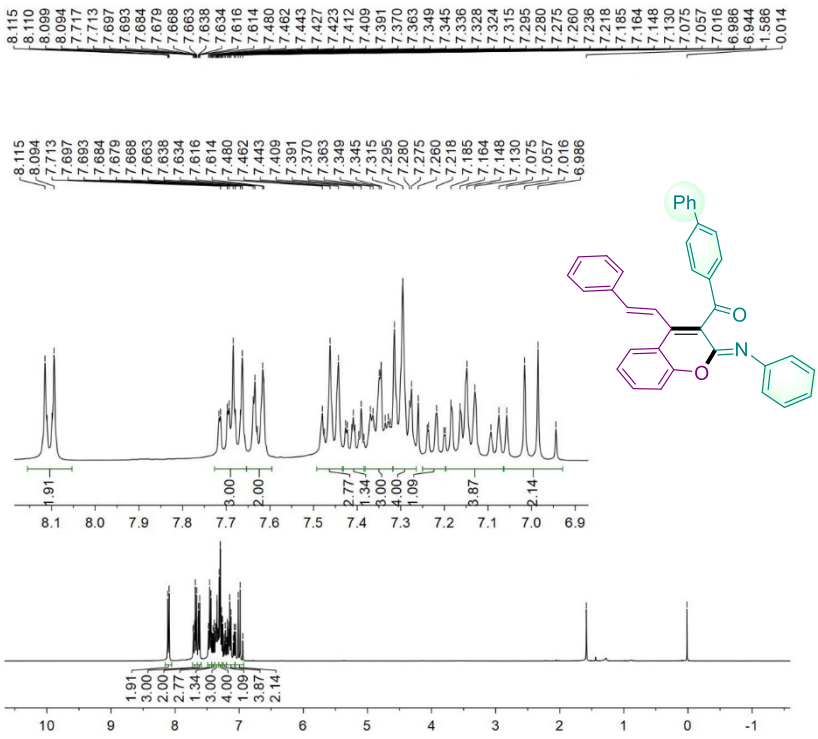


^{1}H NMR Spectra of compound 3ac



^{13}C NMR Spectra of compound 3ac

[1,1'-Biphenyl]-4-yl((*Z*)-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)methanone (Figure 2, compound 3ad)



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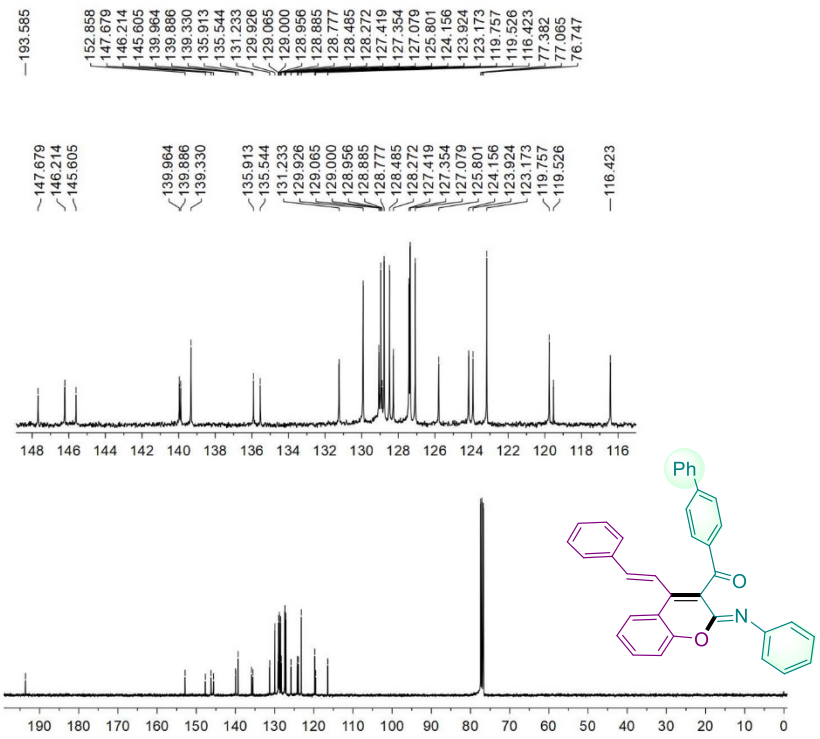
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	296.7
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14	Number of Scans	4
15	Receiver Gain	101.0
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	3.9977
20	Acquisition Date	2020-07-21T23:06:56
21	Modification Date	2020-07-21T23:06:46
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8196.7
25	Lowest Frequency	-1637.2
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

^{1}H NMR Spectra of compound 3ad



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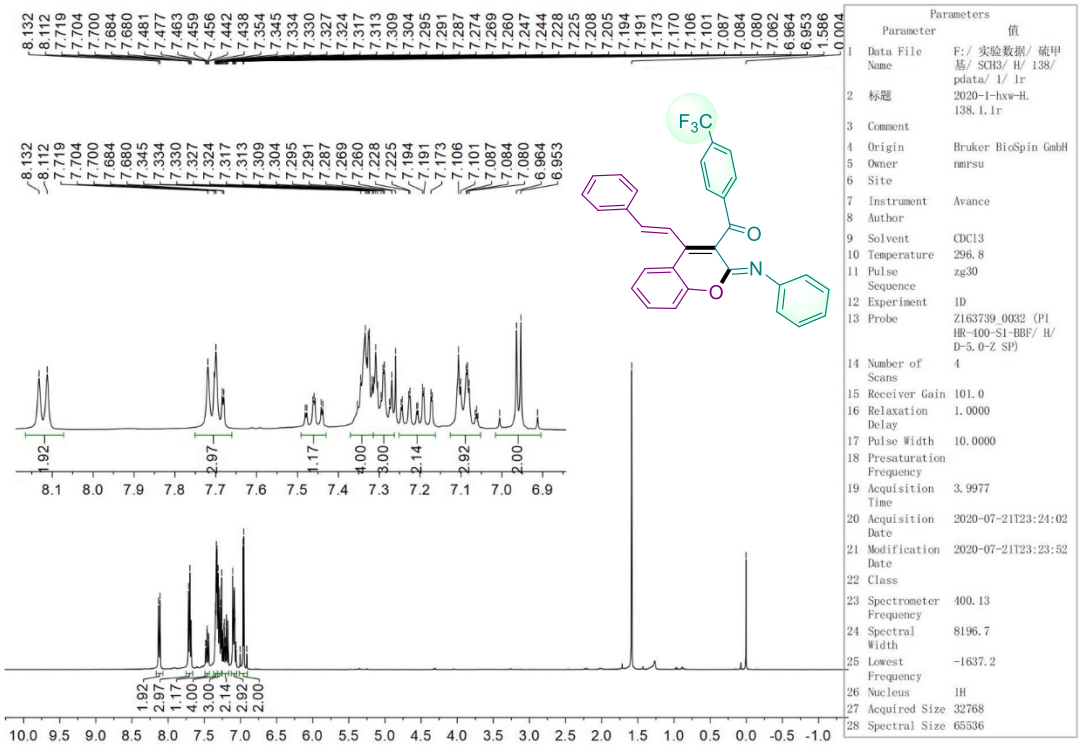
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14	Number of Scans	719
15	Receiver Gain	16.3
16	Relaxation Delay	2.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	1.3763
20	Acquisition Date	2020-07-26T11:58:21
21	Modification Date	2020-07-26T11:58:06
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	23809.5
25	Lowest Frequency	-1843.5
26	Nucleus	13C
27	Acquired Size	32768
28	Spectral Size	32768

^{13}C NMR Spectra of compound 3ad

((*Z*)-2-(Phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)(4-(trifluoromethyl)phenyl)methanone (Figure 2, compound 3ae)



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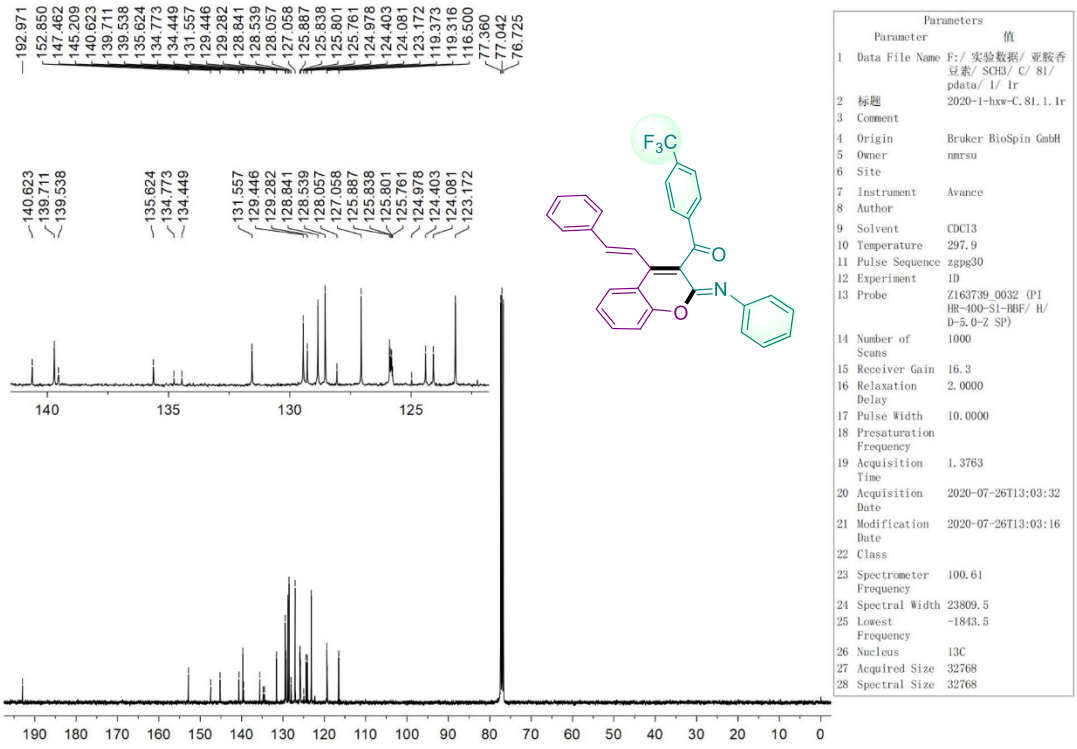
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	296.8
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14	Number of Scans	4
15	Receiver Gain	101.0
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	3.9977
20	Acquisition Date	2020-07-21T23:24:02
21	Modification Date	2020-07-21T23:23:52
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8196.7
25	Lowest Frequency	-1637.2
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

^{1}H NMR Spectra of compound 3ae



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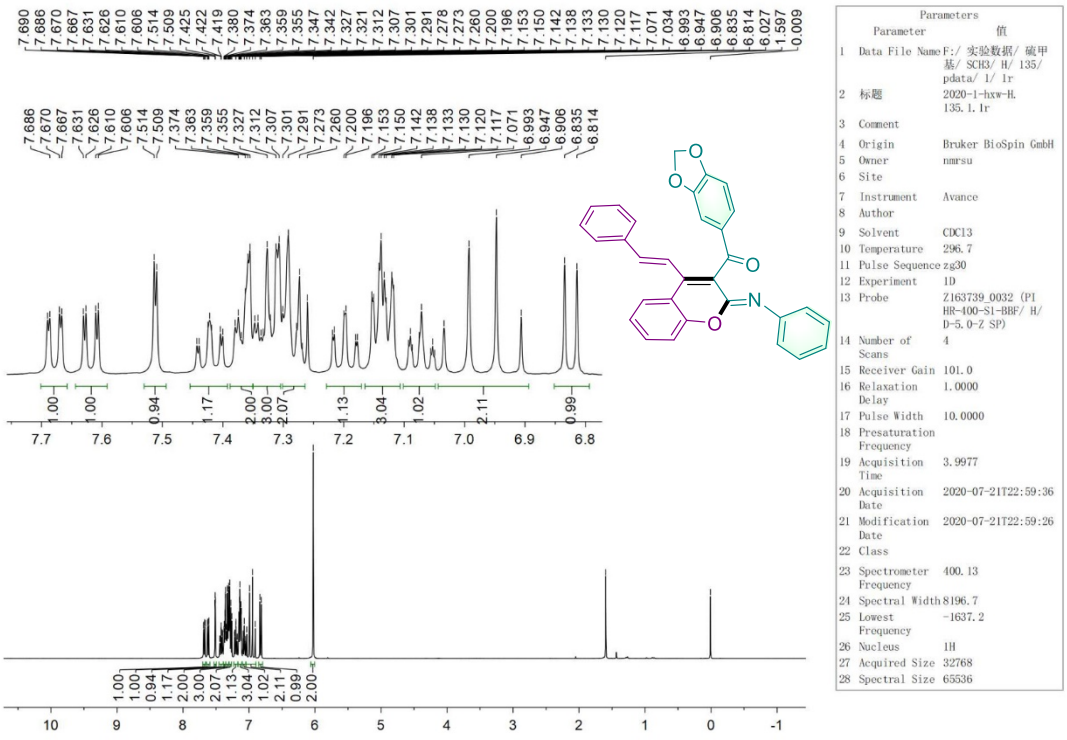
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	297.9
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14	Number of Scans	1000
15	Receiver Gain	16.3
16	Relaxation Delay	2.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	1.3763
20	Acquisition Date	2020-07-26T13:03:32
21	Modification Date	2020-07-26T13:03:16
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	23809.5
25	Lowest Frequency	-1843.5
26	Nucleus	13C
27	Acquired Size	32768
28	Spectral Size	32768

^{13}C NMR Spectra of compound 3ae

Benzo[*d*][1,3]dioxol-5-yl((*Z*)-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)methanone (Figure 2, compound 3af)



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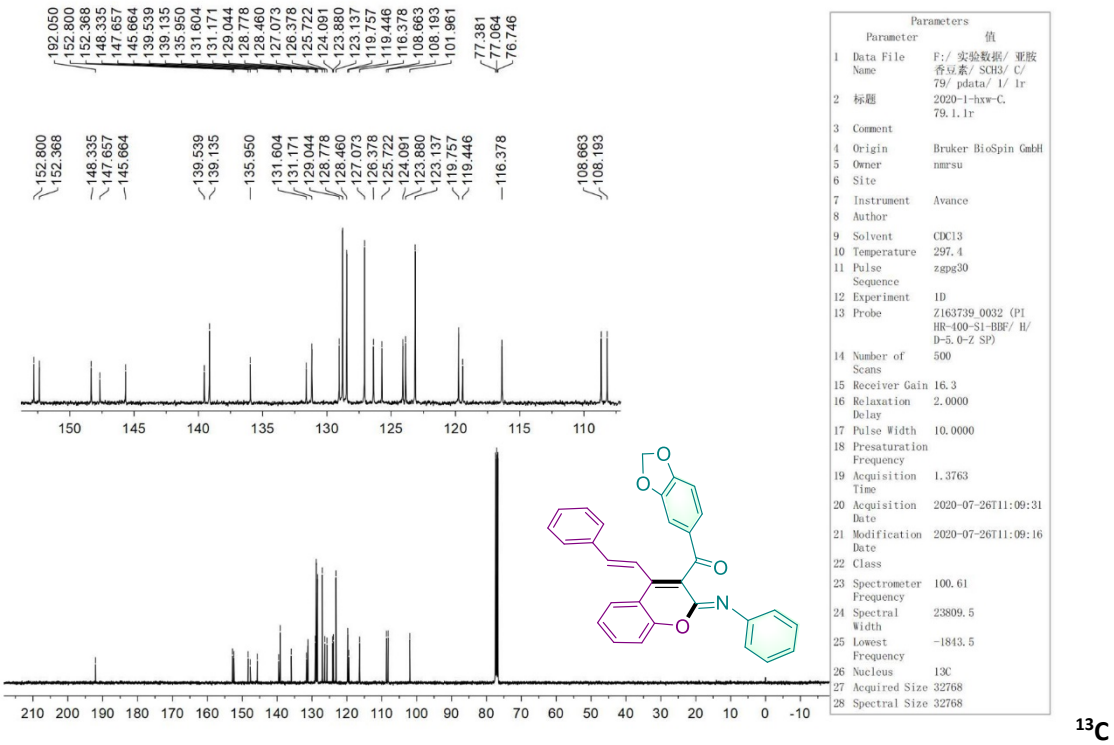
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	296.7
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14	Number of Scans	4
15	Receiver Gain	101.0
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	3.9977
20	Acquisition Date	2020-07-21T22:59:36
21	Modification Date	2020-07-21T22:59:26
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8196.7
25	Lowest Frequency	-1637.2
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

^{1}H NMR Spectra of compound 3af



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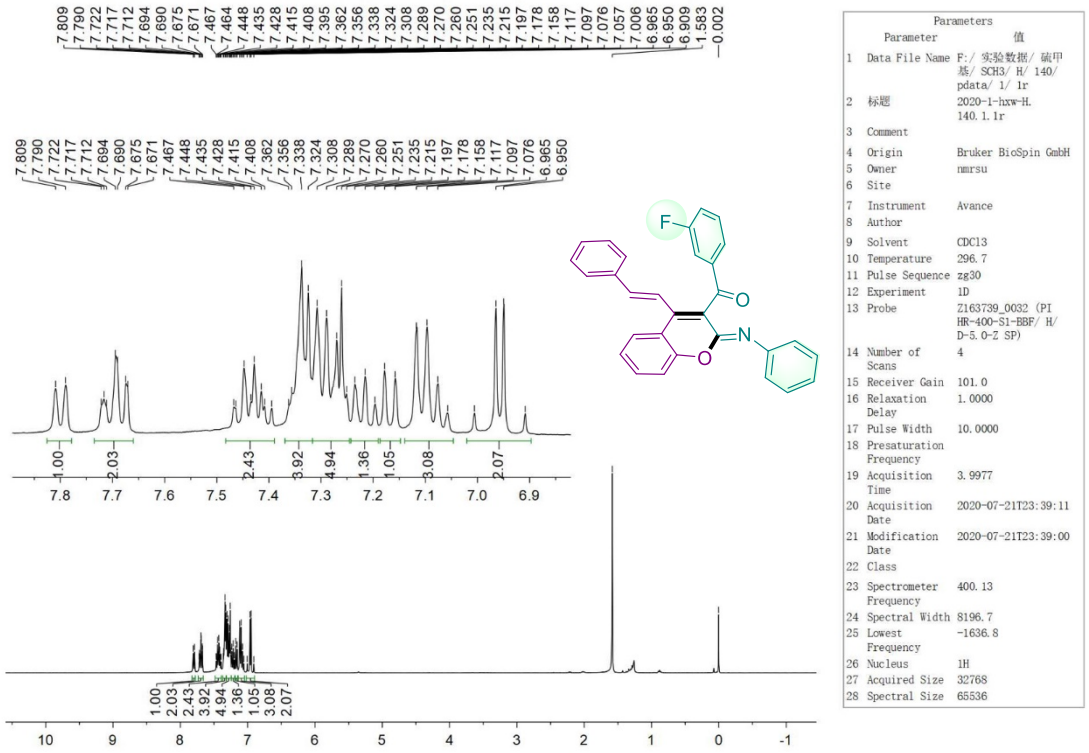
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	297.4
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14	Number of Scans	500
15	Receiver Gain	16.3
16	Relaxation Delay	2.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	1.3763
20	Acquisition Date	2020-07-26T11:09:31
21	Modification Date	2020-07-26T11:09:16
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	23809.5
25	Lowest Frequency	-1843.5
26	Nucleus	13C
27	Acquired Size	32768
28	Spectral Size	32768

^{13}C NMR Spectra of compound 3af

(3-Fluorophenyl)((*Z*)-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)methanone (Figure 2, compound 3ag)



