Supporting information for

Planar, fluorescent push-pull system that comprises benzofuran and iminocoumarin moieties

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TABLE OF CONTENTS:

General information

All chemicals were used as received unless otherwise noted. Reagent grade solvents (MeCN, CH_2Cl_2, hexane, toluene) were distilled prior to use. All reported NMR spectra were recorded on 500 MHz spectrometer unless otherwise noted. Chemical shifts (δ ppm) were determined with TMS as the internal reference; *J* values are given in Hz. UV-vis absorption spectra were recorded in THF. Chromatography was performed on silica (Kieselgel 60, 200-400 mesh) and dry column vacuum chromatography (DCVC) was performed on preparative thin layer chromatography silica (Merck 107747). Mass spectra were obtained via EI or electrospray MS. Electronic absorption spectra were collected on a UV-VIS absorption spectrometer Lambda 35 (Perkin Elmer, Rodgau, Germany). The spectra were corrected with solvent absorption spectra. Steady-state fluorescence emission spectra were collected on an FLS920-stm spectrometer (Edinburgh Instruments, Livingstone, United Kingdom). The spectra were corrected for the detector response. Fluorescence decays were also acquired on the FLS920-stm spectrometer using Time Correlated Single Photon Counting (TCSPC) technique with a sub-nanosecond pulsed LED (EPLED 320) as an excitation source. Fluorescence decay times were determined from the decays using the least squares fitting method. The fitting was assumed to be correct when the goodness-of-fit value χ^2 was lower than 1.2. Fluorescence quantum yields were measured on a C9920-02G absolute QY measurement system from Hamamatsu (Hamamatsu Photonics Deutschland GmbH, Herrsching am Ammersee, Germany). All measurements were executed using 3ml quartz cuvette (Hellma GmbH, Jena, Germany) with 1 cm light path. All measurements were executed for samples with OD below 0.15.

Computational methods

Calculations have been performed at **PM6** and **DFT** using the *Gaussian 09* and *SPARTAN'04* software. All geometries have been calculated primarily at the **PM6** semi-empirical level and subsequently iterated at the **B3LYP/6-31G(d,p)** theory level. Geometries of **(6)** and **(7)** have been optimized also at **MP2/6-31G(d,p)** level, but no significant differences have been observed in comparison to **B3LYP/6-31G(d,p)**. Vibrational analysis for optimized geometries has been done at the **B3LYP/6-31G(d,p)** level. **HOMO** and **LUMO** orbitals, as well as their density maps have been generated at **M06-2X/6-31(d)** theory level.

Tab. S1. Ground state energy of **HOMO** and **LUMO** orbitals calculated at **M06-2X/6-31(d)**.

Compound	E_{HOMO} [eV]	E_{LUMO} [eV]	$\Delta E_{LUMO-HOMO}$ [eV]
6	- 6.5	- 1.5	5.0
7	- 6.4	- 1.2	5.2
8	- 6.4	- 1.4	5.0
9	- 6.4	- 1.3	5.1
10	- 7.1	- 2.2	4.9
11	- 6.8	- 2.0	4.8
12	- 6.8	- 2.2	4.4
13	- 7.0	- 2.3	4.7
14	- 6.8	- 1.8	5.0
15	- 6.7	- 1.7	5.0

Tab. S2. Ground state energy of **HOMO(-1)** and **LUMO(+1)** orbitals calculated at **M06-2X/6-31(d)**.

Compound	$E_{HOMO(-1)}$ [eV]	$E_{LUMO(+1)}$ [eV]	$\Delta E_{LUMO-HOMO}$ [eV]
6	- 7.1	- 0.2	6.9
7	- 7.0	0.0	7.0
8	- 7.0	0.1	6.9
9	- 7.1	- 0.1	7.0
10	- 7.8	- 0.7	7.1
11	- 7.4	- 0.5	6.9
12	- 7.1	- 0.5	6.6
13	- 7.8	- 0.7	7.1
14	- 7.5	- 0.4	7.1
15	- 7.4	- 0.4	7.0

NMR information

Almost all spectra have been recorded at Bruker DRX 500 MHz. In some cases Varian VNMRS 600 MHz and Bruker Avance III 400 MHz spectrometers have been used. Solvent ($CDCl_3$) a priori to measurements was deacidified by passing through short column packed with basic Al_2O_3. One dimensional ^1H proton spectra have been recorded by *homonuclear spin echo* sequence utilizing $180^{(120)}$-$180^{(240)}$-$180^{(120)}$ composite pulse (pulse sequence attached below).

One dimensional ^{13}C carbon spectra have been recorded by standard zgpg pulse program available in *Bruker TopSpin3.2* library.

Two dimensional ^1H - ^1H and ^1H - ^{13}C experiments have been carried out by standard *Bruker TopSpin3.2* pulse sequences:

^1H - ^1H DQF-COSY – **cosydfetgp.2**

^1H - ^1H TOCSY – **mlevetgp**

^1H - ^1H NOESY – **noesyph** *(d8 = 450 ms)*

^1H - ^{13}C HSQC – **hsqcedetgp**

Tab. S3. Homonuclear spin echo sequence for *Bruker TopSpin* software.

```
;zgsecp.3
;avance-version (12/01/11)
;homonuclear spin echo sequence
;utilizing composite pulse 180(120)-180(240)-180(120) for RF field
;inhomogenity and offset compensation
;A. Leniak
;Institute of Organic Chemistry Polish Academy of Sciences
;Warsaw 2014
;
;$CLASS=HighRes
;$DIM=1D
;$TYPE=
;$SUBTYPE=
;$COMMENT=

"p2=p1*2"

#include <Avance.incl>

1 ze
2 d1
  p1 ph1
  d20
  p2 ph2
  4u
  p2 ph3
```

```
  4u
  p2 ph2
  d20
  go=2 ph31
  30m mc #0 to 2 F0(zd)

exit

ph1=0 0 0 0 2 2 2 2 1 1 1 1 3 3 3 3
ph2=(12) 4 7 10 1 4 7 10 1 4 7 10 1 4 7 10 1
ph3=(12) 8 11 2 5 8 11 2 5 8 11 2 5 8 11 2 5
ph31=0 2 0 2 2 0 2 0 1 3 1 3 3 1 3 1

;pl1 : f1 channel - power level for pulse (default)
;p1 : f1 channel -  90 degree high power pulse
;p2 : f1 channel -  180 degree high power pulse
;d1 : relaxation delay; 1-5 * T1
;d20: delay for spin echo (default 2ms)
;ns: 8 * n
;td0: number of loops

;$Id: zgsecp.3,v 1.0 2014/07/18 13:35:23 ber Exp $
```

Solvent dependent Stokes shifts

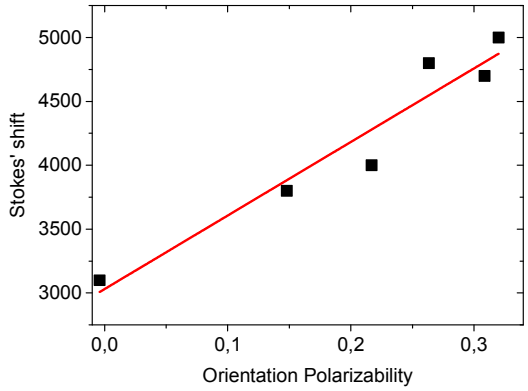


Fig. S1. Lippert-Mataga plot for compound (**10)** in various solvents (R2 = 0.91281 while PCC parameter = 0.96449).

Tab. S4. Photophysical properties of compound **10** in various solvents.

Compd	Solvent	λ_{abs} (nm)	ε (M^{-1} cm^{-1})	λ_{em} (nm)	Φ (%)	$\Delta\nu$ (cm^{-1})	τ (ns) λ_{ex}=405 nm	k_f (10^8 s^{-1})	k_{nr} (10^8 s^{-1})
10	n-Hexan	458	22500	535	70	3100	3.8	1.8	0.8
	CHCl3	460	35000	558	92	3800	5.6	1.6	0.2
	DCM	463	31000	569	94	4000	6.2	1.5	0.1
	MeOH	456	30000	582	78	4700	7.5	1.1	0.3
	DMSO	463	31000	596	60	4800	6.6	0.9	0.6
	H_2O			601	5	5000	2.3	0.2	4.1

Elucidation of the structure of compound 6.

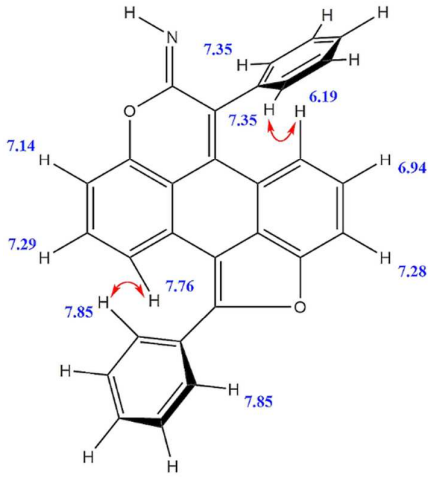
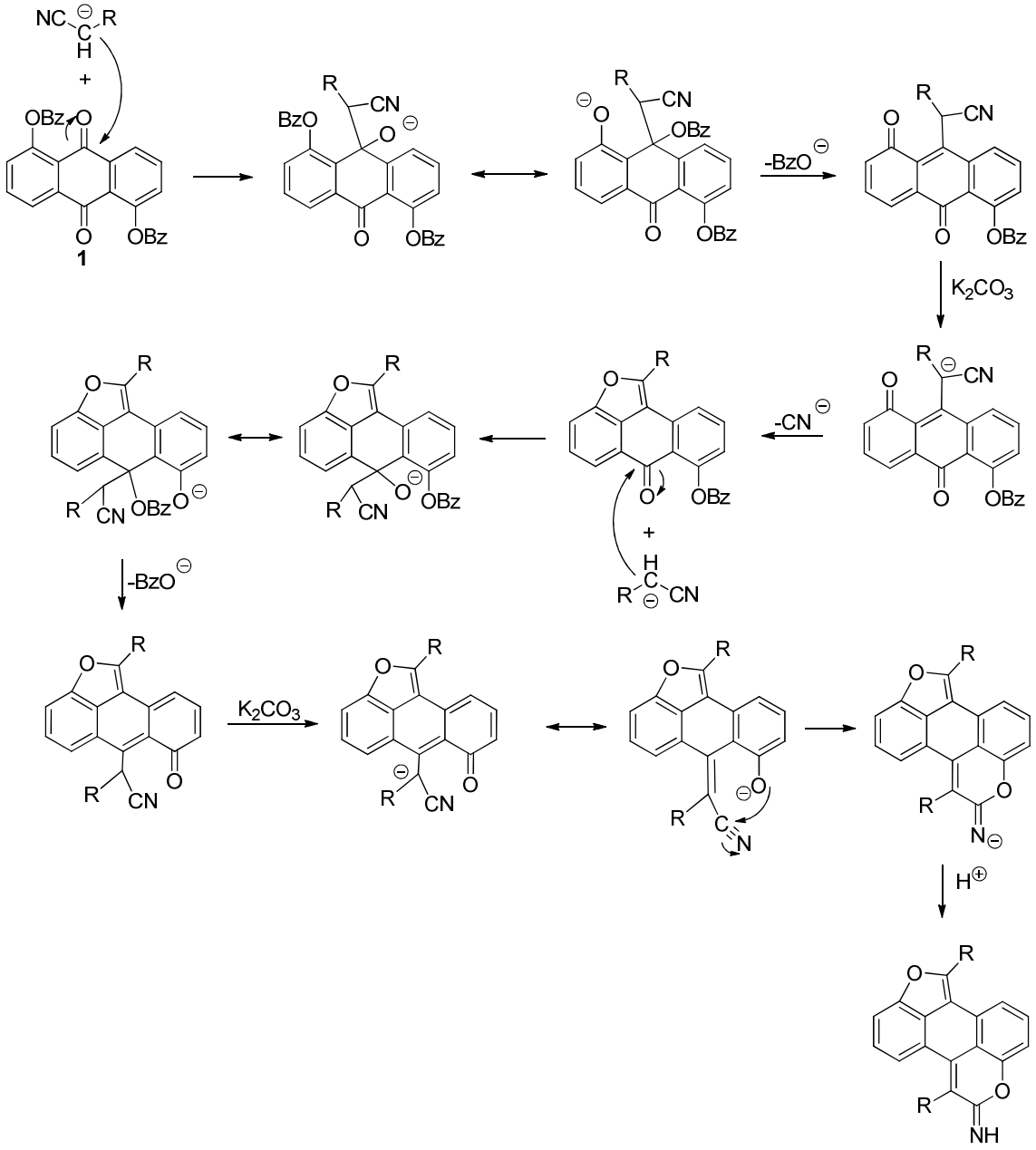


Fig. S2. ^{1}H chemical shifts of **6** ($CDCl_3$ solution). Ambiguous chemical shift descriptions of meta and para positions in phenyl substituents were not described (higher order spin systems); red arrows indicate the most important NOE effects.

Structure identification and signal assignments have been performed by employing ^{1}H and ^{13}C 1D NMR, DQF-COSY (Double Quantum Filtered COSY, allowing for the suppression of diagonal peaks), 2D TOCSY, 2D NOESY, ^{13}C,^{1}H-gHSQC ($^{1}J_{C-H}$=145 Hz) and ^{13}C,^{1}H-gHMBC ($^{3}J_{C-H}$=8 Hz). All signals corresponding to compound **6** can be found on the ^{1}H 1D spectrum within 6.1-7.9 ppm chemical shift range. By the use of DQF-COSY and 2D TOCSY spectra, four distinct spin systems have been found: two AA'MM'N systems of phenyl substituents and two AMX spin systems of the core fragment. The vicinity of the respective spin systems was revealed by the usage of 2D NOESY technique (strong cross peaks at 7.76 ppm x 7.86 ppm and 6.19 ppm x 7.35 ppm). The signal at 6.19 ppm corresponds to a core proton which is strongly shielded by the almost perpendicular aromatic ring (phenyl substituent at 72° angle). By contrast, the proton at 7.86 ppm is deshielded by the other phenyl substituent that is twisted only by 34° in respect to the molecular plane. Chemical shift anisotropy has been observed for the proton signal at 7.14 ppm. This particular signal was quite broad at 1D ^{1}H 600 MHz spectrum and it was getting sharper with decreasing of the external field frequency(500 MHz and 400 MHz). Unfortunately, the N-H proton has not been observed, probably due to the fast *cis-trans* isomerization (the difference in potential energy between the two isomers calculated at B3LYP/6-31G(d,p) is only 3 kcal/mol) or due to the vicinity of a highly polarized quadrupolar nitrogen atom. ^{13}C,^{1}H-gHSQC technique was used to assign all of the ^{13}C signals of C-H carbon atoms. Tertiary carbon signals were distinguished by the use of ^{13}C,^{1}H-gHMBC which also allowed to connect all of the spin systems into a single molecule. Three peaks at 152.20 ppm, 152.41 ppm and 153.50 ppm correspond to aromatic carbon atoms linked to a heteroatom: the former two to the benzofuran fragment and the last one to the imino ether ring. The signal of C=NH carbon could not be found in the ^{13}C spectrum, probably due to the

vicinity of the strongly quadrupolar nitrogen atom. Any attempts to obtain 1D or 2D nitrogen (^{15}N and ^{14}N) spectra were unsuccessful.



Scheme S1. Proposed mechanism for the formation of furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-imine skeleton.

General procedure for synthesis of benzofuranoiminocoumarins.

To the mixture of **di-O-benzoyl-1,5-dihydroxyantraquinone (1)** (5 mmol) and $\mathbf{K_2CO_3}$ (50 mmol) in 50 ml of dry **DMSO**, 30 mmol of respective phenylacetonitrile was added under argon atmosphere and the resulting suspension was stirred vigorously at 60°C for 1 hour.

After completion the reaction mixture was poured into 1.50 dm^3 of **diethyl ether**. Resulting mixture was then filtered, solids were washed with diethyl ether. Filtrate has been cooled to **-78°C**. Under these conditions crystals of **DMSO/Et_2O** were started to deposit. For the most part the two runs of filtration were enough to remove majority of **DMSO**. The remaining **diethyl ether** was removed under reduced pressure on a rotatory evaporator.

Resulting concentrated solution was diluted with 50 ml of **MeOH** and after that formation of a precipitate could be observed*. It was filtered off and washed with small amount of cold **MeOH**. Recrystallization from **DCM/cyclohexane** gave pure derivative of respective **benzofuranoiminocoumarin**.

CAUTION: Cyanide is one of the most lethal poisons known. A significant proportion of fatalities among fire victims is due to cyanide poisoning, as blood cyanide concentrations reach a level of 23-26 μM. Reaction can be carried out only in well-ventilated fume hood. Reaction mixture should not be acidified to prevent evolution of HCN.

General procedure for synthesis of N-substituted benzofuranoiminocoumarin.

Solution of respective **benzofuranoiminocoumarin** (0.5 mmol) in mixture of dry **dichloromethane** (90 ml) and dry **triethylamine** (10 ml) was stirred under **argon** atmosphere. Appropriate **acid chloride** or **anhydride** (0.7 mmol) was added by dropwise manner.

The progress of the reaction was monitored by **TLC** and after full conversion reaction was quenched with **300 ml 0.1M** solution of **$NaHCO_3$**. Resulting two-phase mixture was separated and water phase was extracted 3 times with dichloromethane (**3 x 50 ml**). Organic extracts were combined and washed with **water** and **brine** (**2 x 100 ml**). Next dried with anhydrous **Na_2SO_4** and evaporated with small amount of **silica gel** (TLC 60). Resulting solid was purified by **DCVC** (**D**ry **C**olumn **V**acuum **C**hromatography). Fractions that contained respective amide were evaporated *in vacuo*. Solids were recrystallized from **DCM** and **EtOH** to gave pure amide.

X-Ray data

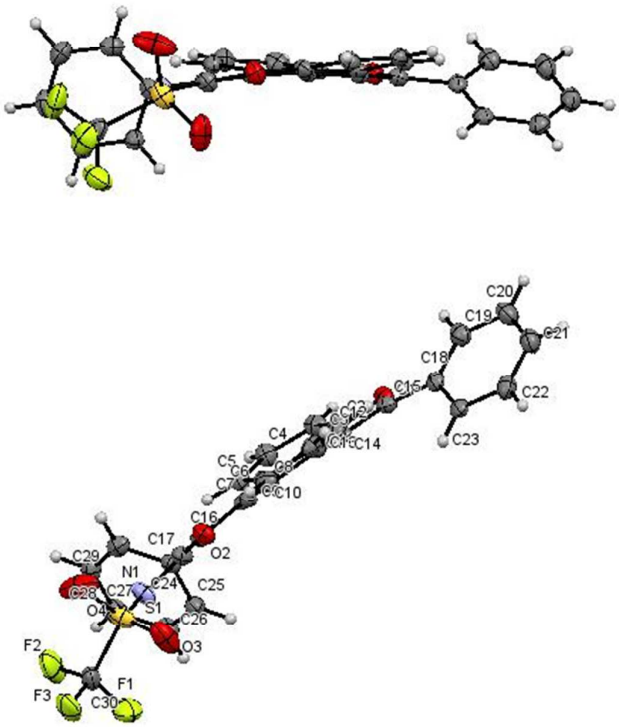


Fig.S3. X-Ray structure of compound **10**.

Crystal data for compound **10**: C30H16NO4F3S ; Mr = 4772.61, triclinic, a = 16.057(4), b = 18.336(5), c = 18.879(5) Å, α = 79.909(13), β = 74.398(12), γ = 79.264(13), V = 5214.0 (2) Å3, T = 152 K, space group P -1 (no. 2), Z = 1, μ = 2.826 mm-1, d = 1.520 g cm-3, F(000) = 2434, 17476 reflections collected, 12827 unique, The final R1 and wR2 (F2) were 0.0675 and 0.2609, 2θ range 2.89 – 66.00 °, GOF = 1.112,

Detailed data (NMR, HRMS, Mp, Yield, DFT MO's)

(6) 1,6-diphenyl-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-imine

Yellow solid (659 mg, 32%); mp (dec.) 240-241°C

^{1}H-NMR ($CDCl_3$, 500 MHz, 303 K) δ 6.20 (d, J = 8.0 Hz, 1H), 6.94 (t, J = 8.1 Hz, 1H), 7.14 (d, J = 7.8, 1H), 7.29 (t, J = 7.3, 1H), 7.30 (d, J = 7.4, 1H), 7.33 – 7.37 (m, 2H), 7.49 – 7.58 (m, 4H), 7.58 – 7.64 (m, 2H), 7.76 (dd, J = 7.9; 1.2, 1H), 7.83 - 7.88 (m, 2H).

^{13}C-NMR ($CDCl_3$, 125 MHz, 303 K) δ 111.39, 111.46, 115.43, 117.62, 118.11, 123.02, 124.73, 125.56, 127.28, 128.79, 128.84, 129.03, 129.29, 129.39, 129.97, 130.08, 130.58, 130.98, 133.00, 136.89, 152.20, 152.41, 153.50.

HRMS (ESI): m/z calculated for $C_{29}H_{17}NO_2$ $[M+H^+]$=412.1338 found 412.1340.

R_f (Al_2O_3; DCM/AcOEt, 19:1): 0.56

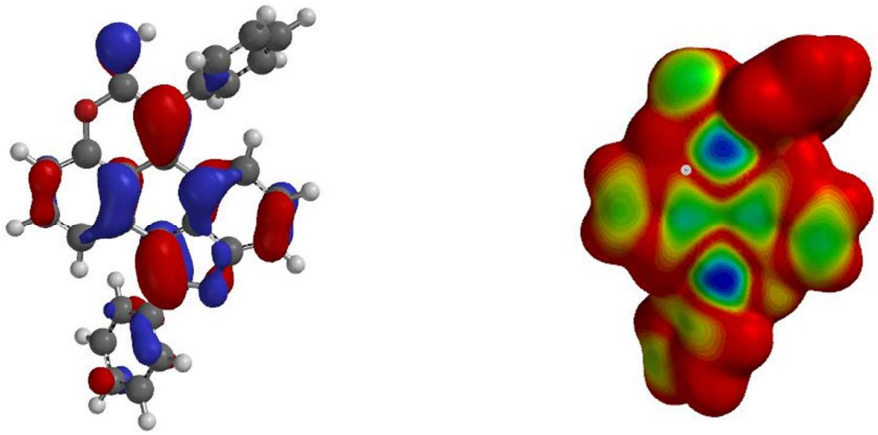


Fig. S 2a. Representation of **HOMO** orbital (*left*) and **HOMO density map** (*right*) for compound **(6)**.

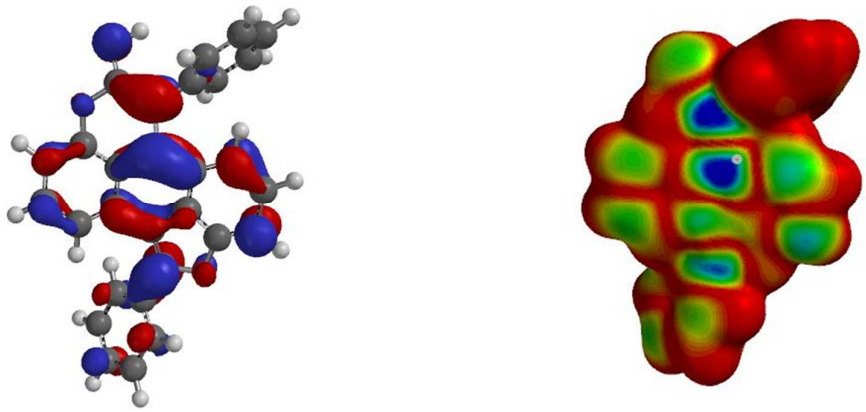


Fig. S 2b. Representation of **LUMO** orbital (*left*) and **LUMO density map** (*right*) for compound **(6)**.

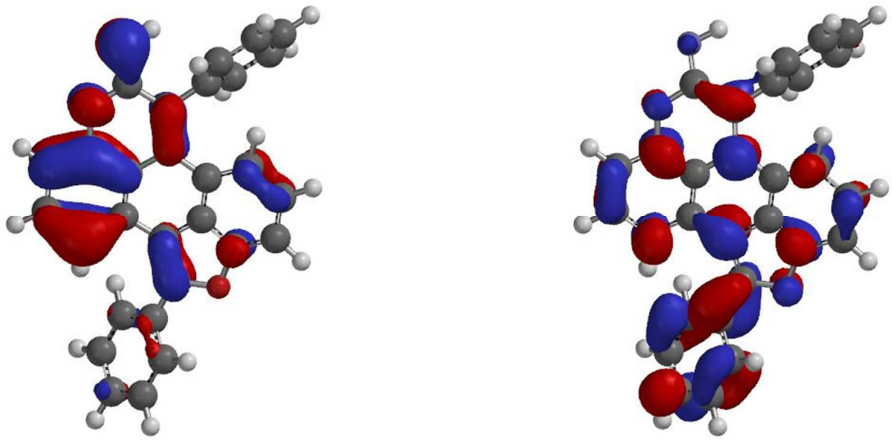


Fig. S 2c. Representation of **HOMO(-1)** orbital (*left*) and **LUMO(+1)** orbital (*right*) for compound **(6)**.

