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Supporting Information

Chiral Phosphoric Acid Catalyzed Asymmetric Hydrolysis of Biaryl Oxazepines for the Synthesis of Axially Chiral Biaryl Amino Phenol Derivatives

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Supporting Information

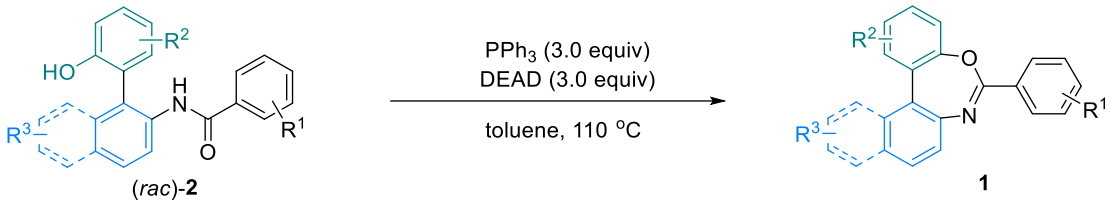
Contents

General methods

All reactions and manipulations involving air-sensitive compounds were carried out using standard Schlenk techniques. Anhydrous toluene and cyclohexane were distilled from CaH_2 under an atmosphere of nitrogen. All reactions were monitored by TLC. TLC analysis was performed by illumination with a UV lamp (254 nm). All flash chromatography was packed with silica-gel as the stationary phase. ^{1}H NMR spectra were recorded on a Bruker AVIII-500 (500 MHz) instrument, and chemical shifts were reported in ppm downfield from internal TMS with the solvent resonance as the internal standard ($CDCl_3$, $\delta = 7.26$ ppm; DMSO, $\delta = 2.49$ ppm). ^{13}C NMR spectra were recorded on a Bruker (126 MHz) instrument, and chemical shifts were reported in ppm downfield from TMS with the solvent resonance as the internal standard ($CDCl_3$, $\delta = 77.00$ ppm; DMSO, $\delta = 39.50$ ppm). ^{19}F NMR spectra were recorded on a Bruker (471 MHz) instrument. Optical rotations were measured on a WZZ-2B polarimeter. High resolution mass spectra (HRMS) (EI+) were recorded on an a Finnigan MAT 95 XP mass spectrometer. The racemic biaryl amides were synthesized according to the literature procedures.[1-3]

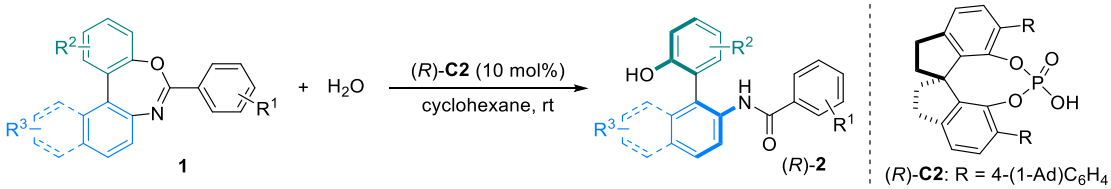
General procedures

General procedure for the Mitsunobu reaction.



To a dried 4 mL tube with a stir bar was added the PPh_3 (0.9 mmol), anhydrous toluene (3.0 mL). And the reaction mixture was stirred at room temperature to form a homogeneous phase. Then DEAD (0.9 mmol) was add and stirred for 2-3 minutes and (*rac*)-**2** (0.3 mmol) was added into the homogeneous mixture. The test tube was sealed and stirred at 110 ℃ for 12 h. Then the reaction mixture was directly purified by column chromatography (PE/DCM/Et_3N = 80:1:1) to afford the desired products **1**.

General procedure for the CPA-catalyzed asymmetric reaction

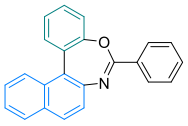


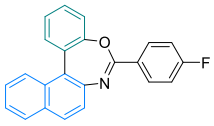
To a dried 4 mL tube with a stir bar was added the (*R*)-**C2** (10 mol%), anhydrous cyclohexane (2 ml) and H_2O (5 μl). Then the reaction mixture was stirred at RT for 2 minutes and **1** (0.1 mmol) was added to the reaction mixture. The test tube was sealed and stirred at room temperature for 1-7 days until the starting material disappeared as indicated by TLC. Then the reaction mixture was carefully filtered, and the solid was washed with petroleum ether 2-3 times to obtain the products (*R*)-**2**.

Procedure for kinetic resolution of racemic biaryl oxazepine **1ai**: To a dried 10 mL tube with a stir bar was added the racemic compound **1ai** (0.1 mmol) and anhydrous toluene (2 ml). The mixture was stirred at RT to form a homogeneous solution. Then this solution was cooled to -10 ℃, H_2O (10 μl) and (*R*)-**C2** (10 mol%) was added. After stirring at -10 ℃ for 2 h, the reaction mixture was directly purified by column chromatography to afford the desired chiral products **1ai** and **2ai**.

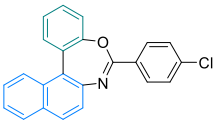
Scope of the Mitsunobu reaction

variation of R^1 group

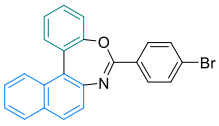

1a, 88%



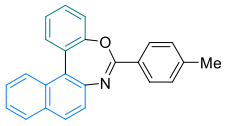
1b, 96%



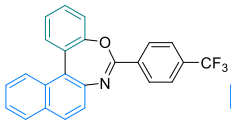
1c, 97%



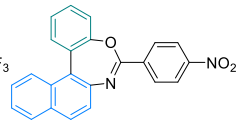
1d, 75%



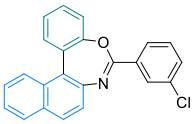
1e, 70%



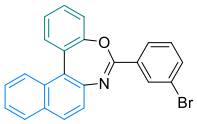
1f, 78%



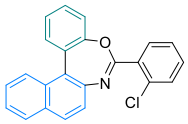
1g, 71%



1h, 81%

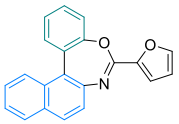


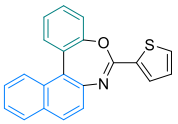
1i, 91%

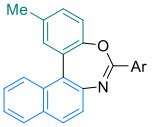


1j, 93%

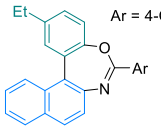
variation of R^2 group


1k, 69%

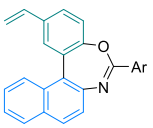

1l, 69%



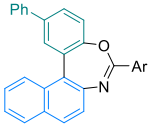
1m, 94%



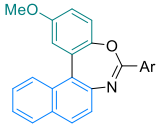
Ar = 4-ClC$_6$H$_4$
1n, 89%



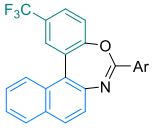
1o, 54%



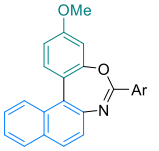
1p, 85%



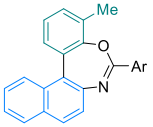
1q, 99%



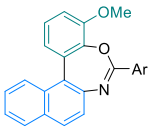
1r, 99%



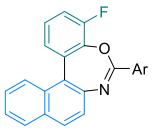
1s, 74%



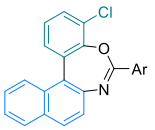
1t, 73%



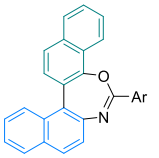
1u, 62%



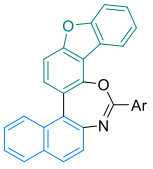
1v, 86%



1w, 86%

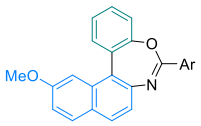


1x, 82%

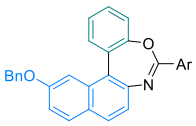


1y, 98%

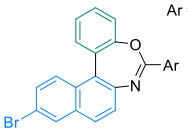
variation of R^3 group



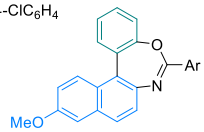
1z, 99%



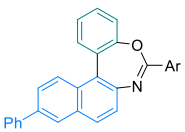
1aa, 93%



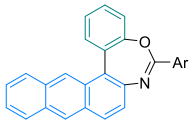
Ar = 4-ClC$_6$H$_4$
1ab, 43%



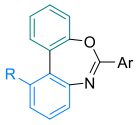
1ac, 80%



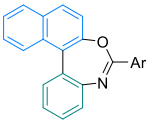
1ad, 50%



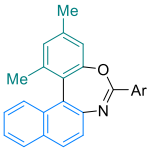
1ae, 79%



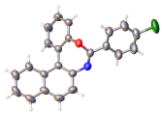
1af, R= Me, 83%
1ag, R= Cl, 84%
Ar = 4-NO$_2$C$_6$H$_4$



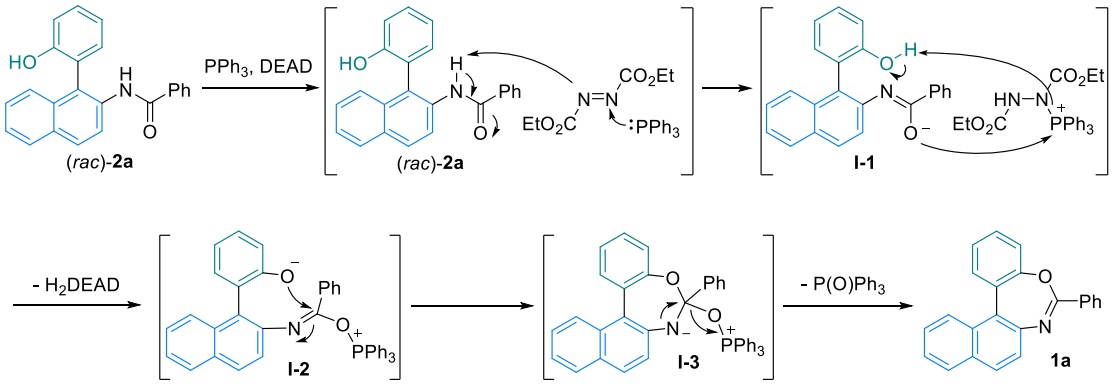
1ah, 90%



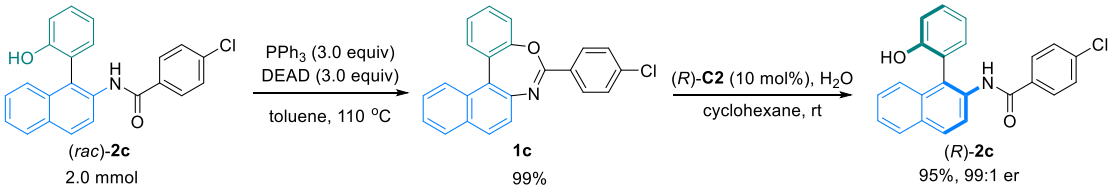
1ai, 60%


crystal structure of **1c**

Proposed mechanism for Mitsunobu reaction:



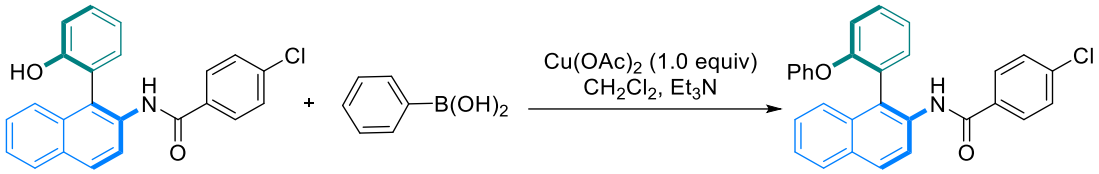
Scale-up synthesis of axially chiral biaryl amide 2c



To a dried 50 mL tube with a stir bar was added the PPh_3 (1.57 g, 6.0 mmol), anhydrous toluene (20.0 mL). It was stirred at room temperature to form a homogeneous phase. Then DEAD (1.04 g, 6.0 mmol) was added and the reaction mixture was stirred at room temperature for 2-3 minutes. To the reaction mixture was added (*rac*)-**2c** (0.74 g, 2 mmol). The test tube was sealed and stirred at 110 ℃ for 12 h. Finally, the reaction mixture was directly subjected to the column chromatography (PE/DCM/Et_3N = 80:1:1) to afford **1c** (0.71 g, 99% yield). To a dried 100 mL tube with a stir bar was added the (*R*)-**C2** (147.0 mg, 10 mol%), anhydrous cyclohexane (40 ml) and H_2O (100 μl). And then it was stirred at room temperature to form a homogeneous phase. Finally, compound **1c** (0.71 g, 2mmol) was added. The test tube was sealed and stirred at room temperature for 3 days. Then the reaction mixture was filtered, and the solid was washed with petroleum ether 2-3 times to afford the product (*R*)-**2c** (0.71 g, 95%, 98:2 er).

Synthetic applications

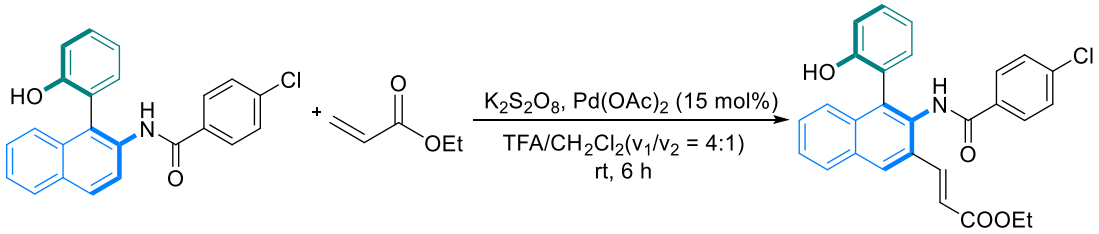
Synthesis of (R)-4-chloro-N-(1-(2-phenoxyphenyl)naphthalen-2-yl)benzamide (3)



(*R*)-**2c** **3**

To a dried 10 mL tube was added compound (*R*)-**2c** (0.1 mmol, 1.0 equiv), $Cu(OAc)_2$ (18 mg, 0.1 mmol), phenylboronic acid (36.5 mg, 0.3 mmol) and activated 4Å molecular sieves (100 mg). Then DCM (2.0 mL) and triethylamine (70 µL, 0.5 mmol) was added to the reaction tube, and the mixture was stirred at room temperature for 12 hours. The reaction mixture was subjected to column chromatography (PE/EA= 5/1) to afford product **3** (38 mg, 84% yield, 98:2 er).

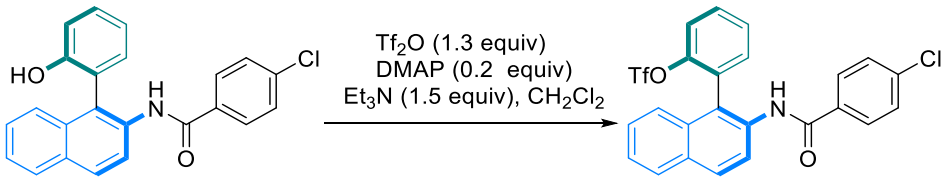
Synthesis of ethyl (R)-3-(3-(4-chlorobenzamido)-4-(2-hydroxyphenyl) naphthalen-2-yl)acrylate (4)



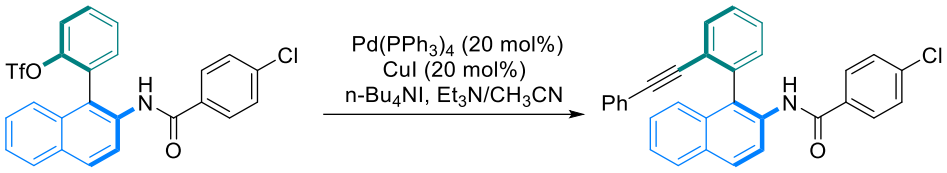
(*R*)-**2c** **4**

To a solution of (*R*)-**2c** (37.4 mg, 0.1 mmol) in TFA and CH_2Cl_2 (v/v = 4:1, 0.5 M) were added ethyl acrylate (44 uL, 4.0 equiv), $Pd(OAc)_2$ (3.4 mg, 15 mol%), and $K_2S_2O_8$ (81 mg, 2.0 equiv). The resulting mixture was stirred at RT for 6 h. After the reaction was completed, the reaction mixture was directly subjected to the column chromatography (DCM/EA = 30:1) to afford the desired products **4** (36 mg, 77%, 99:1 er).

Synthesis of (R)-4-chloro-N-(1-(2-(phenylethynyl)phenyl)naphthalen-2-yl)benzamide (5)



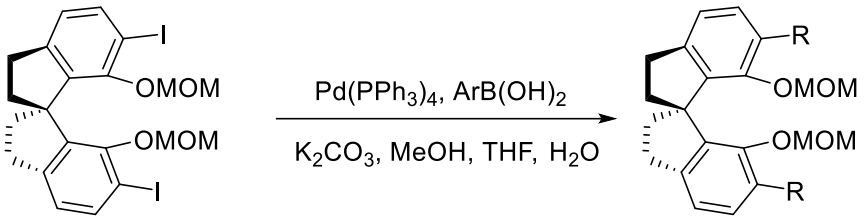
(*R*)-**2c** **5'**



5' **5**

To a solution of (*R*)-**2c** (37.4 mg, 0.1mmol) and DMAP (2.6 mg, 20 mol%) in dry DCM (1.3 mL), Et_3N (22 μL, 1.5 equiv) was added at room temperature under N_2 atmosphere. The reaction mixture was stirred at 0 ℃ for 5 minutes. Tf_2O (22.1 μL, 1.3 equiv) was added dropwise. The resulting reaction mixture was stirred at room temperature for 20 h. Then the mixture solution was concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel using (PE/DCM = 1/1) to give of **5′** (50.5 mg, 99% yield). To a dried 4 mL tube with a stir bar was added the **5′** (50.5 mg, 0.1 mmol), CuI (20 mol%), n-Bu_4NI (98.7 mg, 3.0 equiv), $Pd(PPh_3)_4$ (20 mol%), Et_3N and CH_3CN (v/v=1:4, 0.2 ml) under N_2 atmosphere. Then ethynylbenzene (13.6 mg, 1.5 equiv) was added dropwise. The resulting reaction mixture was stirred at 80 ℃ for 0.5 h and then concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (PE/DCM = 5/1) to give product **5** (23.5 mg, 52% yield, 96:4 er).

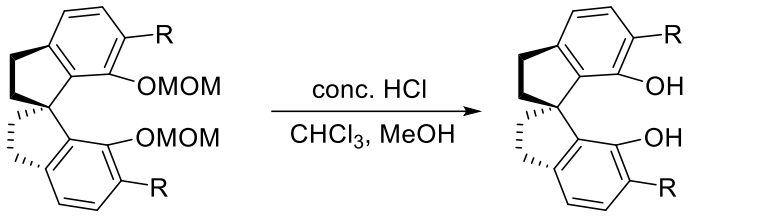
Synthesis of chiral phosphoric acid catalyst [4]



(*R*)-**6** (*R*)-**7**

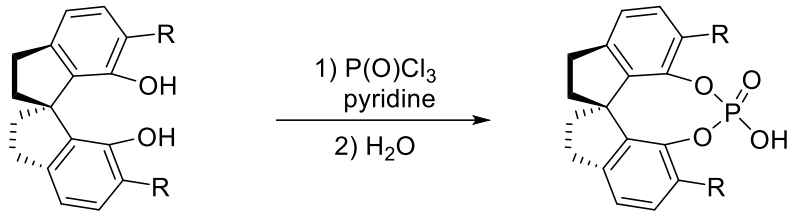
To a solution of (*R*)-**6** (0.8 g, 1.35 mmol), (4-((3r,5r,7r)-adamantan-1-yl)phenyl)boronic acid (1.38 g, 5.4 mmol) and $Pd(PPh_3)_4$ (234 mg, 0.20 mmol) in THF (40 mL) and MeOH (2mL) was added aqueous K_2CO_3 (2 M, 5 mL). The reaction mixture was heated at reflux for 22 h and then the mixture was cooled to ambient temperature, diluted by CH_2Cl_2, washed with brine, dried over Na_2SO_4 and purified by

column chromatography (PE:EA= 15:1) to give (*R*)-**7** (0.66 g, 64% yield) as a white solid.



(*R*)-**7**:R = 4-(1-Ad)C_6H_4 (*R*)-**8**:R = 4-(1-Ad)C_6H_4

To a solution of (*R*)-**7** (650 mg, 0.854 mmol) in 6 mL $CHCl_3$ and 10 mL MeOH, conc. HCl (6.0 mL) was added and the mixture was heated at reflux for 3 h. After cooled to ambient temperature, the mixture was poured into water, extracted by CH_2Cl_2 and the combined organic phase was washed with saturated $NaHCO_3$ and brine, dried over Na_2SO_4. The solvent was removed, and the residue was purified by chromatography (PE:DCM v/v = 2:1) to give (*R*)-**8** (430 mg, 75% yield) as a white solid.

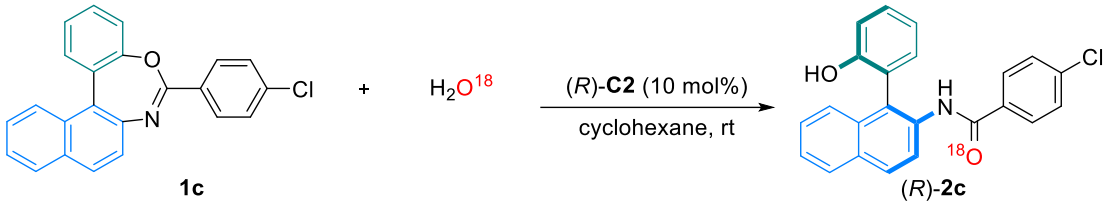


(*R*)-**8**:R = 4-(1-Ad)C_6H_4 (*R*)-**C2**: R = 4-(1-Ad)C_6H_4

To a 50 mL oven-dried Schlenk flask containing (*R*)-**8** (430 mg, 0.63 mmol) was added 2 mL anhydrous pyridine and freshly distilled $P(O)Cl_3$ (193.5 mg, 1.26 mmol) under a nitrogen atmosphere. The mixture was stirred under 90 ℃ for 12 h. After cooling to room temperature, 2 mL of H_2O was added. The mixture was stirred for another 12 h under 90 ℃, then cooled by an ice-bath, followed by slow addition of 16 ml 3N HCl. After stirring for 1 h, the mixture was extracted by CH_2Cl_2 (20 mL ×4). The combined organic layer was concentrated and purified by chromatography on silica gel (first petroleum ether/ethyl acetate = 1:1, then MeOH/CH_2Cl_2 = 1:5) to give white solid. The white solid was dissolved with 45 mL CH_2Cl_2, washed with 3N HCl (25 mL × 3), distilled water (25 mL × 3), and dried under vacuum to give (*R*)-**C2** (410 mg, 87.4% yield).

Mechanism Studies

Detection of the ^{18}O-labeled product via GC-MS



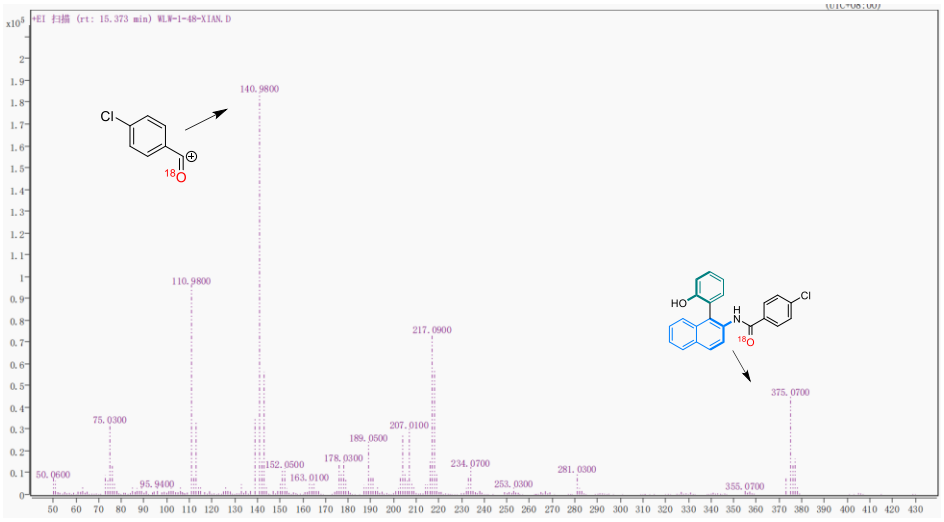


Figure S1. The GC-MS Spectra of ^{18}O-Labeled Product.

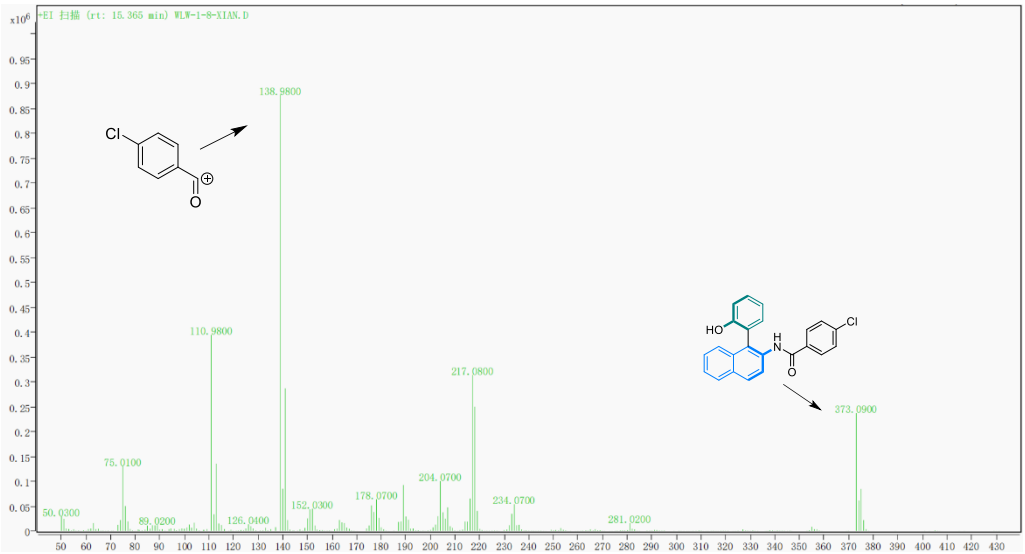


Figure S2. The GC-MS Spectra of Products Unlabeled with ^{18}O

Determination of the rotational barriers

The specified biaryl amino phenol (2 mg) was dissolved in toluene (1.0 mL) and heated at indicated temperature. Aliquots (< 0.1 mL) were diluted with ^{i}PrOH (1.0 mL) and directly analyzed by chiral HPLC to determine the enantiomeric ratio at the specified time. The rotational barrier ($\Delta G^{\neq}$), rate constants for enantiomerization (k_{ent}) and

racemization (k_{rac}), and half-life for racemization ($t_{1/2rac}$) were calculated based on the following equations,

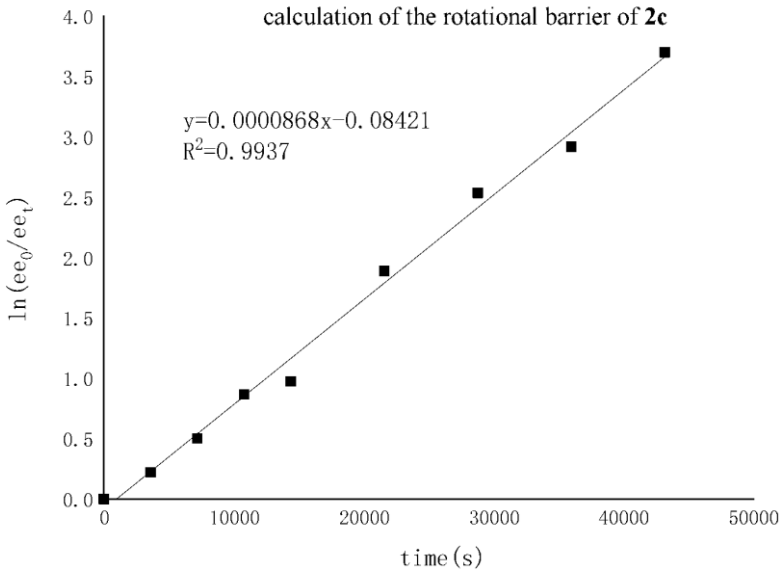
$$t_{1/2rac} = \ln 2/k_{rac}$$

$$\Delta G^{\neq} = -RT\ln(k_{ent}h/k_BT)$$

where the transmission coefficient κ is set as 1, Boltzmann constant k_B = 1.3806503 $\times 10^{-23}$ J/K, Planck constant h = 6.62606876 $\times$ 10^{-34} J·s, idea gas constant R = 8.314472 J/(mol·K).[5]

Table. Change of enantiomer ratio with time for **2c** (120 ℃ in toluene)

t/s	ee(%)	ln (ee_0/ee_t)
0	95.180	0
3600(1 h)	76.266	0.22154
7200(2 h)	57.542	0.50325
10800(3 h)	40.020	0.86639
14400(4 h)	35.906	0.97486
21600(6 h)	14.370	1.89063
28800(8 h)	7.532	2.53661
36000(10 h)	5.138	2.91911
43200(12 h)	2.348	3.70221



$Ln(ee_0/ee_t) = 2k_{ent}t + C$

k_{ent} = 1/2 slope = 0.0000434 s^{-1}

$k_{rac} = 2k_{ent}$ = 0.0000868 s^{-1}

$t_{1/2rac} = \ln 2/k_{rac}$ = 7986 s = 2.22 h

$\Delta G^{\neq} = -RT\ln(k_{ent}h/k_BT)$ = 31.1 kcal/mol

DFT calculations

Conformational sampling

Conformational sampling of the phosphoric acid catalyst was carried out at GFN2-xTB[6–8] level of theory using the CREST program version 2.12 by Grimme and co-workers.[9,10] The conformers and rotamers ensemble was generated using the iterative

metadynamics based on genetic z-matrix crossing algorithm (iMTD-GC). Conformers were further optimized at GFN2-xTB level with very tight (*-opt vtight*) optimization. Due to the large size of the phosphoric acid catalyst, the lowest energy conformer was chosen and further optimized at density functional theory (DFT) level and used for the mechanistic studies.

Density functional theory (DFT) calculations

DFT calculations were carried out using the *Gaussian 16* rev. B.01 program.[11] The global hybrid functional M06-2X[12] with Karlsruhe basis set of double-ζ valence def2-SVP[13,14] for all atoms were employed for all gas-phase optimizations. Single point (SP) corrections were performed using M06-2X functional and def2-TZVP[13] basis set for all atoms. The implicit SMD continuum solvation model[15] was used to account for the solvent effect of cyclohexane solvent that was used in the experimental reactions. Gibbs energies were evaluated at the room temperature (reaction condition), using the entropic quasi-harmonic treatment scheme of Grimme,[16] at a cut off frequency of 100 cm^{-1}. The free energies were further corrected using standard concentration of 1 mol/L, which was used in solvation calculations. Data analysis was carried out using the GoodVibes code version 3.1.1.[16] Gibbs energies evaluated at SMD(cyclohexane)-M06-2X/def2-TZVP//M06-2X/def2-SVP level of theory are given in kcal mol^{-1} and used for discussion throughout.

Non-covalent interactions (NCIs) were analyzed using NCIPLOT[17] calculations. The *.wfn* files for NCIPLOT were generated at M06-2X/def2-SVP level of theory. NCI indices calculated with NCIPLOT were visualized at a gradient isosurface value of *s = 0.5* au. These are colored according to the sign of the second eigenvalue (λ_2) of the Laplacian of the density ($\nabla^2\rho$) over the range of –0.1 (blue = attractive) to +0.1 (red = repulsive). Molecular orbitals are visualized using an isosurface value of 0.05 au throughout. All molecular structures and molecular orbitals were visualized using *PyMOL* software.[18]

Computational rotational barriers studies

The rotational barriers for the enantiomerization of the substrate **1a** and the addition product **INT3** (Scheme S1) were studied computationally. First, a dihedral angle scan

along the axial C–C carbon bond was performed at M06-2X/def2-SVP in gas phase. The relaxed PES energy profile is shown in Figure S3. This gives an estimate of the rotational barrier of 20.0 kcal mol^{-1}. Using the structure with highest energy on this PES (i.e., structure 4 in Figure S3) as the initial guess structure for TS search, we successfully located the *true* TS for the enantiomerization via rotation along the axial C–C bond. After single point energy correction at higher basis set and with solvent effect at SMD(cyclohexane)-M06-2X/def2-TZVP, substrate **1a** was found to have a rotational barrier/enantiomerization barrier of $\Delta G^{\ddagger}$ = 17.4 kcal mol^{-1}.

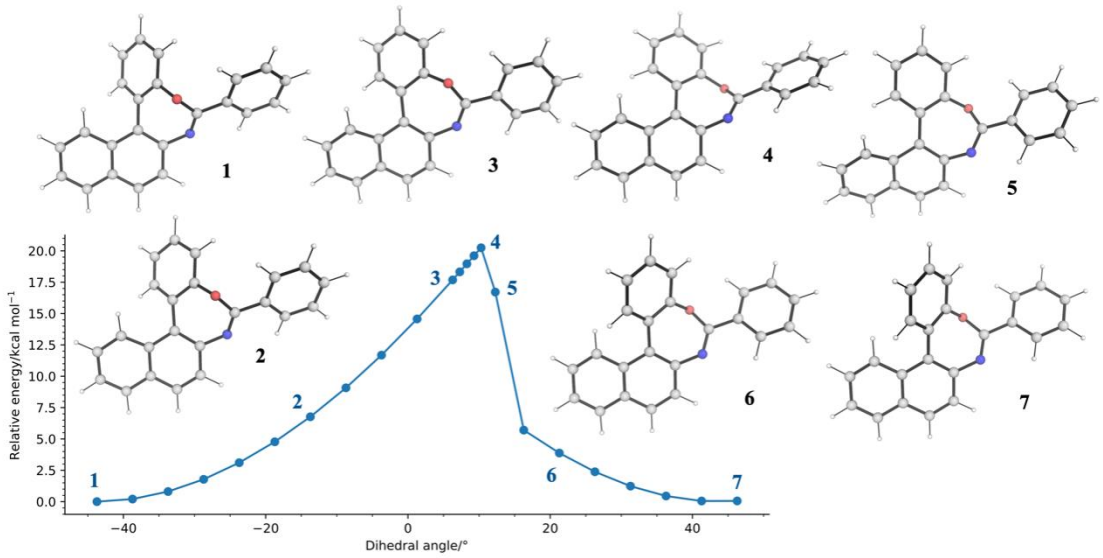


Figure S3. Relaxed potential energy surface (PES) scan for the dihedral angle along the C–C axial bond of substrate **1a**, computed at M06-2X/def2-SVP level of theory.

For intermediate **INT3**, we similarly studied the rotational barrier by first performing a dihedral angle scan along the axial C–C bond. The relaxed PES scan for **INT3** is shown in Figure S4. The highest energy structure on the scan PES was used as initial guess structure to locate the true TS for enantiomerization, which has a solvent corrected rotational barrier/enantiomerization barrier of $\Delta G^{\ddagger}$ = 24.2 kcal mol^{-1} (**TS_rot2**, Figure S5).

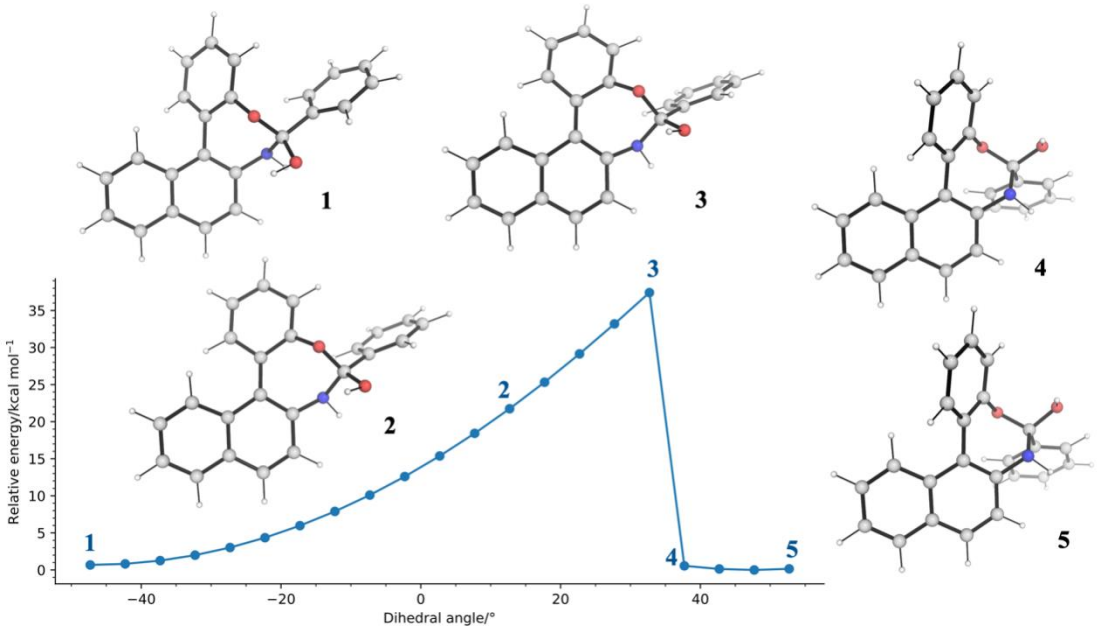
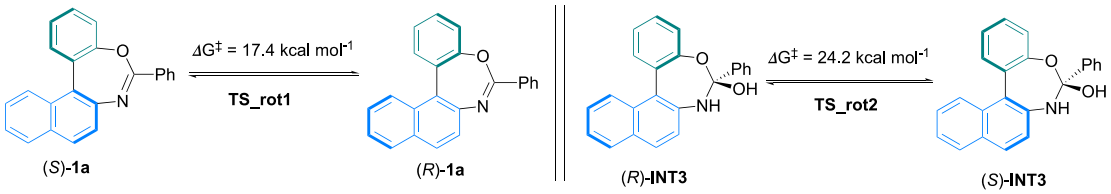


Figure S4. Relaxed potential energy surface (PES) scan for the dihedral angle along the C–C axial bond of intermediate **INT3**, computed at M06-2X/def2-SVP level of theory.

Figure S5 shows the DFT optimized structures of the transition states of the enantiomerization of these structures. The TSs for the enantiomerization for each of these structures have been successfully located and verified by intrinsic reaction coordinate (IRC)[19,20] analyses (see attached IRC movies).



Scheme S1. Computed rotational barriers for the enantiomerization of substrate **1a** and intermediate **INT3**.

TS_rot1	TS_rot2
$\Delta G^{\ddagger}$ = 17.4 kcal mol^{-1}	$\Delta G^{\ddagger}$ = 24.2 kcal mol^{-1}

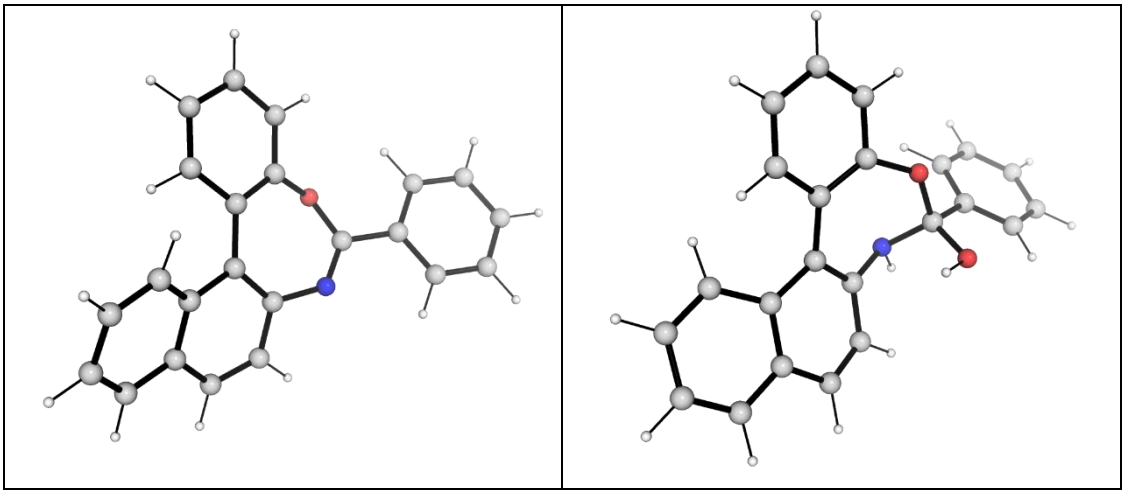


Figure S5. DFT-optimized transition state structures for the enantiomerization of substrate **1a** (**TS_rot1**) and intermediate **INT3** (**TS_rot2**). Computed rotational barriers are taken relative to each structure as reference zero. Rotational barriers are calculated at SMD(cyclohexane)-M06-2X/def2-TZVP//M06-2X/def2-SVP level of theory at room temperature and are given in kcal mol^{-1}.

The computed enantiomerization barrier for substrate **1a** at 17.4 kcal mol^{-1} translates to a half-life of about 1 second at room temperature using simple transition state theory for estimation. Thus, substrate **1a** is expected to enantiomerize rapidly at the reaction condition and no enantiomeric excess (ee) can be observed at the reaction condition. On the other hand, the enantiomerization barrier of 24.2 kcal mol^{-1} for **INT3** gives a half-life of about 17.5 hours, allowing (*R*)-**INT3** to react away via (*R*)-**TS2** (much lower barrier) more rapidly than it has time to enantiomerize to (*S*)-**INT3** via **TS_rot2** (Figure 3, main text).

We additionally studied the rotational barrier for substrate **1ai**, a relaxed PES dihedral angle scan along the C–C axial axis estimates a rotational barrier of ~60 kcal mol^{-1} for substrate **1ai** (Figure S6). However, using the highest energy as a guess for TS location, no TS could be successfully located. This is expected and is consistent with previous study of such substrates that the presence of ortho-substituents on the biaryls provide steric hinderance to prevent the ease of enantiomerization via rotation along the C–C axial axis[21] (the methyl group here provides even more steric hinderance than the hydroxyl group in the earlier study). We further estimated the rotational barrier by using the highest energy structure (structure 3 in Figure S6) directly (without further optimization) and running frequency calculations in gas-phase at M06-2X/def2-SVP

followed by solvent correction at SMD(cyclohexane)-M06-2X/def2-TZVP. This gives an estimated barrier of 62.5 kcal mol^{-1}. Therefore, substrate **1ai** is not expected to racemize under reaction conditions at room temperature (or other synthetically useful temperature, e.g., half-life of 115 days at 400 ºC).

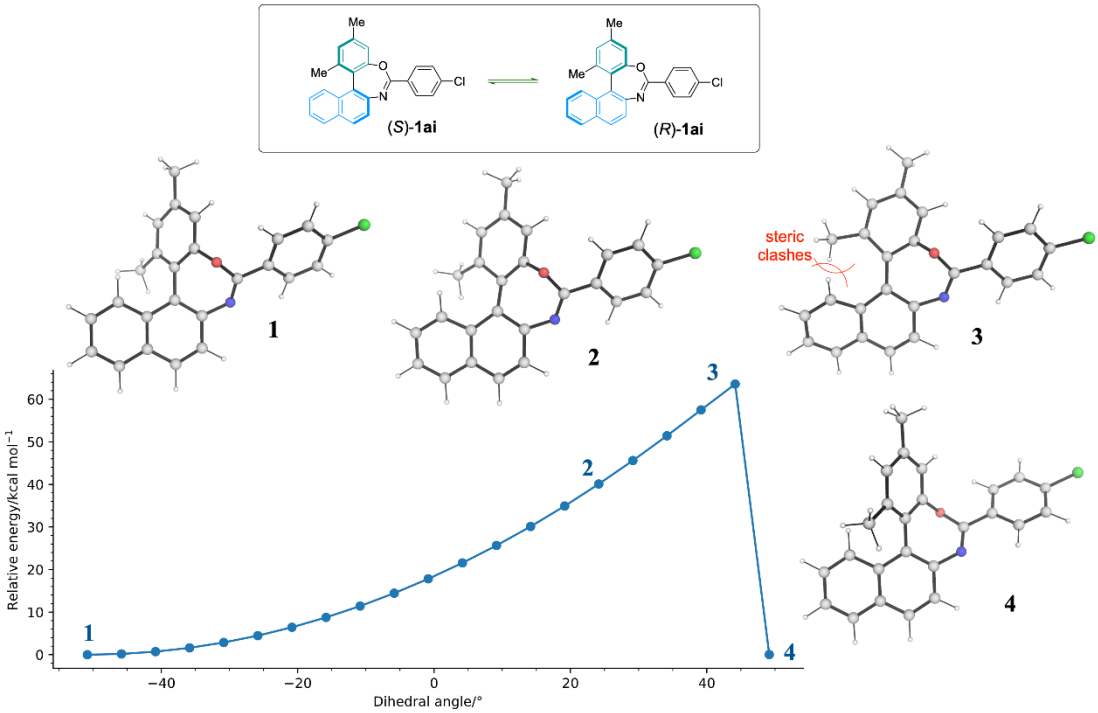


Figure S6. Relaxed potential energy surface (PES) scan for the dihedral angle along the C–C axial bond of substrate **1ai**, computed at M06-2X/def2-SVP level of theory.

Similarly, we studied the rotational barriers for the amide product arising from the reaction of substrate **1a**. The relaxed PES scan (Figure S7) suggests that the barriers for enantiomerization are > 30 kcal mol^{-1}, indicating that the product will be enantiostable at room temperature. The direct location of the TS for enantiomerization using the highest energy structures (structures 3 and 6, Figure S7) as initial guesses was unsuccessful; direct frequency calculations using these structures with solvent correction at SMD(cyclohexane)-M06-2X/def2-TZVP estimated the barriers to be 41.8 kcal mol^{-1} and 34.7 kcal mol^{-1}, respectively, suggesting that the product is enantiostable at room temperature (and may be stable up to 150 ºC with a half-life of ~18 hours).

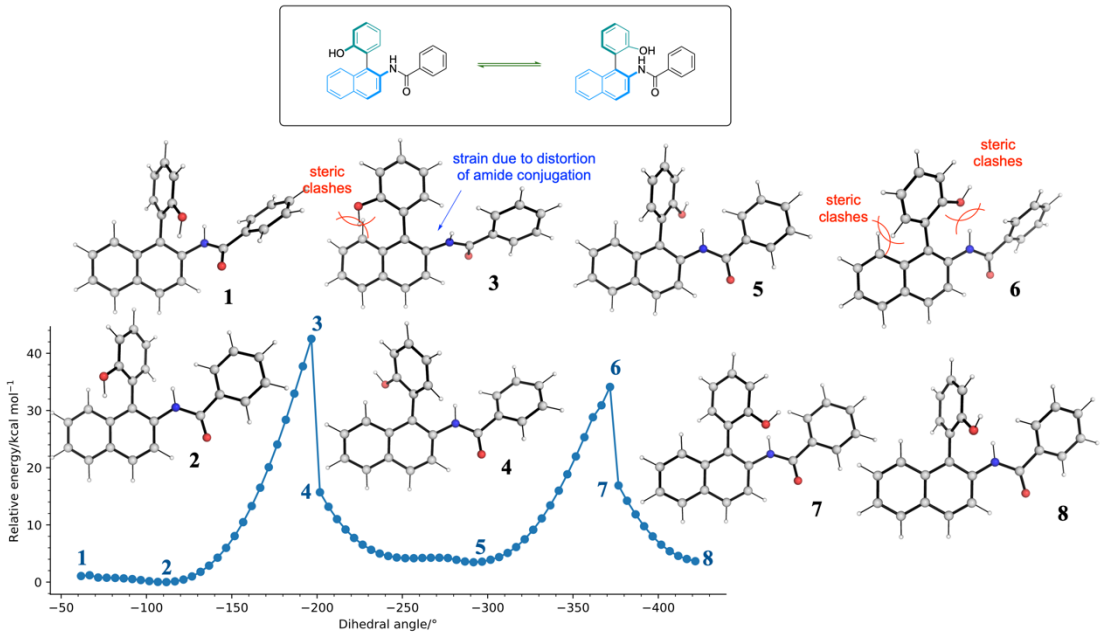
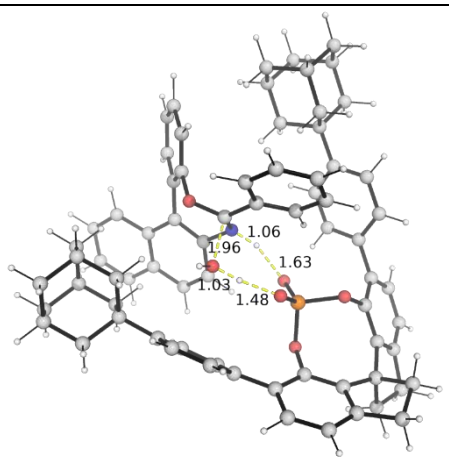
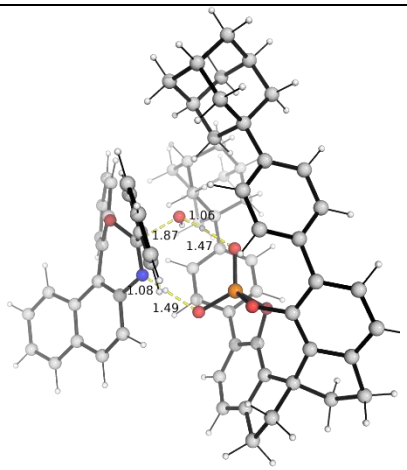
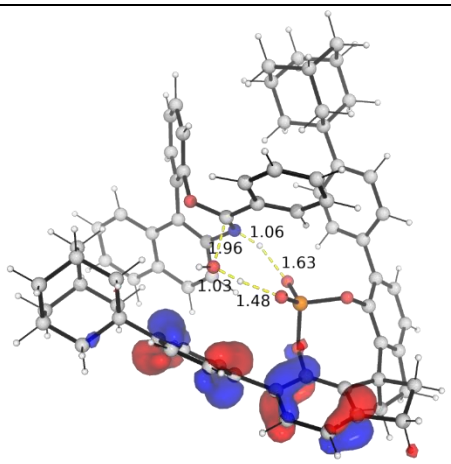
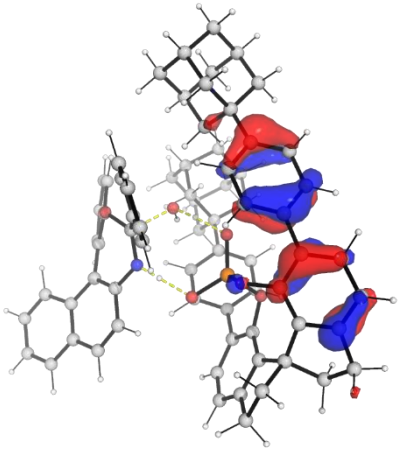
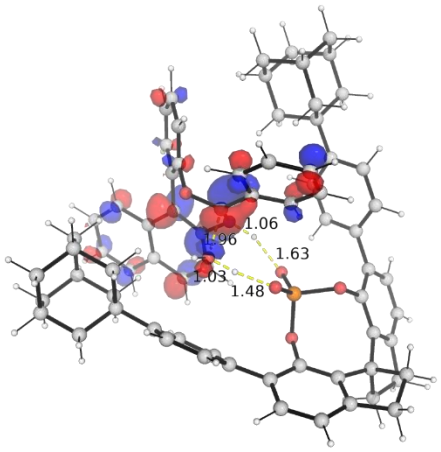
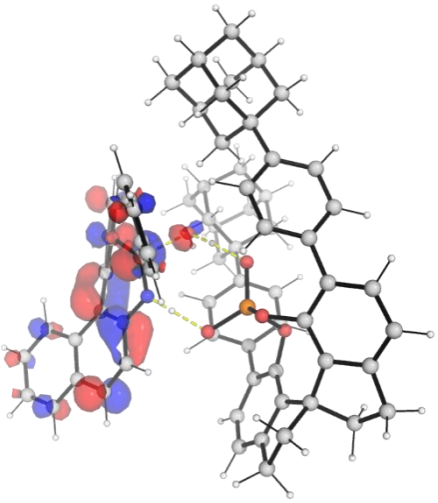
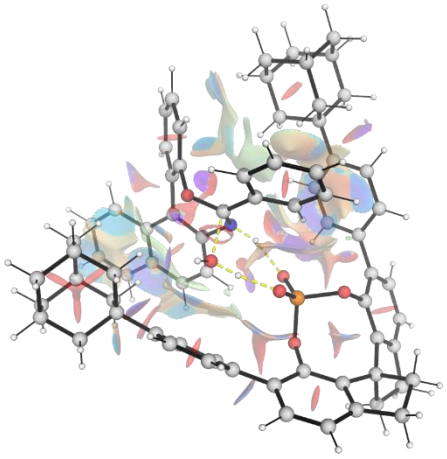
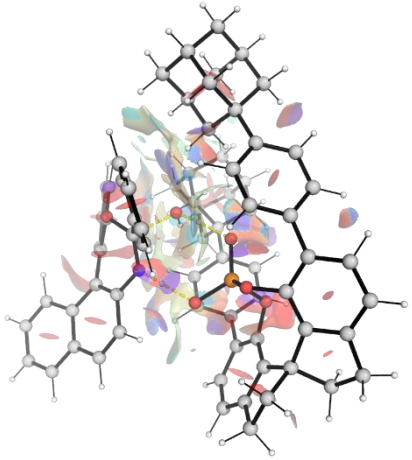
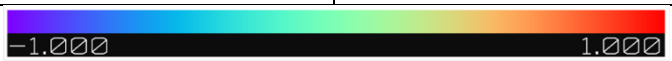
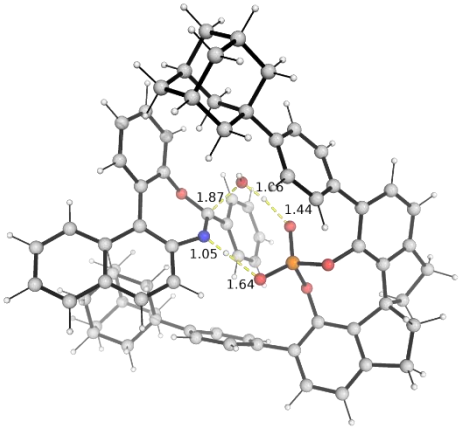
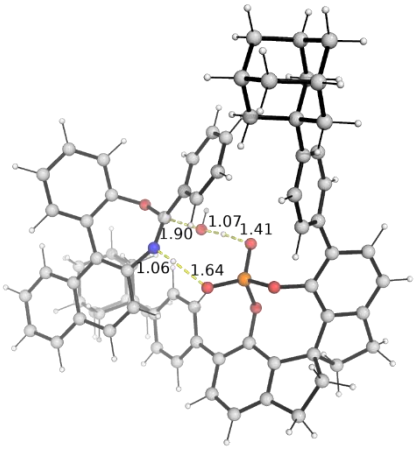
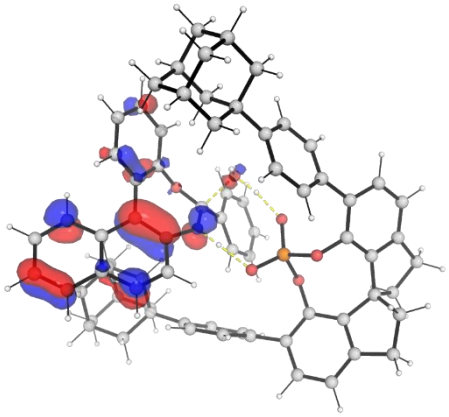
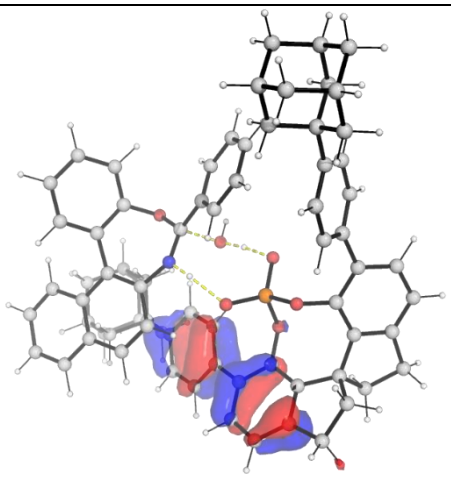


Figure S7. Relaxed potential energy surface (PES) scan for the dihedral angle along the C–C axial bond of the amide product of **2a**, computed at M06-2X/def2-SVP level of theory.

Enantioselectivity determining transition state

From the overall Gibbs energy profile (Figure 3, main text), we see that the enantioselectivity-determining step is the initial phosphoric acid catalyzed addition of water to the bridged biaryl substrate. For each of the enantiomers, (*R*)-**1a** and (*S*)-**1a**, the water molecule can add either to the Re or the Si face of the imine group, giving rise to a total of 4 distinct transition states (TSs). Due to the bulky side groups on the chiral phosphoric acid catalyst, conformational rigidity is determined by the phosphoric acid moiety, which has to be oriented with the imine group in specific spatial arrangement for the catalyzed water addition. This gives rise to only limited conformational freedom in the possible TSs. Figure S8 shows the DFT-optimized TS structures, their HOMO and LUMO plots as well as non-covalent interaction (NCI) plots and their activation barriers relative to substrate **1a**. The frontier molecular orbitals (FMOs) in these TSs have quite similar structure, where the coefficients of the HOMOs are predominantly on the acid catalyst and the coefficients of the LUMOs are predominantly on the substrate. This potentially reflects similar electronic influences in these TSs. The NCI plots suggest that (*R*)-**TS-Si** may be most favorable as it has the least steric repulsions.

	(*R*)-**TS1-Si**	(*R*)-**TS1-Re**
ΔG‡	16.5 kcal mol^{-1}	27.8 kcal mol^{-1}
DFT structure		
HOMO		
LUMO		

NCI		
		
	(*S*)-**TS1-Si**	(*S*)-**TS1-Re**
ΔG‡	20.6 kcal mol^{-1}	24.0 kcal mol^{-1}
DFT structure		
HOMO		

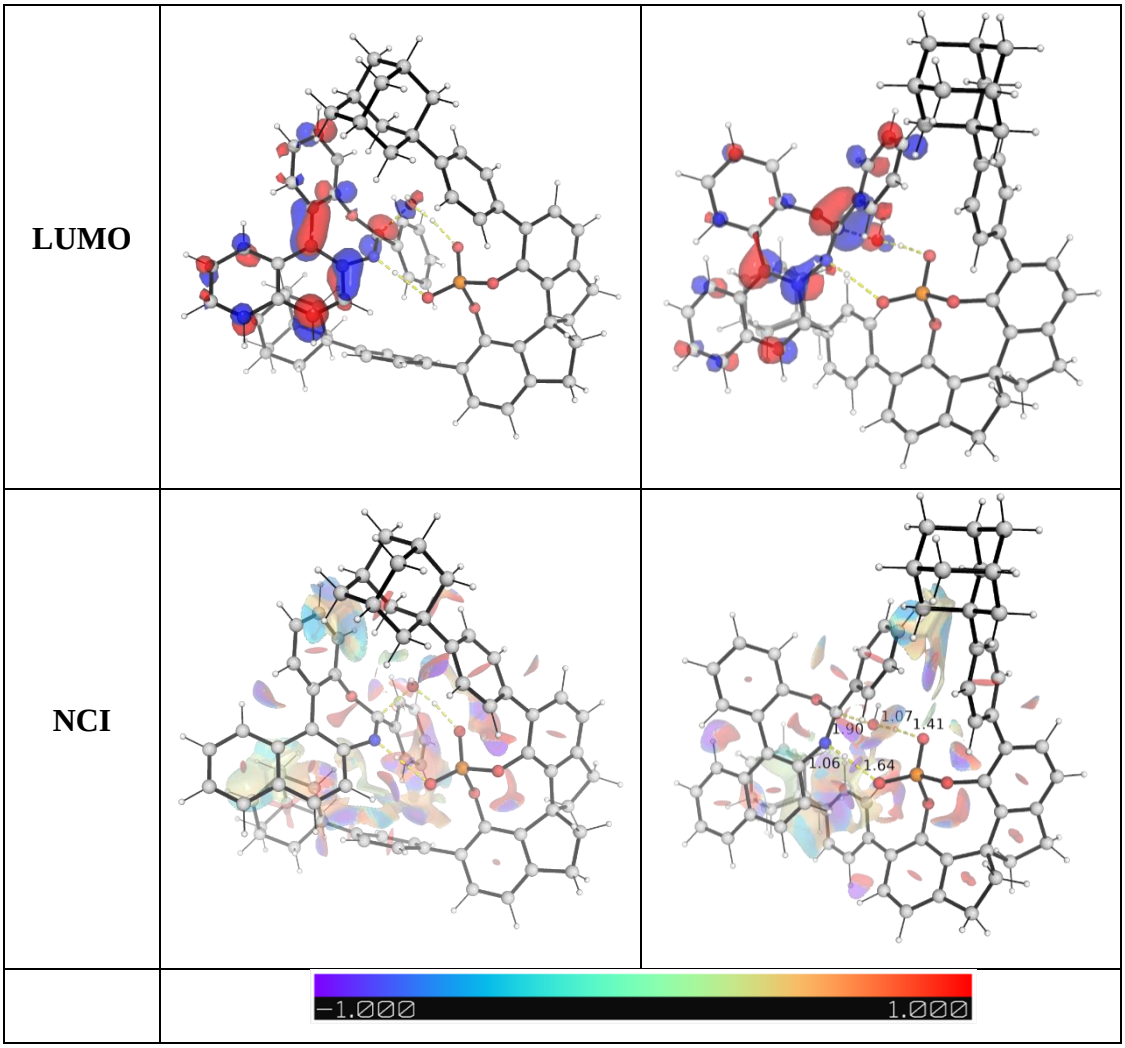


Figure S8. DFT-optimized TS structures, their HOMOs and LUMOs (isosurface value = 0.05 au) and non-covalent interaction (NCI) plots. Key bond distances are given in Å. Activation barriers ($\Delta G^{\ddagger}$) are given in kcal mol^{-1} and taken relative to the starting materials.

Transition state structures for the product formation

The DFT-optimized TS structures for the phosphoric acid catalyzed ring opening of intermediate from the addition of water (most favorable pathway) is shown in Figure S9.

	(R)-**TS2**	*(S)*-**TS2**
$\Delta G^{\ddagger}$	8.6 kcal mol^{-1}	9.3 kcal mol^{-1}

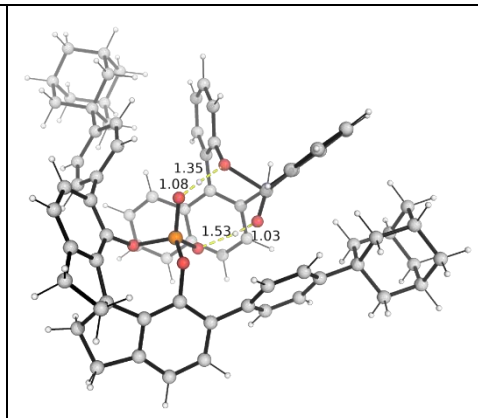
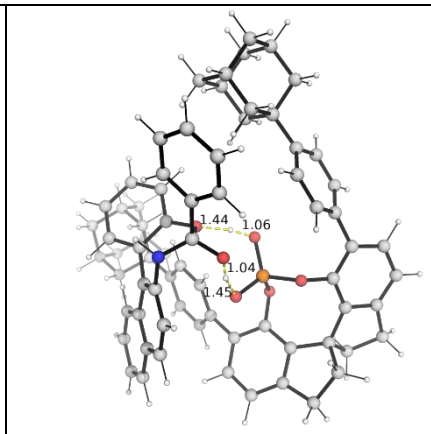
DFT structure		

Figure S9. DFT-optimized transition state structures for the acid-catalyzed ring opening of intermediate (R)-INT3. Activation barriers are taken relative to the sum of substrates as reference zero.

Optimized structures and absolute energies, zero-point energies

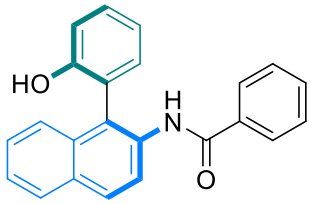
Geometries of all optimized structures (in .xyz format with their associated energy in Hartrees) and movies of relevant IRC analyses are included in a separate folder named *DFT_structures* with an associated readme.txt file. All these data have been deposited with this Supporting Information and uploaded to zenodo.org (DOI: 10.5281/zenodo. 7602173; https://zenodo.org/record/7602173).

Absolute values (in Hartrees) for SCF energy, zero-point vibrational energy (ZPE), enthalpy and quasi-harmonic Gibbs free energy for M06-2X/def2-SVP optimized structures and single point corrections in SMD(cyclohexane) using M06-2X/def2-TZVP functional are also included.

Reaction in cyclohexane at room temperature						
Structures	**E/au**	**ZPE/au**	**H/au**	**T.S/au**	**qh-G/au**	**SP SMD(cyclohexane) M06-2X/def2-TZVP**
water	-76.323214	0.021594	-76.29784	0.018411	-76.316251	-76.429369
R-C2_cat	-2537.734548	0.904737	-2536.788	0.112701	-2536.891851	-2540.331660
R-1a	-1014.316428	0.318103	-1013.98	0.061097	-1014.038693	-1015.442466

TS_rot1	-1014.288938	0.317502	-1013.9537	0.059473	-1014.011176	-1015.414776
S-1a	-1014.316428	0.318103	-1013.98	0.061097	-1014.038693	-1015.442466
R-INT1-Si	-3628.443719	1.249654	-3627.1316	0.151665	-3627.271814	-3632.238532
R-TS1-Si	-3628.432378	1.249944	-3627.1215	0.147361	-3627.258434	-3632.223761
R-INT2-Si	-3628.466462	1.253748	-3627.1515	0.149859	-3627.289614	-3632.253218
R-TS1-Re	-3628.409266	1.249009	-3627.0991	0.150678	-3627.237514	-3632.203605
S-INT1-Si	-3628.437162	1.248541	-3627.1255	0.155334	-3627.267942	-3632.237811
S-TS1-Si	-3628.421475	1.249543	-3627.1108	0.149913	-3627.248844	-3632.215960
S-INT2-Si	-3628.452169	1.253174	-3627.1376	0.151228	-3627.276462	-3632.245884
S-TS1-Re	-3628.414063	1.250004	-3627.103	0.149414	-3627.24093	-3632.211044
R-INT3	-1090.675017	0.34626	-1090.309	0.064039	-1090.370238	-1091.891815
TS_rot2	-1090.6364	0.345853	-1090.2714	0.062758	-1090.331538	-1091.853314
S-INT3	-1090.676097	0.3467	-1090.3098	0.063627	-1090.370726	-1091.893308
R-INT4	-3628.448013	1.251648	-3627.1348	0.15264	-3627.274171	-3632.240326
R-TS2	-3628.442394	1.248294	-3627.1331	0.149825	-3627.27096	-3632.233872
R-INT5	-3628.470656	1.250559	-3627.1577	0.153929	-3627.298814	-3632.263293
S-INT4	-3628.452779	1.253011	-3627.1384	0.150978	-3627.27698	-3632.244778
S-TS2	-3628.43978	1.247804	-3627.131	0.150125	-3627.268982	-3632.232122
S-INT5	-3628.469607	1.250918	-3627.1563	0.1545	-3627.297551	-3632.263464
R-2a	-1090.690151	0.345055	-1090.3241	0.068524	-1090.388493	-1091.911672

Characterization data of the catalytic reaction products



2a

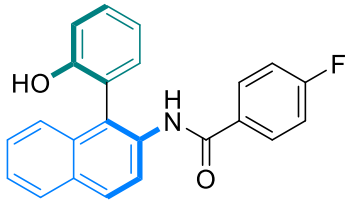
(R)-N-(1-(2-hydroxyphenyl)naphthalen-2-yl)benzamide (2a): white solid, m.p. = 240-241 °C, 33.5 mg, 99% yield

^{1}H NMR (500 MHz, DMSO) δ 9.77 (s, 1H), 9.21 (s, 1H), 7.97 (d, *J* = 8.3 Hz, 3H), 7.67 (d, *J* = 7.6 Hz, 2H), 7.59 – 7.38 (m, 6H), 7.32 (t, *J* = 7.9 Hz, 1H), 7.18 (d, *J* = 7.5 Hz, 1H), 7.09 (d, 1H), 6.95 (t, *J* = 7.4 Hz, 1H);

^{13}C NMR (126 MHz, DMSO) δ 165.5, 155.3, 135.0, 133.8, 132.8, 132.7, 132.1, 131.7, 123.0, 129.7, 129.0, 128.3, 128.0, 127.5, 126.6, 126.3, 125.6, 124.6, 122.6, 119.7, 116.4;

HRMS (ESI, m/z): calcd. for $[M+Na]^+$: 362.1151, found: 362.1150;

HPLC analysis: 96:4 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{minor} = 15.6 min, t_{major} = 18.2 min), $[\alpha]_D^{25}$ = −53.00 (c = 0.2, acetone).



2b

(R)-4-fluoro-N-(1-(2-hydroxyphenyl)naphthalen-2-yl)benzamide (2b): white solid, m.p. = 220-221 °C, 34.9 mg, 98% yield

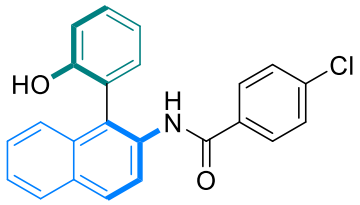
^{1}H NMR (500 MHz, DMSO) δ 9.68 (s, 1H), 9.32 (s, 1H), 7.97 (d, *J* = 8.4 Hz, 2H), 7.86 (d, *J* = 8.8 Hz, 1H), 7.73 (dd, *J* = 8.6, 5.5 Hz, 2H), 7.50 – 7.47 (m, 1H), 7.46 – 7.41 (m, 2H), 7.31 – 7.26 (m, 3H), 7.14 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.04 (d, *J* = 8.1 Hz, 1H), 6.92 (t, *J* = 7.4 Hz, 1H);

^{13}C NMR (126 MHz, DMSO) δ 165.1 (d, *J* = 249.8 Hz), 164.7, 155.4, 133.8, 132.8, 132.6, 131.9, 131.6, 130.6, 130.3 (d, *J* = 9.8 Hz), 129.9, 128.4, 128.0, 126.6, 126.5, 125.7, 125.3, 122.8, 119.6, 116.3, 115.9 (d, *J* = 21.8 Hz);

^{19}F NMR (471 MHz, DMSO) δ -108.7 (s, 1F);

HRMS (ESI, m/z): calcd. for $[M+Na]^+$: 380.1057, found: 380.1055;

HPLC analysis: 98:2 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{minor} = 18.2 min, t_{major} = 22.9 min), $[\alpha]_D^{25}$ = +162.00 (c = 0.2, acetone), $[\alpha]_D^{25}$ = +162.00 (c = 0.2, acetone).



2c

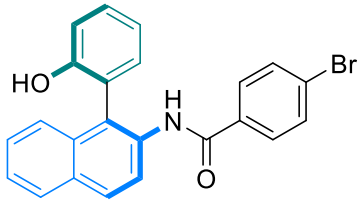
(R)-4-chloro-N-(1-(2-hydroxyphenyl)naphthalen-2-yl)benzamide (2c): white solid, m.p. = 250-251 °C, 36.9 mg, 99% yield

^{1}H NMR (500 MHz, DMSO) δ 9.66 (s, 1H), 9.42 (s, 1H), 7.97 (d, *J* = 8.6 Hz, 2H), 7.84 (d, *J* = 8.8 Hz, 1H), 7.69 (d, *J* = 8.5 Hz, 2H), 7.55 – 7.39 (m, 5H), 7.32 – 7.25 (m, 1H), 7.18 – 7.11 (m, 1H), 7.05 (d, *J* = 8.1 Hz, 1H), 6.92 (t, *J* = 7.5 Hz, 1H);

^{13}C NMR (126 MHz, DMSO) δ 164.8, 155.4, 136.8, 133.8, 133.7, 132.8, 132.6, 131.9, 130.8, 129.9, 129.6, 129.0, 128.3, 128.0, 126.6, 126.5, 125.7, 125.4, 122.8, 119.5, 116.3.

HRMS (ESI, m/z): calcd. for $[M+H]^+$: 374.0942, found: 374.0940;

HPLC analysis: 99:1 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{minor} = 22.4 min, t_{major} = 26.7 min), $[\alpha]_D^{25}$ = +96.00 (c = 0.2, acetone).



2d

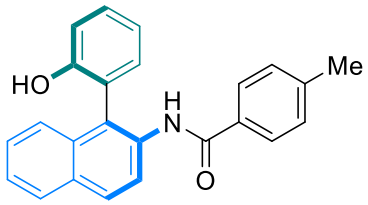
(R)-4-bromo-N-(1-(2-hydroxyphenyl)naphthalen-2-yl)benzamide (2d): white solid, m.p. = 259-260 °C, 41.3 mg, 99% yield

^{1}H NMR (500 MHz, DMSO) δ 9.65 (s, 1H), 9.42 (s, 1H), 7.97 (d, *J* = 8.4 Hz, 2H), 7.84 (d, *J* = 8.8 Hz, 1H), 7.70 – 7.55 (m, 4H), 7.53 – 7.37 (m, 3H), 7.28 (t, *J* = 7.7 Hz, 1H), 7.14 (d, *J* = 7.5 Hz, 1H), 7.04 (d, *J* = 8.1 Hz, 1H), 6.91 (t, *J* = 7.4 Hz, 1H);

^{13}C NMR (126 MHz, DMSO) δ 164.9, 155.4, 134.2, 133.7, 132.8, 132.5, 131.9, 131.8, 130.8, 129.9, 129.7, 128.3, 128.0, 126.6, 126.5, 125.8, 125.7, 125.4, 122.7, 119.5, 116.3;

HRMS (ESI, m/z): calcd. for $[M+H]^+$: 418.0437, found: 418.0433;

HPLC analysis: 98:2 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{minor} = 21.6 min, t_{major} = 24.9 min), $[\alpha]_D^{25}$ = −65.00 (c = 0.2, acetone).



2e

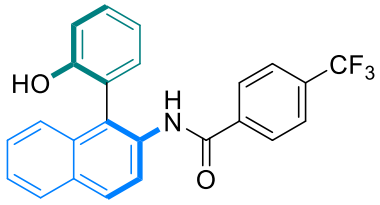
(R)-N-(1-(2-hydroxyphenyl)naphthalen-2-yl)-4-methylbenzamide (2e): white solid, m.p. = 249-250 °C, 34.9 mg, 99% yield

^{1}H NMR (500 MHz, DMSO) δ 9.80 (s, 1H), 9.06 (s, 1H), 8.05 – 7.93 (m, 3H), 7.59 – 7.53 (m, 2H), 7.51 – 7.40 (m, 3H), 7.35 – 7.29 (m, 1H), 7.25 (d, *J* = 7.8 Hz, 2H), 7.17 (dd, *J* = 7.5, 1.8 Hz, 1H), 7.09 (d, *J* = 8.0 Hz, 1H), 6.95 (t, *J* = 7.4 Hz, 1H), 2.34 (s, 3H);

^{13}C NMR (126 MHz, DMSO) δ 165.2, 155.3, 142.2, 133.9, 132.8, 132.7, 132.1, 131.6, 130.0, 129.6, 129.2, 128.3, 128.0, 127.4, 126.6, 126.3, 125.5, 124.3, 122.6, 119.8, 116.4, 21.4;

HRMS (ESI, m/z): calcd. for $[M+Na]^+$: 376.1308, found: 376.1306;

HPLC analysis: 92:8 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{minor} = 24.2 min, t_{major} = 26.6 min), $[\alpha]_D^{25}$ = +116.00 (c = 0.2, acetone).



2f

(R)-N-(1-(2-hydroxyphenyl)naphthalen-2-yl)-4-(trifluoromethyl)benzamide (2f): white solid, m.p. = 239-240 °C, 40.3 mg, 99% yield

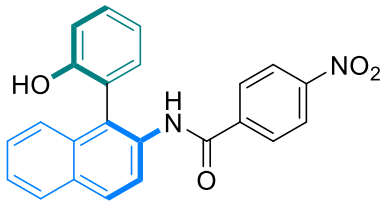
^{1}H NMR (500 MHz, DMSO) δ 9.65 (s, 1H), 9.62 (s, 1H), 7.99 (d, *J* = 8.2 Hz, 2H), 7.92 – 7.74 (m, 5H), 7.52 – 7.46 (m, 3H), 7.28 (t, *J* = 7.8 Hz, 1H), 7.16 (d, *J* = 7.5 Hz, 1H), 7.05 (d, *J* = 8.2 Hz, 1H), 6.92 (t, *J* = 7.6 Hz, 1H);

^{13}C NMR (126 MHz, DMSO) δ 164.9, 155.4, 139.0, 133.6, 132.8, 132.5, 132.1, 131.8 (q, *J* = 32.0 Hz), 131.4, 129.9, 128.7, 128.6, 128.4, 128.1, 126.6, 126.5, 125.9 (q, *J* = 3.4 Hz), 125.6, 124.3 (q, *J* = 273.0 Hz), 122.8, 119.5, 116.3;

^{19}F NMR (471 MHz, DMSO) δ -61.3 (s, 3F);

HRMS (ESI, m/z): calcd. for $[M+Na]^+$: 430.1025, found: 430.1023;

HPLC analysis: 98:2 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{minor} = 16.2 min, t_{major} = 18.2 min), $[\alpha]_D^{25}$ = −73.50 (c = 0.2, acetone).



2g

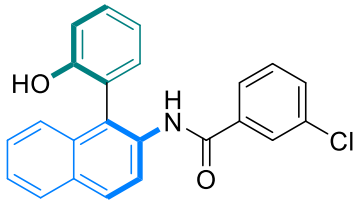
(R)-N-(1-(2-hydroxyphenyl)naphthalen-2-yl)-4-nitrobenzamide (2g): white solid, m.p. = 275-276 °C, 38.0 mg, 99% yield

^{1}H NMR (500 MHz, DMSO) δ 9.79 (s, 1H), 9.58 (s, 1H), 8.28 (d, *J* = 8.3 Hz, 2H), 7.99 (d, *J* = 8.4 Hz, 2H), 7.90 (d, *J* = 8.2 Hz, 2H), 7.77 (d, *J* = 8.5 Hz, 1H), 7.52 – 7.46 (m, 3H), 7.27 (t, *J* = 7.9 Hz, 1H), 7.14 (d, *J* = 7.5 Hz, 1H), 7.03 (d, *J* = 8.0 Hz, 1H), 6.90 (t, *J* = 7.5 Hz, 1H);

^{13}C NMR (126 MHz, DMSO) δ 164.5, 155.4, 149.5, 140.8, 133.4, 132.8, 132.4, 132.1, 131.8, 129.8, 129.2, 128.3, 128.1, 126.6, 126.5, 125.9, 125.8, 124.0, 122.8, 119.4, 116.2;

HRMS (ESI, m/z): calcd. for $[M+Na]^+$: 407.1002, found: 407.0997;

HPLC analysis: 99:1 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{minor} = 33.1 min, t_{major} = 35.5 min), $[\alpha]_D^{25}$ = +148.00 (c = 0.2, acetone).



2h

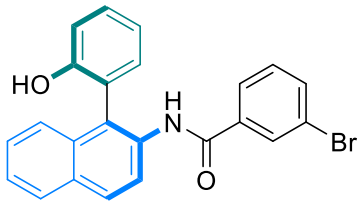
(R)-3-chloro-N-(1-(2-hydroxyphenyl)naphthalen-2-yl)benzamide (2h): white solid, m.p. = 191-192 °C, 36.9 mg, 99% yield

^{1}H NMR (500 MHz, DMSO) δ 9.64 (s, 1H), 9.50 (s, 1H), 7.98 (d, *J* = 8.4 Hz, 2H), 7.82 (d, *J* = 8.8 Hz, 1H), 7.69 – 7.57 (m, 3H), 7.52 – 7.40 (m, 4H), 7.33 – 7.26 (m, 1H), 7.15 (dd, *J* = 7.6, 1.8 Hz, 1H), 7.05 (d, *J* = 8.1 Hz, 1H), 6.95 – 6.89 (m, 1H);

^{13}C NMR (126 MHz, DMSO) δ 164.6, 155.4, 137.2, 133.7, 133.6, 132.8, 132.5, 132.0, 131.8, 131.1, 130.9, 129.8, 128.3, 128.0, 127.6, 126.6, 126.5, 126.4, 125.8, 125.5, 122.8, 119.5, 116.2;

HRMS (ESI, m/z): calcd. for $[M+H]^+$: 374.0942, found: 374.0942;

HPLC analysis: 97:3 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{minor} = 15.9 min, t_{major} = 18.9 min), $[\alpha]_D^{25}$ = +144.00 (c = 0.2, acetone), $[\alpha]_D^{25}$ = +144.00 (c = 0.2, acetone).



2i

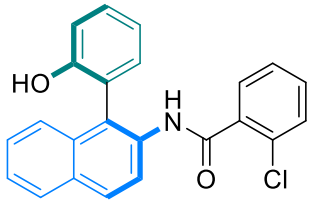
(R)-3-bromo-N-(1-(2-hydroxyphenyl)naphthalen-2-yl)benzamide (2i): white solid, m.p. = 211-212 °C, 41.3 mg, 99% yield

^{1}H NMR (500 MHz, DMSO) δ 9.64 (s, 1H), 9.50 (s, 1H), 7.98 (d, *J* = 8.5 Hz, 2H), 7.86 – 7.76 (m, 2H), 7.73 (d, *J* = 7.9 Hz, 1H), 7.67 (d, *J* = 7.7 Hz, 1H), 7.50 – 7.41 (m, 4H), 7.30 (t, *J* = 7.9 Hz, 1H), 7.15 (d, *J* = 7.6 Hz, 1H), 7.06 (d, *J* = 8.2 Hz, 1H), 6.93 (t, *J* = 7.7 Hz, 1H);

^{13}C NMR (126 MHz, DMSO) δ 164.5, 155.4, 137.4, 134.7, 133.6, 132.8, 132.5, 132.0, 131.1, 131.0, 130.5, 129.8, 128.3, 128.0, 126.7, 126.6, 126.5, 125.8, 125.5, 122.8, 122.2, 119.5, 116.2;

HRMS (ESI, m/z): calcd. for $[M+H]^+$: 418.0437, found: 418.0434;

HPLC analysis: 98:2 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{minor} = 17.3min, t_{major} = 20.6 min), $[\alpha]_D^{25}$ = −54.50 (c = 0.2, acetone).



2j

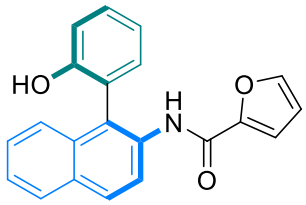
(R)-2-chloro-N-(1-(2-hydroxyphenyl)naphthalen-2-yl)benzamide (2j): white solid, m.p. = 228-229 °C, 36.9 mg, 99% yield

^{1}H NMR (500 MHz, DMSO) δ 9.51 (s, 1H), 9.44 (s, 1H), 7.98 (t, *J* = 8.1 Hz, 2H), 7.90 (d, *J* = 8.8 Hz, 1H), 7.52 – 7.39 (m, 5H), 7.36 – 7.31 (m, 3H), 7.15 (d, *J* = 7.5 Hz, 1H), 7.04 (d, *J* = 8.2 Hz, 1H), 6.96 (t, *J* = 7.5 Hz, 1H);

^{13}C NMR (126 MHz, DMSO) δ165.4, 155.7, 136.8, 133.5, 132.9, 132.6, 131.8, 131.6, 130.7, 130.4, 130.2, 129.8, 129.6, 128.3, 128.0, 127.5, 126.6, 126.5, 125.8, 125.1, 122.8, 119.5, 116.2;

HRMS (ESI, m/z): calcd. for $[M+H]^+$: 374.0942, found: 374.0940;

HPLC analysis: 97:3 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{minor} = 23.2min, t_{major} = 26.4 min), $[\alpha]_D^{25}$ =−102.50(c = 0.2, acetone).



2k

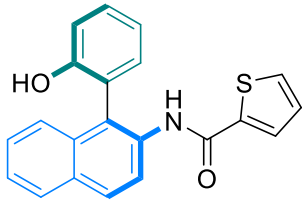
(R)-N-(1-(2-hydroxyphenyl)naphthalen-2-yl)furan-2-carboxamide(2k):white solid, m.p. = 170-171 °C, 32.6 mg, 99% yield

^{1}H NMR (500 MHz, DMSO) δ 9.91 (s, 1H), 8.85 (s, 1H), 8.15 (d, *J* = 8.8 Hz, 1H), 7.98 – 7.94 (m, 2H), 7.81 – 7.78 (m, 1H), 7.50 – 7.33 (m, 4H), 7.19 – 7.10 (m, 3H), 7.04 – 6.96 (m, 1H), 6.65 (dd, *J* = 3.5, 1.8 Hz, 1H);

^{13}C NMR (126 MHz, DMSO) δ 155.8, 155.1, 147.4, 145.9, 132.8, 132.5, 132.4, 131.1, 130.0, 128.1, 127.9, 127.5, 126.5, 125.9, 125.2, 122.6, 121.7, 119.7, 116.2, 115.1, 112.7;

HRMS (ESI, m/z): calcd. for $[M+Na]^+$:352.0944, found: 352.0942;

HPLC analysis: 97:3 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{minor} =18.4min, t_{major} = 22.2 min), $[\alpha]_D^{25} = -110.50$ (c = 0.2, acetone).



2l

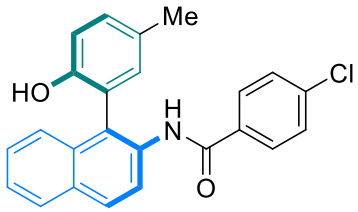
(R)-N-(1-(2-hydroxyphenyl)naphthalen-2-yl)thiophene-2-carboxamide (2l): white solid, m.p. = 240-241 °C, 34.1 mg, 99% yield

^{1}H NMR (500 MHz, DMSO) δ9.75 (s, 1H), 9.19 (s, 1H), 8.00 – 7.94 (m, 2H), 7.90 (d, *J* = 8.8 Hz, 1H), 7.81 (dd, *J* = 5.0, 1.2 Hz, 1H), 7.53 – 7.47 (m, 2H), 7.45 – 7.40 (m, 2H), 7.33 – 7.27 (m, 1H), 7.18 – 7.11 (m, 2H), 7.07 (dd, *J* = 8.2, 1.2 Hz, 1H), 6.97 – 6.90 (m, 1H);

^{13}C NMR (126 MHz, DMSO) δ160.2, 155.3, 139.9, 133.4, 132.8, 132.7, 132.0, 131.7, 130.0, 129.9, 129.0, 128.6, 128.3, 128.1, 126.6, 126.4, 125.7, 124.7, 122.5, 119.7, 116.4;

HRMS (ESI, m/z): calcd. for $[M+Na]^+$:368.0716, found: 368.0715;

HPLC analysis: 97:3 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{minor} =18.1min, t_{major} = 21.5 min), $[\alpha]_D^{25} = -114.00$ (c = 0.2, acetone).