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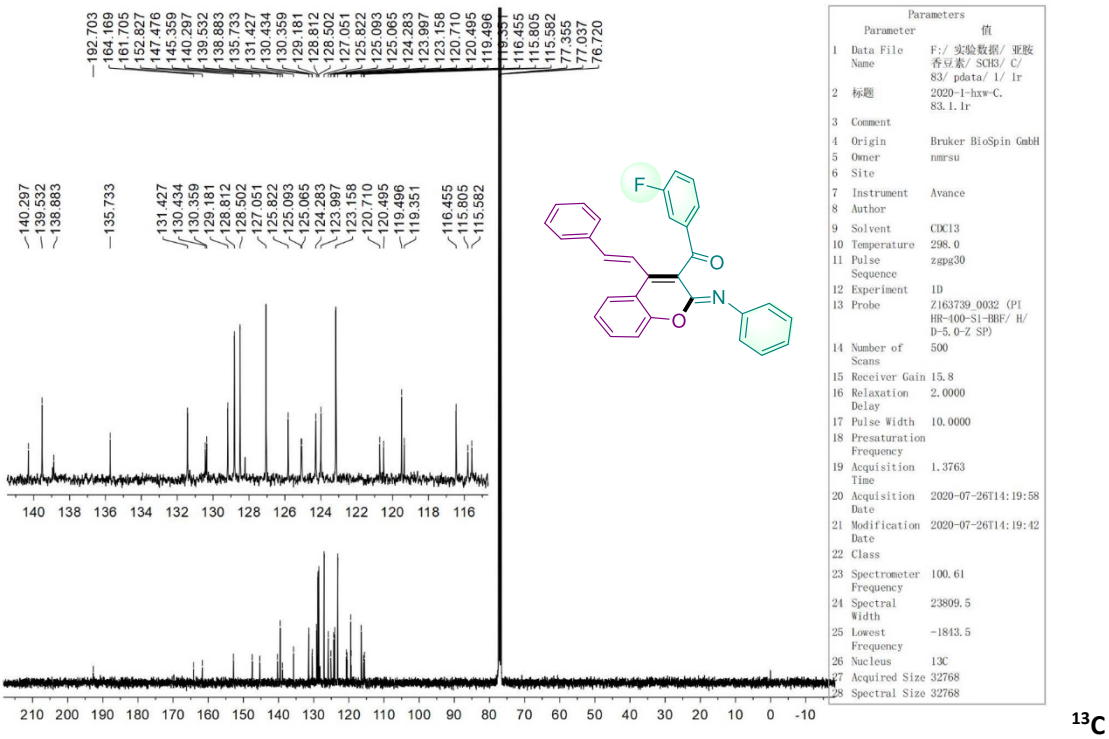
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	296. 7
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5. 0-Z SP)
14	Number of Scans	4
15	Receiver Gain	101. 0
16	Relaxation Delay	1. 0000
17	Pulse Width	10. 0000
18	Presaturation Frequency	
19	Acquisition Time	3. 9977
20	Acquisition Date	2020-07-21T23:39:11
21	Modification Date	2020-07-21T23:39:00
22	Class	
23	Spectrometer Frequency	400. 13
24	Spectral Width	8196. 7
25	Lowest Frequency	-1636. 8
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

^{1}H NMR Spectra of compound 3ag



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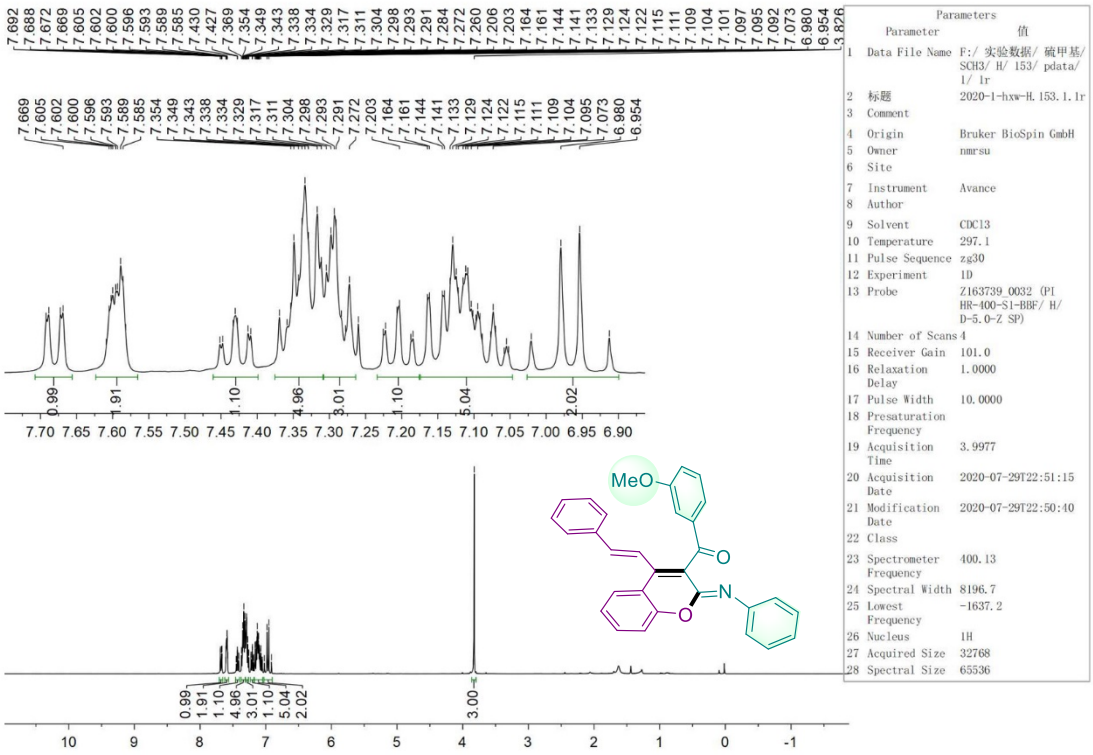
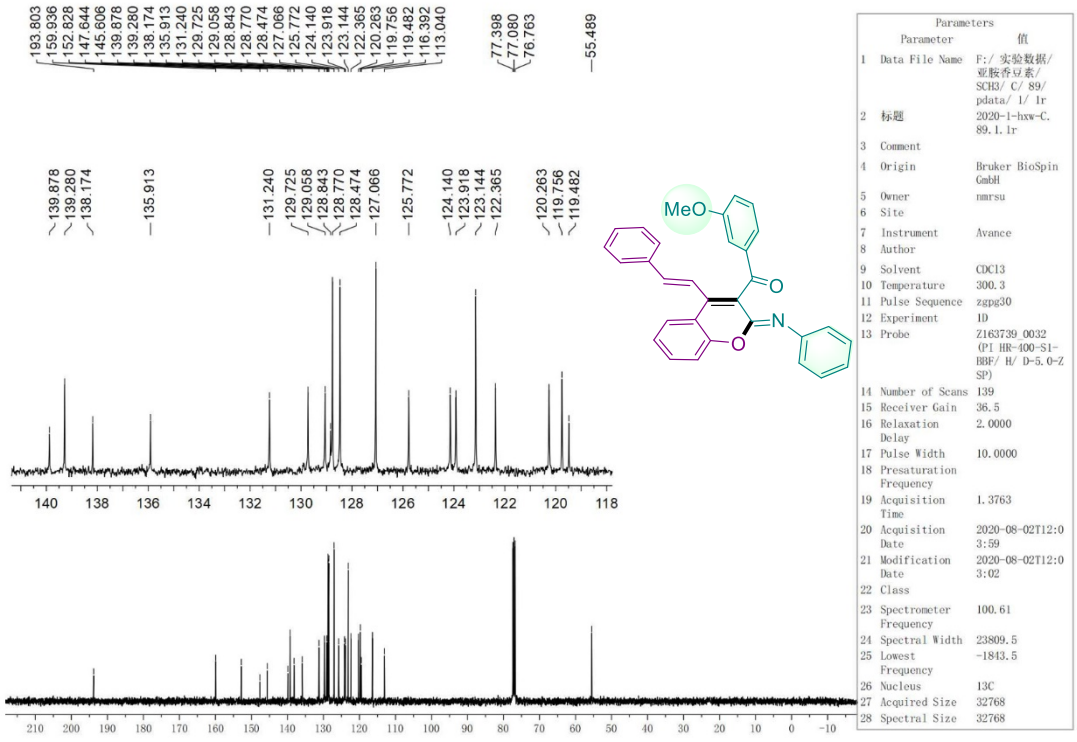
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	298. 0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5. 0-Z SP)
14	Number of Scans	500
15	Receiver Gain	15. 8
16	Relaxation Delay	2. 0000
17	Pulse Width	10. 0000
18	Presaturation Frequency	
19	Acquisition Time	1. 3763
20	Acquisition Date	2020-07-26T14:19:58
21	Modification Date	2020-07-26T14:19:42
22	Class	
23	Spectrometer Frequency	100. 61
24	Spectral Width	23809. 5
25	Lowest Frequency	-1843. 5
26	Nucleus	13C
27	Acquired Size	32768
28	Spectral Size	32768

^{13}C NMR Spectra of compound 3ag

(3-Methoxyphenyl)((*Z*)-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)methanone (Figure 2, compound 3ah)

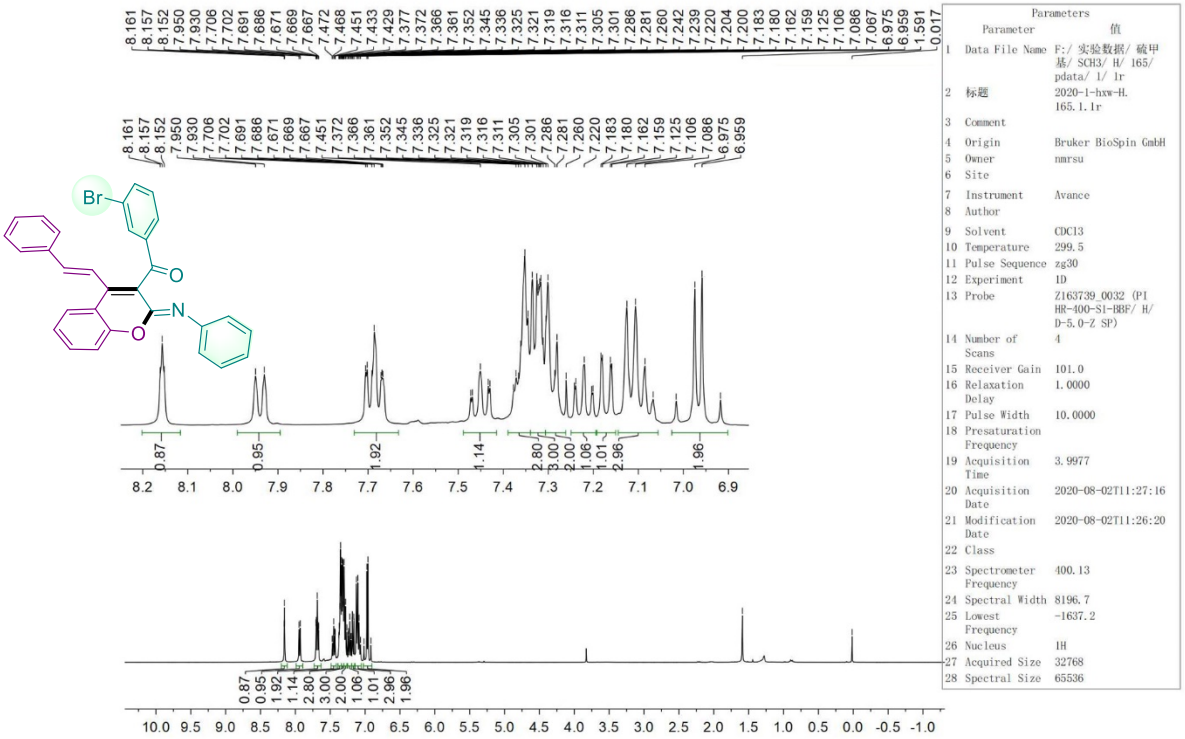


^{1}H NMR Spectra of compound 3ah

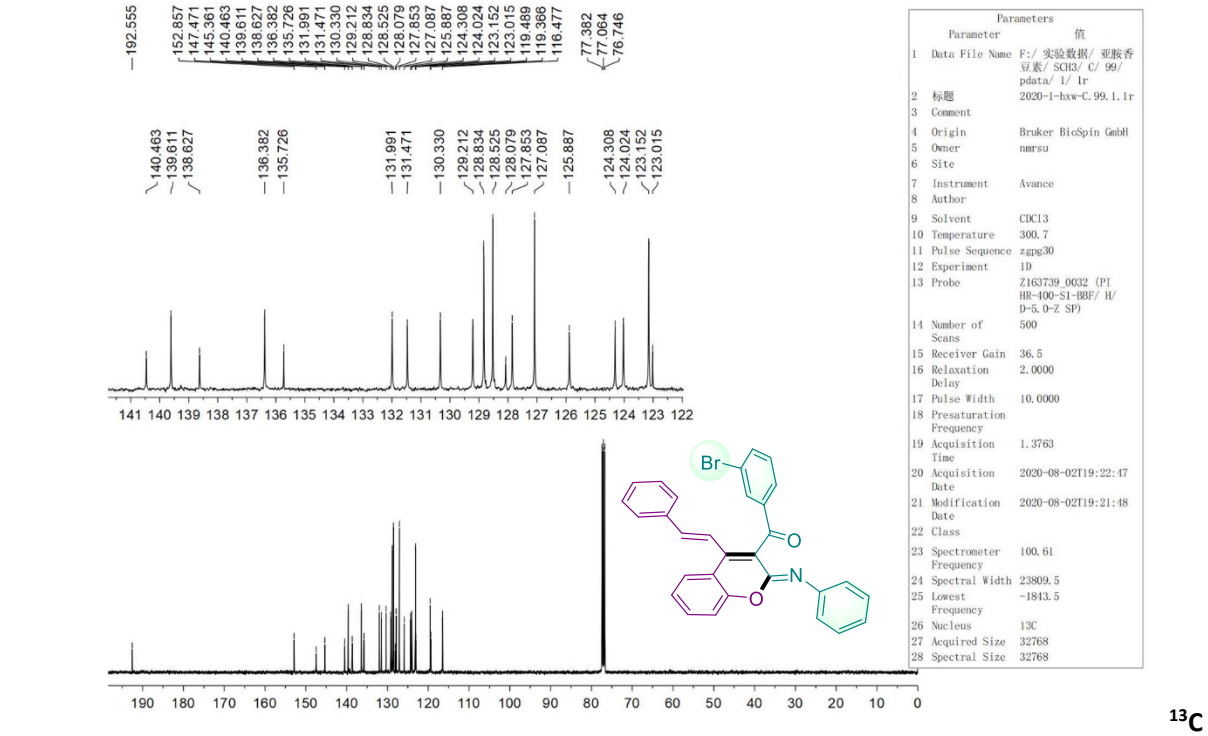


^{13}C NMR Spectra of compound 3ah

(3-Bromophenyl)((*Z*)-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)methanone (Figure 2, compound 3ai)

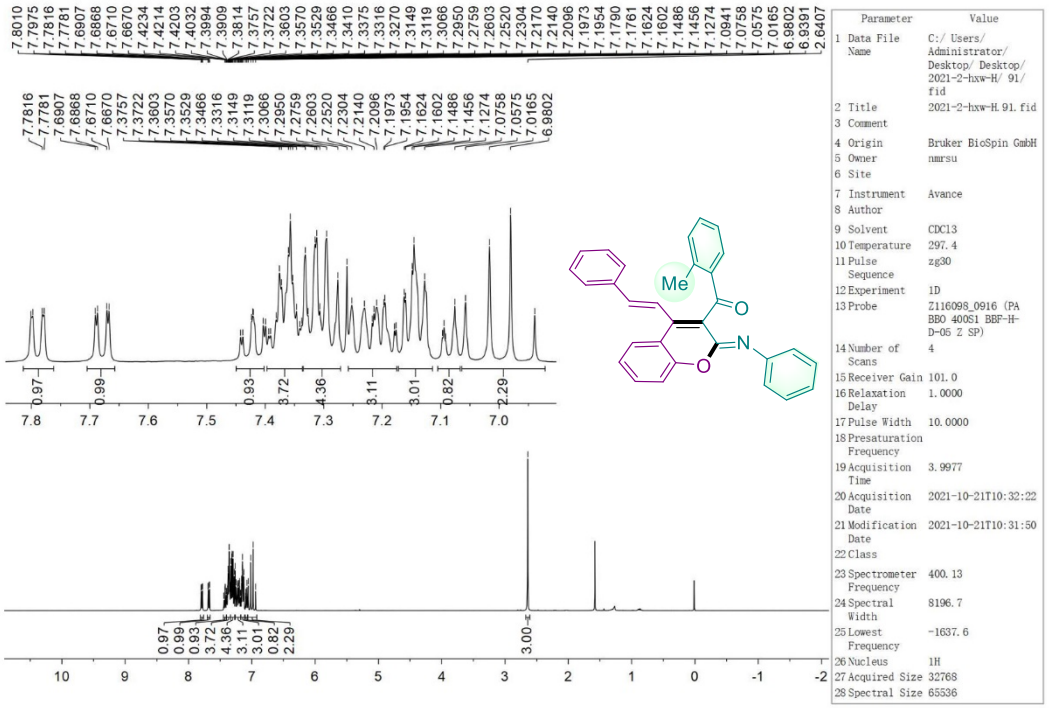


^{1}H NMR Spectra of compound 3ai



^{13}C NMR Spectra of compound 3ai

((*Z*)-2-(Phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)(*o*-tolyl)methanone (Figure 2, compound 3aj)



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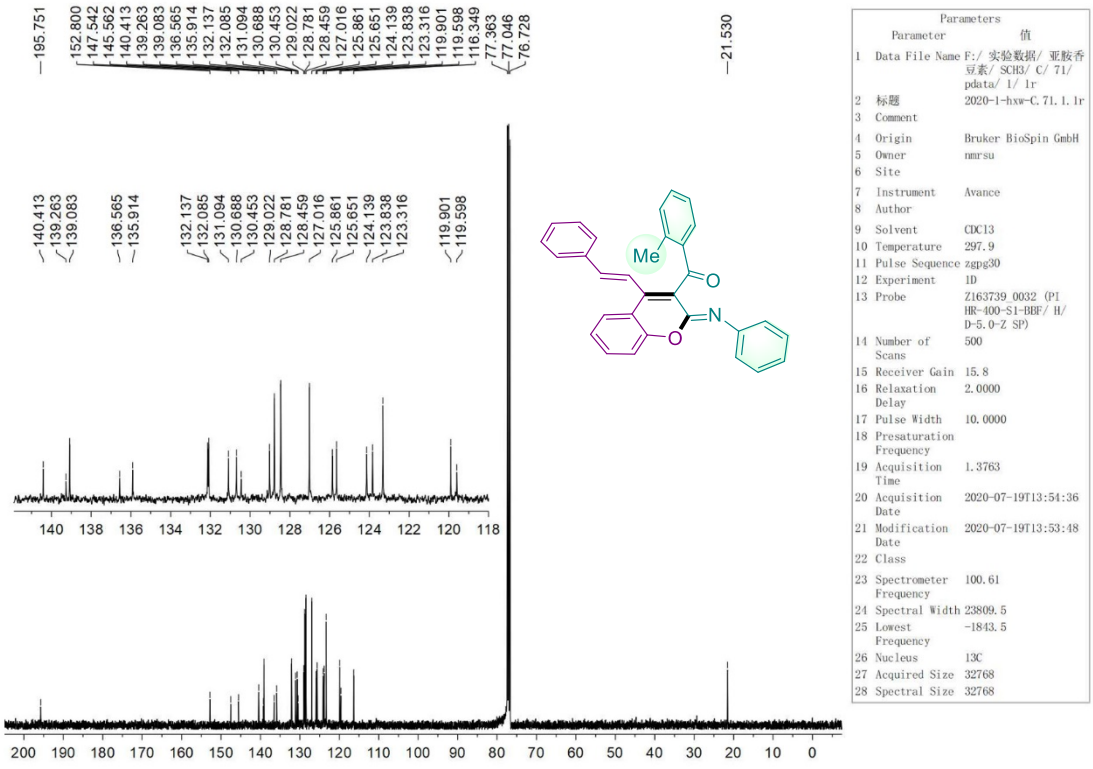
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	297.4
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z116098_0916 (PABBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2021-10-21T10:32:22
21 Modification Date	2021-10-21T10:31:50
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.6
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