(7) 1,6-Di-p-tolyl-7*H*-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-imine

Yellow solid (568 mg, 26%); mp (dec.) 256–258 °C

^{1}H-NMR ($CDCl_3$, 500 MHz, 303 K) δ 2.48 (s, 3H), 2.50 (s, 3H), 6.32 (d, J = 8.2 Hz, 1H), 6.97 (t, J = 8.2 Hz, 1H), 7.15 (d, J = 8.2 Hz, 1H), 7.23 – 7.26 (m, 2H), 7.28 – 7.34 (m, 2H), 7.37 (d, J = 8.2 Hz, 2H), 7.41 (d, J = 7.6 Hz, 2H), 7.75 (m, 3H).

^{13}C-NMR ($CDCl_3$, 125 MHz, 303 K) δ 21.50, 21.58, 111.19, 111.28, 115.32, 117.73, 118.11, 123.02, 124.85, 125.43, 127.47, 128.16, 128.55, 128.75, 129.23, 129.45, 129.58, 129.77, 130.01, 130.49, 131.33, 133.00, 133.83, 138.91, 140.28, 152.41, 152.56, 153.54.

HRMS (ESI): m/z calculated for $C_{31}H_{22}NO_2$ [M+H+] = 440.1653; found: 440.1651.

R_f (Al_2O_3; DCM/AcOEt, 19:1): 0.67.

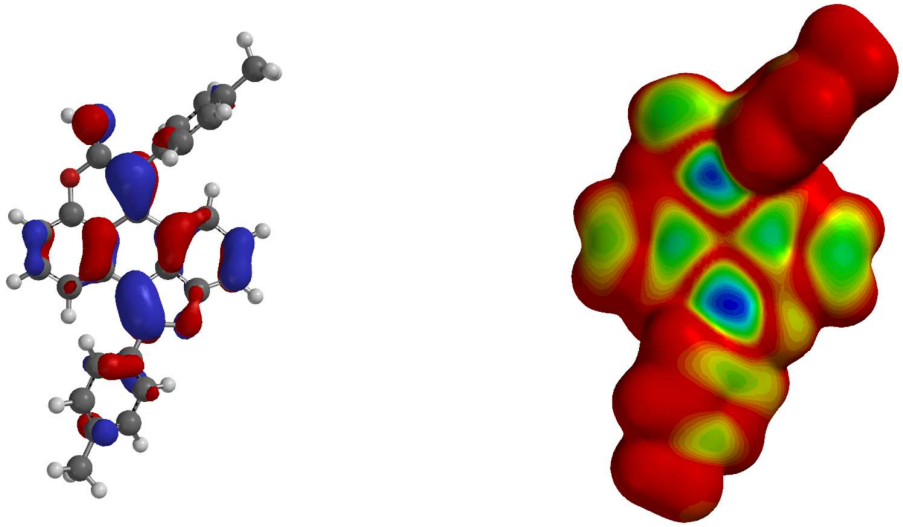


Fig. S 3a. Representation of **HOMO** orbital (*left*) and **HOMO density map** (*right*) for compound **(7)**.

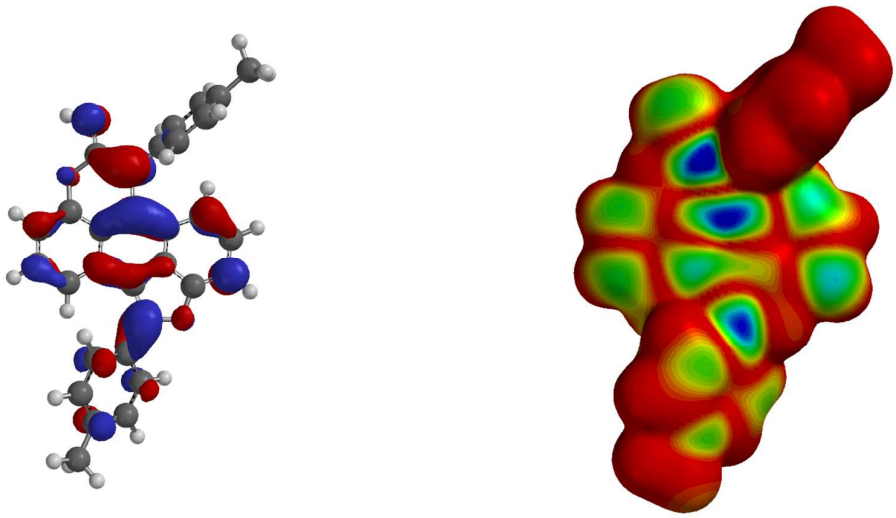


Fig. S 3b. Representation of **LUMO** orbital (*left*) and **LUMO density map** (*right*) for compound **(7)**.

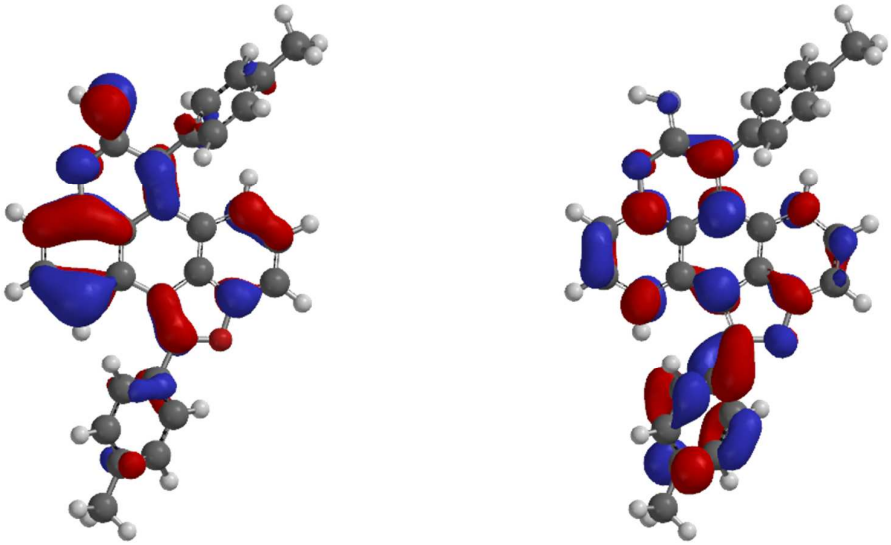


Fig. S 3c. Representation of **HOMO(-1)** orbital (*left*) and **LUMO(+1)** orbital (*right*) for compound **(7)**.

(8) 1,6-Bis(4-methoxyphenyl)-7*H*-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-imine

Yellow solid (493 mg, 21%); mp (dec.) 229-231°C

^{1}H-NMR ($CDCl_3$, 500 MHz, 303 K) δ 3.92 (s, 3H), 3.93 (s, 3H), 6.34 (d, J = 8.0 Hz, 1H), 6.99 (t, J = 8.0 Hz, 1H), 7.08 (d, J = 8.2 Hz, 2H), 7.03 - 7.11 (m, 3H), 7.27 (d, J = 11.0 Hz, 2H), 7.25 - 7.29 (m, 2H), 7.76 (d, J = 8.0 Hz, 1H), 7.81 (d, J = 8.4 Hz, 2H).

^{13}C-NMR ($CDCl_3$, 125 MHz, 303 K) δ 55.40, 55.45, 110.77, 111.22, 114.37, 115.21, 116.09, 117.74, 117.94, 122.97, 123.32, 124.79, 125.36, 127.57, 128.88, 129.55, 130.02, 130.36, 130.72, 133.34, 152.34, 152.51, 153.55, 160.11, 160.96.

HRMS (ESI): m/z calculated for $C_{31}H_{22}NO_4$ $[M+H^+]$ = 472.1545; found: 472.1549.

R_f (Al_2O_3; DCM/AcOEt, 19:1): 0.46.

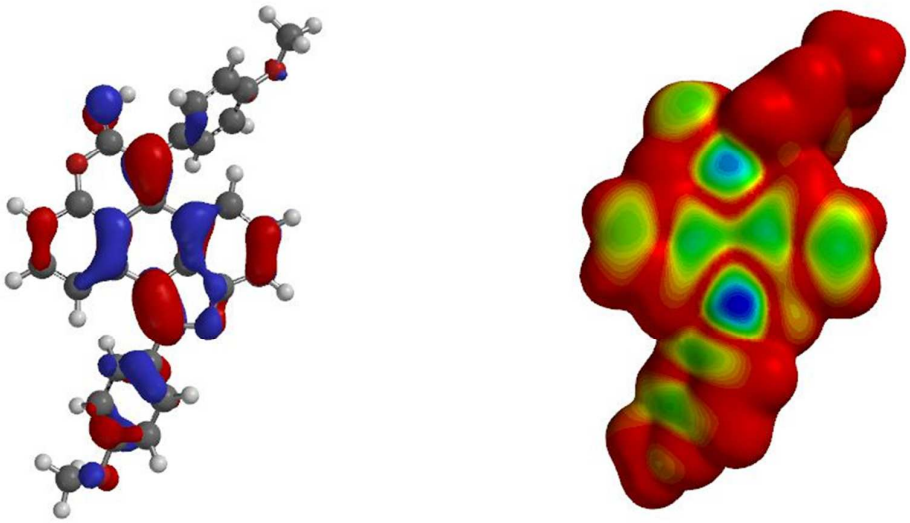


Fig. S 4a. Representation of **HOMO** orbital (*left*) and **HOMO density map** (*right*) for compound **(8)**.

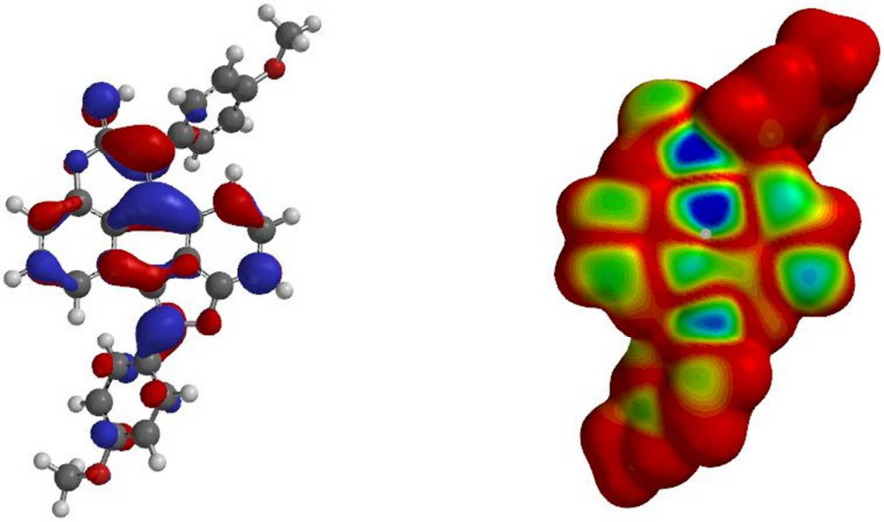


Fig. S 4b. Representation of **LUMO** orbital (*left*) and **LUMO density map** (*right*) for compound **(8)**.

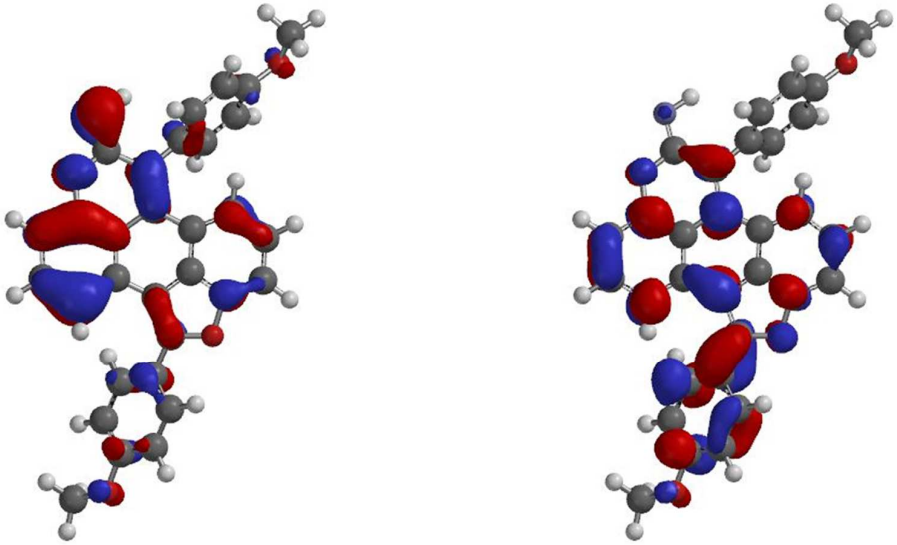


Fig. S 4c. Representation of **HOMO(-1)** orbital (*left*) and **LUMO(+1)** orbital (*right*) for compound **(8)**.

(9) 1,6-Bis(3,4-dimethoxyphenyl)-7*H*-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-imine

Orange crystals (411 mg, 15%); mp (dec.) 128–130 °C

^{1}H-NMR ($CDCl_3$, 500 MHz, 303 K) δ 3.86 (s, 3H), 3.96 (s, 3H), 4.00 (s, 3H), 4.01 (s, 3H), 6.38 (d, J = 7.8 Hz, 1H), 6.85 (d, J = 1.9 Hz, 1H), 6.93 (dd, J = 8.3 Hz; 1.9 Hz, 1H), 7.01 (t, J = 8.3 Hz, 1H), 7.05 (d, J = 8.3 Hz, 1H), 7.12 (d, J = 8.3 Hz, 1H), 7.17 (d, J = 8.3 Hz, 1H), 7.34 (t, J = 7.8 Hz, 1H), 7.38 (d, J = 1.9 Hz, 2H), 7.50 (dd, J = 8.3 Hz; 1.9 Hz, 1H), 7.86 (d, J = 7.8, 1H).

^{13}C-NMR ($CDCl_3$, 125 MHz, 303 K) δ 56.05, 56.07, 56.11, 56.16, 110.90, 111.32, 111.37, 111.73, 112.04, 113.12, 115.34, 117.78, 118.14, 121.74, 122.07, 123.14, 123.47, 124.71, 125.60, 127.62, 129.04, 129.06, 129.56, 130.06, 133.31, 149.25, 149.62, 150.67, 150.98, 152.35, 152.55, 153.63.

HRMS (ESI): m/z calculated for $C_{33}H_{26}NO_6$ [M+H+] = 536.1762; found: 536.1760.

R_f (Al_2O_3; DCM/AcOEt, 19:1): 0.51.

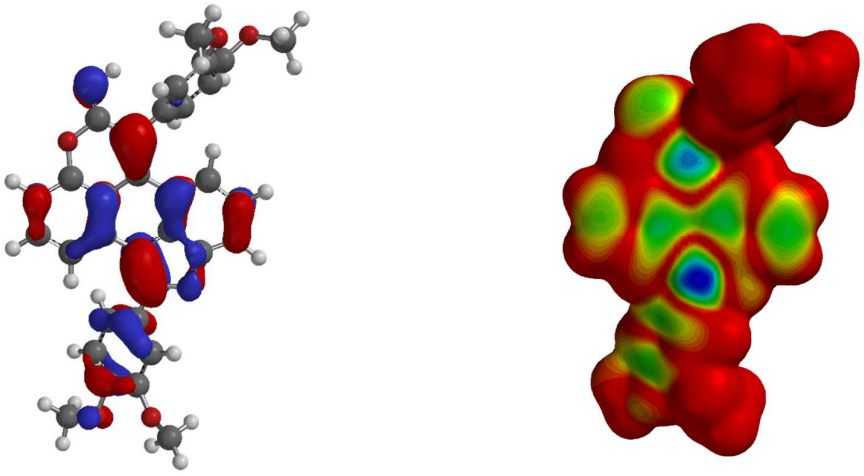


Fig. S 5a. Representation of **HOMO** orbital (*left*) and **HOMO density map** (*right*) for compound **(9)**.

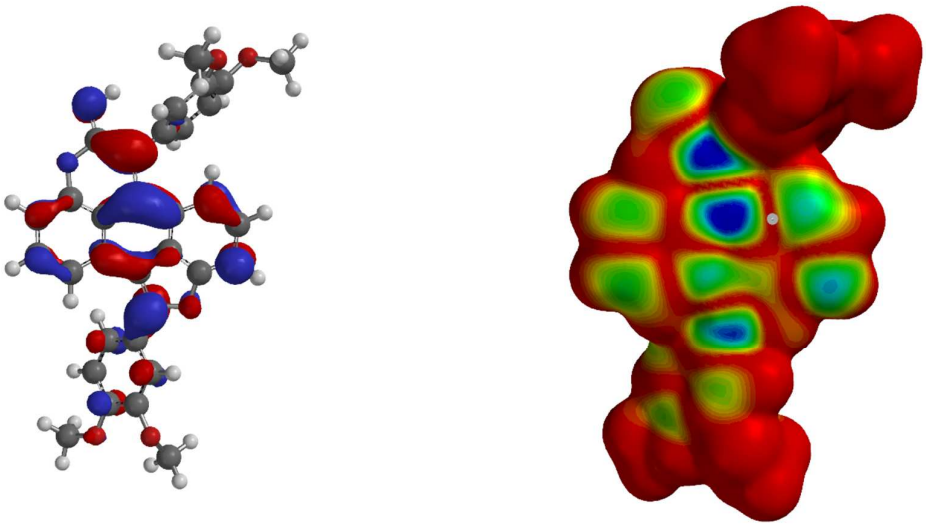


Fig. S 5b. Representation of **LUMO** orbital (*left*) and **LUMO density map** (*right*) for compound **(9)**.

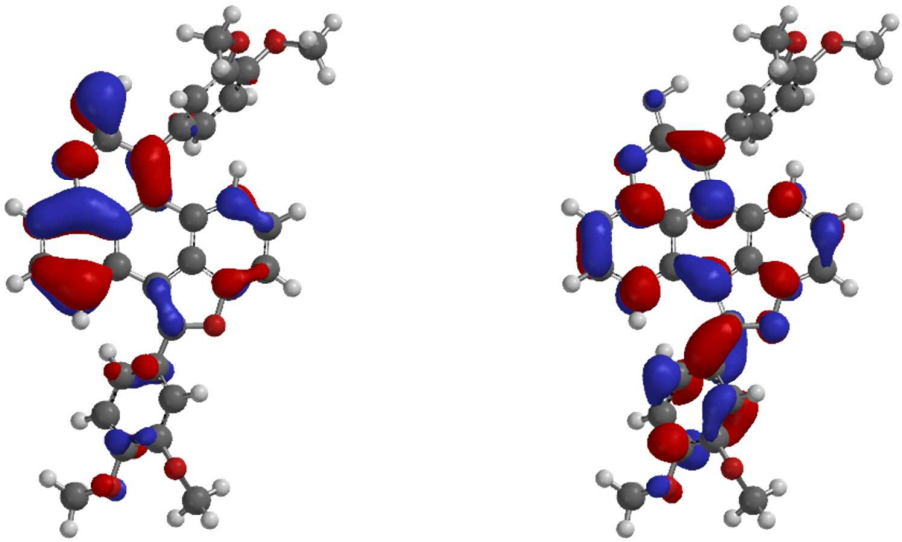


Fig. S 5c. Representation of **HOMO(-1)** orbital (*left*) and **LUMO(+1)** orbital (*right*) for compound **(9)**.

(10) *N*-(1,6-diphenyl-7*H*-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-ylidene)-1,1,1-trifluoromethanesulfonamide

Orange-red solid (201 mg, 71%); mp (dec.) 245-246°C

^{1}H-NMR ($CDCl_3$, 500 MHz, 303 K) δ 6.52 (d, J = 8 Hz, 1H), 7.06 (t, J = 8 Hz, 1H), 7.31 – 7.35 (m, 2H), 7.48 (d, J = 8 Hz, 1H), 7.51 – 7.65 (m, 7H), 7.90 – 7.94 (m, 2H), 8.09 (d, J = 7.8 Hz, 2H).

^{13}C-NMR ($CDCl_3$, 125 MHz, 303 K) δ 111.22, 113.92, 116.25, 117.67, 118.27, 120.21, 120.29, 122.87, 123.42, 125.50, 126.17, 128.45, 128.73, 129.11, 129.19, 129.38, 129.88, 129.93, 130.30, 130.89, 131.83, 134.80, 143.25, 152.51, 152.98, 155.01, 162.29.

HRMS (ESI): m/z calculated for $C_{30}H_{16}NO_4F_3NaS$ $[M+Na^+]$ = 566.0643; found: 566.0650.

R_f (SiO_2; DCM/Hexane, 7:3): 0.41.

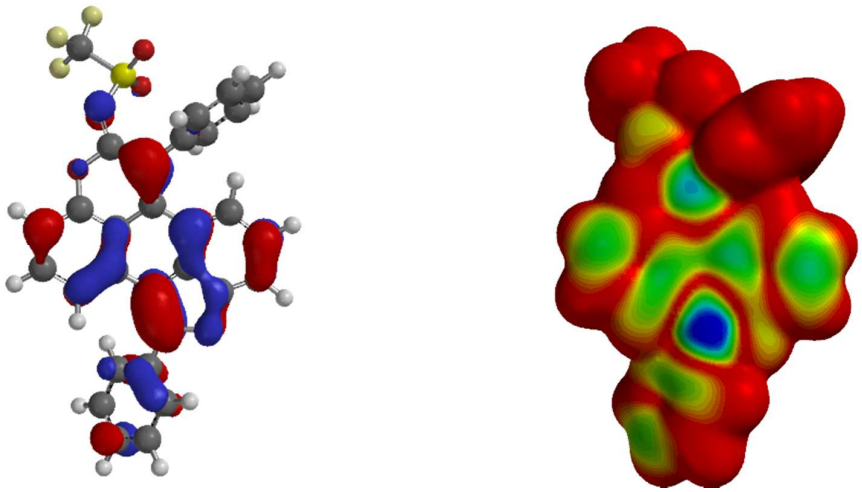


Fig. S 6a. Representation of **HOMO** orbital (*left*) and **HOMO density map** (*right*) for compound **(10)**.

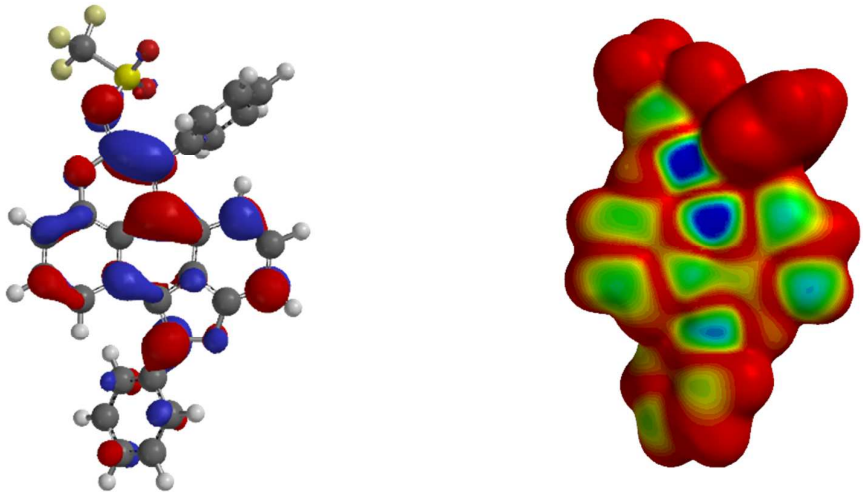


Fig. S 6b. Representation of **LUMO** orbital (*left*) and **LUMO density map** (*right*) for compound **(10)**.

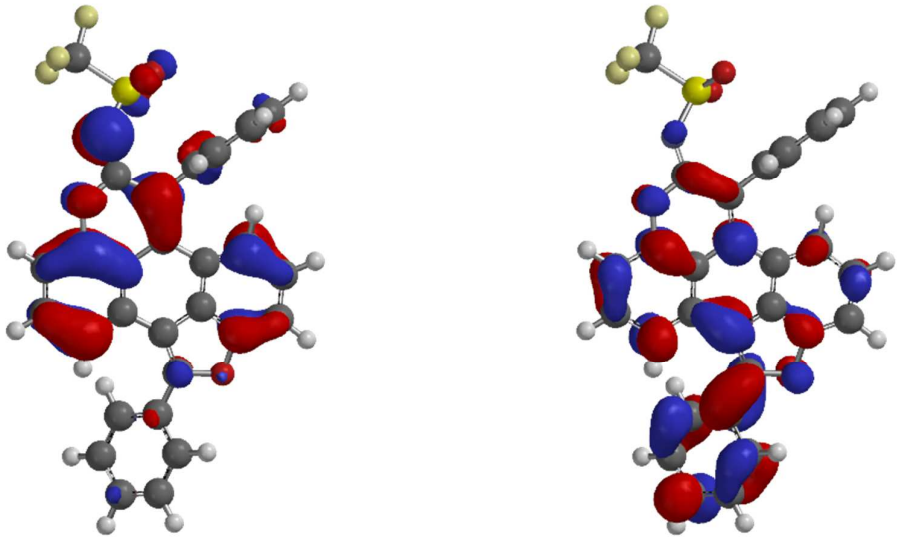


Fig. S 6c. Representation of **HOMO(-1)** orbital (*left*) and **LUMO(+1)** orbital (*right*) for compound **(10).**

(11) *N*-(1,6-di-p-tolyl-7*H*-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-ylidene)-1,1,1-trifluoromethanesulfonamide

Orange-red crystals (208 mg, 73%); mp (dec.) 278-280°C

^{1}H-NMR ($CDCl_3$, 500 MHz, 303 K) δ 2.50 (s, 3H), 2.51 (s, 3H), 6.58 (d, J = 8.2 Hz, 1H), 7.06 (t, J = 8.2 Hz, 1H), 7.20 (d, J = 7.9 Hz, 2H), 7.35 (d, J = 7.9 Hz, 2H), 7.42 (d, J = 7.9 Hz, 2H), 7.46 (d, J = 8.0 Hz, 1H), 7.49 – 7.57 (m, 2H), 7.80 (d, J = 8.0 Hz, 2H), 8.09 (d, J = 7.9 Hz, 1H).