2m

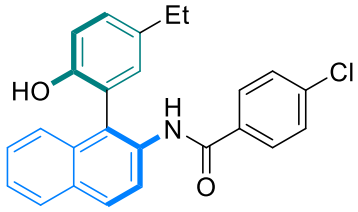
(R)-4-chloro-N-(1-(2-hydroxy-5-methylphenyl)naphthalen-2-yl)benzamide (2m): white solid, m.p. = 189-190 °C, 35.6 mg, 92% yield

^{1}H NMR (500 MHz, DMSO) δ 9.51 (s, 1H), 9.36 (s, 1H), 7.96 (d, *J* = 7.3 Hz, 2H), 7.88 (d, *J* = 8.8 Hz, 1H), 7.69 (d, *J* = 8.5 Hz, 2H), 7.54 (d, *J* = 8.5 Hz, 2H), 7.51 – 7.47 (m, 2H), 7.45 – 7.40 (m, 1H), 7.10 (dd, *J* = 8.3, 2.2 Hz, 1H), 6.96 (t, 2H), 2.21 (s, 3H);

^{13}C NMR (126 MHz, DMSO) δ 164.8, 153.0, 136.9, 133.9, 133.6, 132.9, 132.8, 131.9, 130.4, 130.3, 129.5, 129.1, 128.3, 128.0, 127.9, 126.6, 126.5, 125.7, 125.0, 122.4, 116.3, 20.6;

HRMS (ESI, m/z):calcd. for $[M+Na]^+$:410.0918, found: 410.0917;

HPLC analysis: 96.5:3.5 er, (CHIRALCEL IF column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{major} = 17.4 min, t_{minor} = 22.5 min), $[\alpha]_D^{25}$ = +108.00 (c = 0.2, acetone).



2n

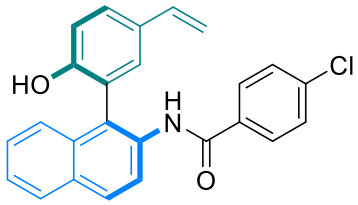
(R)-4-chloro-N-(1-(5-ethyl-2-hydroxyphenyl)naphthalen-2-yl)benzamide(2n): white solid, m.p. = 187-188 °C, 36.5 mg, 91% yield

^{1}H NMR (500 MHz, DMSO) δ 9.50 (s, 1H), 9.43 (s, 1H), 7.98 (d, *J* = 8.4 Hz, 2H), 7.88 (d, *J* = 8.8 Hz, 1H), 7.71 (d, *J* = 8.1 Hz, 2H), 7.54 (d, *J* = 8.3 Hz, 2H), 7.52 – 7.48 (m, 2H), 7.44 (dd, *J* = 8.7, 6.4 Hz, 1H), 7.13 (dd, *J* = 8.2, 2.2 Hz, 1H), 7.01 – 6.97 (m, 2H), 2.53 – 2.48 (q, *J* = 7.5Hz, 2H), 1.08 (t, *J* = 7.5 Hz, 3H);

^{13}C NMR (126 MHz, DMSO) δ 164.5, 152.9, 136.5, 134.2, 133.5, 133.3, 132.4, 131.5, 131.2, 130.6, 129.2, 128.8, 128.6, 128.0, 127.6, 126.4, 126.2, 125.4, 125.0, 122.1, 115.9, 27.4, 16.0;

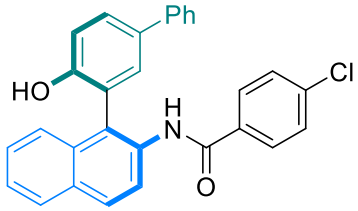
HRMS (ESI, m/z): calcd. for $[M+Na]^+$:424.1075, found: 424.1072;

HPLC analysis: 95:5 er, (CHIRALCEL IF column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{major} = 18.2 min, t_{minor} = 22.5 min), $[\alpha]_D^{25}$ = −55.00 (c = 0.2, acetone).



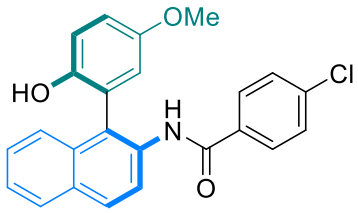
2o

(R)-4-chloro-N-(1-(2-hydroxy-5-vinylphenyl)naphthalen-2-yl)benzamide(2o):
white solid, m.p. = 179-180 °C, 37.9 mg, 95% yield
^{1}H NMR (500 MHz, DMSO) δ 9.82 (s, 1H), 9.48 (s, 1H), 7.98 (d, *J* = 8.5 Hz, 2H), 7.82 (d, *J* = 8.5 Hz, 1H), 7.68 (d, *J* = 8.1 Hz, 2H), 7.51 (d, *J* = 8.0 Hz, 3H), 7.47 – 7.43 (m, 2H), 7.40 (d, *J* = 8.7 Hz, 1H), 7.26 (s, 1H), 7.00 (d, *J* = 8.5 Hz, 1H), δ 6.62 (dd, *J* = 17.5, 11.0 Hz, 1H)., 5.57 (d, *J* = 17.5 Hz, 1H), 5.04 (d, *J* = 11.0 Hz, 1H);
^{13}C NMR (126 MHz, DMSO) δ 165.0, 155.5, 136.8, 136.7, 133.9, 133.8, 132.8, 132.0, 130.7, 130.6, 129.6, 129.0, 128.8, 128.4, 128.1, 127.7, 126.7, 126.5, 125.8, 125.6, 122.9, 116.4, 111.7;
HRMS (ESI, m/z): calcd. for $[M+Na]^+$:422.0918, found: 422.0915;
HPLC analysis: 93:7 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{minor} =21.3min, t_{major} =26.5 min), $[\alpha]_D^{25}$ = +106.00 (c = 0.2, acetone).



2p

(R)-4-chloro-N-(1-(4-hydroxy-[1,1'-biphenyl]-3-yl)naphthalen-2yl)benzamide(2p):
white solid, m.p. = 215-216 °C, 44.4 mg, 99% yield
^{1}H NMR (500 MHz, DMSO) δ 9.80 (s, 1H), 9.65 (s, 1H), 7.99 (dd, *J* = 8.5, 4.5 Hz, 2H), 7.80 (d, *J* = 8.7 Hz, 1H), 7.72 (d, *J* = 8.4 Hz, 2H), 7.60 (dd, *J* = 8.5, 2.4 Hz, 1H), 7.54 (dd, *J* = 8.5, 3.3 Hz, 3H), 7.49 (dd, *J* = 8.2, 6.3 Hz, 3H), 7.46 – 7.42 (m, 2H), 7.36 (t, *J* = 7.6 Hz, 2H), 7.24 (t, *J* = 7.4 Hz, 1H), 7.12 (d, *J* = 8.4 Hz, 1H);
^{13}C NMR (126 MHz, DMSO) δ 165.2, 155.3, 140.4, 136.8, 133.9, 133.8, 132.8, 132.1, 131.5, 131.4, 130.7, 129.7, 129.3, 128.9, 128.4, 128.2, 128.1, 127.0, 126.7, 126.6, 126.5, 126.1, 125.9, 123.4, 116.8;
HRMS (ESI, m/z): calcd. for $[M+Na]^+$:472.1075, found: 472.1070;
HPLC analysis: 93:7 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{minor} =26.5min, t_{major} =33.4 min), $[\alpha]_D^{25}$ = +145.00 (c = 0.2, acetone).



2q

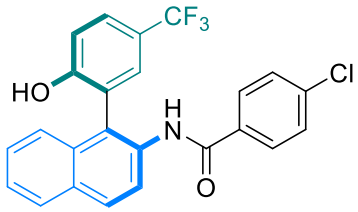
(R)-4-chloro-N-(1-(2-hydroxy-5-methoxyphenyl)naphthalen-2-yl)benzamide(2q): white solid, m.p. = 139-140 °C, 39.5 mg, 98% yield

^{1}H NMR (500 MHz, DMSO) δ 9.46 (s, 1H), 9.24 (s, 1H), 7.97 (d, *J* = 8.4 Hz, 2H), 7.83 (d, *J* = 8.8 Hz, 1H), 7.71 (d, *J* = 8.0 Hz, 2H), 7.54 (d, *J* = 8.2 Hz, 2H), 7.50 (d, *J* = 8.6 Hz, 2H), 7.45 (d, *J* = 7.7 Hz, 1H), 6.96 (d, *J* = 8.8 Hz, 1H), 6.88 (d, *J* = 9.0 Hz, 1H), 6.71 (s, 1H), 3.62 (s, 3H);

^{13}C NMR (126 MHz, DMSO) δ 164.9, 152.4, 149.1, 136.9, 133.8, 133.7, 132.7, 131.9, 130.7, 129.6, 129.1, 128.4, 128.1, 126.7, 126.6, 125.8, 125.4, 123.3, 117.2, 117.0, 115.6, 55.8;

HRMS (ESI, m/z): calcd. for $[M+Na]^+$:426.0867, found: 426.0867;

HPLC analysis: 96:4 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{major} =26.1 min, t_{minor} = 30.3 min), $[\alpha]_D^{25}$ = +32.00 (c = 0.2, acetone).



2r

(R)-4-chloro-N-(1-(2-hydroxy-5-(trifluoromethyl)phenyl)naphthalen-2-yl)benzamide(2r): white solid, m.p. = 195-196 °C, 39.7 mg, 90% yield

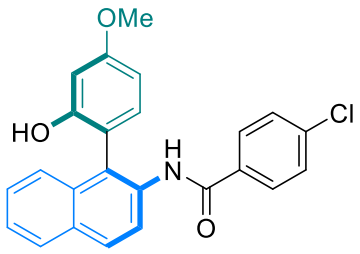
^{1}H NMR (500 MHz, DMSO) δ 10.40 (s, 1H), 9.85 (s, 1H), 8.01 (t, *J* = 7.7 Hz, 2H), 7.69 (dd, *J* = 11.3, 8.5 Hz, 3H), 7.60 (dd, *J* = 8.7, 2.4 Hz, 1H), 7.51 (dd, *J* = 7.9, 5.7 Hz, 3H), 7.48 – 7.44 (m, 2H), 7.41 (d, *J* = 8.4 Hz, 1H), 7.15 (d, *J* = 8.6 Hz, 1H);

^{13}C NMR (126 MHz, DMSO) δ 165.5, 159.1, 136.7, 134.1, 133.8, 132.4, 132.1, 131.1, 129.8, 129.5(q, *J* = 7.3 Hz), 128.8, 128.7, 128.5, 127.0, 126.9, 126.8, 126.2, 126.1, 125.2 (q, *J* = 271.3 Hz), 123.8, 119.8(q, *J* = 31.8 Hz), 116.6;

^{19}F NMR (471 MHz, DMSO) δ -59.5 (s, 3F);

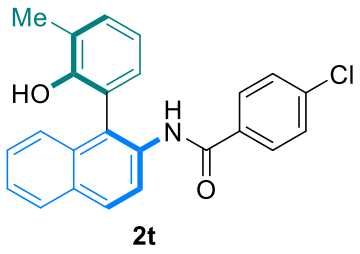
HRMS (ESI, m/z): calcd. for $[M+Na]^+$:464.0636, found: 464.0630;

HPLC analysis: 98:2 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{major} =11.8 min, t_{minor} = 13.8 min), $[\alpha]_D^{25}$ = −60.00 (c = 0.2, acetone).



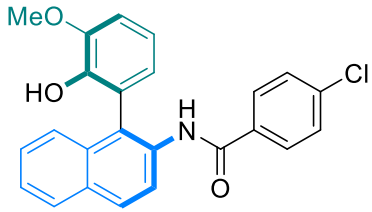
2s

(R)-4-chloro-N-(1-(2-hydroxy-4-methoxyphenyl)naphthalen-2-yl)benzamide(2s):
white solid, m.p. = 209-210 °C, 37.4 mg, 93% yield
^{1}H NMR (500 MHz, DMSO) δ 9.74 (s, 1H), 9.36 (s, 1H), 7.95 – 7.86 (m, 3H), 7.73 (d, *J* = 8.1 Hz, 2H), 7.60 – 7.37 (m, 5H), 7.06 (d, *J* = 8.3 Hz, 1H), 6.62 (s, 1H), 6.57 – 6.48 (m, 1H), 3.76 (s, 3H);
^{13}C NMR (126 MHz, DMSO) δ 164.7, 160.6, 156.3, 136.9, 133.9, 133.8, 133.2, 133.1, 131.9, 130.2, 129.6, 129.1, 128.2, 127.8, 126.6, 126.5, 125.6, 125.0, 115.1, 105.4, 102.0, 55.5;
HRMS (ESI, m/z): calcd. for $[M+Na]^+$:426.0867, found: 426.0864;
HPLC analysis: 98:2 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{minor} =26.2 min, t_{major}=31.0 min), $[\alpha]_D^{25}$ = −84.00 (c = 0.2, acetone).



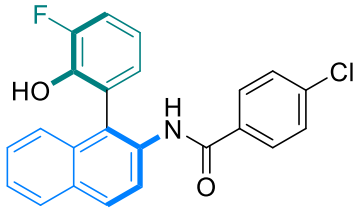
2t

(R)-4-chloro-N-(1-(2-hydroxy-3-methylphenyl)naphthalen-2-yl)benzamide(2t):
white solid, m.p. = 217-218 °C, 36.7 mg, 95% yield
^{1}H NMR (500 MHz, DMSO) δ 9.36 (s, 1H), 7.98 (dd, *J* = 8.5, 5.9 Hz, 2H), 7.90 (d, *J* = 8.8 Hz, 1H), 7.66 (t, *J* = 8.3 Hz, 2H), 7.53 (d, *J* = 8.3 Hz, 2H), 7.51 – 7.47 (m, 1H), 7.45 – 7.39 (m, 2H), 7.23 – 7.17 (m, 1H), 6.95 (dd, *J* = 7.5, 1.8 Hz, 1H), 6.87 (t, *J* = 7.4 Hz, 1H), 2.28 (s, 3H);
^{13}C NMR (126 MHz, DMSO) δ 164.9, 153.1, 136.9, 133.9, 133.8, 133.0, 131.9, 131.3, 130.4, 130.0, 129.6, 129.1, 128.4, 128.2, 126.7, 126.5, 126.0, 125.8, 125.0, 123.7, 120.2, 17.4;
HRMS (ESI, m/z): calcd. for $[M+Na]^+$:410.0918, found: 410.0913;
HPLC analysis: 96.5:3.5 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{minor} =9.2 min, t_{major}= 15.4 min), $[\alpha]_D^{25}$ = −74.50(c = 0.2, acetone).



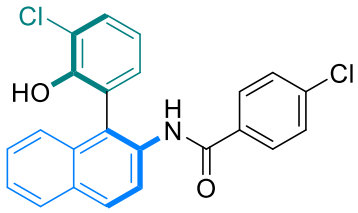
2u

(R)-4-chloro-N-(1-(2-hydroxy-3-methoxyphenyl)naphthalen-2-yl)benzamide(2u):
white solid, m.p. = 159-160 °C, 38.6 mg, 96% yield
^{1}H NMR (500 MHz, DMSO) δ 9.35 (s, 1H), 8.83 (s, 1H), 7.97 (dd, *J* = 8.5, 3.2 Hz, 2H), 7.86 (d, *J* = 8.8 Hz, 1H), 7.69 (dd, *J* = 8.5, 2.3 Hz, 2H), 7.55 – 7.38 (m, 5H), 7.06 (dd, *J* = 8.2, 1.5 Hz, 1H), 6.89 (t, *J* = 7.9 Hz, 1H), 6.77 – 6.72 (m, 1H), 3.87 (s, 3H);
^{13}C NMR (126 MHz, DMSO) δ 164.8, 148.3, 144.5, 136.8, 133.8, 133.6, 132.7, 131.8, 130.2, 129.6, 129.0, 128.3, 128.0, 126.6, 126.5, 125.7, 125.2, 123.9, 123.0, 119.5, 111.9, 56.3;
HRMS (ESI, m/z): calcd. for $[M+Na]^+$:426.0867, found: 426.0864;
HPLC analysis: 99:1 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{minor} =30.5 min, t_{major}= 51.9 min), $[\alpha]_D^{25}$ = +32.00 (c = 0.2, acetone).



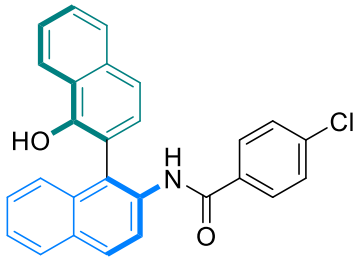
2v

(R)-4-chloro-N-(1-(3-fluoro-2-hydroxyphenyl)naphthalen-2-yl)benzamide(2v):
white solid, m.p. = 219-220 °C, 38.3 mg, 98% yield
^{1}H NMR (400 MHz, DMSO) δ 9.61 (s, 1H), 9.58 (s, 1H), 7.99 (dd, *J* = 8.5, 4.9 Hz, 2H), 7.76 (d, *J* = 8.7 Hz, 1H), 7.71 (d, *J* = 8.1 Hz, 2H), 7.55 – 7.48 (m, 3H), 7.48 – 7.38 (m, 2H), 7.29 – 7.20 (m, 1H), 6.95 (d, *J* = 7.6 Hz, 1H), 6.92 – 6.85 (m, 1H);
^{13}C NMR (126 MHz, DMSO) δ 165.2, 152.3 (d, *J* = 239.0 Hz),143.3(d, *J* = 14.4 Hz), 136.8, 134.0, 133.8, 132.6, 132.0, 130.3(d, *J* = 2.6 Hz), 129.8, 128.9, 128.4(d, *J* = 4.0 Hz), 127.7(d, *J* = 2.8 Hz), 126.8, 126.5(d, *J* = 2.9 Hz), 126.3, 126.1, 125.9, 119.5(d, *J* = 7.3 Hz), 116.0, 115.8;
^{19}F NMR (471 MHz, DMSO) δ -135.0 (s, 1F);
HRMS (ESI, m/z): calcd. for $[M+Na]^+$:414.0668, found: 414.0664;
HPLC analysis: 99:1 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{minor} =26.3 min, t_{major}= 28.3 min), $[\alpha]_D^{25}$ = +28.00 (c = 0.2, acetone).



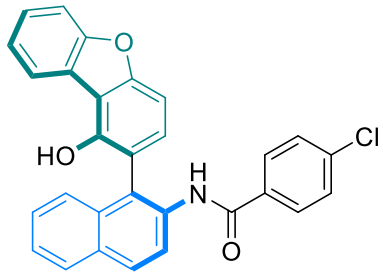
2w

(R)-4-chloro-N-(1-(3-chloro-2-hydroxyphenyl)naphthalen-2-yl)benzamide(2w):
white solid, m.p. = 231-232 °C, 40.3 mg, 99% yield
^{1}H NMR (500 MHz, DMSO) δ 9.69 (s, 1H), 9.17 (s, 1H), 8.00 (dd, *J* = 8.7, 6.8 Hz, 2H), 7.75 (d, *J* = 8.8 Hz, 1H), 7.70 (d, *J* = 8.5 Hz, 2H), 7.55 – 7.49 (m, 3H), 7.48 – 7.42 (m, 2H), 7.37 (d, *J* = 8.4 Hz, 1H), 7.08 (dd, *J* = 7.6, 1.7 Hz, 1H), 6.94 (t, *J* = 7.8 Hz, 1H);
^{13}C NMR (126 MHz, DMSO) δ 165.4, 151.2, 136.8, 134.1, 133.8, 132.6, 132.0, 131.1, 130.6, 130.0, 129.8, 128.9, 128.6, 128.4, 126.9, 126.3, 126.2, 126.1, 126.0, 121.7, 120.8;
HRMS (ESI, m/z): calcd. for $[M+Na]^+$:430.0372, found: 430.0369;
HPLC analysis: 97:3 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{minor} =23.6 min, t_{major}= 27.9 min), $[\alpha]_D^{25}$ = +61.00 (c = 0.2, acetone).



2x

(R)-4-chloro-N-(1'-hydroxy-[1,2'-binaphthalen]-2-yl)benzamide(2x):
white solid, m.p. = 228-229 °C, 41.0 mg, 97% yield
^{1}H NMR (500 MHz, DMSO) δ 9.59 (s, 1H), 9.25 (s, 1H), 8.31 (q, 1H), 8.02 (dd, *J* = 11.4, 8.5 Hz, 2H), 7.89 (t, *J* = 7.2 Hz, 2H), 7.70 – 7.63 (m, 2H), 7.57 – 7.47 (m, 4H), 7.46 – 7.38 (m, 4H), 7.22 (d, *J* = 8.3 Hz, 1H);
^{13}C NMR (126 MHz, DMSO) δ 165.2, 150.6, 136.8, 134.7, 134.4, 133.7, 133.0, 132.1, 130.6, 130.0, 129.7, 128.9, 128.5, 128.4, 128.1, 126.8, 126.7, 126.5, 126.0, 125.8, 125.7, 125.6, 122.9, 119.8, 117.7;
HRMS (ESI, m/z): calcd. for $[M+Na]^+$:446.0918, found: 446.0914;
HPLC analysis: 96:4 er ee, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{major} =27.29 min, t_{minor}=29.06 min), $[\alpha]_D^{25}$ = −94.00 (c = 0.2, acetone).



2y

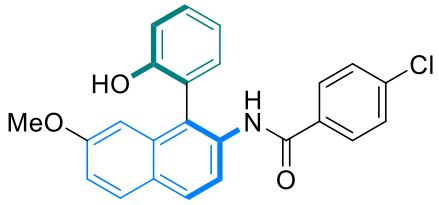
(R)-4-chloro-N-(1-(1-hydroxydibenzo[b,d]furan-2-yl)naphthalen-2-yl)benzamide (2y): white solid, m.p. = 247-248 °C, 45.8 mg, 99% yield

^{1}H NMR (500 MHz, DMSO) δ 9.66 (s, 1H), 9.41 (s, 1H), 8.17 (d, *J* = 7.4 Hz, 1H), 8.06 – 7.96 (m, 2H), 7.90 (d, *J* = 8.6 Hz, 1H), 7.68 (d, *J* = 8.6 Hz, 3H), 7.54 – 7.36 (m, 7H), 7.32 – 7.16 (m, 2H);

^{13}C NMR (126 MHz, DMSO) δ 165.4, 157.1, 155.4, 151.4, 136.7, 134.9, 133.8, 133.4, 132.1, 131.4, 129.7, 128.8, 128.6, 128.6, 128.5, 126.9, 126.8, 126.3, 125.8, 125.7, 123.8, 123.5, 123.0, 118.1, 113.8, 111.7, 103.8;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:464.1048, found: 464.1044;

HPLC analysis: 93:7 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{minor}=16.86 min, t_{major}=26.54 min), $[\alpha]_D^{25}$ = +65.00 (c = 0.2, acetone).



2z

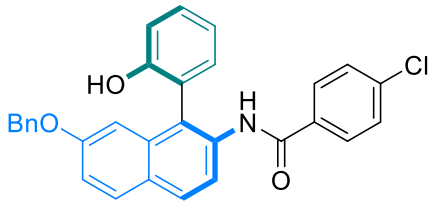
(R)-4-chloro-N-(1-(2-hydroxyphenyl)-7-methoxynaphthalen-2-yl)benzamide (2z): white solid, m.p. = 171-172 °C, 39.8 mg, 99% yield

^{1}H NMR (500 MHz, DMSO) δ 9.69 (s, 1H), 9.35 (s, 1H), 7.90 (dd, *J* = 8.9, 4.1 Hz, 2H), 7.69 (t, *J* = 9.2 Hz, 3H), 7.52 (d, *J* = 8.2 Hz, 2H), 7.28 (t, *J* = 7.6 Hz, 1H), 7.21 – 7.14 (m, 2H), 7.05 (d, *J* = 8.1 Hz, 1H), 6.92 (t, *J* = 7.4 Hz, 1H), 6.79 (d, *J* = 2.6 Hz, 1H), 3.64 (s, 3H);

^{13}C NMR (126 MHz, DMSO) δ 164.6, 157.7, 155.3, 136.8, 134.2, 134.1, 133.8, 132.5, 130.0, 129.9, 129.5, 129.4, 129.0, 127.8, 127.3, 122.9, 122.8, 119.6, 117.5, 116.4, 105.6, 55.3;

HRMS (ESI, m/z): calcd. for $[M+Na]^+$:426.0867, found: 426.0865;

HPLC analysis: 96:4 er, (CHIRALCEL OD column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{major}=10.76 min, t_{minor}=12.32 min), $[\alpha]_D^{25}$ = −58.00 (c = 0.2, acetone).



2aa

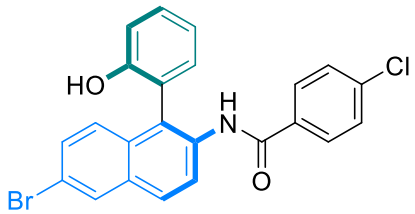
(R)-N-(7-(benzyloxy)-1-(2-hydroxyphenyl)naphthalen-2-yl)-4-chlorobenzamide (2aa): white solid, m.p. = 162-163 °C, 47.4 mg, 99% yield

^{1}H NMR (500 MHz, DMSO) δ 9.68 (s, 1H), 9.34 (s, 1H), 7.90 (t, *J* = 8.9 Hz, 2H), 7.74 – 7.62 (m, 3H), 7.55 – 7.48 (m, 2H), 7.37 – 7.27 (m, 6H), 7.25 (dd, *J* = 8.9, 2.5 Hz, 1H), 7.09 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.06 (dd, *J* = 8.2, 1.1 Hz, 1H), 6.96 – 6.85 (m, 2H), δ 5.00 (d, *J* = 11.5 Hz, 2H);

^{13}C NMR (126 MHz, DMSO) δ 164.6, 156.7, 155.2, 137.1, 136.8, 134.2, 134.1, 133.8, 132.5, 130.0, 129.8, 129.5, 129.4, 129.0, 128.9, 128.4, 128.4, 128.3, 127.7, 127.4, 122.8, 119.6, 117.8, 116.4, 107.3, 69.7;

HRMS (ESI, m/z): calcd. for $[M+Na]^+$:502.1180, found: 502.1177;

HPLC analysis: 97:3 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{minor}=19.5 min, t_{major}=25.1 min), $[\alpha]_D^{25}$ = −108.00 (c = 0.2, acetone).



2ab

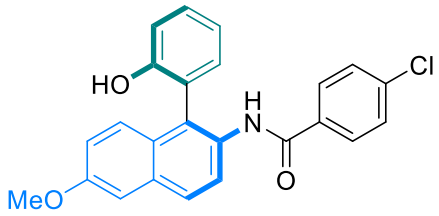
(R)-N-(6-bromo-1-(2-hydroxyphenyl)naphthalen-2-yl)-4-chlorobenzamide(2ab): white solid, m.p. = 95-96 °C, 40.6 mg, 90% yield

^{1}H NMR (500 MHz, DMSO) δ 8.23 (t, *J* = 1.5Hz, 1H), 7.99 – 7.91 (m, 2H), 7.76 (d, *J* = 8.6 Hz, 2H), 7.55 (d, *J* = 1.2 Hz, 2H), 7.35 (d, *J* = 8.3 Hz, 2H), 7.19 – 7.14 (m, 1H), 7.08 (dd, *J* = 7.6, 1.8 Hz, 1H), 7.03 (dd, *J* = 8.3, 1.2 Hz, 1H), 6.78 – 6.72 (m, 1H);

^{13}C NMR (126 MHz, DMSO) δ163.8, 158.4, 136.5, 134.3, 133.3, 132.8, 132.7, 131.4, 130.5, 129.7, 129.5, 129.2, 128.9, 128.8, 128.6, 126.4, 125.5, 122.6, 118.4, 117.5, 116.8.

HRMS (ESI, m/z): calcd. for $[M+H]^+$:452.0047, found: 452.0041;

HPLC analysis: 97:3 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{minor}=19.4 min, t_{major}=32.3 min), $[\alpha]_D^{25}$ = −54.00 (c = 0.2, acetone).



2ac

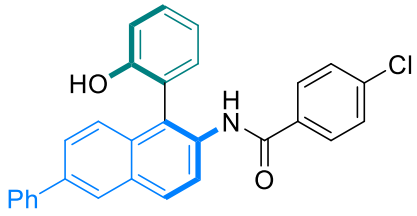
(R)-4-chloro-N-(1-(2-hydroxyphenyl)-6-methoxynaphthalen-2-yl)benzamide(2ac): white solid, m.p. = 209-210 °C, 39.8 mg, 99% yield

^{1}H NMR (500 MHz, DMSO) δ 9.65 (s, 1H), 9.41 (s, 1H), 7.87 (d, *J* = 8.8 Hz, 1H), 7.74 (d, *J* = 8.8 Hz, 1H), 7.69 (d, *J* = 8.2 Hz, 2H), 7.52 (d, *J* = 8.4 Hz, 2H), 7.39 (d, *J* = 2.6 Hz, 1H), 7.36 (d, *J* = 9.2 Hz, 1H), 7.27 (td, *J* = 7.7, 1.7 Hz, 1H), 7.13 (d, *J* = 7.5 Hz, 1H), 7.10 (dd, *J* = 9.2, 2.6 Hz, 1H), 7.03 (d, *J* = 8.1 Hz, 1H), 6.89 (t, *J* = 7.4 Hz, 1H), 3.89 (s, 3H);

^{13}C NMR (126 MHz, DMSO) δ 164.8, 157.3, 155.3, 136.7, 133.9, 133.3, 132.5, 131.6, 131.3, 129.7, 129.6, 128.9, 128.2, 128.0, 126.8, 126.2, 123.0, 119.4, 119.0, 116.2, 106.6, 55.7;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:404.1048, found: 404.1044;

HPLC analysis: 96:4 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{minor}=28.6 min, t_{major}=38.8 min), $[\alpha]_D^{25}$ = −98.00 (c = 0.2, acetone).



2ad

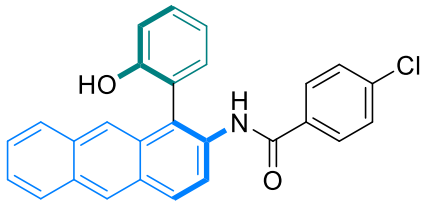
(R)-4-chloro-N-(1-(2-hydroxyphenyl)-6-phenylnaphthalen-2-yl)benzamide(2ad): white solid, m.p. = 219-220 °C, 42.2 mg, 94% yield

^{1}H NMR (500 MHz, DMSO) δ 9.73 (s, 1H), 9.43 (s, 1H), 8.28 (d, *J* = 1.9 Hz, 1H), 8.06 (d, *J* = 8.8 Hz, 1H), 7.88 (d, *J* = 8.8 Hz, 1H), 7.84 – 7.80 (m, 2H), 7.78 (dd, *J* = 8.9, 2.0 Hz, 1H), 7.70 (d, *J* = 8.5 Hz, 2H), 7.55 – 7.51 (m, 5H), 7.40 (t, *J* = 7.3 Hz, 1H), 7.30 (td, *J* = 7.8, 1.7 Hz, 1H), 7.18 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.06 (d, *J* = 8.2 Hz, 1H), 6.93 (t, *J* = 7.4 Hz, 1H);

^{13}C NMR (126 MHz, DMSO) δ 164.8, 155.4, 140.3, 137.3, 136.9, 133.9, 133.8, 132.6, 132.2, 132.1, 130.6, 130.0, 129.6, 129.5, 129.0, 128.4, 128.1, 127.4, 127.3, 125.8, 125.8, 125.7, 122.7, 119.6, 116.4;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:450.1255, found: 450.1250;

HPLC analysis: 97:3 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{minor}=34.01 min, t_{major}=36.19), $[\alpha]_D^{25}$ = +87.00 (c = 0.2, acetone).



2ae

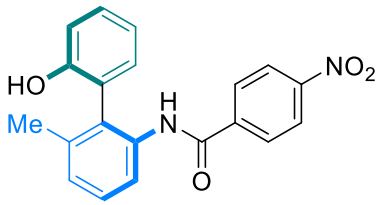
(R)-4-chloro-N-(1-(2-hydroxyphenyl)anthracen-2-yl)benzamide(2ae): yellow solid, m.p. = 251-252 °C, 41.8 mg, 99% yield

^{1}H NMR (500 MHz, DMSO) δ 9.74 (s, 1H), 9.46 (s, 1H), 8.64 (s, 1H), 8.15 (d, *J* = 9.1 Hz, 1H), 8.09 (d, *J* = 8.4 Hz, 1H), 8.05 (s, 1H), 7.89 – 7.84 (m, 2H), 7.72 (d, *J* = 8.1 Hz, 2H), 7.57 – 7.42 (m, 4H), 7.35 (t, *J* = 7.8 Hz, 1H), 7.24 (d, *J* = 7.5 Hz, 1H), 7.11 (d, *J* = 8.2 Hz, 1H), 6.98 (t, *J* = 7.4 Hz, 1H);

^{13}C NMR (126 MHz, DMSO) δ 164.8, 155.5, 136.9, 133.7, 133.1, 132.6, 131.6, 131.2, 131.1, 130.3, 130.0, 129.9, 129.6, 129.0, 128.6, 128.3, 128.2, 126.7, 126.2, 126.0, 125.6, 124.9, 122.8, 119.7, 116.5;

HRMS (ESI, m/z): calcd. for $[M+Na]^+$:446.0918, found: 446.0915;

HPLC analysis: 98:2 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{minor}=19.4 min, t_{major}=21.9 min), $[\alpha]_D^{25}$ = −74.00 (c = 0.2, acetone).



2af

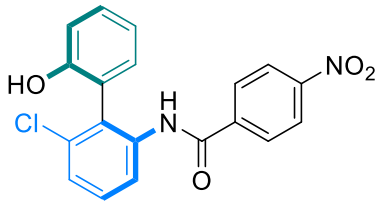
(R)-N-(2'-hydroxy-6-methyl-[1,1'-biphenyl]-2-yl)-4-nitrobenzamide(2af): yellow solid, m.p. = 149-150 °C, 34.4 mg, 99% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.25 (d, *J* = 8.2 Hz, 1H), 8.20 – 8.07 (m, 2H), 7.78 (s, 1H), 7.57 (d, *J* = 8.7 Hz, 2H), 7.44 – 7.38 (m, 1H), 7.35 (t, *J* = 7.9 Hz, 1H), 7.17 – 7.07 (m, 4H), 5.49 (s, 1H), 2.12 (s, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 163.1, 153.2, 149.6, 140.0, 138.6, 135.8, 130.8, 130.6, 129.4, 127.9, 127.1, 126.4, 123.9, 121.9, 121.7, 118.9, 116.7, 20.3;

HRMS (ESI, m/z): calcd. for $[M+Na]^+$:371.1002, found: 371.0999;

HPLC analysis: 94:6 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{major}=16.3 min, t_{minor}=22.0min), $[\alpha]_D^{25}$ = +112.00 (c = 0.2, acetone).



2ag

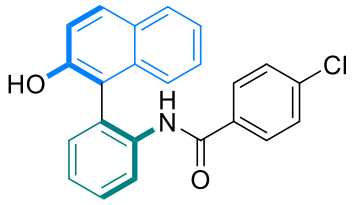
(S)-N-(6-chloro-2'-hydroxy-[1,1'-biphenyl]-2-yl)-4-nitrobenzamide (2ag): white solid, m.p. = 190-191 °C, 36.1 mg, 98% yield

^{1}H NMR (500 MHz, DMSO) δ 9.69 (s, 1H), 9.66 (s, 1H), 8.25 (d, *J* = 8.5 Hz, 2H), 7.81 (d, *J* = 8.5 Hz, 2H), 7.60 (d, *J* = 7.8 Hz, 1H), 7.50 – 7.40 (m, 2H), 7.22 – 7.16 (m, 1H), 7.08 (dd, *J* = 7.6, 1.6 Hz, 1H), 6.93 (d, *J* = 8.1 Hz, 1H), 6.83 (t, *J* = 7.4 Hz, 1H);

^{13}C NMR (126 MHz, DMSO) δ 164.3, 154.9, 149.5, 140.6, 137.9, 134.5, 134.2, 131.7, 130.0, 129.2, 129.1, 127.5, 125.8, 124.0, 122.5, 119.1, 116.0;

HRMS (ESI, m/z): calcd. for $[M+Na]^+$:371.1002, found: 371.0999;

HPLC analysis: 95:5 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{major}=16.3 min, t_{minor}=22.4 min), $[\alpha]_D^{25}$ = −48.00 (c = 0.2, acetone).



2ah

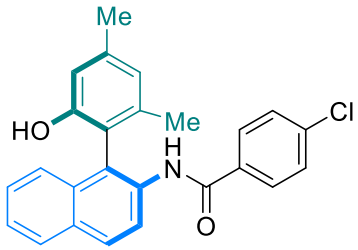
(R)-4-chloro-N-(2-(2-hydroxynaphthalen-1-yl)phenyl)benzamide (2ah): white solid, m.p. = 180-181 °C, 34.4mg, 92% yield

^{1}H NMR (500 MHz, DMSO) δ 8.99 (s, 1H), 7.94 (d, *J* = 8.1 Hz, 1H), 7.83 (t, *J* = 8.2 Hz, 2H), 7.53 – 7.44 (m, 1H), 7.39 (s, 4H), 7.36 – 7.22 (m, 7H);

^{13}C NMR (126 MHz, DMSO) δ 164.4, 152.5, 137.0, 136.6, 134.1, 133.7, 132.8, 130.5, 130.0, 129.3, 128.9, 128.6, 128.5, 128.1, 126.8, 125.4, 125.2, 124.7, 123.1, 118.7, 117.4;

HRMS (ESI, m/z): calcd. for $[M+Na]^+$: 396.0762, found: 396.0761;

HPLC analysis: 92:8 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{minor} = 16.9 min, t_{major} = 21.3 min), $[\alpha]_D^{25}$ = +100.00 (c = 0.2, acetone).



2ai

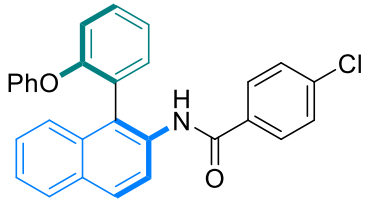
(R)-4-chloro-N-(1-(2-hydroxy-4,6-dimethylphenyl)naphthalen-2-yl)benzamide (2ai): white solid, m.p. = 190-192 °C, 39.7 mg, 99% yield; For kinetic resolution: 49% yield.

^{1}H NMR (500 MHz, DMSO) δ 9.16 (s, 1H), 8.97 (s, 1H), 8.02 (d, *J* = 8.8 Hz, 1H), 7.96 (d, *J* = 8.5 Hz, 2H), 7.63 (d, *J* = 8.5 Hz, 2H), 7.53 (d, *J* = 8.5 Hz, 2H), 7.49 – 7.44 (m, 1H), 7.42 – 7.37 (m, 1H), 7.26 (d, *J* = 8.4 Hz, 1H), 6.68 (d, *J* = 13.3 Hz, 2H), 2.28 (s, 3H), 1.75 (s, 3H);

^{13}C NMR (126 MHz, DMSO) δ 164.7, 155.6, 138.8, 138.7, 136.9, 134.1, 134.0, 132.7, 131.7, 129.6, 129.1, 128.5, 128.3, 127.8, 126.7, 125.8, 125.6, 124.2, 122.4, 119.2, 114.3, 21.5, 20.1;

HRMS (ESI, m/z): calcd. for $[M+Na]^+$:424.1075, found: 424.1072;

HPLC analysis: 51:49 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{major}=14.6 min, t_{minor}=17.7min), $[\alpha]_D^{25}$ = +50.00 (c = 0.2, acetone); For kinetic resolution: 95:5 er, $[\alpha]_D^{25}$ = +162.00 (c = 0.2, acetone).



3

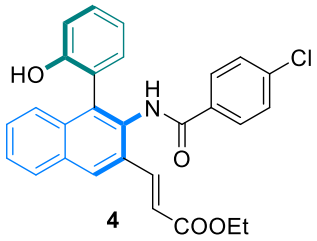
(R)-4-chloro-N-(1-(2-phenoxyphenyl)naphthalen-2-yl)benzamide (3): white solid, m.p. = 131-132 °C, 76.0 mg, 84% yield

^{1}H NMR (500 MHz, DMSO) δ 9.74 (s, 1H), 7.96 (t, *J* = 8.5 Hz, 2H), 7.74 (d, *J* = 8.3 Hz, 2H), 7.69 (d, *J* = 8.7 Hz, 1H), 7.54 (dd, *J* = 8.7, 2.4 Hz, 3H), 7.51 – 7.43 (m, 2H), 7.43 – 7.36 (m, 2H), 7.23 (t, *J* = 7.5 Hz, 1H), 7.19 (t, *J* = 7.8 Hz, 2H), 6.98 (t, *J* = 7.4 Hz, 1H), 6.91 (d, *J* = 8.2 Hz, 1H), 6.82 (d, *J* = 8.0 Hz, 2H);

^{13}C NMR (126 MHz, DMSO) δ 165.2, 156.5, 155.4, 136.8, 134.1, 133.9, 133.4, 132.7, 132.0, 130.7, 130.2, 130.1, 129.9, 128.9, 128.5, 128.4, 127.1, 126.8, 126.3, 126.1, 126.0, 123.9, 123.4, 119.5, 118.1;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:450.1255, found: 450.1244);

HPLC analysis: 98:2 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{major}= 22.2min, t_{minor}=58.5min), $[\alpha]_D^{25}$ = +150.00 (c = 0.2, acetone).



4

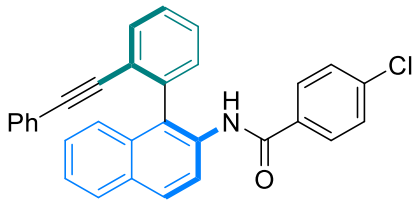
Ethyl(R,E)-3-(3-(4-chlorobenzamido)-4-(2-hydroxyphenyl)naphthalen-2-yl)acrylate (4) : white solid, m.p. = 109-110 °C, 36.0 mg, 77% yield

^{1}H NMR (500 MHz, DMSO) δ 9.96 (s, 1H), 9.49 (s, 1H), 8.64 (s, 1H), 8.08 (d, *J* = 8.0 Hz, 1H), 7.87 (d, *J* = 16.0 Hz, 1H), 7.69 (d, *J* = 8.5 Hz, 2H), 7.62 – 7.56 (m, 1H), 7.54 (d, *J* = 8.5 Hz, 2H), 7.52 – 7.47 (m, 1H), 7.42 (d, *J* = 8.5 Hz, 1H), 7.24 (td, *J* = 7.7, 1.8 Hz, 1H), 7.09 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.00 (d, *J* = 8.1 Hz, 1H), δ 6.86 (d, *J* = 3.5 Hz, 1H), 6.83 (d, *J* = 5.5 Hz, 2H), 4.18 (q, *J* = 7.0 Hz, 2H), 1.24 (t, *J* = 7.0 Hz, 3H);

^{13}C NMR (126 MHz, DMSO) δ 166.7, 166.1, 155.3, 141.8, 136.8, 136.3, 133.7, 133.5, 132.9, 132.4, 131.6, 131.1, 129.8, 129.6, 129.1, 128.9, 127.7, 127.0, 126.9, 126.9, 123.4, 119.9, 119.1, 115.9, 60.6, 14.6;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:472.1310, found: 472.1298;

HPLC analysis: 99:1 er, (CHIRALCEL OD column, *n*-hexane/*i*-PrOH = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, t_{major}= 24.5min, t_{minor}= 26.7min), $[\alpha]_D^{25}$ = +22.00 (c = 0.2, acetone).



5

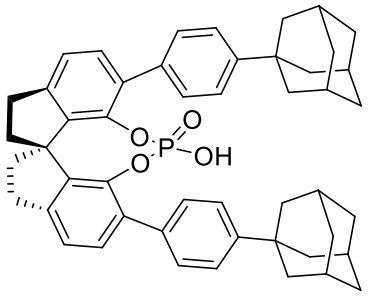
(R)-4-chloro-N-(1-(2-(phenylethynyl)phenyl)naphthalen-2-yl)benzamide (5): yellow solid, m.p. = 120-122 °C, 25.8 mg, 52% yield,

^{1}H NMR (500 MHz,$CDCl_3$) δ 8.61 (d, *J* = 8.8 Hz, 1H), 8.01 (d, *J* = 8.9 Hz, 1H), 7.91 (d, *J* = 8.1 Hz, 1H), 7.87 – 7.78 (m, 2H), 7.58 – 7.53 (m, 2H), 7.49 (d, *J* = 8.2 Hz, 2H), 7.47 – 7.42 (m, 2H), 7.42 – 7.37 (m, 2H), 7.33 (d, *J* = 8.1 Hz, 2H), 7.17 (d, *J* = 7.2 Hz, 1H), 7.13 (t, *J* = 7.5 Hz, 2H), 6.89 (d, *J* = 7.5 Hz, 2H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 164.2, 138.2, 138.0, 133.4, 133.2, 132.6, 132.5, 131.6, 131.4, 131.1, 129.2, 129.0, 128.9, 128.8, 128.5, 128.3, 128.2, 128.1, 126.6, 126.5, 125.8, 125.1, 124.4, 122.3, 120.7, 93.8, 87.2;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:458.1306, found: 458.1294;

HPLC analysis: 96:4 er, (CHIRALCEL OD column, *n*-hexane/*i*-PrOH = 80/20, flow rate = 1.0 mL/min, λ = 254 nm, t_{major}= 16.3min, t_{minor}= 23.7min), $[\alpha]_D^{25}$ = −116.00 (c = 0.2, acetone).



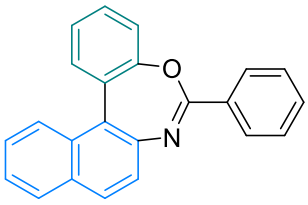
(*R*)-**C2**

1,10-bis(4-((3S,5S,7S)-adamantan-1-yl)phenyl)-12-hydroxy-4,5,6,7-tetrahydrodiindeno[7,1-de:1',7'-fg][1,3,2]dioxaphosphocine 12-oxide (*R*)-C2: white solid, m.p. > 300 °C, 410.0 mg, 87.4% yield,

^{1}H NMR (500 MHz, DMSO) δ 7.39 (d, *J* = 8.5 Hz, 4H), 7.33 – 7.28 (m, 4H), 7.24 (d, *J* = 7.6 Hz, 2H), 7.17 (d, *J* = 7.7 Hz, 2H), 3.16 – 3.06 (m, 2H), 2.85 (dd, *J* = 16.0, 7.5 Hz, 2H), 2.31 (dd, *J* = 12.0, 6.5 Hz, 2H), 2.04 (t, *J* = 3.2 Hz, 6H), 1.85 (d, *J* = 3.0 Hz, 13H), 1.72 (d, *J* = 3.3 Hz, 13H);

^{13}C NMR (126 MHz, DMSO) δ 149.5, 145.2, 143.2, 143.1, 141.2, 135.7, 134.3, 130.2, 129.4, 124.7, 122.4, 59.8, 43.1, 39.1, 36.7, 36.0, 28.8;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:735.3598, found: 735.3586.



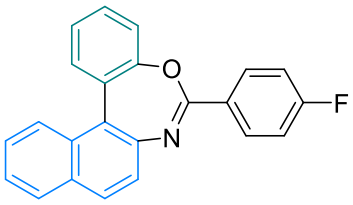
1a

6-phenylbenzo[f]naphtho[2,1-d][1,3]oxazepane (1a): white solid, m.p. = 55-56 °C, 85.0 mg, 88% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.43 – 8.37 (m, 2H), 8.31 – 8.26 (m, 1H), 7.94 – 7.87 (m, 2H), 7.79 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.59 – 7.49 (m, 6H), 7.47 – 7.42 (m, 1H), 7.39 – 7.30 (m, 2H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.7, 157.3, 142.0, 132.8, 132.2, 132.1, 131.8, 131.4, 129.8, 129.3, 129.2, 128.8, 128.6, 128.4, 127.7, 126.5, 126.4, 126.1, 125.5, 124.9, 121.4;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:322.1226, found: 322.1224.



1b

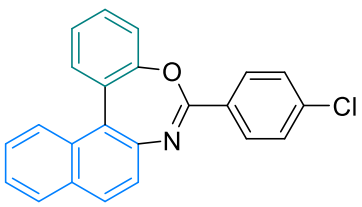
6-(4-fluorophenyl)benzo[f]naphtho[2,1-d][1,3]oxazepane (1b): white solid, m.p. = 147-148 °C, 97.7 mg, 96% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.44 – 8.34 (m, 2H), 8.32 – 8.22 (m, 1H), 7.95 – 7.87 (m, 2H), 7.83 – 7.73 (m, 1H), 7.56 – 7.49 (m, 3H), 7.47 – 7.42 (m, 1H), 7.34 (t, *J* = 7.6 Hz, 2H), 7.19 (t, *J* = 8.7 Hz, 2H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 165.2(d, *J* = 253.4 Hz), 157.6, 156.3, 141.9, 132.9, 132.2, 131.6 (d, *J* = 8.9 Hz), 131.4, 129.9, 129.2, 128.8, 128.4, 127.6, 126.6, 126.4, 126.0, 125.6, 125.0, 121.3, 115.8, 115.7;

^{19}F NMR (471 MHz, $CDCl_3$) δ -107.6. (s, 1F);

HRMS (ESI, m/z): calcd. for $[M+H]^+$:340.1132, found: 340.1131.



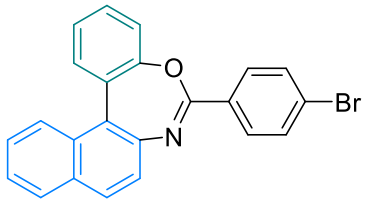
1c

6-(4-chlorophenyl)benzo[f]naphtho[2,1-d][1,3]oxazepane (1c): white solid, m.p. = 183-184 °C, 103.0 mg, 97% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.32 (s, 1H), 8.30 (s, 1H), 8.29 – 8.25 (m, 1H), 7.94 – 7.87 (m, 2H), 7.78 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.56 – 7.43 (m, 6H), 7.37 – 7.29 (m, 2H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.5, 156.3, 141.8, 138.1, 132.3, 132.2, 131.4, 130.7, 130.6, 129.9, 129.2, 128.9, 128.8, 128.4, 127.7, 126.6, 126.4, 126.0, 125.6, 125.0, 121.3;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:356.0837, found: 356.0833.



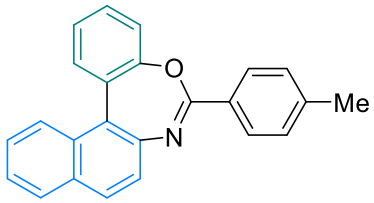
1d

6-(4-bromophenyl)benzo[f]naphtho[2,1-d][1,3]oxazepane (1d): white solid, m.p. = 164-165 °C, 89.7 mg, 75% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.31 – 8.26 (m, 1H), 8.24 (d, *J* = 8.2 Hz, 2H), 7.90 (t, *J* = 8.5 Hz, 2H), 7.78 (d, *J* = 7.7 Hz, 1H), 7.64 (d, *J* = 8.2 Hz, 2H), 7.57 – 7.48 (m, 3H), 7.45 (t, *J* = 7.8 Hz, 1H), 7.33 (q, *J* = 7.8 Hz, 2H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.5, 156.4, 141.8, 132.9, 132.3, 131.9, 131.4, 131.1, 130.7, 129.9, 129.2, 128.9, 128.4, 127.7, 126.7, 126.6, 126.4, 126.0, 125.6, 125.0, 121.3;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:400.0332, found: 400.0326.



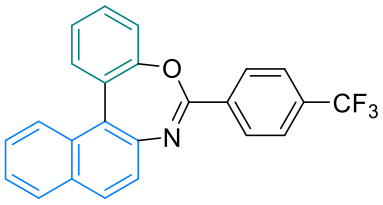
1e

6-(p-tolyl)benzo[f]naphtho[2,1-d][1,3]oxazepane (1e): white solid, m.p. = 135-136 °C, 70.3 mg, 70% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.32 – 8.25 (m, 3H), 7.93 – 7.88 (m, 2H), 7.79 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.56 (d, *J* = 8.7 Hz, 1H), 7.52 – 7.49 (m, 2H), 7.46 – 7.41 (m, 1H), 7.38 – 7.30 (m, 4H), 2.45 (s, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.7, 157.5, 142.4, 142.2, 132.8, 132.7, 132.1, 131.5, 129.7, 129.5, 129.4, 129.3, 128.7, 128.4, 127.6, 126.5, 126.4, 126.1, 125.4, 124.8, 121.4, 21.7;

HRMS (ESI, m/z): calcd. for $[M+Na]^+$:358.1202, found: 358.1199.



1f

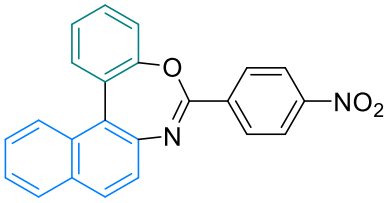
6-(4-(trifluoromethyl)phenyl)benzo[f]naphtho[2,1-d][1,3]oxazepane (1f): white solid, m.p. = 109-110 °C, 91.0 mg, 78%yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.49 (d, *J* = 8.1 Hz, 2H), 8.28 (d, *J* = 7.4 Hz, 1H), 7.92 (s, 2H), 7.77 (d, *J* = 9.1 Hz, 3H), 7.54 – 7.45 (m, 4H), 7.34 (d, *J* = 8.5 Hz, 2H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.5, 155.7, 141.6, 135.5, 133.0, 132.4, 131.3, 130.0, 129.5, 129.4, 129.1, 128.9, 128.4, 127.9, 126.7, 126.5, 126.0, 125.8, 125.6(q, *J* = 3.2 Hz), 125.1, 123.9 (q, *J* = 274.5Hz), 121.2;

^{19}F NMR (471 MHz, $CDCl_3$) δ -62.8. (s, 3F);

HRMS (ESI, m/z): calcd. for $[M+H]^+$:390.1100, found: 390.1089.



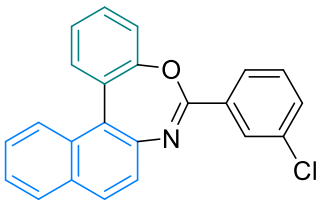
1g

6-(4-nitrophenyl)benzo[f]naphtho[2,1-d][1,3]oxazepane (1g): yellow solid, m.p. = 189-190 °C, 78.0 mg, 71% yield

^{1}H NMR (500 MHz,$CDCl_3$) δ 8.56 – 8.49 (m, 2H), 8.37 – 8.31 (m, 2H), 8.29 – 8.25 (m, 1H), 7.92 (dd, *J* = 9.0, 4.5 Hz, 2H), 7.79 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.56 – 7.51 (m, 3H), 7.50 – 7.45 (m, 1H), 7.39 – 7.31 (m, 2H);

^{13}C NMR (126 MHz,$CDCl_3$) δ 157.3, 154.9, 149.5, 141.3, 137.9, 133.1, 132.5, 131.3, 130.1, 130.0, 129.0, 128.9, 128.4, 128.1, 126.7, 126.5, 126.0, 125.9, 125.3, 123.7, 121.1;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:367.1077, found: 367.1072.



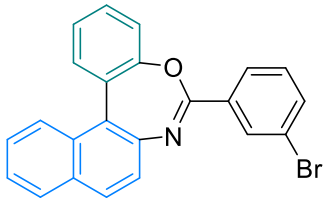
1h

6-(3-chlorophenyl)benzo[f]naphtho[2,1-d][1,3]oxazepane (1h): white solid, m.p. = 70-71 °C, 86.3 mg, 81% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.36 (d, *J* = 1.9 Hz, 1H), 8.27 (t, *J* = 8.4 Hz, 2H), 7.91 (t, *J* = 7.7 Hz, 2H), 7.81 – 7.76 (m, 1H), 7.55 – 7.43 (m, 6H), 7.37 – 7.32 (m, 2H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.5, 155.8, 141.7, 134.7, 134.0, 132.9, 132.3, 131.7, 131.4, 130.0, 129.9, 129.2, 129.1, 128.9, 128.4, 127.8, 127.3, 126.6, 126.4, 126.0, 125.7, 125.1, 121.3;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:356.0837, found: 356.0832.



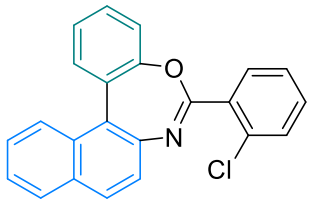
1i

6-(3-bromophenyl)benzo[f]naphtho[2,1-d][1,3]oxazepane (1i): white solid, m.p. = 60-61 °C, 108.9 mg, 91% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.52 (t, *J* = 1.8 Hz, 1H), 8.33 – 8.25 (m, 2H), 7.91 (dd, *J* = 9.2, 6.1 Hz, 2H), 7.78 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.67 (dt, *J* = 7.7, 1.4 Hz, 1H), 7.57 – 7.50 (m, 3H), 7.49 – 7.44 (m, 1H), 7.42 – 7.32 (m, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.5, 155.7, 141.7, 134.6, 134.2, 132.9, 132.4, 132.2, 131.4, 130.1, 130.0, 129.1, 128.9, 128.4, 127.8, 127.7, 126.6, 126.4, 126.0, 125.7, 125.1, 122.8, 121.3;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:400.0332, found: 400.0326.



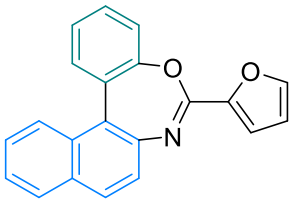
1j

6-(2-chlorophenyl)benzo[f]naphtho[2,1-d][1,3]oxazepane (1j): white solid, m.p. = 50-51 °C, 99.0 mg, 93% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.29 (dd, *J* = 6.3, 3.5 Hz, 1H), 7.95 – 7.88 (m, 3H), 7.82 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.56 (d, *J* = 8.7 Hz, 1H), 7.54 – 7.49 (m, 3H), 7.49 – 7.41 (m, 2H), 7.40 – 7.33 (m, 2H), 7.20 (dd, *J* = 8.1, 1.4 Hz, 1H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.8, 155.7, 141.5, 133.8, 132.8, 132.4, 132.3, 131.6, 131.5, 131.3, 131.1, 129.9, 128.9, 128.8, 128.4, 127.6, 126.6, 126.5, 126.4, 125.9, 125.7, 125.1, 121.6;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:356.0837, found: 356.0834.



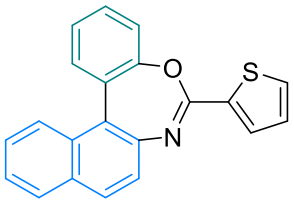
1k

6-(furan-2-yl)benzo[f]naphtho[2,1-d][1,3]oxazepane (1k): white solid, m.p. = 146-147 °C, 64.4 mg, 69% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.3 – 8.2 (m, 1H), 7.9 – 7.9 (m, 2H), 7.8 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.7 (s, 1H), 7.6 (d, *J* = 8.7 Hz, 1H), 7.5 – 7.4 (m, 3H), 7.4 – 7.3 (m, 3H), 6.6 (dd, *J* = 3.4, 1.7 Hz, 1H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.7, 149.0, 146.7, 146.6, 141.4, 133.0, 132.3, 131.4, 130.0, 129.0, 128.9, 128.4, 127.6, 126.5, 126.4, 126.1, 125.6, 125.2, 121.1, 117.0, 112.2;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:312.1019, found: 312.1015.



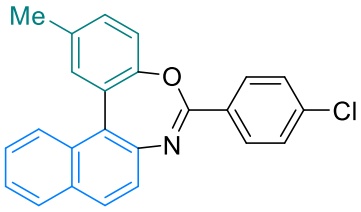
1l

6-(thiophen-2-yl)benzo[f]naphtho[2,1-d][1,3]oxazepane (1l): white solid, m.p. = 100-101 °C, 67.7 mg, 69% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.3 – 8.2 (m, 1H), 8.0 (dd, *J* = 3.7, 1.2 Hz, 1H), 7.9 – 7.9 (m, 2H), 7.8 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.6 – 7.5 (m, 2H), 7.5 – 7.5 (m, 2H), 7.5 – 7.4 (m, 1H), 7.4 – 7.3 (m, 2H), 7.2 (dd, *J* = 5.0, 3.7 Hz, 1H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.6, 153.4, 141.8, 137.2, 133.0, 132.2, 131.8, 131.6, 131.5, 129.9, 129.1, 128.8, 128.4, 128.1, 127.6, 126.5, 126.4, 126.1, 125.5, 125.1, 121.4;

HRMS (ESI, m/z): calcd. for $[M+Na]^+$:350.0610, found:350.0612.



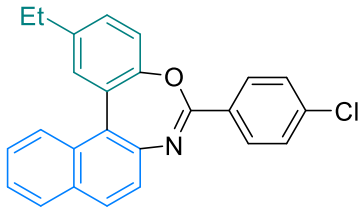
1m

6-(4-chlorophenyl)-2-methylbenzo[f]naphtho[2,1-d][1,3]oxazepane (1m): white solid, m.p. = 130-131 °C, 104.0 mg, 94% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.3 (d, *J* = 8.5 Hz, 3H), 7.9 – 7.9 (m, 2H), 7.6 – 7.5 (m, 6H), 7.2 (dd, *J* = 8.3, 2.1 Hz, 1H), 7.2 (d, *J* = 8.3 Hz, 1H), 2.4 (s, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 156.5, 155.5, 141.8, 138.0, 134.6, 133.1, 132.3, 131.4, 130.7, 130.6, 130.5, 128.9, 128.8, 128.7, 128.4, 127.8, 126.5, 126.4, 126.0, 125.5, 120.9, 21.0;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:370.0993, found: 370.0990.



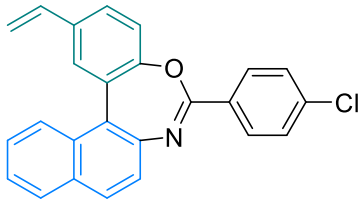
1n

6-(4-chlorophenyl)-2-ethylbenzo[f]naphtho[2,1-d][1,3]oxazepane (1n): white solid, m.p. = 139-140 °C, 102.3 mg, 89% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.39 – 8.25 (m, 3H), 7.97 – 7.87 (m, 2H), 7.63 (d, *J* = 2.1 Hz, 1H), 7.58 – 7.49 (m, 5H), 7.29 (d, *J* = 1.8 Hz, 1H), 7.25 (d, *J* = 8.3 Hz, 1H), 2.73 (q, *J* = 7.5 Hz, 2H), 1.29 (t, *J* = 7.5 Hz, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 156.4, 155.6, 141.8, 140.9, 138.0, 132.3, 132.1, 131.4, 130.7, 130.6, 129.4, 128.9, 128.8, 128.7, 128.4, 127.9, 126.5, 126.4, 126.0, 125.5, 120.9, 28.4, 15.8;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:384.1150, found: 384.1147.



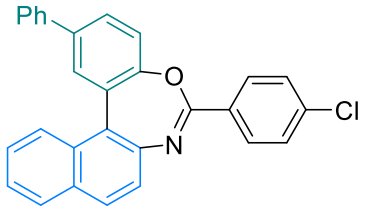
1o

6-(4-chlorophenyl)-2-vinylbenzo[f]naphtho[2,1-d][1,3]oxazepane (1o): white solid, m.p. = 50-51 °C, 61.7 mg, 54% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.28 (d, *J* = 8.5 Hz, 3H), 7.92 – 7.86 (m, 2H), 7.77 (d, *J* = 2.2 Hz, 1H), 7.54 – 7.42 (m, 6H), 7.24 (d, *J* = 1.3 Hz, 1H), 6.73 (dd, *J* = 17.5 Hz, 11.0 Hz, 1H), 5.70 (d, *J* = 17.5 Hz, 1H), 5.26 (d, *J* = 11.0 Hz, 1H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.1, 156.2, 141.9, 138.1, 135.7, 134.6, 132.3, 131.4, 130.7, 130.6, 130.5, 129.2, 129.0, 128.9, 128.4, 127.5, 127.4, 126.7, 126.2, 126.0, 125.6, 121.4, 114.5;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:382.0993, found: 382.0988.



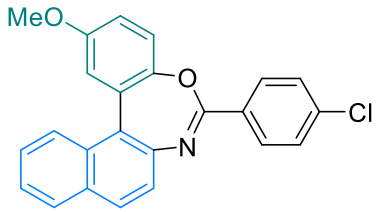
1p

6-(4-chlorophenyl)-2-phenylbenzo[f]naphtho[2,1-d][1,3]oxazepane (1p): white solid, m.p. = 139-140 °C, 109.9 mg, 85% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.38 – 8.31 (m, 3H), 8.00 (d, *J* = 2.1 Hz, 1H), 7.93 (dd, *J* = 9.0, 5.5 Hz, 2H), 7.66 (dd, *J* = 8.5, 2.5Hz, 1H), 7.62 – 7.54 (m, 3H), 7.56 – 7.47 (m, 4H), 7.44 (t, *J* = 7.8 Hz, 2H), 7.40 – 7.34 (m, 2H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.0, 156.3, 142.0, 140.0, 138.2, 132.3, 131.5, 131.4, 130.6, 130.5, 129.4, 129.0, 128.9, 128.8, 128.7, 128.6, 128.5, 127.7, 127.5, 127.2, 126.8, 126.3, 126.0, 125.7, 121.6;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:432.1150, found: 432.1142.



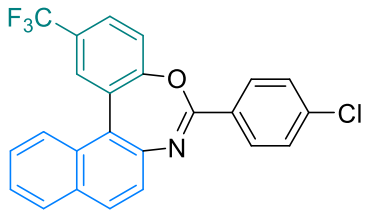
1q

6-(4-chlorophenyl)-2-methoxybenzo[f]naphtho[2,1-d][1,3]oxazepane (1q): white solid, m.p. = 135-136 °C, 114.3 mg, 99% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.38 – 8.34 (m, 1H), 8.29 (d, *J* = 8.6 Hz, 2H), 7.94 – 7.84 (m, 2H), 7.53 – 7.46 (m, 5H), 7.29 (d, *J* = 3.1 Hz, 1H), 7.22 (d, *J* = 8.9 Hz, 1H), 6.98 (dd, *J* = 8.9, 3.1 Hz, 1H), 3.80 (s, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 156.7, 156.5, 151.3, 142.0, 138.1, 132.3, 131.4, 130.7, 130.6, 129.8, 129.0, 128.9, 128.5, 127.5, 126.6, 126.3, 126.0, 125.6, 121.8, 117.2, 115.6, 55.9;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:386.0942, found: 386.0939.



1r

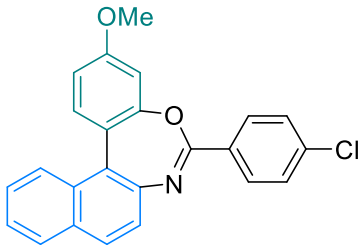
6-(4-chlorophenyl)-2-(trifluoromethyl)benzo[f]naphtho[2,1-d][1,3]oxazepane (1r): white solid, m.p. = 109-110 °C, 125.8 mg, 99% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.32 – 8.23 (m, 1H), 8.15 (d, *J* = 8.1 Hz, 1H), 8.08 – 8.06 (m, 2H), 7.94 (d, *J* = 8.3 Hz, 2H), 7.71 (dd, *J* = 8.5, 2.1 Hz, 1H), 7.60 – 7.46 (m, 5H), 7.42 (d, *J* = 8.5 Hz, 1H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 159.5, 155.7, 142.0, 138.5, 132.4, 131.1, 130.6, 130.2, 130.1, 129.9, 129.7, 129.1, 128.7, 127.6 (q, *J* = 33.0 Hz), 127.3, 126.8, 126.2, 126.0, 125.9, 125.5, 123.9 (q, *J* = 272.8Hz), 122.1;

^{19}F NMR (471 MHz, $CDCl_3$) δ -61.9 (s, 3F);

HRMS (ESI, m/z): calcd. for $[M+H]^+$:424.0711, found: 424.0705.



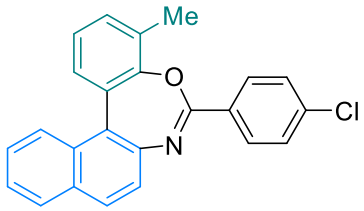
1s

6-(4-chlorophenyl)-3-methoxybenzo[f]naphtho[2,1-d][1,3]oxazepane(1s): white solid, m.p. = 209-210 °C, 85.5 mg, 74% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.29 (d, *J* = 8.3 Hz, 2H), 8.26 – 8.21 (m, 1H), 7.92 – 7.88 (m, 1H), 7.85 (d, *J* = 8.7 Hz, 1H), 7.67 (d, *J* = 8.7 Hz, 1H), 7.54 – 7.45 (m, 5H), 6.92 (dd, *J* = 8.8, 2.5 Hz, 1H), 6.84 (d, *J* = 2.5 Hz, 1H), 3.86 (s, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 161.3, 158.3, 155.6, 141.2, 138.0, 133.2, 132.3, 131.4, 130.7, 130.5, 128.9, 128.4, 128.2, 127.6, 126.5, 126.4, 126.0, 125.5, 121.4, 111.1, 106.7, 55.7;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:386.0942, found: 386.0938.



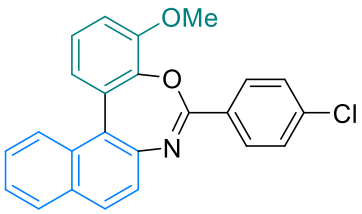
1t

6-(4-chlorophenyl)-4-methylbenzo[f]naphtho[2,1-d][1,3]oxazepane(1t): white solid, m.p. = 104-105 °C, 80.8 mg, 73% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.7 Hz, 3H), 7.93 – 7.85 (m, 2H), 7.57 (d, *J* = 2.1 Hz, 1H), 7.55 – 7.48 (m, 3H), 7.47 (d, *J* = 8.6 Hz, 2H), 7.27 – 7.17 (m, 2H), 2.40 (s, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.4, 157.3, 141.8, 137.5, 132.4, 132.3, 131.6, 131.3, 130.8, 130.6, 130.4, 128.9, 128.7, 128.5, 128.3, 128.2, 126.5, 126.4, 126.0, 125.6, 124.6, 17.6;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:370.0993, found: 370.0990.



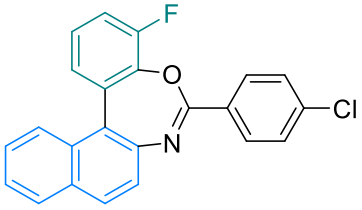
1u

6-(4-chlorophenyl)-4-methoxybenzo[f]naphtho[2,1-d][1,3]oxazepane (1u): white solid, m.p. = 185-186 °C, 71.6 mg, 62% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.56 (s, 1H), 8.54 (s, 1H), 8.30 – 8.22 (m, 1H), 7.92 – 7.85 (m, 2H), 7.52 – 7.47 (m, 3H), 7.45 (d, *J* = 1.9 Hz, 1H), 7.44 (d, *J* = 1.9 Hz, 1H), 7.30 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.24 (t, *J* = 8.0 Hz, 1H), 7.01 (dd, *J* = 8.1, 1.5 Hz, 1H), 3.93 (s, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.7, 151.7, 147.3, 141.9, 137.9, 132.3, 131.6, 131.5, 131.0, 130.4, 128.8, 128.4, 128.3, 128.0, 126.5, 126.4, 126.0, 125.6, 124.9, 124.4, 111.8, 56.0;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:386.0942, found: 386.0940.



1v

6-(4-chlorophenyl)-4-fluorobenzo[f]naphtho[2,1-d][1,3]oxazepane (1v)

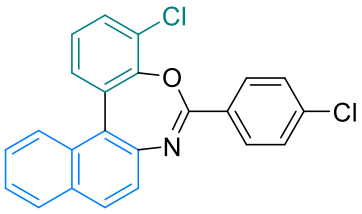
: white solid, m.p. = 157-158 °C, 96.2 mg, 86% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.42 (d, *J* = 8.7 Hz, 2H), 8.23 (dd, *J* = 6.3, 3.4 Hz, 1H), 7.91 (dd, *J* = 9.0, 2.5 Hz, 2H), 7.55 – 7.49 (m, 4H), 7.47 (d, *J* = 8.7 Hz, 2H), 7.31 – 7.25 (m, 1H), 7.23 (dd, *J* = 10.1, 8.4 Hz, 1H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 156.7, 154.4(d, J = 248.9 Hz), 145.5(d, J = 12.3 Hz), 141.8, 138.4, 132.3, 131.7, 131.4, 131.0 (d, J = 3.9Hz), 130.3, 129.3, 128.8, 128.5, 127.8(d, J = 3.5 Hz), 127.1(d, J = 2.5Hz), 126.8, 126.1(d, J = 7.4 Hz), 125.8, 125.2 (d, J = 7.8Hz), 116.2, 116.1;

^{19}F NMR (471 MHz, $CDCl_3$) δ -130.9 (s, 1F);

HRMS (ESI, m/z): calcd. for $[M+H]^+$:374.0742, found: 374.0737.



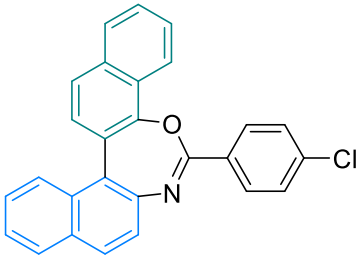
1w

4-chloro-6-(4-chlorophenyl)benzo[f]naphtho[2,1-d][1,3]oxazepane (1w): white solid, m.p. = 160-161 °C, 100.3 mg, 86% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.49 – 8.42 (m, 2H), 8.19 – 8.09 (m, 1H), 7.94 – 7.82 (m, 2H), 7.61 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.55 – 7.41 (m, 6H), 7.23 (t, *J* = 7.9 Hz, 1H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.0, 153.9, 141.7, 138.1, 132.4, 131.5, 131.4, 131.3, 130.9, 130.8, 130.1, 129.3, 128.5, 128.4, 127.1, 126.7, 126.5, 126.0, 125.9, 125.8, 125.3;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:390.0447, found: 390.0441.



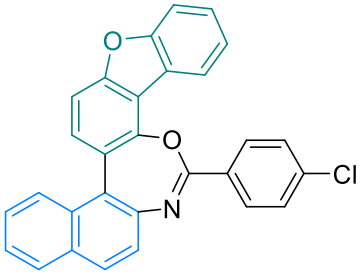
1x

6-(4-chlorophenyl)dinaphtho[2,1-d:2',1'-f][1,3]oxazepane(1x): white solid, m.p. = 185-186 °C, 99.6 mg, 82% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.51 – 8.46 (m, 1H), 8.31 – 8.25 (m, 2H), 8.23 – 8.18 (m, 1H), 7.95 – 7.88 (m, 3H), 7.80 (q, *J* = 8.6 Hz, 2H), 7.59 – 7.55 (m, 3H), 7.53 – 7.49 (m, 2H), 7.47 (d, *J* = 8.6 Hz, 2H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.1, 153.1, 142.0, 137.6, 134.6, 132.3, 131.8, 131.4, 130.4, 129.4, 129.0, 128.6, 128.5, 127.9, 127.8, 127.5, 126.9, 126.7, 126.6, 126.5, 125.9, 125.8, 124.5, 124.5, 122.0;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:406.0993, found: 406.0987.



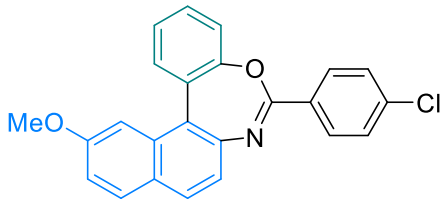
1y

15-(4-chlorophenyl)benzo[2,3]benzofuro[5,4-f]naphtho[2,1-d][1,3]oxazepane(1y): white solid, m.p. = 190-191 °C, 130.8 mg, 98% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.34 (d, *J* = 7.8 Hz, 1H), 8.19 (d, *J* = 8.2 Hz, 2H), 8.10 (d, *J* = 8.1 Hz, 1H), 7.90 (dd, *J* = 8.3, 4.6 Hz, 2H), 7.76 (d, *J* = 8.6 Hz, 1H), 7.63 (d, *J* = 8.3 Hz, 1H), 7.56 – 7.50 (m, 5H), 7.43 – 7.36 (m, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.7, 157.1, 156.2, 154.7, 141.2, 137.6, 132.5, 132.0, 131.8, 131.5, 130.8, 128.7, 128.6, 128.5, 128.4, 128.0, 127.5, 126.6, 126.3, 125.7, 123.6, 123.0, 122.5, 122.2, 117.1, 111.9, 108.4;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:446.0942, found: 446.0943.



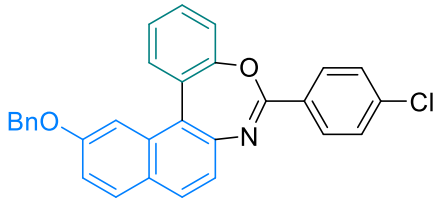
1z

6-(4-chlorophenyl)-12-methoxybenzo[f]naphtho[2,1-d][1,3]oxazepane(1z): white solid, m.p. = 139-140 °C, 114.3 mg, 99% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.31 (d, *J* = 8.3 Hz, 2H), 7.86 (d, *J* = 7.9 Hz, 1H), 7.81 (dd, *J* = 8.8, 3.7 Hz, 2H), 7.66 (s, 1H), 7.52 – 7.37 (m, 4H), 7.36 – 7.28 (m, 2H), 7.21 – 7.15 (m, 1H), 3.85 (s, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 158.4, 157.4, 156.2, 142.4, 138.1, 132.7, 132.2, 130.7, 130.6, 129.9, 129.8, 129.5, 128.9, 128.6, 127.6, 126.5, 125.0, 123.7, 121.4, 117.6, 105.7, 55.3;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:386.0942, found: 386.0937.



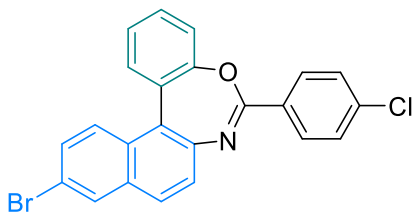
1aa

12-(benzyloxy)-6-(4-chlorophenyl)benzo[f]naphtho[2,1-d][1,3]oxazepane(1aa): white solid, m.p. = 142-143 °C, 128.6 mg, 93% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.3 Hz, 2H), 7.82 (dd, *J* = 8.8, 4.7 Hz, 2H), 7.66 (d, *J* = 2.3 Hz, 1H), 7.60 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.48 (d, *J* = 8.5 Hz, 2H), 7.47 – 7.37 (m, 6H), 7.36 (d, *J* = 7.0 Hz, 1H), 7.31 (d, *J* = 8.1 Hz, 1H), 7.30 – 7.24 (m, 1H), 7.21 (t, *J* = 7.5 Hz, 1H), 5.15 (d, *J* = 12.0 Hz, 1H), 5.12 (d, *J* = 12.0 Hz, 1H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.4, 157.3, 156.2, 142.4, 138.1, 136.9, 132.5, 132.2, 130.7, 130.6, 130.0, 129.7, 129.4, 128.9, 128.7, 128.6, 128.0, 127.7, 127.4, 126.5, 125.1, 123.8, 121.3, 118.2, 107.1, 69.8;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:462.1255, found: 462.1248.



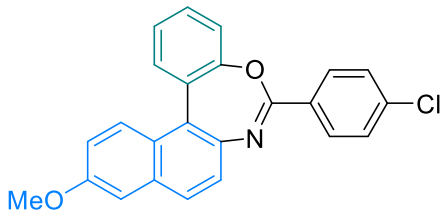
1ab

11-bromo-6-(4-chlorophenyl)benzo[f]naphtho[2,1-d][1,3]oxazepane(1ab): white solid, m.p. = 205-206 °C, 55.7 mg, 43% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.6 Hz, 2H), 8.12 (d, *J* = 9.1 Hz, 1H), 8.05 (d, *J* = 2.1 Hz, 1H), 7.79 (d, *J* = 8.7 Hz, 1H), 7.70 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.59 – 7.51 (m, 2H), 7.50 – 7.44 (m, 3H), 7.37 – 7.30 (m, 2H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.5, 156.5, 142.0, 138.3, 133.4, 132.7, 130.6, 130.5, 130.3, 130.2, 129.9, 129.7, 128.9, 128.7, 128.2, 128.0, 127.7, 127.2, 125.2, 121.4, 119.7;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:433.9942, found: 433.9935.



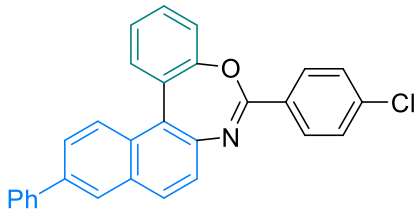
1ac

6-(4-chlorophenyl)-11-methoxybenzo[f]naphtho[2,1-d][1,3]oxazepane(1ac): white solid, m.p. = 172-173 °C, 92.4 mg, 80% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.3 Hz, 2H), 8.17 (d, *J* = 9.3 Hz, 1H), 7.78 (d, *J* = 8.7 Hz, 1H), 7.76 – 7.69 (m, 1H), 7.54 – 7.40 (m, 4H), 7.35 – 7.28 (m, 2H), 7.21 (d, *J* = 2.7 Hz, 1H), 7.17 (dd, *J* = 9.3, 2.6 Hz, 1H), 3.96 (s, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.4, 157.3, 155.6, 140.0, 137.9, 133.7, 132.9, 130.8, 130.4, 129.9, 129.3, 128.9, 128.1, 128.0, 127.7, 126.6, 126.5, 125.0, 121.3, 118.9, 106.6, 55.4;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:386.0942, found: 386.0938.



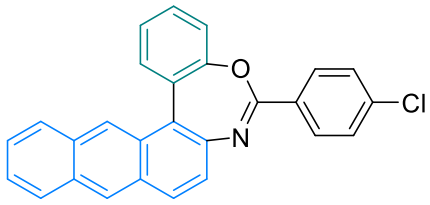
1ad

6-(4-chlorophenyl)-11-phenylbenzo[f]naphtho[2,1-d][1,3]oxazepane(1ad): white solid, m.p. = 139-140 °C, 64.7 mg, 50% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.33 (t, *J* = 8.7 Hz, 3H), 8.11 (s, 1H), 7.94 (d, *J* = 8.7 Hz, 1H), 7.84 – 7.72 (m, 4H), 7.59 – 7.44 (m, 6H), 7.44 – 7.31 (m, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.5, 156.2, 141.8, 140.6, 138.2, 138.1, 132.9, 132.6, 130.7, 130.6, 130.5, 130.0, 129.2, 129.1, 129.0, 128.9, 127.7, 127.6, 127.3, 127.0, 126.5, 126.2, 126.1, 125.1, 121.3;

HRMS (ESI, m/z): calcd. for $[M+Na]^+$:454.0969, found: 454.0966.



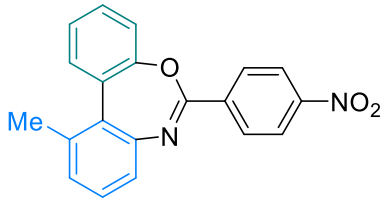
1ae

6-(4-chlorophenyl)anthra[2,1-d]benzo[f][1,3]oxazepane(1ae): white solid, m.p. = 140-141 °C, 96.0 mg, 79% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.83 (s, 1H), 8.47 (s, 1H), 8.33 (d, *J* = 8.2 Hz, 2H), 8.04 (dd, *J* = 8.6, 3.3 Hz, 2H), 7.94 (d, *J* = 7.9 Hz, 2H), 7.52 – 7.45 (m, 6H), 7.40 (t, *J* = 7.5 Hz, 1H), 7.36 (d, *J* = 8.1 Hz, 1H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.2, 156.0, 141.3, 138.1, 132.8, 132.0, 131.2, 130.7, 130.6, 130.5, 130.1, 129.7, 129.5, 129.2, 128.9, 128.5, 127.9, 127.1, 126.6, 126.2, 125.8, 125.7, 125.5, 125.2, 121.4;

HRMS (ESI, m/z): calcd. for $[M+H]^+$:406.0993, found: 406.0987.



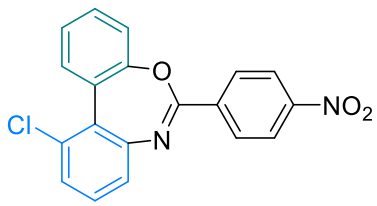
1af

11-methyl-6-(4-nitrophenyl)dibenzo[d,f][1,3]oxazepane(1af): yellow solid, m.p. = 210-211 °C, 82.17 mg, 83% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.49 (d, *J* = 8.5 Hz, 2H), 8.34 (d, *J* = 8.6 Hz, 2H), 7.56 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.43 – 7.33 (m, 2H), 7.31 – 7.26 (m, 4H), 2.55 (s, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.1, 154.9, 149.5, 144.1, 138.1, 136.5, 132.0, 131.2, 129.9, 129.6, 129.5, 129.3, 128.0, 125.0, 124.9, 123.7, 120.6, 22.1;

HRMS (ESI, m/z): calcd. for $[M+Na]^+$:353.0897, found: 353.0901.



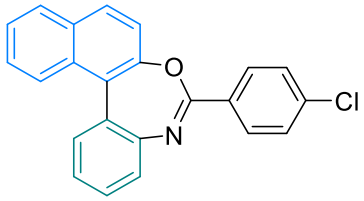
1ag

11-chloro-6-(4-nitrophenyl)dibenzo[d,f][1,3]oxazepane (1ag): white solid, m.p. = 198-199 °C, 88.2 mg, 84% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.50 (s, 1H), 8.48 (s, 1H), 8.35 (d, *J* = 8.5 Hz, 2H), 7.98 (d, *J* = 7.8 Hz, 1H), 7.49 – 7.41 (m, 2H), 7.38 (t, 2H), 7.33 (t, *J* = 7.7 Hz, 1H), 7.28 (d, *J* = 3.4 Hz, 1H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 156.9, 156.1, 149.8, 145.3, 137.6, 132.7, 132.3, 130.2, 130.1, 130.0, 128.8, 128.7, 127.5, 126.0, 125.0, 123.8, 120.5;

HRMS (ESI, m/z): calcd. for $[M+Na]^+$:373.0350, found: 373.0354.



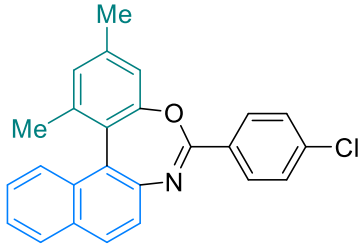
1ah

6-(4-chlorophenyl)benzo[d]naphtho[1,2-f][1,3]oxazepane (1ah): white solid, m.p. = 50-52°C, 96.0mg, 90% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.29 – 8.21 (m, 3H), 7.88 – 7.78 (m, 3H), 7.56 – 7.43 (m, 6H), 7.39 (d, *J* = 8.9 Hz, 1H), 7.37 – 7.31 (m, 1H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.1, 156.0, 145.5, 138.1, 132.4, 131.9, 131.8, 130.7, 130.4, 130.1, 129.8, 128.9, 128.4, 128.3, 127.1, 126.7, 126.1, 125.8, 125.5, 124.7, 120.0;

HRMS (ESI, m/z): calcd. for $[M+H]^+$: 356.0837, found: 356.0836.



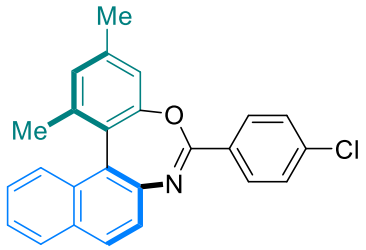
(*rac*)-**1ai**

6-(4-chlorophenyl)-1,3-dimethylbenzo[f]naphtho[2,1-d][1,3]oxazepane(1ai): white solid, m.p. = 140-141 °C, 68.9 mg, 60% yield; For kinetic resolution, 49% yield, 96:4 er

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.29 (d, *J* = 8.2 Hz, 2H), 7.93 – 7.84 (m, 2H), 7.68 – 7.62 (m, 1H), 7.53 (d, *J* = 8.7 Hz, 1H), 7.47 (dd, *J* = 8.9, 5.0 Hz, 4H), 7.01 (s, 1H), 6.96 (s, 1H), 2.38 (s, 3H), 2.00 (s, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 159.9, 157.8, 143.0, 139.4, 139.3, 138.0, 131.4, 131.3, 130.8, 130.4, 129.1, 128.9, 128.4, 128.3, 127.3, 127.1, 126.3, 125.4, 125.3, 125.0, 118.6, 21.9, 21.1;

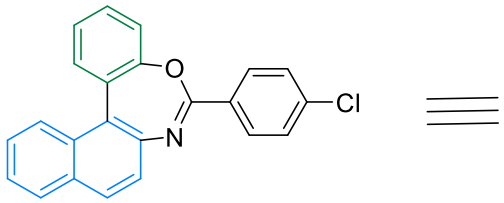
HRMS (ESI, m/z): calcd. for $[M+H]^+$:384.1150, found: 384.1140.