^{1}H NMR Spectra of compound 3aj



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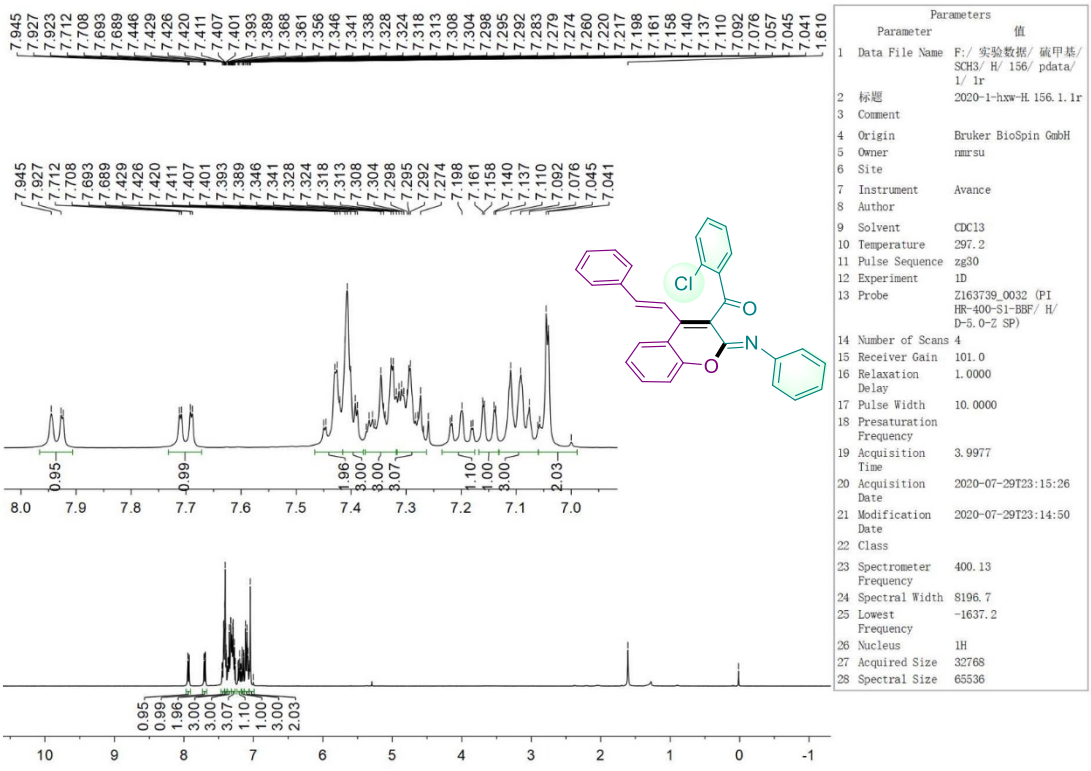
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	297.9
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	500
15 Receiver Gain	15.8
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2020-07-19T13:54:36
21 Modification Date	2020-07-19T13:53:48
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1843.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

^{13}C NMR Spectra of compound 3aj

(2-Chlorophenyl)((*Z*)-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)methanone (Figure 2, compound 3ak)



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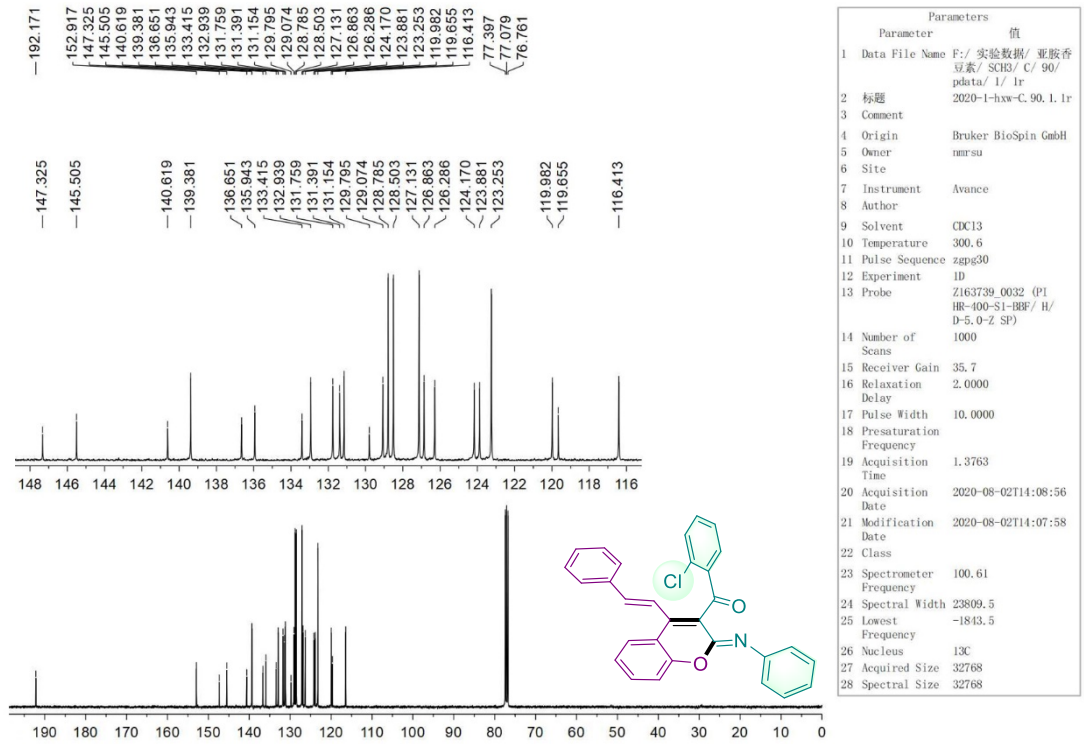
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	297.2
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14	Number of Scans	4
15	Receiver Gain	101.0
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	3.9977
20	Acquisition Date	2020-07-29T23:15:26
21	Modification Date	2020-07-29T23:14:50
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8196.7
25	Lowest Frequency	-1637.2
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

^{1}H NMR Spectra of compound 3ak



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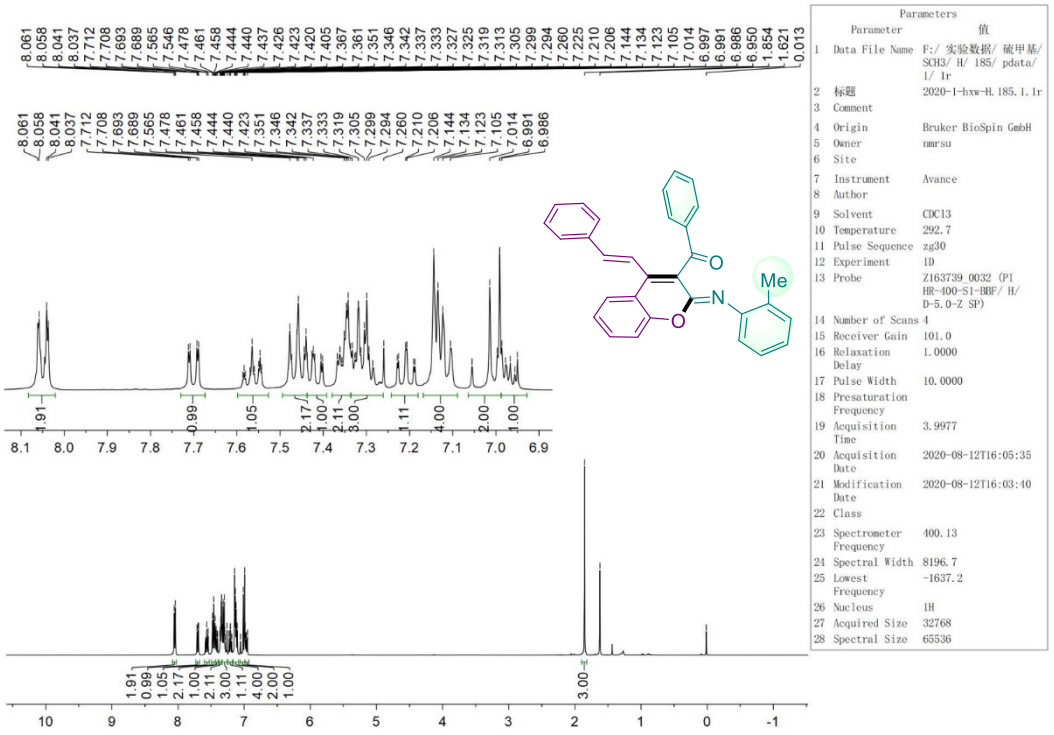
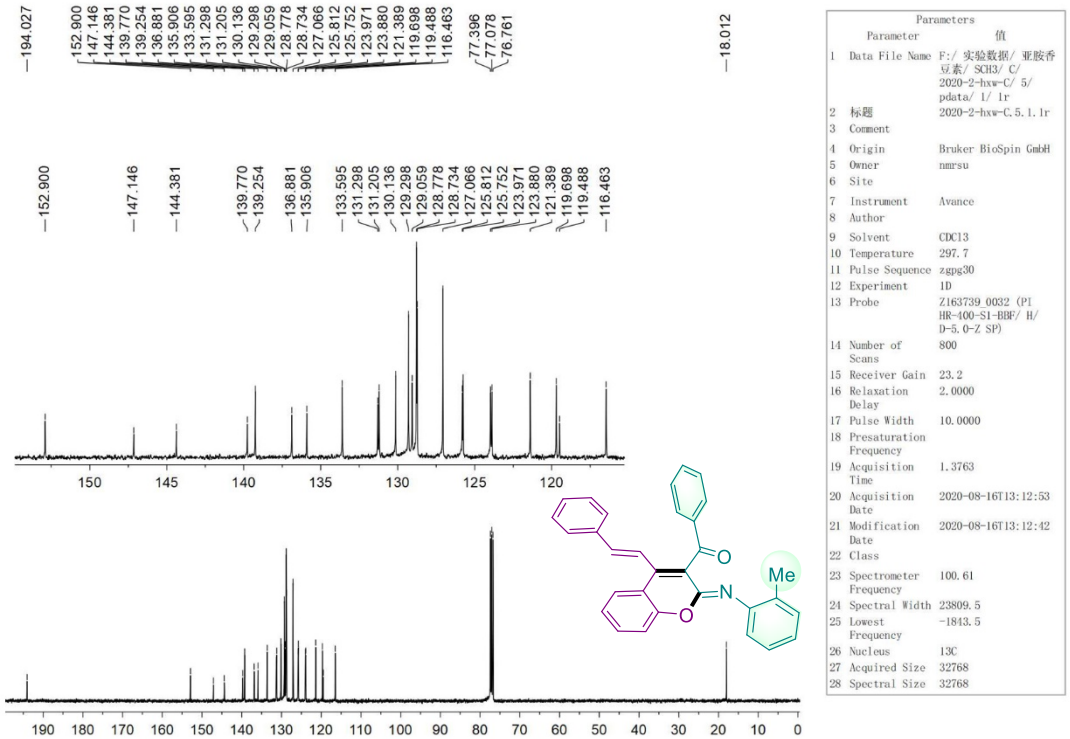
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	300.6
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14	Number of Scans	1000
15	Receiver Gain	35.7
16	Relaxation Delay	2.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	1.3763
20	Acquisition Date	2020-08-02T14:08:56
21	Modification Date	2020-08-02T14:07:58
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	23809.5
25	Lowest Frequency	-1843.5
26	Nucleus	13C
27	Acquired Size	32768
28	Spectral Size	32768

^{13}C NMR Spectra of compound 3ak

Phenyl((*Z*)-4-((*E*)-styryl)-2-(*o*-tolylimino)-2*H*-chromen-3-yl)methanone (Figure 2, compound 3al)

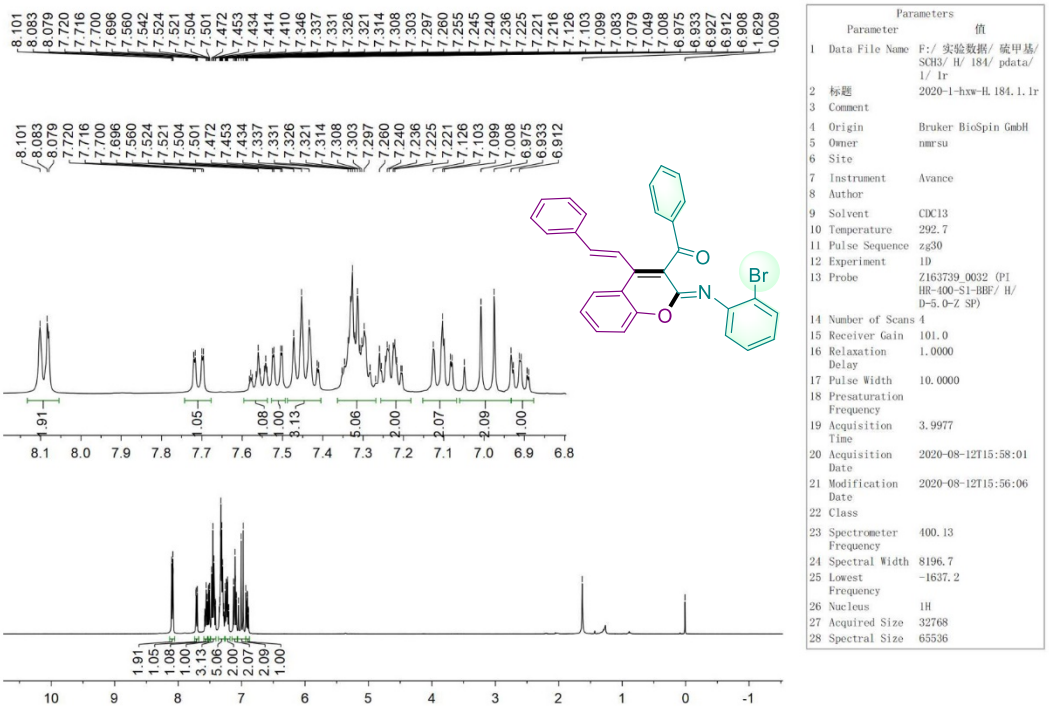


^{1}H NMR Spectra of compound 3al



^{13}C NMR Spectra of compound 3al

((*Z*)-2-((2-Bromophenyl)imino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)(phenyl)methanone (Figure 2, compound 3am)



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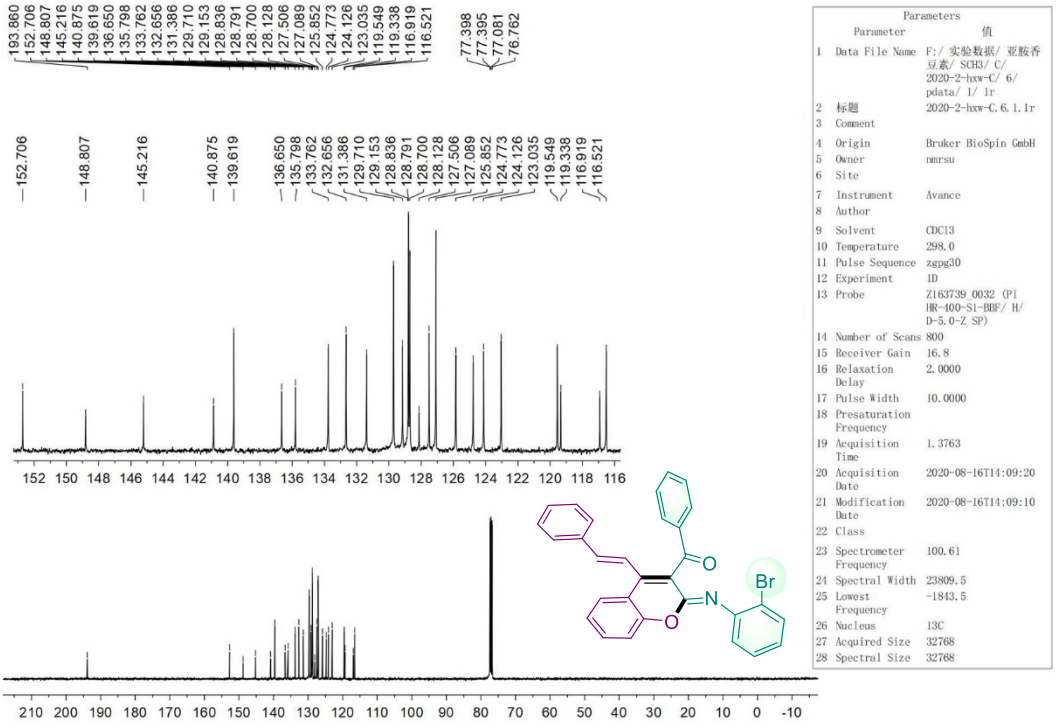
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	292.7
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14	Number of Scans	4
15	Receiver Gain	101.0
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	3.9977
20	Acquisition Date	2020-08-12T15:58:01
21	Modification Date	2020-08-12T15:56:06
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8196.7
25	Lowest Frequency	-1637.2
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

^{1}H NMR Spectra of compound 3am



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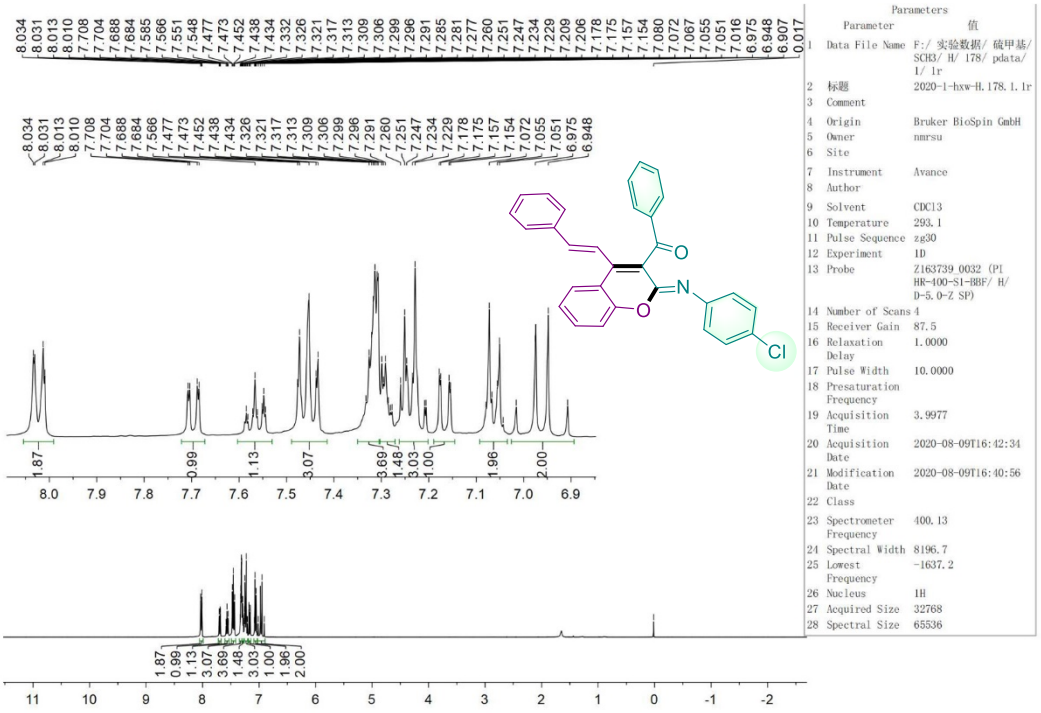
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14	Number of Scans	800
15	Receiver Gain	16.8
16	Relaxation Delay	2.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	1.3763
20	Acquisition Date	2020-08-16T14:09:20
21	Modification Date	2020-08-16T14:09:10
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	23809.5
25	Lowest Frequency	-1843.5
26	Nucleus	13C
27	Acquired Size	32768
28	Spectral Size	32768