^{13}C-NMR ($CDCl_3$, 125 MHz, 303 K) δ 21.54, 21.67, 110.87, 113.70, 116.01, 117.72, 118.33, 120.17, 120.26, 122.79, 123.45, 125.45, 125.95, 127.40, 128.56, 128.61, 129.22, 129.87, 130.05, 130.54, 131.66, 131.71, 138.95, 141.39, 143.35, 152.41, 152.92, 155.34, 162.48.

HRMS (EI): m/z calculated for $C_{32}H_{20}NO_4F_3S$ [$M^{\cdot+}$] = 571.1063; found: 571.1063.

R_f SiO_2; (DCM/Hexane, 7:3): 0.44.

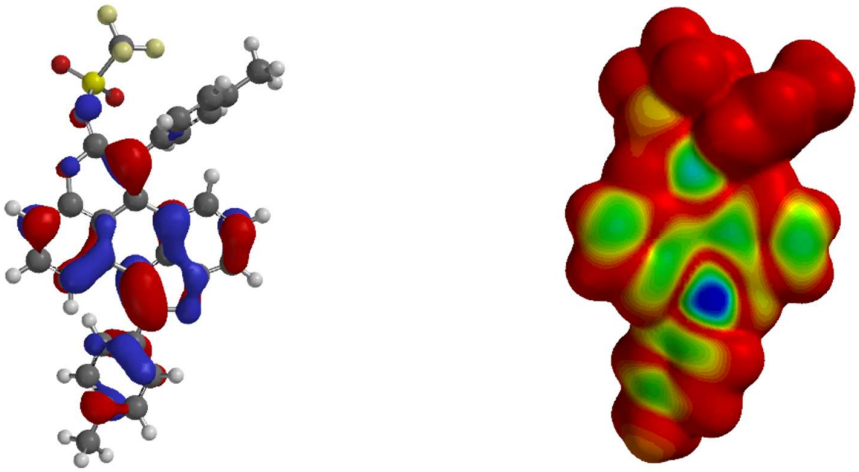


Fig. S 7a. Representation of **HOMO** orbital (*left*) and **HOMO density map** (*right*) for compound **(11)**.

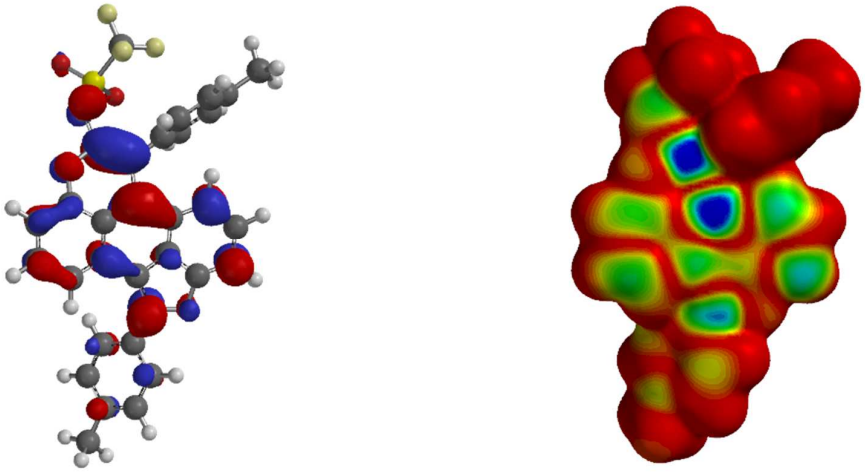


Fig. S 7b. Representation of **LUMO** orbital (*left*) and **LUMO density map** (*right*) for compound **(11)**.

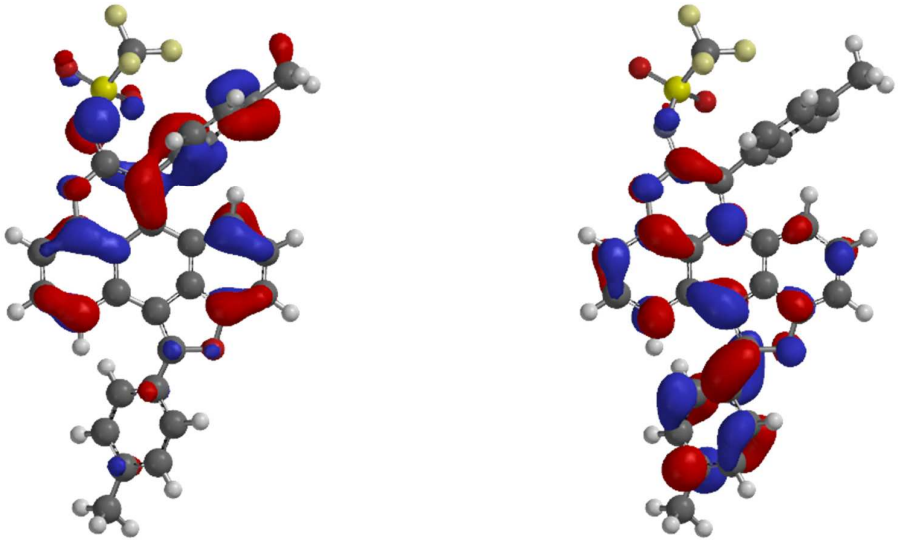


Fig. S 7c. Representation of **HOMO(-1)** orbital (*left*) and **LUMO(+1)** orbital (*right*) for compound **(11).**

(12) *N*-(1,6-bis(4-methoxyphenyl)-7*H*-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-ylidene)-1,1,1-trifluoromethanesulfonamide

Vermilion crystals (229mg, 76%); mp (dec.) 263-264°C

^{1}H-NMR ($CDCl_3$, 500 MHz, 303 K) δ 3.93 (s, 3H), 3.95 (s, 3H), 6.62 (d, J = 8.4 Hz, 1H), 7.05 – 7.10 (m, 3H), 7.12 (d, J = 8.7 Hz, 2H), 7.23 (d, J = 8.4 Hz, 2H), 7.46 (d, J = 7.7 Hz, 1H), 7.51 (m, 1H), 7.54 (t, J = 8 Hz, 1H), 7.86 (d, J = 8.7 Hz, 2H), 8.07 (d, J = 7.7 Hz, 1H).

^{13}C-NMR ($CDCl_3$, 125 MHz, 303 K) δ 55.37, 55.55, 110.43, 113.60, 114.67, 115.27, 115.86, 117.74, 118.38, 119.94, 120.28, 122.24, 122.46, 123.38, 125.32, 125.86, 126.85, 128.67, 130.20, 130.31, 130.81, 131.65, 143.56, 152.36, 152.93, , 155.37, 160.17, 161.66, 162.63.

HRMS (EI): m/z calculated for $C_{32}H_{20}O_6NF_3S$ [$M^{\cdot+}$] = 603.0981; found: 603.0963.

Rf (SiO_2; DCM/Hexane, 4:1): 0.53.

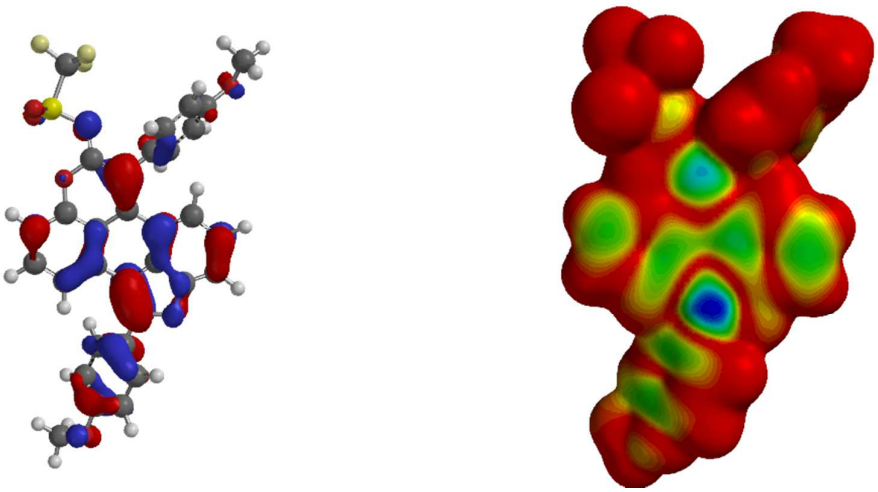


Fig. S 8a. Representation of **HOMO** orbital (*left*) and **HOMO density map** (*right*) for compound **(12)**.

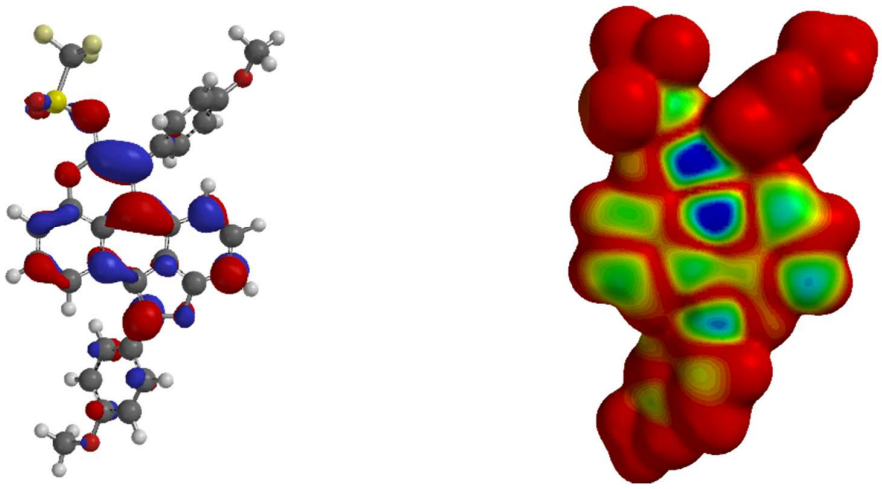


Fig. S 8b. Representation of **LUMO** orbital (*left*) and **LUMO density map** (*right*) for compound **(12)**.

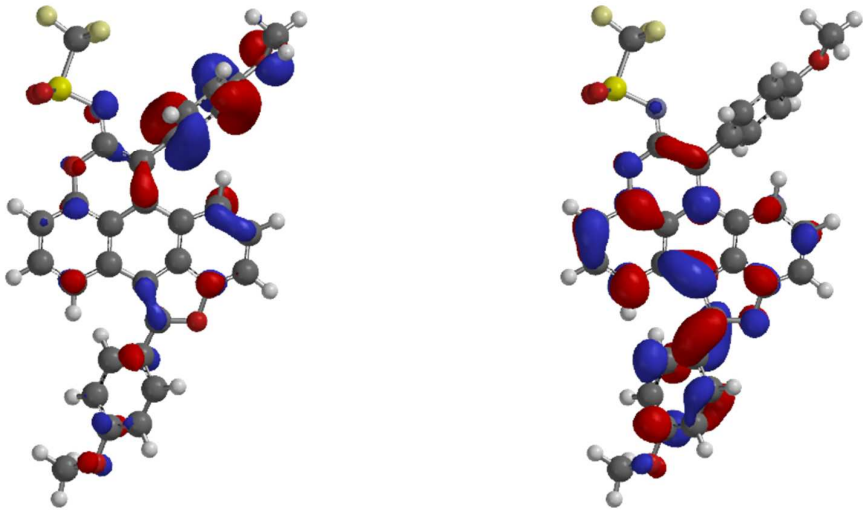


Fig. S 8c. Representation of **HOMO(-1)** orbital (*left*) and **LUMO(+1)** orbital (*right*) for compound **(12).**

(13) *N*-(1,6-bis(3,4-dimethoxyphenyl)-7*H*-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-ylidene)-1,1,1-trifluoromethanesulfonamide

Red solid (206 mg, 62%); mp (dec.) 245-247°C

^{1}H-NMR ($CDCl_3$, 500 MHz, 303 K) δ 3.85 (s, 3H), 3.97 (s, 3H), 4.00 (s, 3H), 4.02 (s, 3H), 6.67 (d, J = 8 Hz, 1H), 6.85 – 6.90 (m, 2H), 7.00 – 7.03 (m, 1H), 7.06 - 7.12 (m, 2H), 7.40 (d, J = 1.7 Hz, 1H), 7.49 (d, J = 8 Hz, 1H), 7.50 – 7.61 (m, 3H), 8.17 (d, J = 8 Hz, 1H).

^{13}C-NMR ($CDCl_3$, 125 MHz, 303 K) δ 55.94, 56.01, 56.13, 56.19, 110.55, 111.42, 111.46, 112.30, 112.57, 113.67, 115.94, 117.72, 118.41, 120.09, 121.93, 122.08, 122.19, 122.58, 123.31, 125.45, 126.00, 126.99, 128.71, 130.19, 131.63, 143.57, 149.47, 149.72, 150.24, 151.38, 152.33, 152.95, 155.36, 162.48.

HRMS (ESI): m/z calculated for $C_{34}H_{24}NO_8F_3NaS$ $[M+Na^+]$ = 686.1072; found: 686.1047.

Rf (SiO_2; DCM/Hexane, 9:1): 0.42.

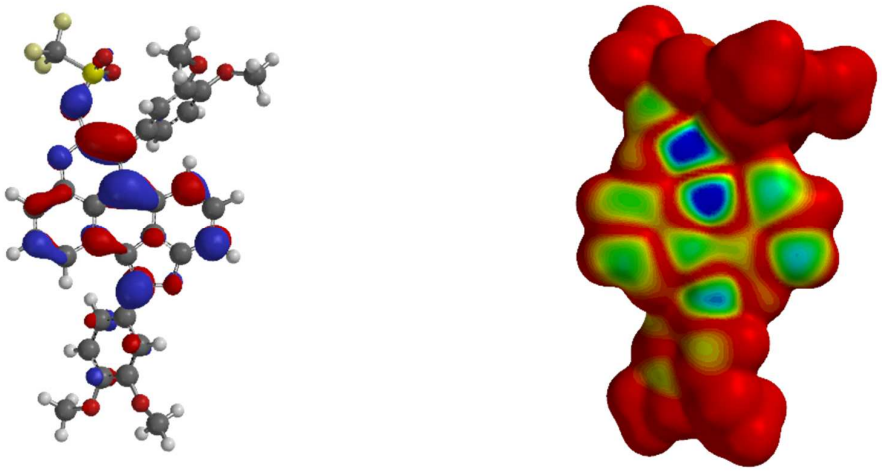


Fig. S 9a. Representation of **HOMO** orbital (*left*) and **HOMO density map** (*right*) for compound **(13)**.

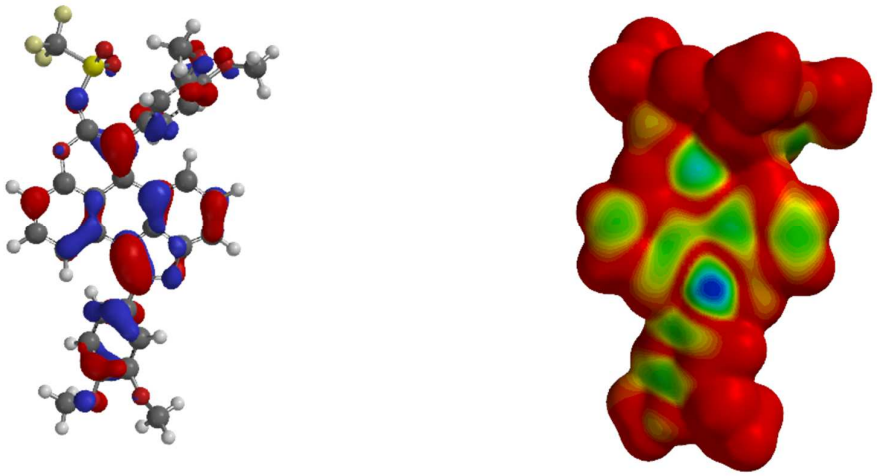


Fig. S 9b. Representation of **LUMO** orbital (*left*) and **LUMO density map** (*right*) for compound **(13)**.

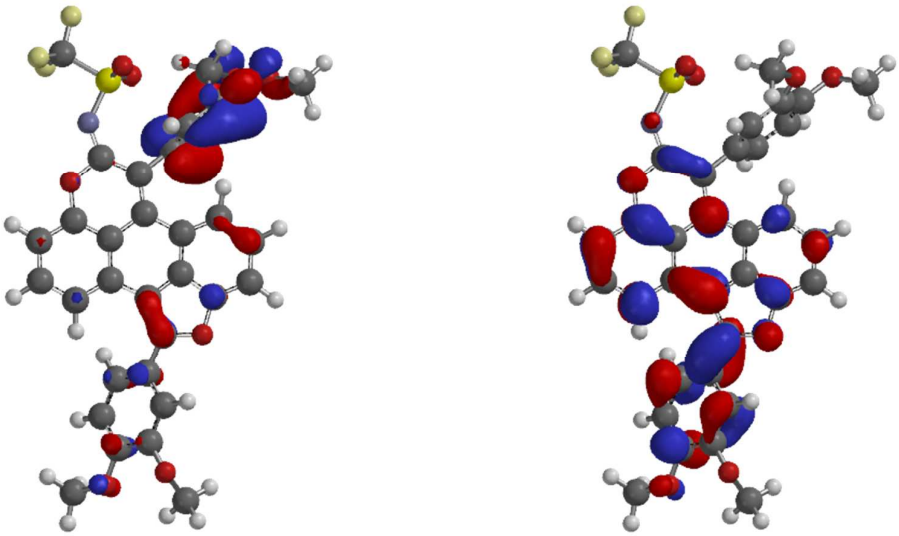


Fig. S 9c. Representation of **HOMO(-1)** orbital (*left*) and **LUMO(+1)** orbital (*right*) for compound **(13).**

(14) *N*-(1,6-diphenyl-7*H*-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-ylidene)-4-methylbenzamide

Yellow crystals (206 mg, 78%); mp (dec.) 185-187°C

^{1}H-NMR ($CDCl_3$, 500 MHz, 303 K) δ 2.38 (s, 3H), 6.35 (d, J = 8.0 Hz), 7.00 (t, J = 8.0 Hz, 1H), 7.07 (d, J = 7.7 Hz, 1H), 7.21 (d, J = 8.0 Hz, 2H), 7.29 (t, J = 8.0 Hz, 1H), 7.37 (d, J = 8.0 Hz, 1H), 7.49 (d, J = 8.3 Hz, 2H), 7.50 – 7.62 (m, 6H), 7.81 – 7.90 (m, 5H).

^{13}C-NMR ($CDCl_3$, 125 MHz, 303 K) δ 21.63, 111.46, 111.93, 115.58, 117.80, 118.84, 123.89, 124.60, 125.35, 125.75, 127.62, 128.62, 128.83, 128.95, 128.98, 129.35, 129.45, 129.51, 129.93, 130.18, 130.92, 131.84, 136.70, 137.00, 143.19, 151.91, 152.51, 152.76, 153.29, 177.94.

HRMS (ESI): m/z calculated for $C_{37}H_{24}NO_3[M+H^+]$ = 530.1756; found: 530.1750.

R_f (SiO_2; DCM): 0.47.

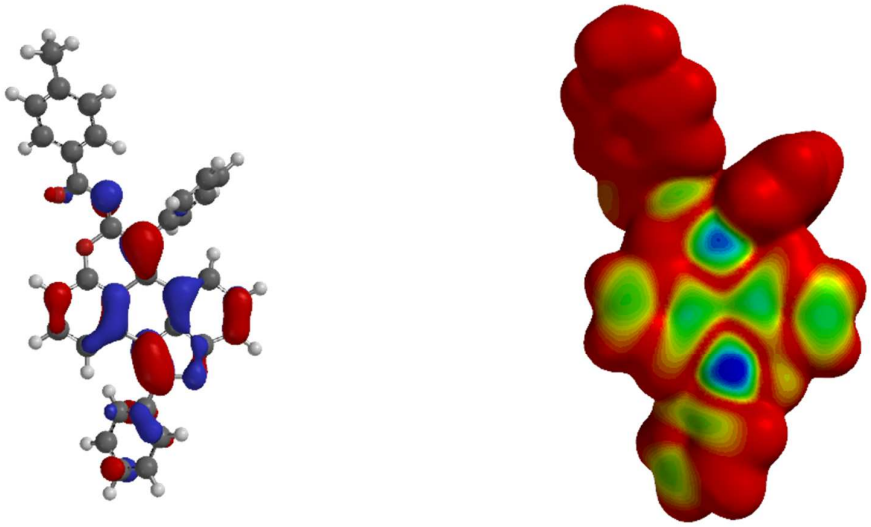


Fig. S 10a. Representation of **HOMO** orbital (*left*) and **HOMO density map** (*right*) for compound **(14)**.

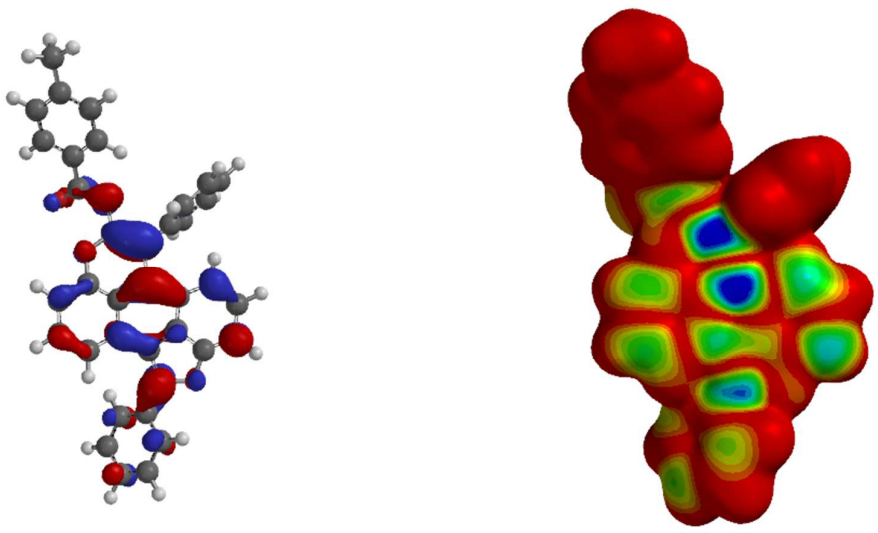


Fig. S 10b. Representation of **LUMO** orbital (*left*) and **LUMO density map** (*right*) for compound **(14)**.

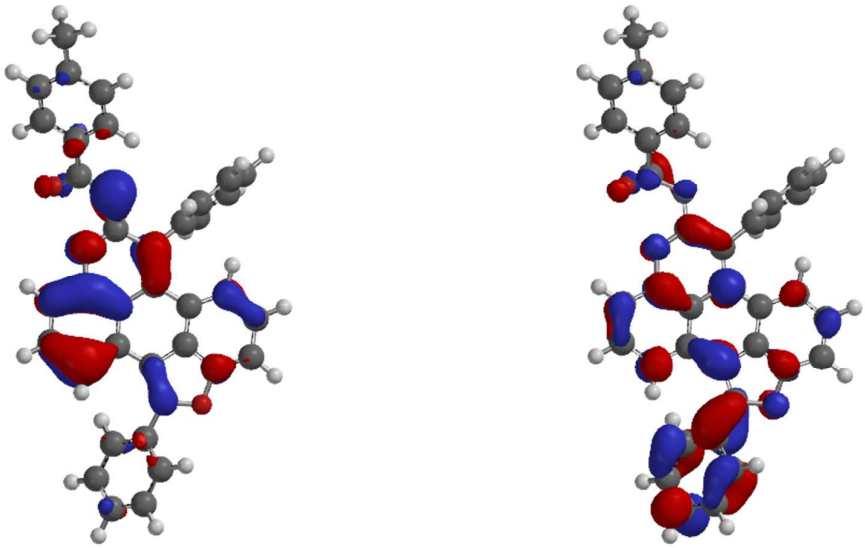


Fig. S 10c. Representation of **HOMO(-1)** orbital (*left*) and **LUMO(+1)** orbital (*right*) for compound **(14).**

(15) *N*-(1,6-diphenyl-7*H*-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-ylidene)-4-methylbenzenesulfonamide

Amber crystals (220 mg, 83%); mp (dec.) 270-271°C

^{1}H-NMR ($CDCl_3$, 500 MHz, 303 K) δ 2.37 (s, 3H), 6.38 (d, J = 8.2Hz, 1H), 7.00 (t, J = 8.0 Hz, 1H), 7.21 (d, J = 8.0 Hz, 2H), 7.31 – 7.34 (m, 2H), 7.40 (d, J = 7.8 Hz, 2H), 7.47 (t, J = 8.0 Hz, 1H), 7.50 – 7.61 (m, 6H), 7.78 (d, J = 8.0 Hz, 2H), 7.86 – 7.90 (m, 2H), 7.98 (d, J = 7.8 Hz, 1H).