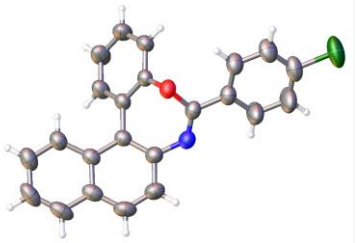


(*S*)-**1ai**

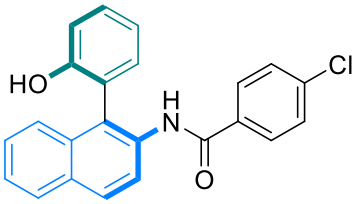
HPLC analysis: 96:4 er, (CHIRALCEL IA column, *n*-hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, t_{major}=4.1 min, t_{minor}=7.7min), $[\alpha]_D^{25}$ = +136.00 (c = 0.2, acetone).

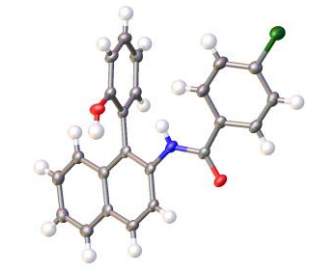
X-ray structure of 1c and 2c





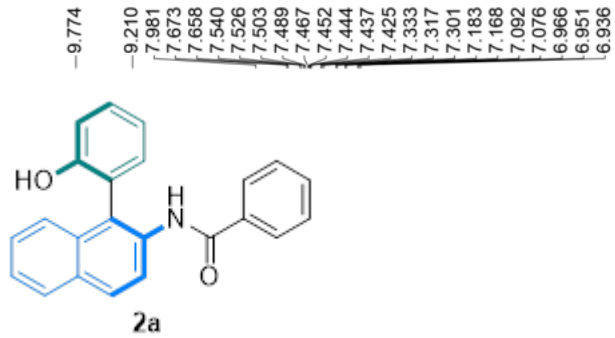
1c Deposition No. CCDC 2256876

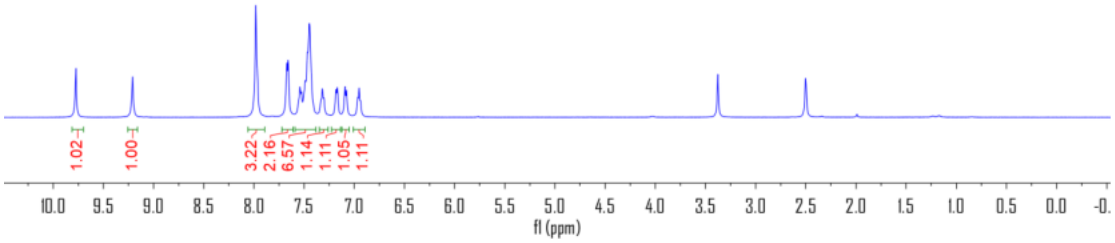


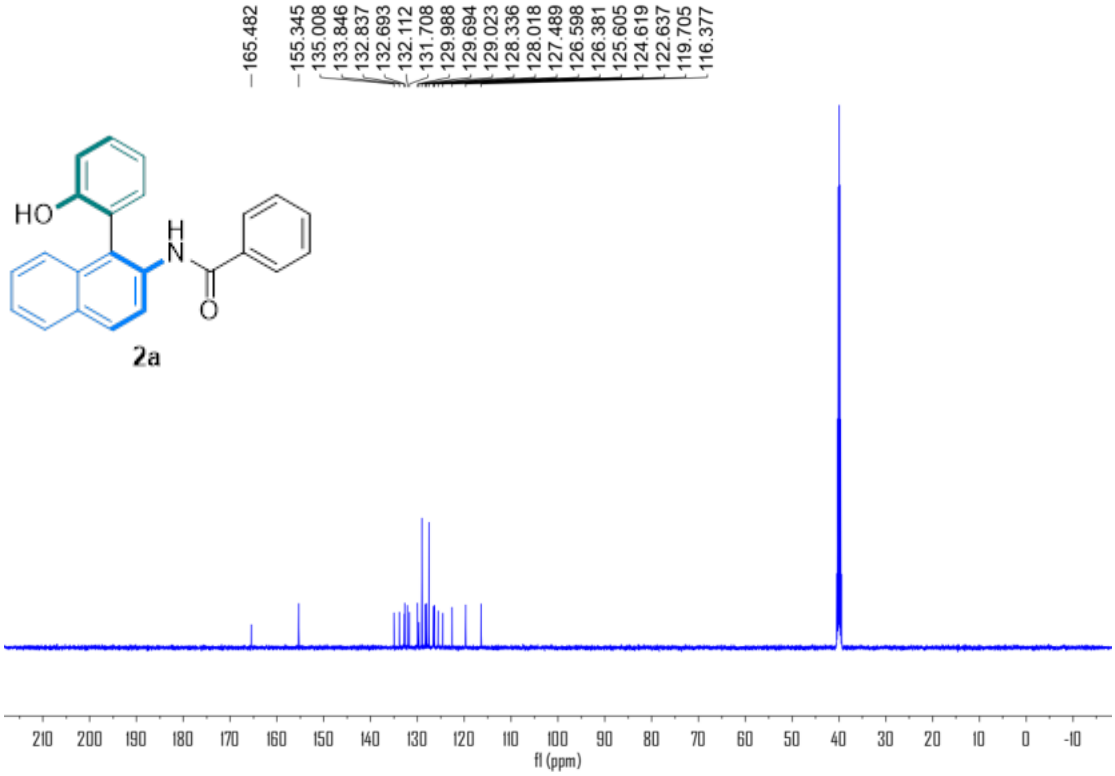


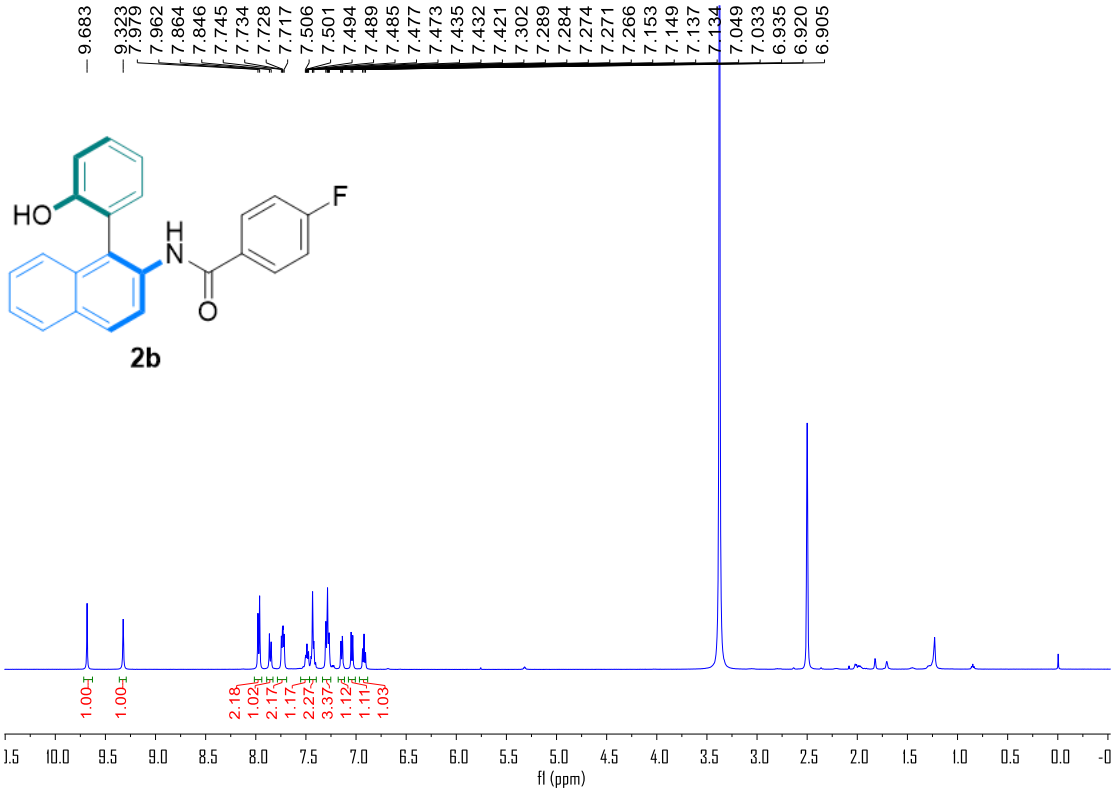
2c Deposition No. CCDC 2256877

^{1}H, ^{13}C, ^{19}F and HPLC charts





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7.846
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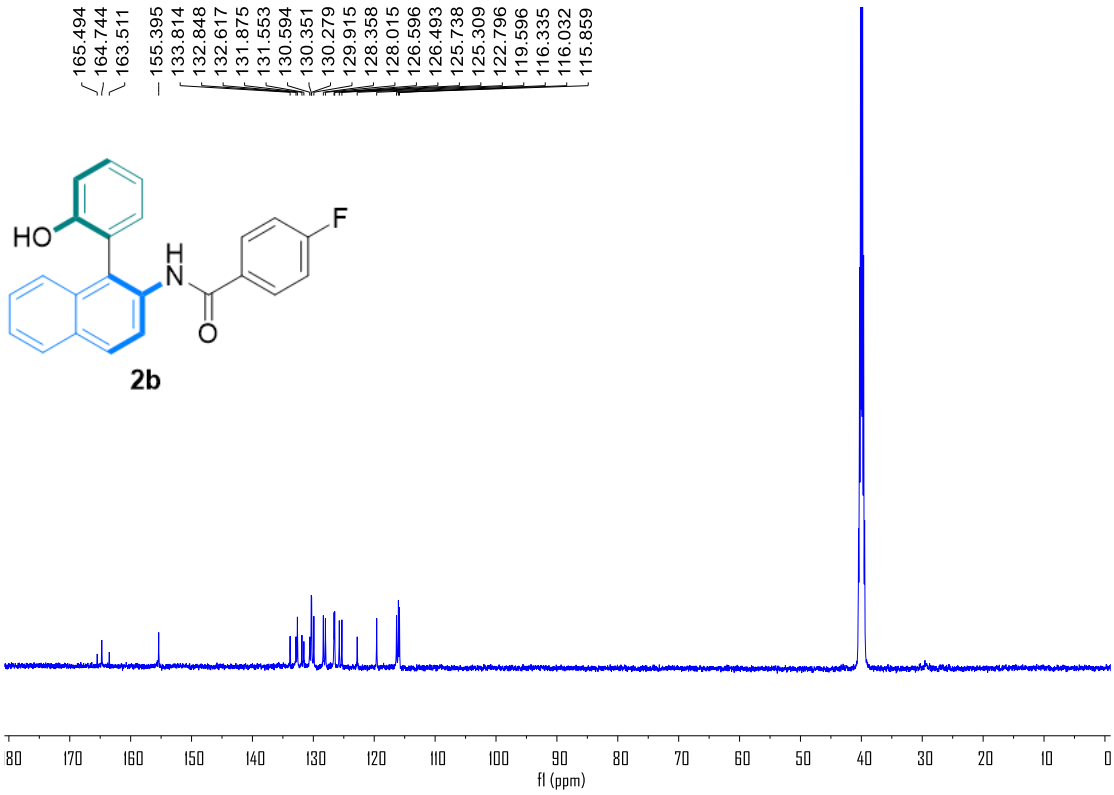
7.734
7.728
7.717
7.506
7.501
7.494
7.489
7.485
7.477
7.473
7.435
7.432
7.421
7.302
7.289
7.284
7.274
7.271
7.266
7.153
7.149
7.137
7.134
7.049
7.033
6.935
6.920
6.905
HO
H
N
O
F
2b
1.00
1.00
2.18
1.02
2.17
1.17
2.27
3.37
1.12
1.11
1.03
f1 (ppm)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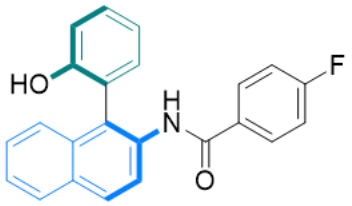
164.744
163.511
155.395
133.814
132.848
132.617
131.875
131.553
130.594
130.351
130.279
129.915
128.358
128.015
126.596
126.493
125.738
125.309
122.796
119.596
116.335
116.032
115.859
HO
H
N
O
F
2b
f1 (ppm)


HO
H
N
O
F

2b

-108.707
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)
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9.416
7.983
7.979
7.964
7.853
7.836
7.701
7.688
7.684
7.532
7.515
7.496
7.492
7.489
7.479
7.476
7.449
7.439
7.436
7.426
7.423
7.305
7.301
7.289
7.286
7.274
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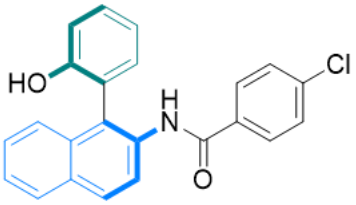
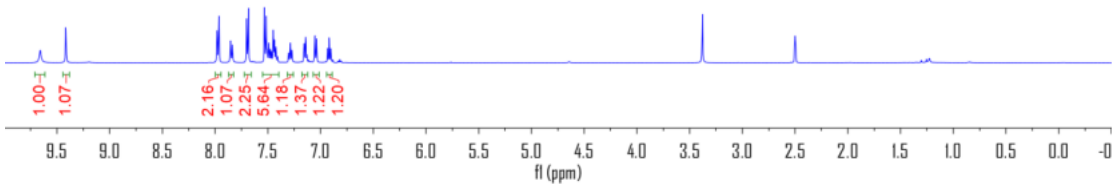
7.157
7.154
7.142
7.139
7.055
7.038
6.933
6.918
6.903


HO
H
N
O
Cl

2c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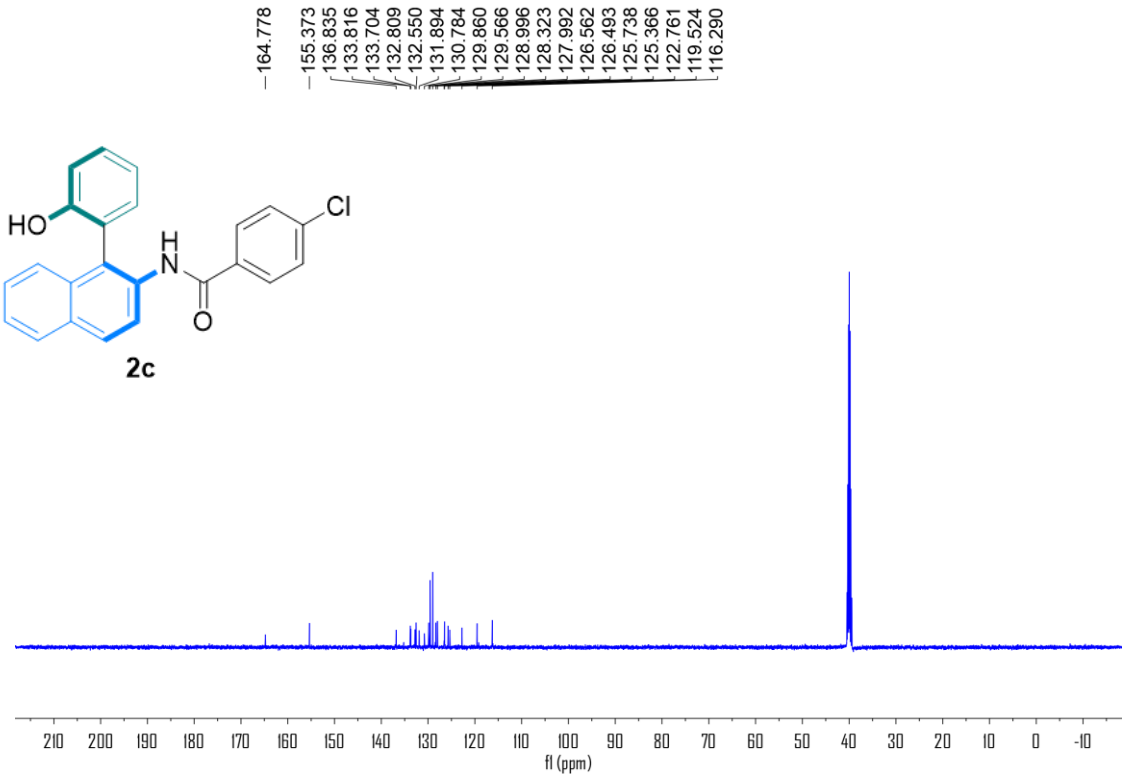
1.07
2.16
1.07
2.25
5.64
1.18
1.37
1.22
1.20
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)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132.550
131.894
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129.566
128.996
128.323
127.992
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126.493
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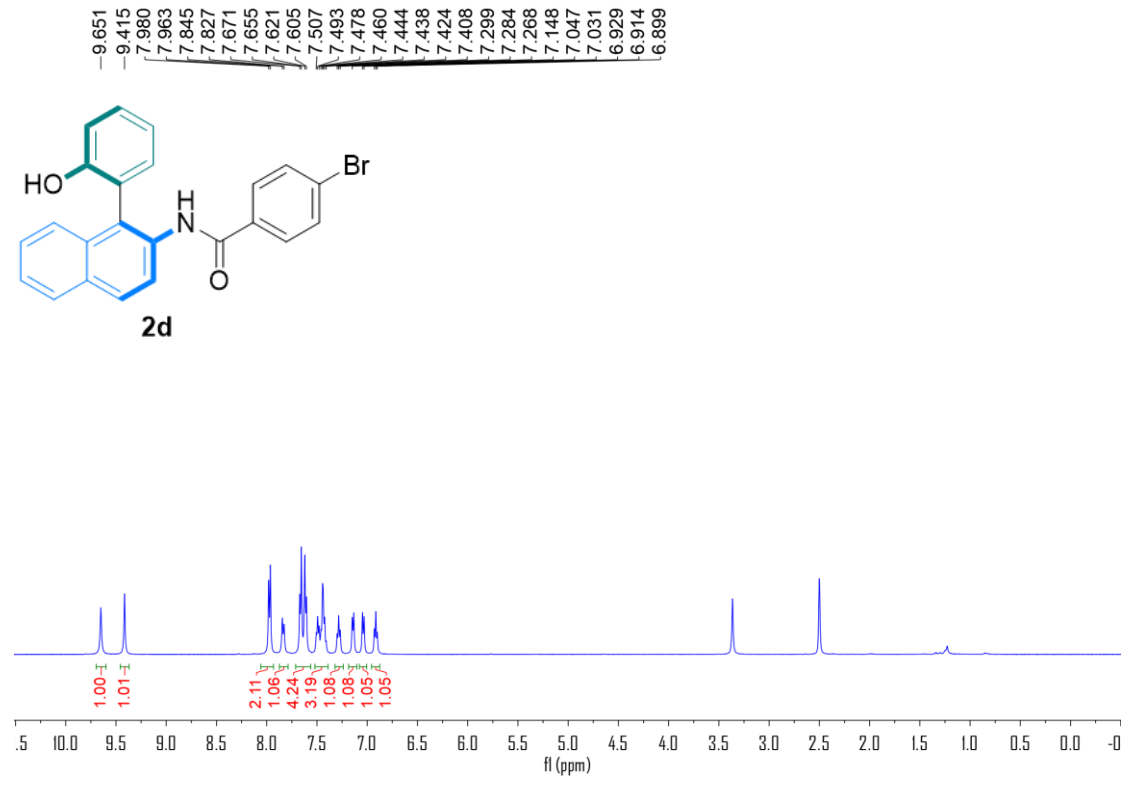
125.366
122.761
119.524
116.290
HO
H
N
O
Cl
2c
f1 (ppm)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9.415
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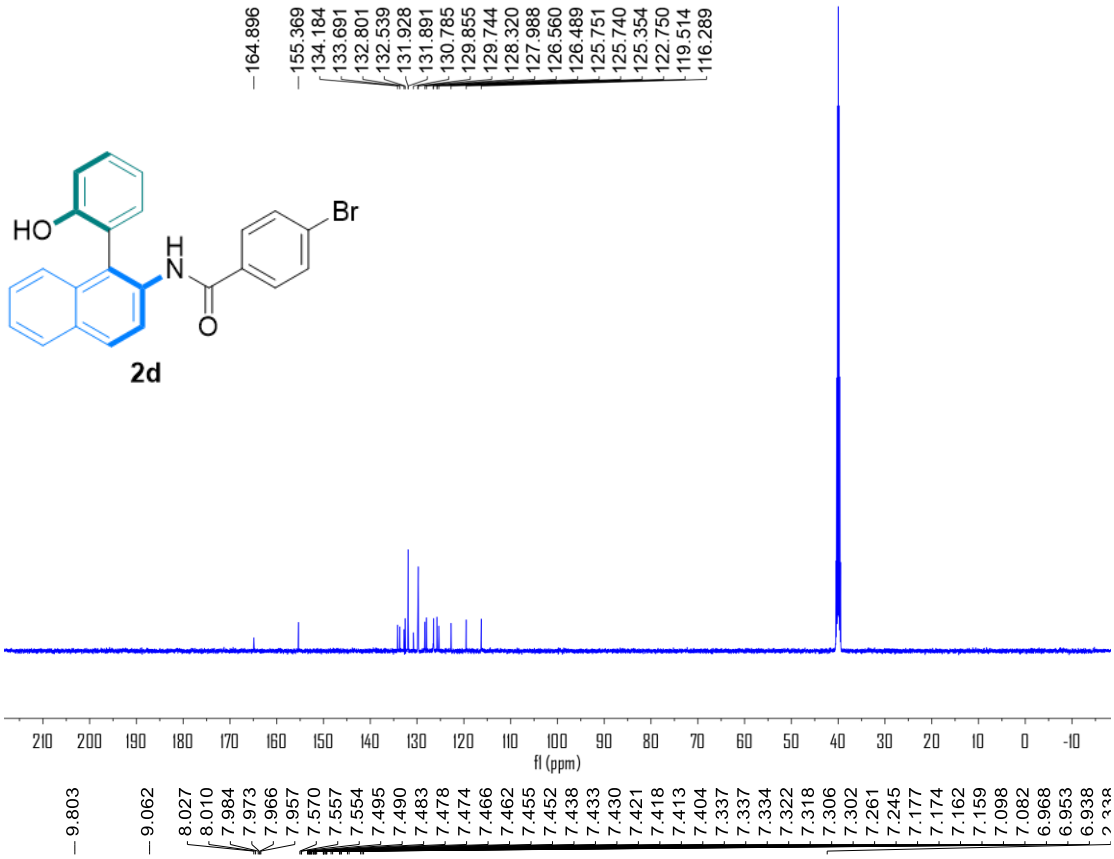
7.963
7.845
7.827
7.671
7.655
7.621
7.605
7.507
7.493
7.478
7.460
7.444
7.438
7.424
7.408
7.299
7.284
7.268
7.148
7.047
7.031
6.929
6.914
6.899
HO
H
N
O
Br
2d
1.00
1.01
2.11
1.06
4.24
3.19
1.08
1.08
1.05
1.05
f1 (ppm)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131.891
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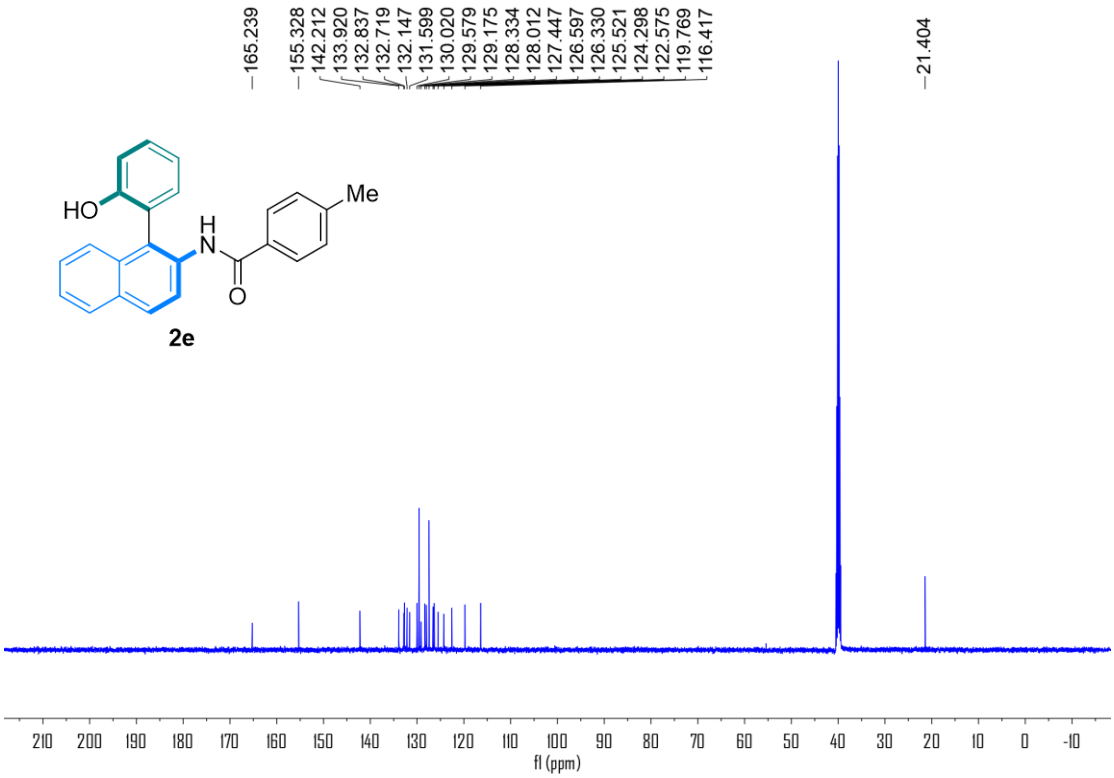
129.855
129.744
128.320
127.988
126.560
126.489
125.751
125.740
125.354
122.750
119.514
116.289
HO
H
N
O
Br
2d
f1 (ppm)
9.803
9.062
8.027
8.010
7.984
7.973
7.966
7.957
7.570
7.557
7.554
7.495
7.490
7.483
7.478
7.474
7.466
7.462
7.455
7.452
7.438
7.433
7.430
7.421
7.418
7.413
7.404
7.337
7.337
7.334
7.322
7.318
7.306
7.302
7.261
7.245
7.177
7.174
7.162
7.159
7.098
7.082
6.968
6.953
6.938
HO
H
N
O
Me
2e
1.00
1.00
3.05
2.05
3.16
1.06
2.06
1.04
1.06
1.03
3.00
f1 (ppm)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132.147
131.599
130.020
129.579
129.175
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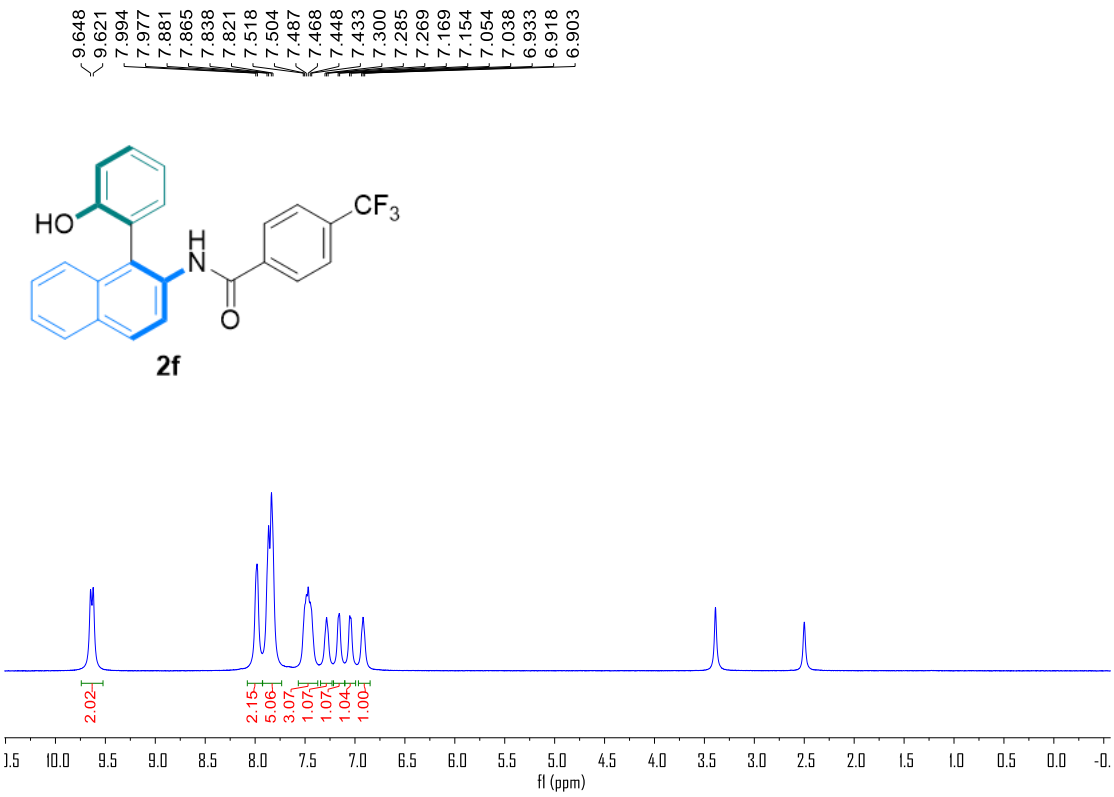
128.012
127.447
126.597
126.330
125.521
124.298
122.575
119.769
116.417
21.404
HO
H
N
O
Me
2e
f1 (ppm)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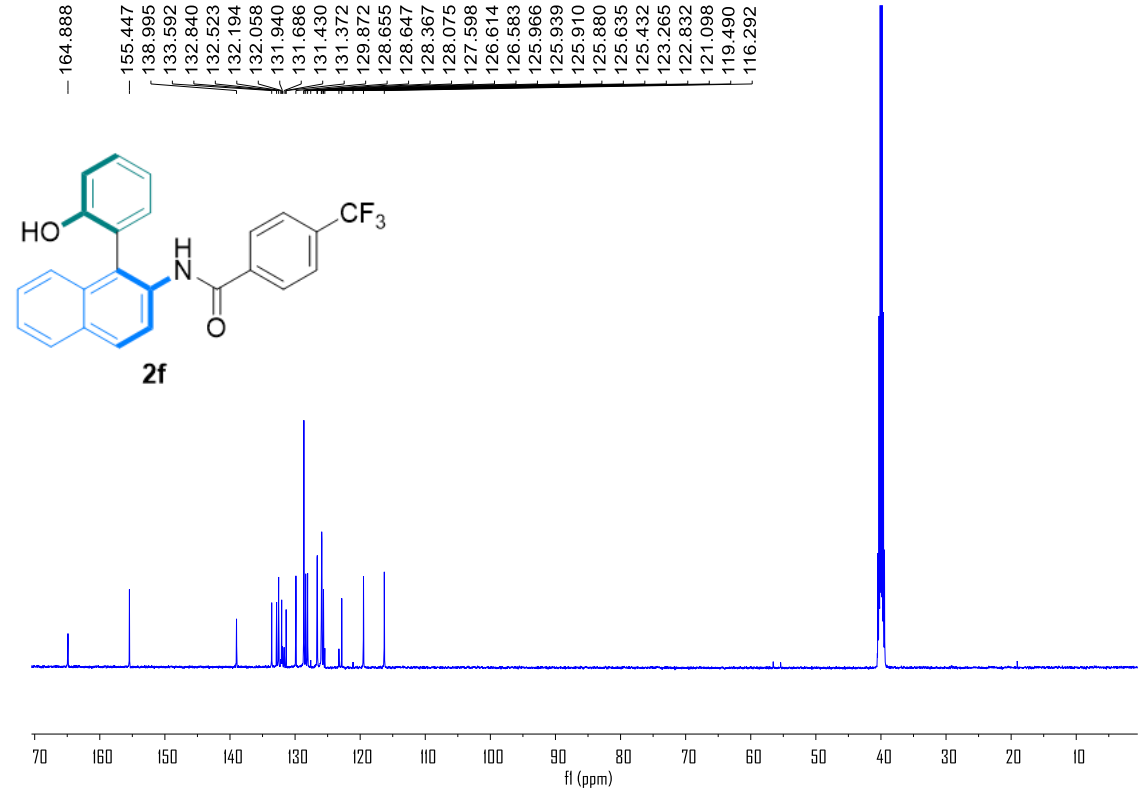
7.865
7.838
7.821
7.518
7.504
7.487
7.468
7.448
7.433
7.300
7.285
7.269
7.169
7.154
7.054
7.038
6.933
6.918
6.903
HO
H
N
O
CF3
2f
2.02
2.15
5.06
3.07
1.07
1.07
1.04
1.00
f1 (ppm)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132.523
132.194
132.058
131.940
131.686
131.430
131.372
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128.655
128.647
128.367
128.075
127.598
126.614
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125.966
125.939
125.910
125.880
125.635
125.432
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122.832
121.098
119.490
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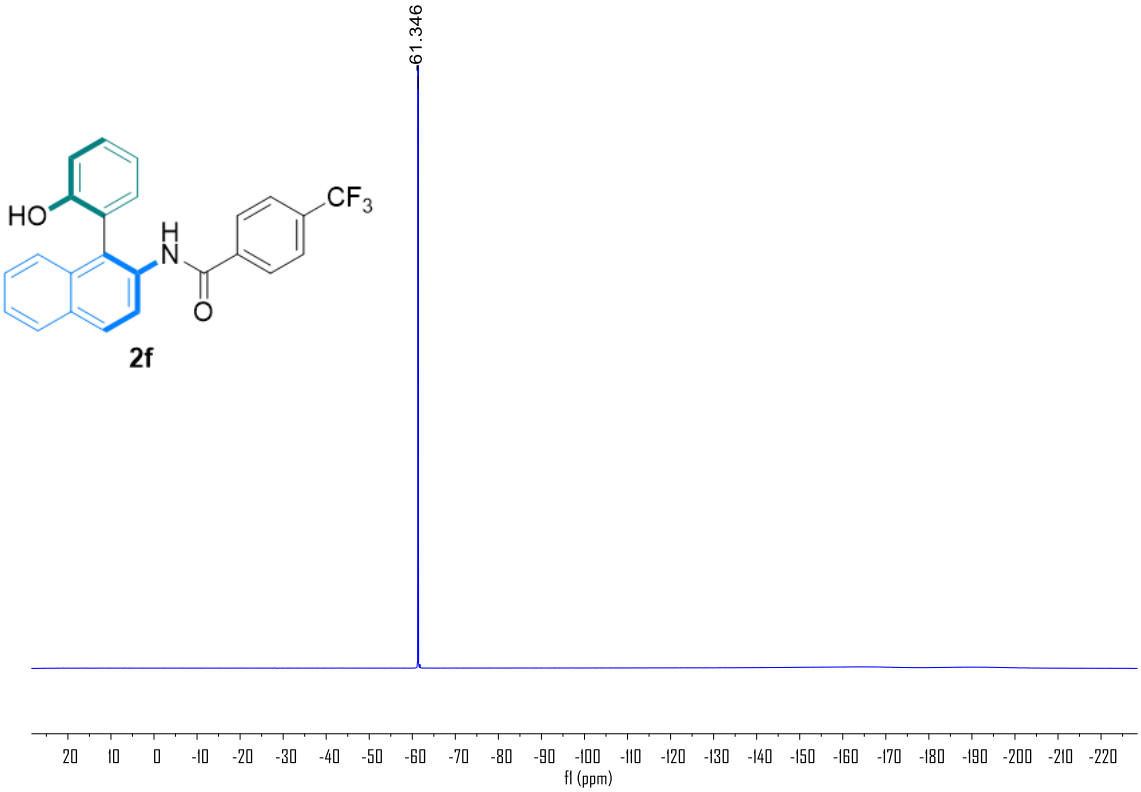
HO
H
N
O
CF3
2f
f1 (ppm)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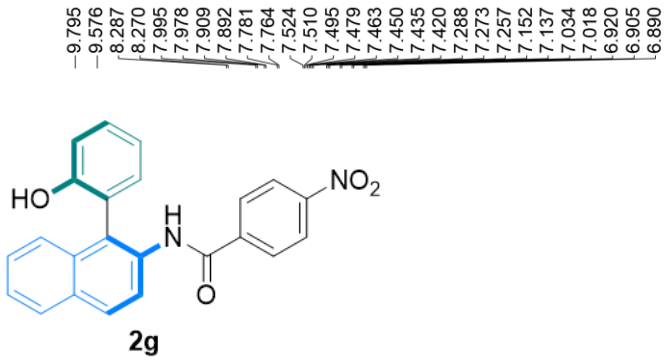
H
N
O
CF3
2f
f1 (ppm)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7.892
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7.510
7.495
7.479
7.463
7.450
7.435
7.420
7.288
7.273
7.257
7.152
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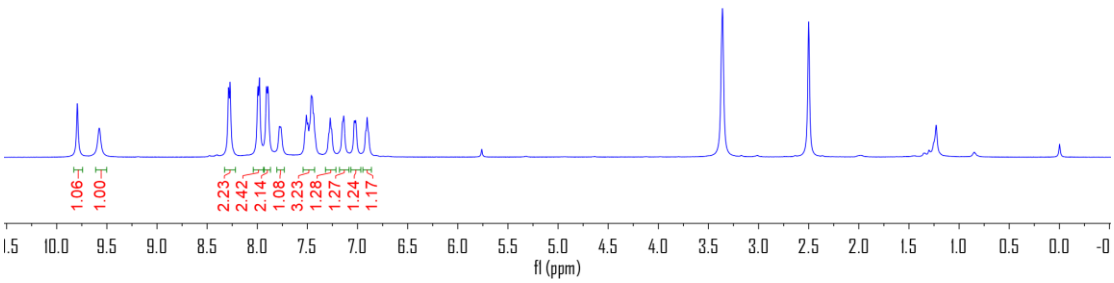
7.034
7.018
6.920
6.905
6.890
HO
H
N
O
NO2

2g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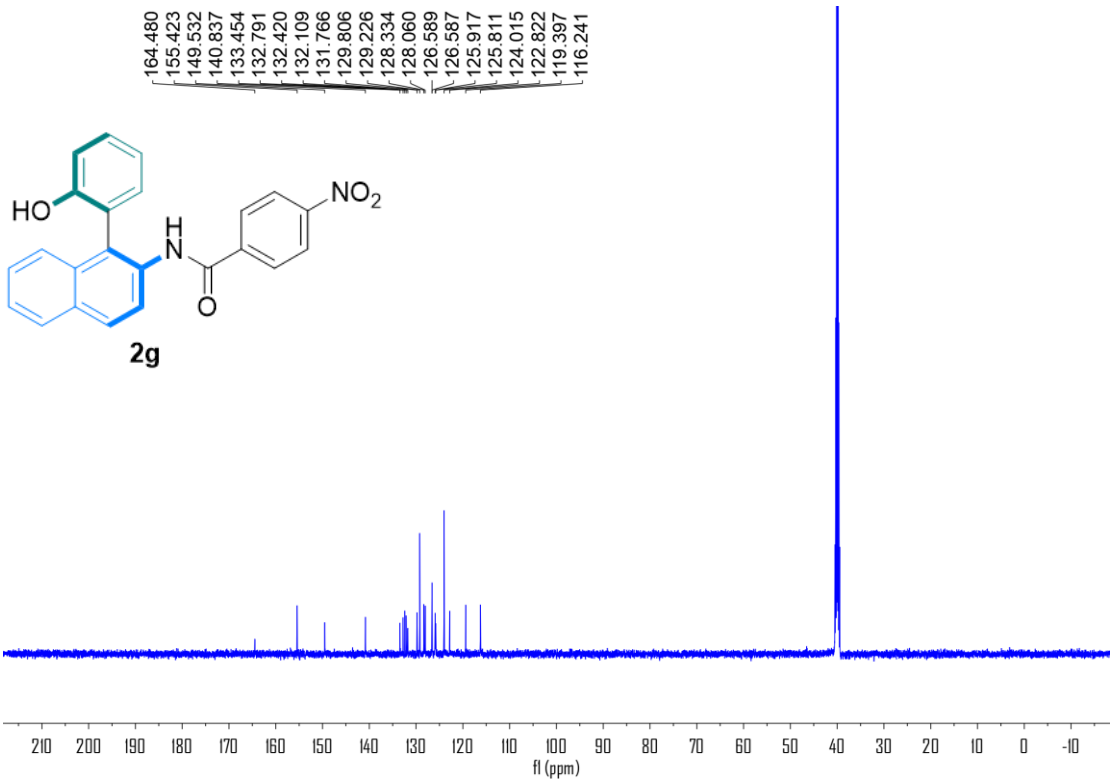
2.14
1.08
3.23
1.28
1.27
1.24
1.17
f1 (ppm)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132.109
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129.806
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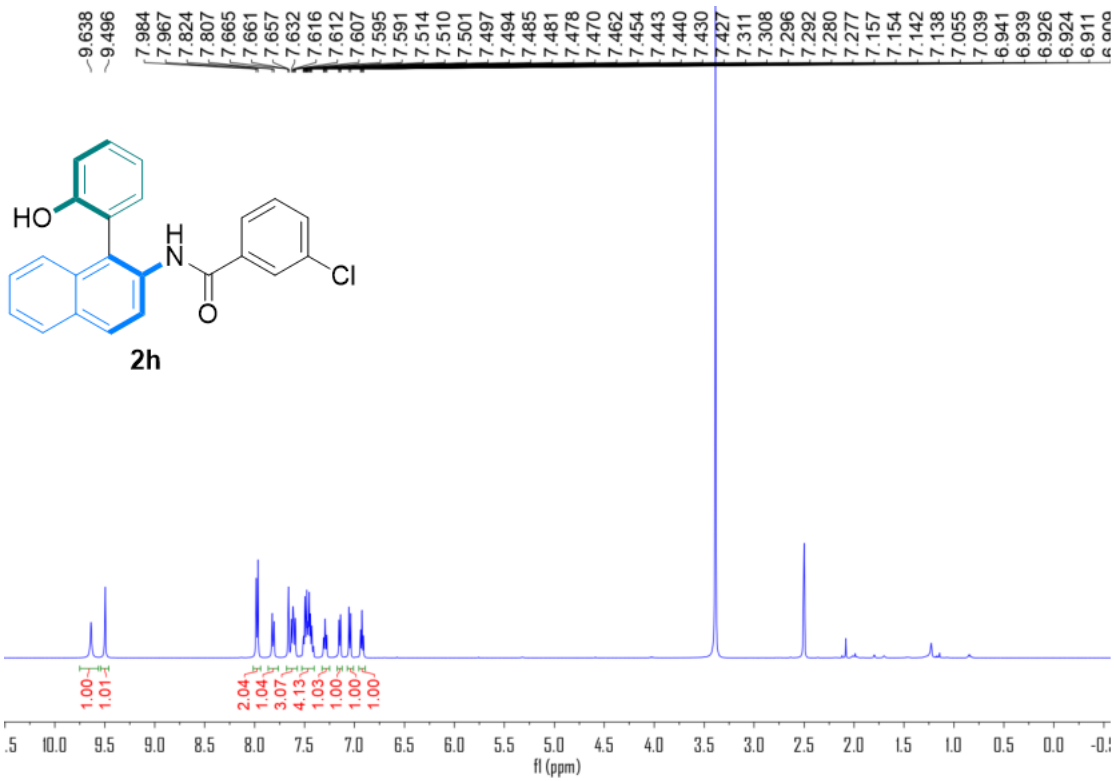
128.334
128.060
126.589
126.587
125.917
125.811
124.015
122.822
119.397
116.241
HO
H
N
O
NO2
f1 (ppm)

2g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7.632
7.616
7.612
7.607
7.595
7.591
7.514
7.510
7.501
7.497
7.494
7.485
7.481
7.478
7.470
7.462
7.454
7.443
7.440
7.430
7.427
7.311
7.308
7.296
7.292
7.280
7.277
7.157
7.154
7.142
7.138
7.055
7.039
6.941
6.939
6.926
6.924
6.911
HO
H
N
O
Cl
2h
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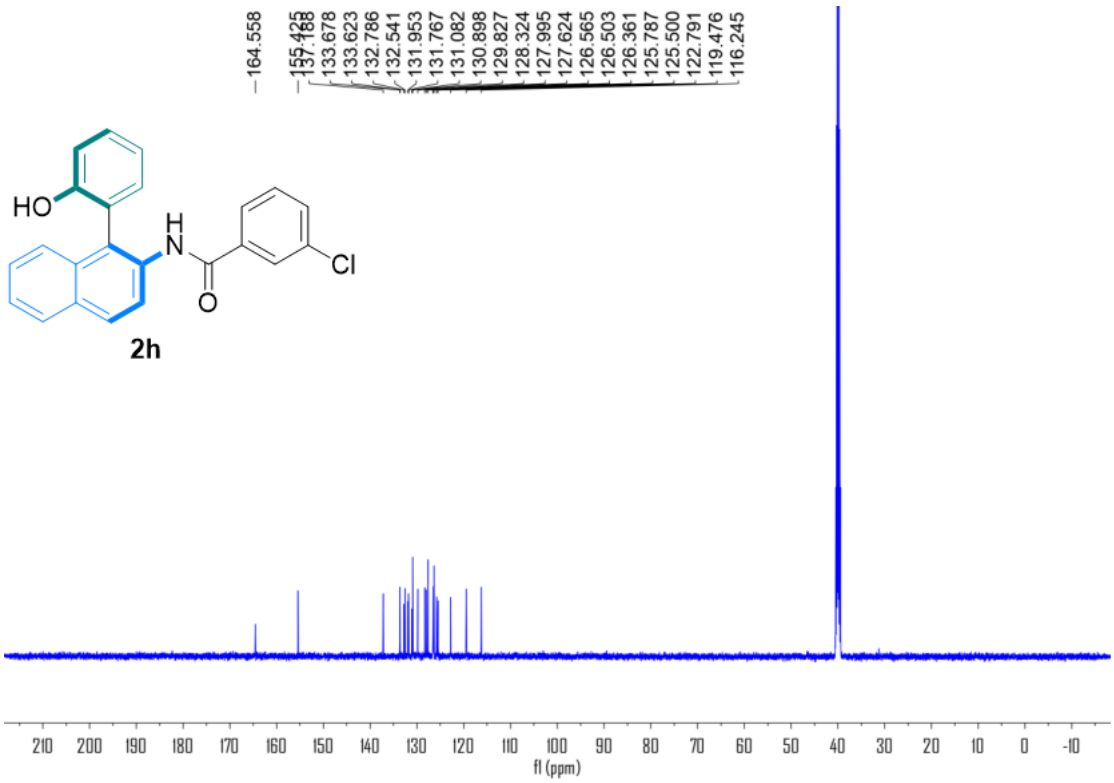
2.04
1.04
3.07
4.13
1.03
1.00
1.00
1.00
f1 (ppm)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132.786
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130.898
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127.995
127.624
126.565
126.503
126.361
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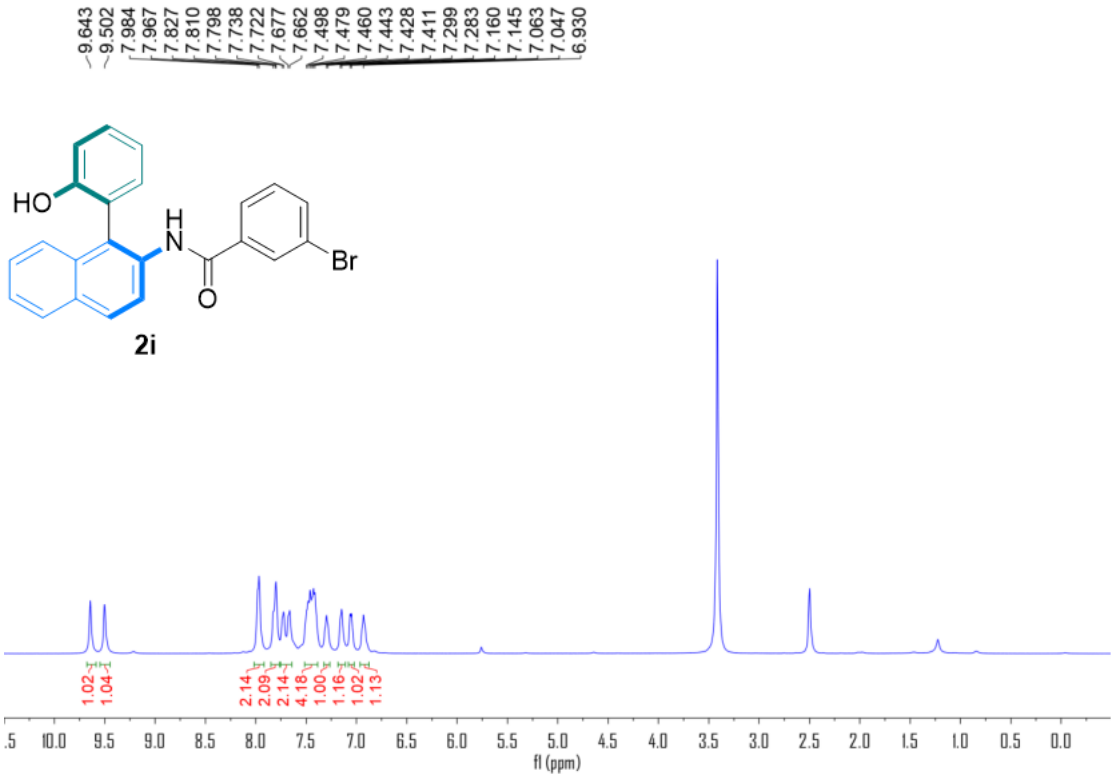
125.500
122.791
119.476
116.245
HO
H
N
O
Cl
2h
f1 (ppm)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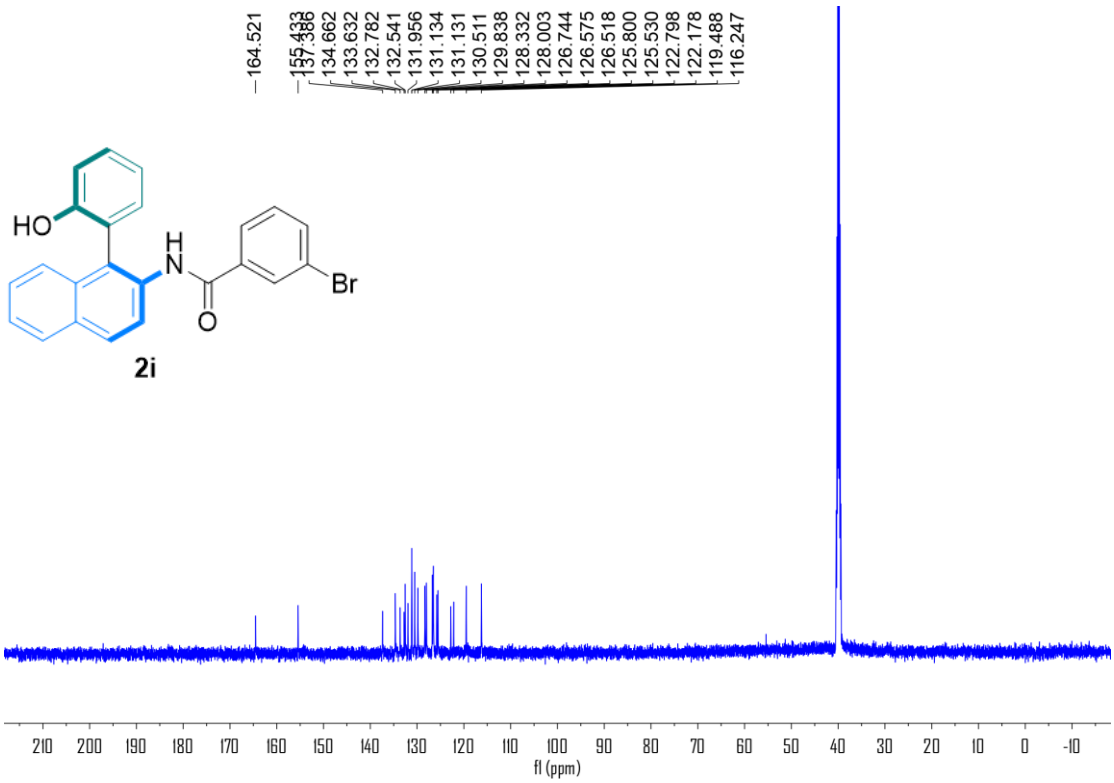
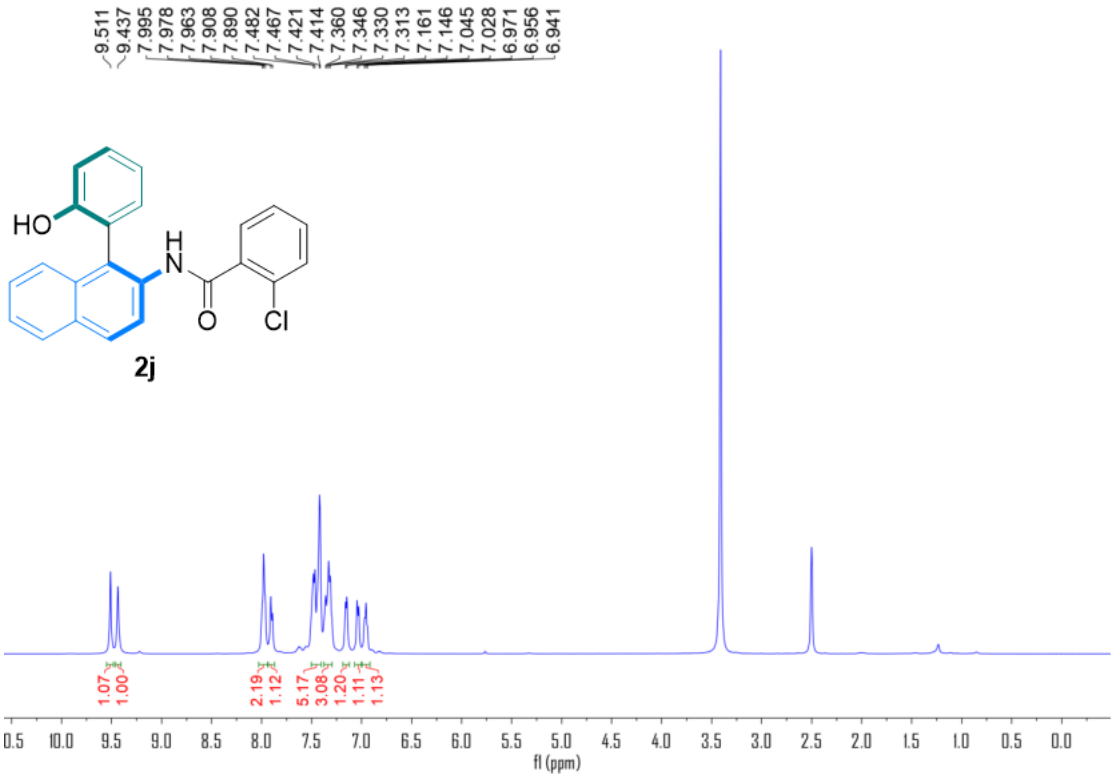
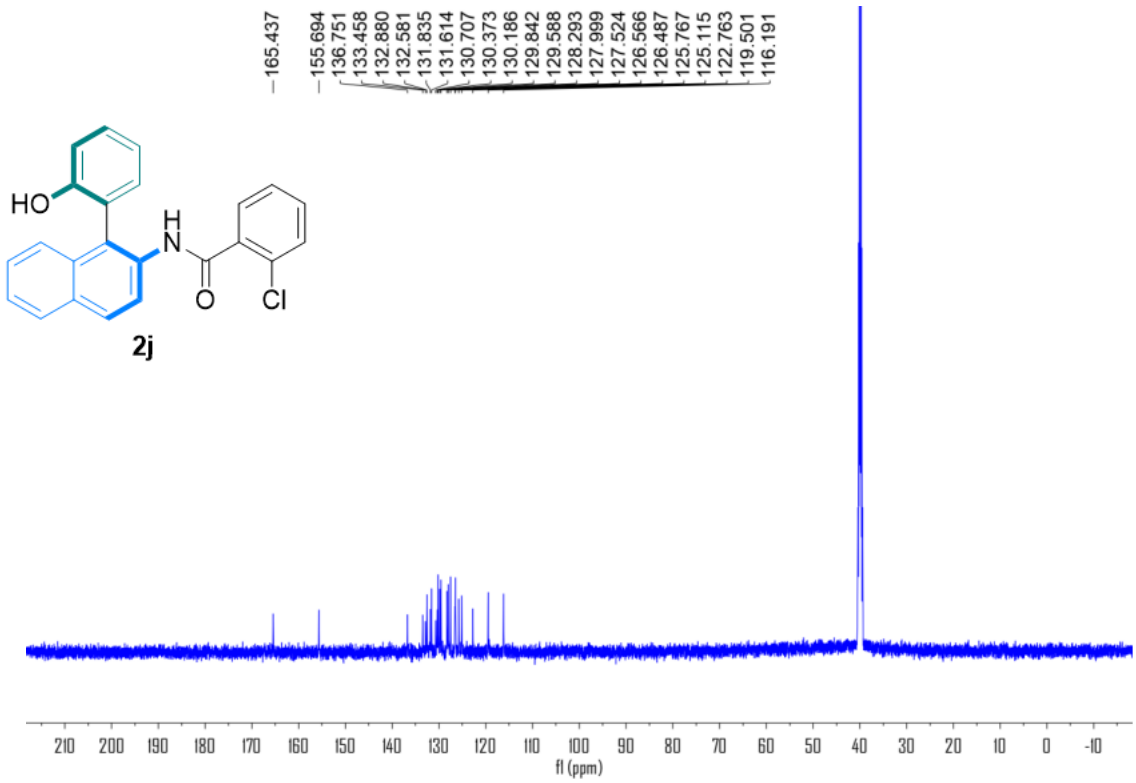
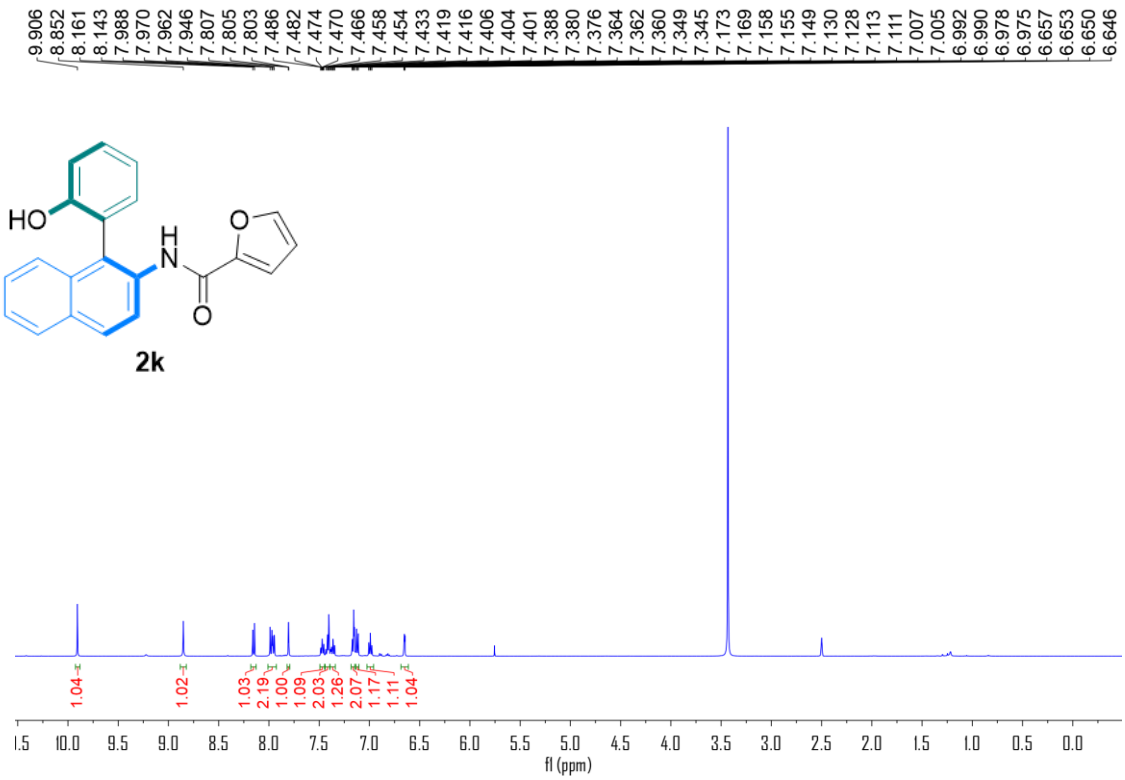
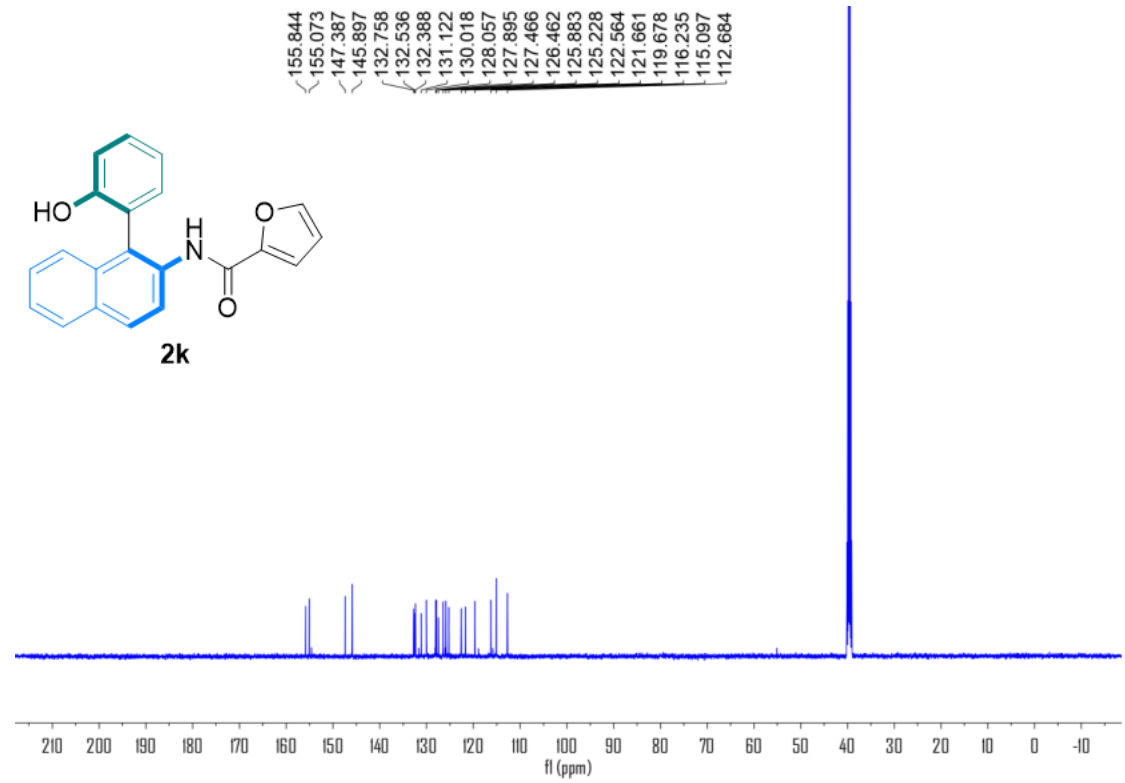
7.827
7.810
7.798
7.738
7.722
7.677
7.662
7.498
7.479
7.460
7.443
7.428
7.411
7.299
7.283
7.160
7.145
7.063
7.047
6.930
HO
H
N
O
Br
2i
1.02
1.04
2.14
2.09
2.14
4.18
1.00
1.16
1.02
1.13
f1 (ppm)

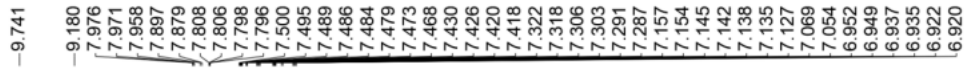

164.521
155.433
137.386
134.662
133.632
132.782
132.541
131.956
131.134
131.131
130.511
129.838
128.332
128.003
126.744
126.575
126.518
125.800
125.530
122.798
122.178
119.488
116.247
HO
H
N
O
Br
2i
f1 (ppm)


9.511
9.437
7.995
7.978
7.963
7.908
7.890
7.482
7.467
7.421
7.414
7.360
7.346
7.330
7.313
7.161
7.146
7.045
7.028
6.971
6.956
6.941
HO
H
N
O
Cl
2j
1.07
1.00
2.19
1.12
5.17
3.08
1.20
1.11
1.13
f1 (ppm)


165.437
155.694
136.751
133.458
132.880
132.581
131.835
131.614
130.707
130.373
130.186
129.842
129.588
128.293
127.999
127.524
126.566
126.487
125.767
125.115
122.763
119.501
116.191
HO
H
N
O
Cl
2j
f1 (ppm)


9.906
8.852
8.161
8.143
7.988
7.970
7.962
7.946
7.807
7.805
7.803
7.486
7.482
7.474
7.470
7.466
7.458
7.454
7.433
7.419
7.416
7.406
7.404
7.401
7.388
7.380
7.376
7.364
7.362
7.360
7.349
7.345
7.173
7.169
7.158
7.155
7.149
7.130
7.128
7.113
7.111
7.007
7.005
6.992
6.990
6.978
6.975
6.657
6.653
6.650
6.646
HO
H
N
O
O
2k
1.04
1.02
1.03
2.19
1.00
1.09
2.03
1.26
2.07
1.17
1.11
1.04
f1 (ppm)


155.844
155.073
147.387
145.897
132.758
132.536
132.388
131.122
130.018
128.057
127.895
127.466
126.462
125.883
125.228
122.564
121.661
119.678
116.235
115.097
112.684
HO
H
N
O
O
2k
f1 (ppm)


9.741
9.180
7.976
7.971
7.958
7.897
7.879
7.808
7.806
7.798
7.796
7.500
7.495
7.489
7.486
7.484
7.479
7.473
7.468
7.430
7.426
7.420
7.418
7.322
7.318
7.306
7.303
7.291
7.287
7.157
7.154
7.145
7.142
7.138
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7.127
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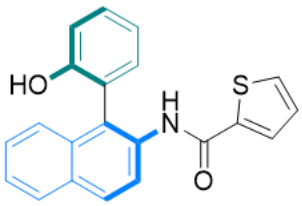
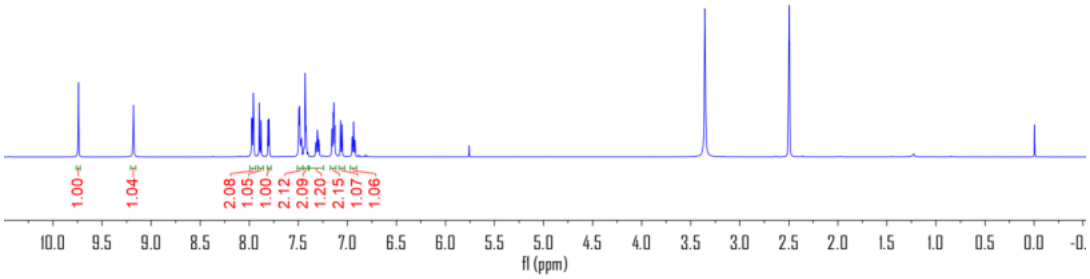
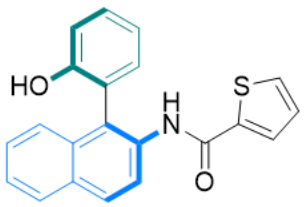
6.949
6.937
6.935
6.922
6.920


HO
H
N
S
O

2l

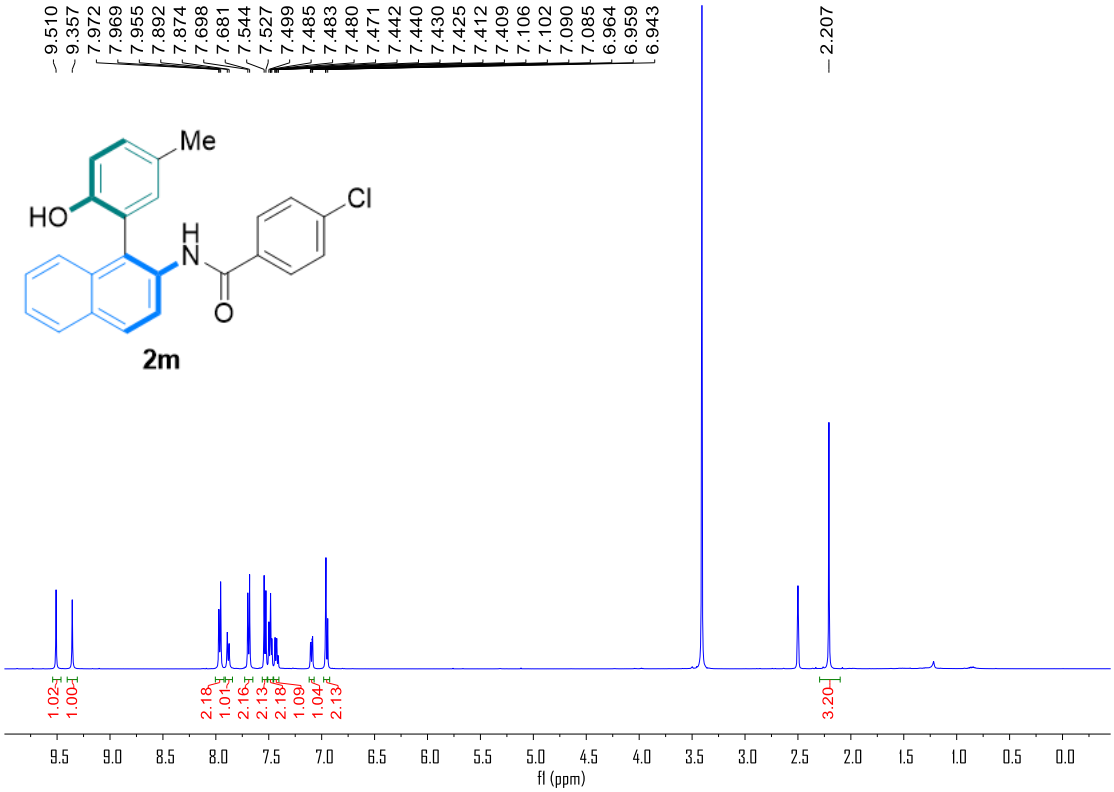

1.00
1.04
2.08
1.05
1.00
2.12
2.09
1.20
2.15
1.07
1.06
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

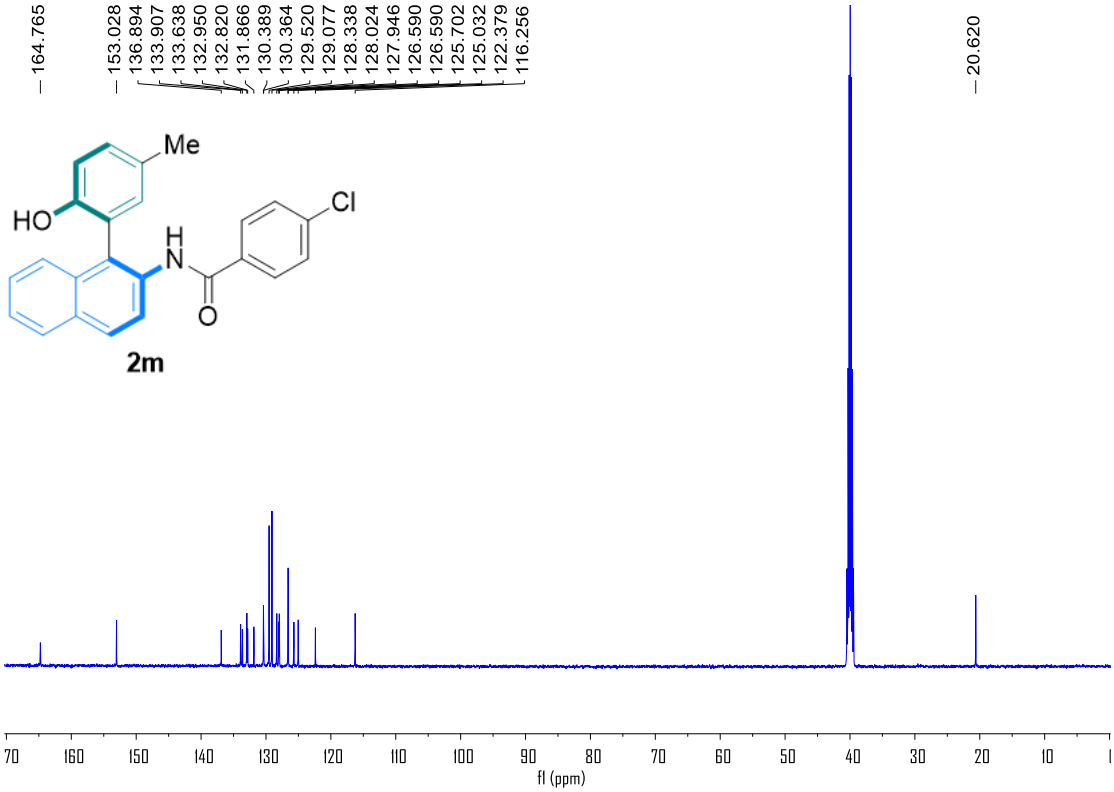

160.174
155.328
139.907
133.393
132.805
132.650
132.087
131.740
129.986
129.916
129.003
128.558
128.342
128.063
126.627
126.435
125.679
124.737
122.532
119.674
116.358


HO
H
N
S
O

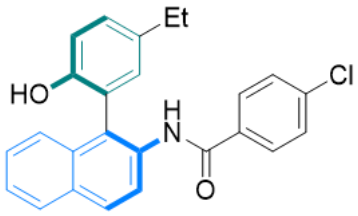
2l

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

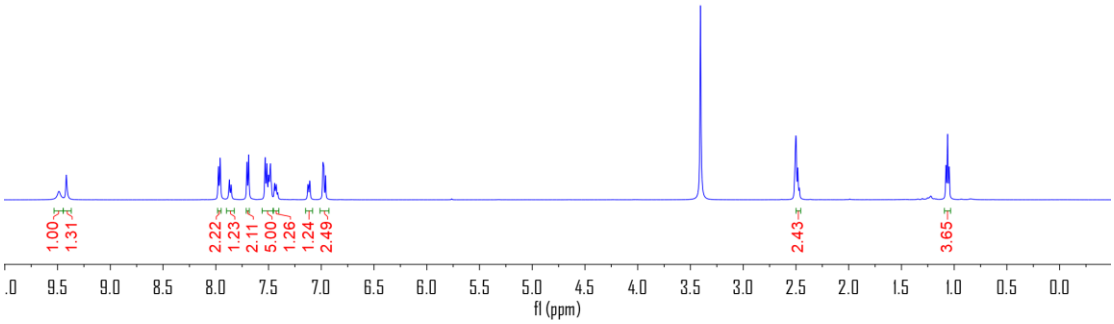

9.510
9.357
7.972
7.969
7.955
7.892
7.874
7.698
7.681
7.544
7.527
7.499
7.485
7.483
7.480
7.471
7.442
7.440
7.430
7.425
7.412
7.409
7.106
7.102
7.090
7.085
6.964
6.959
6.943
2.207
Me
HO
H
N
O
Cl
2m
1.02
1.00
2.18
1.01
2.16
2.13
2.18
1.09
1.04
2.13
3.20
fl (ppm)


164.765
153.028
136.894
133.907
133.638
132.950
132.820
131.866
130.389
130.364
129.520
129.077
128.338
128.024
127.946
126.590
126.590
125.702
125.032
122.379
116.256
20.620
Me
HO
H
N
O
Cl
2m
fl (ppm)

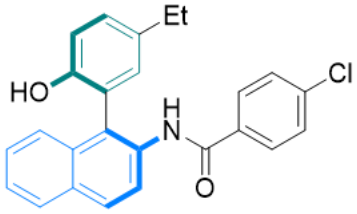

9.487
9.416
7.975
7.958
7.872
7.854
7.705
7.688
7.532
7.516
7.500
7.488
7.482
7.473
7.443
7.431
7.426
7.412
7.127
7.123
7.111
7.106
6.985
6.981
6.976
6.959
2.511
2.498
2.482
2.467
1.078
1.062
1.047


Et
HO
H
N
O
Cl

2n

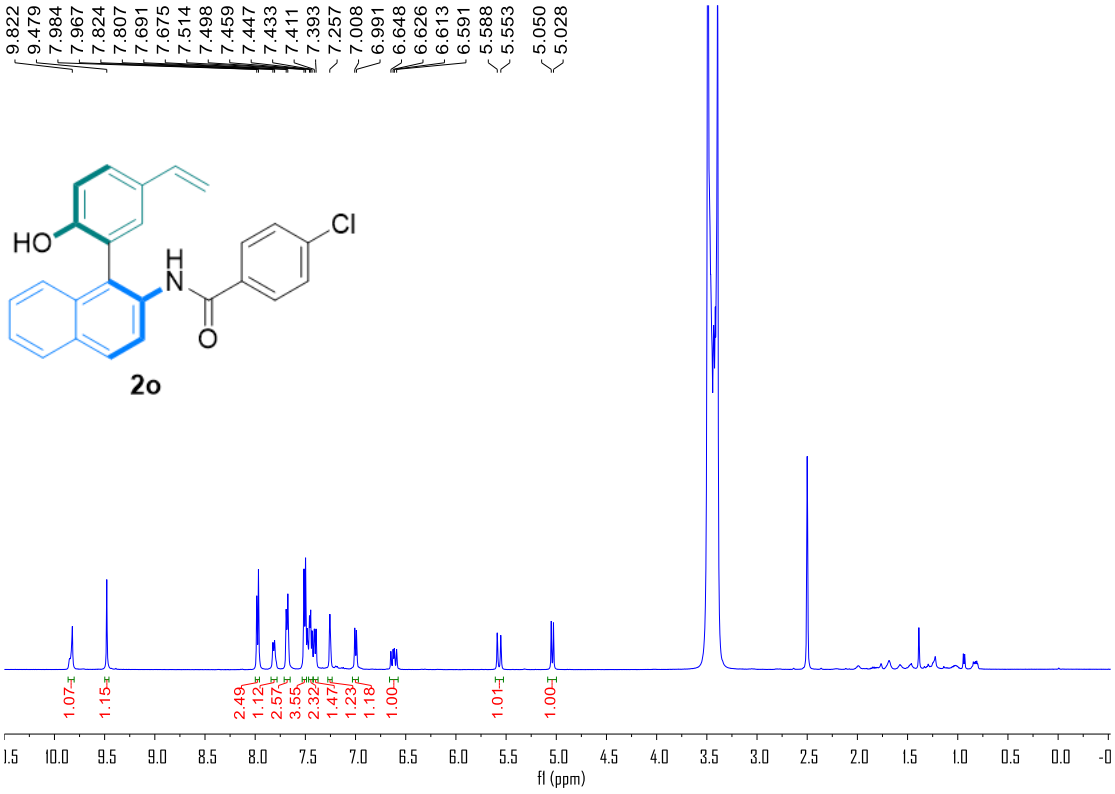

1.00
1.31
2.22
1.23
2.11
5.00
1.26
1.24
2.49
2.43
3.65
f1 (ppm)

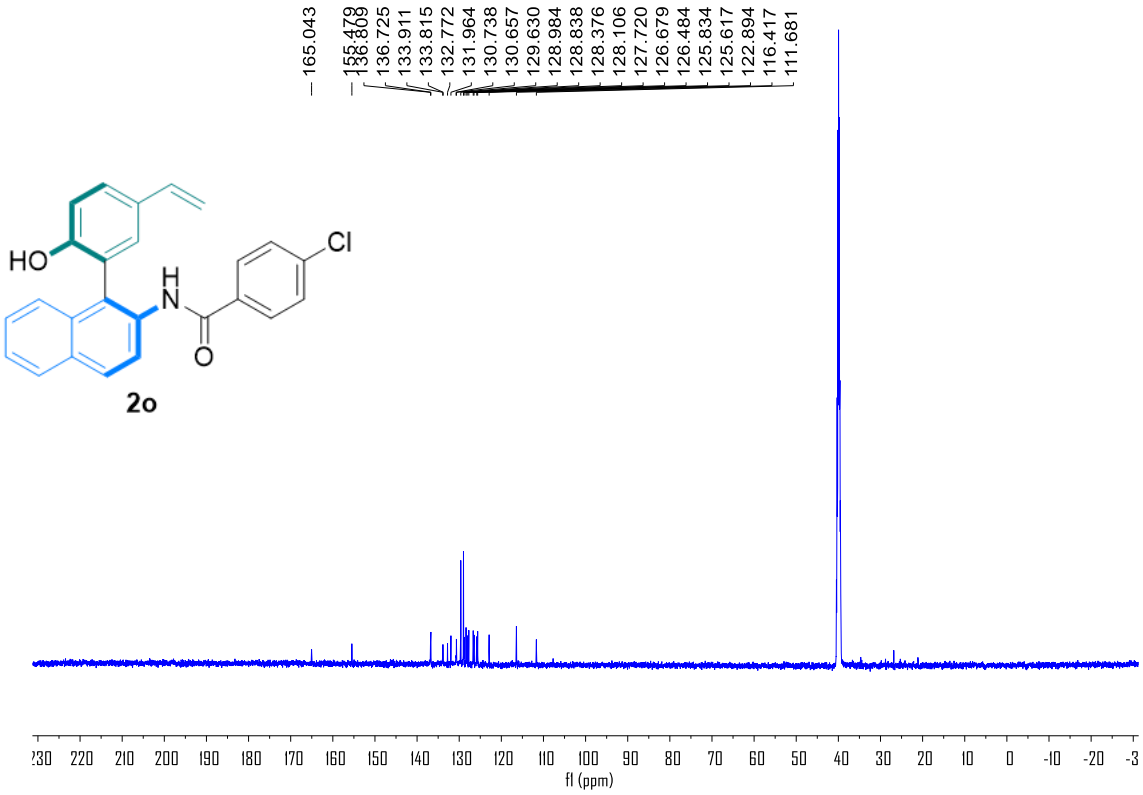

164.496
152.906
136.523
134.233
133.485
133.270
132.416
131.531
131.207
130.559
129.219
128.826
128.650
127.970
127.601
126.372
126.198
125.373
124.936
122.084
115.890
27.443
16.033

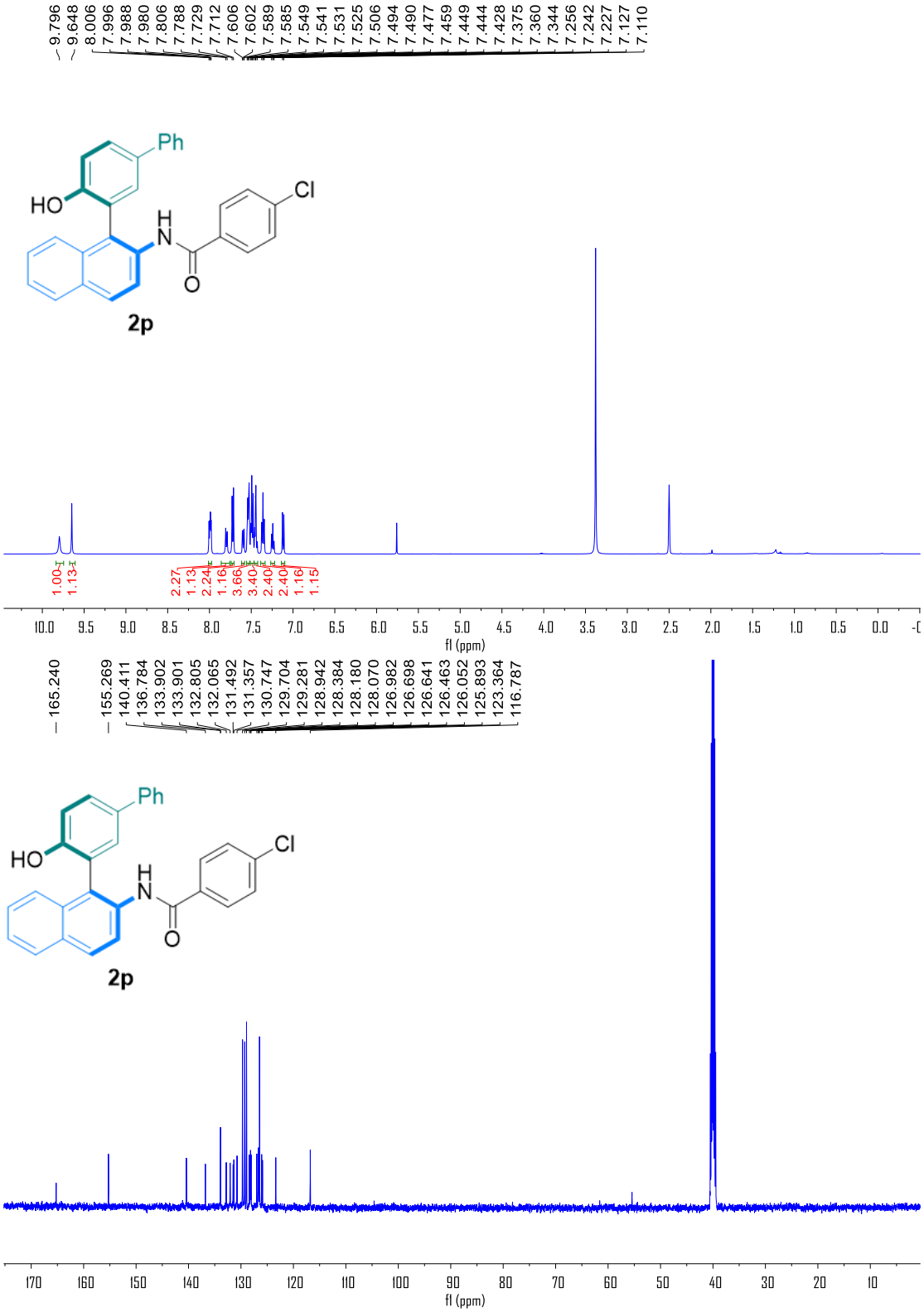

Et
HO
H
N
O
Cl

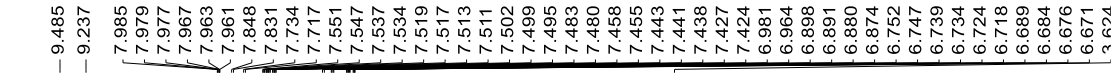
2n

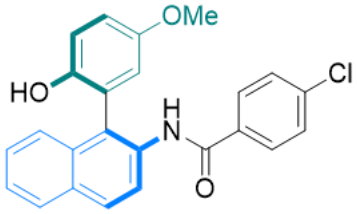
f1 (ppm)


9.822
9.479
7.984
7.967
7.824
7.807
7.691
7.675
7.514
7.498
7.459
7.447
7.433
7.411
7.393
7.257
7.008
6.991
6.648
6.626
6.613
6.591
5.588
5.553
5.050
5.028
HO
H
N
O
Cl
2o
1.07
1.15
2.49
1.12
2.57
3.55
2.32
1.47
1.23
1.18
1.00
1.01
1.00
f1 (ppm)


165.043
155.479
136.809
136.725
133.911
133.815
132.772
131.964
130.738
130.657
129.630
128.984
128.838
128.376
128.106
127.720
126.679
126.484
125.834
125.617
122.894
116.417
111.681
HO
H
N
O
Cl
2o
f1 (ppm)