^{13}C NMR Spectra of compound 3am

((*Z*)-2-((4-Chlorophenyl)imino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)(phenyl)methanone (Figure 2, compound 3an)



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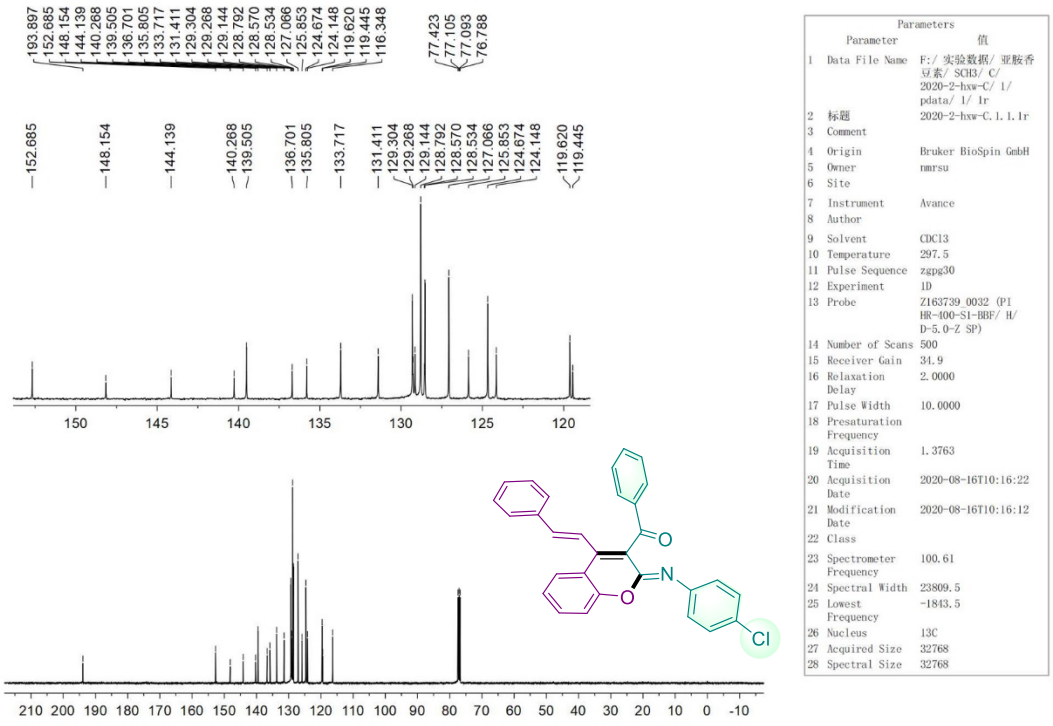
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	293.1
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14	Number of Scans	4
15	Receiver Gain	87.5
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	3.9977
20	Acquisition Date	2020-08-09T16:42:34
21	Modification Date	2020-08-09T16:40:56
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8196.7
25	Lowest Frequency	-1637.2
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

^{1}H NMR Spectra of compound 3an



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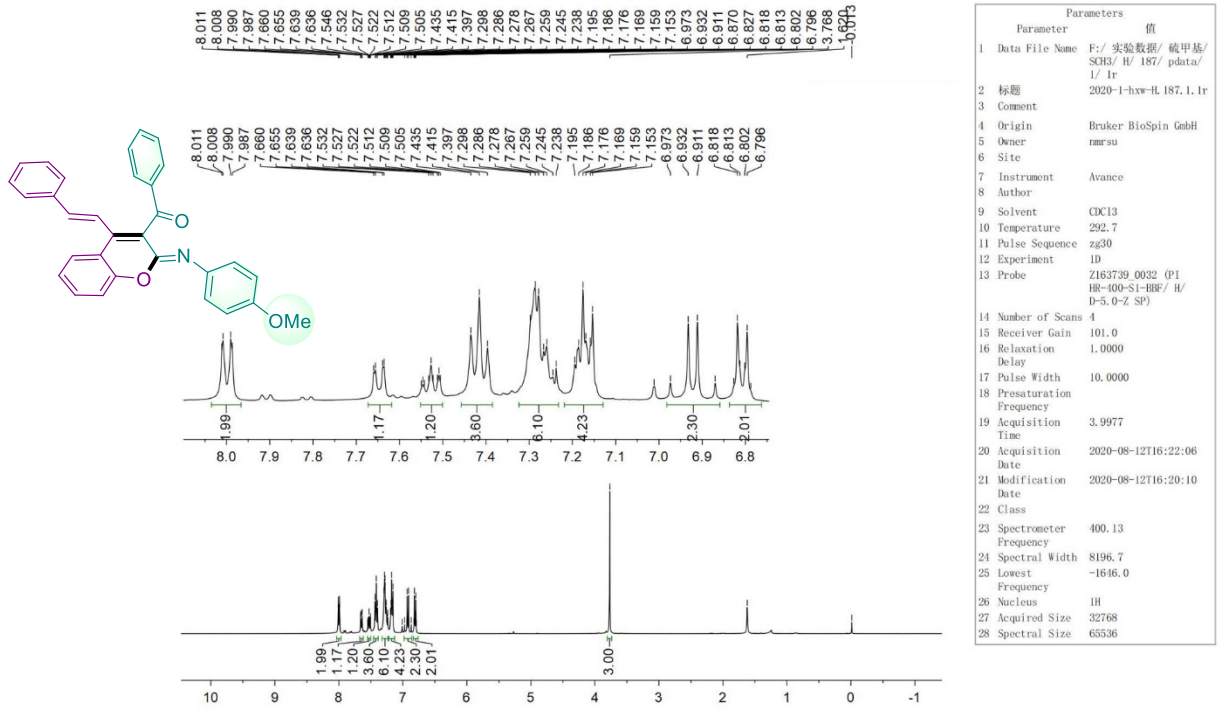
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	297.5
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14	Number of Scans	500
15	Receiver Gain	34.9
16	Relaxation Delay	2.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	1.3763
20	Acquisition Date	2020-08-16T10:16:22
21	Modification Date	2020-08-16T10:16:12
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	23809.5
25	Lowest Frequency	-1843.5
26	Nucleus	13C
27	Acquired Size	32768
28	Spectral Size	32768

^{13}C NMR Spectra of compound 3an

((*Z*)-2-((4-Methoxyphenyl)imino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)(phenyl)methanone (Figure 2, compound 3ao)



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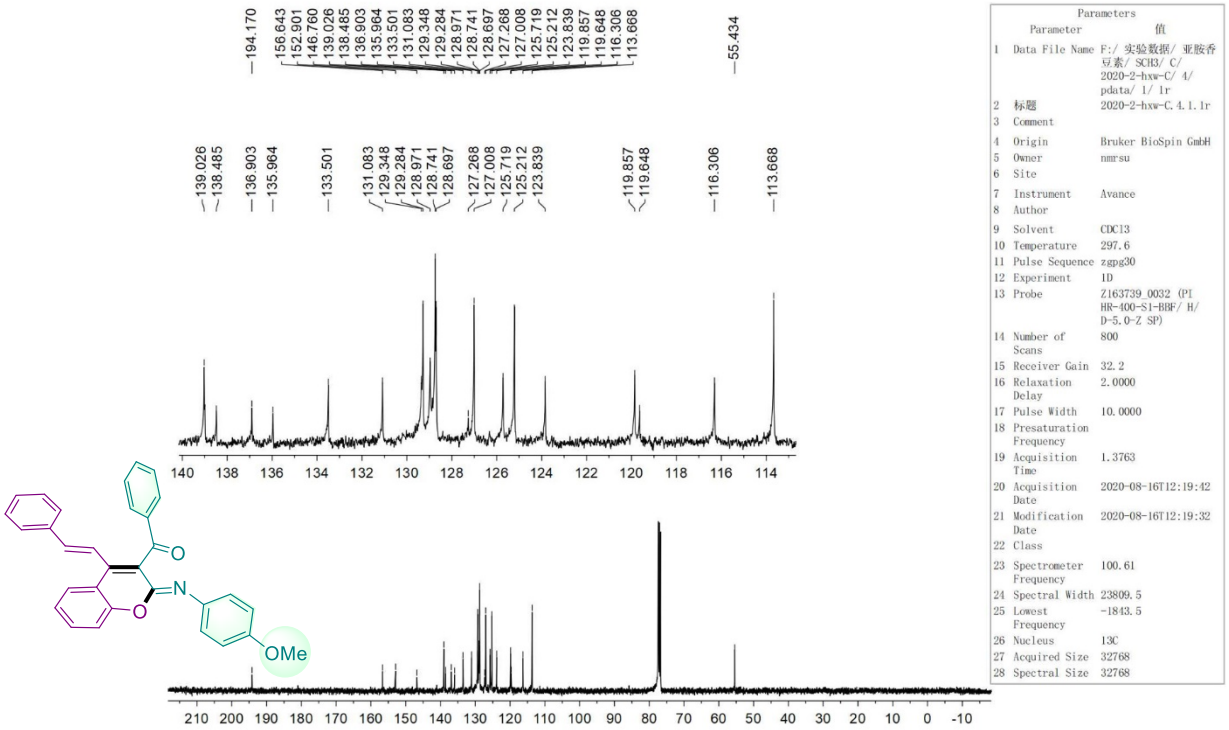
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	292.7
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14	Number of Scans	4
15	Receiver Gain	101.0
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	3.9977
20	Acquisition Date	2020-08-12T16:22:06
21	Modification Date	2020-08-12T16:20:10
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8196.7
25	Lowest Frequency	-1646.0
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

^{1}H NMR Spectra of compound 3ao



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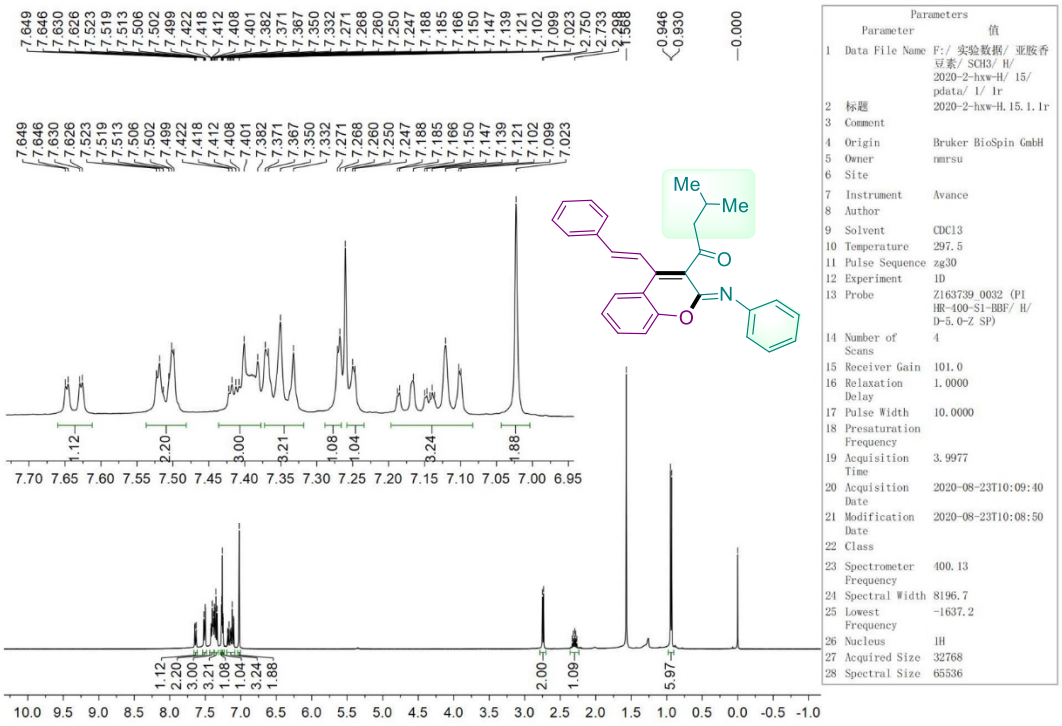
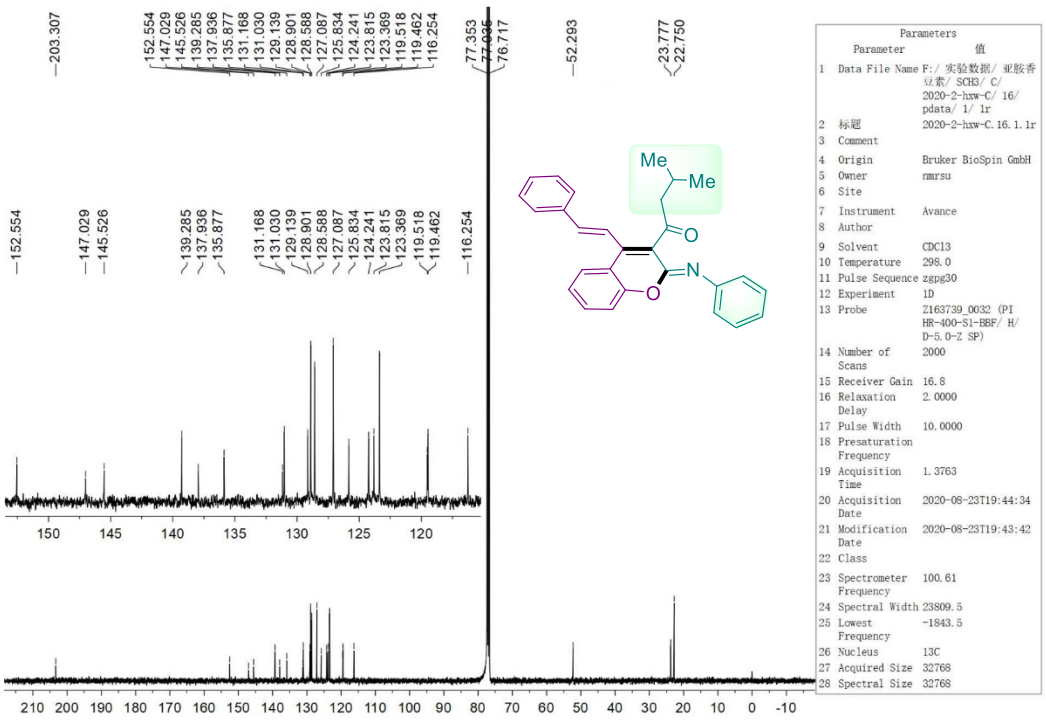
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	297.6
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14	Number of Scans	800
15	Receiver Gain	32.2
16	Relaxation Delay	2.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	1.3763
20	Acquisition Date	2020-08-16T12:19:42
21	Modification Date	2020-08-16T12:19:32
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	23809.5
25	Lowest Frequency	-1843.5
26	Nucleus	13C
27	Acquired Size	32768
28	Spectral Size	32768

^{13}C NMR Spectra of compound 3ao

3-Methyl-1-((*Z*)-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)butan-1-one (Figure 2, compound 3ap)

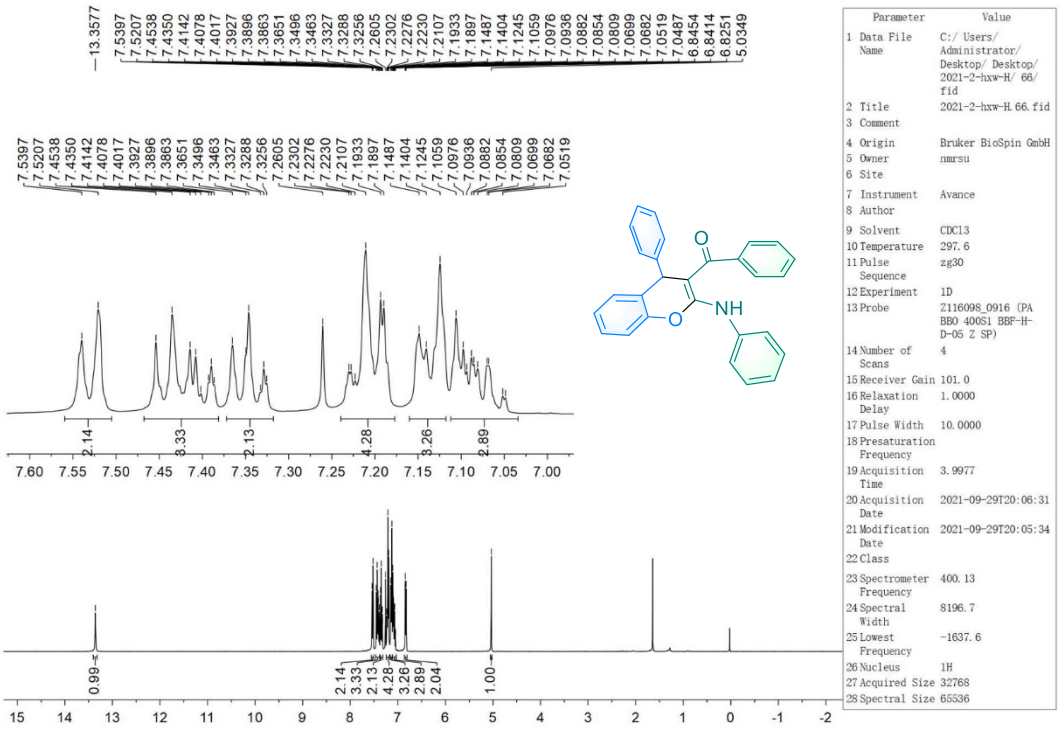


^{1}H NMR Spectra of compound 3ap



^{13}C NMR Spectra of compound 3ap

Phenyl(4-phenyl-2-(phenylamino)-4*H*-chromen-3-yl)methanone (Figure 3, compound 5aa)