^{13}C-NMR ($CDCl_3$, 125 MHz, 303 K) δ 21.48, 99.99, 111.29, 112.99, 115.94, 118.00, 119.72, 123.95, 124.49, 124.84, 125.96, 126.85, 128.07, 128.73, 128.77, 129.01, 129.10, 129.57, 129.66, 129.86, 130.58, 130.60, 131.05, 135.86, 140.04, 140.36, 142.42, 152.50, 153.11, 153.92, 159.22.

HRMS (ESI): m/z calculated for $C_{37}H_{24}NO_3[M+H^+]$ = 530.1750; found: 530.1756.

R_f (SiO_2; DCM/AcOEt, 99:1): 0.44.

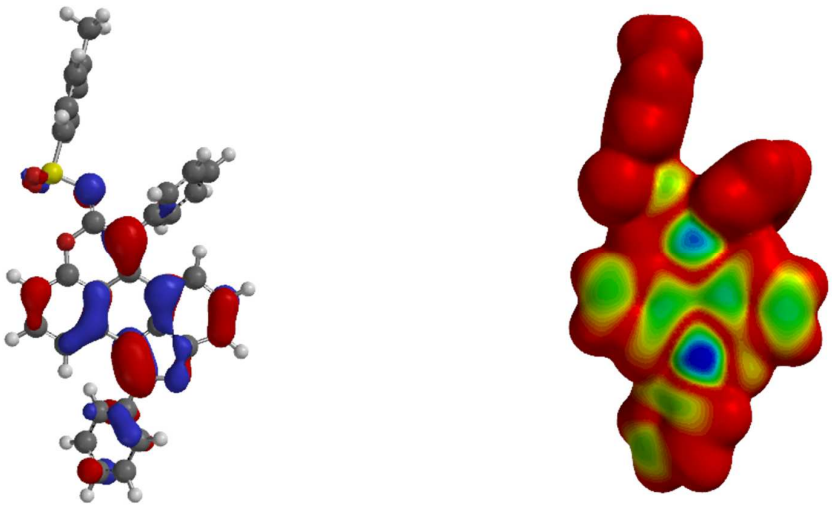


Fig. S 11a. Representation of **HOMO** orbital (*left*) and **HOMO density map** (*right*) for compound **(15)**.

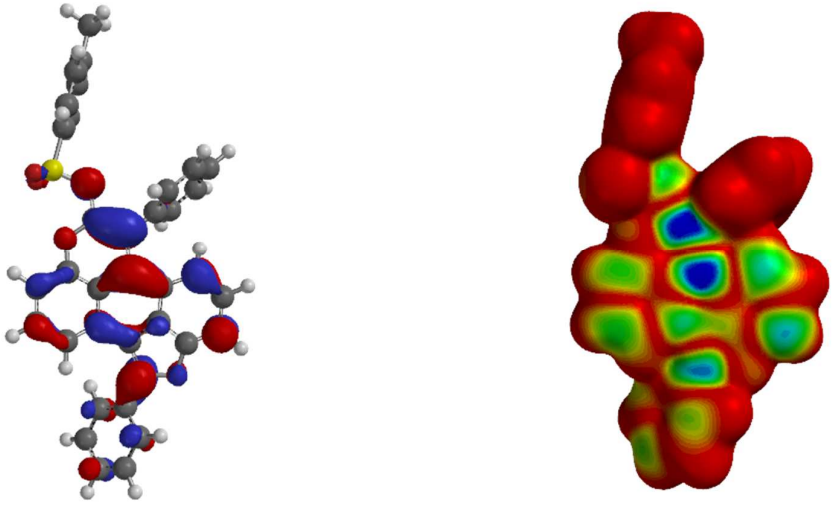


Fig. S 11b. Representation of **LUMO** orbital (*left*) and **LUMO density map** (*right*) for compound **(15)**.

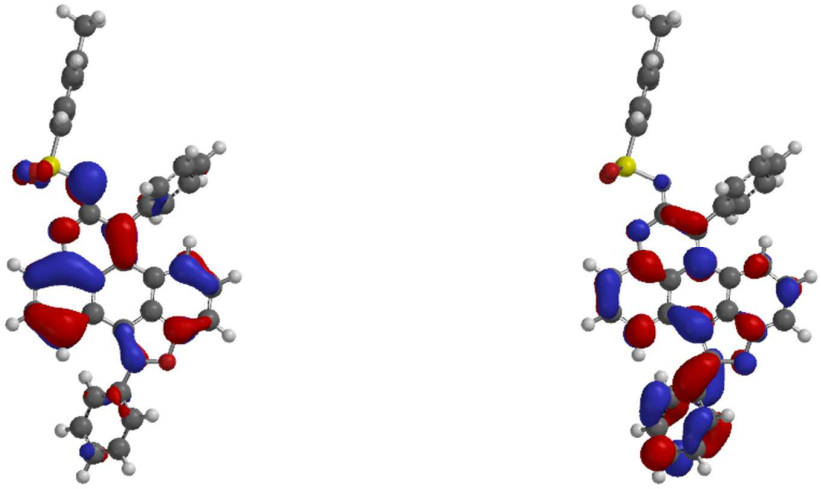
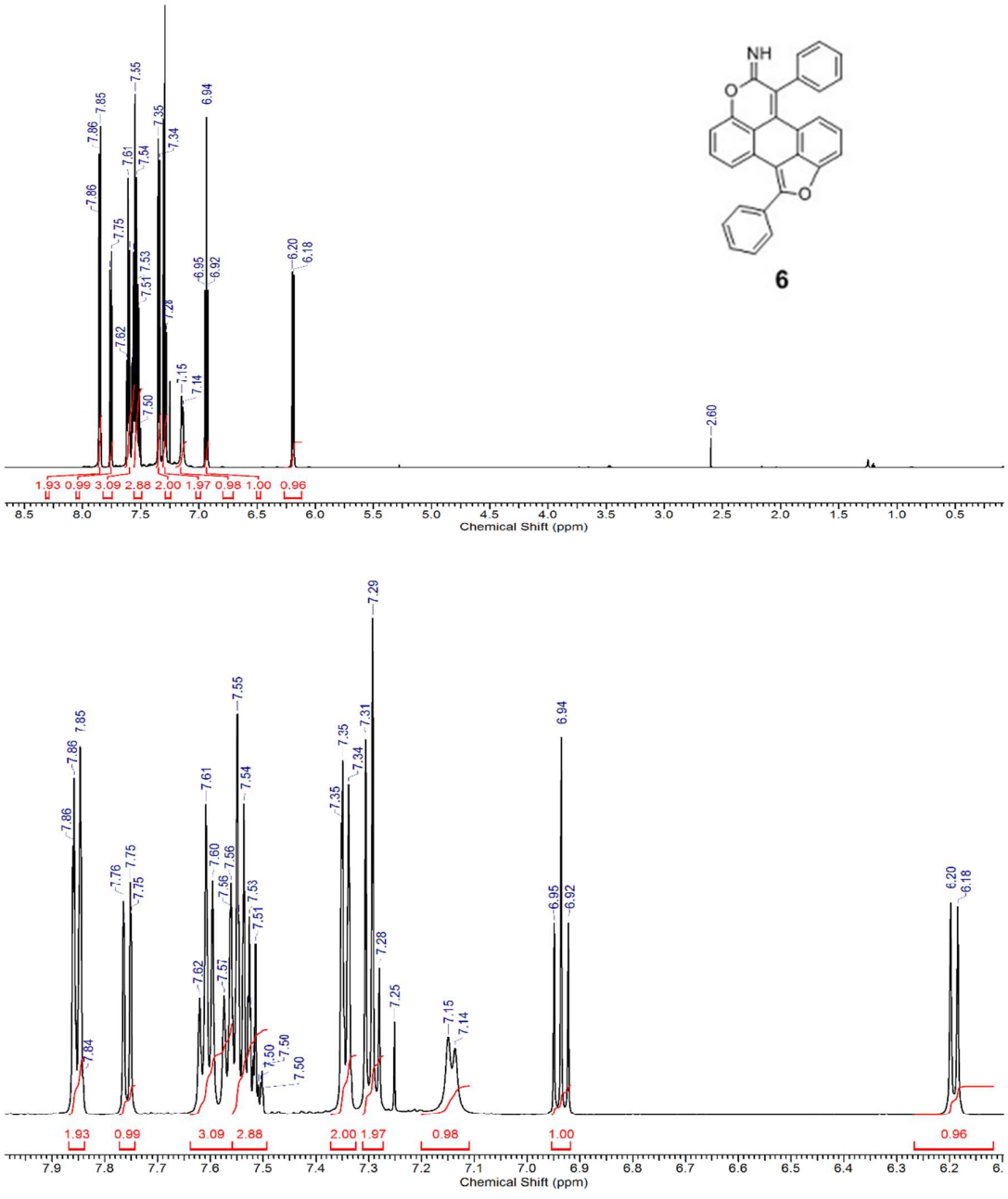


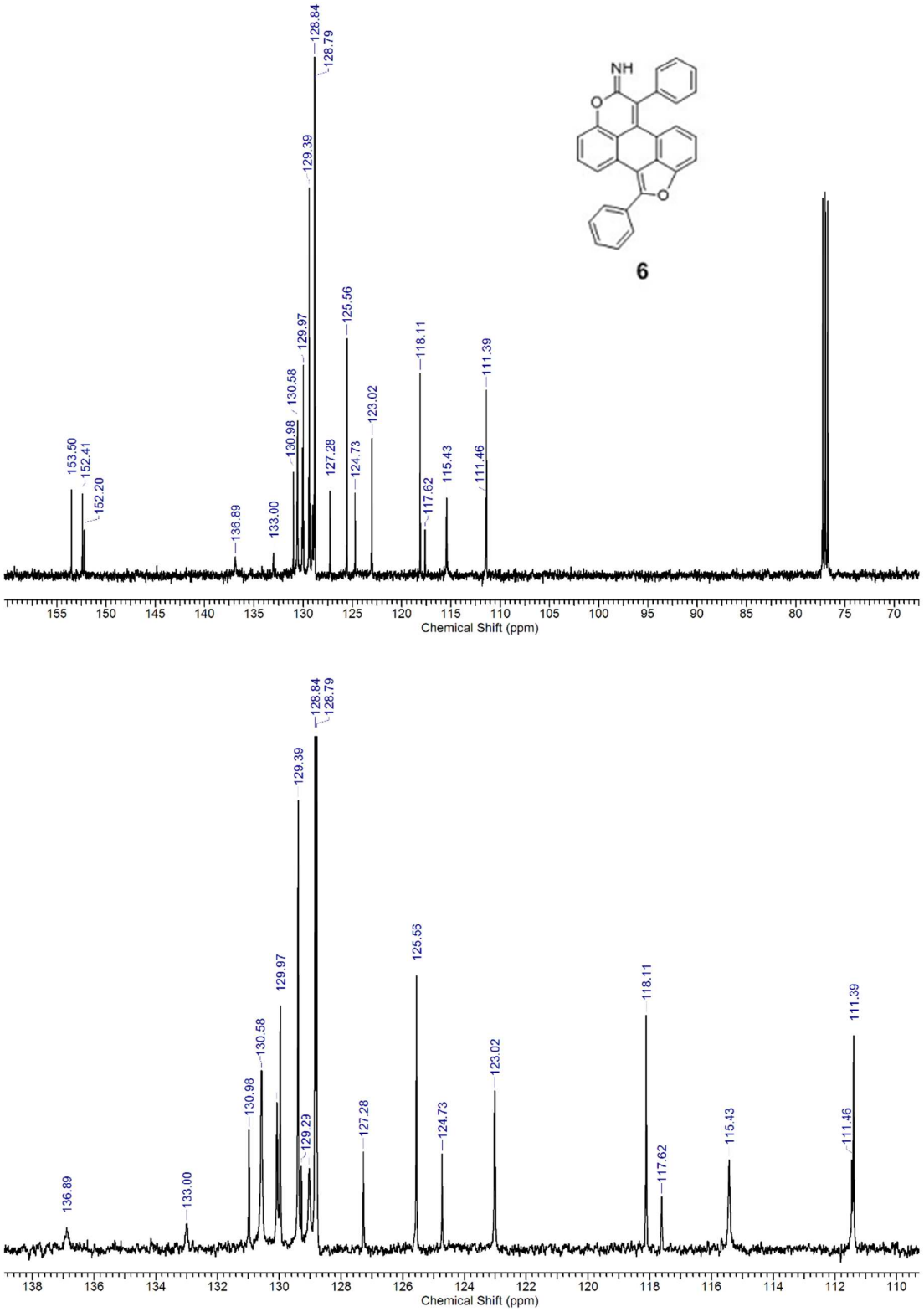
Fig. S 11c. Representation of **HOMO(-1)** orbital (*left*) and **LUMO(+1)** orbital (*right*) for compound **(15).**

NMR Spectra

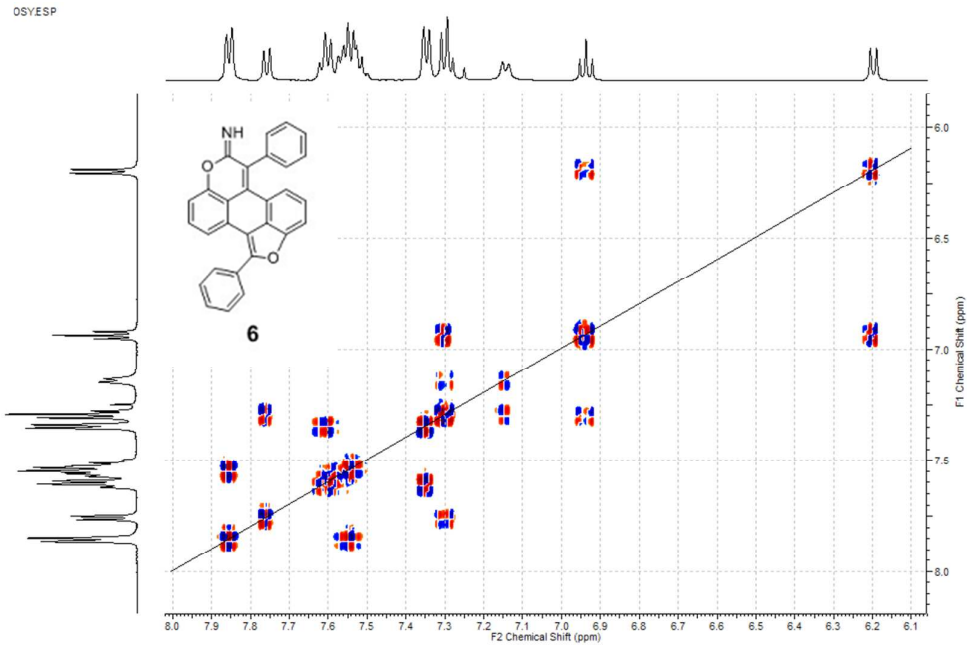
(6) 1,6-Diphenyl-7*H*-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-imine



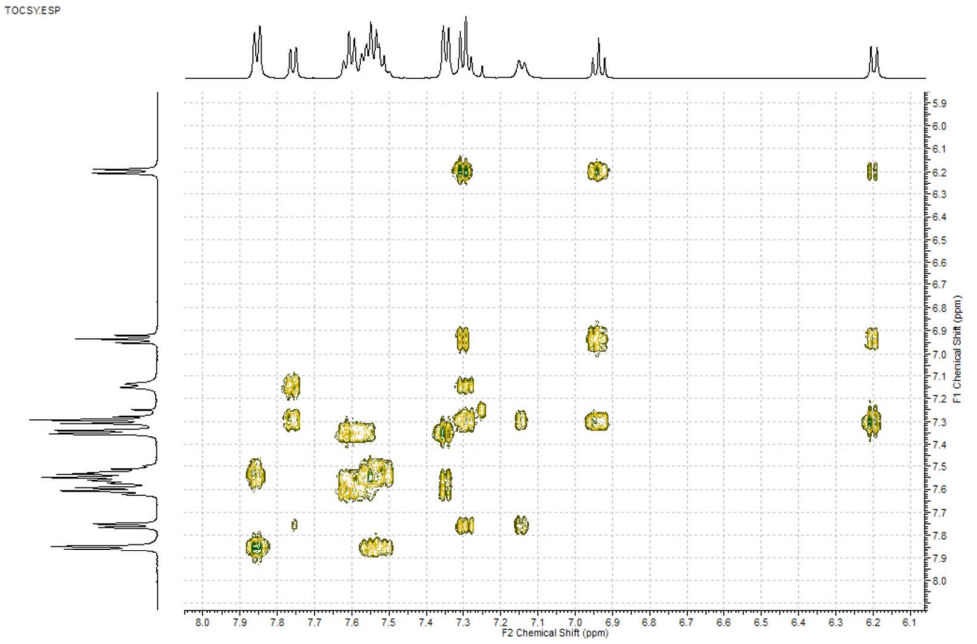
^{1}H NMR (600 MHz) spectrum of compound **(6)**. Whole spectrum at the top of the page, zoomed one at the bottom.



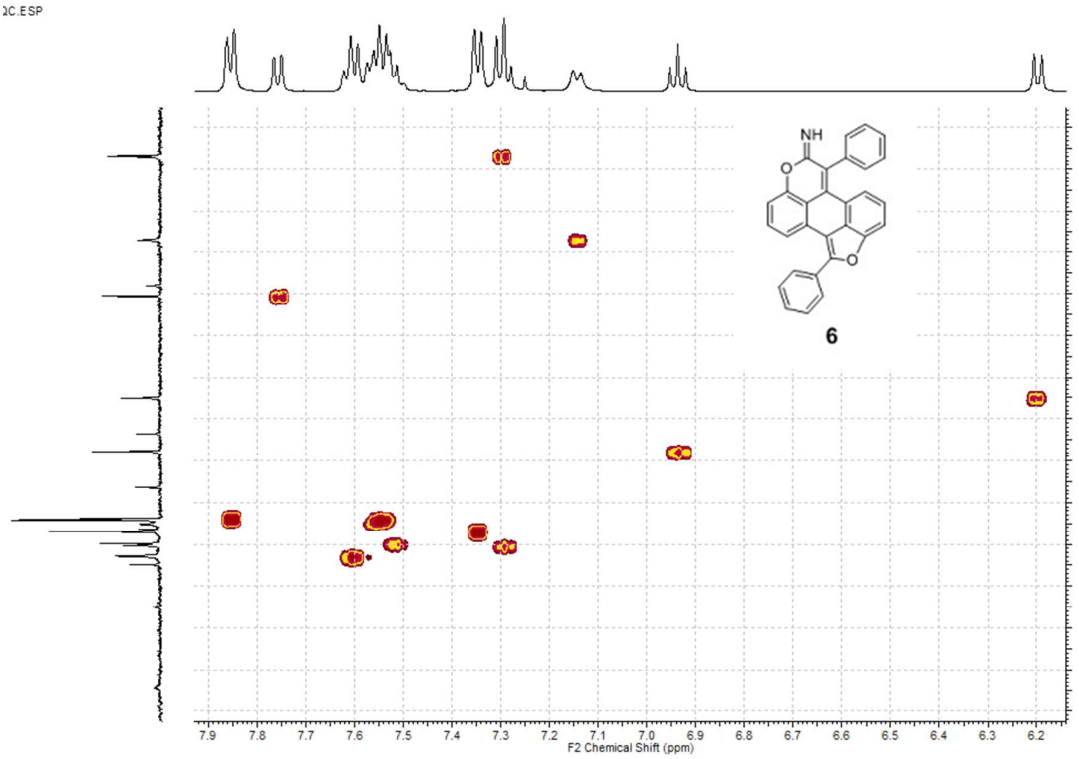
^{13}C NMR (125 MHz) spectrum of compound **(6)**. Whole spectrum at the top of the page, zoomed one at the bottom.



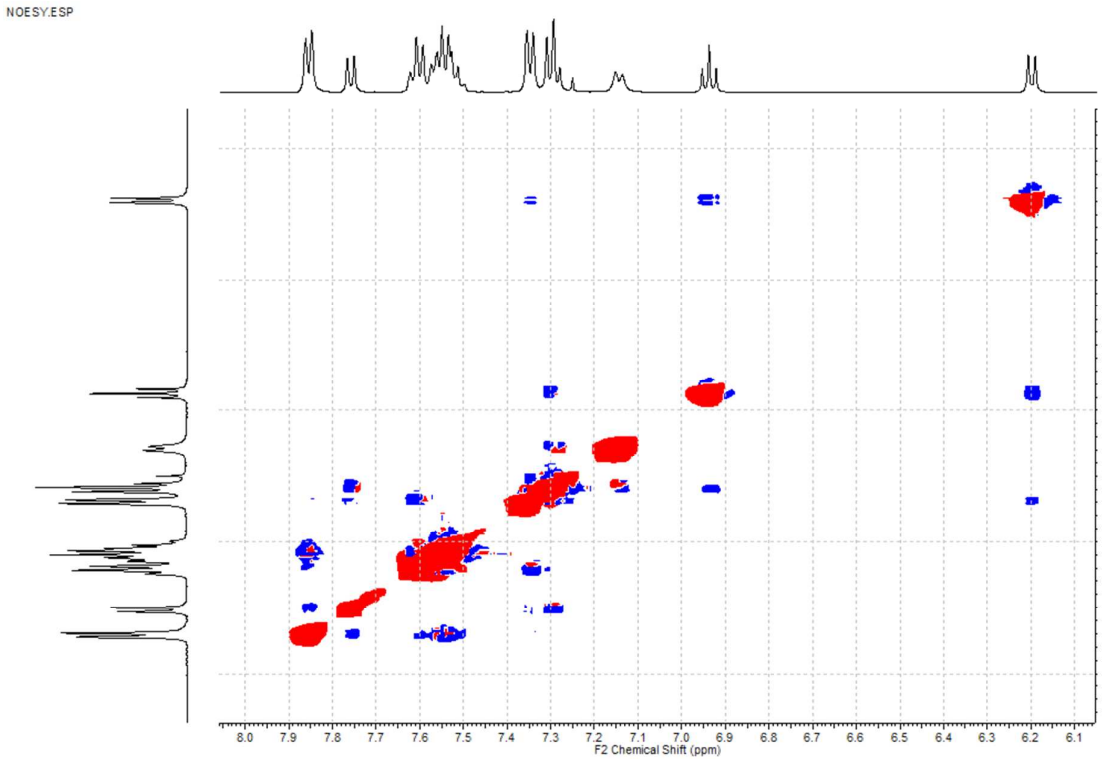
^{1}H-^{1}H DQF-COSY NMR (500 MHz) spectrum of compound **(6)**.



^{1}H-^{1}H 2D TOCSY NMR (500 MHz) spectrum of compound **(6)**.

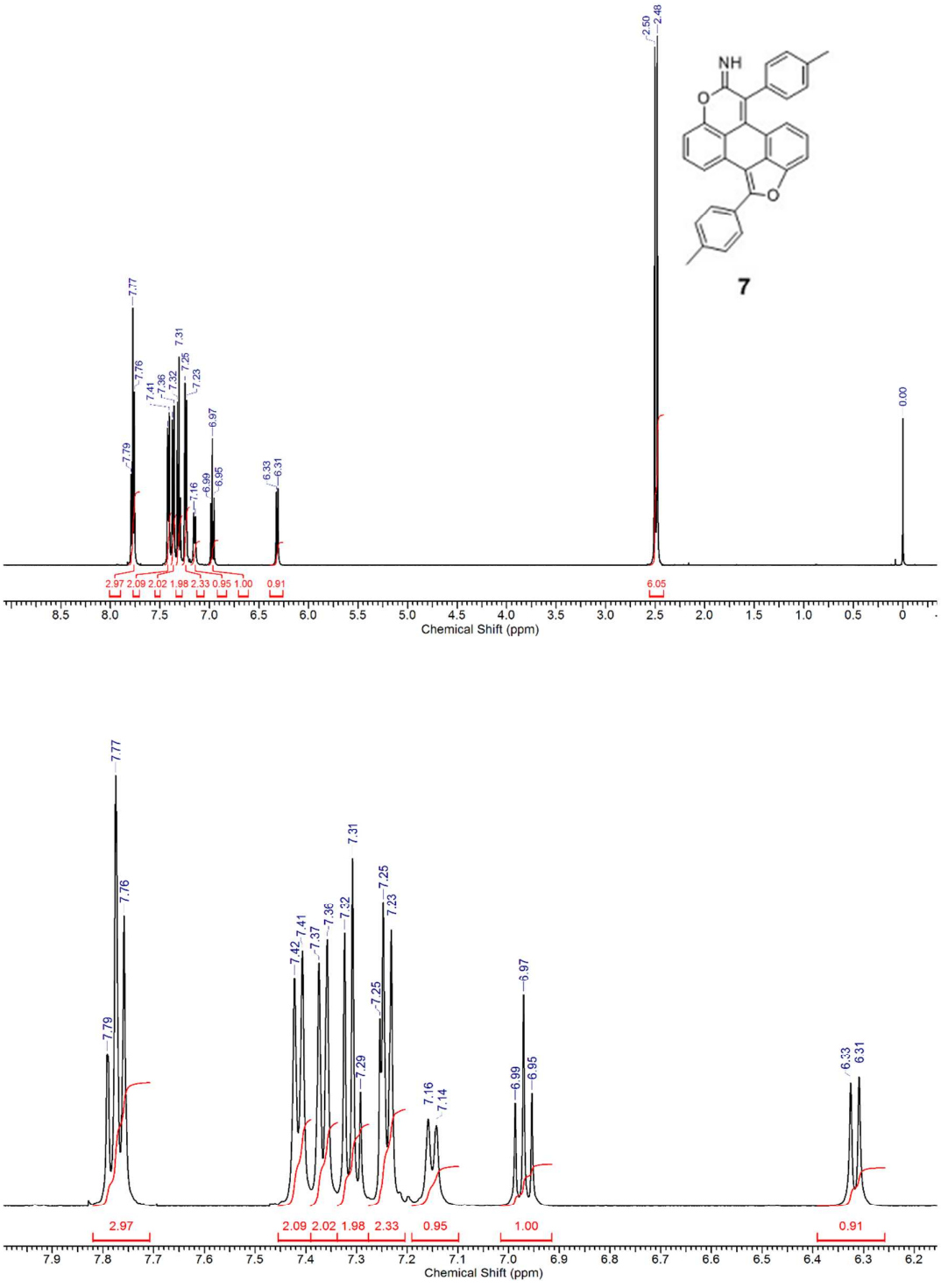


^{1}H-^{13}C 2D HSQC NMR (500 MHz) spectrum of compound **(6)**.