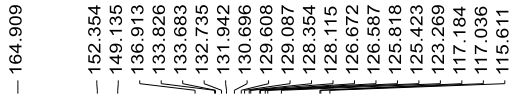

9.796
9.648
8.006
7.996
7.988
7.980
7.806
7.788
7.729
7.712
7.606
7.602
7.589
7.585
7.549
7.541
7.531
7.525
7.506
7.494
7.490
7.477
7.459
7.449
7.444
7.428
7.375
7.360
7.344
7.256
7.242
7.227
7.127
7.110
Ph
HO
H
N
O
Cl
2p
1.00
1.13
2.27
1.13
2.24
1.16
3.66
3.40
2.40
2.40
1.16
1.15
f1 (ppm)
165.240
155.269
140.411
136.784
133.902
133.901
132.805
132.065
131.492
131.357
130.747
129.704
129.281
128.942
128.384
128.180
128.070
126.982
126.698
126.641
126.463
126.052
125.893
123.364
116.787
Ph
HO
H
N
O
Cl
2p
f1 (ppm)


9.485
9.237
7.985
7.979
7.977
7.967
7.963
7.961
7.848
7.831
7.734
7.717
7.551
7.547
7.537
7.534
7.519
7.517
7.513
7.511
7.502
7.499
7.495
7.483
7.480
7.458
7.455
7.443
7.441
7.438
7.427
7.424
6.981
6.964
6.898
6.891
6.880
6.874
6.752
6.747
6.739
6.734
6.724
6.718
6.689
6.684
6.676
6.671


OMe
HO
H
N
O
Cl

2q

1.03
1.00
2.16
1.05
2.15
2.09
2.14
1.06
1.06
1.07
2.60
3.14
f1 (ppm)


164.909
152.354
149.135
136.913
133.826
133.683
132.735
131.942
130.696
129.608
129.087
128.354
128.115
126.672
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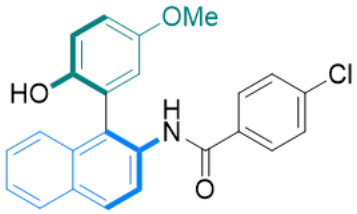
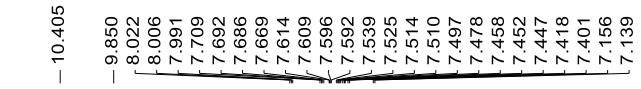
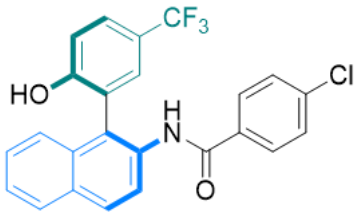
125.423
123.269
117.184
117.036
115.611
55.796


OMe
HO
H
N
O
Cl

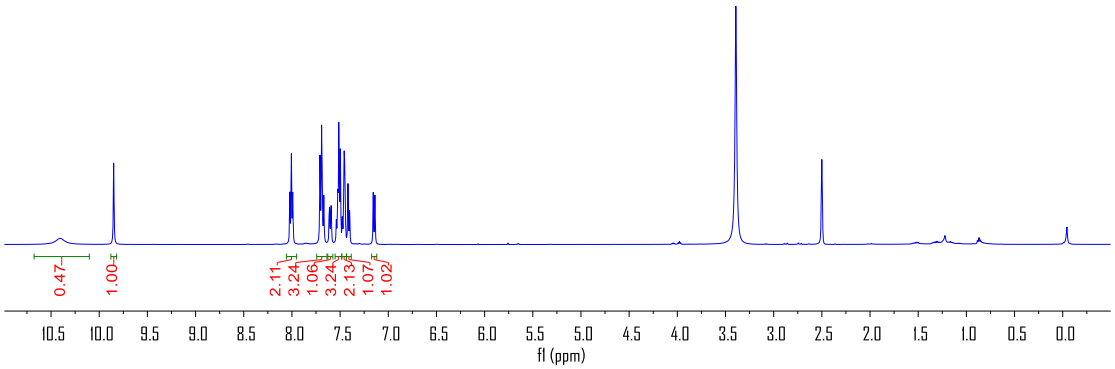
2q

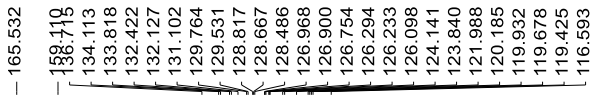
f1 (ppm)


10.405
9.850
8.022
8.006
7.991
7.709
7.692
7.686
7.669
7.614
7.609
7.596
7.592
7.539
7.525
7.514
7.510
7.497
7.478
7.458
7.452
7.447
7.418
7.401
7.156
7.139


CF3
HO
H
N
O
Cl

2r


0.47
1.00
2.11
3.24
1.06
3.24
2.13
1.07
1.02
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


165.532
158.110
138.115
134.113
133.818
132.422
132.127
131.102
129.764
129.531
128.817
128.667
128.486
126.968
126.900
126.754
126.294
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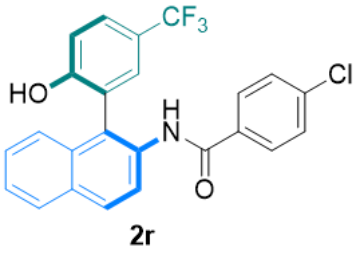
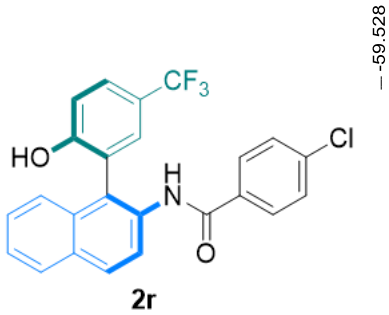
126.098
124.141
123.840
121.988
120.185
119.932
119.678
119.425
116.593


CF3
HO
H
N
O
Cl

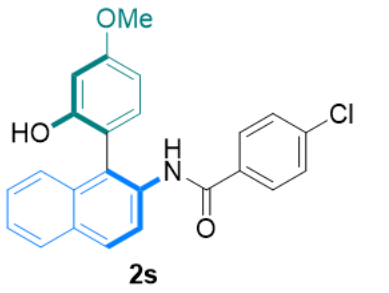
2r

170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

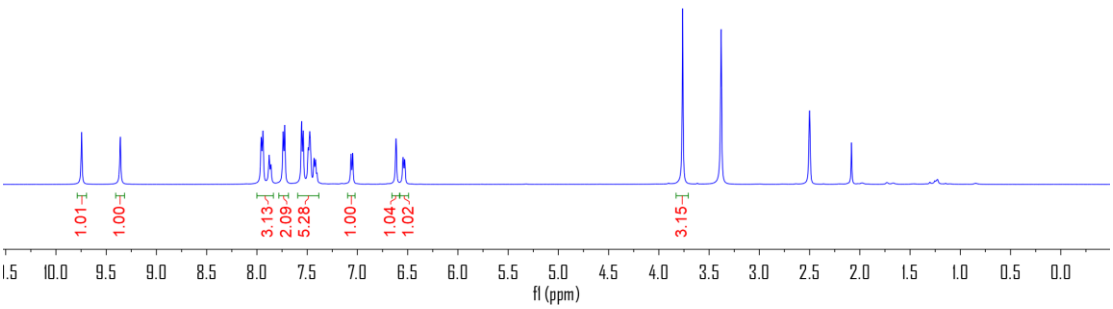

CF3
HO
H
N
O
Cl

2r

-59.528
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)
9.744
9.360
7.957
7.940
7.878
7.861
7.739
7.723
7.556
7.540
7.489
7.474
7.432
7.417
7.063
7.047
6.616
6.546
6.530
3.763


OMe
HO
H
N
O
Cl

2s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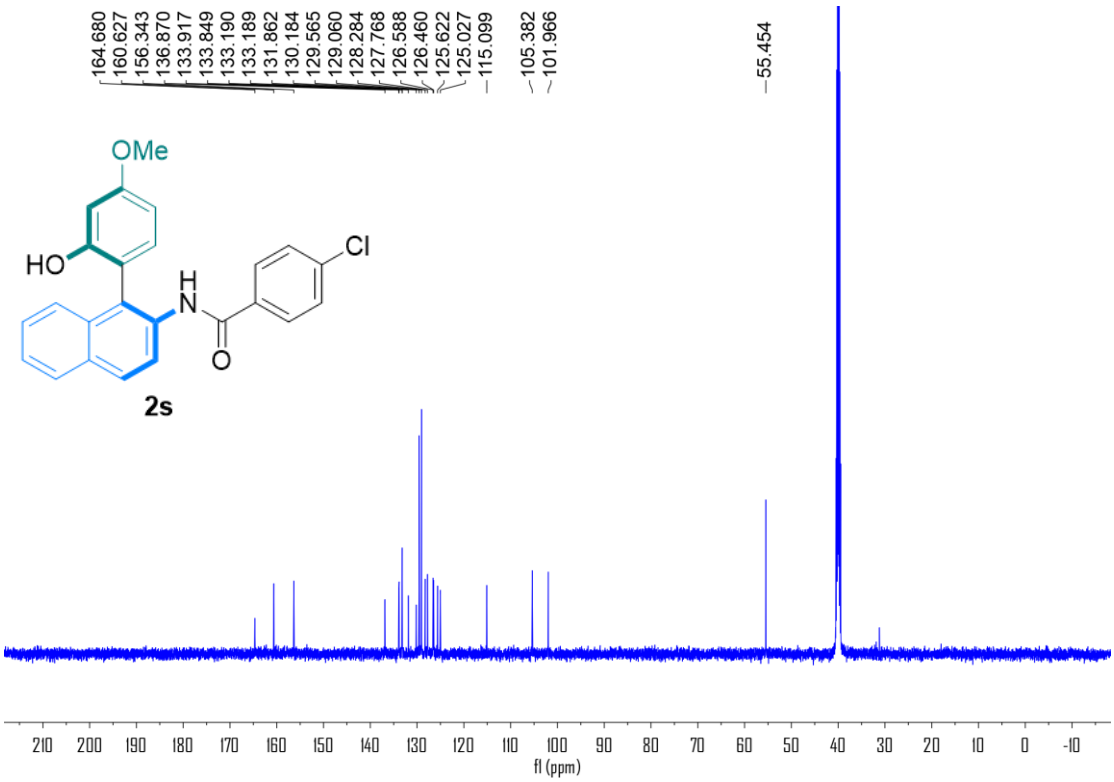
1.00
3.13
2.09
5.28
1.00
1.04
1.02
3.15
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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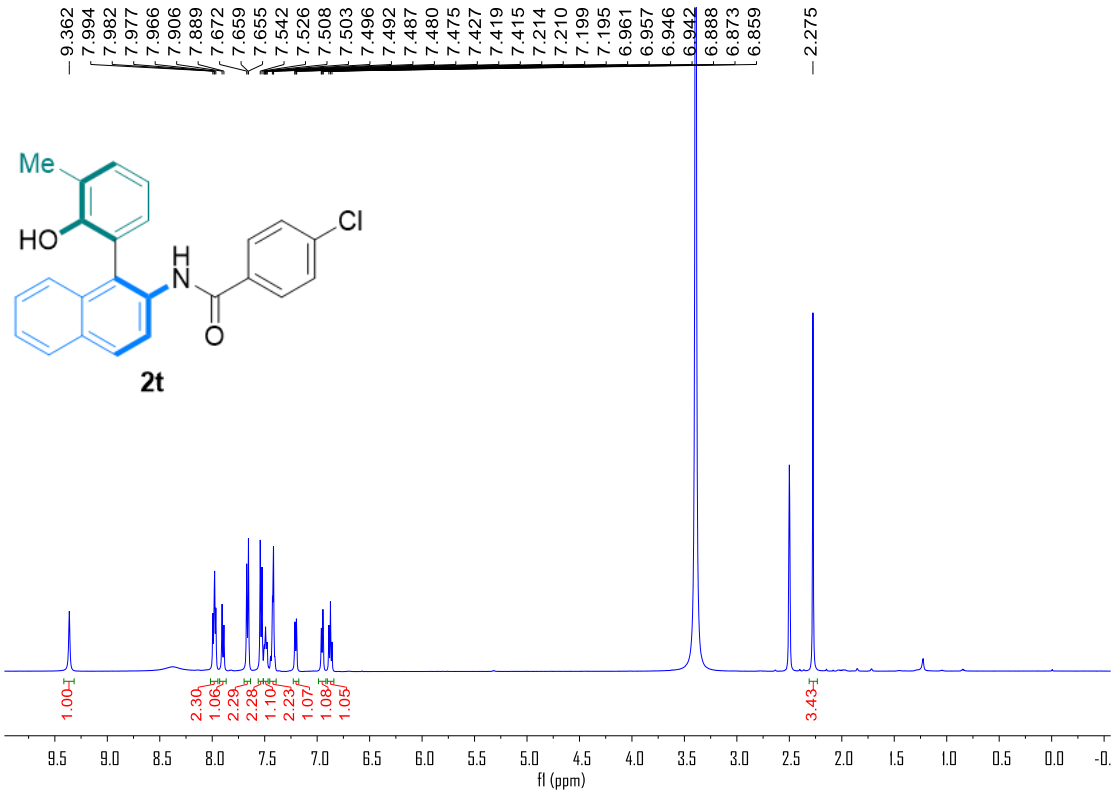
133.190
133.189
131.862
130.184
129.565
129.060
128.284
127.768
126.588
126.460
125.622
125.027
115.099
105.382
101.966
55.454
OMe
HO
H
N
O
Cl
2s
f1 (ppm)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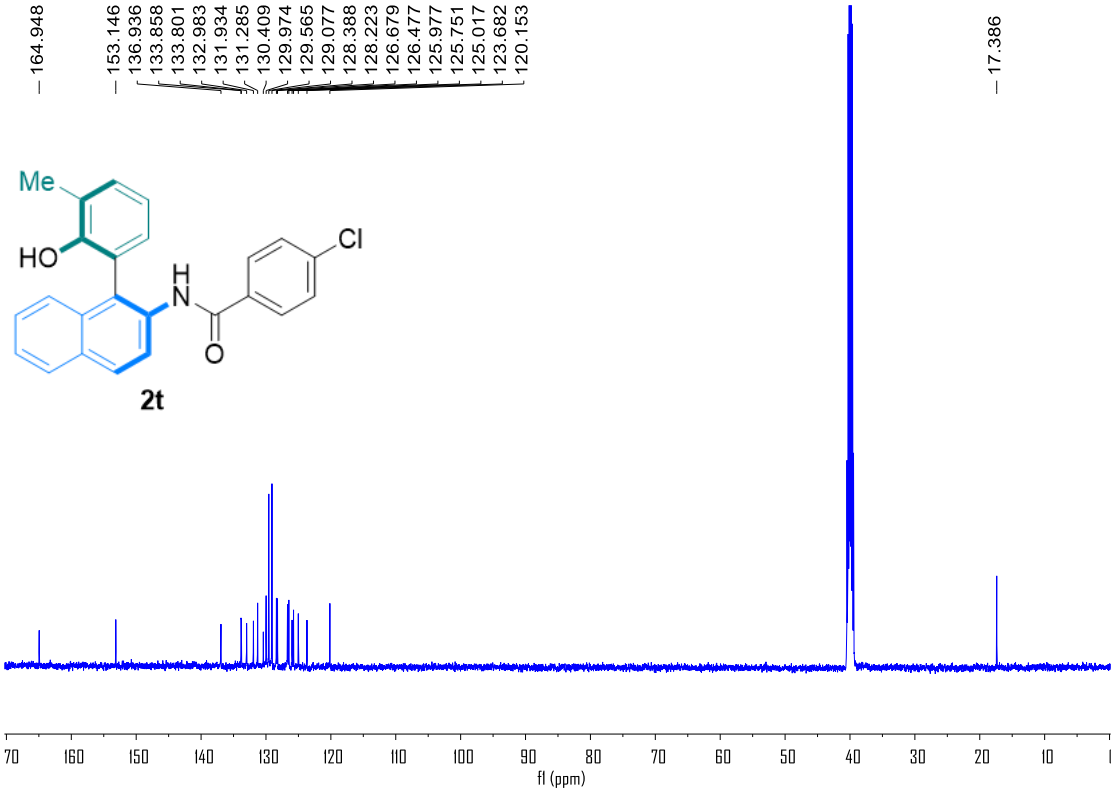
7.889
7.672
7.659
7.655
7.542
7.526
7.508
7.503
7.496
7.492
7.487
7.480
7.475
7.427
7.419
7.415
7.214
7.210
7.199
7.195
6.961
6.957
6.946
6.942
6.888
6.873
6.859
2.275
Me
HO
H
N
O
Cl
2t
1.00
2.30
1.06
2.29
2.28
1.10
2.23
1.07
1.08
1.05
3.43
f1 (ppm)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153.146
136.936
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133.801
132.983
131.934
131.285
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129.974
129.565
129.077
128.388
128.223
126.679
126.477
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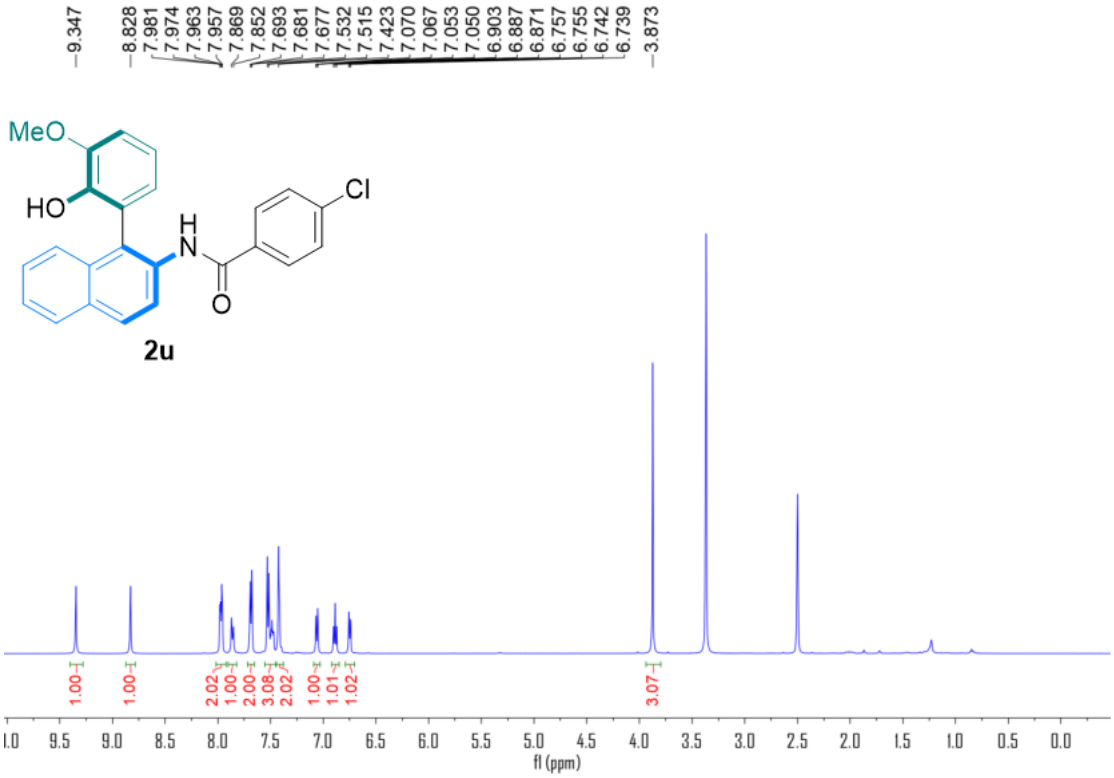
125.017
123.682
120.153
17.386
Me
HO
H
N
O
Cl
2t
f1 (ppm)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7.974
7.963
7.957
7.869
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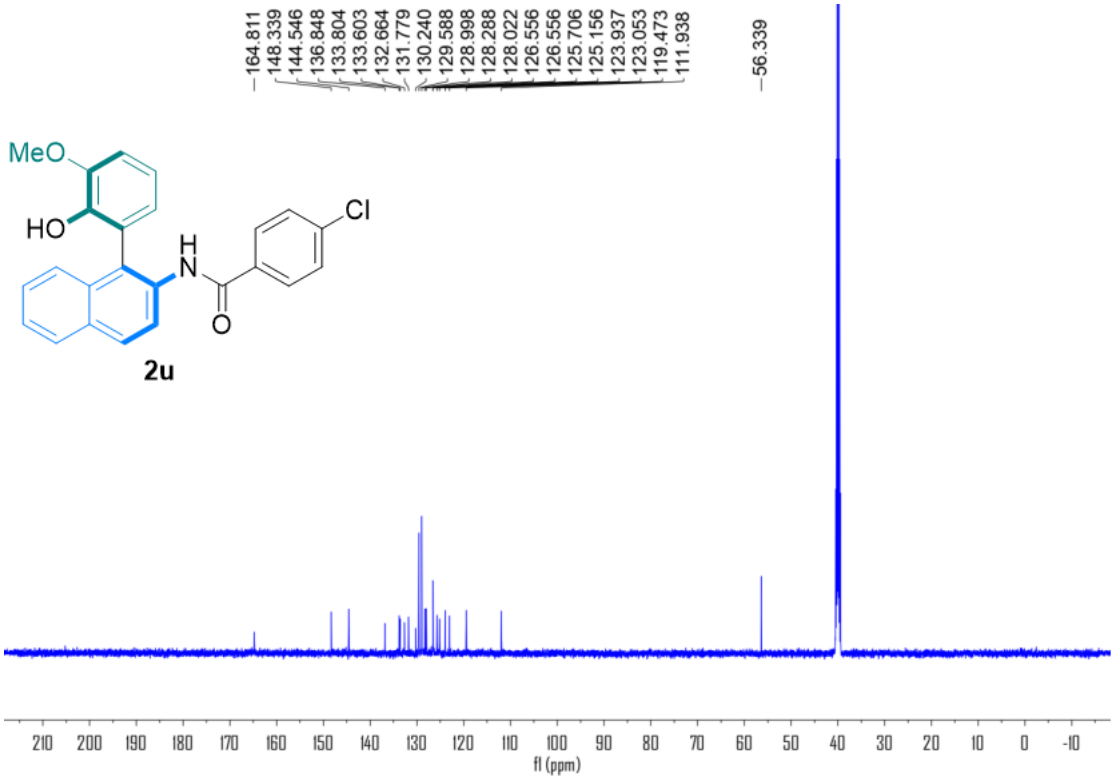
7.693
7.681
7.677
7.532
7.515
7.423
7.070
7.067
7.053
7.050
6.903
6.887
6.871
6.757
6.755
6.742
6.739
3.873
MeO
HO
H
N
O
Cl
2u
1.00
1.00
2.02
1.00
2.00
3.08
2.02
1.00
1.01
1.02
3.07
f1 (ppm)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148.339
144.546
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133.603
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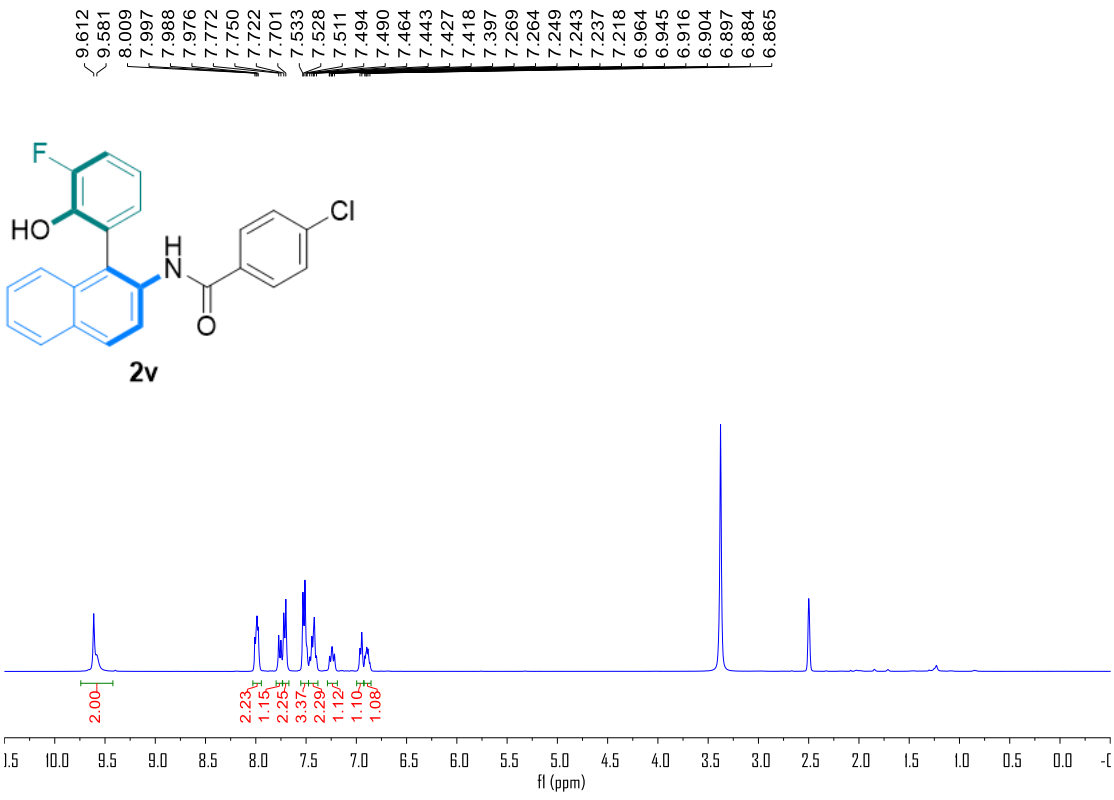
130.240
129.588
128.998
128.288
128.022
126.556
126.556
125.706
125.156
123.937
123.053
119.473
111.938
56.339
MeO
HO
H
N
O
Cl
2u
f1 (ppm)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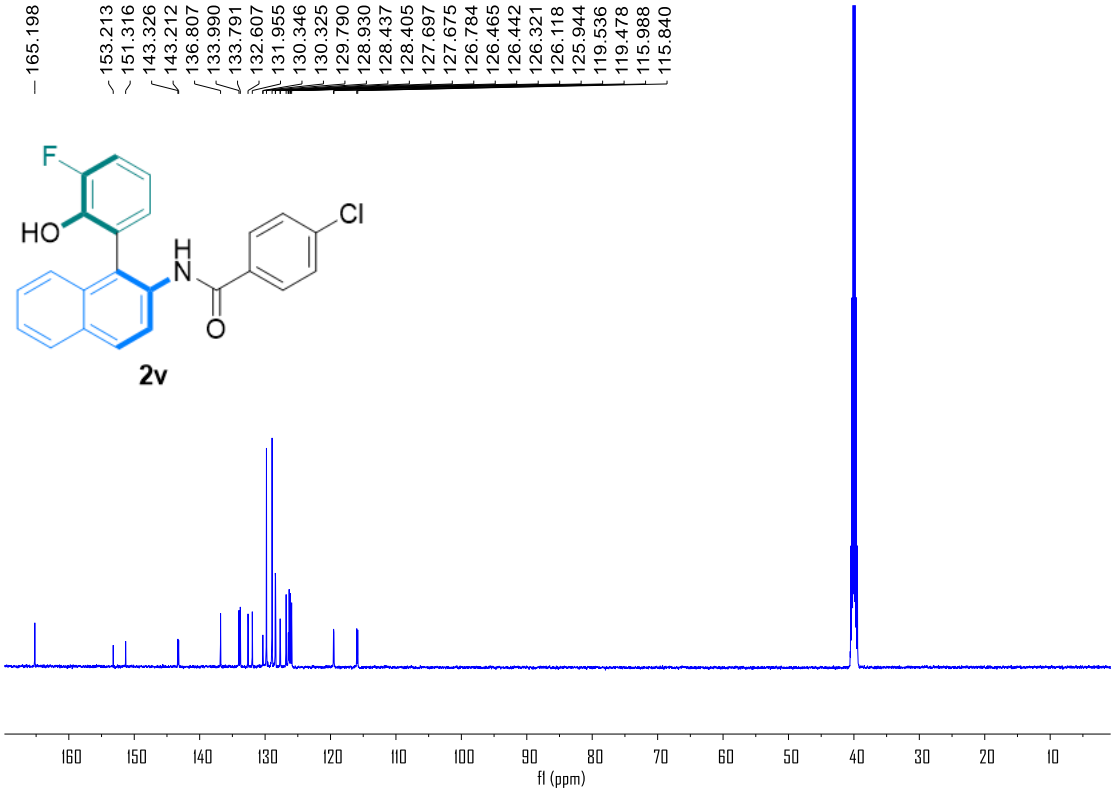
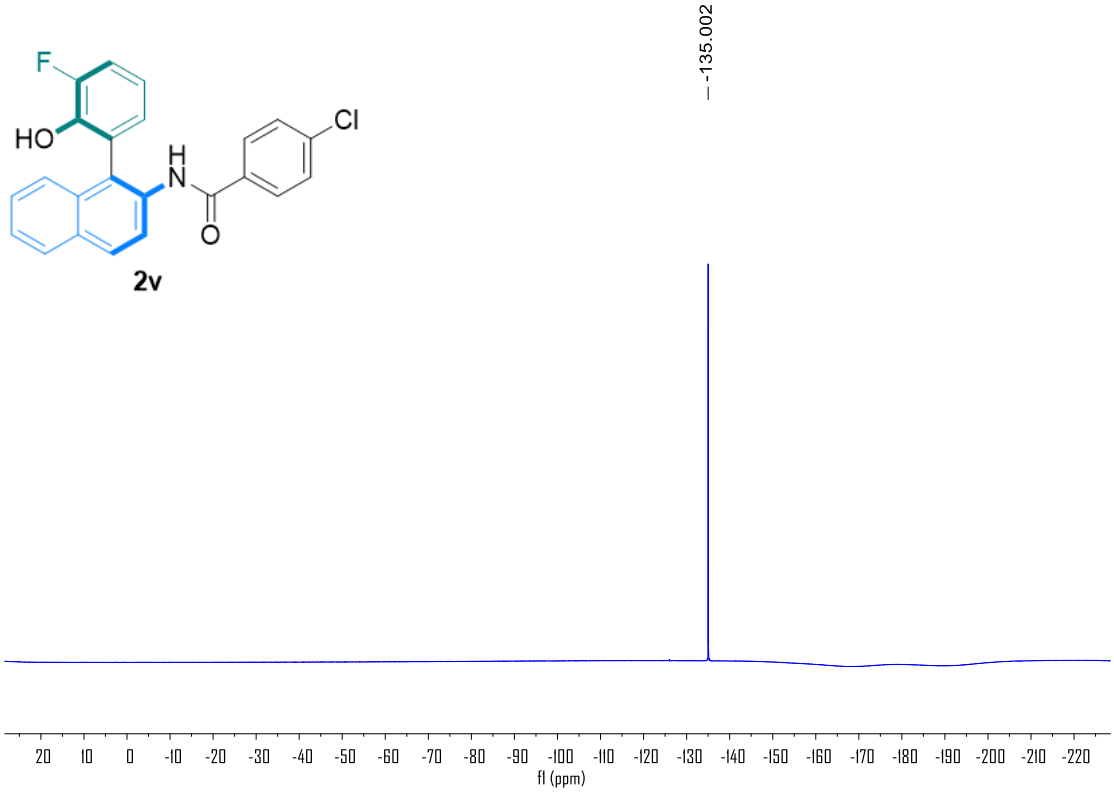
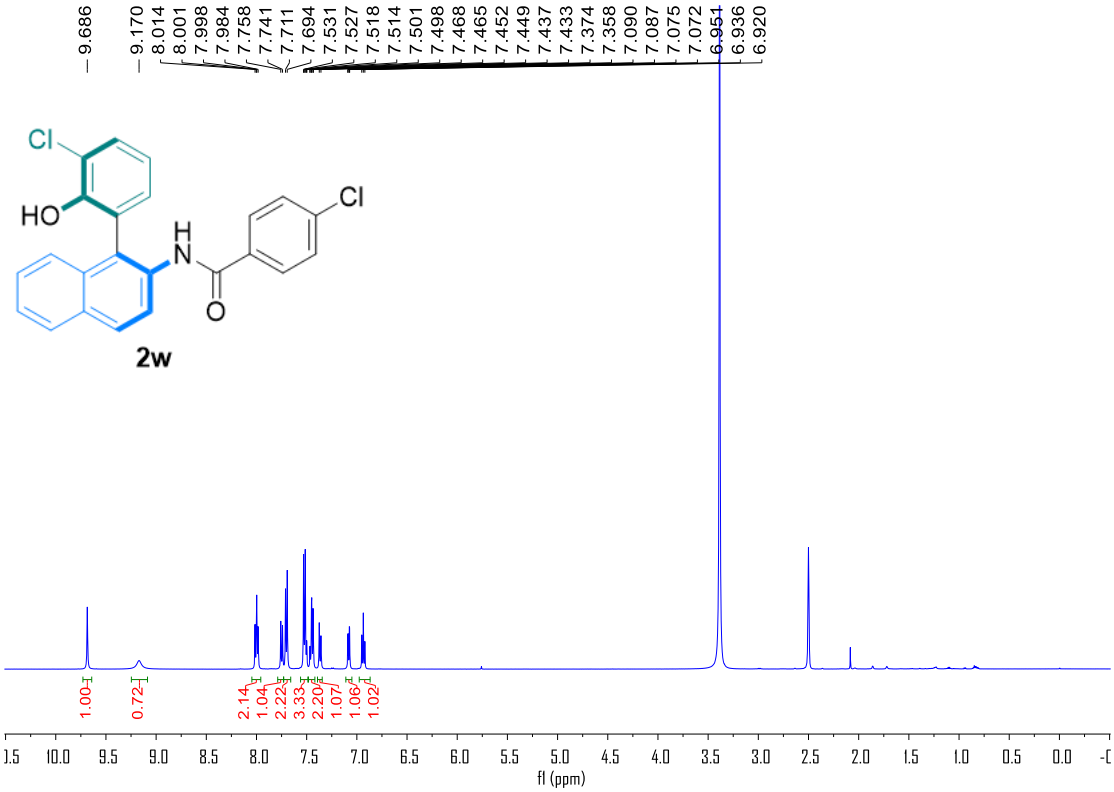
9.581
8.009
7.997
7.988
7.976
7.772
7.750
7.722
7.701
7.533
7.528
7.511
7.494
7.490
7.464
7.443
7.427
7.418
7.397
7.269
7.264
7.249
7.243
7.237
7.218
6.964
6.945
6.916
6.904
6.897
6.884
6.865
F
HO
H
N
O
Cl
2v
2.00
2.23
1.15
2.25
3.37
2.29
1.12
1.10
1.08
f1 (ppm)


165.198
153.213
151.316
143.326
143.212
136.807
133.990
133.791
132.607
131.955
130.346
130.325
129.790
128.930
128.437
128.405
127.697
127.675
126.784
126.465
126.442
126.321
126.118
125.944
119.536
119.478
115.988
115.840
F
HO
H
N
O
Cl
2v
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


-135.002
F
HO
H
N
O
Cl
2v
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-220
f1 (ppm)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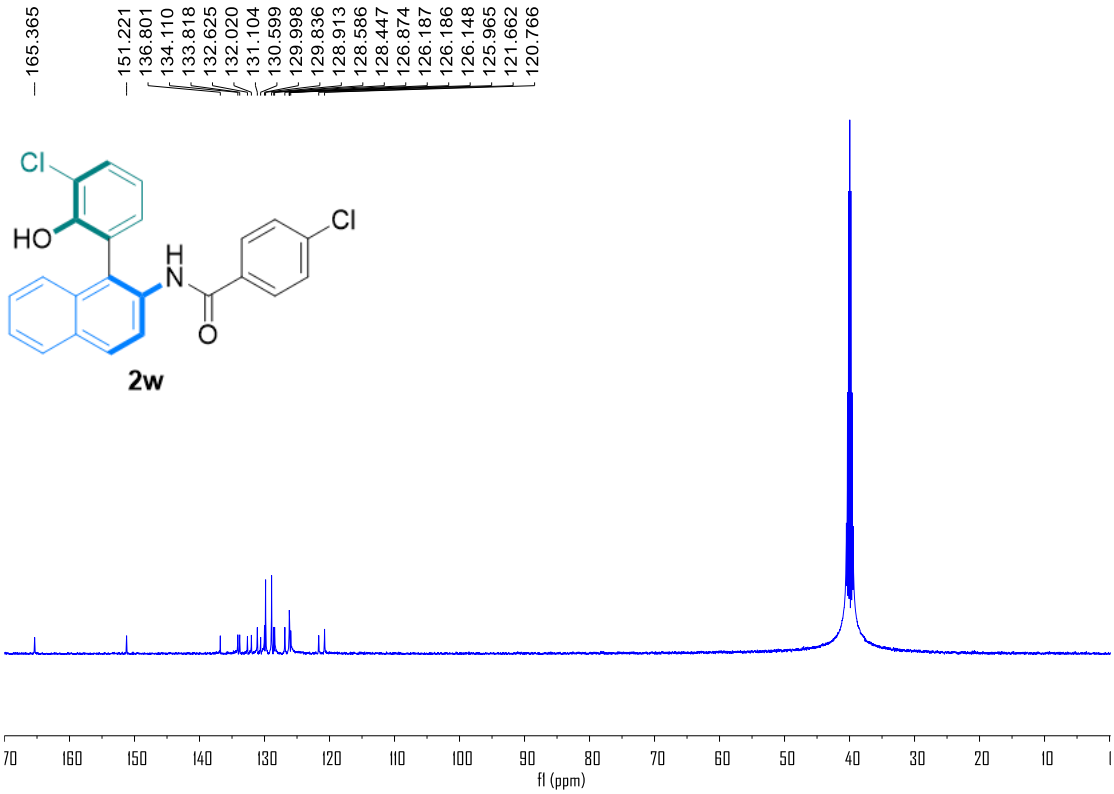
9.170
8.014
8.001
7.998
7.984
7.758
7.741
7.711
7.694
7.531
7.527
7.518
7.514
7.501
7.498
7.468
7.465
7.452
7.449
7.437
7.433
7.374
7.358
7.090
7.087
7.075
7.072
6.951
6.936
6.920
Cl
HO
H
N
O
Cl
2w
1.00
0.72
2.14
1.04
2.22
3.33
2.20
1.07
1.06
1.02
f1 (ppm)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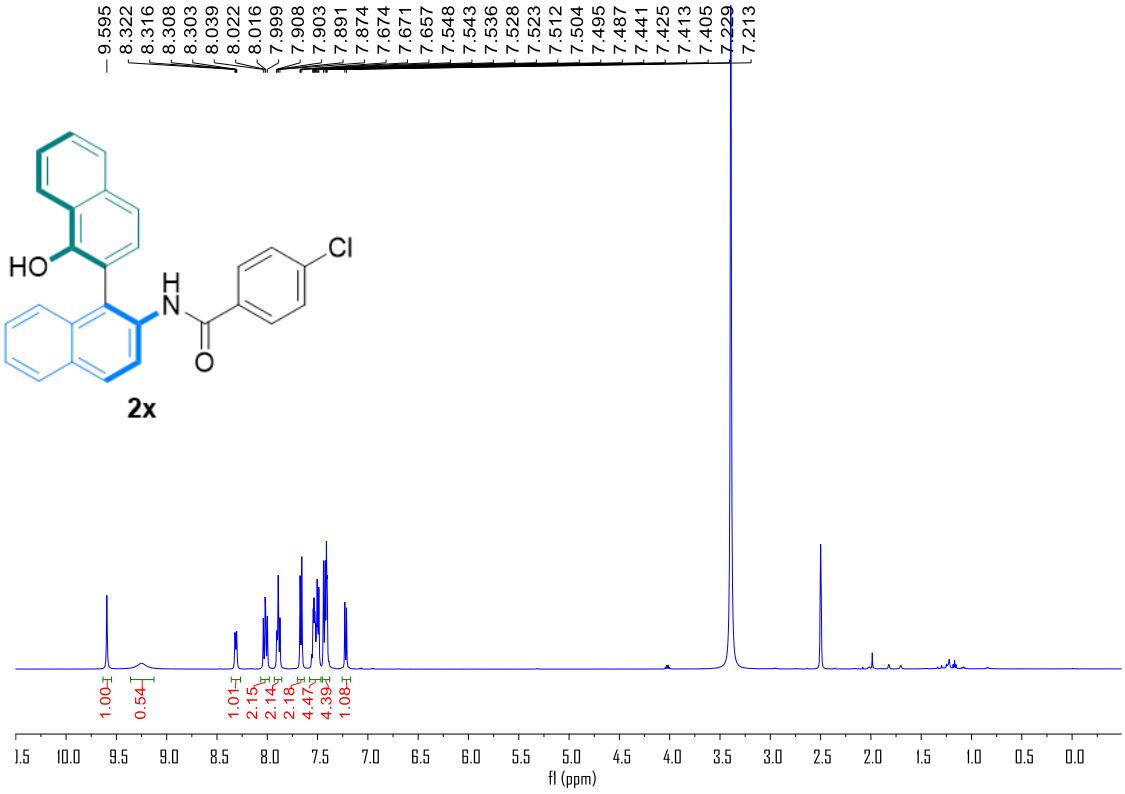
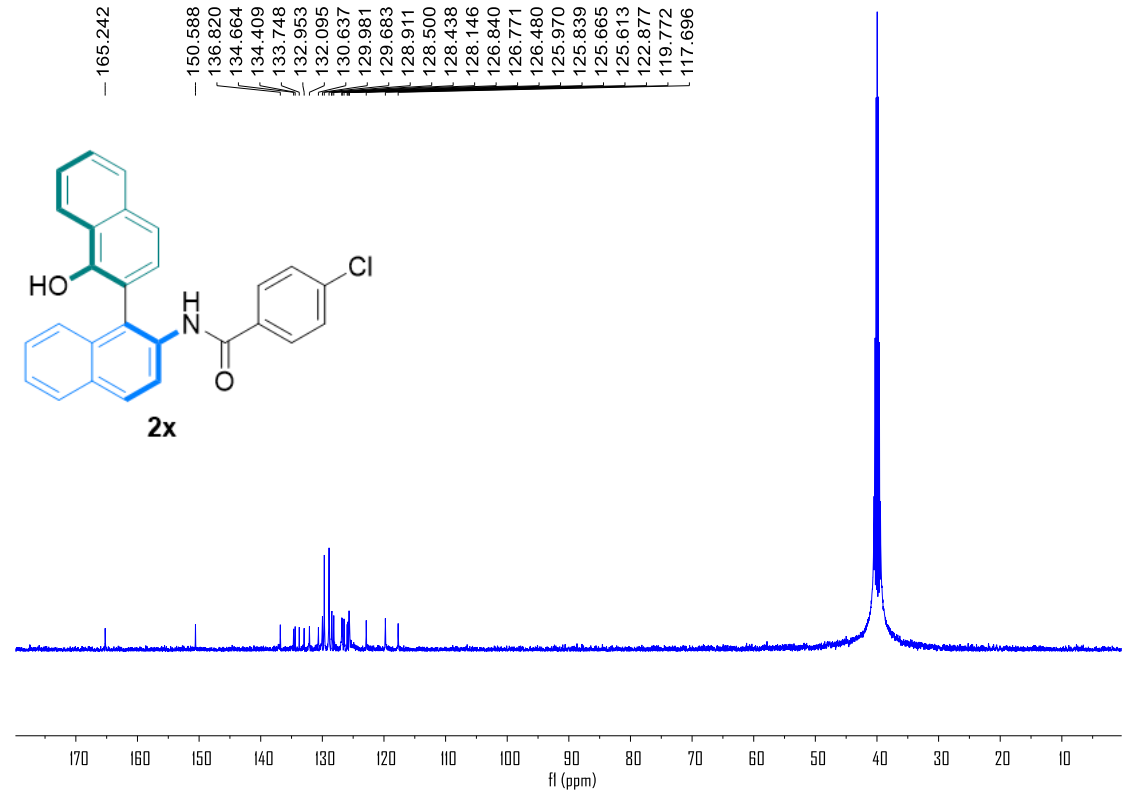
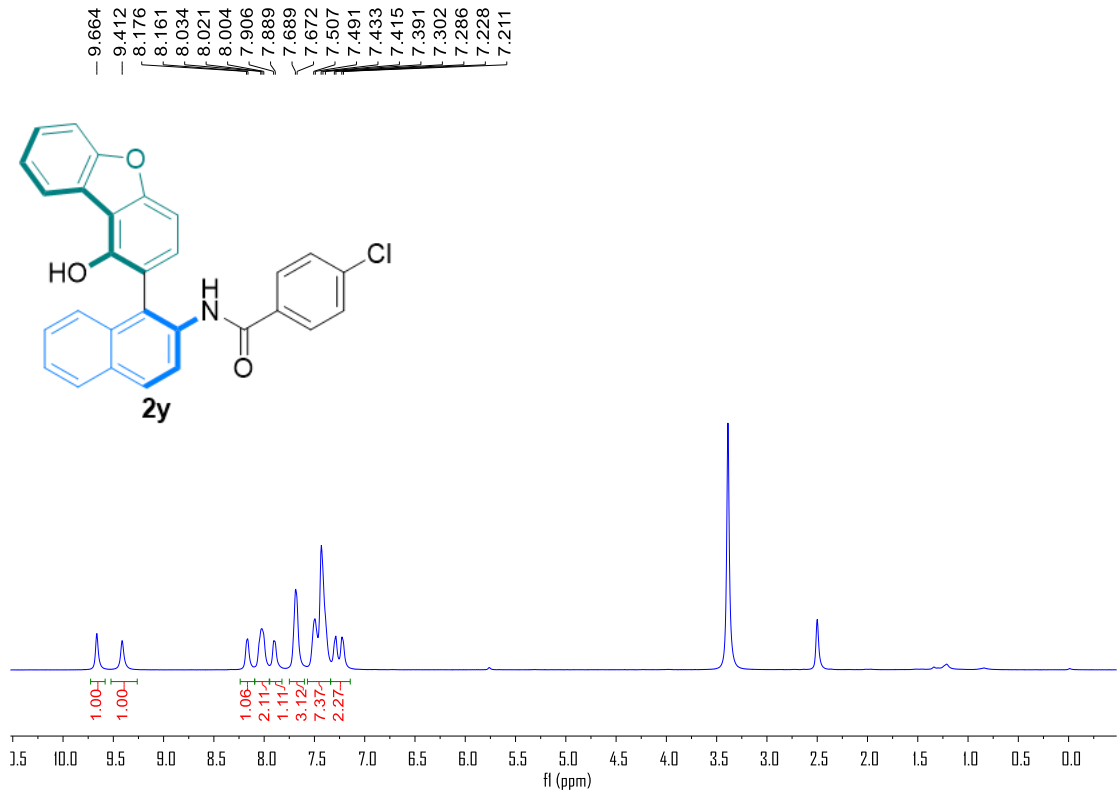
136.801
134.110
133.818
132.625
132.020
131.104
130.599
129.998
129.836
128.913
128.586
128.447
126.874
126.187
126.186
126.148
125.965
121.662
120.766
Cl
HO
H
N
O
Cl
2w
f1 (ppm)


9.595
8.322
8.316
8.308
8.303
8.039
8.022
8.016
7.999
7.908
7.903
7.891
7.874
7.674
7.671
7.657
7.548
7.543
7.536
7.528
7.523
7.512
7.504
7.495
7.487
7.441
7.425
7.413
7.405
7.229
7.213
HO
H
N
O
Cl
2x
1.00
0.54
1.01
2.15
2.14
2.18
4.47
4.39
1.08
f1 (ppm)


165.242
150.588
136.820
134.664
134.409
133.748
132.953
132.095
130.637
129.981
129.683
128.911
128.500
128.438
128.146
126.840
126.771
126.480
125.970
125.839
125.665
125.613
122.877
119.772
117.696
HO
H
N
O
Cl
2x
f1 (ppm)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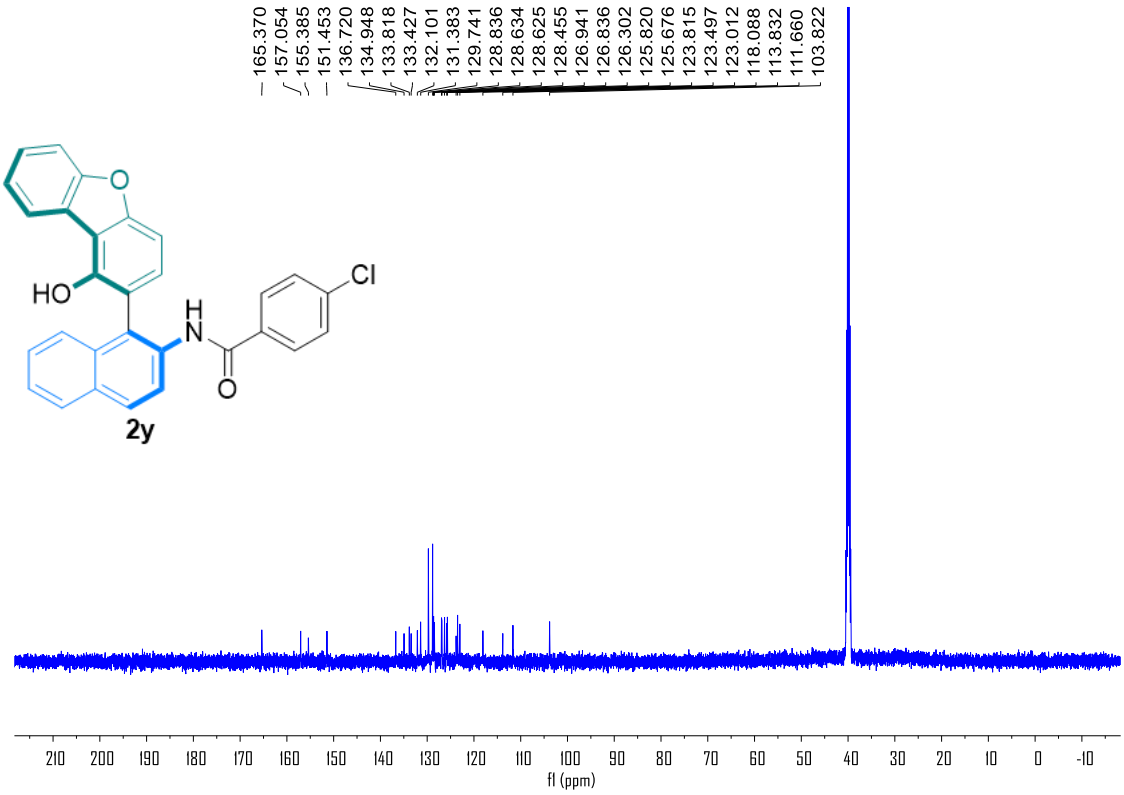
8.176
8.161
8.034
8.021
8.004
7.906
7.889
7.689
7.672
7.507
7.491
7.433
7.415
7.391
7.302
7.286
7.228
7.211
HO
H
N
O
Cl
2y
1.00
1.00
1.06
2.11
1.11
3.12
7.37
2.27
f1 (ppm)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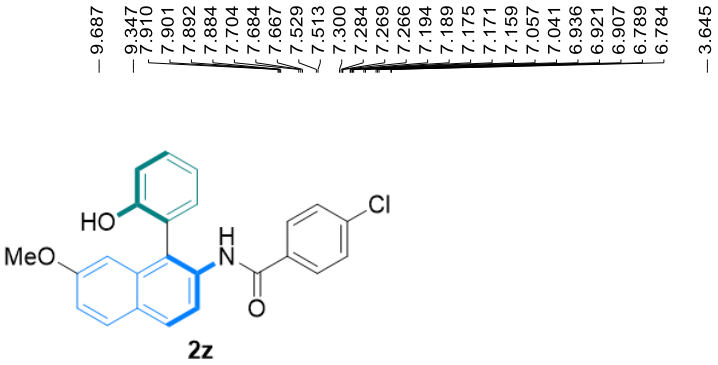
155.385
151.453
136.720
134.948
133.818
133.427
132.101
131.383
129.741
128.836
128.634
128.625
128.455
126.941
126.836
126.302
125.820
125.676
123.815
123.497
123.012
118.088
113.832
111.660
103.822
HO
H
N
O
Cl
2y
f1 (ppm)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9.347
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7.901
7.892
7.884
7.704
7.684
7.667
7.529
7.513
7.300
7.284
7.269
7.266
7.194
7.189
7.175
7.171
7.159
7.057
7.041
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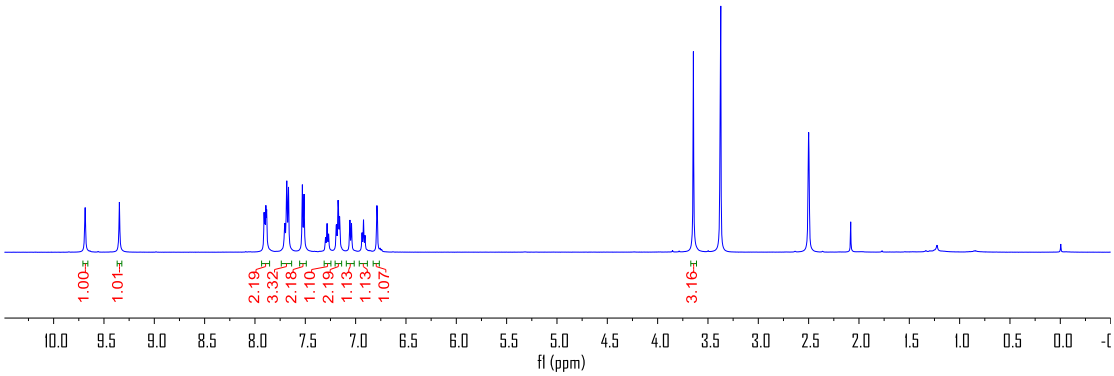
6.921
6.907
6.789
6.784
3.645
HO
MeO
H
N
O
Cl

2z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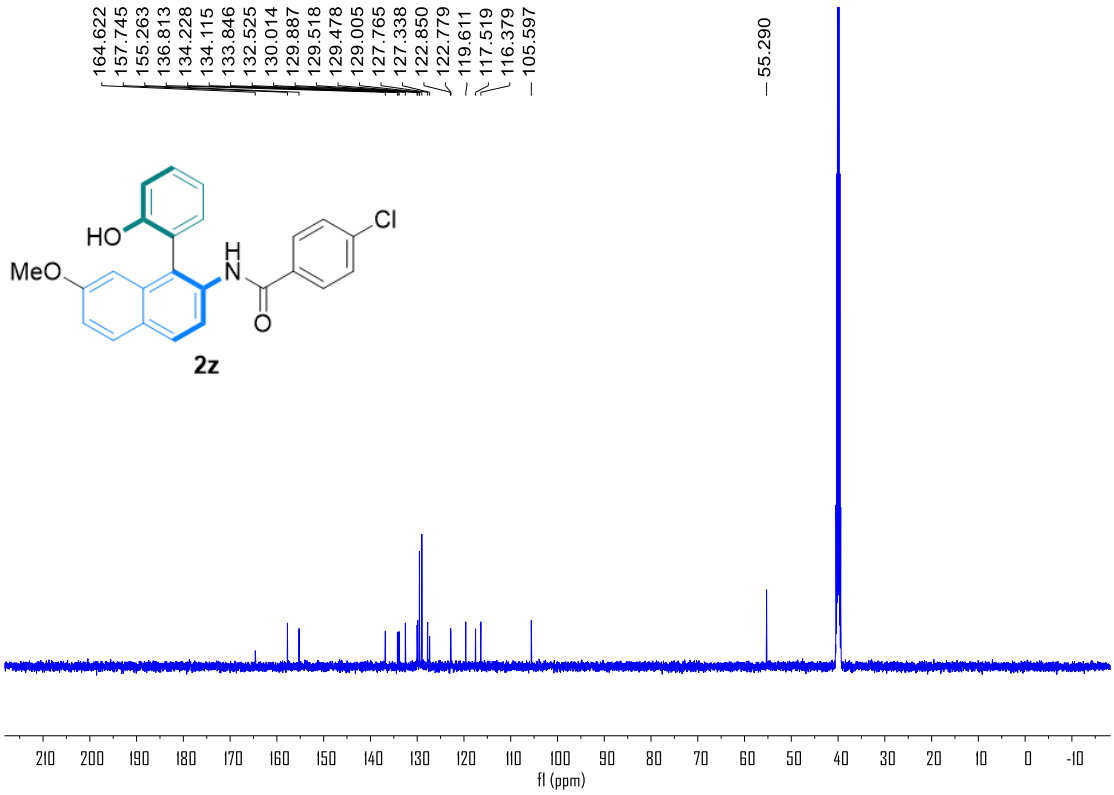
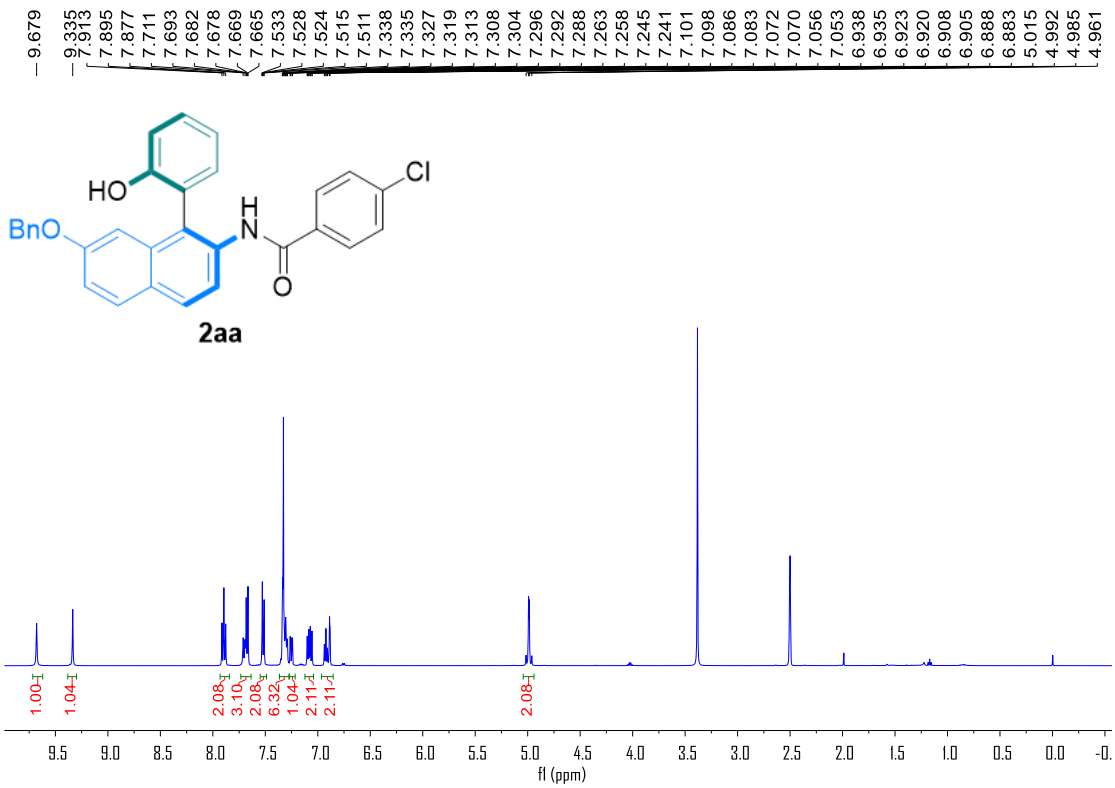
2.19
3.32
2.18
1.10
2.19
1.13
1.13
1.07
3.16
f1 (ppm)


164.622
157.745
155.263
136.813
134.228
134.115
133.846
132.525
130.014
129.887
129.518
129.478
129.005
127.765
127.338
122.850
122.779
119.611
117.519
116.379
105.597
55.290
HO
MeO
H
N
O
Cl
f1 (ppm)

2z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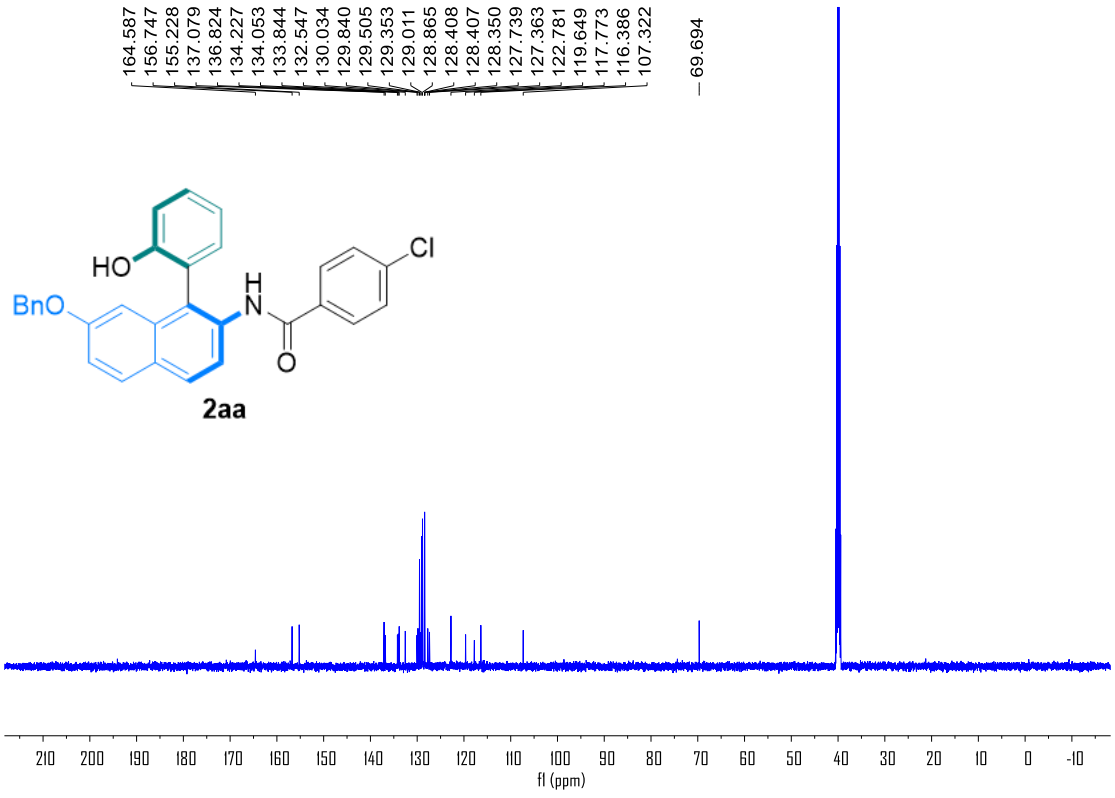
7.895
7.877
7.711
7.693
7.682
7.678
7.669
7.665
7.533
7.528
7.524
7.515
7.511
7.338
7.335
7.327
7.319
7.313
7.308
7.304
7.296
7.292
7.288
7.263
7.258
7.245
7.241
7.101
7.098
7.086
7.083
7.072
7.070
7.056
7.053
6.938
6.935
6.923
6.920
6.908
6.905
6.888
6.883
5.015
4.992
4.985
4.961
HO
BnO
H
N
O
Cl
2aa
1.00
1.04
2.08
3.10
2.08
6.32
1.04
2.11
2.11
2.08
fl (ppm)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156.747
155.228
137.079
136.824
134.227
134.053
133.844
132.547
130.034
129.840
129.505
129.353
129.011
128.865
128.408
128.407
128.350
127.739
127.363
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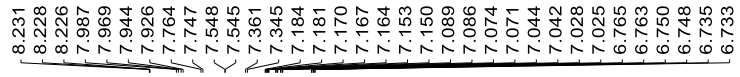
117.773
116.386
107.322
69.694
HO
BnO
H
N
O
Cl
2aa
fl (ppm)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8.228
8.226
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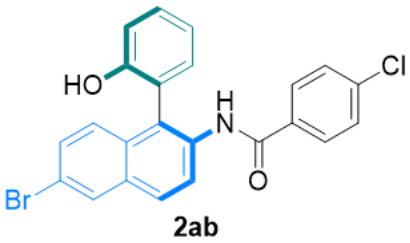
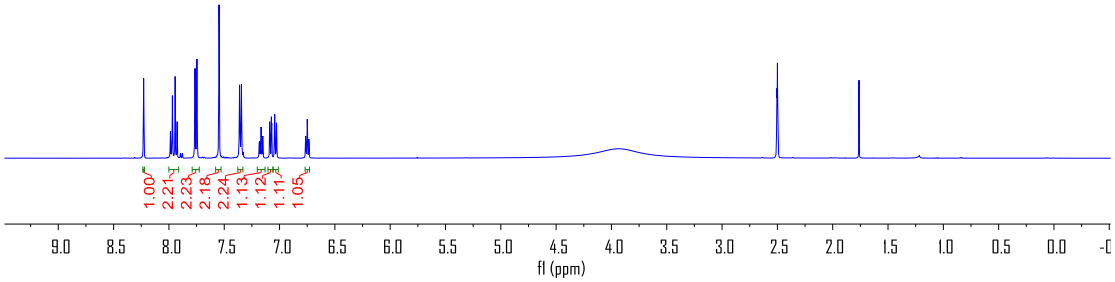
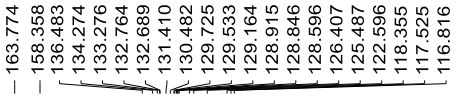
7.969
7.944
7.926
7.764
7.747
7.548
7.545
7.361
7.345
7.184
7.181
7.170
7.167
7.164
7.153
7.150
7.089
7.086
7.074
7.071
7.044
7.042
7.028
7.025
6.765
6.763
6.750
6.748
6.735
6.733


HO
H
N
O
Cl
Br

2ab


1.00
2.21
2.23
2.18
2.24
1.13
1.12
1.11
1.05
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


163.774
158.358
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134.274
133.276
132.764
132.689
131.410
130.482
129.725
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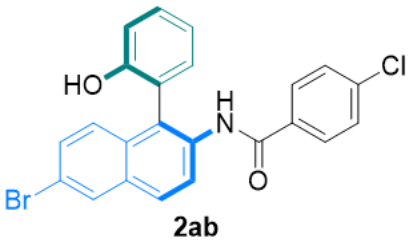
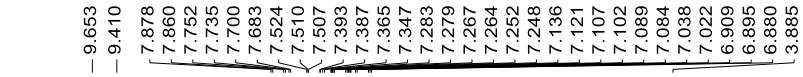
126.407
125.487
122.596
118.355
117.525
116.816


HO
H
N
O
Cl
Br

2ab

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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9.410
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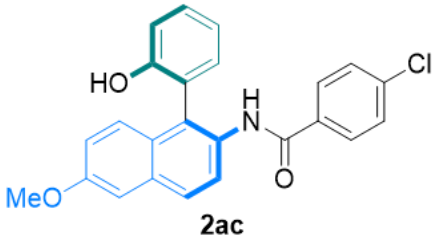
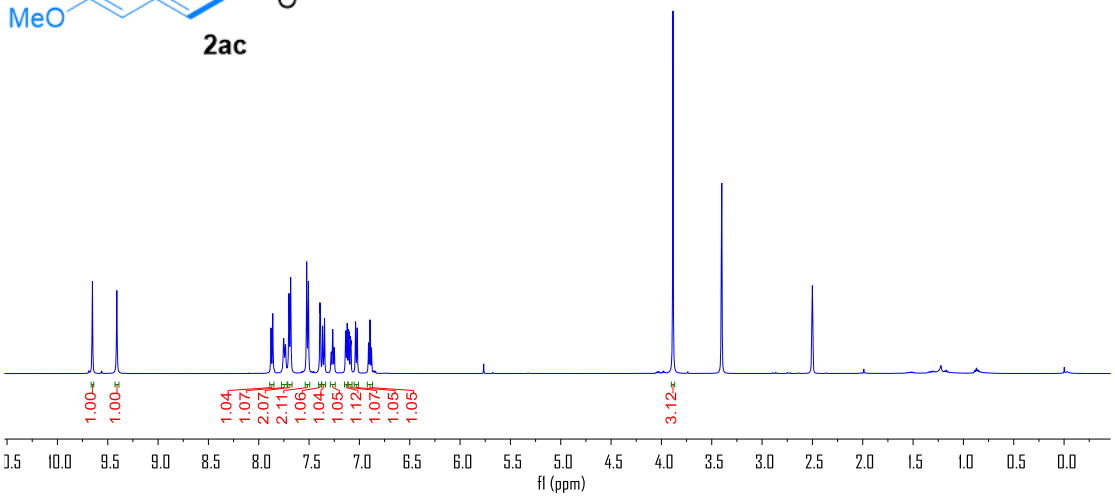
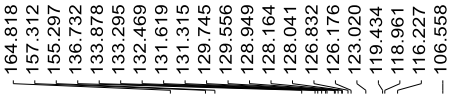
7.860
7.752
7.735
7.700
7.683
7.524
7.510
7.507
7.393
7.387
7.365
7.347
7.283
7.279
7.267
7.264
7.252
7.248
7.136
7.121
7.107
7.102
7.089
7.084
7.038
7.022
6.909
6.895
6.880
3.885


HO
H
N
O
Cl
MeO

2ac


1.00
1.00
1.04
1.07
2.07
2.11
1.06
1.04
1.05
1.12
1.07
1.05
1.05
3.12
f1 (ppm)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157.312
155.297
136.732
133.878
133.295
132.469
131.619
131.315
129.745
129.556
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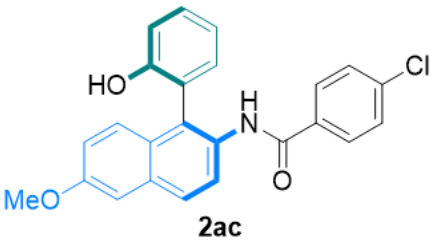
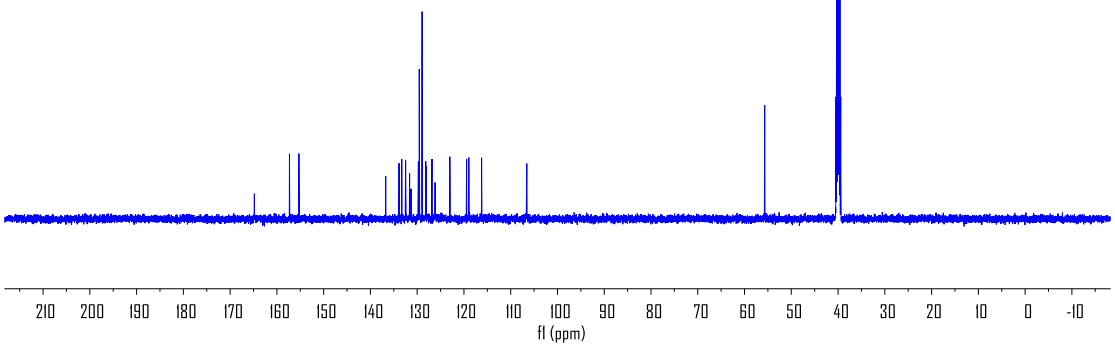
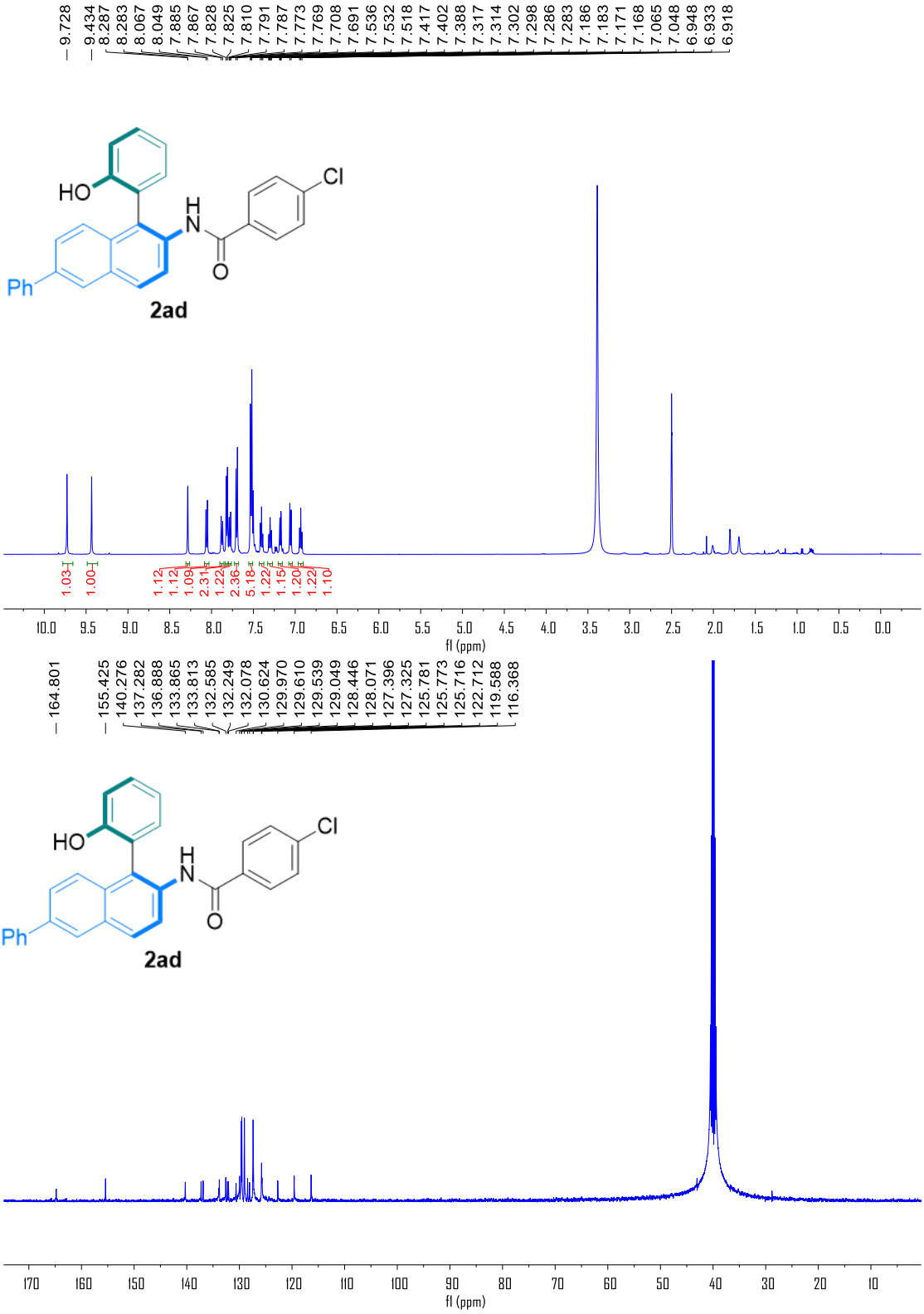
128.164
128.041
126.832
126.176
123.020
119.434
118.961
116.227
106.558
55.690


HO
H
N
O
Cl
MeO

2ac


f1 (ppm)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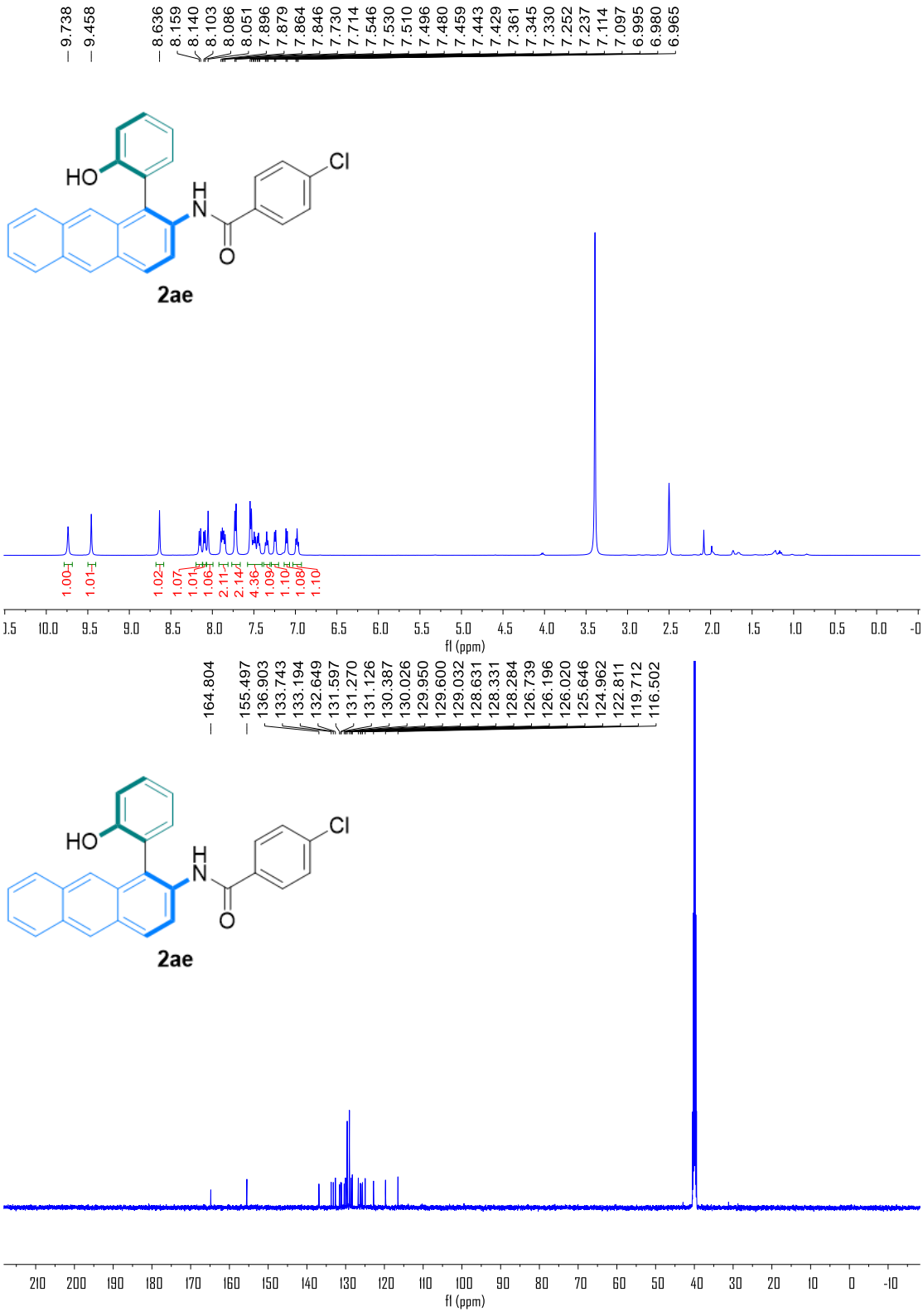
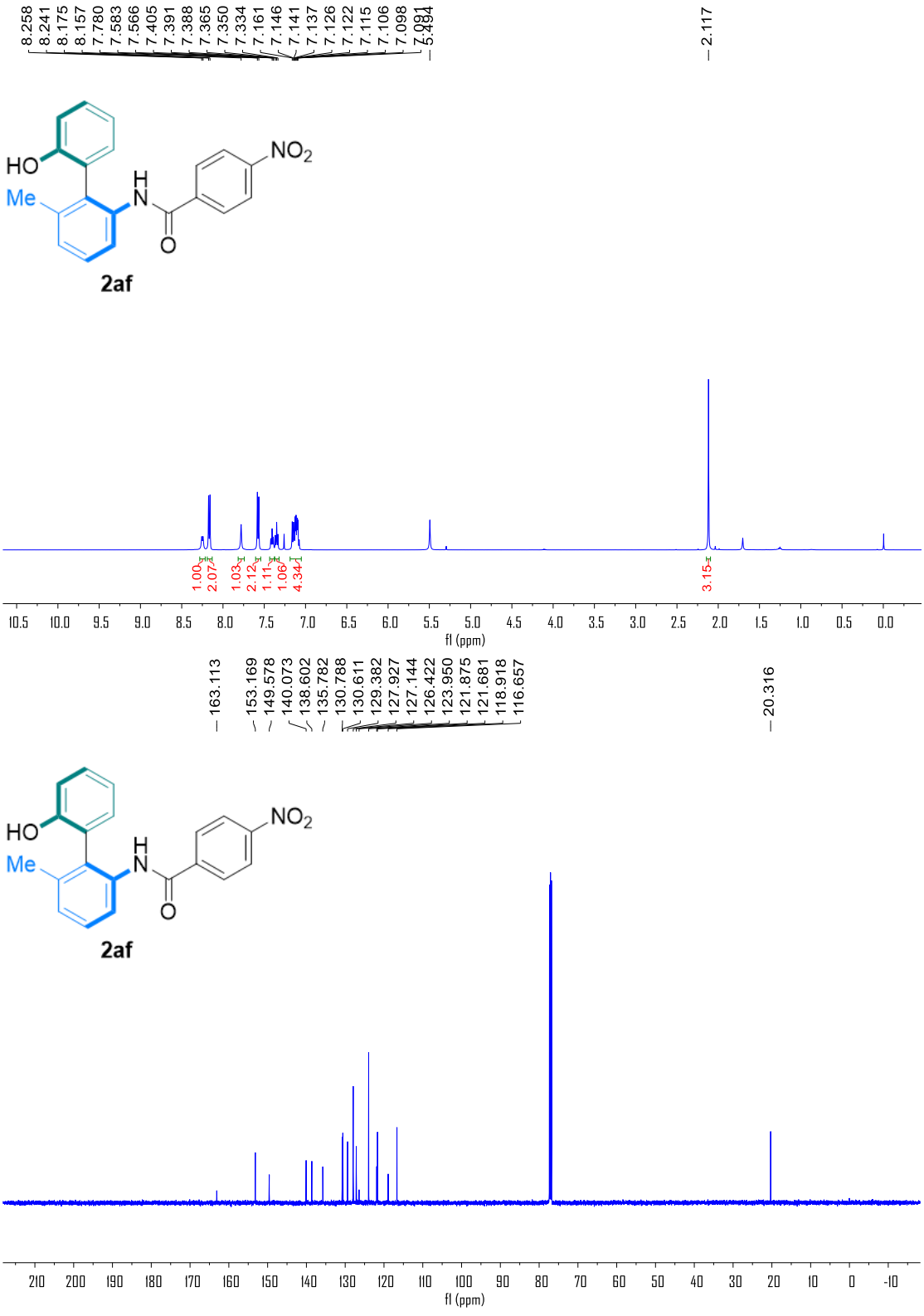
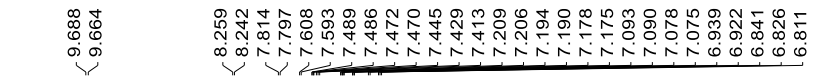
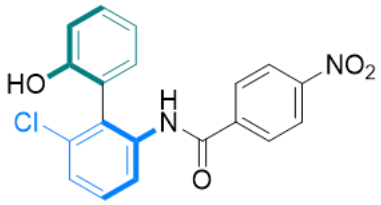
9.434
8.287
8.283
8.067
8.049
7.885
7.867
7.828
7.825
7.810
7.791
7.787
7.773
7.769
7.708
7.691
7.536
7.532
7.518
7.417
7.402
7.388
7.317
7.314
7.302
7.298
7.286
7.283
7.186
7.183
7.171
7.168
7.065
7.048
6.948
6.933
6.918
HO
H
N
O
Cl
Ph
2ad
1.03
1.00
1.12
1.12
1.09
2.31
1.22
2.36
5.18
1.22
1.15
1.20
1.22
1.10
f1 (ppm)
164.801
155.425
140.276
137.282
136.888
133.865
133.813
132.585
132.249
132.078
130.624
129.970
129.610
129.539
129.049
128.446
128.071
127.396
127.325
125.781
125.773
125.716
122.712
119.588
116.368
HO
H
N
O
Cl
Ph
2ad
f1 (ppm)

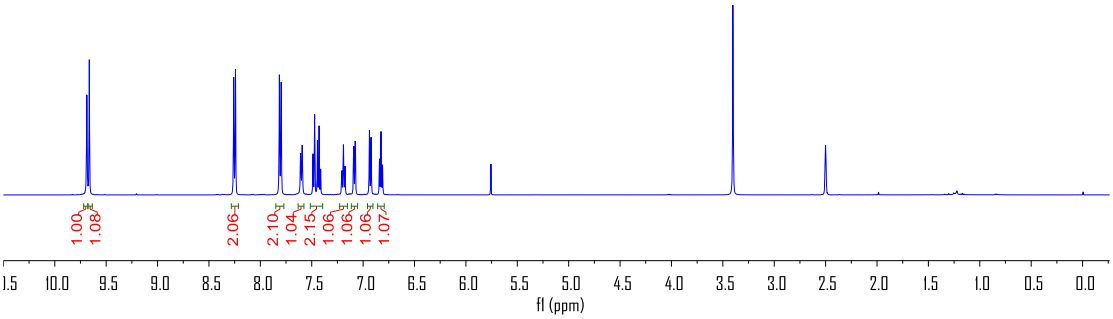

9.738
9.458
8.636
8.159
8.140
8.103
8.086
8.051
7.896
7.879
7.864
7.846
7.730
7.714
7.546
7.530
7.510
7.496
7.480
7.459
7.443
7.429
7.361
7.345
7.330
7.252
7.237
7.114
7.097
6.995
6.980
6.965
HO
H
N
O
Cl
2ae
1.00
1.01
1.02
1.07
1.01
1.06
2.11
2.14
4.36
1.09
1.10
1.08
1.10
f1 (ppm)
164.804
155.497
136.903
133.743
133.194
132.649
131.597
131.270
131.126
130.387
130.026
129.950
129.600
129.032
128.631
128.331
128.284
126.739
126.196
126.020
125.646
124.962
122.811
119.712
116.502
HO
H
N
O
Cl
2ae
f1 (ppm)

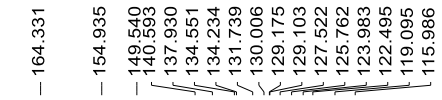

8.258
8.241
8.175
8.157
7.780
7.583
7.566
7.405
7.391
7.388
7.365
7.350
7.334
7.161
7.146
7.141
7.137
7.126
7.122
7.115
7.106
7.098
7.091
5.494
2.117
HO
Me
H
N
O
NO2
2af
1.00
2.07
1.03
2.12
1.11
1.06
4.34
3.15
fl (ppm)
163.113
153.169
149.578
140.073
138.602
135.782
130.788
130.611
129.382
127.927
127.144
126.422
123.950
121.875
121.681
118.918
116.657
20.316
HO
Me
H
N
O
NO2
2af
fl (ppm)

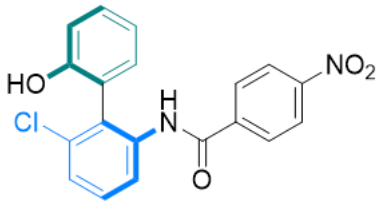

9.688
9.664
8.259
8.242
7.814
7.797
7.608
7.593
7.489
7.486
7.472
7.470
7.445
7.429
7.413
7.209
7.206
7.194
7.190
7.178
7.175
7.093
7.090
7.078
7.075
6.939
6.922
6.841
6.826
6.811