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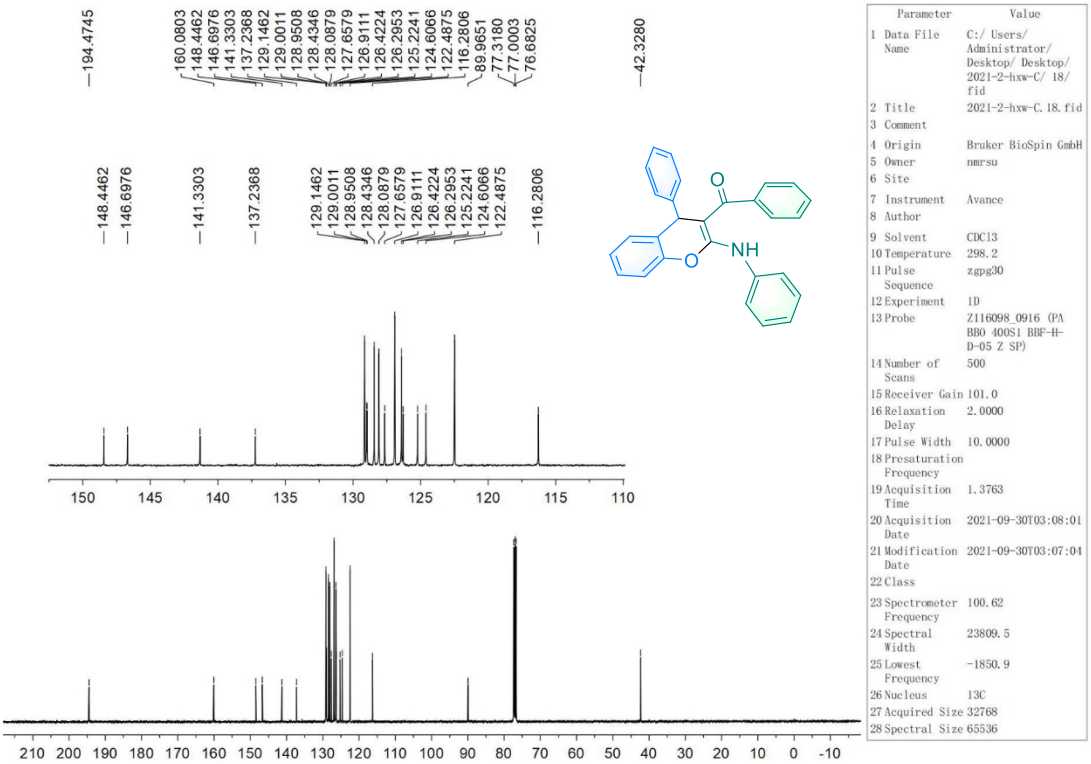
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	297. 6
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z116098_0916 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	4
15 Receiver Gain	101. 0
16 Relaxation Delay	1. 0000
17 Pulse Width	10. 0000
18 Presaturation Frequency	
19 Acquisition Time	3. 9977
20 Acquisition Date	2021-09-29T20:06:31
21 Modification Date	2021-09-29T20:05:34
22 Class	
23 Spectrometer Frequency	400. 13
24 Spectral Width	8196. 7
25 Lowest Frequency	-1637. 6
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

^{1}H NMR Spectra of compound 5aa



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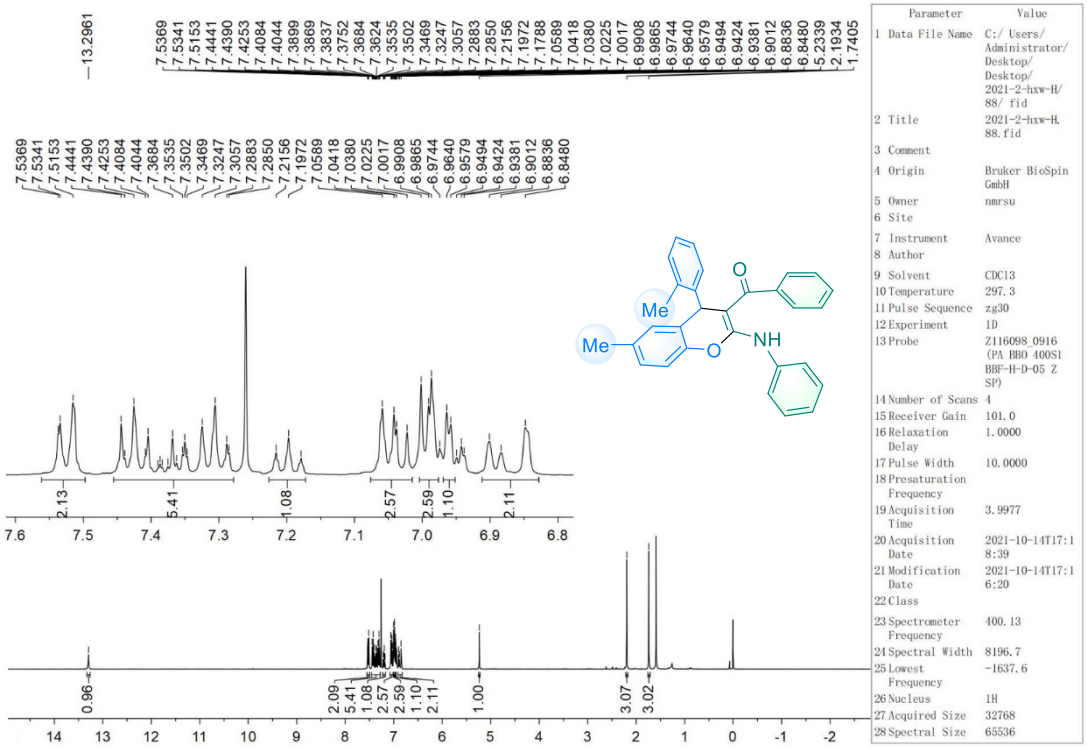
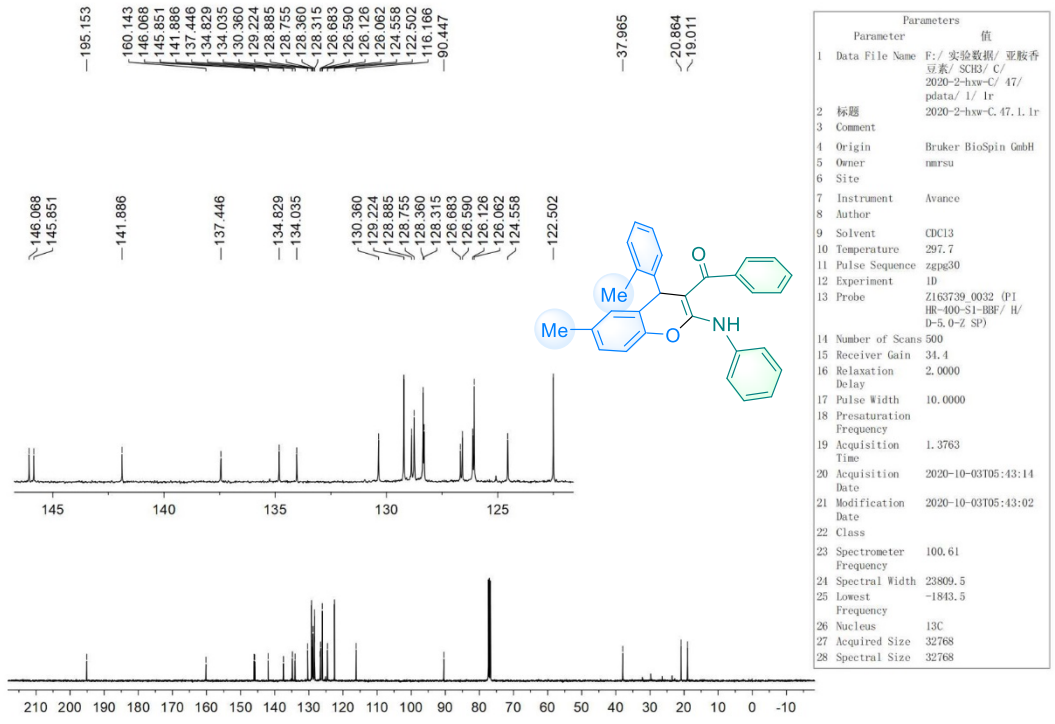
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	298. 2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z116098_0916 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	500
15 Receiver Gain	101. 0
16 Relaxation Delay	2. 0000
17 Pulse Width	10. 0000
18 Presaturation Frequency	
19 Acquisition Time	1. 3763
20 Acquisition Date	2021-09-30T03:08:01
21 Modification Date	2021-09-30T03:07:04
22 Class	
23 Spectrometer Frequency	100. 62
24 Spectral Width	23809. 5
25 Lowest Frequency	-1850. 9
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	65536

^{13}C NMR Spectra of compound 5aa

(6-Methyl-2-(phenylamino)-4-(*o*-tolyl)-4*H*-chromen-3-yl)(phenyl)methanone (Figure 3, compound 5ba)

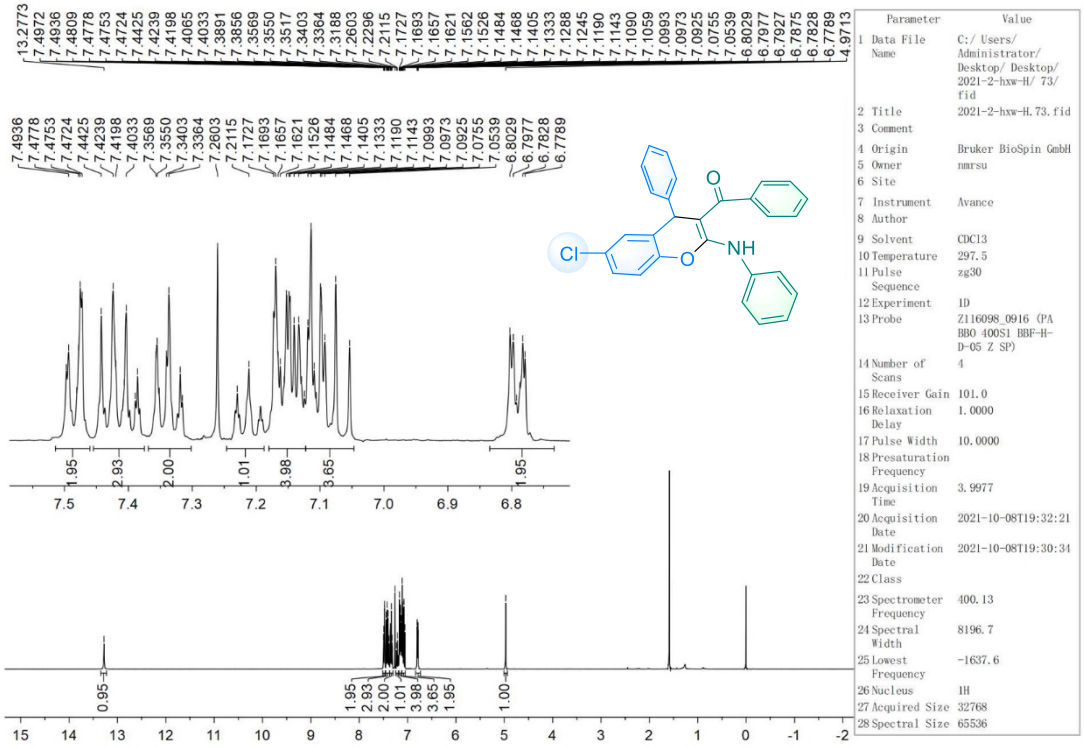


^{1}H NMR Spectra of compound 5ba

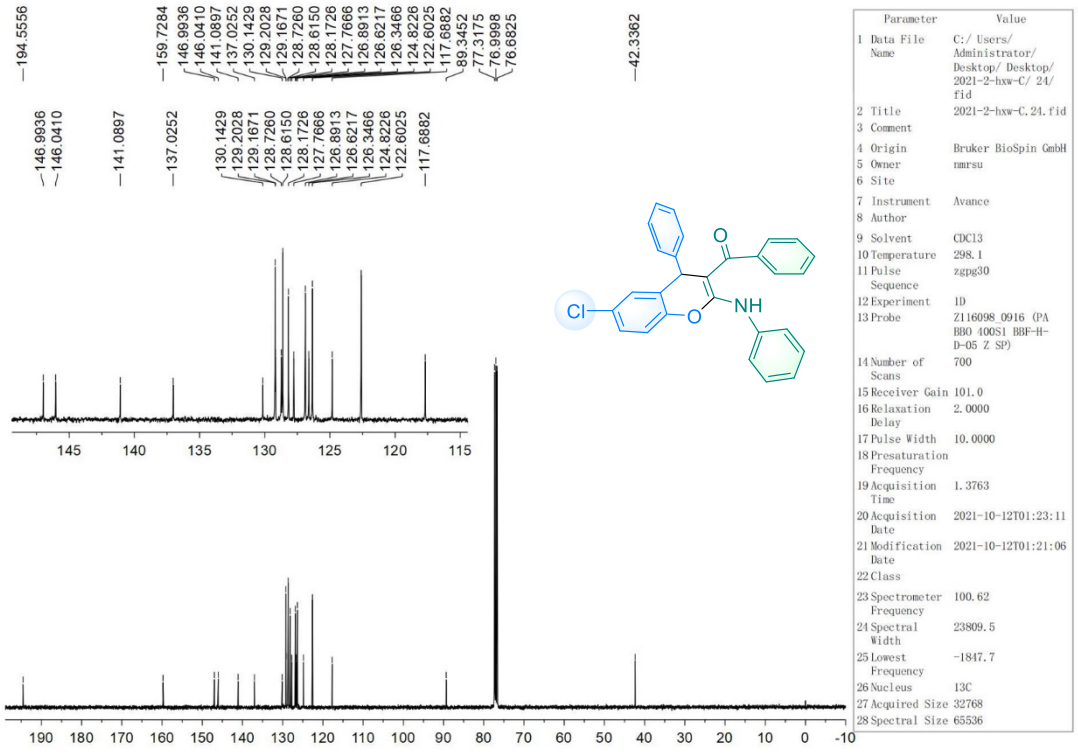


^{13}C NMR Spectra of compound 5ba

(6-Chloro-4-phenyl-2-(phenylamino)-4*H*-chromen-3-yl)(phenyl)methanone (Figure 3, compound 5ca)

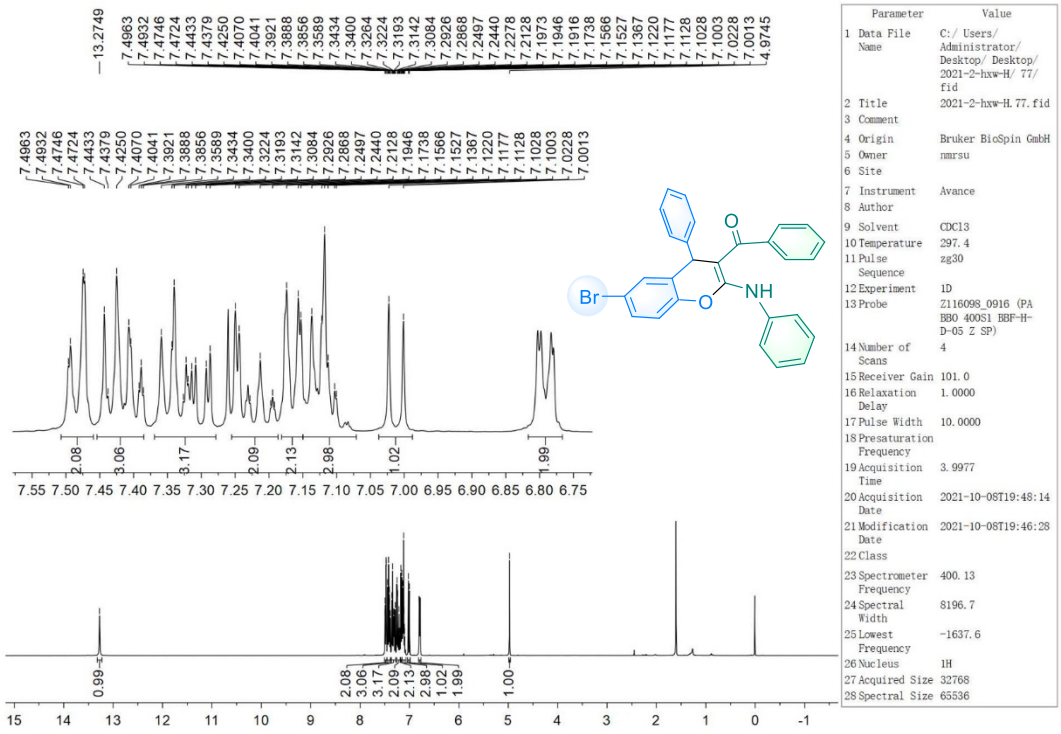


^{1}H NMR Spectra of compound 5ca

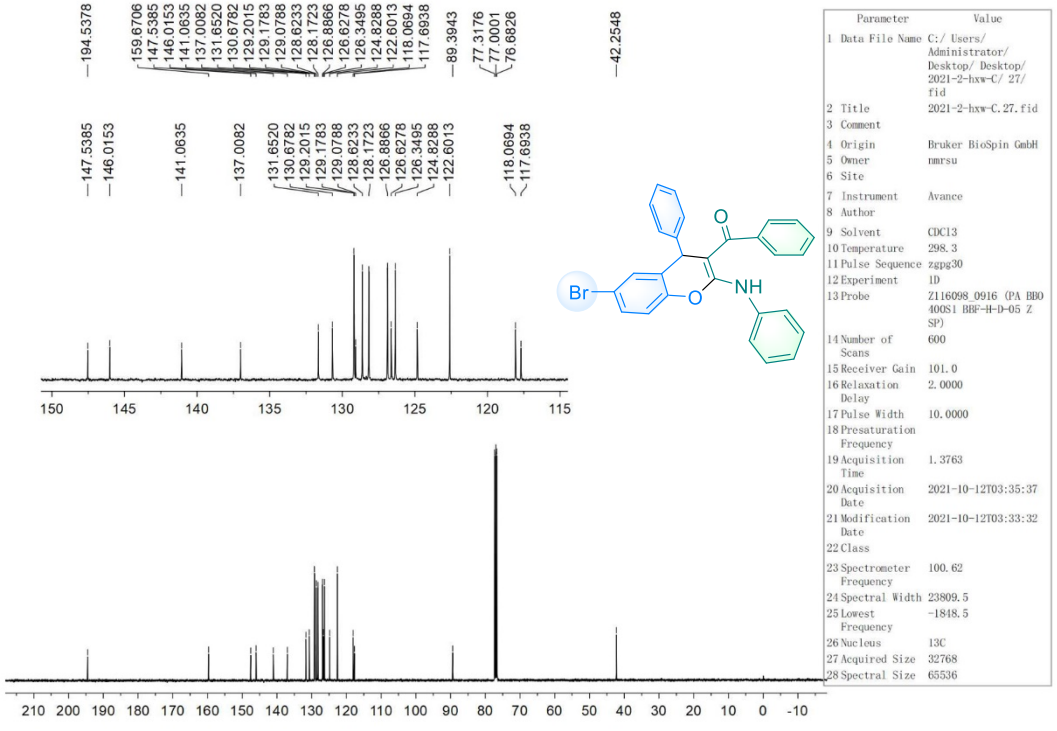


^{13}C NMR Spectra of compound 5ca

(6-Bromo-4-phenyl-2-(phenylamino)-4*H*-chromen-3-yl)(phenyl)methanone (Figure 3, compound 5da)