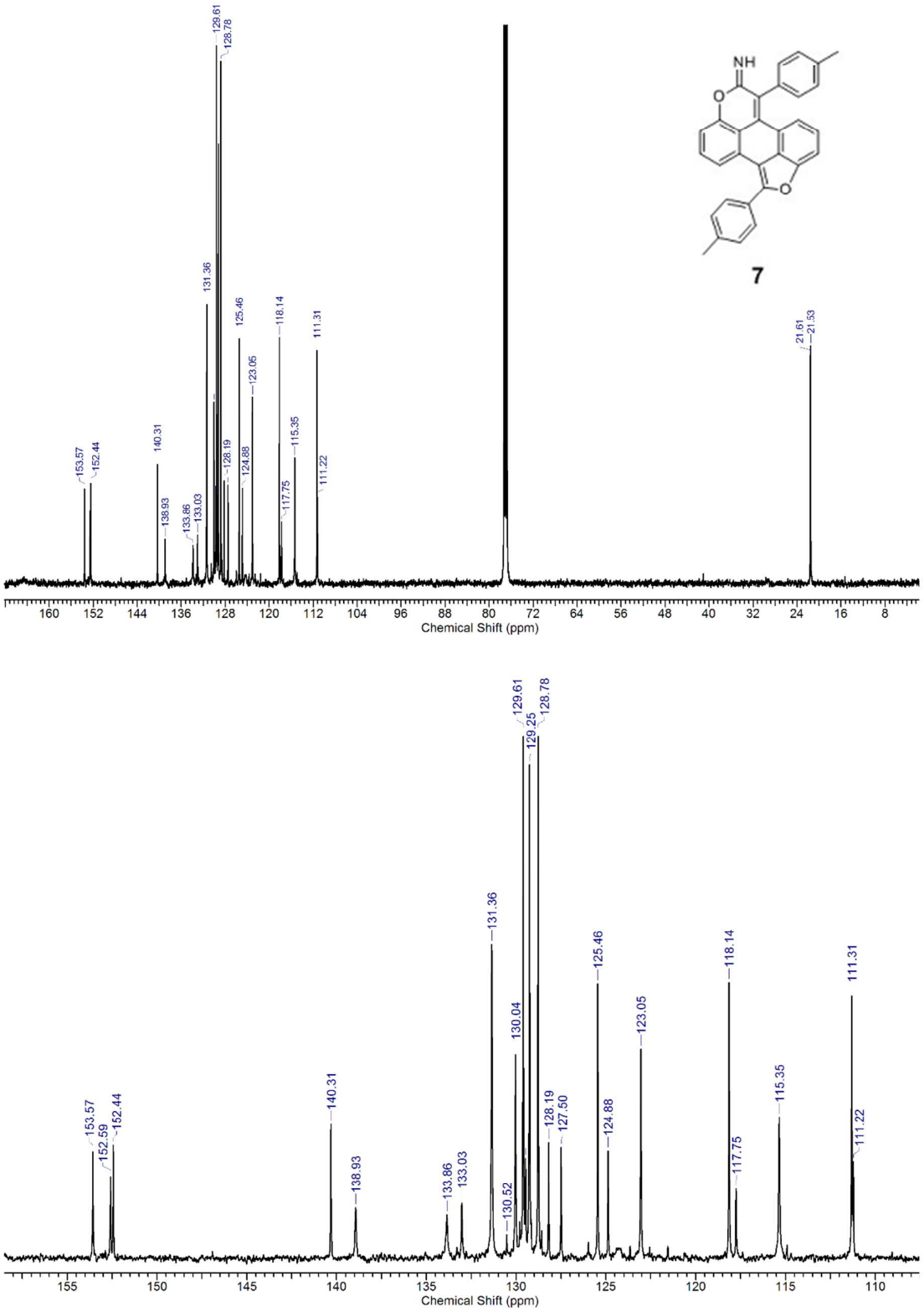


^{1}H-^{1}H 2D NOESY (500 MHz) spectrum of compound **(6)**.

(7) 1,6-Di-p-tolyl-7*H*-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-imine

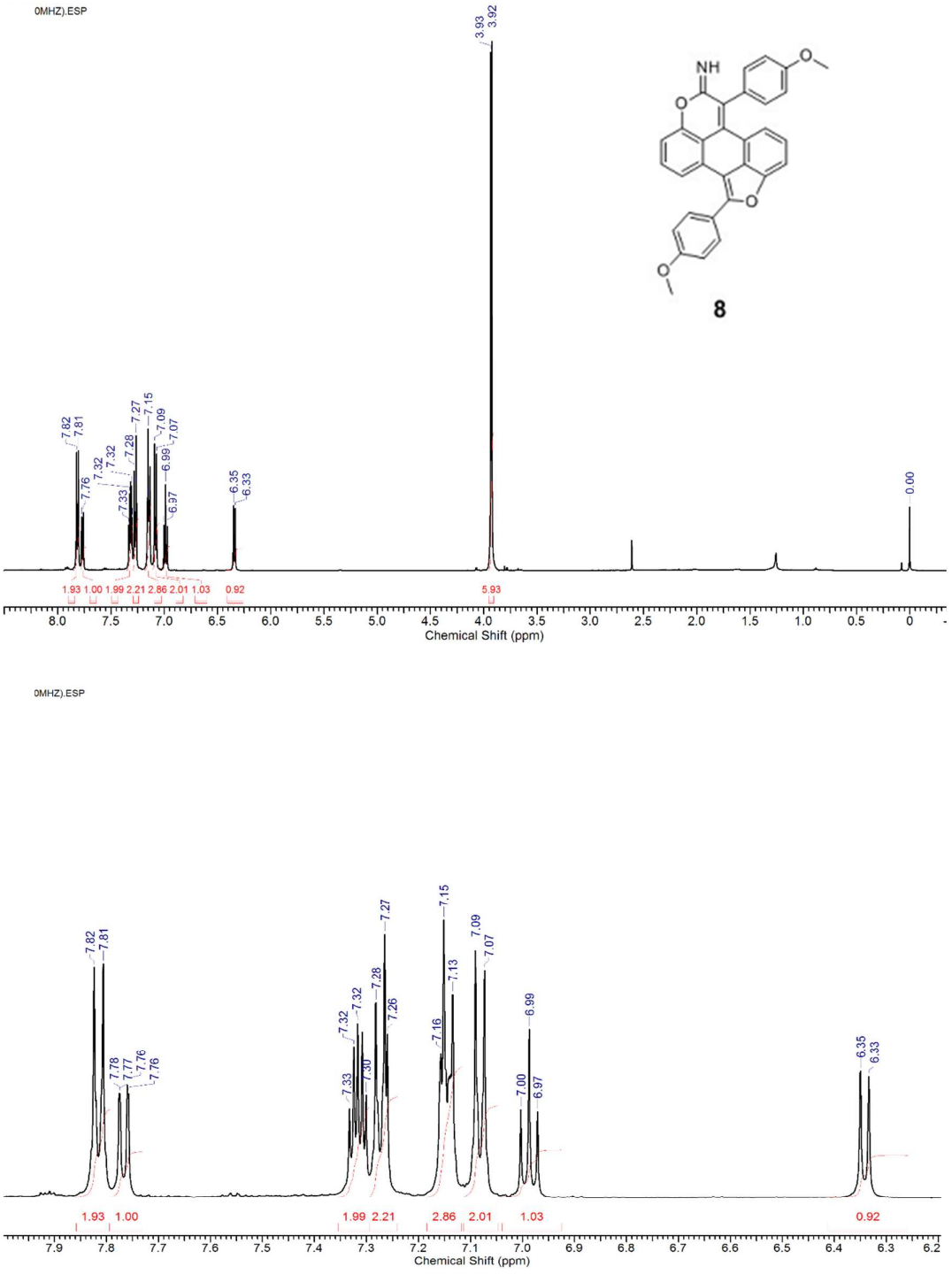


^{1}H NMR (500 MHz) spectrum of compound **(7)**. Whole spectrum at the top of the page, zoomed one at the bottom.

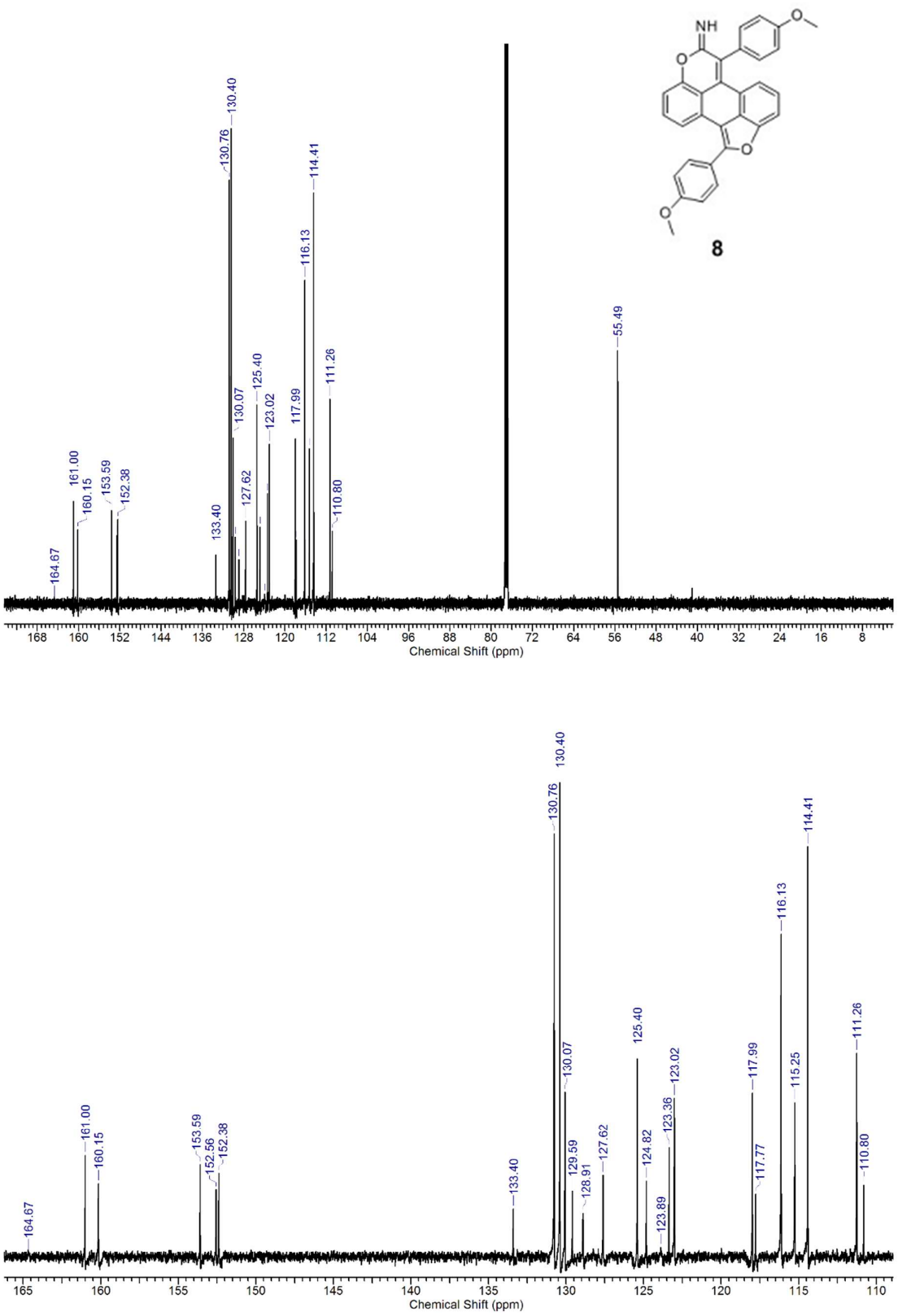


^{13}C NMR (125 MHz) spectrum of compound **(7)**. Whole spectrum at the top of the page, zoomed one at the bottom.

(8) 1,6-Bis(4-methoxyphenyl)-7*H*-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-imine

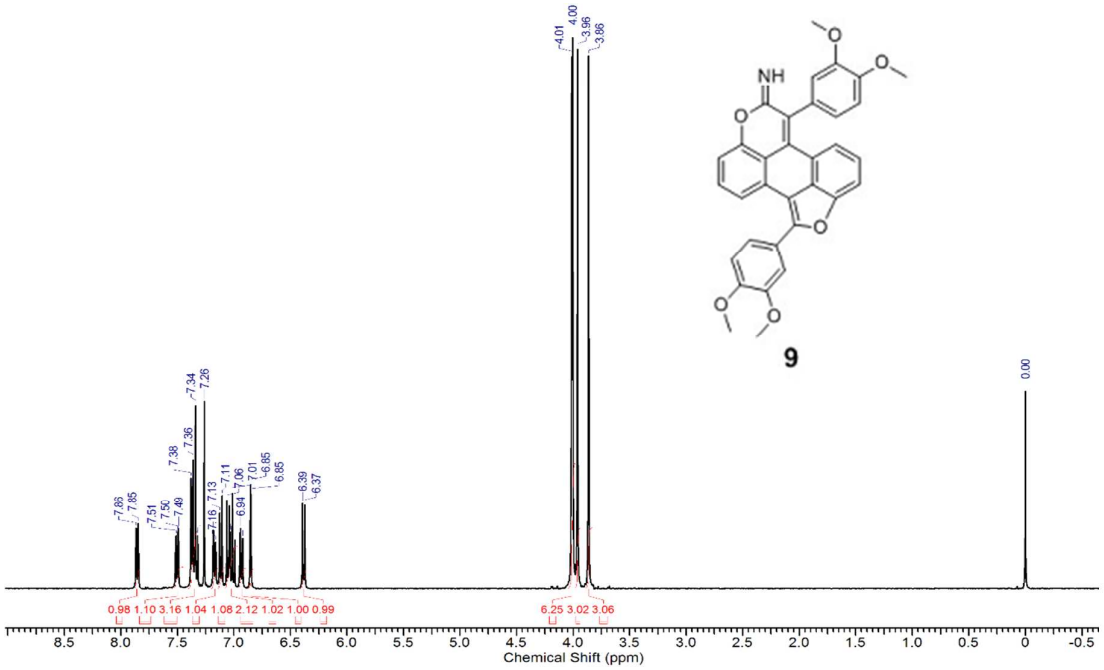


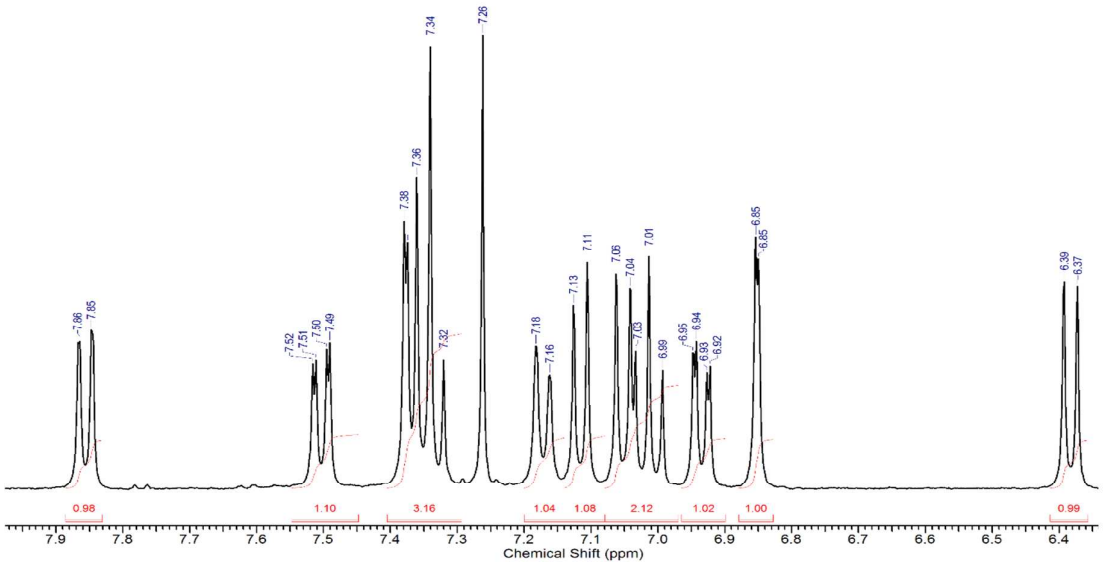
^{1}H NMR (500 MHz) spectrum of compound **(8)**. Whole spectrum at the top of the page, zoomed one at the bottom.



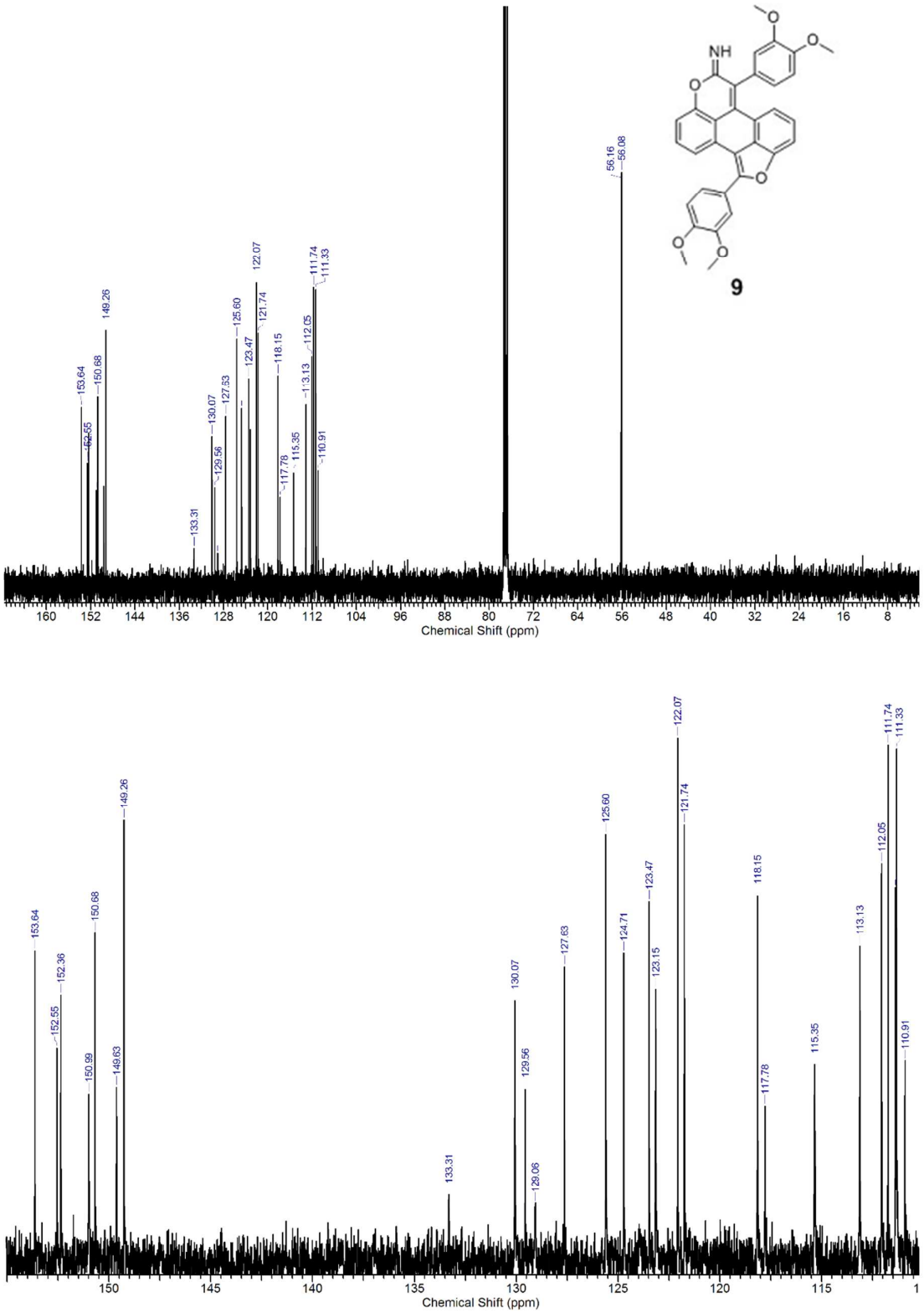
^{13}C NMR (125 MHz) spectrum of compound **(8)**. Whole spectrum at the top of the page, zoomed one at the bottom.

(9) 1,6-Bis(3,4-dimethoxyphenyl)-7*H*-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-imine



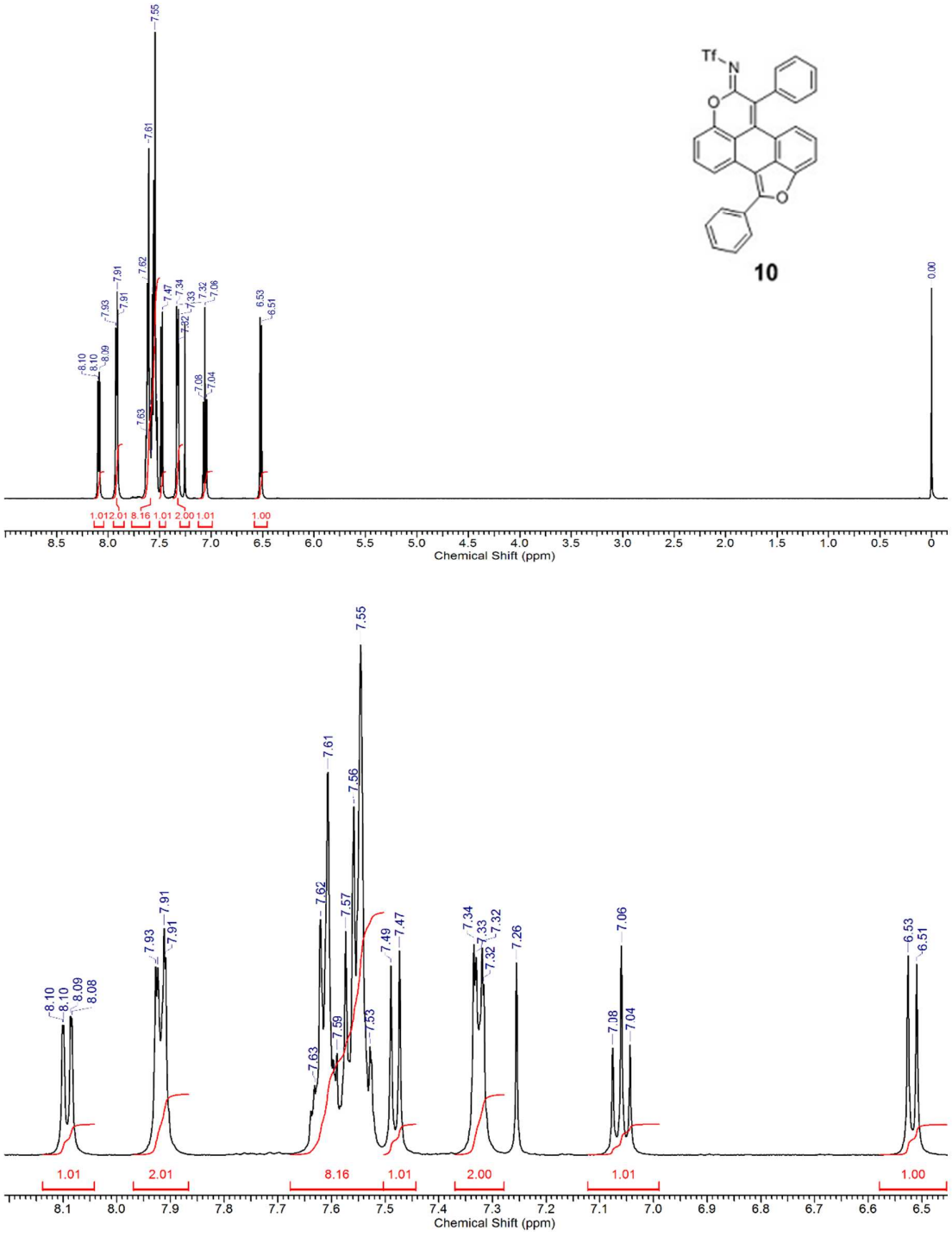


^{1}H NMR (500 MHz) spectrum of compound **(9)**. Whole spectrum at the top of the page, zoomed one at the bottom.