HO
Cl
H
N
O
NO2

2ag

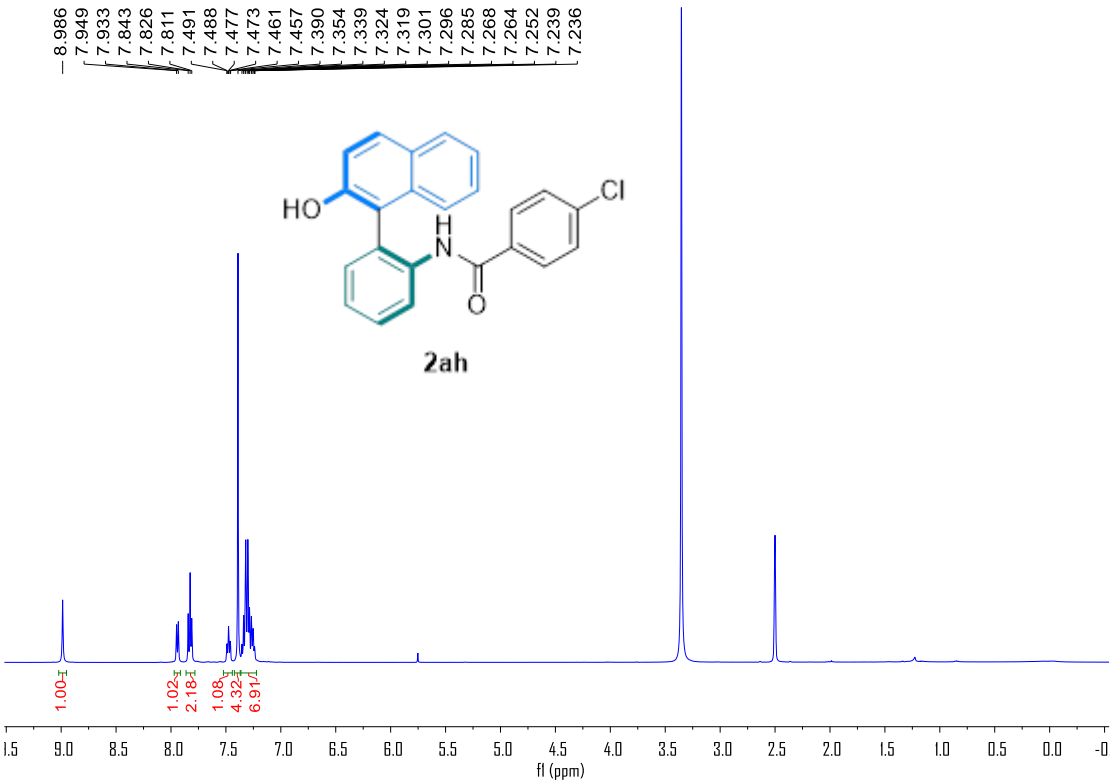

1.00
1.08
2.06
2.10
1.04
2.15
1.06
1.06
1.06
1.07
f1 (ppm)

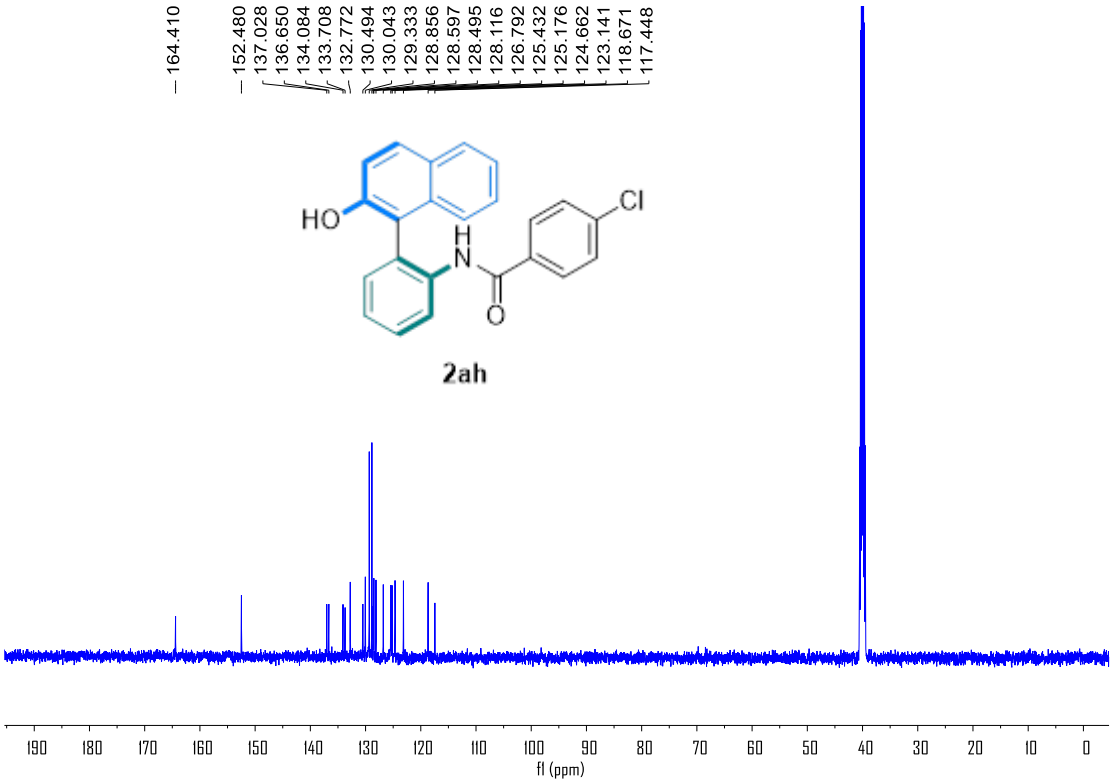

164.331
154.935
149.540
140.593
137.930
134.551
134.234
131.739
130.006
129.175
129.103
127.522
125.762
123.983
122.495
119.095
115.986

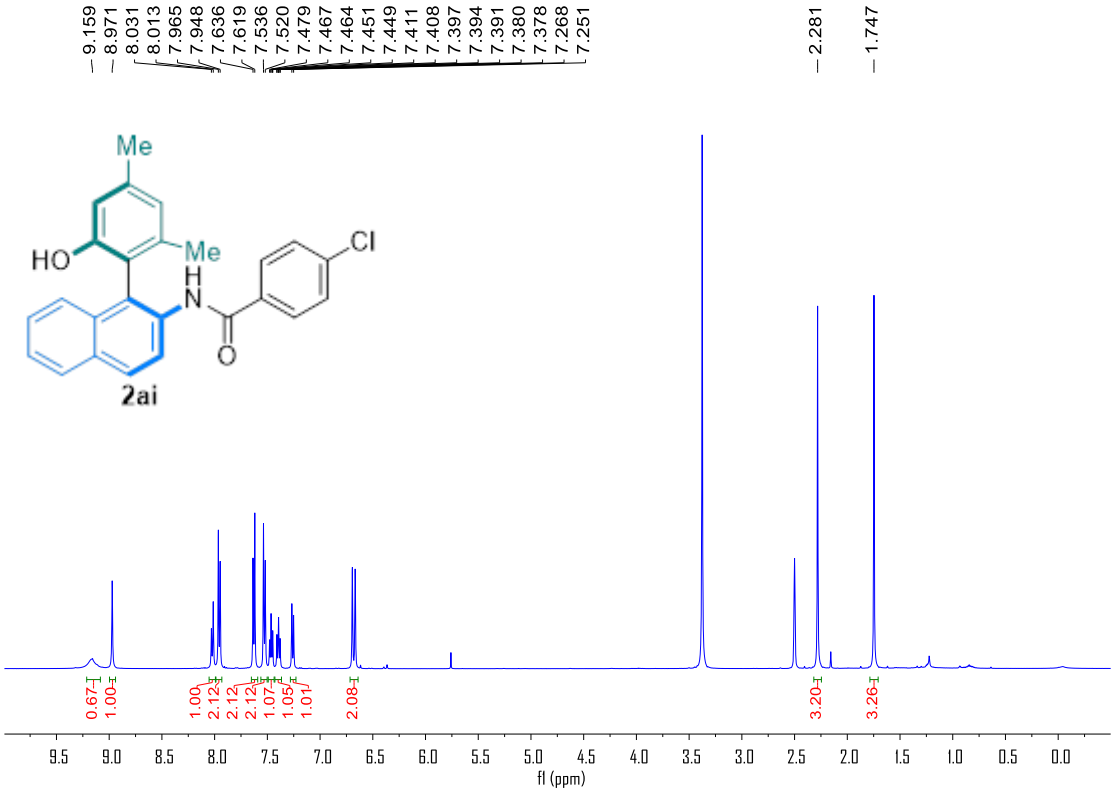

HO
Cl
H
N
O
NO2

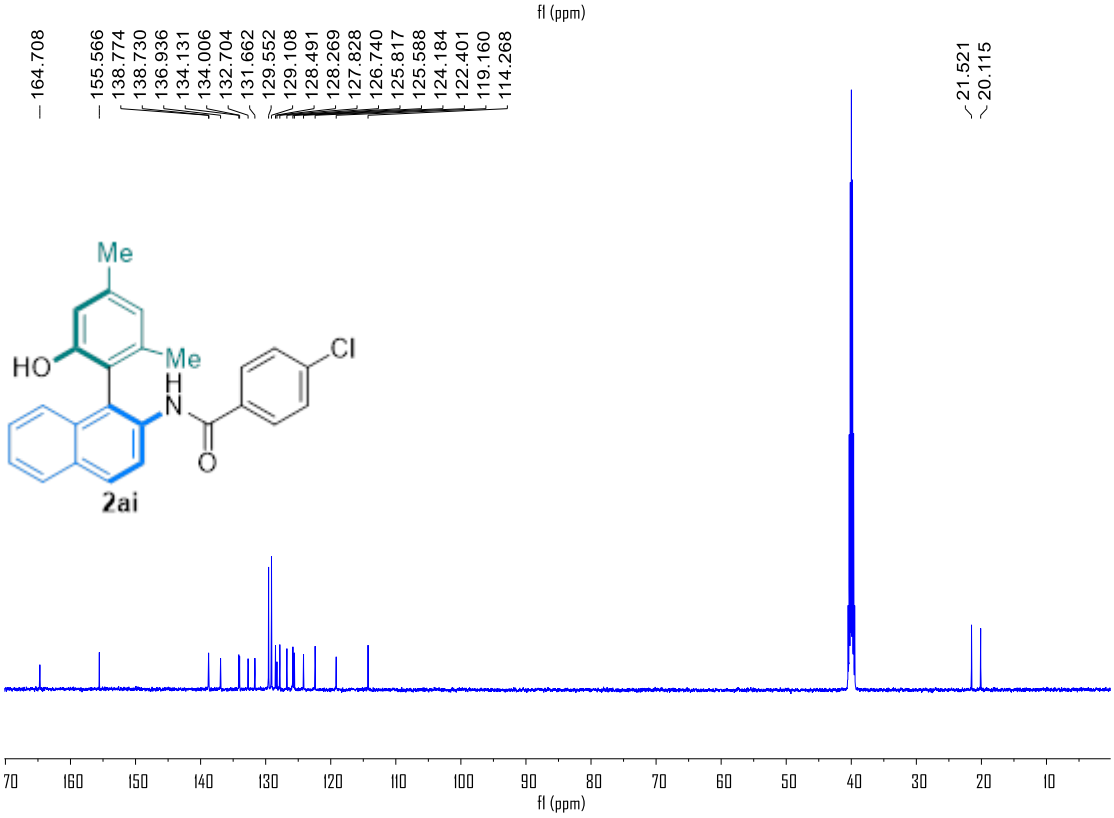
2ag

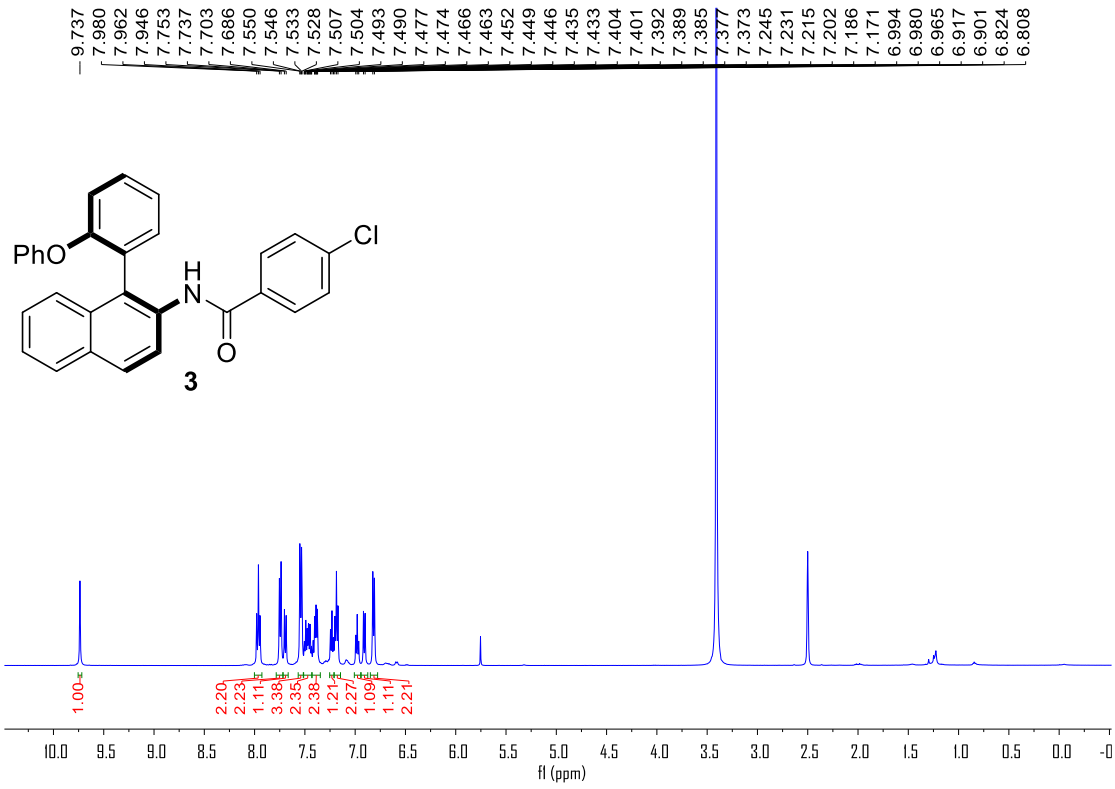
f1 (ppm)

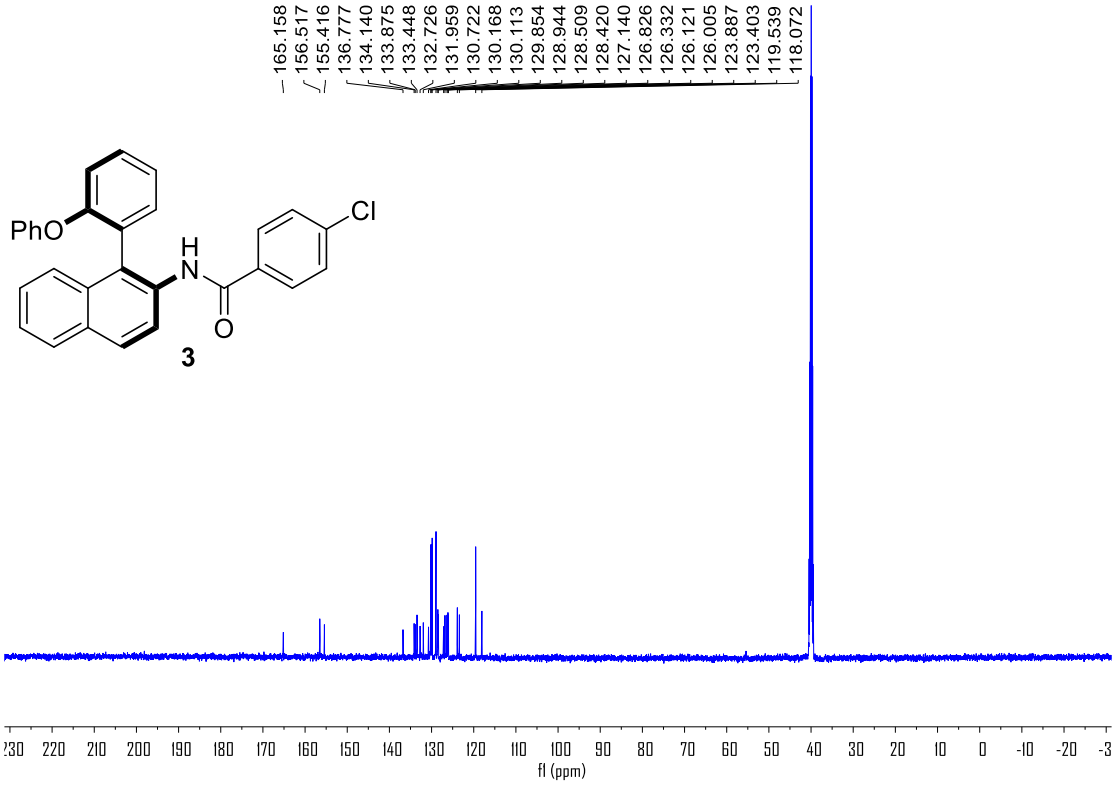

8.986
7.949
7.933
7.843
7.826
7.811
7.491
7.488
7.477
7.473
7.461
7.457
7.390
7.354
7.339
7.324
7.319
7.301
7.296
7.285
7.268
7.264
7.252
7.239
7.236
HO
H
N
O
Cl
2ah
1.00
1.02
2.18
1.08
4.32
6.91
f1 (ppm)

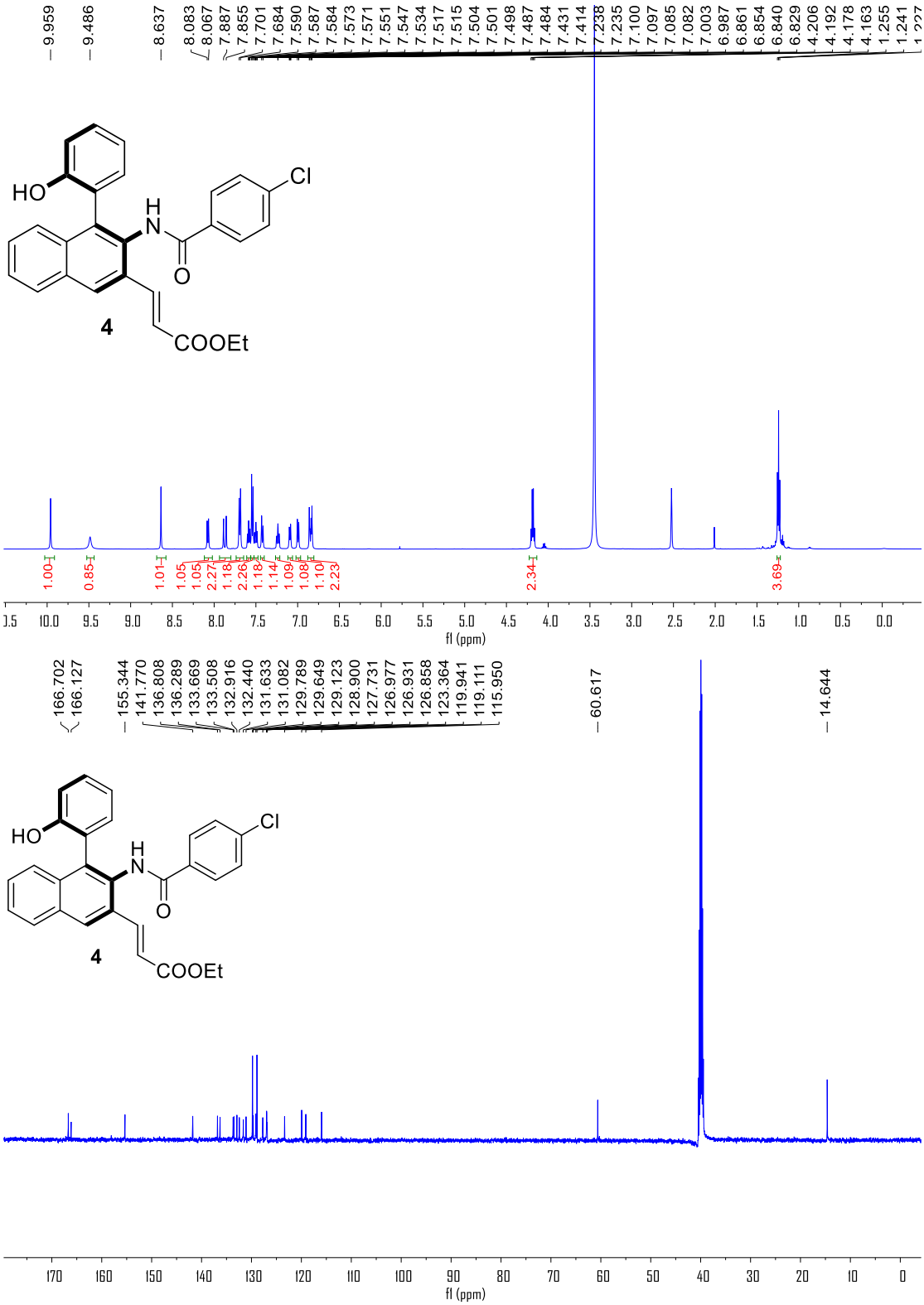

164.410
152.480
137.028
136.650
134.084
133.708
132.772
130.494
130.043
129.333
128.856
128.597
128.495
128.116
126.792
125.432
125.176
124.662
123.141
118.671
117.448
HO
H
N
O
Cl
2ah
f1 (ppm)


9.159
8.971
8.031
8.013
7.965
7.948
7.636
7.619
7.536
7.520
7.479
7.467
7.464
7.451
7.449
7.411
7.408
7.397
7.394
7.391
7.380
7.378
7.268
7.251
2.281
1.747
Me
HO
Me
H
N
O
Cl
2ai
0.67
1.00
1.00
2.12
2.12
2.12
1.07
1.05
1.01
2.08
3.20
3.26
fl (ppm)


164.708
155.566
138.774
138.730
136.936
134.131
134.006
132.704
131.662
129.552
129.108
128.491
128.269
127.828
126.740
125.817
125.588
124.184
122.401
119.160
114.268
21.521
20.115
Me
HO
Me
H
N
O
Cl
2ai
fl (ppm)


9.737
7.980
7.962
7.946
7.753
7.737
7.703
7.686
7.550
7.546
7.533
7.528
7.507
7.504
7.493
7.490
7.477
7.474
7.466
7.463
7.452
7.449
7.446
7.435
7.433
7.404
7.401
7.392
7.389
7.385
7.377
7.373
7.245
7.231
7.215
7.202
7.186
7.171
6.994
6.980
6.965
6.917
6.901
6.824
6.808
PhO
H
N
O
Cl
3
1.00
2.20
2.23
1.11
3.38
2.35
2.38
1.21
2.27
1.09
1.11
2.21
f1 (ppm)


165.158
156.517
155.416
136.777
134.140
133.875
133.448
132.726
131.959
130.722
130.168
130.113
129.854
128.944
128.509
128.420
127.140
126.826
126.332
126.121
126.005
123.887
123.403
119.539
118.072
PhO
H
N
O
Cl
3
f1 (ppm)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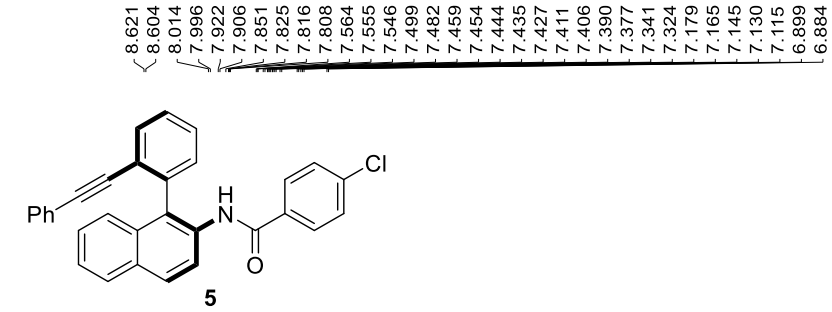
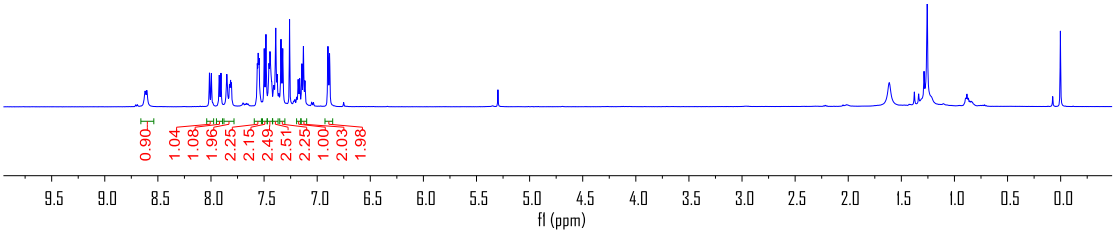
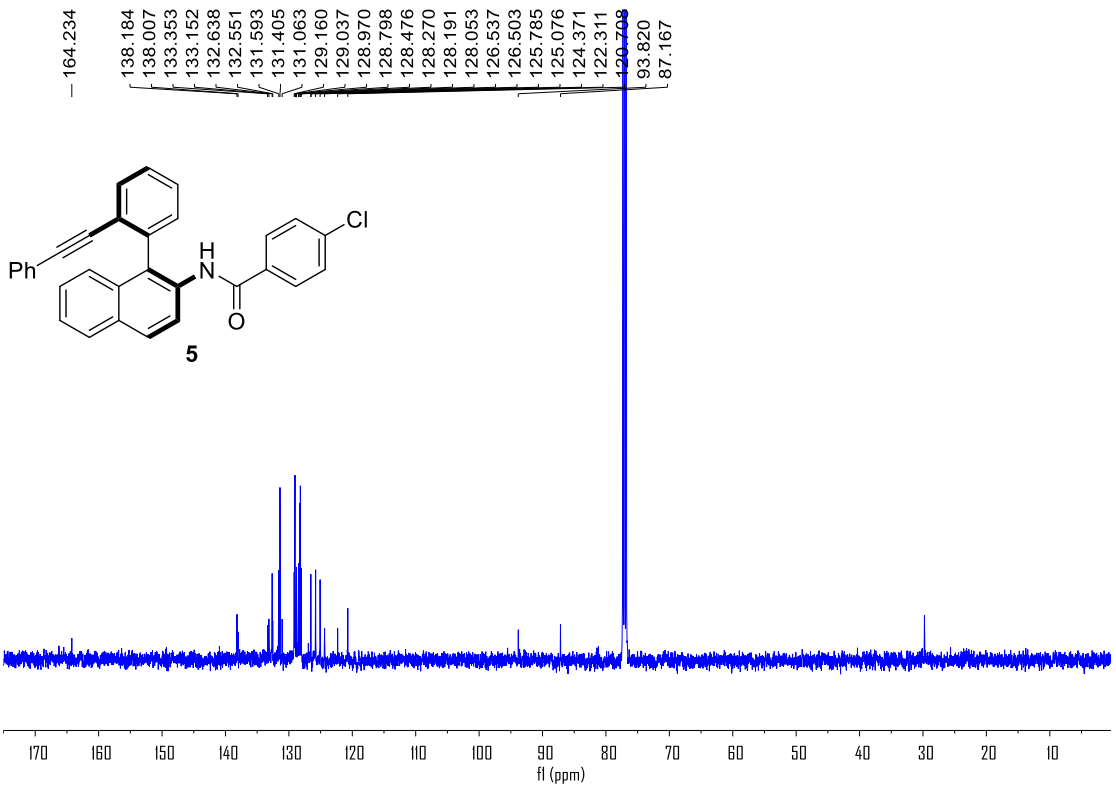
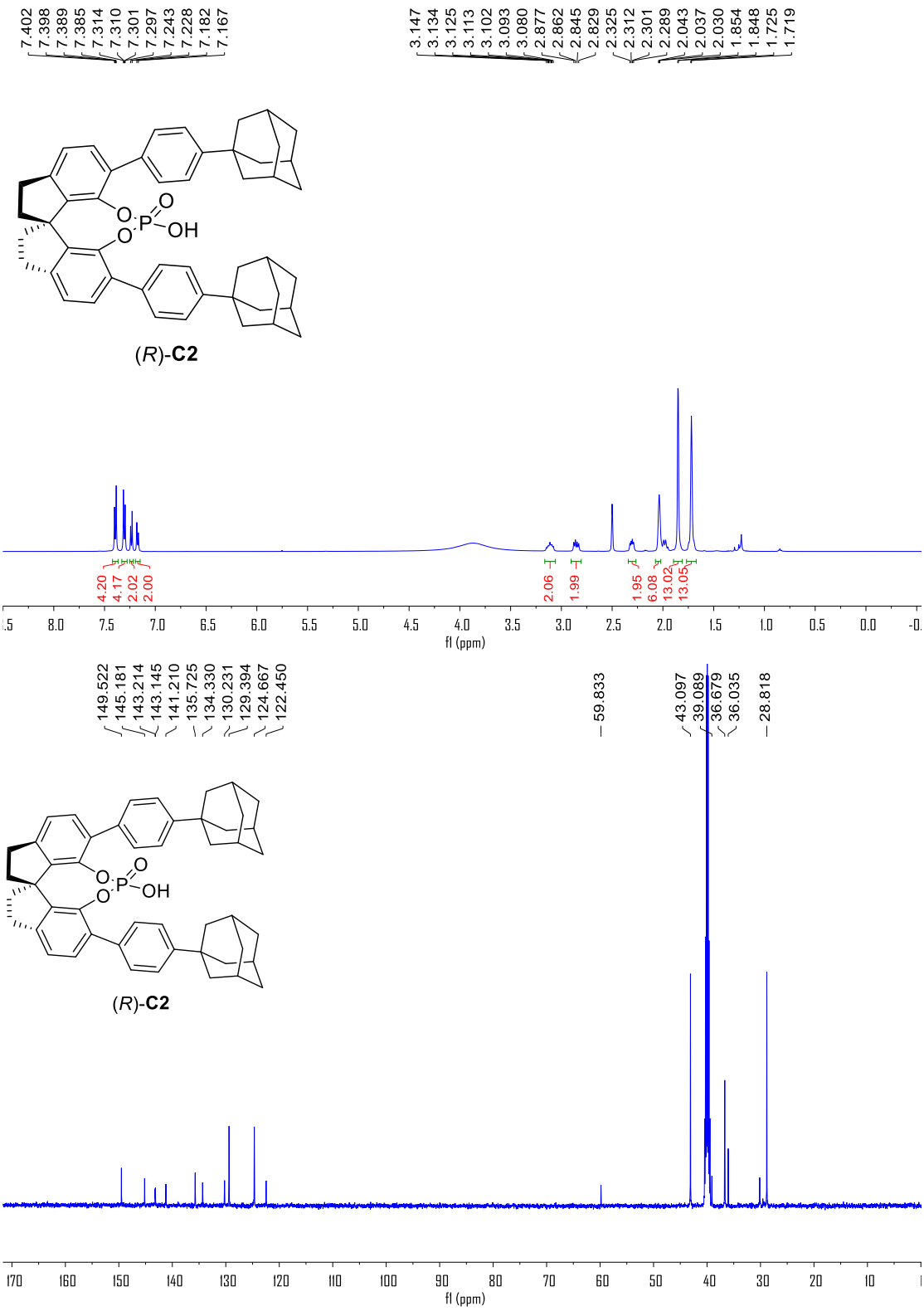
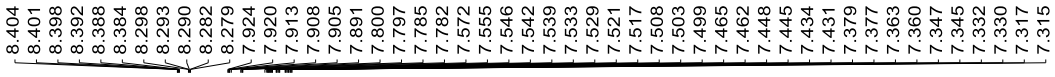
9.486
8.637
8.083
8.067
7.887
7.855
7.701
7.684
7.590
7.587
7.584
7.573
7.571
7.551
7.547
7.534
7.517
7.515
7.504
7.501
7.498
7.487
7.484
7.431
7.414
7.238
7.235
7.100
7.097
7.085
7.082
7.003
6.987
6.861
6.854
6.840
6.829
4.206
4.192
4.178
4.163
1.255
1.241
HO
H
N
O
Cl
4
COOEt
1.00
0.85
1.01
1.05
1.05
2.27
1.18
2.26
1.18
1.14
1.09
1.08
1.10
2.23
2.34
3.69
fl (ppm)
166.702
166.127
155.344
141.770
136.808
136.289
133.669
133.508
132.916
132.440
131.633
131.082
129.789
129.649
129.123
128.900
127.731
126.977
126.931
126.858
123.364
119.941
119.111
115.950
60.617
14.644
HO
H
N
O
Cl
4
COOEt
fl (ppm)


8.621
8.604
8.014
7.996
7.922
7.906
7.851
7.825
7.816
7.808
7.564
7.555
7.546
7.499
7.482
7.459
7.454
7.444
7.435
7.427
7.411
7.406
7.390
7.377
7.341
7.324
7.179
7.165
7.145
7.130
7.115
6.899
6.884
Ph
H
N
O
Cl
5


0.90
1.04
1.08
1.96
2.25
2.15
2.49
2.51
2.25
1.00
2.03
1.98
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


164.234
138.184
138.007
133.353
133.152
132.638
132.551
131.593
131.405
131.063
129.160
129.037
128.970
128.798
128.476
128.270
128.191
128.053
126.537
126.503
125.785
125.076
124.371
122.311
120.708
93.820
87.167
Ph
H
N
O
Cl
5
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


7.402
7.398
7.389
7.385
7.314
7.310
7.301
7.297
7.243
7.228
7.182
7.167
3.147
3.134
3.125
3.113
3.102
3.093
3.080
2.877
2.862
2.845
2.829
2.325
2.312
2.301
2.289
2.043
2.037
2.030
1.854
1.848
1.725
1.719
O
O
P
OH
O
(R)-C2
4.20
4.17
2.02
2.00
2.06
1.99
1.95
6.08
13.02
13.05
f1 (ppm)
149.522
145.181
143.214
143.145
141.210
135.725
134.330
130.231
129.394
124.667
122.450
59.833
43.097
39.089
36.679
36.035
28.818
O
O
P
OH
O
(R)-C2
f1 (ppm)


8.404
8.401
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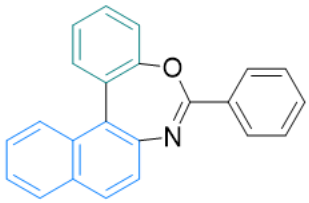
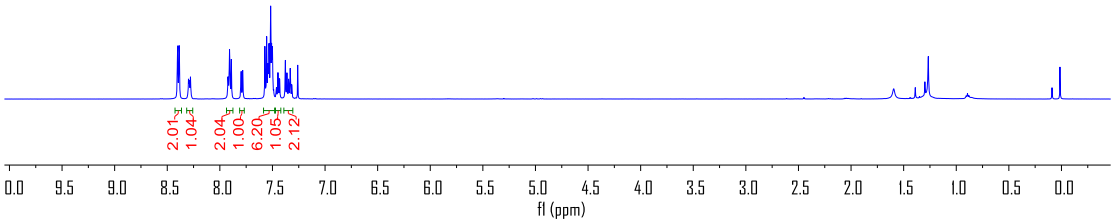
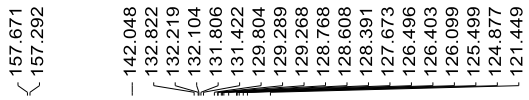
8.392
8.388
8.384
8.298
8.293
8.290
8.282
8.279
7.924
7.920
7.913
7.908
7.905
7.891
7.800
7.797
7.785
7.782
7.572
7.555
7.546
7.542
7.539
7.533
7.529
7.521
7.517
7.508
7.503
7.499
7.465
7.462
7.448
7.445
7.434
7.431
7.379
7.377
7.363
7.360
7.347
7.345
7.332
7.330
7.317
7.315


O
N

1a


2.01
1.04
2.04
1.00
6.20
1.05
2.12
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


157.671
157.292
142.048
132.822
132.219
132.104
131.806
131.422
129.804
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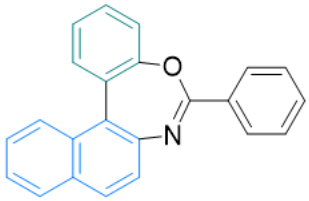
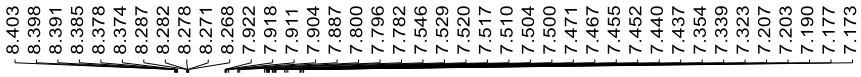
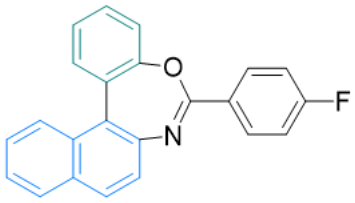
129.268
128.768
128.608
128.391
127.673
126.496
126.403
126.099
125.499
124.877
121.449


O
N

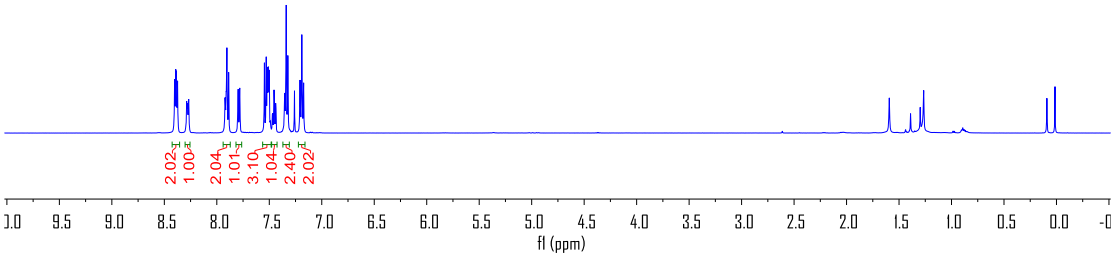
1a

160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

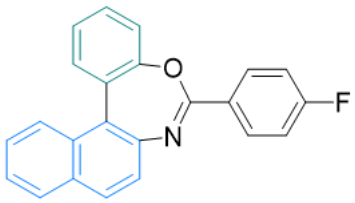

8.403
8.398
8.391
8.385
8.378
8.374
8.287
8.282
8.278
8.271
8.268
7.922
7.918
7.911
7.904
7.887
7.800
7.796
7.782
7.546
7.529
7.520
7.517
7.510
7.504
7.500
7.471
7.467
7.455
7.452
7.440
7.437
7.354
7.339
7.323
7.207
7.203
7.190
7.177
7.173


O
N
F

1b

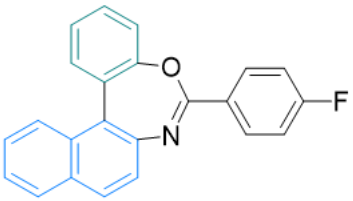

2.02
1.00
2.04
1.01
3.10
1.04
2.40
2.02
f1 (ppm)


166.160
164.149
157.559
156.343
141.900
132.913
132.230
131.603
131.532
131.408
129.851
129.219
128.839
128.409
127.604
126.556
126.385
126.035
125.556
124.990
121.290
115.826
115.652


O
N
F

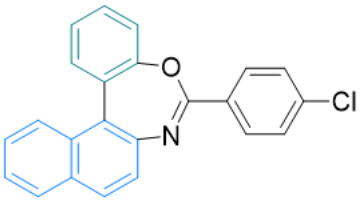
1b

f1 (ppm)

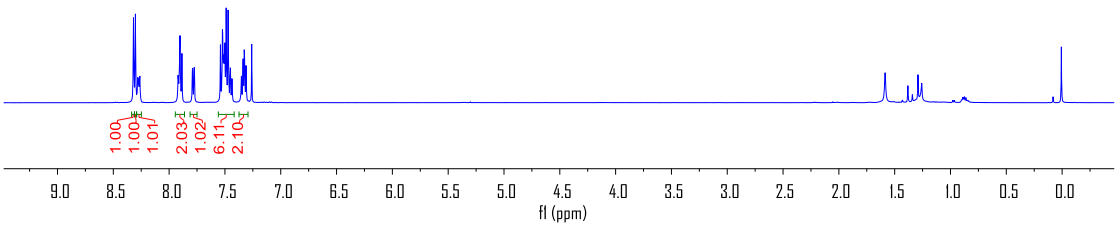

O
N
F

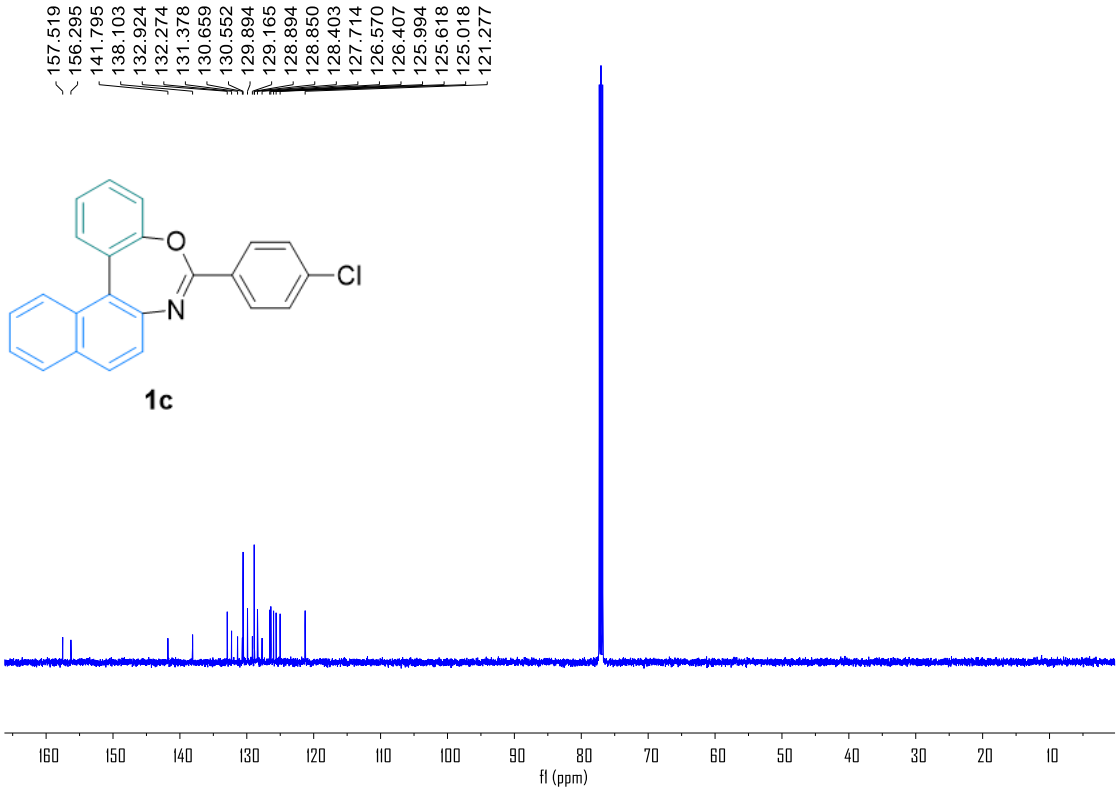
1b

-107.568
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)
8.319 8.302 8.281 8.273 8.262 7.920 7.916 7.911 7.908 7.902 7.886 7.792 7.789 7.777 7.773 7.540 7.529 7.523 7.520 7.515 7.511 7.508 7.505 7.500 7.489 7.485 7.476 7.471 7.466 7.454 7.451 7.439 7.435 7.355 7.352 7.339 7.337 7.328 7.325 7.322 7.312 7.309

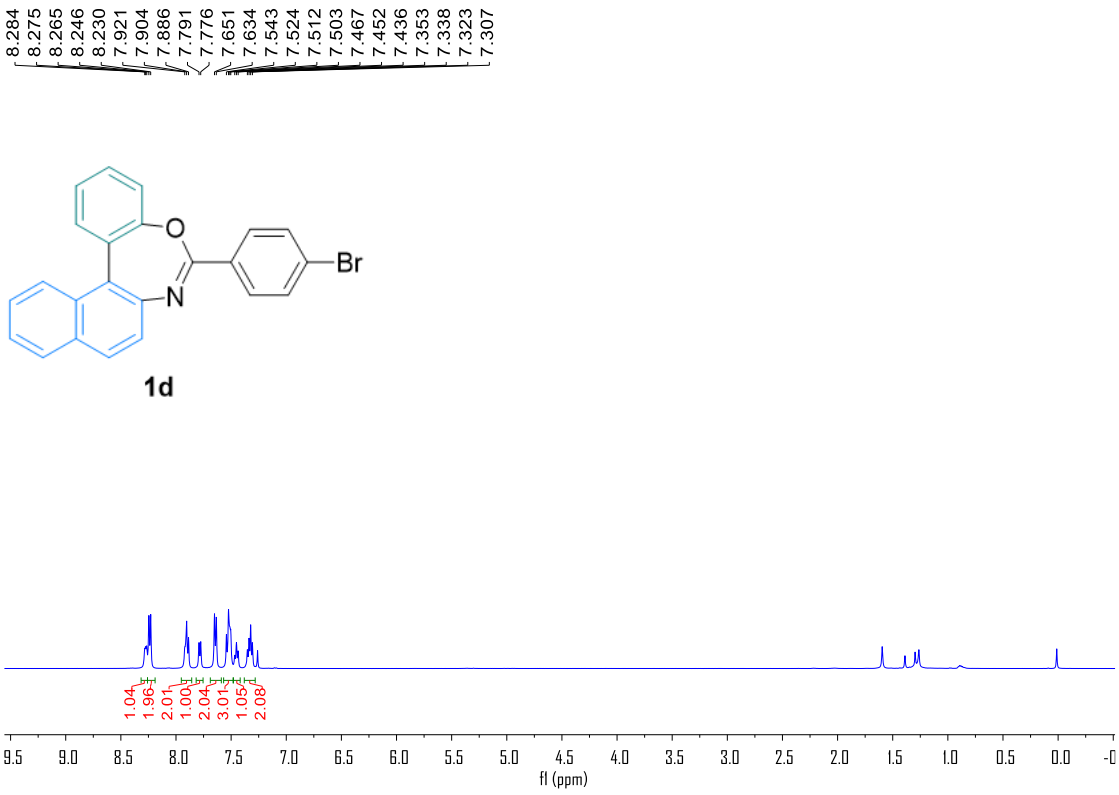

O
N
Cl

1c

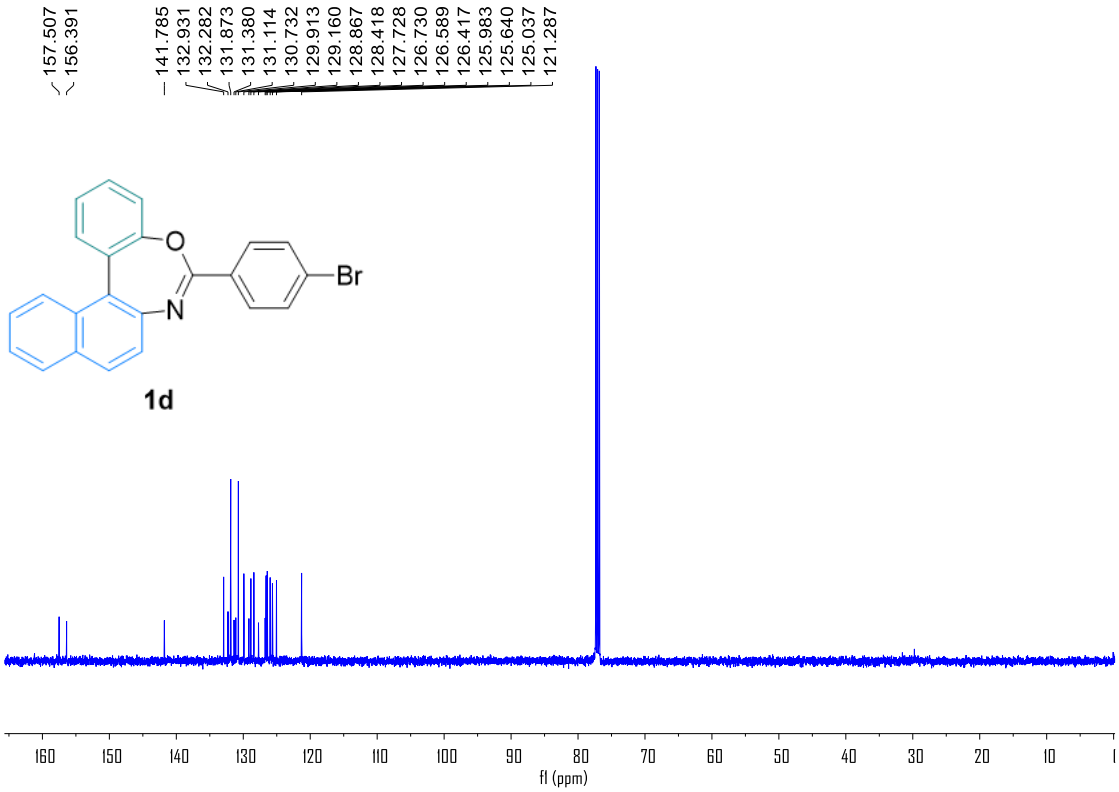

1.00 1.00 1.01 2.03 1.02 6.11 2.10
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

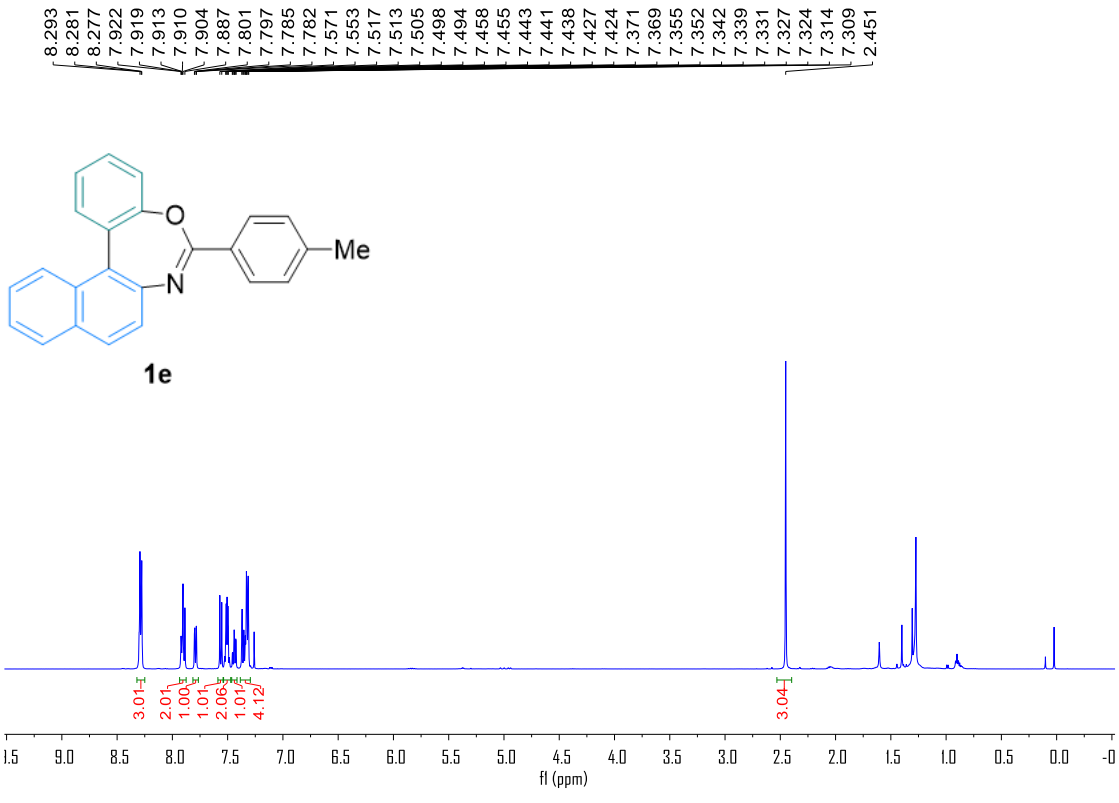

157.519
156.295
141.795
138.103
132.924
132.274
131.378
130.659
130.552
129.894
129.165
128.894
128.850
128.403
127.714
126.570
126.407
125.994
125.618
125.018
121.277
O
N
Cl
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

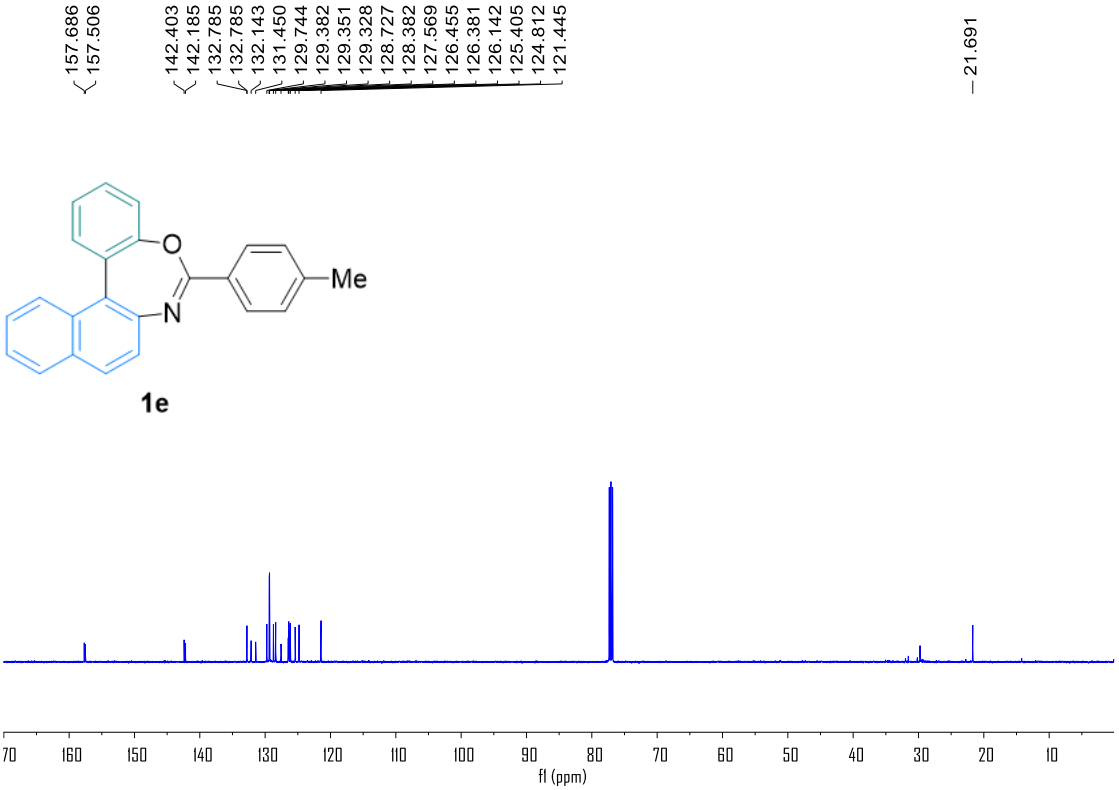
1c

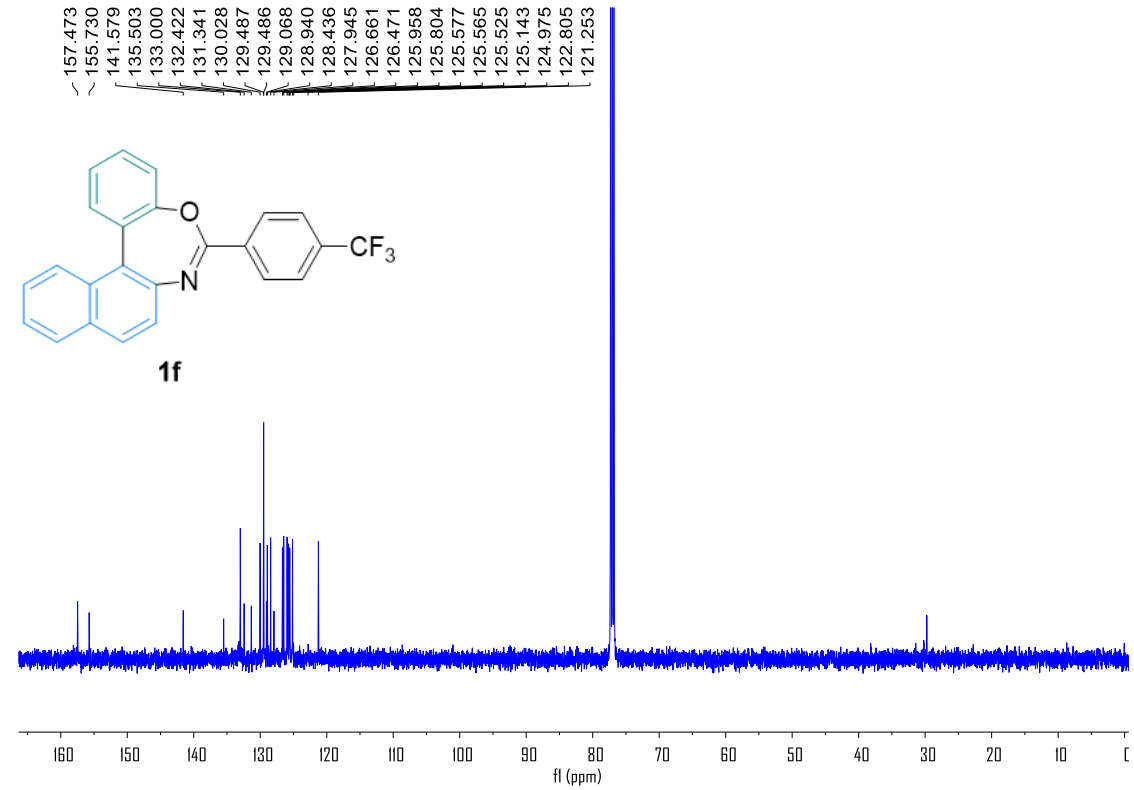

8.284
8.275
8.265
8.246
8.230
7.921
7.904
7.886
7.791
7.776
7.651
7.634
7.543
7.524
7.512
7.503
7.467
7.452
7.436
7.353
7.338
7.323
7.307
O
N
Br
1.04
1.96
2.01
1.00
2.04
3.01
1.05
2.08
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

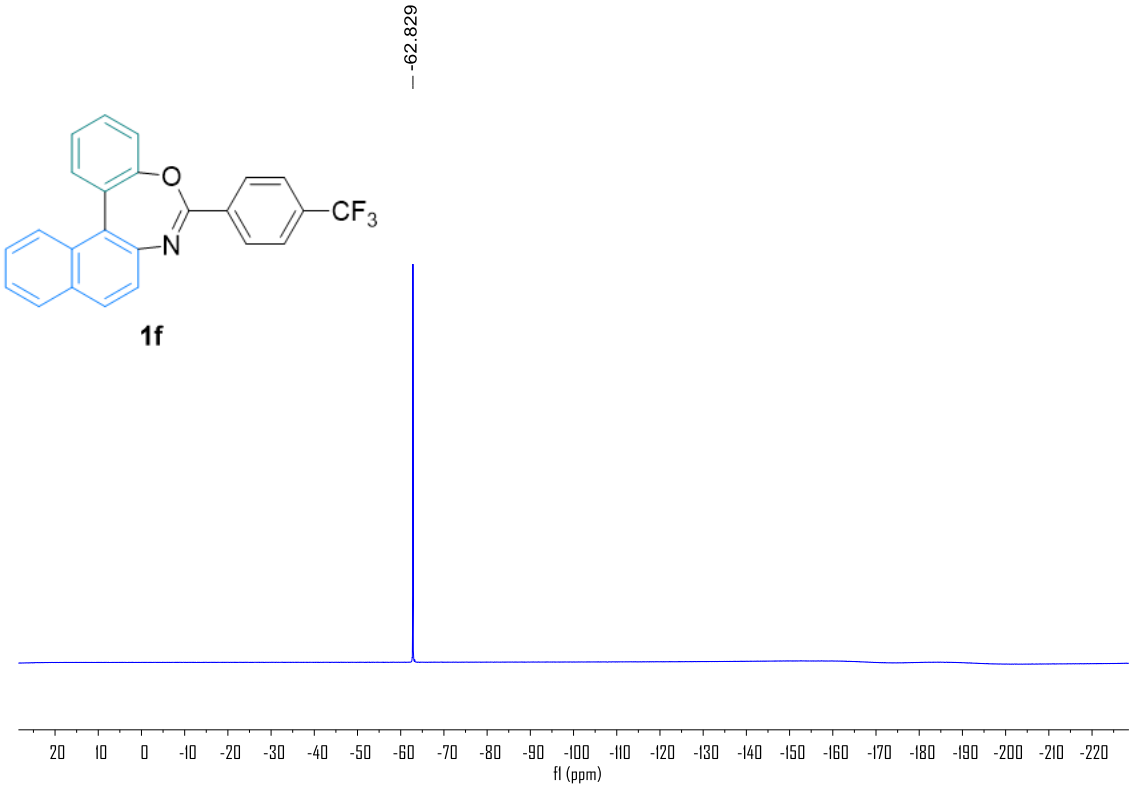
1d

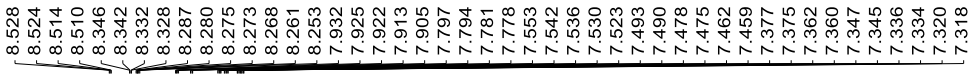

157.507
156.391
141.785
132.931
132.282
131.873
131.380
131.114
130.732
129.913
129.160
128.867
128.418
127.728
126.730
126.589
126.417
125.983
125.640
125.037
121.287
O
N
Br
1d
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

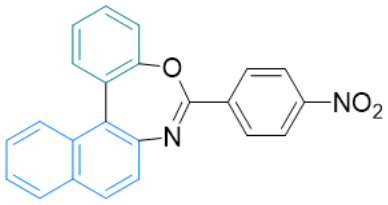

8.293
8.281
8.277
7.922
7.919
7.913
7.910
7.904
7.887
7.801
7.797
7.785
7.782
7.571
7.553
7.517
7.513
7.505
7.498
7.494
7.458
7.455
7.443
7.441
7.438
7.427
7.424
7.371
7.369
7.355
7.352
7.342
7.339
7.331
7.327
7.324
7.314
7.309
2.451
O
N
Me
1e
3.01
2.01
1.00
1.01
2.06
1.01
4.12
3.04
f1 (ppm)


157.686
157.506
142.403
142.185
132.785
132.785
132.143
131.450
129.744
129.382
129.351
129.328
128.727
128.382
127.569
126.455
126.381
126.142
125.405
124.812
121.445
21.691
O
N
Me
1e
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)
8.495
8.479
8.287
8.273
7.919
7.779
7.761
7.563
7.545
7.531
7.518
7.478
7.463
7.447
7.364
7.346
7.329
O
N
CF3
1f
2.16
1.00
2.22
3.10
3.20
1.14
2.10
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)

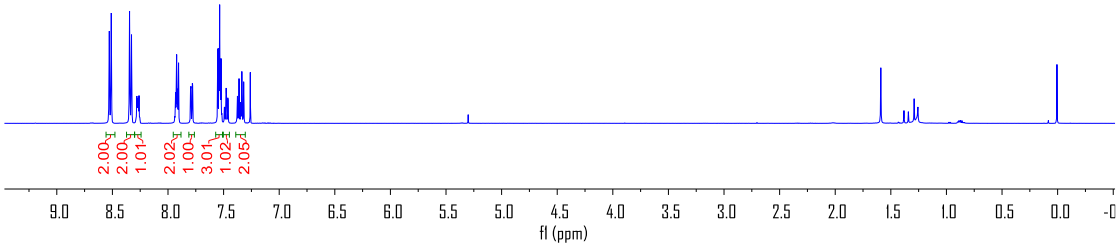

157.473
155.730
141.579
135.503
133.000
132.422
131.341
130.028
129.487
129.486
129.068
128.940
128.436
127.945
126.661
126.471
125.958
125.804
125.577
125.565
125.525
125.143
124.975
122.805
121.253
O
N
CF3
1f
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


-62.829
O
N
CF3
1f
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-220
f1 (ppm)

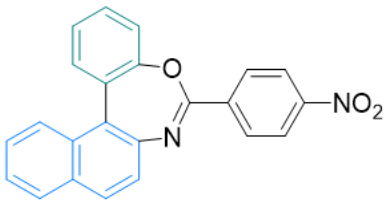

8.528
8.524
8.514
8.510
8.346
8.342
8.332
8.328
8.287
8.280
8.275
8.273
8.268
8.261
8.253
7.932
7.925
7.922
7.913
7.905
7.797
7.794
7.781
7.778
7.553
7.542
7.536
7.530
7.523
7.493
7.490
7.478
7.475
7.462
7.459
7.377
7.375
7.362
7.360
7.347
7.345
7.336
7.334
7.320
7.318


O
N
NO2

1g

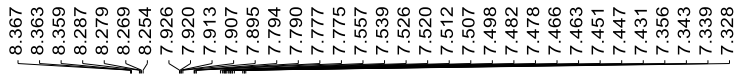

2.00
2.00
1.01
2.02
1.00
3.01
1.02
2.05
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

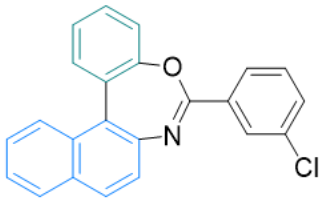

157.381
154.927
149.594
141.362
137.948
133.119
132.570
131.295
130.180
130.028
129.044
128.966
128.454
128.151
126.765
126.525
126.019
125.908
125.305
123.750
121.149


O
N
NO2

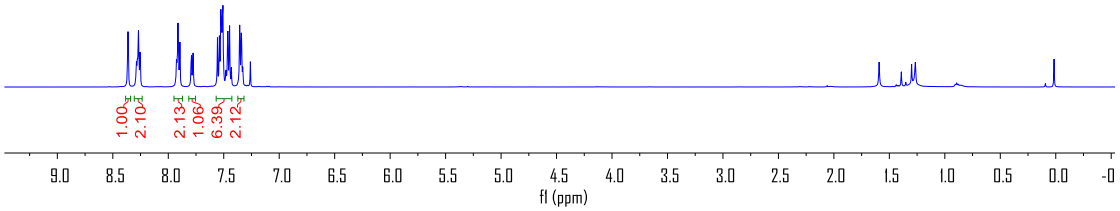
1g

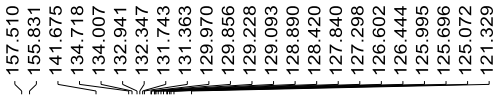
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

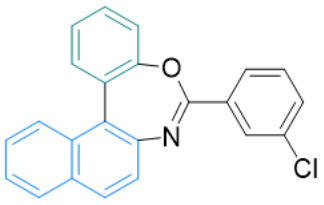

8.367
8.363
8.359
8.287
8.279
8.269
8.254
7.926
7.920
7.913
7.907
7.895
7.794
7.790
7.777
7.775
7.557
7.539
7.526
7.520
7.512
7.507
7.498
7.482
7.478
7.466
7.463
7.451
7.447
7.431
7.356
7.343
7.339
7.328


O
N
Cl

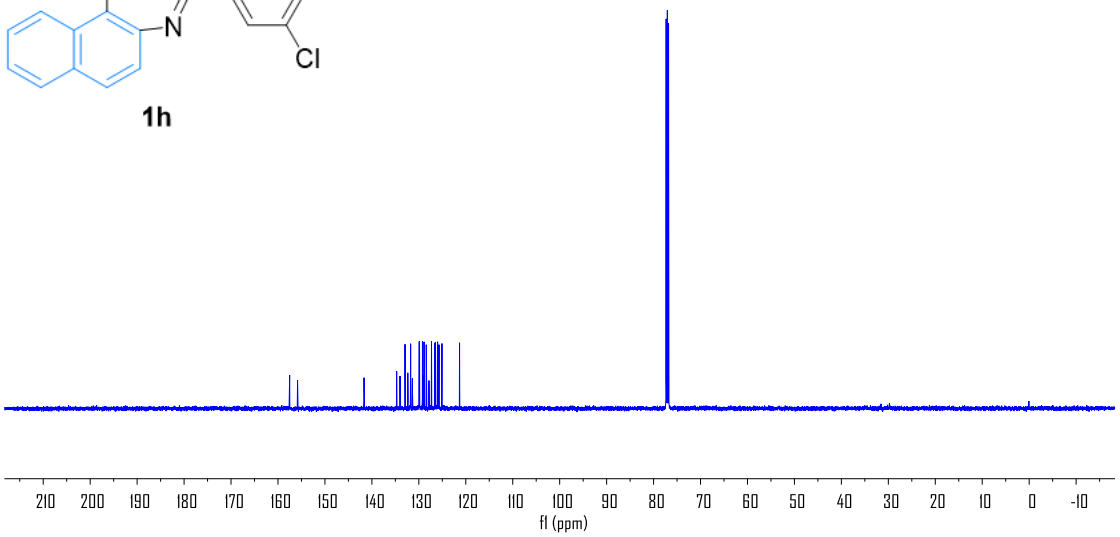
1h

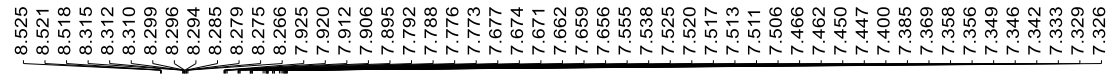

1.00
2.10
2.13
1.06
6.39
2.12
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)

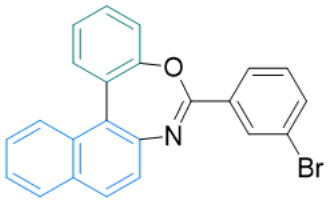

157.510
155.831
141.675
134.718
134.007
132.941
132.347
131.743
131.363
129.970
129.856
129.228
129.093
128.890
128.420
127.840
127.298
126.602
126.444
125.995
125.696
125.072
121.329


O
N
Cl

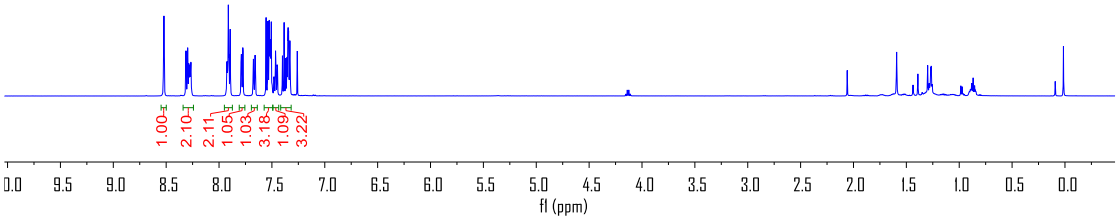
1h

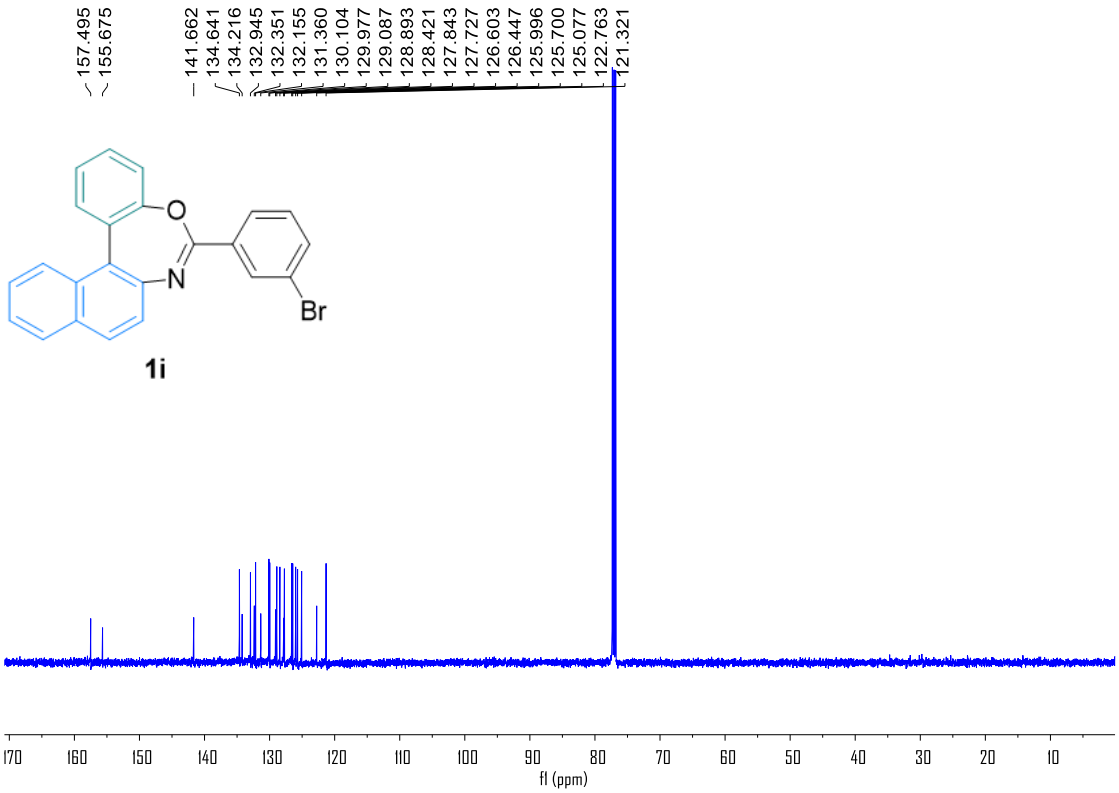

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.525
8.521
8.518
8.315
8.312
8.310
8.299
8.296
8.294
8.285
8.279
8.275
8.266
7.925
7.920
7.912
7.906
7.895
7.792
7.788
7.776
7.773
7.677
7.674
7.671
7.662
7.659
7.656
7.555
7.538
7.525
7.520
7.517
7.513
7.511
7.506
7.466
7.462
7.450
7.447
7.400
7.385
7.369
7.358
7.356
7.349
7.346
7.342
7.333
7.329
7.326


O
N
Br

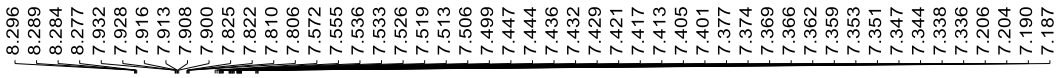
1i

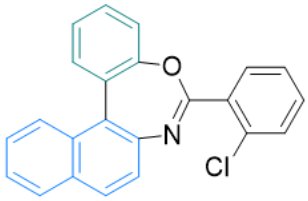

1.00
2.10
2.11
1.05
1.03
3.18
1.09
3.22
fl (ppm)


157.495
155.675
141.662
134.641
134.216
132.945
132.351
132.155
131.360
130.104
129.977
129.087
128.893
128.421
127.843
127.727
126.603
126.447
125.996
125.700
125.077
122.763
121.321
fl (ppm)

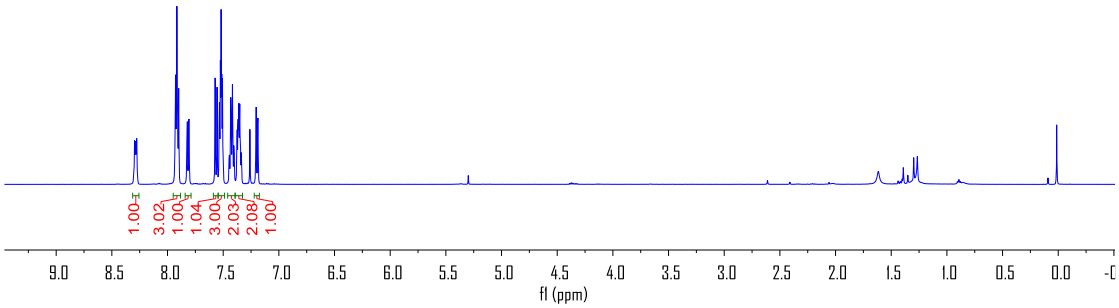
O
N
Br

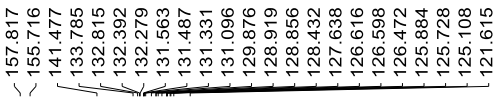
1i

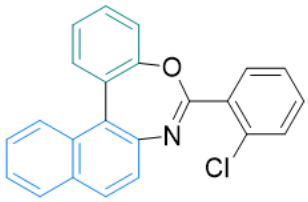

8.296
8.289
8.284
8.277
7.932
7.928
7.916
7.913
7.908
7.900
7.825
7.822
7.810
7.806
7.572
7.555
7.536
7.533
7.526
7.519
7.513
7.506
7.499
7.447
7.444
7.436
7.432
7.429
7.421
7.417
7.413
7.405
7.401
7.377
7.374
7.369
7.366
7.362
7.359
7.353
7.351
7.347
7.344
7.338
7.336
7.206
7.204
7.190
7.187


O
N
Cl

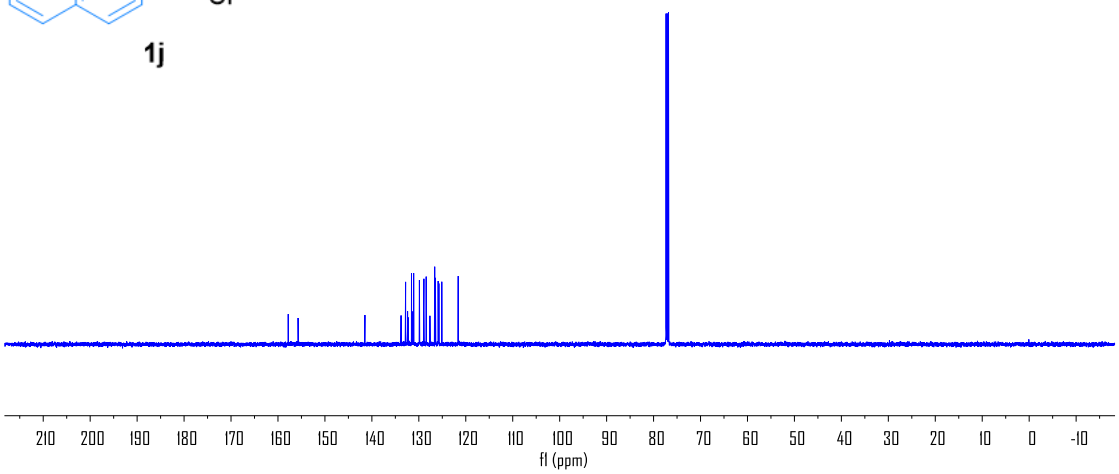
1j

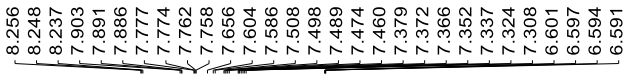

1.00
3.02
1.00
1.04
3.00
2.03
2.08
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

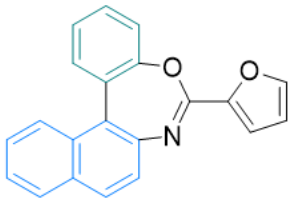

157.817
155.716
141.477
133.785
132.815
132.392
132.279
131.563
131.487
131.331
131.096
129.876
128.919
128.856
128.432
127.638
126.616
126.598
126.472
125.884
125.728
125.108
121.615


O
N
Cl

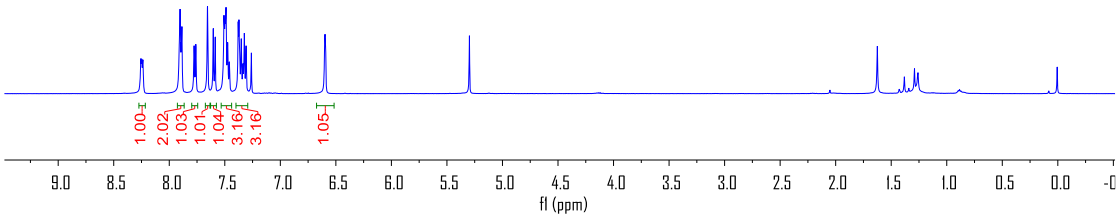
1j

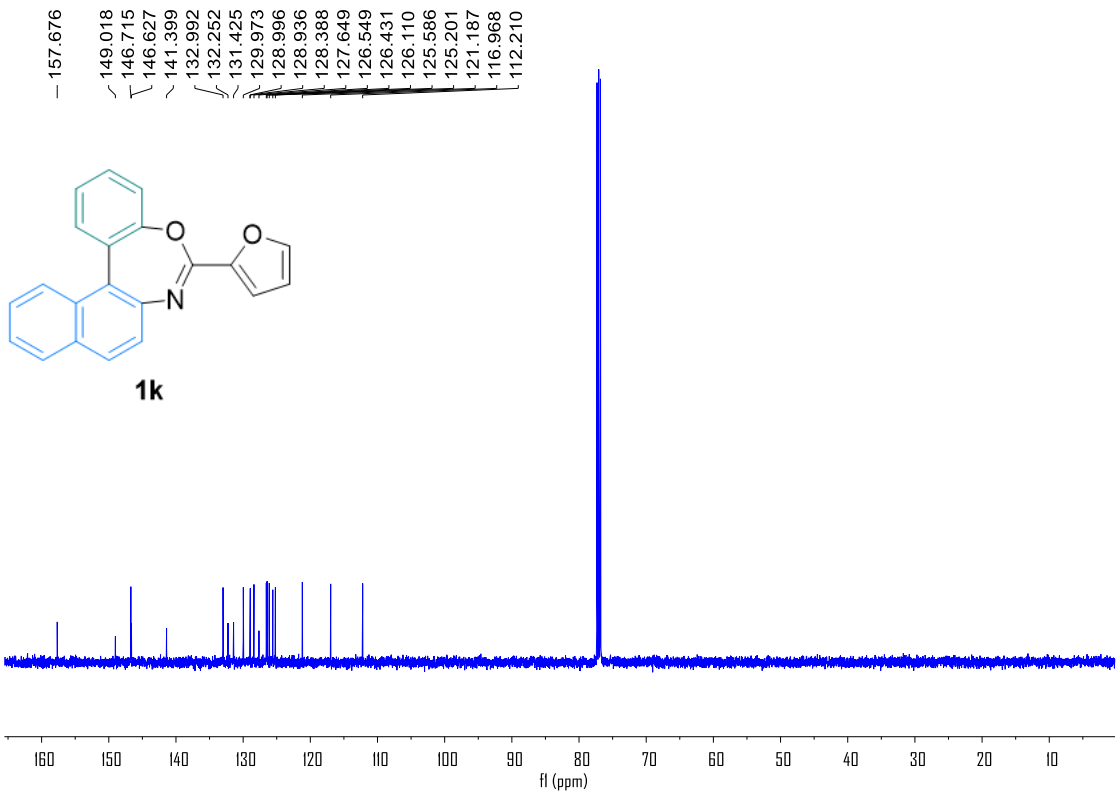

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.256
8.248
8.237
7.903
7.891
7.886
7.777
7.774
7.762
7.758
7.656
7.604
7.586
7.508
7.498
7.489
7.474
7.460
7.379
7.372
7.366
7.352
7.337
7.324
7.308
6.601
6.597
6.594
6.591


O
O
N

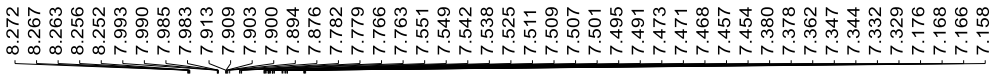
1k

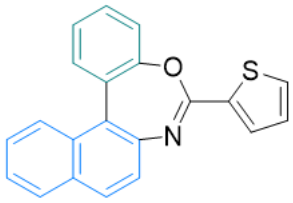

1.00
2.02
1.03
1.01
1.04
3.16
3.16
1.05
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


157.676
149.018
146.715
146.627
141.399
132.992
132.252
131.425
129.973
128.996
128.936
128.388
127.649
126.549
126.431
126.110
125.586
125.201
121.187
116.968
112.210
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

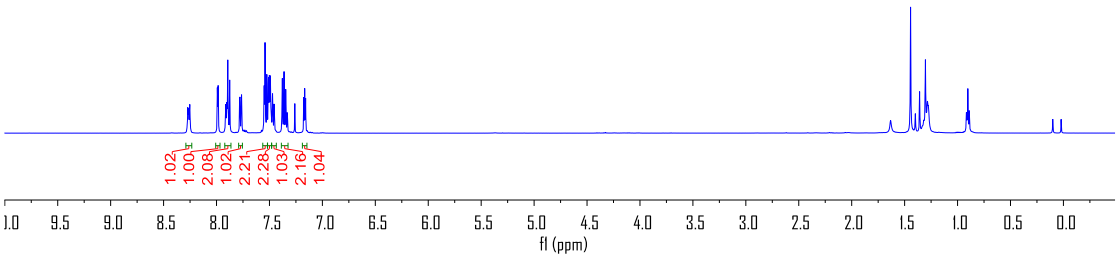
O
O
N

1k

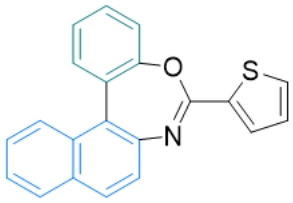

8.272
8.267
8.263
8.256
8.252
7.993
7.990
7.985
7.983
7.913
7.909
7.903
7.900
7.894
7.876
7.782
7.779
7.766
7.763
7.551
7.549
7.542
7.538
7.525
7.511
7.509
7.507
7.501
7.495
7.491
7.473
7.471
7.468
7.457
7.454
7.380
7.378
7.362
7.347
7.344
7.332
7.329
7.176
7.168
7.166
7.158


O
S
N

1l

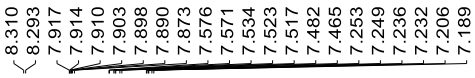

1.02
1.00
2.08
1.02
2.21
2.28
1.03
2.16
1.04
f1 (ppm)

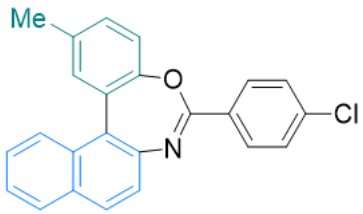

157.628
153.384
141.786
137.167
132.997
132.244
131.762
131.622
131.505
129.920
129.132
128.847
128.411
128.092
127.643
126.531
126.437
126.079
125.513
125.118
121.433


O
S
N

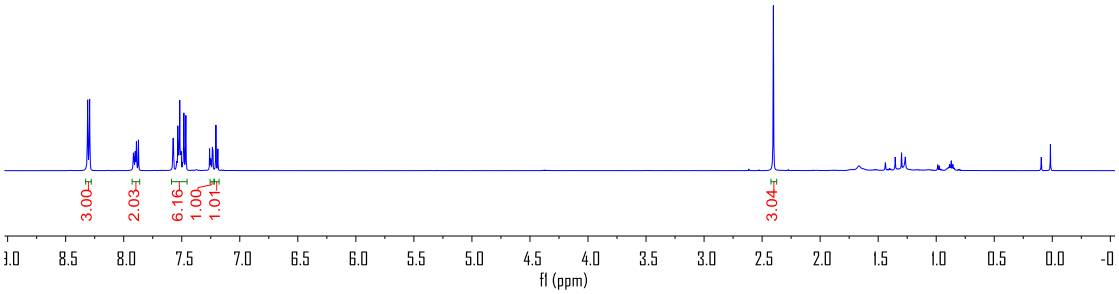
1l

f1 (ppm)

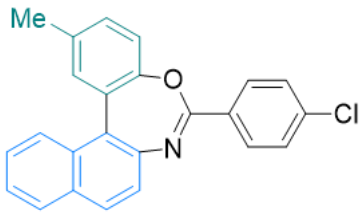

8.310
8.293
7.917
7.914
7.910
7.903
7.898
7.890
7.873
7.576
7.571
7.534
7.523
7.517
7.482
7.465
7.253
7.249
7.236
7.232
7.206
7.189
2.403


Me
O
N
Cl

1m

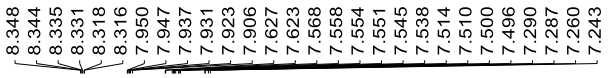

3.00
2.03
6.16
1.00
1.01
3.04
f1 (ppm)

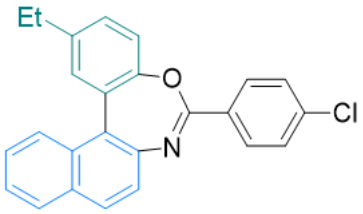

156.470
155.475
141.848
138.029
134.607
133.141
132.270
131.394
130.703
130.573
130.555
128.865
128.753
128.710
128.397
127.804
126.527
126.476
126.018
125.547
120.886
21.044