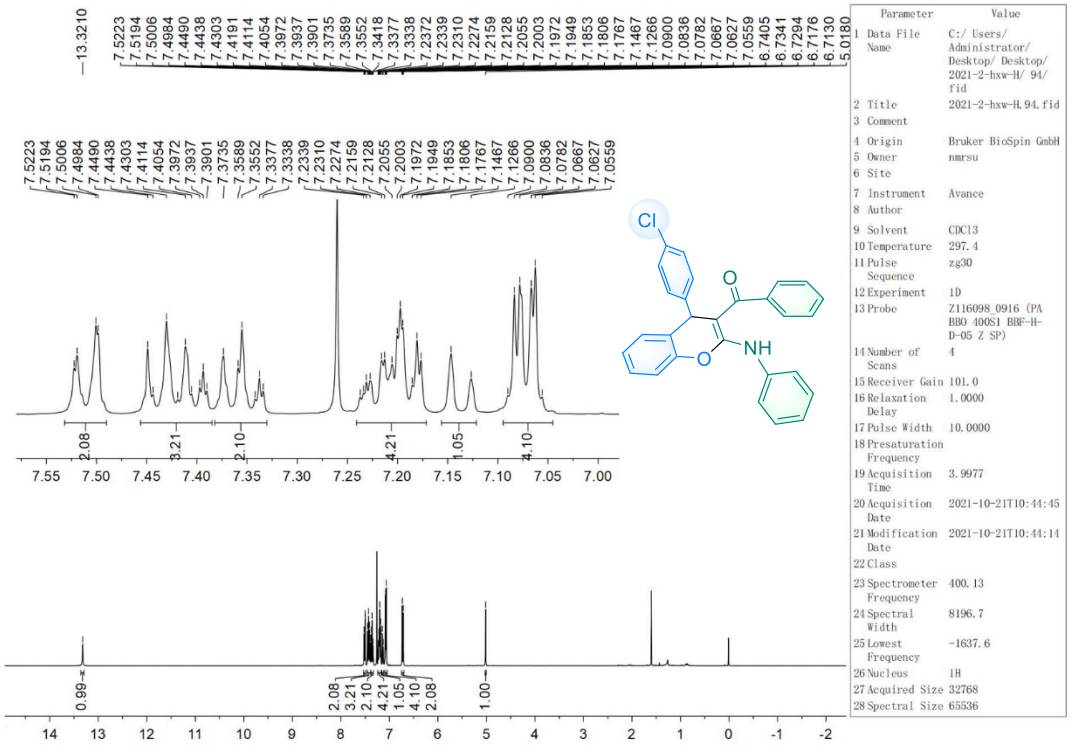


^{1}H NMR Spectra of compound 5da

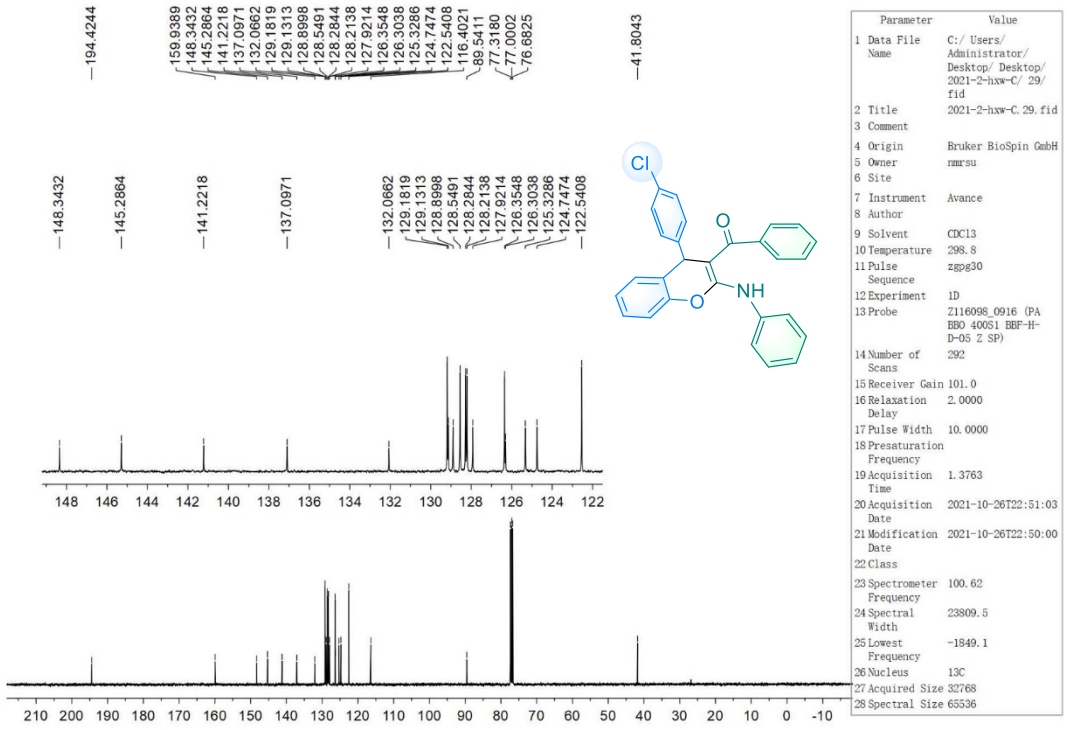


^{13}C NMR Spectra of compound 5da

(4-(4-Chlorophenyl)-2-(phenylamino)-4*H*-chromen-3-yl)(phenyl)methanone (Figure 3, compound 5ea)

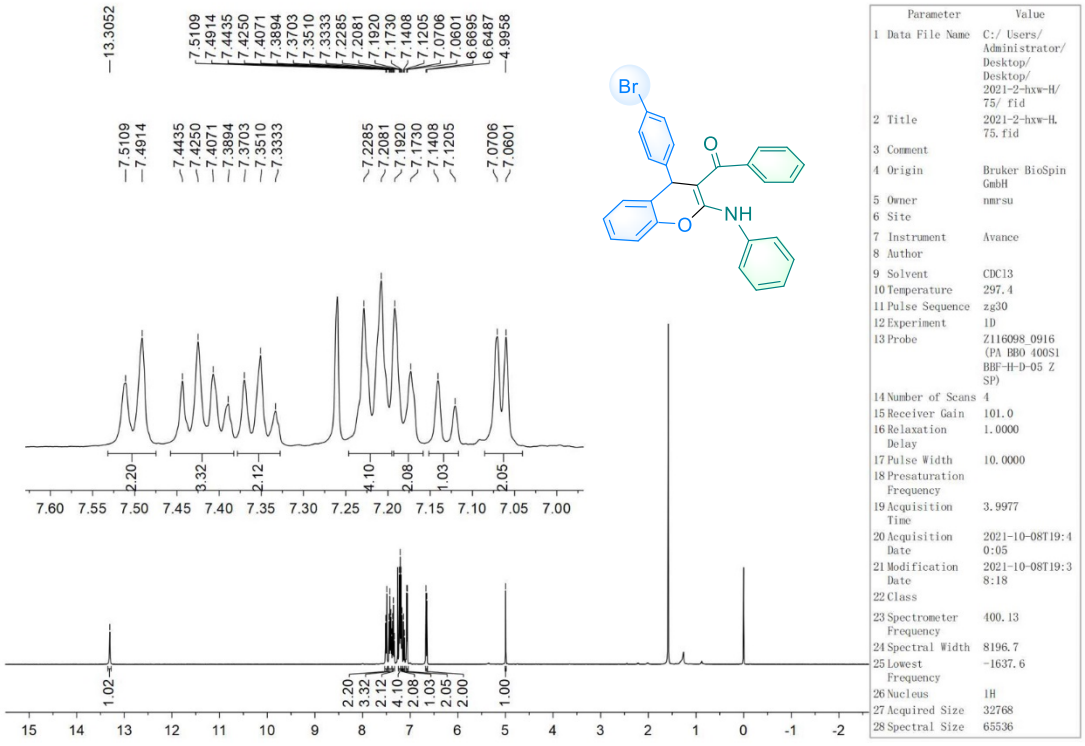


^{1}H NMR Spectra of compound 5ea

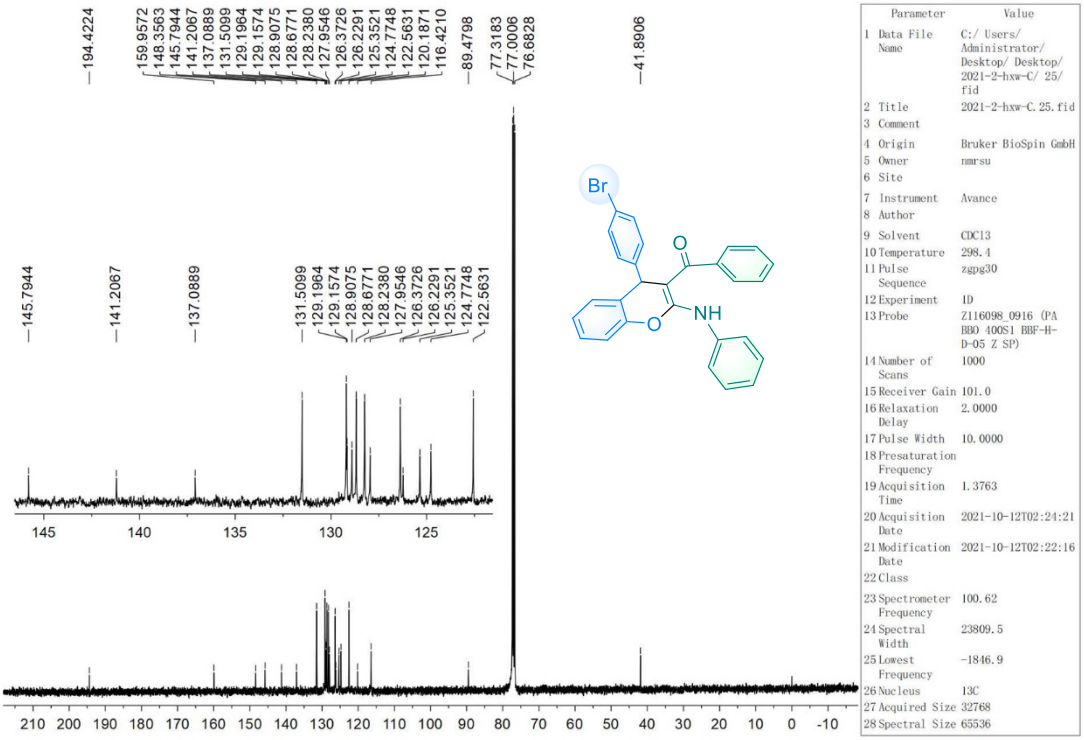


^{13}C NMR Spectra of compound 5ea

(4-(4-bromophenyl)-2-(phenylamino)-4H-chromen-3-yl)(phenyl)methanone (Figure 3, compound 5fa)

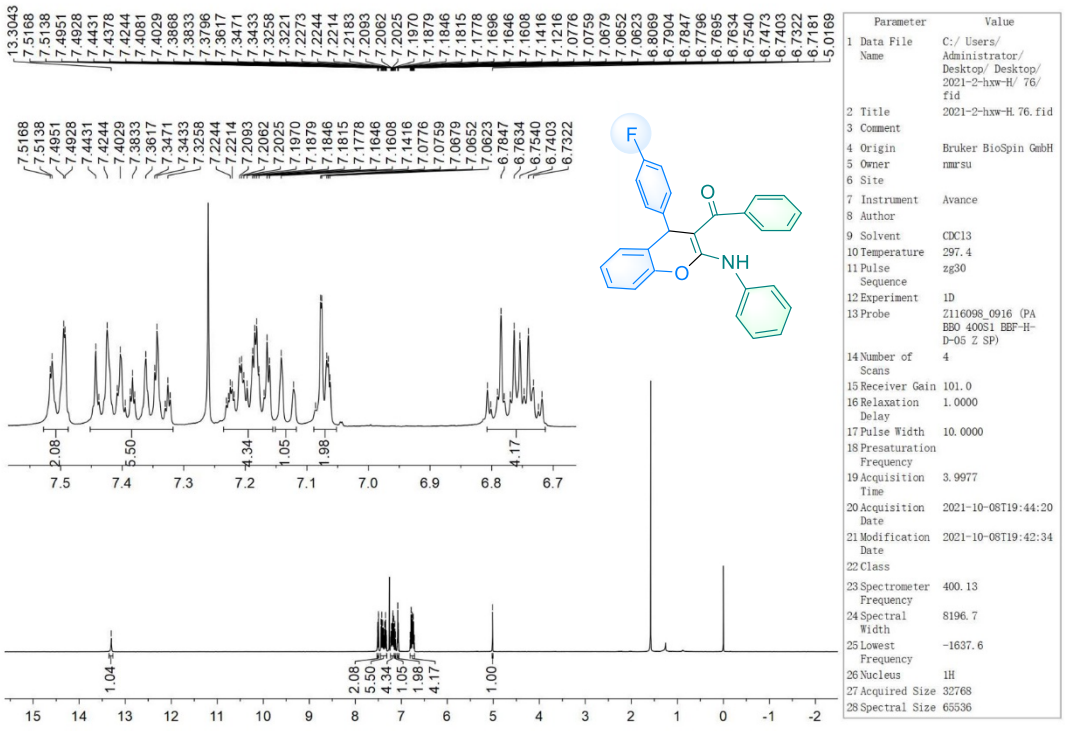


^{1}H NMR Spectra of compound 5fa

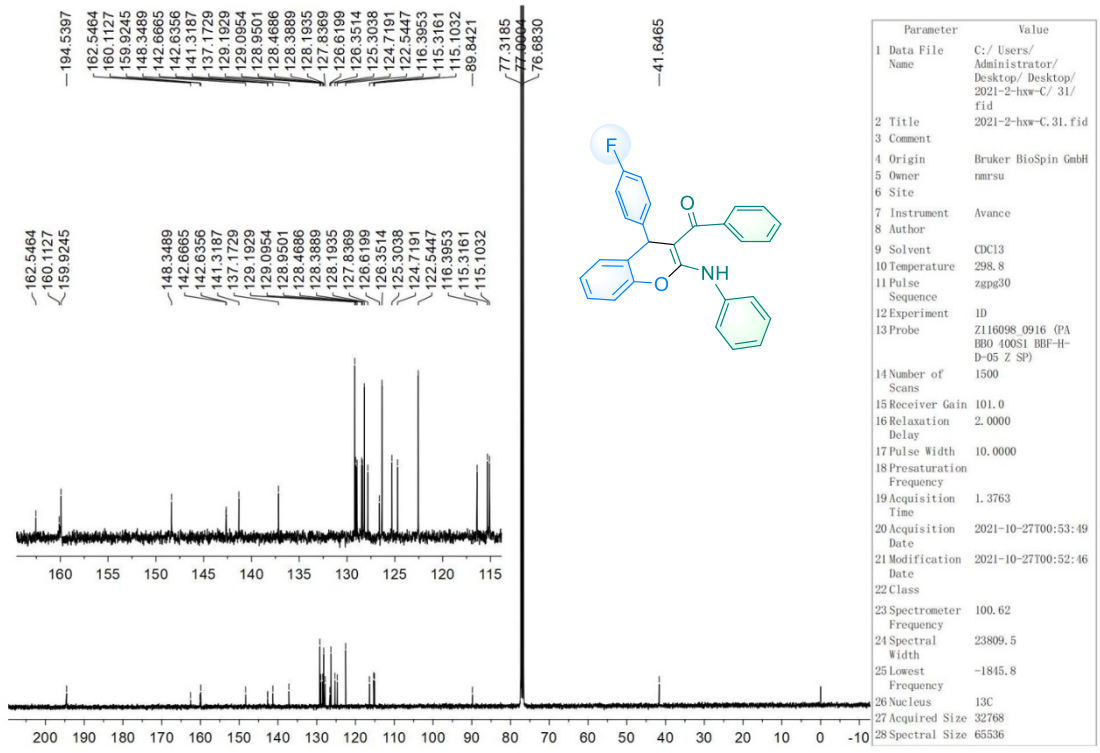


^{13}C NMR Spectra of compound 5fa

(4-(4-Fluorophenyl)-2-(phenylamino)-4*H*-chromen-3-yl)(phenyl)methanone (Figure 3, compound 5ga)

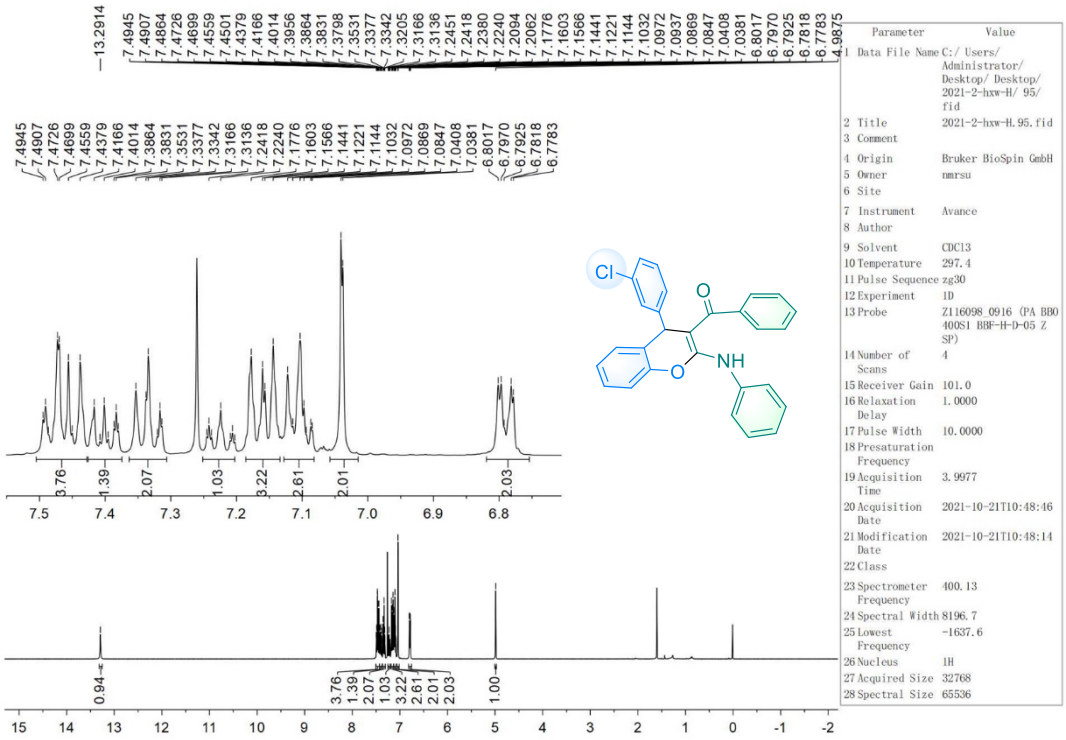


^{1}H NMR Spectra of compound 5ga

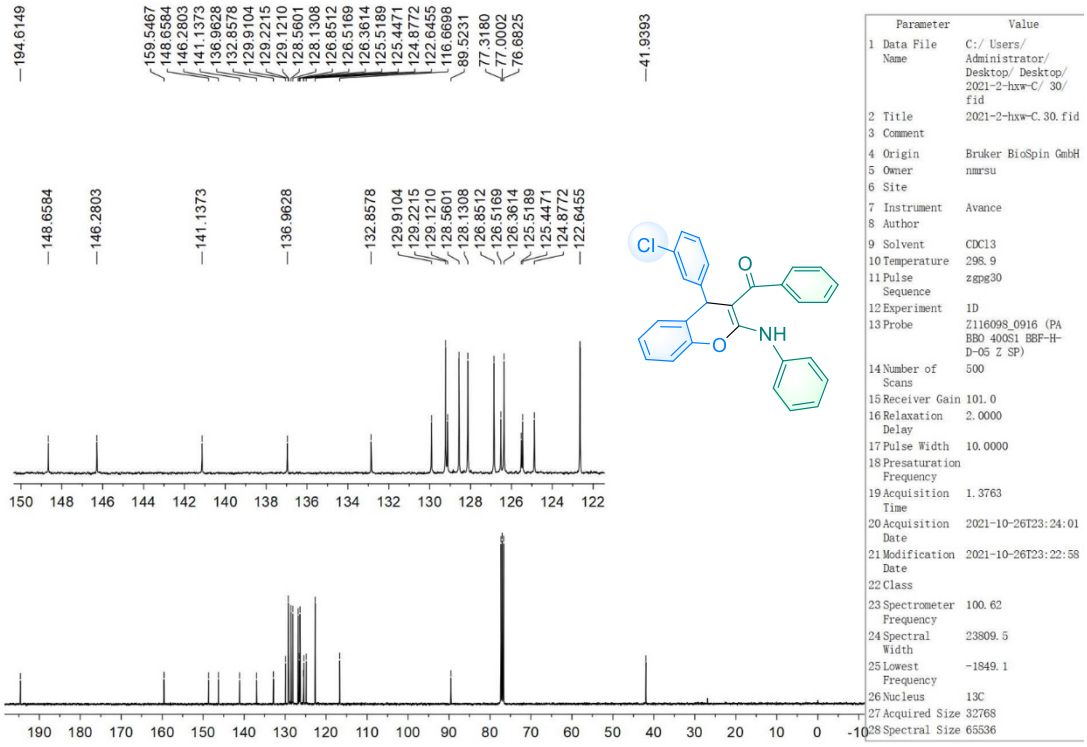


^{13}C NMR Spectra of compound 5ga

(4-(3-Chlorophenyl)-2-(phenylamino)-4*H*-chromen-3-yl)(phenyl)methanone (Figure 3, compound 5ha)