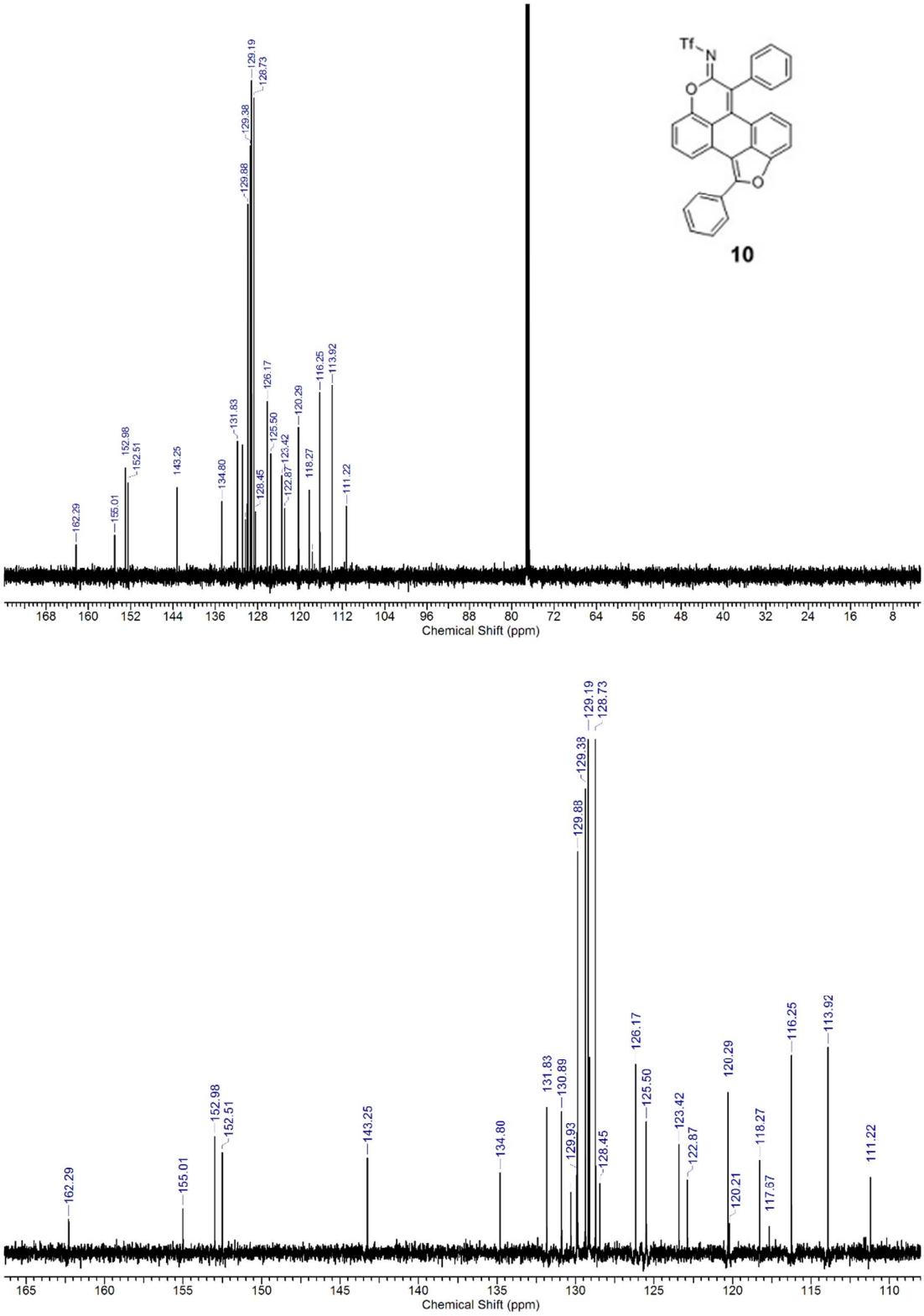


^{13}C NMR (125 MHz) spectrum of compound **(9)**. Whole spectrum at the top of the page, zoomed one at the bottom.

(10) *N*-(1,6-diphenyl-7*H*-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-ylidene)-1,1,1-trifluoromethanesulfonamide

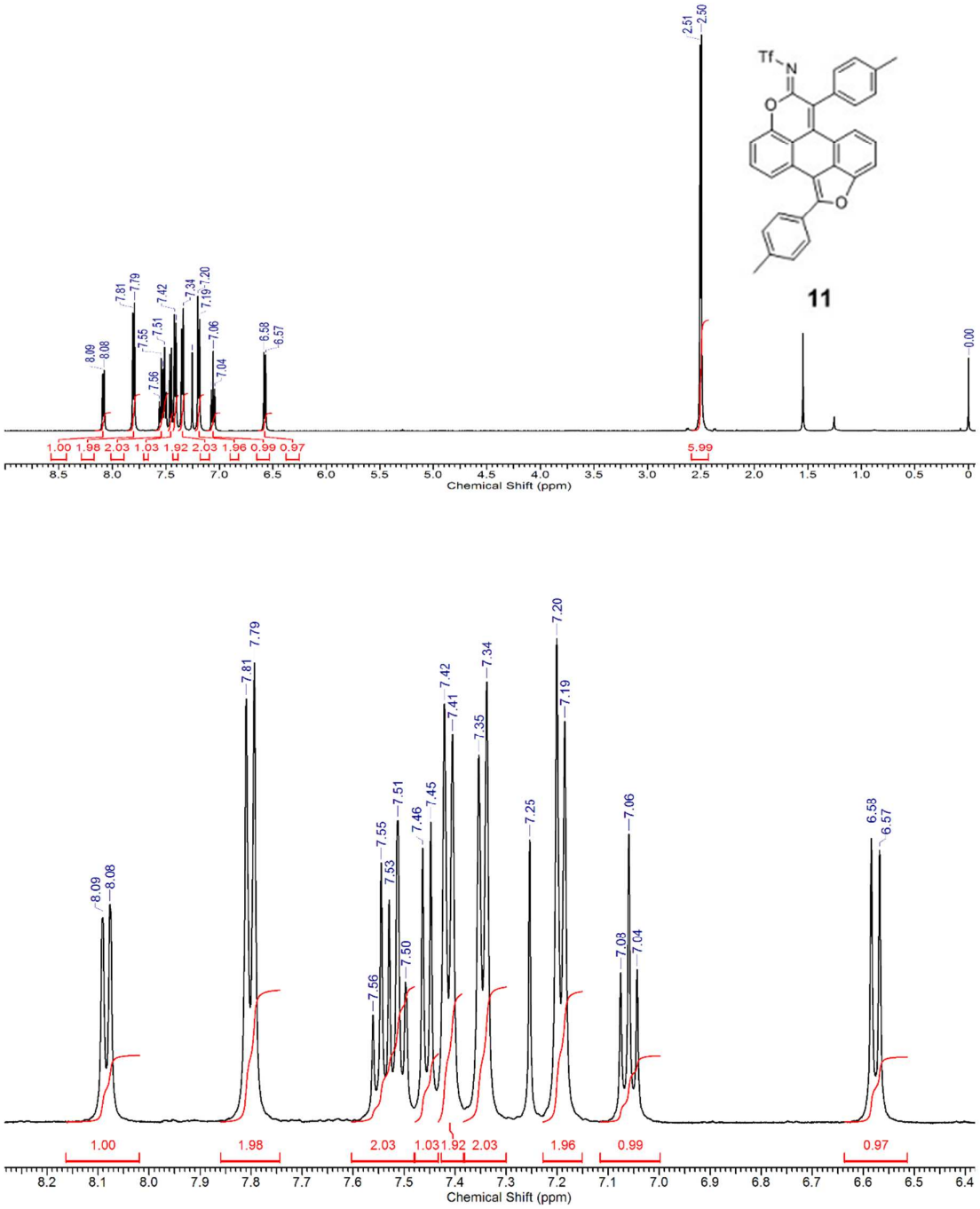


^{1}H NMR (500 MHz) spectrum of compound **(10)**. Whole spectrum at the top of the page, zoomed one at the bottom.

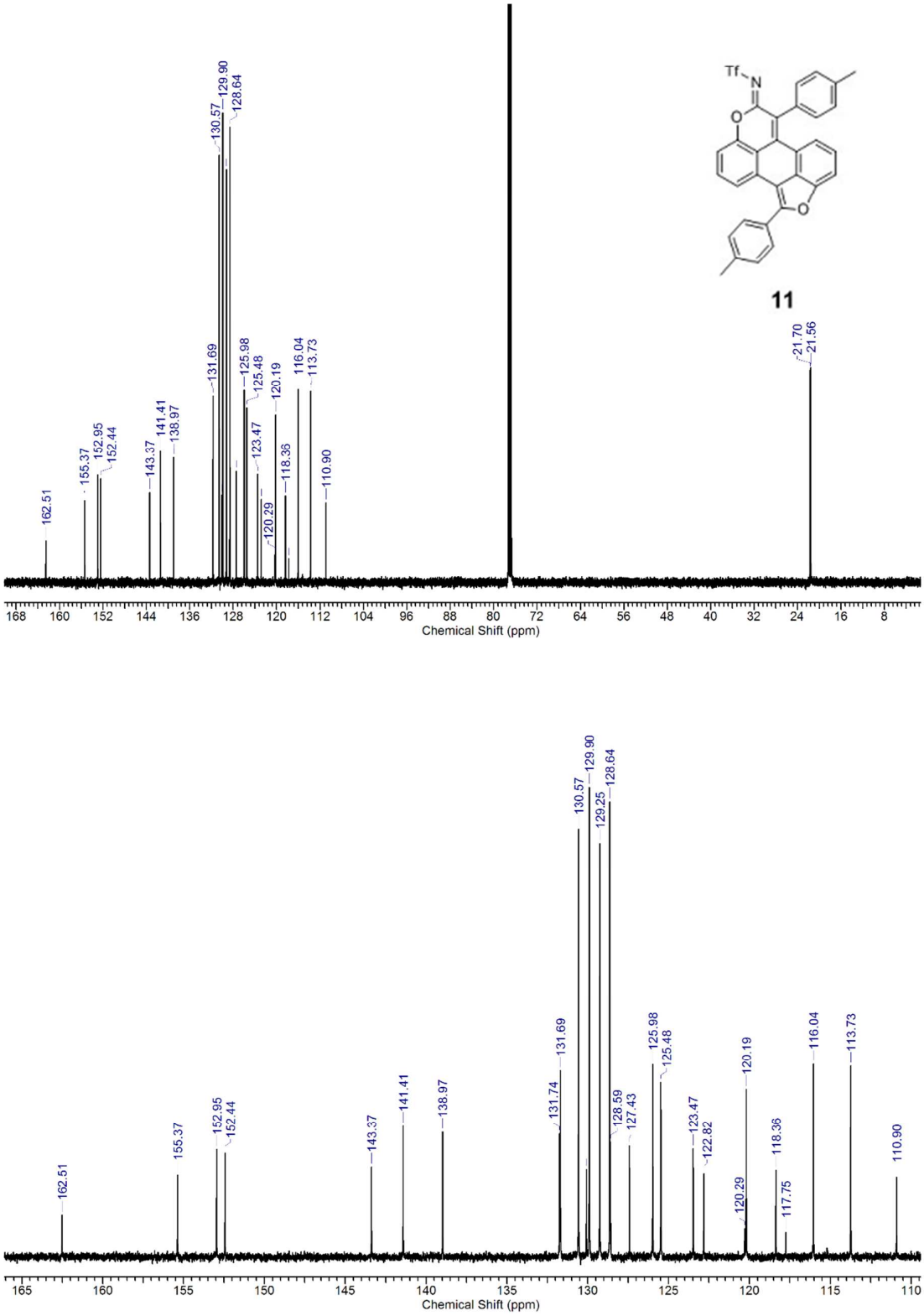


^{13}C NMR (125 MHz) spectrum of compound **(10)**. Whole spectrum at the top of the page, zoomed one at the bottom.

(11) *N*-(1,6-di-p-tolyl-7*H*-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-ylidene)-1,1,1-trifluoromethanesulfonamide

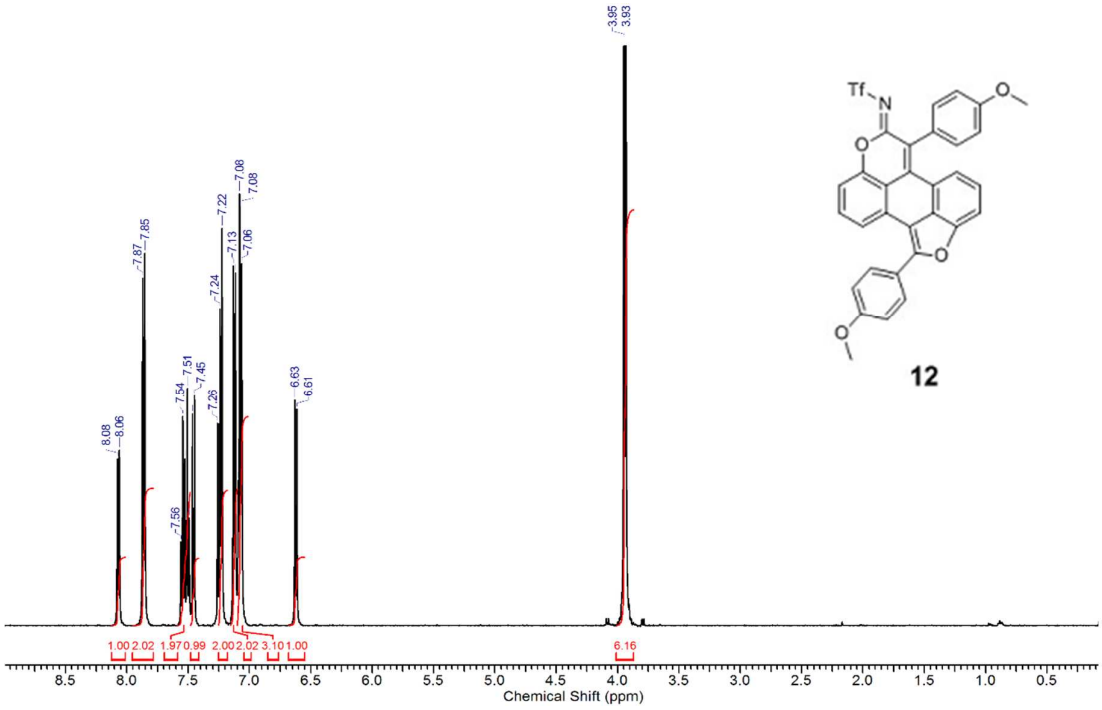


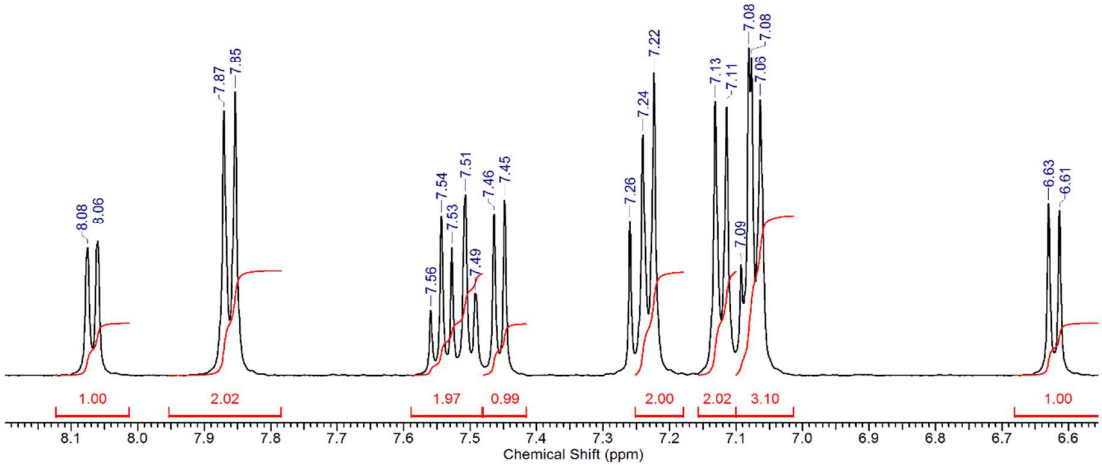
^{1}H NMR (500 MHz) spectrum of compound **(11)**. Whole spectrum at the top of the page, zoomed one at the bottom.



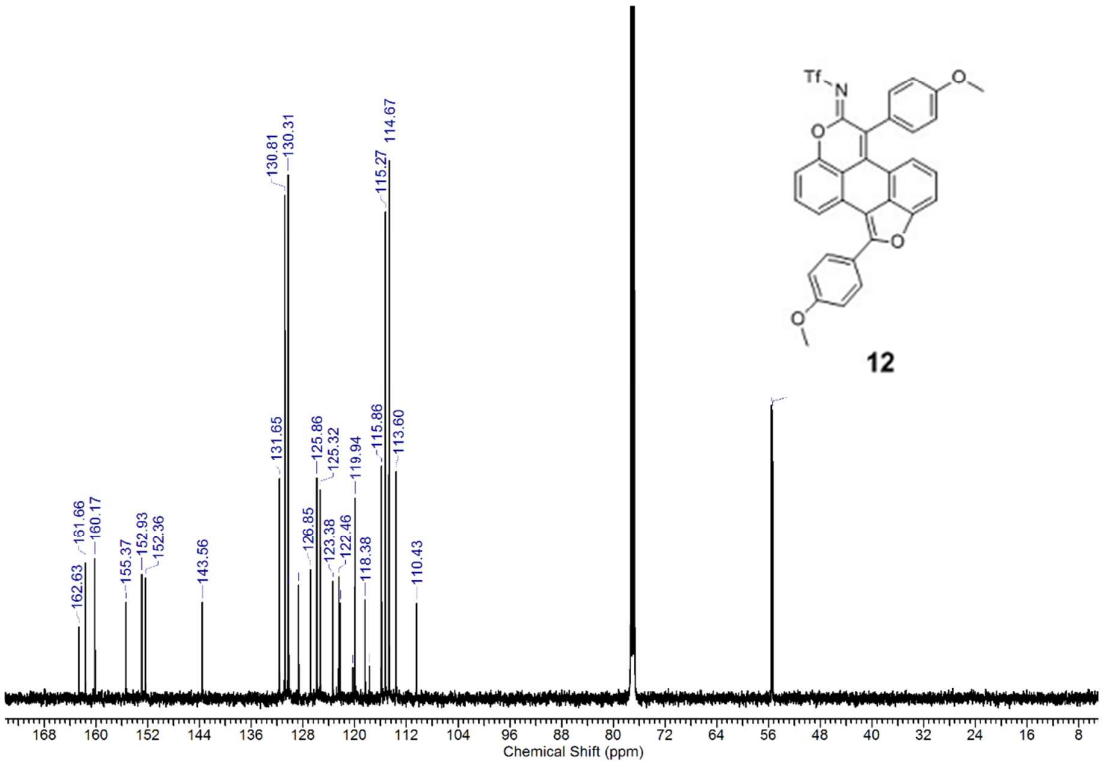
^{13}C NMR (125 MHz) spectrum of compound **(11)**. Whole spectrum at the top of the page, zoomed one at the bottom.

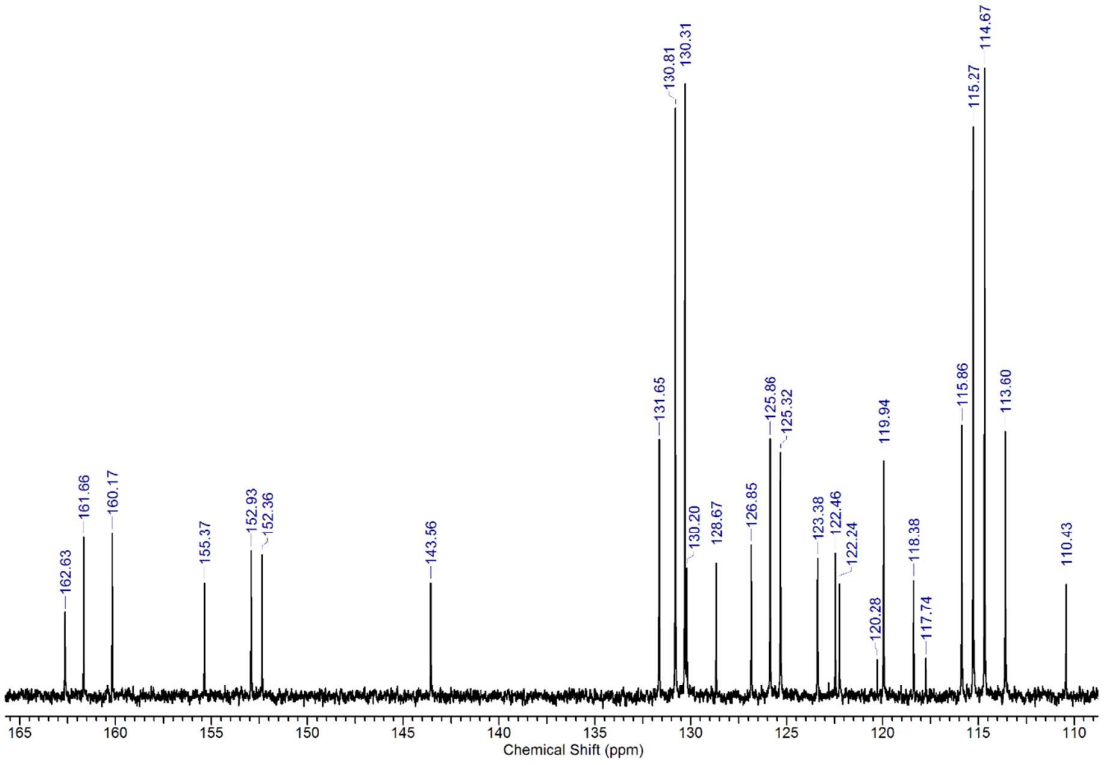
(12) *N*-(1,6-bis(4-methoxyphenyl)-7*H*-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-ylidene)-1,1,1-trifluoromethanesulfonamide





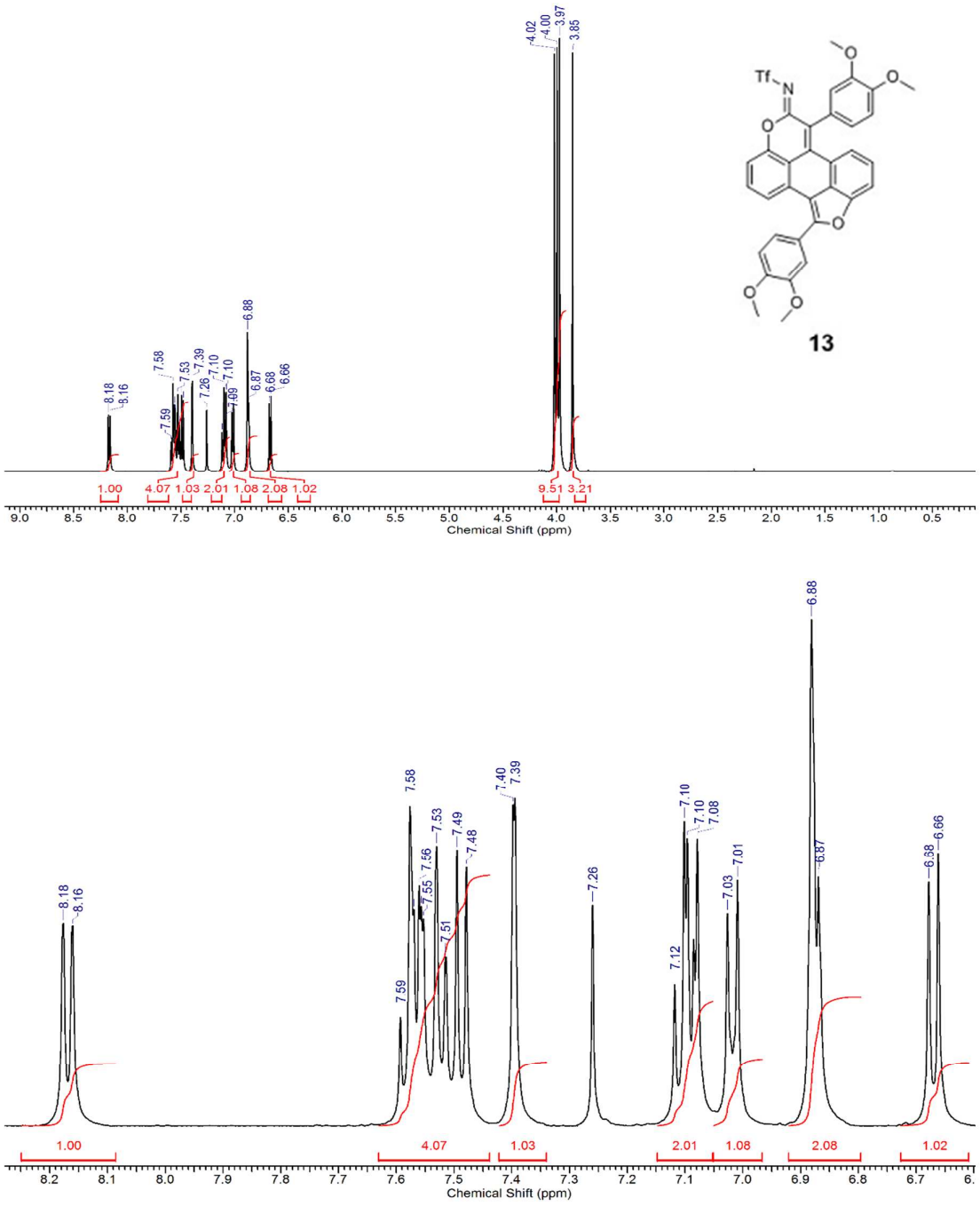
^{1}H NMR (500 MHz) spectrum of compound **(12)**. Whole spectrum at the top of the page, zoomed one at the bottom.