Me
O
N
Cl

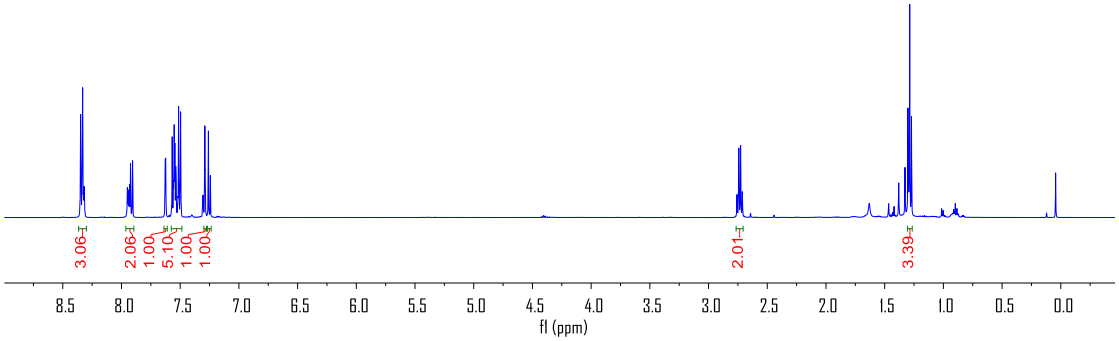
1m

f1 (ppm)

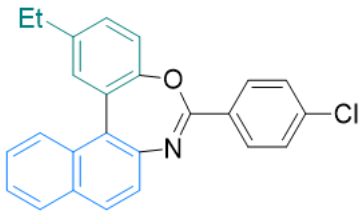

8.348
8.344
8.335
8.331
8.318
8.316
7.950
7.947
7.937
7.931
7.923
7.906
7.627
7.623
7.568
7.558
7.554
7.551
7.545
7.538
7.514
7.510
7.500
7.496
7.290
7.287
7.260
7.243
2.757
2.742
2.727
2.712
1.302
1.287
1.272


Et
O
N
Cl

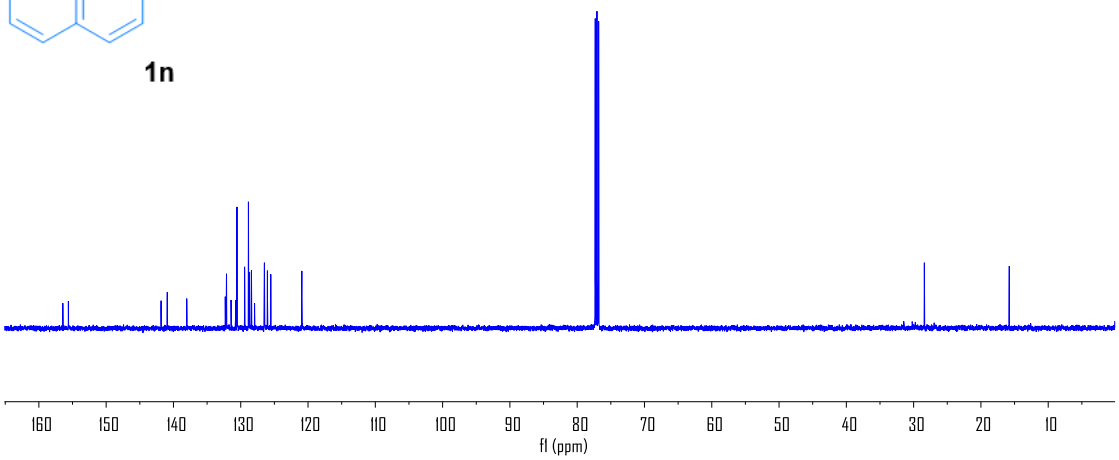
1n

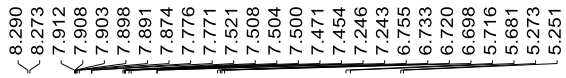

3.06
2.06
1.00
5.10
1.00
1.00
2.01
3.39
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

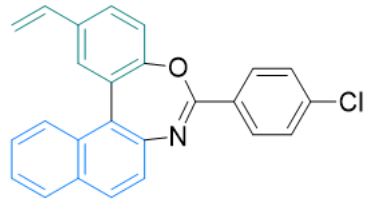

156.442
155.612
141.835
140.918
138.027
132.299
132.114
131.439
130.748
130.559
129.425
128.858
128.775
128.687
128.408
127.946
126.495
126.477
126.034
125.535
120.917
28.406
15.787


Et
O
N
Cl

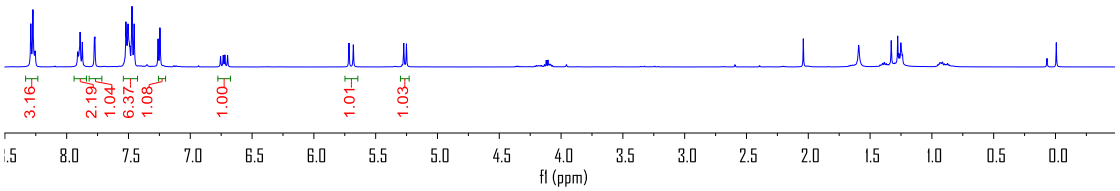
1n


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

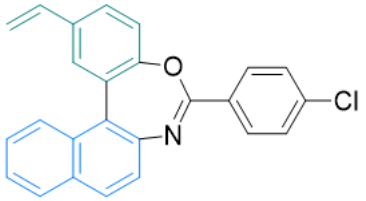

8.290
8.273
7.912
7.908
7.903
7.898
7.891
7.874
7.776
7.771
7.521
7.508
7.504
7.500
7.471
7.454
7.246
7.243
6.755
6.733
6.720
6.698
5.716
5.681
5.273
5.251


O
N
Cl

1o

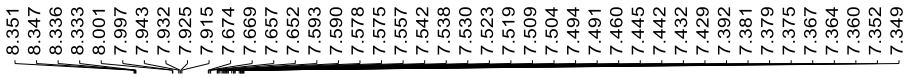

3.16
2.19
1.04
6.37
1.08
1.00
1.01
1.03
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

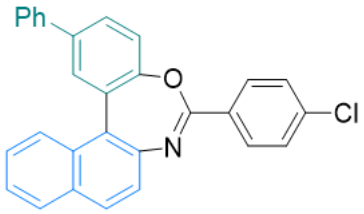

157.102
156.150
141.878
138.144
135.708
134.613
132.299
131.375
130.758
130.589
130.544
129.151
128.926
128.905
128.455
127.489
127.385
126.702
126.247
125.985
125.644
121.387
114.536


O
N
Cl

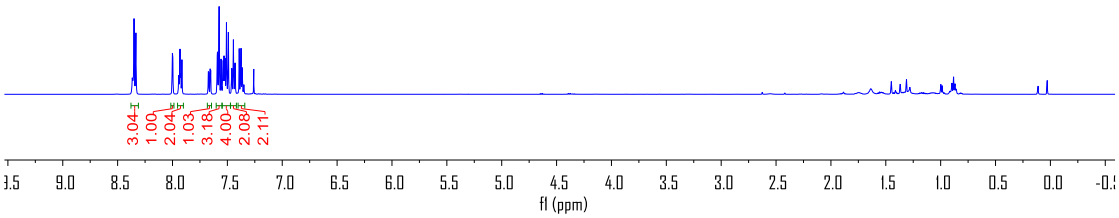
1o

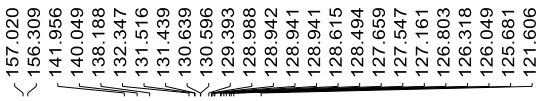
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

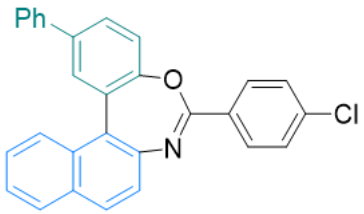

8.351
8.347
8.336
8.333
8.001
7.997
7.943
7.932
7.925
7.915
7.674
7.669
7.657
7.652
7.593
7.590
7.578
7.575
7.557
7.542
7.538
7.530
7.523
7.519
7.509
7.504
7.494
7.491
7.460
7.445
7.442
7.432
7.429
7.392
7.381
7.379
7.375
7.367
7.364
7.360
7.352
7.349


Ph
O
N
Cl

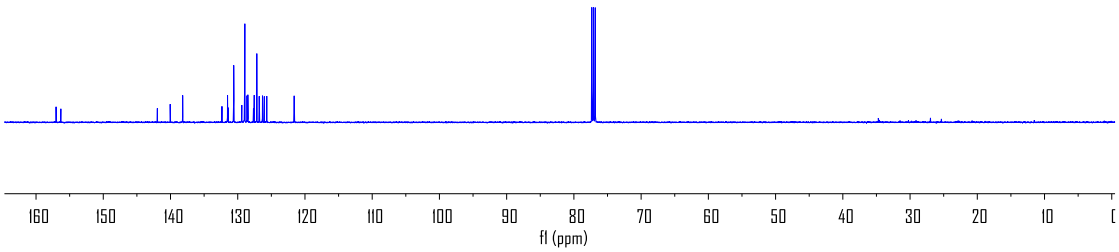
1p

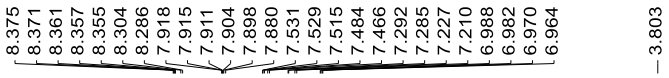

3.04
1.00
2.04
1.03
3.18
4.00
2.08
2.11
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

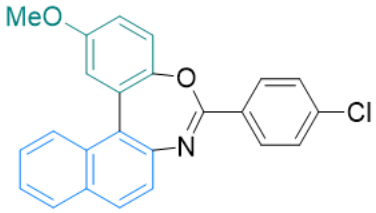

157.020
156.309
141.956
140.049
138.188
132.347
131.516
131.439
130.639
130.596
129.393
128.988
128.942
128.941
128.941
128.615
128.494
127.659
127.547
127.161
126.803
126.318
126.049
125.681
121.606


Ph
O
N
Cl

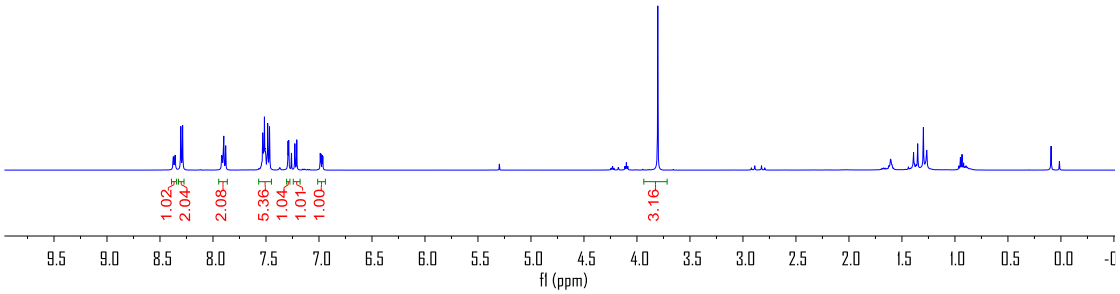
1p


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

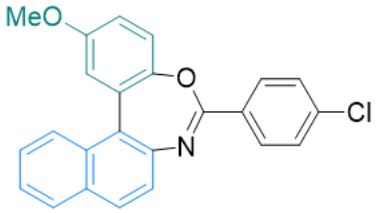

8.375
8.371
8.361
8.357
8.355
8.304
8.286
7.918
7.915
7.911
7.904
7.898
7.880
7.531
7.529
7.515
7.484
7.466
7.292
7.285
7.227
7.210
6.988
6.982
6.970
6.964
3.803


MeO
O
N
Cl

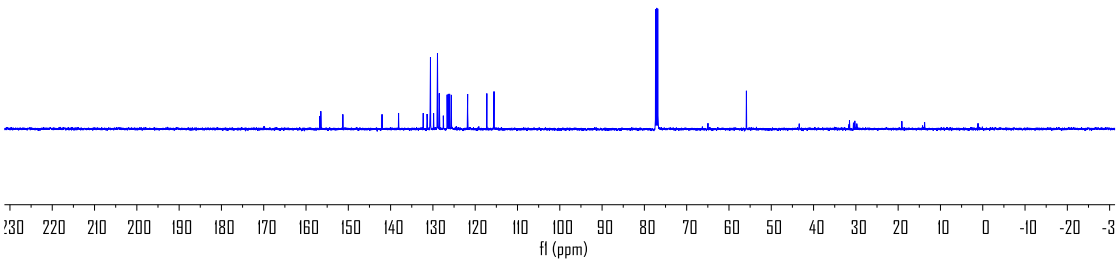
1q

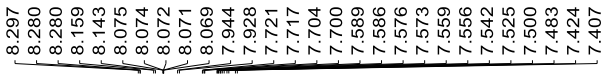

1.02
2.04
2.08
5.36
1.04
1.01
1.00
3.16
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


156.709
156.498
151.289
142.030
138.119
132.291
131.376
130.676
130.579
129.834
128.958
128.919
128.492
127.538
126.638
126.348
126.041
125.630
121.783
117.248
115.553
55.876


MeO
O
N
Cl

1q


230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -3
f1 (ppm)


8.297
8.280
8.280
8.159
8.143
8.075
8.074
8.072
8.071
8.069
7.944
7.928
7.721
7.717
7.704
7.700
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7.573
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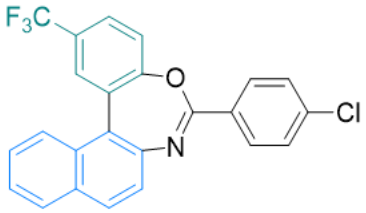
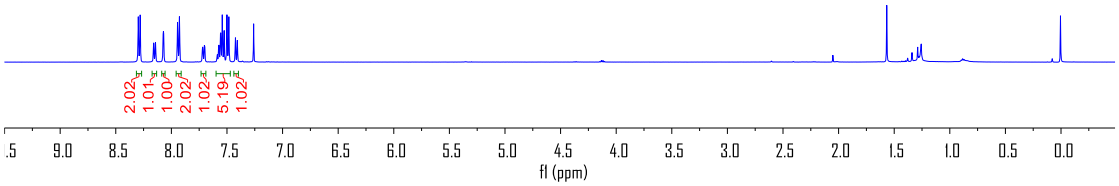
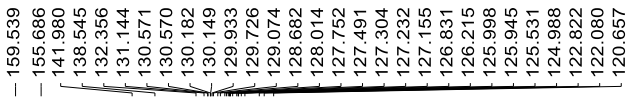
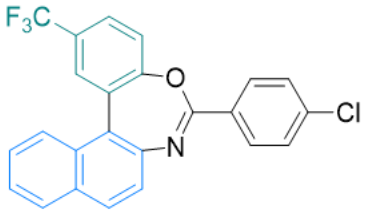
7.556
7.542
7.525
7.500
7.483
7.424
7.407


F3C
O
N
Cl

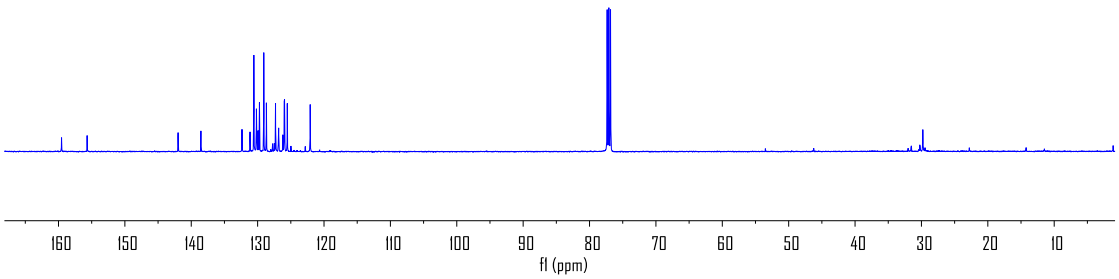
1r


2.02
1.01
1.00
2.02
1.02
5.19
1.02
f1 (ppm)


159.539
155.686
141.980
138.545
132.356
131.144
130.571
130.570
130.182
130.149
129.933
129.726
129.074
128.682
128.014
127.752
127.491
127.304
127.232
127.155
126.831
126.215
125.998
125.945
125.531
124.988
122.822
122.080
120.657

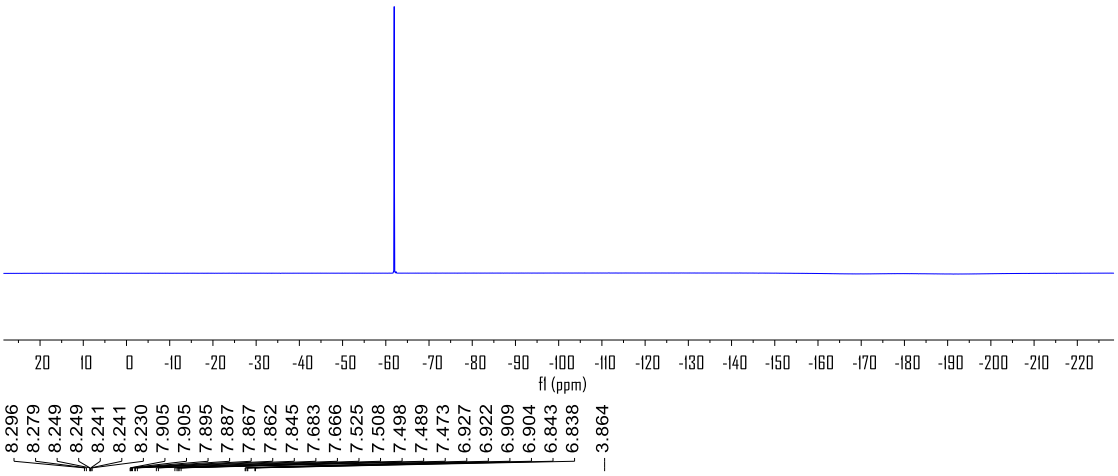

F3C
O
N
Cl

1r


f1 (ppm)


F3C
O
N
Cl
-61.944

1r


20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)
8.296
8.279
8.249
8.249
8.241
8.241
8.230
7.905
7.905
7.895
7.887
7.867
7.862
7.845
7.683
7.666
7.525
7.508
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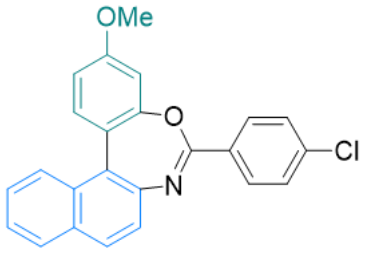
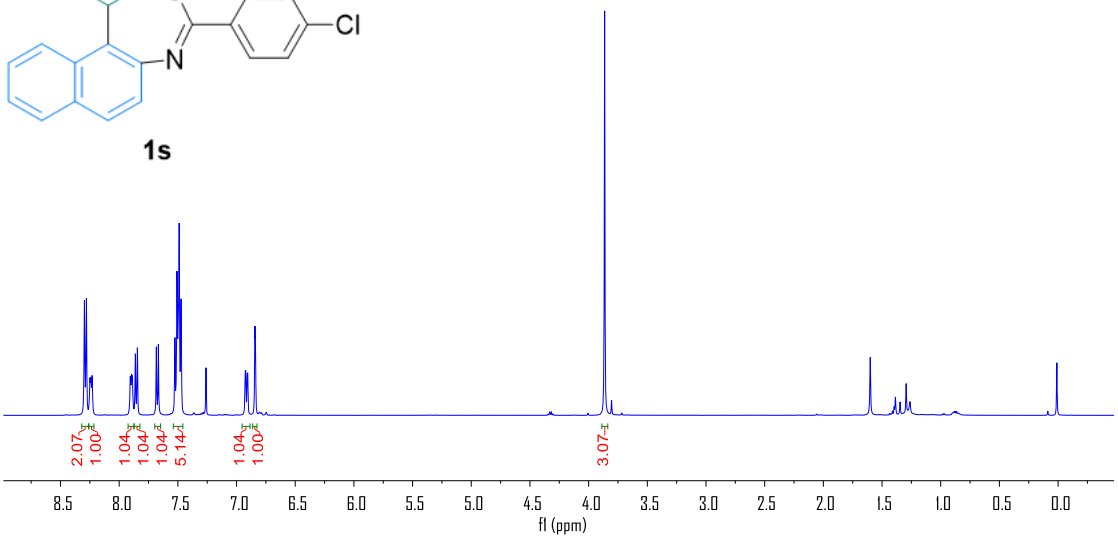
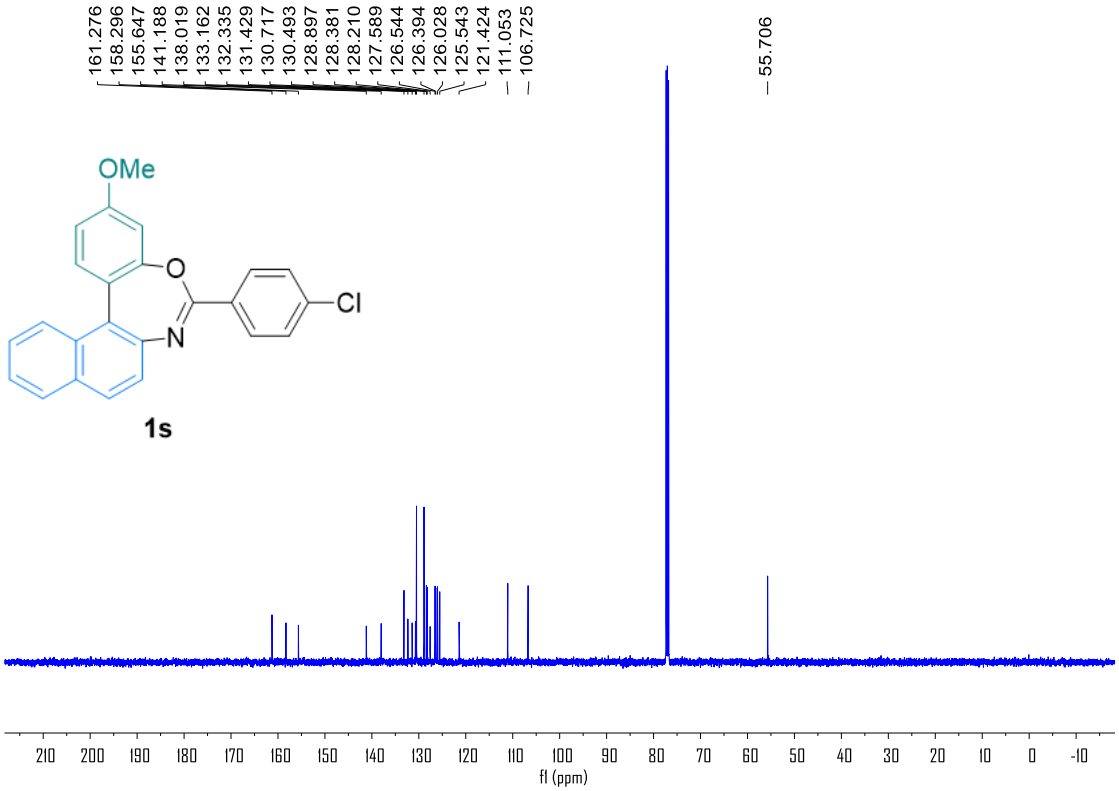
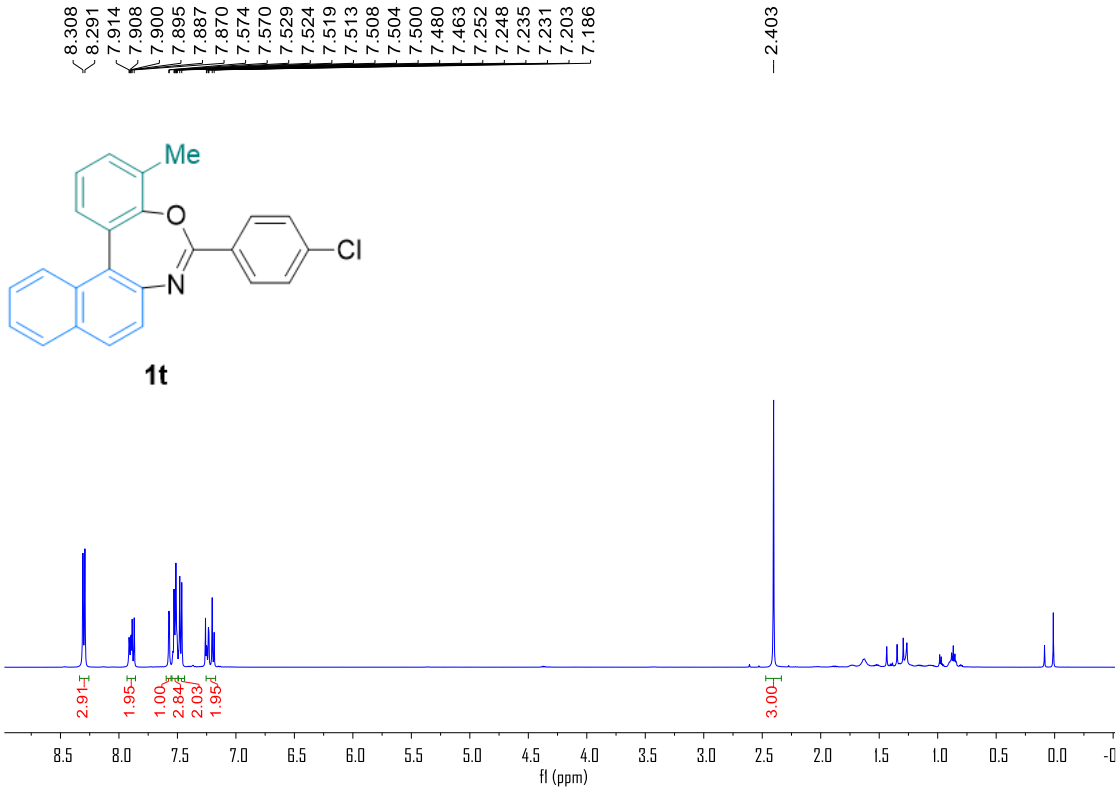
6.909
6.904
6.843
6.838
3.864

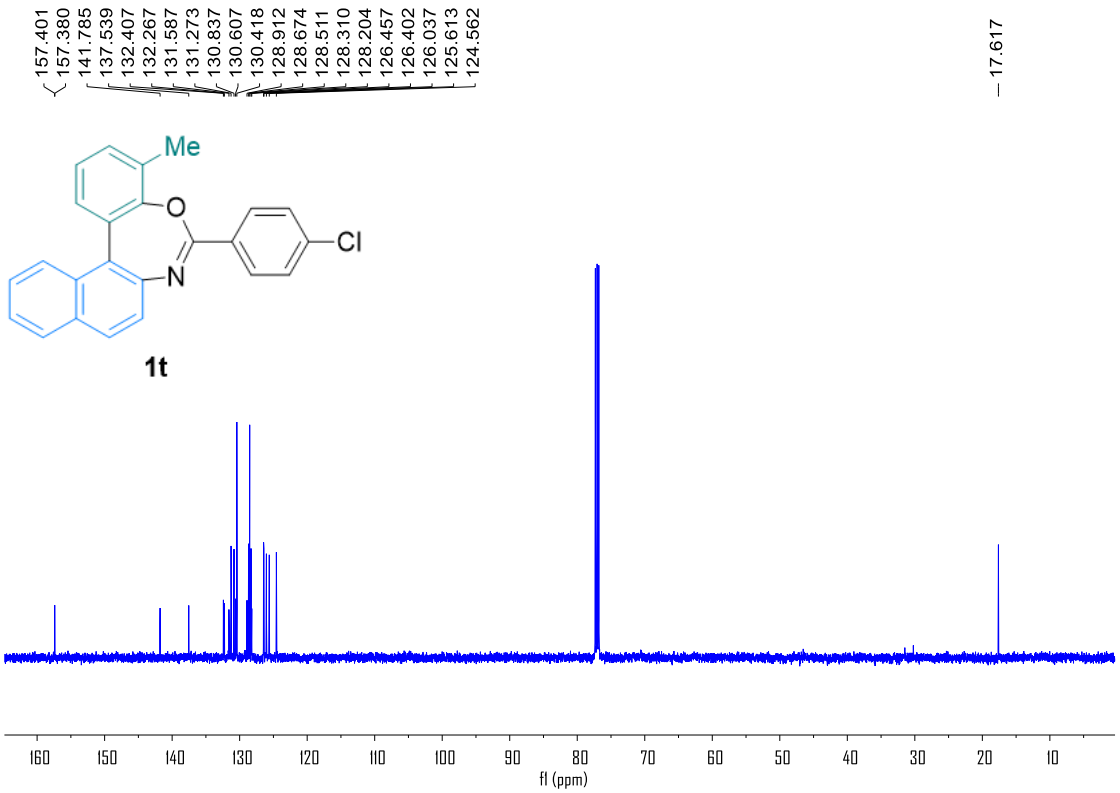

OMe
O
N
Cl

1s

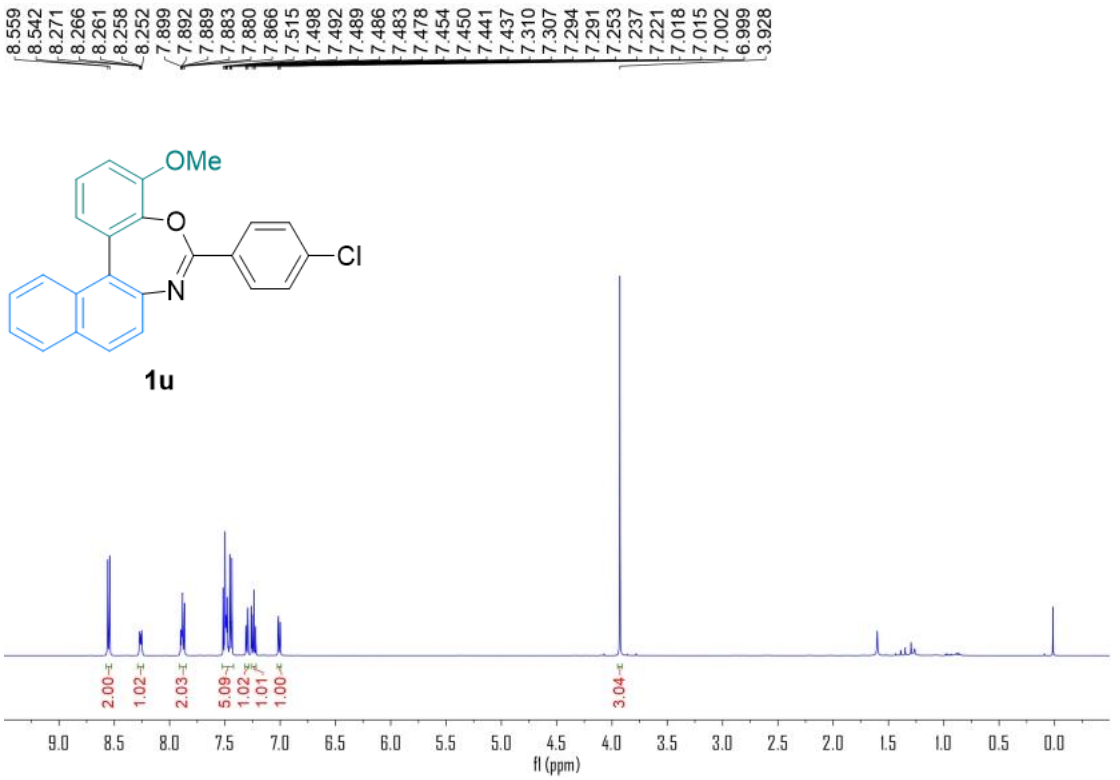

2.07
1.00
1.04
1.04
1.04
5.14
1.04
1.00
3.07
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


161.276
158.296
155.647
141.188
138.019
133.162
132.335
131.429
130.717
130.493
128.897
128.381
128.210
127.589
126.544
126.394
126.028
125.543
121.424
111.053
106.725
55.706
OMe
O
N
Cl
1s
f1 (ppm)

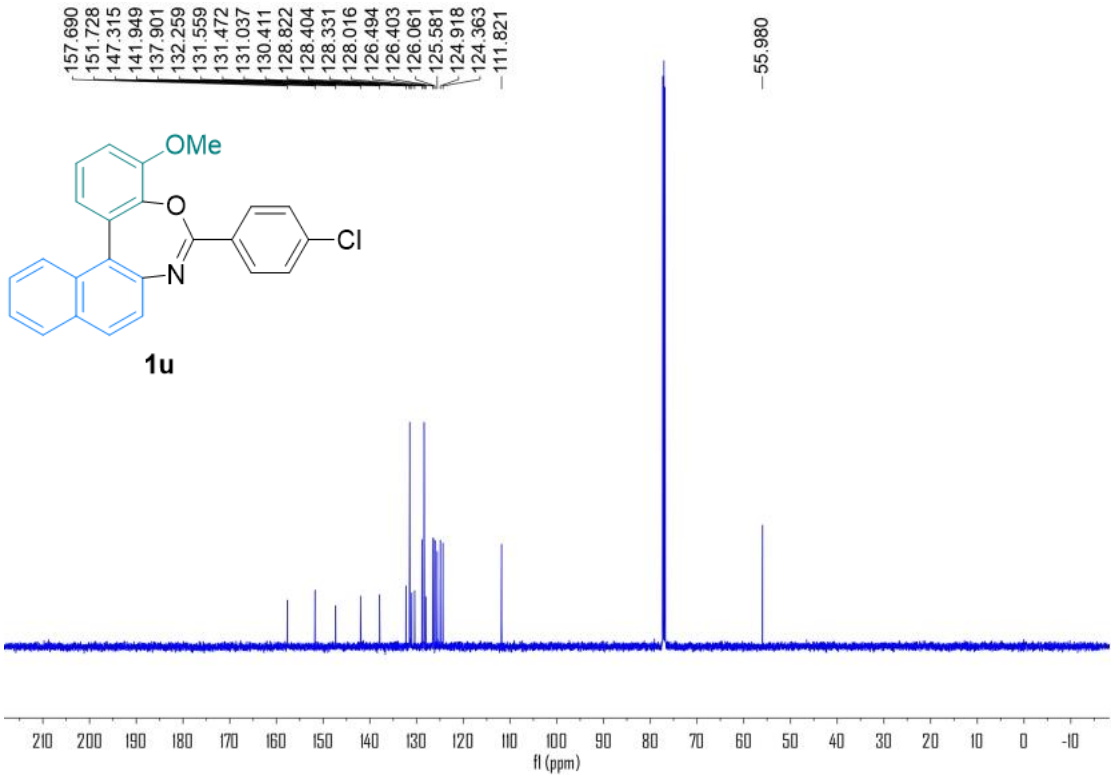

8.308
8.291
7.914
7.908
7.900
7.895
7.887
7.870
7.574
7.570
7.529
7.524
7.519
7.513
7.508
7.504
7.500
7.480
7.463
7.252
7.248
7.235
7.231
7.203
7.186
2.403
Me
O
N
Cl
1t
2.91
1.95
1.00
2.84
2.03
1.95
3.00
f1 (ppm)


157.401
157.380
141.785
137.539
132.407
132.267
131.587
131.273
130.837
130.607
130.418
128.912
128.674
128.511
128.310
128.204
126.457
126.402
126.037
125.613
124.562
17.617
Me
O
N
Cl
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

1t


8.559
8.542
8.271
8.266
8.261
8.258
8.252
7.899
7.892
7.889
7.883
7.880
7.866
7.515
7.498
7.492
7.489
7.486
7.483
7.478
7.454
7.450
7.441
7.437
7.310
7.307
7.294
7.291
7.253
7.237
7.221
7.018
7.015
7.002
6.999
3.928
OMe
O
N
Cl
2.00
1.02
2.03
5.09
1.02
1.01
1.00
3.04
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

1u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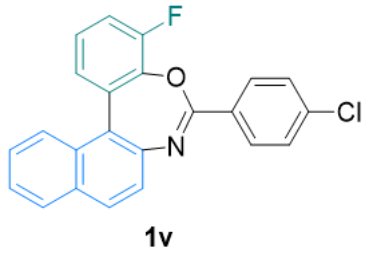
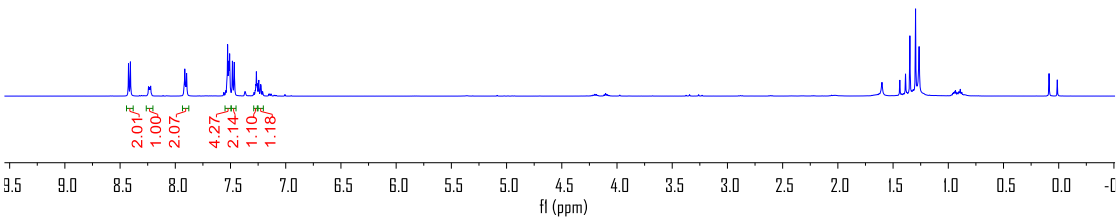
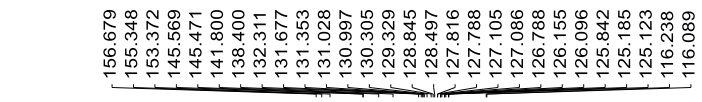
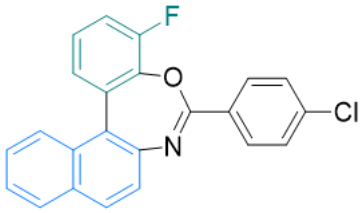
151.728
147.315
141.949
137.901
132.259
131.559
131.472
131.037
130.411
128.822
128.404
128.331
128.016
126.494
126.403
126.061
125.581
124.918
124.363
111.821
55.980
OMe
O
N
Cl
1u
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.424
8.406
8.242
8.236
8.230
8.223
7.920
7.914
7.907
7.901
7.897
7.543
7.534
7.532
7.526
7.519
7.514
7.508
7.500
7.483
7.466
7.287
7.276
7.270
7.266
7.256
7.244
7.231
7.227
7.223
7.210
7.207

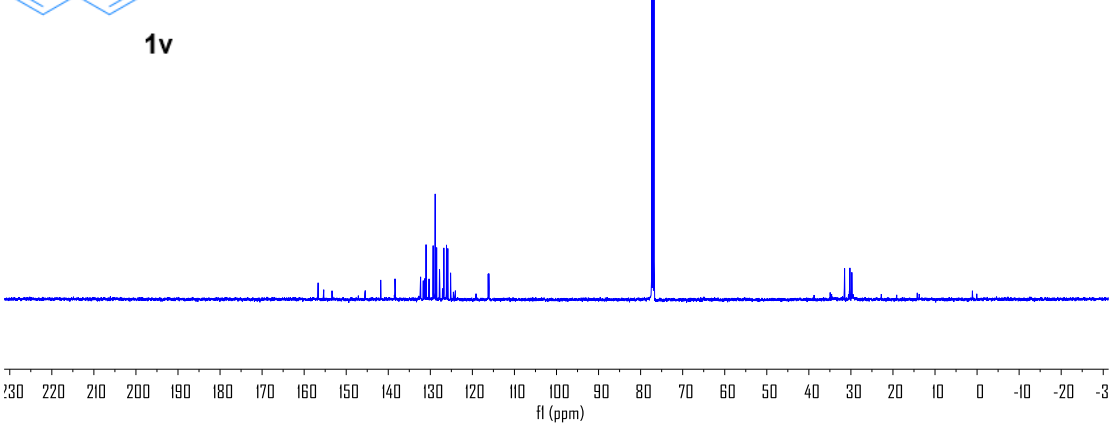

F
O
N
Cl
1v

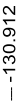

2.01
1.00
2.07
4.27
2.14
1.10
1.18
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

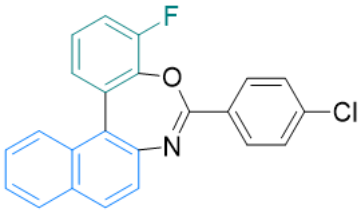

156.679
155.348
153.372
145.569
145.471
141.800
138.400
132.311
131.677
131.353
131.028
130.997
130.305
129.329
128.845
128.497
127.816
127.788
127.105
127.086
126.788
126.155
126.096
125.842
125.185
125.123
116.238
116.089


F
O
N
Cl

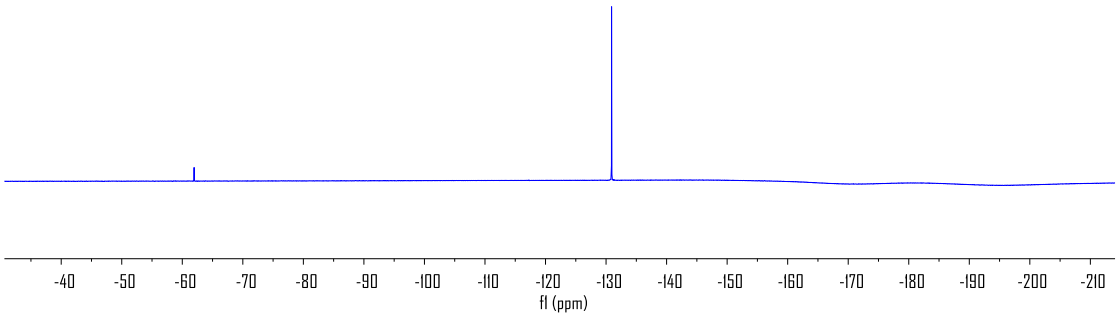
1v

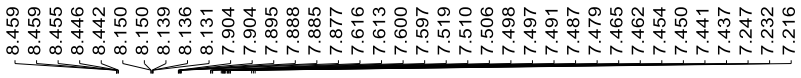

230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -3
f1 (ppm)

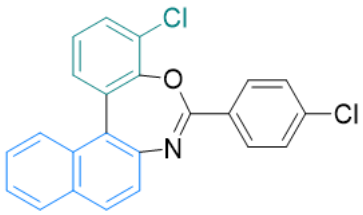

-130.912


F
O
N
Cl

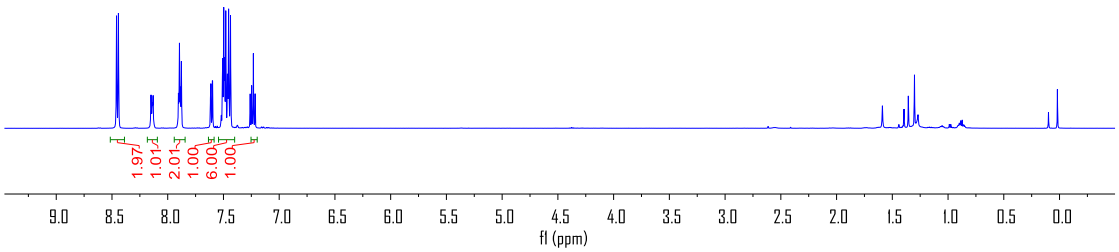
1v

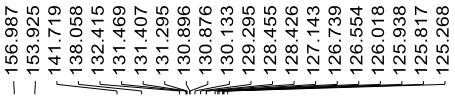

-40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

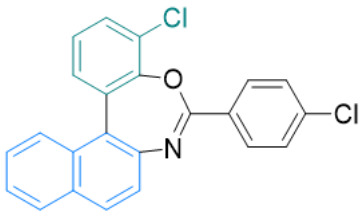

8.459
8.459
8.455
8.446
8.442
8.150
8.150
8.139
8.136
8.131
7.904
7.904
7.895
7.888
7.885
7.877
7.616
7.613
7.600
7.597
7.519
7.510
7.506
7.498
7.497
7.491
7.487
7.479
7.465
7.462
7.454
7.450
7.441
7.437
7.247
7.232
7.216


Cl
O
N
Cl

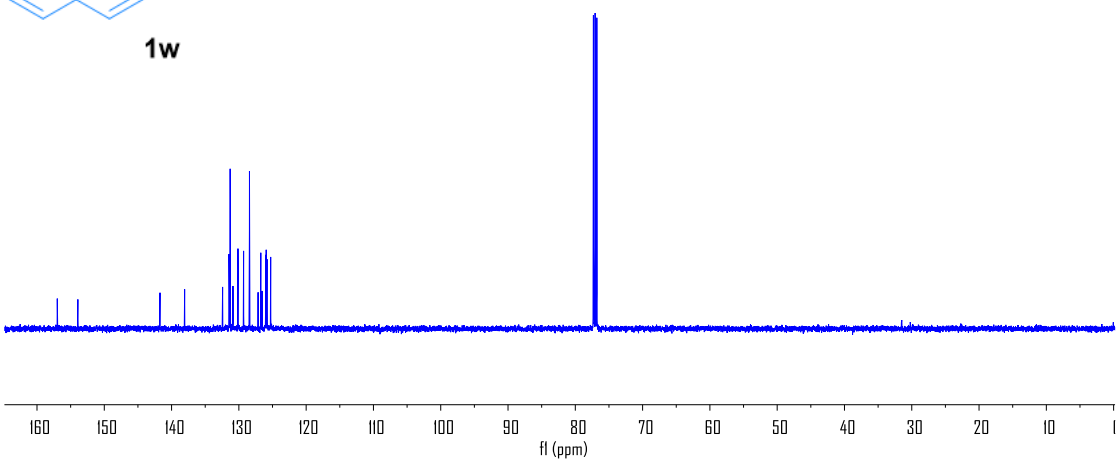
1w

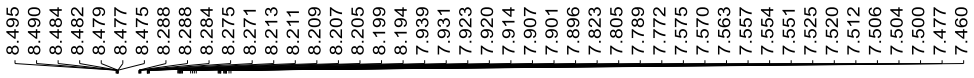

1.97
1.01
2.01
1.00
6.00
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

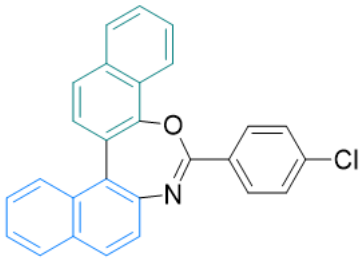

156.987
153.925
141.719
138.058
132.415
131.469
131.407
131.295
130.896
130.876
130.133
129.295
128.455
128.426
127.143
126.739
126.554
126.018
125.938
125.817
125.268


Cl
O
N
Cl

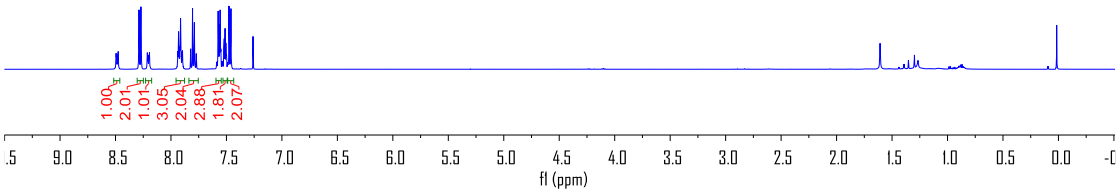
1w

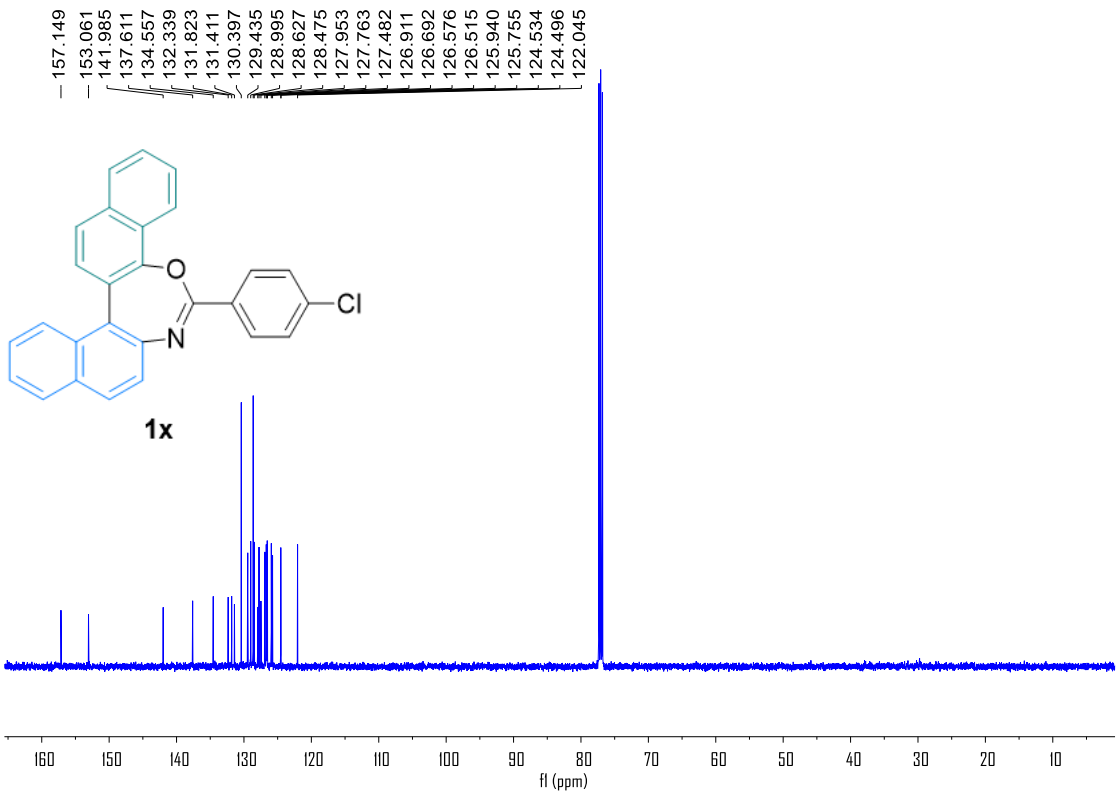

160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.495
8.490
8.484
8.482
8.479
8.477
8.475
8.288
8.288
8.284
8.275
8.271
8.213
8.211
8.209
8.207
8.205
8.199
8.194
7.939
7.931
7.923
7.920
7.914
7.907
7.901
7.896
7.823
7.805
7.789
7.772
7.575
7.570
7.563
7.557
7.554
7.551
7.525
7.520
7.512
7.506
7.504
7.500
7.477
7.460

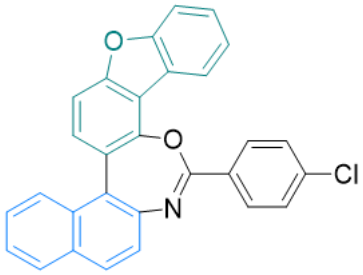

O
N
Cl

1x

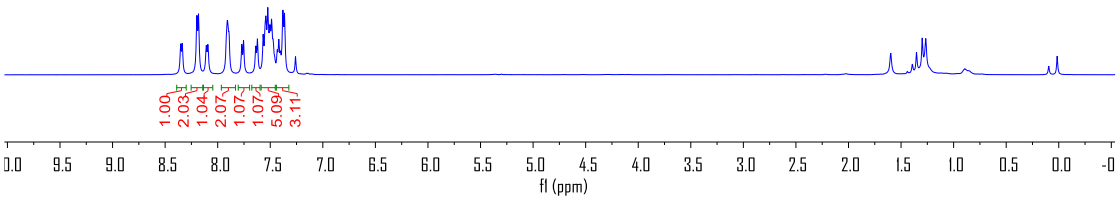

1.00
2.01
1.01
3.05
2.04
2.88
1.81
2.07
.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)

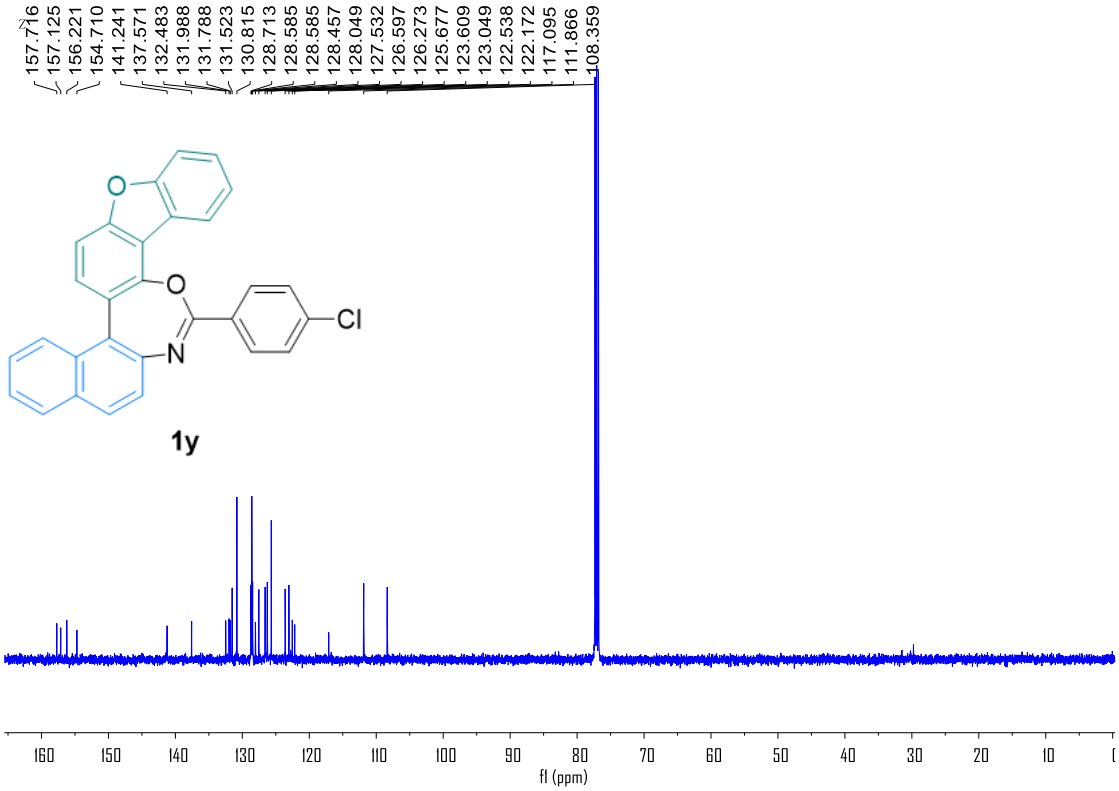

157.149
153.061
141.985
137.611
134.557
132.339
131.823
131.411
130.397
129.435
128.995
128.627
128.475
127.953
127.763
127.482
126.911
126.692
126.576
126.515
125.940
125.755
124.534
124.496
122.045
O
N
Cl
1x
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


8.352
8.337
8.198
8.182
8.109
8.093
7.918
7.908
7.901
7.892
7.771
7.754
7.638
7.622
7.567
7.550
7.542
7.523
7.503
7.487
7.472
7.434
7.419
7.404
7.380
7.364

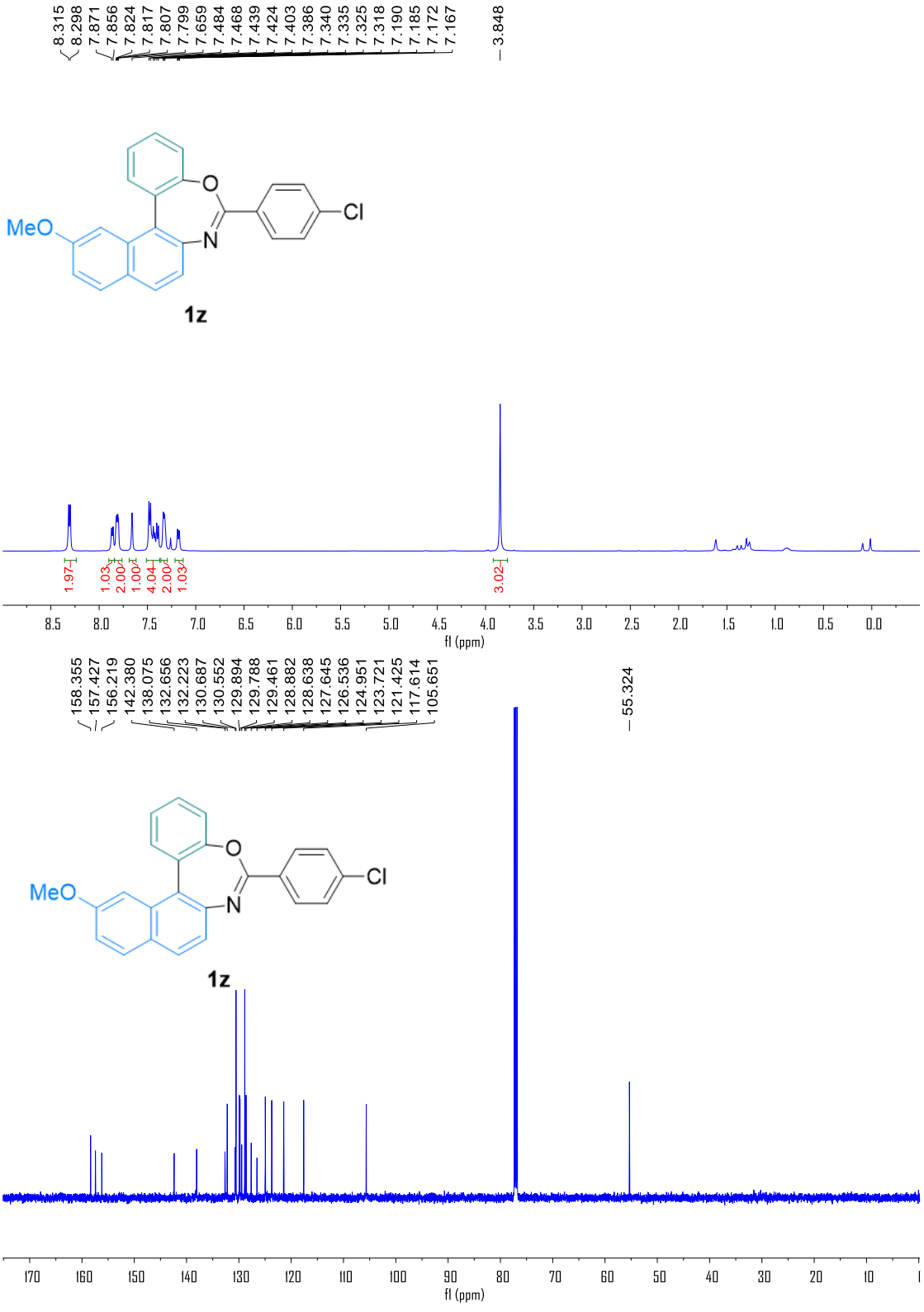

O
O
N
Cl

1y


1.00
2.03
1.04
2.07
1.07
1.07
5.09
3.11
f1 (ppm)


157.716
157.125
156.221
154.710
141.241
137.571
132.483
131.988
131.788
131.523
130.815
128.713
128.585
128.585
128.457
128.049
127.532
126.597
126.273
125.677
123.609
123.049
122.538
122.172
117.095
111.866
108.359
O
O
N
Cl
f1 (ppm)

1y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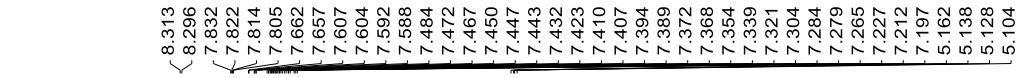
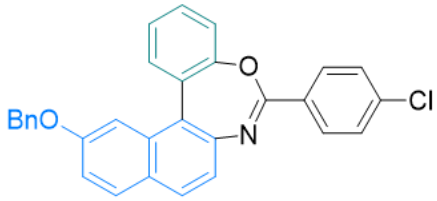
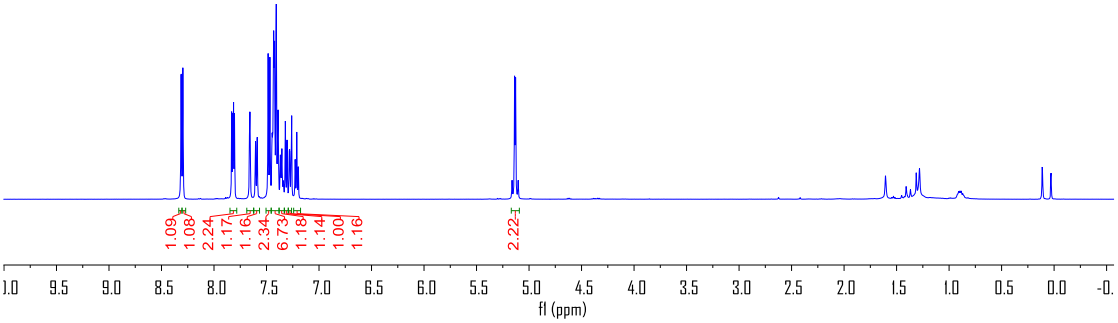
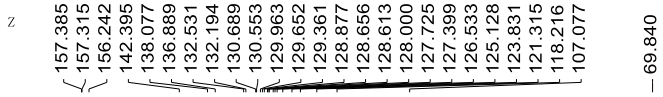
8.298
7.871
7.856
7.824
7.817
7.807
7.799
7.659
7.484
7.468
7.439
7.424
7.403
7.386
7.340
7.335
7.325
7.318
7.190
7.185
7.172
7.167
3.848
MeO
O
N
Cl
1z
1.97
1.03
2.00
1.00
4.04
2.00
1.03
3.02
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
158.355
157.427
156.219
142.380
138.075
132.656
132.223
130.687
130.552
129.894
129.788
129.461
128.882
128.638
127.645
126.536
124.951
123.721
121.425
117.614
105.651
55.324
MeO
O
N
Cl
1z
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

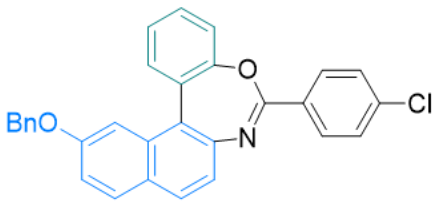

8.313
8.296
7.832
7.822
7.814
7.805
7.662
7.657
7.607
7.604
7.592
7.588
7.484
7.472
7.467
7.450
7.447
7.443
7.432
7.423
7.410
7.407
7.394
7.389
7.372
7.368
7.354
7.339
7.321
7.304
7.284
7.279
7.265
7.227
7.212
7.197
5.162
5.138
5.128
5.104


BnO
O
N
Cl

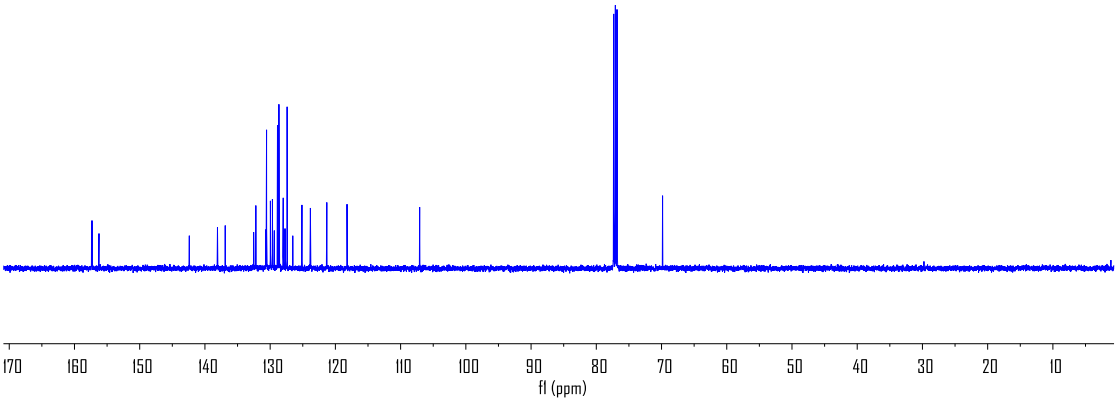
1aa

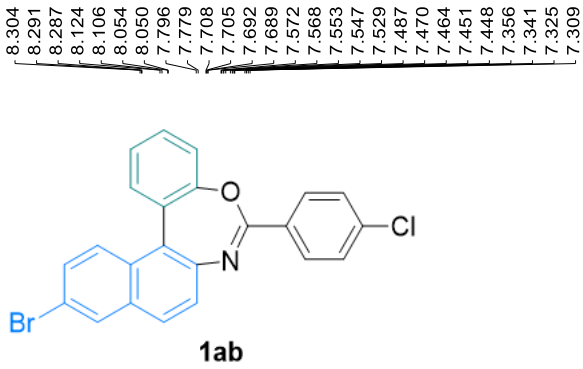

1.09
1.08
2.24
1.17
1.16
2.34
6.73
1.18
1.14
1.00
1.16
2.22
f1 (ppm)

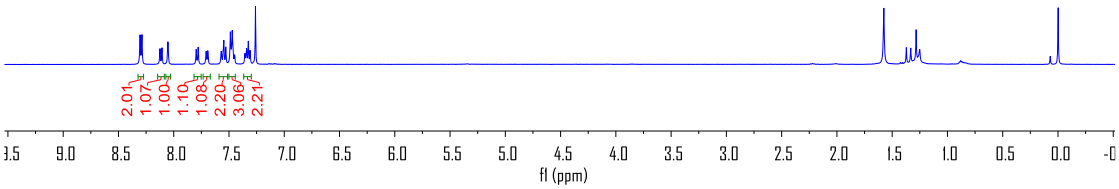

157.385
157.315
156.242
142.395
138.077
136.889
132.531
132.194
130.689
130.553
129.963
129.652
129.361
128.877
128.656
128.613
128.000
127.725
127.399
126.533
125.128
123.831
121.315
118.216
107.077
69.840

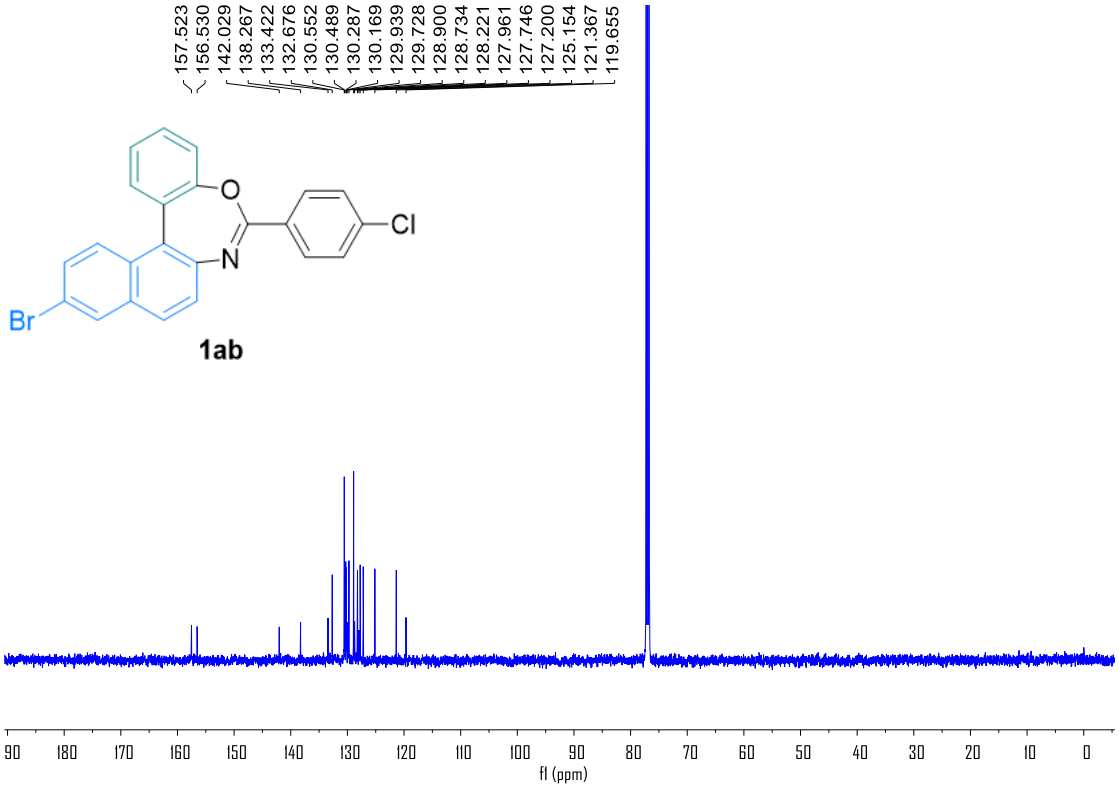

BnO
O
N
Cl

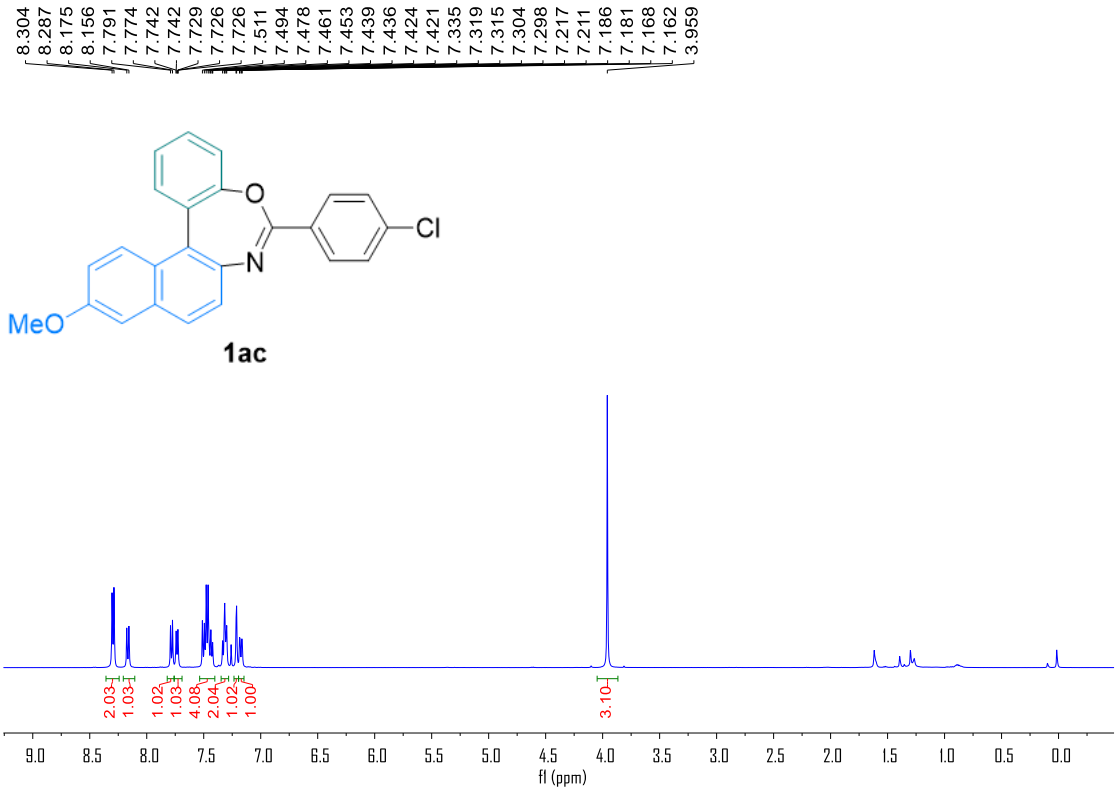
1aa

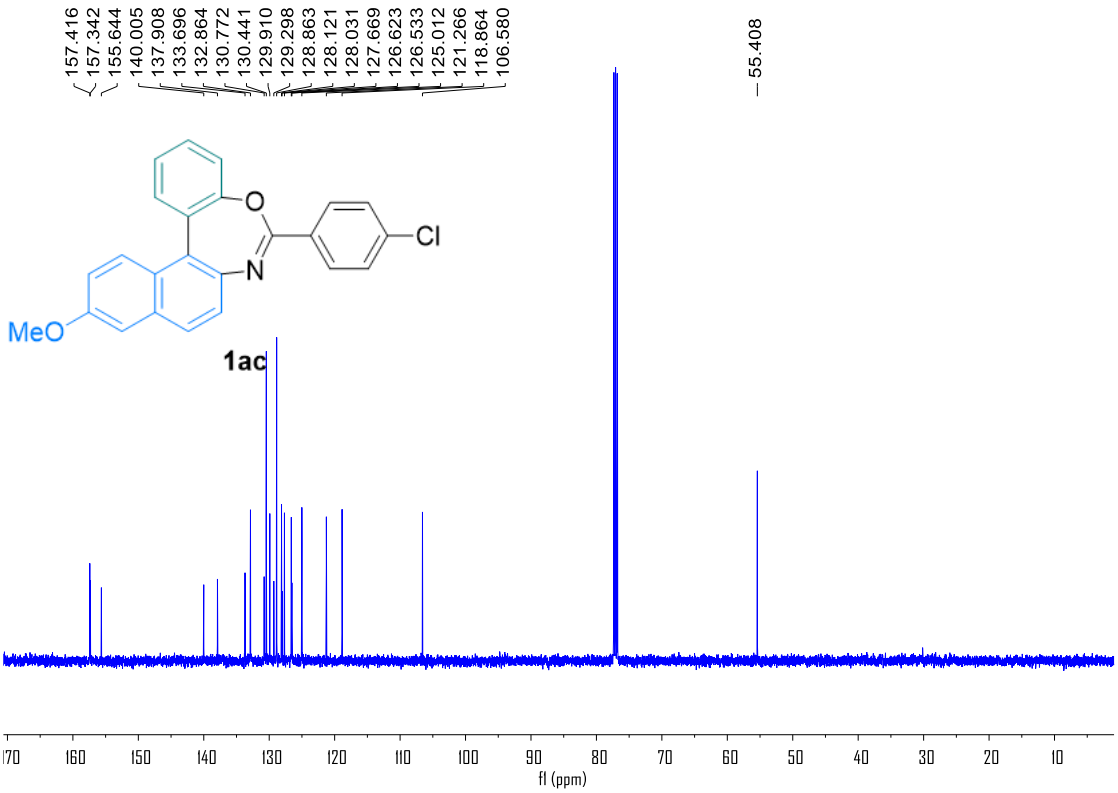

f1 (ppm)

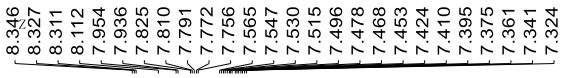

8.304
8.291
8.287
8.124
8.106
8.054
8.050
7.796
7.779
7.708
7.705
7.692
7.689
7.572
7.568
7.553
7.547
7.529
7.487
7.470
7.464
7.451
7.448
7.356
7.341
7.325
7.309
O
N
Cl
Br
1ab


2.01
1.07
1.00
1.10
1.08
2.20
3.06
2.21
f1 (ppm)


157.523
156.530
142.029
138.267
133.422
132.676
130.552
130.489
130.287
130.169
129.939
129.728
128.900
128.734
128.221
127.961
127.746
127.200
125.154
121.367
119.655
O
N
Cl
Br
1ab
f1 (ppm)


8.304
8.287
8.175
8.156
7.791
7.774
7.742
7.742
7.729
7.726
7.726
7.511
7.494
7.478
7.461
7.453
7.439
7.436
7.424
7.421
7.335
7.319
7.315
7.304
7.298
7.217
7.211
7.186
7.181
7.168
7.162
3.959
O
N
Cl
MeO
1ac
2.03
1.03
1.02
1.03
4.08
2.04
1.02
1.00
3.10
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


157.416
157.342
155.644
140.005
137.908
133.696
132.864
130.772
130.441
129.910
129.298
128.863
128.121
128.031
127.669
126.623
126.533
125.012
121.266
118.864
106.580
55.408
O
N
Cl
MeO
1ac
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.346
8.327
8.311
8.112
7.954
7.936
7.825
7.810
7.791
7.772
7.756
7.565
7.547
7.530
7.515
7.496
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7.468
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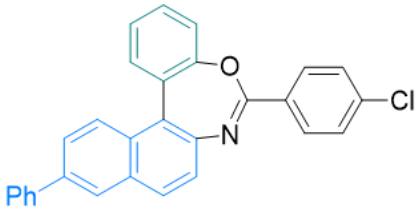
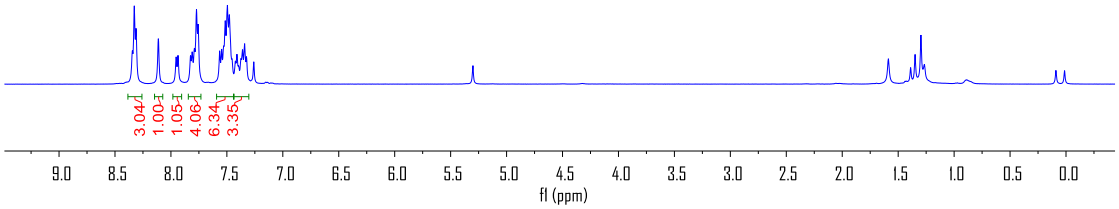
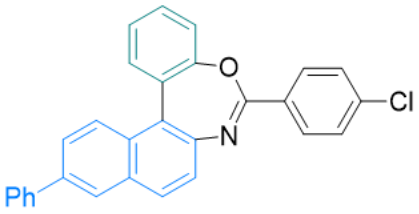
7.424
7.410
7.395
7.375
7.361
7.341
7.324


O
N
Cl
Ph

1ad

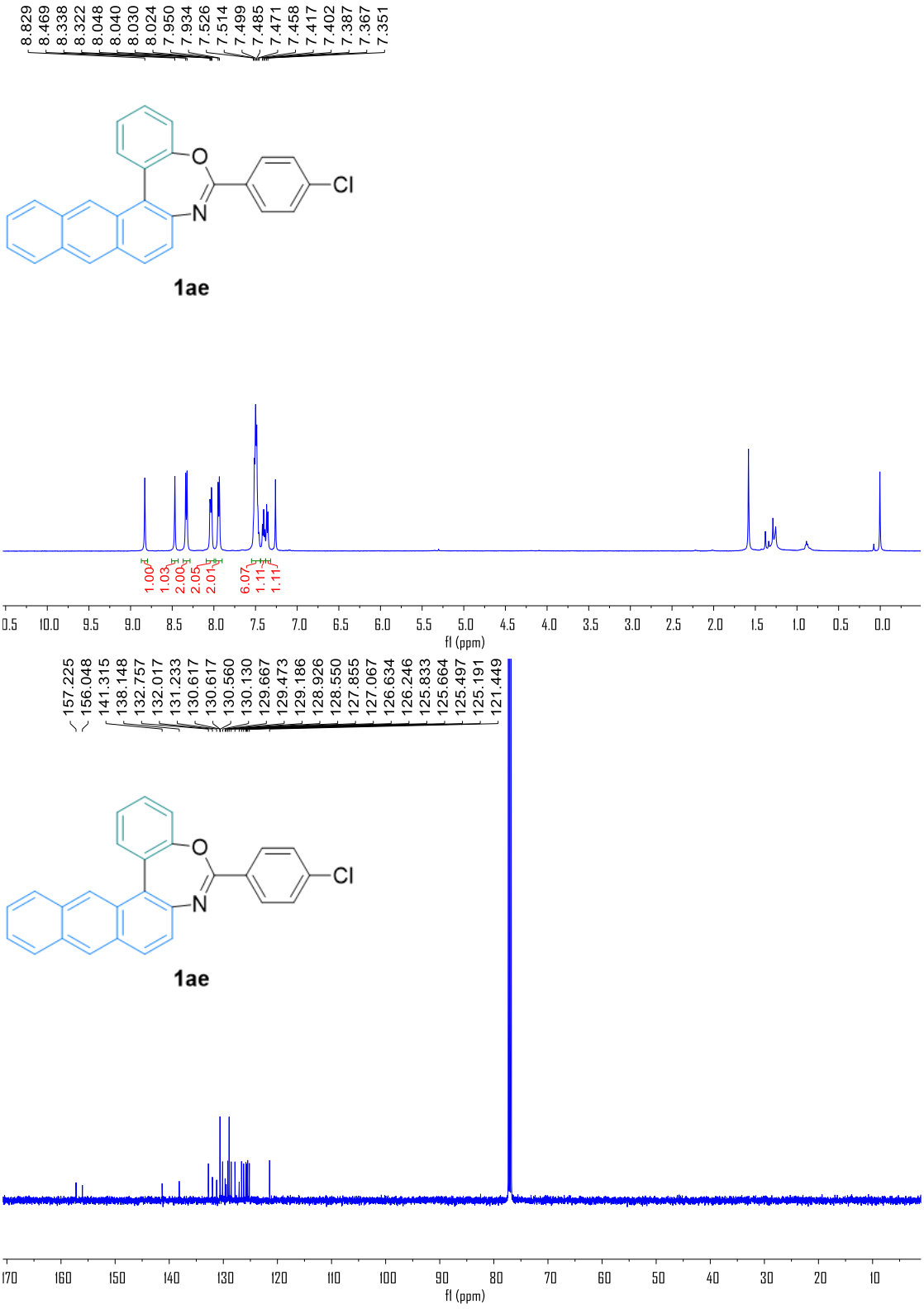

3.04
1.00
1.05
4.06
6.34
3.35
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

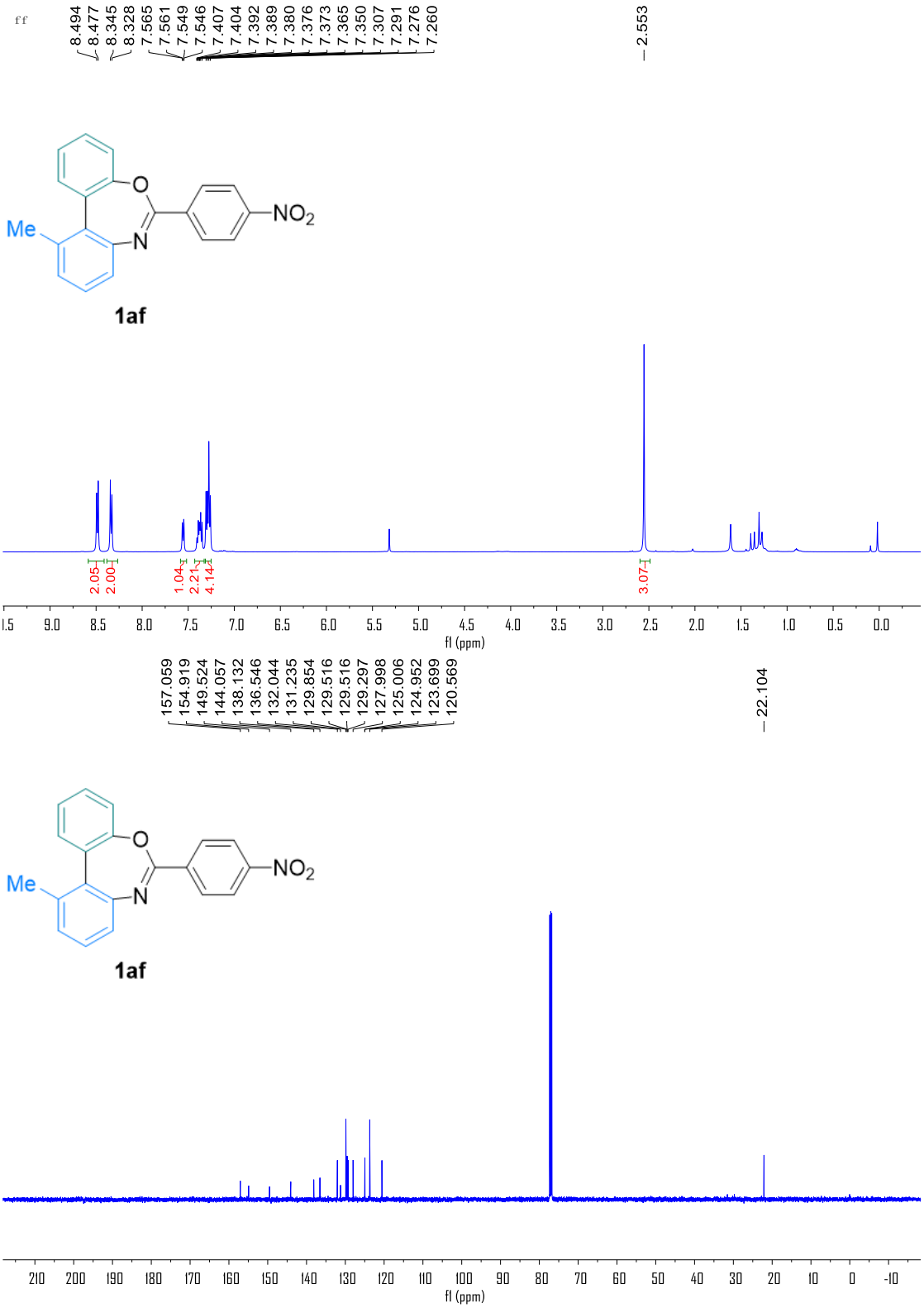

157.489
156.246
141.836
140.568
138.173
138.126
132.887
132.591
130.659
130.566
130.566
129.986
129.156
129.099
128.969
128.913
127.715
127.562
127.335
127.046
126.498
126.166
126.105
125.096
121.322