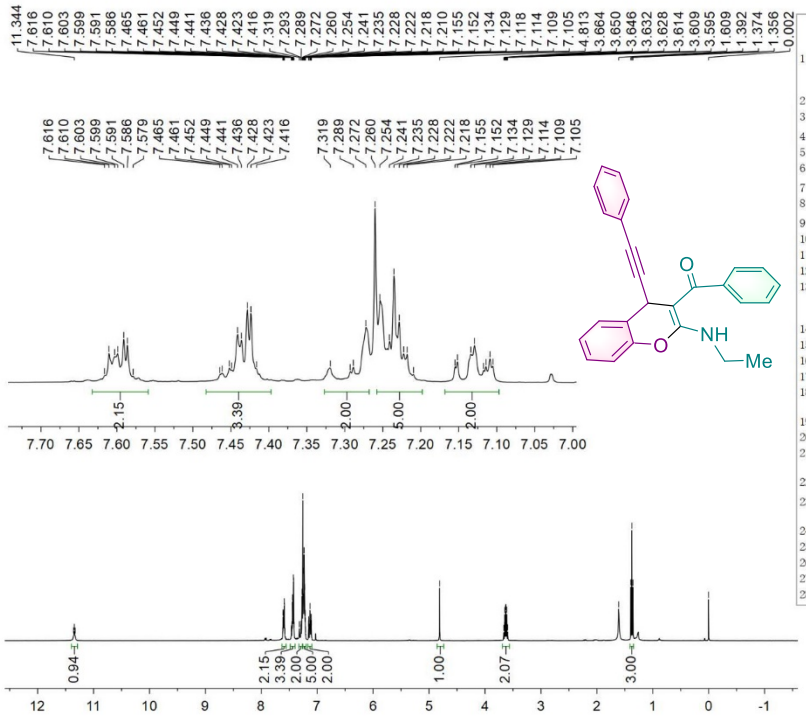


^{1}H NMR Spectra of compound 5ha



^{13}C NMR Spectra of compound 5ha

(2-(Ethylamino)-4-(phenylethynyl)-4*H*-chromen-3-yl)(phenyl)methanone (Figure 3, compound 6aq)



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8	Author	
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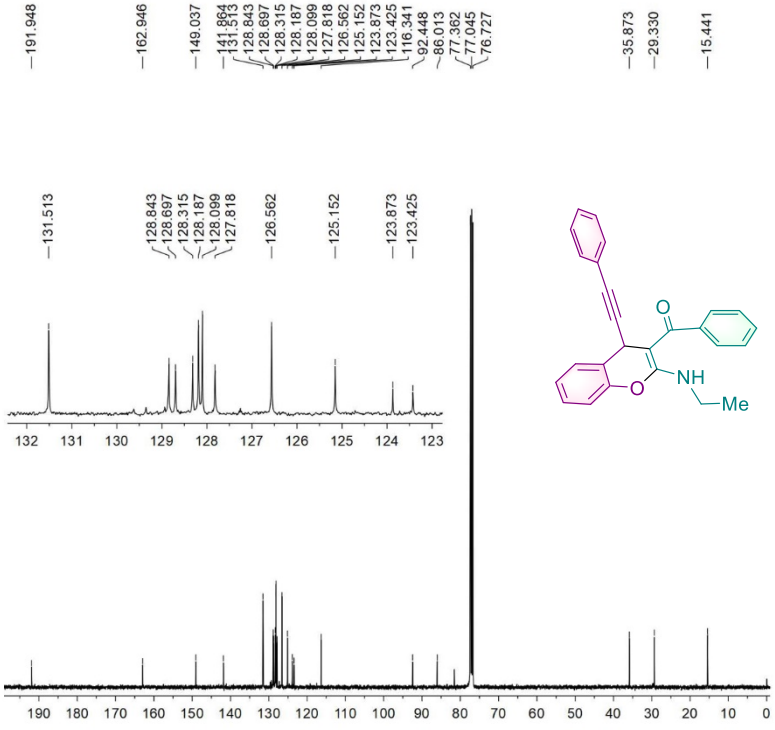
25	Lowest Frequency	-1637.2
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

^{1}H NMR Spectra of compound 6aq



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7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
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11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
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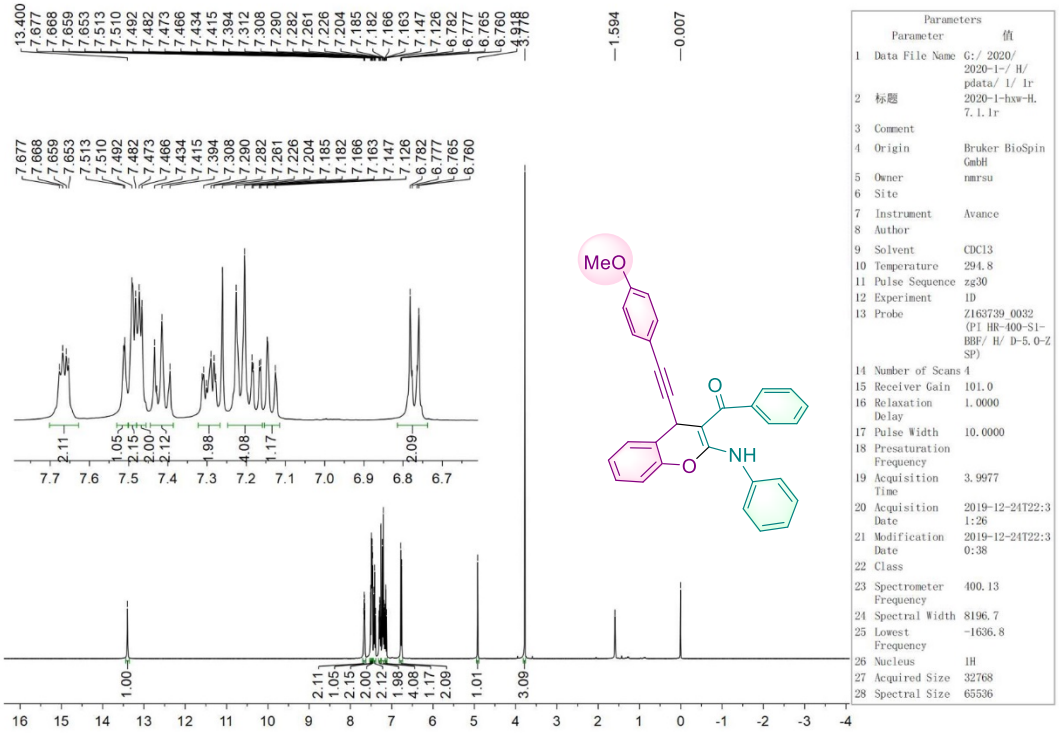
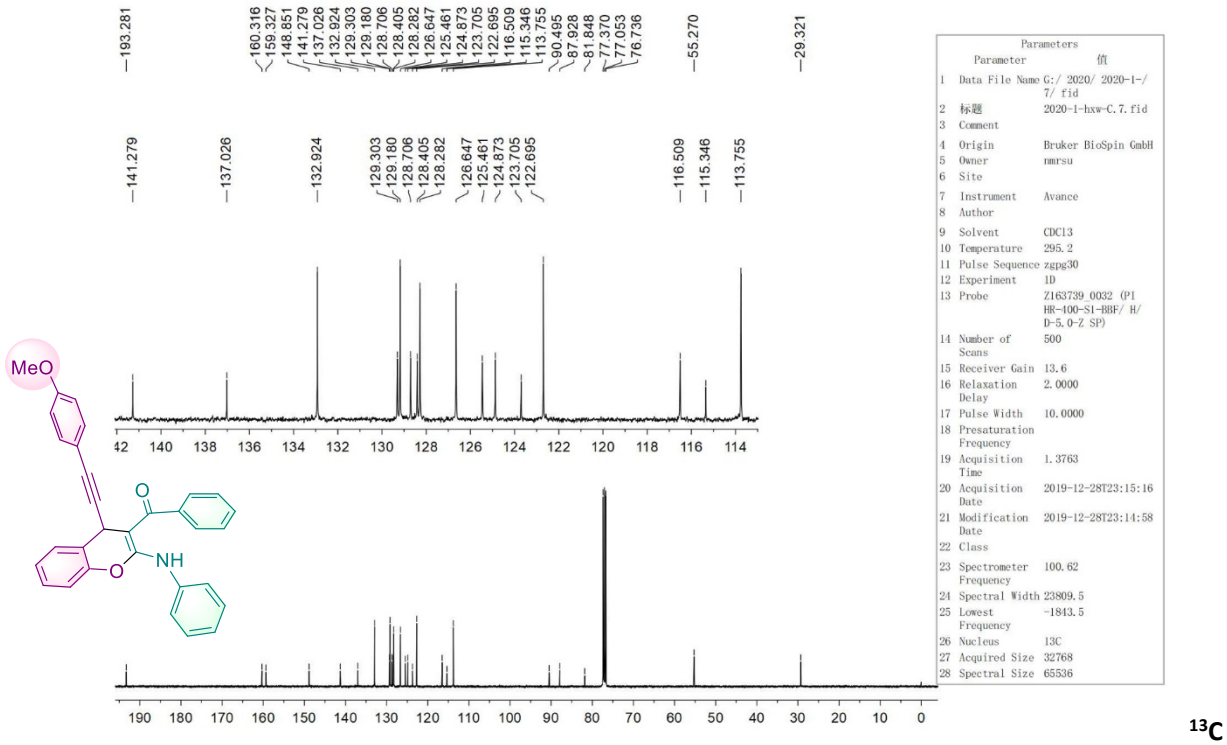
15	Receiver Gain	38.2
16	Relaxation Delay	2.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	1.3763
20	Acquisition Date	2020-09-20T19:36:37
21	Modification Date	2020-09-20T19:36:02
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	23809.5
25	Lowest Frequency	-1843.5
26	Nucleus	13C
27	Acquired Size	32768
28	Spectral Size	32768

^{13}C NMR Spectra of compound 6aq

(4-((4-Methoxyphenyl)ethynyl)-2-(phenylamino)-4*H*-chromen-3-yl)(phenyl)methanone (Figure 3, compound 6ia)

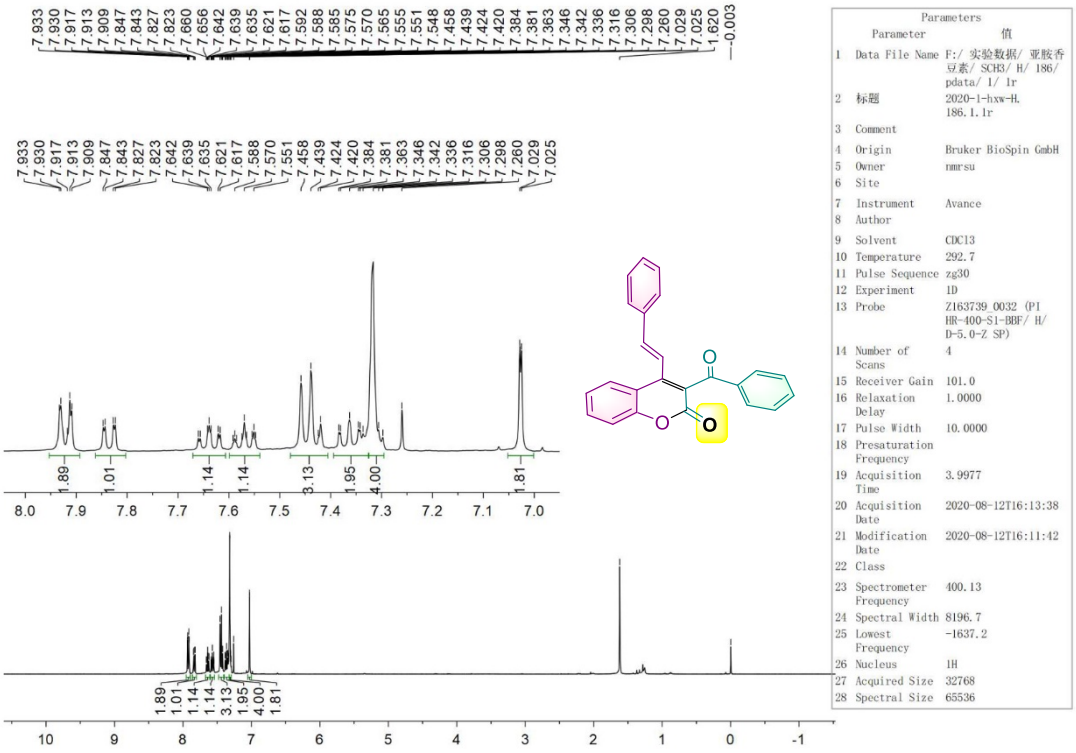


^{1}H NMR Spectra of compound 6ia



^{13}C NMR Spectra of compound 6ia

(*E*)-3-Benzoyl-4-styryl-2*H*-chromen-2-one (Figure 5, compound 8)



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7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
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21	Modification Date	2020-08-12T16:11:42
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23	Spectrometer Frequency	400.13
24	Spectral Width	8196.7
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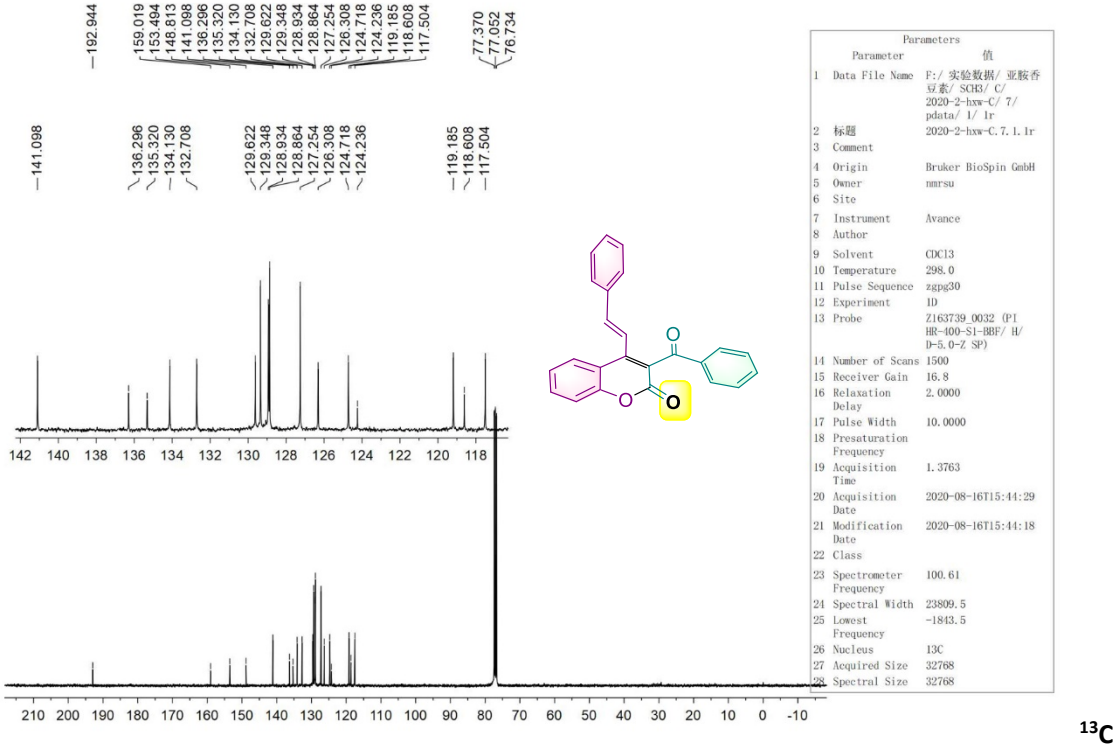
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

^{1}H NMR Spectra of compound 8



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4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
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19	Acquisition Time	1.3763
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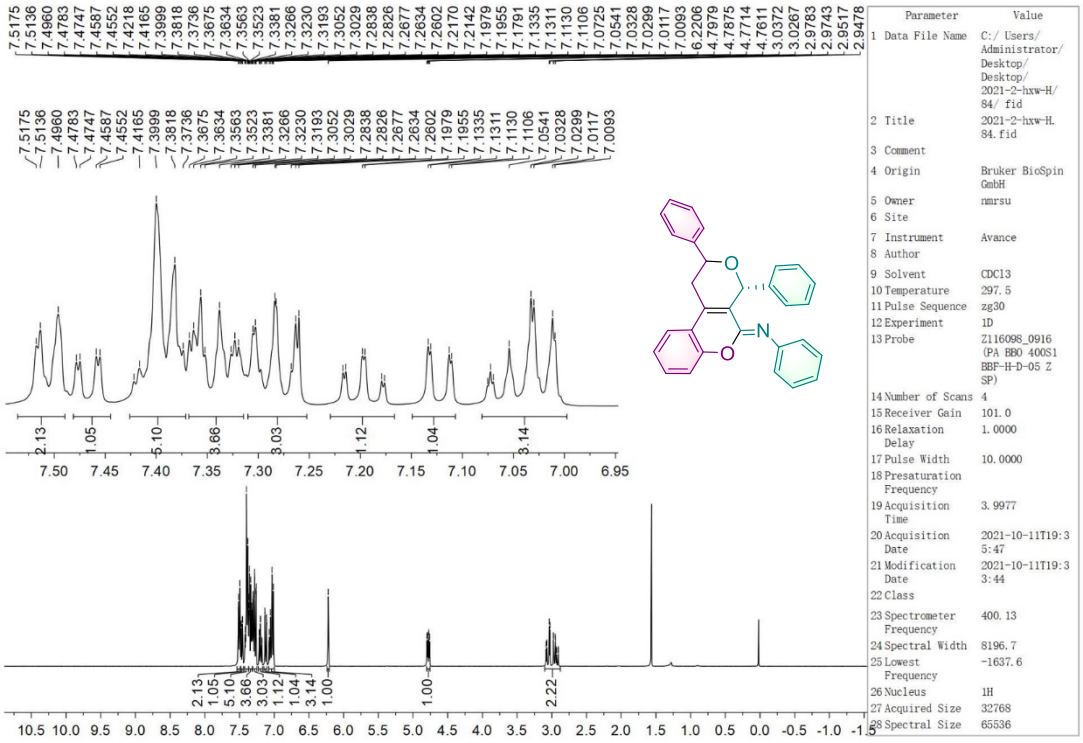
21	Modification Date	2020-08-16T15:44:18
22	Class	
23	Spectrometer Frequency	100.61
24	Spectral Width	23809.5
25	Lowest Frequency	-1843.5
26	Nucleus	13C
27	Acquired Size	32768
28	Spectral Size	32768

^{13}C NMR Spectra of compound 8

(*Z*)-*N*,2,4-Triphenyl-1,4-dihydro-2*H*,5*H*-pyrano[3,4-*c*]chromen-5-imine (Figure 5, compound 9aa)