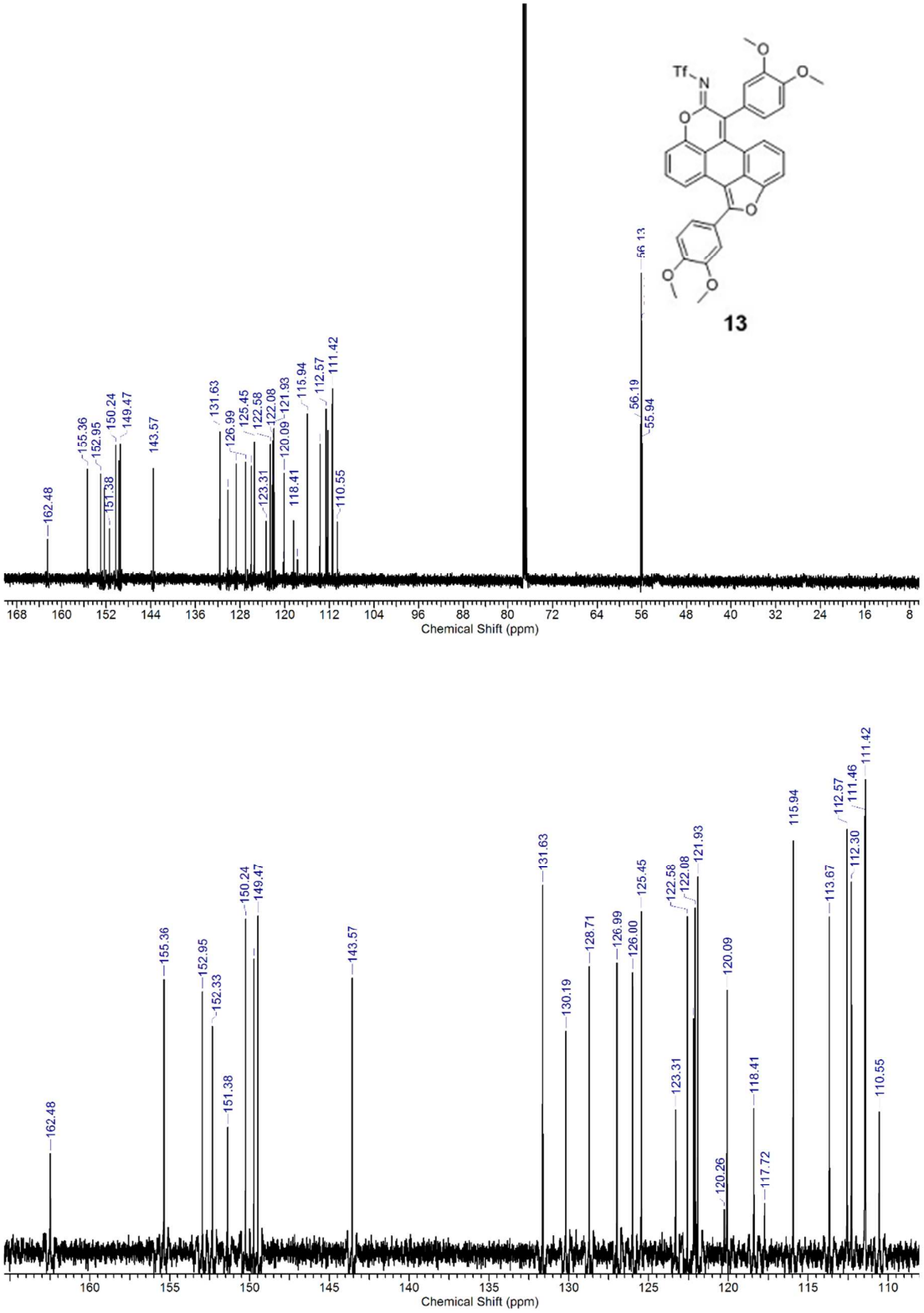


^{13}C NMR (125 MHz) spectrum of compound **(12)**. Whole spectrum at the top of the page, zoomed one at the bottom.

(13) *N*-(1,6-bis(3,4-dimethoxyphenyl)-7*H*-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-ylidene)-1,1,1-trifluoromethanesulfonamide

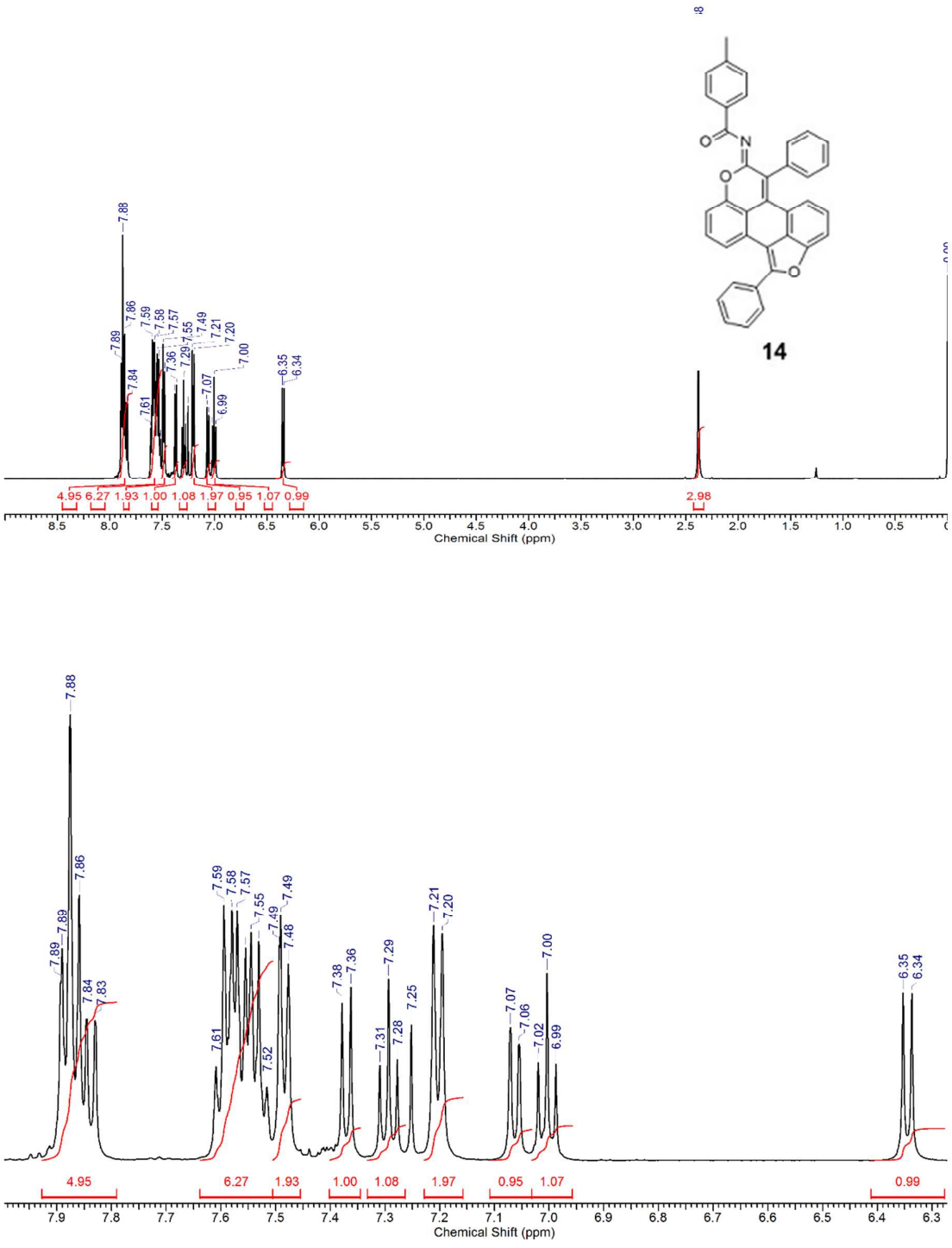


^{1}H NMR (500 MHz) spectrum of compound **(13)**. Whole spectrum at the top of the page, zoomed one at the bottom.

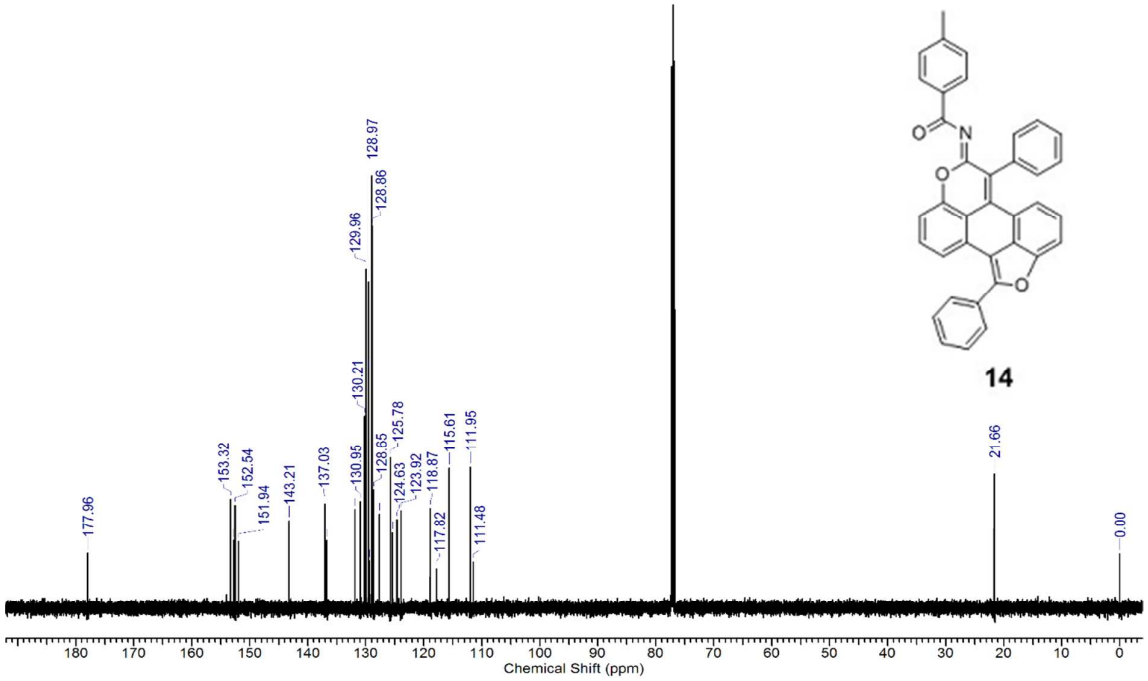


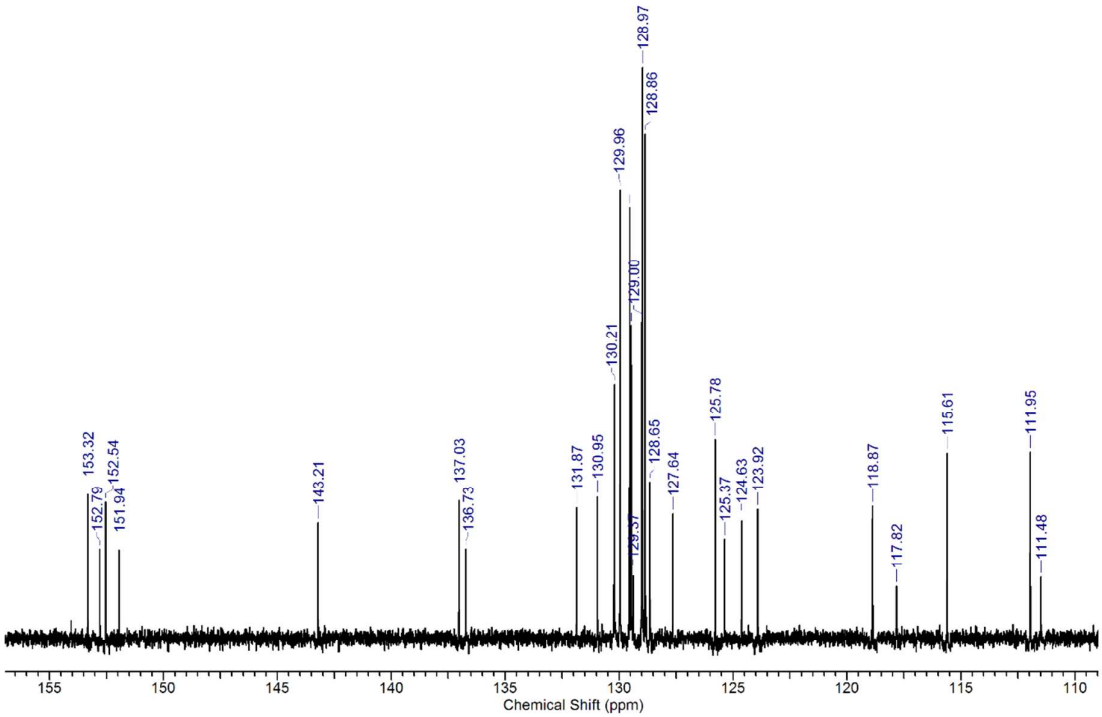
^{13}C NMR (125 MHz) spectrum of compound **(13)**. Whole spectrum at the top of the page, zoomed one at the bottom.

(14) *N*-(1,6-diphenyl-7*H*-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-ylidene)-4-methylbenzamide



^{1}H NMR (500 MHz) spectrum of compound **(14)**. Whole spectrum at the top of the page, zoomed one at the bottom.

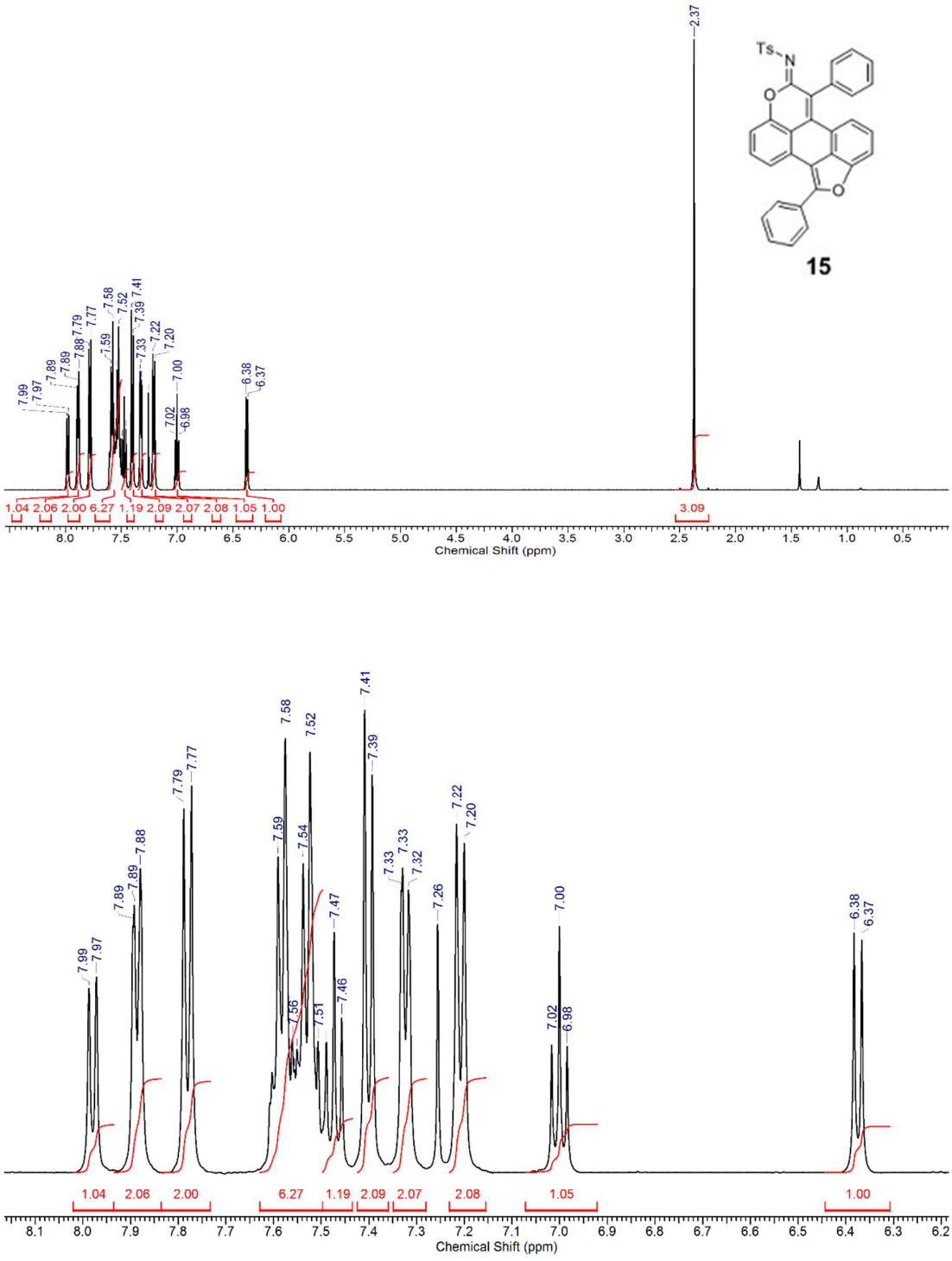




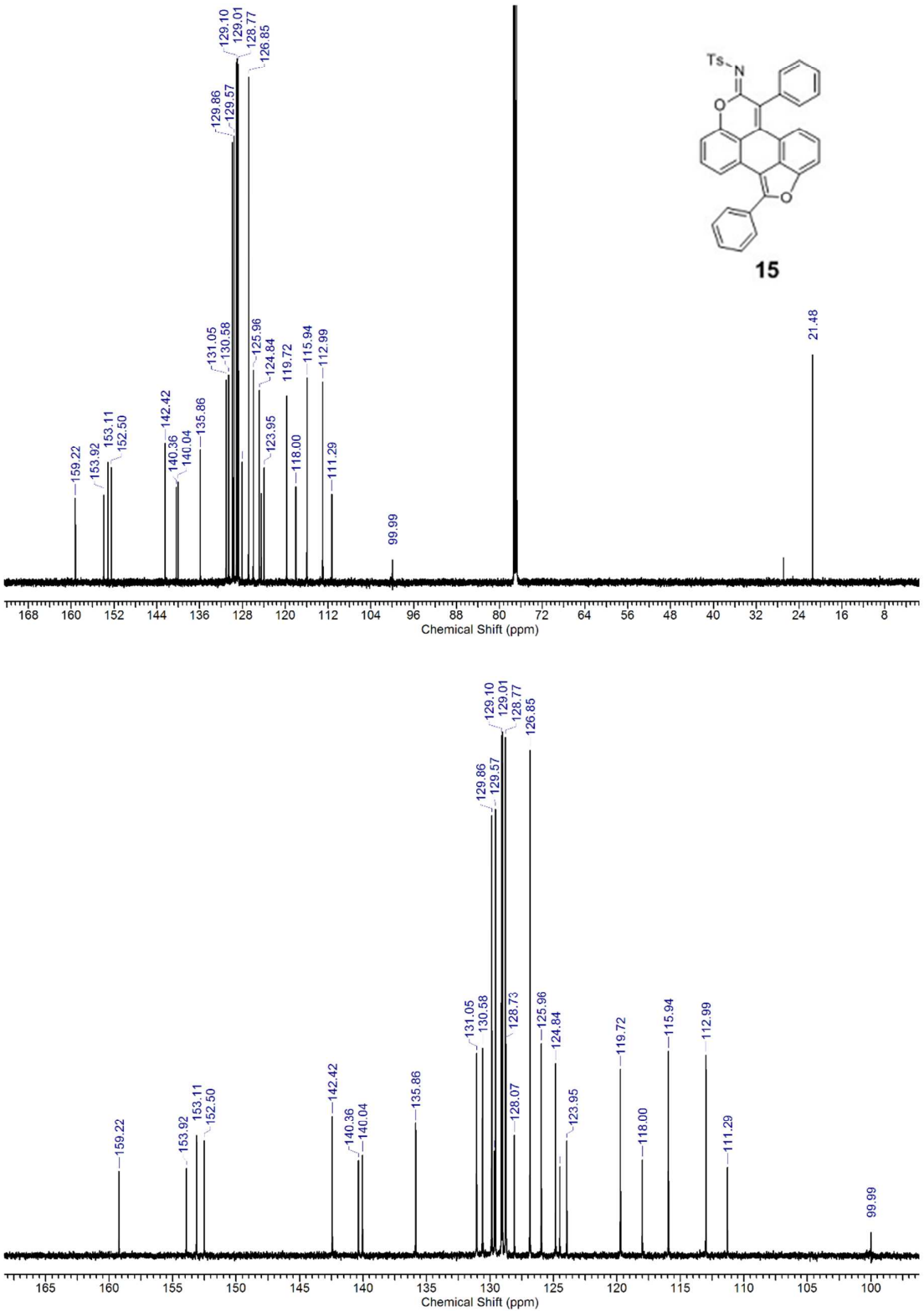
14

^{13}C NMR (125 MHz) spectrum of compound **(14)**. Whole spectrum at the top of the page, zoomed one at the bottom.

(15) *N*-(1,6-diphenyl-7*H*-furo[4',3',2':4,5]naphtho[1,2,3- *de*]chromen-7-ylidene)-4-methylbenzenesulfonamide



^{1}H NMR (500 MHz) spectrum of compound **(15)**. Whole spectrum at the top of the page, zoomed one at the bottom.



^{13}C NMR (125 MHz) spectrum of compound **(15)**. Whole spectrum at the top of the page, zoomed one at the bottom.

Cartesian coordinates for optimized geometries of compounds 6-15.