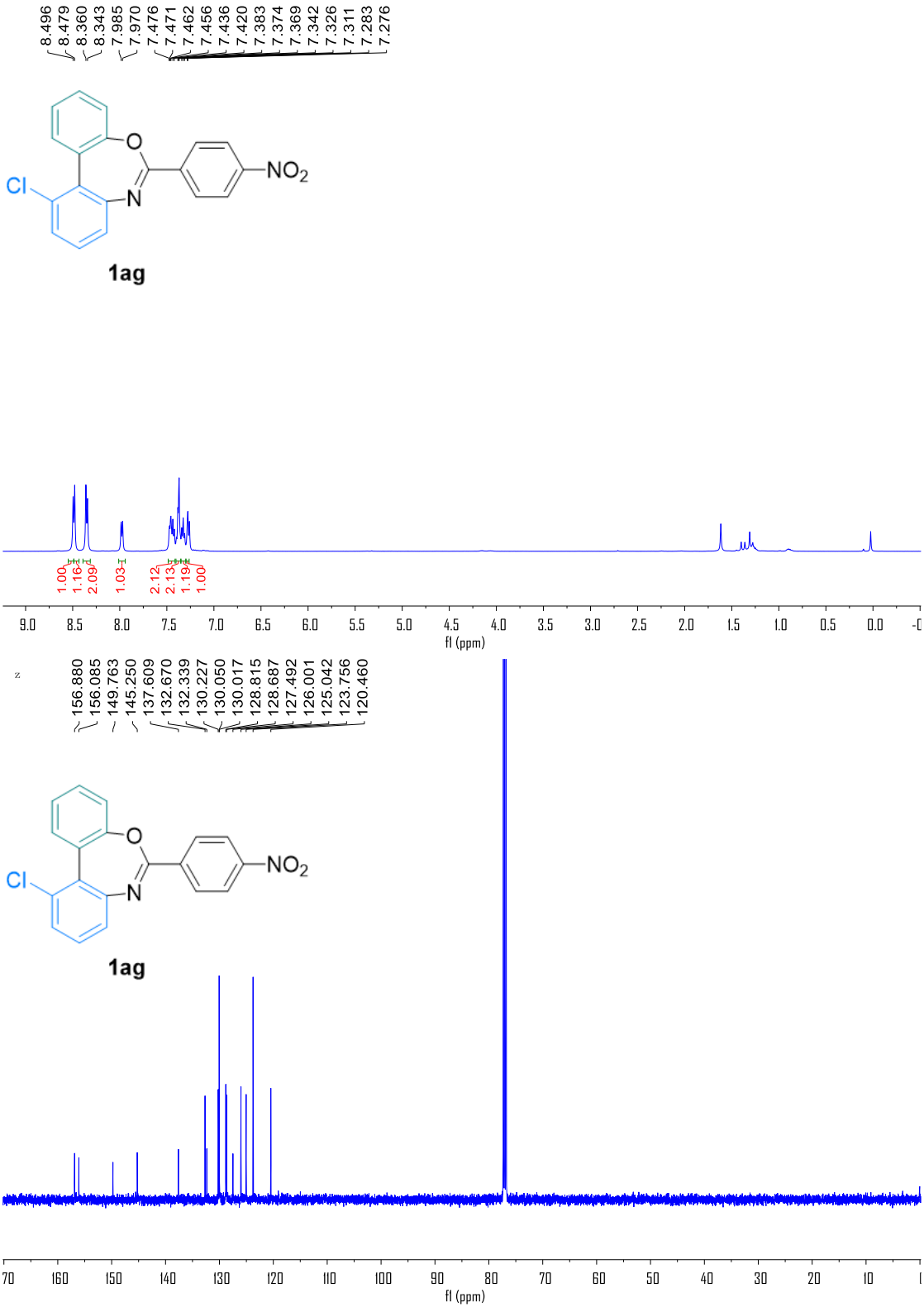

O
N
Cl
Ph

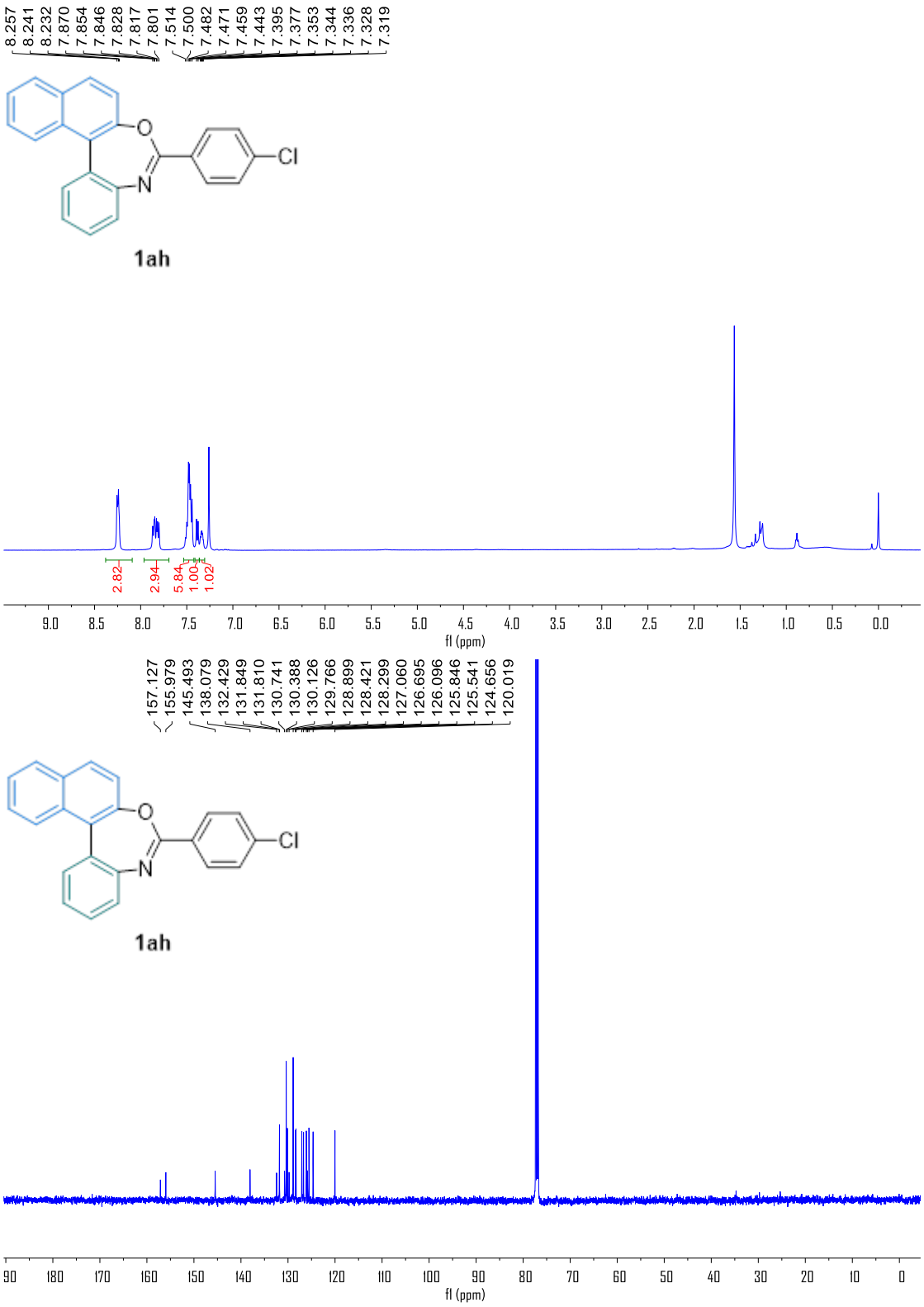
1ad

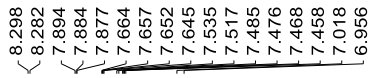
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

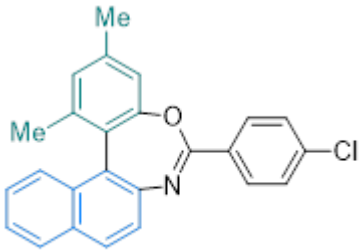

8.829
8.469
8.338
8.322
8.048
8.040
8.030
8.024
7.950
7.934
7.526
7.514
7.499
7.485
7.471
7.458
7.417
7.402
7.387
7.367
7.351
O
N
Cl
1ae
1.00
1.03
2.00
2.05
2.01
6.07
1.11
1.11
f1 (ppm)
157.225
156.048
141.315
138.148
132.757
132.017
131.233
130.617
130.560
130.130
129.667
129.473
129.186
128.926
128.550
127.855
127.067
126.634
126.246
125.833
125.664
125.497
125.191
121.449
O
N
Cl
1ae
f1 (ppm)


ff
8.494
8.477
8.345
8.328
7.565
7.561
7.549
7.546
7.407
7.404
7.392
7.389
7.380
7.376
7.373
7.365
7.350
7.307
7.291
7.276
7.260
2.553
Me
O
N
NO2
1af
2.05
2.00
1.04
2.21
4.14
3.07
fl (ppm)
157.059
154.919
149.524
144.057
138.132
136.546
132.044
131.235
129.854
129.516
129.516
129.297
127.998
125.006
124.952
123.699
120.569
22.104
Me
O
N
NO2
1af
fl (ppm)

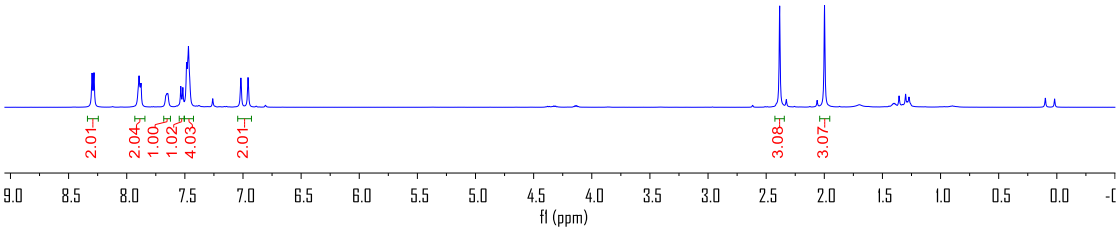

8.496
8.479
8.360
8.343
7.985
7.970
7.476
7.471
7.462
7.456
7.436
7.420
7.383
7.374
7.369
7.342
7.326
7.311
7.283
7.276
O
N
Cl
NO2
1ag
1.00
1.16
2.09
1.03
2.12
2.13
1.19
1.00
f1 (ppm)
156.880
156.085
149.763
145.250
137.609
132.670
132.339
130.227
130.050
130.017
128.815
128.687
127.492
126.001
125.042
123.756
120.460
O
N
Cl
NO2
1ag
f1 (ppm)


8.257
8.241
8.232
7.870
7.854
7.846
7.828
7.817
7.801
7.514
7.500
7.482
7.471
7.459
7.443
7.395
7.377
7.353
7.344
7.336
7.328
7.319
O
N
Cl
1ah
2.82
2.94
5.84
1.00
1.02
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
157.127
155.979
145.493
138.079
132.429
131.849
131.810
130.741
130.388
130.126
129.766
128.899
128.421
128.299
127.060
126.695
126.096
125.846
125.541
124.656
120.019
O
N
Cl
1ah
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

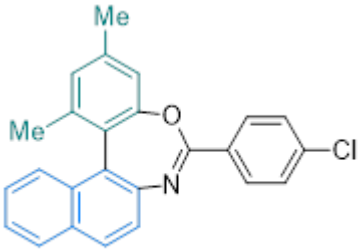

8.298
8.282
7.894
7.884
7.877
7.664
7.657
7.652
7.645
7.535
7.517
7.485
7.476
7.468
7.458
7.018
6.956
2.384
1.998


Me
Me
O
N
Cl

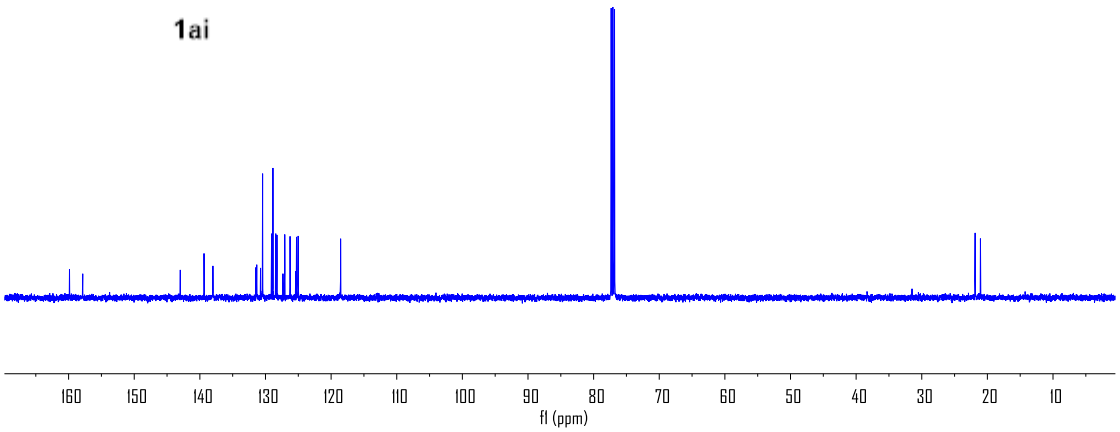
1ai

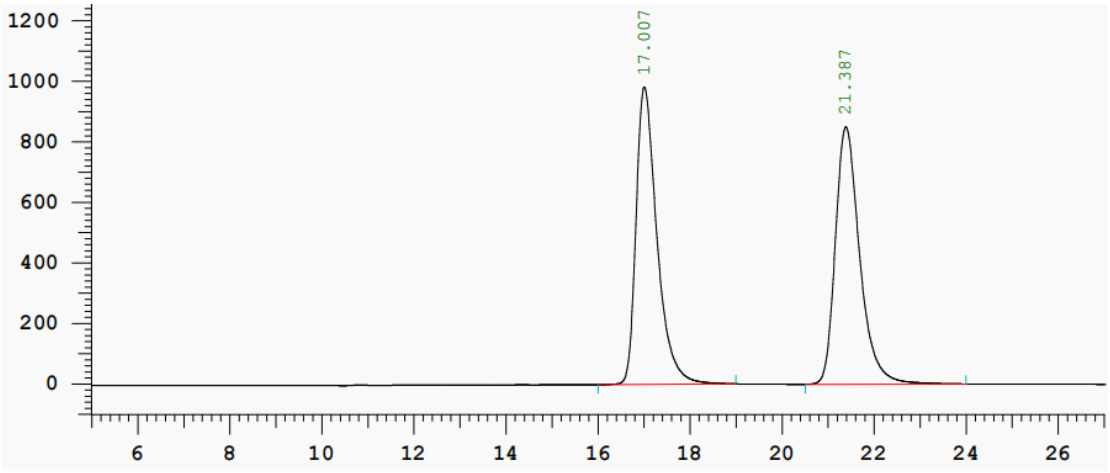

2.01
2.04
1.00
1.02
4.03
2.01
3.08
3.07
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


159.865
157.846
142.983
139.366
139.348
138.012
131.445
131.332
130.751
130.441
129.071
128.865
128.432
128.256
127.337
127.063
126.256
125.402
125.274
125.023
118.555
21.866
21.059

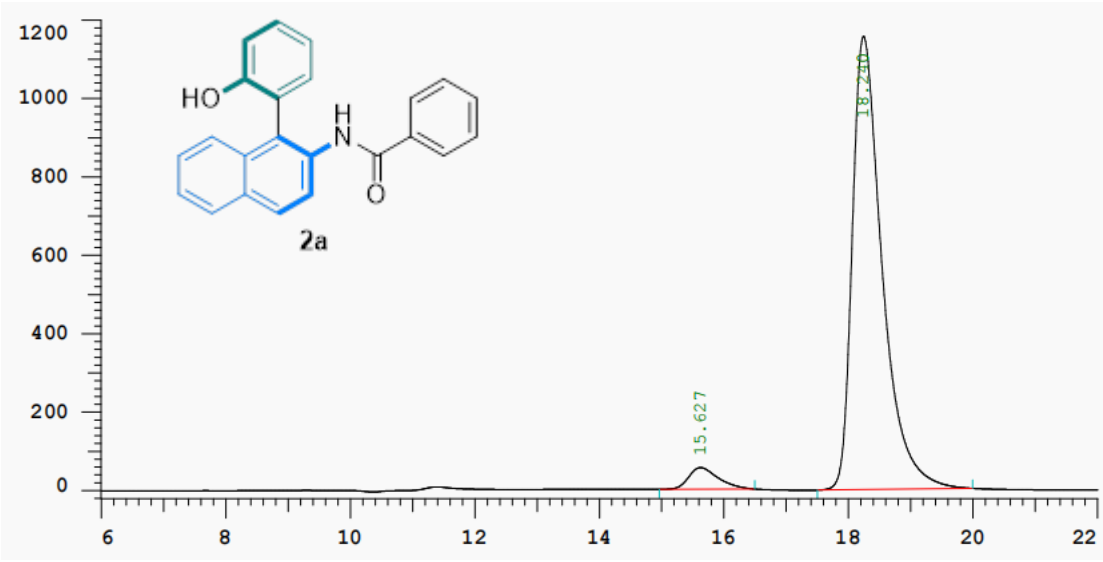

Me
Me
O
N
Cl

1ai

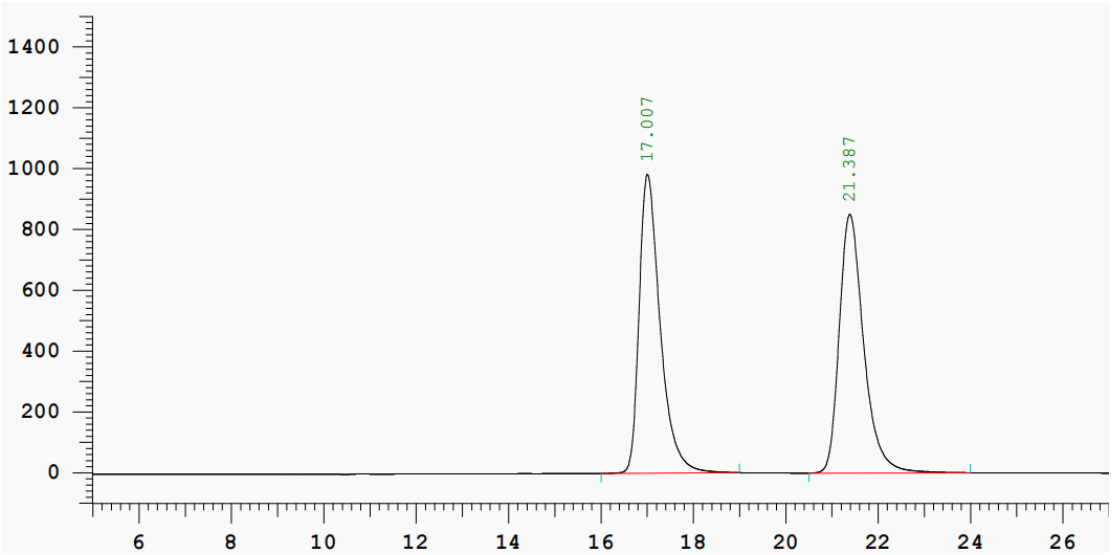

160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)



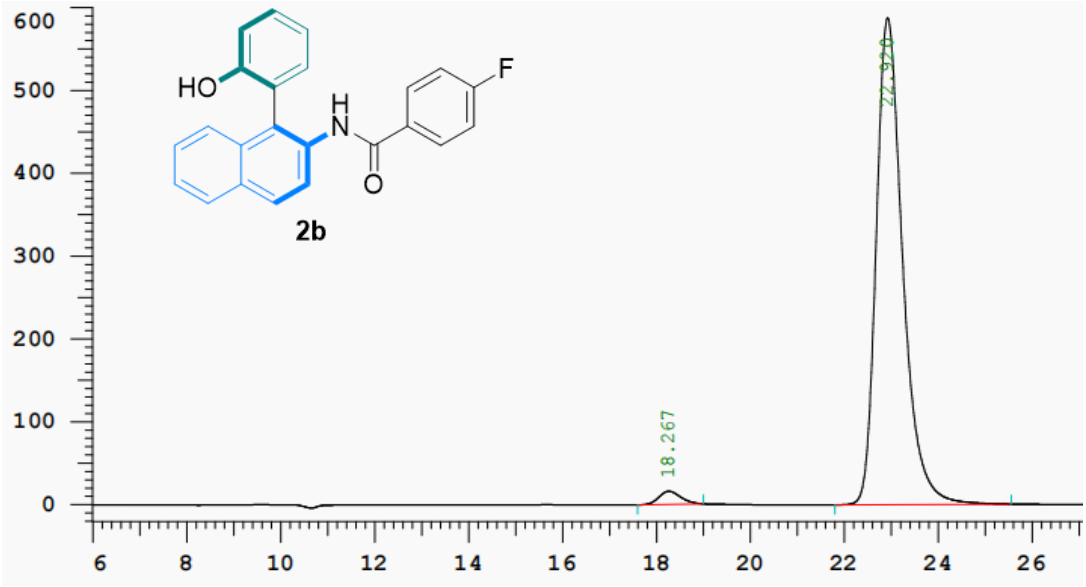
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	17.007	31084559	982380	49.884	53.599
2	21.387	31228712	850445	50.116	46.401
Total		62313271	1832825	100.000	100.000



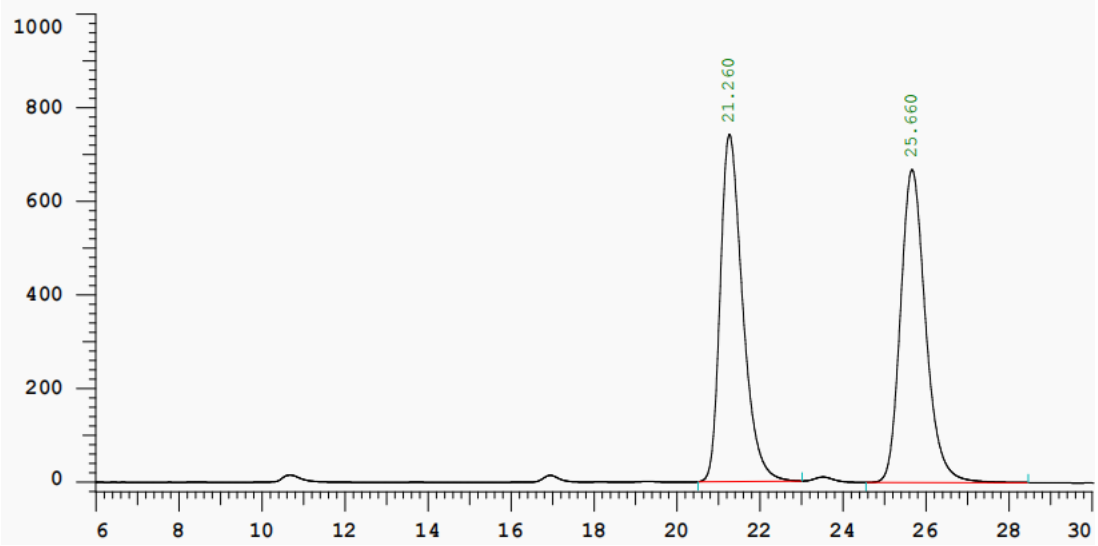
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	15.627	1813245	55048	4.492	4.546
2	18.240	38556974	1155838	95.508	95.454
Total		40370219	1210886	100.000	100.000



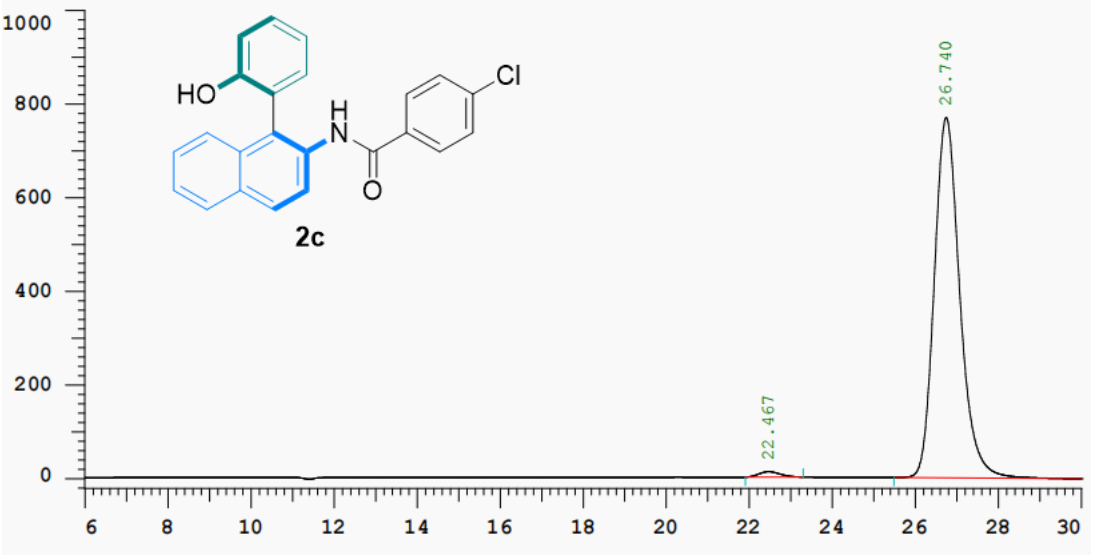
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	17.007	31084559	982380	49.884	53.590
2	21.387	31228712	850445	50.116	46.410
Total		62313271	1832825	100.000	100.000



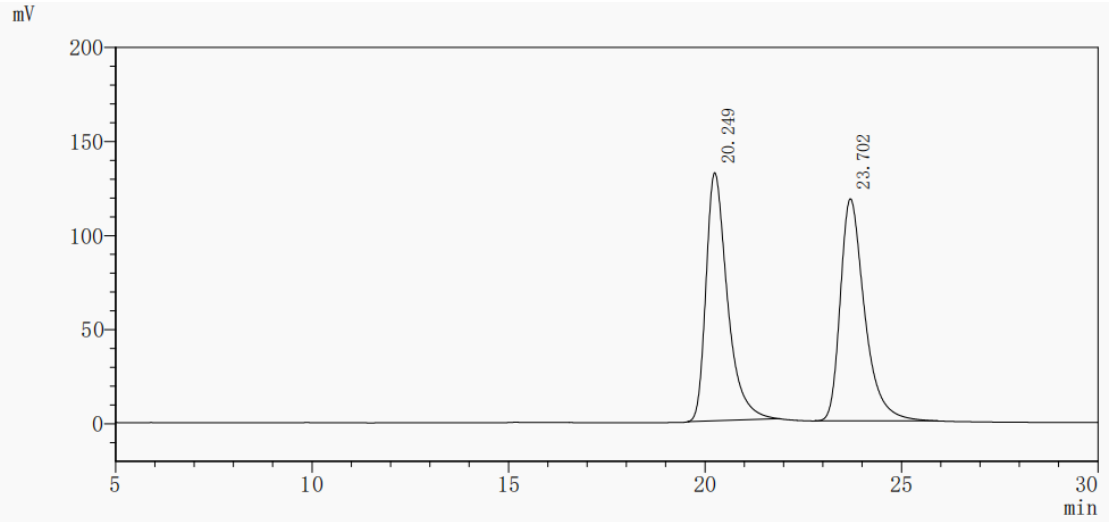
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	18.267	511485	15888	2.184	2.635
2	22.920	22908346	586916	97.816	97.365
Total		23419831	602804	100.000	100.000



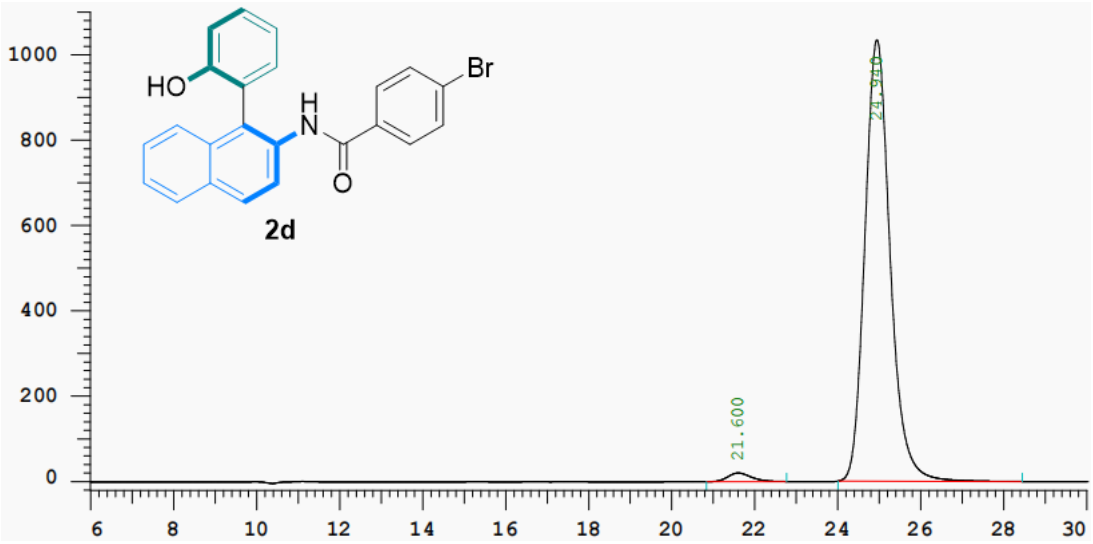
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	21.260	27780700	741451	49.719	52.596
2	25.660	28094760	668244	50.281	47.404
Total		55875460	1409695	100.000	100.000



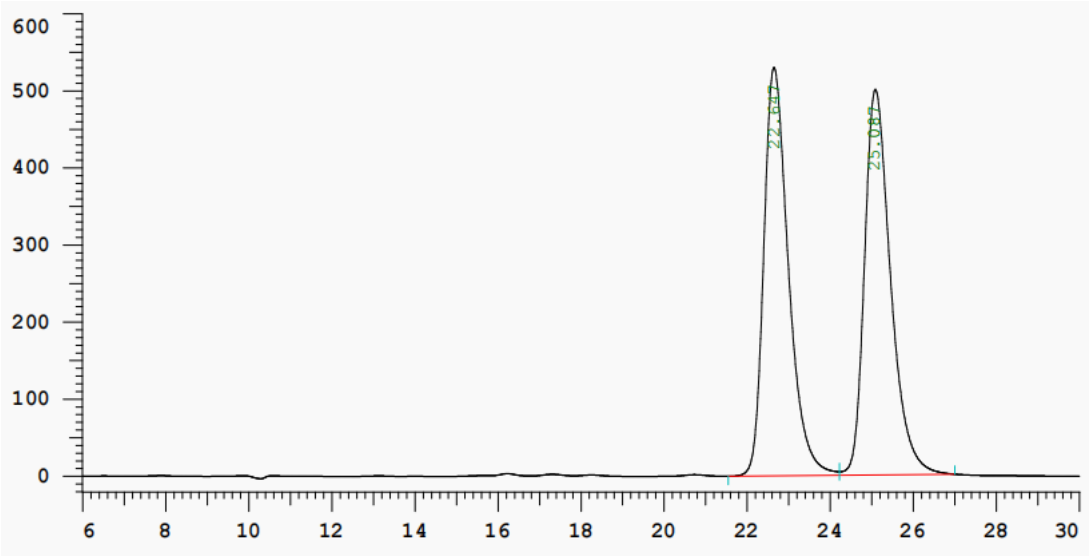
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	22.467	423384	11730	1.275	1.502
2	26.740	32795642	768765	98.725	98.498
Total		33219026	780495	100.000	100.000



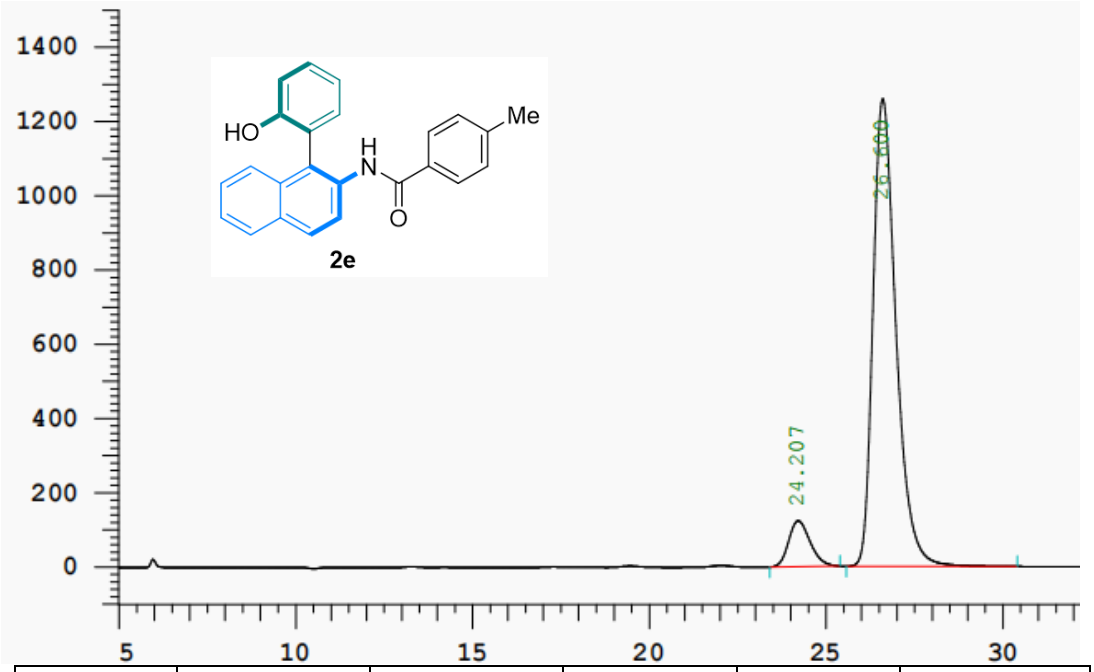
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	20.249	5013065	131958	49.628	52.765
2	23.702	5088189	118128	50.372	47.235
Total		10101254	250085	100.000	100.000



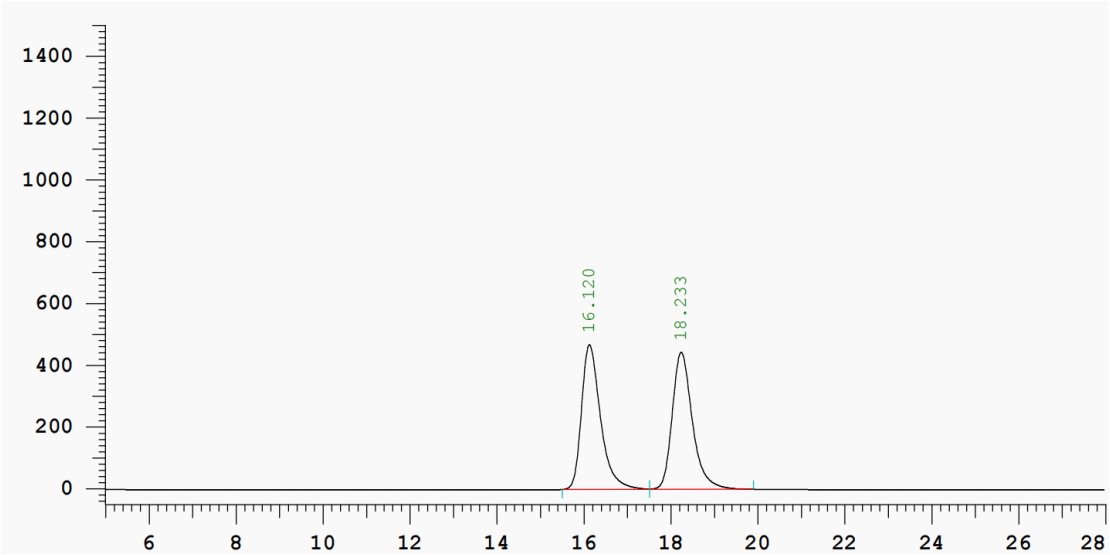
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	21.600	790488	20179	1.778	1.914
2	24.940	43660712	1033816	98.222	98.086
Total		44451200	1053995	100.000	100.000



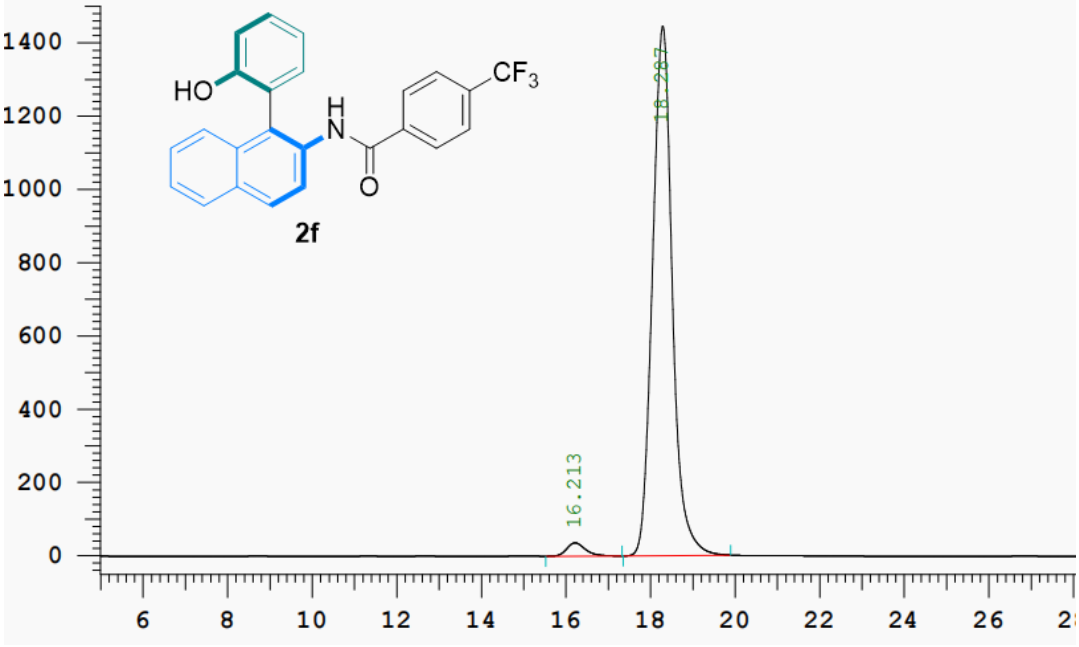
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	22.647	21830471	529484	50.056	51.437
2	25.087	21781319	499880	49.944	48.563
Total		43611790	1029364	100.000	100.000



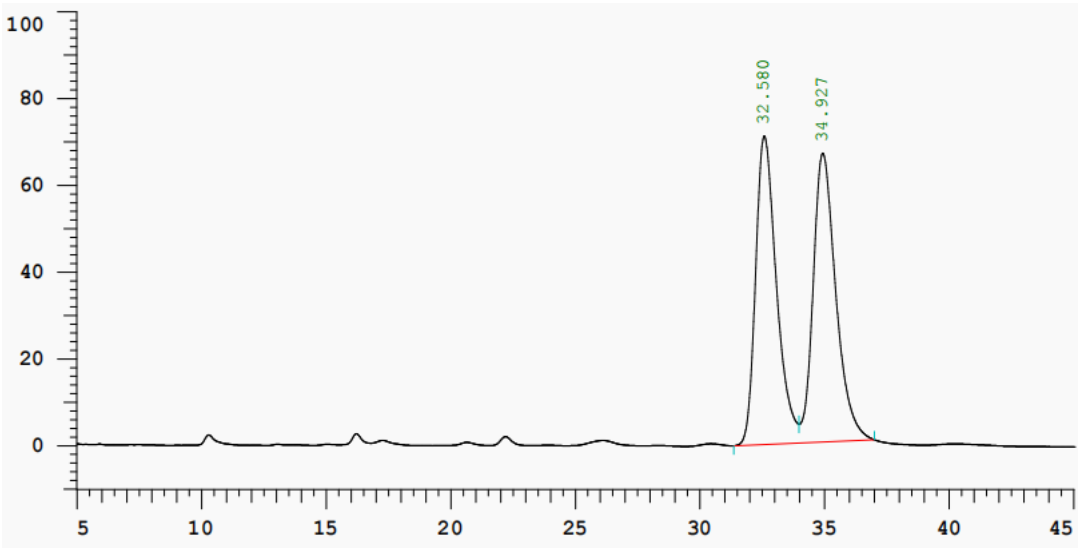
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	24.207	5197136	123500	8.430	8.936
2	26.600	56456181	1258523	91.570	91.064
Total		61653317	1382023	100.000	100.000



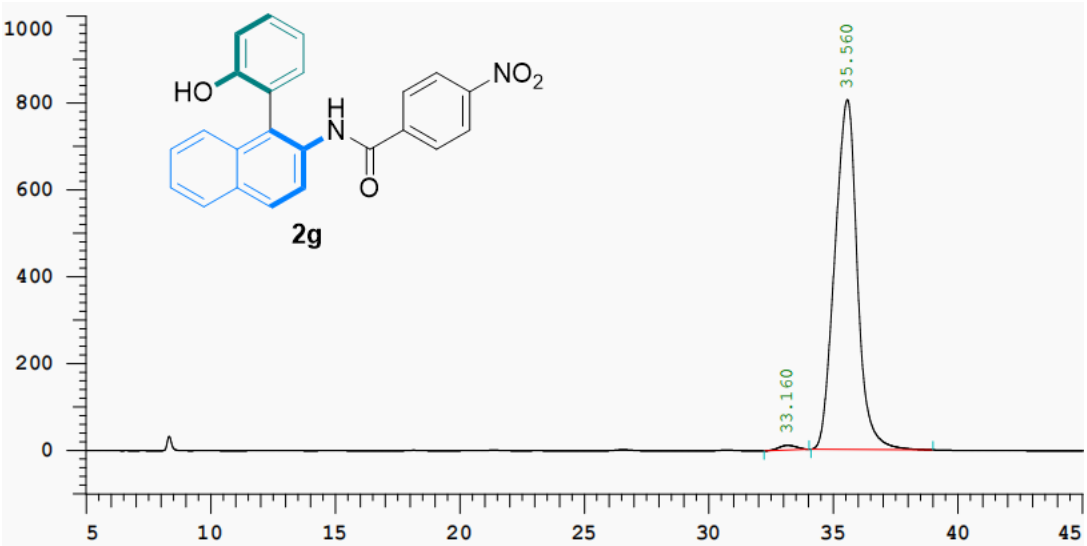
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	16.120	14281020	468032	49.944	51.342
2	18.233	14313326	443564	50.056	48.658
Total		28594346	911596	100.000	100.000



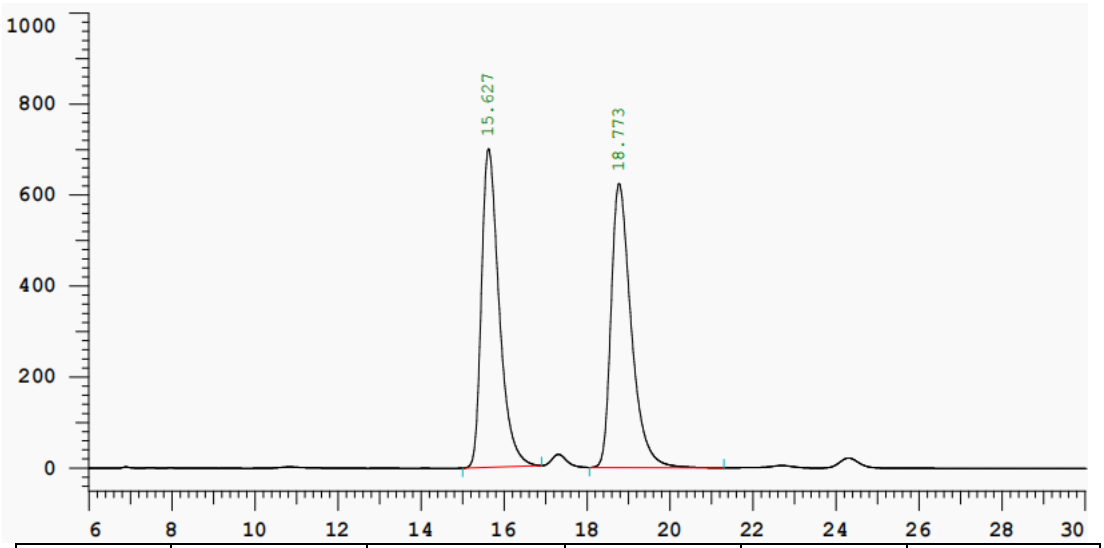
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	16.213	1115979	36336	2.335	2.454
2	18.287	46684682	1444194	97.665	97.546
Total		47800661	1480530	100.000	100.000



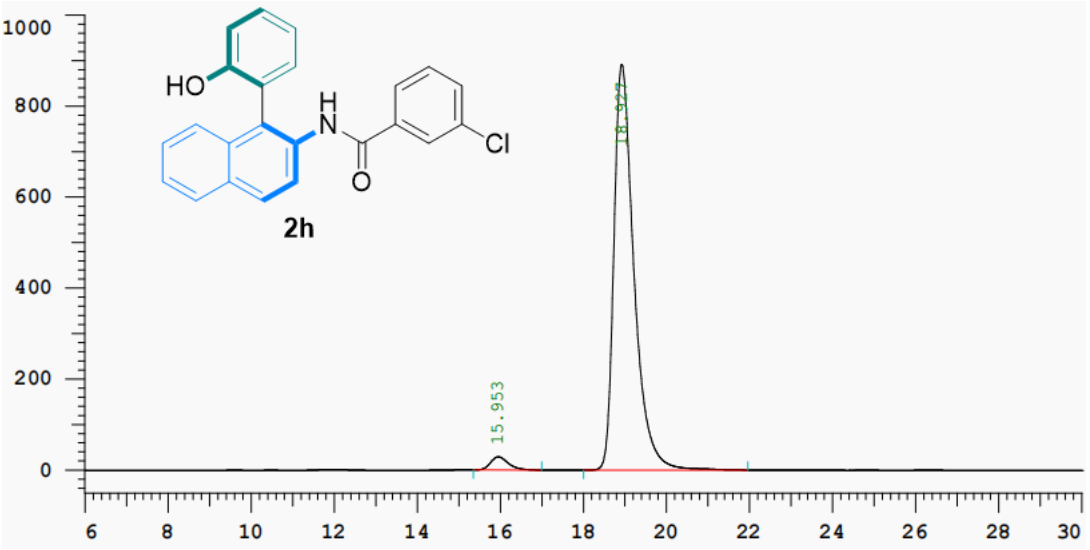
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	32.580	4107591	71029	49.431	51.645
2	34.927	4202085	66502	50.569	48.355
Total		8309676	137531	100.000	100.000



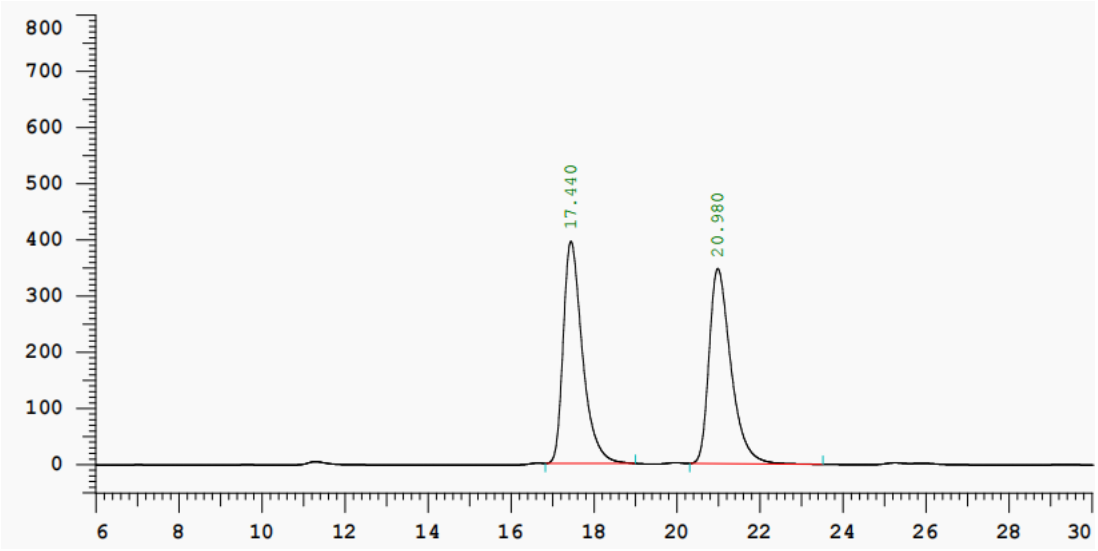
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	33.160	537638	10912	1.054	1.338
2	35.560	50456422	804848	98.946	98.662
Total		50994060	815760	100.000	100.00



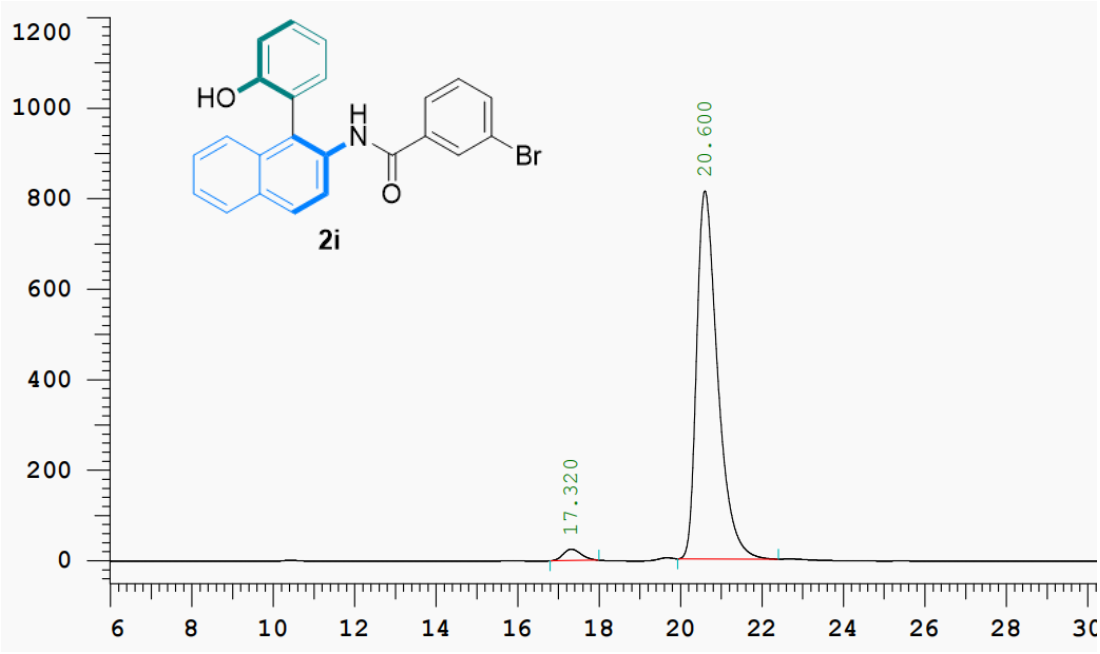
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	15.627	20694581	699614	49.629	52.868
2	18.773	21003568	623684	50.371	47.132
Total		41698149	1323298	100.000	100.000



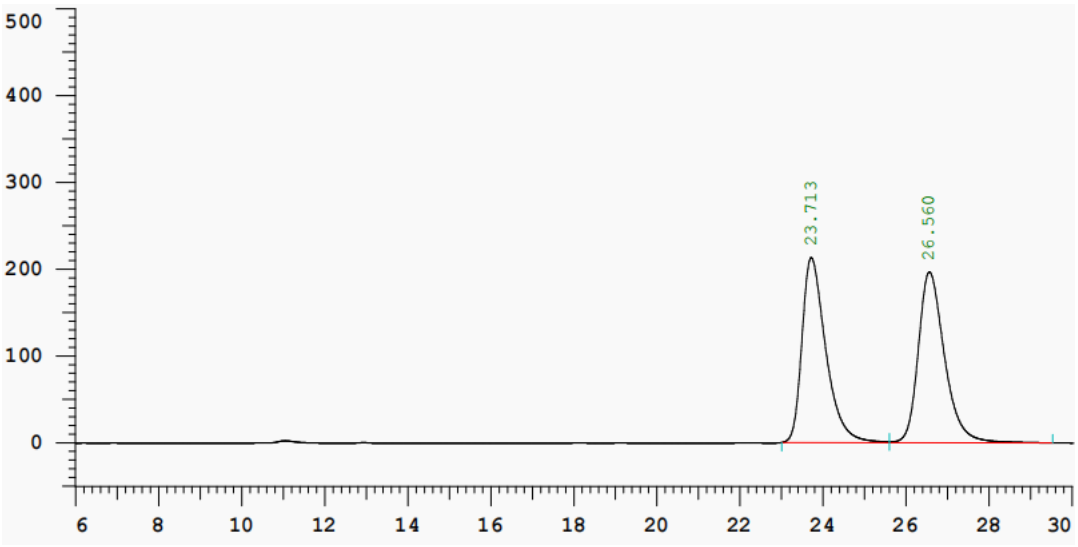
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	15.953	873812	28971	2.846	3.148
2	18.927	29824442	891210	97.154	96.852
Total		30698254	920181	100.000	100.000



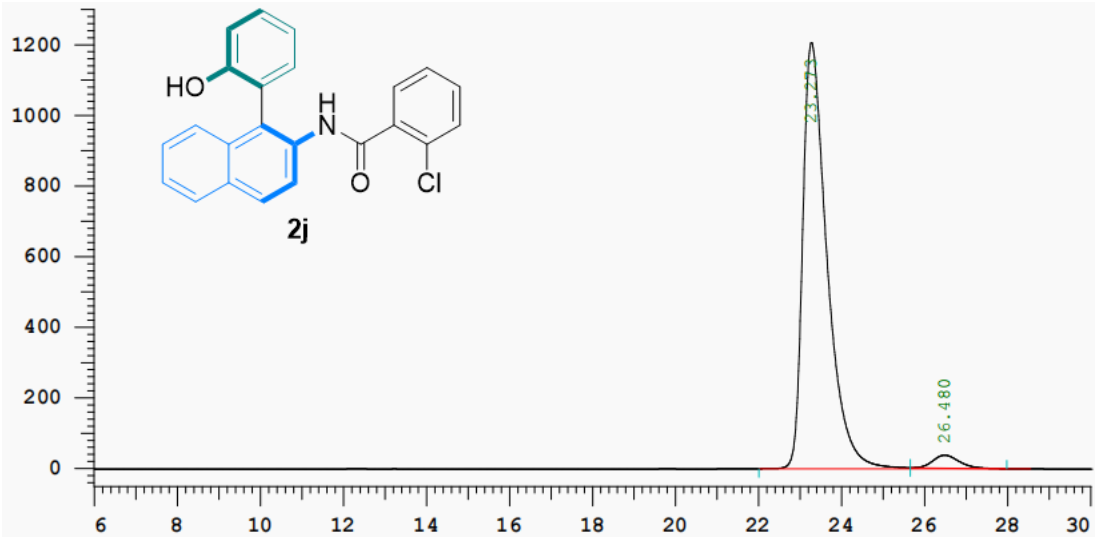
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	17.440	12697534	394779	50.017	53.222
2	20.980	12689077	346977	49.983	46.778
Total		25386611	741756	100.000	100.000



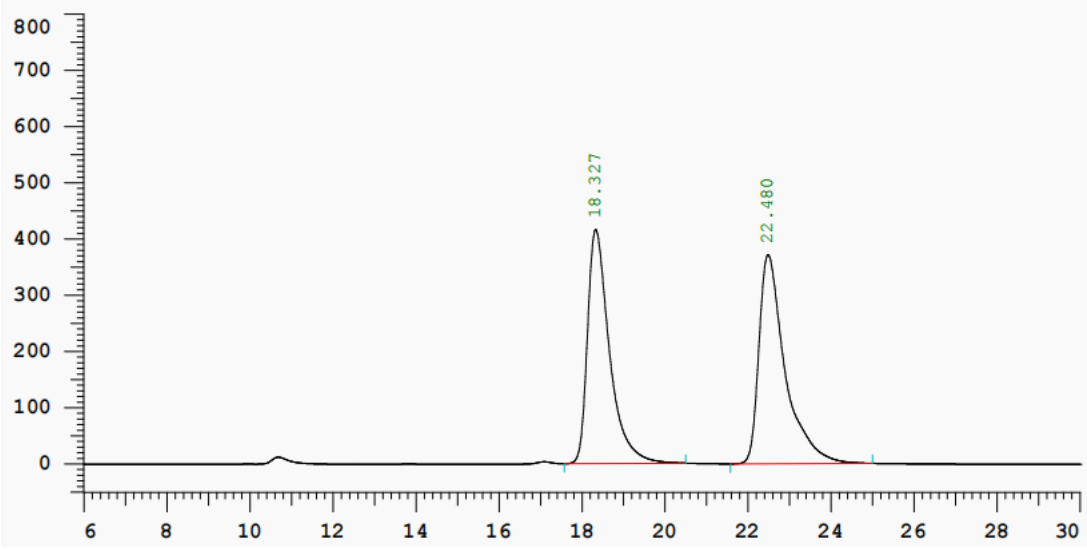
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	17.320	769853	25210	2.471	3.008
2	20.600	29054737	812820	97.529	96.992
Total		29824590	838030	100.000	100.000



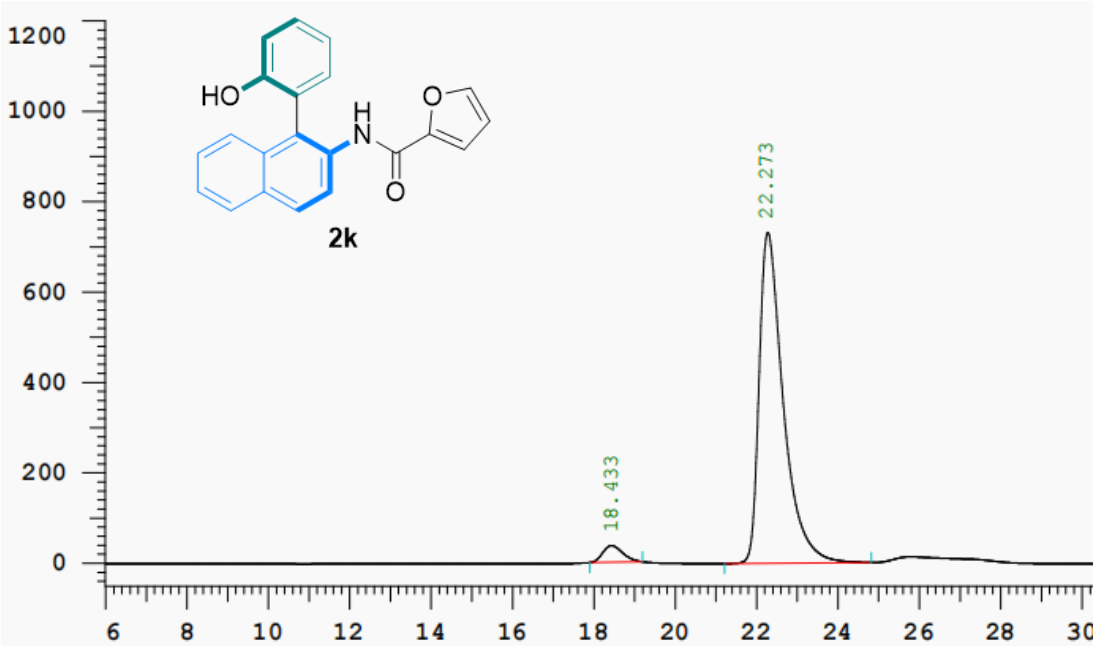
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	23.713	8526928	212990	49.628	51.978
2	26.560	8654689	196777	50.372	48.022
Total		17181617	409767	100.000	100.000



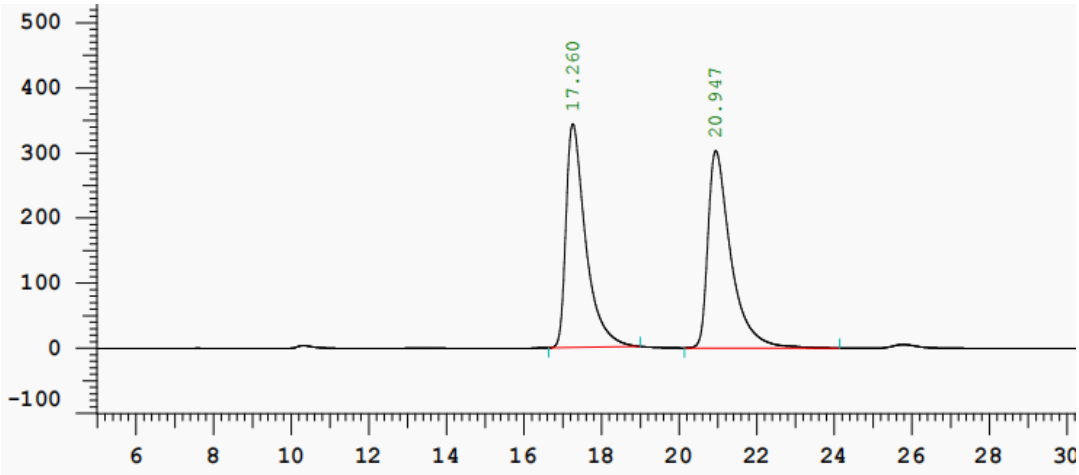
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	23.273	49154995	1206029	96.845	97.050
2	26.480	1601158	36650	3.155	2.950
Total		50756153	1242679	100.000	100.000



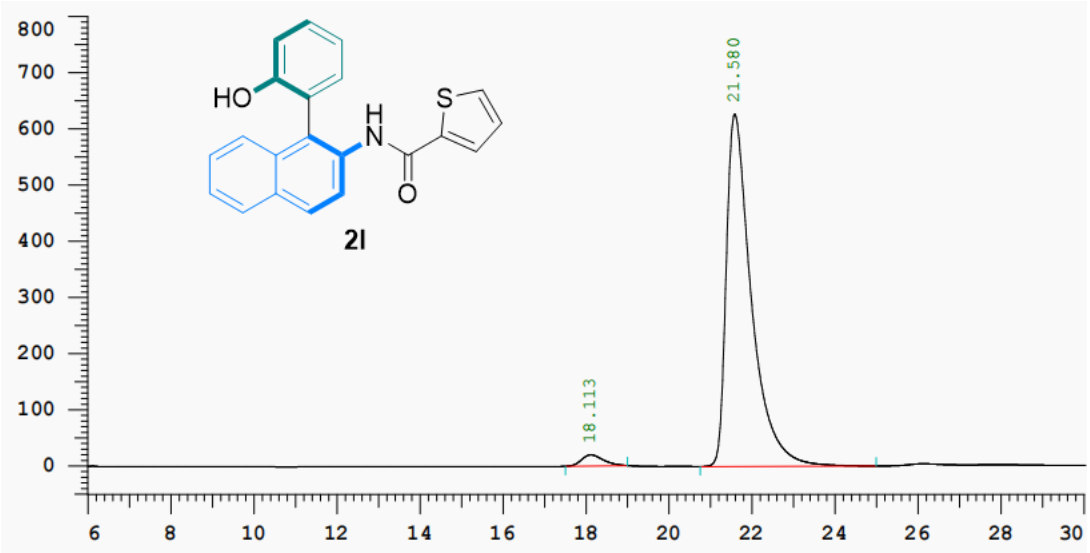
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	18.327	15288670	415792	48.480	52.812
2	22.480	16247479	371504	51.520	47.188
Total		31536149	787296	100.000	100.000



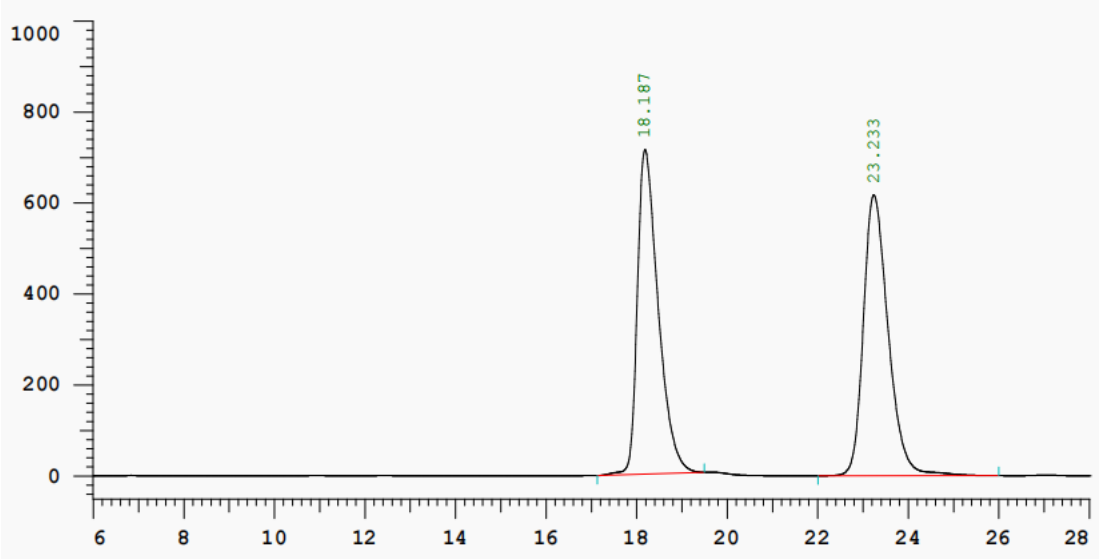
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	18.433	1253985	36954	4.010	5.052
2	22.273	30017377	731435	95.990	94.948
Total		31271362	768389	100.000	100.000



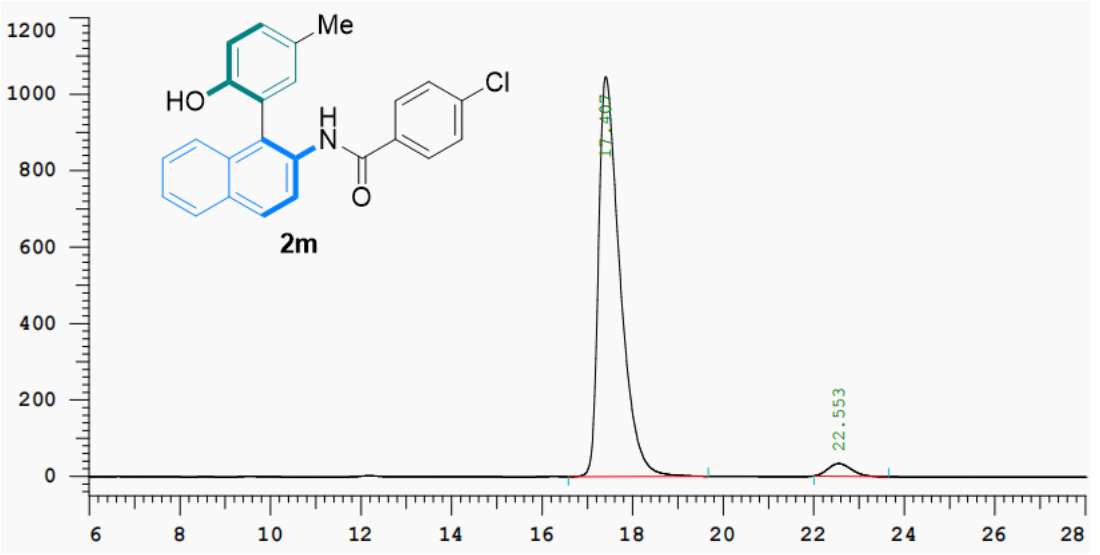
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	17.260	12089392	343635	49.385	53.155
2	20.947	12390425	302834	50.615	46.845
Total		50075777	646469	100.000	100.000



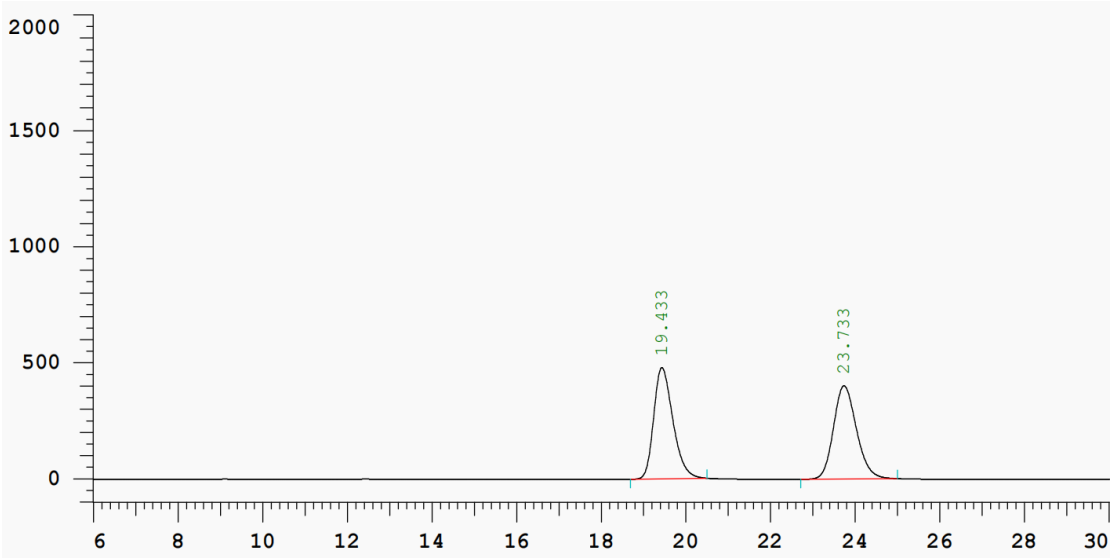
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	18.113	724051	19841	2.676	3.069
2	21.580	26328312	626484	97.324	96.931
Total		27052363	646325	100.000	100.000



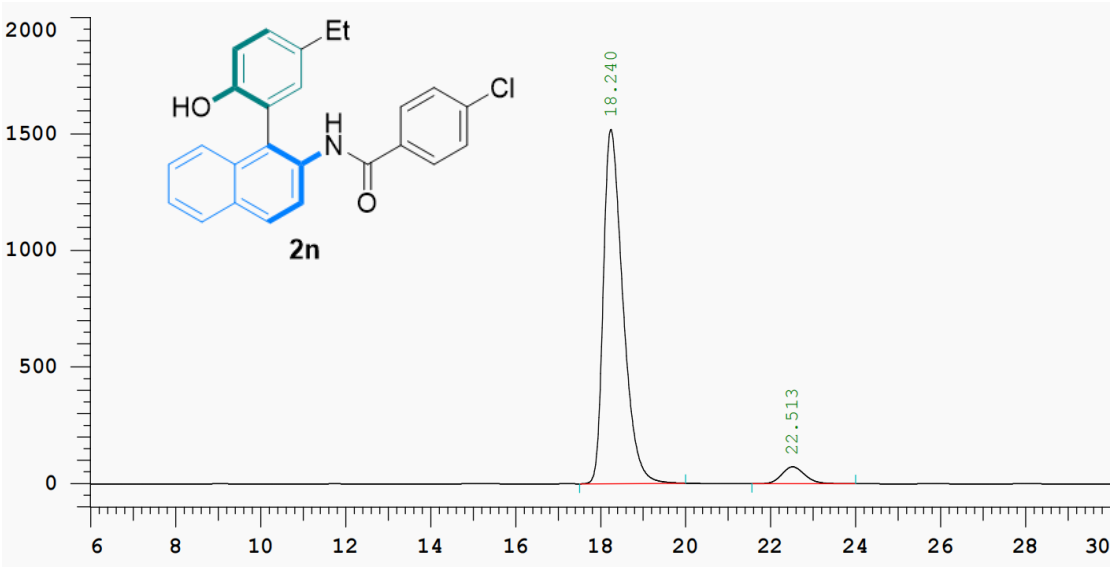
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	18.187	22752535	712578	49.190	53.585
2	23.233	23501585	617217	50.810	46.415
Total		46254120	1329795	100.000	100.000



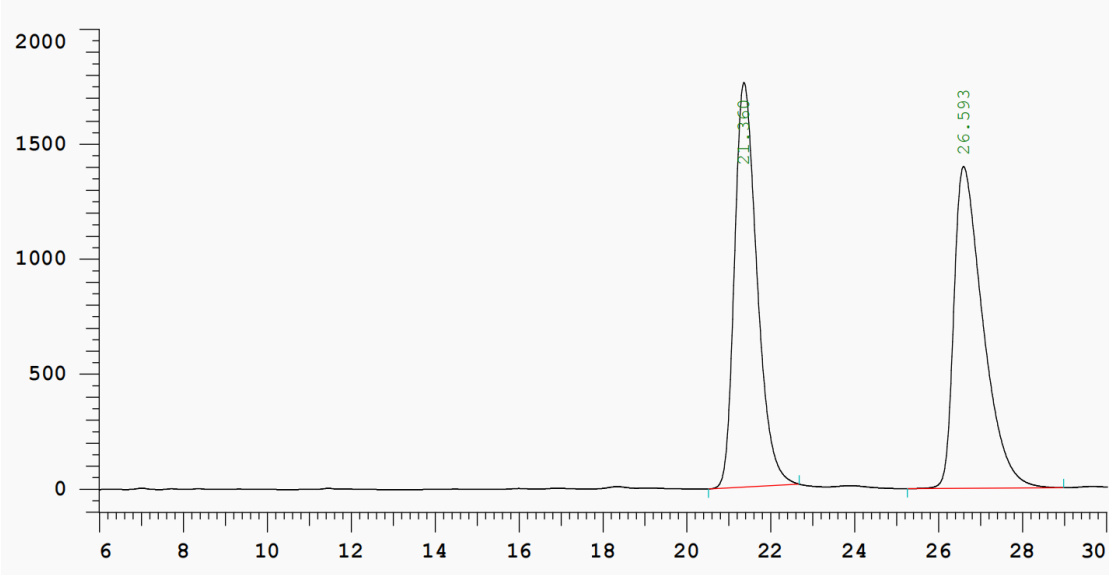
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	17.407	34357580	1045314	96.649	96.936
2	22.553	1191291	33040	3.351	3.064
Total		35548871	1078354	100.000	100.000



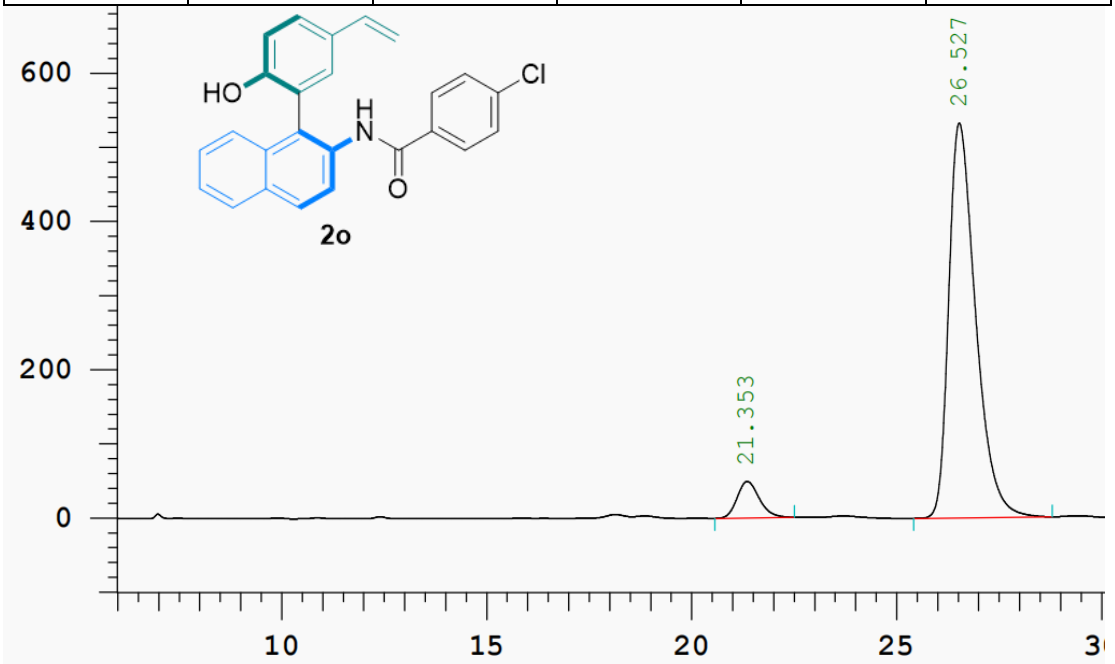
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	19.433	15114291	479369	49.930	54.396
2	23.733	15156624	401885	50.070	45.604
Total		30270915	881254	100.000	100.000



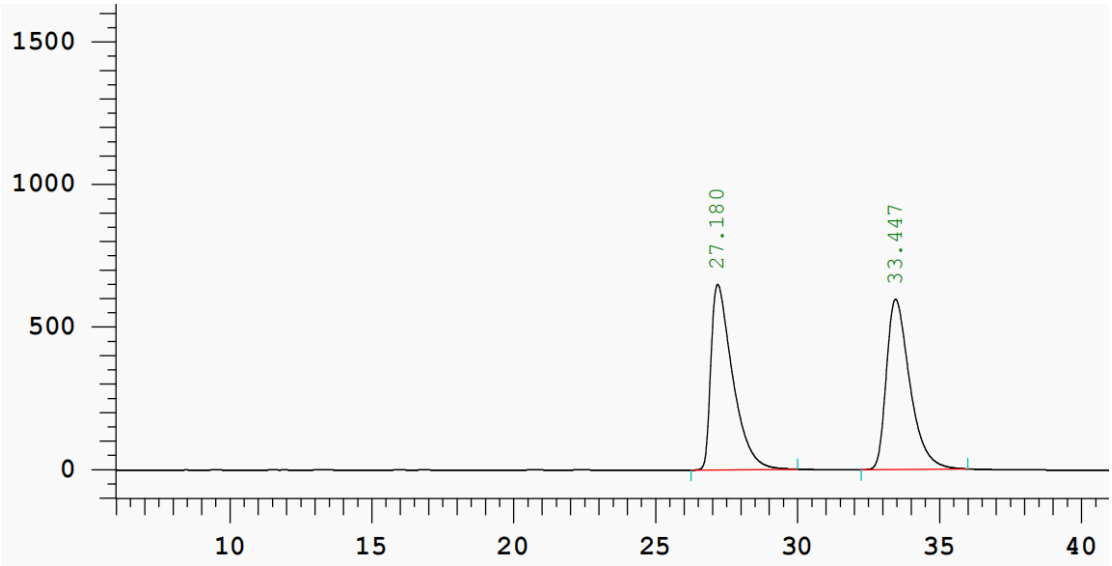
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	18.240	48449561	1519122	94.606	95.427
2	22.513	2762270	72800	5.394	4.573
Total		51211831	1591922	100.000	100.000



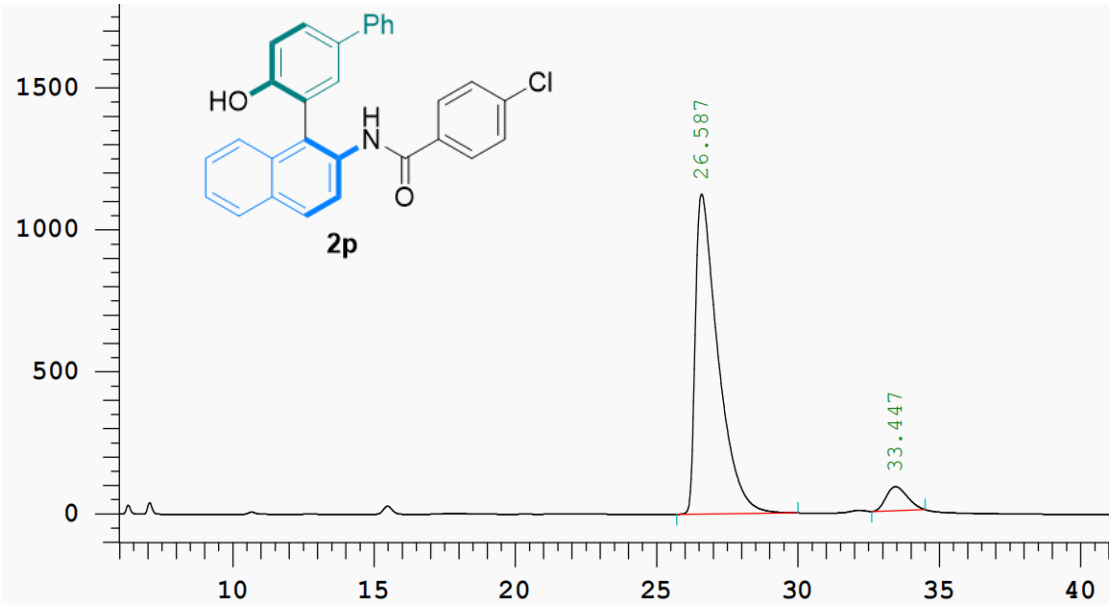
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	21.360	65428495	1758031	49.301	55.694
2	26.593	67282841	1398559	50.699	44.306
Total		132711336	3156590	100.000	100.000



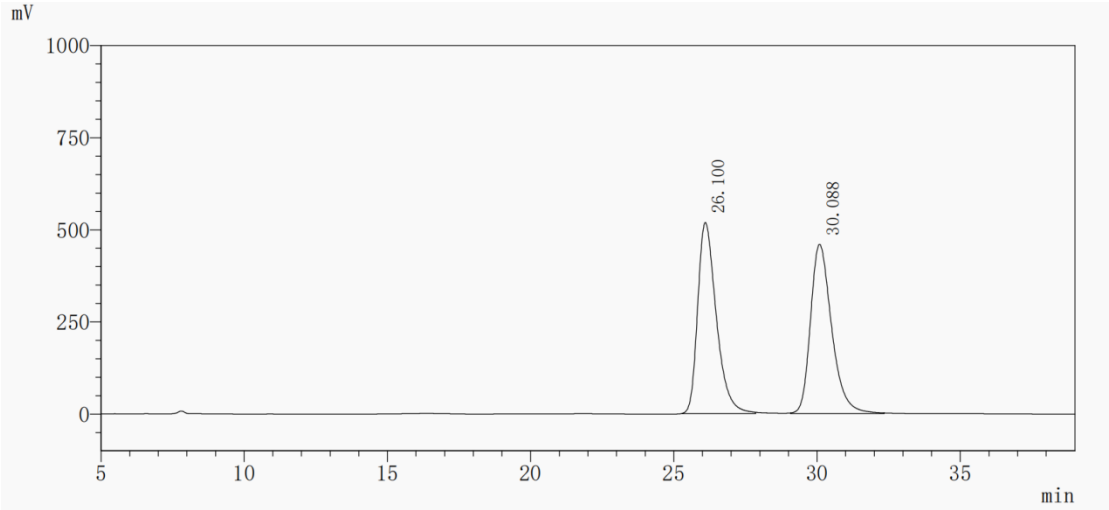
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	21.353	1837339	49202	7.072	8.465
2	26.527	24143490	532016	92.928	91.535
Total		25980829	581218	100.000	100.000



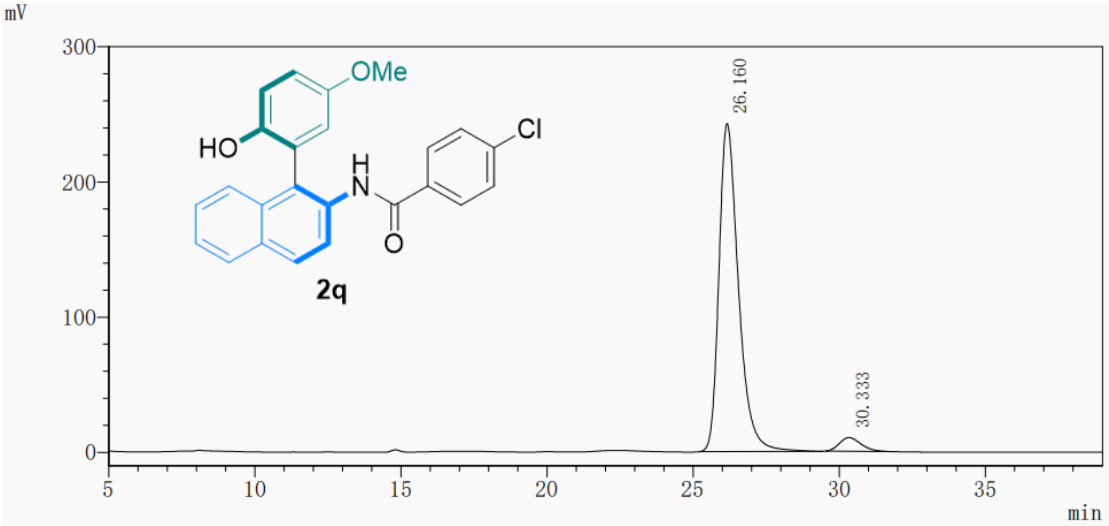
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	27.180	34341985	649538	50.171	52.135
2	33.447	34107845	596347	49.829	47.865
Total		68449830	1245885	100.000	100.000



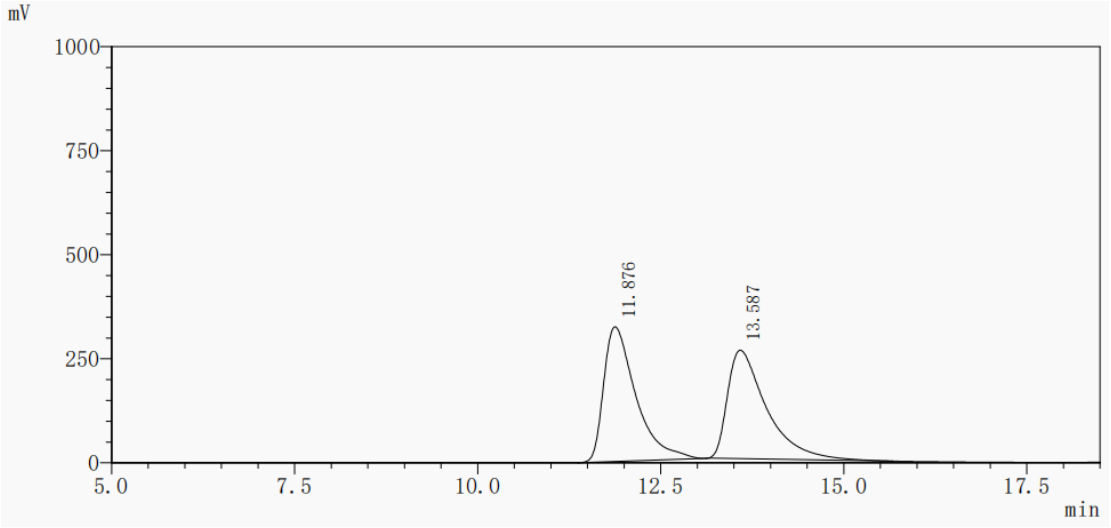
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	26.587	62347233	1125676	93.447	93.029
2	33.447	4371768	84350	6.553	6.971
Total		66719001	1210026	100.000	100.000



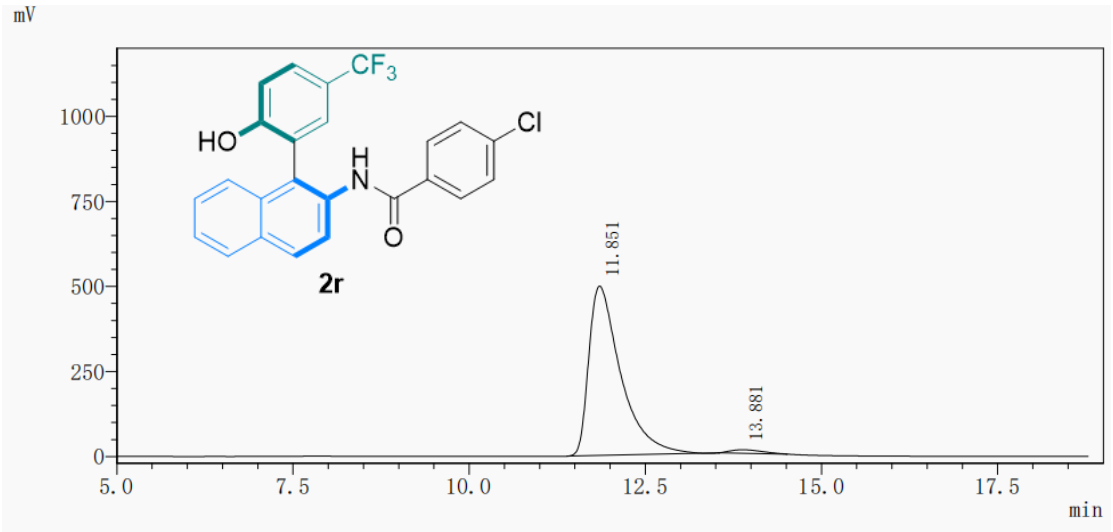
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	26.100	23528097	519203	49.790	53.029
2	30.088	23726774	459898	50.210	46.971
Total		47254871	979100	100.000	100.000



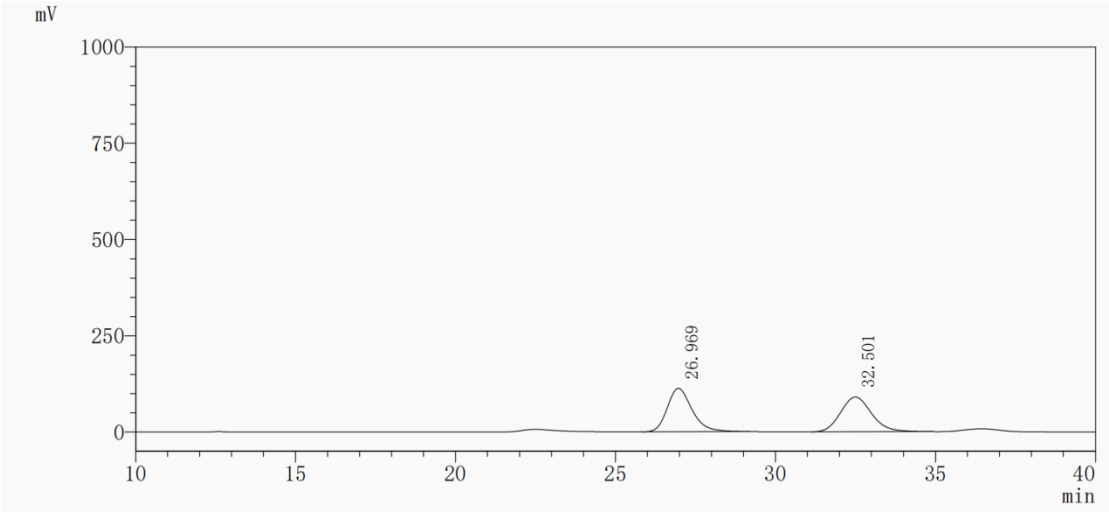
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	26.160	11246452	242733	95.571	95.995
2	30.333	521173	10127	4.429	4.005
Total		11767625	252860	100.000	100.000