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7 Instrument	Avance
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11 Pulse Sequence	zg30
12 Experiment	1D
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22 Class	
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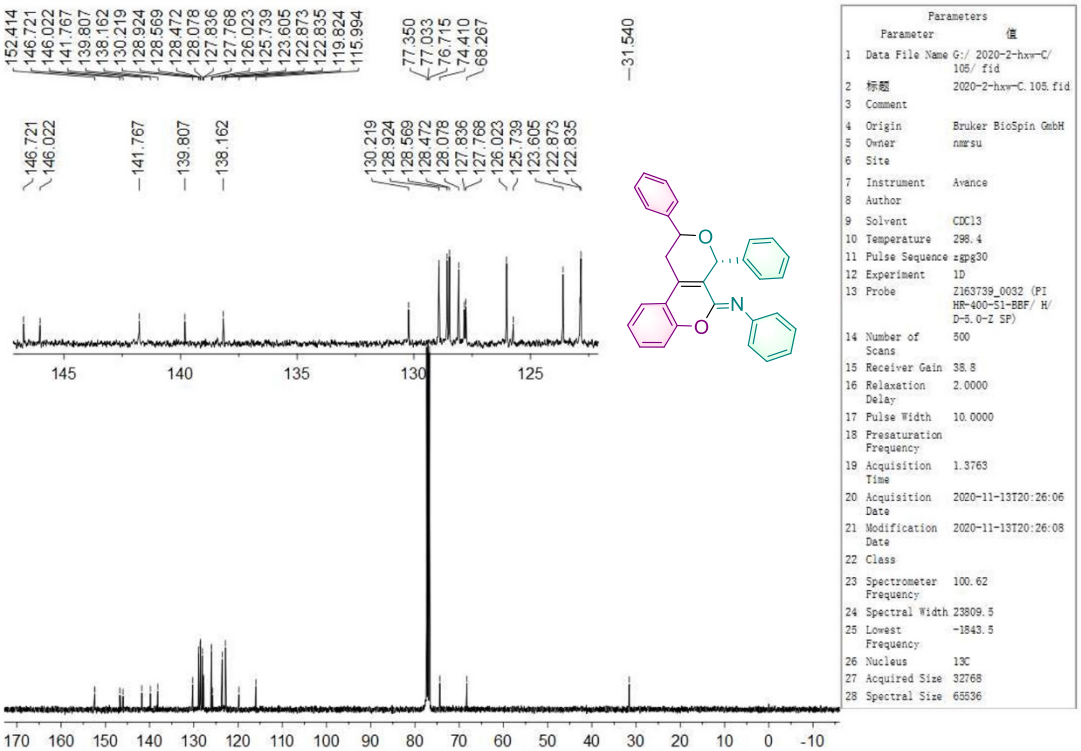
25 Lowest Frequency	-1637.6
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

^{1}H NMR Spectra of compound 9aa



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8	Author	
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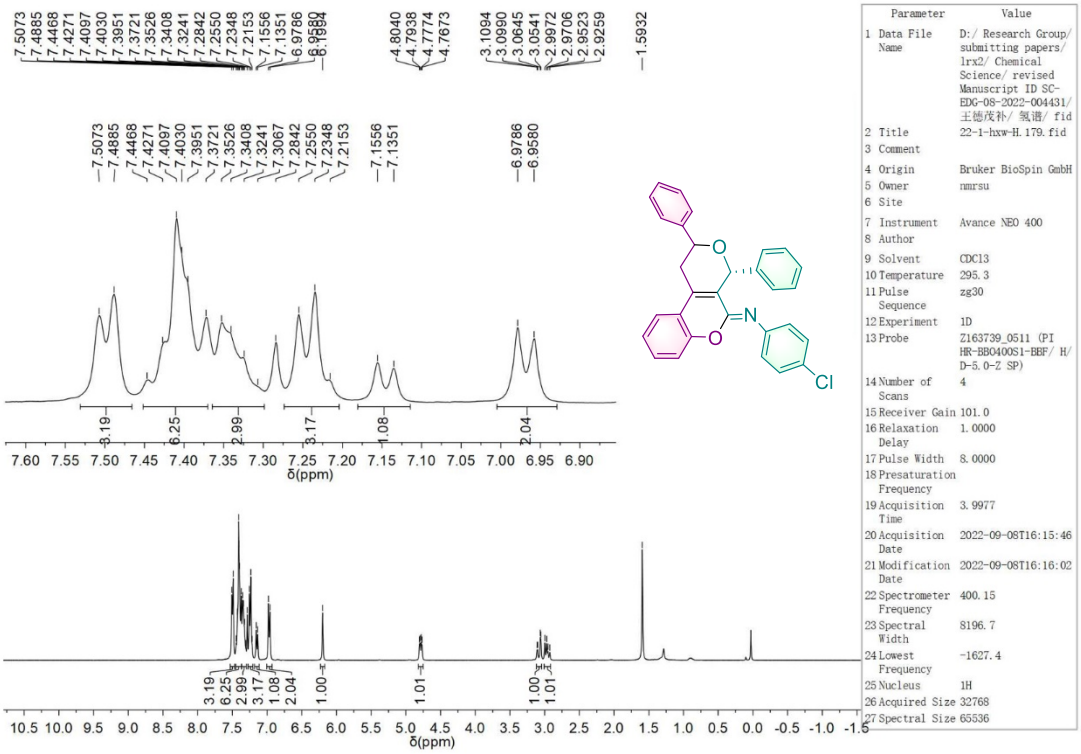
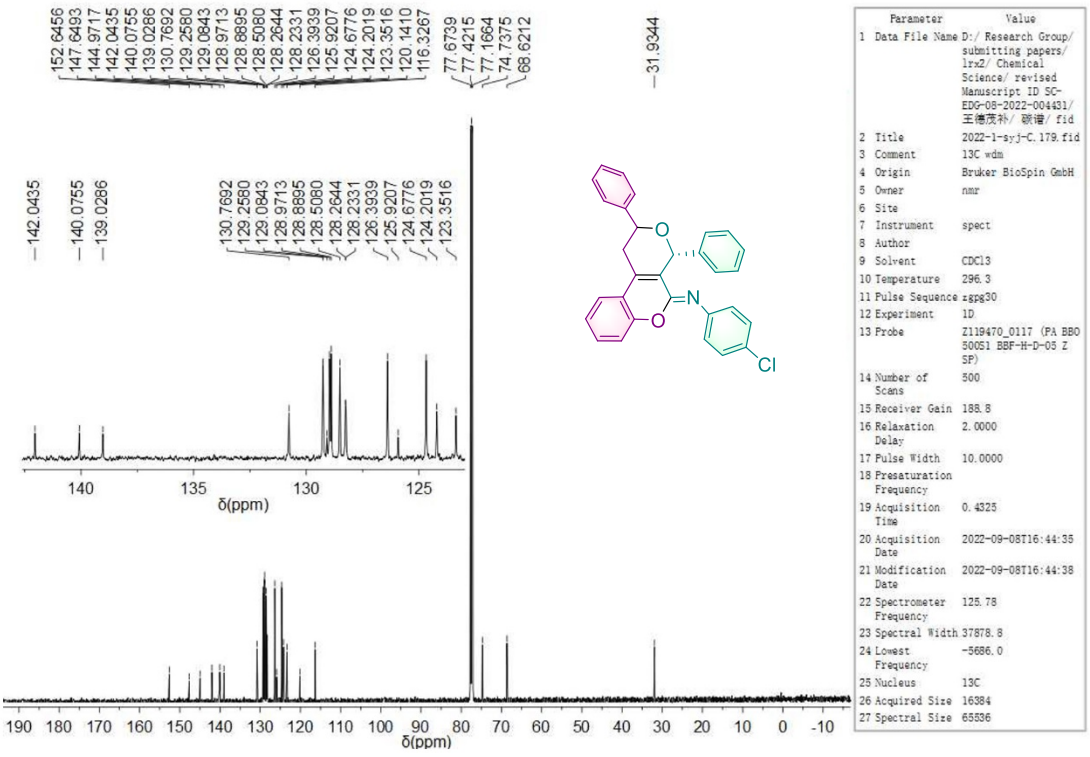
14	Number of Scans	500
15	Receiver Gain	38.8
16	Relaxation Delay	2.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	1.3763
20	Acquisition Date	2020-11-13T20:26:06
21	Modification Date	2020-11-13T20:26:08
22	Class	
23	Spectrometer Frequency	100.62
24	Spectral Width	23809.5
25	Lowest Frequency	-1843.5
26	Nucleus	13C
27	Acquired Size	32768
28	Spectral Size	65536

^{13}C NMR Spectra of compound 9aa

(*Z*)-*N*-(4-Chlorophenyl)-2,4-diphenyl-1,4-dihydro-2*H*,5*H*-pyrano[3,4-*c*]chromen-5-imine (Figure 5, compound 9an)

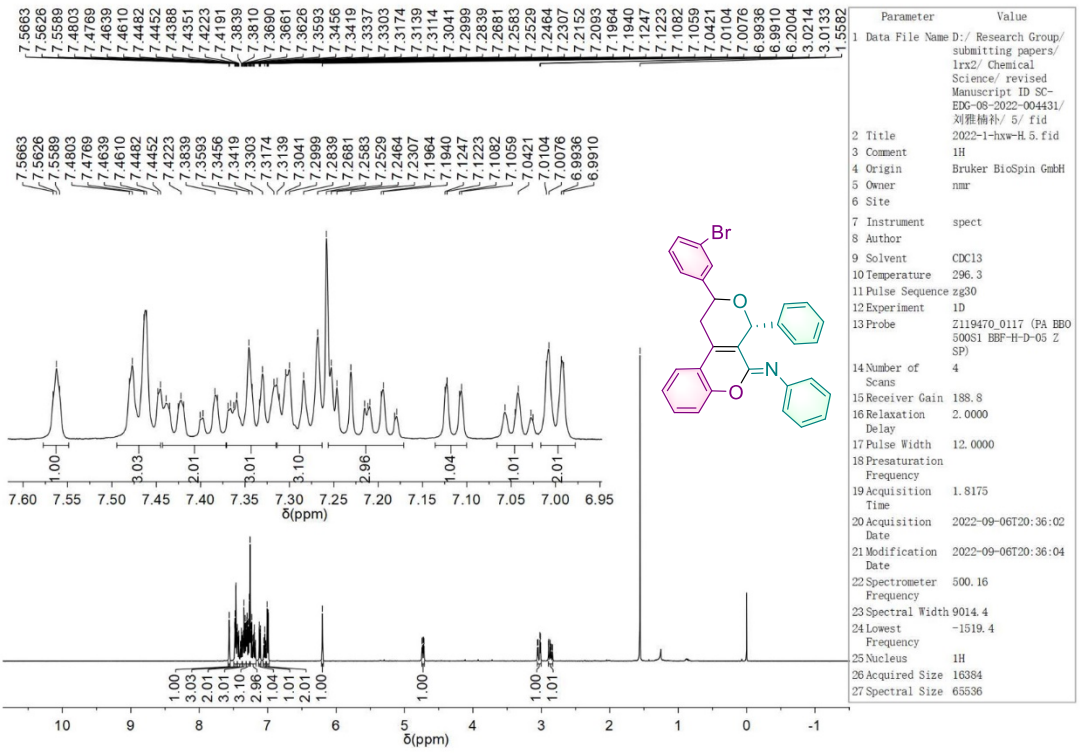


^{1}H NMR Spectra of compound 9an



^{13}C NMR Spectra of compound 9an

(*Z*)-2-(3-Bromophenyl)-*N*,4-diphenyl-1,4-dihydro-2*H*,5*H*-pyrano[3,4-*c*]chromen-5-imine (Figure 5, compound 9qa)



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5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	296. 3
11 Pulse Sequence	zg30
12 Experiment	1D
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23 Spectral Width	9014. 4
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25 Nucleus	1H
26 Acquired Size	16384
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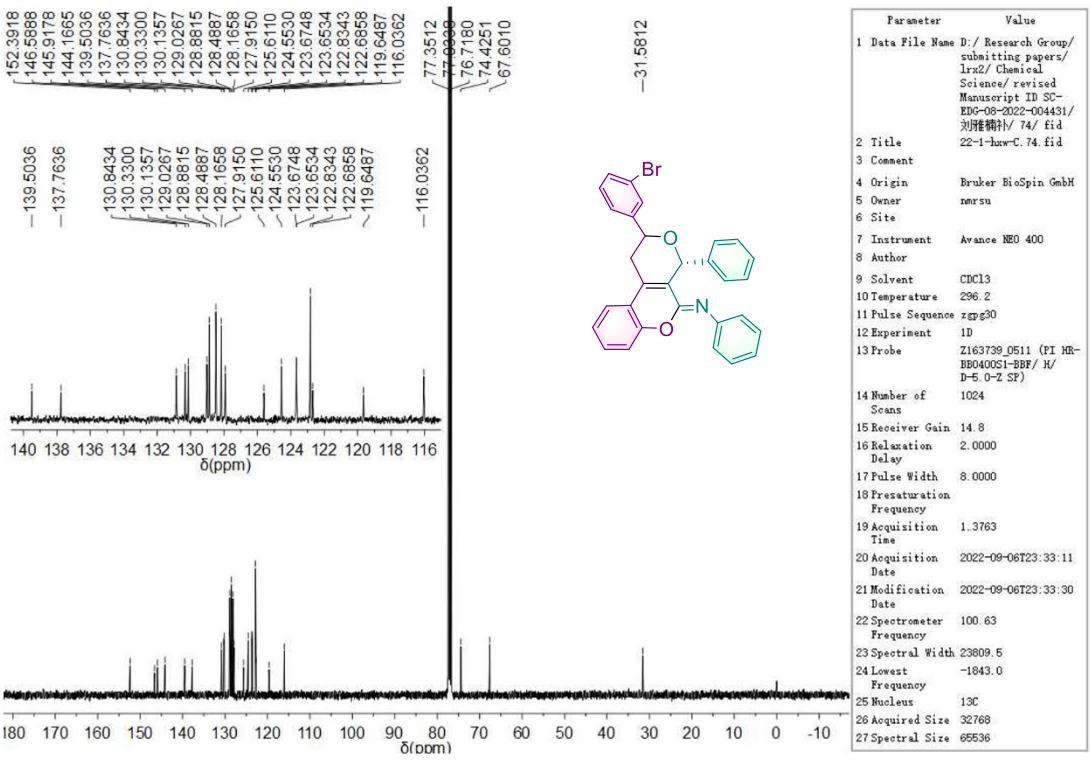
^{1}H NMR Spectra of compound 9qa



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5 Owner	nmrsu
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8 Author	
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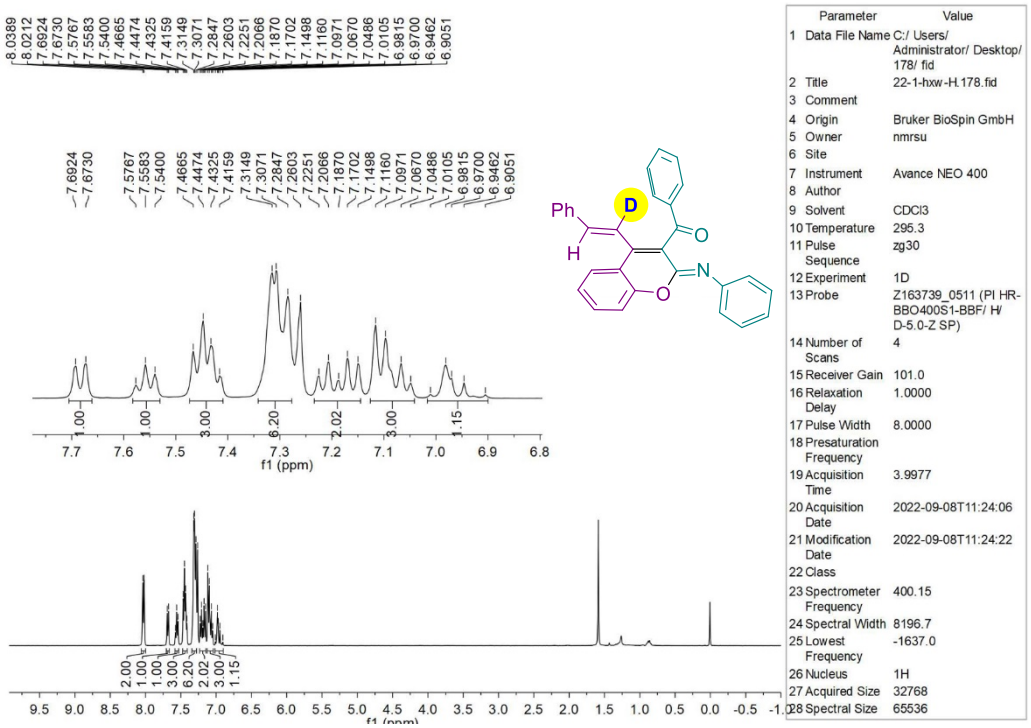
25 Nucleus	13C
26 Acquired Size	32768
27 Spectral Size	65536

^{13}C NMR Spectra of compound 9qa

Phenyl((*Z*)-2-(phenylimino)-4-((*E*)-styryl)-2*H*-chromen-3-yl)methanone (Scheme 4, compound 3aa-*d*)



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12	Experiment	1D
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17	Pulse Width	8.0000
18	Presaturation Frequency	
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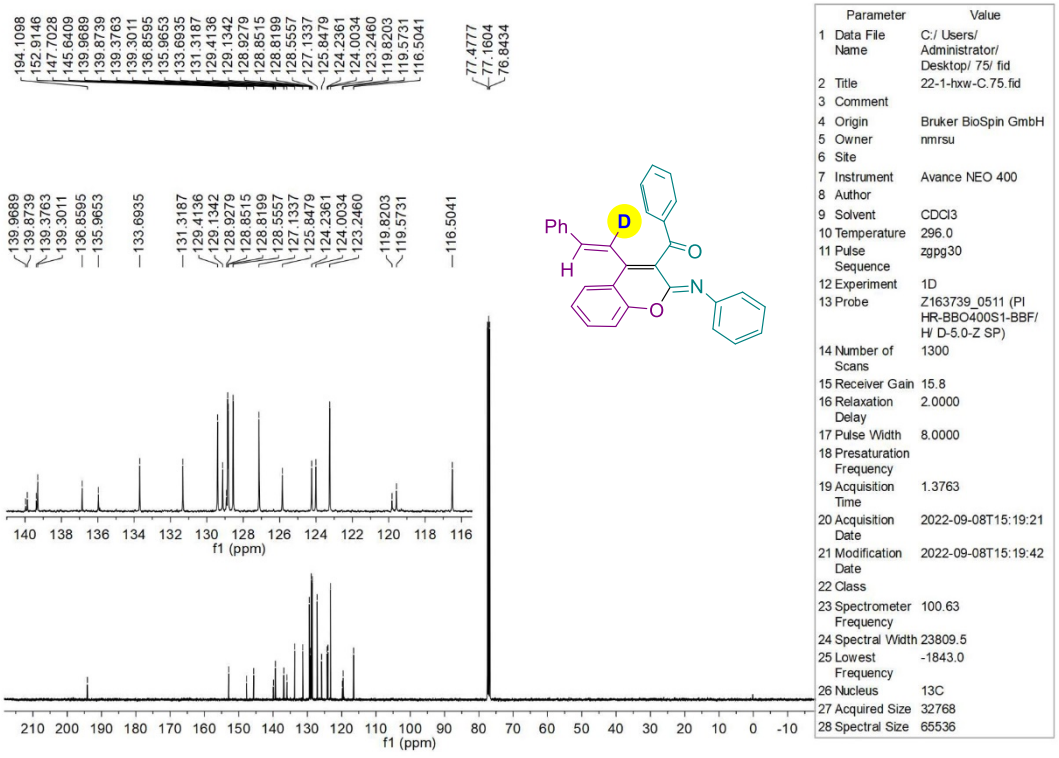
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536

^{1}H NMR Spectra of compound 3aa-*d*



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8	Author	
9	Solvent	CDCl3
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11	Pulse Sequence	zgpg30
12	Experiment	1D
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16	Relaxation Delay	2.0000
17	Pulse Width	8.0000
18	Presaturation Frequency	
19	Acquisition Time	1.3763
20	Acquisition Date	2022-09-08T15:19:21
21	Modification Date	2022-09-08T15:19:42
22	Class	
23	Spectrometer Frequency	100.63
24	Spectral Width	23809.5
25	Lowest Frequency	-1843.0
26	Nucleus	13C
27	Acquired Size	32768
28	Spectral Size	65536

^{13}C NMR Spectra of compound 3aa-*d*

19. References

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