(6) 1,6-Diphenyl-*7H*-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-imine

Element	x	y	z
C	6.812957	-0.005357	0.544425
C	5.834157	0.682056	1.262003
C	6.441409	-1.003287	-0.356154
C	4.488798	0.381146	1.072733
C	5.097419	-1.306433	-0.549733
C	4.109251	-0.604353	0.152933
C	0.490169	-1.173170	-0.230786
C	-0.888036	-0.968437	-0.308638
C	1.086596	-2.423554	-0.317332
C	-1.647246	-2.123776	-0.550368
C	0.345717	-3.575182	-0.526991
C	-1.032713	-3.382656	-0.653192
C	1.148457	1.198584	-0.172066
C	-0.248901	1.470876	-0.201319
C	1.533496	-0.207996	-0.093198
C	-1.317439	0.443934	-0.165881
C	2.066943	2.244581	-0.282985
C	1.633935	3.563558	-0.379251
C	-0.637013	2.814147	-0.264879
C	0.277869	3.858454	-0.355653
C	-2.609952	0.852515	-0.012500
O	-1.949047	3.182058	-0.258835
C	-2.960734	2.279277	-0.035357
C	2.696102	-0.934995	-0.043376
O	2.436336	-2.281876	-0.190828
N	-4.153831	2.693005	0.100789
C	-3.748810	-0.073682	0.221994
C	-4.762561	-0.228344	-0.726904
C	-3.803573	-0.808382	1.409180
C	-5.792449	-1.139985	-0.510034
C	-4.838689	-1.712924	1.631501
C	-5.830084	-1.888285	0.666843
H	7.862694	0.228966	0.694784
H	6.119645	1.444834	1.980622
H	7.201495	-1.546536	-0.909773
H	3.725517	0.893146	1.653017
H	4.801847	-2.084011	-1.247906
H	-2.721818	-2.074880	-0.668386
H	0.801633	-4.556247	-0.603079
H	-1.664802	-4.245728	-0.838686
H	-4.737246	0.366288	-1.635565
H	-3.019258	-0.679630	2.150924
H	-6.569836	-1.263272	-1.258502
H	-4.868828	-2.283147	2.555494
H	-6.634145	-2.599040	0.834846
H	-4.180734	3.712620	0.033392
H	2.359939	4.365622	-0.470898
H	-0.095822	4.875284	-0.413005
H	3.127778	2.023246	-0.315573

(7) 1,6-Di-p-tolyl-*7H*-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-imine

Element	x	y	z
C	-0.456400	-3.933303	0.328379
C	-1.796201	-3.568005	0.349981
C	-2.157203	-2.226705	0.278189
C	-1.186704	-1.220803	0.198394
C	0.201197	-1.569801	0.220992
C	0.514299	-2.937901	0.260584
C	-1.500506	0.201197	0.149702
C	-0.406707	1.105798	0.293507
C	0.961893	0.824299	0.358105
C	1.322995	-0.602999	0.209096
C	-0.931009	2.390397	0.396714
C	-0.128410	3.497897	0.604120
C	1.243390	3.232398	0.707618
C	1.784492	1.943299	0.589911
C	2.603496	-1.083297	0.066193
C	2.869898	-2.521896	0.056985
O	1.804099	-3.378499	0.249581
C	-2.633407	0.991196	0.115307
O	-2.291109	2.328195	0.280715
C	3.812695	-0.233194	-0.131803
N	4.038399	-3.012794	-0.088118
C	-4.063207	0.760895	-0.074794
C	-4.536506	-0.181701	-0.998799
C	-5.903706	-0.369302	-1.186899
C	-6.845907	0.375993	-0.470195
C	-6.368308	1.330089	0.439811
C	-5.006808	1.525790	0.634111
C	4.019893	0.421313	-1.349099
C	5.152192	1.209216	-1.551895
C	6.113693	1.366412	-0.548695
C	5.904894	0.699905	0.666502
C	4.780795	-0.094598	0.869698
C	7.352791	2.199315	-0.771990
C	-8.327407	0.171392	-0.668095
H	4.004600	-4.033394	-0.049724
H	6.639994	0.797501	1.464402
H	4.650796	-0.615004	1.815495
H	3.285293	0.317517	-2.144899
H	5.289891	1.707822	-2.510092
H	8.238492	1.564317	-0.913394
H	7.559591	2.853010	0.084813
H	7.256590	2.831420	-1.661987
H	-0.139899	-4.971803	0.366873
H	-2.565200	-4.333906	0.418477
H	-3.205903	-1.953506	0.303591
H	2.855392	1.833200	0.688010
H	1.924289	4.061498	0.884722
H	-0.530512	4.503296	0.690826
H	-4.662009	2.272686	1.343915
H	-7.077708	1.930885	1.007314
H	-6.243105	-1.101498	-1.917603
H	-3.830106	-0.751096	-1.597002
H	-8.530006	-0.561104	-1.456899

H	-8.806906	-0.188514	0.252203
H	-8.827608	1.108893	-0.944390

(8) 1,6-Bis(4-methoxyphenyl)-*7H*-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-imine

Element	x	y	z
C	0.122510	-1.634099	-0.277450
C	-1.233234	-1.201943	-0.306483
C	0.359945	-3.013050	-0.330423
C	-2.259871	-2.134450	-0.458537
C	-0.667959	-3.942535	-0.463810
C	-1.976064	-3.493898	-0.542043
C	1.047301	0.711781	-0.357318
C	-0.299289	1.075300	-0.332656
C	1.300797	-0.741258	-0.207513
C	-1.453221	0.239814	-0.240374
C	1.946076	1.772117	-0.550719
C	1.488948	3.092873	-0.665104
C	-0.740145	2.387499	-0.432711
C	0.139065	3.443775	-0.598190
C	-2.521921	1.099627	-0.227169
O	-2.099432	2.406725	-0.357134
C	2.527620	-1.304100	-0.021154
O	1.608479	-3.537865	-0.269065
C	2.709896	-2.769616	0.001778
N	3.777007	-3.423221	0.208046
C	3.765439	-0.517528	0.212033
C	4.782285	-0.465773	-0.739640
C	3.935018	0.190479	1.410145
C	5.931057	0.297932	-0.532543
C	5.069690	0.948967	1.632405
C	6.073782	1.013575	0.657448
C	-3.965412	0.944058	-0.071784
C	-4.848819	1.797511	-0.752490
C	-4.494652	-0.012036	0.796340
C	-6.214705	1.669325	-0.592761
C	-5.869327	-0.152993	0.962887
C	-6.735880	0.687880	0.261169
O	7.142924	1.789864	0.962969
O	-8.087025	0.637821	0.343559
C	-8.657027	-0.329097	1.199162
C	8.187461	1.865239	0.017466
H	-3.284665	-1.790397	-0.535225
H	-0.408304	-4.993983	-0.507738
H	-2.784429	-4.207530	-0.665343
H	3.011027	1.599392	-0.624957
H	2.224320	3.877512	-0.809843
H	-0.196622	4.471031	-0.680149
H	4.543517	-2.777707	0.394839
H	4.670772	-1.018869	-1.668655
H	3.151788	0.152734	2.161906
H	6.696322	0.324596	-1.299318
H	5.210251	1.504249	2.553646
H	-4.447217	2.559590	-1.412572
H	-3.821106	-0.645790	1.366285
H	-6.910032	2.314574	-1.118879

H	-6.247191	-0.901937	1.648396
H	-8.378142	-1.344178	0.893124
H	-8.353625	-0.167784	2.240124
H	-9.736257	-0.208083	1.113741
H	8.629259	0.879034	-0.166992
H	7.836090	2.287442	-0.931450
H	8.939434	2.524044	0.450321

(9) 1,6-Bis(3,4-dimethoxyphenyl)-*7H*-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-imine

Element	x	y	z
C	6.775182	-0.073989	0.268425
C	5.883764	0.760258	0.949917
C	6.262253	-1.143586	-0.504873
C	4.507172	0.557778	0.850827
C	4.891330	-1.331396	-0.598215
C	3.986425	-0.475052	0.059847
C	0.316515	-0.851051	-0.073928
C	-1.057416	-0.580660	-0.072872
C	0.842097	-2.139768	-0.120035
C	-1.885237	-1.717242	-0.167732
C	0.035378	-3.263339	-0.196952
C	-1.342555	-3.010279	-0.228140
C	1.081644	1.481444	-0.178229
C	-0.308618	1.822124	-0.131485
C	1.410266	0.065808	-0.058004
C	-1.419182	0.852989	0.003350
C	2.036134	2.484674	-0.390492
C	1.656183	3.817842	-0.524226
C	-0.640921	3.184720	-0.238310
C	0.317917	4.178586	-0.435892
C	-2.693317	1.341759	0.176836
O	-1.924492	3.626148	-0.169042
C	-2.974936	2.787068	0.140523
C	2.550275	-0.717729	-0.036783
O	2.208116	-2.066860	-0.090322
N	-4.084360	3.388409	0.326951
C	-3.892505	0.493612	0.449249
C	-4.854428	0.285944	-0.556463
C	-4.099476	-0.063641	1.713763
C	-5.992007	-0.488303	-0.315058
C	-5.228452	-0.848919	1.955000
C	-6.172930	-1.077976	0.958701
O	8.130023	0.059174	0.283452
H	6.253891	1.568809	1.568590
O	7.090258	-1.959434	-1.233996
H	3.837113	1.197315	1.414156
H	4.530397	-2.152025	-1.207203
H	-2.959493	-1.617777	-0.203719
H	0.439307	-4.268517	-0.238354
H	-2.025471	-3.851273	-0.299933
H	3.081103	2.215070	-0.470870
H	2.410609	4.579959	-0.694153
H	-0.013127	5.207564	-0.517926
H	-4.699071	0.739921	-1.527646
H	-3.372500	0.102152	2.501839

O	-6.977716	-0.718464	-1.230038
H	-5.405034	-1.293324	2.929187
O	-7.295571	-1.801707	1.269996
C	7.926680	-2.840682	-0.477804
C	8.693454	1.137217	1.018809
C	-6.872374	-0.096063	-2.503682
C	-7.465962	-3.039874	0.573979
H	-8.365024	-3.497805	0.990679
H	-6.610026	-3.705153	0.746746
H	-7.597769	-2.883888	-0.499885
H	-7.769067	-0.386277	-3.052419
H	-5.985909	-0.440614	-3.050707
H	-6.839002	0.996416	-2.415010
H	8.471326	-3.440442	-1.209357
H	7.323541	-3.503627	0.155429
H	8.637215	-2.287325	0.142700
H	9.771833	1.067366	0.871982
H	8.467802	1.058117	2.089503
H	8.338992	2.105744	0.645697
H	-4.810166	2.706244	0.541293

(10) *N*-(1,6-diphenyl-*7H*-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-ylidene)-1,1,1-trifluoromethanesulfonamide

Element	x	y	z
C	8.111205	1.689878	0.642896
C	6.927906	2.214682	1.166195
C	8.085303	0.475377	-0.046502
C	5.723105	1.537283	0.993797
C	6.884602	-0.206221	-0.223100
C	5.683602	0.324782	0.282499
C	2.391299	-1.314713	-0.073997
C	1.012199	-1.541711	-0.202297
C	3.326397	-2.337914	0.060704
C	0.642096	-2.904310	-0.224294
C	2.967895	-3.674614	0.053907
C	1.598094	-3.923712	-0.100992
C	2.329804	1.116987	-0.364002
C	0.905203	0.952189	-0.429901
C	3.102701	-0.079614	-0.074000
C	0.178801	-0.320409	-0.292699
C	2.894706	2.367585	-0.635104
C	2.096608	3.469386	-0.941306
C	0.148205	2.103190	-0.702203
C	0.714607	3.349589	-0.966206
C	-1.212999	-0.299707	-0.265099
O	-1.210095	2.070893	-0.717503
C	-1.929597	0.958295	-0.384101
C	4.433701	-0.413416	0.113301
O	4.575799	-1.791116	0.180503
N	-3.185597	1.265697	-0.282601
C	-2.036702	-1.542705	-0.165796
C	-2.519003	-2.151306	-1.333395
C	-2.303602	-2.135002	1.075605
C	-3.236905	-3.343505	-1.262292
C	-3.024205	-3.326301	1.144908
C	-3.486006	-3.935202	-0.022791

H	9.049206	2.219377	0.779195
H	6.944308	3.146383	1.723494
H	9.003402	0.058475	-0.449201
H	4.813506	1.930786	1.434496
H	6.864200	-1.150022	-0.756899
H	-0.386304	-3.200208	-0.346393
H	3.693894	-4.473415	0.153608
H	1.253493	-4.952511	-0.124990
H	3.971506	2.476084	-0.625405
H	2.559609	4.427785	-1.153808
H	0.059509	4.186790	-1.176707
H	-2.325702	-1.689909	-2.297096
H	-1.952801	-1.656801	1.983504
H	-3.608106	-3.804306	-2.172492
H	-3.231505	-3.773099	2.112309
H	-4.049808	-4.861601	0.033611
S	-4.473098	0.458900	0.320701
O	-4.284598	0.079503	1.724702
O	-5.082400	-0.468900	-0.633297
C	-5.615995	1.932903	0.360398
F	-5.140593	2.884303	1.166596
F	-6.798296	1.517406	0.829299
F	-5.787495	2.436101	-0.863703

(11) *N*-(1,6-di-p-tolyl-*7H*-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-ylidene)-1,1,1-trifluoromethanesulfonamide

Element	x	y	z
C	8.168108	0.598102	0.535498
C	7.077408	1.315702	1.041798
C	7.906608	-0.604397	-0.140203
C	5.771708	0.861303	0.874198
C	6.609008	-1.067597	-0.314203
C	5.514408	-0.331697	0.179097
C	1.985507	-1.369495	-0.151404
C	0.586507	-1.350595	-0.265805
C	2.730407	-2.542296	-0.053205
C	-0.013393	-2.627995	-0.332606
C	2.145806	-3.795596	-0.096806
C	0.752906	-3.799695	-0.251606
C	2.345208	1.034005	-0.433703
C	0.911608	1.119705	-0.472303
C	2.900708	-0.277596	-0.146904
C	-0.021392	-0.001094	-0.305304
C	3.111709	2.163305	-0.736902
C	2.510009	3.380505	-1.058902
C	0.359809	2.379506	-0.758303
C	1.128509	3.502506	-1.064502
C	-1.389292	0.269806	-0.213204
O	-0.981291	2.583106	-0.733903
C	-1.874292	1.628106	-0.334604
C	4.156807	-0.840696	0.015896
O	4.057107	-2.222896	0.060396
N	-3.064492	2.149507	-0.240204

C	-2.403893	-0.821394	-0.095905
C	-3.055493	-1.286393	-1.246006
C	-2.651294	-1.465794	1.123595
C	-3.909793	-2.386793	-1.181606
C	-3.506594	-2.561894	1.180494
C	-4.147094	-3.045393	0.030793
C	9.583108	1.090502	0.711499
H	7.252408	2.237602	1.589599
H	8.735608	-1.184898	-0.536903
H	4.949508	1.418503	1.310298
H	6.429607	-2.000297	-0.837704
H	-1.077094	-2.738294	-0.460106
H	2.723006	-4.710596	-0.028706
H	0.236806	-4.752595	-0.309007
H	4.191309	2.085204	-0.743102
H	3.128710	4.239905	-1.297401
H	0.624509	4.436706	-1.282601
H	-2.875893	-0.798292	-2.199405
H	-2.169994	-1.104995	2.025095
H	-4.398893	-2.736592	-2.087007
H	-3.684794	-3.048195	2.135993
C	-5.100894	-4.213093	0.108592
S	-4.238992	1.926307	0.864896
O	-4.863592	3.223207	1.107997
O	-3.824593	1.097206	2.002996
C	-5.572893	0.960508	-0.075505
F	-6.744292	1.577808	0.077495
F	-5.674393	-0.277793	0.412994
F	-5.286692	0.895308	-1.382205
H	-5.169194	-4.741092	-0.847108
H	-6.111094	-3.873193	0.367492
H	-4.794695	-4.931394	0.875092
H	9.616309	2.018101	1.288499
H	10.059409	1.281102	-0.257101
H	10.199908	0.348601	1.230899

(12) *N*-(1,6-bis(4-methoxyphenyl)-*7H*-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-ylidene)-1,1,1-trifluoromethanesulfonamide

Element	x	y	z
C	-8.039005	0.532508	-0.257702
C	-6.979804	1.087109	-0.985600
C	-7.790907	-0.539896	0.613094
C	-5.692304	0.577506	-0.828900
C	-6.509208	-1.039998	0.758194
C	-5.426707	-0.480497	0.049497
C	-1.938808	-1.653802	0.300797
C	-0.540508	-1.693504	0.336498
C	-2.737810	-2.789502	0.386692
C	0.012790	-2.978906	0.508994
C	-2.203512	-4.054503	0.542088
C	-0.803712	-4.113005	0.608790

C	-2.171105	0.786198	0.286005
C	-0.736105	0.804796	0.283606
C	-2.800407	-0.522701	0.212799
C	0.130494	-0.384305	0.228703
C	-2.873104	1.989499	0.408108
C	-2.208102	3.209798	0.499713
C	-0.120303	2.063995	0.347411
C	-0.821902	3.259096	0.456614
C	1.497694	-0.204406	0.092405
O	1.239197	2.188394	0.317613
C	2.054896	1.128793	0.136410
C	-4.086407	-1.035199	0.192096
O	-4.051209	-2.416400	0.313492
N	3.332596	1.334992	0.028312
C	2.483193	-1.297507	-0.143998
C	3.398392	-1.682211	0.836502
C	2.540594	-1.937403	-1.391300
C	4.330991	-2.694512	0.604600
C	3.466293	-2.939703	-1.640402
C	4.368891	-3.329108	-0.641202
O	-9.327505	0.950910	-0.330202
H	-7.145102	1.899511	-1.685097
H	-8.624109	-0.963996	1.167192
H	-4.887203	0.994007	-1.428398
H	-6.331510	-1.872000	1.433991
H	1.082890	-3.116307	0.574995
H	-2.821813	-4.944503	0.616485
H	-0.326913	-5.080906	0.741187
H	-3.956204	1.969700	0.451507
H	-2.778001	4.129998	0.601515
H	-0.268001	4.191595	0.509018
H	3.391891	-1.184714	1.803404
H	1.849195	-1.643099	-2.178000
H	5.024489	-2.964615	1.393900
H	3.514893	-3.430400	-2.609004
O	5.238490	-4.320308	-0.978505
S	3.975498	2.836191	0.103418
O	3.929798	3.392786	1.438620
O	3.641201	3.649895	-1.045580
C	5.750498	2.306589	-0.157182
F	6.512500	3.405288	-0.128878
F	5.908199	1.704093	-1.336884
F	6.154996	1.479285	0.810216
C	6.205289	-4.728812	-0.022805
C	-9.648702	2.030513	-1.196799
H	-10.722702	2.191614	-1.084200
H	-9.424601	1.781116	-2.242400
H	-9.110301	2.943711	-0.910296
H	6.793688	-5.509612	-0.509807
H	6.864490	-3.896514	0.257998
H	5.728187	-5.140315	0.877193

(13) *N*-(1,6-bis(3,4-dimethoxyphenyl)-*7H*-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-ylidene)-1,1,1-trifluoromethanesulfonamide

Element	x	y	z
C	7.878900	0.734598	0.338603
C	6.823600	1.407699	0.962904
C	7.605299	-0.444801	-0.397897
C	5.515300	0.941100	0.840803
C	6.299599	-0.897200	-0.512298
C	5.227999	-0.204100	0.085702
C	1.699998	-1.274597	-0.113999
C	0.298298	-1.270996	-0.161599
C	2.461397	-2.440698	-0.091000
C	-0.292803	-2.552395	-0.228200
C	1.888496	-3.698797	-0.142500
C	0.488496	-3.716096	-0.221401
C	2.017400	1.145603	-0.312198
C	0.582200	1.209804	-0.324198
C	2.601099	-0.170598	-0.114298
C	-0.329901	0.068105	-0.170999
C	2.760701	2.308903	-0.540097
C	2.134802	3.537503	-0.747696
C	0.005801	2.476705	-0.505597
C	0.750802	3.635504	-0.719396
C	-1.699601	0.303106	-0.051299
O	-1.341899	2.648106	-0.496397
C	-2.226000	1.646206	-0.208198
C	3.870099	-0.722699	-0.030998
O	3.788797	-2.107499	-0.032099
N	-3.425200	2.140907	-0.155398
C	-2.657602	-0.785994	0.297701
C	-3.504402	-1.339193	-0.674000
C	-2.685303	-1.288995	1.601800
C	-4.378903	-2.381092	-0.352201
C	-3.527804	-2.351994	1.916900
C	-4.365904	-2.915693	0.957099
O	9.179500	1.127997	0.376304
H	7.013701	2.295398	1.553804
O	8.593699	-1.112502	-1.072798
H	4.718700	1.459800	1.362203
H	6.121398	-1.795600	-1.091599
H	-1.362803	-2.666495	-0.296900
H	2.478095	-4.608398	-0.131901
H	-0.018905	-4.673896	-0.276101
H	3.840701	2.249002	-0.572197
H	2.734703	4.423903	-0.928396
H	0.228303	4.574505	-0.859796
H	-3.498802	-0.929892	-1.675600
H	-2.044402	-0.858095	2.363501
O	-5.269204	-2.929791	-1.224601
H	-3.566504	-2.759795	2.921499

O	-5.215905	-3.914993	1.351598
S	-4.910500	1.536208	0.120501
O	-5.077801	0.903408	1.429201
O	-5.483501	0.924009	-1.085699
C	-5.764599	3.188509	0.263102
F	-5.267499	3.890608	1.284103
F	-7.063399	2.958110	0.485902
F	-5.636698	3.894210	-0.861997
C	9.572898	-1.776203	-0.265598
C	9.506201	2.322897	1.075705
C	-5.485503	-2.266390	-2.469701
C	-5.102006	-5.168692	0.674298
H	-5.788206	-5.847492	1.184497
H	-4.080606	-5.564193	0.755098
H	-5.379505	-5.086792	-0.379202
H	-6.326103	-2.782589	-2.935502
H	-4.608903	-2.349690	-3.125401
H	-5.732402	-1.212290	-2.313500
H	10.237698	-2.289603	-0.962398
H	9.099097	-2.515103	0.392702
H	10.148699	-1.065704	0.333603
H	10.581501	2.454796	0.953505
H	9.269401	2.242796	2.143705
H	8.984102	3.189397	0.652505

(14) *N*-(1,6-diphenyl-*7H*-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-ylidene)-4-methylbenzamide

Element	x	y	z
C	-8.188304	2.310882	-0.018110
C	-7.078304	2.594283	-0.816109
C	-8.153703	1.219482	0.852891
C	-5.936703	1.799585	-0.738908
C	-7.015301	0.422784	0.935893
C	-5.884001	0.712086	0.150893
C	-2.772097	-1.278008	0.213597
C	-1.426496	-1.662705	0.145098
C	-3.817896	-2.182010	0.379397
C	-1.199094	-3.047005	0.284900
C	-3.603593	-3.544509	0.509798
C	-2.262392	-3.946007	0.462900
C	-2.400502	1.147593	0.105396
C	-1.010701	0.813796	-0.009903
C	-3.335800	0.030891	0.145296
C	-0.461698	-0.558004	-0.049502
C	-2.784405	2.489192	0.218094
C	-1.841406	3.514494	0.179394
C	-0.104303	1.886397	-0.071903
C	-0.494106	3.221297	0.018995
C	0.894102	-0.715401	-0.257001
O	1.235298	1.686100	-0.223702
C	1.772900	0.440201	-0.384701

C	-4.704999	-0.150012	0.225995
O	-5.003197	-1.498412	0.387996
N	3.036301	0.316903	-0.580100
C	1.591105	-2.029500	-0.404199
C	2.267906	-2.607598	0.678802
C	1.601607	-2.687101	-1.640799
C	2.922808	-3.830297	0.532603
C	2.259910	-3.908300	-1.787697
C	2.918410	-4.485198	-0.700996
H	-9.077406	2.930880	-0.080711
H	-7.105805	3.427083	-1.512410
H	-9.016203	0.989081	1.471091
H	-5.091703	2.001387	-1.388107
H	-6.989300	-0.425815	1.610693
H	-0.198193	-3.448303	0.262901
H	-4.414592	-4.251511	0.641998
H	-2.029590	-5.001206	0.565601
H	-3.830505	2.732390	0.351193
H	-2.162909	4.547394	0.268893
H	0.268393	3.989398	-0.038205
H	2.272704	-2.098297	1.638002
H	1.090707	-2.238402	-2.487299
H	3.438408	-4.270395	1.381304
H	2.259812	-4.407101	-2.752497
H	3.430312	-5.436197	-0.814995
C	3.877899	1.384904	-0.908700
C	5.225999	1.329008	-0.262199
O	3.587998	2.256503	-1.719701
C	6.120097	2.386209	-0.487499
C	7.376797	2.383312	0.104302
C	7.782798	1.325514	0.934503
C	5.621800	0.269609	0.562602
C	6.885800	0.272612	1.151303
C	9.155598	1.327017	1.563304
H	5.802596	3.198908	-1.132200
H	8.058795	3.211013	-0.076798
H	4.937802	-0.555892	0.726002
H	7.183201	-0.557787	1.787004
H	9.941298	1.262218	0.801205
H	9.334195	2.248918	2.128203
H	9.284699	0.483417	2.246705

(15) *N*-(1,6-diphenyl-*7H*-furo[4',3',2':4,5]naphtho[1,2,3-*de*]chromen-7-ylidene)-4-methylbenzenesulfonamide

Element	x	y	z
C	-8.607603	1.885207	-0.528396
C	-7.445003	2.255807	-1.206795
C	-8.592104	0.771807	0.314904
C	-6.270503	1.526006	-1.037195
C	-7.421304	0.039506	0.489704
C	-6.239204	0.417106	-0.173395

C	-3.033504	-1.387695	0.160905
C	-1.667304	-1.690595	0.229705
C	-4.033004	-2.355895	0.203504
C	-1.370104	-3.059896	0.385305
C	-3.749505	-3.704795	0.340904
C	-2.388605	-4.023995	0.438204
C	-2.802503	1.056505	0.156005
C	-1.390303	0.806305	0.188606
C	-3.666304	-0.112995	0.062205
C	-0.757504	-0.527395	0.157306
C	-3.274203	2.370005	0.263906
C	-2.395703	3.447405	0.365306
C	-0.552103	1.930405	0.264006
C	-1.023303	3.237505	0.352606
C	0.620496	-0.603096	0.076106
O	0.807997	1.804404	0.265206
C	1.428297	0.604904	0.123306
C	-5.023204	-0.376794	-0.001695
O	-5.252704	-1.743894	0.100804
N	2.720897	0.552904	0.054006
C	1.396496	-1.867796	-0.097794
C	2.106196	-2.432597	0.970606
C	1.443596	-2.491996	-1.351495
C	2.824996	-3.614297	0.794306
C	2.168996	-3.669996	-1.528795
C	2.856396	-4.237397	-0.454995
H	-9.522203	2.454807	-0.662696
H	-7.455203	3.106207	-1.881795
H	-9.494904	0.474007	0.839704
H	-5.380503	1.795306	-1.595695
H	-7.409304	-0.825794	1.143304
H	-0.349404	-3.397296	0.475705
H	-4.524605	-4.461695	0.378404
H	-2.104005	-5.064396	0.558904
H	-4.341103	2.549806	0.283805
H	-2.786703	4.456305	0.450906
H	-0.305102	4.046805	0.413607
H	2.091396	-1.943397	1.939506
H	0.906697	-2.051795	-2.186495
H	3.366195	-4.044797	1.631806
H	2.197496	-4.142796	-2.506195
H	3.419796	-5.155797	-0.591795
S	3.618497	1.983304	0.130807
O	3.495597	2.588103	1.465707
O	3.377998	2.794804	-1.071993
C	5.267297	1.290903	-0.001093
C	5.975297	0.981803	1.158907
C	5.831998	1.095403	-1.260993
C	7.261497	0.457002	1.049007
C	7.852197	0.242503	-0.203793
C	7.118298	0.569003	-1.352993
C	9.258897	-0.295298	-0.313692
H	9.390597	-0.888698	-1.223293
H	9.515597	-0.924298	0.543608

H	9.990698	0.521302	-0.349492
H	7.562198	0.412903	-2.332793
H	7.817497	0.213602	1.950708
H	5.522597	1.161703	2.127707
H	5.270498	1.362104	-2.149393