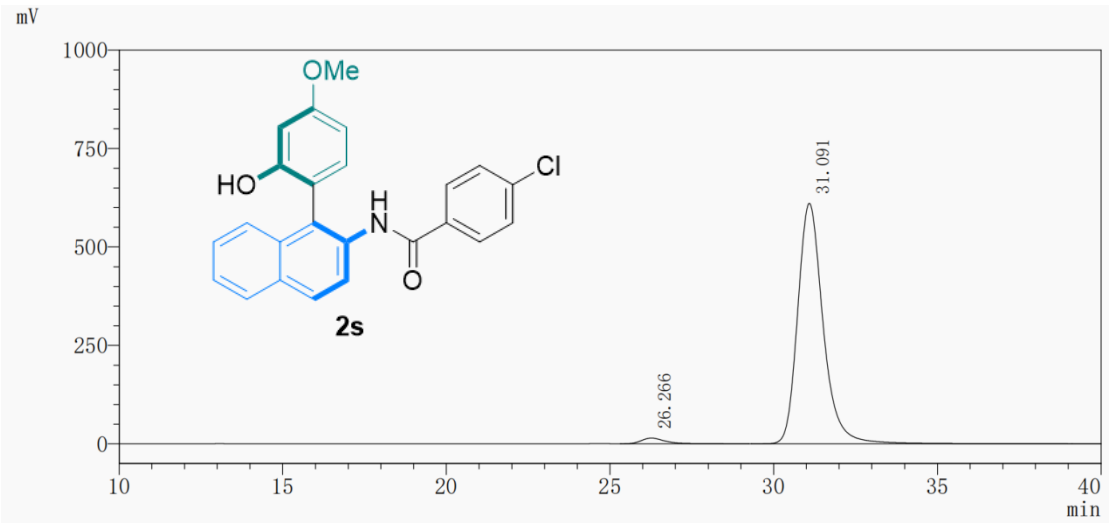
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	11.876	9910933	323520	50.634	55.382
2	13.587	9662698	260643	49.366	44.618
Total		19573632	584163	100.000	100.000



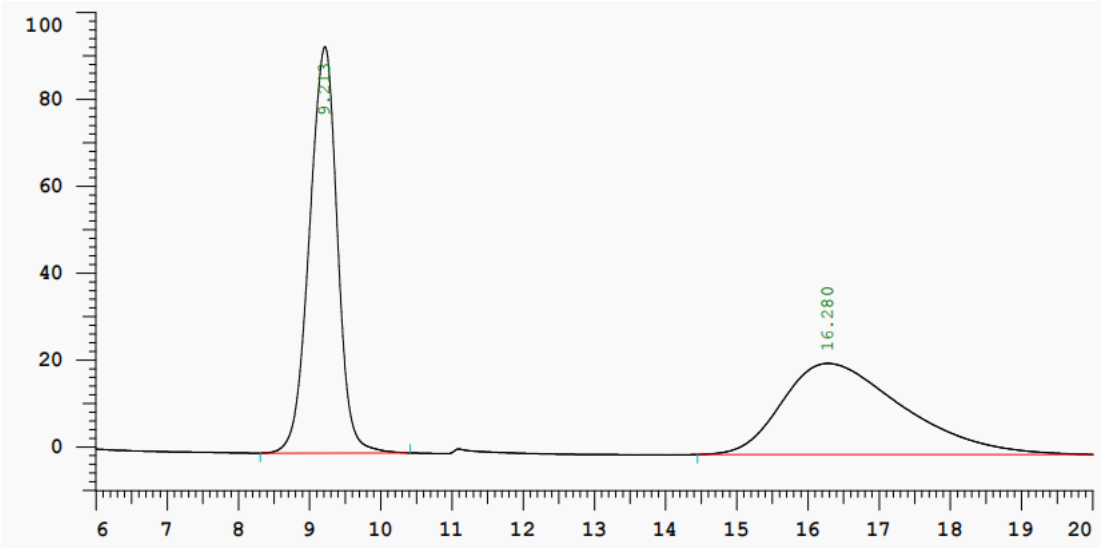
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	11.851	15724735	497987	97.960	97.965
2	13.881	327488	10346	2.040	2.035
Total		16052223	508333	100.000	100.000



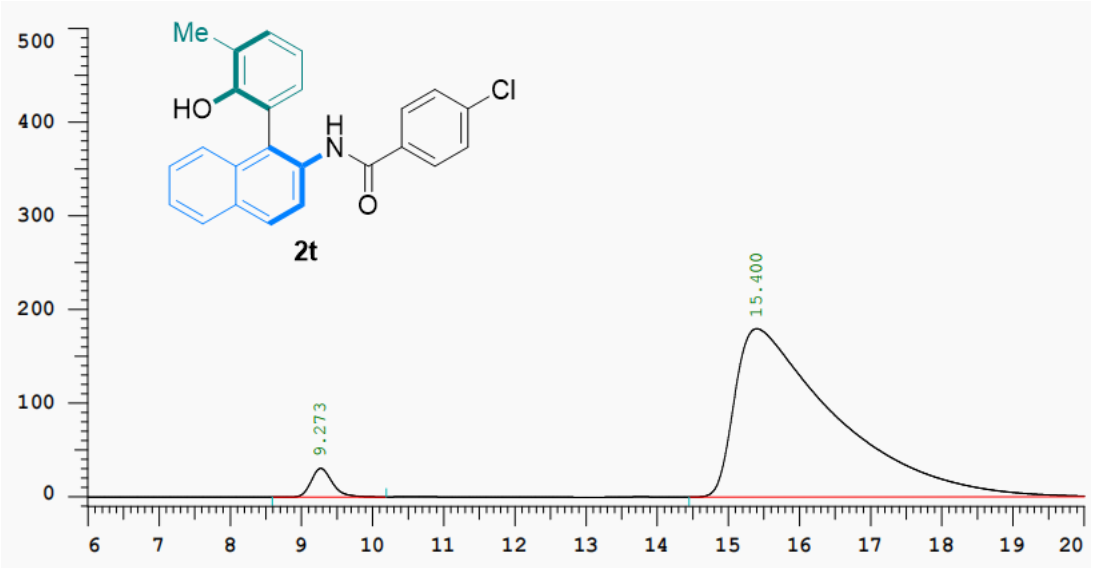
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	26.969	6053015	112695	50.025	55.593
2	32.501	6047007	90020	49.975	44.407
Total		12100022	202715	100.000	100.000



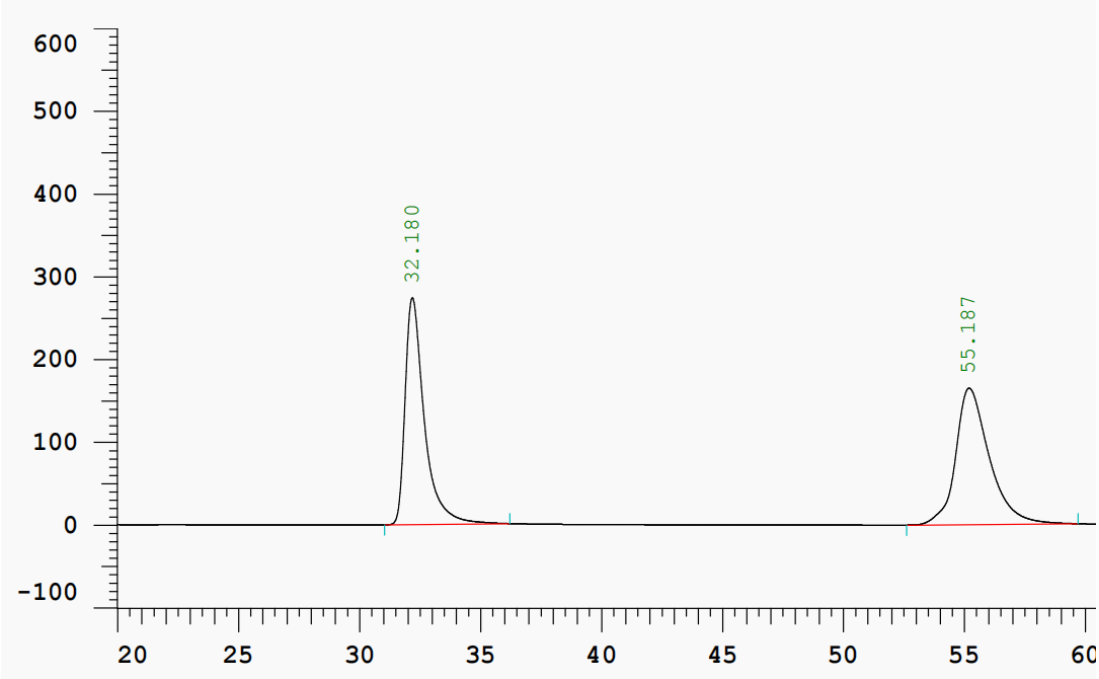
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	26.266	730431	14391	2.156	2.303
2	31.091	33153261	610497	97.844	97.697
Total		33883691	624887	100.000	100.000



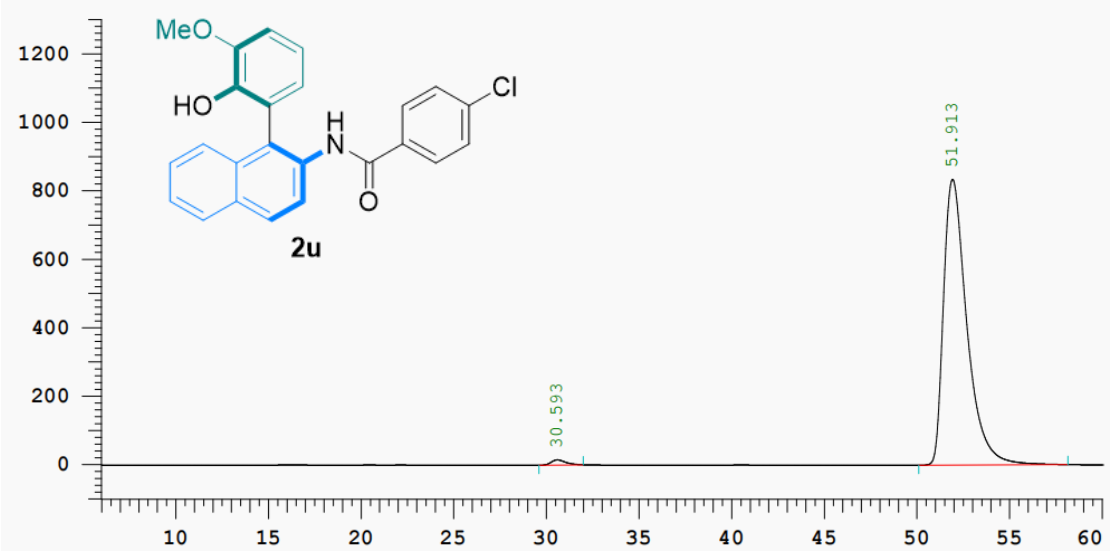
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	9.213	2552141	93458	50.719	81.683
2	16.280	2479825	20957	49.281	18.317
Total		5031966	114415	100.000	100.000



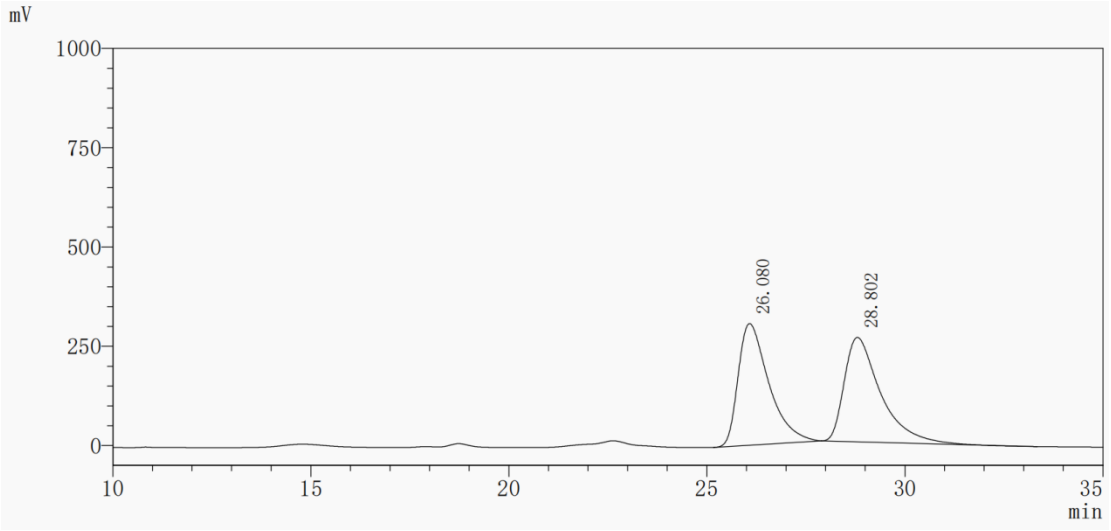
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	9.273	635181	30747	3.466	14.610
2	15.400	17688270	179699	96.534	85.390
Total		18323451	210446	100.000	100.000



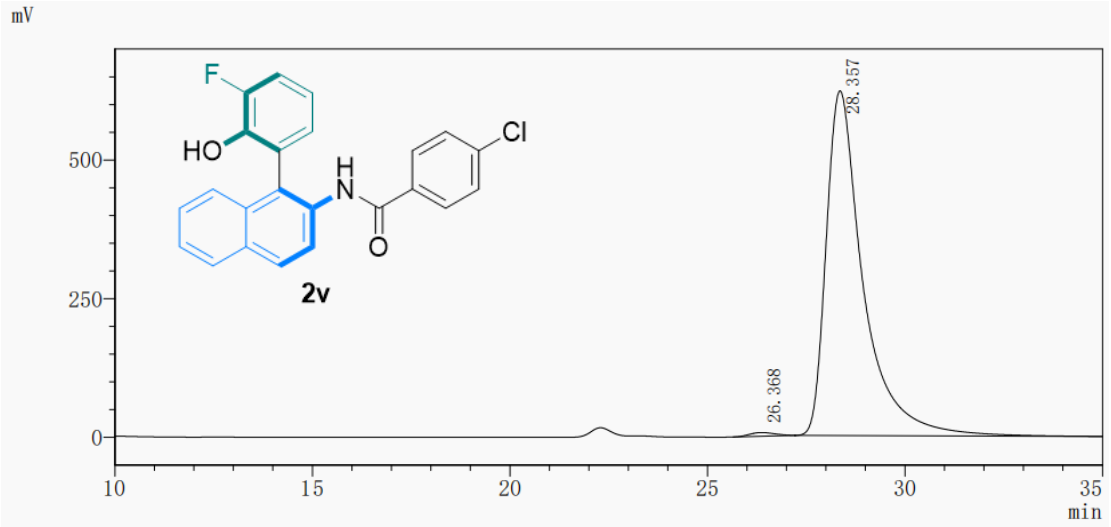
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	32.180	15020628	273750	48.578	62.419
2	55.187	15900162	164818	51.422	37.581
Total		30920790	438568	100.000	100.000



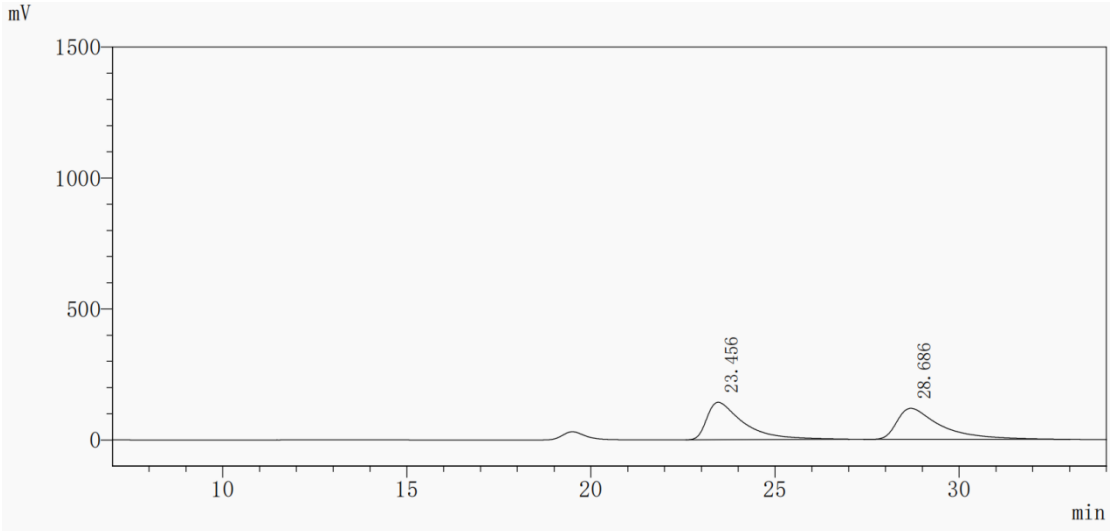
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	30.593	807374	15099	1.100	1.778
2	51.593	72598630	833846	98.900	98.222
Total		73406004	848945	100.000	100.000



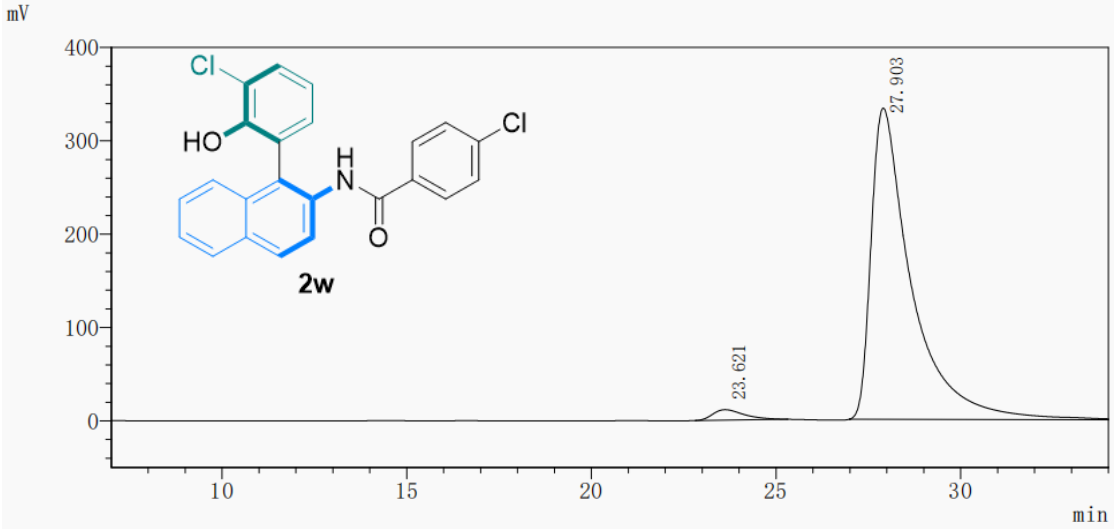
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	26.080	16491719	306278	49.628	53.812
2	28.802	16739195	262886	50.372	46.188
Total		33230914	569164	100.000	100.000



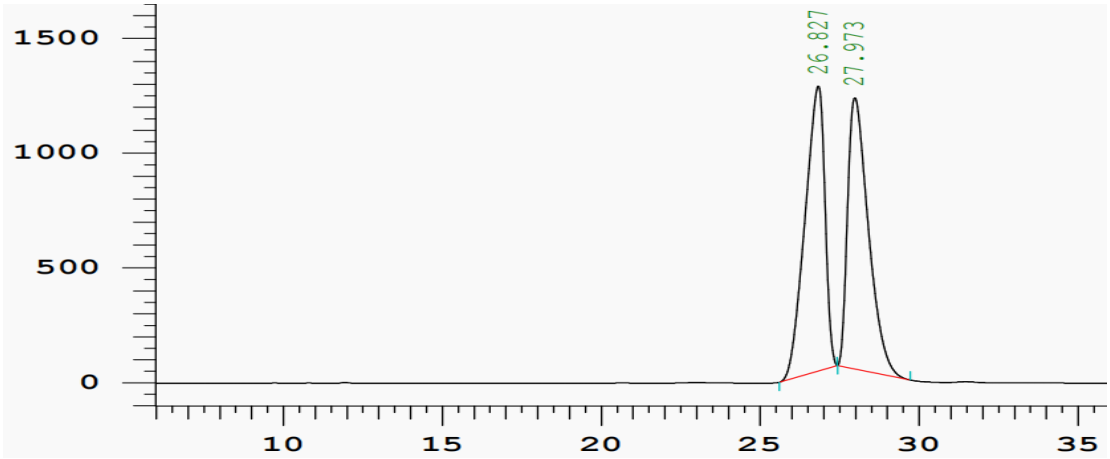
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	26.368	298092	6721	0.729	1.070
2	28.357	40574314	621444	99.271	98.930
Total		40872406	628166	100.000	100.000



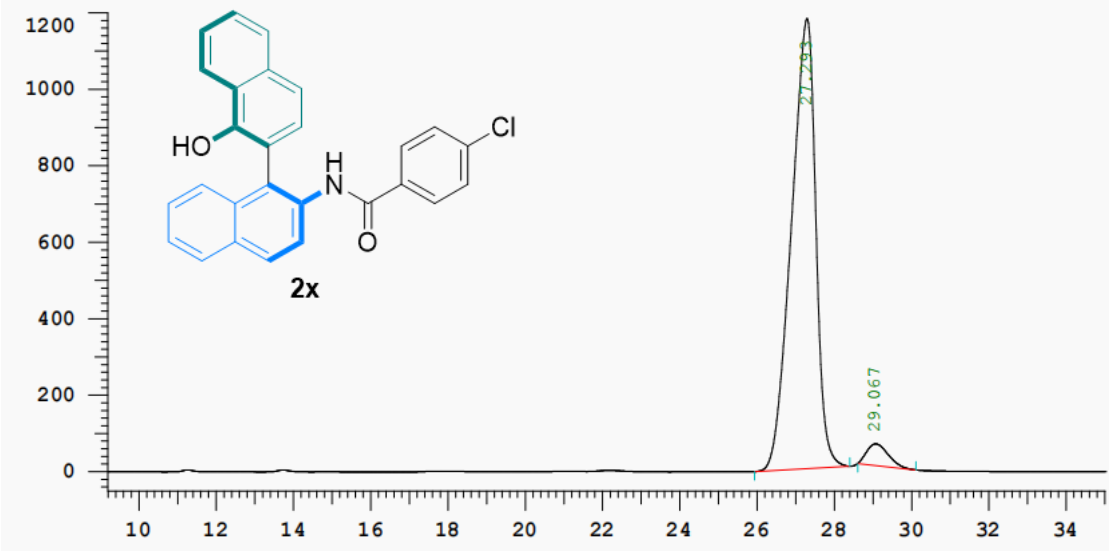
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	23.456	9799308	142811	50.198	54.706
2	28.686	9722037	118242	49.802	45.294
Total		19521345	261053	100.000	100.000



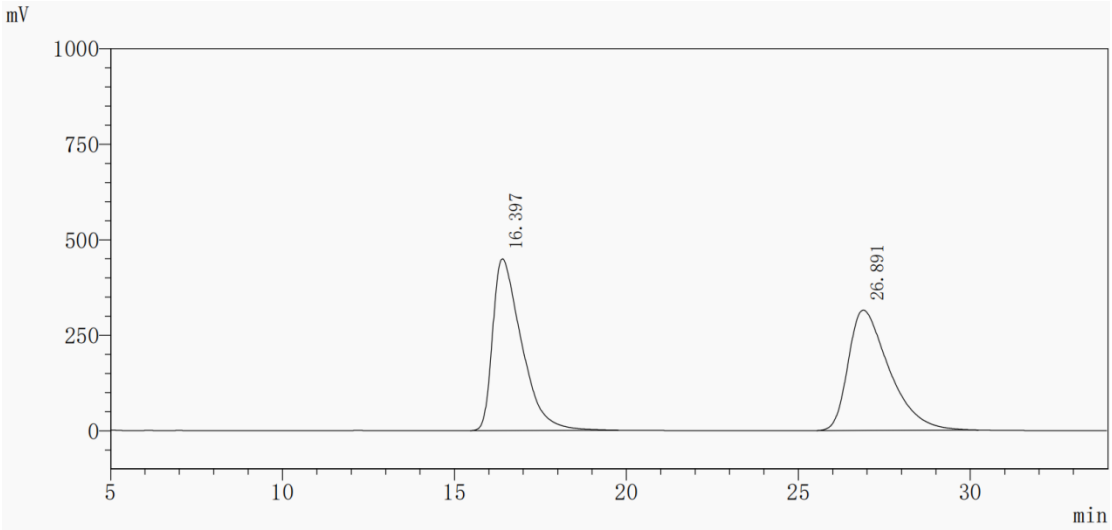
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	23.621	662488	11214	2.533	3.253
2	27.903	25495647	333500	97.467	96.747
Total		26158136	344714	100.000	100.000



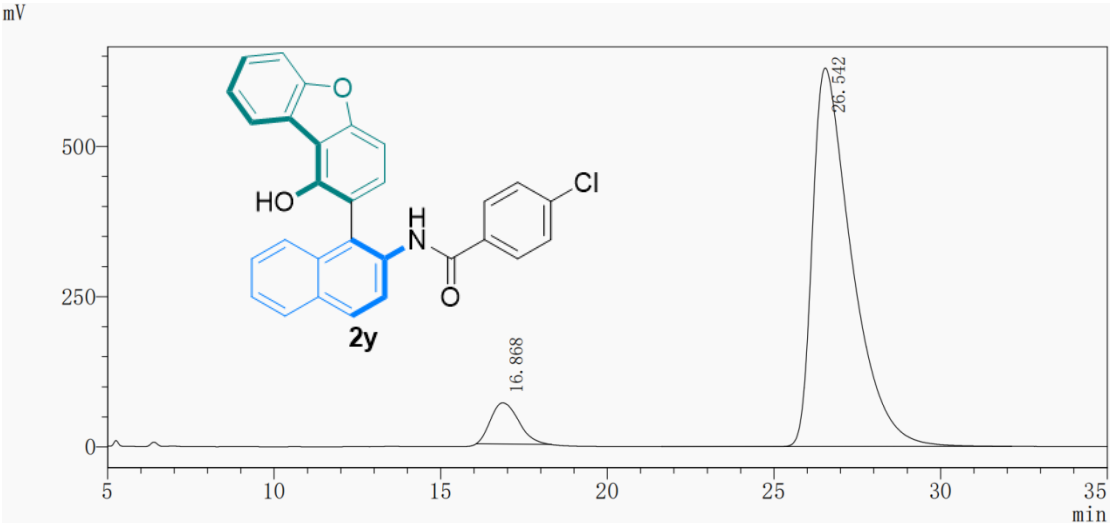
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	26.827	53048064	1239727	50.046	51.238
2	27.973	52950676	1179796	49.954	48.762
Total		105998740	2419523	100.000	100.000



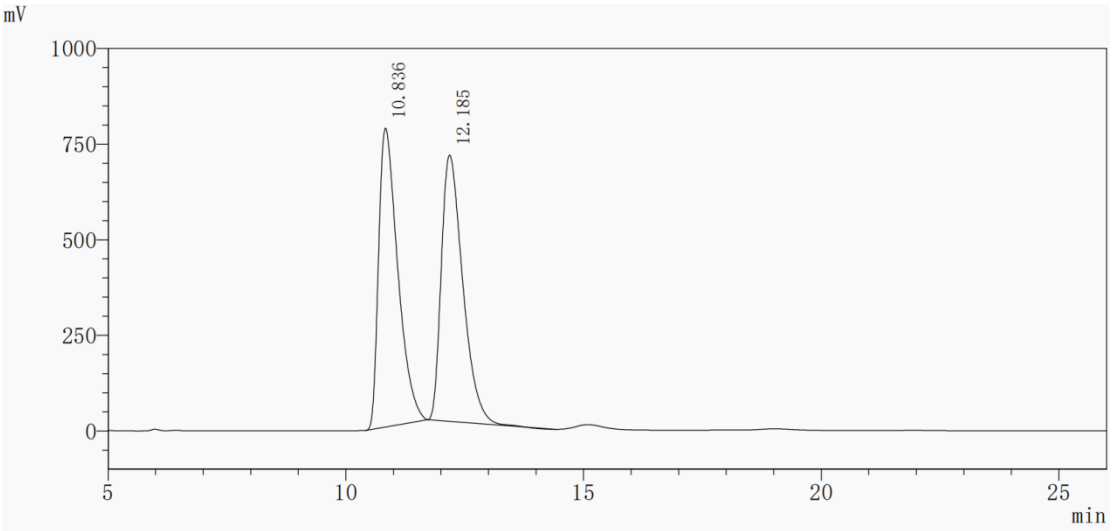
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	27.293	51399147	1175905	95.899	95.405
2	29.067	2197879	56630	4.101	4.595
Total		53597026	1232535	100.000	100.000



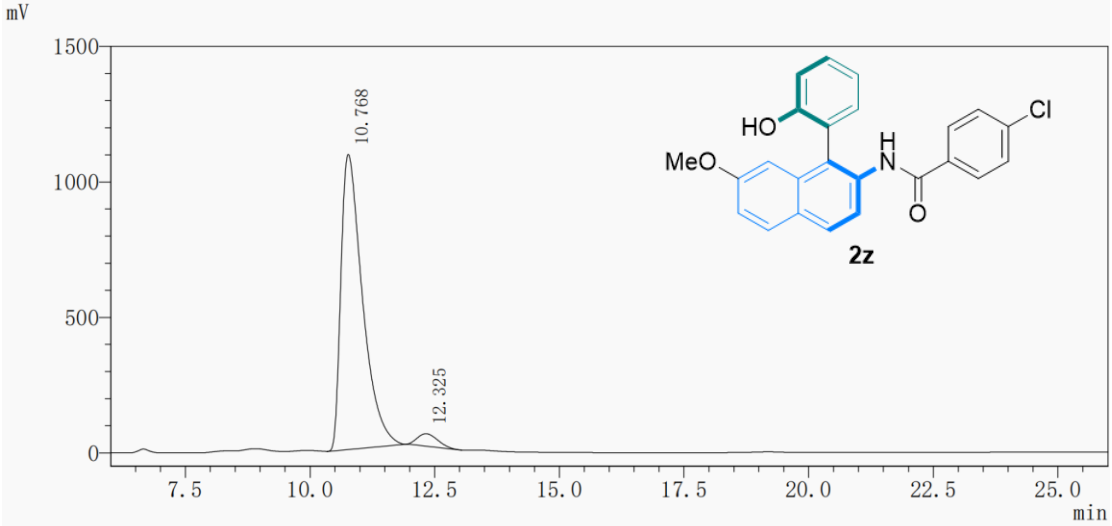
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	16.397	26242106	449287	50.203	58.788
2	26.891	26029898	314962	49.797	41.212
Total		52272004	764248	100.000	100.000



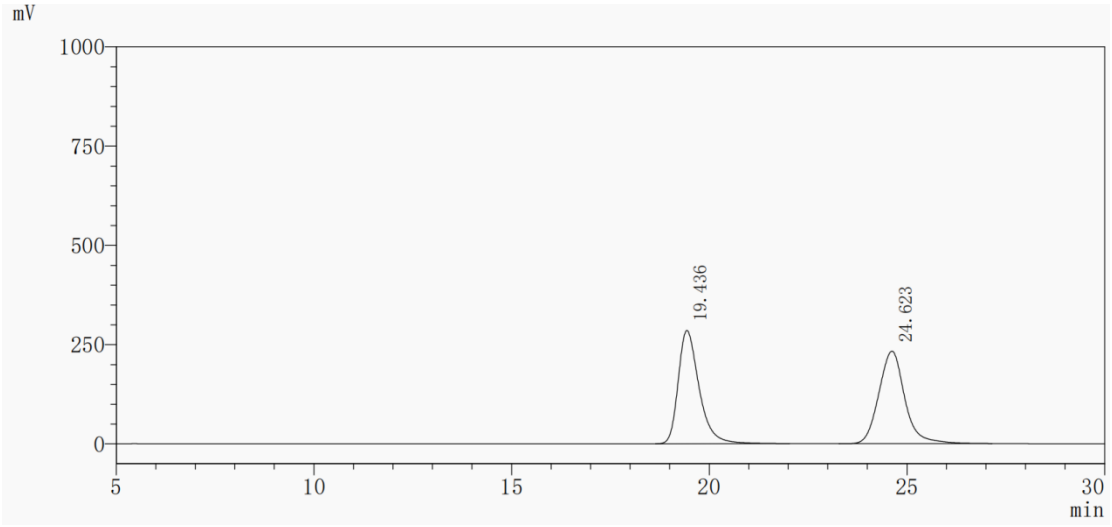
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	16.868	3996950	68610	7.194	9.827
2	26.542	51562499	629570	92.806	90.173
Total		55559449	698181	100.000	100.000



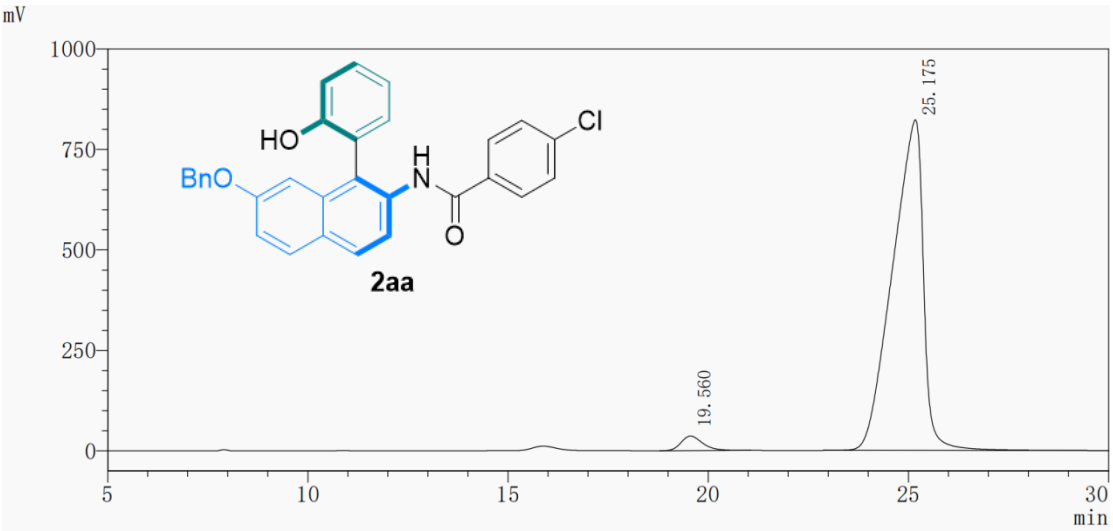
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	10.836	21867318	781224	50.052	52.882
2	12.185	21821687	696072	49.948	47.118
Total		43689004	1477296	100.000	100.000



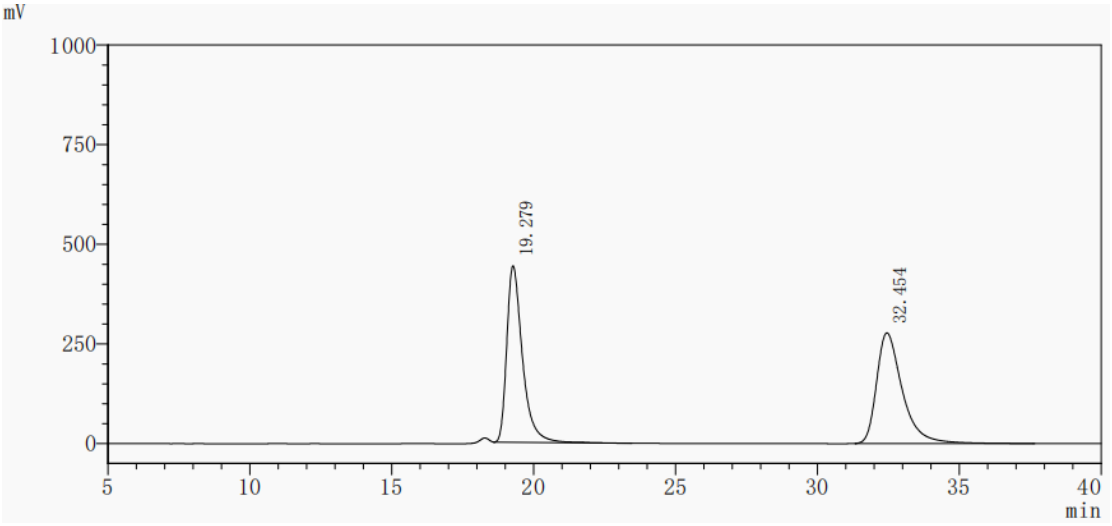
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	10.768	32822001	1089745	96.200	95.986
2	12.325	1296599	45577	3.800	4.014
Total		34118600	1135323	100.000	100.000



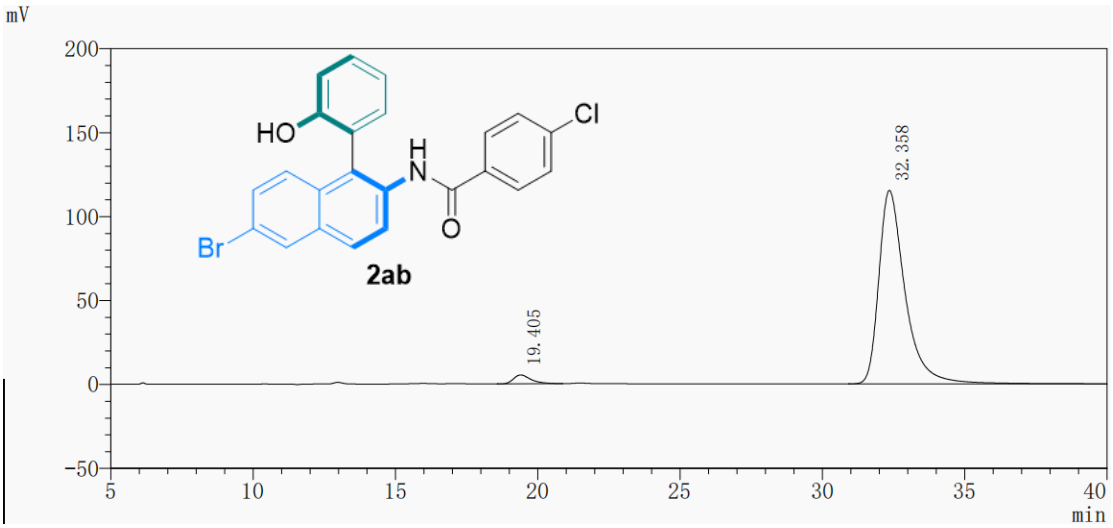
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	19.436	10531239	285393	49.759	55.046
2	24.623	10633273	233068	50.241	44.954
Total		21164512	518461	100.000	100.000



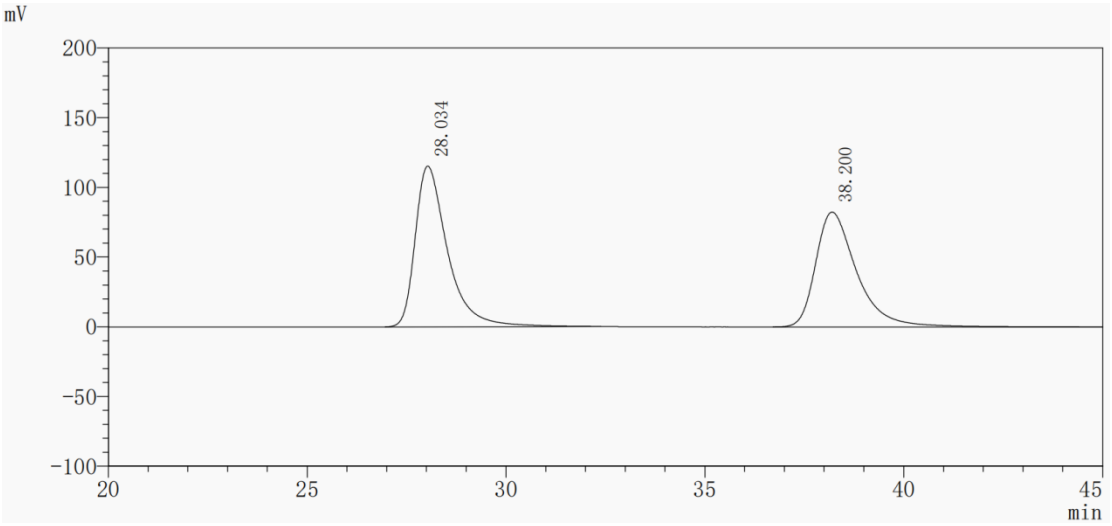
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	19.560	1371065	36280	3.006	4.223
2	25.175	44246060	822829	96.994	95.777
Total		45617126	859110	100.000	100.000



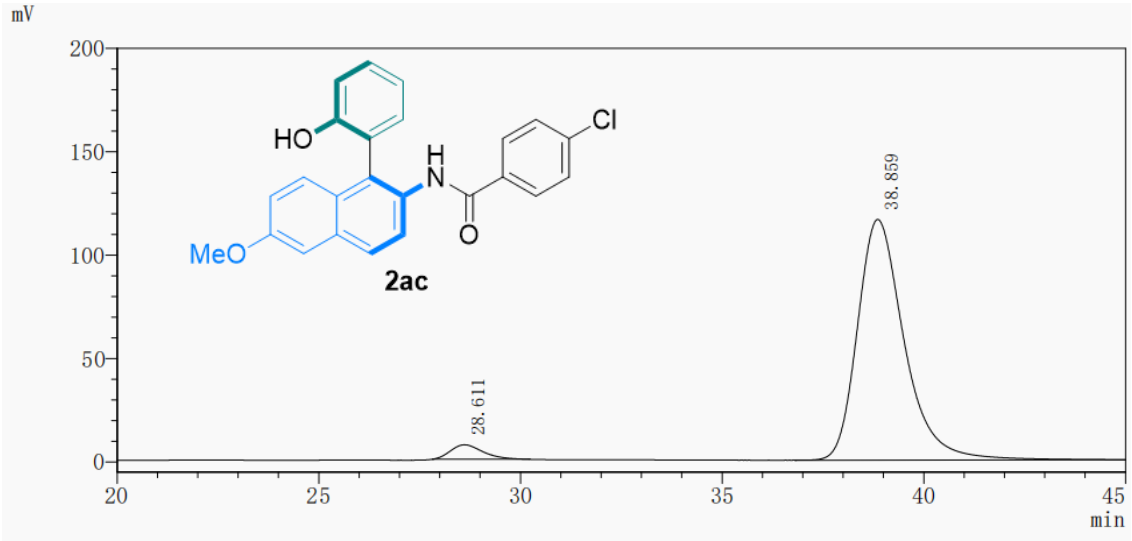
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	19.279	17056320	443124	49.381	61.489
2	32.454	17483839	277535	50.619	38.511
Total		34540159	720659	100.000	100.000



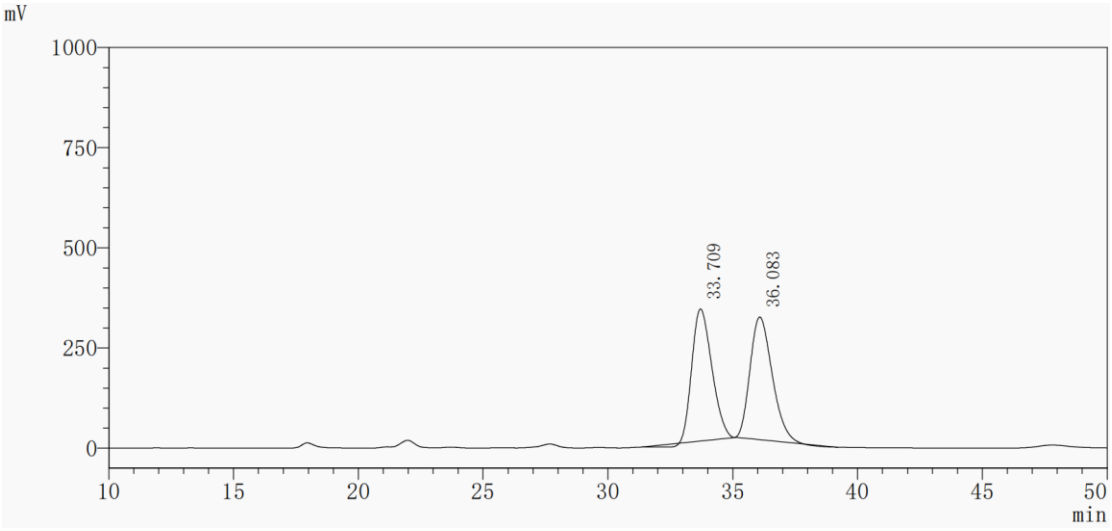
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	19.405	229700	5338	2.999	4.425
2	32.358	7428880	115297	97.001	95.575
Total		7658579	120636	100.000	100.000



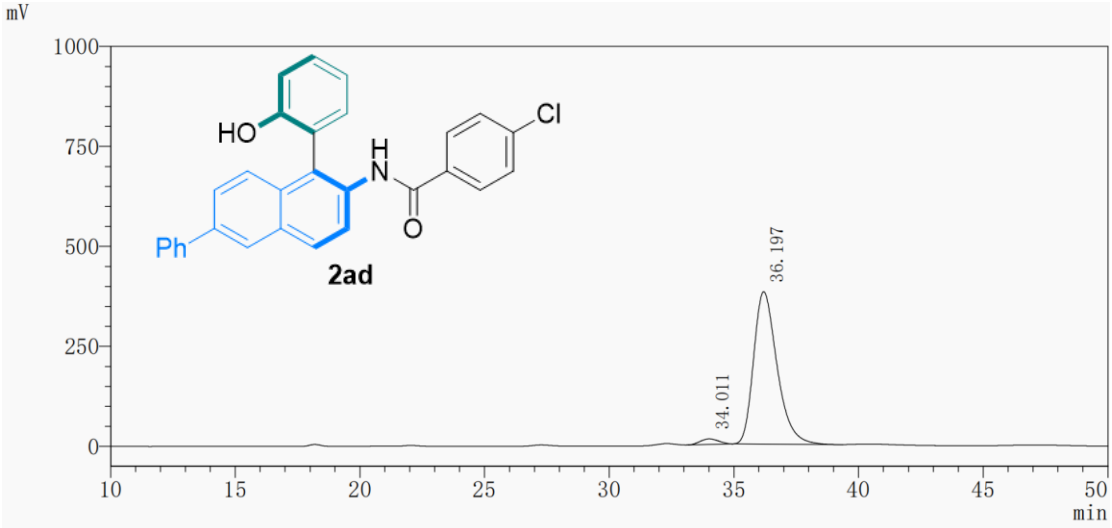
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	28.034	6521261	115273	52.367	58.313
2	38.200	5931837	82407	47.633	41.687
Total		12453097	197680	100.000	100.000



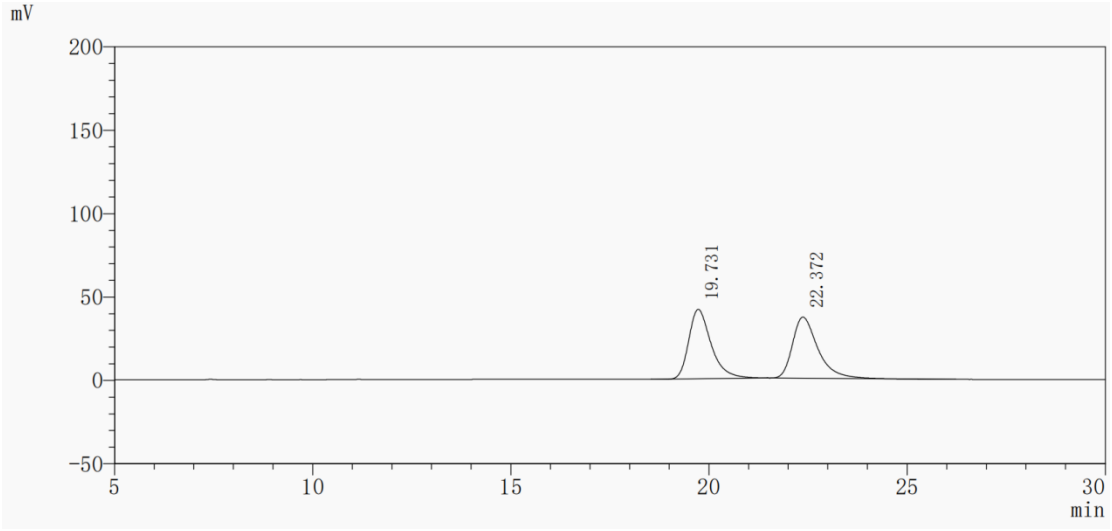
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	28.611	392826	7002	4.015	5.673
2	38.859	9390558	116436	95.985	94.327
Total		9783384	123438	100.000	100.000



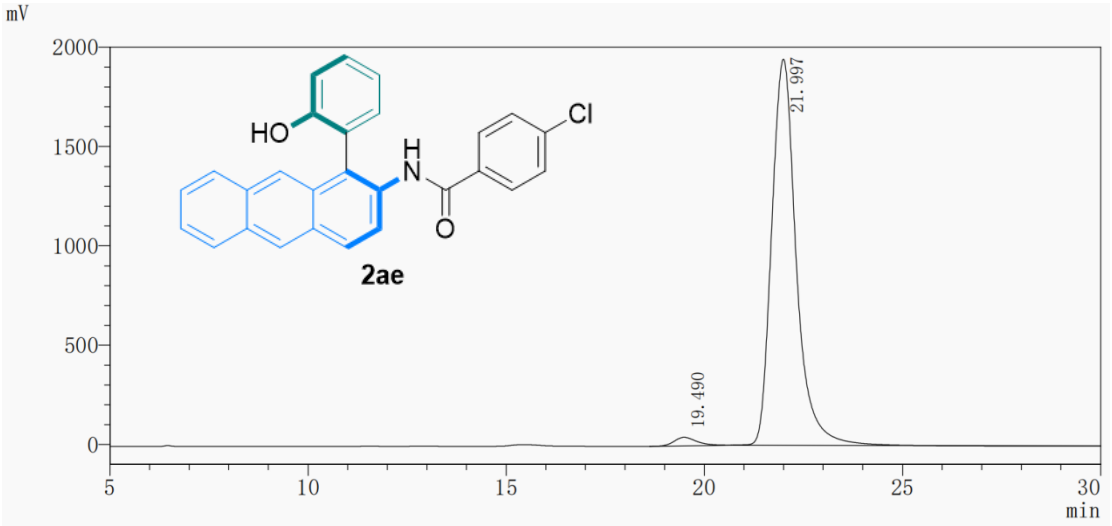
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	33.709	18106585	329697	49.057	51.867
2	36.083	18802662	305957	50.943	48.133
Total		36909247	635654	100.000	100.000



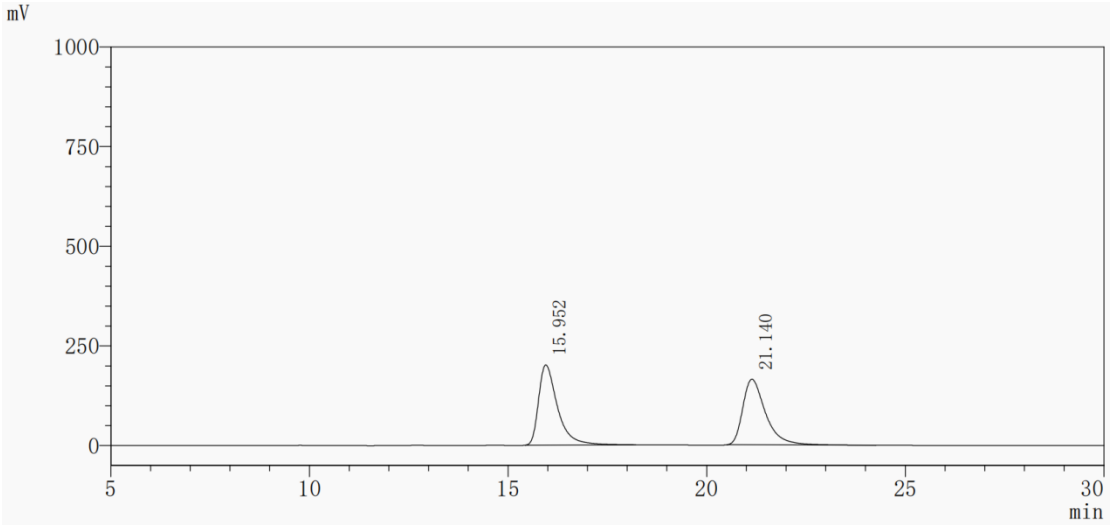
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	34.011	703499	13836	2.747	3.505
2	36.197	24908861	380915	97.253	96.495
Total		25612360	394752	100.000	100.000



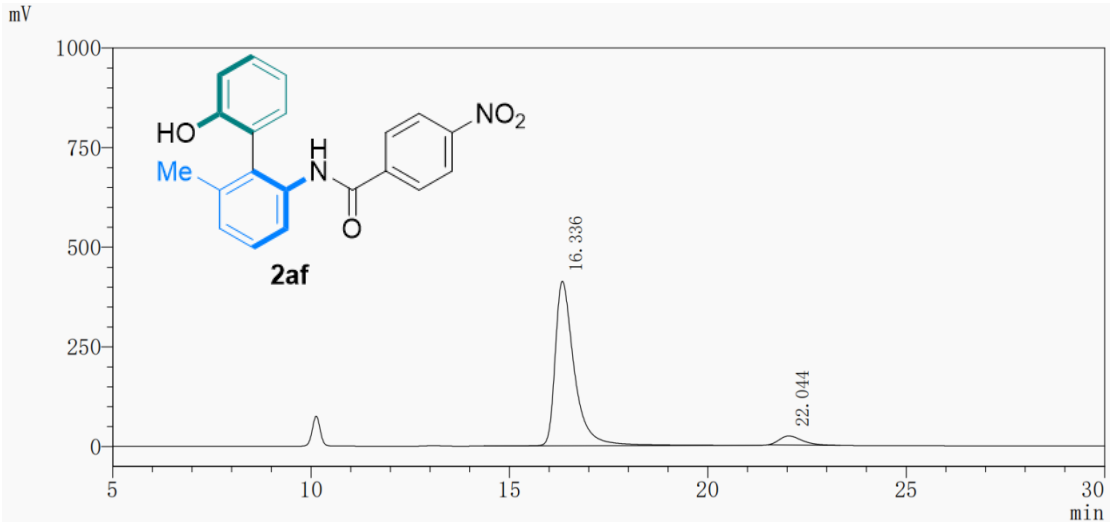
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	19.731	1640871	41659	49.973	53.179
2	22.372	1642656	36679	50.027	46.821
Total		3283526	78338	100.000	100.000



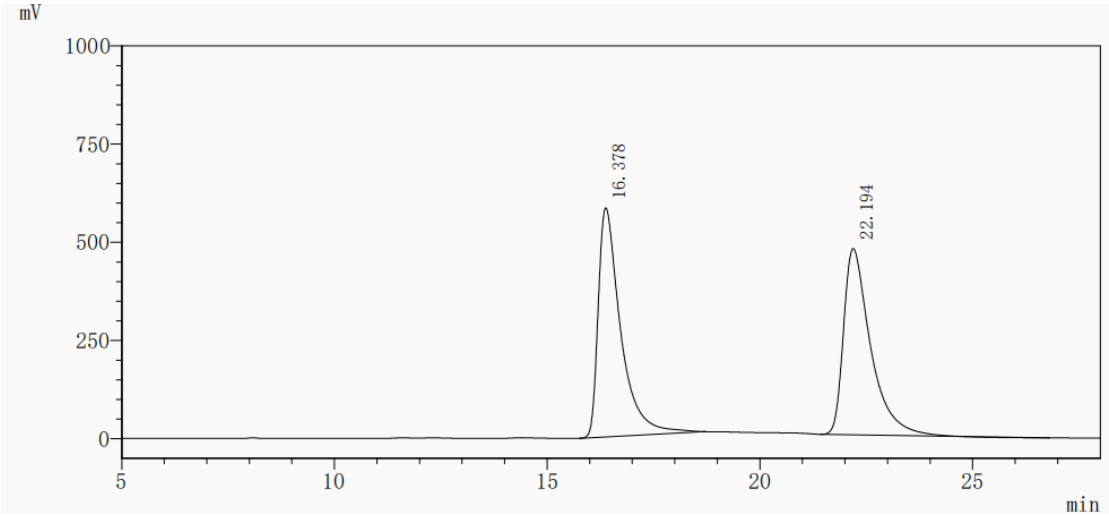
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	19.490	1679220	42532	1.974	2.142
2	21.997	83403066	1943122	98.026	97.858
Total		85082286	1985654	100.000	100.000



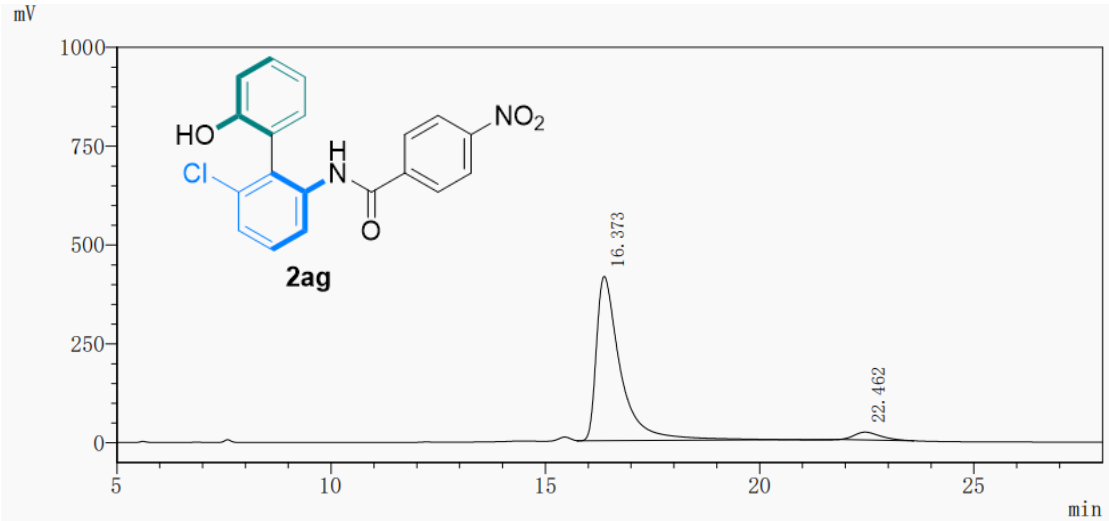
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	15.952	6684644	201369	50.363	54.994
2	21.140	6588161	164795	49.637	45.006
Total		13272805	366164	100.000	100.000



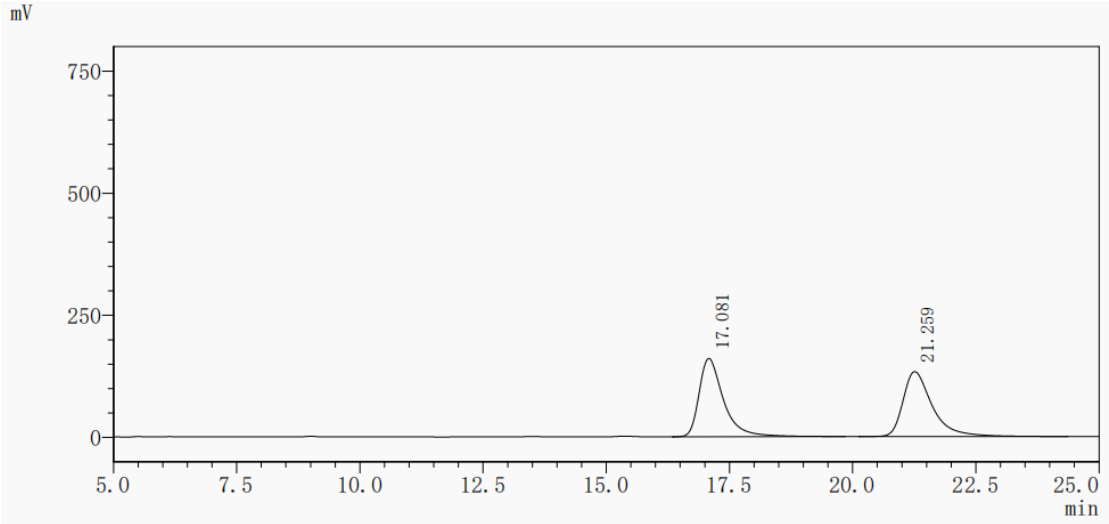
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	16.336	13923168	413052	94.013	94.833
2	22.044	886733	22503	5.987	5.167
Total		14809901	435555	100.000	100.000



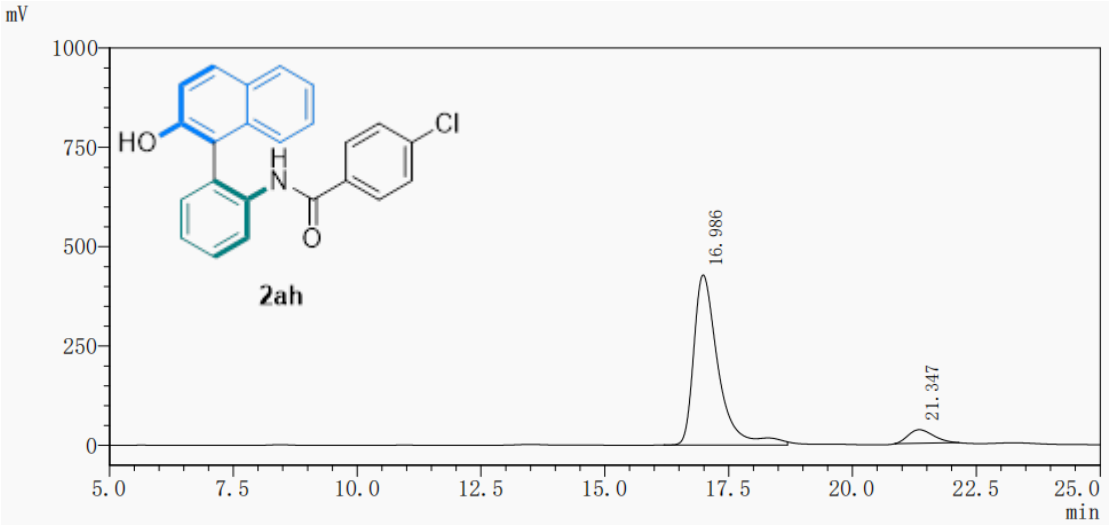
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	16.378	21430737	582885	50.541	55.135
2	22.194	20972063	474306	49.459	44.865
Total		42402799	1057191	100.000	100.000



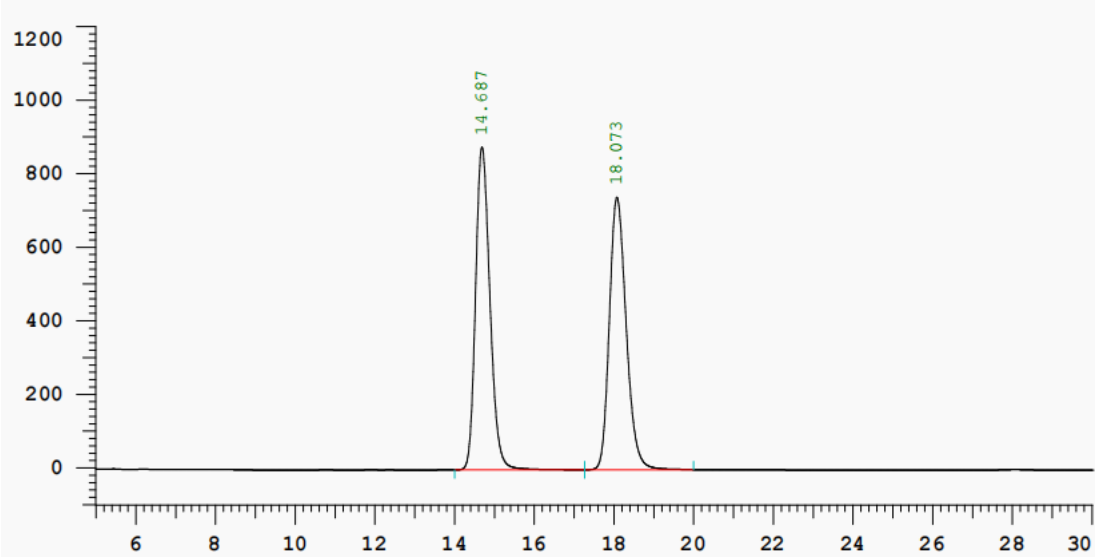
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	16.373	16257081	415207	94.975	95.426
2	22.462	860139	19900	5.025	4.574
Total		17117220	435106	100.000	100.000



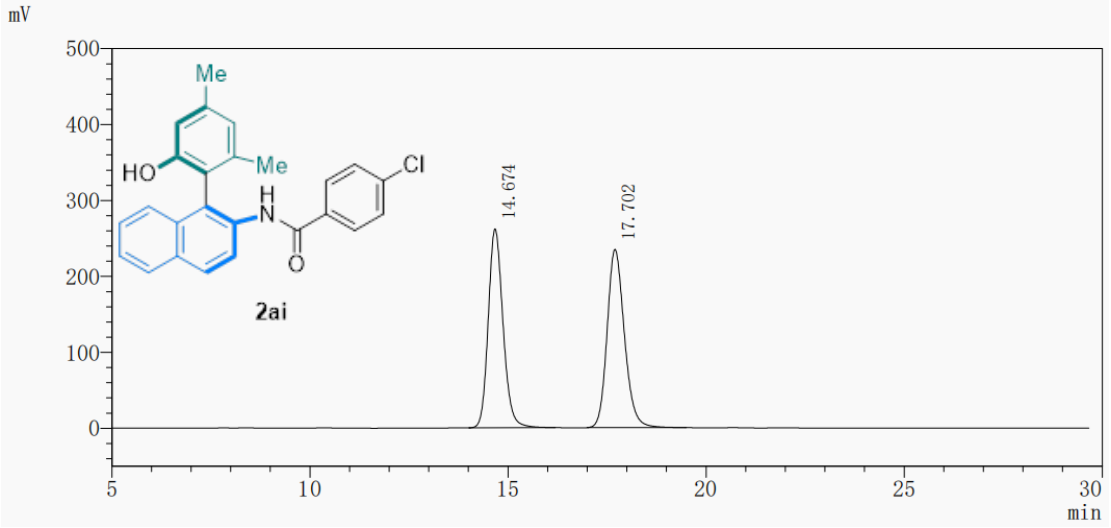
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	17.081	5514191	160236	50.108	54.685
2	21.259	5490439	132783	49.892	45.315
Total		11004629	293019	100.000	100.000



Peaks#	Ret.Time	Area	Height	Area%	Height%
1	16.986	14698046	428238	92.324	92.594
2	21.347	1222008	34253	7.676	7.406
Total		15920054	462491	100.000	100.000

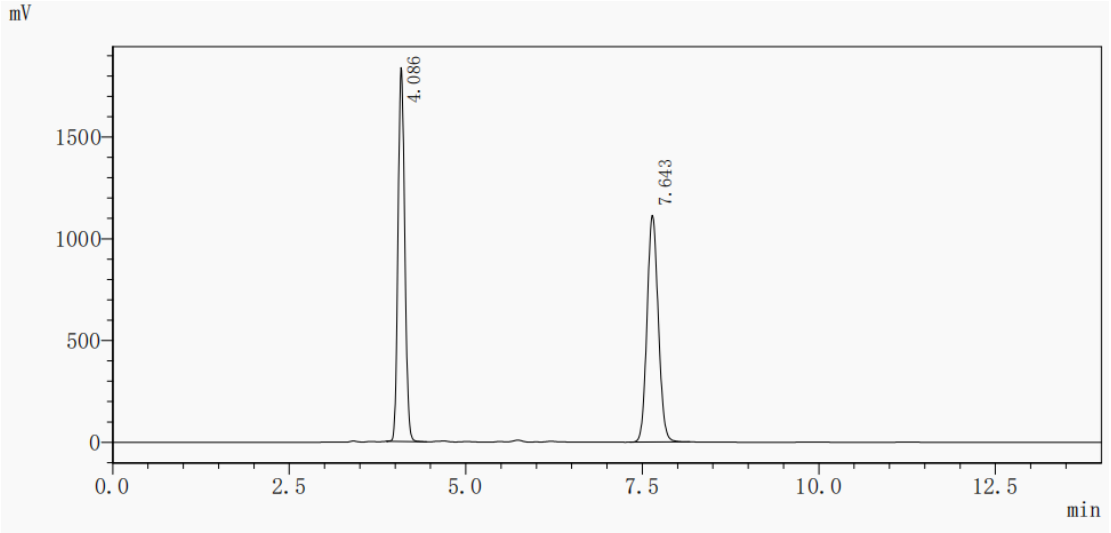


Peaks#	Ret.Time	Area	Height	Area%	Height%
1	14.687	21919152	877224	50.254	54.244
2	18.073	21697571	739931	49.746	45.756
Total		43616723	1617155	100.000	100.000

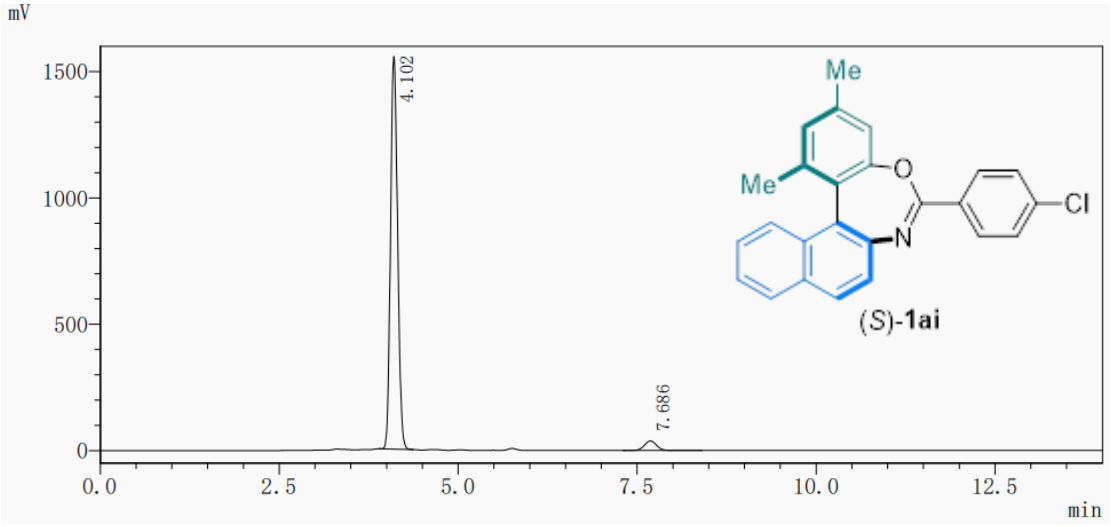


Peaks#	Ret.Time	Area	Height	Area%	Height%
1	14.674	6792476	261912	48.822	52.730
2	17.702	7120224	234793	51.178	47.270
Total		13912699	496706	100.000	100.000

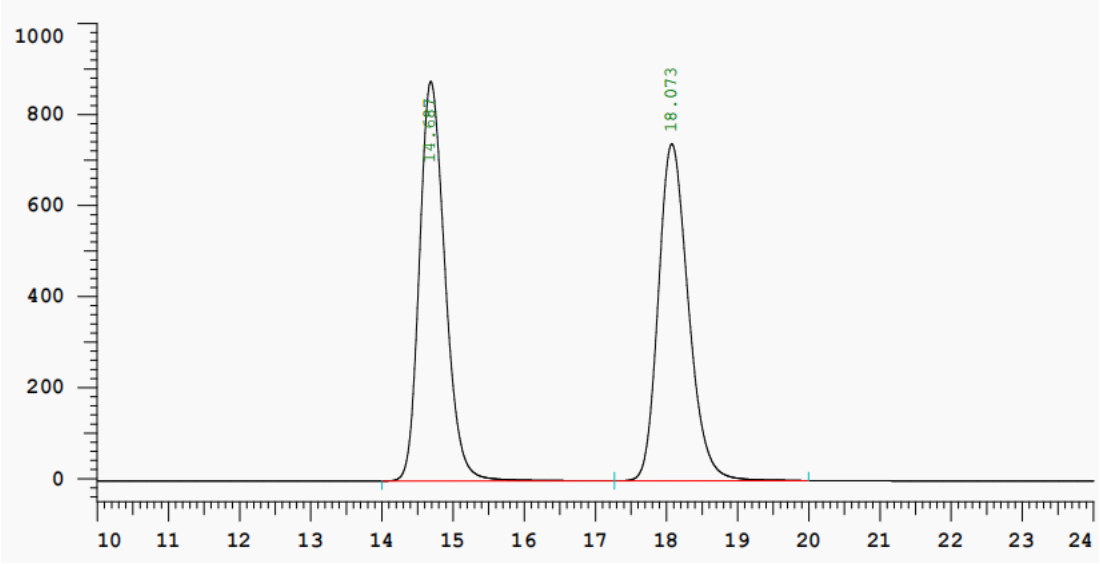
Kinetic resolution of racemic biaryl oxazepane **1ai**



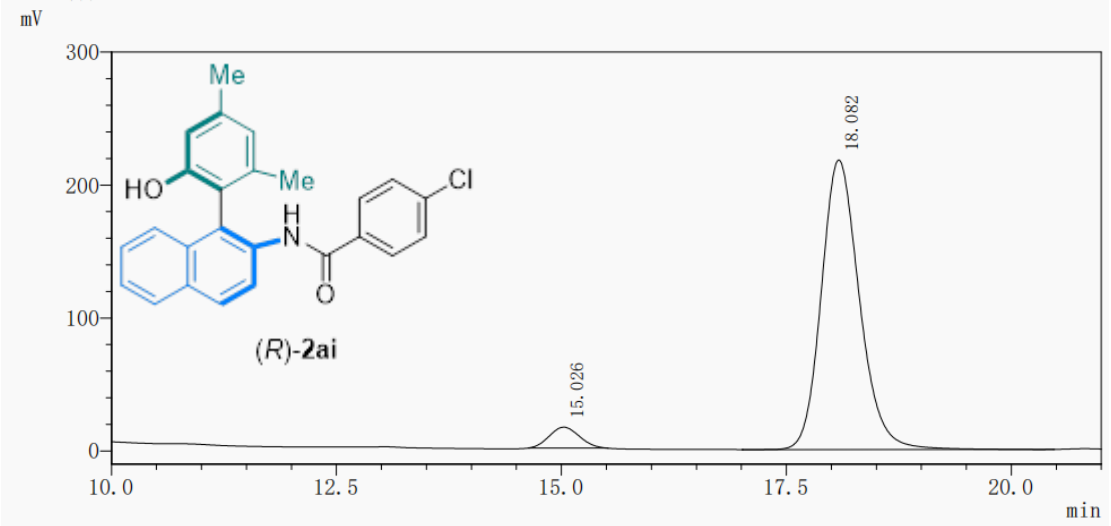
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	4.086	12179945	1836906	49.712	62.238
2	7.643	12321155	1114519	50.288	37.762
Total		24501100	2951426	100.000	100.000



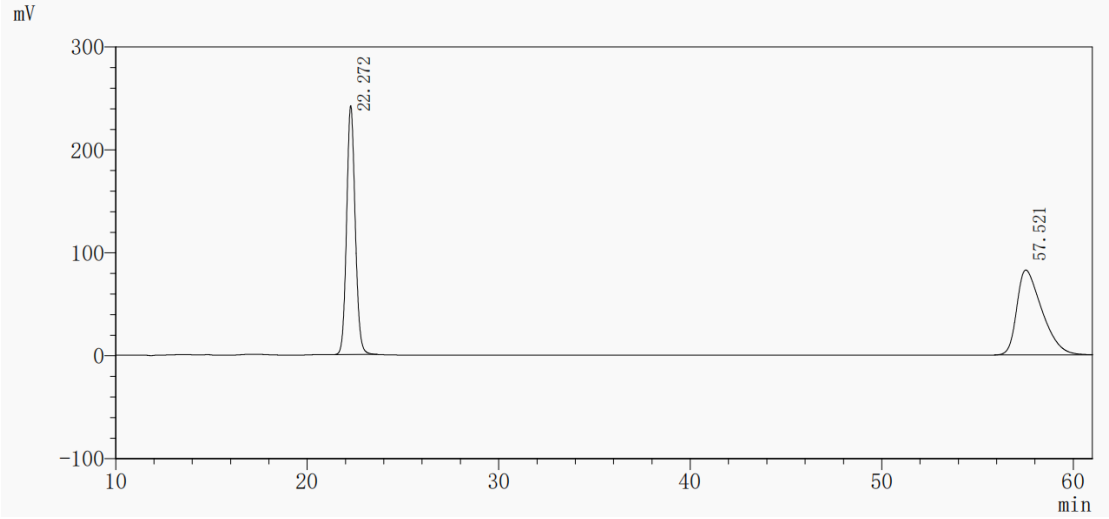
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	4.102	10686658	1554579	95.981	97.619
2	7.686	447468	37924	4.019	2.381
Total		11134127	1592503	100.000	100.000



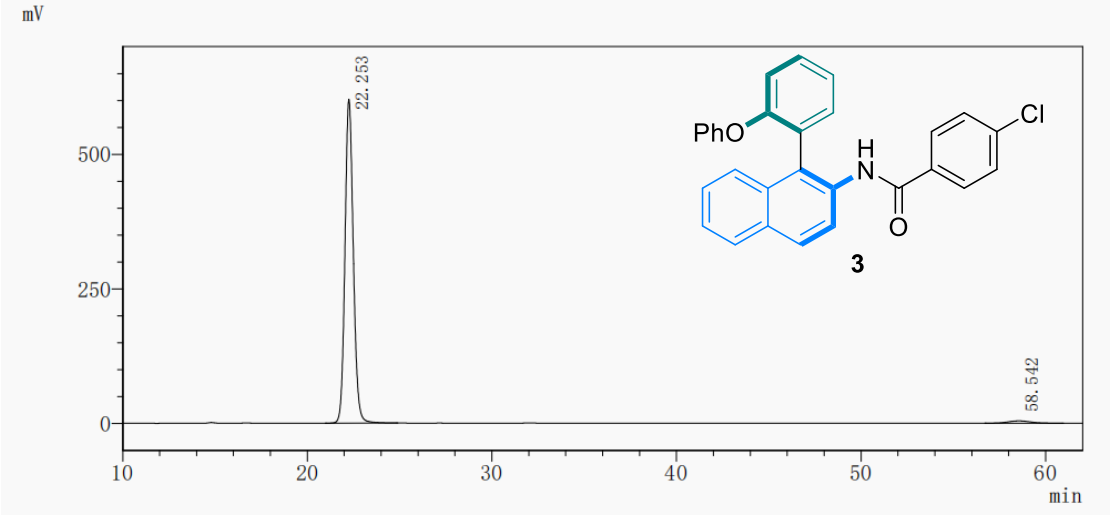
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	14.687	21919152	877224	50.254	54.244
2	18.073	21697571	739931	49.746	45.756
Total		43616723	1617155	100.000	100.000



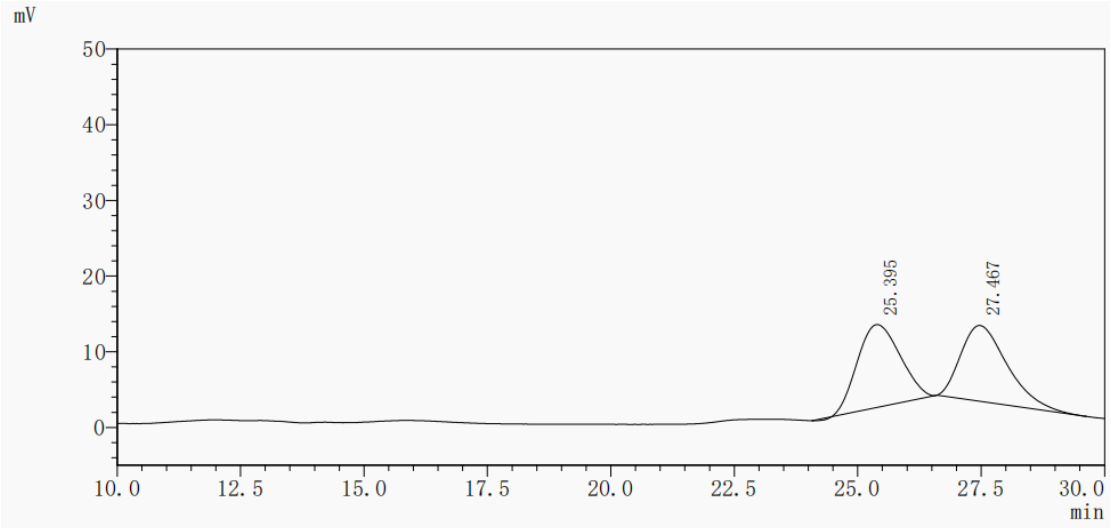
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	15.026	366616	15751	5.404	6.742
2	18.082	6418073	217877	94.596	93.258
Total		6784689	233628	100.000	100.000



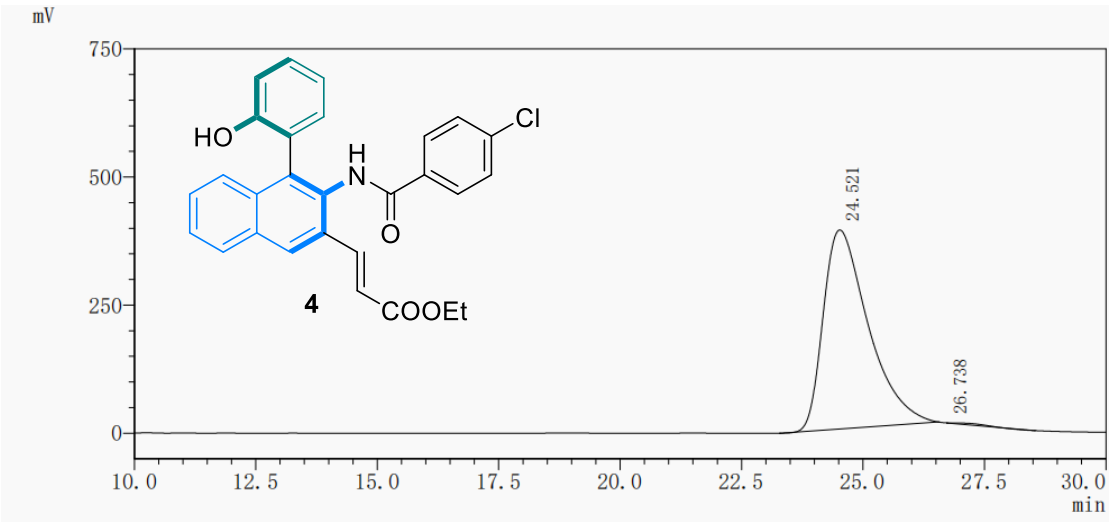
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	22.272	7538779	241850	50.000	74.550
2	57.521	7538703	82561	50.000	25.450
Total		15077482	324411	100.000	100.000



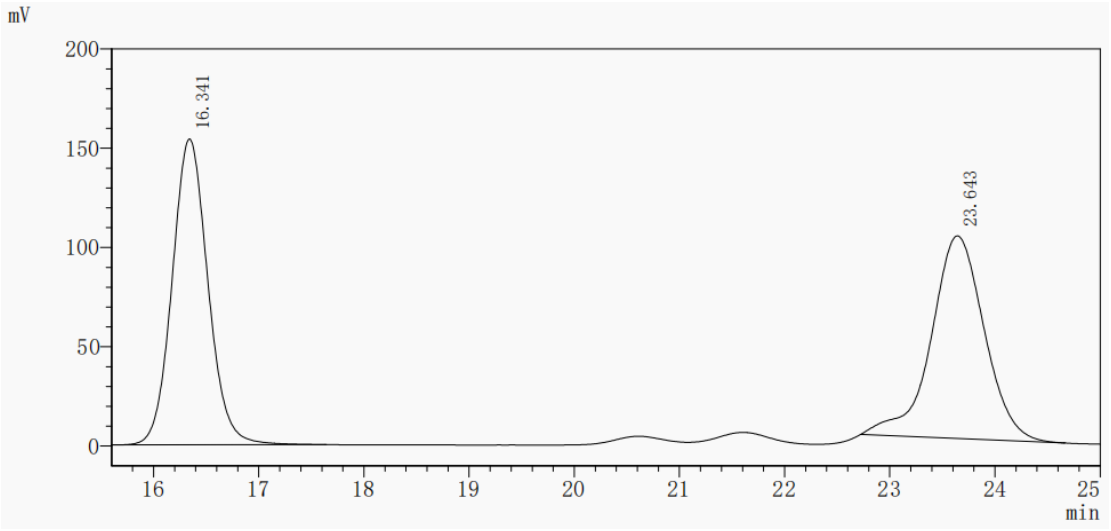
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	22.253	18898468	601464	98.121	99.291
2	58.542	361975	4293	1.879	0.709
Total		19260443	605756	100.000	100.000



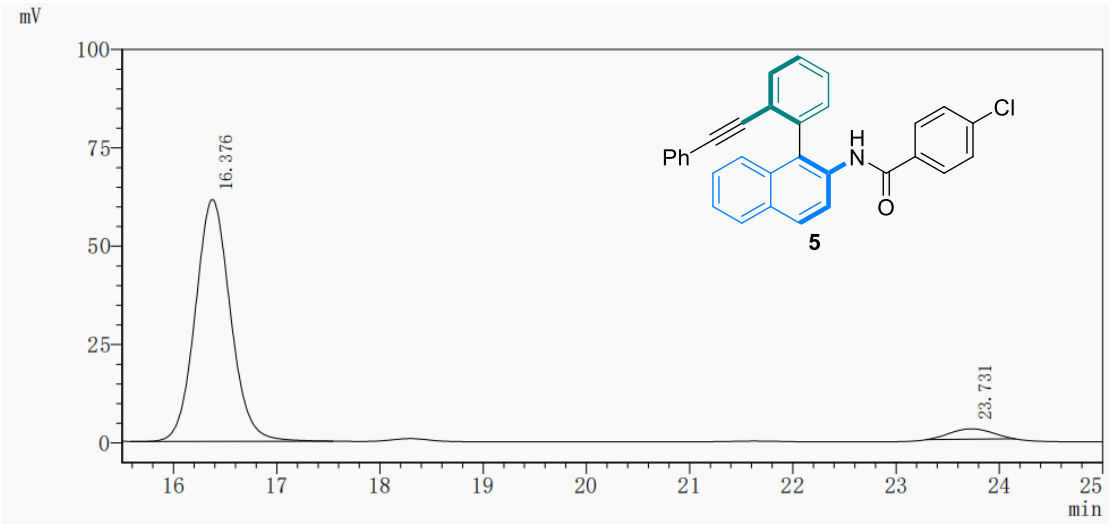
Peaks#	Ret.Time	Area	Height	Area%	Height%
1	25.395	656405	10940	49.868	52.195
2	27.467	659888	10019	50.132	47.805
Total		1316293	20959	100.000	100.000



Peaks#	Ret.Time	Area	Height	Area%	Height%
1	24.521	25065324	388505	99.628	99.983
2	26.738	93662	65	0.372	0.017
Total		25158986	388570	100.000	100.000



Peaks#	Ret.Time	Area	Height	Area%	Height%
1	16.341	3643237	154066	50.395	60.160
2	23.643	3586055	102029	49.605	39.840
Total		7229292	256095	100.000	100.000



Peaks#	Ret.Time	Area	Height	Area%	Height%
1	16.376	1455369	61489	95.241	95.942
2	23.731	72729	2601	4.759	4.058
Total		1528098	64090	100.000	100.000

References

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